

SUPPLEMENTARY INFORMATION

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In silico analysis of druggability, pharmacokinetics, and target identification of key molecules from *Cassia angustifolia* and *Cassia acutifolia*

OUAHAB Ammar*¹, FETNI Samira¹, MEGUELLATI Mohammed Islam¹, LAKHZOUM Hadjer¹
¹Department of Pharmacy, Faculty of Medicine, University of Batna 2. Algeria

*Corresponding author: a.ouahab@univ-batna2.dz ; ouahab.am@gmail.com

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PDB files of the docking results are attached as a ZIP file.

7. Xyz Cartesian coordinates of the complex of Rhein with Human Liver Carboxylesterase 1
8. Xyz Cartesian coordinates of the complex of Isorhamnetin with Estrogen receptor β
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11. Xyz Cartesian coordinates of the complex of 6-Hydroxymusicin with Carbonic anhydrase II
12. Xyz Cartesian coordinates of the complex of Kaempferol with Carbonic anhydrase II

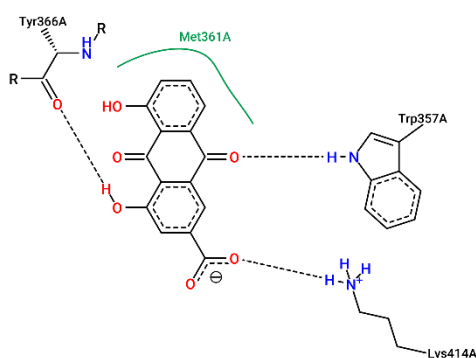


Figure S1. Two-dimensional diagrams of Rhein with Human Liver Carboxylesterase 1

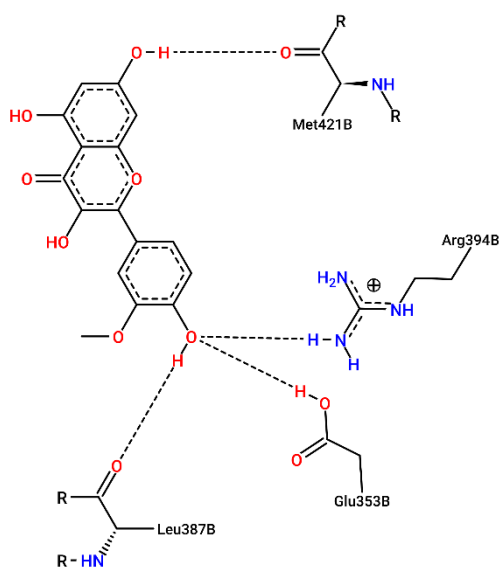


Figure S2. Two-dimensional diagrams of Isorhamnetin with Estrogen receptor β

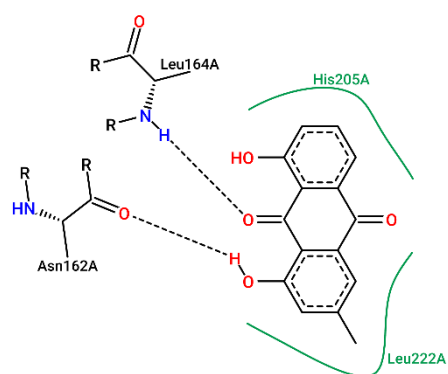


Figure S3. Two-dimensional diagrams of Chrysophanol with Stromelysin-1

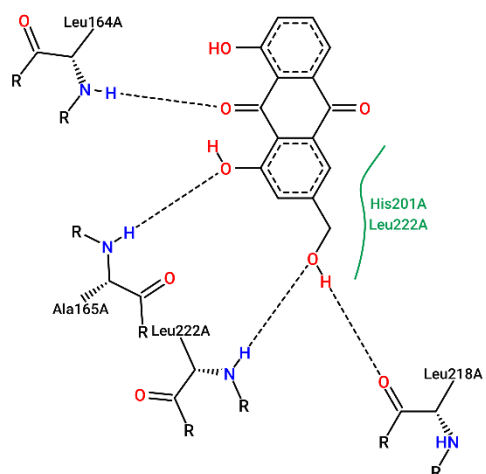


Figure S4. Two-dimensional diagrams of Aloe-Emodin with Stromelysin-1

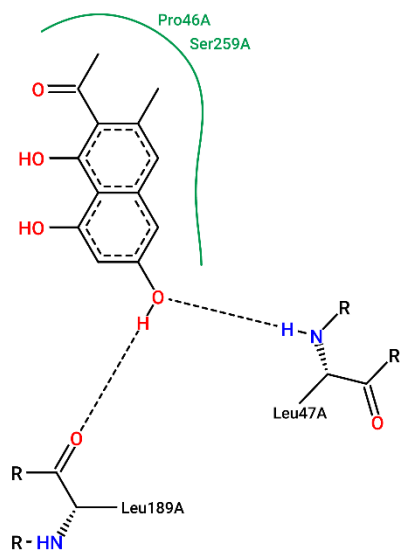


Figure S5. Two-dimensional diagrams of 6-Hydroxymusicin with Carbonic anhydrase II

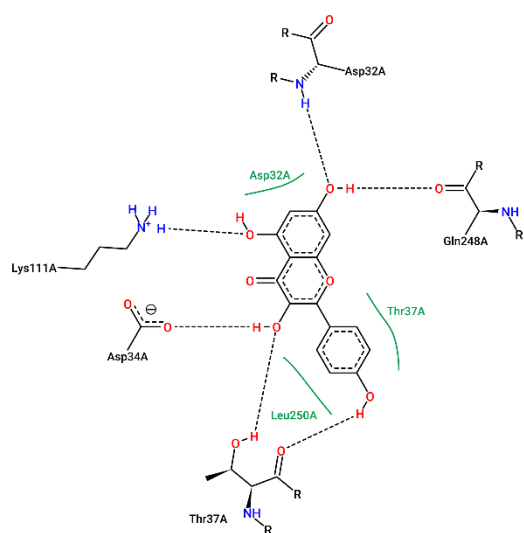


Figure S6. Two-dimensional diagrams of Kaempferol with Carbonic anhydrase II

PDB files of the docking results are attached as a ZIP file.

Xyz Cartesian coordinates of the complex of Rhein with Human Liver Carboxylesterase 1

N	-29.23000	42.20600	72.18600
H	-28.73300	42.80200	72.84900
H	-30.08500	42.64400	71.84400
H	-28.73700	42.12900	71.29600
C	-29.49100	40.87000	72.79900
C	-28.19900	40.18200	73.26500
O	-27.56500	40.62300	74.23100
C	-30.23800	39.97400	71.80200
O	-29.55500	39.89300	70.56200
H	-30.01700	39.33800	69.94500
N	-27.80900	39.10500	72.58500
H	-28.36600	38.78100	71.79400
C	-26.59600	38.38100	72.95400
C	-25.75700	38.01600	71.73500
O	-26.29600	37.68400	70.67900
C	-26.95200	37.11000	73.72400
O	-25.77800	36.43200	74.13900
H	-25.99900	35.64200	74.61800
N	-24.41900	38.05900	71.87400
C	-23.52800	37.72800	70.76100
C	-23.88600	36.37000	70.16100
O	-24.25100	35.43900	70.87600
C	-22.14600	37.72300	71.41300
C	-22.29700	38.67200	72.54600
C	-23.64300	38.30600	73.10000
N	-23.78800	36.24700	68.83400
C	-24.10400	34.99600	68.14500
C	-23.10800	33.87900	68.47800
O	-21.89700	34.11500	68.49700
C	-24.02300	35.38500	66.66500
C	-24.25100	36.85500	66.66600
C	-23.48300	37.31200	67.86700
N	-23.61600	32.67700	68.75400
H	-24.62800	32.55400	68.77400
C	-22.75200	31.53500	69.02800
C	-23.20600	30.38100	68.15600
O	-24.30800	29.86300	68.29400
C	-22.78700	31.08400	70.49600

C	-21.92900	29.84400	70.67400
C	-22.26800	32.17000	71.38000
N	-22.33800	29.98700	67.24400
H	-21.43500	30.45800	67.18200
C	-22.63100	28.90900	66.33200
C	-21.82500	27.68100	66.68100
O	-20.65700	27.77200	67.06800
C	-22.26200	29.31600	64.91400
C	-22.31800	28.11700	63.98100
C	-23.18700	30.41300	64.45700
N	-22.44600	26.52300	66.55100
H	-23.42700	26.49100	66.27300
C	-21.71800	25.30200	66.80800
C	-21.28200	24.72300	65.45900
O	-22.12000	24.39000	64.61100
C	-22.58200	24.29800	67.56300
C	-21.86300	22.98600	67.79600
O	-21.89400	22.12600	66.89100
O	-21.24400	22.81900	68.87200
N	-19.96900	24.64500	65.25000
H	-19.32800	24.98100	65.96900
C	-19.43100	24.09100	64.02000
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O	-19.26100	22.19300	65.45200
C	-18.20800	24.89400	63.49800
O	-17.02200	24.47200	64.17700
H	-16.27400	24.96300	63.85800
C	-18.40500	26.38800	63.72800
N	-18.34400	22.00000	63.44800
H	-18.13400	22.42500	62.54500
C	-17.92400	20.64600	63.73400
C	-16.80500	20.60600	64.75400
O	-16.80100	19.74900	65.63200
C	-17.43400	19.93500	62.46200
C	-17.01600	18.50400	62.79500
C	-18.52700	19.95700	61.40100
N	-15.86200	21.53500	64.63600
H	-15.94800	22.23400	63.89800
C	-14.70600	21.58700	65.52900
C	-14.92600	22.28200	66.86900
O	-14.00700	22.34800	67.69600
C	-13.52100	22.25700	64.83200
C	-12.99900	21.50200	63.65000

N	-13.12000	20.13400	63.52800
H	-13.59900	19.52300	64.19000
C	-12.30100	21.91500	62.56700
C	-12.51900	19.73900	62.42000
N	-12.01300	20.80000	61.81900
H	-11.49300	20.79300	60.94200
N	-16.13000	22.80100	67.08600
H	-16.85700	22.72100	66.37500
C	-16.40900	23.48100	68.33500
C	-17.21700	24.73700	68.11000
O	-17.39800	25.16000	66.97300
N	-17.68500	25.34700	69.19500
H	-17.46000	24.95900	70.11100
C	-18.51000	26.55200	69.12600
C	-17.72300	27.83100	68.87200
O	-16.62500	27.99100	69.40100
C	-19.29800	26.69600	70.43000
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C	-22.11000	24.70000	72.22100
N	-23.09000	24.59100	71.09200
H	-23.80100	23.87500	71.24000
H	-22.60600	24.44200	70.20600
H	-23.52200	25.49500	70.89900
N	-18.27700	28.72900	68.05100
H	-19.16900	28.51100	67.60700
C	-17.63500	30.02200	67.77100
C	-18.56600	31.15700	68.17000
O	-19.78400	31.06100	68.02900
C	-17.23400	30.19500	66.28700
C	-16.05500	29.31300	65.97300
C	-18.38000	29.84600	65.39300
N	-17.96700	32.22500	68.68200
H	-16.94900	32.22500	68.74400
C	-18.68700	33.39700	69.16000
C	-18.43800	34.56800	68.22700
O	-17.29500	34.93500	67.98600
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C	-18.69700	34.90300	71.40900
C	-18.17900	36.20600	70.84500
C	-20.20800	34.88500	71.44700
N	-19.50600	35.15300	67.70200
H	-20.43900	34.81400	67.93600

C	-19.34900	36.27500	66.79600
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O	-19.92600	37.75300	68.59500
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C	-21.75200	40.32400	65.90500
O	-21.65400	40.06900	64.70700
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H	-16.43700	44.91800	64.11300
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H	-17.20200	45.13100	65.59600
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H	-22.76400	41.20100	67.42500
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O	-22.86800	43.79800	65.76300
C	-25.09300	41.70000	66.41400
C	-25.80700	40.40100	66.58500
C	-25.97400	39.85000	67.84700
C	-26.34500	39.74300	65.48000
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C	-24.88300	44.96100	62.39700
O	-25.25100	44.24400	61.46500
C	-22.40400	44.58100	62.37300
C	-22.20800	45.94300	61.73700
C	-21.19600	44.20600	63.21900
N	-25.51300	46.08300	62.72500
H	-25.18300	46.63700	63.51600
C	-26.66900	46.52700	61.96500
C	-26.26400	47.40400	60.80000
O	-25.26600	48.11600	60.86900
C	-27.63900	47.29000	62.86000
O	-28.43500	46.39300	63.61600

H	-29.03900	46.86800	64.17400
N	-27.03300	47.33300	59.71900
H	-27.83000	46.69700	59.71000
C	-26.75500	48.14800	58.54900
C	-27.97900	48.90600	58.07200
O	-29.06400	48.33600	57.90900
C	-26.22700	47.31100	57.39200
C	-25.87100	48.21500	56.20800
C	-24.80700	49.21200	56.64900
C	-25.38000	47.39100	55.03100
N	-27.76900	50.20200	57.85300
H	-26.83400	50.56700	58.03600
C	-28.77800	51.13900	57.37100
C	-29.86000	50.50000	56.50700
O	-29.56900	49.98500	55.42900
C	-28.08800	52.23100	56.55500
C	-29.02900	53.27500	56.01400
C	-29.58900	54.14600	57.11500
O	-29.09800	55.29200	57.26700
O	-30.50500	53.67300	57.83600
N	-31.10400	50.54000	56.97500
H	-31.29200	50.96800	57.88200
C	-32.19800	49.97700	56.20000
C	-32.46500	48.48800	56.35500
O	-33.22100	47.89600	55.57000
N	-31.85300	47.86400	57.35700
H	-31.23400	48.38500	57.97900
C	-32.06400	46.44100	57.56800
C	-32.31900	46.10600	59.02200
O	-31.44600	46.25900	59.87700
C	-30.87800	45.64800	57.03200
C	-30.68000	45.80900	55.56300
C	-29.87600	46.82400	55.06500
C	-31.34500	44.98800	54.67200
C	-29.74100	47.01700	53.69400
C	-31.21700	45.17200	53.30500
C	-30.41500	46.18700	52.81500
N	-33.54000	45.65400	59.28500
H	-34.20100	45.55200	58.51500
C	-33.97100	45.29900	60.62400
C	-33.01500	44.32300	61.28300
O	-32.33800	44.66500	62.25100
C	-35.36200	44.70200	60.56600

N	-32.97200	43.10700	60.74700
H	-33.56200	42.91000	59.93900
C	-32.11900	42.04200	61.26300
C	-30.63000	42.34000	61.15800
O	-30.10300	42.57600	60.07100
C	-32.40900	40.73300	60.52100
C	-31.39600	39.61400	60.77100
C	-31.58800	38.94400	62.11200
O	-32.59800	38.28600	62.34500
N	-30.61900	39.10900	63.00300
H	-30.74900	38.65700	63.90800
H	-29.78000	39.65600	62.80900
N	-29.93000	42.32800	62.29500
C	-28.49600	42.59300	62.29900
C	-27.71200	41.41000	61.71900
O	-28.12600	40.25400	61.83800
C	-28.20300	42.82000	63.77800
C	-29.17600	41.90200	64.44600
C	-30.43500	42.18000	63.66900
N	-26.58200	41.71300	61.08900
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C	-24.76800	40.15400	61.54400
O	-24.16500	40.91200	62.30100
C	-24.91000	41.28600	59.32800
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C	-25.83600	41.94200	58.33400
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C	-23.74900	38.16700	62.52100
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O	-22.32800	37.26800	60.81600
C	-24.32400	36.81700	62.91400
N	-21.37200	38.64900	62.32500
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O	-19.07200	37.82700	63.81100
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C	-20.24000	40.80000	60.58400
C	-17.97800	39.85000	61.03700
C	-19.62600	42.14800	60.28400
N	-18.29600	36.89000	61.91400

H	-18.36900	36.84900	60.89700
C	-17.32700	36.03200	62.58800
C	-15.96200	36.22400	61.96100
O	-15.79000	36.00200	60.76000
C	-17.73200	34.57300	62.47000
C	-19.11000	34.29900	62.95600
C	-20.19800	34.44500	62.10600
C	-19.32600	33.89600	64.27200
C	-21.48800	34.19000	62.55400
C	-20.61400	33.63800	64.73400
C	-21.69800	33.78500	63.87100
N	-14.99400	36.62700	62.78200
H	-15.20800	36.75900	63.77100
C	-13.63900	36.88600	62.31200
C	-12.59800	35.90500	62.82200
O	-12.50600	35.65400	64.02100
C	-13.21700	38.29300	62.72200
C	-14.14600	39.42200	62.28900
C	-13.67700	40.74800	62.88200
C	-14.18000	39.48100	60.77100
N	-11.80800	35.35900	61.90400
H	-11.94200	35.58700	60.91900
C	-10.75500	34.44000	62.29500
C	-11.12000	33.00200	62.59700
O	-10.59300	32.40700	63.53300
N	-12.03100	32.43300	61.82500
H	-12.48800	32.96600	61.08500
C	-12.37200	31.04000	62.04500
C	-11.27000	30.26600	61.34200
O	-10.99800	30.50800	60.15900
C	-13.73600	30.67200	61.41800
C	-14.86000	31.40600	62.15800
C	-13.95100	29.15500	61.47300
C	-16.24900	31.00200	61.70600
N	-10.59800	29.34900	62.06300
C	-9.51500	28.55000	61.47900
C	-10.08900	27.38900	60.66100
O	-10.92900	26.64200	61.15300
C	-8.75700	28.07000	62.71000
C	-9.87500	27.78500	63.66600
C	-10.79500	28.99900	63.48300
N	-9.65700	27.24400	59.41400
H	-8.97100	27.89700	59.03600

C	-10.15700	26.15800	58.58400
C	-9.04600	25.16900	58.27700
O	-9.21200	24.26900	57.46000
C	-10.75200	26.70300	57.28300
C	-9.74500	27.31700	56.36900
C	-8.96200	26.51700	55.53900
C	-9.54400	28.69400	56.36900
C	-7.99200	27.07700	54.72000
C	-8.57600	29.27300	55.55600
C	-7.79500	28.46400	54.72800
N	-7.91300	25.34100	58.94600
H	-7.84300	26.10800	59.61500
C	-6.76600	24.46300	58.75000
C	-5.82200	24.53100	59.93800
O	-5.89400	25.45300	60.74600
C	-6.01900	24.85400	57.49200
N	-4.94900	23.53700	60.04400
H	-4.97700	22.78000	59.36000
C	-3.95300	23.49200	61.10500
C	-2.89000	24.51000	60.68300
O	-2.52600	24.56400	59.50700
C	-3.35500	22.08800	61.17500
C	-2.31400	21.89500	62.24900
C	-1.91400	20.43200	62.32700
C	-0.91400	20.18800	63.44700
N	-1.45500	20.55400	64.79100
H	-0.78400	20.39000	65.54200
H	-2.33500	20.07300	64.97500
H	-1.78900	21.51800	64.80100
N	-2.38600	25.33500	61.61900
C	-1.37000	26.31500	61.20600
C	-0.19400	25.63700	60.50100
O	0.49100	24.80000	61.09400
C	-0.97200	26.97800	62.52500
C	-2.22500	26.88100	63.34000
C	-2.68800	25.47100	63.05300
N	0.04800	25.98700	59.22100
C	1.14400	25.39400	58.44700
C	2.53800	25.84300	58.90700
O	3.28200	26.47700	58.14800
C	0.81300	25.82500	57.01700
C	0.21100	27.16800	57.21100
C	-0.68700	26.98000	58.41100

N	2.87800	25.50000	60.15000
H	2.21200	24.96600	60.70900
C	4.16500	25.85600	60.74700
C	5.10800	24.66000	60.84900
O	4.71800	23.49900	60.62700
C	3.96300	26.42800	62.15000
C	2.88700	27.49700	62.26900
C	2.74300	27.93900	63.70900
C	3.25100	28.65900	61.38700
N	6.35300	24.95800	61.20300
H	6.61100	25.92800	61.38300
C	7.34400	23.91200	61.33400
C	7.40000	22.97900	60.14000
O	7.44700	23.42100	58.99100
N	7.37000	21.66600	60.38400
C	7.42600	20.68600	59.30100
C	6.28300	20.80700	58.30700
O	6.39100	20.32600	57.18700
C	7.39900	19.35700	60.04900
C	6.50100	19.65500	61.18200
C	7.01800	21.00700	61.65400
N	5.19100	21.44700	58.71200
H	5.16000	21.84600	59.65000
C	4.03700	21.58600	57.83200
C	4.23200	22.56200	56.68200
O	3.41800	22.61800	55.75100
C	2.80500	21.97500	58.64500
C	2.31600	20.80500	59.48700
C	0.99000	21.14300	60.12900
C	2.17500	19.58600	58.59400
N	5.31700	23.32600	56.75200
H	5.94300	23.23200	57.55200
C	5.63000	24.29100	55.71500
C	5.83900	23.57200	54.37200
O	6.36600	22.46800	54.33500
C	6.87700	25.07800	56.12400
C	7.15200	26.29300	55.25900
C	8.38400	27.02600	55.72900
N	8.13400	27.91200	56.86300
H	7.16900	28.17500	57.06400
C	9.09400	28.39600	57.65000
N	10.36800	28.07300	57.43900
H	11.10300	28.44400	58.04100

H	10.60700	27.43300	56.68200
N	8.78400	29.22700	58.63300
H	9.51900	29.59800	59.23500
H	7.80800	29.47500	58.79500
N	5.40900	24.19400	53.27600
H	4.97300	25.11100	53.37000
C	5.54100	23.60500	51.93700
C	4.87000	22.23600	51.84300
O	5.41400	21.31400	51.24500
C	7.01400	23.43300	51.54100
C	7.84700	24.65900	51.73000
C	7.52000	25.84700	51.08800
C	8.95800	24.62900	52.55800
C	8.28800	26.99300	51.27000
C	9.73300	25.76500	52.74800
C	9.39800	26.95300	52.10500
N	3.69900	22.09400	52.44700
H	3.29400	22.88200	52.95200
C	2.98200	20.82300	52.39900
C	1.48100	21.09100	52.41000
O	1.03400	22.16100	52.83900
C	3.32400	19.92700	53.60800
O	2.53700	20.32400	54.73700
H	1.61600	20.24900	54.51700
C	4.80000	20.04700	53.96100
N	0.68300	20.12400	51.94200
C	-0.77800	20.24000	51.89000
C	-1.37100	20.68000	53.22200
O	-0.88200	20.29400	54.27400
C	-1.20800	18.83500	51.50700
C	-0.09400	18.39800	50.62800
C	1.12000	18.83600	51.38800
N	-2.44100	21.49000	53.19200
C	-3.05900	21.95000	54.44100
C	-3.78500	20.82300	55.18700
O	-4.47700	20.00100	54.57800
C	-4.01600	23.04100	53.96500
C	-4.49500	22.50300	52.65800
C	-3.21300	21.95100	52.01900
N	-3.62400	20.79200	56.50600
H	-3.03400	21.49600	56.95000
C	-4.26700	19.78000	57.33600
C	-5.41400	20.33300	58.16900

O	-5.41900	21.50300	58.55200
C	-3.23900	19.13500	58.24300
C	-2.33900	18.17800	57.50900
C	-1.22600	17.66100	58.38000
O	-1.46300	17.13800	59.47400
N	0.00300	17.80300	57.90400
H	0.75700	17.45300	58.49400
H	0.19900	18.23500	57.00100
N	-6.40800	19.48900	58.46700
C	-7.58800	19.86500	59.25500
C	-7.24700	20.53200	60.58400
O	-6.28400	20.14800	61.25000
C	-8.30100	18.53700	59.45200
C	-7.92200	17.77100	58.22300
C	-6.45500	18.06300	58.11000
N	-8.03900	21.53000	60.96500
H	-8.81900	21.80200	60.36600
C	-7.82100	22.24700	62.21800
C	-8.16700	21.36300	63.41500
O	-9.03900	20.50100	63.32400
C	-8.66500	23.51600	62.24000
N	-7.48200	21.56800	64.53400
H	-6.76500	22.29200	64.56400
C	-7.75000	20.76300	65.72000
C	-8.96600	21.34800	66.42200
O	-9.06600	22.56000	66.57900
C	-6.53600	20.77200	66.66500
C	-6.33700	19.47300	67.49500
C	-7.06200	19.45600	68.86400
O	-8.26800	19.78200	68.92700
O	-6.42200	19.09600	69.88100
N	-9.91800	20.49200	66.83000
C	-11.14800	20.89900	67.52400
C	-10.90900	21.49900	68.91500
O	-10.00500	21.08700	69.62900
C	-11.95100	19.60600	67.56600
C	-10.89400	18.55200	67.56000
C	-9.94300	19.05000	66.53500
N	-11.73200	22.46900	69.30000
H	-12.49000	22.75500	68.68000
C	-11.57700	23.13700	70.59300
C	-12.63800	22.78800	71.62800
O	-13.79900	22.59100	71.29500

C	-11.52600	24.64800	70.37700
C	-12.58400	25.17100	69.44500
C	-13.80100	25.69500	69.78800
C	-12.49200	25.26800	68.02100
N	-14.46500	26.12200	68.66500
H	-15.38800	26.55600	68.65100
C	-13.68600	25.87100	67.56600
C	-11.51600	24.90700	67.08400
C	-13.92800	26.12300	66.21100
C	-11.75800	25.15800	65.73500
C	-12.95500	25.76000	65.31400
N	-12.22300	22.75200	72.89100
H	-11.25500	23.00200	73.09300
C	-13.09100	22.37100	74.00200
C	-14.19100	23.30100	74.47700
O	-15.16200	22.83700	75.09600
C	-12.24300	21.96100	75.20100
O	-11.55400	20.75100	74.92000
H	-11.02600	20.49600	75.66700
N	-14.08400	24.59800	74.21900
H	-13.27300	24.97000	73.72500
C	-15.16900	25.48300	74.66700
C	-15.72500	26.35900	73.55200
O	-15.90000	25.91500	72.42400
C	-14.68200	26.36000	75.82600
C	-14.23600	25.58100	77.01400
C	-12.89700	25.23300	77.16700
C	-15.15800	25.16700	77.98000
C	-12.47300	24.48200	78.27100
C	-14.74700	24.41400	79.08900
C	-13.40000	24.07200	79.23300
N	-16.03300	27.60100	73.89600
H	-15.94000	27.88200	74.87200
C	-16.49600	28.56700	72.93000
C	-15.32800	29.43300	72.46400
O	-14.70200	30.10600	73.26000
C	-17.59100	29.44700	73.52000
C	-17.88500	30.62400	72.58700
C	-18.82700	28.60400	73.73000
N	-15.03300	29.38200	71.16800
H	-15.58700	28.77400	70.56400
C	-13.95000	30.15900	70.57400
C	-14.45000	31.51900	70.10400

O	-15.51100	31.61800	69.48400
C	-13.33800	29.39400	69.39000
C	-12.36400	30.20300	68.55300
C	-11.81000	29.37600	67.41100
C	-10.82300	28.30300	67.87700
N	-9.51600	28.86600	68.32100
H	-8.85800	28.15100	68.63200
H	-9.65100	29.57400	69.04300
H	-9.10400	29.44800	67.59200
N	-13.67900	32.56300	70.39600
H	-12.81300	32.41700	70.91500
C	-14.04900	33.91000	69.98900
C	-13.55100	34.22200	68.60300
O	-12.35400	34.36200	68.39500
C	-13.46300	34.94000	70.94400
C	-14.20200	34.99900	72.24600
O	-14.73700	33.98700	72.70500
N	-14.22700	36.17400	72.86400
H	-13.80100	36.99700	72.43700
N	-14.47000	34.32700	67.65500
H	-15.45100	34.16600	67.88500
C	-14.10200	34.66700	66.29400
C	-14.41800	36.15300	66.16400
O	-15.24400	36.55500	65.34600
C	-14.92100	33.86100	65.31800
N	-13.73800	36.96600	66.96900
H	-13.02200	36.57500	67.58200
C	-13.99100	38.39800	66.99600
C	-12.86300	39.35800	66.63500
O	-13.07100	40.56800	66.65100
C	-14.53200	38.80200	68.38100
O	-13.64600	38.32200	69.40500
H	-13.98000	38.57100	70.25900
C	-15.91000	38.20400	68.59800
N	-11.67800	38.84000	66.32900
H	-11.55200	37.82800	66.35400
C	-10.55300	39.69500	65.95800
C	-10.23300	39.42500	64.51100
O	-10.51700	38.34600	64.00800
C	-9.31600	39.35500	66.77900
O	-9.59300	39.36400	68.16200
H	-8.82100	39.15200	68.67400
N	-9.65200	40.39900	63.82500

H	-9.47500	41.30200	64.26600
C	-9.26900	40.17300	62.44100
C	-8.03000	39.28400	62.50100
O	-7.13200	39.52000	63.29400
C	-8.95600	41.49900	61.75200
C	-10.19900	42.27200	61.40200
C	-11.03900	41.84100	60.37300
C	-10.56800	43.40200	62.12300
C	-12.22200	42.51600	60.07300
C	-11.74500	44.08400	61.83500
C	-12.56900	43.63500	60.81000
O	-13.75100	44.28800	60.54000
H	-14.31400	43.98100	59.83900
N	-7.98800	38.21900	61.69600
C	-6.81000	37.35000	61.73600
C	-5.59700	37.97300	61.03900
O	-5.73000	38.94200	60.29600
C	-7.30000	36.09800	61.02500
C	-8.26200	36.66000	60.00700
C	-9.03600	37.65700	60.82500
N	-4.39400	37.43500	61.28400
C	-3.19000	37.97400	60.64500
C	-3.29500	37.66400	59.17000
O	-4.10200	36.82800	58.77600
C	-2.06400	37.15900	61.26800
C	-2.62300	36.70500	62.56300
C	-4.04600	36.36800	62.23300
N	-2.49300	38.32700	58.34700
H	-1.86800	39.04500	58.71300
C	-2.50500	38.02800	56.91500
C	-1.23700	37.20800	56.69200
O	-0.26700	37.37200	57.43900
C	-2.50300	39.32000	56.08200
C	-1.25800	40.17800	56.17600
S	-1.47400	41.71500	55.24000
C	-0.48100	42.83600	56.18900
N	-1.23800	36.31000	55.70900
H	-2.06400	36.19400	55.12200
C	-0.04800	35.48900	55.47400
C	1.16000	36.34900	55.12000
O	1.03800	37.36500	54.42700
C	-0.28600	34.46800	54.36600
S	-1.74000	33.39700	54.60900

N	2.32200	35.92700	55.60500
H	2.33700	35.06800	56.15400
C	3.57200	36.63300	55.38900
C	3.71800	37.17300	53.97700
O	3.57000	36.44400	52.99500
C	4.74600	35.72800	55.69300
O	4.49400	35.03000	56.91800
H	3.70400	34.51200	56.81700
C	6.00100	36.55000	55.85400
N	4.01800	38.46500	53.89100
H	4.15200	38.99600	54.75200
C	4.16300	39.15200	52.61400
C	4.86000	40.46200	52.87800
O	5.13400	40.80000	54.02800
C	2.78400	39.44600	52.01700
C	1.85800	40.21500	52.97300
C	0.42600	40.34900	52.46200
O	0.10100	41.25000	51.68300
N	-0.43600	39.43900	52.90000
H	-0.16700	38.69500	53.54400
H	-1.39300	39.52900	52.55900
N	5.14800	41.19600	51.80800
H	4.91800	40.84300	50.87900
C	5.78700	42.49700	51.94400
C	4.80100	43.33400	52.74200
O	3.76100	43.74100	52.23400
C	6.01300	43.12900	50.57300
C	6.64600	44.50700	50.65800
O	6.57000	45.15900	51.72700
O	7.21000	44.94700	49.63600
N	5.12100	43.61000	54.00600
C	4.22900	44.40300	54.85500
C	3.88300	45.73900	54.21300
O	2.76000	46.22400	54.31200
C	5.04200	44.57100	56.13000
C	6.42900	44.67800	55.59100
C	6.47400	43.56000	54.58000
N	4.86400	46.32400	53.54600
H	5.77200	45.86300	53.48800
C	4.67800	47.60100	52.89800
C	3.64700	47.48000	51.77400
O	2.58500	48.10200	51.82900
C	6.02500	48.08400	52.36800

C	6.15600	49.59200	52.28700
C	7.61000	50.03900	52.48600
C	8.10100	49.75000	53.91500
N	9.51400	50.18700	54.15200
H	9.84000	49.99500	55.09900
H	9.63300	51.17300	53.92000
H	10.14200	49.77500	53.46200
N	3.95400	46.66600	50.76800
H	4.84400	46.16800	50.79200
C	3.05900	46.45900	49.62500
C	1.67000	45.96100	50.03000
O	0.66000	46.31700	49.41200
C	3.69000	45.47000	48.64100
N	1.62700	45.12800	51.06300
H	2.49000	44.86500	51.53900
C	0.36100	44.59000	51.51800
C	-0.58800	45.66600	51.99800
O	-1.75100	45.72100	51.59100
N	-0.10100	46.53300	52.87300
H	0.86700	46.45700	53.18500
C	-0.94700	47.58700	53.38400
C	-1.42100	48.47700	52.25700
O	-2.56000	48.92400	52.25600
C	-0.20100	48.42000	54.41800
C	-1.01900	49.58700	54.93100
C	-0.42700	50.20900	56.17900
O	-0.42500	49.59500	57.25300
N	0.08500	51.43300	56.04700
H	0.48400	51.85200	56.88700
H	0.08300	51.93900	55.16100
N	-0.55300	48.71400	51.28300
H	0.37100	48.28400	51.31000
C	-0.91400	49.58300	50.18000
C	-2.02700	49.03500	49.32000
O	-2.94100	49.76900	48.95600
C	0.30200	49.90200	49.30500
C	0.00100	50.88000	48.15500
C	-0.80000	52.05500	48.67600
C	1.29200	51.35800	47.51400
N	-1.96200	47.75200	48.98800
H	-1.18200	47.18000	49.31200
C	-3.00600	47.16000	48.15900
C	-4.31700	47.08800	48.92600

O	-5.39000	47.19800	48.33900
C	-2.61600	45.75900	47.69900
C	-3.61100	45.14400	46.71300
C	-3.65900	46.00300	45.45500
C	-3.21300	43.70900	46.37400
N	-4.23300	46.91100	50.24000
H	-3.31700	46.83400	50.68200
C	-5.43600	46.82600	51.05300
C	-6.18000	48.14700	51.03700
O	-7.39800	48.18000	50.86700
C	-5.09300	46.45600	52.49600
O	-6.26700	46.40400	53.29500
H	-6.05400	46.17400	54.19200
N	-5.44300	49.23800	51.20800
H	-4.43500	49.14400	51.33000
C	-6.04200	50.56600	51.22500
C	-6.69300	50.90300	49.88700
O	-7.75200	51.53300	49.84800
C	-4.98300	51.61300	51.55800
C	-4.16200	51.27300	52.78100
C	-3.13100	52.33100	53.10900
O	-2.33800	52.69100	52.20700
O	-3.11400	52.79400	54.27100
N	-6.06700	50.47200	48.79800
H	-5.20300	49.93900	48.89900
C	-6.58300	50.74100	47.46400
C	-7.80100	49.89500	47.09700
O	-8.63700	50.32000	46.30200
C	-5.48400	50.50500	46.43100
C	-4.26200	51.41600	46.49000
C	-3.09100	50.77100	45.75900
C	-4.61400	52.75300	45.88800
N	-7.90600	48.70400	47.67400
H	-7.19900	48.41100	48.34800
C	-9.01200	47.80600	47.36400
C	-10.15400	47.74100	48.37300
O	-11.28700	47.41500	48.00300
C	-8.47700	46.39200	47.15000
C	-7.87300	46.16500	45.80300
C	-7.82300	47.18900	44.86300
C	-7.38000	44.90900	45.46000
C	-7.29500	46.96800	43.59400
C	-6.85100	44.67300	44.20500

C	-6.80900	45.70800	43.26300
N	-9.85700	48.03400	49.63700
H	-8.90200	48.30300	49.87300
C	-10.86200	47.98100	50.69600
C	-12.14100	48.75700	50.37500
O	-12.10000	49.87900	49.87500
C	-10.29200	48.49000	52.03400
O	-11.30900	48.43200	53.03800
H	-10.95800	48.74600	53.86300
C	-9.81200	49.91300	51.90000
N	-13.27900	48.14300	50.66900
H	-13.24900	47.21400	51.08800
C	-14.56400	48.76000	50.40900
C	-15.10300	49.40800	51.66700
O	-16.27500	49.78000	51.71600
C	-15.56200	47.71400	49.92300
C	-15.98000	46.74200	51.02400
O	-15.14400	46.17000	51.71700
N	-17.28100	46.55000	51.17800
H	-17.56000	45.90100	51.91300
H	-17.97600	47.02500	50.60200
N	-14.26800	49.54500	52.69300
H	-13.30300	49.22300	52.62200
C	-14.75300	50.16200	53.92000
C	-14.17700	51.54200	54.18200
O	-13.16300	51.92600	53.60700
C	-14.53000	49.24400	55.13000
C	-13.10400	48.98300	55.52000
C	-13.06600	48.13600	56.78900
N	-12.66700	46.74900	56.54700
H	-11.78100	46.58300	56.07000
C	-13.38600	45.69100	56.90900
N	-14.54900	45.85900	57.51800
H	-14.89800	46.80300	57.68200
H	-15.10100	45.04700	57.79600
N	-12.93200	44.46400	56.69600
H	-12.03600	44.33500	56.22700
H	-13.48400	43.65200	56.97400
N	-14.85800	52.28100	55.04900
H	-15.68300	51.87100	55.48700
C	-14.49400	53.64500	55.41000
C	-13.04600	53.83800	55.82900
O	-12.36800	54.74500	55.35000

C	-15.39800	54.13200	56.54700
C	-15.01700	53.59400	57.94000
C	-14.90600	52.06100	57.99800
C	-14.17300	51.61100	59.26900
N	-13.92900	50.13200	59.32900
H	-13.44200	49.83300	60.17400
H	-13.43400	49.81400	58.49600
H	-14.80200	49.61700	59.21500
N	-12.58300	52.97900	56.72800
H	-13.19300	52.22900	57.05300
C	-11.23500	53.07200	57.26500
C	-10.49900	51.74900	57.10000
O	-10.95400	50.71800	57.59700
C	-11.33100	53.43700	58.74800
C	-10.04500	53.91100	59.37300
C	-9.52000	55.16500	58.71200
O	-9.02500	55.06800	57.56500
O	-9.61500	56.24700	59.33900
N	-9.36300	51.77400	56.40800
H	-9.02400	52.65400	56.02000
C	-8.60300	50.55200	56.20200
C	-8.15700	49.98200	57.54100
O	-7.73300	50.71000	58.43300
C	-7.39100	50.81400	55.29500
C	-6.64400	49.53100	54.91300
O	-5.63000	49.18000	55.52500
N	-7.14900	48.82600	53.90300
H	-7.98600	49.11600	53.39800
H	-6.65200	47.97200	53.64900
N	-8.29100	48.66900	57.67400
H	-8.67800	48.13600	56.89500
C	-7.90900	47.95800	58.88300
C	-6.48200	47.44900	58.70000
O	-6.21000	46.66600	57.78700
C	-8.82700	46.72700	59.12200
C	-10.29700	47.15500	59.20500
C	-8.38900	45.98300	60.36800
C	-10.64000	48.01700	60.39000
N	-5.54700	47.90000	59.55000
C	-4.15500	47.45100	59.44700
C	-4.08000	46.01500	59.97200
O	-4.87100	45.62700	60.83500
C	-3.41600	48.44200	60.33200

C	-4.40300	48.65800	61.42700
C	-5.70500	48.84500	60.66700
N	-3.13600	45.23400	59.45700
H	-2.48800	45.61600	58.76800
C	-3.01300	43.83800	59.86200
C	-1.62800	43.44000	60.34900
O	-0.66800	44.20000	60.25000
C	-3.40000	42.93400	58.69300
C	-4.78400	43.16200	58.08800
C	-4.84800	42.48000	56.74100
C	-5.86400	42.63700	59.01600
N	-1.54200	42.22700	60.87400
H	-2.38700	41.65800	60.93100
C	-0.29600	41.67400	61.37200
C	0.11900	40.58100	60.39700
O	-0.72500	39.99100	59.72800
C	-0.51300	41.08600	62.76900
C	-0.00100	41.94900	63.90700
C	-0.49300	43.38200	63.80500
C	0.35300	44.31800	64.68100
N	0.04600	45.76600	64.43800
H	0.60800	46.38800	65.02000
H	-0.95000	45.95500	64.55500
H	0.14300	46.00100	63.45000
N	1.41400	40.32700	60.29000
H	2.08500	40.86700	60.83500
C	1.88000	39.28100	59.39800
C	2.05800	38.02100	60.22800
O	2.33300	38.09800	61.42600
C	3.22300	39.64600	58.77000
C	3.29300	40.77800	57.75800
C	4.70500	40.83800	57.21000
C	2.30300	40.54700	56.63200
N	1.89800	36.86200	59.59700
H	1.64500	36.85800	58.60900
C	2.07800	35.60400	60.29500
C	1.97500	34.40800	59.37400
O	1.33300	34.46700	58.33200
C	1.04700	35.46000	61.40200
O	1.29800	34.28400	62.14700
H	0.65300	34.19400	62.83900
N	2.62800	33.32000	59.75800
H	3.18200	33.34300	60.61400

C	2.56600	32.09700	58.97900
C	1.27600	31.39700	59.37300
O	0.74300	30.57800	58.62900
C	3.78700	31.23200	59.26300
C	4.87800	31.45600	58.24500
C	6.26300	31.17600	58.76200
O	6.46100	30.14500	59.42800
O	7.16600	31.98400	58.48300
N	0.78000	31.75100	60.55400
H	1.30200	32.42100	61.11900
C	-0.47400	31.22700	61.08000
C	-1.52100	32.15800	60.49500
O	-1.89000	33.15600	61.12000
C	-0.48200	31.31800	62.60700
C	-1.79200	30.85300	63.21100
O	-2.55600	30.16300	62.51000
O	-2.05000	31.16500	64.39000
N	-1.99700	31.82800	59.29500
H	-1.68500	30.96100	58.85800
C	-2.95400	32.67500	58.58800
C	-4.06800	31.96300	57.82800
O	-4.77200	32.59100	57.03900
C	-2.18900	33.52700	57.60100
S	-1.38500	32.46600	56.37100
N	-4.22800	30.66500	58.03300
H	-3.61400	30.16800	58.67800
C	-5.28400	29.95300	57.33300
C	-6.62100	30.13500	58.04800
O	-7.13800	29.22000	58.69100
C	-4.92700	28.47300	57.19900
C	-3.71100	28.26200	56.29700
C	-3.40800	26.78400	56.13600
C	-3.99300	28.88800	54.94800
N	-7.16400	31.34500	57.92400
H	-6.66500	32.04900	57.38000
C	-8.43900	31.71000	58.53100
C	-9.40100	32.22500	57.48400
O	-9.03100	32.43000	56.32500
C	-8.24300	32.80100	59.57700
C	-7.38900	32.36200	60.73100
C	-5.99800	32.28100	60.61000
C	-7.97700	31.95700	61.92600
C	-5.21800	31.80000	61.65600

C	-7.21600	31.47400	62.97100
C	-5.83900	31.39200	62.83900
O	-5.10200	30.87300	63.88400
H	-4.15800	30.81700	63.79400
N	-10.64300	32.42600	57.90500
H	-10.88000	32.20700	58.87200
C	-11.67400	32.95000	57.02600
C	-12.65800	33.74100	57.88100
O	-12.77100	33.50400	59.09100
C	-12.37700	31.80700	56.27700
C	-13.05100	30.62100	56.98100
C	-14.34500	31.04100	57.67400
C	-13.37500	29.56500	55.93100
N	-13.33600	34.70200	57.26400
H	-13.16500	34.87900	56.27400
C	-14.31800	35.50700	57.97300
C	-15.68800	35.21300	57.38700
O	-15.80900	34.97600	56.18400
C	-13.98500	36.98500	57.83000
C	-12.58900	37.29500	58.29200
O	-12.10000	36.68000	59.24300
N	-11.93500	38.25300	57.63500
H	-10.98700	38.46300	57.94900
H	-12.33900	38.76200	56.84900
N	-16.71900	35.22300	58.22900
H	-16.55900	35.43400	59.21400
C	-18.07500	34.93800	57.76800
C	-19.09100	36.04600	58.06100
O	-19.19800	36.52900	59.18700
C	-18.59200	33.63200	58.39800
C	-17.75400	32.44700	57.90800
C	-20.04800	33.44300	58.06500
C	-18.13400	31.11800	58.52600
N	-19.83800	36.44000	57.03400
H	-19.68700	36.01000	56.12200
C	-20.87100	37.47100	57.16800
C	-22.22900	36.90000	56.79500
O	-22.55400	36.82100	55.61600
C	-20.58800	38.66100	56.24800
C	-19.25600	39.31000	56.48900
C	-18.09400	38.78100	55.93200
C	-19.14700	40.43600	57.30000
C	-16.85200	39.35600	56.17600

C	-17.90500	41.02100	57.55200
C	-16.76200	40.47300	56.98500
O	-15.53100	41.04000	57.23000
H	-14.74900	40.66500	56.84200
N	-23.02100	36.48900	57.77900
H	-22.70800	36.55100	58.74800
C	-24.34300	35.94800	57.46900
C	-25.45900	36.92300	57.82900
O	-25.47100	37.50600	58.91400
C	-24.61100	34.61800	58.18600
O	-25.91700	34.16000	57.83200
H	-25.96500	34.05500	56.88900
C	-24.53400	34.78600	59.69600
N	-26.40600	37.12600	56.90900
C	-27.51000	38.04300	57.17000
C	-28.70500	37.31300	57.76700
O	-29.69400	37.93500	58.14400
C	-27.80700	38.60700	55.78600
C	-27.63600	37.40500	54.92900
C	-26.37500	36.74400	55.48600
N	-28.59600	35.99400	57.86900
H	-27.72800	35.54500	57.57600
C	-29.68300	35.16400	58.38900
C	-29.95000	35.29100	59.88400
O	-29.07900	35.68900	60.64700
C	-29.42400	33.69900	58.03500
N	-31.17000	34.96500	60.29400
H	-31.87100	34.68100	59.61000
C	-31.52100	35.00700	61.70200
C	-31.12600	33.64200	62.24300
O	-31.86800	32.66900	62.12000
C	-33.02000	35.24500	61.86600
C	-33.47300	35.17900	63.31300
O	-32.63200	35.39400	64.22100
O	-34.68000	34.92900	63.53900
N	-29.93900	33.57500	62.83500
H	-29.38000	34.42400	62.91900
C	-29.41000	32.32300	63.36900
C	-30.28200	31.59800	64.40200
O	-29.98700	30.45900	64.79300
C	-28.00800	32.56900	63.93200
C	-26.98400	32.94700	62.85900
C	-25.65400	33.28300	63.49800

C	-26.83400	31.79600	61.88000
N	-31.36400	32.25000	64.82300
H	-31.55500	33.18100	64.45300
C	-32.28500	31.67400	65.79800
C	-33.28200	30.73100	65.12500
O	-34.20100	30.22300	65.76400
C	-33.05500	32.76900	66.52700
O	-33.82300	33.51900	65.57900
H	-34.42700	32.93800	65.13200
C	-32.09200	33.69400	67.24000
N	-33.09200	30.50800	63.83000
H	-32.32500	30.98100	63.35200
C	-33.94700	29.60900	63.07600
C	-33.21800	29.08100	61.85700
O	-32.17200	29.61100	61.48600
C	-35.23400	30.31900	62.67600
C	-35.05600	31.72900	62.20100
C	-36.39600	32.44200	62.18900
C	-36.94300	32.55500	63.59300
N	-38.36600	32.95100	63.58100
H	-38.73500	33.02700	64.52900
H	-38.92700	32.31900	63.01000
H	-38.51200	33.81000	63.05100
N	-33.76300	28.03300	61.24500
H	-34.63800	27.64900	61.60300
C	-33.14300	27.41700	60.07500
C	-33.18400	28.32700	58.85600
O	-34.19700	28.96700	58.57500
C	-33.83700	26.09800	59.73200
C	-33.02000	25.21300	58.79700
C	-33.88900	24.44200	57.81200
C	-34.91400	23.54400	58.49700
N	-35.77800	22.86900	57.47100
H	-36.46300	22.26800	57.92900
H	-35.22500	22.36000	56.78200
H	-36.21900	23.54000	56.84200
N	-32.07800	28.37700	58.13200
H	-31.27300	27.81700	58.41300
C	-31.98400	29.20700	56.95100
C	-30.97000	28.62100	56.01400
O	-29.89200	28.21700	56.43400
C	-31.53500	30.61100	57.31500
C	-32.65000	31.62500	57.21800

O	-33.35300	31.71800	56.19800
N	-32.81100	32.41200	58.27700
H	-32.23400	32.33600	59.11400
H	-33.56400	33.09700	58.21100
N	-31.31200	28.58700	54.73600
H	-32.22400	28.94500	54.45300
C	-30.41500	28.05100	53.72800
C	-30.23300	29.06500	52.61000
O	-30.86300	28.97200	51.55300
C	-30.96500	26.72300	53.18900
C	-30.43200	25.48100	53.92300
C	-30.50200	25.65200	55.43000
N	-29.84800	24.57700	56.17100
H	-29.57300	23.73800	55.66000
C	-29.59100	24.63100	57.47400
N	-29.92700	25.70200	58.16700
H	-29.73000	25.74300	59.16700
H	-30.37500	26.48500	57.69200
N	-29.00900	23.61400	58.09100
H	-28.81200	23.65500	59.09100
H	-28.74900	22.78600	57.55500
N	-29.36000	30.03900	52.86200
H	-28.87000	30.04200	53.75700
C	-29.08000	31.10100	51.90300
C	-27.94700	30.76200	50.95500
O	-27.07200	29.97200	51.28100
C	-28.72800	32.39200	52.64000
C	-29.81900	33.00800	53.51100
C	-29.38300	34.38800	54.02300
C	-31.07500	33.13400	52.68900
N	-27.95900	31.34500	49.75300
C	-26.86600	31.04100	48.83300
C	-25.55600	31.54200	49.44800
O	-25.53700	32.54500	50.17500
C	-27.26600	31.78900	47.56500
C	-28.07400	32.92200	48.08400
C	-28.91600	32.27700	49.14200
N	-24.46900	30.83200	49.16100
H	-24.55300	30.02700	48.54000
C	-23.15800	31.17000	49.70800
C	-22.14800	31.58600	48.63800
O	-21.99200	30.92400	47.60900
C	-22.59200	29.97400	50.52000

C	-21.33400	30.38200	51.27500
C	-23.65800	29.46700	51.49300
N	-21.47400	32.70200	48.89800
H	-21.66900	33.19800	49.76800
C	-20.47000	33.24700	47.99500
C	-19.12000	33.36300	48.71800
O	-18.96500	34.14000	49.67100
C	-20.90800	34.62700	47.49400
C	-22.21400	34.63400	46.72400
S	-22.67300	36.27700	46.09600
C	-21.49400	36.48900	44.74700
N	-18.14900	32.57800	48.26100
H	-18.34200	31.95200	47.47900
C	-16.81700	32.59000	48.84900
C	-15.90900	33.51100	48.02600
O	-15.74900	33.31500	46.81500
C	-16.23000	31.15600	48.88400
C	-14.87600	31.14300	49.61400
C	-17.22600	30.22400	49.56000
N	-15.32300	34.51100	48.68500
H	-15.48800	34.60800	49.68700
C	-14.45200	35.47000	48.01400
C	-12.95600	35.18000	48.12100
O	-12.43400	34.98800	49.21800
C	-14.72200	36.86900	48.55100
C	-13.74900	37.88300	48.03800
C	-12.66500	38.40200	48.70000
C	-13.75100	38.48300	46.74200
N	-11.99600	39.29100	47.88900
H	-11.15800	39.81300	48.14400
C	-12.64200	39.35800	46.68200
C	-14.58300	38.36700	45.62400
C	-12.34800	40.11100	45.54400
C	-14.29300	39.11400	44.49500
C	-13.18300	39.97700	44.46200
N	-12.26700	35.17000	46.97900
H	-12.76000	35.34000	46.10200
C	-10.82100	34.92200	46.94600
C	-10.08600	36.17700	46.48900
O	-10.09100	36.50700	45.30300
C	-10.46700	33.76600	45.99400
C	-11.19000	32.49400	46.43800
C	-8.97100	33.54300	45.99200

C	-10.86300	31.27000	45.60300
N	-9.45100	36.86400	47.44000
H	-9.46800	36.50600	48.39500
C	-8.73000	38.11000	47.17200
C	-7.56500	37.96200	46.21600
O	-6.93400	36.91300	46.15000
C	-8.18400	38.69800	48.46500
C	-6.95500	38.00600	48.95500
N	-6.98000	37.06800	49.96100
H	-7.80800	36.78900	50.48800
C	-5.67100	38.07200	48.53300
C	-5.76300	36.58500	50.13800
N	-4.95100	37.17700	49.28100
H	-3.95100	36.99700	49.19000
N	-7.26000	39.03400	45.49900
H	-7.80900	39.88800	45.60300
C	-6.14900	38.99800	44.56700
C	-4.87600	39.51400	45.20700
O	-4.81800	39.73200	46.41200
N	-3.85200	39.72400	44.39600
H	-3.94800	39.54300	43.39700
C	-2.59500	40.21000	44.92600
C	-1.43900	39.42900	44.34100
O	-0.42300	39.21600	44.99400
N	-1.61200	38.98800	43.10100
H	-2.49100	39.18400	42.62100
C	-0.58200	38.23500	42.41200
C	-0.04500	37.03200	43.15400
O	1.09200	36.63000	42.93200
N	-0.85400	36.44700	44.02800
H	-1.79500	36.81500	44.16600
C	-0.41800	35.28600	44.79300
C	0.77500	35.65600	45.67700
O	1.38300	34.78600	46.29300
C	-0.03000	34.15100	43.84800
C	-1.07700	33.77300	42.79900
C	-0.53500	32.65800	41.94200
C	-2.37300	33.33500	43.46600
N	1.10100	36.94900	45.72800
H	0.55200	37.61100	45.18000
C	2.21300	37.46100	46.53600
C	1.74200	38.28800	47.74700
O	2.39900	38.30600	48.78800

C	3.14300	38.34300	45.68700
C	3.94500	37.63800	44.59600
S	5.06900	36.35000	45.17900
C	6.12100	37.26800	46.39300
N	0.61400	38.97900	47.61100
H	0.10000	38.92900	46.73100
C	0.09700	39.80600	48.69400
C	-1.41500	39.73100	48.74400
O	-2.04300	39.23000	47.81600
C	0.49800	41.29100	48.50500
C	2.01300	41.44500	48.61900
C	0.00300	41.80000	47.15400
N	-1.99700	40.24400	49.82300
H	-1.42600	40.65400	50.56200
C	-3.44100	40.22200	49.95300
C	-3.91500	39.66300	51.27900
O	-3.15400	39.01400	51.99300
N	-5.17900	39.91800	51.60800
H	-5.75400	40.46200	50.96500
C	-5.77500	39.44600	52.86000
C	-7.28900	39.38300	52.72200
O	-7.86600	40.05200	51.86000
C	-5.40700	40.37700	53.99500
N	-7.93500	38.58600	53.57100
H	-7.41000	38.06300	54.27200
C	-9.39000	38.45400	53.50800
C	-10.05100	39.66600	54.12600
O	-10.97200	40.23500	53.54400
C	-9.84700	37.18900	54.22300
N	-9.56000	40.05900	55.30000
H	-8.78100	39.53600	55.70000
C	-10.08400	41.20400	56.04400
C	-10.25200	42.49200	55.23000
O	-11.06100	43.35200	55.57500
C	-9.19700	41.47600	57.25700
O	-9.31400	40.43300	58.20100
H	-8.76200	40.60200	58.95600
N	-9.48800	42.62700	54.15400
H	-8.82700	41.88800	53.91400
C	-9.57400	43.80900	53.30800
C	-11.00100	43.99800	52.79900
O	-11.50500	45.12600	52.71500
C	-8.60600	43.69300	52.09400

O	-7.26400	43.95300	52.52700
H	-7.02700	43.34200	53.21400
C	-8.98600	44.67400	50.99100
N	-11.65400	42.88500	52.48200
H	-11.19600	41.98300	52.61400
C	-13.00400	42.92500	51.95200
C	-14.05500	42.66400	53.01900
O	-14.11900	41.58700	53.59800
C	-13.10900	41.93500	50.79400
C	-11.93700	42.08100	49.84400
C	-10.68000	41.56900	50.17500
C	-12.06100	42.78600	48.64700
C	-9.58900	41.75400	49.34600
C	-10.95800	42.97900	47.80700
C	-9.72800	42.45800	48.16300
O	-8.63300	42.61000	47.33300
H	-7.78800	42.25200	47.57800
N	-14.85900	43.68900	53.28200
H	-14.72700	44.55500	52.76000
C	-15.91700	43.63700	54.27600
C	-17.21600	43.22200	53.59000
O	-17.68300	43.89800	52.67600
C	-16.07100	45.01500	54.91100
C	-17.15500	45.05100	55.95700
O	-17.42200	46.14400	56.49900
O	-17.74100	43.98300	56.24000
N	-17.80700	42.11900	54.03700
H	-17.40400	41.60800	54.82200
C	-19.02600	41.64100	53.40800
C	-20.35300	42.11500	53.97300
O	-21.40400	41.71600	53.47600
N	-20.31000	42.97300	54.98900
H	-19.40000	43.28600	55.32800
C	-21.51800	43.48600	55.64000
C	-22.63200	43.96900	54.70500
O	-23.80700	43.62500	54.89600
C	-21.15600	44.62300	56.59900
C	-22.36100	45.27600	57.28200
C	-23.04300	44.26500	58.19300
C	-21.92300	46.46800	58.08300
N	-22.26700	44.76800	53.70500
H	-21.28200	45.00900	53.59000
C	-23.24800	45.30500	52.77200

C	-23.82900	44.24600	51.84700
O	-25.05100	44.08300	51.77800
C	-22.63300	46.43200	51.95600
N	-22.96000	43.52100	51.14300
H	-21.96000	43.68800	51.25800
C	-23.41200	42.49000	50.20900
C	-24.32600	41.47500	50.86900
O	-25.33000	41.07200	50.29200
C	-22.22200	41.77200	49.57700
C	-22.53000	40.59200	48.65200
C	-23.59600	40.96200	47.63200
C	-21.24200	40.16700	47.96300
N	-23.97900	41.06500	52.08300
H	-23.13100	41.43300	52.51400
C	-24.78900	40.10000	52.80700
C	-26.16000	40.68400	53.13000
O	-27.18700	40.03800	52.90900
C	-24.08700	39.68300	54.08100
N	-26.18800	41.90400	53.65300
H	-25.31600	42.40500	53.82300
C	-27.47000	42.53100	53.98600
C	-28.32100	42.81100	52.73700
O	-29.47900	42.41200	52.66000
C	-27.24200	43.82700	54.77100
N	-27.73700	43.47800	51.75200
H	-26.76200	43.76300	51.84600
C	-28.46800	43.80900	50.54000
C	-28.94800	42.65100	49.67800
O	-30.00200	42.76100	49.07300
C	-27.64600	44.75300	49.66700
C	-27.58200	46.15100	50.19100
N	-28.31500	47.18200	49.64900
H	-28.94000	47.10300	48.84600
C	-26.89300	46.68400	51.23000
C	-28.08300	48.29000	50.33100
N	-27.22300	48.01300	51.29600
H	-26.86300	48.68000	51.97900
N	-28.21100	41.54700	49.60900
H	-27.35300	41.46600	50.15500
C	-28.64100	40.44800	48.74300
C	-29.04200	39.15700	49.42600
O	-29.35500	38.16100	48.77800
C	-27.57200	40.16900	47.69100

C	-27.60700	41.15300	46.55800
C	-29.00100	41.27500	45.96500
O	-29.68000	40.23400	45.84600
O	-29.41800	42.40000	45.60900
N	-29.03500	39.18000	50.74600
H	-28.74800	40.03200	51.22800
C	-29.42500	38.02300	51.52400
C	-28.65300	36.76500	51.19000
O	-29.23200	35.74300	50.84100
C	-30.90400	37.76300	51.34600
C	-31.53300	37.25500	52.59800
O	-32.16400	36.20000	52.60600
N	-31.36000	38.00200	53.68600
H	-31.79000	37.65400	54.54300
H	-30.83600	38.87700	53.67900
N	-27.33600	36.85200	51.30700
H	-26.92400	37.74100	51.59100
C	-26.46500	35.72900	51.04500
C	-25.37200	35.73000	52.09900
O	-25.08300	36.75600	52.71700
C	-25.81400	35.84400	49.67500
C	-26.87700	35.95000	48.60600
C	-24.92300	37.05800	49.63300
N	-24.77600	34.56800	52.31700
H	-25.08000	33.74000	51.80400
C	-23.69500	34.46000	53.27800
C	-22.42700	34.77800	52.50500
O	-22.22200	34.28000	51.39500
C	-23.60200	33.03600	53.85500
C	-22.36100	32.89900	54.72200
C	-24.84800	32.73600	54.66600
N	-21.59100	35.63300	53.07300
H	-21.82000	36.04400	53.97800
C	-20.35200	35.98600	52.41300
C	-19.19400	35.43500	53.22800
O	-19.09900	35.67600	54.44000
C	-20.20400	37.51500	52.26200
C	-18.87300	37.84900	51.58900
C	-21.35900	38.06300	51.45200
N	-18.32800	34.68000	52.55200
H	-18.48800	34.52200	51.55700
C	-17.16200	34.07200	53.17800
C	-15.89300	34.52300	52.47100

O	-15.73100	34.30200	51.27000
C	-17.23000	32.52500	53.11600
C	-16.00900	31.92100	53.76800
C	-18.47500	32.03300	53.81600
N	-15.00600	35.17700	53.21600
H	-15.22700	35.36300	54.19400
C	-13.72700	35.63800	52.68200
C	-12.66300	34.71600	53.28400
O	-12.64700	34.48400	54.50300
C	-13.44800	37.11100	53.06900
O	-13.55600	37.26900	54.48800
H	-13.38500	38.17300	54.72500
C	-14.44600	38.03500	52.38300
N	-11.79600	34.17800	52.42500
H	-11.86200	34.42500	51.43800
C	-10.75300	33.24500	52.85300
C	-9.34100	33.73100	52.57400
O	-9.12700	34.58600	51.72300
C	-10.89700	31.89800	52.13700
C	-10.52100	32.06100	50.66200
C	-12.32400	31.39000	52.26500
C	-10.51300	30.77600	49.87900
N	-8.37900	33.17100	53.29300
H	-8.62300	32.47900	54.00100
C	-6.98700	33.52100	53.09400
C	-6.23800	32.26400	52.71500
O	-6.61800	31.16900	53.11500
C	-6.40500	34.13100	54.35700
C	-6.92300	35.54200	54.57600
C	-6.28000	36.26800	55.74700
O	-6.50400	37.46800	55.93700
N	-5.48500	35.54800	56.53900
H	-5.05400	36.03500	57.32500
H	-5.30000	34.55700	56.38200
N	-5.19200	32.41100	51.91500
H	-4.93700	33.34300	51.58800
C	-4.40100	31.26200	51.49500
C	-2.94700	31.68700	51.49000
O	-2.64900	32.87300	51.30800
C	-4.81200	30.82000	50.09800
C	-4.89400	31.96800	49.12300
C	-6.01100	32.78800	49.08200
C	-3.84300	32.24800	48.25500

C	-6.08400	33.85600	48.20100
C	-3.90500	33.31300	47.37300
C	-5.02800	34.11200	47.35100
O	-5.09700	35.17400	46.47900
H	-4.37000	35.35000	45.89400
N	-2.04700	30.73000	51.69500
H	-2.36200	29.77000	51.83800
C	-0.61600	31.02600	51.72000
C	-0.17800	31.74000	50.44500
O	-0.68600	31.46900	49.36400
C	0.18800	29.73100	51.91800
C	0.17500	29.20500	53.35300
C	0.82000	27.83900	53.46700
N	-0.12000	26.75000	53.21600
H	-1.09900	26.99200	53.06200
C	0.21600	25.46200	53.17500
N	1.47300	25.08400	53.36700
H	1.73000	24.09700	53.33600
H	2.18600	25.79100	53.54700
N	-0.70900	24.54400	52.94200
H	-0.45200	23.55700	52.91100
H	-1.67600	24.83500	52.79400
N	0.77300	32.65400	50.58400
H	1.16900	32.81600	51.51000
C	1.27100	33.43500	49.45900
C	2.78600	33.27600	49.27100
O	3.48600	32.73900	50.13700
C	0.93600	34.91500	49.69300
C	-0.52200	35.25000	50.03700
C	-0.60600	36.57300	50.78400
C	-1.34500	35.29700	48.76300
N	3.27800	33.75500	48.13000
H	2.64100	34.17100	47.45100
C	4.69600	33.70000	47.82800
C	5.38800	32.37100	48.06000
O	4.86300	31.30800	47.72600
N	6.58900	32.43800	48.62400
H	6.97400	33.35100	48.86800
C	7.36600	31.24700	48.90100
C	6.53000	30.24300	49.68200
O	6.39800	29.08500	49.28400
C	8.62600	31.58700	49.71400
C	9.47500	32.59800	48.95800

C	9.45100	30.34700	49.94800
C	10.79600	32.89200	49.63400
N	5.95800	30.69600	50.79000
H	6.09200	31.67200	51.05300
C	5.14300	29.83700	51.64300
C	4.05300	29.04200	50.93900
O	3.76100	27.91000	51.33200
C	4.48200	30.66300	52.73900
C	5.42800	31.19100	53.75400
C	5.81900	30.58100	54.90600
C	6.11600	32.44200	53.70500
N	6.71100	31.37400	55.58400
H	7.15300	31.14400	56.47400
C	6.91000	32.52400	54.86900
C	6.14000	33.50200	52.79000
C	7.71900	33.62800	55.14100
C	6.94400	34.59700	53.06000
C	7.72200	34.65100	54.22600
N	3.44700	29.62400	49.90900
H	3.73700	30.55100	49.59700
C	2.37000	28.92900	49.23300
C	2.60000	28.54400	47.79600
O	1.74000	27.92900	47.17100
N	3.75700	28.87800	47.25100
H	4.46900	29.36600	47.79500
C	3.99100	28.53400	45.86200
C	5.38300	28.03000	45.53000
O	5.69000	27.78700	44.36500
C	3.60100	29.72800	44.98500
C	2.14600	30.04200	45.04900
C	1.21800	29.17800	44.48600
C	1.68700	31.14700	45.74700
C	-0.15800	29.40600	44.62200
C	0.31200	31.38600	45.88900
C	-0.60900	30.50900	45.32400
N	6.21900	27.86100	46.54700
H	5.91400	28.08700	47.49400
C	7.56600	27.35600	46.32500
C	7.47600	25.96700	45.70400
O	6.72000	25.12400	46.17200
C	8.34400	27.29500	47.65100
C	9.67900	26.62900	47.53200
C	9.83200	25.29300	47.86500

C	10.77000	27.31700	47.00700
C	11.05700	24.64600	47.66800
C	11.99300	26.68200	46.80700
C	12.13700	25.34300	47.13600
N	8.24200	25.72400	44.64800
H	8.86400	26.45000	44.29400
C	8.19700	24.41800	43.99000
C	9.54500	23.95200	43.45600
O	10.27600	24.72700	42.84100
C	7.19600	24.44400	42.83100
O	7.23600	23.22200	42.11700
H	6.61500	23.23800	41.39800
N	9.86300	22.68300	43.68400
H	9.21500	22.09100	44.20400
C	11.11700	22.12100	43.20700
C	10.85700	21.42500	41.89100
O	11.77500	20.89700	41.26900
C	11.69500	21.06800	44.18500
O	10.73400	20.02100	44.38500
H	11.08800	19.37500	44.98500
C	12.04700	21.70200	45.52100
N	9.59700	21.41300	41.47600
H	8.87500	21.87200	42.03200
C	9.24000	20.75100	40.23600
C	9.13100	19.23400	40.35900
O	8.98100	18.53200	39.35900
N	9.21200	18.70800	41.57400
H	9.35200	19.31400	42.38300
C	9.10100	17.26700	41.75600
C	8.30900	16.90600	43.01700
O	7.71700	17.77100	43.65400
C	10.49400	16.63200	41.78200
C	11.27800	17.00300	43.00900
O	12.49600	16.74900	43.02900
O	10.67800	17.53900	43.96000
N	8.31500	15.63400	43.39100
H	8.86900	14.95600	42.86800
C	7.54100	15.19900	44.53800
C	8.00500	15.69300	45.90000
O	7.23600	15.65100	46.86300
C	7.41600	13.66500	44.55100
C	8.57300	12.89100	45.18600
C	9.81100	12.80100	44.30500

O	10.72200	12.02200	44.66900
O	9.87500	13.49500	43.26600
N	9.24100	16.16800	46.00400
H	9.85300	16.19600	45.18800
C	9.71700	16.65100	47.30300
C	9.08500	17.99300	47.68800
O	9.10200	18.39300	48.85800
C	11.24500	16.74500	47.31200
C	11.92800	15.41600	47.18100
N	11.70700	14.37900	48.06300
H	11.09300	14.41600	48.87700
C	12.80300	14.95000	46.26200
C	12.41600	13.33100	47.68700
N	13.09000	13.64900	46.59800
H	13.72100	13.03000	46.08900
N	8.51100	18.67000	46.69800
H	8.54300	18.28200	45.75500
C	7.83800	19.94600	46.91000
C	7.05800	20.34100	45.65000
O	7.44300	21.26400	44.91600
C	8.85500	21.03000	47.26800
O	8.19700	22.24200	47.58200
H	8.82900	22.91600	47.80400
N	5.95900	19.63100	45.40800
H	5.69400	18.89200	46.05900
C	5.12300	19.87700	44.24200
C	4.80200	21.34000	44.03300
O	5.13500	21.91200	42.99600
C	3.81500	19.10800	44.35000
C	3.94000	17.62500	44.13500
C	2.56900	17.03300	43.96500
N	2.64500	15.72200	43.34900
H	2.31100	15.62300	42.39000
C	3.12200	14.64500	43.95700
N	3.55700	14.73400	45.20800
H	3.92400	13.90500	45.67600
H	3.51300	15.62300	45.70600
N	3.17900	13.48600	43.30700
H	3.54600	12.65700	43.77500
H	2.84500	13.41800	42.34600
N	4.13600	21.93200	45.01900
H	3.88200	21.39400	45.84700
C	3.76500	23.33200	44.93500

C	2.26400	23.54600	45.01100
O	1.50500	22.61500	45.27500
N	1.84100	24.78400	44.78800
H	2.52700	25.51100	44.58600
C	0.43100	25.13800	44.82200
C	-0.21300	25.02200	46.19400
O	-1.43200	24.87100	46.30800
C	-0.34900	24.28000	43.83800
C	0.10600	24.47600	42.42800
O	0.44700	25.59100	42.03000
N	0.10100	23.40000	41.64600
H	-0.18100	22.47700	41.97600
H	0.41200	23.53400	40.68400
N	0.60200	25.09500	47.23400
H	1.60400	25.21300	47.08300
C	0.08500	25.00900	48.58600
C	-1.10000	25.96300	48.74700
O	-2.10300	25.62100	49.38500
C	1.19500	25.35600	49.56700
C	2.46900	24.70300	49.17200
C	3.65300	25.31500	48.90100
C	2.67800	23.30400	48.94600
N	4.59100	24.38900	48.51700
H	5.55600	24.59400	48.26000
C	4.01900	23.14400	48.53600
C	1.86000	22.16600	49.05100
C	4.56700	21.89400	48.22900
C	2.40200	20.92600	48.74900
C	3.74500	20.80000	48.34200
N	-0.98600	27.14900	48.14700
H	-0.13800	27.36400	47.62200
C	-2.04600	28.14300	48.22600
C	-3.38300	27.68300	47.66500
O	-4.42600	27.87300	48.29500
N	-3.35700	27.08300	46.47800
H	-2.46600	26.96200	45.99700
C	-4.57700	26.59700	45.85500
C	-5.17300	25.49700	46.71400
O	-6.39300	25.37100	46.82500
C	-4.29100	26.07100	44.44800
C	-3.87200	27.13600	43.48300
N	-4.49900	28.36300	43.41300
H	-5.29400	28.65300	43.98300

C	-2.88200	27.16600	42.56100
C	-3.90900	29.10400	42.49200
N	-2.92500	28.40200	41.96000
H	-2.29800	28.72400	41.22300
N	-4.30300	24.70000	47.32600
H	-3.30400	24.84700	47.18500
C	-4.75000	23.62500	48.19000
C	-5.47000	24.19600	49.39900
O	-6.46600	23.62400	49.85900
C	-3.56600	22.77700	48.63000
C	-2.99800	21.97700	47.46100
C	-1.94800	20.99100	47.96500
C	-4.15000	21.25300	46.74800
N	-4.96100	25.32400	49.90200
H	-4.12300	25.72100	49.47600
C	-5.56700	26.00800	51.04400
C	-6.96800	26.46700	50.62700
O	-7.93600	26.39200	51.40500
C	-4.73700	27.23200	51.47000
C	-3.37800	26.86100	52.06900
O	-3.23500	25.74900	52.62400
O	-2.45400	27.70400	52.00300
N	-7.06900	26.94500	49.39000
H	-6.24000	26.99200	48.79800
C	-8.34700	27.40000	48.87300
C	-9.27100	26.19900	48.83300
O	-10.34500	26.22500	49.42200
C	-8.16100	28.02800	47.49200
C	-7.24300	29.24200	47.55400
C	-6.87400	29.79900	46.19500
O	-6.84400	29.07600	45.19500
N	-6.56100	31.08900	46.15800
H	-6.58600	31.68600	46.98400
H	-6.31200	31.46400	45.24300
N	-8.85400	25.13100	48.16600
H	-7.95800	25.14400	47.68000
C	-9.69100	23.93900	48.13600
C	-10.06900	23.55100	49.57500
O	-11.20300	23.16500	49.84000
C	-8.97100	22.74400	47.44600
C	-9.63000	21.43400	47.84400
C	-9.04600	22.89900	45.94100
N	-9.12500	23.68200	50.50200

H	-8.20500	24.02800	50.22900
C	-9.37100	23.34300	51.90300
C	-10.51300	24.13300	52.52400
O	-11.32200	23.58300	53.26800
C	-8.10700	23.55500	52.72100
N	-10.57000	25.42800	52.23500
H	-9.86900	25.84000	51.61800
C	-11.62300	26.26500	52.79000
C	-12.99000	25.92600	52.18400
O	-14.02800	26.10000	52.83300
C	-11.29000	27.72000	52.56800
N	-12.99900	25.44200	50.94500
H	-12.12000	25.31900	50.44200
C	-14.25700	25.08700	50.30200
C	-14.82500	23.85100	50.97100
O	-16.05200	23.69500	51.07300
C	-14.05300	24.83700	48.81000
C	-13.78400	26.12700	48.03300
C	-13.41900	25.80500	46.59500
C	-15.00500	27.02000	48.10400
N	-13.93400	22.97000	51.42500
H	-12.93800	23.14100	51.28400
C	-14.36700	21.76600	52.12000
C	-14.85700	22.16100	53.50400
O	-15.82500	21.59800	53.99800
C	-13.23500	20.74700	52.25100
C	-12.97100	19.95900	50.99300
C	-11.92800	18.87000	51.21300
N	-11.42500	18.33800	49.94600
H	-10.46100	18.55400	49.69300
C	-12.13300	17.59200	49.09700
N	-13.39500	17.26500	49.36500
H	-13.93600	16.69400	48.71600
H	-13.82100	17.58000	50.23700
N	-11.57800	17.18200	47.96200
H	-12.11900	16.61100	47.31300
H	-10.61100	17.43300	47.75700
N	-14.19600	23.12200	54.13700
H	-13.38200	23.55800	53.70500
C	-14.64200	23.54400	55.44600
C	-16.06800	24.05300	55.30500
O	-16.93800	23.72500	56.11800
C	-13.77500	24.66600	55.99900

C	-14.17400	25.06000	57.39900
C	-13.70100	24.53100	58.56700
C	-15.18300	26.01000	57.77200
N	-14.35300	25.08600	59.63800
H	-14.18400	24.85700	60.61800
C	-15.26800	25.99800	59.18000
C	-16.02600	26.86700	57.05100
C	-16.15800	26.80900	59.88300
C	-16.91200	27.67200	57.75000
C	-16.96900	27.63800	59.15300
N	-16.30100	24.85800	54.27000
H	-15.53500	25.08800	53.63700
C	-17.62800	25.42100	54.01800
C	-18.66300	24.32300	53.78900
O	-19.76300	24.36800	54.33400
C	-17.61400	26.38100	52.79300
C	-19.04200	26.80700	52.42000
C	-16.77600	27.60300	53.11600
N	-18.31300	23.33600	52.98100
H	-17.39300	23.34200	52.54000
C	-19.23300	22.24400	52.72000
C	-19.66400	21.55400	54.01500
O	-20.77800	21.05400	54.11700
C	-18.57900	21.21000	51.80800
C	-19.48600	20.04000	51.48500
C	-18.77500	18.94400	50.73100
O	-17.95500	18.20500	51.29600
N	-19.07100	18.83300	49.43800
H	-18.59000	18.09200	48.92800
H	-19.74500	19.44100	48.97300
N	-18.78200	21.52800	55.00400
H	-17.87700	21.98400	54.88500
C	-19.08800	20.86100	56.24900
C	-19.63700	21.73800	57.34900
O	-20.24600	21.23000	58.28400
C	-17.84600	20.14900	56.77000
C	-17.41600	19.00300	55.88400
O	-18.10200	18.74300	54.88000
O	-16.39100	18.35500	56.18400
N	-19.45000	23.04900	57.24200
H	-18.99100	23.43100	56.41500
C	-19.89800	23.94500	58.30300
C	-20.82000	25.10900	57.95500

O	-21.54800	25.60700	58.82300
C	-18.67100	24.51700	59.01500
C	-17.79400	23.44300	59.61500
O	-18.13000	22.85700	60.65400
N	-16.66100	23.16800	58.96200
H	-16.38400	23.65000	58.10700
H	-16.06900	22.44300	59.36700
N	-20.80300	25.55200	56.70500
H	-20.22700	25.08500	56.00500
C	-21.60900	26.70700	56.33500
C	-23.10800	26.65100	56.65200
O	-23.78500	27.68000	56.60500
C	-21.41400	27.06400	54.85100
C	-21.69600	28.55200	54.65000
C	-22.32000	26.21800	53.98000
C	-20.86400	29.45900	55.52100
N	-23.63300	25.47700	56.98900
H	-23.04400	24.64500	57.02900
C	-25.05000	25.38300	57.30100
C	-25.31300	25.93100	58.69100
O	-26.40500	26.41400	58.96700
C	-25.51400	23.95800	57.21600
N	-24.31600	25.85200	59.56800
H	-23.43100	25.43300	59.28100
C	-24.46000	26.35300	60.93500
C	-24.56800	27.87700	60.93900
O	-24.94500	28.48700	61.94300
C	-23.26000	25.93800	61.78900
O	-23.31000	24.56900	62.12900
H	-22.56500	24.31100	62.65900
N	-24.23200	28.48800	59.81000
H	-23.92500	27.93300	59.01100
C	-24.29400	29.93100	59.69500
C	-25.42600	30.39800	58.79700
O	-25.45600	31.55300	58.39100
C	-22.97200	30.47500	59.16900
C	-21.80600	30.23400	60.08700
C	-21.13400	29.02100	60.07300
C	-21.36700	31.23800	60.95300
C	-20.03900	28.81200	60.90300
C	-20.27700	31.03900	61.78500
C	-19.60900	29.82700	61.76300
N	-26.35000	29.50000	58.48200

H	-26.26700	28.54400	58.82900
C	-27.47500	29.86800	57.64900
C	-27.23200	29.70300	56.16800
O	-28.01800	30.17600	55.35100
N	-26.15100	29.03100	55.80400
H	-25.52100	28.64900	56.50900
C	-25.87000	28.84300	54.39300
C	-26.35800	27.51800	53.84100
O	-26.67500	26.59700	54.59300
N	-26.42300	27.42300	52.51700
H	-26.17000	28.23200	51.95000
C	-26.84500	26.19600	51.85000
C	-25.63300	25.59600	51.14600
O	-25.22700	26.06200	50.09300
C	-27.94900	26.49900	50.83500
C	-28.21200	25.33800	49.89500
O	-27.69800	24.23400	50.10000
N	-29.01700	25.57900	48.85800
H	-29.44200	26.49100	48.68900
H	-29.19400	24.79800	48.22600
N	-25.03400	24.55300	51.72600
C	-23.86000	23.94000	51.09300
C	-24.11000	23.46100	49.67200
O	-23.16500	23.22200	48.91800
C	-23.51800	22.79200	52.03400
C	-24.85300	22.44800	52.63100
C	-25.44200	23.79800	52.91800
N	-25.38200	23.33000	49.31200
H	-26.12200	23.55600	49.97600
C	-25.72500	22.86800	47.98300
C	-25.66300	23.95400	46.93500
O	-25.83700	23.68200	45.74800
N	-25.40800	25.18500	47.36700
H	-25.26900	25.34400	48.36500
C	-25.32300	26.31300	46.44800
C	-24.18300	27.28500	46.80600
O	-24.42300	28.41700	47.24900
C	-26.66500	27.05600	46.42400
O	-26.72200	28.02000	45.38000
H	-27.55300	28.48000	45.36500
N	-22.94300	26.84400	46.60300
H	-22.79700	25.90300	46.23800
C	-21.79200	27.68800	46.89600

C	-21.18100	28.27700	45.63100
O	-20.80900	27.55300	44.71400
C	-20.70900	26.91600	47.66900
C	-19.38600	27.68000	47.64000
C	-21.16400	26.72200	49.10500
N	-21.08800	29.60200	45.60300
H	-21.42000	30.13000	46.41000
C	-20.53400	30.33400	44.47400
C	-19.16000	30.86600	44.85800
O	-19.02100	31.49700	45.91000
C	-21.43200	31.54300	44.12600
O	-22.76300	31.09200	43.84900
H	-23.10800	30.62100	44.59800
C	-20.88000	32.29700	42.92700
N	-18.14400	30.60900	44.03400
H	-18.30300	30.05400	43.19300
C	-16.80000	31.11800	44.32600
C	-16.48900	32.24600	43.36400
O	-16.73900	32.13500	42.16500
C	-15.67600	30.05700	44.16300
C	-15.66300	29.50500	42.73200
C	-15.84800	28.95200	45.18800
C	-14.39100	28.72900	42.36300
N	-15.96800	33.34600	43.89000
H	-15.81800	33.40500	44.89700
C	-15.61100	34.46400	43.04100
C	-14.37700	35.18200	43.57400
O	-14.09500	35.16500	44.77600
C	-16.79700	35.42000	42.87700
C	-17.19800	36.14200	44.13100
C	-17.39300	35.45700	45.32300
C	-17.46000	37.51400	44.09700
C	-17.85100	36.12800	46.46200
C	-17.91600	38.18900	45.22700
C	-18.11300	37.49300	46.41100
N	-13.62100	35.77800	42.65900
H	-13.89300	35.74200	41.67700
C	-12.41500	36.47800	43.04400
C	-11.95800	37.40100	41.94200
O	-12.37000	37.25200	40.79800
N	-11.09100	38.34300	42.29200
H	-10.77200	38.37800	43.26000
C	-10.57600	39.32700	41.35300

C	-9.05600	39.22000	41.19400
O	-8.33100	38.96200	42.15500
C	-10.96800	40.72800	41.85800
C	-10.70100	41.91600	40.92500
C	-9.27600	42.45400	41.00900
O	-8.62800	42.29700	42.06800
O	-8.81000	43.05200	40.01400
N	-8.58200	39.41400	39.96800
H	-9.23700	39.59500	39.20800
C	-7.15300	39.37600	39.67600
C	-6.57000	38.00100	39.94900
O	-7.02100	37.00700	39.37700
C	-6.43400	40.42700	40.51800
O	-5.06000	40.45600	40.21100
H	-4.61300	41.11000	40.73500
N	-5.56000	37.94400	40.81500
H	-5.21400	38.80500	41.23900
C	-4.94100	36.67100	41.16700
C	-6.04600	35.75800	41.69300
O	-6.00800	34.54800	41.49100
C	-3.88000	36.87900	42.22900
N	-7.03600	36.36200	42.35400
H	-7.00200	37.37300	42.48200
C	-8.16000	35.61800	42.89600
C	-9.03900	35.09600	41.78100
O	-9.62500	34.02100	41.88500
N	-9.14400	35.87400	40.71100
H	-8.67000	36.77700	40.68900
C	-9.93100	35.44200	39.57400
C	-9.16400	34.31200	38.91700
O	-9.75700	33.36700	38.38800
N	-7.83600	34.41800	38.96200
H	-7.42900	35.24000	39.40800
C	-6.93700	33.41200	38.40200
C	-7.14300	32.12700	39.19800
O	-7.16200	31.02600	38.64600
C	-5.48200	33.88900	38.53100
C	-4.41600	33.05600	37.80200
C	-3.78000	31.97800	38.67800
O	-3.50100	32.25000	39.86600
O	-3.53800	30.86000	38.17200
N	-7.30700	32.28500	40.50400
H	-7.28100	33.22400	40.90100

C	-7.52300	31.15000	41.38000
C	-8.84700	30.46100	41.05400
O	-8.91800	29.22600	40.98100
C	-7.51300	31.60300	42.84400
O	-6.19900	31.93300	43.25700
H	-6.19300	32.21400	44.16500
N	-9.89800	31.25400	40.86200
H	-9.79200	32.26500	40.94100
C	-11.19500	30.68500	40.54100
C	-11.07100	29.87600	39.24900
O	-11.56000	28.74500	39.14900
C	-12.25300	31.78800	40.38900
C	-13.47700	31.24900	39.68400
C	-12.64500	32.30600	41.75600
N	-10.38500	30.44800	38.27200
H	-9.98700	31.37600	38.41500
C	-10.18900	29.77500	36.99900
C	-9.51900	28.40400	37.18100
O	-9.98400	27.38600	36.63700
C	-9.34100	30.65400	36.08600
O	-9.30200	30.11000	34.78100
H	-8.77400	30.65800	34.21200
N	-8.42500	28.39100	37.94700
H	-8.10400	29.26800	38.35800
C	-7.66900	27.16800	38.22000
C	-8.55300	26.13700	38.90000
O	-8.54000	24.97400	38.53100
C	-6.44200	27.44200	39.12800
C	-5.69300	26.15000	39.39400
C	-5.51900	28.44700	38.47900
N	-9.32000	26.56800	39.89600
H	-9.28300	27.55000	40.16900
C	-10.21300	25.66000	40.60500
C	-11.26200	25.06900	39.66500
O	-11.69700	23.92800	39.84100
C	-10.92300	26.37700	41.75300
C	-10.13600	26.75300	43.00400
C	-11.08100	27.42900	43.97600
C	-9.51600	25.52600	43.64000
N	-11.67900	25.84100	38.67000
H	-11.30600	26.78400	38.56100
C	-12.66900	25.33500	37.73800
C	-12.07700	24.22500	36.88900

O	-12.80500	23.42500	36.30900
C	-13.18800	26.42700	36.80600
C	-14.27000	25.85500	35.91700
C	-13.73900	27.58400	37.61600
N	-10.75400	24.17400	36.81700
H	-10.19700	24.86400	37.32200
C	-10.08200	23.14900	36.02900
C	-9.49600	22.01700	36.86900
O	-8.93600	21.07200	36.31800
C	-8.95400	23.76600	35.20500
C	-9.30900	24.80000	34.13900
C	-8.03500	25.35100	33.53500
C	-10.15000	24.16100	33.06500
N	-9.62700	22.09400	38.19200
H	-10.12900	22.88000	38.60600
C	-9.05800	21.06200	39.05500
C	-10.04100	20.03800	39.61600
O	-11.09700	20.39300	40.13200
C	-8.30400	21.71600	40.21600
O	-7.66000	20.74400	41.02800
H	-7.19200	21.15000	41.74800
N	-9.68900	18.74400	39.52900
C	-10.49600	17.62300	40.01700
C	-10.66300	17.73200	41.52400
O	-11.62300	17.22800	42.09900
C	-9.65000	16.40700	39.66800
C	-8.87000	16.85400	38.51100
C	-8.47400	18.24700	38.87300
N	-9.70100	18.39000	42.15800
H	-8.93700	18.79700	41.61800
C	-9.70800	18.54500	43.59600
C	-10.83600	19.43200	44.08100
O	-11.31700	19.26400	45.19800
C	-8.36800	19.10700	44.06500
C	-7.14700	18.22100	43.81600
C	-5.87200	18.97400	44.19400
C	-7.28300	16.93400	44.61800
N	-11.26400	20.37600	43.25100
H	-10.84000	20.47000	42.32800
C	-12.33400	21.27700	43.65000
C	-13.70300	20.77900	43.19200
O	-14.73500	21.33800	43.56000
C	-12.06400	22.66000	43.09900

N	-13.69600	19.72100	42.38800
H	-12.79800	19.31500	42.12500
C	-14.91600	19.11300	41.86400
C	-15.90700	18.84900	42.98900
O	-15.57100	18.19900	43.97800
C	-14.56400	17.79800	41.16600
C	-15.72500	17.07900	40.51400
C	-15.24000	15.83900	39.74800
C	-16.38900	15.13300	39.00000
N	-15.95500	13.87500	38.30300
H	-16.71500	13.40800	37.80800
H	-15.50000	13.23700	38.95600
H	-15.17200	14.05900	37.67600
N	-17.12300	19.36200	42.84100
H	-17.33000	19.90000	41.99900
C	-18.17900	19.18500	43.84100
C	-18.02100	19.98500	45.13000
O	-18.54600	19.60100	46.16800
C	-18.34400	17.70500	44.19700
C	-18.81000	16.87700	43.02000
O	-19.80000	17.21700	42.35900
N	-18.10200	15.78100	42.74800
H	-17.28600	15.50100	43.29300
H	-18.41600	15.22300	41.95400
N	-17.30300	21.09600	45.07000
H	-16.87000	21.37400	44.18900
C	-17.13000	21.91900	46.25100
C	-17.77200	23.27500	46.01400
O	-17.98100	24.04700	46.95400
C	-15.64800	22.06400	46.59000
C	-14.99600	20.79900	47.15500
C	-13.51000	21.03800	47.35700
C	-15.65500	20.42200	48.47300
N	-18.07300	23.56000	44.74700
H	-17.83300	22.88500	44.02100
C	-18.73400	24.80300	44.36100
C	-19.70700	24.50500	43.23600
O	-19.61000	23.46700	42.57100
C	-17.73900	25.88400	43.92500
C	-16.99600	25.56600	42.67000
C	-15.85900	24.76500	42.70100
C	-17.42600	26.07500	41.45300
C	-15.16100	24.47700	41.53000

C	-16.73600	25.79300	40.27900
C	-15.60100	24.99300	40.31400
N	-20.63800	25.42700	43.01900
H	-20.62500	26.28700	43.56800
C	-21.67400	25.24000	42.01800
C	-21.80900	26.38000	41.02300
O	-22.69300	26.34800	40.16300
C	-23.00200	25.03200	42.73000
C	-22.93100	24.04200	43.85100
N	-22.87900	22.68100	43.63900
H	-22.89500	22.22500	42.72700
C	-22.88100	24.21700	45.19000
C	-22.80600	22.06100	44.80100
N	-22.80500	22.96900	45.75900
H	-22.75600	22.77500	46.75900
N	-20.94900	27.38500	41.15000
H	-20.25900	27.35000	41.90000
C	-20.95700	28.53400	40.25600
C	-19.61600	29.19800	40.42600
O	-18.94200	28.96600	41.42300
C	-22.05900	29.51200	40.63800
C	-23.41800	28.87600	40.67500
C	-24.42400	29.74900	41.34800
N	-25.54800	28.96700	41.84300
H	-25.90600	29.18600	42.77300
C	-26.13800	27.99000	41.16800
N	-25.71600	27.65100	39.95800
H	-24.91500	28.13100	39.54800
H	-26.17000	26.89900	39.43900
N	-27.17500	27.36900	41.69800
H	-27.50000	27.63000	42.62900
H	-27.62900	26.61700	41.17900
N	-19.22700	30.02800	39.46300
H	-19.84000	30.19700	38.66500
C	-17.94000	30.69700	39.53400
C	-17.91200	31.97700	38.73000
O	-18.46800	32.04200	37.63300
C	-16.85300	29.76500	39.04600
N	-17.25800	32.99000	39.29500
H	-16.84200	32.84800	40.21500
C	-17.10900	34.29500	38.65700
C	-15.64000	34.69700	38.70900
O	-14.99200	34.56200	39.74100

C	-17.89000	35.40600	39.39700
C	-19.35900	35.03500	39.56300
C	-17.80700	36.70100	38.61400
C	-20.12400	36.06100	40.39000
N	-15.11600	35.18900	37.59800
H	-15.69100	35.25300	36.75800
C	-13.73200	35.64000	37.55400
C	-13.72000	37.12500	37.20500
O	-14.14900	37.51600	36.12200
C	-12.93600	34.85800	36.50700
O	-12.63800	33.55500	36.96100
H	-12.14400	33.06900	36.31100
N	-13.23900	37.95200	38.12600
H	-12.90600	37.57500	39.01300
C	-13.17800	39.39100	37.89100
C	-11.79000	39.87300	37.46700
O	-10.92000	40.12000	38.30100
C	-13.61500	40.15200	39.14400
C	-15.07200	39.98700	39.48700
C	-15.40400	40.53400	40.86200
O	-14.84500	41.58800	41.23100
O	-16.22800	39.92100	41.57300
N	-11.58900	40.00300	36.16100
H	-12.33700	39.76200	35.51100
C	-10.31900	40.48400	35.64500
C	-9.16600	39.54900	35.98400
O	-8.26300	39.93500	36.73000
C	-10.01300	41.88200	36.21100
O	-11.05400	42.80800	35.92100
H	-10.86500	43.67100	36.27000
N	-9.20200	38.33200	35.43600
H	-9.98800	38.07700	34.83800
C	-8.14500	37.36100	35.67300
C	-8.56700	35.92000	35.43300
O	-9.58100	35.48400	35.96500
N	-7.80300	35.18300	34.62500
H	-6.98600	35.61300	34.19100
C	-8.09900	33.77500	34.34000
C	-6.85100	32.88300	34.27100
O	-5.73400	33.32900	34.53000
C	-8.90400	33.59500	33.02700
C	-10.32300	34.06700	33.21800
C	-8.24900	34.35200	31.90400

N	-7.06300	31.61900	33.91000
H	-8.01500	31.34200	33.67100
C	-6.01000	30.60200	33.83500
C	-4.94500	30.82800	32.78200
O	-3.76000	30.66600	33.05800
C	-6.64000	29.23500	33.62600
N	-5.36800	31.17700	31.57100
H	-6.36900	31.27500	31.40300
C	-4.43400	31.42300	30.47600
C	-3.52800	32.62000	30.78500
O	-2.49200	32.79200	30.13200
C	-5.20000	31.69100	29.19300
C	-6.32800	30.70500	28.91400
C	-7.05400	31.11700	27.63800
C	-5.76200	29.30400	28.79300
N	-3.94500	33.44100	31.76500
H	-4.83800	33.23800	32.21400
C	-3.18700	34.61700	32.22800
C	-1.82500	34.11100	32.70700
O	-1.48100	34.10900	33.89900
C	-3.94600	35.38000	33.39000
O	-5.11900	36.02300	32.87300
H	-5.57400	36.48100	33.57000
C	-3.05900	36.45100	34.03900
N	-1.08000	33.65800	31.70900
H	-1.49700	33.70200	30.77900
C	0.26000	33.10700	31.78700
C	1.11200	33.52900	32.97000
O	1.54000	32.68400	33.74000
C	0.98700	33.42900	30.47100
O	0.11500	33.20400	29.37000
H	0.56400	33.40300	28.55700
N	1.35000	34.83000	33.10100
H	0.94500	35.47400	32.42200
C	2.17000	35.37100	34.18200
C	2.09300	34.67600	35.56400
O	3.11700	34.53300	36.25000
C	1.87800	36.88600	34.32700
C	0.39900	37.14600	34.09300
C	2.30500	37.38600	35.69600
N	0.89700	34.24100	35.96400
H	0.09100	34.37800	35.35400
C	0.70800	33.57100	37.25600

C	0.82300	32.05100	37.18500
O	0.69600	31.36900	38.20700
C	-0.65700	33.92500	37.84800
C	-0.86500	35.36400	38.30300
C	-2.24400	35.50700	38.92900
C	0.21500	35.73600	39.30100
N	1.05900	31.52900	35.98200
H	1.15200	32.15900	35.18500
C	1.19000	30.09200	35.75800
C	2.54500	29.73100	35.15300
O	2.72500	29.76600	33.94000
C	0.08000	29.58300	34.82100
C	0.19400	28.07600	34.64800
C	-1.28400	29.96200	35.38200
N	3.49200	29.37600	36.01300
H	3.26900	29.35800	37.00800
C	4.84000	29.01000	35.58800
C	4.82400	27.75500	34.72700
O	4.17100	26.77000	35.06800
C	5.72700	28.75100	36.80600
C	5.66000	29.81400	37.88400
C	6.80900	30.81400	37.81800
C	6.71000	31.79000	36.63800
N	7.37400	31.31000	35.38100
H	7.30800	31.95900	34.59700
H	7.01400	30.39300	35.11600
H	8.34800	31.06900	35.56300
N	5.55600	27.79100	33.61800
H	6.06900	28.64200	33.38900
C	5.64400	26.64300	32.72000
C	7.11800	26.32500	32.43400
O	7.97800	27.20100	32.50500
C	4.88000	26.93300	31.42600
C	3.44300	27.38100	31.67100
C	2.73600	27.76400	30.37400
C	1.40600	28.48300	30.63900
N	1.57800	29.85300	31.23000
H	0.69400	30.33100	31.40600
H	2.18900	30.42500	30.64700
H	2.14300	29.81300	32.07800
N	7.40400	25.06800	32.12400
H	6.65700	24.37600	32.06700
C	8.77500	24.67400	31.86600

C	9.34700	24.10500	33.14400
O	8.59300	23.68700	34.01600
N	10.66700	24.08600	33.27200
H	11.24900	24.44400	32.51500
C	11.30200	23.56000	34.48000
C	11.35100	24.64100	35.57400
O	11.87100	25.73200	35.35800
C	12.71000	23.05000	34.13300
C	13.43200	22.45700	35.32500
O	12.77300	21.79200	36.14800
O	14.66400	22.64200	35.43100
N	10.79700	24.34000	36.74400
H	10.37900	23.41900	36.87600
C	10.77400	25.30000	37.84400
C	12.00500	25.15800	38.74900
O	12.29600	26.03200	39.57500
C	9.48700	25.12900	38.68200
C	9.44500	26.14800	39.80200
C	8.28800	25.30000	37.80100
N	12.73100	24.05800	38.57200
H	12.43800	23.38900	37.86000
C	13.93000	23.76600	39.35400
C	14.89400	24.95600	39.44800
O	15.39500	25.28200	40.52000
C	14.64500	22.56500	38.74200
C	15.70000	21.92800	39.62700
C	15.08200	21.30700	40.86000
C	15.98600	20.23300	41.42600
N	16.11100	19.07100	40.50000
H	16.72000	18.34700	40.88100
H	16.41900	19.36600	39.57300
H	15.19600	18.69400	40.25100
N	15.18700	25.60100	38.31400
C	16.09200	26.75500	38.29600
C	15.66800	27.89500	39.22100
O	16.49700	28.47900	39.91500
C	16.07700	27.16900	36.83300
C	15.97800	25.83600	36.13900
C	14.92700	25.11900	36.94500
N	14.37800	28.21400	39.22000
H	13.73800	27.69700	38.61700
C	13.85700	29.28400	40.05900
C	13.94400	28.84500	41.51500

O	14.27300	29.64200	42.39200
C	12.40500	29.59700	39.66800
C	11.67200	30.85200	40.18300
C	10.71600	30.49300	41.29900
C	12.67500	31.90100	40.64600
N	13.66000	27.56900	41.76600
H	13.39300	26.96000	40.99300
C	13.71900	27.01700	43.11500
C	15.10400	27.23300	43.69500
O	15.24500	27.68300	44.83400
C	13.41300	25.55500	43.08000
N	16.12100	26.91000	42.89500
H	15.91100	26.53600	41.96900
C	17.51800	27.06600	43.28100
C	17.87300	28.52700	43.48900
O	18.52400	28.88100	44.47500
C	18.40900	26.45500	42.21400
C	18.48100	24.94600	42.32000
C	19.04200	24.27800	41.07700
O	20.09300	24.72200	40.55900
O	18.42600	23.29100	40.62400
N	17.44800	29.37800	42.56000
H	16.93600	29.02800	41.75000
C	17.70700	30.80700	42.68900
C	17.19600	31.22300	44.07300
O	17.84200	31.99800	44.78200
C	16.97300	31.60500	41.59000
C	17.66700	31.65000	40.19900
C	16.89000	32.46300	39.11900
O	16.27800	33.50000	39.40600
N	16.94400	31.99300	37.87500
H	16.43600	32.52500	37.16800
H	17.44800	31.13900	37.63900
N	16.04600	30.67900	44.46500
H	15.56900	30.01800	43.85200
C	15.46000	31.01300	45.75300
C	16.23800	30.41500	46.91800
O	16.48600	31.09400	47.92500
C	14.00000	30.55000	45.83500
C	13.19700	31.20600	44.70700
C	13.40600	30.92700	47.19100
C	11.71400	30.91000	44.72600
N	16.63000	29.15100	46.78000

H	16.39700	28.64700	45.92400
C	17.38500	28.47100	47.82600
C	18.68200	29.22000	48.12200
O	19.01400	29.47700	49.28100
C	17.68700	27.03600	47.40800
N	19.41700	29.58100	47.08000
H	19.10800	29.35600	46.13500
C	20.66600	30.29900	47.28600
C	20.43000	31.63400	47.98900
O	21.11400	31.94600	48.95000
C	21.40200	30.54500	45.94900
C	21.67500	29.20800	45.26300
C	22.72100	31.26600	46.19400
C	22.31800	29.33500	43.92800
N	19.46100	32.41400	47.52600
H	18.90000	32.10700	46.73200
C	19.19300	33.70600	48.14400
C	18.91400	33.58000	49.64300
O	19.29000	34.45400	50.43300
C	17.98000	34.42700	47.46800
O	18.24300	34.61600	46.07000
H	18.40100	33.77000	45.66900
C	17.72400	35.80200	48.12000
N	18.25800	32.49000	50.03000
H	17.99100	31.79500	49.33300
C	17.91100	32.26500	51.43200
C	19.07400	31.70700	52.23300
O	18.97400	31.53700	53.44700
C	16.72900	31.33100	51.52600
N	20.17200	31.41100	51.54500
H	20.18600	31.55600	50.53600
C	21.35300	30.88300	52.20900
C	21.34600	29.38600	52.40900
O	21.76900	28.91100	53.45800
N	20.88000	28.65200	51.39700
H	20.57200	29.13400	50.55200
C	20.78800	27.18700	51.43600
C	21.66700	26.48200	50.40200
O	22.14700	27.10200	49.45100
C	19.34000	26.74500	51.19000
S	18.17300	26.91700	52.57700
N	21.88000	25.18200	50.59100
H	21.50300	24.72400	51.42000

C	22.65000	24.40400	49.62100
C	21.67700	24.10700	48.48600
O	20.52500	24.51500	48.53600
C	23.10800	23.07200	50.20000
C	24.24300	23.12100	51.19100
C	24.54400	21.69400	51.63400
C	25.46600	21.62600	52.83400
N	25.27200	20.31600	53.51900
H	25.89300	20.27000	54.32700
H	25.39700	19.52500	52.88800
H	24.29700	20.14800	53.76800
N	22.12100	23.38600	47.47000
H	23.08600	23.05600	47.46000
C	21.22700	23.06600	46.36700
C	21.52900	21.69000	45.80100
O	21.20200	21.39300	44.66300
C	21.32900	24.12500	45.24800
O	22.70200	24.46000	45.02100
H	23.18200	23.67600	44.78100
C	20.56400	25.37500	45.63100
N	22.13800	20.85200	46.62800
H	22.34500	21.17000	47.57500
C	22.52600	19.50100	46.25100
C	21.42300	18.66900	45.59900
O	21.65000	18.06400	44.55000
C	23.06900	18.75500	47.46800
O	23.93700	19.63000	48.20100
H	23.44600	20.39500	48.47700
C	23.85400	17.53100	47.02700
N	20.24700	18.61500	46.22600
H	20.13700	19.10000	47.11600
C	19.10500	17.87500	45.66900
C	17.85000	18.61900	46.08500
O	17.87700	19.40600	47.03300
C	18.97400	16.42200	46.21400
O	18.65100	16.46300	47.60600
H	18.57100	15.57700	47.93800
C	20.25800	15.63500	46.02000
N	16.75300	18.37100	45.38000
H	16.79400	17.71500	44.60000
C	15.48800	19.02400	45.70400
C	15.14700	18.82400	47.17400
O	14.78600	19.76900	47.86900

C	14.34900	18.45900	44.84700
O	14.51700	18.77500	43.47400
H	13.81100	18.42500	42.94300
N	15.26300	17.58400	47.63600
H	15.57300	16.84500	47.00500
C	14.95800	17.25200	49.02200
C	15.80900	18.09500	49.96400
O	15.34300	18.55600	51.01000
C	15.20500	15.76400	49.27000
N	17.06200	18.29700	49.58500
H	17.39500	17.89500	48.70800
C	17.96400	19.08100	50.40000
C	17.48400	20.52300	50.45800
O	17.43700	21.11700	51.53100
C	19.39000	19.02800	49.83900
C	20.31100	19.88400	50.67900
C	19.87600	17.60100	49.83400
N	17.12400	21.09000	49.30900
H	17.18700	20.56000	48.44000
C	16.64000	22.46600	49.28600
C	15.43100	22.62800	50.21000
O	15.44500	23.45700	51.13000
C	16.26500	22.88200	47.86400
C	17.46400	23.14600	46.98800
S	17.06900	23.86900	45.37700
C	16.97900	22.41300	44.35200
N	14.39700	21.82500	49.97800
H	14.45000	21.14700	49.21800
C	13.19400	21.89700	50.78800
C	13.49500	21.71200	52.26300
O	12.99700	22.46900	53.09600
C	12.14200	20.85500	50.34200
C	10.87600	20.98900	51.17400
C	11.79600	21.07500	48.88900
N	14.30900	20.71800	52.59400
H	14.70200	20.12100	51.86700
C	14.64500	20.47500	53.99200
C	15.27000	21.71500	54.62500
O	15.02500	22.01900	55.80000
C	15.62200	19.30600	54.12700
C	16.14700	19.12400	55.51900
N	15.34600	18.73600	56.57400
H	14.35700	18.49600	56.50600

C	17.37600	19.33600	56.04200
C	16.05800	18.72400	57.68500
N	17.29300	19.08500	57.39100
H	18.06100	19.16500	58.05700
N	16.07300	22.42900	53.83500
H	16.21500	22.12200	52.87300
C	16.75700	23.63500	54.29800
C	15.84200	24.85000	54.47100
O	15.92100	25.55300	55.47900
C	17.89400	23.98400	53.34500
S	18.81400	25.46500	53.85400
N	14.98500	25.11300	53.49000
H	14.96700	24.52600	52.65600
C	14.07600	26.23700	53.60700
C	13.09000	25.97800	54.73900
O	12.64300	26.90900	55.41300
C	13.34400	26.45600	52.29400
C	14.24400	27.05000	51.21100
C	13.57400	26.94400	49.85800
C	14.56000	28.49400	51.55300
N	12.75100	24.71000	54.95500
H	13.13700	23.97600	54.36100
C	11.83300	24.35800	56.03300
C	12.39200	24.81100	57.37100
O	11.63900	25.07200	58.30700
C	11.60700	22.85000	56.09300
C	10.70200	22.30800	55.01400
C	9.53100	21.53300	55.60400
N	8.65700	20.99700	54.56100
H	7.73200	21.41400	54.45800
C	8.98200	20.00400	53.73700
N	10.16900	19.42300	53.83000
H	10.83000	19.73700	54.54000
H	10.41800	18.66200	53.19800
N	8.12200	19.59600	52.81300
H	7.20800	20.04300	52.74100
H	8.37100	18.83500	52.18100
N	13.71500	24.90900	57.45100
H	14.27500	24.70300	56.62400
C	14.39400	25.30100	58.67900
C	14.55900	26.79800	58.88100
O	14.83400	27.24100	59.98700
C	15.76300	24.63700	58.74200

C	15.72000	23.11900	58.70000
C	17.11400	22.50200	58.67300
O	17.88700	22.63900	59.62800
N	17.44400	21.82500	57.57400
H	16.80600	21.71200	56.78600
H	18.37700	21.41200	57.55600
N	14.40100	27.58200	57.82100
H	14.19000	27.16600	56.91400
C	14.52600	29.03200	57.93700
C	13.39100	29.59900	58.78600
O	12.40100	28.92100	59.04000
C	14.50000	29.67100	56.55200
C	15.65500	29.25900	55.66800
C	16.96200	29.71300	56.26200
C	18.12700	29.36600	55.35900
N	19.41400	29.76400	55.99200
H	20.19900	29.53000	55.38400
H	19.52100	29.35800	56.92200
H	19.41800	30.75000	56.25500
N	13.54200	30.84200	59.22800
H	14.39000	31.35700	58.99000
C	12.52000	31.48900	60.04800
C	11.69700	32.42900	59.19200
O	12.14700	32.85700	58.13100
C	13.12200	32.32600	61.19700
O	13.84800	33.43500	60.65500
H	13.27100	33.96500	60.11800
C	14.04100	31.48100	62.05300
N	10.50000	32.75500	59.66600
H	10.19500	32.37600	60.56200
C	9.62200	33.64000	58.93100
C	10.36700	34.87300	58.45200
O	10.26700	35.25700	57.28700
C	8.43100	34.06300	59.78900
C	7.50600	35.02800	59.05600
C	6.26700	35.37500	59.84700
O	5.19100	34.81700	59.54300
O	6.36800	36.20200	60.77800
N	11.12800	35.49200	59.34200
H	11.19800	35.13600	60.29500
C	11.86200	36.68100	58.95100
C	12.92700	36.43300	57.89200
O	13.15700	37.29100	57.04300

C	12.46000	37.35900	60.18100
C	11.43000	38.22200	60.89200
C	11.94000	38.84100	62.18000
O	13.10400	39.30900	62.20600
O	11.16400	38.87300	63.16500
N	13.56500	35.26600	57.91500
H	13.33700	34.57600	58.63100
C	14.58900	34.96900	56.92000
C	13.94100	34.83100	55.54200
O	14.44900	35.35000	54.54100
C	15.32300	33.68500	57.28800
C	15.81500	33.66700	58.71700
C	16.89900	32.63900	58.96400
O	18.04400	32.84900	58.50000
O	16.60700	31.62100	59.61900
N	12.81200	34.13000	55.50000
H	12.44800	33.72000	56.36000
C	12.08600	33.93500	54.26000
C	11.45800	35.25000	53.84400
O	11.30600	35.53100	52.65800
C	11.00900	32.86700	54.43700
C	11.54900	31.45100	54.64200
C	10.38100	30.48500	54.70100
C	12.50400	31.08700	53.50400
N	11.08400	36.06400	54.81900
H	11.20300	35.78700	55.79300
C	10.50300	37.35500	54.49200
C	11.59300	38.23600	53.89600
O	11.36900	38.91100	52.89600
C	9.91300	38.02200	55.73700
C	9.48400	39.48500	55.59000
C	8.55000	39.63200	54.40700
C	8.82100	39.95400	56.87000
N	12.77900	38.21900	54.49700
H	12.92700	37.63500	55.32000
C	13.86300	39.03500	53.97700
C	14.34500	38.46400	52.64700
O	14.86000	39.19300	51.80800
C	15.01600	39.15100	54.99200
C	15.99500	37.99700	55.02100
C	17.23200	38.30400	55.87200
O	17.86000	39.36700	55.64700
O	17.58300	37.48300	56.76000

N	14.16400	37.16400	52.44400
H	13.74600	36.59100	53.17700
C	14.55900	36.55000	51.18000
C	13.59500	37.01600	50.09300
O	14.00000	37.28400	48.95700
C	14.49100	35.02400	51.23400
O	15.47800	34.53300	52.14400
H	15.43600	33.58500	52.17800
C	14.74100	34.44300	49.86100
N	12.31700	37.09700	50.46400
H	12.07400	36.84100	51.42100
C	11.24900	37.53300	49.57200
C	11.52100	38.96400	49.13000
O	11.41500	39.29300	47.94300
C	9.88100	37.51300	50.28200
O	9.62200	36.20600	50.80500
H	8.77900	36.19400	51.24300
C	8.77900	37.88500	49.31200
N	11.87200	39.81300	50.09100
H	11.94100	39.47900	51.05200
C	12.15900	41.20800	49.80000
C	13.34800	41.38400	48.85800
O	13.39000	42.33300	48.08300
C	12.38500	41.97200	51.10400
C	11.12300	42.13000	51.96800
C	11.47400	42.66500	53.34000
C	10.14500	43.05200	51.27000
N	14.30600	40.46600	48.90000
H	14.22700	39.68200	49.54700
C	15.47000	40.57000	48.02800
C	15.19200	40.19800	46.57700
O	15.78600	40.77300	45.66800
C	16.60800	39.68700	48.52800
C	17.27300	40.12100	49.81200
C	18.54200	39.30100	49.99200
C	19.05300	39.28800	51.42000
N	20.31600	38.49500	51.50500
H	20.66000	38.48600	52.46500
H	21.02200	38.83000	50.85000
H	20.20100	37.55300	51.13200
N	14.30800	39.22800	46.35700
H	13.84500	38.78800	47.15200
C	13.98300	38.77600	45.00300

C	13.25300	39.85300	44.20300
O	13.25300	39.83100	42.96900
C	13.11300	37.51800	45.05800
C	13.67000	36.34800	45.88100
S	15.03300	35.43700	45.11600
C	14.16800	34.50500	43.84100
N	12.63100	40.79000	44.91600
H	12.67300	40.74100	45.93400
C	11.89000	41.88700	44.29400
C	10.95000	41.36000	43.21900
O	10.96200	41.82700	42.07800
C	12.86000	42.90600	43.68700
C	13.82800	43.50200	44.69000
C	14.75300	44.52200	44.04900
C	15.70500	45.10900	45.08300
N	16.55000	46.21800	44.54800
H	17.18800	46.61100	45.24000
H	15.97000	46.94800	44.13500
H	17.05900	45.91700	43.71700
N	10.13200	40.38500	43.59200
H	10.16300	40.04800	44.55400
C	9.19200	39.78700	42.65800
C	8.23300	40.82100	42.06800
O	7.95300	40.80800	40.87200
C	8.37600	38.68800	43.35000
C	9.20400	37.56000	43.91100
C	9.48400	37.49300	45.27700
C	9.66500	36.54100	43.08200
C	10.20800	36.42100	45.81000
C	10.39000	35.46500	43.60000
C	10.66000	35.40400	44.96700
N	7.74400	41.72200	42.91200
H	8.04300	41.70000	43.88700
C	6.79400	42.74000	42.48600
C	7.28700	43.71300	41.41000
O	6.69100	43.80100	40.33900
C	6.29800	43.51700	43.70900
C	5.80500	42.62400	44.85800
C	5.38400	43.48200	46.04000
C	4.65000	41.75300	44.38300
N	8.36900	44.43700	41.67700
H	8.84800	44.31800	42.57000
C	8.88000	45.40300	40.70300

C	9.46400	44.80700	39.42800
O	9.95400	43.67300	39.41800
C	9.92100	46.31700	41.35300
O	9.29500	47.29900	42.16000
H	9.94100	47.86600	42.56400
N	9.40400	45.60000	38.35800
H	8.98600	46.52500	38.46200
C	9.90800	45.20800	37.04400
C	11.31800	45.74700	36.81600
O	11.54300	46.96100	36.86800
C	8.97600	45.73600	35.94400
C	9.33300	45.46800	34.47400
C	9.40900	43.97100	34.21800
C	8.28400	46.10300	33.57100
N	12.26100	44.84000	36.56200
H	12.00400	43.85300	36.53100
C	13.65400	45.22000	36.32600
C	13.79200	45.89000	34.96100
O	13.40400	45.32500	33.93400
C	14.56100	43.98800	36.38300
C	16.03500	44.34400	36.28300
O	16.83900	43.45400	35.92400
O	16.38800	45.51100	36.57000
N	14.35900	47.09000	34.95300
H	14.68600	47.49800	35.82900
C	14.52100	47.83100	33.71300
C	15.76100	47.48500	32.89500
O	15.75100	47.63200	31.67200
C	14.49600	49.33700	34.00100
C	13.12800	49.93700	34.34000
C	13.27700	51.41500	34.66300
C	12.18700	49.74000	33.16200
N	16.82500	47.02200	33.54400
H	16.79600	46.89200	34.55500
C	18.03600	46.70100	32.79300
C	18.38900	45.22700	32.67300
O	17.69800	44.35600	33.20100
C	19.23300	47.46800	33.35700
C	19.66800	47.07100	34.74200
C	20.86900	47.87800	35.19900
O	20.76400	49.07700	35.46300
N	22.02300	47.22700	35.27700
H	22.11000	46.23400	35.05800

H	22.83000	47.76900	35.58400
N	19.48400	44.96400	31.96700
H	20.02600	45.73300	31.57200
C	19.91700	43.60100	31.75200
C	19.03400	42.98800	30.68800
O	18.07000	43.61000	30.23900
N	19.35900	41.77000	30.27800
H	20.17300	41.30700	30.68300
C	18.57800	41.07900	29.26200
C	17.17200	40.78300	29.80100
O	17.02300	40.17400	30.86300
C	19.28300	39.77500	28.87500
C	18.67500	39.12100	27.64900
O	17.49000	38.72300	27.70600
O	19.38900	39.00600	26.62700
N	16.12600	41.22200	29.07300
C	14.70600	41.04400	29.41100
C	14.25600	39.62200	29.79600
O	13.80900	39.39200	30.92400
C	13.99500	41.54600	28.15700
C	14.88000	42.65200	27.71500
C	16.26200	42.04500	27.85600
N	14.36600	38.68600	28.85200
H	14.75100	38.95100	27.94500
C	13.95800	37.29200	29.06100
C	14.54900	36.66400	30.29900
O	13.99300	35.71800	30.85300
C	14.33200	36.44100	27.85700
C	13.58100	36.79600	26.60700
C	14.20100	36.08500	25.43900
N	15.61900	36.41500	25.33400
H	16.01800	37.03100	26.04200
C	16.42500	35.96600	24.37700
N	15.95500	35.15800	23.43300
H	14.97500	34.87600	23.44900
H	16.57300	34.81300	22.69900
N	17.70000	36.33300	24.35600
H	18.06100	36.95300	25.08100
H	18.31800	35.98800	23.62200
N	15.69200	37.17800	30.72800
H	16.12700	37.94500	30.21600
C	16.32900	36.65400	31.92500
C	15.64400	37.17400	33.17500

O	15.41500	36.42300	34.13000
C	17.79700	37.06000	31.98600
C	18.67300	36.50800	30.88900
C	20.14600	36.74300	31.16400
O	20.54100	37.91300	31.37800
O	20.90600	35.75200	31.15800
N	15.31600	38.45600	33.16000
H	15.50000	39.01400	32.32600
C	14.69700	39.07600	34.31600
C	13.92200	38.08500	35.18000
O	13.15500	37.24600	34.71800
C	13.85500	40.27700	33.90300
O	14.54300	41.47300	34.26700
H	14.01800	42.22200	34.01000
N	14.19200	38.19100	36.46600
H	14.81700	38.93900	36.76600
C	13.65400	37.30800	37.47300
C	12.17200	36.99800	37.51800
O	11.28700	37.89000	37.50800
C	14.16900	37.77100	38.82800
C	13.18000	37.76000	39.93800
C	13.03300	36.40300	40.56800
O	12.25400	36.23700	41.50200
N	13.76600	35.39600	40.07500
H	14.41300	35.53400	39.29900
H	13.66600	34.47500	40.50200
N	11.89400	35.69400	37.51300
C	10.62900	34.98400	37.56500
C	9.86100	35.47100	38.74100
O	10.15600	36.49400	39.33700
C	11.06400	33.53700	37.72200
C	12.21700	33.48300	36.81600
C	12.94500	34.81700	36.97300
N	8.83700	34.72500	39.03300
H	8.64400	33.91300	38.44600
C	7.96800	34.98900	40.13900
C	7.51200	33.56200	40.16500
O	7.63000	32.87100	39.16100
C	6.83100	35.91800	39.71600
C	7.12900	36.69200	38.42500
C	7.21700	35.74900	37.21700
C	6.04600	37.69700	38.19000
N	7.02700	33.10000	41.28900

H	6.97900	33.70300	42.11000
C	6.56200	31.74200	41.36600
C	5.05300	31.84700	41.33000
O	4.52400	32.92100	41.53600
C	7.03500	31.13100	42.67700
C	6.88900	31.99700	43.93700
C	7.84200	31.43300	44.96700
C	7.23000	33.47600	43.70200
N	4.35700	30.75600	41.06800
H	4.83600	29.87700	40.87400
C	2.90900	30.81500	41.05800
C	2.34600	29.44000	40.79300
O	2.93800	28.42600	41.15800
N	1.19800	29.40700	40.14000
H	0.76400	30.28500	39.85400
C	0.53900	28.15800	39.82000
C	1.44800	27.28500	38.96800
O	2.07600	27.76900	38.03600
C	-0.75400	28.43700	39.05100
O	-1.55800	29.35000	39.80400
H	-2.36100	29.52300	39.32700
C	-1.53500	27.15800	38.81800
N	1.52800	26.00000	39.29300
H	1.01000	25.65200	40.10000
C	2.34800	25.07900	38.51000
C	1.53100	23.83500	38.18300
O	0.49800	23.58700	38.80700
C	3.66000	24.67000	39.26300
C	4.46000	25.91400	39.60000
C	3.34700	23.86300	40.52500
N	1.97200	23.07000	37.18900
H	2.81700	23.34000	36.68500
C	1.26600	21.85000	36.80700
C	1.84700	20.72100	37.65400
O	2.73100	19.99800	37.20600
C	1.48700	21.51600	35.31200
C	1.15400	22.73200	34.44400
C	0.64800	20.30800	34.91700
C	-0.24500	23.22200	34.61000
N	1.33100	20.57000	38.87000
H	0.56300	21.17900	39.15300
C	1.81600	19.57100	39.81800
C	1.33900	18.11900	39.66600

O	1.88100	17.20500	40.30200
C	1.47600	20.02700	41.22600
C	-0.00800	20.10100	41.45200
O	-0.43300	20.08000	42.62200
O	-0.75200	20.18300	40.45400
N	0.32700	17.89500	38.84500
H	-0.10100	18.66300	38.32800
C	-0.16300	16.54300	38.69300
C	-1.07600	16.15700	39.84600
O	-1.37700	14.97600	40.03700
N	-1.50800	17.14600	40.62600
H	-1.19800	18.09900	40.43700
C	-2.41200	16.90300	41.74200
C	-3.56200	17.91500	41.68100
O	-4.72700	17.54800	41.84900
C	-1.67700	17.03400	43.07400
C	-0.54500	16.02900	43.29800
S	-0.99600	14.52200	44.20300
C	-1.65300	15.25800	45.73500
N	-3.24100	19.18600	41.44200
H	-2.26000	19.44000	41.32400
C	-4.26400	20.22200	41.34600
C	-4.55500	20.46300	39.86600
O	-5.69900	20.65000	39.46900
C	-3.77500	21.50700	41.99700
C	-4.77600	22.65800	41.97000
C	-5.83900	22.48500	43.03800
C	-4.02600	23.94700	42.17700
N	-3.50300	20.47800	39.05700
H	-2.57200	20.36900	39.46000
C	-3.62700	20.64500	37.61000
C	-2.85500	19.47400	37.00700
O	-1.69700	19.25100	37.35900
C	-3.00700	21.96700	37.14100
C	-3.74500	23.27000	37.46300
C	-2.92000	24.44900	36.97400
C	-5.11700	23.26900	36.80900
N	-3.49000	18.72000	36.11700
H	-4.45100	18.94400	35.85700
C	-2.82600	17.57900	35.51100
C	-2.13800	17.96500	34.21600
O	-1.39500	17.18400	33.63400
C	-3.83100	16.46100	35.28400

C	-4.42100	15.99900	36.62000
C	-5.54400	14.99600	36.39200
C	-3.31300	15.40100	37.47300
N	-2.39500	19.18200	33.77200
H	-3.05500	19.76700	34.28500
C	-1.76700	19.71200	32.57700
C	-2.08100	21.19300	32.48900
O	-2.78800	21.72500	33.34400
C	-2.22400	18.96100	31.32700
C	-3.68600	18.64300	31.26200
C	-3.97200	17.72500	30.07900
C	-3.16600	16.43400	30.18000
N	-3.48000	15.49700	29.06600
H	-2.94100	14.63400	29.13400
H	-3.35300	15.94400	28.15800
H	-4.48100	15.30700	29.01200
N	-1.55100	21.86900	31.47900
H	-0.98100	21.38300	30.78700
C	-1.77900	23.30100	31.35400
C	-3.23100	23.65900	31.12600
O	-3.99600	22.87600	30.57200
C	-0.98300	23.90500	30.19700
O	-1.62200	23.58000	28.95400
H	-2.51300	23.91100	28.94800
C	0.43600	23.37800	30.20700
N	-3.63400	24.85600	31.57300
C	-5.01600	25.29700	31.38900
C	-5.29300	25.26000	29.89100
O	-6.37900	24.89300	29.44600
C	-4.99100	26.71900	31.93800
C	-3.97400	26.62700	33.02400
C	-2.87700	25.82200	32.38900
N	-4.27100	25.63400	29.12700
H	-3.40300	25.91900	29.58100
C	-4.33400	25.65600	27.67200
C	-4.70300	24.28100	27.11700
O	-5.29400	24.17800	26.04600
C	-2.98100	26.09200	27.10100
C	-2.56900	27.54800	27.39800
C	-2.21900	27.81500	28.86500
O	-1.52800	26.97700	29.47900
O	-2.61600	28.87800	29.39800
N	-4.34400	23.23300	27.85500

H	-3.85100	23.40000	28.73200
C	-4.62600	21.85200	27.46200
C	-5.95100	21.34500	28.02100
O	-6.71000	20.68400	27.32300
C	-3.52700	20.91300	27.96100
C	-2.15500	21.10300	27.34500
C	-1.09300	20.26600	28.05000
O	-1.27300	19.03400	28.16700
O	-0.07800	20.83900	28.49300
N	-6.21300	21.64200	29.29100
H	-5.54200	22.20100	29.81700
C	-7.43100	21.19200	29.95300
C	-8.72500	21.76500	29.38200
O	-9.75700	21.09400	29.40100
C	-7.34900	21.48400	31.45600
C	-6.39200	20.56900	32.22800
C	-6.27600	21.01100	33.67000
C	-6.89800	19.14600	32.15300
N	-8.67800	22.98900	28.86300
H	-7.79500	23.50000	28.85900
C	-9.87300	23.61300	28.29800
C	-10.26200	22.96400	26.98400
O	-11.43200	22.62400	26.77500
C	-9.64600	25.10300	28.07200
C	-9.39800	25.88300	29.34100
C	-9.54200	27.36100	29.11800
O	-8.91900	27.92000	28.22000
N	-10.37200	28.00700	29.92800
H	-10.47000	29.01100	29.77700
H	-10.89000	27.54300	30.67400
N	-9.29200	22.80300	26.09500
H	-8.34900	23.12700	26.31100
C	-9.56000	22.16900	24.81700
C	-9.66200	20.65500	25.05700
O	-8.97700	19.89900	24.36300
C	-8.41400	22.45300	23.84300
N	-10.49800	20.20900	25.99700
H	-11.07600	20.85800	26.53100
C	-10.56400	18.82000	26.23500
C	-11.70800	18.17800	27.05100
O	-12.81900	18.06700	26.56300
C	-9.19300	18.34900	26.78900
C	-8.76800	17.01200	26.25400

C	-7.90400	16.29100	27.23700
O	-8.46600	15.53600	28.07100
O	-6.67300	16.51100	27.19400
N	-11.39800	17.89600	28.32700
H	-10.58000	18.34200	28.74200
C	-12.19300	16.96600	29.15300
C	-13.57600	17.23900	29.52900
O	-13.93400	18.37600	29.78400
C	-11.42200	16.51600	30.43300
C	-10.73900	15.14100	30.28900
C	-11.68500	14.10200	30.85200
N	-11.48100	12.79000	30.27200
H	-10.90000	12.71700	29.43700
C	-12.00800	11.68000	30.76700
N	-12.76200	11.73300	31.85300
H	-13.16800	10.87800	32.23400
H	-12.93700	12.62300	32.32000
N	-11.78100	10.52600	30.16200
H	-12.18700	9.67100	30.54300
H	-11.20000	10.48500	29.32500
N	-14.33700	16.13600	29.51900
H	-13.83200	15.27400	29.31200
C	-15.76500	15.96000	29.75400
C	-16.17700	16.11700	31.21700
O	-17.14000	15.50000	31.68300
C	-16.08400	14.55200	29.22200
C	-14.94700	13.98900	28.34200
O	-14.41400	14.69800	27.48500
N	-14.56900	12.72700	28.56600
H	-13.81800	12.35500	27.98500
H	-15.01000	12.14100	29.27500
N	-15.46200	16.98200	31.91900
H	-14.71600	17.48900	31.44300
C	-15.68200	17.25200	33.34000
C	-17.09200	17.61500	33.80900
O	-18.08200	17.48000	33.08200
C	-14.74700	18.37300	33.80700
C	-14.93300	19.67900	33.06700
C	-14.43400	20.87500	33.58900
C	-15.56000	19.70800	31.82100
C	-14.55500	22.08200	32.87500
C	-15.68600	20.89600	31.10100
C	-15.18300	22.08800	31.62700

N	-17.12900	18.08100	35.05800
H	-16.24500	18.12600	35.56500
C	-18.32900	18.53400	35.76500
C	-18.31500	20.06500	35.67800
O	-17.68100	20.73800	36.49400
C	-18.25300	18.09000	37.23500
C	-19.32900	18.65700	38.11400
N	-19.21600	18.69600	39.48700
H	-18.41600	18.35800	40.02200
C	-20.53700	19.19900	37.82200
C	-20.30400	19.23900	40.00400
N	-21.12200	19.55200	39.01400
H	-22.03900	19.98600	39.11800
N	-19.01100	20.60300	34.68300
H	-19.52300	19.98500	34.05400
C	-19.07300	22.04300	34.45300
C	-20.02400	22.77800	35.38000
O	-20.83100	22.16600	36.07000
C	-19.52100	22.33000	33.02500
O	-20.77000	21.67000	32.78500
H	-21.04900	21.84900	31.89500
C	-18.50100	21.82300	32.03700
N	-19.92600	24.10100	35.38300
H	-19.22400	24.54700	34.79300
C	-20.79200	24.93500	36.20400
C	-20.91000	26.29600	35.55000
O	-20.03400	26.69800	34.79400
C	-20.21500	25.15900	37.61000
C	-20.16900	23.85700	38.37900
C	-18.84000	25.77500	37.50000
N	-22.00500	27.02100	35.82000
C	-22.15500	28.34400	35.21800
C	-20.89600	29.13900	35.53900
O	-20.41500	29.11900	36.66800
C	-23.38800	28.89000	35.91700
C	-24.20400	27.66700	36.10100
C	-23.20400	26.65800	36.58900
N	-20.36100	29.83300	34.54600
H	-20.81100	29.83300	33.63100
C	-19.14200	30.59400	34.74600
C	-19.29900	32.02300	34.23100
O	-19.74200	32.23600	33.10200
C	-17.99800	29.88300	34.00700

C	-16.58100	30.33800	34.32800
C	-15.50600	29.83700	33.59800
C	-16.31000	31.26300	35.34400
C	-14.20200	30.23900	33.85800
C	-15.00200	31.67400	35.61200
C	-13.95300	31.15400	34.86000
O	-12.64700	31.53800	35.08500
H	-11.93100	31.18300	34.57200
N	-18.95100	33.00000	35.06500
H	-18.62900	32.76200	36.00300
C	-19.01900	34.40400	34.67100
C	-17.59300	34.95200	34.59700
O	-16.85900	34.93000	35.58800
C	-19.81800	35.22000	35.68800
C	-20.01400	36.66900	35.27200
S	-20.64400	37.74300	36.57600
C	-22.33800	37.20700	36.68500
N	-17.20100	35.43300	33.42200
H	-17.85000	35.41500	32.63500
C	-15.86300	35.98700	33.22900
C	-15.94800	37.43900	32.76000
O	-16.65000	37.75100	31.80200
C	-15.07600	35.15900	32.20200
C	-13.74300	35.81700	31.90300
C	-14.84900	33.77100	32.74500
N	-15.23600	38.32900	33.43400
H	-14.65100	38.03900	34.21700
C	-15.30200	39.71800	33.04200
C	-14.01500	40.49600	33.18900
O	-13.11000	40.10400	33.92700
N	-13.95300	41.62000	32.48300
H	-14.75300	41.88100	31.90700
C	-12.79000	42.49300	32.49800
C	-13.27600	43.91800	32.67700
O	-14.47100	44.18700	32.55700
C	-12.03200	42.42000	31.15900
C	-12.90700	43.00200	30.04200
C	-11.68700	40.96700	30.83600
C	-12.18200	43.23400	28.74000
N	-12.35300	44.82800	32.96500
H	-11.38200	44.53700	33.08200
C	-12.70100	46.23400	33.11700
C	-12.31800	46.94000	31.82600

O	-11.68400	46.33700	30.96000
C	-11.96400	46.84100	34.30400
C	-12.54900	46.39900	35.62600
O	-12.01000	46.68900	36.69400
N	-13.66700	45.69200	35.55900
H	-14.11400	45.45200	34.67400
H	-14.06200	45.39400	36.45100
N	-12.70300	48.20500	31.68700
H	-13.21600	48.65800	32.44300
C	-12.40400	48.95900	30.47000
C	-10.91700	49.22800	30.26700
O	-10.39700	49.04500	29.17000
C	-13.16200	50.28700	30.46800
C	-13.13100	50.99600	29.13000
C	-13.65500	50.08300	28.02900
C	-13.84200	50.85700	26.74700
N	-14.65100	52.08100	27.01200
H	-14.77700	52.60400	26.14600
H	-14.24700	52.65500	27.75200
H	-15.54000	51.86400	27.46300
N	-10.24400	49.66900	31.32400
H	-10.74000	49.80700	32.20500
C	-8.81800	49.96100	31.26200
C	-8.05800	49.19800	32.35900
O	-7.75300	49.75400	33.41700
C	-8.60300	51.46900	31.40700
C	-9.23600	52.27400	30.28400
C	-9.15500	53.77700	30.49800
O	-8.13500	54.29600	30.94200
N	-10.22900	54.48300	30.16400
H	-11.07700	54.05200	29.79500
H	-10.17500	55.49100	30.30800
N	-7.75000	47.92900	32.09400
H	-8.01000	47.53600	31.18900
C	-7.05100	47.08300	33.06000
C	-5.65100	47.55200	33.45600
O	-5.24300	47.38500	34.60700
C	-6.97600	45.63900	32.54500
C	-8.31700	44.90700	32.47100
C	-8.97000	44.71900	33.83000
O	-8.40300	45.19200	34.83500
O	-10.05300	44.09800	33.89700
N	-4.91300	48.12900	32.51200

H	-5.30000	48.24000	31.57500
C	-3.55600	48.60900	32.78700
C	-3.52900	50.13800	32.79300
O	-2.48600	50.75600	32.58900
C	-2.59400	48.07400	31.72300
C	-1.20700	47.79400	32.23800
C	-0.10400	48.45200	31.70800
C	-1.00300	46.87100	33.25600
C	1.17800	48.19500	32.18700
C	0.27800	46.61100	33.73800
C	1.36600	47.27500	33.20200
N	-4.68900	50.73300	33.05400
H	-5.50700	50.15800	33.25300
C	-4.82300	52.17900	33.06300
C	-4.04900	52.98400	34.09000
O	-3.62100	54.09500	33.78300
N	-3.87200	52.46500	35.30100
H	-4.24900	51.54300	35.52000
C	-3.13700	53.21500	36.32000
C	-2.61400	52.40000	37.50600
O	-1.40100	52.31700	37.71500
C	-3.99900	54.35600	36.86900
C	-3.26400	55.18800	37.88400
C	-2.27200	56.09200	37.63300
C	-3.40900	55.14000	39.31500
N	-1.78800	56.60700	38.81400
H	-1.04400	57.30000	38.89700
C	-2.46700	56.03900	39.86200
C	-4.24000	54.42000	40.18900
C	-2.33000	56.24000	41.24300
C	-4.10100	54.62100	41.56900
C	-3.15200	55.52400	42.07600
N	-3.53400	51.82400	38.28400
H	-4.51800	51.93500	38.04000
C	-3.19200	51.03800	39.47500
C	-2.00400	50.09000	39.33200
O	-1.07800	50.12100	40.14700
C	-4.40400	50.23100	39.95100
C	-4.11300	49.21000	41.06200
C	-3.75000	49.91800	42.35600
C	-5.32800	48.34100	41.27200
N	-2.03700	49.23600	38.31600
H	-2.83100	49.23600	37.67500

C	-0.94300	48.30300	38.11800
C	0.35000	49.03900	37.76700
O	1.32800	48.95400	38.50800
C	-1.27500	47.26200	37.02500
C	-2.53200	46.48700	37.41900
C	-0.10900	46.29500	36.85100
C	-2.93600	45.43200	36.41900
N	0.37400	49.78300	36.64500
C	1.60200	50.49700	36.28800
C	2.16900	51.32500	37.43900
O	3.38600	51.39800	37.61300
C	1.16600	51.35500	35.10800
C	0.13100	50.50300	34.45700
C	-0.67400	50.03000	35.63800
N	1.28600	51.94000	38.22200
H	0.29100	51.84000	38.02000
C	1.70100	52.75500	39.36300
C	2.45200	51.92900	40.40300
O	3.43600	52.38600	40.98700
C	0.47500	53.40400	40.01100
C	0.76000	54.22600	41.26900
S	0.86700	53.25500	42.78700
C	-0.85000	52.74200	42.94800
N	1.98000	50.70700	40.62500
H	1.16900	50.38500	40.09700
C	2.58800	49.81700	41.60100
C	3.83900	49.10700	41.10400
O	4.67100	48.70100	41.91000
C	1.57200	48.77600	42.07100
C	0.33800	49.25600	42.83500
C	-0.54500	48.05500	43.12000
C	0.74100	49.94400	44.13100
N	3.97600	48.93700	39.79300
H	3.25100	49.27200	39.15900
C	5.16200	48.27200	39.25700
C	6.23400	49.29200	38.93400
O	7.34100	48.93800	38.51800
C	4.82000	47.46000	38.00500
C	4.16700	46.13700	38.33100
S	4.54100	44.84100	37.15400
C	2.90800	44.45200	36.58100
N	5.89700	50.56100	39.15400
H	4.97000	50.76500	39.52700

C	6.80200	51.66800	38.88200
C	7.17600	51.62400	37.41200
O	8.34600	51.68600	37.04800
C	8.05600	51.56400	39.75300
O	7.74000	51.73800	41.12300
H	8.51800	51.67300	41.66400
N	6.16300	51.49900	36.56900
H	5.21400	51.43600	36.93700
C	6.37100	51.44900	35.13600
C	6.89100	52.82100	34.72500
O	6.38000	53.84700	35.18000
C	5.04500	51.16500	34.44400
C	5.14500	50.38500	33.15800
C	5.36200	49.00600	33.16800
C	4.96000	51.01800	31.93000
C	5.38200	48.27500	31.98300
C	4.97900	50.30000	30.74000
C	5.18700	48.93200	30.77300
O	5.18500	48.23300	29.59000
H	5.05200	48.68200	28.76300
N	7.93000	52.85900	33.87500
C	8.53400	54.11100	33.39400
C	7.65600	54.91700	32.42800
O	7.74500	54.76100	31.20500
C	9.83100	53.63500	32.73500
C	10.16400	52.39000	33.50400
C	8.81500	51.71800	33.58600
N	6.81600	55.78200	32.98700
H	6.79300	55.86300	34.00400
C	5.92500	56.62000	32.19000
C	5.75700	57.99600	32.83200
O	4.65100	58.52700	32.90700
C	4.55700	55.95100	32.04400
C	4.54600	54.62300	31.29200
C	3.13800	54.06400	31.28800
C	5.04900	54.82800	29.87200
N	6.86700	58.56400	33.29100
H	7.75100	58.06500	33.19200
C	6.86900	59.87300	33.93000
C	6.69000	61.01000	32.92200
O	6.45000	62.16000	33.30100
C	8.18200	60.05400	34.68600
O	9.27800	59.67300	33.87100

H	10.09500	59.78600	34.34200
N	6.79900	60.67600	31.63900
H	6.97800	59.70100	31.39800
C	6.67100	61.65500	30.56200
C	5.22400	61.96300	30.18200
O	4.88800	63.10300	29.85900
C	7.41300	61.15700	29.31500
C	8.87100	60.79100	29.55400
C	9.67700	61.94800	30.11000
O	9.70500	63.01300	29.46100
O	10.28300	61.79200	31.19200
N	4.37100	60.94600	30.22400
H	4.69200	60.02600	30.52400
C	2.98600	61.13900	29.84500
C	2.90000	60.99600	28.33500
O	1.85600	61.24500	27.72600
N	4.01600	60.58400	27.73500
H	4.83900	60.38800	28.30600
C	4.10200	60.40300	26.29100
C	5.09300	59.30600	25.90200
O	6.07100	59.05300	26.60700
C	4.52300	61.71200	25.63400
C	5.91500	62.16300	26.03700
C	6.21200	63.59000	25.61600
O	7.31100	64.10100	25.84400
N	5.23000	64.24400	25.00300
H	4.32100	63.82100	24.81400
H	5.43000	65.20300	24.72000
N	4.83200	58.67000	24.76300
H	4.00700	58.93900	24.22700
C	5.68400	57.60300	24.25400
C	5.73900	57.70300	22.72200
O	4.93000	58.40700	22.11000
C	5.11300	56.24300	24.66900
C	6.09800	55.09500	24.89000
C	6.88200	55.35700	26.16400
C	5.35000	53.78000	24.99700
N	6.68800	57.00000	22.10700
H	7.32800	56.43500	22.66500
C	6.83600	57.01800	20.65100
C	7.16100	55.62900	20.09200
O	7.82300	54.82000	20.74700
C	7.94300	57.98800	20.24900

C	9.32600	57.44100	20.54300
O	9.59300	57.09600	21.71200
O	10.14600	57.35400	19.60400
N	6.69600	55.37400	18.87200
H	6.16400	56.10200	18.39500
C	6.90800	54.10600	18.18200
C	8.18000	53.35800	18.54500
O	8.17700	52.12900	18.61700
C	6.87900	54.33100	16.67600
C	5.48600	54.49100	16.11900
C	4.69600	53.20300	16.17800
O	3.54000	53.15200	15.75600
N	5.31800	52.14700	16.70000
H	6.27500	52.18900	17.04900
H	4.78500	51.27800	16.74000
N	9.27200	54.08900	18.75100
H	9.22800	55.10400	18.65500
C	10.53000	53.45000	19.11300
C	10.54600	53.05600	20.58500
O	10.65700	51.87300	20.91200
C	11.72400	54.36200	18.80600
C	12.28600	54.19800	17.39600
C	13.68500	54.79500	17.27900
C	14.32100	54.47900	15.92800
N	15.72500	54.98400	15.82900
H	16.15000	54.77300	14.92600
H	16.29800	54.63300	16.59700
H	15.77300	55.98200	16.03400
N	10.43300	54.04000	21.47300
H	10.34300	55.00400	21.15100
C	10.43700	53.75400	22.90100
C	9.42400	52.67300	23.22100
O	9.62000	51.87600	24.13600
C	10.09500	54.99300	23.72700
O	11.16300	55.93800	23.62200
H	10.95000	56.70800	24.13600
C	9.89600	54.62200	25.18500
N	8.33500	52.65500	22.46200
H	8.22500	53.35200	21.72600
C	7.29700	51.65900	22.66200
C	7.91500	50.27300	22.55200
O	7.91300	49.50200	23.51500
C	6.21200	51.82800	21.61900

N	8.45200	49.97000	21.37300
H	8.42900	50.66300	20.62500
C	9.07100	48.67800	21.12200
C	10.17500	48.36600	22.11500
O	10.46600	47.20300	22.38500
C	9.61100	48.62500	19.69500
C	8.50800	48.52700	18.66700
S	9.09900	48.42500	16.98700
C	8.59800	50.04300	16.36700
N	10.78800	49.40800	22.66100
H	10.51400	50.35200	22.39000
C	11.84600	49.22200	23.64100
C	11.20000	48.70800	24.93200
O	11.60400	47.67800	25.48500
C	12.56500	50.55100	23.89600
O	13.69300	50.37300	24.73600
H	14.13900	51.19700	24.89400
N	10.18300	49.43500	25.39000
H	9.90800	50.26900	24.87100
C	9.44500	49.09200	26.60100
C	8.78000	47.73000	26.46400
O	8.97600	46.85100	27.30000
C	8.37500	50.15200	26.88300
C	8.49400	50.94100	28.18900
C	7.44900	52.04200	28.22600
C	8.32300	50.00700	29.36700
N	7.99800	47.55800	25.40100
H	7.88700	48.32100	24.73300
C	7.29700	46.30100	25.17300
C	8.21800	45.07700	25.18400
O	7.76700	43.96800	25.47100
C	6.52000	46.35700	23.85400
C	5.67200	45.12200	23.52900
C	4.69500	44.85200	24.65800
C	4.92800	45.34100	22.22500
N	9.49900	45.26700	24.87300
H	9.82400	46.20200	24.62800
C	10.44700	44.15200	24.87800
C	10.93200	43.88700	26.29700
O	11.15700	42.74300	26.68600
C	11.64900	44.44800	23.97500
C	12.79100	43.46700	24.14200
C	14.07700	43.76300	24.49700

C	12.74100	42.03900	23.97800
N	14.82800	42.61300	24.56500
H	15.81700	42.56600	24.80900
C	14.03600	41.54400	24.25400
C	11.73000	41.13700	23.62700
C	14.34400	40.18000	24.18900
C	12.04100	39.77800	23.56300
C	13.33900	39.31600	23.84400
N	11.09600	44.95500	27.06600
H	10.90100	45.88100	26.68400
C	11.54800	44.83300	28.44300
C	10.38600	44.35600	29.31300
O	10.57900	43.82200	30.40600
C	12.05100	46.18900	28.94500
C	13.11200	46.82300	28.06300
C	13.56100	48.16400	28.62300
C	14.60900	48.81700	27.72900
N	14.99200	50.17500	28.21700
H	15.69300	50.61200	27.61900
H	15.30100	50.14600	29.18900
H	14.17300	50.77400	28.32600
N	9.17400	44.55100	28.80900
H	9.08700	44.98700	27.89100
C	7.96300	44.16400	29.52100
C	7.67800	42.68200	29.33300
O	6.63300	42.18500	29.74900
C	6.77900	44.97600	28.99800
O	7.09800	46.35600	28.93400
H	6.36200	46.86100	28.60900
N	8.61600	41.98500	28.70200
H	9.46300	42.46200	28.39400
C	8.47200	40.56000	28.43700
C	7.90900	39.76300	29.61500
O	6.95300	39.00400	29.45500
C	9.81800	39.96200	28.02600
C	9.68600	38.60700	27.37500
C	9.12900	38.48200	26.10600
C	10.10600	37.45000	28.03000
C	8.99300	37.23800	25.50100
C	9.97400	36.19900	27.43500
C	9.41700	36.10300	26.17000
O	9.28500	34.87500	25.56600
H	9.57600	34.09600	26.02500

N	8.49400	39.92100	30.81500
C	8.00400	39.18300	31.98600
C	6.54900	39.49200	32.36800
O	6.06500	39.05200	33.41800
C	8.99700	39.57900	33.07800
C	9.40100	40.96300	32.67500
C	9.60200	40.81700	31.19100
N	5.86200	40.24700	31.51300
H	6.32600	40.58100	30.66800
C	4.46900	40.61200	31.74300
C	3.59500	40.29400	30.53800
O	2.42900	39.93700	30.69200
C	4.35300	42.10000	32.08400
C	4.71800	42.49600	33.51800
C	4.71100	44.00700	33.66500
C	3.72900	41.86300	34.48400
N	4.15400	40.42200	29.34000
H	5.12700	40.72000	29.26800
C	3.39600	40.14200	28.12700
C	3.87100	38.87400	27.43500
O	3.07900	38.15800	26.82600
C	3.48900	41.30200	27.12800
C	2.87400	42.55100	27.72900
C	4.93700	41.54000	26.75000
N	5.16700	38.60300	27.53000
H	5.77100	39.24200	28.04800
C	5.75100	37.41800	26.91500
C	5.57700	37.41800	25.40300
O	5.01200	36.48700	24.83200
C	5.12900	36.14700	27.50300
S	5.41900	35.91600	29.27200
N	6.06500	38.47200	24.75800
H	6.51000	39.21900	25.29100
C	5.98000	38.58800	23.30700
C	7.40100	38.57900	22.74700
O	8.26300	39.32300	23.21600
C	5.29200	39.90500	22.88400
C	3.99100	40.09300	23.66000
C	4.98200	39.87100	21.39700
C	3.30300	41.40800	23.38200
N	7.64200	37.73300	21.75100
H	6.88800	37.13600	21.41200
C	8.96200	37.63700	21.12900

C	9.38200	38.98900	20.56300
O	8.54200	39.75700	20.09000
C	8.94000	36.59400	20.02200
N	10.68200	39.27100	20.60100
H	11.33100	38.58400	20.98400
C	11.19700	40.54300	20.10600
C	11.00000	40.74300	18.60600
O	10.98400	41.87500	18.13100
C	12.68000	40.68800	20.45200
C	13.23000	42.07900	20.18600
C	14.62800	42.25000	20.75800
C	15.13200	43.67600	20.55800
N	14.23500	44.68700	21.19900
H	14.57200	45.64000	21.06500
H	14.09400	44.48100	22.18800
H	13.27400	44.58600	20.87400
N	10.85300	39.65300	17.86000
H	10.88300	38.73400	18.30100
C	10.64900	39.75500	16.41600
C	9.19000	40.06400	16.10200
O	8.85200	40.45800	14.98500
C	11.05600	38.45600	15.70500
C	10.36600	37.19400	16.21800
C	11.14300	36.51300	17.33600
O	11.38900	37.16000	18.37700
O	11.51300	35.32800	17.17200
N	8.32900	39.88500	17.09900
H	8.67700	39.56300	18.00200
C	6.90400	40.13600	16.93800
C	6.55900	41.57900	17.29500
O	5.66600	42.17700	16.69600
C	6.11300	39.18500	17.83500
C	6.40600	37.69100	17.68400
C	5.68300	36.91500	18.77300
C	5.97200	37.22000	16.30700
N	7.28600	42.12000	18.27100
H	8.02300	41.55300	18.69100
C	7.09000	43.48200	18.77800
C	6.65400	44.52600	17.74500
O	5.60300	45.15100	17.89400
C	8.37800	44.01200	19.48900
C	8.79500	43.07100	20.62700
C	8.13400	45.41300	20.03500

C	7.83900	43.03700	21.80600
N	7.45500	44.73400	16.68700
C	7.11100	45.72200	15.65700
C	5.70400	45.56000	15.08700
O	4.94400	46.52400	15.00100
C	8.19000	45.50000	14.60200
C	9.36400	45.05700	15.42000
C	8.72900	44.06800	16.36000
N	5.36900	44.33500	14.69800
H	6.04800	43.58000	14.79700
C	4.06000	44.04000	14.13400
C	2.97200	44.39700	15.13700
O	1.98800	45.05100	14.79000
C	3.95900	42.55600	13.77800
C	2.78500	42.23500	12.86700
C	2.64500	40.75100	12.58300
O	3.68000	40.08500	12.36000
O	1.49700	40.25500	12.57000
N	3.16100	43.95800	16.38000
H	4.00100	43.41700	16.58500
C	2.21500	44.21900	17.46100
C	2.15100	45.71200	17.77600
O	1.07700	46.31400	17.74500
C	2.62300	43.44400	18.70400
N	3.30700	46.29700	18.08100
H	4.15500	45.73000	18.09400
C	3.41000	47.72200	18.39800
C	2.70700	48.57400	17.34200
O	1.93900	49.48600	17.65800
C	4.88900	48.16700	18.46700
O	5.59000	47.36500	19.42500
H	6.49900	47.63800	19.46700
C	4.99000	49.63400	18.86600
N	2.98400	48.26300	16.08300
H	3.62900	47.49500	15.89800
C	2.40300	48.97500	14.95700
C	0.87400	48.93100	14.97600
O	0.21000	49.95600	14.82700
C	2.92600	48.36300	13.65400
C	2.49900	49.08600	12.39300
C	2.86400	50.55600	12.42000
O	3.99700	50.88600	12.83600
O	2.01900	51.38300	12.01500

N	0.32400	47.73500	15.16500
H	0.93500	46.93000	15.30200
C	-1.12200	47.53100	15.18400
C	-1.85700	48.52300	16.07500
O	-2.83100	49.14600	15.65400
C	-1.43800	46.10800	15.64500
C	-2.90200	45.71200	15.52500
C	-3.32300	45.51300	14.07500
C	-4.68500	44.83300	13.98500
N	-5.05700	44.48700	12.58700
H	-5.96800	44.03200	12.52700
H	-4.33400	43.92000	12.14400
H	-5.01600	45.30700	11.98200
N	-1.38600	48.66400	17.30800
H	-0.56600	48.12900	17.59400
C	-2.01600	49.56700	18.25900
C	-1.58200	51.01700	18.09500
O	-2.41100	51.89500	17.85600
C	-1.71900	49.11900	19.69700
C	-2.50700	47.91200	20.18500
C	-2.32900	46.64800	19.61500
C	-3.41600	48.03500	21.23900
C	-3.03600	45.53300	20.08900
C	-4.12800	46.92900	21.71800
C	-3.93400	45.68200	21.14000
O	-4.63200	44.59400	21.62100
H	-5.24600	44.69600	22.33900
N	-0.28000	51.25800	18.22100
H	0.35000	50.47300	18.38700
C	0.28200	52.60400	18.13000
C	0.36500	53.20500	16.72500
O	0.66400	54.39300	16.57000
C	1.67000	52.60700	18.76600
C	1.71100	51.97300	20.15400
C	3.13000	51.96800	20.66600
C	0.80300	52.74200	21.09600
N	0.10000	52.39000	15.70800
H	-0.14400	51.41700	15.89000
C	0.15600	52.87600	14.33900
C	-1.06100	53.69000	13.93700
O	-1.24800	54.00300	12.76100
N	-1.89400	54.03000	14.91500
H	-1.69500	53.74100	15.87300

C	-3.08300	54.80900	14.63000
C	-2.72400	56.21700	14.20400
O	-2.83500	56.56700	13.02800
N	-2.29100	57.02500	15.16800
H	-2.23000	56.67000	16.12200
C	-1.90100	58.40400	14.89900
C	-0.45400	58.66100	15.31600
O	0.27700	57.73200	15.66800
C	-2.81900	59.40300	15.63300
O	-2.97300	58.99400	16.99700
H	-3.53800	59.60900	17.44900
C	-4.18500	59.47300	14.96100
N	-0.05000	59.92800	15.27500
H	-0.71000	60.65100	14.98900
C	1.31200	60.31000	15.62900
C	1.37800	61.01600	16.97800
O	2.46000	61.37200	17.44500
C	1.88800	61.22700	14.55100
C	1.53300	60.76900	13.15300
O	1.89800	59.62900	12.78800
O	0.88400	61.55000	12.42200
N	0.22200	61.22300	17.59900
H	-0.64400	60.91300	17.15900
C	0.16700	61.88500	18.89700
C	1.01500	61.09900	19.89300
O	0.88000	59.88200	19.99700
C	-1.27900	61.94100	19.39300
C	-1.44800	62.84700	20.59900
O	-0.58400	62.81100	21.49900
O	-2.45200	63.59100	20.65200
N	1.89100	61.78700	20.61800
H	1.97000	62.79500	20.48400
C	2.74300	61.12600	21.60400
C	1.95900	60.73800	22.85800
O	2.44200	59.97600	23.70000
C	3.91500	62.02600	22.01100
O	3.45600	63.37900	22.13600
H	2.76200	63.42700	22.78300
C	5.02200	61.94900	20.97800
N	0.74800	61.27500	22.97600
H	0.42200	61.91700	22.25400
C	-0.12900	60.97800	24.10100
C	-0.99700	59.78600	23.72400

O	-0.98000	58.76200	24.40600
C	-1.03800	62.17400	24.43800
C	-2.09800	61.76100	25.44800
C	-0.20100	63.30900	24.99300
N	-1.75000	59.91700	22.63400
H	-1.72700	60.79200	22.11100
C	-2.60600	58.83000	22.17600
C	-1.81700	57.52400	22.11300
O	-2.38800	56.43700	22.18700
C	-3.18700	59.14800	20.80100
C	-4.23700	60.23800	20.80900
C	-4.93500	60.31000	19.46500
C	-6.08600	61.30400	19.47200
N	-6.79100	61.31700	18.15200
H	-7.56300	61.98400	18.15700
H	-7.10100	60.38400	17.88200
H	-6.14500	61.49400	17.38200
N	-0.50200	57.64100	21.97100
H	-0.08800	58.57000	21.89400
C	0.36200	56.46900	21.92300
C	0.42100	55.87100	23.32100
O	-0.01100	54.73800	23.53600
C	1.77600	56.85100	21.46800
C	1.92700	57.08300	19.97300
C	3.36100	57.47000	19.63700
C	3.58800	57.52800	18.13600
N	3.37500	56.20200	17.48800
H	3.52700	56.24100	16.48000
H	2.45300	55.82600	17.70900
H	3.95100	55.48100	17.92200
N	0.96000	56.63900	24.26500
H	1.30800	57.56400	24.01300
C	1.06600	56.19500	25.64900
C	-0.15400	55.36700	26.04000
O	-0.02300	54.24500	26.52500
C	1.16600	57.40100	26.58200
C	0.81700	57.07600	28.02700
C	0.50800	58.33100	28.82400
C	0.01700	57.99400	30.22300
N	-0.29000	59.22000	31.00600
H	-0.61900	58.99400	31.94500
H	-0.95100	59.82000	30.51400
H	0.50900	59.85400	31.03400

N	-1.33800	55.93200	25.81400
H	-1.36600	56.86000	25.39200
C	-2.59700	55.27500	26.14700
C	-2.82700	53.98600	25.36600
O	-3.06600	52.94000	25.95900
C	-3.77100	56.23000	25.91200
C	-3.54200	57.60500	26.52100
O	-2.95200	57.67800	27.62100
O	-3.96400	58.61000	25.90300
N	-2.77200	54.05400	24.04000
H	-2.58600	54.94800	23.58600
C	-2.97600	52.85700	23.22700
C	-1.99200	51.76400	23.62300
O	-2.27900	50.57600	23.47500
C	-2.81300	53.17300	21.73800
C	-4.05700	53.62500	20.96500
C	-3.68500	53.89300	19.51600
C	-5.13200	52.54800	21.03000
N	-0.82900	52.17300	24.12000
H	-0.64800	53.17300	24.20500
C	0.19100	51.22900	24.54500
C	-0.34400	50.47300	25.74600
O	-0.06300	49.28800	25.91700
C	1.47700	51.96500	24.92400
C	2.59800	51.05200	25.35000
C	3.04500	50.03600	24.50800
C	3.21200	51.21100	26.59100
C	4.09100	49.18700	24.89800
C	4.25900	50.37000	26.99100
C	4.69900	49.35600	26.14200
N	-1.12200	51.16900	26.57400
H	-1.30400	52.15100	26.36800
C	-1.72600	50.57400	27.77000
C	-2.80100	49.55700	27.37200
O	-2.92100	48.49300	27.98400
C	-2.35000	51.66000	28.65800
C	-1.46300	52.79100	29.18900
C	-2.29900	53.70000	30.07000
C	-0.29300	52.23300	29.97700
N	-3.58500	49.88600	26.35000
H	-3.46300	50.78600	25.88700
C	-4.61400	48.97000	25.89000
C	-3.89800	47.73200	25.37400

O	-4.39900	46.61500	25.48200
C	-5.44500	49.60200	24.76800
C	-6.14300	50.87600	25.20800
O	-6.84100	50.84700	26.24400
O	-5.99800	51.90800	24.52100
N	-2.71300	47.94800	24.81500
H	-2.36000	48.90300	24.75200
C	-1.90700	46.85800	24.29100
C	-1.70900	45.88100	25.43200
O	-2.20600	44.75600	25.39400
C	-0.55200	47.38800	23.80500
C	0.44000	46.45700	23.08700
C	1.17700	45.56900	24.07100
C	-0.30800	45.62800	22.06400
N	-0.99700	46.33100	26.45800
H	-0.63100	47.28300	26.42900
C	-0.72500	45.50400	27.62000
C	-1.98300	44.86000	28.19200
O	-2.06100	43.63400	28.31400
C	-0.02700	46.33200	28.70700
C	1.37400	46.70400	28.22000
C	0.03700	45.55800	30.01200
C	2.17800	47.50000	29.21300
N	-2.97300	45.68300	28.52300
H	-2.85800	46.68600	28.37400
C	-4.22200	45.18400	29.09500
C	-4.91200	44.09300	28.26600
O	-5.55500	43.20600	28.81500
C	-5.17600	46.34400	29.32900
N	-4.77800	44.15500	26.94800
H	-4.22900	44.90900	26.53600
C	-5.40100	43.16400	26.07700
C	-4.71400	41.81000	26.16100
O	-5.36900	40.76800	26.14000
C	-5.38900	43.66200	24.63100
C	-6.54700	44.59800	24.32700
O	-6.81700	45.52200	25.12700
O	-7.19000	44.41100	23.27500
N	-3.39000	41.83600	26.26300
H	-2.91500	42.73800	26.28500
C	-2.59100	40.61600	26.34500
C	-2.71400	39.92600	27.70000
O	-2.61100	38.70300	27.78300

C	-1.08700	40.90900	26.10400
C	-0.29200	39.62100	26.15100
C	-0.89200	41.60100	24.76800
N	-2.93900	40.71100	28.75300
H	-3.03700	41.71600	28.60800
C	-3.05000	40.17600	30.11200
C	-4.44800	39.80300	30.62700
O	-4.56700	38.97400	31.53500
C	-2.42100	41.15200	31.10800
C	-0.94000	41.39100	30.91100
S	-0.12300	41.80800	32.46900
C	-0.43000	43.55600	32.59800
N	-5.49700	40.40600	30.07100
H	-5.35000	41.07100	29.31200
C	-6.85900	40.12800	30.53400
C	-7.86500	39.94800	29.40900
O	-8.51000	38.90200	29.28600
C	-7.35300	41.26200	31.43500
C	-6.35100	41.70500	32.46100
C	-5.35900	42.61300	32.13100
C	-6.40100	41.21200	33.76200
C	-4.43200	43.02200	33.08000
C	-5.47900	41.61500	34.71600
C	-4.49600	42.52100	34.37800
N	-7.99800	40.99300	28.60300
H	-7.43100	41.82400	28.77000
C	-8.92700	40.98500	27.49200
C	-9.00500	39.71800	26.66600
O	-9.99400	38.98900	26.74300
N	-7.97100	39.44200	25.87900
H	-7.15600	40.05500	25.87600
C	-7.99800	38.26900	25.02200
C	-8.13700	36.94000	25.75600
O	-8.99400	36.12400	25.39800
C	-6.76200	38.22000	24.11600
C	-6.88900	37.07100	23.13100
C	-6.63000	39.53100	23.36800
N	-7.30500	36.70400	26.79300
C	-7.33800	35.46200	27.58100
C	-8.72800	35.21500	28.14500
O	-9.24000	34.09500	28.11300
C	-6.32700	35.72500	28.69400
C	-5.37300	36.68400	28.07800

C	-6.28500	37.62400	27.32400
N	-9.32800	36.27800	28.66200
H	-8.84700	37.17700	28.65600
C	-10.65000	36.18600	29.23300
C	-11.67900	35.68300	28.22800
O	-12.42600	34.75100	28.52700
C	-11.06300	37.54400	29.78100
O	-10.18600	37.93000	30.82200
H	-10.44400	38.77800	31.16400
N	-11.71400	36.28300	27.03900
H	-11.05800	37.03800	26.84100
C	-12.67800	35.87900	26.00700
C	-12.42700	34.46000	25.48200
O	-13.37200	33.71400	25.19300
C	-12.67600	36.87000	24.80500
C	-13.55800	36.34000	23.67300
C	-13.17700	38.23300	25.25800
N	-11.15900	34.08700	25.35000
H	-10.40900	34.73700	25.58500
C	-10.84000	32.75200	24.87000
C	-11.43600	31.76700	25.85300
O	-12.13900	30.82900	25.46200
C	-9.33200	32.52600	24.79800
C	-8.71700	33.47200	23.76200
C	-9.05500	31.07700	24.45200
C	-7.21300	33.36700	23.62500
N	-11.15100	31.99900	27.13400
H	-10.55300	32.79200	27.36800
C	-11.66100	31.16300	28.21200
C	-13.18500	31.07500	28.12000
O	-13.75100	29.97800	28.10200
C	-11.25200	31.73500	29.57500
C	-12.01100	31.04700	30.69200
C	-9.76200	31.56200	29.76100
N	-13.84300	32.23000	28.04400
H	-13.31800	33.10400	28.06100
C	-15.30000	32.27400	27.93700
C	-15.77300	31.37100	26.80200
O	-16.63900	30.50500	26.98500
C	-15.76600	33.70200	27.68700
N	-15.19900	31.58200	25.62300
H	-14.49000	32.31000	25.53100
C	-15.56800	30.78900	24.46300

C	-15.36500	29.31600	24.76600
O	-16.28500	28.51200	24.61700
C	-14.72900	31.20000	23.25100
C	-15.10300	32.55600	22.67000
C	-14.20900	32.91100	21.50800
N	-14.60200	34.17000	20.89400
H	-15.50100	34.57200	21.15800
C	-13.85900	34.82700	20.01000
N	-12.68600	34.33500	19.64300
H	-12.11600	34.83900	18.96400
H	-12.36200	33.45100	20.03500
N	-14.28100	35.97900	19.49900
H	-13.71100	36.48300	18.82000
H	-15.18500	36.35800	19.78200
N	-14.16400	28.96900	25.21000
H	-13.44800	29.68500	25.33000
C	-13.85100	27.58500	25.52800
C	-14.85500	26.97000	26.49000
O	-15.21500	25.79900	26.35500
C	-12.44200	27.49500	26.10500
C	-11.37100	27.61600	25.03600
O	-10.23600	28.00000	25.31600
N	-11.72700	27.27200	23.80500
H	-12.66800	26.95400	23.57300
H	-11.00700	27.35300	23.08700
N	-15.31100	27.76100	27.45500
H	-14.98100	28.72400	27.51200
C	-16.27500	27.27500	28.43300
C	-17.61600	27.12300	27.74400
O	-18.29200	26.10800	27.89700
C	-16.40300	28.25900	29.58900
C	-17.31600	27.79900	30.68200
N	-16.87700	27.04900	31.75100
H	-15.91600	26.74300	31.90200
C	-18.64300	27.97900	30.86900
C	-17.89600	26.78800	32.55000
N	-18.98000	27.34100	32.03800
H	-19.91500	27.30100	32.44400
N	-17.99900	28.14400	26.98600
H	-17.39900	28.96600	26.91400
C	-19.26100	28.11200	26.25500
C	-19.30600	26.85000	25.39800
O	-20.25100	26.06600	25.48100

C	-19.38100	29.33900	25.35100
C	-20.60500	29.33000	24.45700
C	-20.40700	30.29500	23.31400
N	-19.29400	29.87000	22.47000
H	-19.05400	28.87900	22.46800
C	-18.57000	30.68100	21.70300
N	-18.82800	31.98300	21.66100
H	-19.59100	32.36400	22.22000
H	-18.27300	32.60500	21.07300
N	-17.57900	30.18600	20.97700
H	-17.38100	29.18600	21.00900
H	-17.02400	30.80800	20.38900
N	-18.26600	26.66500	24.58200
H	-17.51900	27.35900	24.57900
C	-18.15100	25.51100	23.69200
C	-18.18800	24.18300	24.45200
O	-18.64000	23.16600	23.92200
C	-16.85700	25.59700	22.86900
C	-16.76800	26.87300	22.03600
O	-17.80900	27.31500	21.50300
O	-15.65200	27.42300	21.90000
N	-17.70000	24.18800	25.68900
H	-17.31200	25.04900	26.07400
C	-17.71400	22.97900	26.49900
C	-19.17700	22.61600	26.74900
O	-19.50300	21.47700	27.07600
C	-16.99300	23.21900	27.81500
N	-20.05500	23.60400	26.59600
H	-19.72500	24.53500	26.34100
C	-21.47700	23.37500	26.78700
C	-22.03700	23.75900	28.14400
O	-23.04800	23.20900	28.58400
N	-21.39900	24.70900	28.81100
H	-20.57500	25.15000	28.40200
C	-21.86600	25.12500	30.11900
C	-22.22900	26.59700	30.10600
O	-21.57200	27.39700	29.43400
C	-20.79000	24.86700	31.14400
N	-23.28100	26.97800	30.85400
C	-23.70100	28.38100	30.90300
C	-22.46900	29.27200	30.93700
O	-21.46600	28.92000	31.55900
C	-24.49500	28.45300	32.20100

C	-25.14000	27.11000	32.25600
C	-24.03100	26.16900	31.83300
N	-22.52900	30.41100	30.26100
H	-23.37700	30.65200	29.74700
C	-21.39100	31.32100	30.24800
C	-21.87900	32.76000	30.14800
O	-22.77700	33.06900	29.36500
C	-20.44400	31.00600	29.05800
O	-20.05700	29.62900	29.10900
H	-19.47800	29.43600	28.38100
C	-19.19600	31.86100	29.11500
N	-21.29200	33.63700	30.94900
H	-20.56200	33.32000	31.58700
C	-21.66700	35.04400	30.93800
C	-20.41500	35.90000	30.94300
O	-19.41200	35.54000	31.55500
C	-22.51800	35.37900	32.17100
C	-23.92600	34.83100	32.12400
C	-24.93900	35.52800	31.46800
C	-24.24200	33.60100	32.71400
C	-26.23600	35.01800	31.39400
C	-25.53800	33.07800	32.64900
C	-26.53000	33.79400	31.98500
O	-27.81400	33.29700	31.89400
H	-28.01500	32.46100	32.29800
N	-20.47200	37.03000	30.25500
H	-21.32200	37.26300	29.74200
C	-19.34300	37.94200	30.22000
C	-19.80700	39.36100	30.50800
O	-20.99300	39.67200	30.37700
C	-18.64300	37.88100	28.86900
C	-17.88200	36.60000	28.65400
S	-16.48200	36.85000	27.54500
C	-15.20100	37.35700	28.69400
N	-18.87600	40.21700	30.92000
H	-17.91300	39.89900	31.02900
C	-19.21200	41.60000	31.21700
C	-17.99000	42.48000	31.04300
O	-16.87000	41.99000	30.97700
C	-19.73900	41.73600	32.65700
C	-18.67900	41.66800	33.74600
C	-18.47800	40.50700	34.49800
C	-17.86500	42.76500	34.01400

C	-17.48600	40.44900	35.48700
C	-16.87800	42.71500	34.99400
C	-16.69000	41.55800	35.72300
O	-15.68100	41.52800	36.66000
H	-15.13500	42.28800	36.82200
N	-18.21200	43.78400	30.95900
H	-19.17100	44.13000	30.98300
C	-17.11700	44.72900	30.83300
C	-17.50100	45.93900	31.67600
O	-18.41800	46.68300	31.33100
C	-16.90400	45.13100	29.37200
C	-15.58600	45.87600	29.12500
C	-15.42400	46.35800	27.68400
O	-14.37600	46.97100	27.36800
O	-16.34700	46.12500	26.86900
N	-16.80100	46.11500	32.79300
H	-16.05300	45.45700	33.01300
C	-17.06200	47.21300	33.71500
C	-16.32800	48.48600	33.30800
O	-15.10000	48.53000	33.30600
C	-16.62900	46.80800	35.12100
C	-17.05000	47.77200	36.18800
C	-18.35700	47.78400	36.65500
C	-16.13800	48.66100	36.73400
C	-18.74900	48.66900	37.65500
C	-16.52000	49.54400	37.72700
C	-17.82900	49.54900	38.19200
N	-17.09400	49.52100	32.98000
H	-18.10700	49.41100	33.02200
C	-16.54700	50.81400	32.56100
C	-17.13500	51.93300	33.39900
O	-18.16100	52.50700	33.03200
C	-16.87700	51.05800	31.09100
C	-18.14700	50.35700	30.65300
C	-18.45900	50.57900	29.19600
O	-17.56600	50.53200	28.35000
N	-19.73200	50.81000	28.88600
H	-20.47200	50.84900	29.58700
H	-19.94300	50.96000	27.90000
N	-16.48800	52.23300	34.52400
H	-15.64400	51.71100	34.75900
C	-16.94400	53.28400	35.43500
C	-15.80500	53.68900	36.36600

O	-15.03300	52.83800	36.80100
C	-18.12300	52.78300	36.27400
C	-18.78500	53.85300	37.10700
C	-19.81200	54.63700	36.58300
C	-18.37200	54.09700	38.41700
C	-20.41600	55.64100	37.34400
C	-18.96700	55.09900	39.18800
C	-19.98700	55.86500	38.64400
O	-20.57400	56.84900	39.40000
H	-21.27300	57.37400	39.02700
N	-15.69600	54.98300	36.66800
H	-16.35900	55.64600	36.26700
C	-14.64800	55.47200	37.56000
C	-15.19300	55.70900	38.95700
O	-15.83600	56.72300	39.21400
C	-14.05500	56.78200	37.04400
C	-12.99800	57.37700	37.97800
C	-12.38000	58.64100	37.38800
N	-11.08500	58.98700	37.98100
H	-10.27000	59.00500	37.36700
C	-10.90100	59.27900	39.26500
N	-11.93000	59.26600	40.10500
H	-11.78900	59.49000	41.09000
H	-12.86000	59.02300	39.76300
N	-9.69000	59.59500	39.71000
H	-9.54900	59.81900	40.69500
H	-8.90000	59.60500	39.06500
N	-14.94200	54.78100	39.88700
C	-15.46400	55.00700	41.23300
C	-14.98300	56.32300	41.83100
O	-13.93500	56.85100	41.45300
C	-14.97700	53.78100	42.00800
C	-13.75400	53.35900	41.26700
C	-14.15700	53.53800	39.83000
N	-15.77500	56.85300	42.75200
H	-16.64000	56.37100	42.99700
C	-15.45000	58.09800	43.42300
C	-14.56500	57.79700	44.61900
O	-14.20700	58.69600	45.37800
C	-16.71800	58.76800	43.91700
O	-17.31400	57.97800	44.92700
H	-18.10800	58.39800	45.23600
N	-14.23100	56.52300	44.79800

H	-14.57500	55.81900	44.14500
C	-13.38300	56.11400	45.91000
C	-11.96200	55.85200	45.42900
O	-11.13700	55.31600	46.17500
C	-13.92400	54.84500	46.56200
C	-15.39400	54.87000	46.81100
C	-16.26200	54.19000	45.96200
C	-15.91300	55.54300	47.90900
C	-17.62800	54.17600	46.20900
C	-17.27800	55.53600	48.16500
C	-18.13800	54.85100	47.31500
N	-11.68800	56.21800	44.17800
H	-12.42600	56.64000	43.61400
C	-10.36800	56.03500	43.59000
C	-9.36400	56.93800	44.29700
O	-9.74300	57.92400	44.93900
C	-10.39900	56.36700	42.09500
O	-11.22900	55.46600	41.37800
H	-11.24800	55.67200	40.45100
N	-8.08400	56.59600	44.18000
H	-7.83700	55.76900	43.63700
C	-7.02400	57.37600	44.81000
C	-6.83500	58.72500	44.10700
O	-7.08400	58.85800	42.90800
C	-5.71200	56.58600	44.79400
O	-4.72300	57.23000	45.57900
H	-3.90900	56.74000	45.56900
N	-6.39600	59.72200	44.86400
H	-6.20600	59.54900	45.85100
C	-6.17900	61.05400	44.32500
C	-5.19000	61.03400	43.16400
O	-5.47900	61.54700	42.08100
C	-5.65000	61.96600	45.42400
C	-6.35700	61.74500	46.74300
O	-7.60400	61.83900	46.76900
O	-5.66900	61.47400	47.75200
N	-4.02700	60.43300	43.40100
H	-3.87100	60.01700	44.31900
C	-2.96200	60.34300	42.40100
C	-3.37600	59.69700	41.07800
O	-2.54800	59.53000	40.17900
C	-1.78000	59.56800	42.98300
C	-1.18100	60.19100	44.22100

S	0.06200	59.12000	44.96500
C	-0.89900	58.32100	46.28000
N	-4.65000	59.33800	40.96100
H	-5.28700	59.51700	41.73700
C	-5.16600	58.69600	39.75800
C	-5.78900	59.70000	38.80000
O	-6.75100	60.38300	39.14500
C	-6.20900	57.64100	40.14700
C	-7.00900	57.04000	38.99200
C	-8.13800	56.16000	39.52900
C	-9.00700	55.58500	38.41400
N	-10.12900	54.74200	38.94300
H	-10.71000	54.35800	38.19800
H	-10.69200	55.26000	39.61800
H	-9.77900	54.00400	39.55400
N	-5.23900	59.80800	37.58100
C	-5.80000	60.75000	36.61300
C	-7.29100	60.48400	36.41900
O	-7.75600	59.35900	36.58600
C	-4.96800	60.49200	35.35400
C	-4.41000	59.10500	35.55700
C	-4.08300	59.09700	37.01200
N	-8.04400	61.52000	36.07700
H	-7.61500	62.43500	35.93600
C	-9.47800	61.35800	35.90200
C	-9.85200	60.76900	34.55700
O	-10.98800	60.35000	34.34900
C	-10.19200	62.69900	36.08300
C	-9.86800	63.75900	35.02900
C	-10.72000	65.00700	35.26400
C	-10.32000	66.17100	34.36600
N	-11.07300	67.41300	34.72400
H	-10.80500	68.19200	34.12300
H	-10.96500	67.64600	35.71100
H	-12.08100	67.25800	34.71000
N	-8.89800	60.72800	33.64300
H	-7.96300	61.07000	33.86700
C	-9.17900	60.19700	32.32100
C	-9.32800	58.67700	32.34300
O	-9.77700	58.07400	31.36300
C	-8.06000	60.58200	31.32200
O	-6.91600	59.73900	31.52100
H	-7.17600	58.83500	31.38700

C	-7.64100	62.03700	31.53700
N	-8.96400	58.05600	33.46400
H	-8.62300	58.60400	34.25400
C	-9.04600	56.60200	33.57900
C	-10.42900	56.13000	34.02700
O	-11.01600	56.68600	34.95600
C	-8.00000	56.05900	34.57200
C	-7.63500	54.62900	34.21100
C	-6.77600	56.93600	34.56700
N	-10.93500	55.09900	33.35900
H	-10.38900	54.68800	32.60200
C	-12.24100	54.53500	33.66800
C	-12.18100	53.01900	33.58100
O	-11.73900	52.46600	32.57100
C	-13.30400	55.05300	32.68500
C	-13.56300	56.52800	32.96000
C	-14.58800	54.24700	32.81400
C	-14.55900	57.14900	32.02500
N	-12.62900	52.34900	34.63900
H	-12.99300	52.85500	35.44600
C	-12.60000	50.90000	34.64600
C	-11.17800	50.40200	34.80700
O	-10.72100	49.53600	34.06000
N	-10.47700	50.97100	35.78300
H	-10.92300	51.69400	36.34700
C	-9.10000	50.60500	36.08000
C	-9.12700	49.24300	36.77100
O	-10.19500	48.71200	37.07500
C	-8.47700	51.66900	37.00200
C	-6.97000	51.48400	37.20400
O	-6.25900	51.14200	36.23100
O	-6.49100	51.70600	38.33800
N	-7.95700	48.66900	37.01100
H	-7.09400	49.13200	36.72500
C	-7.90200	47.38600	37.67800
C	-8.50000	47.58100	39.07600
O	-8.21100	48.57100	39.74600
C	-6.44800	46.89800	37.76800
C	-6.31700	45.44500	38.11600
N	-6.80300	44.43900	37.30800
H	-7.27200	44.57700	36.41300
C	-5.77300	44.83100	39.19400
C	-6.56700	43.26900	37.87300

N	-5.94300	43.47900	39.01900
H	-5.63700	42.75400	39.66800
N	-9.36000	46.64900	39.48800
H	-9.58800	45.87400	38.86500
C	-9.98300	46.70800	40.80300
C	-11.18300	47.63200	40.97300
O	-11.82900	47.62400	42.02100
N	-11.49700	48.41500	39.94500
H	-10.94800	48.35300	39.08800
C	-12.60800	49.36100	40.01100
C	-13.98600	48.76800	40.27400
O	-14.77400	49.33900	41.02500
C	-12.64500	50.21600	38.73600
C	-11.63000	51.35900	38.76600
O	-10.80000	51.40100	39.71200
O	-11.66500	52.21300	37.84300
N	-14.28300	47.62900	39.66700
H	-13.59500	47.18000	39.06200
C	-15.59000	47.01600	39.86100
C	-15.74500	46.45800	41.27200
O	-16.82600	46.02400	41.65700
C	-15.82100	45.90400	38.82500
C	-15.27900	44.51300	39.18200
C	-13.78100	44.50000	39.46700
O	-13.06600	45.41900	38.99800
O	-13.31800	43.55800	40.15000
N	-14.66300	46.48200	42.04300
H	-13.79500	46.87200	41.67600
C	-14.69300	45.96200	43.40100
C	-15.55900	46.77300	44.35300
O	-16.21400	46.20900	45.22800
C	-13.27600	45.84800	43.95900
C	-12.50200	44.64600	43.41400
C	-11.06800	44.67400	43.92900
C	-13.19500	43.36500	43.82900
N	-15.57800	48.09000	44.18500
H	-15.02500	48.51400	43.44000
C	-16.38400	48.93400	45.05800
C	-17.87700	48.68900	44.85300
O	-18.66500	48.76500	45.79800
C	-16.03000	50.39800	44.82300
C	-14.58200	50.68000	45.00200
C	-13.68200	50.40200	43.98800

C	-14.09700	51.13400	46.22300
C	-12.31900	50.56700	44.18700
C	-12.73300	51.30100	46.43100
C	-11.84500	51.01500	45.41100
N	-18.26000	48.38500	43.61900
H	-17.56500	48.34000	42.87400
C	-19.65300	48.11500	43.31400
C	-20.04300	46.73000	43.81800
O	-21.09000	46.56100	44.44200
C	-19.89300	48.21200	41.80900
O	-19.84200	49.56100	41.37800
H	-19.99100	49.62100	40.44200
N	-19.19000	45.74300	43.56400
H	-18.32700	45.94800	43.06100
C	-19.45900	44.37500	43.98800
C	-19.65500	44.21700	45.49700
O	-20.58000	43.52800	45.93300
C	-18.34500	43.43200	43.52700
C	-18.49600	42.08800	44.20500
C	-18.40400	43.27300	42.01600
N	-18.79100	44.83800	46.29600
H	-18.02500	45.37900	45.89500
C	-18.93700	44.74600	47.74800
C	-19.60200	45.98600	48.33200
O	-19.33500	46.35100	49.47600
C	-17.59300	44.54800	48.44400
C	-17.01900	43.18400	48.27800
C	-16.36400	42.82300	47.10200
C	-17.11600	42.25500	49.30300
C	-15.80900	41.55200	46.94600
C	-16.56700	40.98200	49.15700
C	-15.91100	40.63200	47.97300
N	-20.45400	46.63400	47.54300
H	-20.61800	46.29600	46.59500
C	-21.15300	47.81500	48.01200
C	-20.37700	48.82800	48.84400
O	-20.72400	49.09600	49.99600
N	-19.32300	49.39700	48.27100
H	-19.05300	49.12400	47.32600
C	-18.54800	50.40900	48.98000
C	-19.44300	51.62300	49.25200
O	-19.35400	52.24400	50.31000
C	-17.32900	50.82900	48.15300

N	-20.31300	51.98200	48.29200
C	-21.20400	53.12600	48.48000
C	-22.02400	53.10000	49.77200
O	-22.54400	54.13600	50.19300
C	-22.08600	53.06900	47.24000
C	-21.12500	52.62000	46.20200
C	-20.39000	51.50000	46.89900
N	-22.13600	51.93100	50.40300
H	-21.66900	51.10800	50.02200
C	-22.91700	51.81100	51.63000
C	-22.09500	51.76600	52.90700
O	-22.64300	51.66700	54.00900
C	-23.80200	50.58600	51.54900
C	-24.65100	50.56100	50.32700
C	-24.14600	50.06800	49.12600
C	-25.94200	51.09400	50.35400
C	-24.91400	50.10700	47.96300
C	-26.71700	51.14100	49.20300
C	-26.20400	50.64700	48.00300
N	-20.78100	51.85000	52.75000
H	-20.39900	51.93100	51.80800
C	-19.87400	51.83000	53.87700
C	-19.07400	53.11400	53.84200
O	-18.94900	53.80900	54.85600
C	-18.93800	50.62700	53.77700
C	-19.64600	49.27500	53.71900
C	-18.61900	48.16800	53.73500
C	-20.58100	49.13600	54.90000
N	-18.52800	53.42700	52.67000
H	-18.66000	52.80400	51.87400
C	-17.74600	54.64300	52.50400
C	-18.69500	55.82600	52.44100
O	-19.90100	55.65900	52.60500
C	-16.88600	54.56700	51.23800
C	-15.81600	53.49000	51.32200
C	-14.62100	53.76600	50.42400
C	-13.48100	52.84100	50.80800
N	-12.20400	53.16400	50.13300
H	-11.43800	52.54200	50.39100
H	-11.94800	54.13800	50.29300
H	-12.32600	53.18500	49.12100
N	-18.16700	57.02000	52.20400
H	-17.16300	57.11700	52.05100

C	-19.03000	58.18900	52.16400
C	-18.94500	59.03500	50.90100
O	-17.91200	59.08100	50.23300
C	-18.75900	59.07100	53.38500
C	-19.89400	60.02300	53.68100
C	-21.24100	59.30400	53.76700
O	-21.41500	58.46600	54.68500
O	-22.12100	59.57100	52.90900
N	-20.05600	59.68800	50.57700
H	-20.89200	59.57700	51.15100
C	-20.09200	60.55400	49.42000
C	-20.59200	59.95300	48.13000
O	-20.70600	60.65200	47.12700
N	-20.89400	58.66700	48.12500
H	-20.79100	58.10700	48.97200
C	-21.37400	58.06300	46.89600
C	-22.55800	58.86200	46.33200
O	-23.44000	59.30300	47.07400
C	-21.77600	56.61300	47.15300
N	-22.55700	59.06900	45.01900
H	-21.77800	58.72100	44.46000
C	-23.64300	59.78200	44.36100
C	-24.75200	58.77100	44.10400
O	-24.49900	57.56800	44.03900
C	-23.17800	60.35700	43.02800
O	-22.85800	59.31500	42.12400
H	-22.56800	59.67300	41.29300
N	-25.97500	59.25800	43.94500
H	-26.12300	60.26600	43.98900
C	-27.10800	58.38000	43.70900
C	-26.88000	57.42200	42.55300
O	-27.41600	56.31800	42.53700
C	-28.36400	59.19900	43.44200
C	-29.61600	58.35400	43.39000
C	-29.69500	57.39600	44.56600
O	-29.53700	57.84300	45.72300
O	-29.91400	56.19300	44.33600
N	-26.08500	57.85000	41.58400
H	-25.67200	58.78000	41.65700
C	-25.78200	57.03000	40.41400
C	-24.83200	55.89200	40.75900
O	-24.97500	54.77100	40.26600
C	-25.16000	57.90600	39.33100

C	-24.24200	57.18400	38.37100
C	-23.54000	58.15200	37.44400
O	-24.22300	58.71700	36.56100
O	-22.31300	58.35600	37.61000
N	-23.85500	56.19700	41.60800
H	-23.79300	57.14800	41.97100
C	-22.87000	55.21100	42.03400
C	-23.53200	54.22900	42.99500
O	-23.21900	53.03800	43.00400
C	-21.69300	55.90700	42.71600
C	-20.39600	55.14100	42.62300
C	-19.28500	55.83200	43.36700
O	-18.11600	55.40300	43.23200
O	-19.59100	56.80500	44.09000
N	-24.44500	54.74500	43.80600
H	-24.64100	55.74500	43.76800
C	-25.16900	53.91400	44.74400
C	-25.94000	52.89300	43.93000
O	-25.89900	51.69300	44.20800
C	-26.14800	54.76000	45.58100
C	-25.34200	55.74200	46.43300
C	-27.02500	53.86200	46.44300
C	-26.15400	56.63100	47.31800
N	-26.62900	53.38400	42.90500
H	-26.60300	54.38700	42.72400
C	-27.41500	52.53100	42.03900
C	-26.58200	51.50500	41.30700
O	-26.97700	50.34800	41.21500
C	-28.19300	53.36600	41.03200
C	-29.60000	53.67000	41.48500
C	-30.38400	54.49100	40.46000
N	-31.81100	54.52400	40.79800
H	-32.46500	54.13200	40.12100
C	-32.31800	55.02900	41.92500
N	-31.52300	55.56100	42.84300
H	-31.91000	55.94700	43.70400
H	-30.51800	55.59900	42.67200
N	-33.62600	54.98000	42.14800
H	-34.01300	55.36600	43.00900
H	-34.23800	54.57100	41.44200
N	-25.42900	51.90900	40.78400
H	-25.12900	52.87800	40.88700
C	-24.59700	50.95400	40.06100

C	-24.25200	49.78600	40.96600
O	-24.17100	48.64800	40.52000
C	-23.30700	51.60500	39.55900
C	-22.41000	50.63400	38.77400
C	-23.14200	50.11200	37.54500
C	-21.12200	51.33200	38.36800
N	-24.06000	50.07400	42.24600
H	-24.15200	51.03900	42.56300
C	-23.72000	49.03600	43.20500
C	-24.90700	48.11100	43.49800
O	-24.75600	46.88400	43.49500
C	-23.20700	49.66700	44.50300
O	-22.76400	48.67600	45.41500
H	-22.44600	49.06700	46.22000
N	-26.08200	48.68500	43.75400
H	-26.16000	49.70200	43.75600
C	-27.25900	47.86700	44.03100
C	-27.46300	46.89800	42.88500
O	-27.77400	45.71900	43.08400
C	-28.50200	48.74100	44.19100
C	-28.54800	49.47600	45.50800
C	-29.80500	50.31300	45.66800
C	-29.85600	50.92200	47.07100
N	-30.97800	51.88100	47.27000
H	-31.01200	52.28700	48.20500
H	-31.86900	51.44400	47.03500
H	-30.95400	52.61400	46.56100
N	-27.26100	47.41400	41.68100
H	-26.98200	48.39300	41.61200
C	-27.41800	46.65200	40.45500
C	-26.44100	45.48100	40.36000
O	-26.85500	44.32200	40.30300
C	-27.24700	47.60200	39.26900
C	-27.46300	46.98200	37.90100
S	-27.64200	48.27300	36.65100
C	-26.11000	49.14700	36.88400
N	-25.14800	45.78900	40.35000
H	-24.87000	46.76800	40.41100
C	-24.11700	44.76100	40.25400
C	-24.33400	43.65700	41.27800
O	-24.25200	42.47100	40.94600
C	-22.69700	45.34000	40.46800
C	-21.67600	44.21000	40.51300

C	-22.35700	46.31200	39.35200
N	-24.60600	44.04200	42.52000
H	-24.66200	45.03600	42.74100
C	-24.82400	43.05800	43.56400
C	-25.99500	42.13600	43.22200
O	-25.87100	40.92000	43.32700
C	-25.04900	43.75500	44.90000
C	-23.87700	44.60900	45.31500
S	-23.97100	45.13100	47.03000
C	-25.08700	46.49100	46.90500
N	-27.12600	42.69800	42.80400
H	-27.19400	43.71300	42.73700
C	-28.26800	41.86700	42.44200
C	-27.85100	40.83600	41.40800
O	-28.17500	39.65400	41.52800
C	-29.38900	42.70500	41.85100
C	-30.47900	43.01900	42.82500
C	-31.81200	43.07200	42.11800
C	-32.88200	43.47100	43.09700
N	-32.68900	42.72700	44.37500
H	-33.41500	42.99800	45.03900
H	-31.75100	42.85300	44.75600
H	-32.65400	41.71800	44.23200
N	-27.14500	41.30400	40.38100
H	-26.93700	42.30200	40.34200
C	-26.65800	40.44300	39.31100
C	-25.79100	39.31700	39.85000
O	-26.01900	38.14600	39.53500
C	-25.86100	41.26800	38.30100
C	-26.69200	41.84100	37.19400
C	-26.35400	43.05600	36.61700
C	-27.79700	41.15300	36.71100
C	-27.10500	43.58200	35.57300
C	-28.55300	41.66400	35.67400
C	-28.20900	42.88300	35.10100
N	-24.78900	39.67300	40.65100
H	-24.63500	40.66000	40.85600
C	-23.90600	38.66800	41.24000
C	-24.75700	37.69100	42.03900
O	-24.81400	36.50700	41.72500
C	-22.85800	39.32000	42.15800
C	-21.51400	39.57900	41.49900
C	-20.29300	39.22500	41.98500

C	-21.26600	40.25500	40.25100
N	-19.29900	39.63200	41.12700
H	-18.30000	39.48400	41.26700
C	-19.86500	40.26700	40.05500
C	-22.08900	40.84900	39.28400
C	-19.26700	40.85000	38.93000
C	-21.49000	41.43100	38.16100
C	-20.09200	41.42400	37.99700
N	-25.43700	38.20000	43.06000
H	-25.35600	39.19600	43.26300
C	-26.29300	37.37400	43.89500
C	-27.23100	36.50100	43.05700
O	-27.33000	35.30100	43.28700
C	-27.09000	38.25500	44.84400
N	-27.92400	37.09700	42.09200
H	-27.82400	38.10100	41.94400
C	-28.82600	36.32800	41.24400
C	-28.09400	35.15000	40.64000
O	-28.58900	34.02400	40.65500
C	-29.37500	37.17300	40.10200
C	-30.52200	38.02800	40.52300
O	-31.17000	37.74900	41.53200
N	-30.80500	39.07200	39.74500
H	-30.26800	39.30300	38.90900
H	-31.59000	39.65700	40.03300
N	-26.92000	35.42900	40.08500
H	-26.58400	36.39200	40.09600
C	-26.10000	34.40400	39.46200
C	-25.78000	33.32800	40.49900
O	-25.77100	32.14100	40.19700
C	-24.80500	35.03700	38.93500
C	-23.90100	34.07400	38.22600
C	-24.26900	33.52900	37.00600
C	-22.68100	33.70300	38.78800
C	-23.43400	32.62100	36.34900
C	-21.83700	32.79600	38.14300
C	-22.21600	32.25500	36.91900
N	-25.54300	33.76600	41.72900
H	-25.60000	34.76800	41.91100
C	-25.20500	32.87600	42.82600
C	-26.37800	32.00900	43.28100
O	-26.18500	30.97000	43.91700
C	-24.68300	33.69800	43.99400

N	-27.59200	32.44900	42.96800
H	-27.68400	33.32000	42.44600
C	-28.79400	31.72300	43.34900
C	-29.19400	30.76200	42.26100
O	-29.42100	29.59000	42.52200
C	-29.95600	32.68800	43.59900
C	-29.93700	33.37100	44.95600
C	-31.10300	34.35200	45.10300
N	-30.85300	35.61600	44.40900
H	-31.02900	35.64800	43.40500
C	-30.41200	36.72900	44.99600
N	-30.16800	36.75600	46.30000
H	-29.83100	37.60700	46.74900
H	-30.32600	35.91600	46.85600
N	-30.20700	37.81900	44.27400
H	-29.87000	38.67000	44.72300
H	-30.39500	37.79800	43.27200
N	-29.26800	31.26500	41.03300
H	-29.02800	32.24400	40.87900
C	-29.68500	30.44700	39.90400
C	-28.58100	30.11900	38.92000
O	-28.64600	29.11700	38.23200
C	-30.81400	31.14000	39.13700
C	-31.86900	31.75100	40.05500
O	-32.37100	31.09900	40.97000
N	-32.21600	33.00900	39.80000
H	-31.80000	33.54900	39.04200
H	-32.92100	33.41700	40.41400
N	-27.55900	30.94900	38.84300
H	-27.50300	31.76600	39.45100
C	-26.52000	30.67300	37.87500
C	-26.92900	31.42400	36.62400
O	-26.59900	31.04500	35.50100
N	-27.68700	32.49300	36.84400
H	-27.94600	32.71000	37.80600
C	-28.16800	33.37200	35.78800
C	-28.32300	34.74000	36.44000
O	-29.09300	34.90300	37.39200
C	-29.52200	32.90800	35.26500
C	-29.99200	33.72600	34.07700
O	-29.84900	34.95000	34.05800
N	-30.56200	33.05500	33.08300
H	-30.68000	32.04200	33.09900

H	-30.87800	33.60500	32.28400
N	-27.59100	35.74200	35.94100
C	-27.68600	37.07800	36.52900
C	-29.04100	37.76100	36.41100
O	-29.41800	38.56200	37.27400
C	-26.57400	37.84700	35.81600
C	-26.46100	37.14400	34.49600
C	-26.56700	35.70000	34.88300
N	-29.78200	37.44300	35.35800
H	-29.44000	36.74900	34.69300
C	-31.07600	38.07000	35.13900
C	-32.05700	37.89900	36.29400
O	-31.95200	36.95900	37.08400
C	-31.65700	37.56300	33.82500
C	-30.74900	37.87600	32.64100
O	-30.50600	39.04400	32.31500
N	-30.22700	36.83300	32.00200
H	-29.62000	37.04200	31.21000
H	-30.42700	35.87000	32.27100
N	-32.99100	38.84200	36.39700
H	-33.01000	39.59400	35.70800
C	-33.98600	38.83500	37.46000
C	-34.75300	40.13800	37.35500
O	-34.27500	41.06600	36.70900
N	-35.91800	40.24000	37.98500
H	-36.26500	39.46700	38.55200
C	-36.69600	41.46700	37.85900
C	-36.07800	42.75400	38.39800
O	-35.49200	42.79000	39.48800
C	-38.11000	41.28400	38.43400
C	-38.22200	40.55400	39.76700
C	-39.68400	40.32100	40.17500
O	-40.49400	39.97900	39.28600
O	-40.02200	40.47000	41.37400
N	-36.22500	43.80800	37.59500
H	-36.71800	43.68800	36.71000
C	-35.70800	45.11900	37.93500
C	-34.31600	45.34200	37.37500
O	-33.63200	46.31000	37.73000
N	-33.89200	44.45500	36.48500
H	-34.50400	43.69000	36.20000
C	-32.56100	44.56700	35.91300
C	-32.56100	44.50400	34.39800

O	-33.43300	43.88700	33.79200
C	-31.66300	43.44500	36.45700
C	-31.40800	43.38200	37.96500
C	-30.91200	41.99500	38.33600
C	-30.40300	44.44900	38.36500
N	-31.57200	45.15300	33.76700
C	-31.44000	45.16800	32.31000
C	-31.18600	43.72300	31.89200
O	-30.59700	42.96600	32.65500
C	-30.20900	46.04000	32.08800
C	-30.20000	46.94300	33.29100
C	-30.54500	46.00200	34.39400
N	-31.62800	43.32200	30.70600
H	-32.12800	43.96500	30.09200
C	-31.38400	41.95200	30.30300
C	-29.92400	41.71700	29.97200
O	-29.34100	42.42800	29.15700
C	-32.18700	41.56300	29.08300
C	-31.95300	40.14700	28.66700
N	-32.49900	39.07600	29.34100
H	-33.13800	39.14200	30.13300
C	-31.17200	39.62100	27.69500
C	-32.06600	37.94900	28.80200
N	-31.25800	38.25300	27.80200
H	-30.77600	37.58100	27.20500
N	-29.35500	40.69600	30.60600
H	-29.92200	40.16400	31.26600
C	-27.96600	40.29300	30.41300
C	-28.04100	39.00400	29.58900
O	-28.45300	37.96100	30.09400
C	-27.34000	40.00700	31.77700
C	-25.86500	39.74700	31.79000
C	-25.10700	39.17500	30.80200
C	-24.97800	39.99600	32.88400
N	-23.80000	39.05300	31.22000
H	-23.03600	38.65800	30.67200
C	-23.69600	39.55000	32.49200
C	-25.14400	40.55200	34.15900
C	-22.58600	39.64600	33.33700
C	-24.03800	40.64500	34.99700
C	-22.77700	40.19400	34.58200
N	-27.66300	39.06600	28.30300
C	-27.69800	37.89500	27.42000

C	-26.62300	36.87800	27.74700
O	-25.59400	37.21500	28.32000
C	-27.49600	38.50700	26.03800
C	-26.56100	39.63500	26.32000
C	-27.14900	40.24600	27.58200
N	-26.85000	35.62700	27.38900
H	-27.72100	35.36500	26.92700
C	-25.83300	34.63700	27.66900
C	-24.71300	34.79300	26.66200
O	-24.94100	35.28600	25.55900
C	-26.39200	33.23000	27.57200
C	-25.34000	32.20900	27.86500
C	-25.90800	30.84000	28.03100
O	-26.93800	30.71400	28.72700
O	-25.32100	29.89000	27.47900
N	-23.50100	34.39500	27.04200
H	-23.36000	34.02900	27.98400
C	-22.37500	34.47900	26.12200
C	-22.38900	33.19100	25.30600
O	-21.59100	32.27900	25.54500
C	-21.04200	34.60800	26.86700
C	-19.85400	34.85400	25.94900
C	-19.49500	36.14700	25.55900
C	-19.11000	33.78800	25.43700
C	-18.42200	36.37000	24.67800
C	-18.04200	33.99900	24.55500
C	-17.70400	35.28900	24.17800
O	-16.66500	35.48400	23.28700
H	-16.43300	36.36800	23.02900
N	-23.33200	33.11900	24.36800
H	-23.97800	33.90200	24.26500
C	-23.48100	31.97100	23.48300
C	-22.80200	32.28500	22.15600
O	-21.82100	33.03000	22.10600
C	-24.96400	31.66700	23.23600
C	-25.74300	32.88500	22.75700
O	-25.17300	33.82700	22.21300
N	-27.05700	32.86200	22.95000
H	-27.57900	33.67800	22.62900
H	-27.53000	32.08000	23.40200
N	-23.34600	31.72800	21.08200
H	-24.16600	31.13100	21.19400
C	-22.80700	31.94400	19.75000

C	-22.73700	33.40600	19.31700
O	-21.74800	33.81600	18.71400
C	-23.61400	31.14400	18.73700
C	-23.44300	29.64900	18.91100
C	-21.97400	29.25500	18.96300
O	-21.16700	29.72900	18.15800
N	-21.61900	28.38200	19.90600
H	-22.28600	27.99000	20.57100
H	-20.63400	28.11800	19.94100
N	-23.77100	34.19200	19.61200
H	-24.57200	33.80300	20.10900
C	-23.77400	35.60700	19.23300
C	-22.73600	36.39000	20.02900
O	-22.43600	37.54700	19.70800
C	-25.14900	36.24700	19.46400
C	-26.24000	35.86500	18.47100
C	-26.73500	34.43500	18.67500
C	-27.95700	34.12800	17.79600
N	-29.13200	35.01600	18.08500
H	-29.94300	34.81200	17.50100
H	-28.87000	35.99900	18.01200
H	-29.37900	34.98100	19.07400
N	-22.19900	35.75300	21.06800
H	-22.50000	34.79900	21.26800
C	-21.19500	36.36900	21.93300
C	-21.70700	37.62700	22.62800
O	-20.98700	38.62100	22.75600
C	-19.93100	36.70400	21.13800
C	-19.03900	35.50700	20.85000
C	-17.78500	35.89800	20.08300
O	-16.87500	35.04700	19.95400
O	-17.71200	37.05600	19.60700
N	-22.95400	37.57900	23.08200
H	-23.51500	36.73800	22.94700
C	-23.51700	38.72400	23.76900
C	-22.94000	38.87000	25.16400
O	-22.57700	37.88100	25.81200
N	-22.84400	40.10500	25.63500
H	-23.13900	40.89200	25.05700
C	-22.32100	40.34500	26.96800
C	-22.90900	41.64100	27.50200
O	-23.55900	42.37600	26.76600
C	-20.79100	40.39500	26.93000

C	-20.23000	41.57300	26.18400
C	-19.84800	42.72700	26.86700
C	-20.10800	41.55300	24.79400
C	-19.35700	43.84100	26.18800
C	-19.61800	42.66300	24.10100
C	-19.24700	43.80500	24.80900
O	-18.78800	44.91900	24.15100
H	-18.53500	45.69700	24.63400
N	-22.69400	41.91600	28.78100
H	-22.13900	41.27500	29.34800
C	-23.24000	43.12200	29.38600
C	-22.21000	44.20900	29.59900
O	-21.14200	43.97300	30.15600
C	-23.89400	42.80100	30.73500
C	-24.56600	43.97100	31.46800
C	-25.75300	44.45000	30.65300
C	-25.02600	43.54600	32.85800
N	-22.54100	45.40700	29.13900
H	-23.42700	45.52300	28.64700
C	-21.67500	46.56000	29.31700
C	-22.21800	47.21300	30.57900
O	-23.34900	47.69500	30.60200
C	-21.79800	47.50300	28.12300
C	-20.48600	47.74100	27.41300
C	-20.67700	48.16000	25.97300
O	-21.42700	49.09000	25.67800
N	-19.99100	47.47500	25.06500
H	-19.36900	46.70400	25.31000
H	-20.12000	47.75800	24.09300
N	-21.42200	47.21100	31.63700
H	-20.48600	46.81200	31.56500
C	-21.87000	47.77100	32.89700
C	-21.25900	49.11900	33.18400
O	-20.05800	49.31300	33.02900
C	-21.54800	46.80800	34.03900
C	-22.21500	45.45900	33.75000
C	-22.01700	47.39000	35.35800
C	-21.72300	44.32700	34.59600
N	-22.10300	50.05200	33.60600
H	-23.09100	49.82400	33.71500
C	-21.64100	51.39100	33.91500
C	-22.82100	52.30700	34.15100
O	-23.94100	51.82700	34.34900

N	-22.58000	53.61700	34.12500
H	-21.63000	53.94300	33.94800
C	-23.63900	54.60000	34.34300
C	-24.81300	54.30800	33.41700
O	-25.95100	54.68200	33.69700
C	-23.11000	55.99400	34.10100
N	-24.51800	53.63800	32.30900
H	-23.54500	53.38900	32.13200
C	-25.52600	53.24500	31.33700
C	-25.21900	51.80200	30.98000
O	-24.37700	51.53200	30.12300
C	-25.44600	54.11600	30.08500
C	-25.85800	55.55200	30.34800
O	-26.99100	55.82000	30.76600
N	-24.94200	56.48800	30.10200
H	-25.21900	57.45400	30.27900
H	-24.00800	56.26700	29.75700
N	-25.89400	50.87700	31.65000
H	-26.58100	51.17000	32.34400
C	-25.68100	49.45700	31.42200
C	-26.57900	48.87800	30.32400
O	-27.79900	49.04700	30.36200
C	-25.90400	48.68100	32.74000
O	-24.96000	49.13600	33.71200
H	-25.09700	48.65900	34.52200
C	-25.72700	47.19100	32.53800
N	-25.96800	48.21300	29.34200
H	-24.95000	48.14300	29.35300
C	-26.70700	47.58000	28.24900
C	-25.90300	46.43800	27.65000
O	-24.70600	46.32100	27.90300
C	-27.05400	48.58000	27.14400
C	-25.86800	49.14300	26.39500
C	-25.17300	50.24600	27.16300
O	-25.79000	51.25700	27.50300
N	-23.88100	50.06200	27.44000
H	-23.37000	49.22500	27.15900
H	-23.41200	50.80600	27.95800
N	-26.56300	45.60000	26.85200
H	-27.55400	45.76100	26.67200
C	-25.90300	44.45600	26.22800
C	-25.18600	44.82600	24.95000
O	-25.53400	45.79900	24.29100

C	-26.90500	43.36200	25.94100
N	-24.18000	44.03200	24.60800
H	-23.94700	43.24600	25.21500
C	-23.39500	44.23900	23.39800
C	-22.97800	42.87100	22.86600
O	-23.42600	41.84000	23.37100
C	-22.16800	45.08100	23.70800
N	-22.12100	42.85700	21.85200
H	-21.78100	43.73800	21.46800
C	-21.66100	41.59800	21.28200
C	-20.20400	41.63800	20.85400
O	-19.65000	42.70500	20.60300
C	-22.52800	41.21700	20.08000
C	-23.94200	40.80200	20.45200
C	-24.82500	40.54400	19.24200
O	-25.71600	39.69800	19.28600
N	-24.58900	41.28000	18.16200
H	-23.85000	41.98200	18.12500
H	-25.18200	41.10700	17.35000
N	-19.59300	40.45900	20.79600
H	-20.11900	39.62800	21.06600
C	-18.20700	40.29100	20.36600
C	-17.13000	41.04900	21.13800
O	-16.27300	41.68900	20.53100
C	-18.09200	40.64600	18.88600
C	-19.02400	39.86000	17.98700
C	-18.78000	40.21500	16.52900
C	-19.51400	39.26400	15.60000
N	-19.07200	39.45300	14.18700
H	-19.56500	38.81400	13.56300
H	-18.06000	39.36500	14.09400
H	-19.17100	40.42300	13.88800
N	-17.15900	40.96900	22.46200
H	-17.89200	40.42400	22.91500
C	-16.16300	41.64600	23.27900
C	-14.74400	41.23500	22.87100
O	-14.43200	40.05000	22.81400
C	-16.39200	41.31300	24.75800
C	-15.34800	41.75700	25.79300
C	-15.19200	43.27100	25.80300
C	-15.78400	41.25800	27.15900
N	-13.89700	42.22000	22.57900
H	-14.23400	43.18200	22.62500

C	-12.50400	41.98400	22.19500
C	-12.29800	41.06100	20.99300
O	-11.17300	40.66400	20.68800
C	-11.73700	41.42300	23.38900
C	-11.66100	42.37100	24.56200
C	-10.81300	43.58000	24.23100
C	-10.71400	44.50800	25.42000
N	-9.81000	45.64600	25.13000
H	-9.74300	46.27200	25.93200
H	-10.09100	46.14400	24.28600
H	-8.89100	45.32800	24.82300
N	-13.38500	40.73100	20.31000
H	-14.28500	41.11300	20.60200
C	-13.34000	39.84000	19.15500
C	-12.17700	40.13000	18.19800
O	-11.46100	39.21800	17.77100
C	-14.66800	39.93300	18.40600
C	-14.83700	38.83400	17.39800
O	-13.98700	38.73000	16.48800
O	-15.81900	38.07200	17.52100
N	-12.00700	41.40700	17.87200
H	-12.64300	42.09800	18.27000
C	-10.95200	41.87000	16.96900
C	-9.55300	41.51700	17.47800
O	-8.73400	40.96000	16.74700
C	-11.08500	43.38800	16.79400
C	-10.00600	44.04500	15.95300
C	-10.32600	45.52200	15.68200
C	-10.24500	46.39400	16.94400
N	-8.84600	46.66200	17.41600
H	-8.79200	47.24100	18.25400
H	-8.28700	47.06700	16.66500
H	-8.34200	45.78600	17.55400
N	-9.29700	41.84500	18.73900
H	-10.03000	42.29900	19.28400
C	-8.01400	41.58400	19.37600
C	-7.71900	40.09300	19.48300
O	-6.64800	39.63100	19.09200
C	-7.98500	42.21200	20.77000
C	-8.08300	43.73600	20.78400
C	-9.46800	44.26200	20.43500
O	-9.66100	45.49400	20.50100
O	-10.36400	43.45900	20.09900

N	-8.67100	39.34200	20.02700
H	-9.53400	39.78100	20.34900
C	-8.50200	37.90400	20.17000
C	-7.90100	37.38200	18.87300
O	-6.87000	36.71200	18.88000
C	-9.85900	37.20900	20.42500
C	-9.67300	35.71100	20.53100
C	-10.47600	37.74600	21.69900
N	-8.54500	37.72900	17.76100
H	-9.37800	38.31300	17.84100
C	-8.10900	37.30900	16.43000
C	-6.67600	37.72500	16.12100
O	-5.82700	36.88900	15.81100
C	-9.04400	37.87700	15.38500
N	-6.41400	39.02200	16.20000
H	-7.15900	39.66900	16.46100
C	-5.08700	39.53800	15.92200
C	-4.01500	38.81700	16.72600
O	-3.01500	38.37000	16.17300
C	-5.02500	41.03700	16.22900
C	-3.63400	41.60600	16.18400
C	-2.95000	41.72100	14.97900
C	-2.99100	41.99800	17.35800
C	-1.64100	42.21700	14.94500
C	-1.68500	42.49400	17.33400
C	-1.00900	42.60300	16.12600
N	-4.22600	38.69900	18.03000
H	-5.09000	39.06100	18.43400
C	-3.24300	38.06000	18.89300
C	-3.09400	36.55200	18.73600
O	-2.08600	35.98100	19.16500
C	-3.53800	38.39700	20.35100
C	-3.23400	39.81500	20.68700
C	-4.13000	40.82300	20.88200
C	-1.93700	40.38200	20.90200
N	-3.47200	41.98300	21.21500
H	-3.91500	42.87900	21.41500
C	-2.12500	41.74000	21.23400
C	-0.63200	39.87300	20.84800
C	-1.06000	42.59600	21.51400
C	0.43200	40.72700	21.12600
C	0.20900	42.07400	21.45500
N	-4.08700	35.90400	18.13200

H	-4.90200	36.42400	17.80600
C	-4.02800	34.46200	17.92900
C	-3.02900	34.14300	16.81500
O	-2.26400	33.17500	16.90300
C	-5.41000	33.89800	17.56200
O	-6.32600	34.15700	18.63300
H	-6.37400	35.09500	18.77800
C	-5.33300	32.39700	17.33000
N	-3.02900	34.97200	15.77400
H	-3.68500	35.75300	15.76200
C	-2.11600	34.79400	14.64900
C	-0.71500	35.23400	15.05400
O	0.23900	34.46800	14.93700
C	-2.58600	35.61900	13.45400
C	-4.08100	35.51500	13.23300
O	-4.64000	34.41400	13.16900
N	-4.74100	36.66400	13.11500
H	-5.74800	36.59400	12.96600
H	-4.28000	37.57200	13.16800
N	-0.59900	36.46700	15.53900
H	-1.43100	37.05200	15.61800
C	0.69000	37.00200	15.96100
C	1.42400	36.04100	16.88900
O	2.62400	35.82300	16.73800
C	0.50800	38.35900	16.65100
C	1.77600	39.07600	17.13000
C	2.79000	39.16800	16.01000
C	1.41500	40.46200	17.61800
N	0.70600	35.46200	17.84600
H	-0.28700	35.68000	17.92900
C	1.31300	34.52000	18.78000
C	1.62600	33.17100	18.13500
O	2.42400	32.39500	18.65900
C	0.40900	34.32800	19.99900
C	0.65400	35.32600	21.09600
C	-0.34200	35.61700	22.02500
C	1.88500	35.97000	21.20900
C	-0.11700	36.53400	23.04900
C	2.12300	36.89000	22.22900
C	1.12000	37.17300	23.15000
N	0.99500	32.89000	17.00000
H	0.32200	33.55600	16.62000
C	1.25200	31.64300	16.29200

C	2.45500	31.87000	15.36600
O	2.52300	31.32700	14.25700
C	0.02600	31.24100	15.48900
N	3.39900	32.68100	15.84500
H	3.26900	33.07900	16.77500
C	4.61200	33.03000	15.10500
C	4.33100	33.35300	13.64300
O	4.64700	34.44700	13.17000
C	5.64600	31.90300	15.19500
C	6.41500	31.85500	16.51300
C	7.37300	30.67400	16.55500
C	8.33100	30.70100	15.37300
N	9.18500	29.48100	15.31100
H	9.82700	29.49900	14.51900
H	8.61700	28.63400	15.30600
H	9.68500	29.33600	16.18800
C	-14.87200	36.26100	74.15700
C	-13.85000	36.25500	75.30500
C	-14.60600	36.27400	76.65100
C	-15.68300	37.38600	76.67800
C	-16.57200	37.29500	75.42900
C	-17.64400	38.36700	75.32700
C	-12.00900	34.84800	76.03500
C	-11.97400	33.50500	76.75500
N	-13.02000	35.06300	75.19600
H	-13.21700	34.38100	74.46400
O	-13.68600	36.47400	77.71700
H	-14.15100	36.48600	78.54500
O	-16.48600	37.25700	77.84500
H	-17.14700	37.93900	77.86200
O	-15.74900	37.38700	74.25200
O	-18.92600	37.79400	75.09000
H	-19.59600	38.46400	75.02600
O	-11.12300	35.67700	76.24000
N	22.30300	-14.60800	94.33800
H	22.68400	-15.36000	93.76400
H	22.35000	-14.82900	95.33300
H	22.90800	-13.78600	94.33600
C	20.94200	-14.28200	93.91800
C	20.93600	-13.83800	92.45800
O	21.68800	-12.93700	92.08000
C	20.37000	-13.15100	94.78100
O	20.96300	-11.90000	94.45400

H	20.60900	-11.19900	94.98900
N	20.09300	-14.46700	91.64200
H	19.50300	-15.21400	92.00900
C	19.99900	-14.10500	90.23100
C	18.95900	-12.99000	90.09900
O	17.80400	-13.15300	90.49800
C	19.58900	-15.31800	89.39400
O	19.90800	-15.11400	88.03000
H	19.65300	-15.86700	87.51000
N	19.36300	-11.84300	89.53000
C	18.51400	-10.66600	89.33000
C	17.08500	-10.97900	88.88900
O	16.86100	-11.83800	88.03000
C	19.28000	-9.87800	88.27600
C	20.69400	-10.20300	88.59100
C	20.63000	-11.68800	88.79700
N	16.09600	-10.27500	89.46900
C	14.69600	-10.50800	89.10500
C	14.45300	-9.99300	87.69200
O	14.71200	-8.81800	87.41000
C	13.91000	-9.68200	90.13000
C	14.91400	-9.28600	91.17300
C	16.20700	-9.16800	90.43000
N	13.98400	-10.85600	86.79800
H	13.82600	-11.82900	87.05900
C	13.69600	-10.40600	85.44300
C	12.22900	-10.56800	85.15100
O	11.70900	-11.67400	85.17200
C	14.47100	-11.17700	84.37400
C	13.89400	-10.85800	82.99900
C	15.93300	-10.78600	84.41500
N	11.56700	-9.45100	84.87400
H	12.06900	-8.56300	84.86600
C	10.14600	-9.46500	84.58200
C	9.85100	-9.14800	83.13100
O	10.53200	-8.34300	82.49200
C	9.37200	-8.46900	85.47400
C	7.93900	-8.31300	84.97400
C	9.37000	-8.96400	86.91400
N	8.81100	-9.79600	82.62900
H	8.29900	-10.44000	83.23100
C	8.37200	-9.62700	81.26100
C	7.20200	-8.65000	81.21100

O	6.17200	-8.87400	81.84300
C	7.93700	-10.97800	80.70800
C	8.13900	-11.08100	79.22300
O	7.58000	-10.24000	78.48500
O	8.86300	-12.00500	78.79500
N	7.36600	-7.55900	80.47500
H	8.25300	-7.40600	79.99500
C	6.30000	-6.57600	80.34100
C	5.96100	-6.47800	78.86200
O	6.72900	-6.93200	78.01900
C	6.72700	-5.18600	80.88600
O	6.71500	-4.21700	79.82900
H	6.97600	-3.36700	80.16200
C	8.11400	-5.25800	81.48800
N	4.80800	-5.89900	78.55200
H	4.21200	-5.54800	79.30100
C	4.36900	-5.75100	77.16400
C	5.49300	-5.27200	76.24000
O	5.78900	-5.89900	75.21200
C	3.20300	-4.74600	77.05800
C	2.72900	-4.65900	75.61800
C	2.07500	-5.15200	78.00600
N	6.11200	-4.15700	76.61700
H	5.82600	-3.69900	77.48200
C	7.18000	-3.57700	75.83200
C	8.48900	-4.37000	75.86600
O	9.42700	-4.07000	75.11700
C	7.42300	-2.14700	76.29600
C	6.25400	-1.23800	76.08400
N	5.58500	-1.15600	74.88400
H	5.80000	-1.70400	74.05100
C	5.65200	-0.35000	76.91100
C	4.62000	-0.25700	74.97800
N	4.63900	0.24600	76.19800
H	4.00500	0.96100	76.55400
N	8.56100	-5.38000	76.72900
H	7.76600	-5.59600	77.33100
C	9.77500	-6.17400	76.81200
C	10.16900	-6.52400	78.23100
O	9.44000	-6.21700	79.16900
N	11.33400	-7.15100	78.38500
H	11.89800	-7.34400	77.55800
C	11.83800	-7.57500	79.69200

C	12.59600	-6.51000	80.46700
O	13.24500	-5.63600	79.89600
C	12.75700	-8.78300	79.53500
C	12.11500	-10.00600	78.90600
C	13.18100	-11.05600	78.63300
C	12.61700	-12.27600	77.91500
N	11.71400	-13.10500	78.76700
H	11.33600	-13.92200	78.28600
H	10.96200	-12.53600	79.15600
H	12.18400	-13.37900	79.63000
N	12.51300	-6.61100	81.78600
H	11.94800	-7.36000	82.18600
C	13.19700	-5.69400	82.68500
C	14.02400	-6.49400	83.68500
O	13.60600	-7.56200	84.15100
C	12.20200	-4.81600	83.46400
C	11.87700	-3.56300	82.67800
C	10.93000	-5.60400	83.72300
N	15.20300	-5.96600	84.00300
H	15.47500	-5.08300	83.57200
C	16.12200	-6.59600	84.94100
C	16.23900	-5.66800	86.13300
O	16.49000	-4.47300	85.96500
C	17.49600	-6.76800	84.28200
C	18.68600	-7.43100	84.99000
C	19.16600	-6.61200	86.18400
C	18.27000	-8.81200	85.40800
N	16.04300	-6.21800	87.32900
H	15.81500	-7.21000	87.39600
C	16.15000	-5.42200	88.54000
C	17.15800	-6.02300	89.50300
O	18.01600	-6.80400	89.10000
N	17.07100	-5.64800	90.77300
H	16.36200	-4.96800	91.04700
C	17.97100	-6.19000	91.78200
C	17.14900	-6.56000	93.00400
O	16.07500	-5.99400	93.23300
C	19.03800	-5.16500	92.18300
C	18.52600	-4.03600	93.07300
C	19.59700	-2.97100	93.33400
C	19.03500	-1.78100	94.12700
N	19.99300	-0.63300	94.27200
H	19.62000	0.15700	94.79800

H	20.32600	-0.32800	93.35800
H	20.87300	-0.95100	94.67900
N	17.64400	-7.52400	93.77600
H	18.51900	-7.97500	93.51000
C	16.96300	-7.95100	94.99500
C	17.56200	-7.22100	96.20500
O	18.78400	-7.07800	96.32600
C	17.10400	-9.46800	95.19200
C	16.06000	-10.28500	94.47900
C	16.42700	-11.24600	93.54700
C	14.71100	-10.10800	94.75200
C	15.46300	-12.01700	92.89600
C	13.73600	-10.87500	94.10600
C	14.11400	-11.82800	93.17800
N	16.69700	-6.73700	97.08700
H	15.69700	-6.84100	96.91800
C	17.15200	-6.06100	98.29000
C	16.36600	-6.64600	99.45200
O	15.13800	-6.66400	99.41900
C	16.91000	-4.54000	98.22100
C	17.19700	-3.91100	99.56600
C	17.80500	-3.92100	97.16700
N	17.07100	-7.15400	100.46100
H	18.09000	-7.13700	100.41800
C	16.41200	-7.73600	101.62900
C	16.32900	-6.70800	102.74100
O	17.20400	-5.85800	102.88200
C	17.16900	-8.96800	102.13800
O	16.88600	-10.12100	101.35900
H	17.35500	-10.88400	101.67400
N	15.26700	-6.77800	103.52900
H	14.55700	-7.49200	103.36900
C	15.11800	-5.83600	104.62000
C	15.13600	-6.54400	105.96400
O	14.55300	-7.62200	106.13600
C	13.82100	-5.03700	104.48300
C	13.65500	-3.97300	105.57300
C	14.66600	-2.85600	105.36400
C	12.24500	-3.42500	105.54800
N	15.82500	-5.91600	106.90700
H	16.28800	-5.03900	106.66900
C	15.95000	-6.41900	108.26100
C	14.63400	-7.02500	108.74600

O	13.62800	-6.32600	108.87500
C	16.38100	-5.26300	109.17400
C	16.36000	-5.55100	110.67200
C	17.22300	-6.73900	111.06500
O	18.39900	-6.79100	110.63700
O	16.72500	-7.61400	111.80900
N	14.64300	-8.33400	108.98500
H	15.49400	-8.87200	108.82000
C	13.45200	-9.00400	109.47900
C	12.48000	-9.58100	108.46300
O	11.33100	-9.87500	108.80800
N	12.91600	-9.74300	107.21600
H	13.86900	-9.47200	106.97500
C	12.04100	-10.30600	106.18800
C	12.72600	-11.35000	105.31400
O	13.76900	-11.09000	104.70500
C	11.46200	-9.20100	105.30900
C	10.57200	-8.25100	106.04900
C	11.11400	-7.22800	106.82200
C	9.18900	-8.38200	105.98100
C	10.29500	-6.34500	107.51700
C	8.36100	-7.50800	106.67000
C	8.91700	-6.48400	107.44100
N	12.11200	-12.53000	105.26000
H	11.24400	-12.64900	105.78300
C	12.61900	-13.66200	104.48900
C	12.77800	-13.35200	103.00500
O	13.87000	-13.44300	102.44800
C	11.68700	-14.85700	104.66700
N	11.66700	-12.98100	102.38100
H	10.80700	-12.90800	102.92500
C	11.61300	-12.67200	100.95600
C	12.20300	-11.30100	100.58400
O	11.66100	-10.25200	100.95100
C	10.15000	-12.75500	100.49300
C	9.93500	-12.60600	99.00400
C	10.50800	-13.76300	98.22400
O	10.10800	-14.91600	98.41800
N	11.45200	-13.46800	97.33400
H	11.83900	-14.25000	96.80700
H	11.78200	-12.51600	97.17400
N	13.32400	-11.29500	99.84300
C	13.90500	-10.00500	99.46600

C	12.95200	-9.30800	98.49700
O	12.24600	-9.95800	97.72100
C	15.22600	-10.40000	98.80800
C	14.87300	-11.68200	98.13500
C	14.04500	-12.40500	99.19600
N	12.92500	-7.98400	98.55500
H	13.52600	-7.50100	99.22300
C	12.05900	-7.20700	97.68800
C	12.71500	-7.00200	96.32600
O	13.90800	-6.68700	96.24200
C	11.76200	-5.83700	98.31100
C	10.86400	-5.04300	97.39500
C	11.12000	-6.01300	99.67700
N	11.93900	-7.20100	95.26200
H	10.97100	-7.49300	95.40000
C	12.43800	-7.01200	93.90500
C	12.24500	-5.53000	93.57800
O	11.13600	-5.00900	93.68900
C	11.65500	-7.87900	92.93400
N	13.32100	-4.84900	93.19300
H	14.21800	-5.32900	93.11900
C	13.24100	-3.42700	92.87500
C	13.57300	-3.11100	91.41600
O	14.45200	-3.72700	90.81700
C	14.19300	-2.61900	93.76600
C	13.86100	-2.87100	95.23700
C	14.09200	-1.14000	93.43000
C	14.81000	-2.17300	96.19600
N	12.86500	-2.14400	90.84700
H	12.13700	-1.67400	91.38500
C	13.10700	-1.74000	89.46900
C	13.18000	-0.21200	89.38000
O	12.30000	0.49600	89.86800
C	12.00800	-2.29300	88.56400
C	11.89300	-3.78700	88.60400
C	11.24000	-4.42100	89.65600
C	12.44400	-4.57000	87.59500
C	11.13400	-5.81500	89.69800
C	12.34200	-5.96200	87.63000
C	11.68400	-6.58200	88.68500
N	14.23700	0.29500	88.75800
H	14.92800	-0.33600	88.35200
C	14.43100	1.73600	88.64300

C	14.47800	2.25700	87.20600
O	15.19900	1.72700	86.36800
C	15.72100	2.12000	89.37000
C	15.78600	1.63000	90.82200
C	17.18100	1.83100	91.39200
C	14.74800	2.37200	91.65000
N	13.69900	3.29500	86.92600
H	13.09500	3.68400	87.65000
C	13.70000	3.88000	85.59900
C	13.07300	3.07700	84.48000
O	13.65800	2.91600	83.40400
N	11.88000	2.55800	84.72600
H	11.45600	2.68100	85.64500
C	11.17000	1.81600	83.70100
C	10.36900	2.87800	82.98600
O	9.61400	3.60900	83.61500
C	10.19100	0.79000	84.30400
C	10.97100	-0.37400	84.92700
C	9.21100	0.31700	83.23500
C	10.10900	-1.56500	85.34000
N	10.54200	3.00300	81.66800
C	9.80000	4.00600	80.89900
C	8.32200	3.63600	80.75400
O	7.99400	2.48500	80.48200
C	10.52500	4.00900	79.55600
C	10.96500	2.59000	79.41600
C	11.48400	2.26700	80.80600
N	7.42800	4.60000	80.95600
H	7.74000	5.53700	81.21200
C	6.00100	4.32300	80.81300
C	5.41600	5.17000	79.69400
O	4.23800	5.04000	79.35300
C	5.24400	4.56000	82.13300
C	5.20300	5.98800	82.57800
C	4.22600	6.85200	82.09600
C	6.12500	6.46700	83.49700
C	4.16600	8.17900	82.52700
C	6.07400	7.79200	83.93600
C	5.09200	8.64900	83.45000
N	6.25700	6.02900	79.12000
H	7.21600	6.08500	79.46300
C	5.85100	6.89000	78.01900
C	7.05200	7.15800	77.12600

O	8.18700	6.90100	77.50800
C	5.30400	8.19300	78.55500
N	6.79300	7.66100	75.93000
H	5.82200	7.81200	75.65600
C	7.85300	8.00500	74.99500
C	8.39100	9.36000	75.45200
O	7.61500	10.24300	75.81600
C	7.28300	8.13400	73.58200
C	8.30600	8.44300	72.50900
C	7.62500	8.61800	71.15900
C	8.63000	8.64200	70.00500
N	9.23200	7.29400	69.72200
H	9.90200	7.31000	68.95300
H	8.50500	6.59800	69.55700
H	9.65300	6.89900	70.56300
N	9.72200	9.54200	75.43400
C	10.39700	10.78100	75.84300
C	9.77900	12.01100	75.17400
O	9.79000	12.12000	73.94900
C	11.83300	10.54700	75.40100
C	11.98200	9.07100	75.54300
C	10.69900	8.55300	74.95500
N	9.24300	12.95900	75.97500
C	8.61000	14.18100	75.46400
C	9.56500	15.24500	74.92400
O	9.59400	16.38000	75.41300
C	7.80600	14.66600	76.66800
C	8.68600	14.29800	77.80300
C	9.14400	12.90400	77.44700
N	10.32400	14.88400	73.89400
H	10.23200	13.94300	73.51200
C	11.28400	15.80400	73.30000
C	10.84200	16.39300	71.96300
O	9.88300	15.94000	71.33800
C	12.62700	15.10000	73.13000
C	12.99200	14.27600	74.35900
C	14.35300	13.65000	74.15600
C	12.97400	15.15400	75.60600
N	11.55900	17.42000	71.53300
H	12.34100	17.76500	72.09000
C	11.23600	18.05200	70.27700
C	9.76600	18.38100	70.16400
O	9.19300	19.00400	71.05700

N	9.12100	17.96400	69.06900
C	7.70000	18.21700	68.82300
C	6.71800	17.62100	69.83000
O	5.52000	17.91600	69.77700
C	7.50000	17.67100	67.41000
C	8.49300	16.58000	67.32800
C	9.71100	17.20300	67.95500
N	7.22200	16.79200	70.73900
H	8.22200	16.58900	70.73100
C	6.37300	16.16600	71.74900
C	6.19100	17.02700	73.00700
O	5.41700	16.68100	73.90900
C	6.93700	14.79800	72.12300
C	6.74300	13.74700	71.03500
C	7.39700	12.44600	71.44300
C	5.26100	13.54800	70.80700
N	6.91000	18.14300	73.05500
H	7.54600	18.35100	72.28500
C	6.82500	19.07900	74.16300
C	5.46000	19.78700	74.08300
O	5.04200	20.22600	73.00700
C	7.97900	20.08600	74.05900
C	8.03100	21.15000	75.14800
C	9.14200	22.17300	74.87700
N	10.49200	21.63500	75.05200
H	10.59100	20.73400	75.52000
C	11.60000	22.24900	74.63800
N	11.52100	23.41900	74.01700
H	10.60500	23.83600	73.85200
H	12.36900	23.88900	73.70000
N	12.79100	21.70700	74.85300
H	12.85200	20.80800	75.33000
H	13.63900	22.17700	74.53600
N	4.77300	19.87800	75.22300
H	5.18700	19.48700	76.06900
C	3.45700	20.50900	75.32300
C	2.39600	19.71000	74.58200
O	1.55000	20.28100	73.88200
C	3.46000	21.93000	74.75700
C	4.52700	22.80800	75.31600
C	4.73500	22.89100	76.68100
C	5.32500	23.56300	74.47100
C	5.73000	23.71400	77.20200

C	6.31800	24.38800	74.97900
C	6.52100	24.46400	76.34700
N	2.44500	18.38900	74.71700
H	3.18200	17.97200	75.28600
C	1.46600	17.52400	74.06800
C	1.27300	16.34000	74.99700
O	2.07200	16.12800	75.91100
C	1.95900	17.01600	72.69500
O	2.49800	15.70300	72.83000
H	1.81700	15.13700	73.17500
C	3.04400	17.91800	72.14500
N	0.20400	15.56200	74.79200
C	-0.06400	14.39500	75.64300
C	0.99200	13.29900	75.48700
O	1.49200	13.06300	74.39800
C	-1.44700	13.95100	75.18500
C	-2.07600	15.25000	74.73700
C	-0.95700	15.86700	73.94400
N	1.32800	12.60100	76.57800
C	2.33600	11.54200	76.52700
C	1.96600	10.36400	75.65600
O	0.83300	9.87700	75.68600
C	2.48600	11.14600	77.98800
C	1.09900	11.28800	78.48800
C	0.67200	12.62200	77.89600
N	2.93900	9.89700	74.88400
H	3.85900	10.33700	74.90700
C	2.70500	8.76800	74.01000
C	3.32400	7.48700	74.51600
O	4.25000	7.50400	75.32400
C	3.20600	9.08500	72.62000
C	2.16100	9.80400	71.81900
C	2.76400	10.68500	70.76500
O	3.48500	10.21200	69.87400
N	2.48200	11.98700	70.85600
H	2.89200	12.58600	70.13900
H	1.88900	12.37600	71.58900
N	2.80900	6.34600	74.04700
C	3.31800	5.04000	74.46800
C	4.82600	4.93100	74.28300
O	5.40500	5.55500	73.38700
C	2.56100	4.07400	73.56800
C	1.29400	4.80500	73.27000

C	1.77100	6.19200	73.01600
N	5.45500	4.13800	75.13900
H	4.92100	3.66800	75.87000
C	6.88800	3.92500	75.05600
C	7.18700	2.93900	73.91100
O	6.38600	2.04800	73.62100
C	7.40400	3.37700	76.39300
N	8.32400	3.11600	73.24600
H	8.93700	3.89100	73.49800
C	8.70900	2.22000	72.16100
C	9.23100	0.95000	72.81200
O	10.01700	1.00300	73.76000
C	9.81000	2.84700	71.31000
C	9.44900	4.20100	70.71400
C	8.47300	4.09000	69.55400
O	7.48100	3.33200	69.67900
O	8.69700	4.76600	68.52000
N	8.80000	-0.21100	72.31600
C	9.22000	-1.50800	72.85200
C	10.71500	-1.78200	72.65700
O	11.30900	-1.32800	71.68000
C	8.34600	-2.47800	72.08100
C	8.23600	-1.80500	70.74600
C	7.97300	-0.37700	71.11100
N	11.32200	-2.53000	73.57500
H	10.78500	-2.89900	74.36000
C	12.75400	-2.83100	73.47200
C	13.09700	-4.27600	73.11800
O	12.47600	-5.22100	73.60300
C	13.47400	-2.41800	74.76200
C	12.84800	-2.93400	76.01600
C	13.08800	-4.13600	76.62500
C	11.88500	-2.25800	76.82800
N	12.33400	-4.24600	77.77200
H	12.33200	-5.04400	78.40800
C	11.58600	-3.10600	77.91800
C	11.24300	-1.01600	76.74000
C	10.67400	-2.75000	78.91300
C	10.34000	-0.66200	77.72500
C	10.06200	-1.52400	78.79900
N	14.11800	-4.42300	72.27900
H	14.60800	-3.58700	71.96200
C	14.57300	-5.72200	71.78900

C	15.08900	-6.77500	72.75700
O	14.69300	-7.93900	72.65300
C	15.61500	-5.52900	70.68700
O	14.97500	-5.23400	69.45400
H	15.62200	-5.11400	68.76900
N	15.96300	-6.41300	73.68700
H	16.27200	-5.44400	73.76500
C	16.47100	-7.43600	74.59500
C	16.01400	-7.27700	76.03400
O	14.82900	-7.06900	76.29000
C	17.99500	-7.48100	74.51200
C	18.50700	-7.76400	73.12900
C	18.89000	-6.72500	72.28500
C	18.57200	-9.07500	72.65500
C	19.33400	-6.98900	70.98300
C	19.01100	-9.35100	71.36000
C	19.39400	-8.30600	70.52100
N	16.94500	-7.40400	76.97200
H	17.90400	-7.61500	76.69600
C	16.63000	-7.25000	78.38600
C	17.09100	-5.86700	78.84500
O	18.27700	-5.55200	78.76700
C	17.33700	-8.34100	79.24700
C	17.32000	-7.94400	80.71600
C	16.63700	-9.68100	79.07700
N	16.15200	-5.04900	79.32000
H	15.18600	-5.37400	79.35300
C	16.46200	-3.69500	79.79700
C	16.80300	-3.67000	81.29300
O	16.03300	-4.13800	82.12900
C	15.27400	-2.75700	79.52000
C	15.48800	-1.30800	79.96400
C	14.23900	-0.44900	79.76900
C	13.96200	-0.09400	78.30500
N	14.80400	1.02300	77.76300
H	14.62000	1.25900	76.78800
H	15.79400	0.81800	77.89700
H	14.71500	1.85100	78.35100
N	17.95900	-3.11100	81.62500
H	18.55300	-2.72600	80.89000
C	18.40600	-3.03100	83.01300
C	17.75800	-1.90600	83.80700
O	18.29000	-0.80400	83.86100

C	19.92900	-2.84500	83.07100
C	20.68200	-4.09900	82.70200
O	20.17500	-4.92700	81.94500
N	21.89900	-4.24100	83.22000
H	22.40800	-5.08900	82.97100
H	22.31900	-3.55500	83.84700
N	16.62000	-2.16700	84.43400
H	16.19000	-3.08900	84.35800
C	15.98900	-1.12400	85.23400
C	16.75900	-1.10300	86.54400
O	16.26800	-1.56400	87.56800
C	14.52800	-1.45200	85.48500
N	17.97100	-0.56000	86.50400
H	18.31300	-0.15700	85.63200
C	18.81700	-0.53300	87.68700
C	19.54200	0.77200	87.96200
O	20.57100	0.77300	88.63300
C	19.87500	-1.65200	87.61900
O	20.49700	-1.64000	86.32800
H	20.89500	-0.79100	86.17800
C	19.23900	-3.00900	87.85900
N	19.01500	1.87800	87.45000
H	18.16800	1.81300	86.88600
C	19.62500	3.18800	87.67900
C	18.55300	4.23800	87.87500
O	17.67800	4.41100	87.02500
C	20.51100	3.60900	86.50100
O	21.73200	2.89100	86.48000
H	22.28100	3.15200	85.75000
N	18.61900	4.93900	88.99600
H	19.35400	4.74200	89.67500
C	17.65500	5.98300	89.26200
C	17.56500	6.86600	88.03700
O	18.58300	7.29100	87.49700
C	18.09300	6.79400	90.46900
C	17.95400	6.00700	91.73400
C	16.69700	5.60300	92.17700
C	19.07000	5.61800	92.46500
C	16.55000	4.82400	93.32100
C	18.93800	4.84000	93.61000
C	17.67200	4.44500	94.03400
O	17.52200	3.67200	95.16900
H	18.29300	3.41200	95.65900

N	16.34000	7.12400	87.55800
C	16.13000	7.96500	86.38200
C	16.23300	9.43600	86.73300
O	16.15000	9.81800	87.90700
C	14.72100	7.59300	85.94900
C	14.04800	7.37500	87.26200
C	15.06500	6.53900	88.00800
N	16.40900	10.28500	85.71100
C	16.52200	11.73400	85.88900
C	15.21100	12.28700	86.42400
O	14.15300	11.68300	86.21800
C	16.78300	12.24000	84.47000
C	17.40000	11.07500	83.78600
C	16.60800	9.91500	84.30200
N	15.27900	13.41800	87.11800
H	16.18900	13.83600	87.31200
C	14.07200	14.06700	87.60500
C	13.80200	15.17000	86.57900
O	14.73300	15.83900	86.13200
C	14.29500	14.66500	88.98700
C	15.25800	15.83000	89.03900
S	15.59000	16.29900	90.75200
C	16.79000	17.59000	90.52200
N	12.54300	15.34000	86.18300
H	11.81100	14.75300	86.58300
C	12.18500	16.34900	85.18700
C	12.83900	17.69900	85.45200
O	13.02500	18.09400	86.60000
C	10.66800	16.51000	85.13300
S	9.76900	14.99000	84.67200
N	13.17900	18.41100	84.38400
H	12.97900	18.04200	83.45400
C	13.83300	19.71200	84.51000
C	13.09500	20.60200	85.49300
O	11.89400	20.81200	85.38100
C	13.92700	20.43700	83.15100
O	14.01200	19.47100	82.09500
H	14.07000	19.91700	81.25800
C	15.17600	21.31100	83.10700
N	13.83400	21.11800	86.46200
H	14.83100	20.90300	86.48200
C	13.28600	21.98000	87.50200
C	14.46000	22.76800	88.06200

O	15.58200	22.65000	87.56300
C	12.68400	21.11800	88.60600
C	13.64200	20.02800	89.03000
C	13.05300	19.04900	90.01900
O	12.97000	19.32400	91.21500
N	12.63900	17.89000	89.52100
H	12.24100	17.22900	90.18900
H	12.70800	17.66200	88.52900
N	14.21200	23.58300	89.08100
H	13.25900	23.68300	89.43200
C	15.29600	24.33400	89.69900
C	16.09400	23.26500	90.43200
O	15.63100	22.72300	91.42800
C	14.74700	25.33000	90.70400
C	15.83200	26.14400	91.35400
O	16.91500	25.57800	91.61700
O	15.59500	27.34500	91.60600
N	17.30400	22.95000	89.94900
C	18.17900	21.93200	90.54100
C	18.48800	22.17000	92.01300
O	18.54800	21.23100	92.81900
C	19.41900	22.01100	89.67000
C	19.48200	23.45500	89.34600
C	18.05300	23.77800	88.99100
N	18.69300	23.43600	92.34900
H	18.64400	24.15000	91.62300
C	18.98500	23.84500	93.71200
C	17.73500	23.54500	94.55700
O	17.78200	22.76000	95.51200
C	19.31000	25.34000	93.71200
C	20.06200	25.84400	94.92200
C	20.79500	27.15000	94.60300
C	21.91400	26.93600	93.57200
N	22.60100	28.21200	93.17600
H	23.34400	28.07000	92.49200
H	22.95200	28.70600	93.99600
H	21.92600	28.90000	92.84300
N	16.61800	24.16300	94.17900
H	16.65400	24.79200	93.37700
C	15.34700	23.97700	94.86500
C	14.95400	22.49900	94.87300
O	14.48600	21.96700	95.88100
C	14.26900	24.79800	94.17400

N	15.14200	21.84300	93.73500
H	15.52500	22.33500	92.92800
C	14.81100	20.43800	93.62300
C	15.56800	19.57500	94.61200
O	14.94800	18.87800	95.41400
N	16.90000	19.61900	94.56900
H	17.36400	20.22300	93.89100
C	17.69800	18.81100	95.48200
C	17.35200	19.03900	96.95000
O	17.38500	18.11000	97.75200
C	19.19400	19.06300	95.30700
C	19.99600	18.15400	96.23500
C	21.43900	18.57700	96.43600
O	22.29500	18.36100	95.57200
N	21.72000	19.18300	97.59200
H	22.69000	19.46700	97.72700
H	21.01300	19.36100	98.30500
N	17.02200	20.27300	97.30700
H	17.00500	21.01200	96.60500
C	16.68300	20.58700	98.69200
C	15.44600	19.85400	99.20000
O	15.47800	19.22800	100.25900
C	16.46200	22.08800	98.86000
C	16.21200	22.49600	100.30800
C	17.46400	22.22800	101.12800
C	15.83700	23.95300	100.36200
N	14.35000	19.95900	98.45400
H	14.37700	20.51200	97.59700
C	13.11500	19.29900	98.84000
C	13.33600	17.78900	98.89100
O	12.75800	17.09600	99.73600
C	12.00300	19.63600	97.84700
C	10.59100	19.14200	98.17000
C	10.17300	19.61100	99.55100
C	9.63400	19.66300	97.12400
N	14.17600	17.28000	97.99000
H	14.61800	17.90000	97.31100
C	14.47400	15.85300	97.95800
C	15.09500	15.45300	99.28600
O	14.74000	14.43100	99.86700
C	15.44400	15.53100	96.82700
O	15.77600	14.15500	96.84000
H	16.38100	13.95400	96.13500

N	16.02100	16.27700	99.76500
H	16.26600	17.11200	99.23300
C	16.69700	16.01800	101.03300
C	15.71300	16.05700	102.20400
O	15.62700	15.10400	102.97600
C	17.81100	17.04800	101.26100
C	18.76700	17.18700	100.08500
C	19.88800	18.19000	100.32500
O	19.59800	19.31100	100.80500
O	21.05600	17.86000	100.01600
N	14.97000	17.15500	102.32700
H	15.07800	17.90500	101.64400
C	14.00500	17.31700	103.41100
C	12.92800	16.22600	103.45700
O	12.57900	15.74300	104.53500
C	13.33500	18.69100	103.31400
C	14.23500	19.92600	103.41300
C	13.45200	21.15500	103.01100
C	14.76700	20.08300	104.82000
N	12.41100	15.83100	102.29600
H	12.75300	16.24800	101.43000
C	11.36400	14.81400	102.23400
C	11.84600	13.36400	102.13200
O	11.11800	12.45200	102.51000
C	10.42300	15.07500	101.04100
C	9.40300	16.17900	101.25800
C	9.34600	16.89400	102.45000
C	8.48100	16.48500	100.25000
C	8.38600	17.89200	102.63400
C	7.52400	17.47600	100.42400
C	7.47400	18.18200	101.61900
N	13.04700	13.12400	101.62200
H	13.65400	13.89200	101.33600
C	13.48200	11.73900	101.47800
C	13.31400	10.93300	102.75100
O	13.27600	11.48300	103.84200
C	14.94100	11.62500	101.02200
O	15.30100	10.24300	100.94700
H	16.20500	10.17200	100.66400
C	15.86000	12.31500	101.98900
N	13.20800	9.61900	102.60900
H	13.24800	9.20900	101.67600
C	13.03600	8.75500	103.76300

C	14.19000	7.77200	103.85800
O	14.26900	6.98300	104.79200
C	11.70600	8.00200	103.65500
C	11.75300	6.85800	102.65000
O	12.21300	7.01600	101.51700
N	11.26000	5.69600	103.06500
H	10.87900	5.56500	104.00200
H	11.29100	4.93000	102.39200
N	15.08500	7.81700	102.88100
H	14.96900	8.48800	102.12100
C	16.22900	6.92100	102.88100
C	17.38600	7.54100	103.67500
O	17.42800	8.75600	103.88800
C	16.66000	6.60900	101.43900
C	17.01200	7.83000	100.63300
C	17.61200	7.50000	99.26800
N	16.62600	7.25400	98.21400
H	16.30400	8.05400	97.67000
C	16.12200	6.06100	97.91700
N	16.50500	4.98900	98.59800
H	17.17700	5.08400	99.35900
H	16.11800	4.07300	98.37000
N	15.24800	5.93800	96.92700
H	14.95300	6.76200	96.40300
H	14.86100	5.02200	96.69900
N	18.30300	6.68800	104.13000
H	18.17700	5.69600	103.92800
C	19.48400	7.08900	104.90400
C	20.21300	8.27200	104.28400
O	20.31000	9.35300	104.85800
C	20.45900	5.91400	104.97800
C	20.62000	5.21900	103.62000
C	21.74900	4.19200	103.56600
C	23.10400	4.85700	103.36700
N	24.13800	3.87200	102.92800
H	25.04600	4.31800	102.79500
H	23.84300	3.36900	102.09100
H	24.20000	3.08400	103.57300
N	20.73700	8.02300	103.09800
H	20.60600	7.09400	102.69800
C	21.48600	8.99500	102.33600
C	20.59100	9.51200	101.22900
O	19.85400	8.73500	100.62200

C	22.68300	8.29500	101.71100
C	22.28400	6.95500	101.07600
C	23.24300	6.49400	99.98900
O	23.22500	7.09300	98.88600
O	24.01500	5.53700	100.23700
N	20.65300	10.80900	100.95200
H	21.26900	11.42200	101.48500
C	19.83300	11.34300	99.88100
C	20.51600	11.03000	98.56200
O	21.74100	11.05700	98.47900
C	19.64800	12.85100	100.00700
C	18.56100	13.37000	99.07800
O	18.40700	14.57200	98.88800
N	17.79400	12.45200	98.50000
H	17.06500	12.80000	97.87700
H	17.92200	11.45200	98.65800
N	19.72000	10.72700	97.54000
H	18.71000	10.72200	97.68200
C	20.25200	10.40100	96.22100
C	20.21400	11.59000	95.27500
O	19.14600	12.05200	94.88100
C	19.46900	9.25500	95.55100
C	19.49200	8.01400	96.43500
C	20.08100	8.93400	94.20100
C	20.88100	7.58000	96.81800
N	21.39000	12.08800	94.87800
C	21.44400	13.23000	93.96800
C	20.88700	12.81600	92.61100
O	21.05400	11.67800	92.17600
C	22.92700	13.54900	93.92400
C	23.52800	12.17300	93.97600
C	22.72800	11.49900	95.06300
N	20.22300	13.74100	91.93800
H	20.12500	14.68100	92.32300
C	19.63600	13.41800	90.65500
C	19.96500	14.40700	89.55300
O	20.25900	15.57900	89.80600
C	18.12000	13.30800	90.80300
C	17.62500	12.25700	91.79500
C	16.11700	12.38100	91.90900
C	18.03000	10.86000	91.35100
N	19.90100	13.91100	88.32300
H	19.65200	12.93000	88.20100

C	20.17300	14.71500	87.14700
C	18.86300	15.23000	86.54100
O	17.80200	14.64200	86.75300
C	20.94800	13.87900	86.13100
C	22.27300	13.37700	86.67100
C	23.15600	12.77600	85.58800
C	24.60200	12.63900	86.08200
N	25.54700	12.07400	85.06300
H	26.50800	11.98300	85.39100
H	25.51400	12.62100	84.20300
H	25.20300	11.18000	84.71300
N	18.94200	16.33700	85.80800
H	19.84800	16.79000	85.68600
C	17.76500	16.91700	85.17500
C	17.66000	16.41600	83.75800
O	18.65700	16.00900	83.16100
C	17.86000	18.43600	85.10300
C	18.01200	19.28900	86.35100
C	17.86300	20.74600	85.93900
C	16.96100	18.92400	87.38600
N	16.45300	16.46100	83.21700
H	15.66600	16.79100	83.77500
C	16.23100	16.05000	81.84700
C	14.76900	16.07900	81.48600
O	13.90400	15.82400	82.32000
C	16.76600	14.64500	81.60100
O	16.66100	14.31200	80.22500
H	16.99500	13.43600	80.07200
N	14.49800	16.41000	80.23200
H	15.26400	16.65400	79.60400
C	13.13600	16.43300	79.73300
C	12.72900	14.97100	79.64400
O	11.54400	14.63800	79.70600
C	13.09000	17.09400	78.35200
C	13.09300	18.61500	78.39400
C	13.16600	19.25900	77.01700
O	12.50800	18.76200	76.06600
O	13.87400	20.28200	76.89400
N	13.74100	14.11300	79.50900
H	14.68600	14.49500	79.46300
C	13.58600	12.66000	79.42200
C	13.48500	12.17300	80.85300
O	14.47700	11.74800	81.43800

C	14.81600	12.05700	78.72300
C	14.77500	10.54000	78.63900
O	13.67600	9.96500	78.53300
O	15.85500	9.92100	78.65700
N	12.27100	12.22900	81.40200
H	11.48400	12.53400	80.82900
C	12.03000	11.86800	82.79700
C	10.76800	11.06700	83.08300
O	10.50100	10.73400	84.23200
C	11.99100	13.15200	83.62900
S	10.74200	14.33100	83.01200
N	9.98500	10.76300	82.06000
H	10.23800	11.05200	81.11500
C	8.76000	10.01300	82.29400
C	9.02700	8.54100	82.63000
O	8.79600	7.64600	81.81400
C	7.82400	10.12800	81.08600
C	7.40600	11.54100	80.65200
C	6.31600	11.42800	79.59900
C	6.89600	12.35800	81.83800
N	9.50900	8.30900	83.84700
H	9.67100	9.10200	84.46700
C	9.81600	6.96800	84.33400
C	9.08200	6.68400	85.64500
O	8.49400	7.58300	86.25300
C	11.32600	6.81100	84.58600
C	12.19800	7.00800	83.36700
C	12.59400	8.28300	82.96100
C	12.60200	5.91500	82.60100
C	13.36800	8.45900	81.82000
C	13.37200	6.07600	81.46300
C	13.75400	7.34600	81.07000
O	14.49600	7.49400	79.91400
H	14.75800	8.36600	79.64400
N	9.12400	5.42600	86.07800
H	9.60700	4.72400	85.51700
C	8.49900	5.02400	87.33200
C	9.33400	3.92400	87.98200
O	9.96000	3.11800	87.29300
C	7.05100	4.54500	87.10200
C	6.69400	3.31400	86.25200
C	7.12300	2.03000	86.93700
C	5.18600	3.28600	86.04000

N	9.36200	3.91600	89.31000
H	8.85400	4.63600	89.82500
C	10.10200	2.90200	90.04600
C	9.11900	1.92300	90.67000
O	8.01200	2.30700	91.05100
C	10.95600	3.55000	91.13100
C	11.94800	4.53200	90.56400
O	12.34100	4.42000	89.40400
N	12.37200	5.49600	91.37800
H	12.04600	5.58900	92.34000
H	13.04400	6.16100	90.99400
N	9.51500	0.65600	90.75600
H	10.43800	0.39600	90.40700
C	8.65400	-0.37300	91.34100
C	9.33800	-1.14000	92.48300
O	10.52100	-1.48800	92.41100
C	8.17600	-1.38700	90.26900
C	7.22800	-0.70100	89.29200
C	7.47200	-2.55600	90.92700
C	6.89400	-1.54800	88.05700
N	8.57600	-1.37900	93.54300
H	7.61400	-1.03900	93.54800
C	9.07000	-2.10900	94.69300
C	8.05800	-3.21200	94.97300
O	6.99600	-2.96500	95.54500
C	9.19900	-1.18400	95.91000
C	10.10200	0.01400	95.69400
C	9.67700	1.11000	94.93600
C	11.38600	0.05200	96.23700
C	10.51400	2.21300	94.72500
C	12.22900	1.14800	96.03200
C	11.78700	2.22300	95.27500
O	12.62000	3.29400	95.05100
H	13.49200	3.30100	95.42800
N	8.37300	-4.42800	94.54600
H	9.25500	-4.58000	94.05700
C	7.47100	-5.54400	94.76900
C	8.05900	-6.54200	95.76100
O	9.22700	-6.93200	95.67000
C	7.12500	-6.27800	93.44600
O	6.14300	-7.28500	93.71100
H	5.37200	-6.88200	94.09400
C	8.36100	-6.92400	92.83200

N	7.25900	-6.94300	96.75100
C	7.75400	-7.90100	97.73400
C	7.32600	-9.30900	97.32100
O	7.79400	-10.30400	97.87700
C	7.08200	-7.43000	99.01500
C	5.72400	-7.02000	98.52200
C	6.02700	-6.28300	97.22700
N	6.44200	-9.37800	96.32900
H	6.11900	-8.51300	95.89600
C	5.92000	-10.64600	95.84100
C	6.99300	-11.60800	95.35700
O	8.09700	-11.20800	94.99600
C	4.92100	-10.39600	94.72700
N	6.65500	-12.89100	95.36600
H	5.73000	-13.15600	95.70400
C	7.56400	-13.93200	94.90800
C	7.23100	-14.12800	93.42900
O	6.35200	-14.91100	93.06500
C	7.32900	-15.21800	95.70800
C	8.25500	-16.34500	95.29700
O	9.48000	-16.11800	95.17800
O	7.75000	-17.46800	95.10700
N	7.93600	-13.38000	92.58800
H	8.65000	-12.76000	92.97100
C	7.73900	-13.40200	91.14700
C	7.68300	-14.79600	90.54100
O	7.11200	-14.99100	89.46700
C	8.83900	-12.57200	90.49700
C	8.79500	-11.16400	91.09400
C	10.06200	-10.39700	90.77600
C	7.55700	-10.44700	90.56800
N	8.26200	-15.76400	91.24500
H	8.70200	-15.52800	92.13400
C	8.29200	-17.15300	90.79300
C	6.88800	-17.72300	90.60600
O	6.68600	-18.65900	89.84100
C	9.01900	-18.03800	91.80800
O	8.17900	-18.22900	92.95000
H	8.63000	-18.77800	93.58000
C	10.31000	-17.38100	92.25700
N	5.92200	-17.15900	91.32100
H	6.15200	-16.38500	91.94500
C	4.54300	-17.61600	91.23800

C	3.57100	-16.45100	91.04100
O	3.96100	-15.27900	91.09100
C	4.19100	-18.40200	92.50400
C	4.52700	-17.67300	93.78900
C	4.68200	-18.63100	94.96100
C	5.88600	-19.55400	94.77300
N	6.16700	-20.40300	95.97500
H	6.97000	-21.01900	95.85000
H	5.34000	-20.93500	96.24700
H	6.27700	-19.82700	96.81000
N	2.30600	-16.78200	90.80600
H	2.04900	-17.76900	90.77300
C	1.27600	-15.77500	90.59400
C	0.99300	-15.02400	91.88800
O	0.99100	-15.60900	92.97200
C	-0.01600	-16.43400	90.10400
C	-1.14500	-15.45800	89.77400
C	-2.50300	-15.99900	90.20900
C	-2.77700	-17.38900	89.63900
N	-4.03800	-17.99900	90.17600
H	-4.22100	-18.92700	89.79500
H	-4.83500	-17.38000	90.02800
H	-4.02900	-18.01700	91.19600
N	0.74700	-13.72500	91.76500
H	0.76700	-13.30500	90.83600
C	0.45000	-12.88300	92.91200
C	-0.36700	-11.68800	92.47700
O	-0.14400	-11.12700	91.40300
C	1.73800	-12.39100	93.56800
C	2.37500	-13.43400	94.44200
O	1.73600	-13.96300	95.34400
N	3.64100	-13.73700	94.18600
H	4.17300	-13.29700	93.43500
H	4.07300	-14.44500	94.77900
N	-1.32400	-11.30300	93.30800
H	-1.47600	-11.82500	94.17100
C	-2.16200	-10.15300	93.01500
C	-2.26100	-9.29700	94.25700
O	-3.32200	-9.18400	94.86900
C	-3.55500	-10.59300	92.55300
C	-3.64800	-10.81900	91.04400
C	-2.80500	-12.00000	90.63100
N	-1.93000	-11.73100	89.48900

H	-0.92800	-11.66000	89.66900
C	-2.34300	-11.57200	88.23400
N	-3.63400	-11.64100	87.92700
H	-4.32200	-11.79500	88.66500
H	-3.95100	-11.51900	86.96500
N	-1.45000	-11.37200	87.27600
H	-0.45900	-11.31900	87.51200
H	-1.76700	-11.25000	86.31400
N	-1.13300	-8.69400	94.62000
H	-0.29500	-8.83400	94.05500
C	-1.05300	-7.84000	95.79800
C	-1.57400	-6.44300	95.52300
O	-1.41600	-5.91300	94.42500
C	0.39300	-7.72800	96.27600
C	1.17000	-9.02100	96.48600
C	2.48800	-8.69200	97.15500
C	0.36800	-9.97400	97.34600
N	-2.20700	-5.82300	96.52200
C	-2.70100	-4.47100	96.25600
C	-1.52800	-3.56500	95.84300
O	-0.40400	-3.71300	96.33400
C	-3.35000	-4.07300	97.58300
C	-2.58300	-4.88800	98.60200
C	-2.43400	-6.21900	97.92100
N	-1.79700	-2.64600	94.92400
H	-2.74600	-2.57700	94.55700
C	-0.77900	-1.73200	94.42300
C	-1.02400	-0.31900	94.92600
O	-2.15600	0.14400	94.96900
C	-0.77400	-1.69900	92.87500
C	0.48000	-1.00600	92.37500
C	-0.87100	-3.10500	92.31900
N	0.04400	0.36500	95.30500
H	0.96200	-0.07600	95.25700
C	-0.06400	1.72800	95.78700
C	0.84400	2.61500	94.94900
O	2.07000	2.50500	95.02400
C	0.32600	1.79900	97.26700
C	-0.72700	1.21000	98.20700
S	-0.30200	1.27700	99.98200
C	-0.69000	3.01700	100.37500
N	0.23400	3.48100	94.13700
H	-0.78600	3.50900	94.12200

C	0.97900	4.39200	93.26800
C	1.11600	5.75800	93.93000
O	0.11800	6.38500	94.28100
C	0.28300	4.55200	91.91200
C	1.16700	5.34700	90.96700
C	-0.03900	3.18400	91.33500
N	2.36000	6.20900	94.08900
H	3.13300	5.64400	93.73600
C	2.66500	7.47700	94.74700
C	3.00100	8.62100	93.80000
O	3.77400	8.45000	92.86500
C	3.82600	7.26100	95.72500
C	4.36000	8.50800	96.36600
C	5.46600	9.21700	95.98900
C	3.82000	9.18400	97.51000
N	5.64900	10.29100	96.83000
H	6.40300	10.97500	96.76300
C	4.65400	10.29300	97.77300
C	2.71400	8.95700	98.34200
C	4.41500	11.17600	98.83700
C	2.47600	9.83800	99.40200
C	3.32300	10.93000	99.63800
N	2.42000	9.78900	94.06600
H	1.78700	9.84900	94.86400
C	2.65100	10.99000	93.26300
C	3.28600	12.02400	94.17600
O	2.62200	12.56300	95.06300
C	1.32800	11.56100	92.72200
C	0.60200	10.48900	91.90600
C	1.60300	12.79700	91.88000
C	-0.75600	10.90500	91.43700
N	4.56700	12.29900	93.96200
H	5.05700	11.84200	93.19300
C	5.28400	13.24200	94.80800
C	4.77500	14.66800	94.71600
O	4.14300	15.05200	93.73800
C	6.77000	13.24500	94.47800
C	7.09700	13.92900	93.18700
N	7.23400	13.24900	91.99600
H	7.16300	12.23800	91.88300
C	7.26700	15.23800	92.89300
C	7.47200	14.11000	91.02400
N	7.49700	15.32400	91.54200

H	7.66100	16.18600	91.02300
N	5.07100	15.44200	95.75500
H	5.59400	15.04400	96.53500
C	4.67300	16.83500	95.81200
C	5.80800	17.71000	95.31800
O	6.79200	17.21400	94.78800
N	5.68100	19.01500	95.50200
H	4.85400	19.38200	95.97300
C	6.70700	19.92500	95.03900
C	6.05700	21.03500	94.24000
O	6.69100	21.67000	93.39800
N	4.77200	21.24900	94.50200
H	4.30300	20.66300	95.19300
C	4.01600	22.29400	93.83200
C	4.00800	22.27400	92.31900
O	3.81600	23.31200	91.69400
N	4.21200	21.10300	91.72800
H	4.36400	20.27800	92.30800
C	4.22600	20.95800	90.27300
C	5.38900	21.69900	89.62000
O	5.44700	21.80100	88.40200
C	2.90800	21.46700	89.68300
C	1.63400	20.96600	90.36500
C	0.42700	21.68500	89.77500
C	1.51900	19.45700	90.20000
N	6.31200	22.20900	90.43200
H	6.20600	22.07800	91.43800
C	7.47500	22.95200	89.93700
C	8.77000	22.16600	90.14400
O	9.75000	22.35700	89.42000
C	7.61100	24.30300	90.66200
C	6.50400	25.32300	90.41800
S	6.48200	25.93300	88.72100
C	8.18500	26.58300	88.58200
N	8.77700	21.29400	91.14600
H	7.93900	21.18000	91.71600
C	9.95800	20.49700	91.44700
C	9.56300	19.14500	92.04700
O	8.38800	18.89400	92.31300
C	10.87700	21.24000	92.45000
C	11.32500	22.58100	91.86400
C	10.14000	21.44600	93.77900
N	10.54300	18.27300	92.25200

H	11.50100	18.51600	92.00200
C	10.25300	16.97500	92.83100
C	10.68100	15.79700	91.97900
O	10.96800	15.94400	90.79100
N	10.72400	14.61500	92.57900
H	10.48200	14.53900	93.56700
C	11.11300	13.42900	91.84000
C	10.56100	12.19900	92.53000
O	10.14400	12.27000	93.68100
C	12.61700	13.34300	91.74700
N	10.56300	11.07100	91.82600
H	10.93300	11.07300	90.87600
C	10.04700	9.83700	92.38800
C	11.09300	9.12600	93.23300
O	10.78000	8.54000	94.27000
C	9.56400	8.92500	91.27400
N	12.34100	9.19300	92.79100
H	12.53900	9.72200	91.94200
C	13.43800	8.53100	93.48600
C	13.64500	9.01600	94.92300
O	14.35800	8.37800	95.70600
C	14.71900	8.70600	92.67900
O	14.46500	8.41800	91.31700
H	15.26300	8.52700	90.81400
N	13.01300	10.13500	95.27100
H	12.43400	10.61400	94.58100
C	13.12800	10.69600	96.61900
C	12.49700	9.76200	97.65600
O	12.87400	9.77600	98.82800
C	12.43000	12.09300	96.72200
O	13.14400	13.06400	95.94300
H	13.17400	12.77000	95.04000
C	12.38200	12.56300	98.16700
N	11.55100	8.94000	97.21400
H	11.30500	8.94800	96.22400
C	10.86000	8.03000	98.11100
C	11.17900	6.55900	97.84000
O	10.89800	6.03400	96.76000
C	9.34700	8.27800	98.02100
C	8.98800	9.75000	98.07400
C	9.31300	10.60000	97.02100
C	8.38200	10.30700	99.19700
C	9.05400	11.95900	97.08600

C	8.12100	11.67700	99.27100
C	8.46300	12.49100	98.20900
O	8.24000	13.84500	98.26500
H	8.47500	14.40500	97.53400
N	11.77400	5.90100	98.82900
H	11.99100	6.39400	99.69500
C	12.12200	4.49700	98.70500
C	10.94900	3.68100	99.22900
O	10.57800	3.80600	100.39500
C	13.38100	4.20100	99.52100
C	13.80800	2.74800	99.42900
O	14.91300	2.41300	99.91900
O	13.03700	1.93900	98.86800
N	10.36700	2.84800	98.37200
H	10.71800	2.77500	97.41700
C	9.23400	2.04200	98.78800
C	9.62000	0.69200	99.36200
O	8.81700	-0.23600	99.37400
N	10.84700	0.58100	99.85800
H	11.46400	1.39300	99.85000
C	11.33200	-0.67600	100.41400
C	10.56600	-1.14700	101.63800
O	9.97600	-2.22200	101.62900
C	12.81800	-0.55900	100.76400
C	13.44300	-1.83900	101.32600
C	13.26600	-2.98300	100.33500
C	14.91500	-1.60900	101.61900
N	10.58500	-0.33800	102.69100
H	11.08800	0.54700	102.62300
C	9.91200	-0.67100	103.94100
C	8.43700	-0.96200	103.75000
O	7.94000	-2.00600	104.17900
C	10.08000	0.46400	104.94200
N	7.74300	-0.02700	103.10600
H	8.22900	0.80400	102.76900
C	6.31200	-0.15100	102.86600
C	5.95100	-1.48500	102.22500
O	5.04400	-2.18100	102.68600
C	5.83700	0.99700	101.98100
C	4.32300	1.18300	101.93300
C	3.79000	1.33600	103.34000
C	3.98300	2.40800	101.10500
N	6.67400	-1.83900	101.16900

H	7.41900	-1.22000	100.84900
C	6.43500	-3.08700	100.45200
C	6.60300	-4.32100	101.34300
O	5.72800	-5.18900	101.39200
C	7.37900	-3.18400	99.24500
N	7.73700	-4.39200	102.03600
H	8.41400	-3.63300	101.95100
C	8.04600	-5.51500	102.91100
C	7.13700	-5.55800	104.13700
O	6.56000	-6.60000	104.45700
C	9.49500	-5.43800	103.34400
N	7.01300	-4.41900	104.81300
H	7.50900	-3.59300	104.47900
C	6.19400	-4.31000	106.01300
C	4.69000	-4.55600	105.83300
O	4.05300	-5.11100	106.72800
C	6.41800	-2.93900	106.66600
C	7.66100	-2.86000	107.49900
N	7.71900	-3.32100	108.79700
H	6.94000	-3.73400	109.31000
C	8.90200	-2.39600	107.21200
C	8.93900	-3.14500	109.27400
N	9.67700	-2.58700	108.33100
H	10.66200	-2.33800	108.41900
N	4.11700	-4.15900	104.69500
H	4.68700	-3.72800	103.96700
C	2.67700	-4.33500	104.47800
C	2.30600	-5.16000	103.25600
O	1.14800	-5.18000	102.83100
C	1.98000	-2.97600	104.38400
C	1.82200	-2.25900	105.71300
C	1.15900	-3.12800	106.77500
O	0.16900	-3.82600	106.45500
O	1.62600	-3.10300	107.93700
N	3.29300	-5.83700	102.69200
H	4.23100	-5.76500	103.08700
C	3.08200	-6.68100	101.52600
C	2.22200	-6.03800	100.42700
O	1.16300	-6.54900	100.05500
C	2.49200	-8.03000	101.96700
C	2.62200	-9.09700	100.89800
O	1.75800	-9.23100	100.02800
N	3.72200	-9.84800	100.94200

H	3.80900	-10.56600	100.22300
H	4.43600	-9.73700	101.66100
N	2.69700	-4.91100	99.91100
H	3.57000	-4.53000	100.27700
C	2.01200	-4.20200	98.84000
C	3.05000	-3.83700	97.79400
O	4.24300	-3.78400	98.09200
C	1.37100	-2.89700	99.33100
C	0.21200	-3.19800	100.24600
C	2.41700	-2.05100	100.02200
N	2.59900	-3.59500	96.56900
H	1.60200	-3.68400	96.37300
C	3.50600	-3.20500	95.50300
C	3.55800	-1.67900	95.47500
O	2.55700	-1.03300	95.17800
C	3.01000	-3.70500	94.13800
C	3.97600	-3.26800	93.05500
C	2.87300	-5.21800	94.15100
N	4.71200	-1.09800	95.79300
H	5.51800	-1.67300	96.03800
C	4.83200	0.35800	95.79400
C	5.41300	0.87400	94.47600
O	6.49700	0.46600	94.05000
C	5.70600	0.85400	96.97200
C	5.79000	2.37500	96.95600
C	5.10900	0.39000	98.28400
N	4.68100	1.77500	93.83400
H	3.79500	2.08000	94.23700
C	5.11900	2.33500	92.56900
C	5.23800	3.85600	92.66200
O	4.25800	4.54000	92.95300
C	4.12100	1.98200	91.43900
C	4.58600	2.59000	90.13100
C	3.98000	0.46500	91.30700
N	6.43700	4.38600	92.43600
H	7.22800	3.77400	92.23600
C	6.63500	5.83600	92.47000
C	6.77500	6.32100	91.02800
O	7.64500	5.85100	90.28400
C	7.89300	6.23200	93.26700
O	9.03900	5.56500	92.72400
H	9.81500	5.80900	93.21500
C	7.72100	5.87300	94.73500

N	5.91100	7.25600	90.63900
H	5.23400	7.61700	91.31100
C	5.90600	7.77900	89.27600
C	6.39000	9.21800	89.18000
O	6.32000	9.97300	90.14900
C	4.48500	7.73400	88.67900
C	3.60300	8.76000	89.38600
C	3.88900	6.34600	88.83200
C	2.23500	8.86900	88.80500
N	6.87600	9.58900	88.00200
H	6.92900	8.90500	87.24700
C	7.33400	10.94600	87.76200
C	6.46800	11.57800	86.67600
O	5.90200	10.87100	85.83800
C	8.80400	10.95300	87.35100
C	9.74400	10.71100	88.51100
C	11.17900	10.99300	88.14900
O	12.08800	10.84000	88.97100
N	11.39700	11.41000	86.90600
H	12.36900	11.60100	86.66100
H	10.64600	11.53600	86.22700
N	6.34800	12.90300	86.69800
H	6.83600	13.43600	87.41800
C	5.53400	13.61200	85.71500
C	6.13300	14.96900	85.38900
O	6.87900	15.53100	86.19100
C	4.10600	13.79300	86.23900
C	4.03700	14.43900	87.60200
C	4.19000	13.68600	88.76000
C	3.84900	15.81200	87.72900
C	4.16100	14.27900	90.00400
C	3.81800	16.42000	88.96700
C	3.97500	15.65000	90.10300
O	3.96000	16.26400	91.33900
H	3.83300	17.20300	91.40700
N	5.79300	15.49300	84.21100
H	5.15200	14.97700	83.60800
C	6.30900	16.78100	83.75600
C	5.97500	17.93000	84.68200
O	4.83100	18.10200	85.09900
C	5.81300	17.07700	82.34200
C	6.63700	16.35800	81.28900
C	6.07300	16.51000	79.91100

N	4.92900	15.63700	79.72000
H	4.73300	14.94000	80.43900
C	4.12300	15.69000	78.66900
N	4.33300	16.58000	77.70300
H	3.71300	16.62100	76.89400
H	5.11800	17.22800	77.76700
N	3.10500	14.84900	78.58600
H	2.48500	14.89000	77.77700
H	2.94400	14.16700	79.32700
N	6.99000	18.72100	85.00000
H	7.91100	18.53700	84.60300
C	6.81500	19.84600	85.90400
C	6.98800	21.19400	85.20500
O	7.41200	21.25700	84.04900
C	7.81500	19.72300	87.06200
C	7.86900	18.34900	87.74500
C	9.09800	18.25500	88.61300
C	6.62200	18.12700	88.56600
N	6.64500	22.26200	85.92200
H	6.28200	22.12800	86.86600
C	6.77100	23.61400	85.40200
C	6.20100	23.86700	84.02000
O	5.11100	23.39300	83.69500
N	6.94200	24.62200	83.20900
H	7.83300	24.98500	83.54900
C	6.51900	24.94600	81.85100
C	6.22500	23.68300	81.05200
O	5.20100	23.57900	80.37500
C	7.60700	25.77400	81.11700
C	7.77500	27.12600	81.81300
C	7.21900	26.01100	79.66000
C	8.81600	28.02500	81.17000
N	7.12700	22.71700	81.15100
H	7.94300	22.86100	81.74600
C	6.98900	21.45900	80.43700
C	5.69100	20.69300	80.68400
O	5.20800	19.99300	79.79700
C	8.16500	20.56500	80.78100
C	9.46700	21.12100	80.33500
C	10.10700	20.88500	79.14200
C	10.31400	21.99500	81.07700
N	11.30300	21.55700	79.10800
H	11.96900	21.54500	78.33600

C	11.45500	22.24700	80.28400
C	10.22100	22.59200	82.33700
C	12.49400	23.07000	80.71600
C	11.25900	23.41300	82.76300
C	12.37700	23.64200	81.95500
N	5.11700	20.81600	81.87400
H	5.52100	21.42200	82.58800
C	3.90400	20.07000	82.13400
C	2.63200	20.86700	82.33000
O	1.54000	20.28700	82.39600
N	2.74800	22.19000	82.40200
H	3.66100	22.63100	82.29400
C	1.56400	23.00500	82.63600
C	1.40500	24.28600	81.82500
O	0.46600	25.05200	82.05000
C	1.45900	23.27900	84.13800
C	1.31100	22.02600	84.94600
C	0.08300	21.37600	85.01800
C	2.41900	21.43000	85.54400
C	-0.04400	20.14800	85.66800
C	2.30600	20.20400	86.19700
C	1.06800	19.56000	86.25500
N	2.30100	24.52200	80.87500
H	3.08000	23.87900	80.73200
C	2.16400	25.70500	80.03900
C	0.85000	25.57800	79.26400
O	0.56200	24.53900	78.66100
C	3.33600	25.81900	79.06400
C	3.14200	26.87100	78.02200
C	2.53800	26.56100	76.81200
C	3.51400	28.18800	78.27200
C	2.30200	27.54900	75.85900
C	3.28600	29.18500	77.33600
C	2.67600	28.86700	76.12100
N	0.04400	26.62800	79.28300
H	0.31600	27.47200	79.78800
C	-1.23300	26.57700	78.58200
C	-1.61300	27.88600	77.92600
O	-1.50100	28.95300	78.53000
C	-2.35100	26.17800	79.53700
O	-3.60500	26.39300	78.92600
H	-4.30200	26.14400	79.52100
N	-2.07700	27.79500	76.68800

H	-2.14600	26.87800	76.24600
C	-2.49000	28.97600	75.94800
C	-3.99400	29.15500	76.11600
O	-4.58000	30.10000	75.59200
C	-2.14800	28.84400	74.44600
O	-2.78900	27.68100	73.90200
H	-2.57900	27.60000	72.97900
C	-0.64700	28.72000	74.25700
N	-4.61200	28.24200	76.85500
H	-4.07700	27.47800	77.26800
C	-6.04100	28.32300	77.07900
C	-6.88100	27.94500	75.87400
O	-8.08300	28.19200	75.85000
N	-6.25100	27.35500	74.86500
H	-5.24600	27.19500	74.92900
C	-6.96600	26.93100	73.66800
C	-6.44900	25.58000	73.14900
O	-5.61400	24.93300	73.78200
C	-6.85700	28.00600	72.59400
C	-5.44800	28.17400	72.07700
O	-5.21300	29.15200	71.33600
O	-4.58000	27.33100	72.39500
N	-6.93500	25.15800	71.99100
H	-7.59100	25.74500	71.47600
C	-6.54200	23.86400	71.44500
C	-5.09100	23.72900	70.98400
O	-4.67700	22.64200	70.58300
C	-7.48000	23.47000	70.29100
C	-7.32600	24.30000	69.00300
C	-7.92100	25.70400	69.08800
O	-7.73100	26.48100	68.13300
O	-8.58000	26.03100	70.09500
N	-4.31300	24.80800	71.03500
H	-4.68800	25.69100	71.38200
C	-2.92400	24.72800	70.59400
C	-1.99200	24.25100	71.69200
O	-0.88400	23.79800	71.42600
C	-2.47600	26.07400	70.03700
C	-3.23200	26.47600	68.81000
N	-3.26900	25.69300	67.67600
H	-2.75600	24.82100	67.54500
C	-4.04100	27.53200	68.56200
C	-4.07200	26.24700	66.78600

N	-4.55400	27.36300	67.29800
H	-5.20200	27.99800	66.83200
N	-2.46400	24.33000	72.92800
H	-3.40100	24.70800	73.07200
C	-1.69800	23.89900	74.08900
C	-2.63600	23.93600	75.30200
O	-2.48200	24.76700	76.19700
C	-0.49600	24.83200	74.29700
O	0.27500	24.44000	75.41700
H	1.01900	25.01700	75.54600
N	-3.61600	23.03900	75.31900
H	-3.69900	22.37300	74.55100
C	-4.57400	22.99100	76.41500
C	-3.90900	23.09000	77.77500
O	-4.34600	23.87000	78.62300
C	-5.39800	21.71200	76.36000
C	-6.42900	21.69500	75.26500
C	-7.33000	20.48400	75.41900
N	-8.50600	20.57500	74.56500
H	-9.41000	20.72800	75.01100
C	-8.47400	20.47100	73.24400
N	-7.32000	20.26200	72.61800
H	-7.29500	20.18200	71.60100
H	-6.45700	20.16200	73.15200
N	-9.59600	20.60100	72.55000
H	-9.57100	20.52100	71.53300
H	-10.48100	20.76100	73.03000
N	-2.85700	22.29400	77.97200
H	-2.54900	21.67900	77.21900
C	-2.13900	22.28400	79.23600
C	-2.32900	20.96700	79.97500
O	-2.77200	19.98100	79.38600
N	-1.98600	20.95100	81.26200
H	-1.61400	21.80600	81.67500
C	-2.11600	19.76600	82.11400
C	-1.37100	18.53700	81.62400
O	-1.82000	17.40300	81.82600
C	-3.58500	19.39200	82.28900
C	-4.36000	20.42600	83.05700
O	-3.82000	21.09700	83.94000
N	-5.64700	20.54700	82.74600
H	-6.17300	21.24900	83.26700
H	-6.09400	19.99200	82.01600

N	-0.23000	18.74900	80.98700
H	0.10900	19.70200	80.85400
C	0.54200	17.62400	80.47600
C	1.03400	16.79200	81.64400
O	1.04700	15.56500	81.58000
C	1.71600	18.12900	79.64200
C	1.31400	19.26700	78.77800
C	1.71300	20.56600	78.89800
C	0.38900	19.22800	77.68700
N	1.09600	21.34400	77.94700
H	1.22600	22.34800	77.82600
C	0.27700	20.54900	77.18800
C	-0.35700	18.21000	77.08300
C	-0.55600	20.87800	76.10800
C	-1.18300	18.53700	76.01000
C	-1.27400	19.86300	75.53500
N	1.42500	17.47100	82.71800
H	1.39300	18.49100	82.71400
C	1.89600	16.76800	83.89500
C	0.85300	15.77600	84.37300
O	1.16700	14.60500	84.62400
N	-0.39000	16.24700	84.48500
H	-0.57100	17.22300	84.25000
C	-1.49700	15.41200	84.93300
C	-1.80000	14.27700	83.95800
O	-2.19600	13.18200	84.36800
C	-2.74800	16.26700	85.14400
C	-2.67000	17.17500	86.33800
N	-2.28600	16.73300	87.58900
H	-2.00300	15.78000	87.81600
C	-2.96000	18.48900	86.47900
C	-2.34200	17.73600	88.44500
N	-2.74900	18.81300	87.79900
H	-2.88500	19.73600	88.21200
N	-1.61500	14.53700	82.66600
H	-1.29200	15.46100	82.37900
C	-1.86900	13.51800	81.65700
C	-0.82300	12.42100	81.78400
O	-1.08400	11.26100	81.44100
C	-1.82500	14.13000	80.26100
C	-2.93500	15.12700	79.93200
C	-2.79100	15.61000	78.49600
C	-4.28300	14.46200	80.13700

N	0.36100	12.79600	82.27600
H	0.50700	13.77600	82.51900
C	1.45400	11.84700	82.47700
C	1.07100	10.90700	83.61800
O	1.40100	9.72200	83.59800
C	2.76200	12.56200	82.84700
C	3.37100	13.34200	81.68600
O	3.18500	12.95200	80.51100
O	4.06800	14.34100	81.96000
N	0.38000	11.44800	84.62000
H	0.15400	12.44200	84.59000
C	-0.06200	10.64900	85.76200
C	-1.05600	9.58900	85.29000
O	-0.95300	8.40800	85.64100
C	-0.70100	11.55600	86.81700
C	0.30200	12.19100	87.76000
C	-0.05400	13.61900	88.13800
O	-1.23000	13.99300	88.17200
N	0.96500	14.42400	88.44300
H	1.93700	14.11500	88.41500
H	0.72600	15.38300	88.69700
N	-2.00900	10.01900	84.47500
H	-2.03900	11.00600	84.21800
C	-3.01000	9.11600	83.94200
C	-2.35500	8.12300	82.98300
O	-2.84600	7.00800	82.78700
C	-4.09800	9.89000	83.18000
C	-5.20800	8.94300	82.76200
C	-4.64100	11.01200	84.04900
N	-1.24800	8.53900	82.38100
H	-0.89100	9.47400	82.57900
C	-0.53600	7.68800	81.44700
C	0.20800	6.62800	82.23200
O	0.27200	5.47000	81.82200
C	0.43300	8.51900	80.62800
N	0.77400	7.03300	83.36700
H	0.69200	8.01200	83.64000
C	1.50700	6.11600	84.22900
C	0.51900	5.10400	84.81700
O	0.83200	3.92100	84.95600
C	2.20200	6.88300	85.33200
N	-0.68200	5.56400	85.15400
H	-0.90200	6.55200	85.03000

C	-1.68200	4.66100	85.69900
C	-2.09300	3.56300	84.71200
O	-2.30000	2.41600	85.11800
C	-2.91000	5.44300	86.16100
C	-2.69000	6.15800	87.49400
C	-3.95200	6.90100	87.88900
C	-2.29700	5.13900	88.56800
N	-2.22100	3.89800	83.42700
H	-2.06300	4.86200	83.13500
C	-2.58700	2.88900	82.43600
C	-1.49400	1.84200	82.35300
O	-1.77500	0.64900	82.21000
C	-2.74900	3.49200	81.05500
C	-3.94800	4.34400	80.88200
C	-3.94800	4.93300	79.48500
N	-5.05100	5.87000	79.31700
H	-4.82700	6.84700	79.12700
C	-6.33100	5.52600	79.39700
N	-6.66400	4.26000	79.63500
H	-5.94100	3.54800	79.73600
H	-7.64700	3.99600	79.69600
N	-7.27400	6.45400	79.26600
H	-7.01900	7.42500	79.08400
H	-8.25700	6.19000	79.32700
N	-0.24300	2.29300	82.42200
H	-0.07400	3.29300	82.52600
C	0.88700	1.37600	82.35100
C	0.76800	0.34500	83.47400
O	1.04800	-0.84500	83.27700
C	2.20500	2.13800	82.49500
C	3.39800	1.26200	82.27100
C	4.09200	1.10500	81.10700
C	4.00800	0.38900	83.22500
N	5.09500	0.19000	81.27500
H	5.75600	-0.10400	80.55600
C	5.06800	-0.26900	82.57000
C	3.76200	0.09600	84.57500
C	5.88800	-1.20300	83.21700
C	4.57800	-0.83200	85.21700
C	5.62600	-1.46800	84.53700
N	0.36400	0.82800	84.65000
H	0.18500	1.82900	84.72800
C	0.16700	-0.00300	85.82600

C	-0.89800	-1.04600	85.49600
O	-0.70400	-2.24100	85.70800
C	-0.28400	0.86500	87.01900
C	-0.91800	0.01000	88.09100
C	0.90900	1.60900	87.58500
N	-2.01700	-0.58900	84.94800
H	-2.11700	0.41200	84.78200
C	-3.10600	-1.48500	84.57800
C	-2.70200	-2.57100	83.58600
O	-3.19000	-3.69500	83.67700
C	-4.27800	-0.69200	83.99700
C	-5.03200	0.16100	85.01900
C	-5.80000	-0.66600	86.04500
O	-6.69200	-1.43500	85.69400
N	-5.45700	-0.50300	87.31900
H	-5.97100	-1.05600	88.00500
H	-4.71700	0.13500	87.61000
N	-1.81700	-2.25100	82.64800
H	-1.42400	-1.31000	82.62000
C	-1.40600	-3.23900	81.66000
C	-0.20100	-4.07800	82.03400
O	0.05400	-5.10500	81.39800
C	-1.07900	-2.58000	80.32500
C	-2.25100	-1.86700	79.72200
O	-3.40200	-2.28600	79.96600
O	-2.01300	-0.88800	78.98300
N	0.54800	-3.66600	83.05000
H	0.28300	-2.84000	83.58600
C	1.75300	-4.40900	83.38800
C	1.93400	-4.90700	84.81400
O	2.46500	-6.00300	85.02200
C	2.98200	-3.57300	83.00700
C	3.17100	-3.45700	81.50600
O	3.59000	-4.40800	80.84600
N	2.85900	-2.29200	80.95900
H	2.51200	-1.50400	81.50600
H	2.98600	-2.21400	79.95000
N	1.49600	-4.11700	85.79100
H	1.01600	-3.24900	85.55300
C	1.68800	-4.46500	87.19400
C	1.45600	-5.93500	87.59300
O	2.03500	-6.41200	88.57400
C	0.86700	-3.52600	88.10900

C	1.63100	-3.29900	89.41200
C	-0.50000	-4.11800	88.39400
C	3.04400	-2.74000	89.21800
N	0.63800	-6.65800	86.83000
H	0.19000	-6.22400	86.02300
C	0.37200	-8.06500	87.13000
C	1.64200	-8.89500	87.00000
O	1.75300	-9.95800	87.60500
C	-0.69200	-8.60600	86.20200
N	2.59300	-8.40300	86.20600
H	2.42200	-7.51900	85.72700
C	3.87100	-9.08100	85.99500
C	4.81100	-8.87100	87.17400
O	5.86700	-9.49500	87.25600
C	4.55200	-8.55600	84.73400
O	3.77600	-8.82700	83.59000
H	4.20000	-8.50000	82.80500
N	4.43900	-7.97500	88.08000
H	3.56400	-7.46400	87.95900
C	5.27000	-7.71900	89.24000
C	4.57800	-8.21200	90.50200
O	4.97300	-7.85600	91.61400
C	5.56600	-6.22800	89.36800
C	6.26900	-5.63900	88.17900
C	5.55000	-5.24000	87.05400
C	7.65100	-5.47400	88.18700
C	6.19700	-4.68300	85.95500
C	8.31100	-4.91900	87.09600
C	7.58200	-4.52200	85.97500
N	3.53900	-9.02500	90.32700
H	3.24800	-9.27800	89.38200
C	2.81500	-9.55600	91.46900
C	1.71100	-8.64200	91.95800
O	1.13600	-8.85400	93.02100
N	1.40200	-7.62300	91.17100
H	1.89600	-7.49500	90.28800
C	0.36600	-6.69000	91.55900
C	-1.00800	-7.04300	91.02700
O	-1.16100	-7.86200	90.11800
N	-2.02200	-6.42300	91.61500
H	-1.83200	-5.77700	92.38100
C	-3.39300	-6.63900	91.19800
C	-3.89200	-5.35700	90.54600

O	-4.22400	-4.38100	91.22700
C	-4.26000	-7.00200	92.40200
C	-5.73600	-7.08900	92.05500
O	-6.10900	-7.27500	90.88900
N	-6.58500	-6.97000	93.07200
H	-7.57600	-7.02800	92.83900
H	-6.27800	-6.81700	94.03200
N	-3.93400	-5.33800	89.20700
C	-4.39900	-4.15400	88.47900
C	-5.80100	-3.79700	88.92000
O	-6.30800	-2.72400	88.60400
C	-4.34900	-4.60000	87.02200
C	-4.58400	-6.08300	87.12000
C	-3.72600	-6.47200	88.29300
N	-6.41400	-4.71100	89.66200
H	-5.92800	-5.57600	89.90000
C	-7.76400	-4.49500	90.13700
C	-7.85500	-3.86900	91.51000
O	-8.95000	-3.61600	91.99900
N	-6.71600	-3.62800	92.14500
H	-5.83000	-3.87600	91.70500
C	-6.71800	-3.01100	93.46700
C	-5.61300	-1.96900	93.52500
O	-4.66200	-2.09200	94.29600
C	-6.50400	-4.05900	94.56900
O	-6.68400	-3.49000	95.86300
H	-6.55200	-4.13800	96.54500
N	-5.74100	-0.94300	92.69800
H	-6.54700	-0.89500	92.07500
C	-4.75100	0.10900	92.66800
C	-5.20100	1.30000	93.50200
O	-6.32600	1.78300	93.36000
C	-4.49300	0.58000	91.23200
C	-3.38900	1.61500	91.23000
C	-4.10700	-0.60300	90.35200
N	-4.31800	1.76200	94.38000
H	-3.41400	1.29700	94.46500
C	-4.60300	2.91200	95.22300
C	-3.62600	4.03500	94.90200
O	-2.41900	3.81000	94.84700
C	-4.46200	2.56900	96.71100
O	-5.56700	1.76300	97.11800
H	-5.48000	1.55100	98.04000

C	-4.42600	3.83500	97.55300
N	-4.14900	5.24100	94.68600
H	-5.16100	5.36300	94.72600
C	-3.30100	6.39000	94.39300
C	-3.18300	7.29200	95.60700
O	-4.18700	7.68100	96.20000
C	-3.84400	7.22700	93.21800
C	-5.32200	7.54000	93.43000
C	-3.62300	6.48800	91.91600
C	-5.90800	8.45000	92.36700
N	-1.95100	7.60900	95.98900
H	-1.15200	7.23700	95.47600
C	-1.73100	8.48000	97.13100
C	-0.55300	9.41200	96.91100
O	0.48100	9.01300	96.36700
C	-1.55400	7.65700	98.42500
C	-0.28000	6.84700	98.49600
C	0.16700	6.10100	97.41000
C	0.44200	6.78300	99.68600
C	1.31000	5.30200	97.51200
C	1.58200	5.98800	99.79500
C	2.01400	5.24700	98.70500
N	-0.73200	10.66500	97.32000
H	-1.62000	10.93300	97.74400
C	0.31700	11.65800	97.17300
C	0.27400	12.70000	98.27700
O	-0.67000	12.74600	99.05700
N	1.29400	13.55000	98.33000
H	2.03800	13.46900	97.63700
C	1.38700	14.59400	99.34300
C	1.53400	15.96700	98.68500
O	2.22200	16.12000	97.66800
C	2.59000	14.31000	100.26000
C	2.75200	15.22300	101.47500
C	3.70800	16.37900	101.24600
O	4.40800	16.40200	100.21500
O	3.77200	17.27300	102.11000
N	0.87800	16.96400	99.26700
H	0.31300	16.77400	100.09500
C	0.94800	18.31900	98.74900
C	0.42400	18.36000	97.30800
O	-0.73700	17.99900	97.04200
C	2.39700	18.81000	98.80300

O	2.45300	20.22100	98.75500
H	3.35200	20.52600	98.78900
N	1.27900	18.80200	96.38400
H	2.21700	19.08500	96.66700
C	0.90100	18.89000	94.97600
C	0.44100	17.51700	94.50600
O	-0.42900	17.40100	93.63700
C	2.08000	19.36800	94.14300
N	1.04100	16.48400	95.09200
H	1.76300	16.65300	95.79200
C	0.68400	15.12200	94.75000
C	-0.68400	14.83600	95.32400
O	-1.45900	14.04900	94.77100
N	-0.97400	15.48300	96.45100
H	-0.28100	16.10500	96.86800
C	-2.26300	15.31400	97.09300
C	-3.28600	15.96300	96.18800
O	-4.36600	15.40200	95.94900
N	-2.93000	17.14400	95.67700
H	-2.02500	17.54100	95.92900
C	-3.79900	17.88200	94.77000
C	-4.02300	17.04500	93.50900
O	-5.13700	16.98100	92.99600
C	-3.16800	19.23400	94.41800
C	-4.04100	20.14600	93.55300
C	-3.79100	19.99000	92.05200
O	-3.68800	18.83700	91.57900
O	-3.71100	21.01900	91.34100
N	-2.96800	16.40000	93.01900
H	-2.06400	16.49400	93.48200
C	-3.08100	15.56000	91.83100
C	-4.10500	14.43700	92.04500
O	-4.97800	14.20100	91.19700
C	-1.72500	14.94400	91.46600
O	-0.78400	15.93400	91.09000
H	0.05600	15.55200	90.86400
N	-3.99600	13.74100	93.17500
H	-3.25500	13.96700	93.83800
C	-4.92900	12.65700	93.47300
C	-6.34500	13.23400	93.52000
O	-7.30600	12.59000	93.09500
C	-4.59000	11.95700	94.83100
C	-5.70300	10.99100	95.21600

C	-3.26900	11.19400	94.71700
N	-6.45100	14.46000	94.02800
H	-5.60600	14.92900	94.35500
C	-7.72900	15.16000	94.13600
C	-8.26200	15.42000	92.73500
O	-9.44800	15.23700	92.46800
C	-7.54300	16.48900	94.88500
O	-8.79000	17.09000	95.20400
H	-8.67500	17.91200	95.66700
N	-7.37300	15.83400	91.83900
H	-6.40200	15.96200	92.12300
C	-7.75400	16.10900	90.46000
C	-8.17100	14.82700	89.74500
O	-9.19300	14.78800	89.06300
C	-6.59200	16.76600	89.66900
C	-6.98300	16.93300	88.21200
C	-6.25300	18.12600	90.26700
N	-7.37200	13.77700	89.89900
H	-6.53600	13.86600	90.47700
C	-7.66600	12.50000	89.25900
C	-8.99000	11.91200	89.72600
O	-9.71800	11.30100	88.94700
C	-6.53900	11.50700	89.53200
C	-5.21100	11.86300	88.87300
C	-4.15100	10.89800	89.34700
C	-5.34400	11.80700	87.36500
N	-9.30000	12.08600	91.00500
H	-8.65800	12.59200	91.61500
C	-10.54600	11.56200	91.54600
C	-11.71400	12.25300	90.84700
O	-12.84000	11.74500	90.83600
C	-10.60800	11.76900	93.07900
C	-12.00700	11.51800	93.59700
C	-9.64900	10.80400	93.75100
N	-11.42100	13.40000	90.23600
H	-10.46300	13.74700	90.27500
C	-12.42300	14.17800	89.51300
C	-12.38400	14.00200	87.99300
O	-13.38100	14.25700	87.32800
C	-12.27100	15.67100	89.82200
C	-12.65100	16.17500	91.20800
C	-12.36400	17.66600	91.29700
C	-14.12300	15.89800	91.47200

N	-11.25600	13.56500	87.43900
H	-10.45900	13.32700	88.02900
C	-11.15400	13.42500	85.98400
C	-11.72500	12.17800	85.30900
O	-11.39700	11.04300	85.67000
C	-9.70100	13.57800	85.52900
O	-9.63000	13.53200	84.10900
H	-8.72800	13.62700	83.82700
N	-12.58100	12.38500	84.29400
C	-13.21600	11.30900	83.52800
C	-12.15600	10.46100	82.82400
O	-12.41800	9.33300	82.42300
C	-14.08200	12.06500	82.52800
C	-14.42600	13.32400	83.26200
C	-13.11400	13.69700	83.88700
N	-10.95900	11.02000	82.67200
H	-10.80700	11.96600	83.02300
C	-9.86000	10.32400	82.02100
C	-9.23400	9.27100	82.91800
O	-8.53400	8.37500	82.43900
C	-8.77400	11.31000	81.61600
C	-9.10700	12.33200	80.53800
C	-7.90000	13.23300	80.30900
C	-9.49600	11.60900	79.25400
N	-9.47600	9.38000	84.22100
H	-10.07000	10.13600	84.56300
C	-8.90200	8.43200	85.16300
C	-9.88900	7.34200	85.55100
O	-9.48700	6.27000	86.01700
C	-8.41200	9.16700	86.40200
N	-11.17800	7.61900	85.36100
H	-11.43800	8.52700	84.97700
C	-12.22700	6.66100	85.68700
C	-11.76200	5.23200	85.42600
O	-11.36500	4.90000	84.31500
C	-13.47900	6.94500	84.85400
C	-14.61600	5.95900	85.10200
C	-15.73600	6.07700	84.06800
C	-16.84300	5.06200	84.35500
N	-17.80900	4.94900	83.23100
H	-18.54700	4.27200	83.42200
H	-17.33200	4.73600	82.35500
H	-18.19800	5.86000	82.98700

N	-11.79500	4.39800	86.45800
H	-12.11200	4.74600	87.36300
C	-11.39300	2.99900	86.34000
C	-9.89000	2.74300	86.33200
O	-9.45600	1.62100	86.05800
C	-12.01100	2.36800	85.08800
C	-13.53200	2.36100	85.12500
O	-14.14500	1.74600	86.00500
N	-14.15000	3.04900	84.16700
H	-15.17000	3.04400	84.19200
H	-13.64400	3.55600	83.44100
N	-9.09000	3.76400	86.62600
H	-9.48800	4.68000	86.83500
C	-7.64500	3.57400	86.65000
C	-7.11900	3.33400	88.06100
O	-5.98800	2.88600	88.24400
C	-6.93500	4.76200	86.01500
C	-7.03300	4.82200	84.49300
C	-6.02400	5.83600	83.98500
C	-6.74100	3.45100	83.88600
N	-7.94800	3.63800	89.05300
H	-8.85900	4.03800	88.83000
C	-7.59700	3.41800	90.44900
C	-8.85900	3.00100	91.21200
O	-9.96100	3.10400	90.68500
C	-6.97600	4.68100	91.06100
C	-7.83300	5.90000	90.94800
C	-7.98800	6.54600	89.73000
C	-8.47100	6.41800	92.06600
C	-8.76700	7.69900	89.63100
C	-9.25000	7.56700	91.97600
C	-9.39900	8.21000	90.76000
N	-8.70300	2.53500	92.44700
H	-7.76900	2.49200	92.85600
C	-9.85000	2.08600	93.22300
C	-10.00400	2.73200	94.58300
O	-11.05500	2.60300	95.21300
C	-9.77000	0.57900	93.38100
C	-9.53300	-0.13200	92.08900
N	-10.44800	-0.12700	91.05900
H	-11.36800	0.31200	91.09000
C	-8.46000	-0.82000	91.63400
C	-9.94900	-0.77900	90.02500

N	-8.74200	-1.21000	90.34800
H	-8.12100	-1.74500	89.74100
N	-8.95800	3.41800	95.03700
H	-8.12000	3.46900	94.45800
C	-8.95800	4.10300	96.33300
C	-7.98400	5.26400	96.20200
O	-7.04700	5.19200	95.40800
C	-8.49500	3.13600	97.42000
C	-9.21400	1.80900	97.32300
C	-8.48400	0.69400	98.00200
N	-9.00400	-0.61600	97.60500
H	-8.33300	-1.31000	97.27700
C	-10.29000	-0.97000	97.64000
N	-11.21600	-0.11500	98.04100
H	-10.93900	0.83300	98.29700
H	-12.19900	-0.38600	98.06800
N	-10.65000	-2.20100	97.30700
H	-9.93600	-2.86000	96.99800
H	-11.63300	-2.47200	97.33400
N	-8.19300	6.33300	96.96100
H	-8.97500	6.34600	97.61500
C	-7.30800	7.49000	96.86300
C	-6.97800	8.13900	98.20700
O	-7.81500	8.19900	99.10300
C	-7.92600	8.52700	95.92800
N	-5.75300	8.62700	98.34300
H	-5.08700	8.54200	97.57500
C	-5.35200	9.27800	99.57000
C	-4.72200	10.62200	99.24400
O	-3.77000	10.69500	98.46700
C	-4.32600	8.41800	100.36000
C	-4.91500	7.03500	100.65000
C	-3.94200	9.11700	101.68100
C	-3.98100	6.12100	101.42500
N	-5.26600	11.68700	99.82300
H	-6.07800	11.56400	100.42800
C	-4.73100	13.02500	99.61400
C	-4.11700	13.51000	100.91000
O	-4.82600	13.77600	101.88000
C	-5.82800	13.99500	99.18800
O	-5.97900	14.00800	97.78000
H	-6.66200	14.61200	97.51500
N	-2.79700	13.62600	100.92700

H	-2.26300	13.39400	100.08900
C	-2.09600	14.07800	102.11700
C	-1.73000	15.55000	102.03300
O	-0.86100	15.93200	101.25200
C	-0.82200	13.25700	102.32000
C	-1.06500	11.79900	102.66800
C	0.21600	10.99500	102.65300
O	1.27200	11.60000	102.94200
O	0.16600	9.77400	102.36700
N	-2.38900	16.37400	102.84000
H	-3.11100	16.00200	103.45700
C	-2.09600	17.80100	102.85600
C	-2.13200	18.39800	101.45400
O	-1.11500	18.89400	100.95900
C	-0.71000	18.05100	103.46700
O	-0.56200	17.39800	104.71600
H	0.29600	17.55300	105.09400
N	-3.29900	18.34400	100.81800
H	-4.10000	17.90600	101.27300
C	-3.44900	18.90000	99.48500
C	-4.67900	18.41500	98.73200
O	-4.88700	17.21000	98.58600
N	-5.50200	19.34900	98.25800
H	-5.29500	20.33300	98.42900
C	-6.69700	18.98800	97.49600
C	-6.87100	19.91700	96.29400
O	-6.01900	20.77200	96.04800
C	-7.97300	19.02300	98.37600
C	-7.87000	17.98200	99.45400
C	-8.16500	20.39300	98.98700
N	-7.96600	19.74900	95.55200
H	-8.64000	19.03100	95.82000
C	-8.23000	20.56300	94.36600
C	-8.88200	21.91700	94.63700
O	-8.69800	22.85100	93.85700
C	-9.06900	19.77300	93.37200
N	-9.65500	22.03200	95.71700
H	-9.81200	21.22200	96.31700
C	-10.28000	23.31400	96.04700
C	-9.19300	24.32500	96.44000
O	-9.46400	25.52500	96.60400
C	-11.27800	23.15700	97.19800
C	-12.60000	22.43600	96.91600

C	-13.47100	22.45100	98.15500
C	-13.32900	23.11900	95.78500
N	-7.96500	23.81200	96.58500
H	-7.84500	22.81000	96.44000
C	-6.77900	24.60500	96.94100
C	-6.38800	25.45200	95.73100
O	-5.41700	25.16500	95.02300
C	-5.56800	23.69200	97.33000
O	-5.94500	22.80800	98.39800
H	-5.21000	22.25400	98.63400
C	-4.38300	24.53700	97.79200
N	-7.17200	26.49800	95.51400
H	-7.94000	26.66600	96.16300
C	-6.99900	27.42000	94.40200
C	-5.56500	27.72400	93.95300
O	-5.31700	27.90200	92.75900
C	-7.72500	28.73500	94.72100
O	-9.11500	28.52000	94.92500
H	-9.56400	29.33400	95.12200
N	-4.62300	27.78500	94.88700
H	-4.86300	27.60800	95.86200
C	-3.24700	28.10400	94.52400
C	-2.72300	27.30200	93.33500
O	-2.08600	27.85900	92.43900
C	-2.28900	27.92100	95.73100
C	-2.40000	26.51400	96.28000
C	-0.85000	28.22600	95.31300
N	-3.00300	26.00300	93.31800
H	-3.55300	25.60000	94.07600
C	-2.53900	25.14400	92.23600
C	-3.47100	25.08100	91.02500
O	-3.09400	24.55100	89.97300
C	-2.29700	23.73100	92.76100
C	-1.05800	23.52900	93.63100
C	-0.91300	22.05300	93.98400
C	0.17100	24.01300	92.88100
N	-4.68200	25.61300	91.17100
H	-4.93900	26.03400	92.06400
C	-5.64900	25.60600	90.07800
C	-5.89100	27.00400	89.50900
O	-6.44800	27.88900	90.16400
C	-6.98500	24.96200	90.51900
C	-8.02800	25.10400	89.42300

C	-6.76100	23.48600	90.82600
N	-5.45000	27.17500	88.26700
H	-5.01200	26.38200	87.79900
C	-5.55600	28.42700	87.53600
C	-6.89100	28.61600	86.82700
O	-7.05400	28.22800	85.67000
C	-4.42300	28.50900	86.51200
C	-3.04300	28.56700	87.12600
C	-2.89300	29.81600	87.97600
C	-1.48800	29.92700	88.53800
N	-1.31700	31.15600	89.35700
H	-0.37200	31.23100	89.73500
H	-2.01800	31.21100	90.09600
H	-1.57400	31.99100	88.83100
N	-7.84700	29.21500	87.52500
H	-7.66100	29.50100	88.48600
C	-9.15800	29.47200	86.94400
C	-9.07400	30.81500	86.21800
O	-8.14100	31.59500	86.43900
C	-10.22600	29.50000	88.04400
C	-10.23700	28.22400	88.87800
C	-11.23000	28.27600	90.01700
C	-11.07200	27.06000	90.93200
N	-9.84600	27.09400	91.79100
H	-9.74100	26.28300	92.40100
H	-9.81500	27.95600	92.33500
H	-9.01200	27.22000	91.21800
N	-10.03400	31.07800	85.34100
H	-10.78900	30.40800	85.19300
C	-10.00700	32.32000	84.59400
C	-9.18200	32.16800	83.33000
O	-8.66000	31.08900	83.04200
N	-9.06600	33.25300	82.57500
H	-9.52600	34.11100	82.88000
C	-8.30900	33.27200	81.32700
C	-6.79700	33.14800	81.57800
O	-6.18200	34.03400	82.17200
C	-8.64700	34.56500	80.57900
C	-7.85900	34.73500	79.30400
O	-7.62000	33.72800	78.60300
O	-7.49500	35.89200	78.99600
N	-6.20700	32.04300	81.12300
H	-6.76800	31.35300	80.62300

C	-4.78000	31.78900	81.31800
C	-3.89100	32.39900	80.24000
O	-2.67300	32.50800	80.41100
C	-4.47700	30.26600	81.36800
C	-5.35400	29.60400	82.41000
C	-4.69000	29.62600	80.00000
N	-4.51000	32.79400	79.13500
H	-5.52300	32.69500	79.07500
C	-3.79200	33.36400	78.00600
C	-2.74100	34.41700	78.39800
O	-1.59700	34.36900	77.93700
C	-4.80700	33.94300	77.01900
C	-4.24700	34.30200	75.65700
C	-3.72900	33.08800	74.91900
C	-3.27600	33.47700	73.52000
N	-4.38900	34.02600	72.67800
H	-4.08500	34.28700	71.74000
H	-4.84700	34.80900	73.14400
H	-5.17300	33.37400	72.64000
N	-3.11200	35.37900	79.25800
C	-2.16000	36.41500	79.67500
C	-0.87600	35.85900	80.28500
O	0.22400	36.30900	79.95200
C	-2.96500	37.23300	80.67300
C	-4.35900	37.13100	80.12200
C	-4.45300	35.66100	79.79600
N	-1.00400	34.88200	81.17700
H	-1.93000	34.53700	81.43200
C	0.18500	34.30700	81.78800
C	1.05800	33.61700	80.73200
O	2.28500	33.64600	80.81500
C	-0.21200	33.32900	82.90000
C	0.88900	32.56300	83.66200
C	1.28900	31.33700	82.85400
C	2.10300	33.46000	83.95200
N	0.41600	33.01700	79.73100
H	-0.60400	33.04100	79.71400
C	1.12400	32.32500	78.65600
C	1.99400	33.29600	77.86500
O	3.17700	33.03800	77.61000
C	0.12500	31.64500	77.72000
N	1.39900	34.41600	77.47800
H	0.42100	34.57600	77.71800

C	2.12200	35.41400	76.71900
C	3.29600	35.94300	77.53300
O	4.38600	36.18300	77.00500
C	1.17300	36.54600	76.32700
C	0.01900	36.07400	75.44900
C	-0.83800	37.21200	74.92000
O	-0.30800	38.06100	74.16800
O	-2.04200	37.25500	75.25400
N	3.08100	36.11400	78.82800
H	2.16800	35.89300	79.22700
C	4.14100	36.61500	79.68000
C	5.36400	35.69300	79.57400
O	6.49200	36.15200	79.37800
C	3.64900	36.69800	81.12400
C	4.47000	37.63200	81.99800
C	3.91700	37.74000	83.40800
O	2.76900	38.15400	83.61100
N	4.73100	37.36300	84.39500
H	4.36000	37.43600	85.34200
H	5.67800	37.02200	84.22800
N	5.13100	34.38900	79.68700
H	4.17500	34.06800	79.83900
C	6.20400	33.40300	79.60000
C	6.89700	33.44300	78.23900
O	8.12100	33.39900	78.14900
C	5.66100	31.98700	79.82300
C	4.87700	31.93800	81.13700
C	6.80800	30.99700	79.83400
C	4.35200	30.57200	81.49900
N	6.09500	33.52000	77.18200
H	5.08500	33.54400	77.32500
C	6.62100	33.57100	75.82600
C	7.60100	34.73200	75.67300
O	8.72600	34.54600	75.19300
C	5.47800	33.71100	74.82500
N	7.18200	35.92700	76.08500
H	6.24700	36.02500	76.48000
C	8.04600	37.09700	75.97700
C	9.34800	36.94900	76.76300
O	10.41500	37.31000	76.27700
C	7.33000	38.35800	76.45300
C	6.09100	38.58900	75.59400
C	8.25900	39.54400	76.35300

C	5.22700	39.72500	76.06500
N	9.26100	36.42100	77.97800
H	8.35000	36.14000	78.34100
C	10.44600	36.23800	78.79700
C	11.41800	35.31800	78.08200
O	12.63600	35.49100	78.16600
C	10.08100	35.63000	80.15500
O	9.23300	36.53800	80.87000
H	8.45100	36.70600	80.35700
C	11.32800	35.36200	80.97400
N	10.87400	34.33500	77.37400
H	9.85900	34.24200	77.34400
C	11.70200	33.38800	76.64000
C	12.12500	33.97200	75.29300
O	12.96900	33.40700	74.59400
C	10.95200	32.08400	76.44200
N	11.52600	35.10100	74.93100
H	10.81400	35.51300	75.53400
C	11.87800	35.75300	73.68200
C	11.10200	35.29300	72.46800
O	11.69100	34.98500	71.43300
N	9.78000	35.26700	72.58200
H	9.34900	35.56000	73.45900
C	8.93400	34.83000	71.48500
C	7.81800	35.81200	71.18200
O	7.32400	36.49400	72.08100
C	8.29800	33.49800	71.83100
S	9.40500	32.06600	71.95500
N	7.41200	35.86800	69.91600
H	7.87600	35.28600	69.21900
C	6.31800	36.74300	69.49900
C	5.02800	36.18900	70.10900
O	4.94600	35.00100	70.41200
C	6.19700	36.74100	67.97500
C	7.42200	37.26200	67.25200
C	7.97300	36.24400	66.25100
C	7.03400	35.99400	65.06600
N	7.70500	35.14900	64.01700
H	7.08000	34.98300	63.22800
H	8.06000	34.27600	64.40700
H	8.59100	35.55500	63.71600
N	4.02200	37.03200	70.30300
H	4.12900	38.01800	70.06300

C	2.76000	36.54800	70.86100
C	1.63600	36.77700	69.85600
O	0.46800	36.91200	70.23100
C	2.40600	37.26100	72.18000
O	2.23500	38.66300	71.93900
H	1.54600	38.79400	71.29800
C	3.50600	37.05100	73.20400
N	2.01100	36.80800	68.57500
H	2.99600	36.66600	68.35300
C	1.07700	37.03500	67.47800
C	-0.19100	36.22100	67.62600
O	-1.29200	36.76400	67.58400
C	1.70100	36.68000	66.12800
O	3.00500	37.27200	66.02100
H	3.39300	37.05100	65.18200
C	0.81600	37.18700	65.00500
N	-0.02700	34.91200	67.78200
H	0.91900	34.53100	67.78500
C	-1.15600	34.00100	67.94900
C	-0.70500	32.88300	68.87200
O	0.49400	32.67600	69.04600
C	-1.58000	33.35800	66.61800
O	-0.57200	32.43600	66.19500
H	-0.83400	32.03900	65.37300
C	-1.78300	34.41500	65.54600
N	-1.64900	32.16300	69.46700
H	-2.63300	32.37500	69.30300
C	-1.27500	31.07000	70.35400
C	-0.32200	30.12300	69.62800
O	0.80600	29.88900	70.07600
C	-2.50700	30.28500	70.79600
O	-3.35400	31.06400	71.61400
H	-4.12100	30.57500	71.88900
N	-0.78800	29.59700	68.49800
H	-1.72000	29.86200	68.17900
C	-0.01500	28.65700	67.70100
C	1.41700	29.10900	67.45200
O	2.31900	28.28400	67.29900
C	-0.71800	28.40400	66.37800
N	1.63400	30.41600	67.41000
H	0.86000	31.06400	67.55300
C	2.97100	30.92900	67.16100
C	3.79700	30.83200	68.43400

O	4.98300	30.49800	68.39300
C	2.90800	32.38600	66.65800
C	4.28800	32.97700	66.57900
C	2.25500	32.42200	65.28700
N	3.16600	31.11000	69.57000
H	2.18400	31.38500	69.54600
C	3.85700	31.02700	70.84500
C	4.32700	29.59600	71.06800
O	5.50400	29.34400	71.33000
C	2.92700	31.43000	71.98900
C	2.48700	32.87700	71.94600
S	1.80400	33.42800	73.52300
C	0.09200	32.94400	73.35800
N	3.39900	28.65500	70.95300
H	2.44200	28.91600	70.71600
C	3.73200	27.26100	71.16100
C	4.86600	26.82300	70.25100
O	5.83600	26.22500	70.71000
C	2.51500	26.34700	70.91300
C	2.86200	24.90800	71.28800
C	1.32900	26.82500	71.72900
N	4.74500	27.12000	68.96100
H	3.92100	27.62800	68.64000
C	5.77000	26.73300	67.99500
C	7.12600	27.25800	68.42900
O	8.12800	26.55000	68.34000
C	5.43000	27.27500	66.60200
C	6.42600	26.89900	65.54800
N	6.65500	25.59400	65.16800
H	6.17300	24.77800	65.54500
C	7.26800	27.65700	64.80400
C	7.59500	25.56300	64.24000
N	7.98400	26.80300	64.00100
H	8.70000	27.08100	63.32900
N	7.14700	28.49800	68.91000
H	6.27300	29.02000	68.97000
C	8.38200	29.13500	69.35400
C	8.97200	28.51800	70.61100
O	10.17800	28.35900	70.71800
C	8.14200	30.61200	69.59800
S	9.65200	31.54900	70.00700
N	8.11500	28.19500	71.57000
H	7.12000	28.37800	71.43900

C	8.57400	27.58500	72.80200
C	9.09800	26.17800	72.52100
O	9.98100	25.69100	73.23100
C	7.44100	27.54700	73.82500
C	7.00700	28.91600	74.35600
C	5.90100	28.74300	75.37400
C	8.19400	29.61900	74.99800
N	8.56500	25.52400	71.48700
H	7.82600	25.96400	70.93800
C	9.02900	24.18400	71.13300
C	10.43300	24.28400	70.55300
O	11.17100	23.30100	70.53800
C	8.11400	23.51600	70.09200
C	6.77400	23.02200	70.62800
C	6.31700	21.71900	69.95900
N	5.10100	21.21400	70.59500
H	5.19400	20.43900	71.25100
C	3.88100	21.69900	70.37400
N	3.70300	22.69400	69.51800
H	4.50200	23.06400	69.00300
H	2.76800	23.06600	69.34900
N	2.84200	21.21800	71.04300
H	2.97900	20.45200	71.70200
H	1.90700	21.59000	70.87400
N	10.78700	25.48000	70.08400
H	10.11600	26.24600	70.15200
C	12.08600	25.74800	69.47800
C	13.20400	25.93800	70.48700
O	14.36400	25.66800	70.19500
C	12.01000	27.01000	68.62700
C	10.90800	27.01000	67.61300
C	11.01200	25.82900	66.68900
O	11.99000	25.69400	65.95000
N	10.00700	24.95300	66.72600
H	9.19800	25.06500	67.33700
H	10.07800	24.15200	66.09900
N	12.85900	26.42300	71.67000
H	11.87700	26.62300	71.86300
C	13.85400	26.67600	72.69900
C	14.47800	25.41100	73.26600
O	13.91000	24.32300	73.18200
C	13.22300	27.47700	73.83200
C	12.60900	28.79100	73.40000

C	13.66000	29.69800	72.83300
C	13.07600	31.03200	72.44700
N	14.12600	31.86800	71.80600
H	13.73100	32.77100	71.54500
H	14.56400	31.39600	71.01500
H	14.95300	31.96600	72.39500
N	15.65600	25.55900	73.85100
H	16.09000	26.48100	73.88700
C	16.33600	24.41900	74.44200
C	15.96300	24.30300	75.90900
O	15.47100	25.26100	76.51100
C	17.86600	24.55900	74.36500
O	18.29600	25.63000	75.21800
H	18.02300	25.45900	76.11200
C	18.29900	24.83000	72.94800
N	16.20400	23.12400	76.47500
H	16.60300	22.37400	75.91000
C	15.91400	22.87400	77.88000
C	16.52300	24.01000	78.68800
O	15.84100	24.65800	79.48200
C	16.51700	21.53500	78.31700
C	16.48600	21.29300	79.80900
C	17.11600	19.96900	80.21500
O	16.38400	18.96500	80.33100
O	18.35100	19.93000	80.41200
N	17.80100	24.27800	78.45300
H	18.30800	23.73600	77.75300
C	18.48900	25.33200	79.17800
C	17.79900	26.69200	79.08900
O	17.76100	27.44000	80.06700
C	19.92900	25.45200	78.68600
C	20.79100	26.27100	79.62200
C	20.55500	25.89800	81.08500
O	20.75100	24.71300	81.44900
O	20.16400	26.79500	81.86800
N	17.24800	27.00800	77.92000
H	17.29800	26.34600	77.14600
C	16.57300	28.28800	77.72800
C	15.28000	28.36300	78.53500
O	14.97100	29.39400	79.14400
C	16.29500	28.51700	76.24200
C	17.55500	28.42300	75.40000
C	17.35100	28.79900	73.94400

O	17.20000	30.00700	73.65000
O	17.34400	27.88200	73.09400
N	14.52800	27.26800	78.55100
H	14.82100	26.44100	78.03100
C	13.29200	27.24800	79.30600
C	13.56900	27.22500	80.80900
O	12.76900	27.71600	81.60500
C	12.43800	26.04900	78.89800
C	11.81900	26.11800	77.49600
C	10.71800	25.08500	77.38200
C	11.23000	27.49100	77.25000
N	14.70700	26.67000	81.20800
H	15.35200	26.27800	80.52200
C	15.03500	26.62100	82.62700
C	15.39500	28.02400	83.10300
O	14.97200	28.45200	84.17500
C	16.19000	25.64800	82.87700
C	16.66400	25.41900	84.31300
C	15.48400	25.22000	85.24400
C	17.58300	24.21500	84.34400
N	16.16600	28.74500	82.29400
H	16.49300	28.34100	81.41600
C	16.54900	30.10500	82.64700
C	15.29300	30.94100	82.76500
O	15.14400	31.72500	83.69700
C	17.46200	30.69200	81.58600
C	18.64900	29.81000	81.31500
C	19.75800	30.54200	80.60600
O	20.77200	29.88900	80.26100
O	19.60900	31.76900	80.40300
N	14.39100	30.77100	81.80700
H	14.58400	30.12500	81.04100
C	13.13700	31.49200	81.83700
C	12.41100	31.04700	83.10200
O	11.86700	31.86600	83.84300
C	12.27700	31.16000	80.60700
O	12.93000	31.64500	79.43200
H	13.78800	31.24300	79.36500
C	10.90800	31.80100	80.71400
N	12.42400	29.74300	83.35800
H	12.90200	29.11000	82.71700
C	11.76600	29.20500	84.54000
C	12.25900	29.89700	85.79700

O	11.49800	30.09200	86.74100
C	12.03000	27.70000	84.69900
O	11.39200	26.98900	83.63300
H	11.72600	27.30000	82.80000
C	11.49300	27.20100	86.03700
N	13.53600	30.26700	85.80100
H	14.10700	30.09200	84.97400
C	14.13800	30.91500	86.95500
C	13.95800	32.42400	87.01200
O	13.87000	32.99100	88.10000
C	15.62100	30.55800	87.03600
C	15.83700	29.06500	87.28800
C	17.31500	28.75900	87.33500
C	15.16600	28.66700	88.59300
N	13.91200	33.08600	85.86200
H	14.01400	32.58600	84.97900
C	13.71500	34.53100	85.86600
C	12.34400	34.78100	86.47400
O	12.14300	35.74100	87.22000
C	13.73700	35.09000	84.44600
C	15.05000	34.93300	83.73200
C	14.89200	35.24600	82.25800
C	16.18400	35.00400	81.51100
N	15.98000	35.10000	80.04800
H	16.85200	34.93700	79.54400
H	15.55500	35.99000	79.78600
H	15.24000	34.47400	79.73000
N	11.41100	33.89000	86.15300
H	11.66500	33.10800	85.54900
C	10.04100	33.98900	86.63200
C	9.91400	33.88600	88.15400
O	8.91700	34.32600	88.71700
C	9.17600	32.90400	85.97600
C	9.25400	32.81700	84.44000
S	8.64100	34.24700	83.51200
C	6.86800	33.95200	83.53100
N	10.91600	33.30700	88.81500
H	11.71900	32.96400	88.28900
C	10.90400	33.14600	90.27600
C	9.52900	32.70300	90.78900
O	8.93100	33.35100	91.65500
C	11.32200	34.45800	90.95300
C	12.69400	34.95200	90.51000

C	13.07100	36.28700	91.13500
C	14.43300	36.75200	90.62400
N	14.88300	38.04600	91.21600
H	15.79300	38.35700	90.87500
H	14.87700	37.99800	92.23500
H	14.17900	38.77100	91.07600
N	9.05000	31.58400	90.24700
H	9.62500	31.10100	89.55600
C	7.74600	31.00500	90.58400
C	7.58200	30.49200	92.01600
O	6.49500	30.58300	92.59100
C	7.43400	29.85200	89.62000
C	7.06600	30.29500	88.23100
C	7.31500	29.46700	87.13900
C	6.44600	31.52300	88.01200
C	6.95200	29.85300	85.84800
C	6.07900	31.91800	86.72600
C	6.33300	31.07900	85.64200
N	8.65800	29.95000	92.58000
H	9.53200	29.93100	92.05500
C	8.63200	29.38000	93.92700
C	8.76300	30.39000	95.07700
O	8.33900	30.11300	96.20500
C	9.73000	28.31200	94.04300
C	9.67200	27.18900	92.99700
C	10.95500	26.37700	93.02800
C	8.45900	26.30900	93.26100
N	9.34200	31.55400	94.79400
H	9.67000	31.73300	93.84500
C	9.51500	32.57800	95.81700
C	8.36700	33.58800	95.79200
O	7.79400	33.86900	94.73700
C	10.85100	33.29800	95.61600
O	11.16100	34.11800	96.72800
H	11.99000	34.56500	96.60300
N	8.03800	34.12900	96.96200
H	8.56000	33.85400	97.79400
C	6.95600	35.10300	97.10000
C	7.46300	36.53800	96.95600
O	8.42000	36.93500	97.62300
C	6.28200	34.93500	98.46700
C	5.07200	35.81500	98.79300
C	3.92100	35.48500	97.85800

C	4.65500	35.58500	100.23500
N	6.81400	37.31100	96.08900
H	6.02700	36.92400	95.56800
C	7.20300	38.70000	95.86700
C	6.59200	39.61900	96.92000
O	5.38000	39.83400	96.93600
C	6.75600	39.16900	94.48200
C	7.24800	40.57300	94.15500
O	6.73700	41.17700	93.18500
O	8.15200	41.07100	94.86100
N	7.44000	40.16300	97.79000
H	8.43300	39.94200	97.71100
C	7.00300	41.06600	98.85500
C	6.41800	42.38400	98.34100
O	5.26000	42.71100	98.62500
C	8.17200	41.37100	99.80100
C	8.39700	40.42300	100.98000
C	9.68600	40.78900	101.70300
C	7.20600	40.51300	101.92300
N	7.22300	43.13900	97.59500
H	8.16700	42.81000	97.39500
C	6.79000	44.42600	97.05600
C	5.86900	44.25700	95.85500
O	5.61900	43.13900	95.39700
C	8.00200	45.27900	96.65600
C	8.68900	44.84300	95.36700
C	9.90900	45.68800	95.04300
O	10.91700	45.63700	95.75100
N	9.82000	46.47500	93.97400
H	8.98600	46.51700	93.38800
H	10.63900	47.04200	93.75600
N	5.37100	45.37700	95.34400
H	5.62100	46.27600	95.75500
C	4.47500	45.33000	94.20700
C	3.03800	45.18600	94.66400
O	2.74100	45.31100	95.85400
N	2.14400	44.92100	93.71800
H	2.45500	44.82600	92.75100
C	0.73000	44.76300	94.02900
C	0.40400	43.29100	94.25300
O	0.78800	42.43300	93.45900
C	-0.12700	45.31700	92.88700
C	-1.60300	45.38600	93.24000

O	-2.22700	44.32200	93.45000
O	-2.13800	46.51300	93.31000
N	-0.30200	42.98000	95.35100
C	-0.68400	41.60500	95.68300
C	-1.35700	40.87900	94.51500
O	-1.06500	39.71000	94.24400
C	-1.62300	41.79600	96.87100
C	-1.01400	42.96800	97.57100
C	-0.72000	43.90800	96.41900
N	-2.25300	41.58200	93.82600
H	-2.44000	42.54700	94.10000
C	-2.97600	41.01800	92.69200
C	-2.13900	40.95100	91.41400
O	-2.41200	40.13400	90.53200
C	-4.24800	41.82400	92.44000
C	-5.30200	41.63000	93.51000
C	-6.32200	42.74700	93.47800
N	-5.71900	44.02600	93.84500
H	-4.73100	44.03100	94.09800
C	-6.37100	45.18400	93.87100
N	-7.65800	45.23400	93.54800
H	-8.15800	46.12300	93.56800
H	-8.14600	44.38000	93.27700
N	-5.73600	46.29500	94.22300
H	-6.23600	47.18400	94.24300
H	-4.74700	46.25700	94.47100
N	-1.12500	41.80800	91.31200
H	-0.94900	42.47200	92.06600
C	-0.26200	41.80900	90.13500
C	0.84300	40.76600	90.22300
O	0.99900	39.95700	89.30900
C	0.36600	43.18700	89.90900
C	-0.53300	44.17100	89.18000
C	0.25800	45.19100	88.38200
O	1.11200	45.87500	88.97900
O	0.02800	45.30800	87.15800
N	1.60600	40.79300	91.31600
H	1.41800	41.49800	92.02800
C	2.70500	39.84600	91.53200
C	2.44200	38.54600	90.79100
O	1.67100	37.70400	91.25700
C	2.88000	39.55100	93.02500
O	3.92400	38.61400	93.24000

H	4.03300	38.43100	94.16600
N	3.08600	38.40000	89.63600
H	3.71700	39.13900	89.32700
C	2.92100	37.22200	88.80000
C	2.66800	35.96100	89.62100
O	3.42000	35.64300	90.55300
C	4.15400	37.01700	87.91300
C	5.37400	36.49800	88.63800
C	6.39500	35.93300	87.68000
O	6.09100	35.03400	86.89600
N	7.61400	36.45700	87.73300
H	7.86600	37.20200	88.38300
H	8.30400	36.07500	87.08600
N	1.57900	35.24700	89.29600
C	1.18000	34.01100	89.97000
C	2.13700	32.87000	89.63600
O	3.24700	32.78700	90.17000
C	-0.22100	33.74900	89.41600
C	-0.71200	35.11500	89.03100
C	0.51300	35.70400	88.38900
N	1.68500	31.98200	88.75200
H	0.75300	32.11600	88.36100
C	2.46500	30.82100	88.31500
C	1.63500	30.05600	87.30700
O	0.75100	30.62400	86.68500
C	2.81600	29.88400	89.49000
C	2.30000	30.13700	90.90200
C	0.80100	29.93300	90.96900
C	3.02300	29.18300	91.83600
N	1.90500	28.76400	87.16500
H	2.62900	28.33400	87.74000
C	1.18200	27.95800	86.20100
C	0.96200	26.59000	86.79800
O	1.85400	26.02200	87.41400
C	1.98300	27.85500	84.90100
C	3.33900	27.15500	84.91800
C	4.04000	27.42800	83.60600
C	4.18800	27.64800	86.07400
N	-0.24400	26.07500	86.62800
H	-0.95000	26.59600	86.10700
C	-0.56600	24.77900	87.17600
C	-1.77600	24.20600	86.48100
O	-1.97200	24.44000	85.28900

N	-2.58600	23.46000	87.22600
H	-2.36300	23.31400	88.21100
C	-3.78300	22.84700	86.67100
C	-4.68600	23.90400	86.06400
O	-4.80300	25.00600	86.58700
C	-4.58300	22.11300	87.74300
O	-3.70500	21.28800	88.51200
H	-4.20300	20.83100	89.17900
C	-5.64800	21.24600	87.09900
N	-5.31600	23.56300	84.94900
H	-5.15900	22.63500	84.55600
C	-6.23000	24.47700	84.26500
C	-7.46200	23.66600	83.92600
O	-7.46800	22.45200	84.13000
C	-5.62400	25.01400	82.94900
C	-4.45000	25.92900	83.24800
C	-5.18900	23.85200	82.06400
N	-8.50800	24.31200	83.42900
H	-8.48300	25.32400	83.30500
C	-9.69000	23.55200	83.06400
C	-9.63000	23.36600	81.54800
O	-10.17300	24.15900	80.79200
C	-10.97000	24.28500	83.47200
C	-10.87800	24.74000	84.93400
C	-12.16400	23.35400	83.30700
C	-10.92200	23.61500	85.95800
N	-8.95300	22.30600	81.11700
H	-8.55200	21.67000	81.80700
C	-8.75800	22.01100	79.69900
C	-9.95000	21.42800	78.94900
O	-9.99300	21.46800	77.71700
C	-7.58100	21.06100	79.53600
C	-7.82400	19.73100	80.20400
O	-7.06100	18.78200	79.93700
O	-8.77800	19.63400	81.00400
N	-10.91200	20.87300	79.67300
H	-10.84600	20.85500	80.69100
C	-12.05600	20.29300	79.00500
C	-11.71300	18.91000	78.50100
O	-12.36100	18.38200	77.60500
N	-10.66700	18.33000	79.07400
H	-10.15100	18.84200	79.78900
C	-10.23000	16.98600	78.71700

C	-10.05900	16.23600	80.04200
O	-10.76900	15.26700	80.32200
C	-8.90100	17.03800	77.95400
C	-8.96200	17.67900	76.55300
S	-9.52100	16.59300	75.17600
C	-8.16400	15.39400	75.10900
N	-9.12400	16.70900	80.86200
H	-8.57300	17.51600	80.56900
C	-8.86100	16.11200	82.16700
C	-9.89100	16.63600	83.15700
O	-10.31800	15.93100	84.06100
C	-7.46500	16.50200	82.64800
C	-7.10200	16.08500	84.07100
C	-6.78900	14.61000	84.09100
C	-5.90600	16.87300	84.54400
N	-10.27000	17.89400	82.97500
H	-9.86100	18.42100	82.20300
C	-11.24600	18.55400	83.83200
C	-12.23400	19.29100	82.95600
O	-11.84600	20.17800	82.19900
C	-10.55700	19.56300	84.75500
C	-9.86000	19.01600	85.99400
C	-8.93600	20.06000	86.56300
C	-10.91000	18.60800	87.01200
N	-13.50800	18.92800	83.05300
H	-13.77600	18.18100	83.69400
C	-14.52300	19.59100	82.24900
C	-14.98300	20.89700	82.88200
O	-15.73700	21.65500	82.27800
C	-15.71200	18.66300	82.01400
C	-15.40200	17.42400	81.16800
C	-16.71500	16.76400	80.75600
C	-14.60000	17.80700	79.93800
N	-14.51500	21.15600	84.10000
H	-13.90700	20.47300	84.55100
C	-14.84500	22.38700	84.81000
C	-14.18800	22.47200	86.17700
O	-13.75300	21.46700	86.72800
C	-16.35700	22.53600	84.95600
C	-17.05200	21.35800	85.57800
C	-18.55500	21.55900	85.49900
C	-18.99800	21.76500	84.05200
N	-20.46100	21.98500	83.92500

H	-20.75700	22.12300	82.95900
H	-20.76700	22.75900	84.51500
H	-20.98400	21.22700	84.36300
N	-14.11100	23.68300	86.71500
H	-14.48500	24.48100	86.20100
C	-13.50600	23.90000	88.01900
C	-13.95900	22.85500	89.03500
O	-15.08600	22.36200	88.97400
C	-13.85600	25.29500	88.56800
O	-15.26500	25.50400	88.44900
H	-15.48100	26.36500	88.78800
C	-13.10900	26.38400	87.80600
N	-13.06700	22.50200	89.98000
C	-13.28500	21.52200	91.05500
C	-14.44500	21.90100	91.98300
O	-15.21800	21.04100	92.42000
C	-11.94500	21.51900	91.79200
C	-10.96300	21.88100	90.72100
C	-11.67400	22.98700	90.00000
N	-14.54400	23.19200	92.28900
H	-13.85900	23.84500	91.90800
C	-15.60100	23.69800	93.15100
C	-16.92800	23.25000	92.55000
O	-17.82100	22.78300	93.26000
C	-15.54400	25.23000	93.22900
C	-14.24000	25.81300	93.80500
C	-12.99400	25.44100	92.99800
O	-13.08300	25.39800	91.75300
O	-11.92000	25.20700	93.60200
N	-17.04500	23.37800	91.23100
H	-16.26800	23.76600	90.69700
C	-18.25800	22.97600	90.53400
C	-18.40500	21.46200	90.52400
O	-19.35300	20.92100	91.08300
C	-18.24000	23.48600	89.09600
C	-18.25100	24.99300	88.96700
C	-18.37700	25.44600	87.52600
O	-19.37000	25.06500	86.87300
O	-17.48800	26.18000	87.04400
N	-17.45600	20.78600	89.88700
H	-16.68900	21.30300	89.45600
C	-17.46900	19.33000	89.78000
C	-17.89000	18.57400	91.03600

O	-18.71000	17.65900	90.96000
C	-16.09500	18.81700	89.34200
C	-15.68900	19.01100	87.88300
C	-14.28600	18.46200	87.67300
C	-16.67700	18.29600	86.97800
N	-17.33200	18.94400	92.18400
H	-16.66900	19.71900	92.19800
C	-17.66100	18.24900	93.42500
C	-19.12300	18.37700	93.84400
O	-19.58500	17.66700	94.74100
C	-16.75800	18.72800	94.56000
C	-16.92200	20.18400	94.93200
C	-16.22700	20.51000	96.23900
O	-15.03100	20.26200	96.40000
N	-16.97800	21.06600	97.18600
H	-16.51000	21.28500	98.06600
H	-17.96800	21.27100	97.05300
N	-19.84800	19.28400	93.19900
H	-19.40400	19.85600	92.48100
C	-21.26200	19.48200	93.49200
C	-22.07600	18.68500	92.47300
O	-23.20000	19.05100	92.12900
C	-21.60700	20.96300	93.40700
N	-21.49400	17.58800	91.99800
H	-20.56700	17.33500	92.34100
C	-22.13300	16.73400	91.00400
C	-21.93800	15.24600	91.30000
O	-20.92900	14.64800	90.91800
C	-21.56700	17.04900	89.62400
C	-22.07300	16.13900	88.53300
C	-21.22600	16.22600	87.28900
O	-21.09400	17.34200	86.73700
O	-20.69000	15.17600	86.87100
N	-22.92300	14.65400	91.96600
H	-23.74000	15.20400	92.23200
C	-22.87300	13.24400	92.32900
C	-23.33500	12.32900	91.19000
O	-24.32000	11.59900	91.32700
C	-23.74100	12.98300	93.57000
C	-23.42400	13.83900	94.80000
C	-23.87200	15.28900	94.62800
N	-23.92700	16.01100	95.89900
H	-24.83300	16.36800	96.20300

C	-22.87800	16.23400	96.68500
N	-21.67500	15.79400	96.33900
H	-20.87000	15.96500	96.94200
H	-21.55400	15.28400	95.46400
N	-23.03500	16.89800	97.82300
H	-22.23000	17.06900	98.42600
H	-23.96000	17.23600	98.08900
N	-22.62800	12.37100	90.06600
H	-21.83300	13.00700	89.99700
C	-22.96800	11.52300	88.92700
C	-21.68600	10.96300	88.32300
O	-21.68200	10.41400	87.22000
C	-23.74100	12.31900	87.87400
C	-25.03900	12.89200	88.41400
O	-25.03000	13.73700	89.31100
N	-26.16400	12.43200	87.86900
H	-26.17100	11.73300	87.12700
H	-27.03600	12.81700	88.23200
N	-20.59600	11.11000	89.06600
H	-20.67000	11.57600	89.97000
C	-19.30000	10.62400	88.62500
C	-18.96300	9.35600	89.40300
O	-19.47700	9.15400	90.50400
C	-18.23400	11.68900	88.88000
C	-16.96100	11.45300	88.12900
C	-16.94500	11.50500	86.73800
C	-15.78200	11.16400	88.80500
C	-15.77500	11.27300	86.03000
C	-14.60300	10.93000	88.10600
C	-14.60000	10.98500	86.71500
N	-18.10500	8.51100	88.83000
H	-17.72200	8.74600	87.91400
C	-17.69100	7.25700	89.46700
C	-16.94100	7.52200	90.78900
O	-15.94300	8.25100	90.81400
C	-16.80300	6.46800	88.49900
C	-16.36600	5.13500	89.02200
N	-15.29600	4.44500	88.49200
H	-14.71800	4.76100	87.71300
C	-16.85000	4.36700	90.02600
C	-15.13700	3.31100	89.15100
N	-16.06600	3.23900	90.08600
H	-16.18300	2.47100	90.74600

N	-17.41600	6.92100	91.88000
H	-18.22200	6.30100	91.79900
C	-16.80200	7.13400	93.19200
C	-16.01000	5.97300	93.76700
O	-16.24200	4.81400	93.42900
C	-17.85000	7.50400	94.23800
O	-18.80900	6.44600	94.33400
H	-18.37600	5.63400	94.57000
C	-18.54400	8.80500	93.86000
N	-15.09100	6.30600	94.66800
H	-14.98000	7.29000	94.91300
C	-14.23800	5.32300	95.31800
C	-13.84200	5.78900	96.71300
O	-13.86500	6.98100	97.00500
C	-12.95500	5.10400	94.50800
C	-13.27900	4.43000	93.19900
C	-12.27900	6.43100	94.25000
N	-13.48300	4.84800	97.59700
C	-13.07200	5.17500	98.96900
C	-12.03100	6.27500	98.88000
O	-11.11900	6.19500	98.05900
C	-12.47900	3.86600	99.46700
C	-13.32800	2.84500	98.77000
C	-13.42000	3.39600	97.36100
N	-12.14900	7.28800	99.72800
H	-12.89000	7.27700	100.42900
C	-11.23000	8.41700	99.66700
C	-10.78400	8.89900	101.04500
O	-11.60600	9.27100	101.87300
C	-11.93100	9.55300	98.91100
C	-11.08300	10.73400	98.49500
C	-11.68500	11.89200	98.01800
C	-9.68800	10.69300	98.55200
C	-10.93100	12.98300	97.60600
C	-8.91900	11.78300	98.13900
C	-9.55200	12.92700	97.66700
O	-8.81700	14.01900	97.25500
H	-7.86900	13.98000	97.29700
N	-9.48000	8.89800	101.28600
H	-8.84000	8.56800	100.56300
C	-8.94000	9.35700	102.56000
C	-8.31700	10.74800	102.37700
O	-7.45300	10.94400	101.52000

C	-7.87600	8.37400	103.06900
C	-7.31800	8.71800	104.44600
S	-5.81800	7.80100	104.88300
C	-6.46800	6.10600	104.93600
N	-8.76600	11.71500	103.17000
H	-9.50100	11.50300	103.84500
C	-8.23300	13.07400	103.10000
C	-7.73500	13.47300	104.48400
O	-8.44100	13.27700	105.47200
C	-9.31000	14.07500	102.64800
C	-8.70500	15.46200	102.49700
C	-9.91900	13.60900	101.33800
N	-6.52700	14.02700	104.56400
H	-5.97500	14.18200	103.72000
C	-6.00200	14.40900	105.86200
C	-4.99200	15.53700	105.86400
O	-4.35300	15.81300	104.84700
N	-4.83900	16.18900	107.01400
H	-5.39300	15.91200	107.82500
C	-3.89400	17.29100	107.13500
C	-3.00900	17.15800	108.37200
O	-3.24000	16.31100	109.22900
C	-4.61300	18.67100	107.19300
C	-5.32600	18.84600	108.53600
C	-5.62400	18.78300	106.06000
C	-5.81400	20.26100	108.78000
N	-1.99100	18.00600	108.44600
H	-1.85500	18.67700	107.68900
C	-1.06400	18.01600	109.56100
C	-1.42000	19.17000	110.48200
O	-2.11300	20.10400	110.07400
C	0.35800	18.18600	109.05000
C	0.79600	17.04000	108.16900
O	1.85000	17.10200	107.53300
N	-0.00400	15.98000	108.13500
H	-0.87600	15.92900	108.66100
H	0.29200	15.20600	107.54000
N	-0.92900	19.11000	111.71700
H	-0.33100	18.32300	111.97000
C	-1.21500	20.13200	112.72800
C	-0.79800	21.54300	112.32700
O	-1.59200	22.47900	112.39200
C	-0.53300	19.76100	114.04100

C	-1.10100	20.47600	115.24800
C	-2.45700	19.90700	115.65500
C	-3.01300	20.67500	116.84700
N	-1.96000	20.90100	117.88700
H	-2.33200	21.41500	118.68500
H	-1.13900	21.36200	117.49500
H	-1.52500	20.02500	118.17600
N	0.45500	21.69300	111.92500
H	1.07300	20.88200	111.90600
C	0.96900	22.98700	111.51100
C	1.47200	22.88700	110.07700
O	2.66900	22.72400	109.84400
C	2.12100	23.40400	112.41900
C	1.76600	23.53500	113.88900
C	2.99300	23.45100	114.77600
O	4.00900	24.08400	114.50400
N	2.90600	22.66600	115.84200
H	2.06200	22.14000	116.06800
H	3.73100	22.60900	116.43900
N	0.55700	22.97200	109.11800
H	-0.42300	23.09500	109.37200
C	0.92600	22.89300	107.71200
C	1.89300	24.00400	107.31700
O	2.80200	23.79700	106.50700
C	-0.32000	22.98200	106.84200
C	-1.16800	21.74200	106.85200
C	-0.44700	20.55400	106.26300
O	0.66500	20.74100	105.71900
O	-0.99300	19.43400	106.33700
N	1.69100	25.18500	107.89600
H	0.92800	25.28700	108.56500
C	2.53200	26.33500	107.59800
C	3.54500	26.59600	108.71300
O	4.03600	27.70800	108.87700
C	1.65200	27.56600	107.38000
C	2.26800	28.58900	106.47500
C	2.75300	29.79100	106.98200
C	2.38600	28.34000	105.11100
C	3.35100	30.73500	106.13900
C	2.98000	29.27300	104.26100
C	3.46500	30.47400	104.77700
N	3.85600	25.55200	109.47200
H	3.42200	24.64800	109.28500

C	4.80300	25.67600	110.56200
C	6.17900	26.17100	110.15900
O	6.48500	27.34700	110.32200
N	7.01600	25.28600	109.62700
H	6.71100	24.32200	109.48900
C	8.36400	25.67800	109.23900
C	8.70600	25.53300	107.75200
O	8.97500	26.52500	107.06300
C	9.38500	24.88300	110.05700
C	10.80500	25.21300	109.70600
C	11.44600	26.39800	109.92300
C	11.74200	24.36900	109.01900
N	12.72300	26.35000	109.41100
H	13.40300	27.10900	109.44400
C	12.93200	25.11800	108.85000
C	11.69200	23.05600	108.52700
C	14.06400	24.59600	108.20800
C	12.82000	22.53800	107.88900
C	13.98900	23.31100	107.73600
N	8.69900	24.29300	107.26800
H	8.43400	23.52700	107.88700
C	9.05600	23.98700	105.88400
C	8.65300	24.99300	104.81700
O	9.51400	25.65800	104.23900
C	8.51900	22.61300	105.48000
C	8.98600	22.17900	104.08900
C	10.47200	21.90300	104.12700
C	8.23500	20.95100	103.64000
N	7.35400	25.09300	104.54800
H	6.69100	24.52500	105.07500
C	6.85600	25.99800	103.51600
C	7.33800	27.44800	103.63900
O	7.95300	27.97600	102.71500
C	5.31400	25.98300	103.45400
C	4.81500	24.54600	103.30100
C	4.83100	26.82800	102.28200
C	3.30300	24.41900	103.23100
N	7.07100	28.11100	104.77800
C	7.50900	29.49900	104.94300
C	8.98400	29.65500	104.61200
O	9.37500	30.54200	103.86200
C	7.23200	29.76900	106.41500
C	6.05300	28.90500	106.69100

C	6.43300	27.62200	106.01000
N	9.79100	28.77100	105.18600
H	9.38400	28.06000	105.79300
C	11.23300	28.77400	104.98500
C	11.60400	28.68900	103.50400
O	12.38300	29.50400	103.01200
C	11.85100	27.61100	105.77500
C	13.36400	27.48100	105.68200
S	13.90900	26.56500	104.22900
C	13.51200	24.89400	104.75100
N	11.04000	27.71200	102.79700
H	10.39900	27.06900	103.26100
C	11.31700	27.53800	101.37300
C	10.84200	28.71400	100.52200
O	11.34300	28.92400	99.41800
C	10.66400	26.26000	100.84200
C	11.23900	24.89700	101.21600
C	10.46100	23.82100	100.49400
C	12.69700	24.82200	100.82900
N	9.86500	29.46700	101.02100
H	9.47000	29.23400	101.93200
C	9.34800	30.62000	100.29100
C	10.03900	31.89300	100.74100
O	9.83500	32.95900	100.16000
C	7.84600	30.77000	100.50700
C	7.00200	29.82200	99.69300
S	5.26600	30.21600	99.90900
C	5.17100	31.79100	99.06100
N	10.84800	31.77400	101.78700
H	10.96100	30.86000	102.22500
C	11.57700	32.91000	102.32500
C	10.60700	33.89400	102.98200
O	10.82600	35.10300	102.96600
C	12.33900	33.59700	101.19600
O	12.82200	32.62900	100.28000
H	13.29700	33.05700	99.57700
N	9.53700	33.36200	103.56500
H	9.42300	32.34900	103.55100
C	8.52000	34.17500	104.22400
C	9.13700	35.16900	105.21000
O	10.06400	34.82900	105.94500
C	7.53200	33.26900	104.96000
C	6.12600	33.81200	104.98900

C	5.39000	33.95800	103.81100
C	5.53400	34.20100	106.18900
C	4.09900	34.47800	103.82600
C	4.24200	34.72500	106.21900
C	3.53200	34.86100	105.03500
O	2.26100	35.38900	105.06900
H	1.87300	35.65100	105.89600
N	8.63300	36.41700	105.22700
C	9.10600	37.49400	106.10800
C	8.79400	37.29000	107.58800
O	7.89900	37.93400	108.13900
C	8.40800	38.73400	105.55000
C	8.24800	38.40500	104.10800
C	7.77500	36.97200	104.16700
N	9.53800	36.39300	108.22500
H	10.25700	35.88700	107.70900
C	9.35300	36.11400	109.64000
C	10.70600	36.06100	110.34300
O	11.07200	35.05200	110.95100
C	8.60500	34.79100	109.83200
C	7.18400	34.72900	109.26200
C	6.57300	33.36700	109.56900
C	6.33500	35.84700	109.85900
N	11.44400	37.16400	110.25100
H	11.07600	37.96100	109.73200
C	12.76200	37.27200	110.86800
C	12.62400	37.57800	112.35500
O	13.38400	37.06800	113.17600
C	13.56800	38.38900	110.19800
O	13.64800	38.19800	108.79600
H	14.14800	38.89100	108.38000
N	11.63900	38.40900	112.68500
H	11.03900	38.77400	111.94600
C	11.38300	38.81900	114.06100
C	10.85300	37.72400	114.98100
O	11.23600	37.65400	116.14900
C	10.41000	40.00000	114.07300
C	10.95900	41.23000	113.39300
C	12.34300	41.57800	113.89700
O	12.49000	41.80500	115.11800
O	13.28300	41.61700	113.07500
N	9.97200	36.87500	114.46200
H	9.69300	36.96600	113.48500

C	9.40500	35.81700	115.28100
C	8.28500	36.37000	116.14400
O	7.87300	35.75800	117.13300
N	7.79300	37.54100	115.75000
H	8.18300	37.97600	114.91400
C	6.72100	38.23200	116.45800
C	5.87100	38.99100	115.44200
O	6.23000	39.06900	114.26600
C	7.32300	39.20400	117.47200
C	8.31500	40.18200	116.85700
C	9.17000	40.88000	117.89400
O	10.02000	41.70800	117.56000
N	8.95400	40.54700	119.16200
H	9.53000	41.01700	119.86000
H	8.25100	39.86200	119.43800
N	4.75400	39.55800	115.88900
H	4.50500	39.48300	116.87500
C	3.88600	40.28600	114.97300
C	2.91000	41.23500	115.67100
O	2.79800	41.24500	116.89800
C	3.11300	39.28300	114.11200
C	2.82200	39.67100	112.66200
C	4.12800	39.97300	111.93500
C	2.07400	38.53100	111.97900
N	2.20600	42.03000	114.87100
H	2.34700	41.96400	113.86300
C	1.23900	42.99400	115.38500
C	0.06300	43.10100	114.42200
O	0.22000	42.89700	113.21900
C	1.88400	44.36900	115.50600
C	1.96400	45.08400	114.16900
O	2.47000	44.47500	113.20100
O	1.51900	46.25000	114.08800
N	-1.10500	43.44900	114.95500
H	-1.15300	43.62700	115.95800
C	-2.32100	43.58600	114.15700
C	-2.13700	44.32800	112.83600
O	-2.89700	44.11900	111.88800
C	-3.40500	44.27500	114.98700
C	-3.96900	43.39300	116.08100
C	-4.79100	42.24700	115.52600
O	-5.09600	41.28700	116.23300
N	-5.16600	42.34800	114.25400

H	-5.71900	41.57700	113.88000
H	-4.91300	43.14400	113.66800
N	-1.13100	45.19400	112.77400
H	-0.53500	45.33400	113.59000
C	-0.86900	45.94600	111.55500
C	-0.16800	45.06900	110.52800
O	-0.76100	44.68800	109.51500
C	-0.00800	47.17300	111.85800
C	-0.70500	48.20600	112.72000
C	-0.66900	49.57300	112.06300
C	-1.52700	50.56700	112.82400
N	-1.55000	51.89100	112.14600
H	-2.12700	52.55900	112.65700
H	-1.84600	51.80900	111.17300
H	-0.60800	52.25000	111.99300
N	1.09600	44.75800	110.79900
H	1.52000	45.11700	111.65400
C	1.89500	43.92000	109.91300
C	1.06400	42.72400	109.47400
O	1.09100	42.32900	108.30900
C	3.15400	43.40000	110.62800
O	3.92000	44.51000	111.11200
H	4.69700	44.18900	111.55400
C	4.00400	42.57100	109.67400
N	0.32700	42.15500	110.42400
H	0.36100	42.53700	111.36900
C	-0.52700	41.00500	110.16000
C	-1.41000	41.30300	108.95900
O	-1.42500	40.55300	107.97800
C	-1.38700	40.70700	111.37700
N	-2.14400	42.40800	109.04300
H	-2.08500	42.98300	109.88300
C	-3.02900	42.81500	107.96400
C	-2.24300	43.15100	106.70100
O	-2.81000	43.19900	105.60800
C	-3.86100	44.02400	108.39200
C	-4.85200	43.72500	109.50100
S	-5.99700	45.08700	109.77900
C	-5.20900	45.90800	111.17300
N	-0.93800	43.37200	106.85600
H	-0.53200	43.30500	107.78900
C	-0.07200	43.70800	105.72700
C	0.54500	42.45900	105.09300

O	0.61500	42.34000	103.86800
C	1.03700	44.66000	106.18500
O	1.78500	45.14700	105.08200
H	2.47300	45.73700	105.36600
N	0.99200	41.53100	105.93000
H	0.91400	41.68700	106.93500
C	1.59100	40.29600	105.44500
C	0.53900	39.44000	104.75800
O	0.79700	38.84200	103.71700
C	2.20700	39.51400	106.60400
C	3.70900	39.27200	106.48800
C	4.21200	38.54000	107.72100
C	3.99100	38.47200	105.23400
N	-0.65200	39.38700	105.34500
H	-0.80800	39.90700	106.20900
C	-1.74000	38.60000	104.77800
C	-2.15500	39.14700	103.41400
O	-2.44800	38.38000	102.49500
C	-2.94300	38.59600	105.72600
C	-4.11500	37.71300	105.28700
C	-3.65300	36.27000	105.15300
C	-5.24100	37.82000	106.29800
N	-2.18400	40.47200	103.28600
H	-1.94300	41.05700	104.08600
C	-2.55300	41.10400	102.02400
C	-1.53300	40.74100	100.95800
O	-1.89500	40.32400	99.86000
C	-2.59800	42.62600	102.16200
C	-3.00600	43.32700	100.88600
C	-2.48100	44.48400	100.38000
C	-4.03200	42.91800	99.96800
N	-3.11300	44.81900	99.20600
H	-2.90400	45.63700	98.63300
C	-4.06900	43.87600	98.93000
C	-4.92300	41.83500	99.92300
C	-4.96200	43.78500	97.85500
C	-5.81200	41.74500	98.85600
C	-5.82300	42.71700	97.83500
N	-0.25600	40.91500	101.28400
H	-0.02200	41.28400	102.20600
C	0.81700	40.59100	100.35400
C	0.81300	39.08900	100.08600
O	1.27500	38.63400	99.03900

C	2.16000	41.03200	100.93400
C	2.22700	42.52800	101.16900
C	3.47100	42.94900	101.93400
C	3.44000	44.45100	102.21000
N	4.60400	44.92800	103.00600
H	4.58300	45.93100	103.19000
H	5.48200	44.66000	102.56100
H	4.68800	44.40200	103.87600
N	0.28200	38.32400	101.03700
H	-0.07200	38.76300	101.88700
C	0.19200	36.87300	100.89700
C	-1.03700	36.52100	100.06900
O	-1.48900	35.37600	100.06800
C	0.08500	36.20000	102.26900
O	1.31400	36.25700	102.96400
H	1.24800	35.84000	103.81500
N	-1.57200	37.51900	99.37100
H	-1.14200	38.44200	99.42500
C	-2.75100	37.34000	98.53200
C	-2.56400	36.22600	97.49900
O	-3.49600	35.46400	97.22400
C	-3.08600	38.64900	97.81700
C	-4.31400	38.57700	96.94200
C	-5.59300	38.57700	97.49800
C	-4.19600	38.50300	95.55400
C	-6.72300	38.50700	96.69300
C	-5.31700	38.43100	94.74100
C	-6.57600	38.43400	95.31500
O	-7.68900	38.37200	94.50900
H	-7.58800	38.32200	93.56600
N	-1.36100	36.12000	96.90400
C	-1.16000	35.05900	95.91400
C	-1.16100	33.65700	96.52500
O	-1.00100	32.66900	95.80900
C	0.18300	35.42900	95.28300
C	0.90300	36.10800	96.39800
C	-0.17000	36.98500	96.99100
N	-1.35100	33.57700	97.84300
H	-1.48700	34.43700	98.37400
C	-1.37100	32.29600	98.55400
C	-2.70500	31.99100	99.24000
O	-3.21800	30.87300	99.15400
C	-0.26200	32.25000	99.61600

C	1.21500	32.26000	99.21000
C	2.08200	32.10000	100.45900
C	1.49200	31.13200	98.23000
N	-3.25500	32.98400	99.92900
H	-2.78900	33.89100	99.95400
C	-4.51000	32.80900	100.65100
C	-5.69300	33.51900	100.00600
O	-6.81800	33.43100	100.50200
C	-4.37600	33.30600	102.10200
C	-3.42800	32.40200	102.87400
C	-3.86400	34.73600	102.11000
N	-5.43400	34.21600	98.90400
H	-4.47700	34.24200	98.55200
C	-6.47300	34.94700	98.17900
C	-7.52700	35.55900	99.09700
O	-8.64700	35.05600	99.20700
C	-7.15200	34.02800	97.15900
S	-6.05800	33.48500	95.84200
N	-7.16200	36.65000	99.75500
H	-6.22100	37.02300	99.62800
C	-8.08100	37.32100	100.65300
C	-8.17600	38.79400	100.28200
O	-7.17000	39.50400	100.24800
C	-7.62000	37.17800	102.11600
C	-7.58700	35.69500	102.50000
C	-8.55800	37.94200	103.03800
C	-7.11100	35.42800	103.91700
N	-9.39400	39.23900	99.99000
H	-10.17800	38.58800	100.02700
C	-9.64800	40.62600	99.61900
C	-9.22500	41.55100	100.74900
O	-9.44200	41.25000	101.92100
C	-11.12200	40.81800	99.31500
N	-8.62700	42.68100	100.39300
H	-8.48800	42.88500	99.40300
C	-8.16600	43.63300	101.39100
C	-9.29200	44.06900	102.32800
O	-9.08700	44.19300	103.53700
C	-7.54300	44.85100	100.70500
C	-6.61600	45.66000	101.60400
C	-5.78200	46.64200	100.79100
C	-4.75300	47.34400	101.65900
N	-3.83700	46.37900	102.33100

H	-3.14600	46.85100	102.91400
H	-3.39000	45.76000	101.65400
H	-4.35900	45.68400	102.86500
N	-10.48000	44.29400	101.77500
H	-10.59500	44.17600	100.76800
C	-11.62400	44.70800	102.58400
C	-12.02700	43.58900	103.54600
O	-12.88700	43.77500	104.40900
C	-12.81600	45.07400	101.69200
C	-13.36400	43.91900	100.86000
C	-12.67800	43.77500	99.51100
O	-11.42800	43.76800	99.46500
O	-13.39700	43.66000	98.49300
N	-11.40200	42.42600	103.38700
H	-10.70700	42.33400	102.64600
C	-11.68200	41.27900	104.24300
C	-10.54400	41.07900	105.24400
O	-10.76200	40.58300	106.35200
C	-11.84700	40.00600	103.40000
C	-13.01000	39.90600	102.40700
C	-12.93000	38.58200	101.66000
C	-14.33300	40.01500	103.14400
N	-9.33500	41.47100	104.84000
H	-9.24200	41.88300	103.91200
C	-8.13500	41.33700	105.66900
C	-8.40000	41.48700	107.17000
O	-8.12300	40.57300	107.94800
C	-7.03900	42.36800	105.25200
C	-6.56900	42.10100	103.81900
C	-5.85400	42.28900	106.20800
C	-5.71700	40.85700	103.65700
N	-8.95100	42.63700	107.59300
C	-9.24000	42.88100	109.01200
C	-10.02900	41.76400	109.69600
O	-9.50700	41.07400	110.57200
C	-10.01500	44.19600	108.98100
C	-9.42500	44.89700	107.79700
C	-9.37500	43.78900	106.77600
N	-11.28600	41.60100	109.29100
H	-11.65000	42.21100	108.55900
C	-12.16100	40.58100	109.85700
C	-11.41600	39.27500	110.08100
O	-11.55400	38.64400	111.13000

C	-13.34700	40.33600	108.92900
C	-14.16300	41.57600	108.64100
C	-15.41000	41.27300	107.83500
O	-15.28100	40.68200	106.74100
O	-16.52000	41.62600	108.29500
N	-10.62700	38.87600	109.08800
H	-10.56600	39.44500	108.24400
C	-9.84800	37.64800	109.17400
C	-8.73800	37.79800	110.21500
O	-8.61100	36.97600	111.12500
C	-9.25000	37.31400	107.81600
N	-7.94100	38.85400	110.08700
H	-8.09600	39.50900	109.32100
C	-6.84900	39.09200	111.02200
C	-7.34300	39.09200	112.46200
O	-6.68200	38.57100	113.35700
C	-6.17500	40.44700	110.76900
O	-5.94000	40.61400	109.36800
H	-6.76900	40.57000	108.90700
C	-4.84600	40.51700	111.50800
N	-8.51400	39.67900	112.67900
H	-9.02800	40.07600	111.89300
C	-9.07700	39.76600	114.01500
C	-9.48500	38.42500	114.59700
O	-9.01400	38.03900	115.66400
C	-10.28000	40.71200	114.02200
C	-10.83600	40.96200	115.41900
C	-9.74500	41.32400	116.42400
O	-9.07500	42.36800	116.24200
O	-9.55400	40.55600	117.39300
N	-10.36900	37.72400	113.89900
H	-10.72400	38.10500	113.02200
C	-10.84700	36.42400	114.35200
C	-9.72800	35.51200	114.86000
O	-9.94800	34.72000	115.77600
C	-11.59400	35.72500	113.21400
C	-12.13500	34.35200	113.56200
C	-13.08600	34.43000	114.73400
C	-13.77300	33.10300	114.97300
N	-14.66000	33.17200	116.16100
H	-15.12300	32.27800	116.32200
H	-15.33200	33.93600	116.08600
H	-14.15700	33.49000	116.98900

N	-8.53500	35.63100	114.27100
H	-8.42000	36.32100	113.52900
C	-7.38200	34.80400	114.65300
C	-6.41500	35.44300	115.64700
O	-6.22900	34.94000	116.75300
C	-6.59100	34.38100	113.40400
C	-7.16900	33.18600	112.67300
C	-8.42200	33.25000	112.06300
C	-6.47100	31.97900	112.61000
C	-8.96500	32.14100	111.41100
C	-7.00900	30.86400	111.96100
C	-8.25400	30.95500	111.36800
O	-8.80000	29.85900	110.74900
H	-9.65600	29.92200	110.34100
N	-5.79600	36.54800	115.24000
H	-6.00500	36.91700	114.31200
C	-4.82600	37.25200	116.07700
C	-5.44600	38.14500	117.15500
O	-4.75800	38.98400	117.74100
C	-3.90100	38.10200	115.19700
C	-3.15700	37.39800	114.06000
C	-2.26700	38.39400	113.34700
C	-2.32700	36.25700	114.61300
N	-6.73500	37.96500	117.42000
H	-7.26300	37.25300	116.91600
C	-7.39500	38.77900	118.42600
C	-7.33900	38.20100	119.82900
O	-7.77400	38.84500	120.78400
N	-6.80500	36.98800	119.95100
H	-6.46000	36.50800	119.12000
C	-6.70400	36.33200	121.24700
C	-6.03100	37.18300	122.30600
O	-6.71000	37.87000	123.06900
N	-4.70100	37.13000	122.36900
H	-4.19500	36.52100	121.72600
C	-3.95300	37.92600	123.33900
C	-3.18900	39.01600	122.60400
O	-3.32600	39.17500	121.39000
C	-2.92800	37.08600	124.13700
O	-1.87200	36.66300	123.26400
H	-1.24300	36.14700	123.75400
C	-3.60200	35.87300	124.77100
N	-2.37600	39.75900	123.34500

H	-2.29600	39.56700	124.34400
C	-1.59700	40.84100	122.76400
C	-0.17100	40.38800	122.46300
O	0.59600	41.09900	121.80600
C	-1.58600	42.03000	123.72200
C	-2.98300	42.44000	124.15200
O	-3.80500	42.77900	123.27300
O	-3.26200	42.41900	125.36900
N	0.16600	39.19300	122.94200
H	-0.53100	38.66500	123.46700
C	1.49000	38.60300	122.75000
C	1.93400	38.65100	121.28500
O	1.34100	37.98800	120.43200
C	1.46800	37.14700	123.22000
C	2.85200	36.53600	123.29900
O	3.71600	36.89600	122.47300
O	3.07100	35.68100	124.18300
N	2.97900	39.42300	120.99400
H	3.43800	39.95100	121.73600
C	3.47600	39.52300	119.62500
C	3.92100	38.15600	119.10200
O	3.86900	37.90000	117.89600
C	4.66400	40.51200	119.51500
O	5.65900	40.18500	120.49300
H	6.38700	40.79100	120.42600
C	4.19300	41.93700	119.72900
N	4.35500	37.28300	120.01000
H	4.37700	37.55900	120.99200
C	4.80000	35.94100	119.63900
C	3.59600	35.02700	119.41600
O	3.52900	34.31300	118.41700
C	5.70500	35.32400	120.72300
C	6.17300	33.95100	120.28300
C	6.89400	36.23000	120.98500
N	2.64700	35.04600	120.34800
H	2.75800	35.63900	121.17000
C	1.45000	34.22700	120.20500
C	0.78900	34.57700	118.88100
O	0.11100	33.74900	118.28000
C	0.45000	34.51000	121.32600
C	0.77300	33.91700	122.68300
C	-0.38100	34.21200	123.63200
C	-0.16100	33.65400	125.02600

N	-1.31400	33.97400	125.92300
H	-1.16600	33.59900	126.86000
H	-2.19800	33.65500	125.52600
H	-1.50500	34.97600	125.94500
N	0.98400	35.81500	118.43800
H	1.56000	36.45300	118.98700
C	0.39700	36.28600	117.18900
C	0.99000	35.59200	115.96900
O	0.26100	34.99100	115.17900
C	0.56800	37.80200	117.06100
C	-0.24800	38.60100	118.07100
C	-0.05700	40.10200	117.89500
C	-0.89600	40.88500	118.89700
N	-2.34900	40.57500	118.77300
H	-2.91100	41.09900	119.44400
H	-2.52100	39.57300	118.85000
H	-2.67900	40.72300	117.81900
N	2.30900	35.67600	115.81000
H	2.86400	36.19600	116.48900
C	2.97300	35.03500	114.67900
C	2.38000	33.64600	114.47200
O	1.95100	33.29200	113.37600
C	4.48100	34.91000	114.94100
C	5.22600	34.03800	113.92600
C	6.68900	33.82000	114.31900
C	7.37200	32.76800	113.43600
N	8.78400	32.48400	113.84400
H	9.23800	31.78400	113.25700
H	8.83100	32.21900	114.82800
H	9.33300	33.34300	113.87600
N	2.34600	32.88000	115.55500
H	2.69500	33.26400	116.43300
C	1.83400	31.51700	115.54800
C	0.39600	31.38500	115.06000
O	0.09100	30.51000	114.25100
C	1.96700	30.92800	116.94900
C	3.34900	31.14800	117.53300
O	4.33400	30.73300	116.88700
O	3.45200	31.73900	118.62900
N	-0.49100	32.23900	115.55400
H	-0.19700	32.93800	116.23600
C	-1.88200	32.18300	115.12700
C	-1.97400	32.56800	113.66400

O	-2.83700	32.08000	112.94200
C	-2.74700	33.11900	115.97200
C	-3.23100	32.54400	117.30400
C	-3.73000	33.66000	118.19500
C	-4.32700	31.52500	117.04600
N	-1.07500	33.44400	113.23100
H	-0.38600	33.81600	113.88500
C	-1.05100	33.88500	111.84400
C	-0.73700	32.68600	110.94500
O	-1.35000	32.50100	109.89000
C	0.00700	34.97600	111.66500
C	0.03000	35.58000	110.28900
C	-1.10900	36.17400	109.75500
C	1.19600	35.56500	109.52900
C	-1.09000	36.74500	108.48500
C	1.23000	36.13400	108.25600
C	0.08400	36.72500	107.73300
N	0.22400	31.87300	111.37700
H	0.70000	32.08900	112.25300
C	0.61300	30.68500	110.63400
C	-0.56900	29.72600	110.59400
O	-0.74700	28.98300	109.62900
C	1.81600	30.01800	111.29800
C	3.09300	30.86100	111.35800
C	4.18900	30.07100	112.06100
C	3.53000	31.25300	109.94900
N	-1.37400	29.73800	111.65000
H	-1.16300	30.34800	112.44000
C	-2.55300	28.89000	111.69100
C	-3.53400	29.46600	110.67700
O	-4.14000	28.74000	109.88400
C	-3.18600	28.91800	113.08100
C	-2.31400	28.27600	114.12900
O	-2.02400	27.06900	114.00500
O	-1.91600	28.97600	115.08000
N	-3.67900	30.78500	110.71900
H	-3.15000	31.31700	111.41100
C	-4.56500	31.49800	109.81400
C	-4.35700	30.93400	108.41300
O	-5.27700	30.38100	107.80600
C	-4.22700	32.99400	109.84700
C	-5.09100	34.01400	109.10100
C	-5.00500	33.82000	107.59400

C	-6.51100	33.87300	109.56900
N	-3.12800	31.06100	107.92100
H	-2.41300	31.50900	108.49400
C	-2.76500	30.58400	106.59400
C	-2.91400	29.07800	106.45200
O	-3.44300	28.58900	105.45400
C	-1.31700	30.96900	106.25900
C	-1.19300	32.49000	106.20900
C	-0.89800	30.35200	104.93300
C	0.20100	32.96900	105.89500
N	-2.44200	28.34500	107.45100
H	-2.01600	28.80900	108.25300
C	-2.51900	26.89300	107.42700
C	-3.95700	26.37900	107.27500
O	-4.18400	25.25200	106.81900
C	-1.89000	26.32900	108.69100
N	-4.93000	27.20000	107.65700
H	-4.69800	28.12000	108.03100
C	-6.32400	26.79700	107.54600
C	-6.88600	27.11400	106.17400
O	-7.75200	26.40700	105.66400
C	-7.15600	27.49300	108.61600
C	-6.91700	26.92100	109.99400
O	-7.32500	25.76800	110.25000
O	-6.31200	27.62600	110.82000
N	-6.38200	28.18300	105.57600
H	-5.66100	28.72700	106.05100
C	-6.83300	28.59800	104.26000
C	-6.33200	27.68000	103.15000
O	-7.10600	27.26200	102.29500
C	-6.38600	30.03600	103.96900
C	-6.65100	30.38600	102.50900
C	-7.13500	30.98900	104.88500
N	-5.04300	27.35700	103.16900
H	-4.44600	27.71400	103.91500
C	-4.47100	26.50000	102.13800
C	-4.78600	25.02700	102.28300
O	-5.04000	24.34600	101.29200
C	-2.95400	26.65600	102.08400
C	-2.49300	28.04900	101.75300
S	-0.73400	28.07800	101.42000
C	-0.08000	27.71200	103.02500
N	-4.77900	24.52400	103.50900

H	-4.60300	25.12600	104.31300
C	-5.02500	23.10400	103.69300
C	-6.23500	22.72900	104.54300
O	-7.03900	21.87500	104.14800
C	-3.76500	22.44200	104.26700
C	-2.48100	22.89300	103.60400
C	-1.79100	24.00800	104.07500
C	-1.95300	22.19300	102.52200
C	-0.59800	24.41400	103.48400
C	-0.75800	22.59700	101.92300
C	-0.08200	23.70800	102.40900
N	-6.36200	23.36500	105.70500
H	-5.67700	24.07400	105.96900
C	-7.46500	23.06200	106.60400
C	-8.86700	23.03700	106.00900
O	-9.43600	21.97200	105.75100
N	-9.42500	24.22000	105.79400
H	-8.89400	25.06400	106.00800
C	-10.76800	24.34900	105.26300
C	-11.01300	23.53800	103.98000
O	-11.92900	22.71100	103.93100
C	-11.10700	25.84800	105.05200
C	-12.59800	26.01600	104.75400
C	-10.71900	26.64200	106.29900
N	-10.19200	23.74900	102.93300
C	-10.35500	23.01500	101.67200
C	-10.53600	21.52000	101.90000
O	-11.52300	20.92700	101.45100
C	-9.05400	23.30600	100.93300
C	-8.71800	24.66900	101.38600
C	-8.99700	24.60700	102.87800
N	-9.57000	20.92900	102.60800
H	-8.79800	21.50100	102.95100
C	-9.56900	19.50300	102.91300
C	-10.86000	18.99500	103.52700
O	-11.46600	18.06100	103.00100
C	-8.40800	19.15500	103.84600
O	-7.17700	19.07500	103.14900
H	-6.45600	18.85900	103.72800
N	-11.27600	19.59300	104.64000
H	-10.73200	20.36100	105.03500
C	-12.50100	19.16200	105.30100
C	-13.69700	19.29200	104.36300

O	-14.56200	18.41100	104.31400
C	-12.76200	19.98200	106.58900
C	-14.18400	19.73600	107.10100
C	-11.74900	19.59000	107.66000
N	-13.74100	20.39600	103.62000
H	-13.00000	21.09100	103.71300
C	-14.82700	20.63100	102.67600
C	-14.88000	19.47600	101.68700
O	-15.91700	18.82200	101.54000
C	-14.63600	21.95900	101.90400
C	-14.81800	23.14000	102.86600
C	-15.61600	22.03300	100.74000
C	-14.63800	24.51100	102.25400
N	-13.75500	19.21800	101.02200
H	-12.93100	19.79400	101.19400
C	-13.67700	18.12900	100.05300
C	-14.21900	16.83100	100.64000
O	-15.03700	16.15200	100.02000
C	-12.23300	17.89000	99.60300
C	-12.17200	16.67900	98.67400
C	-11.69900	19.13700	98.91400
N	-13.75500	16.49700	101.84000
H	-13.07800	17.10700	102.29800
C	-14.18900	15.28000	102.51900
C	-15.69700	15.28000	102.71600
O	-16.35900	14.26200	102.49800
C	-13.48800	15.14900	103.86200
N	-16.23900	16.42100	103.13400
H	-15.63900	17.22700	103.31300
C	-17.67700	16.53600	103.34000
C	-18.42700	16.21600	102.05700
O	-19.26900	15.31600	102.03500
C	-18.03600	17.94000	103.81800
C	-17.72200	18.16100	105.28200
C	-18.13200	19.54500	105.74000
N	-18.11000	19.65800	107.19300
H	-18.15000	18.79900	107.74200
C	-18.04100	20.81100	107.84300
N	-17.98500	21.94600	107.16500
H	-17.93200	22.83300	107.66500
H	-18.00000	21.93400	106.14500
N	-18.02100	20.82700	109.16700
H	-17.96800	21.71400	109.66700

H	-18.06400	19.95200	109.69000
N	-18.11000	16.94400	100.98800
H	-17.40000	17.67200	101.07200
C	-18.75800	16.72200	99.69700
C	-18.65300	15.26000	99.26600
O	-19.64100	14.65500	98.84900
C	-18.13700	17.61500	98.61800
C	-18.18300	19.08600	98.98200
O	-17.37100	19.56800	99.77000
N	-19.14700	19.80700	98.41600
H	-19.17800	20.79700	98.66100
H	-19.82000	19.40700	97.76200
N	-17.45500	14.69500	99.36600
H	-16.66600	15.24000	99.71500
C	-17.25900	13.31100	98.98300
C	-18.17800	12.42900	99.80800
O	-18.73900	11.45100	99.31100
C	-15.81900	12.88900	99.21600
C	-15.49100	11.56200	98.61700
N	-15.50700	11.33800	97.25800
H	-15.71600	12.04000	96.54800
C	-15.17000	10.37800	99.19000
C	-15.21000	10.07400	97.01700
N	-15.00100	9.47000	98.17400
H	-14.75400	8.48800	98.29300
N	-18.30900	12.77700	101.08200
H	-17.78800	13.58200	101.43000
C	-19.17100	12.04900	101.99600
C	-20.59400	12.15000	101.46500
O	-21.24300	11.14100	101.18300
C	-19.09800	12.68200	103.38900
C	-20.13500	12.15300	104.38400
C	-20.22900	13.04900	105.61500
N	-20.70600	14.38400	105.27700
H	-21.21100	14.50100	104.39900
C	-20.52600	15.46000	106.03900
N	-19.87500	15.37000	107.19500
H	-19.73700	16.19500	107.77900
H	-19.51300	14.46700	107.50100
N	-20.99700	16.63400	105.64100
H	-20.85900	17.45900	106.22500
H	-21.49600	16.70300	104.75400
N	-21.06300	13.38700	101.32500

H	-20.46100	14.17400	101.56800
C	-22.40400	13.65300	100.83800
C	-22.65200	12.99600	99.48700
O	-23.78100	12.63200	99.16300
C	-22.63900	15.16100	100.74400
C	-22.54100	15.85700	102.09900
O	-22.80900	15.20200	103.13300
O	-22.21200	17.06700	102.13100
N	-21.59300	12.84000	98.70200
H	-20.68300	13.17300	99.02100
C	-21.69900	12.20400	97.39500
C	-22.06600	10.72600	97.56400
O	-22.36900	10.03700	96.58800
C	-20.37900	12.33500	96.64400
N	-22.02700	10.24300	98.80500
H	-21.75500	10.85400	99.57500
C	-22.36700	8.85800	99.07600
C	-21.18400	7.90800	99.08700
O	-21.34700	6.69900	99.28500
N	-19.98400	8.44900	98.89300
H	-19.90500	9.45700	98.75900
C	-18.77900	7.62600	98.86800
C	-18.03700	7.53500	100.20100
O	-17.99800	8.48900	100.98700
C	-17.84100	8.13500	97.78800
N	-17.43700	6.37000	100.47000
C	-16.67900	6.10800	101.69700
C	-15.60100	7.16900	101.92400
O	-14.69500	7.33000	101.09800
C	-16.08800	4.72300	101.43900
C	-17.13700	4.06600	100.60600
C	-17.50400	5.16400	99.63000
N	-15.68800	7.87800	103.04500
H	-16.43900	7.68500	103.70800
C	-14.72100	8.92700	103.33400
C	-14.06800	8.82100	104.71000
O	-14.72100	8.48900	105.69400
C	-15.39100	10.30500	103.20500
O	-16.01700	10.40200	101.92100
H	-16.65600	9.70500	101.83000
C	-14.37000	11.41800	103.35000
N	-12.77100	9.11600	104.76200
H	-12.29700	9.37800	103.89800

C	-11.99500	9.08200	106.00000
C	-11.10400	10.31400	106.09600
O	-10.55200	10.75400	105.09500
C	-11.10700	7.83200	106.03800
C	-11.86900	6.53800	106.19100
C	-12.41400	6.16600	107.42000
C	-12.08300	5.70600	105.10000
C	-13.15800	4.99800	107.55700
C	-12.82500	4.53600	105.22400
C	-13.36100	4.18600	106.45400
O	-14.10900	3.03200	106.56500
H	-14.47600	2.79200	107.40800
N	-10.97000	10.87300	107.29400
H	-11.48600	10.48800	108.08500
C	-10.09800	12.02900	107.50400
C	-9.14400	11.78300	108.67300
O	-9.35600	10.86200	109.46700
C	-10.90800	13.29400	107.77200
C	-11.37400	14.00000	106.52300
S	-11.87100	15.70000	106.86200
C	-10.54400	16.60700	106.11800
N	-8.09000	12.59400	108.77100
H	-7.96000	13.32900	108.07600
C	-7.11600	12.45100	109.85500
C	-6.29700	13.71200	110.03400
O	-6.14300	14.50200	109.10900
C	-6.13700	11.29900	109.58500
C	-5.07400	11.61800	108.54100
C	-5.09600	11.00700	107.28400
C	-4.06400	12.55600	108.79600
C	-4.14700	11.32000	106.31500
C	-3.11600	12.87700	107.82900
C	-3.16400	12.25400	106.59500
O	-2.22300	12.54900	105.63800
H	-1.54900	13.19000	105.83000
N	-5.75500	13.89600	111.22500
H	-5.93400	13.23000	111.97600
C	-4.90800	15.04200	111.46100
C	-3.63500	14.53900	112.11300
O	-3.64600	14.12600	113.27600
C	-5.58000	16.06500	112.36600
C	-4.71400	17.30100	112.56200
C	-5.39000	18.35900	113.39400

O	-4.79100	19.44800	113.57200
O	-6.52100	18.09900	113.87000
N	-2.54500	14.56200	111.35100
H	-2.61700	14.91200	110.39600
C	-1.25000	14.10200	111.83800
C	-0.59500	15.18000	112.68500
O	-0.42700	16.31500	112.23500
C	-0.33800	13.76500	110.66800
C	0.92500	13.07600	111.06900
C	0.96000	11.69600	111.20900
C	2.08900	13.80800	111.29300
C	2.14000	11.04900	111.56300
C	3.27500	13.17500	111.64800
C	3.30200	11.79000	111.78200
N	-0.21700	14.81000	113.90600
H	-0.37400	13.84600	114.20000
C	0.41500	15.73800	114.83700
C	1.58400	15.08200	115.56200
O	1.45600	14.64800	116.69900
C	-0.62500	16.23100	115.84100
C	-1.87400	15.35600	115.86400
C	-2.98700	15.92700	116.71900
O	-2.84000	16.05500	117.93700
N	-4.11000	16.27600	116.08600
H	-4.23200	16.17000	115.07900
H	-4.85900	16.66000	116.66200
N	2.72400	15.01100	114.88700
H	2.76400	15.39100	113.94100
C	3.91700	14.40800	115.45400
C	5.13800	15.15300	114.93100
O	5.05900	15.83400	113.90700
C	4.00500	12.94500	115.03600
C	5.06300	12.15600	115.77200
C	4.83500	11.68800	117.06900
C	6.29100	11.86800	115.17300
C	5.79500	10.94900	117.75000
C	7.26000	11.13300	115.84500
C	7.00300	10.67300	117.13400
O	7.94400	9.91900	117.79700
H	7.76900	9.60500	118.67600
N	6.26100	15.03800	115.63600
H	6.26000	14.48800	116.49500
C	7.49700	15.68800	115.19900

C	8.58700	14.63900	115.02700
O	9.20300	14.19900	115.99800
C	7.95700	16.74600	116.20200
C	9.11900	17.57800	115.69100
C	9.33400	18.79900	116.57400
N	10.31600	19.74200	116.03300
H	10.01000	20.69800	115.85500
C	11.57900	19.43400	115.75900
N	12.02800	18.20100	115.97000
H	11.39800	17.48700	116.33500
H	12.99800	17.96500	115.76000
N	12.39900	20.36300	115.28400
H	12.05400	21.30900	115.12200
H	13.36900	20.12700	115.07400
N	8.83400	14.21800	113.77800
C	9.85600	13.21100	113.50600
C	11.25700	13.68200	113.85800
O	11.57500	14.86800	113.75100
C	9.68000	12.94600	112.01600
C	9.24200	14.27100	111.49900
C	8.22000	14.68500	112.52300
N	12.08600	12.73800	114.28600
H	11.74200	11.78000	114.35900
C	13.46500	13.01500	114.65500
C	14.27900	13.33000	113.41300
O	15.40300	13.81900	113.50100
C	14.06600	11.79800	115.34300
O	14.03900	10.67900	114.47300
H	14.41400	9.91900	114.90300
N	13.70400	13.02900	112.25500
H	12.77000	12.62000	112.25900
C	14.36300	13.26400	110.98100
C	14.08900	14.68000	110.47100
O	14.15200	14.93200	109.27000
C	13.87100	12.25300	109.94800
C	13.75800	10.85400	110.47300
C	12.51300	10.29700	110.73800
C	14.89200	10.07500	110.67100
C	12.40000	8.97600	111.19000
C	14.78900	8.75600	111.12200
C	13.54000	8.20800	111.38000
N	13.77800	15.59900	111.37900
H	13.73400	15.33500	112.36300

C	13.49900	16.97700	110.99600
C	14.81600	17.71800	110.79400
O	15.86600	17.25200	111.23600
C	12.67500	17.68200	112.08400
O	11.40900	17.06900	112.28700
H	10.89900	17.50500	112.96000
N	14.75700	18.86300	110.11900
H	13.85700	19.18500	109.76400
C	15.95000	19.67100	109.87300
C	16.37200	20.34600	111.17300
O	15.53000	20.69400	112.00000
C	15.66700	20.73600	108.80400
O	16.79200	21.58100	108.59300
H	16.61700	22.24000	107.93200
N	17.67300	20.53400	111.35200
H	18.32600	20.23300	110.62900
C	18.18700	21.16200	112.56200
C	17.70400	22.59600	112.71900
O	17.51600	23.07900	113.83500
C	19.71600	21.15900	112.55800
C	20.29600	19.77000	112.40300
O	19.72500	18.82100	112.98300
O	21.33000	19.62700	111.71300
N	17.50800	23.27400	111.59700
H	17.66700	22.81300	110.70100
C	17.07200	24.66000	111.61600
C	15.58000	24.80200	111.89000
O	15.01600	25.89300	111.77200
C	17.44500	25.32200	110.29000
C	18.95400	25.35500	110.05000
S	19.43200	25.85900	108.38700
C	19.71700	24.24600	107.60800
N	14.95300	23.69500	112.27500
H	15.49000	22.83300	112.37000
C	13.52200	23.66900	112.56700
C	13.24500	23.81100	114.06700
O	13.64900	22.96400	114.86500
C	12.92000	22.35500	112.04500
C	11.43700	22.14000	112.33600
C	10.99900	20.76700	111.83800
C	9.54200	20.47800	112.14900
N	9.16300	19.11000	111.70300
H	8.18400	18.91600	111.91200

H	9.78000	18.40100	112.09900
H	9.37300	18.96500	110.71600
N	12.55100	24.88800	114.46800
C	12.23800	25.10200	115.88400
C	11.54000	23.88600	116.45900
O	10.53200	23.42800	115.93000
C	11.34200	26.33300	115.86000
C	10.70200	26.26300	114.51400
C	11.85400	25.87200	113.62900
N	12.08900	23.37100	117.54800
H	12.91300	23.82300	117.94500
C	11.55800	22.18200	118.19800
C	10.08600	22.25700	118.62600
O	9.47200	21.23000	118.93700
C	12.45000	21.83100	119.39400
C	13.92500	21.66900	119.01500
C	14.79300	21.27400	120.20700
C	16.24700	21.05000	119.79200
N	17.09800	20.57900	120.92600
H	18.06800	20.43000	120.64900
H	16.70600	19.74200	121.35700
H	17.03700	21.21600	121.72100
N	9.51200	23.45700	118.63000
H	10.05100	24.27800	118.35300
C	8.11600	23.60600	119.02800
C	7.17300	23.26200	117.88300
O	6.00700	22.94000	118.10700
C	7.80400	25.03400	119.46700
O	7.57300	25.84600	118.30900
H	6.84400	25.48800	117.81500
C	8.96700	25.60500	120.25500
N	7.67400	23.34100	116.65500
H	8.64600	23.62300	116.52500
C	6.85500	23.03000	115.49100
C	6.60900	21.52700	115.41200
O	7.54200	20.74000	115.25200
C	7.52800	23.50800	114.18800
C	6.66900	23.13700	112.99600
C	7.73200	25.00500	114.23200
N	5.34400	21.14400	115.53000
H	4.62500	21.85700	115.65300
C	4.94300	19.74400	115.49000
C	3.89500	19.54700	114.40700

O	2.98500	20.36000	114.26800
C	4.35400	19.31700	116.84900
C	5.47100	19.25700	117.89000
C	3.63900	17.98100	116.72500
C	4.97700	19.05500	119.30400
N	4.01800	18.47000	113.64100
H	4.78700	17.81700	113.79200
C	3.05000	18.22900	112.58700
C	3.15800	19.25100	111.46800
O	2.15700	19.78200	110.97800
N	4.39600	19.52500	111.07600
H	5.16700	19.05300	111.54900
C	4.71500	20.46100	110.00900
C	4.43200	19.79600	108.65000
O	4.22100	18.58000	108.56500
C	6.19000	20.85600	110.14100
C	6.60400	21.94700	109.17700
O	5.76100	22.80100	108.82900
O	7.79200	21.96500	108.78400
N	4.41900	20.60200	107.59400
H	4.59500	21.59700	107.73700
C	4.16300	20.12400	106.23500
C	5.09500	18.97800	105.81300
O	6.31700	19.15200	105.74400
C	4.31500	21.28800	105.25100
C	3.82500	20.98700	103.86800
N	2.49900	20.74100	103.58500
H	1.74400	20.71800	104.27000
C	4.48100	20.92200	102.68500
C	2.36000	20.54000	102.28600
N	3.54700	20.64500	101.71600
H	3.73900	20.53800	100.72000
N	4.50900	17.81300	105.53600
H	3.49700	17.72800	105.62700
C	5.28500	16.66100	105.10600
C	5.76000	15.72300	106.20400
O	6.25800	14.63100	105.91700
N	5.60600	16.13300	107.46000
H	5.17200	17.03800	107.64300
C	6.04700	15.31000	108.57900
C	5.53400	13.87300	108.58300
O	6.24900	12.95700	108.99100
C	5.68500	15.97400	109.90400

C	6.68400	17.03200	110.31400
O	7.90500	16.80300	110.17300
O	6.25400	18.09200	110.79600
N	4.30400	13.66800	108.13200
H	3.74800	14.45600	107.79900
C	3.74200	12.32600	108.10900
C	4.42300	11.42600	107.08000
O	4.25200	10.20900	107.10800
C	2.23900	12.38500	107.81800
C	1.83800	12.36000	106.33500
C	2.33600	13.56100	105.53700
O	2.68900	14.59500	106.14500
O	2.35800	13.46600	104.29100
N	5.19500	12.02200	106.17400
H	5.31500	13.03400	106.21000
C	5.87200	11.26000	105.13200
C	6.79600	10.18800	105.68800
O	6.83700	9.06200	105.17800
C	6.66300	12.19900	104.21800
C	5.84100	13.17300	103.36100
C	6.79500	14.04200	102.52400
C	4.87600	12.40100	102.46000
N	7.52900	10.53900	106.74100
H	7.43300	11.48000	107.12200
C	8.46600	9.61100	107.36400
C	7.77700	8.38900	107.98200
O	8.32900	7.29000	107.97900
C	9.29500	10.34900	108.41400
C	9.97900	11.57000	107.88200
C	9.30600	12.78300	107.81100
C	11.28700	11.50300	107.41500
C	9.92700	13.91500	107.28000
C	11.91300	12.62600	106.88400
C	11.22900	13.83500	106.81700
N	6.57200	8.58300	108.50500
H	6.16600	9.51900	108.48900
C	5.81800	7.49200	109.10000
C	5.13700	6.65000	108.01200
O	5.01800	5.43100	108.14100
C	4.76500	8.04500	110.06600
O	5.36500	8.71200	111.16300
H	4.71200	9.05500	111.76200
N	4.69400	7.30200	106.94200

H	4.81900	8.31200	106.88200
C	4.03100	6.59300	105.85200
C	5.02600	5.75300	105.05000
O	4.72900	4.62000	104.66200
C	3.29800	7.57800	104.88900
C	2.71500	6.82400	103.70100
C	2.18400	8.30000	105.62700
N	6.20900	6.30100	104.80300
H	6.42300	7.23600	105.15000
C	7.19800	5.56400	104.03700
C	8.20800	4.86600	104.91300
O	9.24800	4.42400	104.43400
C	7.91500	6.47500	103.04200
C	7.12100	6.75100	101.80300
C	6.45800	7.96200	101.63800
C	7.01100	5.78500	100.81300
C	5.69500	8.21000	100.50400
C	6.25000	6.02200	99.67600
C	5.59000	7.23900	99.52300
N	7.89800	4.77800	106.19900
H	7.03300	5.19800	106.53900
C	8.77700	4.09000	107.13100
C	10.24400	4.48000	107.18900
O	11.12500	3.61800	107.10600
N	10.50500	5.77500	107.34200
H	9.72900	6.43500	107.38800
C	11.86300	6.27600	107.44600
C	12.57000	5.58300	108.61900
O	13.78500	5.39100	108.59700
C	11.84600	7.78700	107.65000
N	11.81500	5.20600	109.66800
C	12.43200	4.53500	110.81600
C	13.17700	3.24100	110.48500
O	14.12100	2.88300	111.18100
C	11.24300	4.29700	111.74500
C	10.41500	5.50300	111.51100
C	10.43400	5.60800	110.00000
N	12.76100	2.54100	109.43200
H	11.97500	2.88100	108.87700
C	13.41900	1.29200	109.06400
C	14.48700	1.43100	107.98000
O	14.94600	0.43000	107.43400
C	12.38800	0.25900	108.62200

C	11.23500	0.13700	109.55300
C	10.16300	1.01000	109.46200
C	11.24600	-0.80500	110.56900
C	9.12200	0.95200	110.37400
C	10.20600	-0.87300	111.49200
C	9.14300	0.00900	111.39500
N	14.88100	2.66600	107.67600
H	14.45400	3.45400	108.16300
C	15.90400	2.92800	106.66800
C	16.89700	3.94500	107.21500
O	18.05400	3.98600	106.80000
C	15.27300	3.47000	105.38300
C	14.17800	2.63400	104.71500
C	13.68400	3.37900	103.50100
C	14.69500	1.27500	104.31100
N	16.43700	4.76900	108.15000
H	15.46300	4.69600	108.44500
C	17.29400	5.77400	108.76300
C	17.71400	5.33700	110.16700
O	17.40500	4.21900	110.59100
C	16.57700	7.12600	108.80300
C	16.40500	7.73200	107.42400
C	16.00700	9.19100	107.48900
C	16.22900	9.86600	106.14400
N	15.87400	11.30500	106.18700
H	16.02300	11.75800	105.28500
H	16.37400	11.78900	106.93300
H	14.91900	11.44300	106.51900
N	18.41200	6.21500	110.88800
H	18.61600	7.13400	110.49400
C	18.89200	5.89000	112.23200
C	18.46500	6.87000	113.30900
O	18.27000	8.05100	113.03900
C	20.41900	5.80500	112.21900
C	20.96000	4.73800	111.28400
C	22.41400	4.96100	110.91500
O	22.97600	4.09600	110.20600
O	22.98900	6.00000	111.32400
N	18.32400	6.37000	114.53400
H	18.48500	5.37500	114.69300
C	17.94300	7.22200	115.65000
C	16.46700	7.24000	116.01100
O	16.06300	7.91500	116.96300

N	15.65600	6.50600	115.25700
H	16.04100	5.96700	114.48200
C	14.22700	6.46000	115.52100
C	13.96000	5.72400	116.82700
O	14.33100	4.55400	116.98100
C	13.50700	5.77000	114.37400
N	13.32400	6.42200	117.76700
H	13.06700	7.38900	117.57000
C	12.98100	5.85500	119.06900
C	11.91600	4.77800	118.89000
O	11.27000	4.71000	117.84900
C	12.45900	6.95200	119.99900
O	11.25400	7.51600	119.51200
H	10.93000	8.19700	120.08900
N	11.73200	3.93000	119.89300
H	12.28800	4.01600	120.74400
C	10.73600	2.87900	119.77700
C	9.36900	3.47800	119.48100
O	8.58100	2.89900	118.73100
C	10.65800	2.06300	121.05700
C	9.90000	0.75800	120.88800
C	10.54700	-0.15200	119.85900
O	11.77600	-0.03000	119.65900
O	9.83900	-0.99700	119.26300
N	9.09000	4.63600	120.08000
H	9.78600	5.04800	120.70100
C	7.81900	5.33900	119.87900
C	7.60500	5.58900	118.38300
O	6.60500	5.17400	117.79300
C	7.86000	6.68000	120.61000
C	6.54400	7.44200	120.65300
C	6.72000	8.87300	121.14000
O	5.73600	9.47300	121.61500
O	7.84400	9.40600	121.03600
N	8.57400	6.27000	117.78400
H	9.37300	6.57300	118.34100
C	8.54600	6.60300	116.37100
C	8.46400	5.34700	115.51700
O	7.65600	5.26100	114.59900
C	9.80200	7.38700	116.01400
C	9.70800	8.16300	114.72600
C	10.93900	9.00900	114.49200
O	10.88700	9.91600	113.63200

O	11.96100	8.76100	115.17200
N	9.30500	4.37200	115.82000
H	9.95700	4.49300	116.59500
C	9.31200	3.12900	115.06300
C	7.93200	2.48700	115.01000
O	7.52100	1.96800	113.97200
C	10.32000	2.11900	115.66600
C	11.73900	2.66900	115.50800
C	10.17400	0.75400	114.99200
C	12.79400	1.80500	116.11000
N	7.21600	2.53000	116.12800
H	7.60000	2.98700	116.95500
C	5.89000	1.93300	116.18600
C	4.81300	2.84600	115.59600
O	3.78600	2.36900	115.09600
C	5.57500	1.52600	117.62800
C	6.63300	0.56800	118.18000
C	6.06400	-0.62100	118.95200
N	5.64100	-0.25300	120.29900
H	6.36300	-0.16300	121.01400
C	4.38100	-0.02600	120.66100
N	3.39700	-0.13400	119.77300
H	2.43100	0.04000	120.05100
H	3.60700	-0.40400	118.81200
N	4.10800	0.32600	121.91200
H	3.14200	0.50000	122.19000
H	4.86300	0.40900	122.59300
N	5.04800	4.15400	115.63600
H	5.89600	4.50400	116.08200
C	4.10100	5.08900	115.04700
C	4.07700	4.80300	113.55200
O	3.01800	4.79300	112.93200
C	4.54100	6.53400	115.28500
C	3.84600	7.60100	114.43300
C	2.34300	7.38900	114.46500
C	4.20900	8.98600	114.94500
N	5.25400	4.56100	112.98100
H	6.09800	4.58200	113.55300
C	5.36600	4.26700	111.55800
C	4.66300	2.96400	111.20600
O	3.84600	2.92000	110.28500
C	6.83200	4.17400	111.14700
O	6.95200	3.71500	109.81200

H	7.86500	3.65700	109.55600
N	4.99100	1.89900	111.93000
H	5.69000	1.98700	112.66700
C	4.36300	0.60700	111.68300
C	2.85800	0.79400	111.64200
O	2.17800	0.34300	110.71300
C	4.69500	-0.38700	112.79800
C	6.08300	-0.99700	112.74800
C	6.15500	-2.18900	113.69500
C	7.47800	-2.92500	113.58200
N	7.51600	-4.10500	114.48900
H	8.40500	-4.59900	114.41300
H	6.72500	-4.72800	114.32700
H	7.31400	-3.84300	115.45400
N	2.36000	1.46900	112.67500
H	3.00600	1.80700	113.38800
C	0.94000	1.75000	112.84100
C	0.36200	2.39800	111.58300
O	-0.61700	1.90700	111.01900
C	0.74200	2.67000	114.05700
C	-0.62800	2.57800	114.72900
S	-0.84300	3.76000	116.10000
C	0.47100	3.22900	117.26100
N	0.97900	3.48900	111.13900
H	1.80200	3.83300	111.63400
C	0.50400	4.20400	109.95900
C	0.47700	3.35800	108.68600
O	-0.51600	3.36600	107.95500
C	1.35200	5.45900	109.68700
C	0.85700	6.15600	108.43700
C	1.27500	6.39900	110.86800
N	1.56000	2.63600	108.41300
H	2.35800	2.66200	109.04700
C	1.61600	1.80800	107.21600
C	0.46000	0.80500	107.21200
O	-0.13000	0.55000	106.17000
C	2.97900	1.10500	107.11800
C	4.15100	2.07300	106.91100
S	5.78700	1.29300	106.74600
C	6.20300	1.05500	108.45100
N	0.13700	0.24900	108.37800
H	0.68700	0.48200	109.20500
C	-0.98300	-0.68700	108.51200

C	-2.21500	0.02000	107.95900
O	-2.84500	-0.43500	107.00100
C	-1.25400	-1.00600	109.99000
C	-0.62700	-2.27800	110.53900
C	-1.46900	-3.50300	110.23600
C	-0.92300	-4.72900	110.96400
N	0.51400	-5.00500	110.64400
H	0.87900	-5.82400	111.13000
H	1.09200	-4.18500	110.82700
H	0.65400	-5.08600	109.63700
N	-2.55500	1.13500	108.59700
H	-1.99600	1.43700	109.39500
C	-3.69400	1.93600	108.19600
C	-3.70900	2.13400	106.68500
O	-4.65000	1.69800	106.00900
C	-3.65400	3.29000	108.90600
C	-4.23200	3.26900	110.30100
C	-3.69300	4.07200	111.30200
C	-5.34300	2.48300	110.60100
C	-4.24800	4.09800	112.57500
C	-5.90600	2.50100	111.87500
C	-5.35700	3.31100	112.86300
N	-2.67100	2.78100	106.15400
H	-1.92100	3.11400	106.76000
C	-2.59500	3.01900	104.71500
C	-2.77100	1.71700	103.92400
O	-3.65700	1.62100	103.07600
C	-1.26600	3.68100	104.34600
C	-1.27000	5.20800	104.31700
C	-0.74000	5.99900	103.33700
C	-1.73500	6.10800	105.34100
N	-0.83800	7.32600	103.68300
H	-0.51300	8.11100	103.11900
C	-1.44300	7.42300	104.90700
C	-2.36500	5.93100	106.58200
C	-1.75800	8.55700	105.66900
C	-2.67800	7.06300	107.34000
C	-2.37200	8.35700	106.87700
N	-1.94200	0.71300	104.20600
H	-1.22800	0.84100	104.92300
C	-2.03600	-0.57200	103.50700
C	-3.42600	-1.18900	103.64100
O	-3.96100	-1.74800	102.67700

C	-0.98400	-1.54200	104.02900
N	-4.00700	-1.10400	104.83700
H	-3.51200	-0.65900	105.61000
C	-5.34600	-1.64300	105.04800
C	-6.31200	-0.94200	104.10100
O	-7.06800	-1.59700	103.37700
C	-5.81000	-1.44000	106.49700
C	-5.17600	-2.42700	107.44900
O	-4.71600	-3.49100	107.03200
N	-5.16100	-2.09000	108.73800
H	-5.54200	-1.20900	109.08300
H	-4.73300	-2.75600	109.38100
N	-6.28100	0.38900	104.10800
H	-5.63800	0.87100	104.73600
C	-7.14900	1.17000	103.23600
C	-6.95200	0.69300	101.80500
O	-7.91600	0.45900	101.08200
C	-6.80300	2.65900	103.33700
C	-7.67400	3.55500	102.49300
C	-9.02900	3.68100	102.75600
C	-7.12100	4.30900	101.46100
C	-9.82300	4.55000	102.00700
C	-7.90400	5.18200	100.70600
C	-9.25800	5.30400	100.97900
N	-5.69200	0.54500	101.41200
H	-4.94000	0.75400	102.06900
C	-5.35500	0.09400	100.07200
C	-6.02900	-1.24000	99.80300
O	-6.54900	-1.47700	98.71500
C	-3.84400	-0.03900	99.93000
N	-6.02300	-2.11200	100.80200
H	-5.57700	-1.86400	101.68500
C	-6.64400	-3.41600	100.65400
C	-8.17100	-3.39400	100.61500
O	-8.76100	-3.96900	99.70700
C	-6.18500	-4.35600	101.77200
C	-4.80300	-4.95600	101.56000
C	-4.43700	-5.94600	102.67100
N	-4.10100	-5.27500	103.92300
H	-4.83200	-5.18900	104.62900
C	-2.90400	-4.76900	104.20400
N	-1.91600	-4.86300	103.32500
H	-0.99800	-4.47500	103.54100

H	-2.07200	-5.34200	102.43800
N	-2.70100	-4.14700	105.35700
H	-1.78300	-3.75900	105.57300
H	-3.46100	-4.07500	106.03300
N	-8.81500	-2.71900	101.56900
H	-8.28600	-2.19800	102.26900
C	-10.27700	-2.72300	101.61500
C	-11.01500	-1.39500	101.57500
O	-12.22500	-1.36200	101.79900
C	-10.74500	-3.45700	102.86700
C	-9.93000	-4.69400	103.15400
O	-9.96800	-5.67100	102.40500
N	-9.17600	-4.65800	104.24600
H	-8.62500	-5.49400	104.44000
H	-9.14500	-3.84900	104.86600
N	-10.32500	-0.30000	101.29800
H	-9.32600	-0.34700	101.09800
C	-11.02500	0.96500	101.28600
C	-11.49800	1.25500	102.69800
O	-12.48800	1.95200	102.91500
N	-10.79100	0.68600	103.66900
H	-10.00700	0.08400	103.41900
C	-11.09800	0.89300	105.08200
C	-9.82200	0.70000	105.88800
O	-9.30600	-0.40900	105.98600
C	-12.14100	-0.09500	105.56900
C	-12.69600	0.29000	106.91400
O	-11.95300	0.69600	107.80700
N	-14.00800	0.16600	107.07100
H	-14.38400	0.42700	107.98300
H	-14.62400	-0.17100	106.33100
N	-9.31100	1.77800	106.49600
C	-8.08000	1.75500	107.29700
C	-8.02300	0.82600	108.51000
O	-6.95300	0.57400	109.05400
C	-7.90400	3.22200	107.68800
C	-9.30800	3.71000	107.77900
C	-9.95300	3.10200	106.56000
N	-9.16400	0.30200	108.92700
H	-10.02900	0.50100	108.42400
C	-9.18800	-0.55500	110.09700
C	-8.56600	-1.93500	109.92500
O	-8.46000	-2.46600	108.81400

C	-10.62000	-0.66600	110.62100
C	-11.10600	0.63300	111.25100
O	-10.53800	1.10700	112.23500
N	-12.15100	1.21800	110.67900
H	-12.62200	0.82500	109.86400
H	-12.47600	2.08800	111.10100
N	-8.13200	-2.49000	111.05300
H	-8.24000	-1.97700	111.92800
C	-7.51000	-3.80100	111.08100
C	-7.24900	-4.20600	112.52200
O	-7.08600	-3.34100	113.39300
N	-7.21600	-5.51000	112.78700
H	-7.36300	-6.18000	112.03200
C	-6.97300	-5.99500	114.13800
C	-5.62800	-5.54500	114.66900
O	-4.61100	-5.65200	113.98400
C	-7.07000	-7.52000	114.19000
C	-8.46600	-8.01200	114.58800
C	-8.61200	-9.52900	114.55200
O	-7.82700	-10.22400	115.24000
O	-9.52000	-10.02100	113.84000
N	-5.63800	-5.03000	115.89300
H	-6.52100	-4.96000	116.39900
C	-4.41900	-4.56500	116.52300
C	-4.19900	-3.07900	116.33200
O	-3.16900	-2.54500	116.74500
N	-5.17100	-2.40500	115.72000
H	-6.01100	-2.90500	115.42700
C	-5.07100	-0.96800	115.45500
C	-6.20200	-0.16600	116.08100
O	-7.32500	-0.65800	116.20300
C	-5.08500	-0.71700	113.94300
C	-3.86700	-1.11400	113.11900
C	-4.24900	-1.20900	111.64800
C	-2.76700	-0.09200	113.34600
N	-5.92500	1.09000	116.47900
C	-6.99400	1.89500	117.07700
C	-8.13100	1.96600	116.06500
O	-7.90100	1.81000	114.86400
C	-6.32600	3.25200	117.29300
C	-4.89200	2.89100	117.52800
C	-4.65000	1.83000	116.47200
N	-9.35300	2.19000	116.52800

H	-9.51100	2.31300	117.52800
C	-10.46500	2.25900	115.59400
C	-10.57700	3.62000	114.92500
O	-10.60800	4.65800	115.59000
C	-11.78500	1.94000	116.27400
C	-12.94400	1.93000	115.33100
N	-13.17900	0.89000	114.45600
H	-12.62500	0.03600	114.39100
C	-13.90300	2.85400	115.08900
C	-14.23500	1.17500	113.71500
N	-14.69300	2.36100	114.07700
H	-15.50100	2.83400	113.67200
N	-10.64700	3.58800	113.59600
H	-10.62700	2.68100	113.12900
C	-10.75100	4.78700	112.78000
C	-12.18900	4.94800	112.30900
O	-12.65600	4.21900	111.43500
C	-9.82500	4.67700	111.56600
C	-9.50700	5.99100	110.90800
C	-10.30700	7.09800	110.84500
C	-8.31800	6.31200	110.17400
N	-9.69100	8.08700	110.11600
H	-10.08000	9.01000	109.92300
C	-8.47200	7.63300	109.69100
C	-7.14000	5.61200	109.87600
C	-7.48700	8.26900	108.92400
C	-6.16100	6.24400	109.11400
C	-6.34300	7.56300	108.64700
N	-12.90500	5.91700	112.88600
C	-14.29800	6.20300	112.55000
C	-14.42500	6.64900	111.11300
O	-13.53400	7.30600	110.58500
C	-14.65400	7.32400	113.50800
C	-13.36900	8.08000	113.59300
C	-12.36900	6.95900	113.77800
N	-15.53100	6.28700	110.47600
H	-16.23000	5.71700	110.95200
C	-15.74700	6.70100	109.10400
C	-16.21300	8.15300	109.16300
O	-16.92000	8.54900	110.09100
C	-16.81700	5.84900	108.43000
C	-16.77400	5.97600	106.92600
C	-18.13300	5.83800	106.27500

O	-18.77100	4.77600	106.43400
O	-18.56200	6.79900	105.59700
N	-15.79700	8.95500	108.19100
H	-15.19100	8.59300	107.45500
C	-16.20400	10.34500	108.17700
C	-17.59500	10.42300	107.56500
O	-17.77200	10.27400	106.34300
C	-15.23700	11.19100	107.35900
C	-15.46200	12.67500	107.50400
C	-14.87300	13.38800	108.54500
C	-16.23700	13.37100	106.58200
C	-15.04300	14.76600	108.65800
C	-16.41900	14.74600	106.68500
C	-15.81900	15.44000	107.72400
O	-15.99400	16.80300	107.83000
H	-15.58300	17.27900	108.54200
N	-18.58100	10.63500	108.43100
H	-18.35500	10.72000	109.42200
C	-19.97300	10.75100	108.01500
C	-20.54300	12.01600	108.64000
O	-19.84600	13.02500	108.74100
C	-20.75800	9.52200	108.48900
C	-20.55100	9.23500	109.95800
O	-20.48300	10.14800	110.78700
N	-20.46200	7.95700	110.29500
H	-20.51800	7.20300	109.61000
H	-20.32200	7.76300	111.28700
N	-21.80000	11.96200	109.07300
H	-22.33300	11.10000	108.95800
C	-22.42800	13.11200	109.70800
C	-21.75600	13.47900	111.02400
O	-21.58700	14.65700	111.31100
C	-23.92000	12.86100	109.93600
C	-24.71200	12.61300	108.65700
C	-24.48600	13.67800	107.57100
O	-24.49900	14.88400	107.83700
N	-24.29400	13.22300	106.33600
H	-24.28300	12.22700	106.11600
H	-24.14400	13.92900	105.61600
N	-21.37200	12.47800	111.81600
H	-21.54600	11.51400	111.53200
C	-20.70300	12.75000	113.08900
C	-19.35700	13.40600	112.84500

O	-18.76800	13.99600	113.75200
C	-20.47000	11.46300	113.88700
C	-21.70100	10.89000	114.56500
C	-22.39700	9.85900	113.69900
C	-23.32800	9.01500	114.54700
N	-22.59800	8.47700	115.73200
H	-23.22400	7.90900	116.30300
H	-22.15400	9.21800	116.27500
H	-21.75800	7.96500	115.46200
N	-18.87800	13.28800	111.61200
H	-19.42800	12.78600	110.91500
C	-17.59600	13.85000	111.22300
C	-16.45700	13.32200	112.09200
O	-15.60300	14.08300	112.55000
C	-17.64000	15.38100	111.28300
C	-18.50600	16.00200	110.20300
C	-18.37000	17.50700	110.14300
O	-18.96000	18.11500	109.22800
O	-17.67300	18.08200	111.00600
N	-16.45400	12.01300	112.31900
H	-17.19400	11.42700	111.93300
C	-15.40100	11.41900	113.11400
C	-14.14100	11.28100	112.28300
O	-14.18800	10.80500	111.15100
N	-13.01300	11.70800	112.84100
H	-13.04500	12.10700	113.77900
C	-11.72900	11.62300	112.15200
C	-10.69400	11.07700	113.12200
O	-10.95300	10.98600	114.31800
C	-11.29200	13.00100	111.66800
C	-10.86800	13.94500	112.77300
C	-9.52900	14.07400	113.12700
C	-11.80400	14.73400	113.44300
C	-9.12900	14.97400	114.11600
C	-11.41600	15.63300	114.43400
C	-10.07700	15.75000	114.76200
O	-9.67900	16.65600	115.71500
H	-10.32900	17.18800	116.15800
N	-9.51700	10.73200	112.61600
H	-9.33800	10.85600	111.61900
C	-8.48200	10.18000	113.47100
C	-7.27900	11.07800	113.67300
O	-6.68400	11.56000	112.71800

C	-8.01300	8.83500	112.91800
C	-6.86500	8.17600	113.68000
C	-7.27600	7.92200	115.11700
C	-6.48200	6.88100	112.99400
N	-6.93200	11.30100	114.93500
H	-7.49500	10.89700	115.68400
C	-5.76800	12.10800	115.27900
C	-4.64000	11.10900	115.43400
O	-4.75900	10.15000	116.20100
C	-5.97600	12.84200	116.60500
C	-7.08500	13.87300	116.58200
C	-7.42000	14.38800	117.96700
O	-7.69100	13.60400	118.88000
N	-7.40900	15.70800	118.13200
H	-7.63500	16.05500	119.06400
H	-7.18500	16.35600	117.37700
N	-3.55400	11.33200	114.70100
H	-3.52300	12.15300	114.09600
C	-2.40500	10.43400	114.73800
C	-1.17900	11.09600	115.35400
O	-0.84700	12.24000	115.02800
C	-2.04000	9.95500	113.31900
C	-3.25200	9.27300	112.67200
C	-0.84200	9.01900	113.38500
C	-3.01400	8.80300	111.25800
N	-0.50500	10.36400	116.23900
H	-0.82600	9.42200	116.46200
C	0.68200	10.89100	116.89000
C	1.13600	10.01800	118.04100
O	0.97200	8.79400	117.99400
N	1.70900	10.64300	119.07000
H	1.82300	11.65600	119.03000
C	2.17900	9.92500	120.25400
C	1.04000	9.05400	120.74700
O	1.21100	7.87100	121.02500
C	2.57900	10.90600	121.32800
N	-0.13100	9.66800	120.84400
H	-0.18300	10.66000	120.61300
C	-1.34000	8.98900	121.26500
C	-2.30600	9.10900	120.09400
O	-2.80000	10.19300	119.79500
C	-1.90900	9.66200	122.52100
C	-3.28100	9.12900	122.91000

O	-3.62100	7.97600	122.63600
N	-4.07200	9.97000	123.57000
H	-3.79100	10.92400	123.79700
H	-4.99100	9.61300	123.83100
N	-2.54500	7.99400	119.41500
H	-2.08300	7.13200	119.70400
C	-3.44600	7.96100	118.26900
C	-4.85800	7.63800	118.73900
O	-5.14600	6.50100	119.10500
C	-2.99600	6.89000	117.25500
O	-1.64000	7.14600	116.86300
H	-1.07700	7.13700	117.62800
C	-3.89800	6.90500	116.02800
N	-5.73700	8.63700	118.72100
H	-5.44100	9.55300	118.38300
C	-7.11800	8.45500	119.17400
C	-8.12500	9.14200	118.25100
O	-7.82300	10.16700	117.63400
C	-7.26600	9.02700	120.58100
C	-7.19900	10.54400	120.60200
C	-6.93700	11.10100	121.97900
O	-7.58000	10.70300	122.95200
N	-5.99200	12.03700	122.07300
H	-5.81500	12.41400	123.00400
H	-5.46000	12.36600	121.26800
N	-9.33000	8.58400	118.17800
H	-9.52300	7.74600	118.72700
C	-10.38400	9.13900	117.33300
C	-11.02400	10.39000	117.92800
O	-11.10200	10.54400	119.14300
C	-11.44800	8.08800	117.08100
N	-11.47500	11.28200	117.05300
H	-11.36100	11.09100	116.05800
C	-12.12700	12.52300	117.45600
C	-13.23100	12.85600	116.45400
O	-13.60300	12.01900	115.62100
C	-11.12100	13.65400	117.51700
N	-13.75700	14.07500	116.53100
H	-13.41000	14.73000	117.23100
C	-14.82500	14.48600	115.62500
C	-14.82000	15.98300	115.32800
O	-14.21300	16.77000	116.05200
C	-16.18200	14.08900	116.20700

C	-16.37400	12.59700	116.38100
C	-17.71000	12.26100	117.01500
O	-18.10700	11.09400	117.07000
N	-18.41100	13.28300	117.50400
H	-18.08300	14.24800	117.45900
H	-19.31000	13.05700	117.93000
N	-15.50500	16.35600	114.25000
H	-15.97200	15.63700	113.69800
C	-15.61900	17.74700	113.82000
C	-14.27200	18.44700	113.64100
O	-13.87200	19.28700	114.44900
C	-16.50400	18.52800	114.80200
C	-17.95900	18.04000	114.85000
C	-18.81400	18.88100	115.80100
C	-20.27300	18.40900	115.83300
N	-21.11900	19.19000	116.79700
H	-22.08900	18.87600	116.81800
H	-21.06300	20.19000	116.60400
H	-20.71100	19.17900	117.73200
N	-13.59200	18.09700	112.55500
H	-14.00100	17.40500	111.92600
C	-12.28900	18.65600	112.22100
C	-12.40900	20.03500	111.56800
O	-13.12000	20.19200	110.58100
C	-11.56500	17.69000	111.28400
C	-10.16200	18.01600	110.78900
C	-9.20300	18.20600	111.94900
C	-9.70900	16.87400	109.91200
N	-11.70700	21.02100	112.12600
H	-11.13500	20.80700	112.94300
C	-11.71800	22.39900	111.62200
C	-13.12500	22.90400	111.32600
O	-13.31300	23.76300	110.46200
C	-10.87100	22.52900	110.34800
C	-9.38000	22.26700	110.51900
C	-8.68900	23.36200	111.30000
C	-7.21500	23.03500	111.48300
N	-6.50700	24.01500	112.35300
H	-5.51800	23.79600	112.47600
H	-6.97500	24.10700	113.25500
H	-6.62900	24.96600	112.00500
N	-14.10500	22.37300	112.05200
H	-13.86900	21.67400	112.75600

C	-15.50400	22.75000	111.88300
C	-15.72100	24.24900	112.06600
O	-16.34800	24.90000	111.23300
C	-16.36800	21.98900	112.87900
C	-17.78700	21.81000	112.39300
O	-18.41900	22.82100	112.01400
O	-18.27100	20.65500	112.38900
N	-15.21600	24.79700	113.16500
H	-14.72600	24.21300	113.84300
C	-15.35600	26.22500	113.40900
C	-14.70700	26.94700	112.24100
O	-15.32300	27.78700	111.58500
C	-14.65200	26.62900	114.70700
C	-14.61500	28.13800	114.92800
C	-13.93000	28.52600	116.24200
C	-13.98100	30.05200	116.46500
N	-13.29600	30.53100	117.71700
H	-13.33000	31.54000	117.86400
H	-12.33000	30.20300	117.73900
H	-13.66700	30.04200	118.53200
N	-13.45400	26.58600	111.98700
H	-13.03000	25.86600	112.57200
C	-12.65600	27.16500	110.91700
C	-13.37200	27.21000	109.56900
O	-13.43100	28.25800	108.92600
C	-11.34000	26.39500	110.78700
C	-10.35900	26.63800	111.93600
C	-10.83200	26.08100	113.26900
O	-10.20100	26.40200	114.29700
O	-11.82200	25.32100	113.29300
N	-13.90900	26.07400	109.13800
H	-13.82100	25.23100	109.70500
C	-14.62200	26.01300	107.86800
C	-15.76500	27.02100	107.88100
O	-15.99600	27.73100	106.90000
C	-15.18600	24.60400	107.62300
C	-15.97900	24.57200	106.33100
C	-14.04800	23.60400	107.57100
N	-16.46500	27.08800	109.01100
H	-16.20600	26.47800	109.78600
C	-17.59000	28.00300	109.18200
C	-17.17800	29.45700	109.00000
O	-17.67000	30.14700	108.10400

C	-18.20300	27.81600	110.55600
N	-16.27800	29.92400	109.85600
H	-15.90400	29.31000	110.58000
C	-15.82000	31.30100	109.77300
C	-15.44400	31.72000	108.35200
O	-15.87400	32.77400	107.87800
C	-14.61800	31.52600	110.68400
C	-13.97000	32.85600	110.48500
C	-14.63900	34.02000	110.82800
C	-12.72300	32.95100	109.87500
C	-14.08000	35.26700	110.56000
C	-12.15200	34.19200	109.60100
C	-12.83300	35.35500	109.94300
N	-14.64800	30.89600	107.67500
H	-14.34100	30.02700	108.11300
C	-14.20500	31.20800	106.32100
C	-15.25200	31.08500	105.22000
O	-15.22800	31.84900	104.25200
C	-12.98700	30.36300	105.96200
C	-11.81100	30.67900	106.81000
C	-11.36800	29.97900	107.89300
C	-10.94700	31.80800	106.67800
N	-10.27900	30.60300	108.44500
H	-9.76200	30.28100	109.26300
C	-9.99900	31.72900	107.71900
C	-10.88000	32.88100	105.78200
C	-8.99500	32.68500	107.88900
C	-9.87900	33.83300	105.95100
C	-8.95100	33.72700	106.99800
N	-16.16500	30.13100	105.34800
H	-16.14600	29.50800	106.15500
C	-17.19300	29.97900	104.33100
C	-17.94000	31.30200	104.19900
O	-18.37400	31.67900	103.10900
C	-18.20000	28.87800	104.70300
O	-17.51300	27.62900	104.84600
H	-18.13500	26.94900	105.07600
C	-19.26300	28.74300	103.62300
N	-18.06400	32.00600	105.32100
H	-17.65500	31.63300	106.17800
C	-18.76000	33.29000	105.38100
C	-17.91600	34.46500	104.89600
O	-18.27700	35.13700	103.92900

C	-19.22500	33.55300	106.81400
C	-20.17800	32.48600	107.31400
O	-20.33700	31.43700	106.68500
N	-20.81300	32.74300	108.45300
H	-20.68200	33.61000	108.97300
H	-21.45400	32.02500	108.79000
N	-16.80100	34.71700	105.57200
H	-16.55600	34.13000	106.36900
C	-15.92300	35.81500	105.19600
C	-15.74600	35.89500	103.68100
O	-15.81900	36.97900	103.09900
C	-14.55500	35.65500	105.86700
C	-13.50100	36.72900	105.56100
C	-14.01300	38.09500	105.98300
C	-12.20800	36.40800	106.29200
N	-15.52300	34.74600	103.04800
H	-15.48700	33.88100	103.58700
C	-15.32800	34.69200	101.60200
C	-16.57600	35.02300	100.79700
O	-16.48200	35.51500	99.67000
C	-14.79800	33.31900	101.20100
C	-13.31500	33.17300	101.37600
C	-12.70900	31.92300	101.28000
C	-12.51700	34.29000	101.61900
C	-11.33300	31.78700	101.42300
C	-11.13900	34.16300	101.76200
C	-10.54600	32.90800	101.66400
N	-17.74200	34.74900	101.37100
H	-17.75600	34.31900	102.29600
C	-19.00200	35.05100	100.70400
C	-19.19200	36.56300	100.76900
O	-20.21300	37.10100	100.33700
C	-20.14800	34.34500	101.40600
N	-18.18100	37.23500	101.31500
H	-17.37100	36.70900	101.64300
C	-18.17400	38.68500	101.46700
C	-19.27400	39.13100	102.42000
O	-19.25700	38.78000	103.60100
C	-18.34100	39.36700	100.10400
C	-17.31800	38.92400	99.06800
C	-17.07500	40.00800	98.03900
C	-16.45300	41.23100	98.70100
N	-16.20400	42.34300	97.74300

H	-15.78800	43.16200	98.18600
H	-17.05800	42.59300	97.24400
H	-15.63800	42.02700	96.95600
N	17.10200	4.42900	20.20000
H	17.54100	3.72900	19.60200
H	16.08800	4.32100	20.22000
H	17.29900	4.25500	21.18600
C	17.48800	5.78300	19.80800
C	16.83100	6.83100	20.70300
O	17.40000	7.89900	20.95000
C	17.10800	6.04300	18.34400
O	15.70900	5.92200	18.13900
H	15.47400	6.08300	17.23300
N	15.62800	6.52400	21.18200
H	15.20500	5.63000	20.93300
C	14.90100	7.43900	22.05500
C	15.14300	7.02300	23.50500
O	15.26800	5.83400	23.80000
C	13.40300	7.39700	21.73700
O	12.71100	8.42000	22.43300
H	11.78200	8.39400	22.23600
N	15.22000	7.99900	24.42700
C	15.45300	7.70700	25.84300
C	14.54200	6.61200	26.39700
O	13.32600	6.64200	26.19400
C	15.21200	9.05600	26.51100
C	15.68200	10.01100	25.48800
C	15.08700	9.45000	24.21700
N	15.12500	5.62300	27.09800
C	14.34800	4.52300	27.68000
C	13.40600	5.09100	28.72700
O	13.72000	6.10700	29.35000
C	15.41300	3.64500	28.33400
C	16.66900	3.98900	27.60400
C	16.55800	5.46500	27.39400
N	12.25400	4.45800	28.91900
H	12.02400	3.64300	28.35000
C	11.31500	4.91800	29.93600
C	10.60800	3.73800	30.56600
O	9.76200	3.12100	29.94500
C	10.26400	5.89300	29.36600
C	9.19300	6.16100	30.40500
C	10.92100	7.20700	28.99500

N	10.96600	3.42700	31.80600
H	11.68000	3.98600	32.27300
C	10.36300	2.30700	32.51500
C	9.44200	2.79700	33.62500
O	9.75200	3.77500	34.30400
C	11.45300	1.41100	33.14400
C	10.81100	0.26600	33.91900
C	12.37700	0.88100	32.06200
N	8.30900	2.12400	33.80700
H	8.08900	1.33300	33.20200
C	7.37800	2.50600	34.86300
C	7.67000	1.71200	36.12300
O	7.66600	0.48600	36.09400
C	5.93300	2.24000	34.44700
C	5.56800	2.92600	33.15200
O	5.95700	4.10000	32.97100
O	4.88300	2.29900	32.31500
N	7.93900	2.40000	37.22700
H	7.96400	3.41900	37.20000
C	8.19900	1.69700	38.47700
C	6.96300	1.85900	39.34600
O	5.95400	2.40100	38.89900
C	9.45500	2.24000	39.22400
O	9.10400	3.36500	40.04200
H	8.43500	3.11100	40.66700
C	10.52800	2.64700	38.22100
N	7.03500	1.38800	40.58100
H	7.90100	0.96200	40.91100
C	5.89300	1.47400	41.46700
C	5.58700	2.89900	41.86900
O	4.42800	3.26700	42.01000
C	6.11100	0.62700	42.72400
C	4.87900	0.67600	43.60800
C	6.42100	-0.80800	42.32000
N	6.61500	3.71400	42.03900
H	7.56600	3.37800	41.88900
C	6.38200	5.09300	42.44100
C	6.45900	6.10600	41.29800
O	6.49500	7.31300	41.53500
C	7.36200	5.48400	43.55300
C	7.37300	4.53300	44.71000
N	6.22000	4.05300	45.29300
H	5.27100	4.27200	44.98900

C	8.39900	3.99900	45.41500
C	6.53300	3.26600	46.30600
N	7.84900	3.21700	46.40100
H	8.37300	2.68400	47.09500
N	6.48500	5.62300	40.06000
H	6.46400	4.61500	39.90300
C	6.54300	6.53700	38.93100
C	7.41000	6.11800	37.75700
O	8.02000	5.05000	37.75700
N	7.46600	6.97700	36.74800
H	6.94200	7.85000	36.80700
C	8.25700	6.70200	35.55900
C	9.68400	7.26200	35.65200
O	9.90900	8.35900	36.17400
C	7.56100	7.28700	34.32500
C	6.14300	6.78400	34.09200
C	5.58800	7.36000	32.79300
C	4.15100	6.92900	32.51900
N	3.99900	5.46900	32.23900
H	3.03800	5.18100	32.05600
H	4.40100	4.91500	32.99500
H	4.61100	5.18500	31.47400
N	10.64400	6.49200	35.14700
H	10.39400	5.58700	34.75000
C	12.04200	6.90200	35.14400
C	12.54300	6.93600	33.71200
O	12.25300	6.04400	32.91200
C	12.93100	5.93600	35.94000
C	12.56400	5.98300	37.39900
C	12.77900	4.52800	35.40000
N	13.30400	7.97700	33.40500
H	13.51100	8.66100	34.13200
C	13.85700	8.18600	32.07500
C	15.36000	7.98000	32.16400
O	16.04400	8.67700	32.91500
C	13.53800	9.62000	31.62200
C	13.88300	10.23100	30.25800
C	15.37400	10.26800	30.06500
C	13.21200	9.44500	29.15900
N	15.86900	7.01200	31.41100
H	15.25400	6.45000	30.82300
C	17.29500	6.75000	31.42000
C	17.91900	7.04500	30.06900

O	17.32200	7.71700	29.22800
N	19.13200	6.55100	29.85800
H	19.59300	6.02200	30.59800
C	19.81500	6.75100	28.59100
C	20.37800	5.41500	28.10100
O	20.59100	4.49900	28.89300
C	20.94500	7.76800	28.75400
C	22.00000	7.33600	29.74000
C	23.25400	8.18700	29.62500
C	24.35900	7.62700	30.51800
N	25.65100	8.36400	30.39100
H	26.38900	7.99000	30.98700
H	25.51800	9.36100	30.56100
H	25.95400	8.39900	29.41800
N	20.59000	5.30800	26.79100
H	20.34900	6.09700	26.19200
C	21.15400	4.10800	26.17400
C	22.65900	4.30100	25.99200
O	23.12300	5.40700	25.72100
C	20.52600	3.86500	24.79900
C	19.20100	3.16200	24.84000
C	18.05200	3.79400	24.38800
C	19.10700	1.85400	25.31300
C	16.83000	3.14000	24.40200
C	17.88900	1.19200	25.33200
C	16.74700	1.83800	24.87400
N	23.42900	3.23500	26.13400
H	23.01600	2.33300	26.37100
C	24.86800	3.35300	25.95100
C	25.38700	2.09500	25.27200
O	25.00300	0.99400	25.65500
C	25.58200	3.53100	27.30000
C	27.07400	3.71400	27.07600
C	24.98100	4.71500	28.05000
N	26.24800	2.25200	24.26700
H	26.53300	3.19200	23.99300
C	26.79300	1.09500	23.54800
C	28.24200	0.78000	23.86700
O	29.09100	1.67100	23.87300
C	26.67500	1.28600	22.03700
O	25.35500	1.03400	21.59600
H	25.28200	1.15300	20.65600
N	28.51800	-0.49800	24.11600

H	27.76100	-1.18200	24.09600
C	29.87100	-0.94800	24.41700
C	30.49900	-1.47400	23.13300
O	29.81900	-2.05700	22.29500
C	29.85100	-2.05500	25.47500
C	31.18300	-2.32600	26.17600
C	31.64700	-1.05900	26.86500
C	31.02500	-3.44100	27.19000
N	31.80000	-1.25100	22.99700
H	32.28200	-0.76100	23.75000
C	32.58300	-1.66300	21.83800
C	31.88700	-2.41200	20.69400
O	31.46800	-1.79700	19.71600
C	33.79700	-2.46900	22.30300
C	34.82500	-2.70400	21.19900
C	35.05900	-1.46100	20.34100
O	35.30000	-0.37300	20.91200
O	35.00200	-1.57700	19.09500
N	31.76500	-3.73000	20.79400
H	32.10100	-4.22300	21.62100
C	31.14200	-4.45700	19.70000
C	29.74900	-5.01800	19.91100
O	29.30700	-5.88700	19.15900
N	29.03900	-4.52600	20.91500
H	29.42900	-3.78700	21.50000
C	27.70800	-5.03500	21.18400
C	26.60500	-4.29300	20.44400
O	26.50900	-3.07600	20.50600
C	27.44600	-5.01800	22.69000
C	28.34800	-5.93200	23.46500
C	29.64800	-5.55400	23.76600
C	27.90800	-7.19300	23.85700
C	30.50100	-6.42300	24.44600
C	28.74800	-8.06600	24.53300
C	30.05000	-7.68300	24.83100
N	25.76800	-5.04600	19.74300
H	25.89900	-6.05800	19.73600
C	24.66800	-4.46900	18.98400
C	23.51000	-4.03100	19.88300
O	22.84400	-3.03300	19.60500
C	24.17700	-5.47200	17.94100
N	23.26100	-4.77900	20.95300
H	23.83200	-5.60400	21.13500

C	22.17900	-4.43300	21.87200
C	22.69400	-3.38800	22.85000
O	23.59900	-3.65500	23.63900
C	21.69700	-5.67700	22.63300
C	20.58800	-5.42400	23.65300
C	19.29300	-4.90500	23.03100
O	18.70500	-5.54500	22.14700
N	18.83600	-3.74400	23.49800
H	19.32000	-3.21700	24.22500
H	17.97100	-3.39700	23.08300
N	22.14800	-2.16700	22.79600
C	22.65000	-1.17200	23.74400
C	22.17600	-1.49800	25.15200
O	21.29500	-2.34300	25.34900
C	22.06700	0.13300	23.21800
C	20.75000	-0.30900	22.65800
C	21.11600	-1.59000	21.91900
N	22.77200	-0.82800	26.12900
H	23.49900	-0.15000	25.89900
C	22.41200	-1.03900	27.52000
C	21.75400	0.23000	28.03900
O	22.24700	1.33400	27.81500
C	23.66100	-1.36900	28.37500
C	23.24300	-1.80700	29.76200
C	24.47600	-2.46000	27.70400
N	20.62400	0.06500	28.70900
H	20.25000	-0.87600	28.83400
C	19.90500	1.19600	29.27000
C	20.48500	1.49600	30.65000
O	20.66700	0.58800	31.46500
C	18.43300	0.87000	29.38000
N	20.77300	2.76700	30.91100
H	20.58900	3.48100	30.20600
C	21.34700	3.15000	32.19000
C	20.53100	4.18200	32.95100
O	20.21300	5.25100	32.43000
C	22.76500	3.69800	32.00800
C	23.65800	2.62400	31.39200
C	23.32800	4.13100	33.34600
C	25.03500	3.12500	31.01700
N	20.20300	3.84800	34.19500
H	20.49500	2.94000	34.55600
C	19.44000	4.73700	35.05900

C	20.29700	5.09400	36.26200
O	20.83400	4.21800	36.94600
C	18.15400	4.05600	35.52600
C	17.26300	3.61200	34.40200
C	17.51600	2.42300	33.72800
C	16.19500	4.41300	33.98900
C	16.72400	2.03900	32.65900
C	15.39500	4.03800	32.91900
C	15.65800	2.84900	32.25000
N	20.42200	6.38600	36.52700
H	19.93600	7.06900	35.94600
C	21.24400	6.84100	37.63500
C	20.46200	7.62000	38.67700
O	19.75300	8.56700	38.34900
C	22.38100	7.71500	37.10400
C	23.27000	7.10700	36.01800
C	24.24900	8.16000	35.54400
C	23.99600	5.88100	36.55200
N	20.59500	7.21300	39.93400
H	21.17900	6.40400	40.14600
C	19.91500	7.91300	41.00700
C	18.44400	7.61000	41.21600
O	17.66000	8.51500	41.53000
N	18.04900	6.35500	41.03000
H	18.71700	5.64700	40.72500
C	16.66300	5.99800	41.26300
C	16.56200	5.87300	42.76800
O	17.30800	5.10600	43.37500
C	16.30900	4.64600	40.66100
C	16.28900	4.74300	39.13400
C	14.97500	4.17400	41.22800
C	16.03400	3.41700	38.44300
N	15.66500	6.64600	43.39800
C	15.50200	6.58300	44.85300
C	14.77200	5.30500	45.25400
O	13.82900	4.89400	44.58000
C	14.67800	7.82900	45.15200
C	13.79900	7.92200	43.95600
C	14.77300	7.66500	42.81800
N	15.22100	4.66500	46.32900
H	16.03100	5.02800	46.83100
C	14.56700	3.44900	46.79700
C	14.04100	3.67700	48.21000

O	13.58200	2.75000	48.88500
C	15.52100	2.23700	46.73600
C	16.68500	2.31000	47.68500
C	16.56800	1.84200	48.99300
C	17.89900	2.84500	47.27200
C	17.64600	1.91000	49.87100
C	18.98000	2.91800	48.13800
C	18.85800	2.45200	49.43900
N	14.08800	4.93300	48.64200
H	14.47100	5.65500	48.03200
C	13.60500	5.30400	49.96700
C	13.42000	6.81200	50.09300
O	13.82600	7.58300	49.22600
C	14.56500	4.80300	51.03400
N	12.79700	7.22600	51.18300
H	12.47200	6.53600	51.86100
C	12.56200	8.63500	51.44200
C	13.85300	9.22900	52.01300
O	14.50900	8.61300	52.85200
C	11.41400	8.75700	52.44700
C	10.99500	10.15100	52.81000
C	9.96300	10.09100	53.93200
C	9.42300	11.46000	54.30100
N	8.69000	12.07700	53.15200
H	8.32700	12.99700	53.40000
H	7.95300	11.46400	52.80400
H	9.27000	12.11500	52.31400
N	14.25400	10.41900	51.54700
C	15.48100	11.02700	52.07300
C	15.49600	10.99600	53.60800
O	14.64200	11.61400	54.24900
C	15.41000	12.45000	51.52400
C	14.79000	12.24000	50.18000
C	13.68000	11.23600	50.46300
N	16.46100	10.27300	54.21400
C	16.60900	10.14100	55.67000
C	17.06700	11.41500	56.37200
O	18.11700	11.43200	57.01700
C	17.63200	9.01900	55.80400
C	18.49800	9.22500	54.62200
C	17.48400	9.46900	53.52400
N	16.26200	12.47200	56.25800
H	15.39200	12.37200	55.73500

C	16.58000	13.76800	56.85400
C	15.74500	14.10000	58.08100
O	14.77400	13.40700	58.40300
C	16.39400	14.87300	55.81500
C	17.01800	14.53600	54.46300
C	16.72300	15.63400	53.44800
C	18.50800	14.33000	54.65500
N	16.14200	15.17600	58.75600
H	16.95600	15.69600	58.42800
C	15.44800	15.62700	59.94300
C	15.24400	14.50200	60.92400
O	16.19000	13.79900	61.26600
N	14.00800	14.29600	61.39100
C	13.71700	13.22700	62.34600
C	13.97700	11.82000	61.80700
O	14.16200	10.89100	62.58300
C	12.24900	13.46500	62.68200
C	11.71700	14.01900	61.40400
C	12.77600	15.00800	61.01700
N	13.99100	11.65900	60.48600
H	13.83700	12.46300	59.87700
C	14.22500	10.34300	59.90100
C	15.65500	9.83000	60.11300
O	15.95200	8.66200	59.84200
C	13.87500	10.34900	58.40700
C	12.37500	10.40600	58.09200
C	12.13000	10.18600	56.61000
C	11.65400	9.33800	58.89200
N	16.53300	10.69700	60.61100
H	16.23500	11.65100	60.81300
C	17.91400	10.30700	60.87300
C	17.97100	9.31900	62.04300
O	17.30900	9.51500	63.06000
C	18.75300	11.53900	61.19700
C	20.21500	11.23200	61.41800
C	20.94100	12.43900	61.96200
N	21.07200	13.50200	60.97500
H	20.88600	13.27900	59.99700
C	21.42100	14.74700	61.28100
N	21.66200	15.07200	62.54500
H	21.93000	16.02800	62.78000
H	21.57100	14.36900	63.27900
N	21.53900	15.66000	60.32800

H	21.80700	16.61600	60.56300
H	21.35400	15.41000	59.35700
N	18.77400	8.27000	61.89700
H	19.32100	8.18800	61.04000
C	18.90500	7.22700	62.91600
C	17.61200	6.43200	63.04200
O	17.28200	5.94000	64.11800
C	19.25400	7.81100	64.29100
C	20.46000	8.69600	64.28700
C	21.63500	8.29500	63.64900
C	20.42900	9.92900	64.93300
C	22.76100	9.10900	63.65500
C	21.54300	10.75000	64.94900
C	22.71400	10.34200	64.31000
N	16.86700	6.33000	61.94700
H	17.16900	6.79500	61.09100
C	15.62200	5.56400	61.94700
C	15.63700	4.70400	60.68500
O	16.29000	5.05200	59.70000
C	14.35700	6.48100	61.92600
O	13.98500	6.77800	60.57200
H	13.81400	5.96200	60.11700
C	14.62900	7.77700	62.64800
N	14.92800	3.56600	60.70100
C	14.89300	2.69100	59.52700
C	14.49000	3.49700	58.30900
O	13.80000	4.50400	58.43900
C	13.84000	1.66100	59.89800
C	13.98800	1.56900	61.38200
C	14.11400	3.01200	61.79300
N	14.92400	3.07500	57.11200
C	14.57700	3.79700	55.88800
C	13.10000	3.62900	55.60800
O	12.51500	2.59900	55.92900
C	15.42000	3.10400	54.83300
C	15.38600	1.69600	55.28900
C	15.65000	1.83700	56.78400
N	12.48800	4.63800	55.01100
H	13.00700	5.48400	54.77500
C	11.08100	4.53900	54.69400
C	10.85400	4.58800	53.20000
O	11.71500	5.03300	52.43700
C	10.30800	5.64100	55.40400

C	9.92600	5.24500	56.81000
C	9.75800	6.43600	57.71600
O	8.98700	7.35500	57.42200
N	10.48400	6.43300	58.83400
H	10.37000	7.24000	59.44800
H	11.12100	5.67400	59.07700
N	9.69400	4.09700	52.75700
C	9.35600	4.08700	51.33500
C	9.51200	5.47400	50.73000
O	9.45300	6.47400	51.44200
C	7.91700	3.60300	51.34000
C	7.91300	2.65200	52.50600
C	8.64400	3.43800	53.55100
N	9.72400	5.53500	49.42200
H	9.77200	4.67000	48.88300
C	9.88900	6.80800	48.74000
C	8.53700	7.35900	48.30800
O	7.60800	6.59600	48.00900
C	10.78800	6.63000	47.53300
N	8.43000	8.68500	48.27900
H	9.23200	9.25500	48.54800
C	7.19500	9.34300	47.87300
C	7.03600	9.26800	46.35800
O	7.93700	9.64800	45.60100
C	7.20800	10.79900	48.32900
C	7.35900	10.95700	49.83200
C	6.04900	10.76100	50.58100
O	5.28100	9.83100	50.23300
O	5.79600	11.54000	51.53000
N	5.87800	8.77400	45.89700
C	5.56400	8.62900	44.47200
C	5.57100	9.94900	43.72100
O	5.02500	10.94100	44.19500
C	4.18600	7.98300	44.49300
C	3.58100	8.55600	45.74000
C	4.70700	8.44000	46.72600
N	6.19900	9.95500	42.55000
H	6.64400	9.10100	42.21500
C	6.26200	11.16000	41.73800
C	5.19500	11.13900	40.64900
O	4.71900	10.07700	40.24900
C	7.66600	11.33700	41.15200
C	8.19800	10.14300	40.45200

C	8.10100	9.86000	39.12000
C	8.91600	9.06000	41.04200
N	8.71800	8.66600	38.84300
H	8.78700	8.23300	37.92200
C	9.22700	8.15100	40.00700
C	9.33100	8.76700	42.34600
C	9.93400	6.96500	40.23600
C	10.03700	7.58700	42.57200
C	10.33100	6.70200	41.52000
N	4.83300	12.32600	40.17300
H	5.31400	13.15900	40.51100
C	3.77300	12.47800	39.18600
C	4.04000	12.33700	37.69600
O	3.19900	11.78200	36.97800
C	3.04500	13.80300	39.42600
O	2.30000	13.74600	40.63300
H	1.84800	14.56800	40.78200
N	5.16200	12.83600	37.19700
H	5.84600	13.29500	37.79800
C	5.38700	12.70800	35.76600
C	6.51900	11.73700	35.47000
O	6.51200	10.61600	35.98100
C	5.62400	14.09100	35.14900
C	4.45000	15.03000	35.31900
C	4.49900	16.08100	36.23400
C	3.26300	14.81200	34.62700
C	3.38000	16.89200	36.45900
C	2.14800	15.61600	34.84700
C	2.20900	16.65600	35.76700
N	7.47300	12.13100	34.63500
H	7.42100	13.05200	34.19900
C	8.59400	11.24900	34.34100
C	9.81400	11.78400	35.07600
O	10.16600	12.95000	34.92200
C	8.89300	11.18600	32.81600
C	10.22700	10.48600	32.56700
C	7.78300	10.43900	32.09600
N	10.44300	10.93500	35.88400
H	10.08900	9.98300	35.98100
C	11.62800	11.33700	36.63400
C	12.90600	11.00100	35.86400
O	13.13300	9.85500	35.47700
C	11.64600	10.64900	38.00200

C	12.85000	11.02500	38.86300
C	12.90700	10.22100	40.15300
C	11.79200	10.58000	41.11700
N	11.92200	11.96000	41.64400
H	11.17200	12.20100	42.29200
H	11.98500	12.63900	40.88500
H	12.83700	12.10600	42.07000
N	13.74200	12.00700	35.65100
H	13.50400	12.93300	36.00700
C	14.99500	11.82900	34.92100
C	16.13600	11.22900	35.72800
O	16.81800	11.92900	36.47600
C	15.45000	13.16500	34.35400
C	14.74100	13.51600	33.08400
O	13.65500	13.00900	32.80300
N	15.36200	14.39800	32.31200
H	16.26200	14.81800	32.54500
H	14.87900	14.63700	31.44600
N	16.35200	9.93200	35.55000
H	15.75600	9.41700	34.90200
C	17.41000	9.22200	36.24900
C	18.68400	9.31200	35.42500
O	19.17200	8.29500	34.93000
C	17.00900	7.77100	36.42900
N	19.23300	10.51700	35.28700
H	18.81300	11.32100	35.75300
C	20.43200	10.69500	34.47300
C	21.60400	11.45300	35.06600
O	22.41100	12.01600	34.32700
C	20.09300	11.36600	33.13900
O	18.88800	12.12500	33.28500
H	18.99300	12.77400	33.97100
C	19.92500	10.32900	32.04400
N	21.70200	11.47400	36.38900
H	20.98400	11.01400	36.94900
C	22.81400	12.14000	37.06400
C	23.26300	11.30000	38.23900
O	22.44500	10.83800	39.04200
C	22.40800	13.51800	37.57700
O	22.21800	14.41700	36.50900
H	21.96500	15.27500	36.82800
N	24.56600	11.09300	38.34300
H	25.20500	11.47600	37.64600

C	25.07700	10.31900	39.45300
C	24.51000	10.92600	40.72600
O	24.54100	12.14200	40.92200
C	26.60100	10.36100	39.45800
C	27.19200	9.54200	38.34600
C	27.09900	8.15500	38.36600
C	27.81400	10.14500	37.25300
C	27.61200	7.37900	37.32400
C	28.33200	9.37900	36.20200
C	28.22600	7.99600	36.24800
O	28.73600	7.21600	35.23500
H	28.66300	6.26900	35.26600
N	23.94200	10.08700	41.59600
C	23.39500	10.65100	42.82600
C	24.56000	11.05700	43.71500
O	25.72900	10.85500	43.36400
C	22.60700	9.48600	43.40600
C	23.47300	8.31900	43.03800
C	23.84700	8.61600	41.59800
N	24.25900	11.66000	44.86600
C	25.32300	12.07300	45.78200
C	25.73100	10.85600	46.59700
O	24.91800	9.95600	46.81200
C	24.64100	13.11800	46.66200
C	23.48300	13.59400	45.82400
C	22.99300	12.33000	45.19500
N	26.98500	10.79900	47.02800
H	27.65300	11.52600	46.77300
C	27.39300	9.68500	47.86900
C	27.09000	10.16400	49.27700
O	27.18900	11.36000	49.55500
C	28.88500	9.36400	47.70700
C	29.80400	10.56600	47.55200
S	31.56200	10.10700	47.35700
C	32.28700	10.98600	48.75100
N	26.68600	9.24000	50.14600
H	26.60800	8.27300	49.83200
C	26.35000	9.55800	51.53200
C	27.49700	10.27900	52.22800
O	28.65600	10.03300	51.91900
C	26.00900	8.27800	52.27900
S	24.55000	7.39100	51.62200
N	27.17600	11.16500	53.16700

H	26.19400	11.31100	53.39900
C	28.20000	11.93500	53.87500
C	29.34400	11.06600	54.38400
O	29.13300	10.02100	55.01200
C	27.61800	12.71700	55.08000
O	26.41100	13.38900	54.69000
H	25.78300	12.74300	54.38900
C	28.62500	13.75200	55.56300
N	30.56100	11.52700	54.10900
H	30.64500	12.41100	53.60700
C	31.77600	10.82800	54.49200
C	32.93600	11.80100	54.36900
O	32.73800	12.96000	54.01000
C	32.00100	9.64800	53.54700
C	31.92800	10.04400	52.08800
C	31.96500	8.85400	51.14600
O	32.99000	8.18900	51.00500
N	30.83900	8.58100	50.49200
H	29.98900	9.13200	50.60900
H	30.86400	7.78100	49.85900
N	34.13900	11.32900	54.69000
H	34.22100	10.36900	55.02500
C	35.34600	12.14700	54.57600
C	35.52800	12.36300	53.08400
O	35.80400	11.42000	52.34700
C	36.56800	11.39500	55.11200
C	37.86100	12.17500	54.93500
O	37.91900	13.04600	54.04500
O	38.82400	11.90900	55.68300
N	35.38300	13.60700	52.61600
C	35.54900	13.83400	51.17800
C	36.94200	13.48400	50.62600
O	37.06600	13.02100	49.49500
C	35.16900	15.30700	51.02100
C	35.58200	15.89600	52.33100
C	35.13200	14.86700	53.33500
N	37.98500	13.68600	51.41800
H	37.84400	14.06600	52.35400
C	39.33100	13.36900	50.96100
C	39.42000	11.86400	50.75900
O	39.62700	11.38100	49.64200
C	40.36100	13.81000	51.99900
C	41.61200	14.44300	51.41500

C	41.90700	15.80300	52.08400
C	40.77000	16.82800	51.84600
N	40.96200	18.12100	52.57900
H	40.21300	18.79600	52.42200
H	41.86900	18.53100	52.35500
H	41.09300	17.95300	53.57700
N	39.24900	11.12900	51.85500
H	39.07400	11.60400	52.74000
C	39.30200	9.67300	51.84200
C	38.33000	9.08100	50.82900
O	38.64800	8.13000	50.12800
C	38.98500	9.14900	53.22500
N	37.13600	9.65400	50.76800
H	36.92900	10.44600	51.37600
C	36.12200	9.17500	49.85400
C	36.55000	9.28900	48.41200
O	36.40200	8.34200	47.64300
N	37.07600	10.44600	48.02700
H	37.17200	11.21200	48.69400
C	37.51600	10.61800	46.64800
C	38.62900	9.63200	46.35900
O	38.62100	8.95600	45.33400
C	38.00900	12.04400	46.40500
C	36.90600	13.04700	46.07900
C	36.28500	12.83200	44.69200
O	35.39200	11.99000	44.50900
N	36.76800	13.59200	43.70600
H	37.50200	14.28400	43.85600
H	36.35500	13.44900	42.78400
N	39.56700	9.53000	47.29200
H	39.49000	10.09000	48.14100
C	40.70200	8.63700	47.13000
C	40.32500	7.18700	46.86200
O	40.84700	6.57100	45.92500
C	41.60800	8.70300	48.35700
C	42.87000	7.84800	48.24800
C	43.60900	8.17600	46.96100
C	43.74000	8.07600	49.45900
N	39.43400	6.63400	47.68300
H	39.04100	7.18500	48.44600
C	39.01400	5.25100	47.50400
C	38.33200	5.07200	46.15100
O	38.60000	4.10600	45.43500

C	38.06300	4.82700	48.62100
C	37.84500	3.31600	48.72400
C	39.14000	2.62400	49.12500
C	36.76000	3.03600	49.74400
N	37.45900	6.01000	45.79900
H	37.28200	6.79000	46.43200
C	36.74800	5.94800	44.52600
C	37.73100	5.96700	43.35700
O	37.50600	5.31200	42.33900
C	35.77600	7.12700	44.39900
O	35.03400	7.05500	43.19200
H	34.43200	7.78500	43.11300
N	38.82500	6.71100	43.49800
H	38.98000	7.22700	44.36400
C	39.80200	6.79200	42.42300
C	40.60000	5.50700	42.30100
O	40.93500	5.09300	41.19400
C	40.74100	7.97900	42.64000
C	40.00500	9.30400	42.77000
C	40.92800	10.51200	42.86600
O	41.95100	10.42900	43.58300
O	40.61300	11.54900	42.23400
N	40.88300	4.87300	43.43800
H	40.54900	5.27200	44.31600
C	41.65200	3.62900	43.48100
C	40.87500	2.40000	43.00800
O	41.46000	1.48500	42.42200
C	42.13800	3.37000	44.90500
C	43.25200	4.22000	45.50900
C	43.26800	4.07900	47.03000
C	44.56500	3.77400	44.92400
N	39.56600	2.38100	43.26500
H	39.14600	3.18200	43.73700
C	38.71200	1.25200	42.89400
C	37.90400	1.36100	41.60900
O	37.48800	0.35100	41.05900
C	37.73400	0.94900	44.02600
C	38.33200	0.17800	45.15600
C	39.65800	-0.23900	45.11000
C	37.56100	-0.15300	46.26500
C	40.20900	-0.97700	46.15500
C	38.10000	-0.89200	47.31600
C	39.43000	-1.30600	47.26300

N	37.66700	2.57000	41.12600
H	38.04600	3.39100	41.59800
C	36.86600	2.72800	39.92300
C	37.39200	1.93300	38.73600
O	38.59300	1.76400	38.56300
C	36.74100	4.20300	39.53000
O	35.84800	4.31300	38.42000
H	35.00000	3.95300	38.65200
C	38.09200	4.77700	39.16100
N	36.47700	1.44500	37.91400
H	35.49100	1.62800	38.09800
C	36.85000	0.65500	36.75700
C	36.58600	1.41400	35.47600
O	36.75900	0.87500	34.38900
C	36.05600	-0.64800	36.74600
C	34.56000	-0.41300	36.67100
O	34.01000	0.41000	37.40400
N	33.89200	-1.14300	35.78900
H	34.34700	-1.82500	35.18200
H	32.88600	-0.98500	35.73900
N	36.15400	2.66200	35.60500
H	36.01500	3.04800	36.53900
C	35.87300	3.49400	34.44100
C	37.12900	4.29500	34.09100
O	37.98900	4.49900	34.94200
C	34.68900	4.42900	34.73500
C	34.75000	5.06100	36.11500
C	33.72900	6.17900	36.34600
N	32.39600	5.72200	36.74500
H	32.14300	5.79600	37.73000
C	31.49600	5.21800	35.91100
N	31.78300	5.09800	34.62100
H	31.09100	4.71000	33.98000
H	32.69900	5.37900	34.27100
N	30.30600	4.85300	36.36600
H	29.61400	4.46500	35.72500
H	30.08500	4.94500	37.35800
N	37.24000	4.72900	32.83800
H	36.49300	4.52200	32.17500
C	38.40200	5.49500	32.38200
C	38.71800	6.70000	33.26500
O	39.79200	6.78600	33.86000
C	38.18800	5.96500	30.93700

C	36.71900	6.19900	30.59000
C	36.52800	7.05100	29.32900
C	36.59500	8.55100	29.63400
N	36.28700	9.40400	28.44400
H	36.33200	10.40300	28.64700
H	35.38400	9.15400	28.04100
H	36.89200	9.16500	27.65800
N	37.77700	7.63100	33.33600
H	36.91200	7.49600	32.81300
C	37.93300	8.84000	34.13300
C	37.13500	8.71200	35.42800
O	36.03200	8.16700	35.42700
C	37.40800	10.03700	33.34400
C	36.05000	9.75000	32.71100
C	35.23700	10.99800	32.38700
O	34.84100	11.72300	33.33500
O	34.98600	11.24600	31.18100
N	37.67900	9.21600	36.53100
H	38.59900	9.65500	36.49400
C	36.95700	9.13800	37.78900
C	35.91300	10.24300	37.83300
O	36.15700	11.36000	37.37100
C	37.90200	9.26300	38.98300
C	37.27900	8.73000	40.27000
O	36.36800	9.33700	40.84600
N	37.75600	7.57400	40.71300
H	37.34000	7.21800	41.57300
H	38.50700	7.07300	40.23800
N	34.75100	9.91700	38.39200
H	34.63100	8.97600	38.76600
C	33.64400	10.85900	38.48800
C	33.58000	11.59100	39.82100
O	33.38200	10.97400	40.86900
C	32.29800	10.14300	38.28200
C	32.31200	9.36800	36.95900
C	31.16300	11.15200	38.33200
C	32.76000	10.17900	35.75700
N	33.73100	12.92400	39.79800
C	33.67800	13.70300	41.03500
C	32.27900	13.57800	41.62500
O	31.28700	13.61800	40.89800
C	33.97200	15.11800	40.55600
C	33.31800	15.13700	39.21200

C	33.77200	13.81500	38.62500
N	32.19600	13.42000	42.93700
H	33.04500	13.39400	43.50200
C	30.89500	13.28400	43.57400
C	30.62900	14.39200	44.57900
O	31.52600	15.15100	44.94000
C	30.78300	11.91600	44.26000
C	30.64400	10.71900	43.31500
C	31.10300	9.45100	44.01400
C	29.20300	10.60100	42.84600
N	29.37700	14.46800	45.01100
H	28.69700	13.79800	44.65000
C	28.92900	15.45700	45.97100
C	28.46700	14.68900	47.20900
O	28.05900	13.52600	47.11200
C	27.76200	16.25900	45.38000
C	27.46700	17.60300	46.06300
C	28.51100	18.65700	45.69000
C	28.04600	20.08600	45.98600
N	29.02600	21.08500	45.43200
H	28.71600	22.03700	45.62900
H	29.19400	20.93900	44.43600
H	29.97300	20.91600	45.77200
N	28.53600	15.34000	48.36600
H	28.88300	16.29900	48.37600
C	28.13000	14.72000	49.61900
C	26.73000	15.15500	50.02300
O	26.36200	16.32600	49.88000
C	29.09000	15.11300	50.73800
C	30.57000	14.78500	50.62600
C	31.29500	15.45800	51.76400
C	30.78700	13.28000	50.66700
N	25.95000	14.22000	50.54300
H	26.29100	13.26300	50.63200
C	24.61300	14.55500	50.98600
C	24.01900	13.47600	51.84300
O	24.34200	12.30000	51.69100
C	23.68000	14.78200	49.80500
O	22.38800	15.14600	50.26600
H	21.80600	15.28800	49.52900
N	23.14700	13.88200	52.75400
H	22.94700	14.87700	52.85100
C	22.47600	12.93300	53.61100

C	21.44800	12.31900	52.68700
O	20.98000	11.20200	52.89700
C	21.82300	13.65400	54.79100
C	22.57600	13.44500	56.08700
C	22.16400	14.39400	57.17700
O	20.95000	14.52500	57.44000
O	23.06400	15.00500	57.78500
N	21.12100	13.06500	51.64000
H	21.54800	13.98500	51.53500
C	20.17000	12.60900	50.63600
C	20.96600	11.71400	49.69100
O	21.54200	12.19100	48.71200
C	19.60300	13.79700	49.86600
C	18.54000	13.39200	48.88400
O	18.33900	12.17600	48.69000
O	17.90500	14.29100	48.30200
N	20.98700	10.41500	49.98000
H	20.45400	10.06300	50.77500
C	21.76400	9.49800	49.16900
C	21.19100	8.09700	48.99400
O	21.85400	7.24100	48.41700
C	23.16300	9.38800	49.77600
S	23.09800	8.80200	51.49500
N	19.98500	7.83500	49.48600
H	19.44900	8.55900	49.96500
C	19.44500	6.49000	49.32600
C	18.93000	6.22400	47.89900
O	17.72200	6.14200	47.64100
C	18.36300	6.22900	50.37800
C	18.86300	6.40800	51.81600
C	17.84700	5.86000	52.79100
C	20.16600	5.68300	51.99400
N	19.89000	6.09300	46.98500
H	20.85900	6.17600	47.29300
C	19.64000	5.83800	45.56900
C	20.38600	4.58700	45.09200
O	21.23000	4.04200	45.80800
C	20.12400	7.02000	44.73200
C	19.44900	8.31600	45.05300
C	19.94200	9.15800	46.04200
C	18.28300	8.68500	44.38800
C	19.28200	10.34000	46.36300
C	17.61800	9.85400	44.69900

C	18.11400	10.67600	45.68700
O	17.40400	11.80300	46.02700
H	17.74600	12.37000	46.70800
N	20.06600	4.14100	43.87900
H	19.33200	4.62100	43.35800
C	20.72700	2.98800	43.26400
C	20.82600	3.24400	41.75500
O	20.05300	4.04200	41.20600
C	19.93600	1.70700	43.54400
C	18.45600	1.65600	43.14500
C	18.33300	1.56100	41.62100
C	17.78400	0.45100	43.80100
N	21.78500	2.59900	41.09300
H	22.41800	1.98300	41.60300
C	21.94900	2.75800	39.64300
C	21.62900	1.44900	38.95500
O	21.97700	0.39100	39.47300
C	23.37900	3.14600	39.29000
C	23.77100	4.49100	39.84700
O	22.95400	5.41700	39.89500
N	25.03400	4.61900	40.25900
H	25.70800	3.85500	40.21900
H	25.29900	5.52900	40.63600
N	20.96700	1.50000	37.80300
H	20.67800	2.40100	37.42300
C	20.65100	0.26600	37.07700
C	21.32400	0.18800	35.69500
O	21.37900	1.17700	34.95900
C	19.11300	0.07000	36.90600
C	18.45300	-0.18400	38.27100
C	18.84100	-1.11800	35.98900
C	16.92200	-0.41700	38.22700
N	21.85700	-0.99100	35.37700
H	21.80700	-1.74300	36.06400
C	22.51200	-1.26800	34.09400
C	21.86400	-2.52600	33.51100
O	22.24900	-3.65400	33.84000
C	24.01000	-1.52200	34.28200
C	24.76000	-0.34600	34.84200
C	24.76800	-0.08100	36.20900
C	25.43900	0.52800	34.00300
C	25.44000	1.03400	36.72700
C	26.10900	1.64300	34.50600

C	26.10600	1.89000	35.86700
O	26.76100	2.99400	36.35600
H	27.21800	3.58200	35.76600
N	20.87300	-2.34500	32.65000
H	20.58800	-1.40200	32.38500
C	20.19700	-3.49800	32.08800
C	20.44300	-3.68600	30.60300
O	20.25600	-2.76600	29.80200
C	18.69000	-3.41600	32.32800
O	18.09400	-4.66900	31.98300
H	18.48000	-5.36200	32.50600
C	18.07200	-2.30600	31.49000
N	20.87700	-4.89300	30.21600
C	21.15800	-5.22600	28.81700
C	19.93200	-5.78100	28.08800
O	19.97200	-6.02400	26.88000
C	22.27400	-6.25400	28.94000
C	21.85000	-7.03400	30.15300
C	21.39500	-5.93900	31.12100
N	18.84300	-5.97100	28.82300
H	18.86300	-5.73100	29.81400
C	17.62000	-6.51500	28.24600
C	16.93100	-5.56500	27.26900
O	17.09600	-4.34400	27.35000
C	16.64600	-6.89200	29.36600
N	16.16900	-6.13100	26.33400
H	16.11400	-7.14800	26.27600
C	15.41200	-5.31200	25.39200
C	14.13800	-4.96200	26.16700
O	13.29100	-5.81600	26.41800
C	15.06900	-6.09800	24.12200
C	14.29400	-5.26200	23.10700
O	14.77000	-4.15900	22.74700
O	13.21000	-5.71100	22.66900
N	14.01300	-3.70300	26.55800
H	14.72800	-3.02100	26.30300
C	12.87400	-3.28600	27.34200
C	11.54200	-3.40300	26.62500
O	10.50300	-3.54700	27.27100
C	13.10600	-1.86400	27.85000
C	14.36700	-1.75200	28.72800
C	14.62800	-0.29800	29.06300
C	14.21800	-2.59200	30.00700

N	11.56400	-3.37200	25.29600
H	12.45700	-3.28100	24.81100
C	10.32600	-3.46700	24.51600
C	9.62900	-4.82100	24.67200
O	8.40800	-4.90100	24.60800
C	10.58200	-3.24800	23.02100
O	10.91900	-4.49900	22.40800
H	11.07800	-4.36300	21.48100
C	11.72600	-2.26600	22.82100
N	10.40600	-5.88100	24.86600
H	11.41700	-5.75400	24.90300
C	9.85400	-7.22200	25.02800
C	10.07500	-7.68700	26.45700
O	10.96500	-7.18500	27.13900
C	10.53100	-8.18300	24.04600
C	10.25900	-7.81400	22.59500
C	11.22200	-8.45900	21.61800
C	10.98400	-7.91300	20.20800
N	12.01700	-8.34700	19.21600
H	11.85800	-7.98300	18.27600
H	12.09700	-9.36400	19.20000
H	12.95300	-8.10800	19.54200
N	9.25800	-8.62900	26.92400
H	8.51700	-8.99600	26.32600
C	9.41000	-9.14300	28.28200
C	10.81400	-9.70200	28.40400
O	11.39400	-10.17600	27.42600
C	8.39100	-10.24400	28.56300
C	8.59200	-10.98200	29.87900
C	9.76600	-11.96500	29.82800
C	9.61900	-12.99800	28.70600
N	10.79200	-13.92900	28.61400
H	10.69400	-14.61700	27.86700
H	10.96700	-14.38500	29.50900
H	11.66400	-13.40900	28.51900
N	11.36100	-9.65300	29.60900
H	10.83200	-9.26400	30.38900
C	12.70800	-10.14900	29.82800
C	12.96000	-10.36400	31.30500
O	12.73300	-9.46400	32.10600
C	13.72800	-9.14500	29.28800
C	14.39800	-9.61700	28.02400
O	14.85400	-10.75200	27.94500

N	14.47900	-8.74100	27.03300
H	14.10000	-7.79600	27.09900
H	14.93300	-9.06100	26.17700
N	13.42300	-11.55300	31.67000
H	13.58200	-12.27300	30.96500
C	13.70500	-11.83500	33.06600
C	15.11400	-12.36900	33.25200
O	15.31300	-13.51800	33.64900
C	12.66200	-12.80500	33.64900
C	11.41800	-12.09800	34.22200
C	10.74100	-11.25900	33.14900
N	9.87000	-10.19400	33.64800
H	10.20400	-9.23400	33.56700
C	8.67500	-10.38700	34.20000
N	8.19500	-11.61400	34.34000
H	8.75600	-12.41400	34.04600
H	7.27900	-11.76200	34.76300
N	7.94400	-9.34500	34.58300
H	8.31400	-8.40000	34.47500
H	7.02800	-9.49300	35.00600
N	16.08500	-11.50600	32.95900
H	15.82300	-10.57600	32.63100
C	17.50700	-11.82300	33.08300
C	17.88200	-11.87100	34.55700
O	17.20100	-11.26700	35.39000
C	18.34400	-10.74300	32.39900
C	18.22300	-10.53900	30.89100
C	18.85800	-9.22500	30.48800
C	18.90000	-11.67800	30.18900
N	18.97300	-12.58300	34.90300
C	19.38200	-12.66200	36.31100
C	19.84400	-11.29100	36.82600
O	20.40300	-10.49100	36.07700
C	20.48900	-13.71800	36.28800
C	21.08600	-13.54800	34.94200
C	19.89000	-13.35300	34.04500
N	19.60100	-11.01800	38.10000
H	19.15100	-11.71900	38.68800
C	19.96900	-9.72600	38.67200
C	21.14700	-9.82100	39.63500
O	21.16300	-10.68000	40.51100
C	18.76700	-9.10900	39.43000
C	19.07500	-7.67800	39.82400

C	17.51600	-9.18300	38.57000
N	22.12600	-8.93500	39.47100
H	22.05400	-8.25500	38.71400
C	23.30000	-8.90500	40.33900
C	23.41700	-7.57100	41.07400
O	23.83900	-6.56800	40.50200
C	24.56800	-9.15200	39.52400
C	24.68800	-10.56100	38.97800
S	26.33200	-10.87500	38.29700
C	27.26900	-11.27500	39.80900
N	23.04300	-7.56600	42.34800
H	22.71200	-8.43400	42.77000
C	23.09100	-6.35500	43.16400
C	24.44600	-6.21300	43.86000
O	24.87400	-7.11800	44.58000
C	21.97900	-6.38800	44.21500
C	21.94500	-5.07400	44.97200
C	20.63900	-6.68000	43.53000
N	25.10900	-5.07400	43.65300
H	24.67700	-4.35100	43.07700
C	26.43800	-4.82400	44.22500
C	26.50600	-3.87700	45.41600
O	26.02500	-2.74600	45.35600
C	27.37300	-4.30400	43.13400
C	28.69000	-3.78800	43.63200
C	29.02800	-2.48600	43.86600
C	29.85600	-4.56100	43.92400
N	30.33500	-2.39600	44.28000
H	30.82600	-1.53300	44.51500
C	30.86900	-3.65600	44.32500
C	30.14900	-5.93400	43.88600
C	32.16000	-4.08100	44.68600
C	31.43300	-6.35800	44.24500
C	32.42200	-5.43100	44.64000
N	27.12500	-4.34500	46.49400
H	27.50100	-5.29300	46.47600
C	27.28400	-3.54300	47.70600
C	28.74800	-3.10700	47.84600
O	29.62000	-3.91600	48.17500
C	26.87900	-4.34200	48.96900
C	25.41500	-4.76700	48.87200
C	27.09300	-3.49500	50.20100
C	24.94400	-5.59500	50.05100

N	29.00900	-1.82800	47.60100
H	28.24300	-1.20100	47.35600
C	30.36300	-1.30200	47.67500
C	30.98500	-1.42800	49.06000
O	30.28100	-1.55100	50.05300
C	30.38500	0.17200	47.24700
C	29.88100	1.11600	48.29300
N	28.65000	1.73200	48.21200
H	27.98400	1.62000	47.44800
C	30.43500	1.53600	49.45600
C	28.46800	2.48900	49.27800
N	29.53800	2.38600	50.04900
H	29.67400	2.86200	50.94100
N	32.31500	-1.39400	49.10400
H	32.84100	-1.30800	48.23400
C	33.03100	-1.47600	50.36000
C	33.51300	-0.09100	50.77300
O	33.18500	0.90800	50.13300
N	34.30800	-0.02800	51.83500
H	34.57400	-0.88800	52.31400
C	34.80500	1.24500	52.32500
C	34.67700	1.31000	53.84100
O	34.32300	2.34000	54.39700
N	34.96100	0.19100	54.49900
H	35.23800	-0.63400	53.96700
C	34.89200	0.09700	55.95200
C	33.62800	0.62000	56.61500
O	33.61900	0.89200	57.82000
N	32.56400	0.75000	55.82700
H	32.64200	0.47600	54.84800
C	31.29100	1.26900	56.31000
C	31.39500	2.75100	56.63700
O	30.41800	3.35500	57.07900
C	30.83300	0.51700	57.55100
C	30.47500	-0.93900	57.33300
C	30.08200	-1.56400	58.65800
C	29.35000	-1.01900	56.31900
N	32.57900	3.32500	56.42400
H	33.34200	2.75400	56.06100
C	32.82700	4.73900	56.69000
C	32.76500	5.57300	55.40000
O	32.26200	6.69700	55.40600
C	34.20800	4.93600	57.34100

C	34.51300	4.11700	58.60200
S	33.39000	4.38200	60.00500
C	33.54200	6.16400	60.25800
N	33.28500	5.02100	54.30200
H	33.67900	4.08200	54.36500
C	33.31300	5.71200	53.00500
C	32.85100	4.82900	51.84900
O	32.51200	3.66300	52.04100
C	34.73900	6.21200	52.65400
C	35.18400	7.26800	53.63900
C	35.70600	5.05300	52.65600
N	32.85100	5.39500	50.64700
H	33.14900	6.36500	50.54800
C	32.43200	4.65100	49.47300
C	31.14400	5.16400	48.85600
O	30.36500	5.86100	49.49700
N	30.92200	4.81700	47.59600
H	31.61400	4.24200	47.11600
C	29.72700	5.22600	46.87200
C	29.46100	4.20500	45.78300
O	30.37200	3.49900	45.34800
C	29.92900	6.58800	46.25300
N	28.21600	4.14000	45.32800
H	27.51100	4.77300	45.70600
C	27.83800	3.18200	44.29900
C	28.30100	3.53600	42.89100
O	28.65400	2.65100	42.11900
C	26.33700	2.99300	44.31100
N	28.30300	4.82400	42.56500
H	28.02200	5.51100	43.26500
C	28.69400	5.28800	41.23800
C	30.11900	4.94700	40.82400
O	30.45400	4.99100	39.63900
C	28.48900	6.78400	41.15600
O	27.19200	7.09800	41.61100
H	27.06300	8.03800	41.55900
N	30.96000	4.61100	41.79300
H	30.63500	4.60400	42.76000
C	32.33700	4.25300	41.49800
C	32.35800	3.08700	40.51500
O	33.14700	3.07200	39.56700
C	33.07400	3.81500	42.76400
O	33.11700	4.90000	43.69500

H	32.22900	5.16800	43.90000
C	34.47700	3.39200	42.44000
N	31.47000	2.12200	40.74400
H	30.82700	2.22900	41.52900
C	31.37300	0.91800	39.92400
C	30.42100	1.03500	38.73900
O	29.20800	1.14800	38.91800
C	30.95800	-0.25500	40.81500
C	31.74600	-0.27600	42.10600
C	31.48200	0.64100	43.11900
C	32.82000	-1.14500	42.27700
C	32.26200	0.69600	44.25500
C	33.61300	-1.09000	43.41500
C	33.32400	-0.16900	44.39400
O	34.09900	-0.11700	45.52100
H	34.83200	-0.71400	45.61700
N	30.98200	1.01400	37.52900
H	31.99600	0.93600	37.45800
C	30.19400	1.09900	36.30400
C	29.81800	-0.31900	35.88500
O	30.68800	-1.18000	35.74700
C	31.00200	1.77200	35.19200
C	30.20900	1.90700	33.89200
O	30.74700	2.44900	32.90000
O	29.04000	1.47200	33.86300
N	28.52600	-0.55200	35.67100
H	27.85200	0.20800	35.76800
C	28.06700	-1.87800	35.30100
C	27.93100	-2.20000	33.82300
O	27.45900	-3.28100	33.47000
N	28.36400	-1.29100	32.95600
H	28.78500	-0.43100	33.30800
C	28.25400	-1.48900	31.51300
C	28.90100	-2.75800	30.94700
O	28.25000	-3.52800	30.23500
C	28.80300	-0.25900	30.78700
C	28.87500	-0.31200	29.26100
C	27.54600	-0.76600	28.67600
C	29.26000	1.05400	28.74300
N	30.17200	-2.98300	31.25200
H	30.67400	-2.32900	31.85300
C	30.85300	-4.15800	30.73300
C	30.20300	-5.45100	31.19900

O	29.80800	-6.27700	30.38200
C	32.31800	-4.14100	31.13700
N	30.09700	-5.62800	32.51300
H	30.43900	-4.90200	33.14300
C	29.50100	-6.83900	33.07500
C	28.09800	-7.08000	32.54400
O	27.72600	-8.21400	32.25400
C	29.46100	-6.75400	34.60500
C	28.71200	-7.83400	35.40200
C	29.25800	-9.20400	35.07800
C	28.84900	-7.55600	36.89300
N	27.32000	-6.01100	32.41500
H	27.68500	-5.09300	32.66700
C	25.95100	-6.12600	31.91900
C	25.91200	-6.64300	30.48600
O	25.15100	-7.56500	30.16600
C	25.25800	-4.78400	31.99700
N	26.73000	-6.04200	29.62500
H	27.33100	-5.28500	29.95000
C	26.78200	-6.44600	28.23000
C	27.46700	-7.80600	28.05300
O	26.92400	-8.70500	27.41200
C	27.49900	-5.38700	27.41500
N	28.65000	-7.95200	28.63800
H	29.02700	-7.17700	29.18400
C	29.42800	-9.17500	28.53000
C	28.81600	-10.47300	29.07600
O	29.17200	-11.54700	28.60800
C	30.80400	-8.95700	29.16800
C	31.77500	-8.22100	28.29300
N	32.37000	-8.79700	27.18900
H	32.19700	-9.74500	26.85400
C	32.28000	-6.96600	28.37600
C	33.19900	-7.92900	26.63300
N	33.16300	-6.81000	27.33400
H	33.70200	-5.96800	27.13500
N	27.91800	-10.41100	30.05400
H	27.63200	-9.50800	30.43200
C	27.33800	-11.65400	30.58900
C	25.80800	-11.69100	30.60600
O	25.20100	-12.60500	31.17800
C	27.86000	-11.94000	32.00200
C	29.32200	-12.34700	32.08200

C	29.64500	-13.59700	31.27700
O	28.73500	-14.42600	31.05900
O	30.82200	-13.75200	30.87900
N	25.19900	-10.68300	29.99000
H	25.77500	-9.95000	29.57500
C	23.75000	-10.57200	29.87700
C	22.97500	-10.70600	31.18000
O	22.08900	-11.54600	31.31300
C	23.24500	-11.59100	28.86200
C	22.19800	-11.01300	27.95600
O	21.01100	-11.02100	28.27500
N	22.63400	-10.47500	26.82600
H	23.61900	-10.46800	26.56100
H	21.92200	-10.08200	26.21000
N	23.32000	-9.84500	32.12900
H	24.06400	-9.17600	31.92800
C	22.69500	-9.80500	33.43700
C	22.41800	-8.34700	33.74700
O	22.97200	-7.45300	33.11300
C	23.63700	-10.34600	34.52100
C	23.90100	-11.83000	34.30300
C	24.94000	-9.55700	34.49700
N	21.55700	-8.10500	34.72000
H	21.11000	-8.88500	35.20200
C	21.23900	-6.74300	35.11300
C	22.11100	-6.39600	36.31500
O	22.08300	-7.09600	37.32600
C	19.75600	-6.61400	35.50500
C	19.45200	-5.18500	35.91700
C	18.87400	-7.04100	34.33300
N	22.89700	-5.33000	36.20500
H	22.89500	-4.78500	35.34300
C	23.76300	-4.93600	37.31200
C	23.14700	-3.81100	38.13500
O	22.76300	-2.77600	37.59100
C	25.15500	-4.48500	36.81200
C	25.99400	-4.02200	37.97600
C	25.85000	-5.63000	36.11000
N	23.05500	-4.02400	39.44700
H	23.38300	-4.91100	39.83000
C	22.49700	-3.02200	40.35300
C	23.48800	-2.61600	41.44200
O	23.87700	-3.44000	42.27900

C	21.22500	-3.52800	41.05000
C	20.68800	-2.45400	41.97400
C	20.18500	-3.90200	40.02200
N	23.89200	-1.34700	41.42400
H	23.54400	-0.73100	40.69000
C	24.81600	-0.80600	42.41900
C	23.99900	0.06800	43.36300
O	23.33900	1.02500	42.92700
C	25.90400	0.05300	41.76300
O	25.29100	1.10300	41.00800
H	24.75300	1.63300	41.58400
C	26.76500	-0.79500	40.84100
N	24.02500	-0.26600	44.65100
H	24.59100	-1.06000	44.95200
C	23.25600	0.48600	45.64300
C	24.11500	1.19300	46.67800
O	25.28100	0.86000	46.87800
C	22.29300	-0.42200	46.41800
C	23.09000	-1.36700	47.32600
C	21.41500	-1.19700	45.44700
C	22.24200	-2.08900	48.34900
N	23.52200	2.17100	47.34500
H	22.55400	2.40800	47.12800
C	24.22100	2.91400	48.38000
C	23.51100	2.72100	49.72100
O	22.39100	2.21900	49.78400
C	24.29800	4.39800	48.00300
C	25.30300	4.67800	46.89000
C	25.48200	6.16100	46.56700
O	26.37700	6.53800	45.80300
N	24.63000	7.00400	47.14300
H	24.74900	7.99400	46.92700
H	23.89100	6.69300	47.77400
N	24.17000	3.11000	50.79700
H	25.10000	3.51800	50.69900
C	23.58700	2.96300	52.11500
C	24.33100	3.89500	53.05200
O	25.51200	4.16400	52.85300
C	23.73300	1.52000	52.58700
C	25.15000	1.00400	52.49300
C	25.70500	0.65600	51.27100
C	25.95200	0.91900	53.62300
C	27.02600	0.23800	51.18000

C	27.27000	0.50800	53.53900
C	27.79800	0.16900	52.31900
O	29.10300	-0.24100	52.23900
H	29.46900	-0.47600	51.39400
N	23.63500	4.38600	54.06900
H	22.66000	4.10900	54.17800
C	24.21800	5.31000	55.03700
C	25.53700	4.82700	55.63000
O	25.72500	3.64100	55.89000
C	23.19900	5.60200	56.14000
C	22.07700	6.46800	55.64000
C	20.99800	6.64100	56.65700
N	19.95400	5.63800	56.51400
H	20.01600	4.98600	55.73200
C	18.92300	5.52400	57.34700
N	18.81400	6.35300	58.37500
H	18.02400	6.26600	59.01400
H	19.52100	7.07300	58.52500
N	18.00100	4.58500	57.15100
H	17.21100	4.49800	57.79000
H	18.08500	3.94700	56.36000
N	26.45200	5.76300	55.84000
H	26.23300	6.73600	55.62600
C	27.75700	5.42600	56.36900
C	28.04300	6.09800	57.69900
O	27.34000	7.02800	58.11800
C	28.82800	5.82500	55.35800
C	28.61100	5.20800	53.97900
C	29.44400	5.93900	52.94700
C	28.95300	3.73000	54.02700
N	29.08600	5.60900	58.36100
H	29.60800	4.82600	57.96700
C	29.49500	6.16800	59.63300
C	28.40200	6.46700	60.63900
O	27.51700	5.64800	60.89500
N	28.46500	7.65500	61.21800
H	29.20200	8.30800	60.95300
C	27.49700	8.03600	62.22500
C	26.06300	7.89300	61.76500
O	25.24000	7.31300	62.46900
C	27.73000	9.47500	62.69000
C	29.13700	9.59600	63.27400
C	26.69600	9.85900	63.73700

C	29.43900	10.95000	63.84500
N	25.77300	8.41300	60.57700
H	26.51500	8.85600	60.03500
C	24.42000	8.36900	60.02400
C	23.87300	6.96200	59.84400
O	22.68900	6.72700	60.05800
C	24.37500	9.09300	58.68100
C	24.72500	10.53900	58.75400
C	23.86400	11.58300	58.89500
C	26.03700	11.11100	58.65000
N	24.55200	12.77500	58.87900
H	24.13400	13.70200	58.96400
C	25.88900	12.51500	58.73000
C	27.32400	10.57400	58.49200
C	26.98300	13.39300	58.65600
C	28.40900	11.44700	58.41700
C	28.22900	12.84000	58.49900
N	24.72900	6.02600	59.45700
H	25.71100	6.25900	59.31000
C	24.26400	4.67300	59.24500
C	24.59100	3.64600	60.30800
O	24.10200	2.52100	60.21900
N	25.38400	3.99600	61.32200
H	25.74500	4.94700	61.39300
C	25.72800	2.99500	62.33000
C	25.75400	3.39800	63.79500
O	26.16900	2.61300	64.65600
C	27.04400	2.33700	61.92900
C	26.93000	1.54000	60.67800
C	26.32900	0.28500	60.70100
C	27.31900	2.07900	59.45800
C	26.10800	-0.42300	59.52500
C	27.10500	1.38400	58.27100
C	26.49600	0.12800	58.30200
N	25.29600	4.61200	64.08200
H	24.97500	5.21900	63.32800
C	25.24500	5.09100	65.46100
C	24.18400	4.31100	66.24300
O	23.01200	4.25600	65.85400
C	24.93200	6.59400	65.49400
C	24.80500	7.15400	66.88000
C	23.56000	7.29800	67.47300
C	25.94200	7.49400	67.61300

C	23.44700	7.77200	68.78400
C	25.84200	7.96800	68.92300
C	24.59000	8.10600	69.51000
N	24.60800	3.71100	67.35000
H	25.58600	3.80900	67.62300
C	23.71500	2.91400	68.18900
C	23.87300	3.18700	69.68600
O	24.99000	3.28400	70.18800
C	23.97800	1.42900	67.92300
O	23.45700	0.62100	68.95900
H	23.62000	-0.30000	68.79400
N	22.76700	3.30500	70.40700
H	21.85100	3.24300	69.96300
C	22.87800	3.52400	71.84400
C	22.66000	2.21600	72.58700
O	22.53500	2.20100	73.80500
C	21.85300	4.53900	72.38800
O	20.53500	4.10600	72.04400
H	20.37300	3.23600	72.38900
C	22.11300	5.93200	71.83500
N	22.60600	1.11600	71.84700
H	22.69800	1.18100	70.83300
C	22.41700	-0.17600	72.47300
C	20.98500	-0.45500	72.87900
O	20.66300	-1.58200	73.27000
N	20.12300	0.55900	72.79800
H	20.44800	1.47000	72.47300
C	18.71900	0.38600	73.16800
C	17.74800	0.79600	72.06300
O	18.15400	1.08100	70.93600
C	18.41000	1.13000	74.47700
C	18.69100	2.62200	74.39800
O	18.96300	3.23400	75.45100
O	18.62200	3.19400	73.29200
N	16.46300	0.82300	72.39400
H	16.19300	0.61700	73.35600
C	15.43400	1.13800	71.42500
C	15.46400	2.54700	70.87000
O	14.89200	2.81000	69.81100
C	14.04600	0.84400	72.00900
C	13.49100	1.86300	73.00200
C	13.97000	1.64800	74.43000
O	13.38900	2.28000	75.34600

O	14.92100	0.85900	74.64300
N	16.13100	3.45800	71.56500
H	16.60400	3.19100	72.42900
C	16.19200	4.84200	71.10000
C	17.07500	5.02400	69.85700
O	16.98600	6.03500	69.16000
C	16.64100	5.73800	72.25400
C	15.73700	5.66000	73.44900
N	14.37500	5.87000	73.36600
H	13.86400	6.09500	72.51200
C	15.99400	5.39200	74.75000
C	13.83600	5.73500	74.56400
N	14.79500	5.44600	75.42200
H	14.66800	5.28800	76.42200
N	17.90500	4.02300	69.57700
H	17.92700	3.21800	70.20300
C	18.78400	4.02600	68.41400
C	19.50800	2.67700	68.29400
O	20.73200	2.58700	68.47600
C	19.80500	5.16800	68.50500
O	20.51700	5.31100	67.28100
H	21.14900	6.01800	67.33700
N	18.73400	1.63700	67.98500
H	17.73500	1.79500	67.85200
C	19.25400	0.28000	67.82800
C	20.51600	0.20500	66.98000
O	21.51200	-0.38100	67.39500
C	18.19400	-0.62400	67.20100
C	17.02600	-0.97000	68.10200
C	16.22500	-2.11300	67.48900
N	15.31500	-2.72400	68.45100
H	15.58300	-3.61900	68.86000
C	14.16000	-2.19000	68.82900
N	13.76800	-1.03100	68.31400
H	12.88000	-0.62100	68.60400
H	14.34500	-0.56200	67.61600
N	13.40800	-2.80200	69.73900
H	12.52000	-2.39200	70.02900
H	13.70900	-3.69300	70.13500
N	20.46300	0.78300	65.78600
H	19.60400	1.24400	65.48600
C	21.61500	0.76500	64.90400
C	21.38800	0.03300	63.59200

O	20.24800	-0.26200	63.21400
N	22.48700	-0.26500	62.90400
H	23.39000	0.00600	63.29300
C	22.46700	-0.96200	61.61800
C	21.57500	-0.30200	60.58100
O	21.00600	-0.99800	59.73400
C	21.99200	-2.41300	61.75700
C	22.93000	-3.27300	62.56000
O	24.15000	-3.08400	62.54100
N	22.36500	-4.25700	63.25700
H	23.00100	-4.84000	63.80100
H	21.35700	-4.41300	63.27300
N	21.43600	1.01900	60.63100
H	21.91900	1.55800	61.35000
C	20.58600	1.69700	59.65000
C	21.10000	1.33900	58.25100
O	20.31600	1.05800	57.33400
C	20.61900	3.21900	59.86000
C	20.56800	3.62800	61.31400
C	21.51500	4.33200	61.99700
C	19.55800	3.28600	62.27100
N	21.16600	4.44600	63.32100
H	21.70900	4.92500	64.03900
C	19.96900	3.81100	63.51700
C	18.34600	2.58400	62.20000
C	19.21400	3.65400	64.68300
C	17.59600	2.43000	63.36000
C	18.03600	2.96300	64.58500
N	22.42600	1.32200	58.11700
H	23.00700	1.54100	58.92600
C	23.06900	1.00100	56.85500
C	22.69500	-0.36400	56.32300
O	22.52900	-0.54900	55.12000
N	22.56400	-1.33400	57.21500
H	22.72300	-1.14300	58.20400
C	22.19500	-2.66700	56.78300
C	20.72400	-2.67800	56.43600
O	20.30200	-3.40500	55.54000
C	22.50600	-3.68900	57.86700
C	23.97400	-3.87800	58.10300
N	24.88100	-3.99600	57.06900
H	24.64900	-3.97900	56.07600
C	24.69400	-3.95600	59.24500

C	26.09600	-4.13400	57.56700
N	26.01200	-4.11200	58.88400
H	26.79700	-4.19700	59.52900
N	19.94000	-1.85400	57.12700
H	20.33600	-1.27100	57.86400
C	18.52100	-1.78600	56.83000
C	18.32000	-1.09800	55.47400
O	17.35300	-1.39200	54.75400
C	17.77800	-1.04200	57.93200
C	17.71200	-1.72600	59.30000
C	16.86100	-0.87700	60.22800
C	17.12100	-3.12600	59.17800
N	19.23700	-0.19200	55.12500
H	19.99600	0.02200	55.77200
C	19.17900	0.50200	53.83600
C	19.43200	-0.50000	52.71000
O	18.85600	-0.41000	51.62500
C	20.24100	1.60400	53.74800
C	19.88400	2.82300	54.55600
O	18.67800	3.06200	54.74200
O	20.80200	3.55300	54.98800
N	20.31900	-1.44900	52.96800
H	20.78900	-1.47700	53.87300
C	20.62100	-2.44600	51.96500
C	19.38200	-3.32000	51.78000
O	18.95600	-3.58000	50.65500
C	21.84600	-3.26200	52.39800
C	23.08900	-2.39400	52.52400
C	24.21300	-3.03700	53.32100
O	23.97600	-3.77300	54.28900
N	25.44900	-2.73300	52.93700
H	26.20300	-3.16400	53.47200
H	25.64400	-2.12700	52.14000
N	18.78800	-3.74600	52.88800
H	19.17400	-3.48400	53.79500
C	17.59400	-4.58200	52.83300
C	16.46500	-3.87800	52.08900
O	15.68600	-4.51600	51.37700
C	17.08800	-4.93300	54.24100
C	15.73300	-5.60200	54.14400
C	18.06700	-5.83800	54.93200
N	16.37700	-2.56300	52.26900
H	17.05000	-2.09600	52.87700

C	15.34100	-1.77700	51.61600
C	15.53500	-1.79000	50.10600
O	14.58100	-2.02700	49.36000
C	15.35400	-0.35100	52.13500
N	16.76100	-1.54200	49.65300
H	17.51100	-1.34300	50.31500
C	17.04700	-1.55100	48.22200
C	16.72200	-2.92400	47.62500
O	16.19500	-3.01000	46.51800
C	18.50700	-1.20100	47.97000
N	17.03500	-3.99400	48.35400
H	17.48500	-3.86800	49.26000
C	16.74500	-5.34200	47.87900
C	15.24500	-5.50000	47.68300
O	14.79900	-6.11900	46.71600
C	17.23800	-6.39000	48.87400
C	18.74900	-6.58800	48.93300
C	19.06600	-7.64800	49.96800
C	19.28100	-6.99200	47.56300
N	14.46700	-4.95400	48.61200
H	14.88700	-4.49000	49.41800
C	13.02000	-5.01400	48.48600
C	12.62300	-4.22400	47.24500
O	11.69400	-4.60400	46.53500
C	12.32400	-4.40300	49.70200
C	12.29500	-5.27000	50.93400
C	11.52900	-4.56400	52.04600
N	11.76600	-5.16600	53.35400
H	12.21800	-4.59500	54.06900
C	11.43000	-6.41000	53.67100
N	10.83500	-7.18700	52.77400
H	10.57700	-8.14300	53.01800
H	10.63100	-6.82400	51.84300
N	11.69600	-6.88200	54.88300
H	11.43800	-7.83800	55.12700
H	12.15300	-6.28500	55.57200
N	13.32500	-3.12500	46.98000
H	14.08800	-2.84600	47.59700
C	13.00400	-2.32000	45.80800
C	13.26200	-3.10400	44.53200
O	12.54400	-2.95100	43.54100
C	13.82000	-1.03600	45.75300
C	13.37900	-0.15900	44.61700

C	12.46400	0.84900	44.67000
C	13.80900	-0.23900	43.24900
N	12.29600	1.40600	43.42300
H	11.66800	2.17700	43.19800
C	13.11000	0.75600	42.53200
C	14.72000	-1.05600	42.56000
C	13.29200	0.95900	41.16000
C	14.90100	-0.85300	41.19500
C	14.19000	0.14700	40.51200
N	14.30000	-3.93200	44.55600
H	14.87600	-3.99300	45.39500
C	14.62400	-4.75000	43.40600
C	13.48700	-5.74500	43.19000
O	12.98400	-5.88900	42.07700
C	15.92800	-5.49500	43.63500
C	16.24200	-6.38400	42.44300
C	17.03900	-4.48900	43.86000
N	13.06400	-6.41200	44.25800
H	13.51100	-6.24400	45.15900
C	11.97300	-7.38100	44.17100
C	10.69600	-6.81600	43.53400
O	10.04300	-7.48100	42.72400
C	11.62600	-7.91400	45.56400
C	12.74200	-8.69800	46.22900
C	13.00200	-10.04200	45.56200
O	12.09400	-10.86100	45.42700
N	14.24900	-10.27600	45.15200
H	15.00200	-9.59700	45.26400
H	14.42300	-11.17600	44.70500
N	10.33800	-5.58900	43.89200
H	10.92000	-5.05300	44.53600
C	9.11700	-5.01300	43.36500
C	9.24000	-4.29600	42.04200
O	8.22700	-3.93600	41.45200
C	8.49900	-4.04300	44.37100
C	8.41900	-4.61800	45.76500
O	8.38700	-5.86000	45.90200
O	8.37500	-3.81900	46.73000
N	10.45100	-4.09100	41.54500
H	11.27900	-4.44300	42.02500
C	10.57000	-3.35000	40.29400
C	11.41100	-3.95200	39.18600
O	11.05900	-3.83900	38.01700

C	11.12400	-1.94700	40.57600
C	10.30400	-1.18500	41.58400
O	9.45500	-0.37800	41.22400
N	10.54900	-1.44300	42.85800
H	11.25600	-2.11500	43.15800
H	9.99400	-0.92700	43.54100
N	12.52300	-4.57500	39.55400
H	12.72800	-4.67800	40.54800
C	13.46100	-5.11700	38.57800
C	12.84500	-5.70200	37.29900
O	13.33900	-5.44000	36.20700
C	14.46000	-6.12200	39.26700
C	15.83900	-5.99500	38.61700
C	13.96600	-7.56000	39.17000
C	16.40900	-4.58900	38.62200
N	11.75600	-6.45200	37.41600
H	11.35700	-6.61900	38.34000
C	11.12000	-7.04300	36.23500
C	10.83100	-5.99400	35.17000
O	10.88700	-6.28100	33.97300
C	9.83100	-7.75300	36.62800
N	10.51600	-4.78200	35.62000
H	10.48200	-4.62900	36.62800
C	10.21700	-3.66300	34.73400
C	11.48300	-3.28600	33.98500
O	11.43300	-2.60900	32.96100
C	9.72700	-2.45700	35.54500
O	8.60000	-2.78800	36.34300
H	8.29600	-2.04100	36.84500
N	12.62200	-3.72500	34.50600
H	12.60000	-4.27900	35.36200
C	13.89900	-3.43000	33.87900
C	14.47000	-4.64500	33.16600
O	15.61700	-4.63700	32.73300
C	14.90400	-2.91100	34.91700
C	14.56500	-1.55100	35.46400
C	13.84800	-1.41900	36.64200
C	14.93600	-0.40200	34.77700
C	13.50400	-0.15700	37.12700
C	14.59500	0.85600	35.25500
C	13.87900	0.97900	36.43000
N	13.66500	-5.69200	33.04800
H	12.72300	-5.65600	33.43800

C	14.12100	-6.88800	32.36600
C	14.88700	-7.81900	33.27400
O	15.69700	-8.62400	32.81400
N	14.62200	-7.70800	34.57100
H	13.93400	-7.02500	34.88700
C	15.29800	-8.54600	35.54400
C	14.33900	-9.51700	36.19600
O	13.16000	-9.21900	36.34900
N	14.84000	-10.68400	36.57900
H	15.82900	-10.88000	36.42700
C	14.00400	-11.68400	37.21000
C	14.12300	-11.60200	38.72500
O	15.13700	-11.99300	39.30400
C	14.40700	-13.06400	36.70500
C	13.78700	-14.17700	37.50500
O	12.70100	-14.03000	38.06700
N	14.46800	-15.31200	37.55100
H	15.36700	-15.43400	37.08600
H	14.04800	-16.06700	38.09300
N	13.07800	-11.08500	39.39100
C	13.06300	-10.94600	40.85100
C	13.25200	-12.25100	41.59900
O	13.47800	-12.24700	42.80900
C	11.70100	-10.32200	41.12700
C	10.87300	-10.83100	40.01300
C	11.78200	-10.68300	38.82400
N	13.15700	-13.36400	40.88100
H	12.96700	-13.30700	39.88000
C	13.32200	-14.66100	41.51100
C	14.74200	-15.18400	41.43600
O	15.02200	-16.27800	41.92100
N	15.63800	-14.40700	40.82800
H	15.33900	-13.51100	40.44200
C	17.03500	-14.80600	40.70100
C	17.97300	-13.62500	40.94500
O	18.73000	-13.21500	40.05800
C	17.29900	-15.40100	39.31300
O	18.51100	-16.15200	39.27700
H	18.67500	-16.52100	38.41700
N	17.92300	-13.08000	42.15400
H	17.26800	-13.44900	42.84300
C	18.78600	-11.96500	42.51400
C	19.99800	-12.45200	43.30600

O	19.86700	-13.21000	44.27000
C	18.01800	-10.91300	43.34200
C	18.98300	-9.88800	43.92300
C	16.99400	-10.22100	42.46000
N	21.17700	-12.01000	42.87900
H	21.19800	-11.39000	42.06900
C	22.44500	-12.36900	43.51300
C	23.05200	-11.11700	44.14800
O	23.09700	-10.05400	43.52100
C	23.46400	-12.90400	42.46500
O	22.84900	-13.91400	41.65300
H	23.47100	-14.24100	41.01300
C	24.66900	-13.49900	43.15100
N	23.50800	-11.22500	45.39100
H	23.42400	-12.10900	45.89400
C	24.12800	-10.07500	46.03100
C	25.58800	-10.37200	46.24900
O	25.93700	-11.43000	46.74500
C	23.51800	-9.75900	47.39000
C	23.50600	-11.03400	48.24000
C	22.15700	-9.09700	47.20000
C	23.25400	-10.79300	49.70800
N	26.43300	-9.42700	45.86300
H	26.06100	-8.57700	45.43900
C	27.87300	-9.55900	46.02300
C	28.48300	-8.20000	46.38000
O	28.04900	-7.15600	45.88800
C	28.50300	-10.11900	44.73700
C	28.35000	-9.22600	43.51900
C	27.10400	-8.69700	43.16300
C	29.45200	-8.94400	42.70900
C	26.96100	-7.90600	42.02000
C	29.31900	-8.15900	41.57300
C	28.07000	-7.63700	41.22500
N	29.47900	-8.21400	47.25500
H	29.79900	-9.10100	47.64400
C	30.11800	-6.97400	47.66300
C	31.56900	-7.22600	48.00800
O	31.99900	-8.37800	48.09200
N	32.32700	-6.16000	48.21800
H	31.91900	-5.22700	48.15600
C	33.73600	-6.31400	48.53600
C	34.09100	-5.65600	49.86700

O	33.54700	-4.60500	50.22600
C	34.56600	-5.74000	47.38800
C	36.03300	-6.11300	47.39300
C	36.88300	-5.11800	48.15500
O	36.58300	-3.90100	48.08600
O	37.85900	-5.55100	48.80300
N	34.99600	-6.30100	50.60000
H	35.39500	-7.16400	50.23100
C	35.44500	-5.82900	51.91100
C	34.24100	-5.57200	52.81900
O	33.55600	-6.51200	53.22900
C	36.28500	-4.55600	51.75700
O	36.96800	-4.23400	52.95700
H	37.48900	-3.44500	52.86200
N	33.97600	-4.31100	53.14000
H	34.57400	-3.56200	52.79200
C	32.83600	-3.99500	53.98600
C	31.57000	-4.46700	53.25800
O	30.61400	-4.94500	53.87400
C	32.77800	-2.50000	54.24100
N	31.58200	-4.32700	51.93500
H	32.39900	-3.92100	51.47800
C	30.44800	-4.74400	51.13500
C	30.36700	-6.24700	51.20600
O	29.30400	-6.84700	51.04100
N	31.52100	-6.85400	51.44800
H	32.37200	-6.30100	51.54700
C	31.58200	-8.29400	51.57300
C	31.00300	-8.67100	52.92200
O	30.29100	-9.66400	53.04300
N	31.30700	-7.86500	53.93500
H	31.90800	-7.05800	53.76900
C	30.79800	-8.11400	55.27600
C	29.27400	-7.98800	55.29900
O	28.59000	-8.72400	56.01100
C	31.41000	-7.12800	56.28100
C	31.01000	-7.41100	57.72900
C	29.94400	-6.46500	58.27100
O	29.24900	-5.78800	57.48200
O	29.79400	-6.41200	59.50600
N	28.75400	-7.04800	54.51600
H	29.37800	-6.47300	53.95000
C	27.32200	-6.81600	54.44400

C	26.63800	-8.02100	53.82800
O	25.60200	-8.47800	54.31800
C	27.03300	-5.57200	53.60900
O	27.57200	-4.41600	54.21900
H	27.39200	-3.64100	53.69900
N	27.21000	-8.53100	52.74400
H	28.05400	-8.10000	52.36600
C	26.64100	-9.70000	52.09300
C	26.59000	-10.83500	53.12100
O	25.58200	-11.51600	53.26300
C	27.48900	-10.12000	50.87100
C	27.00200	-11.44900	50.31600
C	27.40100	-9.05500	49.80200
N	27.68000	-11.00900	53.85600
H	28.48400	-10.40000	53.70100
C	27.76400	-12.04400	54.87800
C	26.71000	-11.86200	55.97600
O	26.20400	-12.84600	56.51800
C	29.16300	-12.04400	55.49800
O	29.29600	-13.07000	56.45800
H	30.16500	-13.07000	56.84300
N	26.38200	-10.60600	56.29400
H	26.84000	-9.84200	55.79800
C	25.38800	-10.27800	57.32900
C	23.96700	-10.52900	56.83300
O	23.10800	-10.98000	57.58100
C	25.50100	-8.79300	57.78900
C	24.40000	-8.46000	58.78000
C	26.85000	-8.54700	58.43200
N	23.72400	-10.22200	55.56800
H	24.46800	-9.82300	54.99600
C	22.41600	-10.44400	54.98400
C	22.17000	-11.95300	54.95400
O	21.03900	-12.42300	55.09700
C	22.38000	-9.86500	53.57000
C	22.49900	-8.33900	53.50700
C	22.57300	-7.86400	52.05800
C	21.29800	-7.71300	54.21100
N	23.24500	-12.71200	54.78200
H	24.15800	-12.26800	54.68300
C	23.15100	-14.15800	54.73100
C	22.64500	-14.74300	56.04400
O	22.04800	-15.82200	56.04500

C	24.52000	-14.78200	54.38500
C	24.51700	-16.27400	54.66700
C	24.83100	-14.53800	52.92300
N	22.87200	-14.03400	57.15200
H	23.35400	-13.13900	57.07400
C	22.45000	-14.50100	58.48000
C	21.24400	-13.74000	59.01100
O	20.78000	-14.00600	60.11800
C	23.57700	-14.32200	59.49800
C	24.99100	-14.80800	59.19100
C	25.93300	-14.37500	60.31300
C	25.00100	-16.30200	59.04300
N	20.74400	-12.78500	58.23700
H	21.15000	-12.62100	57.31600
C	19.62400	-11.96800	58.68300
C	18.24400	-12.48100	58.28000
O	17.94700	-12.65300	57.09500
C	19.81200	-10.53200	58.18900
O	18.77900	-9.69100	58.66700
H	18.89600	-8.79900	58.36000
N	17.38000	-12.73300	59.27600
C	16.01400	-13.22400	59.07000
C	15.18700	-12.25900	58.21500
O	14.30000	-12.66600	57.46100
C	15.48100	-13.33900	60.49500
C	16.70500	-13.68500	61.27700
C	17.71300	-12.72000	60.71100
N	15.48600	-10.97500	58.34500
H	16.23200	-10.69800	58.98300
C	14.77700	-9.95900	57.60200
C	14.98100	-10.12300	56.10700
O	14.02200	-10.03700	55.33300
C	15.26500	-8.57100	58.01500
C	15.04000	-8.11100	59.45400
C	15.70200	-6.76000	59.65000
C	13.54500	-8.02900	59.75600
N	16.22900	-10.36700	55.71100
H	16.95600	-10.47000	56.41900
C	16.59800	-10.49300	54.30400
C	16.24700	-11.80400	53.61200
O	16.39600	-11.92400	52.39400
C	18.08500	-10.20900	54.13800
N	15.79600	-12.79300	54.37100

H	15.71500	-12.66500	55.38000
C	15.41600	-14.06400	53.76500
C	14.39600	-13.78000	52.65500
O	13.41700	-13.06000	52.88100
C	14.79400	-14.97300	54.82800
C	14.28300	-16.31400	54.31700
C	13.64500	-17.12300	55.44900
C	14.62800	-17.34700	56.60100
N	14.01800	-18.08400	57.73900
H	14.67300	-18.23300	58.50700
H	13.61100	-18.96600	57.42800
H	13.17100	-17.61800	58.06500
N	14.63900	-14.32100	51.46400
H	15.48400	-14.87900	51.34400
C	13.74100	-14.14800	50.31700
C	14.00600	-12.90300	49.48000
O	13.24700	-12.58900	48.56900
C	12.26700	-14.11700	50.75300
C	11.85900	-15.33400	51.56800
O	12.29600	-16.45700	51.30000
N	10.99400	-15.11700	52.56000
H	10.72000	-15.93300	53.10700
H	10.63300	-14.18900	52.78100
N	15.07600	-12.19000	49.78500
H	15.68000	-12.48600	50.55200
C	15.39900	-10.98600	49.03500
C	16.53700	-11.25400	48.06500
O	16.90600	-10.39200	47.26900
C	15.76900	-9.85900	50.00100
C	14.56700	-9.44500	50.85000
C	14.99300	-8.54300	52.00200
C	13.55900	-8.75100	49.94200
N	17.08000	-12.46200	48.14400
H	16.71700	-13.11800	48.83600
C	18.17300	-12.88900	47.28200
C	18.20000	-14.41200	47.19600
O	17.59000	-15.11300	48.01700
C	19.52400	-12.36000	47.79600
C	19.86000	-12.78900	49.19100
C	19.17000	-12.26800	50.27800
C	20.86900	-13.71500	49.41900
C	19.48200	-12.66500	51.57500
C	21.19000	-14.11900	50.71500

C	20.49600	-13.59200	51.79400
N	18.93100	-14.92600	46.21600
H	19.46100	-14.30400	45.60600
C	18.98800	-16.36100	45.99800
C	20.40400	-16.91800	45.88300
O	20.59000	-18.13300	45.80400
C	18.18400	-16.66600	44.73700
C	16.88200	-15.92700	44.67500
N	15.77200	-16.30800	45.39700
H	15.70800	-17.14100	45.98300
C	16.53900	-14.77900	44.04100
C	14.80400	-15.42900	45.21400
N	15.24500	-14.49000	44.39400
H	14.71000	-13.68200	44.07600
N	21.39200	-16.02500	45.86500
H	21.15300	-15.03500	45.92400
C	22.80600	-16.39700	45.76400
C	23.62200	-15.24800	46.35700
O	23.22900	-14.08300	46.24700
C	23.19200	-16.60700	44.30000
C	22.13500	-17.36200	43.49600
C	22.52500	-17.50500	42.03500
N	21.46200	-18.08000	41.20800
H	21.19400	-17.56900	40.36700
C	20.81700	-19.21600	41.46500
N	21.09800	-19.93600	42.53900
H	21.80900	-19.60600	43.19100
H	20.60400	-20.80600	42.73600
N	19.89700	-19.64300	40.62100
H	19.68000	-19.08800	39.79300
H	19.40300	-20.51300	40.81800
N	24.75400	-15.56500	46.98000
H	25.05000	-16.54000	47.02700
C	25.57400	-14.52900	47.59600
C	27.08600	-14.68700	47.39900
O	27.62700	-15.79200	47.47300
C	25.24700	-14.45000	49.08300
N	27.76200	-13.56400	47.15700
H	27.25100	-12.68300	47.11200
C	29.21000	-13.55000	46.95400
C	29.90300	-12.57700	47.88900
O	29.62900	-11.37800	47.85200
C	29.60300	-13.12500	45.51100

C	29.04700	-14.12000	44.49100
C	31.12400	-13.03100	45.39500
C	29.36400	-13.75900	43.07200
N	30.80100	-13.09500	48.71900
H	30.95800	-14.10300	48.71300
C	31.56800	-12.26500	49.63700
C	33.00600	-12.24900	49.14900
O	33.65500	-13.29800	49.09500
C	31.51800	-12.81800	51.06100
O	30.38600	-12.33100	51.75500
H	30.35500	-12.67500	52.64000
N	33.48400	-11.05400	48.79200
H	32.86600	-10.24600	48.87100
C	34.84500	-10.83600	48.29400
C	35.71300	-10.10200	49.31900
O	35.58900	-8.89300	49.48900
C	34.80000	-10.01300	47.00200
C	34.03500	-10.66300	45.85400
C	33.85800	-9.72100	44.66300
O	34.81900	-9.00100	44.31400
O	32.76300	-9.70600	44.06700
N	36.59300	-10.83100	49.99500
H	36.65200	-11.83300	49.81600
C	37.47700	-10.23100	50.98800
C	36.69400	-9.58100	52.11100
O	36.76500	-8.36700	52.28200
C	38.36200	-9.16900	50.33700
O	39.13000	-9.72300	49.28000
H	39.68000	-9.06300	48.87500
N	35.94200	-10.37800	52.86900
H	35.91100	-11.37900	52.67600
C	35.16600	-9.82900	53.96900
C	33.92500	-10.62300	54.34000
O	33.05900	-10.86100	53.49900
N	33.83800	-11.03200	55.60300
H	34.59200	-10.80200	56.25000
C	32.70000	-11.79800	56.08900
C	32.25500	-11.25300	57.43800
O	32.89000	-10.35700	57.97300
C	33.05200	-13.28500	56.24100
C	33.45900	-13.86300	54.89400
C	34.15500	-13.45900	57.26600
N	31.17300	-11.79700	57.99000

H	30.70100	-12.56000	57.50400
C	30.63900	-11.33700	59.27000
C	31.52400	-11.65000	60.46300
O	31.42800	-10.99300	61.48700
C	29.25500	-11.91800	59.48800
N	32.37200	-12.66400	60.34700
H	32.38500	-13.21300	59.48700
C	33.28900	-13.00600	61.43600
C	34.45600	-12.01000	61.46400
O	35.18700	-11.93900	62.45500
C	33.83700	-14.42000	61.26400
C	32.91100	-15.59700	61.56000
C	33.54000	-16.87500	61.02900
C	32.67900	-15.70600	63.05200
N	34.63900	-11.26400	60.36600
H	34.02600	-11.41300	59.56400
C	35.69100	-10.23700	60.27200
C	35.37100	-9.20200	61.36300
O	34.84900	-8.11100	61.09700
C	35.71200	-9.52700	58.86200
O	36.10700	-10.45900	57.84400
H	35.49700	-11.18800	57.84500
C	36.69600	-8.35100	58.86000
N	35.68100	-9.59300	62.59400
H	36.11200	-10.51100	62.70600
C	35.44900	-8.80300	63.79200
C	35.42900	-7.28800	63.60300
O	34.38700	-6.65600	63.75100
C	36.50400	-9.16300	64.83800
O	36.76100	-10.55500	64.81900
H	37.41700	-10.77900	65.46900
N	36.58700	-6.72000	63.28500
H	37.40200	-7.31900	63.15500
C	36.74800	-5.28400	63.11300
C	35.49700	-4.49500	62.72200
O	35.38400	-3.31700	63.05500
C	37.88000	-4.98300	62.10100
C	37.51700	-5.53600	60.73400
C	38.14200	-3.49100	62.03400
N	34.55400	-5.12400	62.03200
H	34.67100	-6.10700	61.78700
C	33.35100	-4.41000	61.62500
C	32.07000	-4.66400	62.42100

O	31.06000	-3.99900	62.18700
C	33.08900	-4.64200	60.13500
C	34.01300	-3.84100	59.21400
C	33.61200	-4.04000	57.76000
C	33.93400	-2.36000	59.58900
N	32.10000	-5.60800	63.35900
H	32.96000	-6.13500	63.50900
C	30.92200	-5.90800	64.18300
C	31.22200	-5.67400	65.67100
O	31.81700	-6.52200	66.32900
C	30.45100	-7.37600	63.97900
C	29.24400	-7.67500	64.87200
C	30.10000	-7.60800	62.51600
N	30.80300	-4.52500	66.19800
H	30.29200	-3.86400	65.61300
C	31.06000	-4.19100	67.59700
C	30.15200	-4.96900	68.54400
O	28.96200	-4.68400	68.66000
C	30.87100	-2.68500	67.84800
C	31.28400	-1.76200	66.69800
C	32.76900	-1.81700	66.34100
C	33.63600	-1.16000	67.39500
N	33.55800	-1.89500	68.68200
H	34.14200	-1.45300	69.39200
H	33.78900	-2.88200	68.56600
H	32.59400	-1.99800	68.99900
N	30.71700	-5.95500	69.22500
H	31.70600	-6.16300	69.08400
C	29.94400	-6.74500	70.17100
C	30.07100	-6.06900	71.53900
O	30.69900	-5.01300	71.66000
C	30.48700	-8.17400	70.21500
C	30.61200	-8.81500	68.84100
C	31.42500	-10.10100	68.89900
C	31.85900	-10.56900	67.51000
N	32.84600	-9.63900	66.86300
H	33.13600	-9.95100	65.93600
H	33.65400	-9.48800	67.46600
H	32.48300	-8.68600	66.83000
N	29.47500	-6.66200	72.56500
H	28.96100	-7.53200	72.42500
C	29.55600	-6.07000	73.88800
C	28.68600	-4.83500	73.99300

O	27.86500	-4.58600	73.11200
N	28.86300	-4.05900	75.06100
H	29.56700	-4.31900	75.75200
C	28.07500	-2.84400	75.27100
C	28.59200	-1.71300	74.39500
O	29.75000	-1.31300	74.50000
C	28.12600	-2.43000	76.74400
C	27.16800	-1.29700	77.06900
O	26.00300	-1.34800	76.61600
O	27.57200	-0.36200	77.79300
N	27.72900	-1.20000	73.52600
H	26.77600	-1.56200	73.48800
C	28.12800	-0.12900	72.62900
C	27.90100	1.24500	73.23300
O	28.43500	2.24400	72.73600
C	27.36500	-0.20300	71.30600
C	27.67600	-1.50700	70.61300
C	25.87700	-0.06800	71.55900
N	27.12000	1.28400	74.31100
H	26.73600	0.41100	74.67200
C	26.79300	2.53200	74.99500
C	27.97700	3.50700	75.13100
O	27.83000	4.70800	74.90900
C	26.18500	2.21500	76.36600
C	25.55800	3.41300	77.09500
C	24.51700	4.12000	76.24900
C	23.63700	5.01800	77.09400
N	22.71400	4.22300	77.95800
H	22.12100	4.82800	78.52700
H	23.22500	3.55300	78.53300
H	22.15900	3.56800	77.40800
N	29.16200	3.00700	75.50500
C	30.31300	3.90400	75.63800
C	30.69800	4.63500	74.34700
O	30.79900	5.86000	74.33200
C	31.41500	2.97100	76.12000
C	30.67100	2.04200	76.98200
C	29.44600	1.71600	76.15100
N	30.90800	3.89500	73.26500
H	30.79900	2.88200	73.31100
C	31.29500	4.53200	72.01000
C	30.27800	5.60700	71.63100
O	30.61000	6.58300	70.95500

C	31.43100	3.47500	70.89400
C	32.16600	3.80200	69.57300
C	31.21700	4.47300	68.59800
C	33.40900	4.67200	69.83900
N	29.04300	5.42800	72.09000
H	28.83800	4.60300	72.65300
C	27.97600	6.37600	71.81100
C	28.21300	7.65500	72.59800
O	28.17800	8.76200	72.04800
C	26.64800	5.77500	72.19600
N	28.44400	7.49000	73.89600
H	28.43900	6.54700	74.28400
C	28.70300	8.61400	74.77800
C	29.89900	9.39500	74.25200
O	29.89800	10.62700	74.23300
C	28.95600	8.10000	76.18900
C	27.67200	7.85900	76.96500
C	27.83100	6.86800	78.11100
O	28.86700	6.91600	78.81200
O	26.90500	6.04700	78.31600
N	30.90800	8.66600	73.79500
H	30.83900	7.64900	73.82100
C	32.10800	9.28200	73.25800
C	31.74900	10.11700	72.02900
O	32.13500	11.28400	71.93100
C	33.13200	8.21000	72.89300
C	34.55900	8.71700	72.90700
C	35.57400	7.60900	72.68400
O	35.58500	6.60900	73.40700
N	36.43800	7.78300	71.68300
H	37.12000	7.03900	71.53300
H	36.42900	8.61000	71.08500
N	31.01000	9.53300	71.09000
H	30.72400	8.56000	71.19800
C	30.60800	10.28300	69.90600
C	29.74100	11.45600	70.34700
O	29.92800	12.58300	69.89200
C	29.80700	9.41700	68.92800
C	30.68700	8.26600	68.43200
C	29.30000	10.27300	67.77300
C	29.98200	7.29100	67.52000
N	28.80300	11.18900	71.25100
H	28.70100	10.23500	71.59700

C	27.91700	12.23100	71.75900
C	28.71200	13.43600	72.26400
O	28.47900	14.57600	71.85000
C	27.05800	11.67300	72.87800
N	29.65100	13.17400	73.16700
H	29.79400	12.21000	73.46800
C	30.48200	14.22400	73.74000
C	31.30100	14.94800	72.69100
O	31.35700	16.17400	72.69400
C	31.44600	13.65800	74.77300
C	30.65800	13.07400	75.93300
C	32.36900	14.73900	75.26900
C	31.51500	12.33500	76.91200
N	31.94700	14.19600	71.80500
H	31.87200	13.18000	71.85700
C	32.76100	14.80400	70.76100
C	31.93100	15.73000	69.88900
O	32.42000	16.75500	69.42000
C	33.42100	13.73900	69.87800
O	34.31300	12.96100	70.68000
H	34.72200	12.30100	70.13300
C	34.20900	14.38100	68.74900
N	30.67400	15.36500	69.66700
H	30.32900	14.49300	70.06800
C	29.77900	16.18200	68.86400
C	29.27300	17.29600	69.75500
O	28.58600	18.20600	69.30800
C	28.62000	15.35400	68.37100
N	29.60800	17.20300	71.03400
H	30.17100	16.41500	71.35300
C	29.18200	18.21000	71.98200
C	27.74200	18.04900	72.42000
O	26.93800	18.96800	72.28600
N	27.40800	16.88200	72.94900
H	28.11000	16.14800	73.03800
C	26.05100	16.63900	73.40300
C	26.05300	16.06400	74.80400
O	26.97300	15.33700	75.17800
C	25.36000	15.65500	72.47900
S	24.83400	16.29600	70.86400
N	25.02900	16.39500	75.58500
H	24.31400	17.03100	75.23200
C	24.91200	15.86300	76.93800

C	24.79600	14.35200	76.78400
O	24.42200	13.85600	75.72200
C	23.65200	16.40400	77.61800
C	23.74600	17.85800	78.06800
C	22.45600	18.65600	77.77800
C	21.22300	18.14200	78.52900
N	20.02100	19.01000	78.27600
H	19.20000	18.66800	78.77600
H	19.83600	19.10900	77.27800
H	20.21300	19.98700	78.49800
N	25.11700	13.60700	77.82900
H	25.43300	14.04500	78.69400
C	25.01600	12.15900	77.73500
C	24.09700	11.64800	78.82500
O	24.19000	10.49800	79.22600
C	26.39100	11.49300	77.89400
O	26.90800	11.77600	79.19600
H	26.30100	11.44400	79.84700
C	27.36000	12.02400	76.85400
N	23.20000	12.50700	79.29000
H	23.15600	13.44500	78.89100
C	22.27900	12.14600	80.35300
C	21.57400	10.81000	80.11700
O	21.57300	9.95600	81.00100
C	21.24000	13.25500	80.56800
O	21.90400	14.52800	80.57500
H	22.34500	14.64700	79.74200
C	20.53300	13.06400	81.90400
N	20.97700	10.62900	78.93800
H	20.99800	11.38400	78.25200
C	20.28700	9.36900	78.59600
C	20.37000	9.12800	77.09300
O	20.60400	10.05800	76.33300
C	18.77500	9.39300	78.92300
O	18.07500	10.04600	77.85000
H	18.24600	9.59800	77.03000
C	18.49900	10.11800	80.25000
N	20.15900	7.88700	76.66900
H	19.97100	7.15200	77.35100
C	20.19100	7.55100	75.24600
C	19.29300	8.48400	74.43000
O	19.73600	9.09800	73.45700
C	19.73100	6.11200	75.03600

O	20.59900	5.22600	75.70100
H	20.31200	4.33000	75.57000
N	18.02900	8.57500	74.83400
H	17.73100	8.02800	75.64200
C	17.05700	9.42400	74.16800
C	17.57800	10.85500	74.09400
O	17.36900	11.54800	73.10100
C	15.74000	9.38500	74.91600
N	18.24800	11.30500	75.14800
H	18.36900	10.70200	75.96200
C	18.81400	12.65200	75.15900
C	19.88800	12.76300	74.07000
O	19.88700	13.69900	73.26900
C	19.44700	12.98200	76.53300
C	20.30000	14.22700	76.43000
C	18.35100	13.18500	77.56800
N	20.80000	11.79600	74.04500
H	20.75400	11.04900	74.73800
C	21.86100	11.77900	73.05300
C	21.28300	11.78400	71.64000
O	21.56900	12.68200	70.84100
C	22.74500	10.54600	73.24100
C	23.53000	10.53600	74.54500
S	24.93000	9.37400	74.53100
C	24.10800	7.84800	74.99500
N	20.46400	10.78300	71.34200
H	20.25500	10.08400	72.05400
C	19.85500	10.65700	70.02200
C	19.18100	11.95500	69.57900
O	19.30900	12.37300	68.41800
C	18.82000	9.49500	70.00000
C	18.20800	9.35300	68.63200
C	19.49500	8.20800	70.37300
N	18.47600	12.59300	70.51200
H	18.43200	12.20500	71.45400
C	17.76700	13.83000	70.22100
C	18.70100	14.98600	69.89800
O	18.38600	15.81900	69.05300
C	16.87200	14.22400	71.39400
C	16.27000	15.58700	71.25300
N	15.23700	15.86000	70.38000
H	14.75700	15.17100	69.80100
C	16.60600	16.77100	71.81700

C	14.96600	17.15200	70.41000
N	15.78300	17.72800	71.27400
H	15.80000	18.72200	71.50100
N	19.84000	15.04100	70.58200
H	20.03800	14.32700	71.28300
C	20.81000	16.10100	70.35000
C	21.51200	15.91100	69.01000
O	21.68400	16.86600	68.24300
C	21.84200	16.11600	71.46700
S	23.16700	17.37500	71.33400
N	21.92800	14.68400	68.72300
H	21.78000	13.92400	69.38700
C	22.59300	14.42900	67.46100
C	21.66300	14.65900	66.27300
O	22.12000	15.03900	65.19800
C	23.16500	13.01100	67.43900
C	24.42900	12.88900	68.29200
C	24.82500	11.44000	68.44800
C	25.54900	13.67900	67.64700
N	20.36100	14.44400	66.44900
H	20.00900	14.12900	67.35300
C	19.44000	14.66400	65.33300
C	19.29700	16.14700	65.04800
O	18.87400	16.54300	63.96900
C	18.05000	14.09500	65.61700
C	17.94500	12.58900	65.56700
C	16.50300	12.16700	65.27100
N	16.32300	10.71900	65.33900
H	16.54200	10.17200	64.50600
C	15.89300	10.06800	66.41500
N	15.58800	10.74000	67.51800
H	15.66500	11.75700	67.53100
H	15.25800	10.24000	68.34400
N	15.79200	8.74200	66.39800
H	16.02600	8.22600	65.55000
H	15.46200	8.24200	67.22400
N	19.66200	16.96800	66.02100
H	20.02500	16.57900	66.89100
C	19.55700	18.40800	65.87800
C	20.78900	19.01200	65.23000
O	20.74100	20.15300	64.78900
C	19.33300	19.04800	67.24600
C	18.13400	18.49700	68.00500

C	16.79800	19.01900	67.49200
O	16.56600	20.22700	67.46500
N	15.90800	18.10700	67.09500
H	15.01300	18.45700	66.75200
H	16.10000	17.10600	67.11700
N	21.88700	18.25900	65.17400
H	21.86600	17.31700	65.56600
C	23.12600	18.75500	64.56100
C	23.03500	18.78400	63.03600
O	22.32800	17.98000	62.43500
C	24.32400	17.88400	64.95700
C	24.68600	17.88200	66.43800
C	25.18800	19.23800	66.89900
C	25.52700	19.23400	68.38400
N	25.96000	20.58100	68.83700
H	26.18700	20.57800	69.83100
H	25.26600	21.29400	68.61200
H	26.73500	20.93500	68.27600
N	23.75900	19.70900	62.41100
H	24.33000	20.35400	62.95700
C	23.74900	19.81400	60.95900
C	24.62400	18.71700	60.37600
O	25.50100	18.19500	61.05700
C	24.30100	21.17000	60.47300
O	25.72800	21.16100	60.53600
H	26.06800	21.99600	60.23700
C	23.79400	22.28100	61.33500
N	24.37900	18.36700	59.11700
H	23.62200	18.82500	58.60900
C	25.17000	17.34300	58.44800
C	26.64900	17.70600	58.57200
O	27.47700	16.85400	58.90100
C	24.78500	17.24700	56.96400
C	25.70200	16.35100	56.11800
C	25.38100	16.38900	54.62000
O	24.30300	15.90000	54.22100
O	26.20800	16.91000	53.83600
N	26.97000	18.97500	58.32000
H	26.23100	19.63200	58.07000
C	28.34400	19.45100	58.39100
C	28.96500	19.27200	59.76800
O	30.15100	18.93500	59.88300
C	28.41700	20.92400	57.99900

C	28.43000	21.20700	56.50300
C	27.13300	20.83100	55.81200
O	26.04200	21.15500	56.34800
O	27.21800	20.22000	54.72000
N	28.17500	19.50700	60.81300
H	27.20800	19.79200	60.66100
C	28.67900	19.36100	62.17500
C	29.04100	17.89900	62.46500
O	30.09600	17.61300	63.04400
C	27.64300	19.84400	63.18800
C	27.17800	21.26300	62.99300
C	26.27900	21.73400	64.12400
O	26.79300	21.96800	65.23600
O	25.05400	21.86300	63.90800
N	28.16400	16.98000	62.05900
H	27.30800	17.27800	61.59100
C	28.40400	15.55900	62.27100
C	29.61400	15.06300	61.46600
O	30.24600	14.06800	61.83700
C	27.15600	14.74600	61.91500
C	25.94400	14.91100	62.84500
C	24.86700	13.90400	62.45600
C	26.35100	14.69300	64.29600
N	29.94700	15.75600	60.37600
H	29.39000	16.56600	60.10400
C	31.09500	15.37100	59.57000
C	32.35300	15.84700	60.29000
O	33.36300	15.13600	60.33600
C	30.99400	15.97700	58.16300
C	32.08900	15.67300	57.12200
C	32.52400	14.23700	57.24800
C	31.58800	15.95600	55.70900
N	32.29300	17.05000	60.86400
H	31.44300	17.60800	60.78800
C	33.44400	17.56900	61.60100
C	33.70300	16.63600	62.78300
O	34.85100	16.31800	63.09000
C	33.19600	18.99200	62.10500
C	33.21800	20.04800	61.02400
C	33.57200	21.43400	61.56000
O	33.61100	22.39500	60.75700
O	33.81600	21.56500	62.78000
N	32.62800	16.20200	63.44200

H	31.70400	16.53000	63.16200
C	32.74900	15.26900	64.55300
C	33.42500	14.01700	63.99300
O	34.29600	13.43000	64.63400
C	31.36500	14.87200	65.12800
O	30.75000	16.00500	65.74600
H	30.65500	16.68300	65.08700
C	31.51500	13.79700	66.17200
N	33.03100	13.62200	62.78300
H	32.31100	14.15200	62.29300
C	33.61200	12.44300	62.14500
C	35.10100	12.59700	61.87100
O	35.83500	11.61300	61.89700
C	32.93800	12.10900	60.80200
O	31.54200	11.87700	61.00600
H	31.15800	12.66000	61.38200
C	33.55100	10.85800	60.20100
N	35.55700	13.81600	61.59400
H	34.91600	14.60900	61.57500
C	36.97900	14.01500	61.31700
C	37.76600	14.03500	62.61800
O	38.87500	13.51600	62.69800
C	37.21100	15.31400	60.53400
C	36.63300	15.41900	59.11200
C	37.11100	16.72100	58.47100
C	37.05400	14.23000	58.26200
N	37.18200	14.63400	63.64300
H	36.26200	15.05800	63.52100
C	37.83100	14.69600	64.93500
C	38.07400	13.27400	65.41200
O	39.14000	12.96600	65.93900
C	36.94300	15.42400	65.93300
C	36.64800	16.85200	65.58000
C	35.72100	17.44400	66.61300
C	35.66100	18.95800	66.52600
N	34.93700	19.50000	67.70600
H	34.89700	20.51800	67.64800
H	35.34400	19.18200	68.58600
H	34.01200	19.08500	67.81300
N	37.08400	12.40400	65.22100
H	36.22300	12.71400	64.77000
C	37.21100	11.01300	65.64700
C	38.51200	10.39400	65.13900

O	39.26400	9.82500	65.92000
C	36.02400	10.17800	65.14800
C	34.63000	10.63600	65.60100
S	34.26400	10.46500	67.36600
C	33.80300	8.76900	67.46100
N	38.77300	10.51800	63.83800
H	38.10600	11.02100	63.25200
C	39.97700	9.96300	63.21400
C	39.88000	8.43900	63.15900
O	40.75000	7.72800	63.67900
C	41.22600	10.34600	64.00500
C	41.52100	11.81800	64.08000
C	42.74800	12.05300	64.94800
C	43.18700	13.50800	64.90400
N	44.43300	13.75400	65.69100
H	44.72800	14.73000	65.66100
H	45.18500	13.13400	65.39000
H	44.32900	13.43100	66.65300
N	38.82900	7.94200	62.51400
H	38.16800	8.58500	62.07900
C	38.59000	6.50400	62.40700
C	39.56300	5.69600	61.54000
O	40.30900	4.86000	62.05500
C	37.16200	6.24400	61.90500
C	36.08000	6.75900	62.82300
C	35.25300	7.81300	62.42300
C	35.86100	6.16700	64.06700
C	34.22300	8.26700	63.24100
C	34.83300	6.61400	64.89800
C	34.01000	7.66700	64.48100
N	39.54500	5.94600	60.23100
H	38.92500	6.67800	59.88400
C	40.37700	5.21600	59.26600
C	41.89300	5.20600	59.50200
O	42.63600	4.59100	58.73600
C	40.09200	5.72800	57.84400
C	40.55700	4.86600	56.65900
C	39.72000	3.59200	56.58300
C	40.41900	5.65100	55.36600
N	42.35800	5.87100	60.55400
H	41.71000	6.36300	61.16900
C	43.78900	5.90300	60.83600
C	44.14300	5.14000	62.11100

O	43.56600	5.39500	63.17300
C	44.26400	7.35200	60.95800
O	45.64800	7.41000	61.26100
H	45.94300	8.31000	61.33700
N	45.08700	4.20400	62.00200
H	45.51200	4.03100	61.09100
C	45.53000	3.41800	63.15600
C	46.36600	4.29400	64.08000
O	47.32900	4.92400	63.64300
C	46.37400	2.21500	62.71700
C	46.99300	1.39300	63.86100
C	45.89300	0.72300	64.67800
C	47.93900	0.35100	63.29800
N	46.00200	4.32400	65.35800
H	45.20300	3.77000	65.66600
C	46.72700	5.13600	66.32400
C	47.89900	4.36000	66.92900
O	47.75900	3.19300	67.30300
C	45.78000	5.60600	67.43200
C	46.18500	6.95000	68.01400
O	45.63300	7.34100	69.06100
O	47.05000	7.62300	67.41600
N	49.05200	5.02200	67.01500
H	49.08800	5.98500	66.68100
C	50.26700	4.42800	67.56700
C	50.43900	4.77800	69.05100
O	50.82900	3.92500	69.85200
C	51.49600	4.91800	66.79000
C	51.50700	4.77300	65.26500
C	52.80200	5.35500	64.71100
C	51.36700	3.31100	64.87800
N	50.15000	6.03300	69.40500
H	49.83000	6.68500	68.68900
C	50.27700	6.50800	70.78800
C	49.03900	6.14800	71.61100
O	47.92000	6.13800	71.09400
C	50.47000	8.03600	70.83400
C	50.77700	8.72000	69.49600
C	52.25600	8.73400	69.13700
O	52.89000	7.68500	69.01100
N	52.81000	9.93200	68.96200
H	53.80100	9.94100	68.72100
H	52.28500	10.80000	69.06600

N	49.25000	5.86000	72.89300
H	50.19900	5.88900	73.26600
C	48.14600	5.50500	73.76800
C	48.02300	4.01000	74.00600
O	48.86200	3.22900	73.55500
N	46.97500	3.61400	74.72300
H	46.32500	4.31700	75.07400
C	46.72200	2.20500	75.02600
C	46.09300	1.55800	73.79000
O	45.11800	2.07200	73.24300
C	45.76900	2.08900	76.22500
C	45.66400	0.67100	76.76300
O	45.26100	-0.23600	76.00500
O	45.98200	0.46400	77.95200
N	46.65200	0.42400	73.33200
C	46.17000	-0.31600	72.15800
C	44.67600	-0.64200	72.19800
O	43.96400	-0.47200	71.20500
C	47.03100	-1.57300	72.17500
C	48.31300	-1.07700	72.74900
C	47.84000	-0.23300	73.90200
N	44.21400	-1.11700	73.35100
H	44.86200	-1.23400	74.13000
C	42.81400	-1.47600	73.53900
C	41.91200	-0.24500	73.60500
O	40.84800	-0.21400	72.98400
C	42.66500	-2.32000	74.80900
C	43.25200	-3.72100	74.68100
C	43.45000	-4.38200	76.03600
N	44.44400	-3.66900	76.83400
H	44.82400	-2.80300	76.45200
C	44.89000	-4.06700	78.02200
N	44.43600	-5.18500	78.57300
H	44.77800	-5.49000	79.48400
H	43.73800	-5.74200	78.08100
N	45.79700	-3.34300	78.66100
H	46.13900	-3.64800	79.57200
H	46.14600	-2.48300	78.23700
N	42.33500	0.77000	74.35300
H	43.22200	0.69300	74.85000
C	41.54800	1.99300	74.47300
C	41.41500	2.70000	73.12500
O	40.41200	3.36400	72.86100

C	42.17400	2.94700	75.50200
C	42.02100	2.49300	76.95300
C	42.40700	3.57200	77.95500
O	43.58500	3.99400	77.96400
O	41.52900	4.00000	78.73600
N	42.43100	2.55500	72.27600
H	43.23800	1.99800	72.55700
C	42.41800	3.17400	70.95300
C	41.19900	2.69700	70.17900
O	41.27000	1.74800	69.40100
C	43.69100	2.81800	70.17400
O	44.84000	3.40200	70.76600
H	45.62800	3.18200	70.28400
N	40.07800	3.37000	70.41000
H	40.10400	4.14400	71.07400
C	38.81700	3.05800	69.76300
C	38.91400	2.57500	68.31800
O	39.53800	3.22600	67.47200
C	37.89700	4.28200	69.78800
C	37.43000	4.72100	71.16700
C	36.44700	3.74700	71.79700
O	35.84000	4.04300	72.82700
N	36.29100	2.57700	71.18300
H	36.79400	2.33200	70.33000
H	35.63200	1.92400	71.60600
N	38.31900	1.41700	68.02900
C	38.29300	0.80100	66.69600
C	37.46100	1.63900	65.69800
O	38.00500	2.42700	64.91800
C	37.66900	-0.56200	66.97100
C	38.33700	-0.91900	68.22500
C	38.15300	0.35900	69.06300
N	36.15000	1.45400	65.74400
H	35.77800	0.77800	66.41100
C	35.20900	2.17400	64.88300
C	33.82300	2.09000	65.51600
O	33.64800	2.24400	66.72800
C	35.12900	1.52900	63.48400
C	36.33600	1.28600	62.56500
C	35.87500	0.46700	61.36100
C	36.94800	2.60400	62.10300
N	32.84500	1.85400	64.65900
H	33.07600	1.79100	63.66800

C	31.45800	1.68000	65.05400
C	30.86700	1.11500	63.78700
O	31.09300	1.65600	62.70400
C	30.78400	3.01000	65.41400
C	30.37400	3.95500	64.28600
C	29.55900	5.11300	64.82900
C	31.61600	4.45300	63.59000
N	30.13300	0.01900	63.91200
H	29.97900	-0.39700	64.83100
C	29.55300	-0.58000	62.73300
C	28.36000	-1.46900	62.98100
O	27.34100	-1.02900	63.50700
N	28.49100	-2.72900	62.58400
H	29.36700	-3.02200	62.15200
C	27.42500	-3.70300	62.74600
C	27.29400	-4.04500	64.21600
O	28.28800	-4.31000	64.89100
C	27.73000	-4.99500	61.95300
O	28.02000	-4.65600	60.59500
H	28.76300	-4.06400	60.58200
C	26.54700	-5.93800	61.97400
N	26.06500	-4.01300	64.71500
H	25.28700	-3.74100	64.11400
C	25.80900	-4.35800	66.10200
C	24.69900	-5.38100	66.06400
O	24.12900	-5.64200	65.00100
C	25.36100	-3.13500	66.94600
C	26.47400	-2.11700	67.00800
C	24.11200	-2.51500	66.35200
N	24.40800	-5.97200	67.21600
H	24.94100	-5.72500	68.05000
C	23.34800	-6.96300	67.31800
C	22.13200	-6.18000	67.78100
O	21.94200	-5.97000	68.96800
C	23.71500	-8.02800	68.35500
C	25.20200	-8.37600	68.22700
C	22.84100	-9.25100	68.16800
C	25.64100	-8.79600	66.82500
N	21.30700	-5.74100	66.84400
H	21.47700	-5.97200	65.86500
C	20.15800	-4.92900	67.21100
C	18.91600	-5.65400	67.69900
O	18.13900	-5.08900	68.46700

C	19.77300	-3.99400	66.05200
C	19.42700	-4.74000	64.77200
O	18.72300	-4.13300	63.93700
O	19.85800	-5.90700	64.59500
N	18.72300	-6.89300	67.26500
H	19.40600	-7.32900	66.64500
C	17.54000	-7.62700	67.67300
C	16.45900	-7.53700	66.60900
O	15.31500	-7.92800	66.83800
N	16.83200	-7.01800	65.43900
H	17.79800	-6.71200	65.32700
C	15.91400	-6.86900	64.30900
C	16.54000	-7.37800	63.01400
O	15.88000	-8.05900	62.23400
C	15.51500	-5.40800	64.14300
C	14.87300	-4.81900	65.38000
S	13.25800	-4.16000	65.01300
C	13.72500	-2.69700	63.94500
N	17.80500	-7.03500	62.78100
H	18.29100	-6.43500	63.44700
C	18.51000	-7.50100	61.59100
C	19.33600	-8.70900	62.01100
O	19.40500	-9.69700	61.29000
C	19.43800	-6.42400	61.03300
C	20.13100	-6.86000	59.73600
C	19.20000	-6.67100	58.57000
C	21.38100	-6.05800	59.51600
N	19.96800	-8.61000	63.18000
H	19.88700	-7.74100	63.70800
C	20.77300	-9.69600	63.73600
C	20.28700	-9.92900	65.15100
O	20.20000	-8.98700	65.93200
C	22.26100	-9.33700	63.78400
C	23.05600	-9.17200	62.48500
C	24.49800	-8.85400	62.82600
C	22.98800	-10.43600	61.65600
N	19.97900	-11.18100	65.47600
H	20.08900	-11.91700	64.77900
C	19.48800	-11.52800	66.80600
C	20.55200	-12.07300	67.75000
O	20.28600	-12.30100	68.92500
C	18.34800	-12.53500	66.69500
C	17.15600	-12.03900	65.88800

C	16.03700	-13.03300	66.02100
C	16.71500	-10.67800	66.39000
N	21.75100	-12.29800	67.22900
H	21.89800	-12.12100	66.23500
C	22.86700	-12.79000	68.03000
C	24.13400	-12.60200	67.21100
O	24.06800	-12.40800	65.99900
C	22.68300	-14.26800	68.38700
C	21.36800	-14.86000	67.91800
C	21.13700	-16.25900	68.46400
C	20.93800	-16.24100	69.96600
N	20.62900	-17.60400	70.46800
H	20.49500	-17.59200	71.47900
H	21.33900	-18.28100	70.18800
H	19.82900	-18.01300	69.98500
N	25.28500	-12.64000	67.86900
H	25.28400	-12.79700	68.87700
C	26.55000	-12.46100	67.17200
C	26.67000	-13.46100	66.03700
O	26.17200	-14.58100	66.13400
C	27.73300	-12.69900	68.09900
O	27.68300	-14.04900	68.57300
H	28.42200	-14.19800	69.15200
C	27.69500	-11.75300	69.27200
N	27.33300	-13.06600	64.94000
C	27.52200	-13.94800	63.78700
C	28.04800	-15.31200	64.23000
O	27.65800	-16.35300	63.70000
C	28.52900	-13.17800	62.94500
C	28.07500	-11.78300	63.14200
C	27.84700	-11.71900	64.64300
N	28.93200	-15.28700	65.21900
H	29.20400	-14.38800	65.61600
C	29.52300	-16.49700	65.75200
C	28.43100	-17.48800	66.18800
O	28.44500	-18.65300	65.79300
C	30.43800	-16.13600	66.92600
C	31.63700	-15.19600	66.59300
C	31.24800	-13.78300	66.10100
O	30.19000	-13.26200	66.50600
O	32.01900	-13.17700	65.32000
N	27.47300	-17.02400	66.98200
H	27.49100	-16.04400	67.26600

C	26.39200	-17.88700	67.45900
C	25.43500	-18.31200	66.34900
O	24.92500	-19.42800	66.36000
C	25.58100	-17.17700	68.54100
C	26.38800	-16.67200	69.71500
C	25.61400	-15.67000	70.55000
O	24.55900	-16.04300	71.10100
O	26.05100	-14.50300	70.65300
N	25.18100	-17.41400	65.40200
H	25.63900	-16.50400	65.44600
C	24.26500	-17.69500	64.30100
C	24.72000	-18.80800	63.37200
O	23.91800	-19.63400	62.95600
C	24.02200	-16.43600	63.47400
C	23.27800	-15.27600	64.12700
C	22.96900	-14.21500	63.07700
C	21.99800	-15.78200	64.73900
N	26.00300	-18.82700	63.03600
H	26.63100	-18.11700	63.41400
C	26.53200	-19.84500	62.13600
C	26.36200	-21.25900	62.65600
O	26.19300	-22.20100	61.87900
C	28.00900	-19.59900	61.86600
C	28.27500	-18.41300	60.98600
C	29.51500	-18.61000	60.15900
O	30.62600	-18.67700	60.68900
N	29.33500	-18.72400	58.84500
H	30.17600	-18.85800	58.28400
H	28.41600	-18.66900	58.40600
N	26.42400	-21.40700	63.97400
H	26.57700	-20.58900	64.56300
C	26.27800	-22.71300	64.59200
C	24.80500	-23.12800	64.63700
O	24.42000	-23.97300	65.44500
C	26.86600	-22.68500	65.99800
N	23.99000	-22.54100	63.76100
H	24.37700	-21.86400	63.10400
C	22.55500	-22.83700	63.71100
C	22.05300	-23.13400	62.29800
O	21.69200	-22.22100	61.55000
C	21.75400	-21.66300	64.28400
C	20.25100	-21.76700	64.07100
C	19.56700	-20.40900	64.08500

O	19.64100	-19.71500	65.12500
O	18.95900	-20.03500	63.05400
N	22.01900	-24.41300	61.94300
H	22.33000	-25.12300	62.60600
C	21.54700	-24.82600	60.62500
C	20.01700	-24.82000	60.59200
O	19.39700	-25.80000	60.17800
C	22.05200	-26.23700	60.28900
C	23.56800	-26.39100	60.18900
C	24.25500	-26.20200	61.53600
N	25.65700	-26.61900	61.51000
H	25.93200	-27.39400	62.11300
C	26.60000	-26.05900	60.75500
N	26.30100	-25.04700	59.95200
H	25.34300	-24.69900	59.91300
H	27.02300	-24.61800	59.37400
N	27.84800	-26.51300	60.80600
H	28.07800	-27.29100	61.42400
H	28.57000	-26.08400	60.22800
N	19.40800	-23.72300	61.03100
H	19.96400	-22.93600	61.36500
C	17.95100	-23.63400	61.03900
C	17.43200	-22.37300	60.36600
O	16.32100	-21.91900	60.63700
C	17.42400	-23.72200	62.47400
C	17.46100	-25.14400	63.02300
O	18.50600	-25.80200	63.01500
N	16.31700	-25.62300	63.50300
H	15.45400	-25.08000	63.51000
H	16.34200	-26.57400	63.87000
N	18.25100	-21.81200	59.48500
H	19.16600	-22.23100	59.32100
C	17.87800	-20.61600	58.74800
C	17.75500	-21.02400	57.28100
O	17.79800	-22.21200	56.95500
C	18.95600	-19.53400	58.90700
C	18.54400	-18.17700	58.38100
C	17.53300	-17.44800	59.00700
C	19.15600	-17.63500	57.25000
C	17.13800	-16.20300	58.51400
C	18.76500	-16.38800	56.74800
C	17.75500	-15.67400	57.38200
N	17.59500	-20.03600	56.40500

H	17.54700	-19.07700	56.75000
C	17.48600	-20.27200	54.97000
C	18.90700	-20.34600	54.40000
O	19.74800	-19.49900	54.70800
C	16.72100	-19.12300	54.31700
C	16.39000	-19.35800	52.87800
N	16.02000	-18.34100	52.02500
H	15.94700	-17.35600	52.27900
C	16.35800	-20.49600	52.14600
C	15.77400	-18.84200	50.82700
N	15.97100	-20.14800	50.87400
H	15.85500	-20.79300	50.09300
N	19.17300	-21.35500	53.57300
H	18.43300	-22.01800	53.34100
C	20.50100	-21.53500	52.99000
C	20.50400	-21.34800	51.48000
O	19.60900	-21.82700	50.79300
C	21.03500	-22.93700	53.29200
O	20.12000	-23.90700	52.77100
H	20.02500	-23.78000	51.83400
C	21.18700	-23.14100	54.79400
N	21.52200	-20.66300	50.96500
H	22.24400	-20.29900	51.58700
C	21.62900	-20.42100	49.52800
C	23.06300	-20.59000	49.01800
O	24.01000	-20.58900	49.80900
C	21.14600	-19.00400	49.18300
C	19.72900	-18.82100	49.66500
C	22.05500	-17.97600	49.81200
N	23.24500	-20.74500	47.68900
C	24.59600	-20.90700	47.14100
C	25.42100	-19.70500	47.57000
O	25.04900	-18.56000	47.30000
C	24.36000	-20.92900	45.63700
C	22.99600	-21.47600	45.51600
C	22.24900	-20.75900	46.60900
N	26.53800	-19.96600	48.23700
H	26.80500	-20.93600	48.40300
C	27.39100	-18.89700	48.73700
C	28.83400	-19.03300	48.27600
O	29.47500	-20.04600	48.56000
C	27.35200	-18.91300	50.27100
C	27.92800	-17.69200	50.95900

C	28.11900	-17.68500	52.33800
C	28.25200	-16.53900	50.24000
C	28.61500	-16.56600	52.98800
C	28.74600	-15.41600	50.87300
C	28.92800	-15.43000	52.25100
O	29.42400	-14.31200	52.89700
H	29.63800	-13.53600	52.39300
N	29.34400	-18.02200	47.56900
H	28.74900	-17.22600	47.33900
C	30.74500	-18.02700	47.11200
C	31.53100	-17.07300	48.02600
O	31.13100	-15.92400	48.20900
C	30.84900	-17.54100	45.66500
C	32.25900	-17.58400	45.10000
S	32.51700	-16.54300	43.62000
C	31.42500	-17.33700	42.42000
N	32.62600	-17.55300	48.61500
H	32.89500	-18.52100	48.43900
C	33.46100	-16.73800	49.51000
C	34.89200	-16.75500	48.99000
O	35.35400	-17.77500	48.49500
C	33.47500	-17.30300	50.95700
C	34.39100	-16.46700	51.84000
C	32.07700	-17.32300	51.52100
N	35.60800	-15.64500	49.10100
H	35.21500	-14.80600	49.52800
C	36.96700	-15.65900	48.59700
C	37.88500	-14.59000	49.13400
O	37.43000	-13.59200	49.68500
N	39.18600	-14.80600	48.96600
H	39.48900	-15.66100	48.49800
C	40.18900	-13.86400	49.42700
C	41.20400	-13.57600	48.31900
O	41.09500	-14.09700	47.21500
C	40.93300	-14.41200	50.66700
C	41.67600	-15.70500	50.31000
C	39.94600	-14.68600	51.78300
C	42.58900	-16.21800	51.41900
N	42.17800	-12.72400	48.62000
H	42.18900	-12.29900	49.54700
C	43.23300	-12.37400	47.67400
C	44.56300	-12.72600	48.31900
O	44.72000	-12.61600	49.53600

C	43.19300	-10.88500	47.34200
C	41.97300	-10.51300	46.54000
O	41.73300	-9.34100	46.24900
N	41.19100	-11.51600	46.17100
H	41.39000	-12.48700	46.41200
H	40.36500	-11.26400	45.62800
N	45.51100	-13.15600	47.49500
H	45.30800	-13.20400	46.49700
C	46.83000	-13.56200	47.96100
C	47.46000	-12.62400	48.98900
O	47.97000	-13.08000	50.00700
C	47.76700	-13.70900	46.75900
C	49.10900	-14.35900	47.06700
C	48.95000	-15.83100	47.40600
C	50.30000	-16.51800	47.42700
N	51.01500	-16.33100	46.12700
H	51.92400	-16.79400	46.14100
H	51.09800	-15.34400	45.88200
H	50.44800	-16.63900	45.33700
N	47.41400	-11.32000	48.71700
H	46.94600	-11.01400	47.86400
C	48.00900	-10.30900	49.59600
C	47.02900	-9.22500	50.06700
O	47.16000	-8.05000	49.69500
C	49.18700	-9.64200	48.88000
C	50.35800	-10.57800	48.58600
C	51.47600	-9.90600	47.80300
O	52.03100	-8.88300	48.21900
N	51.81500	-10.48400	46.66300
H	52.56500	-10.03300	46.13800
H	51.35700	-11.32800	46.32000
N	46.06600	-9.62800	50.90100
H	46.04700	-10.60900	51.17900
C	45.03500	-8.73500	51.43800
C	45.56200	-7.49100	52.14400
O	44.94200	-6.43000	52.09400
C	44.14000	-9.49500	52.41700
C	43.26900	-10.56200	51.79000
C	42.14600	-9.99600	50.94300
O	42.00500	-8.75700	50.87100
O	41.39700	-10.79900	50.34800
N	46.69800	-7.62300	52.81100
H	47.18200	-8.52100	52.81400

C	47.26100	-6.49900	53.53800
C	48.57300	-6.07900	52.89400
O	49.45400	-5.51900	53.54900
C	47.48700	-6.90600	54.99200
C	47.41200	-5.77300	55.95700
C	48.51100	-5.43300	56.73000
C	46.23400	-5.05800	56.11300
C	48.43700	-4.39100	57.65500
C	46.15000	-4.01800	57.03200
C	47.25300	-3.68300	57.80600
N	48.68000	-6.33400	51.59600
H	47.89700	-6.76300	51.10200
C	49.89300	-6.01200	50.86900
C	50.23800	-4.55400	50.61900
O	51.42200	-4.23600	50.50000
N	49.24500	-3.67200	50.53100
H	48.28000	-3.98300	50.64100
C	49.52800	-2.26600	50.27800
C	48.37000	-1.30100	50.58200
O	48.44100	-0.50900	51.52500
C	49.95500	-2.09500	48.81000
C	50.32900	-0.71300	48.43300
C	51.48600	-0.06800	48.73300
C	49.53200	0.20900	47.69100
N	51.46300	1.20500	48.22100
H	52.21100	1.89300	48.30800
C	50.27200	1.40100	47.57500
C	48.25700	0.14300	47.11100
C	49.78800	2.52100	46.90100
C	47.77300	1.25600	46.44000
C	48.53900	2.43100	46.34000
N	47.31200	-1.38700	49.77400
H	47.30800	-2.10900	49.05400
C	46.16100	-0.49800	49.87100
C	45.72700	-0.21200	51.29400
O	45.59400	0.94200	51.69000
C	44.98200	-1.07100	49.09100
C	43.66700	-0.30300	49.21800
C	43.85700	1.10200	48.73600
C	42.59600	-0.96600	48.40200
N	45.50800	-1.25800	52.07300
H	45.64600	-2.20200	51.71200
C	45.07100	-1.05900	53.44100

C	46.13700	-0.45000	54.34100
O	45.86500	0.50700	55.05600
C	44.54600	-2.37000	54.07100
C	43.36300	-2.89500	53.24200
C	44.06500	-2.10100	55.51500
C	42.72300	-4.12700	53.78800
N	47.35700	-1.00900	54.34300
C	48.38900	-0.42800	55.20200
C	48.69400	1.00900	54.81000
O	49.15100	1.80400	55.63300
C	49.57300	-1.36400	54.99300
C	48.91500	-2.66700	54.78100
C	47.80000	-2.31200	53.82300
N	48.43500	1.34000	53.55000
H	48.05900	0.63500	52.91600
C	48.67700	2.68800	53.05500
C	47.60300	3.64800	53.56900
O	47.90300	4.59300	54.29900
C	48.71400	2.67700	51.51900
C	48.87800	4.03800	50.86300
S	47.30100	4.85400	50.54100
C	47.51700	5.39200	48.82300
N	46.35000	3.38700	53.20700
H	46.16500	2.57400	52.61900
C	45.23100	4.22800	53.62500
C	45.18100	4.49600	55.12900
O	44.53800	5.45800	55.56500
C	43.90600	3.59500	53.20600
C	43.72800	3.23500	51.73500
C	42.35800	2.60500	51.54900
C	43.88600	4.46600	50.86100
N	45.84300	3.65000	55.91800
H	46.35600	2.87500	55.49800
C	45.85000	3.80800	57.36900
C	47.16500	4.34600	57.89900
O	47.33900	4.49300	59.10600
C	45.52900	2.48200	58.05600
C	44.05000	2.12400	58.06700
S	43.74400	0.46500	58.71800
C	44.28300	0.68000	60.43700
N	48.09300	4.63000	56.99700
H	47.90200	4.45900	56.01000
C	49.37900	5.18200	57.39200

C	50.16300	4.25100	58.31100
O	50.78600	4.69200	59.27900
C	49.16500	6.52600	58.08500
O	48.39000	7.39300	57.27400
H	48.25700	8.22900	57.70500
N	50.13400	2.96200	58.00200
H	49.59600	2.65300	57.19300
C	50.85600	1.98000	58.79600
C	52.33600	2.34500	58.79200
O	52.89600	2.66400	57.74300
C	50.67200	0.59000	58.19300
C	50.39000	-0.48400	59.21300
C	49.17100	-0.52300	59.89200
C	51.33600	-1.46900	59.48900
C	48.89900	-1.52100	60.81600
C	51.07700	-2.47200	60.41300
C	49.85600	-2.49400	61.07100
O	49.59000	-3.50000	61.96900
H	48.75400	-3.51500	62.42000
N	52.99100	2.29700	59.96600
C	54.41800	2.62600	60.10100
C	55.34500	1.55900	59.51000
O	55.89200	0.72700	60.23800
C	54.58900	2.76500	61.60900
C	53.67100	1.71500	62.12100
C	52.42400	1.91000	61.27100
N	55.51900	1.59100	58.19000
H	55.04500	2.31200	57.64600
C	56.36900	0.62500	57.49800
C	57.04900	1.27300	56.30200
O	56.93300	0.80900	55.16700
C	55.54000	-0.57900	57.03900
C	55.00800	-1.47400	58.16100
C	54.05700	-2.50100	57.58900
C	56.17000	-2.14800	58.86900
N	57.75800	2.35800	56.57700
H	57.80400	2.68400	57.54200
C	58.47200	3.09900	55.55300
C	59.84800	2.49800	55.27200
O	60.23300	2.31000	54.11600
C	58.60200	4.56100	55.98900
O	58.62200	4.66400	57.40600
H	58.70300	5.57100	57.67700

N	60.57800	2.18900	56.34000
H	60.19300	2.36700	57.26700
C	61.90900	1.60500	56.23200
C	61.86900	0.22700	55.57400
O	62.87700	-0.47700	55.52900
C	62.56000	1.51400	57.61700
C	61.75500	0.74300	58.66400
C	60.42700	1.41100	59.02200
O	60.43200	2.61000	59.39100
O	59.37800	0.73000	58.94200
N	60.69200	-0.14400	55.07600
H	59.89400	0.48300	55.17400
C	60.50900	-1.41500	54.39700
C	60.98200	-2.68500	55.08200
O	61.20100	-3.69500	54.41400
N	61.14900	-2.65800	56.39800
H	60.97300	-1.79700	56.91600
C	61.58400	-3.85600	57.10500
C	61.17700	-3.85700	58.56900
O	60.82800	-2.81900	59.13000
C	63.10000	-4.05200	56.96400
C	63.96700	-2.91000	57.47200
C	65.42200	-3.05700	57.04800
O	66.29100	-2.30900	57.49500
N	65.69100	-4.02100	56.17500
H	64.97100	-4.64100	55.80500
H	66.66600	-4.11900	55.89100
N	61.21600	-5.04000	59.17500
H	61.53200	-5.85300	58.64600
C	60.82400	-5.21800	60.56600
C	61.64400	-6.31100	61.24200
O	62.34400	-7.07700	60.58600
C	59.33700	-5.59000	60.63100
C	58.40100	-4.76600	61.52000
C	58.36900	-3.31900	61.04900
C	57.00800	-5.37300	61.47200
N	61.54400	-6.37500	62.56400
H	60.94900	-5.70100	63.04600
C	62.25500	-7.37500	63.35200
C	61.34400	-7.87700	64.47600
O	60.47000	-7.14600	64.95000
C	63.53700	-6.77900	63.94600
C	63.26500	-5.81100	65.08500

O	62.63900	-4.75800	64.84800
O	63.68100	-6.10800	66.22500
N	61.55600	-9.12100	64.89400
H	62.30200	-9.66300	64.45800
C	60.76400	-9.74500	65.95200
C	60.22000	-8.80000	67.02200
O	59.03100	-8.85000	67.34700
C	61.58300	-10.84700	66.61500
C	61.88300	-12.00200	65.68100
C	60.65300	-12.82900	65.37000
O	60.65000	-13.62400	64.43300
N	59.60500	-12.65700	66.16800
H	58.77700	-13.21400	65.95900
H	59.60700	-11.99700	66.94600
N	61.07800	-7.94400	67.57300
H	62.05200	-7.94300	67.26900
C	60.64700	-7.00600	68.60600
C	59.66100	-5.95700	68.10000
O	58.55900	-5.83600	68.62600
C	61.85100	-6.30500	69.23200
C	62.49000	-7.05500	70.38500
C	63.62200	-6.23200	70.98100
C	64.23300	-6.88400	72.20000
N	65.45600	-6.15200	72.60300
H	65.86800	-6.59200	73.42600
H	65.27700	-5.15900	72.74900
H	66.12400	-6.07100	71.83600
N	60.05900	-5.19600	67.08500
H	60.98700	-5.34100	66.68700
C	59.19600	-4.15500	66.52600
C	57.89600	-4.75300	66.00300
O	56.88600	-4.05700	65.87000
C	59.89000	-3.42300	65.37000
O	61.15600	-2.92300	65.81500
H	61.69000	-3.64800	66.11800
C	59.03700	-2.26600	64.88700
N	57.93700	-6.04800	65.70300
H	58.81200	-6.55500	65.83200
C	56.77800	-6.76700	65.19700
C	55.79400	-7.02600	66.33200
O	54.62500	-6.64400	66.24100
C	57.21600	-8.07900	64.56800
N	56.26300	-7.67700	67.39700

H	57.23600	-7.98200	67.41000
C	55.40800	-7.96000	68.54400
C	54.78200	-6.66800	69.04100
O	53.61000	-6.63000	69.41100
C	56.21100	-8.57500	69.68300
C	56.60400	-10.01700	69.48400
S	57.44000	-10.66200	70.95100
C	59.14400	-10.57600	70.41600
N	55.58800	-5.61100	69.04500
H	56.54600	-5.72800	68.71400
C	55.16600	-4.29400	69.50100
C	54.19000	-3.66900	68.52100
O	53.22000	-3.02300	68.91600
C	56.38800	-3.39300	69.66600
O	56.01900	-2.11700	70.15500
H	56.77900	-1.55700	70.25800
N	54.45500	-3.86200	67.23700
H	55.28300	-4.39300	66.96900
C	53.58100	-3.32700	66.20600
C	52.24100	-4.04000	66.34200
O	51.18100	-3.40700	66.36100
C	54.16100	-3.60100	64.82100
C	53.87400	-2.54300	63.75500
C	54.29300	-3.07800	62.39900
C	52.40600	-2.17700	63.75100
N	52.30900	-5.36500	66.45200
H	53.22700	-5.81000	66.44400
C	51.12400	-6.20800	66.58300
C	50.23000	-5.76500	67.73800
O	49.01500	-5.64600	67.58600
C	51.54400	-7.66600	66.78100
C	50.46700	-8.72100	66.53100
C	49.93100	-8.58400	65.11100
C	51.05600	-10.10200	66.75000
N	50.83100	-5.52000	68.89500
H	51.84100	-5.63600	68.97700
C	50.05600	-5.08700	70.04700
C	49.32100	-3.77800	69.75300
O	48.16400	-3.62300	70.13600
C	50.95800	-4.91800	71.27400
C	50.21200	-4.45500	72.50100
C	50.55200	-3.41900	73.32200
C	48.99300	-5.00000	73.02900

N	49.62300	-3.28300	74.32400
H	49.64900	-2.58200	75.06400
C	48.65600	-4.24100	74.16900
C	48.15500	-6.05700	72.65100
C	47.51500	-4.50400	74.93500
C	47.02000	-6.31700	73.41400
C	46.71300	-5.54300	74.54200
N	49.98700	-2.84400	69.07200
H	50.94500	-3.03200	68.77600
C	49.37400	-1.55300	68.73900
C	48.23200	-1.71200	67.75100
O	47.27800	-0.92900	67.74200
C	50.39600	-0.59900	68.11500
C	51.49500	-0.11900	69.02900
C	52.39100	0.83200	68.26700
C	53.68100	1.10700	69.00800
N	54.59400	1.94800	68.18400
H	55.46400	2.13300	68.68400
H	54.14200	2.81000	67.88000
H	54.76600	1.53300	67.26800
N	48.34500	-2.72500	66.90500
H	49.15700	-3.33900	66.96600
C	47.33800	-2.97900	65.89500
C	46.11300	-3.67400	66.47600
O	45.17600	-4.00500	65.74900
C	47.94900	-3.82100	64.78100
O	49.14600	-3.21900	64.33100
H	49.52700	-3.74400	63.63700
N	46.12300	-3.87800	67.79000
H	46.92900	-3.56100	68.32800
C	45.02500	-4.53900	68.49600
C	43.64100	-4.20400	67.94700
O	42.82900	-5.09900	67.71800
C	45.05900	-4.17900	69.97700
C	44.08700	-4.97200	70.80400
C	44.45100	-6.20300	71.33700
C	42.79400	-4.50400	71.03400
C	43.55600	-6.95400	72.08100
C	41.88700	-5.24600	71.77500
C	42.27500	-6.47200	72.29600
O	41.38500	-7.22700	73.02500
H	40.50700	-6.89600	73.17200
N	43.34500	-2.91000	67.74800

C	42.03100	-2.53500	67.22000
C	41.90800	-2.87100	65.73800
O	41.34300	-2.09800	64.96300
C	41.97800	-1.03500	67.48000
C	43.40500	-0.63300	67.27400
C	44.15500	-1.71000	68.02900
N	42.44200	-4.02800	65.35500
H	42.88700	-4.61900	66.05700
C	42.41500	-4.48400	63.96600
C	42.37900	-6.00400	63.85800
O	41.61600	-6.56500	63.06800
C	43.65200	-3.98200	63.21700
C	43.48800	-2.82100	62.24100
C	44.84000	-2.47300	61.64800
C	42.50700	-3.20400	61.14900
N	43.22100	-6.66000	64.65000
H	43.81600	-6.12900	65.28600
C	43.32000	-8.10900	64.63900
C	42.96100	-8.69700	65.99200
O	42.83800	-9.91500	66.14000
C	44.74500	-8.54400	64.26800
C	45.07500	-8.08300	62.85300
C	45.73200	-7.96000	65.26100
N	42.80700	-7.82000	66.97800
H	42.94500	-6.82900	66.78200
C	42.44700	-8.22800	68.33000
C	43.23100	-9.45400	68.77900
O	42.78900	-10.58500	68.60200
C	40.95300	-8.53800	68.39400
S	39.90700	-7.33300	67.54600
N	44.40100	-9.23200	69.35600
H	44.73500	-8.27500	69.47200
C	45.21200	-10.33900	69.82400
C	45.66100	-10.04900	71.23700
O	46.38800	-9.09000	71.47000
C	46.45300	-10.53800	68.93900
C	46.01400	-10.86100	67.50900
C	47.33000	-11.65000	69.51400
C	47.15900	-11.02000	66.53800
N	45.22000	-10.86800	72.18200
H	44.60400	-11.64200	71.93300
C	45.60600	-10.67300	73.57100
C	47.11400	-10.51100	73.61800

O	47.84200	-11.25600	72.96300
C	45.18400	-11.86200	74.39400
N	47.57800	-9.53600	74.39000
H	46.92000	-8.96400	74.92000
C	49.00400	-9.26500	74.49800
C	49.82200	-10.50900	74.84600
O	50.90500	-10.72100	74.29900
C	49.24200	-8.16800	75.53300
C	50.62900	-7.56900	75.46500
C	50.74800	-6.32900	76.32700
C	52.09700	-5.66800	76.12900
N	52.30900	-5.33000	74.69400
H	53.21700	-4.88500	74.56100
H	51.54900	-4.75900	74.32300
H	52.19500	-6.14500	74.09200
N	49.29600	-11.33300	75.74600
H	48.39200	-11.10200	76.15800
C	49.97000	-12.55900	76.16400
C	50.11200	-13.58200	75.03700
O	50.79300	-14.59700	75.19400
C	49.22500	-13.20400	77.34100
C	47.73800	-13.41600	77.10600
C	46.89600	-12.18600	77.45400
O	47.28600	-11.05200	77.08300
O	45.83100	-12.35500	78.09300
N	49.47400	-13.31300	73.90200
H	48.93200	-12.45200	73.82800
C	49.53000	-14.22000	72.75900
C	50.55900	-13.78000	71.72300
O	51.21400	-14.61300	71.09200
C	48.15200	-14.31300	72.10300
C	47.04800	-14.86000	73.00900
C	45.71400	-14.81600	72.28200
C	47.38600	-16.28000	73.41900
N	50.69700	-12.46700	71.56300
H	50.12800	-11.84400	72.13600
C	51.62600	-11.87900	70.60400
C	52.88500	-12.71100	70.30000
O	53.08800	-13.13200	69.16400
C	52.06400	-10.46500	71.06000
C	50.83400	-9.60400	71.35300
C	52.91900	-9.81500	69.98700
C	49.94700	-9.36500	70.15800

N	53.73700	-12.96800	71.30900
C	54.95500	-13.74800	71.07600
C	54.73800	-15.04000	70.30400
O	55.39600	-15.28100	69.29200
C	55.47000	-14.00900	72.48400
C	55.02600	-12.81500	73.22200
C	53.60800	-12.65100	72.74100
N	53.82100	-15.87400	70.78000
H	53.29300	-15.63100	71.61800
C	53.57300	-17.13500	70.10000
C	53.14900	-16.88600	68.66100
O	53.62100	-17.55300	67.73800
C	52.49600	-17.95600	70.82100
C	52.37200	-19.37800	70.26200
C	51.38900	-20.25000	71.02400
O	51.48000	-20.31300	72.27200
O	50.53200	-20.88400	70.37000
N	52.26300	-15.91500	68.47400
H	51.91900	-15.39100	69.27800
C	51.77400	-15.58400	67.14600
C	52.89800	-15.08600	66.25100
O	53.07600	-15.58000	65.13900
C	50.67700	-14.53700	67.24100
N	53.65800	-14.10900	66.73800
H	53.46800	-13.74600	67.67200
C	54.75500	-13.54700	65.96500
C	55.84100	-14.57400	65.70700
O	56.50400	-14.53500	64.67400
C	55.39100	-12.34900	66.67500
O	54.38400	-11.37800	66.98400
H	54.77900	-10.63500	67.42500
C	56.42800	-11.70500	65.77500
N	56.02800	-15.49200	66.64700
H	55.45600	-15.47000	67.49100
C	57.03700	-16.53000	66.49200
C	56.61700	-17.53800	65.42600
O	57.45200	-18.24800	64.86700
C	57.27100	-17.24400	67.83100
C	58.29900	-18.38700	67.80100
C	59.63400	-18.00500	67.14800
O	60.15100	-16.89700	67.42700
O	60.17100	-18.82500	66.36300
N	55.32200	-17.58500	65.13200

H	54.67900	-16.95400	65.61000
C	54.80000	-18.52100	64.13900
C	55.00900	-18.06700	62.70200
O	55.37800	-18.86700	61.84600
C	53.30300	-18.76600	64.37100
C	52.66300	-19.74200	63.38100
C	53.17000	-21.16400	63.58300
C	52.51500	-22.13400	62.60900
N	52.90100	-23.54900	62.87200
H	52.46200	-24.19900	62.22000
H	52.70600	-23.81000	63.83800
H	53.91500	-23.65900	62.87500
N	54.76000	-16.78700	62.44100
H	54.45700	-16.17300	63.19800
C	54.91000	-16.24100	61.09700
C	56.30300	-15.70400	60.81600
O	56.87900	-15.97100	59.76100
C	53.88800	-15.12300	60.85300
C	52.47300	-15.60700	60.60700
C	51.76600	-16.29500	61.59100
C	51.83700	-15.36900	59.39100
C	50.46300	-16.72700	61.37000
C	50.53700	-15.80200	59.16100
C	49.85600	-16.47800	60.15400
O	48.56400	-16.90100	59.93800
H	48.14700	-16.73000	59.10200
N	56.84900	-14.94800	61.75900
H	56.34000	-14.77300	62.62600
C	58.16500	-14.36900	61.56600
C	59.32000	-15.26800	61.99300
O	60.48800	-14.92600	61.79500
C	58.23700	-13.02700	62.28700
C	57.08000	-12.10200	61.90800
C	57.38200	-10.69500	62.39200
C	56.88000	-12.10600	60.40200
N	58.99800	-16.42100	62.56800
H	58.01800	-16.66300	62.71500
C	60.04400	-17.33600	62.98600
C	60.84900	-17.82100	61.79300
O	61.87600	-18.48500	61.96000
N	60.37300	-17.48600	60.59000
H	59.51600	-16.93600	60.53400
C	61.04000	-17.88100	59.35700

C	62.48700	-17.42500	59.26100
O	63.24000	-17.54300	60.22400
N	62.89200	-16.90400	58.10700
H	62.24000	-16.81700	57.32800
C	64.27400	-16.45600	57.95900
C	64.55200	-15.27400	58.87900
O	63.65200	-14.76700	59.55900
C	64.62100	-16.01000	56.50000
O	63.70500	-14.99000	56.08800
H	63.91600	-14.71900	55.20200
C	64.58500	-17.19700	55.52400
N	65.81500	-14.85200	58.88400
H	66.49200	-15.34000	58.29700
C	66.27600	-13.73000	59.68500
C	66.22400	-12.51100	58.78200
O	66.56900	-11.40000	59.18300
C	67.70800	-13.98300	60.15000
C	67.90700	-15.39500	60.67600
O	67.24700	-15.76500	61.67200
O	68.72400	-16.13500	60.08500
N	65.79400	-12.75100	57.54900
H	65.55100	-13.70900	57.29600
C	65.65400	-11.71000	56.54300
C	64.64900	-10.71700	57.10500
O	63.46300	-11.03700	57.22900
C	65.11000	-12.31900	55.25000
C	65.20100	-11.37200	54.07100
O	64.85000	-10.17900	54.22600
O	65.61700	-11.83200	52.98400
N	65.11000	-9.51900	57.45100
H	66.09700	-9.29900	57.31800
C	64.21600	-8.51900	58.01800
C	63.16400	-8.02500	57.03800
O	62.17300	-7.42300	57.43800
C	64.99300	-7.31800	58.56300
O	65.84300	-6.79400	57.53900
H	66.32500	-6.04900	57.87700
C	65.82900	-7.73800	59.76100
N	63.37600	-8.26800	55.75100
H	64.22500	-8.74700	55.45200
C	62.39000	-7.84700	54.77000
C	61.30400	-8.91600	54.67100
O	60.12300	-8.59400	54.55000

C	63.02400	-7.59300	53.38200
C	61.94400	-7.47300	52.32100
C	63.82900	-6.30800	53.42300
N	61.69200	-10.18700	54.73600
H	62.68100	-10.41700	54.83300
C	60.69600	-11.24800	54.66800
C	59.76400	-11.10200	55.86200
O	58.55600	-11.30900	55.74700
C	61.34500	-12.63300	54.69400
C	62.06200	-13.04300	53.41300
C	62.49200	-14.50600	53.50400
C	63.44400	-14.93500	52.38900
N	63.94200	-16.33700	52.61900
H	64.57800	-16.62300	51.87500
H	63.17200	-16.99700	52.73200
H	64.36900	-16.43900	53.54000
N	60.32600	-10.73300	57.00900
H	61.33200	-10.56600	57.04500
C	59.52400	-10.56400	58.21700
C	58.42200	-9.52300	58.02700
O	57.34300	-9.64900	58.59500
C	60.41000	-10.16400	59.40000
C	61.43300	-11.21100	59.80600
C	62.08600	-10.85400	61.13700
C	63.14700	-11.87100	61.53300
N	62.61700	-13.26100	61.62700
H	63.32800	-13.94300	61.89200
H	62.15700	-13.53400	60.75900
H	61.81800	-13.30400	62.26000
N	58.68800	-8.48800	57.24000
H	59.60400	-8.40400	56.79900
C	57.67200	-7.47300	57.00700
C	56.53500	-8.08800	56.19700
O	55.36400	-7.90000	56.51700
C	58.24600	-6.28600	56.23900
C	57.19300	-5.25000	55.87200
C	57.65800	-4.34700	54.74200
C	57.93800	-5.13500	53.46600
N	56.73500	-5.82700	52.94500
H	56.92200	-6.35400	52.09200
H	55.96600	-5.17100	52.80900
H	56.31800	-6.42400	53.65900
N	56.89000	-8.81800	55.14400

H	57.88000	-8.93000	54.92700
C	55.89600	-9.46300	54.29200
C	55.10800	-10.48900	55.09400
O	53.88000	-10.51000	55.03900
C	56.56100	-10.16300	53.10400
C	57.34500	-9.21200	52.21600
O	56.86800	-8.08300	51.97200
O	58.43100	-9.61000	51.74400
N	55.81600	-11.34000	55.83300
H	56.83400	-11.27500	55.82400
C	55.17900	-12.36300	56.65600
C	54.28800	-11.74300	57.72400
O	53.31500	-12.35900	58.16700
C	56.23100	-13.22500	57.34200
C	57.09600	-14.09100	56.43800
C	58.17000	-14.77100	57.27500
C	56.22100	-15.10900	55.71900
N	54.64400	-10.53500	58.15400
H	55.48000	-10.09700	57.76700
C	53.87200	-9.82100	59.16300
C	52.59300	-9.33100	58.49300
O	51.52800	-9.28100	59.11300
C	54.66500	-8.62500	59.70900
C	53.92300	-7.83500	60.75800
C	53.71800	-8.36000	62.03100
C	53.40400	-6.57800	60.46400
C	53.00800	-7.64800	62.99500
C	52.69100	-5.85800	61.42300
C	52.49400	-6.39400	62.68900
N	52.71100	-8.96200	57.22100
H	53.62400	-9.01000	56.77000
C	51.56700	-8.49300	56.46200
C	50.67600	-9.67800	56.10700
O	49.52900	-9.50700	55.68900
C	52.02700	-7.76700	55.20100
C	52.76500	-6.46300	55.48900
C	53.07900	-5.74700	54.17800
C	51.90400	-5.59200	56.40000
N	51.22300	-10.88000	56.26200
H	52.19500	-10.95100	56.56400
C	50.46500	-12.09700	56.01000
C	49.71900	-12.37900	57.30800
O	48.51700	-12.65800	57.31400

C	51.39700	-13.26900	55.68700
C	51.75700	-13.34900	54.21200
O	50.84500	-13.19700	53.36500
O	52.94500	-13.58400	53.90000
N	50.46400	-12.29100	58.40600
H	51.45400	-12.06600	58.30400
C	49.93700	-12.50000	59.74400
C	48.59900	-11.76900	59.81500
O	47.55900	-12.38500	60.02800
C	50.93400	-11.93300	60.77100
C	50.82300	-12.03800	62.30300
C	49.57300	-11.34600	62.80300
C	50.82600	-13.47800	62.71500
N	48.63200	-10.45900	59.59500
H	49.52500	-10.01600	59.37800
C	47.42900	-9.63700	59.65500
C	46.37400	-10.01800	58.62800
O	45.20000	-10.16000	58.97000
C	47.77800	-8.15100	59.49500
C	48.56700	-7.69200	60.71900
C	46.50900	-7.32400	59.29900
C	49.02100	-6.27000	60.64200
N	46.78700	-10.17800	57.37500
H	47.77200	-10.03400	57.15300
C	45.86400	-10.55500	56.31100
C	45.11700	-11.82200	56.70100
O	43.90600	-11.93600	56.47800
C	46.61900	-10.77900	55.02400
N	45.84100	-12.77100	57.28900
H	46.83700	-12.61400	57.44600
C	45.24100	-14.03100	57.71400
C	44.15200	-13.85400	58.76800
O	43.05100	-14.38400	58.61100
C	46.31300	-14.99100	58.24600
C	47.02300	-15.75500	57.13400
O	46.57700	-15.66500	55.96700
O	48.02000	-16.45400	57.42500
N	44.45500	-13.10600	59.83000
H	45.38000	-12.68000	59.88100
C	43.50900	-12.87200	60.92800
C	42.29000	-12.01900	60.53300
O	41.19400	-12.18500	61.08500
C	44.22000	-12.19400	62.13800

C	43.28000	-12.11900	63.33300
C	45.47100	-12.96600	62.51200
N	42.47100	-11.11100	59.57800
H	43.38700	-11.01400	59.14100
C	41.37300	-10.25300	59.15000
C	40.56000	-10.79600	57.98500
O	39.39400	-10.43100	57.82700
C	41.88700	-8.87500	58.74800
C	42.48100	-8.06200	59.85600
S	42.40200	-6.34100	59.39500
C	43.52100	-6.28200	58.03600
N	41.16200	-11.64500	57.15700
H	42.12600	-11.93000	57.32800
C	40.43900	-12.16500	56.00600
C	40.50900	-13.67100	55.80000
O	39.49400	-14.35900	55.82200
C	40.92600	-11.47500	54.72800
C	40.76200	-9.98700	54.73800
C	41.78400	-9.16200	55.20400
C	39.58400	-9.40300	54.28300
C	41.63600	-7.77000	55.21600
C	39.42500	-8.01700	54.29100
C	40.45300	-7.20000	54.75700
N	41.71400	-14.17100	55.57300
H	42.52400	-13.55100	55.57000
C	41.89700	-15.58700	55.32900
C	41.16700	-16.53200	56.25200
O	40.26800	-17.24000	55.82000
N	41.54800	-16.55000	57.52100
H	42.28500	-15.91800	57.83400
C	40.93000	-17.45700	58.47300
C	39.41400	-17.27000	58.59400
O	38.64900	-18.19200	58.30200
C	41.61000	-17.34100	59.85800
C	41.01100	-18.34600	60.83000
C	43.09900	-17.60100	59.71300
N	38.95600	-16.07000	58.99200
C	37.51300	-15.83500	59.12600
C	36.73900	-16.35400	57.91300
O	35.72900	-17.04600	58.05600
C	37.41600	-14.31700	59.23100
C	38.71700	-13.92500	59.80200
C	39.69000	-14.79600	59.06000

N	37.23200	-16.01200	56.72500
H	38.08200	-15.44900	56.69400
C	36.61200	-16.40600	55.46900
C	36.43700	-17.89700	55.29400
O	35.35600	-18.35300	54.92300
C	37.40800	-15.86100	54.28600
O	37.06200	-14.51700	54.02200
H	37.55700	-14.17800	53.28600
N	37.48700	-18.66600	55.54100
H	38.36900	-18.25000	55.84100
C	37.37300	-20.10500	55.38200
C	36.36900	-20.68800	56.37300
O	35.51800	-21.49300	55.99200
C	38.74600	-20.79100	55.54200
C	38.57500	-22.26500	55.93700
C	39.50600	-20.69200	54.23000
N	36.45500	-20.27000	57.63400
H	37.17300	-19.59200	57.88900
C	35.54200	-20.76300	58.65700
C	34.09800	-20.55900	58.22200
O	33.25700	-21.44000	58.38300
C	35.78100	-20.05600	60.00700
C	37.13300	-20.49300	60.57800
C	34.66700	-20.39100	60.98400
C	37.50000	-19.84400	61.90200
N	33.80900	-19.39700	57.65700
H	34.53600	-18.69000	57.54600
C	32.45600	-19.12700	57.19400
C	32.03100	-20.15800	56.14900
O	31.03000	-20.84400	56.33900
C	32.33700	-17.69300	56.61600
C	31.05000	-17.54500	55.81600
C	32.34900	-16.68800	57.75700
N	32.79800	-20.27400	55.06400
H	33.62400	-19.68200	54.97900
C	32.49400	-21.22400	53.98900
C	32.24000	-22.63400	54.54100
O	31.30100	-23.33500	54.12900
C	33.64200	-21.25800	52.98600
N	33.09200	-23.04300	55.47000
H	33.85000	-22.42500	55.76000
C	32.96800	-24.34700	56.08100
C	31.65200	-24.47000	56.79900

O	30.87800	-25.37800	56.52300
C	34.09800	-24.56300	57.06700
C	35.43300	-24.72400	56.40400
C	36.44700	-25.06600	57.44000
N	37.70700	-25.47400	56.85000
H	37.76900	-25.55500	55.83500
C	38.78000	-25.74500	57.57500
N	38.71400	-25.63700	58.89800
H	39.54100	-25.84600	59.45700
H	37.84800	-25.34500	59.35200
N	39.90800	-26.12500	56.98400
H	40.73500	-26.33400	57.54300
H	39.95900	-26.20800	55.96900
N	31.40800	-23.56000	57.73600
H	32.10700	-22.84500	57.93500
C	30.16000	-23.56800	58.48200
C	28.97900	-23.58300	57.51600
O	27.99300	-24.28500	57.74500
C	30.05800	-22.34100	59.38800
C	30.88700	-22.47100	60.64800
O	32.10300	-22.30500	60.63000
N	30.22500	-22.77400	61.75600
H	30.78400	-22.86200	62.60500
H	29.21400	-22.91200	61.77100
N	29.07900	-22.81000	56.43700
H	29.91800	-22.24400	56.30600
C	28.01800	-22.75200	55.43600
C	27.89600	-24.11700	54.75700
O	26.79400	-24.65000	54.57600
C	28.33700	-21.69300	54.38300
C	27.24800	-21.50100	53.37500
N	26.08500	-20.82000	53.65600
H	25.86200	-20.37800	54.54800
C	27.13700	-21.92200	52.09300
C	25.30300	-20.82700	52.59200
N	25.91900	-21.48900	51.63000
H	25.55000	-21.65200	50.69300
N	29.03900	-24.67400	54.37200
H	29.91600	-24.17700	54.52700
C	29.06100	-25.97700	53.73500
C	28.40200	-27.01600	54.63900
O	27.53000	-27.76700	54.20000
C	30.49800	-26.39300	53.45200

C	30.63400	-27.83900	53.06300
C	32.03600	-28.30900	53.34200
N	32.36200	-28.22800	54.76200
H	31.59300	-28.11600	55.42300
C	33.60000	-28.29100	55.25100
N	34.64500	-28.43200	54.43700
H	34.49400	-28.49100	53.43000
H	35.59300	-28.48000	54.81100
N	33.79600	-28.21400	56.56000
H	32.99600	-28.10600	57.18300
H	34.74400	-28.26200	56.93400
N	28.81600	-27.05000	55.90200
H	29.53000	-26.39100	56.21400
C	28.26800	-28.01200	56.84800
C	26.76500	-27.85900	57.08200
O	26.08700	-28.82500	57.44700
C	29.01000	-27.93000	58.18500
C	30.47400	-28.33200	58.07200
O	30.83900	-29.00700	57.08100
O	31.25600	-27.98400	58.98500
N	26.24400	-26.65200	56.87600
H	26.85400	-25.89000	56.58100
C	24.81800	-26.39300	57.06300
C	24.02900	-27.01400	55.91600
O	22.80100	-26.97400	55.90200
C	24.56200	-24.91000	57.12400
N	24.75600	-27.56800	54.94700
H	25.77400	-27.52900	55.00400
C	24.13500	-28.22600	53.81200
C	23.86900	-27.40800	52.56200
O	23.03100	-27.79200	51.75200
N	24.56800	-26.29700	52.37500
H	25.27400	-26.01600	53.05600
C	24.32500	-25.47700	51.19300
C	25.56000	-25.32400	50.31100
O	26.68900	-25.25500	50.80600
C	23.80600	-24.11600	51.61300
N	25.35900	-25.26300	48.98400
C	26.43900	-25.11600	48.00200
C	27.40000	-23.99600	48.38800
O	26.99700	-22.83500	48.52300
C	25.68800	-24.80400	46.71000
C	24.40300	-25.52300	46.88900

C	24.04700	-25.21700	48.31900
N	28.66600	-24.34800	48.56800
H	28.93600	-25.32300	48.44000
C	29.67600	-23.37500	48.94400
C	30.80400	-23.42400	47.92800
O	31.11900	-24.48300	47.39100
C	30.24400	-23.67400	50.35300
O	29.18500	-23.64500	51.31900
H	29.53400	-23.82800	52.18400
C	31.29200	-22.64400	50.73900
N	31.40600	-22.27000	47.66700
H	31.08900	-21.43000	48.15200
C	32.50500	-22.15700	46.71200
C	33.48100	-21.12800	47.25000
O	33.05300	-20.10400	47.77800
C	31.98200	-21.68100	45.35800
C	31.18300	-22.70900	44.59500
C	31.81000	-23.58300	43.71400
C	29.80000	-22.81400	44.75200
C	31.08500	-24.53700	43.00800
C	29.06600	-23.76800	44.04800
C	29.72000	-24.62400	43.18000
O	29.02800	-25.59000	42.49500
H	29.47700	-26.17800	41.89900
N	34.78000	-21.40200	47.12200
H	35.05800	-22.28300	46.68900
C	35.82000	-20.48000	47.58200
C	36.82300	-20.18900	46.48200
O	36.82000	-20.83900	45.43800
C	36.56700	-21.03700	48.79500
C	35.81200	-20.90700	50.08800
S	36.84500	-21.15600	51.54200
C	37.38200	-19.50000	51.84900
N	37.68300	-19.20300	46.71500
H	37.63400	-18.68900	47.59400
C	38.69300	-18.84900	45.73200
C	39.77000	-17.95300	46.32300
O	39.58800	-17.37300	47.39000
C	38.04300	-18.14300	44.54100
C	37.56900	-16.73700	44.82900
C	36.20500	-16.43000	44.88300
C	38.48800	-15.70200	45.02100
C	35.77800	-15.12000	45.11600

C	38.07600	-14.40200	45.25700
C	36.72600	-14.11200	45.29900
O	36.34100	-12.80900	45.49800
H	36.98600	-12.12300	45.62300
N	40.89200	-17.85000	45.61900
H	40.98500	-18.38900	44.75800
C	41.99300	-16.99300	46.03700
C	42.48600	-16.25800	44.79300
O	42.99900	-16.88200	43.86500
C	43.12500	-17.82100	46.63100
C	44.03600	-17.01700	47.53100
C	45.23400	-17.80900	48.00200
O	45.80000	-17.45900	49.06700
O	45.61400	-18.77400	47.29800
N	42.32100	-14.93700	44.76800
H	41.89100	-14.47600	45.57000
C	42.74000	-14.12700	43.62000
C	44.20700	-13.73900	43.73200
O	44.60500	-13.03500	44.66400
C	41.89100	-12.86500	43.52000
C	42.01600	-12.16000	42.20900
C	41.40900	-12.67300	41.07100
C	42.73300	-10.97700	42.10800
C	41.51300	-12.01300	39.84500
C	42.84500	-10.31000	40.89300
C	42.23400	-10.82900	39.76000
N	44.99900	-14.19700	42.76700
H	44.58600	-14.74700	42.01400
C	46.43600	-13.94300	42.74400
C	46.85000	-13.32900	41.40900
O	47.28000	-14.03300	40.49800
C	47.16600	-15.26700	42.98200
C	46.53000	-16.07300	44.12800
C	46.82300	-17.57300	44.07900
O	46.70200	-18.20900	43.02500
N	47.18900	-18.14800	45.23000
H	47.38400	-19.14900	45.19700
H	47.28900	-17.62400	46.09900
N	46.71000	-12.01200	41.29900
H	46.35200	-11.48600	42.09600
C	47.05200	-11.29400	40.07600
C	47.27300	-9.81800	40.39700
O	46.71300	-9.29400	41.36200

C	45.91400	-11.41700	39.05700
C	46.25700	-10.91800	37.66900
C	46.91200	-11.74400	36.75600
C	45.93800	-9.62100	37.27000
C	47.24300	-11.29400	35.47300
C	46.26400	-9.15500	35.98400
C	46.91800	-10.00100	35.09200
O	47.25200	-9.56200	33.82900
H	47.69800	-10.13900	33.22000
N	48.09000	-9.14800	39.59100
H	48.54000	-9.62900	38.81200
C	48.34800	-7.73300	39.81100
C	47.80200	-6.90100	38.65600
O	48.48000	-6.68800	37.65400
C	49.84700	-7.47400	39.97900
C	50.18100	-6.02300	40.32500
C	51.67300	-5.84200	40.56400
N	52.01800	-4.50400	41.04800
H	52.40600	-4.42500	41.98800
C	51.86100	-3.38400	40.34700
N	51.35900	-3.42800	39.11700
H	51.09000	-4.32400	38.71100
H	51.23900	-2.56900	38.58000
N	52.21100	-2.21700	40.87500
H	52.59600	-2.18300	41.81900
H	52.09100	-1.35800	40.33800
N	46.56400	-6.40800	38.78800
C	45.98000	-5.60100	37.71400
C	46.91600	-4.46700	37.29500
O	47.69900	-3.96400	38.10600
C	44.67000	-5.10800	38.32800
C	44.98600	-5.05700	39.80500
C	45.74100	-6.34000	40.00900
N	46.83400	-4.07600	36.02500
H	46.15900	-4.53300	35.41100
C	47.67800	-3.01500	35.48100
C	47.18700	-1.64700	35.89800
O	47.91900	-0.66300	35.82200
C	47.70400	-3.09000	33.95700
O	46.43100	-2.81600	33.40900
H	46.44700	-2.86300	32.46000
N	45.93800	-1.59200	36.34000
H	45.38800	-2.45000	36.38200

C	45.33300	-0.34300	36.76600
C	45.70300	0.03000	38.20900
O	45.08200	0.91200	38.80500
C	43.82100	-0.44400	36.62300
C	43.38400	-1.19000	35.40000
C	43.11300	-2.55100	35.46300
C	43.24300	-0.53400	34.18100
C	42.70500	-3.24900	34.32900
C	42.83600	-1.22100	33.04200
C	42.56600	-2.58200	33.11900
N	46.71300	-0.63900	38.76500
H	47.18300	-1.36600	38.22600
C	47.16500	-0.35800	40.12600
C	47.79500	1.03000	40.21000
O	48.30100	1.55400	39.22000
C	48.19600	-1.39500	40.57500
O	47.64600	-2.69700	40.58600
H	48.28600	-3.34100	40.86500
N	47.75100	1.62800	41.39200
H	47.29100	1.16300	42.17400
C	48.35100	2.93900	41.58800
C	49.85200	2.81300	41.35100
O	50.42900	1.73500	41.52500
C	48.09800	3.43400	43.01300
O	48.95400	4.51800	43.33600
H	48.79700	4.82500	44.22100
N	50.48100	3.90900	40.95100
H	49.95200	4.77100	40.82100
C	51.91300	3.90200	40.69500
C	52.68600	3.65000	41.98400
O	53.67400	2.91500	41.99600
C	52.35100	5.23800	40.08000
C	51.78000	5.45800	38.68000
O	51.96200	4.56500	37.82000
O	51.16000	6.52300	38.43800
N	52.21700	4.25000	43.07100
H	51.37700	4.82400	42.99600
C	52.86600	4.11300	44.36800
C	52.76000	2.70800	44.94800
O	53.02700	2.50100	46.13000
C	52.25500	5.09900	45.35600
C	52.14200	6.50900	44.83400
S	51.18700	7.54600	45.95200

C	49.52100	6.82000	45.76800
N	52.37700	1.74100	44.12700
H	52.17900	1.95500	43.15000
C	52.23700	0.37700	44.61000
C	53.34700	-0.51700	44.08800
O	53.49200	-0.70100	42.88400
C	50.88000	-0.17200	44.18700
C	50.64400	-1.64000	44.49000
C	49.35600	-2.07200	43.80300
C	49.10000	-3.55600	43.89500
N	47.84500	-3.90500	43.16400
H	47.67200	-4.90800	43.22600
H	47.86300	-3.57900	42.19700
H	47.04800	-3.35900	43.49100
N	54.16100	-1.07500	44.99700
C	55.26300	-1.96000	44.60800
C	54.80000	-3.09400	43.70800
O	53.83600	-3.79400	44.01700
C	55.81300	-2.45400	45.95200
C	54.70100	-2.18700	46.92800
C	54.13700	-0.88600	46.45400
N	55.49600	-3.26100	42.58900
H	56.29000	-2.64800	42.40700
C	55.16400	-4.29100	41.61100
C	55.23400	-5.69900	42.17300
O	54.74100	-6.63900	41.55700
C	56.07900	-4.17200	40.38800
C	55.79900	-2.94100	39.52100
C	56.71700	-2.89600	38.29800
C	56.17100	-1.98400	37.19700
N	55.99500	-0.57000	37.63900
H	55.63100	0.03800	36.90500
H	56.86500	-0.19800	38.02000
H	55.41100	-0.52100	38.47400
N	55.83800	-5.84400	43.34600
H	56.22900	-5.02500	43.81100
C	55.95300	-7.15200	43.98300
C	54.68300	-7.54500	44.74400
O	54.52900	-8.69600	45.14600
C	57.14800	-7.18900	44.95300
O	57.03900	-6.11700	45.89800
H	56.22400	-6.20700	46.37800
C	58.44300	-7.04600	44.19000

N	53.78500	-6.58300	44.95500
H	53.98200	-5.63800	44.62400
C	52.52200	-6.84600	45.64900
C	51.54900	-7.38000	44.61300
O	51.16000	-6.66200	43.69300
C	51.92000	-5.57100	46.25300
C	50.66300	-5.92300	47.01600
C	52.92800	-4.89100	47.15900
N	51.16100	-8.64000	44.76800
H	51.50300	-9.16500	45.57300
C	50.26300	-9.29800	43.82800
C	49.01600	-9.81800	44.53100
O	49.10900	-10.55400	45.51000
C	51.01400	-10.45700	43.12400
C	52.20000	-9.87000	42.34700
C	50.09200	-11.21800	42.19500
C	53.16200	-10.89200	41.75700
N	47.84800	-9.42900	44.03400
H	47.81800	-8.81900	43.21700
C	46.61400	-9.87400	44.65600
C	46.34300	-9.08600	45.92300
O	45.94000	-9.65300	46.94800
N	46.57700	-7.77300	45.83300
H	46.91400	-7.41100	44.94100
C	46.38300	-6.81800	46.92600
C	44.89600	-6.60000	47.16400
O	44.07600	-6.91900	46.30300
C	47.06200	-5.49100	46.56700
C	47.03800	-4.48700	47.70800
O	47.16800	-4.91600	48.87700
O	46.90600	-3.26800	47.43400
N	44.54400	-6.05500	48.32300
H	45.26500	-5.79100	48.99400
C	43.13700	-5.82800	48.65100
C	42.41500	-5.09600	47.53400
O	42.89000	-4.07700	47.04300
C	42.99800	-5.02600	49.94500
C	41.61300	-5.03800	50.51500
N	40.98200	-6.19700	50.91300
H	41.37800	-7.13500	50.85000
C	40.74200	-4.03100	50.76900
C	39.78400	-5.90500	51.38900
N	39.61400	-4.59700	51.31200

H	38.78000	-4.08900	51.60800
N	41.27200	-5.64100	47.13000
H	40.94800	-6.50400	47.56600
C	40.47800	-5.03300	46.08200
C	40.95300	-5.26900	44.66500
O	40.29800	-4.83000	43.73400
N	42.07300	-5.96100	44.48700
H	42.57200	-6.32400	45.29900
C	42.60500	-6.21300	43.14400
C	41.68100	-6.97500	42.19700
O	41.72400	-6.76400	40.99100
C	43.94900	-6.95200	43.22900
C	45.12300	-6.00800	43.41900
O	44.89500	-4.77400	43.47500
O	46.27200	-6.49700	43.51000
N	40.84800	-7.85600	42.73500
H	40.83700	-7.98400	43.74700
C	39.95100	-8.64100	41.90400
C	38.83300	-7.80000	41.30800
O	38.23400	-8.17500	40.29700
C	39.35000	-9.79900	42.70700
C	38.10200	-9.46300	43.51900
C	38.33600	-8.41500	44.60300
O	39.50900	-8.06400	44.86200
O	37.33500	-7.95100	45.20400
N	38.55900	-6.66000	41.93100
H	39.10000	-6.39800	42.75500
C	37.49900	-5.77500	41.46000
C	37.62500	-5.45700	39.98300
O	36.61500	-5.35200	39.27500
C	37.48900	-4.46400	42.25500
C	36.95400	-4.52300	43.69000
C	36.99400	-3.13300	44.30200
C	35.53200	-5.06300	43.69700
N	38.86100	-5.31500	39.51400
H	39.65900	-5.44400	40.13600
C	39.07800	-4.97800	38.12300
C	38.62500	-6.05900	37.16300
O	38.13200	-5.76000	36.07200
C	40.53800	-4.60400	37.90900
C	40.94600	-3.39900	38.68800
C	41.44000	-3.52500	39.98000
C	40.73500	-2.12100	38.17300

C	41.71200	-2.39100	40.75100
C	41.00100	-0.98700	38.93700
C	41.48900	-1.12000	40.22700
N	38.77400	-7.31600	37.56400
H	39.19800	-7.51500	38.47000
C	38.33300	-8.41100	36.71200
C	36.81000	-8.52300	36.80800
O	36.11300	-8.50300	35.79400
C	39.00400	-9.72700	37.13300
O	40.38200	-9.74900	36.76800
H	40.79700	-10.56300	37.02800
N	36.29700	-8.61000	38.03300
H	36.92200	-8.60100	38.83900
C	34.86000	-8.71800	38.24500
C	34.08300	-7.68800	37.43700
O	33.10400	-8.02600	36.78100
C	34.47200	-8.54500	39.73800
C	32.95000	-8.51900	39.88200
C	35.04700	-9.68300	40.56400
N	34.51000	-6.43200	37.46700
H	35.34300	-6.18000	38.00000
C	33.77000	-5.42100	36.72700
C	34.28600	-5.07500	35.34100
O	33.85300	-4.08700	34.74900
C	33.61400	-4.15400	37.56800
C	32.59700	-4.29200	38.66600
C	32.96900	-4.72700	39.93500
C	31.25300	-4.02100	38.42200
C	32.00700	-4.88700	40.94700
C	30.29100	-4.18100	39.42100
C	30.66800	-4.61300	40.68300
N	35.18800	-5.91000	34.82300
H	35.49500	-6.71300	35.37200
C	35.74700	-5.70500	33.49200
C	36.44600	-4.38500	33.18900
O	36.14000	-3.72700	32.19400
N	37.39100	-3.99000	34.03400
H	37.61100	-4.56200	34.84900
C	38.11600	-2.74600	33.80600
C	38.79300	-2.77400	32.42400
O	38.83700	-1.75600	31.72700
C	39.15800	-2.52800	34.91000
N	39.32900	-3.94200	32.01500

C	39.99400	-4.07800	30.71700
C	39.17500	-3.60800	29.51100
O	39.74800	-3.29300	28.46700
C	40.29900	-5.57000	30.64800
C	40.60100	-5.89200	32.05800
C	39.48900	-5.18200	32.79700
N	37.84800	-3.55900	29.64500
H	37.42400	-3.81800	30.53600
C	36.99100	-3.14000	28.53500
C	36.48800	-1.71400	28.64900
O	35.64000	-1.29700	27.86300
C	35.78200	-4.06700	28.40400
C	36.14100	-5.51200	28.28000
C	36.46800	-6.25800	29.40100
C	36.20100	-6.11700	27.03600
C	36.85300	-7.58800	29.28300
C	36.58600	-7.44500	26.90800
C	36.91300	-8.18000	28.02900
N	36.99500	-0.96600	29.62300
H	37.69100	-1.36800	30.25100
C	36.57700	0.41900	29.81200
C	37.79400	1.31100	29.96400
O	37.76900	2.48200	29.59500
C	35.69700	0.53500	31.05000
C	34.38200	-0.24400	31.00800
C	33.76400	-0.27600	32.39500
C	33.43400	0.39400	30.00600
N	38.85500	0.74500	30.52600
H	38.79200	-0.22600	30.83300
C	40.10200	1.46400	30.71700
C	41.11400	0.99600	29.67600
O	40.92700	-0.04400	29.04600
C	40.65800	1.20800	32.11500
C	39.88600	1.88300	33.22400
C	40.64800	1.80800	34.52900
C	39.97500	2.65100	35.57800
N	40.87100	2.88700	36.73300
H	40.41500	3.45800	37.44400
H	41.76000	3.29200	36.44100
H	41.21900	2.01100	37.12300
N	42.18700	1.76000	29.50000
H	42.29200	2.60600	30.05900
C	43.21700	1.41800	28.52700

C	44.39500	0.73400	29.19800
O	44.46200	0.66800	30.42100
C	43.68100	2.68200	27.81500
C	42.53800	3.40300	27.11700
C	42.93700	4.75600	26.55100
O	42.05800	5.43200	25.96600
O	44.12300	5.14300	26.68900
N	45.30800	0.19900	28.39700
H	45.18600	0.24500	27.38500
C	46.47800	-0.45100	28.95500
C	46.41800	-1.94900	29.18500
O	47.45400	-2.60400	29.23500
N	45.22400	-2.50700	29.33200
H	44.38400	-1.93100	29.27600
C	45.10700	-3.94200	29.57300
C	45.75700	-4.74200	28.44500
O	45.67700	-4.35700	27.27600
C	43.63000	-4.33700	29.72200
N	46.40500	-5.85000	28.80500
H	46.44200	-6.10100	29.79300
C	47.06300	-6.71500	27.83200
C	46.11200	-7.84100	27.48700
O	45.07600	-7.99100	28.12800
C	48.34500	-7.29900	28.41900
O	48.05700	-8.15000	29.51000
H	48.85500	-8.51400	29.87500
N	46.46700	-8.63600	26.48200
H	47.34900	-8.46300	25.99900
C	45.62500	-9.75200	26.05100
C	45.35300	-10.72100	27.19200
O	44.28100	-11.32000	27.26500
C	46.27700	-10.49600	24.87700
C	47.75300	-10.86500	25.09600
C	48.34100	-11.74500	23.97300
O	47.86300	-12.89500	23.79300
O	49.28500	-11.28900	23.27500
N	46.32600	-10.86000	28.08800
H	47.18400	-10.32000	27.97200
C	46.20800	-11.75900	29.23200
C	45.23400	-11.26100	30.30600
O	44.45400	-12.04100	30.86200
C	47.59100	-11.99700	29.85200
C	47.59400	-11.97500	31.37000

C	48.85300	-12.56100	31.96500
O	49.07100	-13.77500	31.78800
O	49.62000	-11.81400	32.61000
N	45.29700	-9.96400	30.59600
H	45.97300	-9.38200	30.10100
C	44.43600	-9.34500	31.59500
C	43.01800	-9.33100	31.04700
O	42.03900	-9.52900	31.77400
C	44.90000	-7.91700	31.86000
C	44.35600	-7.30500	33.12600
C	44.96300	-5.94400	33.40300
O	44.74800	-5.41100	34.51200
O	45.65700	-5.40400	32.51000
N	42.91200	-9.09000	29.74900
H	43.75100	-8.91900	29.19400
C	41.61500	-9.06800	29.11600
C	41.02900	-10.45100	29.25700
O	39.87300	-10.60300	29.64200
C	41.72800	-8.71200	27.63500
C	42.15900	-7.25100	27.50100
C	40.40500	-8.96200	26.93800
C	42.47200	-6.83800	26.09900
N	41.83600	-11.46500	28.96400
H	42.79400	-11.27900	28.66600
C	41.36600	-12.83800	29.06500
C	40.94500	-13.18000	30.49500
O	39.93900	-13.86300	30.70800
C	42.44400	-13.81600	28.57400
C	42.03200	-15.29000	28.65500
C	42.87100	-16.19600	27.75400
N	44.30800	-15.94900	27.88100
H	44.78600	-16.32800	28.69800
C	45.03300	-15.26100	26.99900
N	44.46200	-14.74900	25.90900
H	43.46500	-14.88800	25.74300
H	45.01700	-14.22300	25.23400
N	46.33200	-15.08000	27.21500
H	46.76900	-15.47200	28.04900
H	46.88700	-14.55400	26.54000
N	41.70400	-12.69400	31.47400
H	42.51800	-12.12400	31.24400
C	41.38700	-12.96500	32.87200
C	40.02800	-12.38700	33.22400

O	39.16200	-13.08600	33.75000
C	42.44000	-12.35600	33.78700
C	42.17200	-12.53500	35.27900
C	42.25500	-14.01100	35.63000
C	43.17600	-11.72300	36.08900
N	39.84100	-11.10700	32.92200
H	40.58900	-10.58300	32.46800
C	38.58800	-10.44300	33.22900
C	37.38600	-11.18000	32.67200
O	36.41600	-11.41000	33.39100
C	38.59300	-9.01300	32.69900
O	37.37100	-8.36500	33.02200
H	37.37400	-7.47400	32.69200
N	37.45000	-11.54900	31.39400
H	38.29000	-11.33500	30.85600
C	36.34400	-12.25400	30.74200
C	36.02100	-13.54000	31.47800
O	34.85900	-13.86800	31.70800
C	36.68700	-12.57200	29.28300
C	37.05900	-11.35500	28.46100
C	37.08400	-11.64200	26.96300
C	35.67900	-11.87600	26.40800
N	35.66100	-12.02000	24.91100
H	34.72400	-12.17600	24.54100
H	36.30100	-12.75400	24.60700
H	36.10300	-11.21800	24.46100
N	37.07000	-14.25800	31.85000
H	38.00300	-13.91200	31.62600
C	36.94600	-15.51700	32.56300
C	36.17100	-15.29400	33.86200
O	35.12000	-15.90100	34.08300
C	38.34800	-16.05100	32.86000
C	38.41400	-17.47600	33.37800
S	40.13200	-17.94200	33.72800
C	40.87900	-17.55500	32.11700
N	36.69400	-14.40900	34.71000
H	37.56100	-13.93700	34.45500
C	36.07000	-14.09200	35.98900
C	34.60600	-13.68400	35.82400
O	33.73800	-14.17400	36.54700
C	36.86000	-12.96700	36.71300
C	36.09100	-12.46600	37.94000
C	38.22500	-13.49300	37.12800

N	34.32700	-12.79500	34.87200
H	35.08100	-12.41600	34.29900
C	32.95400	-12.35800	34.64100
C	32.02400	-13.51500	34.30400
O	30.85600	-13.49900	34.69700
C	32.89800	-11.30000	33.54600
C	33.44700	-9.96200	33.99600
S	33.14500	-8.64700	32.81200
C	34.48300	-8.95500	31.66600
N	32.53500	-14.51300	33.58200
H	33.50100	-14.45000	33.26100
C	31.74200	-15.69900	33.23800
C	31.40900	-16.45200	34.52400
O	30.26300	-16.80400	34.77100
C	32.53100	-16.64100	32.32900
C	32.33000	-16.45800	30.83600
C	30.94800	-16.88000	30.38100
C	30.91300	-17.02000	28.86300
N	31.46000	-15.82400	28.15100
H	31.43700	-15.91800	27.13600
H	32.40300	-15.60800	28.47500
H	30.98200	-14.97400	28.44900
N	32.43000	-16.70700	35.33300
H	33.36600	-16.40100	35.06600
C	32.24600	-17.41200	36.59100
C	31.21600	-16.73100	37.48000
O	30.29400	-17.37700	37.97500
C	33.57500	-17.50400	37.34300
C	34.47800	-18.60300	36.85800
C	35.83400	-18.36000	36.63800
C	33.98500	-19.88800	36.65500
C	36.68500	-19.38100	36.22400
C	34.82900	-20.91400	36.24300
C	36.18400	-20.65900	36.02700
N	31.38100	-15.42700	37.68700
H	32.16900	-14.94800	37.25100
C	30.46000	-14.66900	38.52300
C	29.03600	-14.71200	37.97500
O	28.07200	-14.86000	38.72800
C	30.93100	-13.21400	38.65800
C	31.75700	-12.92700	39.91500
C	31.56400	-11.90500	40.80100
C	32.91800	-13.63900	40.38100

N	32.52700	-11.93300	41.78200
H	32.60100	-11.27500	42.55800
C	33.37000	-12.98600	41.54900
C	33.62100	-14.76300	39.92300
C	34.48700	-13.41500	42.26200
C	34.73500	-15.18900	40.63300
C	35.15600	-14.51500	41.79000
N	28.90300	-14.59400	36.66100
H	29.73300	-14.47800	36.07900
C	27.58600	-14.62800	36.03700
C	26.99100	-16.04000	36.01300
O	25.78300	-16.20100	36.08600
C	27.66600	-14.06100	34.62800
N	27.83500	-17.06200	35.90100
H	28.83600	-16.88000	35.82600
C	27.35100	-18.44300	35.88400
C	26.77700	-18.74700	37.24800
O	25.79700	-19.49200	37.37600
C	28.48500	-19.43700	35.59000
C	28.83900	-19.50300	34.11900
O	28.11900	-18.96300	33.27600
N	29.94400	-20.17900	33.79900
H	30.54000	-20.62600	34.49600
H	30.18200	-20.22300	32.80800
N	27.40600	-18.17000	38.26900
H	28.21900	-17.58300	38.08500
C	26.96100	-18.35700	39.64100
C	25.59500	-17.66600	39.77100
O	24.61700	-18.26600	40.22700
C	27.98300	-17.74100	40.60000
C	27.70800	-18.01800	42.04700
C	27.66100	-19.32000	42.52400
C	27.51300	-16.97200	42.94500
C	27.42500	-19.57900	43.87600
C	27.27600	-17.22100	44.29800
C	27.23400	-18.52900	44.76000
N	25.53000	-16.41000	39.33400
H	26.36500	-15.97300	38.94400
C	24.29300	-15.64700	39.40100
C	23.17100	-16.41700	38.72400
O	22.01700	-16.35900	39.14700
C	24.47500	-14.28500	38.72900
N	23.51800	-17.14800	37.67300

H	24.49600	-17.17100	37.38500
C	22.54000	-17.91800	36.92000
C	22.09300	-19.22500	37.55600
O	20.88900	-19.47100	37.68300
C	23.07700	-18.21000	35.52000
C	22.75300	-17.14600	34.49400
C	23.22300	-17.57100	33.12000
N	24.67200	-17.48600	32.99600
H	25.20900	-18.35100	33.05000
C	25.33800	-16.34700	32.81600
N	24.67400	-15.19600	32.73600
H	25.18400	-14.32400	32.59800
H	23.65700	-15.19000	32.81400
N	26.66400	-16.35500	32.71400
H	27.17400	-15.48300	32.57600
H	27.17300	-17.23700	32.77500
N	23.05200	-20.05500	37.96700
H	24.03000	-19.77800	37.88500
C	22.71400	-21.35400	38.53200
C	23.26700	-21.68200	39.91500
O	23.14000	-22.81300	40.37100
C	23.16500	-22.45100	37.57000
C	23.18500	-21.99200	36.12600
O	22.15400	-21.63300	35.56000
N	24.36600	-21.99900	35.52100
H	24.37900	-21.69000	34.54900
H	25.22100	-22.29700	35.99000
N	23.87900	-20.72500	40.59400
H	23.96500	-19.78400	40.20900
C	24.42500	-21.04600	41.89900
C	25.53800	-22.06600	41.72800
O	25.75600	-22.93500	42.57900
N	26.23400	-21.95200	40.59700
H	25.97000	-21.21400	39.94400
C	27.35200	-22.82000	40.23700
C	28.15700	-22.05600	39.18900
O	27.70100	-21.85600	38.06300
C	26.84500	-24.13400	39.63900
C	27.95700	-25.15700	39.45000
O	29.02200	-24.84000	38.91700
N	27.71000	-26.38800	39.88000
H	26.82900	-26.65000	40.32100
H	28.45500	-27.07300	39.75300

N	29.38000	-21.64300	39.53800
C	30.25600	-20.88600	38.63500
C	30.69400	-21.58000	37.35000
O	31.07400	-20.91900	36.38100
C	31.44300	-20.54000	39.52800
C	31.54900	-21.75700	40.38700
C	30.10600	-22.05400	40.75400
N	30.63400	-22.90600	37.33800
H	30.27100	-23.39600	38.15600
C	31.07500	-23.67700	36.18200
C	30.34600	-23.39600	34.87700
O	29.18900	-22.96700	34.86600
C	31.03100	-25.16700	36.51400
C	32.12500	-25.57200	37.48600
O	33.30200	-25.63500	37.12500
N	31.74600	-25.83100	38.73300
H	30.77200	-25.77900	39.03200
H	32.48100	-26.10300	39.38600
N	31.05300	-23.63000	33.77600
H	32.00800	-23.97800	33.86000
C	30.49300	-23.40000	32.45800
C	31.41100	-23.86700	31.34100
O	32.62200	-24.00500	31.52100
N	30.82800	-24.11900	30.17600
H	29.81900	-23.99800	30.08600
C	31.59400	-24.56300	29.02900
C	32.64500	-23.52700	28.67400
O	32.35100	-22.33900	28.54600
C	30.65900	-24.81200	27.84500
C	29.48900	-23.84000	27.78100
C	28.44400	-24.21700	26.73000
O	27.96300	-25.37500	26.74500
O	28.09500	-23.34600	25.89400
N	33.88100	-23.99300	28.53700
H	34.06100	-24.98700	28.67700
C	34.97800	-23.11300	28.19200
C	35.63400	-22.47100	29.39800
O	36.29900	-21.43700	29.27000
N	35.45800	-23.08000	30.56800
H	34.90600	-23.93700	30.60500
C	36.03400	-22.55200	31.79800
C	36.66200	-23.66900	32.60700
O	36.15000	-24.79200	32.62200

C	34.94900	-21.87500	32.63200
C	34.39700	-20.55800	32.10000
C	33.18300	-20.14700	32.90500
C	35.48200	-19.50600	32.17700
N	37.77800	-23.37800	33.29900
C	38.45600	-24.39100	34.11000
C	37.46500	-24.89700	35.13200
O	36.54200	-24.16900	35.49800
C	39.59100	-23.61600	34.76400
C	39.84000	-22.50500	33.82400
C	38.45700	-22.08200	33.41400
N	37.64000	-26.12900	35.59700
H	38.42100	-26.69500	35.26600
C	36.71200	-26.66900	36.58200
C	36.88500	-26.06500	37.96400
O	37.98300	-26.04200	38.52000
C	36.84700	-28.17200	36.72300
C	35.91500	-28.74400	37.74000
N	34.54600	-28.73900	37.57200
H	34.05300	-28.38300	36.75300
C	36.14500	-29.29700	38.95300
C	33.97300	-29.26800	38.63800
N	34.92000	-29.61500	39.49200
H	34.76700	-30.04800	40.40300
N	35.78300	-25.59300	38.52200
H	34.90100	-25.64700	38.01200
C	35.80500	-25.00200	39.84100
C	35.11200	-25.99300	40.78100
O	33.89100	-26.11000	40.79700
C	35.06600	-23.66000	39.79800
C	35.27900	-22.76800	40.98500
C	35.53100	-23.15400	42.26500
C	35.13000	-21.34000	41.01800
N	35.54000	-22.05700	43.09600
H	35.70300	-22.07900	44.10300
C	35.29600	-20.93100	42.35600
C	34.86400	-20.36600	40.04200
C	35.20300	-19.59300	42.75200
C	34.77000	-19.03100	40.43700
C	34.93900	-18.66100	41.78300
N	35.89600	-26.74700	41.55700
C	35.31500	-27.71900	42.48700
C	34.43000	-27.04100	43.52800

O	34.54700	-25.83700	43.77100
C	36.54400	-28.35800	43.12100
C	37.53800	-27.23700	43.12700
C	37.35700	-26.66600	41.73300
N	33.54100	-27.81100	44.14100
H	33.47000	-28.79800	43.89300
C	32.67100	-27.26200	45.16000
C	33.42700	-27.33300	46.47900
O	34.22300	-28.24200	46.70100
C	31.38700	-28.07300	45.27000
C	30.26900	-27.31100	45.95400
C	29.14900	-28.20200	46.44700
O	28.62400	-29.01500	45.65700
O	28.78700	-28.07900	47.63500
N	33.19400	-26.37100	47.36100
H	32.53200	-25.62600	47.14400
C	33.88300	-26.38400	48.63300
C	33.18800	-27.37500	49.55300
O	32.45700	-26.98600	50.46400
C	33.87900	-24.99200	49.26800
C	34.82000	-24.86000	50.44500
C	36.19200	-24.70400	50.25100
C	34.34300	-24.92400	51.75500
C	37.06400	-24.61500	51.32500
C	35.21200	-24.84100	52.84300
C	36.57200	-24.68600	52.62000
O	37.44000	-24.60700	53.69300
H	37.10300	-24.65600	54.58000
N	33.39900	-28.66100	49.29500
H	33.97900	-28.92600	48.49900
C	32.81200	-29.69800	50.13400
C	33.81900	-30.09600	51.20900
O	34.58000	-29.25600	51.69700
C	32.42900	-30.92100	49.30200
C	33.56000	-31.41100	48.44000
O	34.69800	-31.50100	48.88600
N	33.25300	-31.74000	47.19900
H	32.30600	-31.66500	46.82800
H	34.02000	-32.07200	46.61400
N	33.83600	-31.37400	51.56900
H	33.20100	-32.03300	51.11800
C	34.74900	-31.84700	52.60000
C	36.21500	-31.89100	52.17900

O	37.10500	-31.83500	53.02900
C	34.29800	-33.21700	53.09300
C	32.96000	-33.18500	53.82000
C	32.97800	-32.26800	55.03000
O	33.79100	-32.43800	55.93800
N	32.07800	-31.29200	55.04900
H	32.09000	-30.67600	55.86200
H	31.40400	-31.15100	54.29600
N	36.46800	-32.00100	50.87700
H	35.69000	-32.06800	50.22000
C	37.83800	-32.02700	50.37000
C	38.37800	-30.61600	50.47600
O	39.58600	-30.39900	50.59600
C	37.88400	-32.45800	48.90000
C	37.78100	-33.94900	48.65000
C	36.41200	-34.49000	49.00700
C	36.25100	-35.91700	48.50800
N	36.43500	-35.98900	47.02700
H	36.32700	-36.94600	46.69200
H	37.32700	-35.58800	46.73800
H	35.81100	-35.34700	46.53800
N	37.45400	-29.66200	50.41800
H	36.47800	-29.93800	50.31200
C	37.76700	-28.24300	50.49900
C	38.47300	-27.73000	49.25100
O	39.49000	-27.04600	49.31800
C	38.59000	-27.96100	51.75600
C	37.78700	-28.21400	53.01700
C	38.47200	-27.72500	54.27100
O	37.81600	-27.73500	55.33500
O	39.65700	-27.33200	54.19500
N	37.91300	-28.07200	48.10200
H	37.07700	-28.65700	48.09700
C	38.48300	-27.61900	46.85800
C	38.12100	-26.16600	46.63900
O	37.01400	-25.72100	46.94400
N	39.06700	-25.40800	46.11700
H	39.97600	-25.81500	45.89500
C	38.82700	-24.00700	45.85700
C	39.51900	-23.67600	44.55400
O	40.33100	-24.45100	44.05300
C	39.37700	-23.15300	46.99500
C	40.88500	-23.08000	47.07000

C	41.58200	-22.03000	46.46900
C	41.61400	-24.03200	47.78600
C	42.96300	-21.92300	46.59000
C	42.99200	-23.93400	47.91000
C	43.65800	-22.87500	47.31500
O	45.01200	-22.73800	47.49300
H	45.48900	-23.39200	47.99100
N	39.20200	-22.52400	43.99800
H	38.53900	-21.89700	44.45400
C	39.80000	-22.16100	42.74200
C	40.84300	-21.07500	42.90800
O	40.63400	-20.08400	43.61700
C	38.70500	-21.72400	41.76500
C	39.14800	-21.36800	40.35100
C	40.12500	-22.41000	39.84200
C	37.92500	-21.27100	39.44800
N	41.99000	-21.28800	42.27300
H	42.11900	-22.15400	41.75000
C	43.06000	-20.31400	42.31000
C	42.92100	-19.55000	41.02600
O	43.01600	-20.12300	39.94500
C	44.40300	-21.00500	42.38100
C	45.01800	-20.89600	43.75000
C	45.93600	-22.04500	44.04700
O	46.81400	-22.37200	43.25500
N	45.74000	-22.67000	45.19600
H	46.36400	-23.45100	45.39800
H	45.01000	-22.39800	45.85400
N	42.67400	-18.25500	41.15300
H	42.62800	-17.84700	42.08700
C	42.46700	-17.40200	39.99900
C	43.63800	-16.47300	39.74100
O	44.21200	-15.90200	40.67000
C	41.18700	-16.58900	40.18800
C	40.00600	-17.55000	40.31300
C	41.00000	-15.61900	39.04500
C	38.72700	-16.88600	40.71400
N	43.98700	-16.33400	38.46500
H	43.46800	-16.84100	37.74800
C	45.09200	-15.47600	38.07000
C	45.57800	-15.82600	36.67500
O	44.80400	-16.32100	35.85100
N	46.85400	-15.56400	36.40700

H	47.43700	-15.13800	37.12800
C	47.43900	-15.87100	35.11000
C	47.16700	-17.33900	34.79200
O	46.76500	-17.67700	33.68100
C	48.92400	-15.60400	35.13800
N	47.38200	-18.20400	35.78000
H	47.72700	-17.85400	36.67400
C	47.14100	-19.63900	35.63000
C	46.05600	-20.06900	36.60900
O	46.33800	-20.35100	37.77100
C	48.41700	-20.42800	35.91400
C	49.54200	-20.06000	34.97500
O	49.41000	-20.17800	33.74900
N	50.66100	-19.60700	35.53900
H	50.77000	-19.51000	36.54900
H	51.42000	-19.35900	34.90500
N	44.81600	-20.12700	36.13700
H	44.64100	-19.90700	35.15700
C	43.70700	-20.49900	36.99500
C	43.44100	-22.00100	37.02700
O	43.12700	-22.60600	36.00700
C	42.42300	-19.77700	36.55000
O	42.68700	-18.37400	36.42000
H	41.89400	-17.92800	36.14500
C	41.30900	-19.99100	37.56800
N	43.57500	-22.60800	38.19800
H	43.87500	-22.07100	39.01200
C	43.29900	-24.03400	38.33700
C	42.81500	-24.36300	39.74200
O	43.02600	-23.59000	40.68200
C	44.52900	-24.88500	37.99700
C	45.67100	-24.83900	39.00200
C	46.55400	-23.62300	38.83100
O	46.88600	-23.24200	37.70700
N	46.95600	-23.01400	39.94500
H	46.68100	-23.32900	40.87500
H	47.55100	-22.19400	39.83000
N	42.16000	-25.51300	39.88000
H	42.02700	-26.11200	39.06500
C	41.63000	-25.93500	41.16700
C	42.73800	-26.24900	42.17500
O	43.91100	-26.32400	41.81900
C	40.71900	-27.13800	40.97900

N	42.35300	-26.41600	43.43700
H	41.36200	-26.32700	43.66300
C	43.29100	-26.72100	44.51100
C	42.50900	-27.20700	45.73500
O	41.28500	-27.33800	45.67600
C	44.09600	-25.48400	44.85500
N	43.20500	-27.46900	46.84000
H	44.21700	-27.33900	46.84100
C	42.53700	-27.94000	48.05100
C	43.07700	-27.38400	49.37700
O	44.21200	-26.92600	49.46100
C	42.57500	-29.46600	48.09300
C	41.70200	-30.15100	47.05100
C	41.82900	-31.67400	47.07600
O	40.93300	-32.39500	46.62500
N	42.95000	-32.16700	47.59400
H	43.03500	-33.18300	47.61100
H	43.69000	-31.57200	47.96600
N	42.23100	-27.43900	50.40200
H	41.30300	-27.82300	50.22600
C	42.52900	-26.99000	51.76500
C	43.07500	-25.57800	52.00200
O	43.91700	-25.38400	52.87900
C	43.46300	-27.97800	52.44300
C	42.94500	-29.38700	52.54300
C	44.01700	-30.25500	53.18300
C	43.74900	-31.73500	53.01900
N	44.92300	-32.49900	53.53000
H	44.74200	-33.49700	53.41900
H	45.16000	-32.25100	54.49100
H	45.79600	-32.21100	53.08900
N	42.58600	-24.60000	51.24600
H	41.89500	-24.83500	50.53300
C	42.99500	-23.19900	51.39000
C	43.08700	-22.73900	52.84900
O	42.13000	-22.87800	53.59600
C	41.98500	-22.32100	50.66700
C	41.99900	-20.82700	50.94700
C	43.30400	-20.22100	50.46300
C	40.81200	-20.18800	50.24100
N	44.22700	-22.18100	53.24800
H	44.99300	-22.09300	52.58000
C	44.42100	-21.68500	54.62300

C	44.19600	-22.71500	55.72100
O	44.14100	-22.36200	56.89800
C	43.49700	-20.49100	54.91100
C	43.70400	-19.28200	54.02600
C	45.08200	-18.70400	54.20900
C	45.31700	-17.60000	53.21600
N	46.71600	-17.14100	53.25200
H	46.87500	-16.39200	52.57800
H	47.36800	-17.91300	53.11500
H	46.99600	-16.86500	54.19300
N	44.06100	-23.97900	55.34000
H	44.12800	-24.20100	54.34700
C	43.82000	-25.06500	56.28800
C	44.69800	-25.01800	57.54800
O	44.20100	-25.13300	58.67100
C	44.01700	-26.39600	55.57200
C	43.49500	-27.56800	56.36600
O	43.98300	-27.79900	57.49300
O	42.59400	-28.26300	55.85100
N	46.00300	-24.84800	57.35100
H	46.34400	-24.75400	56.39400
C	46.97200	-24.79000	58.45000
C	46.79100	-23.55700	59.34000
O	46.84900	-23.64600	60.57300
C	48.39100	-24.79800	57.88000
C	49.48500	-24.65100	58.92500
C	50.88000	-24.56000	58.28300
C	51.13600	-23.21900	57.56700
N	51.27700	-22.05500	58.50700
H	51.44600	-21.16800	58.03300
H	52.00100	-22.23700	59.20200
H	50.46600	-21.98700	59.12200
N	46.58300	-22.40800	58.70300
H	46.55500	-22.41000	57.68300
C	46.39400	-21.14700	59.40700
C	45.16900	-21.14800	60.33000
O	45.24100	-20.64500	61.45600
C	46.28500	-19.99500	58.40200
C	47.57500	-19.67000	57.66700
C	47.93500	-20.68800	56.59700
O	48.93600	-20.46600	55.87800
O	47.22200	-21.70500	56.46600
N	44.05300	-21.70800	59.86100

H	44.04800	-22.10800	58.92300
C	42.83700	-21.75800	60.67100
C	43.04300	-22.61000	61.91700
O	42.53100	-22.30100	62.99000
C	41.65100	-22.32500	59.88000
C	40.41100	-22.38600	60.76800
C	41.38700	-21.45200	58.67400
N	43.79600	-23.69200	61.77500
H	44.19200	-23.92000	60.86300
C	44.05800	-24.55200	62.91300
C	44.85200	-23.76700	63.95800
O	44.54100	-23.78700	65.14800
C	44.83400	-25.77400	62.46700
N	45.87400	-23.05600	63.50600
H	46.08900	-23.05000	62.50900
C	46.68800	-22.28500	64.42700
C	45.90200	-21.23000	65.19200
O	45.93000	-21.20000	66.42300
C	47.84100	-21.60000	63.69500
C	48.68900	-20.76600	64.59200
C	49.37500	-21.35000	65.64800
C	48.74900	-19.38600	64.43100
C	50.10600	-20.57200	66.54200
C	49.48000	-18.59800	65.32100
C	50.15900	-19.19700	66.38100
N	45.21000	-20.36000	64.46300
H	45.21300	-20.43800	63.44600
C	44.44900	-19.29800	65.10100
C	43.28200	-19.80000	65.94900
O	43.02100	-19.25600	67.02200
C	43.97600	-18.27300	64.05500
C	45.12400	-17.50500	63.43900
C	45.68000	-17.70600	62.20600
C	45.91600	-16.49200	64.07200
N	46.77200	-16.88700	62.03600
H	47.36100	-16.84900	61.20400
C	46.93900	-16.13100	63.16700
C	45.86400	-15.85400	65.32000
C	47.90300	-15.16200	63.46900
C	46.82300	-14.88900	65.62300
C	47.82900	-14.55300	64.69900
N	42.58300	-20.83600	65.49500
H	42.82200	-21.26500	64.60100

C	41.46800	-21.35500	66.28800
C	42.04900	-21.81400	67.61200
O	41.51200	-21.52400	68.68100
C	40.76900	-22.57200	65.62200
O	40.04500	-22.14900	64.46200
H	40.65900	-21.75000	63.85600
C	39.79300	-23.20600	66.58500
N	43.16900	-22.51900	67.52400
H	43.57200	-22.69700	66.60400
C	43.83600	-23.04300	68.69800
C	44.42400	-21.96600	69.60900
O	44.24600	-22.00500	70.83000
C	44.92700	-24.01100	68.26700
C	45.72400	-24.52100	69.43200
O	45.16000	-24.91900	70.45400
N	47.04500	-24.51900	69.29200
H	47.51100	-24.19000	68.44700
H	47.58700	-24.86600	70.08400
N	45.13000	-21.01000	69.01700
H	45.25200	-21.03200	68.00500
C	45.73300	-19.93100	69.78600
C	44.66200	-19.07200	70.45100
O	44.79200	-18.70600	71.61300
C	46.60700	-19.06400	68.87300
C	47.24200	-17.81300	69.48400
C	48.24100	-18.19300	70.56500
C	47.92500	-17.02500	68.38400
N	43.60400	-18.76100	69.70900
H	43.55500	-19.11100	68.75200
C	42.50900	-17.93600	70.21500
C	41.69500	-18.59100	71.33000
O	40.92600	-17.91600	72.01600
C	41.57000	-17.54600	69.06900
C	42.04200	-16.36600	68.26500
C	41.65500	-16.21800	66.93500
C	42.84900	-15.38900	68.83800
C	42.06500	-15.11500	66.18700
C	43.26300	-14.28100	68.09900
C	42.87000	-14.14400	66.77200
N	41.85400	-19.89900	71.50800
H	42.49500	-20.41200	70.90300
C	41.12800	-20.61500	72.55300
C	41.64200	-20.15000	73.91500

O	41.25800	-20.68300	74.96200
C	41.33400	-22.10500	72.39300
N	42.51200	-19.14200	73.87100
H	42.75900	-18.76800	72.95500
C	43.13800	-18.53500	75.04600
C	44.07300	-19.50600	75.75300
O	44.23300	-20.63900	75.23900
C	42.08200	-18.02400	76.03500
C	42.28400	-16.56600	76.43400
C	42.02600	-16.35700	77.91500
C	43.05600	-17.10200	78.75800
N	42.85700	-16.87000	80.21400
H	43.54600	-17.36800	80.77800
H	41.90600	-17.10400	80.50000
H	42.85000	-15.87400	80.43300
O	44.63700	-19.11200	76.80200
O	3.46300	54.08600	34.80000
H	4.00000	53.80500	35.56000
C	2.51800	54.98000	35.20700
C	2.49700	55.53700	36.49200
C	1.49800	56.44700	36.84100
C	3.53700	55.15400	37.46900
C	1.46400	57.04200	38.19200
C	0.51800	56.80100	35.90500
O	0.58700	57.84100	38.49800
C	2.50300	56.66000	39.16900
C	3.50300	55.75000	38.82000
C	2.48300	57.21600	40.45400
C	4.48200	55.39600	39.75600
C	4.45800	55.95200	41.03500
C	3.46100	56.86100	41.38300
C	0.54100	56.24400	34.62500
C	1.53900	55.33600	34.27800
O	4.41400	54.35800	37.16200
O	5.48700	54.51500	39.48400
H	5.38100	54.13500	38.59900
C	-0.47600	56.61100	33.65400
O	-0.80500	57.76700	33.36400
O	-1.05600	55.52600	33.07100
H	-1.82900	55.20600	33.58400

Xyz Cartesian coordinates of the complex of Isorhamnetin with Estrogen receptor β

N	-10.96500	38.50100	81.45200
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H	-11.13300	38.63000	82.45000
H	-10.15900	39.03900	81.13300
H	-10.61700	37.56500	81.24700
C	-12.18800	38.82000	80.66000
C	-11.93600	38.62700	79.16600
O	-12.85800	38.34500	78.39900
C	-12.62900	40.26400	80.92500
C	-11.74800	41.40600	80.40100
C	-12.40600	42.74400	80.72600
C	-10.35900	41.33100	81.02000
N	-10.68000	38.77600	78.75900
H	-9.95900	39.00500	79.44400
C	-10.30600	38.62100	77.36000
C	-10.43100	37.17100	76.90500
O	-10.56100	36.89300	75.71300
C	-8.88000	39.10900	77.15200
N	-10.39700	36.24800	77.85900
H	-10.30400	36.53900	78.83200
C	-10.49000	34.82800	77.54600
C	-11.92300	34.33900	77.32600
O	-12.14000	33.18900	76.93800
C	-9.82900	34.01100	78.65800
C	-8.35400	34.34500	78.89600
C	-7.77100	33.39400	79.92900
C	-7.59300	34.24100	77.58500
N	-12.89800	35.21100	77.56600
H	-12.66200	36.15300	77.87800
C	-14.29900	34.84300	77.39100
C	-14.87900	35.39800	76.09500
O	-16.00700	35.07900	75.72600
C	-15.12700	35.33900	78.58100
O	-15.02800	36.74700	78.72100
H	-15.54100	37.05500	79.45900
N	-14.10400	36.23100	75.40900
H	-13.17800	36.46100	75.77000
C	-14.54600	36.82400	74.15300
C	-14.73500	35.76000	73.08000
O	-14.04000	34.74500	73.06600
C	-13.52100	37.84800	73.65500
C	-13.34100	39.16300	74.41500
C	-12.21100	39.96500	73.77700
C	-14.63700	39.95700	74.38200
N	-15.68100	35.99300	72.18000

H	-16.24900	36.83700	72.25500
C	-15.92000	35.06200	71.08700
C	-14.95700	35.47400	69.98000
O	-14.26100	36.48100	70.10900
C	-17.35500	35.17100	70.55200
O	-17.56800	36.48600	70.02300
H	-18.45600	36.55300	69.69200
C	-18.36000	34.90300	71.66700
N	-14.91500	34.70600	68.89800
H	-15.51100	33.88000	68.84300
C	-14.02800	35.02900	67.78700
C	-14.38300	36.39100	67.19900
O	-13.50900	37.22600	66.95600
C	-14.12100	33.95600	66.71400
N	-15.67500	36.61200	66.98200
H	-16.34900	35.88300	67.21700
C	-16.15600	37.86700	66.41700
C	-15.80800	39.06600	67.28500
O	-15.42700	40.11900	66.77600
C	-17.67100	37.80500	66.21600
C	-18.07900	36.74800	65.21200
O	-17.64400	36.83900	64.04400
O	-18.83200	35.82400	65.59000
N	-15.94600	38.90700	68.59600
H	-16.27400	38.01300	68.96200
C	-15.63700	39.98800	69.51700
C	-14.14200	40.26800	69.52000
O	-13.72200	41.41400	69.65300
C	-16.09800	39.62900	70.93000
C	-17.59700	39.42200	71.05100
C	-18.00800	39.00100	72.44500
O	-17.51700	38.00300	72.97300
N	-18.91400	39.76100	73.05200
H	-19.19100	39.47700	73.99200
H	-19.32100	40.58800	72.61500
N	-13.34500	39.21000	69.38300
H	-13.75900	38.28200	69.29700
C	-11.89300	39.35000	69.35300
C	-11.52600	40.20100	68.13900
O	-10.75800	41.15700	68.24900
C	-11.23300	37.97000	69.24600
C	-9.70300	37.97600	69.22300
S	-8.92000	38.45700	70.78600

C	-8.23500	39.98100	70.34400
N	-12.09100	39.84500	66.98700
H	-12.72000	39.04200	66.97600
C	-11.84400	40.56300	65.73400
C	-12.27500	42.02200	65.81100
O	-11.51900	42.92800	65.45100
C	-12.59400	39.90400	64.55600
C	-12.52400	40.79900	63.32800
C	-11.98900	38.54800	64.24700
N	-13.49800	42.24900	66.28000
H	-14.08200	41.46200	66.56300
C	-14.01600	43.60600	66.39500
C	-13.10600	44.44000	67.29000
O	-12.81600	45.59700	66.99000
C	-15.43600	43.58000	66.96800
O	-16.29300	42.80400	66.14900
H	-17.17400	42.78800	66.50400
N	-12.65300	43.83700	68.38500
H	-12.93100	42.87300	68.56900
C	-11.77000	44.51200	69.33200
C	-10.46700	44.93500	68.65100
O	-10.05000	46.09100	68.74100
C	-11.47000	43.58500	70.50800
N	-9.82600	43.99300	67.96900
H	-10.21400	43.05100	67.92300
C	-8.57400	44.29000	67.28500
C	-8.76700	45.33800	66.19500
O	-7.97400	46.27200	66.07200
C	-7.97600	43.00300	66.70400
C	-7.62200	41.95600	67.76500
C	-6.96000	40.74800	67.11300
C	-6.68000	42.58600	68.80400
N	-9.82400	45.20200	65.40400
H	-10.46000	44.41500	65.53300
C	-10.07400	46.17800	64.35200
C	-10.23500	47.57500	64.94500
O	-9.65800	48.54000	64.44600
C	-11.32500	45.79400	63.55600
C	-11.15700	44.55100	62.68400
C	-12.50000	44.16400	62.06800
C	-10.12400	44.83500	61.60000
N	-11.01300	47.67500	66.01800
H	-11.46000	46.83600	66.38600

C	-11.24500	48.95300	66.68400
C	-9.96900	49.54900	67.25600
O	-9.80500	50.76700	67.29400
C	-12.25600	48.78600	67.81800
C	-13.68200	48.90500	67.34700
O	-14.12900	48.05400	66.54700
O	-14.35400	49.86400	67.77900
N	-9.07300	48.67900	67.70300
H	-9.27600	47.68200	67.62600
C	-7.80900	49.09400	68.30100
C	-6.75600	49.62000	67.32600
O	-5.76500	50.20700	67.75300
C	-7.22700	47.92900	69.09100
N	-6.96100	49.41100	66.02600
H	-7.81400	48.93900	65.72600
C	-5.99100	49.84300	65.01700
C	-5.50000	51.27700	65.13900
O	-6.28500	52.21400	65.29300
C	-6.55000	49.61700	63.60400
C	-6.40900	48.18500	63.12400
C	-4.95400	47.77700	62.98600
O	-4.35200	48.03600	61.91700
O	-4.40800	47.21600	63.95900
N	-4.17500	51.46900	65.06600
C	-3.59800	52.80800	65.17000
C	-3.78300	53.60800	63.88500
O	-4.08300	53.05700	62.82800
C	-2.13000	52.52400	65.46400
C	-1.88300	51.27100	64.65600
C	-3.11800	50.44200	64.96500
N	-3.60000	54.92900	63.96400
C	-3.75200	55.77700	62.78200
C	-2.53000	55.68000	61.87500
O	-1.44500	55.30400	62.32200
C	-3.90100	57.16500	63.38600
C	-2.96900	57.09300	64.56100
C	-3.30600	55.73600	65.16100
N	-2.70400	56.00300	60.60000
H	-3.63100	56.26800	60.26700
C	-1.58500	55.98200	59.67600
C	-0.97900	57.37500	59.70400
O	-1.62800	58.35900	59.33400
C	-2.03100	55.64500	58.24700

C	-2.50400	54.19400	58.18400
C	-0.88300	55.86400	57.27800
C	-2.75000	53.69400	56.77100
N	0.26600	57.46600	60.15000
H	0.76800	56.62300	60.42800
C	0.91900	58.75700	60.24500
C	1.58800	59.18100	58.95300
O	1.84200	58.35700	58.07100
C	1.94600	58.74000	61.38100
C	1.35900	58.38000	62.75300
C	2.39400	58.63500	63.84500
C	0.11200	59.21900	63.01100
N	1.85300	60.48100	58.85000
H	1.57900	61.10000	59.61300
C	2.51900	61.05300	57.69000
C	3.96500	61.37100	58.02100
O	4.30400	61.64900	59.17200
C	1.82700	62.34800	57.23600
C	0.64500	62.10600	56.34100
C	-0.53200	61.57000	56.84200
C	0.72800	62.34800	54.97700
C	-1.59300	61.27300	56.00500
C	-0.32600	62.05400	54.13400
C	-1.48000	61.51300	54.65200
O	-2.51200	61.17600	53.80800
H	-2.43400	61.34100	52.87600
N	4.81500	61.31600	57.00200
H	4.47100	61.04200	56.08200
C	6.22500	61.63600	57.16500
C	6.22800	63.15900	57.31300
O	5.36800	63.83300	56.75100
C	7.00300	61.19700	55.91800
O	8.38200	61.48400	56.02900
H	8.86400	61.21200	55.25700
N	7.17800	63.70000	58.06600
H	7.88400	63.10200	58.49500
C	7.22300	65.14200	58.28600
C	8.28600	65.86200	57.45700
O	9.43800	65.43200	57.39600
C	7.45400	65.42500	59.77600
C	6.72600	66.65400	60.31200
C	6.88200	66.81500	61.81600
O	6.62900	65.83400	62.55100

O	7.25000	67.92300	62.26200
N	7.87900	66.96100	56.82400
H	6.90200	67.23900	56.91200
C	8.76800	67.78800	56.00800
C	7.97200	68.77000	55.14900
O	6.74100	68.72200	55.10800
C	9.66700	66.91900	55.11300
C	8.94600	66.12200	54.04400
C	8.35200	66.75300	52.95500
C	8.87600	64.73700	54.11600
C	7.71000	66.02500	51.97000
C	8.23800	64.00000	53.13700
C	7.65700	64.64900	52.06600
O	7.02300	63.91700	51.08800
H	6.98700	62.97000	51.15400
N	16.97800	65.36400	51.66300
H	17.93900	65.61600	51.89200
H	16.46600	66.14400	51.25100
H	16.92900	64.72000	50.87300
C	16.30800	64.83200	52.84400
C	17.05400	63.61300	53.37300
O	17.49800	62.76400	52.59900
C	14.87200	64.45500	52.50200
N	17.20600	63.53600	54.69100
H	16.84200	64.28100	55.28400
C	17.88600	62.40100	55.29900
C	16.87000	61.26600	55.37600
O	15.91600	61.32200	56.15700
C	18.38800	62.76500	56.69900
O	19.16100	61.71400	57.25600
H	19.47200	61.94000	58.12500
N	17.06900	60.24500	54.54700
H	17.87700	60.25900	53.92400
C	16.16000	59.10600	54.50700
C	15.99500	58.47600	55.88900
O	14.87600	58.20100	56.32100
C	16.67000	58.06800	53.50400
C	15.60900	57.08100	53.03900
S	14.09300	57.90400	52.49500
C	14.56900	58.53300	50.87400
N	17.10900	58.26000	56.58200
H	18.00800	58.50800	56.16800
C	17.07900	57.67700	57.92100

C	16.39000	58.60800	58.91000
O	15.62200	58.16400	59.76200
C	18.49600	57.37500	58.40800
C	19.08500	56.10900	57.82700
S	18.00900	54.69900	58.12700
C	17.97500	54.65500	59.91000
N	16.67200	59.90200	58.80200
H	17.33200	60.22300	58.09300
C	16.04200	60.85700	59.69100
C	14.53300	60.77600	59.55600
O	13.80200	60.77900	60.54700
N	14.06500	60.69200	58.31500
H	14.72300	60.69000	57.53500
C	12.63800	60.60300	58.03900
C	12.03100	59.32700	58.61600
O	11.01300	59.36300	59.30700
C	12.38900	60.63500	56.52700
C	12.72800	61.93800	55.80300
C	12.42800	61.78900	54.31100
C	11.92000	63.07900	56.41000
N	12.66200	58.20100	58.31700
H	13.50600	58.24200	57.74600
C	12.18300	56.90500	58.78200
C	12.18600	56.78500	60.29900
O	11.23000	56.27900	60.88100
C	13.02400	55.79000	58.16400
C	12.92300	55.70600	56.64000
C	13.78700	54.56500	56.11900
C	11.47000	55.50200	56.24000
N	13.24900	57.25500	60.94400
H	14.01900	57.67100	60.42100
C	13.31500	57.17600	62.40100
C	12.32600	58.11800	63.08200
O	11.75900	57.76900	64.11700
C	14.72600	57.48600	62.93000
O	15.15100	58.76100	62.43900
H	16.02200	58.95200	62.76600
C	15.70400	56.41800	62.49100
N	12.11800	59.31100	62.52100
H	12.61800	59.57100	61.67100
C	11.17100	60.24500	63.12800
C	9.77700	59.65900	63.00800
O	8.96100	59.77100	63.92400

C	11.22100	61.62000	62.44000
C	10.15800	62.59100	62.97100
O	8.99900	62.57100	62.54200
N	10.55400	63.44000	63.91500
H	9.84700	64.08500	64.26800
H	11.51000	63.45700	64.26900
N	9.50600	59.02500	61.87200
H	10.21900	58.96400	61.14500
C	8.20300	58.41800	61.65700
C	7.99900	57.28400	62.65500
O	6.96000	57.20500	63.29500
C	8.09300	57.88600	60.22500
C	6.83400	57.08300	59.89300
C	5.57800	57.95200	59.99800
C	6.97700	56.53200	58.47600
N	8.99100	56.40700	62.77800
H	9.83000	56.51300	62.20800
C	8.89500	55.29200	63.72000
C	8.73900	55.81500	65.14900
O	8.00700	55.23600	65.94600
C	10.13400	54.40100	63.61200
N	9.42400	56.90900	65.48100
H	10.03000	57.35800	64.79400
C	9.30800	57.46800	66.82900
C	7.88100	57.90500	67.14600
O	7.36200	57.59500	68.21500
C	10.25700	58.65600	67.01900
C	11.71300	58.24000	67.07400
O	11.99700	57.02500	67.16300
O	12.58300	59.13500	67.03800
N	7.23900	58.62700	66.22500
H	7.71000	58.87200	65.35400
C	5.86700	59.06900	66.45600
C	4.88500	57.89700	66.47800
O	3.87500	57.93500	67.19000
C	5.42500	60.08100	65.38400
C	5.83400	61.52600	65.67900
C	5.36300	62.47000	64.56500
N	6.07800	62.21800	63.32000
H	7.09700	62.19300	63.35600
C	5.49700	62.01900	62.14300
N	4.17900	62.04400	62.03700
H	3.60900	62.23100	62.86200

H	3.73300	61.89100	61.13300
N	6.23900	61.77500	61.06800
H	7.25600	61.75600	61.15000
H	5.79300	61.62200	60.16400
N	5.16100	56.85700	65.69500
H	5.99700	56.86900	65.11000
C	4.26900	55.69600	65.67000
C	4.32000	54.92000	66.98300
O	3.33500	54.30500	67.38600
C	4.63600	54.74300	64.52600
C	4.21600	55.21700	63.13600
C	4.50600	54.16800	62.07900
O	5.65700	54.09900	61.61200
O	3.58600	53.40200	61.73200
N	5.47100	54.94700	67.64500
H	6.25400	55.48300	67.26900
C	5.63400	54.22200	68.90200
C	4.61100	54.65500	69.93500
O	4.05200	53.82900	70.65300
C	7.05300	54.41000	69.45300
C	8.11900	53.51900	68.81100
C	9.50000	53.89300	69.33000
C	7.80900	52.05800	69.12800
N	4.36200	55.95800	69.99800
H	4.86500	56.59100	69.37700
C	3.39300	56.50200	70.92800
C	2.03800	55.86500	70.68100
O	1.35400	55.45400	71.61700
C	3.27300	58.03400	70.74900
C	2.38100	58.61100	71.82300
C	4.66400	58.66200	70.77300
N	1.65000	55.78200	69.41000
H	2.25900	56.14900	68.67800
C	0.37100	55.17700	69.03800
C	0.38300	53.66200	69.20900
O	-0.65500	53.04700	69.44300
C	0.02800	55.54500	67.59400
C	-0.27000	57.00000	67.41300
N	-1.46000	57.56800	67.81500
H	-2.24800	57.06200	68.22000
C	0.49000	58.01400	66.93700
C	-1.42100	58.87000	67.59300
N	-0.24900	59.16600	67.06100

H	0.05800	60.09900	66.78600
N	1.55800	53.05600	69.09800
H	2.39600	53.60000	68.89300
C	1.64900	51.61100	69.27000
C	1.26600	51.21400	70.69900
O	0.61800	50.18900	70.92500
C	3.06700	51.12600	68.97100
C	3.19000	49.61700	69.06700
S	4.84700	48.99800	68.80900
C	5.25600	49.72600	67.20700
N	1.67000	52.02800	71.66300
H	2.20700	52.86200	71.42500
C	1.35800	51.74800	73.06300
C	-0.14400	51.79200	73.30500
O	-0.68100	50.94100	74.01100
C	2.07900	52.73300	73.99400
C	3.56200	52.36300	74.05500
C	1.48200	52.68400	75.39300
C	4.41300	53.39100	74.75000
N	-0.82800	52.76700	72.70700
H	-0.33400	53.45200	72.13500
C	-2.27700	52.86700	72.86100
C	-2.93900	51.64400	72.25600
O	-3.89400	51.10000	72.80900
C	-2.81400	54.11900	72.16800
C	-2.36700	55.38000	72.84900
O	-2.25900	55.41900	74.08000
N	-2.11100	56.42600	72.06800
H	-1.80700	57.28300	72.53100
H	-2.20000	56.39400	71.05200
N	-2.43300	51.22400	71.10200
H	-1.65600	51.73300	70.68000
C	-2.96900	50.04900	70.43000
C	-2.74300	48.80600	71.29400
O	-3.65500	47.99900	71.49600
C	-2.28800	49.86700	69.06900
C	-2.42200	48.48100	68.52800
C	-3.52600	47.92500	67.94500
C	-1.43500	47.44100	68.59900
N	-3.28500	46.60000	67.65200
H	-3.94800	45.96000	67.21500
C	-2.01000	46.28100	68.04200
C	-0.11700	47.38400	69.07900

C	-1.31600	45.06800	67.95600
C	0.57000	46.17900	68.99500
C	-0.03100	45.03800	68.43700
N	-1.52900	48.65800	71.81300
H	-0.81900	49.36900	71.63500
C	-1.18900	47.49400	72.63600
C	-2.11200	47.39000	73.84700
O	-2.58600	46.30900	74.19100
C	0.26900	47.57500	73.08400
N	-2.36500	48.52200	74.49000
H	-1.93700	49.39000	74.16700
C	-3.24400	48.54300	75.64900
C	-4.65700	48.09400	75.27500
O	-5.42600	47.66800	76.14100
C	-3.26200	49.94800	76.25400
C	-1.98200	50.29200	77.00800
C	-1.83800	51.79200	77.22300
C	-3.09300	52.41100	77.81700
N	-3.46400	51.80200	79.12000
H	-4.30600	52.21700	79.51900
H	-2.68700	51.84300	79.77900
H	-3.55700	50.78900	79.03900
N	-4.99500	48.17400	73.98700
H	-4.31600	48.52900	73.31300
C	-6.31900	47.76300	73.52200
C	-6.37200	46.30000	73.07700
O	-7.43800	45.79100	72.74900
C	-6.79500	48.65900	72.37100
C	-6.85100	50.14400	72.71300
C	-8.27800	50.69200	72.72700
N	-8.90000	50.68600	71.40500
H	-8.37800	50.27200	70.63300
C	-10.10500	51.18700	71.14500
N	-10.81800	51.73800	72.11900
H	-11.74200	52.12200	71.92000
H	-10.43800	51.77300	73.06500
N	-10.60000	51.14100	69.91400
H	-11.52400	51.52500	69.71500
H	-10.05200	50.71700	69.16500
N	-5.22700	45.62400	73.05300
H	-4.35700	46.08900	73.31100
C	-5.21100	44.22100	72.66000
C	-5.70800	43.42600	73.85800

O	-5.11500	43.46700	74.93100
C	-3.79000	43.74800	72.27800
C	-3.78800	42.25300	72.04400
C	-3.32400	44.47600	71.02500
N	-6.81600	42.69400	73.68500
C	-7.39100	41.89500	74.76700
C	-6.36400	41.10400	75.57100
O	-5.57900	40.33300	75.01000
C	-8.38200	40.99200	74.03300
C	-8.86900	41.88100	72.93600
C	-7.57400	42.51200	72.43700
N	-6.37000	41.31600	76.88400
H	-7.02300	41.99200	77.28000
C	-5.46200	40.60100	77.76400
C	-4.13700	41.26700	78.08500
O	-3.52300	40.97100	79.11000
N	-3.69100	42.16900	77.21700
H	-4.25100	42.39300	76.39500
C	-2.41500	42.84300	77.42000
C	-2.34700	43.64900	78.71900
O	-1.36200	43.56100	79.45400
C	-2.12400	43.75400	76.23100
C	-0.72100	44.29200	76.20700
C	0.33600	43.49000	75.79700
C	-0.45900	45.59900	76.58800
C	1.62800	43.98600	75.76700
C	0.83800	46.10100	76.56000
C	1.87800	45.29400	76.14800
N	-3.38500	44.43200	79.01100
H	-4.18800	44.46700	78.38300
C	-3.37500	45.24100	80.22900
C	-3.51000	44.44900	81.53200
O	-3.33000	45.00800	82.61700
C	-4.47400	46.33600	80.19700
C	-4.17900	47.32600	79.07700
C	-5.85000	45.70500	80.01600
N	-3.82200	43.15800	81.44100
H	-3.97600	42.73700	80.52500
C	-3.94600	42.33800	82.65000
C	-2.55800	41.91700	83.12000
O	-2.38500	41.40200	84.23000
C	-4.78500	41.08600	82.38700
C	-6.20000	41.40800	81.96400

O	-6.82700	42.29900	82.57700
O	-6.69000	40.75600	81.02000
N	-1.56600	42.13400	82.26600
H	-1.76900	42.54900	81.35700
C	-0.19300	41.79100	82.60400
C	0.39800	42.90600	83.45900
O	-0.19300	43.98700	83.56700
C	0.63500	41.62900	81.32600
C	0.19900	40.52200	80.35200
C	1.02600	40.61400	79.06800
C	0.38900	39.16400	81.00400
N	1.55000	42.63900	84.07100
H	1.96500	41.71300	83.96500
C	2.23800	43.63700	84.89200
C	2.85400	44.66700	83.95100
O	3.08400	44.37600	82.77000
C	3.39400	43.01900	85.71200
O	4.39300	42.50900	84.82300
H	5.10300	42.12900	85.32700
C	2.88900	41.88600	86.59900
N	3.12500	45.86000	84.47200
H	2.90800	46.03500	85.45300
C	3.72700	46.92700	83.67300
C	5.06500	46.44500	83.09900
O	5.35400	46.64000	81.92200
C	3.94100	48.17600	84.54400
C	4.58100	49.40000	83.88000
C	3.66600	49.93700	82.78300
C	4.83200	50.47700	84.93400
N	5.86500	45.80700	83.94600
H	5.55400	45.68800	84.91000
C	7.16800	45.26800	83.56500
C	7.07100	44.30600	82.37400
O	7.85200	44.38900	81.42200
C	7.78500	44.55400	84.77600
C	8.98000	43.70800	84.45200
N	8.87500	42.45900	83.87200
H	8.00300	42.01000	83.59200
C	10.30200	43.91700	84.65600
C	10.08100	41.93600	83.73700
N	10.96500	42.79900	84.20500
H	11.97500	42.65900	84.22800
N	6.11100	43.39200	82.42800

H	5.49000	43.35800	83.23700
C	5.93700	42.44000	81.34500
C	5.40400	43.12600	80.09000
O	5.72200	42.71500	78.97500
C	5.01000	41.30100	81.78300
C	5.68600	40.35500	82.77400
O	6.90400	40.51800	83.01100
O	5.01200	39.45100	83.30900
N	4.59400	44.16700	80.26800
H	4.33800	44.45300	81.21300
C	4.06900	44.90300	79.12300
C	5.23100	45.56800	78.38700
O	5.31600	45.51700	77.15800
C	3.06500	45.97100	79.57900
C	1.68100	45.41500	79.94200
C	0.72000	46.49200	80.42800
O	0.59800	47.54800	79.81400
N	0.03000	46.22200	81.52900
H	-0.61400	46.94300	81.85400
H	0.13100	45.34500	82.03900
N	6.12700	46.19100	79.14500
H	6.00600	46.19900	80.15800
C	7.28300	46.86500	78.55600
C	8.20500	45.87000	77.85400
O	8.69400	46.13000	76.75200
C	8.11700	47.59800	79.61900
C	9.30900	48.28500	78.95300
C	7.26100	48.61200	80.34900
N	8.44600	44.73600	78.50100
H	8.01400	44.57100	79.41000
C	9.32100	43.72800	77.92500
C	8.77100	43.24200	76.59000
O	9.51600	43.12700	75.62600
C	9.50600	42.54900	78.89500
C	10.37200	41.45600	78.34800
N	9.88400	40.45500	77.53500
H	8.90800	40.34100	77.26100
C	11.70400	41.23600	78.45700
C	10.87900	39.66600	77.16600
N	11.99300	40.11900	77.71100
H	12.91900	39.70600	77.59700
N	7.47100	42.97200	76.52300
H	6.88700	43.09200	77.35000

C	6.87100	42.50500	75.27400
C	7.00500	43.53600	74.16000
O	7.35800	43.19700	73.03000
C	5.39100	42.15700	75.48400
C	5.13100	40.89200	76.31300
C	3.63700	40.68800	76.49600
C	5.74300	39.67400	75.60900
N	6.70900	44.79500	74.46900
H	6.40100	45.02400	75.41400
C	6.82100	45.84900	73.47200
C	8.26800	46.10000	73.06900
O	8.54600	46.33000	71.89500
C	6.17800	47.15000	73.98100
C	4.64900	47.13800	73.89400
C	4.04900	48.26100	74.74400
C	4.23900	47.28000	72.42800
N	9.19800	46.05000	74.02300
H	8.93100	45.85300	74.98800
C	10.60300	46.27900	73.68200
C	11.08600	45.17400	72.73500
O	11.93200	45.39600	71.86500
C	11.48100	46.29300	74.94300
C	12.97400	46.40400	74.63400
C	13.84200	46.49200	75.87900
O	13.65500	45.66200	76.79500
O	14.71800	47.38300	75.93500
N	10.54300	43.97700	72.91400
H	9.84900	43.84700	73.65000
C	10.92100	42.84700	72.07900
C	10.28900	42.87600	70.68300
O	10.91000	42.47400	69.69600
C	10.51200	41.54200	72.77600
O	10.64600	40.43100	71.90300
H	10.39300	39.62300	72.33400
N	9.06900	43.39100	70.59700
H	8.64000	43.81100	71.42100
C	8.33600	43.36300	69.33900
C	8.06900	44.65400	68.56900
O	7.50100	44.59900	67.48300
C	7.00500	42.65600	69.58100
N	8.47900	45.80100	69.08900
H	9.00800	45.81600	69.96100
C	8.15900	47.04600	68.39100

C	8.55900	47.10400	66.92100
O	7.76800	47.54800	66.09700
C	8.74100	48.26000	69.12700
C	10.21600	48.36400	69.06000
C	11.12300	47.76400	69.89100
C	10.97800	49.09000	68.08900
N	12.40300	48.07500	69.49600
H	13.25800	47.75500	69.95000
C	12.34100	48.88700	68.39100
C	10.64000	49.89000	66.99000
C	13.36600	49.45800	67.63800
C	11.65800	50.45500	66.24100
C	13.00500	50.23700	66.56800
N	9.76400	46.66700	66.56800
H	10.40600	46.28200	67.26100
C	10.14100	46.75400	65.16000
C	9.38000	45.75200	64.29400
O	9.07700	46.04900	63.13700
C	11.65400	46.59400	64.98400
C	12.17400	46.90800	63.57600
C	11.71100	48.29700	63.14800
C	13.68300	46.82100	63.55500
N	9.06000	44.57400	64.83200
H	9.35300	44.35100	65.78300
C	8.28600	43.59900	64.05300
C	6.89300	44.17400	63.80000
O	6.31200	43.99700	62.72500
C	8.13300	42.27500	64.81100
C	9.41600	41.46100	64.93100
C	9.22200	40.21700	65.77000
O	8.74300	39.20000	65.23100
O	9.52200	40.26500	66.97700
N	6.35600	44.84800	64.81300
H	6.88100	44.95100	65.68100
C	5.03200	45.44100	64.70400
C	5.04200	46.57000	63.67100
O	4.12500	46.67400	62.84900
C	4.54700	45.95200	66.08800
C	4.30400	44.74000	67.01000
C	3.25700	46.78900	65.91500
C	4.22600	45.09600	68.50400
N	6.07200	47.40700	63.69500
H	6.80500	47.30500	64.39700

C	6.14200	48.47700	62.70100
C	6.29100	47.86700	61.30700
O	5.66500	48.32700	60.34200
C	7.33000	49.40800	62.97000
C	7.24600	50.34700	64.17800
C	8.48300	51.25300	64.20000
C	5.96800	51.18900	64.08500
N	7.11900	46.82900	61.19100
H	7.60600	46.47300	62.01300
C	7.33100	46.19900	59.88700
C	6.12700	45.46200	59.30300
O	5.89400	45.53700	58.10100
C	8.54500	45.26400	59.93600
C	9.87500	46.00700	60.07200
S	11.29600	44.88500	60.15300
C	12.65000	46.05200	59.89200
N	5.36100	44.74100	60.11800
H	5.57900	44.66900	61.11200
C	4.20300	44.05700	59.55500
C	3.16100	45.12100	59.15400
O	2.40100	44.93100	58.19700
C	3.60000	43.01300	60.53300
C	2.63800	42.09600	59.75600
C	2.88200	43.70800	61.69000
C	2.10600	40.91400	60.53700
N	3.15000	46.24800	59.86700
H	3.78400	46.35500	60.65900
C	2.23500	47.32700	59.51900
C	2.64800	47.88700	58.16000
O	1.81600	48.11800	57.28200
N	3.95200	48.08500	57.98600
H	4.58500	47.86600	58.75500
C	4.51700	48.60300	56.74100
C	4.22000	47.67600	55.57100
O	3.78300	48.12400	54.50200
C	6.03500	48.77000	56.87700
C	6.83200	49.05600	55.59900
C	6.41200	50.39900	54.99800
C	8.31400	49.06300	55.93700
N	4.46500	46.38300	55.76400
H	4.82800	46.06200	56.66200
C	4.21700	45.42900	54.69900
C	2.73400	45.42500	54.34200

O	2.36200	45.36500	53.16400
C	4.65500	44.02100	55.11500
C	4.24300	43.02200	54.05800
C	6.16600	43.99500	55.29700
N	1.89100	45.50100	55.36300
H	2.26200	45.55200	56.31200
C	0.45300	45.51300	55.16400
C	-0.01200	46.68800	54.30300
O	-0.75200	46.50200	53.33400
C	-0.27300	45.54600	56.51400
C	-1.74000	45.80000	56.37800
C	-2.41500	46.92400	56.75100
C	-2.71400	44.92100	55.79600
N	-3.74800	46.80100	56.43800
H	-4.46600	47.50400	56.61400
C	-3.95600	45.58000	55.85100
C	-2.65300	43.64100	55.23800
C	-5.12900	45.00400	55.36400
C	-3.80900	43.07200	54.75900
C	-5.03500	43.75300	54.82300
N	0.41000	47.90000	54.63100
H	1.02900	48.04700	55.42900
C	-0.04000	49.01100	53.81400
C	0.69900	49.11700	52.48100
O	0.35700	49.94700	51.64800
C	0.02200	50.33000	54.59500
C	1.30800	50.61500	55.30600
C	1.19000	51.88000	56.16600
N	2.50900	52.31900	56.60000
H	3.02800	52.94500	55.98400
C	3.08000	51.96100	57.74000
N	2.43300	51.16500	58.58400
H	1.48600	50.85000	58.37400
H	2.87300	50.88900	59.46200
N	4.31400	52.37200	58.01400
H	4.81100	52.98300	57.36600
H	4.75400	52.09600	58.89200
N	1.69500	48.25900	52.26800
H	1.94300	47.58600	52.99300
C	2.43800	48.26900	51.00900
C	1.86800	47.22400	50.04000
O	2.25700	47.16800	48.87100
C	3.92800	47.97400	51.24600

O	4.58200	49.01500	51.95600
H	5.50300	48.83300	52.10200
N	0.94200	46.40200	50.52000
H	0.63100	46.50300	51.48600
C	0.36200	45.35400	49.68100
C	-0.17600	45.81000	48.33700
O	-0.03800	45.09900	47.34200
C	-0.75900	44.62400	50.41400
C	-0.30400	43.44400	51.23200
S	-1.72600	42.47600	51.69600
C	-3.03500	43.60900	51.29600
N	-0.79800	46.98500	48.30300
H	-0.88100	47.54000	49.15500
C	-1.36200	47.48500	47.05600
C	-0.40300	48.31900	46.22600
O	-0.82300	49.01100	45.29800
C	-2.63400	48.28500	47.34200
C	-3.74300	47.44000	47.95600
C	-5.05900	48.18600	48.05500
O	-5.08900	49.25800	48.69600
O	-6.06400	47.69900	47.49000
N	0.88400	48.24200	46.54700
H	1.16900	47.64100	47.32000
C	1.89600	48.99400	45.82200
C	3.10800	48.13400	45.47900
O	4.19600	48.31100	46.03900
C	2.32500	50.19900	46.64900
C	1.18200	51.07400	47.05600
N	0.56400	51.94100	46.18100
H	0.83900	52.09600	45.21100
C	0.51100	51.17500	48.22500
C	-0.44100	52.54000	46.79600
N	-0.49600	52.09200	48.03800
H	-1.17500	52.38000	48.74300
N	2.92800	47.18500	44.54500
C	3.98500	46.27800	44.09500
C	5.27800	47.03600	43.83500
O	5.26900	48.09100	43.19900
C	3.40400	45.68900	42.81300
C	1.94700	45.60900	43.12500
C	1.66400	46.92600	43.82700
N	6.38400	46.50600	44.34300
H	6.32700	45.64500	44.88600

C	7.67200	47.13800	44.13400
C	7.96600	48.34100	45.00200
O	9.05100	48.91800	44.92100
N	7.01800	48.73300	45.83900
H	6.13400	48.22600	45.88400
C	7.24100	49.88800	46.69400
C	6.80800	49.67900	48.14200
O	5.95200	48.83900	48.44100
C	6.52700	51.10500	46.10900
C	7.00400	51.45000	44.70300
C	6.33000	52.69500	44.18300
C	6.81900	53.03100	42.78300
N	6.19300	54.28600	42.29500
H	6.52100	54.51100	41.35600
H	6.34200	55.05900	42.94300
H	5.17500	54.24300	42.33900
N	7.42000	50.45300	49.03400
H	8.12700	51.11300	48.71000
C	7.11600	50.39200	50.46100
C	6.43000	51.68200	50.89300
O	6.98600	52.77300	50.75800
C	8.40200	50.18800	51.27100
C	9.07200	48.83500	50.98200
C	10.42200	48.75200	51.69000
C	8.15000	47.70400	51.44300
N	5.21600	51.54900	51.40700
H	4.81000	50.61800	51.49800
C	4.45100	52.70700	51.84400
C	4.72300	52.99200	53.32000
O	3.93800	52.63000	54.19500
C	2.96100	52.46700	51.62200
C	2.04500	53.68800	51.70500
C	2.52900	54.74800	50.74300
C	0.62900	53.28400	51.35200
N	5.85600	53.62600	53.58600
H	6.48600	53.87100	52.82200
C	6.21500	53.97700	54.95000
C	5.14900	54.94500	55.43800
O	4.74300	54.91300	56.59900
C	7.60100	54.62100	54.97000
C	8.71800	53.63800	54.76000
C	9.18900	52.87600	55.81600
C	9.26100	53.44100	53.50000

C	10.18500	51.93100	55.61700
C	10.25500	52.49800	53.29400
C	10.71500	51.74400	54.35000
N	4.67200	55.78100	54.51900
H	5.04600	55.73700	53.57100
C	3.63100	56.75900	54.82300
C	2.96000	57.17000	53.50700
O	3.54000	57.01000	52.44100
C	4.24600	57.97400	55.49900
N	1.72700	57.70100	53.56900
C	1.03000	58.11400	52.34400
C	1.87100	59.07200	51.50800
O	1.75600	59.10600	50.27700
C	-0.23800	58.77100	52.87700
C	-0.50500	57.99000	54.12500
C	0.87300	57.91900	54.74900
N	2.72600	59.83600	52.18800
H	2.76900	59.74000	53.20300
C	3.60100	60.80200	51.54000
C	5.05400	60.34100	51.53100
O	5.96400	61.13900	51.32600
C	3.49300	62.16600	52.23700
C	4.10700	62.16900	53.63300
O	3.97300	61.20500	54.38800
N	4.76800	63.27100	53.98600
H	5.17900	63.27300	54.92000
H	4.87900	64.06900	53.36100
N	5.27100	59.05000	51.76100
H	4.47900	58.43600	51.95000
C	6.61700	58.49600	51.74900
C	6.56400	57.07200	51.18500
O	6.71100	56.08600	51.91200
C	7.21600	58.50400	53.16400
C	8.72500	58.23900	53.27300
C	9.50700	59.31200	52.52300
C	9.13700	58.22400	54.73000
N	6.32900	56.98400	49.87700
H	6.19400	57.84400	49.34600
C	6.25700	55.70800	49.17300
C	7.61100	55.56500	48.48100
O	7.94100	56.34100	47.58200
C	5.11100	55.74500	48.15400
C	4.76200	54.51100	47.31300

C	4.45800	53.31800	48.19700
C	3.55900	54.83800	46.45100
N	8.39900	54.58500	48.91100
H	8.06500	53.95800	49.64300
C	9.73200	54.38900	48.35600
C	9.93000	53.08400	47.60200
O	9.35900	52.05000	47.95200
C	10.77500	54.45900	49.47800
C	10.72400	55.64000	50.45200
C	11.85900	55.50300	51.46100
C	10.83600	56.95200	49.69200
N	10.76100	53.13700	46.56700
H	11.19500	54.02500	46.31400
C	11.05900	51.94600	45.79200
C	12.43400	51.42200	46.18100
O	13.14800	52.03300	46.97900
C	11.02300	52.24500	44.29200
C	12.05300	53.27400	43.87700
O	13.25800	53.04100	44.11500
O	11.65400	54.31600	43.30800
N	12.80000	50.29200	45.59500
H	12.16200	49.86000	44.92700
C	14.07100	49.64100	45.86300
C	15.30400	50.53500	45.72300
O	16.16600	50.55900	46.60200
C	14.20700	48.43600	44.93700
C	15.47500	47.65800	45.12800
C	15.48400	46.41300	44.26800
N	16.53100	45.51000	44.72100
H	16.25500	44.59500	45.07600
C	17.82500	45.80700	44.69900
N	18.22600	46.98200	44.23400
H	17.54300	47.65000	43.87700
H	19.22000	47.21000	44.21700
N	18.71300	44.93900	45.16300
H	18.40400	44.03500	45.52100
H	19.70700	45.16700	45.14600
N	15.39700	51.26500	44.61800
H	14.65300	51.21900	43.92100
C	16.54700	52.13300	44.38500
C	16.71200	53.21800	45.45000
O	17.83200	53.54500	45.84200
C	16.44500	52.77300	42.99900

C	16.31200	51.74400	41.89400
O	17.14300	50.84300	41.76500
N	15.26300	51.87100	41.08900
H	14.57500	52.61700	41.19600
H	15.17400	51.17900	40.34500
N	15.60200	53.77500	45.92100
H	14.69600	53.47100	45.56400
C	15.66200	54.81600	46.94200
C	16.19900	54.28100	48.26500
O	16.39100	55.03800	49.21700
C	14.28000	55.42600	47.15400
C	13.80800	56.26700	45.99100
C	12.37800	56.72200	46.15700
O	11.45400	55.90800	46.16100
N	12.18600	58.02900	46.30500
H	12.95100	58.70300	46.30200
H	11.22000	58.33600	46.41700
N	16.43700	52.97400	48.31700
H	16.25000	52.39400	47.49900
C	16.96000	52.36400	49.52500
C	18.47200	52.25500	49.47500
O	19.12500	52.11400	50.50700
N	19.03300	52.32400	48.27100
H	18.43800	52.44400	47.45100
C	20.48000	52.23200	48.09500
C	21.17900	53.49700	48.59100
O	22.40500	53.56200	48.63500
C	20.82100	52.00800	46.62200
C	20.27800	50.71900	46.03000
C	20.68400	50.60000	44.56900
C	20.15800	49.32700	43.93400
N	20.52700	49.23100	42.49000
H	20.17300	48.37500	42.06300
H	21.53400	49.32200	42.35800
H	20.22200	50.05600	41.97400
N	20.39700	54.49900	48.97200
H	19.38400	54.38800	48.92100
C	20.95400	55.75600	49.46200
C	21.52800	55.69400	50.88000
O	22.06800	56.68300	51.38000
C	19.89200	56.85600	49.38900
O	18.72800	56.51300	50.12700
H	18.06900	57.19600	50.08200

N	21.40900	54.53500	51.52600
H	20.93800	53.75800	51.06200
C	21.93200	54.33900	52.88200
C	22.52700	52.92600	52.94300
O	21.81700	51.96400	52.67700
C	20.80400	54.42800	53.93200
C	21.37000	54.18900	55.32800
C	20.13000	55.77600	53.83900
N	23.80500	52.78400	53.30900
H	24.36000	53.60300	53.55800
C	24.40400	51.45400	53.35100
C	23.64200	50.44300	54.22300
O	23.26300	50.72300	55.36500
C	25.87400	51.47000	53.79600
C	26.50600	50.10400	53.56300
C	27.97100	50.07700	53.86100
O	28.50200	51.17400	54.09000
O	28.59200	48.98600	53.86500
N	23.43100	49.26100	53.65100
H	23.77100	49.11500	52.70000
C	22.73900	48.16400	54.31400
C	21.23200	48.29800	54.38700
O	20.58000	47.47900	55.02700
N	20.66500	49.32700	53.76900
H	21.24100	50.00100	53.26500
C	19.21800	49.49000	53.81300
C	18.53900	48.68600	52.70500
O	17.47200	48.10600	52.90400
C	18.83300	50.97000	53.68800
C	17.34400	51.22900	53.76900
S	16.94200	52.96900	53.50800
C	17.04300	53.60100	55.15400
N	19.17400	48.62800	51.53700
H	20.07500	49.09400	51.43200
C	18.60000	47.90700	50.40100
C	18.26200	46.43800	50.68000
O	17.24400	45.93600	50.21200
C	19.52800	48.03800	49.14500
C	20.79600	47.21700	49.32800
C	18.79100	47.61600	47.91300
N	19.09700	45.75100	51.45200
H	19.91900	46.20800	51.84500
C	18.84000	44.34400	51.73800

C	17.55700	44.19600	52.53500
O	16.78400	43.27100	52.29700
C	19.98200	43.70800	52.54500
C	21.36900	43.85000	51.95000
C	21.80700	45.29200	51.88200
O	21.46900	46.05000	52.81200
O	22.49100	45.66200	50.90800
N	17.33400	45.10900	53.47800
H	18.01200	45.85700	53.62700
C	16.12900	45.05100	54.30100
C	14.90900	45.38000	53.44000
O	13.89000	44.70000	53.51600
C	16.23200	46.02600	55.49200
C	17.49100	45.70500	56.29900
C	15.01400	45.88600	56.39100
C	17.68600	46.59300	57.50000
N	15.02800	46.41800	52.61400
H	15.90000	46.94600	52.60900
C	13.94800	46.82600	51.71300
C	13.47400	45.62400	50.89700
O	12.26900	45.37300	50.78100
C	14.43600	47.89500	50.73000
C	14.07800	49.30300	51.10900
C	13.38000	50.10200	50.21900
C	14.49000	49.85200	52.31500
C	13.10300	51.41800	50.51100
C	14.21300	51.18400	52.61800
C	13.51900	51.96500	51.71000
N	14.43200	44.89400	50.32200
H	15.40800	45.15800	50.45600
C	14.11700	43.73000	49.50800
C	13.37700	42.68100	50.31500
O	12.47600	42.03100	49.80800
C	15.38800	43.11200	48.91600
C	16.00400	43.97200	47.81600
O	15.25000	44.68400	47.11300
O	17.24200	43.92000	47.64600
N	13.76300	42.50800	51.57300
H	14.53900	43.05400	51.94600
C	13.07900	41.53800	52.42400
C	11.63400	41.98400	52.68100
O	10.69900	41.18200	52.60700
C	13.82600	41.37800	53.75100

C	15.18000	40.69000	53.60500
S	15.96000	40.31200	55.18900
C	16.59700	41.86700	55.65900
N	11.45700	43.26600	52.97300
H	12.26700	43.88400	53.02100
C	10.12500	43.80900	53.22700
C	9.25400	43.71300	51.97900
O	8.08100	43.33600	52.06000
C	10.23300	45.26200	53.70200
C	10.85500	45.39600	55.10000
C	11.29000	46.82600	55.34100
C	9.84800	44.96400	56.15600
N	9.83300	44.04300	50.82700
H	10.80300	44.35900	50.83300
C	9.11700	43.96600	49.55000
C	8.67200	42.53100	49.23500
O	7.57100	42.30400	48.73000
C	10.01000	44.50600	48.42100
C	10.18200	46.03100	48.44200
C	11.28600	46.47400	47.49400
C	8.85800	46.67600	48.06100
N	9.52300	41.55700	49.54000
H	10.42600	41.78800	49.95400
C	9.18000	40.16100	49.29000
C	8.04900	39.72700	50.21800
O	7.17000	38.95500	49.83100
C	10.40600	39.26900	49.50200
N	8.07000	40.22900	51.44600
H	8.82200	40.86100	51.72000
C	7.03600	39.88900	52.40300
C	5.70900	40.47500	51.94100
O	4.66500	39.84200	52.07000
C	7.34200	40.45100	53.79200
O	8.66300	40.05400	54.18300
H	9.29200	40.38300	53.55200
C	6.32800	39.92000	54.80900
N	5.75400	41.68900	51.40100
H	6.64900	42.17100	51.31500
C	4.53700	42.33800	50.93000
C	3.91900	41.54000	49.77700
O	2.69700	41.36600	49.71400
C	4.84100	43.77000	50.48300
O	3.64800	44.54100	50.49100

H	3.83700	45.43000	50.21400
N	4.77000	41.05700	48.87500
H	5.76600	41.24800	48.98700
C	4.32900	40.26300	47.72900
C	3.70400	38.95300	48.19800
O	2.71000	38.49100	47.63700
C	5.51400	39.95200	46.81200
O	6.12100	41.14700	46.35400
H	6.85700	40.95400	45.78500
N	4.30600	38.34700	49.21800
H	5.14300	38.76500	49.62300
C	3.79400	37.09600	49.77000
C	2.38700	37.32500	50.32000
O	1.47700	36.54000	50.05400
C	4.72800	36.57900	50.87500
C	4.20000	35.37000	51.64700
C	4.05200	34.12600	50.78100
N	3.61800	32.97000	51.56700
H	3.66100	33.04100	52.58400
C	3.17100	31.83200	51.04100
N	3.09800	31.69400	49.72300
H	3.39200	32.46000	49.11700
H	2.75500	30.82200	49.32000
N	2.78800	30.83500	51.82900
H	2.84400	30.94100	52.84200
H	2.44500	29.96300	51.42600
N	2.20600	38.40000	51.08500
H	2.99400	39.01500	51.28700
C	0.88900	38.70600	51.63800
C	-0.10700	38.92000	50.51000
O	-1.24900	38.46600	50.58000
C	0.92700	39.96600	52.51100
C	1.38500	39.71500	53.92000
C	1.30500	38.44900	54.47500
C	1.86700	40.75400	54.69900
C	1.69800	38.22000	55.78900
C	2.26100	40.53300	56.00900
C	2.17700	39.26600	56.55300
N	0.33000	39.62300	49.47400
H	1.28600	39.97900	49.48000
C	-0.52500	39.89700	48.32900
C	-0.85000	38.57300	47.63700
O	-1.99100	38.32300	47.26400

C	0.18700	40.85600	47.36900
C	-0.70300	41.44600	46.28700
C	-0.01500	42.63300	45.62300
N	1.33100	42.30200	45.16200
H	1.42800	41.56800	44.46000
C	2.43900	42.89700	45.59900
N	2.37100	43.85600	46.51600
H	3.22000	44.31200	46.85100
H	1.46500	44.12800	46.89700
N	3.61600	42.54400	45.10400
H	4.46500	43.00000	45.43900
H	3.66800	41.80800	44.40000
N	0.15700	37.71700	47.50400
H	1.07800	37.97500	47.85700
C	-0.02000	36.42000	46.86700
C	-1.02600	35.55500	47.62600
O	-1.80100	34.81400	47.01600
C	1.33100	35.70700	46.76800
C	1.25300	34.24400	46.37600
S	2.87600	33.56300	45.95700
C	3.71400	33.62500	47.53300
N	-1.01800	35.66000	48.95400
H	-0.35300	36.29600	49.39400
C	-1.92900	34.89500	49.80000
C	-3.25600	35.60800	49.98500
O	-4.18400	35.05400	50.57800
C	-1.33700	34.67900	51.18800
C	-0.11200	33.80700	51.25500
S	0.40200	33.72000	52.98600
C	-0.96100	32.79600	53.68700
N	-3.34300	36.84600	49.51300
H	-2.54200	37.27100	49.04600
C	-4.58400	37.59800	49.66200
C	-4.87900	37.78300	51.16100
O	-6.00200	37.54500	51.61900
C	-5.73000	36.82400	48.99900
C	-6.76400	37.73000	48.37200
O	-7.36500	38.57400	49.04000
N	-6.98100	37.55600	47.07400
H	-6.48400	36.85800	46.52100
H	-7.67900	38.16800	46.65100
N	-3.86500	38.19100	51.92200
H	-2.95500	38.35500	51.49200

C	-4.02500	38.41000	53.36100
C	-5.20400	39.33800	53.62200
O	-5.29400	40.41300	53.03100
C	-2.76600	39.04100	53.96100
C	-2.81400	39.22400	55.48400
C	-2.80100	37.85700	56.16000
C	-1.62900	40.05000	55.94800
N	-6.09500	38.92400	54.51700
H	-5.95200	38.02600	54.97900
C	-7.27100	39.71700	54.85700
C	-7.00300	40.61700	56.05900
O	-6.21400	40.26900	56.93800
C	-8.44900	38.78800	55.16400
C	-8.83900	37.87800	54.00900
C	-9.38400	38.65400	52.82600
O	-10.36300	39.39300	52.95700
N	-8.75300	38.49400	51.66300
H	-9.12000	39.01600	50.86700
H	-7.94400	37.88300	51.55500
N	-7.66200	41.77000	56.09700
H	-8.30000	42.01000	55.33900
C	-7.48500	42.69500	57.20700
C	-7.72500	42.07500	58.57500
O	-7.02300	42.39900	59.54100
N	-8.71300	41.18800	58.66500
H	-9.25900	40.96600	57.83300
C	-9.03400	40.52500	59.92300
C	-7.88800	39.60600	60.34400
O	-7.64800	39.41100	61.53300
C	-10.31200	39.68300	59.79400
C	-11.60900	40.44500	59.49400
C	-11.66000	41.00900	58.08500
O	-11.07200	40.39300	57.16800
O	-12.30500	42.06100	57.89200
N	-7.20500	39.02400	59.36200
H	-7.47400	39.20300	58.39500
C	-6.07800	38.13400	59.63600
C	-4.85900	38.96500	60.03000
O	-4.09800	38.58900	60.92000
C	-5.74400	37.29100	58.40100
C	-6.86300	36.35700	57.93800
C	-6.50700	35.62700	56.65400
O	-5.98700	36.28000	55.72500

O	-6.75200	34.40400	56.56700
N	-4.67300	40.09400	59.35500
H	-5.32600	40.34700	58.61300
C	-3.55400	40.97800	59.65500
C	-3.56200	41.40500	61.12200
O	-2.54000	41.30100	61.80600
C	-3.60500	42.21800	58.76300
C	-2.75500	43.36400	59.26000
C	-1.37500	43.30000	59.20500
C	-3.34900	44.51200	59.77500
C	-0.59600	44.35400	59.64800
C	-2.57900	45.57200	60.22000
C	-1.20000	45.49600	60.15700
N	-4.70000	41.89000	61.62200
H	-5.53400	41.96100	61.03900
C	-4.73200	42.31700	63.01800
C	-4.50100	41.15000	63.98000
O	-3.93900	41.34300	65.05600
C	-6.04900	43.06500	63.38300
C	-6.17200	44.32000	62.52400
C	-7.25200	42.15900	63.21100
N	-4.92200	39.94400	63.60900
H	-5.41200	39.82100	62.72300
C	-4.67600	38.79500	64.48300
C	-3.17500	38.53200	64.53800
O	-2.61600	38.29300	65.61100
C	-5.39100	37.54100	63.97400
S	-7.16600	37.53300	64.31800
N	-2.52900	38.58300	63.37400
H	-3.05100	38.78900	62.52200
C	-1.08900	38.35100	63.29000
C	-0.29400	39.39400	64.05800
O	0.66800	39.05800	64.74200
C	-0.62900	38.34800	61.83100
C	-1.04700	37.13200	61.00500
C	-0.52100	37.31100	59.58000
C	-0.49100	35.84500	61.64500
N	-0.69200	40.65900	63.95500
H	-1.50500	40.89200	63.38500
C	0.03400	41.71600	64.65800
C	-0.05600	41.53900	66.17300
O	0.90300	41.82100	66.89000
C	-0.49600	43.10300	64.26900

C	0.57700	44.17300	64.32200
C	0.00700	45.56500	64.51600
C	-1.13100	45.84600	63.58200
N	-1.69500	47.20200	63.85200
H	-2.46900	47.39300	63.21600
H	-0.98000	47.92800	63.81100
H	-1.96600	47.31500	64.82900
N	-1.20600	41.07800	66.66400
H	-1.98000	40.88700	66.02800
C	-1.38100	40.84000	68.10000
C	-0.56500	39.61800	68.54100
O	-0.05000	39.56700	69.66000
C	-2.85700	40.62400	68.42900
O	-3.56100	41.85600	68.38900
H	-4.47900	41.72200	68.59400
N	-0.46500	38.62300	67.66700
H	-0.94100	38.68500	66.76700
C	0.32400	37.44300	67.99200
C	1.78300	37.85600	68.17900
O	2.44400	37.39000	69.10200
C	0.22200	36.37300	66.88000
C	-1.15500	35.69000	66.94800
C	1.34300	35.33700	67.03800
C	-1.41500	34.71200	65.79300
N	2.28800	38.71300	67.29400
H	1.70100	39.04200	66.52800
C	3.67600	39.19700	67.39600
C	3.90300	39.86300	68.76200
O	4.88200	39.58000	69.46800
C	3.98900	40.22100	66.26000
C	4.00300	39.49900	64.90400
C	5.34100	40.92600	66.51900
C	4.19800	40.42700	63.69400
N	2.98900	40.75000	69.13000
H	2.21100	40.94600	68.50000
C	3.05800	41.45700	70.40700
C	3.16700	40.50600	71.60000
O	4.01000	40.67900	72.47600
C	1.80100	42.32900	70.58100
C	1.68000	43.00000	71.95400
C	2.84700	43.97000	72.12300
C	0.34400	43.74300	72.06900
N	2.30100	39.50300	71.63800

H	1.63400	39.38700	70.87500
C	2.28700	38.56100	72.75400
C	3.36500	37.47300	72.70100
O	3.82600	37.00300	73.74000
C	0.90000	37.90200	72.85100
C	-0.27600	38.84800	73.18400
C	-1.59800	38.11400	73.02300
C	-0.14100	39.36100	74.59800
N	3.78800	37.09900	71.50200
H	3.43300	37.57200	70.67100
C	4.75800	36.01600	71.35800
C	6.24700	36.33500	71.28300
O	7.06000	35.58200	71.80700
C	4.38300	35.16900	70.13500
C	5.39900	34.06800	69.84400
O	6.19600	34.16500	68.91500
N	5.36700	33.02200	70.64100
H	4.70500	32.94100	71.41300
H	6.04600	32.28600	70.44700
N	6.61100	37.43600	70.63700
H	5.89700	38.06200	70.26500
C	8.02000	37.75900	70.45400
C	8.93300	37.74100	71.67600
O	10.04000	37.20900	71.60400
C	8.14900	39.09100	69.71600
O	7.62400	38.94300	68.40300
H	7.70400	39.77100	67.94400
N	8.48100	38.30600	72.78900
H	7.55100	38.72400	72.81300
C	9.32500	38.32300	73.97600
C	8.89300	37.37100	75.07800
O	9.45100	37.40200	76.16900
N	7.92400	36.50600	74.79800
H	7.52200	36.48400	73.86100
C	7.42900	35.58800	75.81700
C	8.46800	34.55200	76.23800
O	8.43100	34.04900	77.36300
C	6.14800	34.85900	75.33600
C	6.50200	33.79600	74.31000
C	5.41100	34.25600	76.52800
N	9.40600	34.25600	75.34300
H	9.40100	34.73200	74.44100
C	10.44000	33.27000	75.61900

C	11.66700	33.87300	76.29500
O	12.64300	33.17000	76.54800
C	10.87100	32.59100	74.31500
C	9.72300	32.05100	73.48900
C	8.97500	30.96300	73.92500
C	9.38500	32.63600	72.27100
C	7.92100	30.47100	73.17400
C	8.33500	32.15400	71.51100
C	7.60500	31.07000	71.96700
O	6.55700	30.59000	71.21300
H	6.34000	31.00100	70.38500
N	11.62300	35.16800	76.58800
H	10.78800	35.71000	76.36500
C	12.75900	35.82000	77.22500
C	12.41800	36.57000	78.50700
O	13.09500	37.53800	78.85600
C	13.45500	36.80000	76.25400
O	12.49400	37.72400	75.72800
H	12.92200	38.32700	75.13100
C	14.09600	36.03900	75.10500
N	11.37500	36.13100	79.20700
H	10.84000	35.33300	78.86500
C	10.98600	36.77600	80.45900
C	11.96500	36.41300	81.56700
O	12.23000	35.23600	81.81800
C	9.57000	36.36900	80.87900
C	8.48900	37.21200	80.26400
C	8.59500	38.59400	80.24900
C	7.35600	36.62800	79.72500
C	7.59000	39.37700	79.70800
C	6.35000	37.40600	79.18600
C	6.46800	38.78200	79.17700
N	12.49400	37.44100	82.22200
H	12.21400	38.38400	81.95300
C	13.45700	37.28600	83.30800
C	13.09800	36.20100	84.32600
O	13.39800	35.01900	84.13300
C	13.62800	38.62800	84.03500
C	14.47100	38.66100	85.31600
C	15.89500	38.23000	85.01000
C	14.44600	40.06200	85.91000
N	12.45100	36.62300	85.40800
H	12.21600	37.61300	85.47900

C	12.06100	35.73600	86.49800
C	11.24900	34.50500	86.10100
O	10.78000	34.37400	84.96700
C	11.28600	36.53300	87.55500
O	12.07600	37.58400	88.09700
H	11.59600	38.07800	88.75200
N	11.11300	33.59700	87.06200
H	11.56800	33.77100	87.95800
C	10.35100	32.36900	86.90500
C	9.55900	32.21600	88.19700
O	9.32600	31.11000	88.68300
C	11.28000	31.17100	86.70200
O	12.21300	31.06200	87.76300
H	12.79000	30.31800	87.63700
N	9.16800	33.35800	88.75300
H	9.42500	34.23600	88.30200
C	8.38700	33.40600	89.98100
C	6.98600	32.89300	89.68400
O	6.64700	32.63500	88.52900
C	8.27500	34.84800	90.50300
O	7.85000	35.70800	89.43700
H	7.01300	35.40600	89.10500
C	9.61000	35.32900	91.03300
N	6.17100	32.75200	90.72400
H	6.50600	32.98200	91.65900
C	4.80600	32.27400	90.54900
C	4.06600	33.27800	89.66300
O	3.26200	32.90800	88.81600
C	4.10300	32.17900	91.90300
C	3.00500	31.12800	92.08100
C	2.13600	31.53800	93.26100
C	2.16300	30.99900	90.82500
N	4.35300	34.55400	89.87900
H	5.03500	34.78900	90.60000
C	3.73000	35.63400	89.12400
C	4.09000	35.50900	87.65100
O	3.24100	35.65800	86.77200
C	4.22900	36.96900	89.65900
C	3.50900	38.18700	89.14100
C	4.12200	39.41000	89.79300
C	3.27600	40.64300	89.63200
N	3.90300	41.75200	90.41400
H	3.32900	42.58800	90.30500

H	4.87800	41.90900	90.15800
H	4.05400	41.50500	91.39200
N	5.36400	35.23400	87.40100
H	6.00500	35.12600	88.18700
C	5.88100	35.08000	86.05100
C	5.19700	33.88300	85.38400
O	4.75000	33.96800	84.24400
C	7.39900	34.87100	86.10800
O	8.02000	35.21500	84.87900
H	8.96000	35.08600	84.91400
N	5.11700	32.76500	86.09800
H	5.51200	32.73700	87.03800
C	4.47100	31.57800	85.55100
C	3.01400	31.89000	85.23400
O	2.47600	31.42100	84.23600
C	4.55200	30.41800	86.54600
C	5.96400	29.92000	86.86400
C	5.89900	28.81900	87.90800
C	6.62200	29.40700	85.59400
N	2.37900	32.68800	86.08700
H	2.87800	33.05000	86.89900
C	0.98300	33.05600	85.88400
C	0.82800	33.93900	84.64300
O	-0.11900	33.78400	83.87000
C	0.44200	33.77900	87.12500
C	0.46000	32.90900	88.38900
C	-0.06700	33.62000	89.62800
O	0.25300	34.81400	89.82100
O	-0.79100	32.97200	90.41700
N	1.76300	34.86000	84.45200
H	2.52400	34.94800	85.12500
C	1.72300	35.75000	83.29600
C	1.89800	34.95300	81.99800
O	1.18000	35.17000	81.03000
C	2.83300	36.79600	83.41200
C	2.70300	37.70600	84.62400
C	2.03000	39.01500	84.29000
O	2.72000	39.93600	83.79500
O	0.80300	39.12000	84.50500
N	2.86300	34.03900	81.98300
H	3.43800	33.90600	82.81500
C	3.11500	33.22400	80.80200
C	1.90800	32.36800	80.45300

O	1.58300	32.19700	79.27900
C	4.35600	32.35200	81.01900
C	5.64400	33.17500	81.02300
C	6.88200	32.35100	81.35700
C	8.11500	33.24800	81.39400
N	9.34300	32.52600	81.84000
H	10.16800	33.12600	81.86500
H	9.51000	31.70000	81.26600
H	9.19300	32.07400	82.74200
N	1.23900	31.83300	81.47200
H	1.56600	31.98800	82.42600
C	0.04700	31.02900	81.24300
C	-1.02000	31.88800	80.56200
O	-1.65800	31.45400	79.60300
C	-0.51900	30.50800	82.56300
C	-1.82300	29.75600	82.37600
O	-1.78000	28.58900	81.92800
O	-2.89300	30.34000	82.66000
N	-1.21400	33.10300	81.07000
H	-0.65800	33.40000	81.87200
C	-2.20100	34.02300	80.51100
C	-1.87300	34.34100	79.05100
O	-2.73700	34.25900	78.18400
C	-2.24100	35.32300	81.32900
C	-3.17100	36.36100	80.77900
N	-4.53600	36.18100	80.71300
H	-5.03700	35.34900	81.02500
C	-2.92900	37.58900	80.26200
C	-5.09500	37.25400	80.18200
N	-4.14100	38.12300	79.89800
H	-4.28200	39.04100	79.47700
N	-0.62300	34.70100	78.78700
H	0.05300	34.75000	79.55000
C	-0.19100	35.03000	77.42700
C	-0.45500	33.88600	76.45300
O	-0.95900	34.10000	75.35100
C	1.30900	35.39300	77.41100
C	1.50500	36.73700	78.11600
C	1.83400	35.42700	75.97200
C	2.95300	37.10500	78.39500
N	-0.12300	32.66700	76.86200
H	0.29400	32.54100	77.78400
C	-0.34700	31.50800	76.01000

C	-1.83200	31.25400	75.82300
O	-2.25900	30.78000	74.77100
C	0.32000	30.26300	76.59800
C	1.80900	30.26200	76.46200
N	2.44800	30.61500	75.29200
H	1.98500	30.91900	74.43600
C	2.78700	29.92700	77.33800
C	3.75400	30.49800	75.45300
N	3.98500	30.08200	76.68400
H	4.90600	29.90400	77.08500
N	-2.61900	31.55700	76.84900
H	-2.20900	31.92100	77.70900
C	-4.06400	31.37400	76.75800
C	-4.62400	32.35400	75.72500
O	-5.44100	31.98400	74.88500
C	-4.72400	31.62200	78.11700
C	-4.87900	30.39500	79.00200
C	-5.44400	30.82200	80.35800
N	-6.19200	29.76700	81.03700
H	-7.19000	29.91500	81.18400
C	-5.66600	28.62800	81.47700
N	-4.37400	28.38200	81.31200
H	-3.97000	27.50800	81.65000
H	-3.78300	29.06700	80.84100
N	-6.43500	27.73600	82.09000
H	-6.03100	26.86200	82.42800
H	-7.42900	27.92500	82.21700
N	-4.18900	33.60700	75.78900
H	-3.52200	33.87700	76.51200
C	-4.66200	34.59900	74.83000
C	-4.20200	34.20000	73.42600
O	-4.98500	34.26200	72.47800
C	-4.14500	36.01800	75.17200
C	-4.61600	37.01700	74.12900
C	-4.66800	36.43900	76.53500
N	-2.94700	33.76700	73.29300
H	-2.33300	33.72600	74.10700
C	-2.45000	33.35100	71.98200
C	-3.32700	32.22900	71.40500
O	-3.62600	32.22900	70.21300
C	-0.98200	32.89700	72.07200
C	0.06900	34.02000	72.17100
C	1.41800	33.44400	72.57600

C	0.18100	34.73400	70.83200
N	-3.74900	31.28000	72.24200
H	-3.47600	31.31100	73.22400
C	-4.60300	30.19300	71.75600
C	-5.91400	30.77600	71.24100
O	-6.46800	30.30500	70.24700
C	-4.92000	29.17600	72.86700
C	-3.74700	28.26200	73.19300
O	-2.80400	28.16100	72.37700
O	-3.77500	27.62700	74.26900
N	-6.40500	31.80100	71.93500
H	-5.89000	32.13500	72.75000
C	-7.65300	32.46400	71.57100
C	-7.54100	33.09300	70.18600
O	-8.45400	32.97900	69.37400
C	-7.99300	33.55000	72.59400
C	-9.48100	33.83500	72.73800
C	-10.06300	33.04900	73.90600
C	-11.55000	33.31800	74.09400
N	-12.40100	32.60700	73.09900
H	-13.39700	32.78700	73.22500
H	-12.20900	31.60500	73.10500
H	-12.10900	32.82700	72.14700
N	-6.42000	33.76100	69.91800
H	-5.69400	33.83400	70.63100
C	-6.21900	34.38900	68.61600
C	-6.10800	33.30600	67.54400
O	-6.53000	33.50300	66.39800
C	-4.95100	35.27600	68.60200
C	-5.05100	36.33700	69.70000
C	-4.80700	35.96100	67.23900
C	-3.85700	37.27800	69.77200
N	-5.52600	32.16700	67.90500
H	-5.15300	32.06300	68.84900
C	-5.41900	31.06800	66.95700
C	-6.84600	30.62800	66.62900
O	-7.18100	30.41800	65.46100
C	-4.66200	29.85300	67.53900
O	-3.29200	30.19400	67.76700
H	-3.24900	30.92800	68.36900
C	-4.73100	28.68200	66.57900
N	-7.68400	30.50400	67.66100
H	-7.34500	30.69400	68.60400

C	-9.08400	30.10000	67.46700
C	-9.78700	31.08500	66.53600
O	-10.57900	30.69400	65.67300
C	-9.85400	30.06600	68.80000
C	-9.37300	28.97200	69.74100
O	-8.82800	27.95000	69.27200
O	-9.56500	29.13200	70.96500
N	-9.48400	32.36600	66.72100
H	-8.81400	32.61100	67.45000
C	-10.07100	33.43100	65.92300
C	-9.63900	33.33600	64.46300
O	-10.44900	33.52600	63.55300
C	-9.66900	34.80600	66.48100
O	-10.01000	34.87200	67.87200
H	-9.56600	34.17700	68.34300
C	-10.37600	35.91300	65.73100
N	-8.35800	33.05300	64.24000
H	-7.72800	32.92900	65.03200
C	-7.83800	32.91700	62.88400
C	-8.52800	31.76900	62.15300
O	-8.93900	31.92000	61.00300
C	-6.32600	32.68000	62.90900
C	-5.47600	33.95200	62.92800
C	-4.01300	33.58800	63.12900
C	-5.66900	34.71000	61.61200
N	-8.65400	30.62700	62.82000
H	-8.28500	30.56000	63.76900
C	-9.30900	29.46400	62.22500
C	-10.78100	29.76900	61.94100
O	-11.33100	29.34500	60.92300
C	-9.22700	28.23100	63.15400
C	-7.81100	27.64000	63.12800
C	-10.25200	27.18700	62.72700
C	-7.37100	27.12400	61.77500
N	-11.41000	30.51100	62.84400
H	-10.90100	30.83400	63.66700
C	-12.80900	30.87400	62.68600
C	-13.00900	31.74700	61.45000
O	-13.96300	31.55800	60.69500
C	-13.30700	31.60400	63.93200
C	-14.69600	32.14000	63.79800
N	-14.95800	33.46300	63.51600
H	-14.25400	34.19000	63.39100

C	-15.90100	31.52600	63.88300
C	-16.26400	33.64200	63.43300
N	-16.85900	32.48200	63.65100
H	-17.86600	32.32300	63.64700
N	-12.10500	32.69600	61.24000
H	-11.33700	32.81300	61.90100
C	-12.19400	33.57500	60.07700
C	-12.05300	32.76900	58.78800
O	-12.74900	33.01900	57.80100
C	-11.09300	34.63500	60.12700
C	-11.16900	35.67300	61.24400
C	-9.90000	36.51700	61.25100
C	-12.40200	36.54900	61.03300
N	-11.14300	31.80200	58.80200
H	-10.60100	31.64000	59.65100
C	-10.90100	30.96800	57.63500
C	-12.06500	30.02400	57.36600
O	-12.38200	29.73200	56.21200
C	-9.61500	30.16800	57.82700
C	-8.37300	31.04000	57.83900
S	-6.89600	30.13200	58.28800
C	-5.77600	31.49600	58.64400
N	-12.68800	29.54000	58.43500
H	-12.36500	29.80500	59.36500
C	-13.82400	28.63700	58.30300
C	-14.98600	29.39300	57.65700
O	-15.63400	28.88800	56.74000
C	-14.22900	28.10500	59.67700
N	-15.23900	30.60700	58.13600
H	-14.67200	30.96900	58.90200
C	-16.30800	31.43100	57.59100
C	-16.01000	31.84600	56.15200
O	-16.90700	32.26600	55.42400
C	-16.52000	32.67800	58.45600
C	-17.33800	32.41800	59.71200
C	-17.71800	33.71400	60.41100
C	-18.82700	33.48600	61.43100
N	-19.14300	34.72700	62.20100
H	-19.88500	34.57400	62.88400
H	-19.36700	35.50200	61.57700
H	-18.30800	35.11200	62.64200
N	-14.75100	31.73600	55.74300
H	-14.03800	31.39800	56.38900

C	-14.37800	32.09300	54.37900
C	-14.68600	30.91600	53.45500
O	-14.57800	31.02200	52.23300
C	-12.89700	32.45400	54.31000
N	-15.06400	29.78900	54.05100
H	-15.11700	29.74900	55.06900
C	-15.40200	28.61400	53.26600
C	-14.28600	27.61400	53.03200
O	-14.47300	26.63600	52.30900
N	-13.12200	27.83900	53.63500
H	-13.01000	28.66100	54.22800
C	-12.00400	26.91800	53.45500
C	-12.27400	25.60700	54.19600
O	-12.92000	25.60200	55.24400
C	-10.70700	27.55100	53.97900
C	-10.29100	28.90100	53.39100
C	-8.93100	29.31500	53.96800
C	-10.21400	28.80600	51.87400
N	-11.79300	24.49600	53.64700
H	-11.29200	24.55000	52.76000
C	-11.97100	23.20000	54.29600
C	-11.05400	23.17200	55.51500
O	-10.19000	24.03700	55.66100
C	-11.56800	22.03500	53.37200
O	-10.18400	22.16100	53.01500
H	-9.65500	22.15900	53.80400
C	-12.41400	22.03800	52.11000
N	-11.23800	22.18400	56.38600
H	-11.97400	21.49700	56.22200
C	-10.39800	22.07300	57.57300
C	-8.92900	22.00300	57.17900
O	-8.08500	22.66600	57.78300
C	-10.75800	20.82700	58.38500
C	-11.98300	20.88000	59.29500
C	-12.10300	19.55200	60.03000
C	-11.85200	22.02900	60.29100
N	-8.62500	21.19600	56.16600
H	-9.36600	20.67200	55.70100
C	-7.24700	21.05000	55.71100
C	-6.67800	22.36400	55.18100
O	-5.50600	22.66800	55.39300
C	-7.14500	19.97700	54.62400
C	-5.76300	19.89100	53.99700

C	-5.66300	18.81400	52.93700
O	-6.49600	18.73600	52.03400
N	-4.63500	17.98100	53.03500
H	-4.56800	17.25600	52.32100
H	-3.94500	18.04600	53.78300
N	-7.50800	23.13400	54.48600
H	-8.46800	22.82400	54.33400
C	-7.07500	24.41400	53.93500
C	-6.88600	25.41900	55.06600
O	-6.02600	26.29400	54.99200
C	-8.10700	24.93200	52.93200
C	-8.32900	23.99500	51.74900
C	-9.43700	24.46500	50.82900
O	-10.43600	25.02200	51.28000
N	-9.27700	24.22100	49.53200
H	-8.44800	23.75900	49.15800
H	-10.02300	24.53700	48.91300
N	-7.70700	25.28500	56.10600
H	-8.41500	24.55100	56.08200
C	-7.63000	26.14800	57.27500
C	-6.29600	25.93600	57.98400
O	-5.58700	26.89500	58.29200
C	-8.76300	25.82600	58.25100
C	-10.14900	26.28500	57.81300
C	-11.23400	25.76000	58.73700
O	-11.11800	25.84800	59.96200
N	-12.29500	25.21000	58.15400
H	-13.02400	24.85700	58.77500
H	-12.39100	25.13700	57.14100
N	-5.95800	24.67600	58.24500
H	-6.58400	23.92000	57.96800
C	-4.70300	24.35900	58.92300
C	-3.49900	24.77300	58.08400
O	-2.49700	25.24800	58.62400
C	-4.60900	22.86100	59.23200
C	-5.76200	22.33200	60.02900
N	-6.28900	23.00200	61.11300
H	-5.96300	23.90200	61.46500
C	-6.47800	21.18900	59.90900
C	-7.28100	22.29600	61.62500
N	-7.41700	21.19100	60.91300
H	-8.10700	20.45900	61.08100
N	-3.59500	24.58500	56.76900

H	-4.44900	24.18000	56.38500
C	-2.50600	24.94500	55.86300
C	-2.26500	26.45300	55.81100
O	-1.12000	26.90500	55.80200
C	-2.79300	24.42100	54.45000
C	-2.60200	22.91400	54.30500
C	-2.96500	22.40300	52.92400
O	-2.75000	21.23100	52.60500
N	-3.52100	23.27600	52.09900
H	-3.69900	24.24500	52.36300
H	-3.76500	22.93200	51.17000
N	-3.34200	27.23300	55.78200
H	-4.27100	26.81100	55.79600
C	-3.21100	28.68200	55.73000
C	-2.68800	29.21900	57.06200
O	-1.86300	30.13100	57.08600
C	-4.55100	29.33700	55.40200
C	-4.44900	30.84600	55.17300
C	-5.79700	31.46100	54.81200
N	-5.70800	32.90000	54.55800
H	-6.06600	33.53000	55.27600
C	-5.19400	33.44700	53.45900
N	-4.71100	32.68300	52.48700
H	-4.31700	33.10200	51.64500
H	-4.72300	31.66800	52.59200
N	-5.17900	34.76700	53.32300
H	-4.78500	35.18600	52.48100
H	-5.55000	35.35400	54.07000
N	-3.17700	28.65600	58.16300
H	-3.88000	27.92100	58.08200
C	-2.72200	29.07400	59.48800
C	-1.20200	28.92500	59.52000
O	-0.47900	29.84600	59.90300
C	-3.35300	28.19800	60.57500
C	-2.87300	28.43600	62.01700
C	-3.28000	29.82400	62.47600
C	-3.48200	27.40200	62.93900
N	-0.72100	27.75700	59.09900
H	-1.36700	27.03300	58.78500
C	0.71200	27.49600	59.08000
C	1.44700	28.47500	58.17900
O	2.47400	29.03600	58.57800
C	0.98800	26.06400	58.63500

N	0.93300	28.68200	56.96800
H	0.09100	28.18100	56.68600
C	1.56200	29.61900	56.03800
C	1.67800	31.01300	56.67600
O	2.70200	31.67600	56.55900
C	0.75200	29.73000	54.73100
C	0.59600	28.43100	53.93700
C	-0.40200	28.56200	52.78400
O	-0.73600	27.57500	52.11800
N	-0.88300	29.78200	52.54700
H	-0.60800	30.59600	53.09600
H	-1.54800	29.86900	51.77900
N	0.62700	31.46000	57.35100
H	-0.20700	30.87900	57.44000
C	0.66300	32.78400	57.96700
C	1.66900	32.86000	59.12300
O	2.41700	33.82800	59.24300
C	-0.72700	33.17500	58.47100
C	-1.83100	33.42900	57.43000
C	-3.14300	33.69800	58.15100
C	-1.47100	34.60800	56.54600
N	1.68900	31.84100	59.97100
H	1.05400	31.05500	59.83600
C	2.61800	31.84000	61.09900
C	4.08800	31.70900	60.69100
O	4.98000	32.20100	61.39100
C	2.24100	30.73200	62.08500
C	0.84000	30.91100	62.67600
C	0.57400	29.85500	63.74800
C	0.72100	32.29500	63.26700
N	4.35300	31.05400	59.56700
H	3.59300	30.65700	59.01500
C	5.73600	30.90400	59.12300
C	6.29100	32.25400	58.68100
O	7.49100	32.51100	58.77300
C	5.84200	29.89000	57.97800
C	5.57900	28.43400	58.39100
C	5.71300	27.51800	57.18100
C	6.55700	28.02900	59.48400
N	5.41500	33.11900	58.19000
H	4.43300	32.85700	58.10300
C	5.85300	34.44100	57.77500
C	6.33800	35.24000	58.98700

O	7.20000	36.10100	58.85400
C	4.71800	35.19600	57.05200
C	4.36100	34.45300	55.76200
C	5.15800	36.62200	56.71700
C	3.22100	35.07900	54.98500
N	5.81300	34.93800	60.17400
H	5.10600	34.20600	60.24400
C	6.24500	35.65200	61.37900
C	7.71100	35.35800	61.65600
O	8.41200	36.15700	62.27800
C	5.40100	35.26200	62.59900
C	3.92100	35.61700	62.49500
C	3.24700	35.39500	63.84100
C	3.78200	37.06300	62.04600
N	8.17500	34.20000	61.20300
H	7.54500	33.54900	60.73500
C	9.57800	33.85600	61.37100
C	10.39000	34.83500	60.51700
O	11.43800	35.32700	60.94200
C	9.82900	32.41900	60.91000
O	11.21500	32.15000	60.88200
H	11.37100	31.25800	60.59600
N	9.90200	35.12400	59.31500
H	9.03700	34.68400	59.00000
C	10.59500	36.06600	58.44200
C	10.54300	37.49200	58.99400
O	11.49500	38.26300	58.85700
C	9.98800	36.05200	57.04200
C	10.65400	37.00500	56.09600
N	11.99500	36.92200	55.77400
H	12.64200	36.21500	56.12200
C	10.17200	38.07500	55.42300
C	12.30800	37.90300	54.94400
N	11.22000	38.61800	54.71500
H	11.16600	39.43900	54.11200
N	9.41900	37.85000	59.60400
H	8.64500	37.19000	59.67500
C	9.29200	39.18400	60.17100
C	10.26400	39.32900	61.33900
O	10.86700	40.39400	61.53600
C	7.84000	39.44700	60.58500
C	6.99600	39.55200	59.30700
C	7.73900	40.72000	61.42100

C	5.54000	39.72700	59.53000
N	10.44200	38.25100	62.10100
H	9.91400	37.40000	61.90800
C	11.39100	38.28200	63.21200
C	12.78500	38.52200	62.63500
O	13.57000	39.32200	63.15700
C	11.37400	36.95000	63.96900
C	12.37900	36.88500	65.11500
C	12.06100	37.93400	66.16300
N	12.00500	37.36500	67.50000
H	12.71000	37.66300	68.17500
C	11.09600	36.48300	67.90000
N	10.15800	36.07300	67.06100
H	9.46000	35.39600	67.36800
H	10.12900	36.44300	66.11100
N	11.13300	36.00300	69.13200
H	10.43500	35.32600	69.43900
H	11.85600	36.31900	69.77900
N	13.08700	37.82300	61.54800
H	12.39500	37.18200	61.16000
C	14.38800	37.95100	60.89400
C	14.64200	39.39500	60.45200
O	15.70800	39.96400	60.70300
C	14.45300	37.02600	59.67300
C	15.78800	37.01000	58.99600
N	16.92500	36.52800	59.60500
H	16.96800	36.13500	60.54500
C	16.17000	37.43000	57.76600
C	17.95200	36.65400	58.78200
N	17.51900	37.19900	57.65800
H	18.09400	37.41300	56.84300
N	13.65800	39.99500	59.79300
H	12.78900	39.49300	59.61100
C	13.81400	41.36700	59.32900
C	14.02600	42.34400	60.47900
O	14.81200	43.28000	60.36400
C	12.59400	41.78300	58.50100
C	12.45400	40.97800	57.22000
S	11.17400	41.64600	56.11000
C	9.72000	41.25500	57.00300
N	13.31500	42.12700	61.58300
H	12.66500	41.34100	61.61200
C	13.44400	42.98400	62.74700

C	14.87000	42.91400	63.28900
O	15.46500	43.93800	63.62600
C	12.42900	42.57000	63.82200
O	12.70000	43.20900	65.05800
H	12.07200	42.95300	65.72300
N	15.42800	41.70800	63.36900
H	14.89800	40.88100	63.09500
C	16.79900	41.57100	63.84900
C	17.78000	42.29400	62.92600
O	18.68000	42.99200	63.39800
C	17.17100	40.09100	63.99400
C	16.47700	39.44300	65.17800
O	16.30100	40.07800	66.21600
N	16.09200	38.17800	65.03500
H	16.23800	37.65100	64.17400
H	15.62600	37.74200	65.83100
N	17.61400	42.12800	61.61500
H	16.87000	41.51900	61.27300
C	18.48600	42.80900	60.66300
C	18.24700	44.31900	60.78900
O	19.17400	45.12100	60.66100
C	18.19600	42.36000	59.22500
C	18.31400	40.85500	58.97200
C	19.54100	40.24600	59.64300
C	20.83400	40.85500	59.13400
N	22.02100	40.20400	59.77500
H	22.89000	40.61300	59.43300
H	22.00700	39.19200	59.65200
H	21.96400	40.23700	60.79300
N	16.99800	44.70300	61.04700
H	16.26000	44.00500	61.13400
C	16.68300	46.11300	61.20500
C	17.37600	46.71000	62.41600
O	17.87800	47.83800	62.36600
N	17.39000	45.95500	63.51200
H	16.93600	45.04200	63.48800
C	18.03500	46.39100	64.75000
C	19.53000	46.54700	64.51500
O	20.13800	47.52300	64.95100
C	17.81500	45.36100	65.85500
C	16.37200	45.05500	66.12900
S	15.55800	46.33400	67.07400
C	15.20600	45.40600	68.54300

N	20.12500	45.56800	63.84100
H	19.57300	44.76900	63.52800
C	21.55100	45.61400	63.54000
C	21.85000	46.88700	62.74900
O	22.83300	47.57900	63.00900
C	21.96200	44.39400	62.71000
C	22.11100	43.09400	63.49500
C	22.33500	41.89600	62.58600
O	23.14600	42.01100	61.64000
O	21.70700	40.83600	62.82000
N	20.99100	47.18300	61.78000
H	20.19600	46.56400	61.62300
C	21.14200	48.36000	60.93100
C	20.98100	49.64600	61.73700
O	21.76900	50.58500	61.60700
C	20.10100	48.31800	59.80700
C	20.24500	49.41800	58.80200
N	19.44100	50.53800	58.80200
H	18.69600	50.72900	59.47100
C	21.09500	49.56500	57.75900
C	19.78800	51.32500	57.79800
N	20.79000	50.75800	57.15000
H	21.26000	51.14300	56.33100
N	19.95000	49.68400	62.57000
H	19.32900	48.87800	62.63500
C	19.69000	50.85300	63.39100
C	20.90100	51.11800	64.27700
O	21.34200	52.26000	64.41100
C	18.44800	50.62200	64.25000
C	17.76300	51.90200	64.73000
C	17.46500	52.79300	63.53500
C	16.48600	51.55400	65.47000
N	21.44200	50.06000	64.87400
H	21.03300	49.13800	64.72600
C	22.61100	50.19500	65.73700
C	23.86200	50.63300	64.98300
O	24.80000	51.14900	65.58300
C	22.89000	48.88700	66.48100
C	22.02600	48.70700	67.70700
C	20.68500	48.35500	67.59500
C	22.54300	48.92700	68.97900
C	19.88300	48.22900	68.71500
C	21.75000	48.80600	70.10500

C	20.42200	48.45700	69.96800
O	19.63300	48.34000	71.09000
H	20.00300	48.49700	71.95100
N	23.88300	50.42400	63.67200
H	23.08800	49.96900	63.22200
C	25.02800	50.83600	62.86600
C	25.06800	52.35900	62.81200
O	26.10400	52.95500	62.52200
C	24.91400	50.28200	61.44300
O	25.02600	48.87100	61.43500
H	24.95500	48.52700	60.55200
N	23.92800	52.98000	63.09800
H	23.10900	52.42300	63.34100
C	23.81300	54.43100	63.07500
C	23.30800	54.95500	64.41700
O	22.34300	55.71500	64.46600
C	22.84400	54.85100	61.97200
C	22.90800	53.96500	60.74300
S	21.84200	54.54000	59.42100
C	23.05200	55.29100	58.33000
N	23.95200	54.54900	65.50500
H	24.74700	53.91600	65.41400
C	23.53600	54.99800	66.83100
C	23.66200	56.50700	66.95700
O	24.49500	57.12300	66.29400
C	24.38100	54.33000	67.91300
C	24.31000	52.81600	67.91100
C	24.91600	52.23900	69.17500
C	25.13400	50.74600	69.03800
N	25.42300	50.11500	70.35200
H	25.57000	49.11000	70.26000
H	24.69500	50.32500	71.03500
H	26.21100	50.56600	70.81700
N	18.40500	58.09300	75.94800
H	18.61700	59.00500	76.35200
H	17.95700	58.17700	75.03600
H	19.25000	57.60100	75.65800
C	17.60600	57.29800	76.87400
C	17.28900	55.93100	76.26900
O	16.83700	55.83400	75.12700
C	16.27900	58.02200	77.22500
C	15.49400	58.32200	75.95400
C	15.45100	57.16800	78.17300

N	17.53000	54.85200	77.03100
C	17.26300	53.48800	76.55700
C	15.79200	53.29300	76.19100
O	14.89900	53.77500	76.88800
C	17.69500	52.62200	77.73900
C	17.42700	53.50900	78.92100
C	17.94800	54.84500	78.44400
N	15.55100	52.58800	75.09000
H	16.33800	52.21300	74.56000
C	14.19400	52.33500	74.61900
C	13.26300	51.83400	75.71600
O	12.10700	52.25400	75.78800
C	14.21300	51.32700	73.47000
C	12.83800	51.02000	72.87600
C	12.18400	52.30700	72.40900
C	12.98600	50.04100	71.72500
N	13.76500	50.93500	76.56200
H	14.72800	50.62200	76.44100
C	12.97000	50.38700	77.65800
C	12.38800	51.49900	78.51900
O	11.19100	51.51400	78.79700
C	13.82800	49.45700	78.53000
C	13.08000	48.77300	79.66200
C	12.81600	49.43400	80.85800
C	12.65400	47.45400	79.53700
C	12.15000	48.79800	81.89900
C	11.98900	46.81200	80.56900
C	11.74000	47.48500	81.74700
O	11.08100	46.83200	82.76900
H	10.80000	45.93100	82.66500
N	13.23700	52.43100	78.94000
H	14.22000	52.37500	78.67400
C	12.77900	53.53100	79.77700
C	11.79800	54.43200	79.05300
O	10.90800	55.00300	79.67300
C	13.96900	54.34400	80.28600
C	14.68700	53.65700	81.43000
O	14.06700	53.49400	82.50400
O	15.86200	53.27500	81.25400
N	11.95400	54.54900	77.73800
H	12.71700	54.05100	77.28000
C	11.05600	55.37600	76.93400
C	9.67500	54.70100	76.87800

O	8.63900	55.35000	77.05800
C	11.63200	55.53900	75.52700
C	11.30600	56.81500	74.75200
C	12.02000	56.79000	73.40400
C	9.81400	56.93500	74.55500
N	9.66000	53.39400	76.63700
H	10.53900	52.90000	76.48500
C	8.39800	52.65600	76.58700
C	7.76300	52.65200	77.97500
O	6.55700	52.85000	78.12200
C	8.64300	51.21500	76.12300
C	9.17300	51.09600	74.69300
C	9.53100	49.64200	74.38000
C	8.13100	51.62400	73.72500
N	8.58400	52.41800	78.99500
H	9.57200	52.24700	78.80900
C	8.10500	52.40000	80.37500
C	7.47400	53.75100	80.71900
O	6.38700	53.81300	81.28300
C	9.27100	52.11600	81.32400
C	8.96500	52.15800	82.82100
C	7.90400	51.12300	83.14500
C	10.23800	51.88300	83.61000
N	8.16800	54.83200	80.37900
H	9.07600	54.71900	79.92800
C	7.66100	56.17800	80.63600
C	6.24600	56.33700	80.08400
O	5.36200	56.85600	80.75900
C	8.59200	57.21000	79.99200
C	8.02200	58.61700	79.84900
C	7.67600	59.26200	81.17400
O	8.46000	59.10500	82.13800
O	6.62700	59.94100	81.24700
N	6.02400	55.86900	78.85900
H	6.78200	55.41700	78.34700
C	4.70900	55.99400	78.23900
C	3.67100	54.98100	78.72100
O	2.49500	55.31300	78.83900
C	4.84300	55.92500	76.71200
C	5.71100	57.02600	76.12000
S	5.70800	57.01800	74.31200
C	6.79200	55.64600	73.97900
N	4.09800	53.75500	79.00900

H	5.08700	53.53200	78.89700
C	3.17900	52.71700	79.48400
C	2.75500	52.95700	80.93300
O	1.65300	52.60000	81.33300
C	3.83700	51.33800	79.39400
C	3.84500	50.57900	78.06400
C	4.84300	49.41900	78.14500
C	2.44000	50.05500	77.76400
N	3.64200	53.55100	81.72000
H	4.54200	53.83700	81.33600
C	3.34900	53.80100	83.12700
C	2.64600	55.13800	83.29900
O	3.22000	56.09100	83.82300
C	4.64700	53.78000	83.93700
C	4.40300	53.85300	85.43100
O	3.25900	53.58400	85.86200
O	5.36200	54.16600	86.16800
N	1.39300	55.19600	82.87100
H	0.96100	54.36100	82.47500
C	0.62300	56.42500	82.95400
C	-0.10300	56.59200	84.28200
O	-0.32000	55.62500	85.01200
C	-0.38300	56.47700	81.80600
N	-0.46700	57.83200	84.59800
H	-0.22100	58.60400	83.97800
C	-1.21100	58.09900	85.81800
C	-2.68300	58.17100	85.44400
O	-3.04500	57.94900	84.28400
C	-0.76000	59.41500	86.47700
C	-0.82700	60.61300	85.58000
N	-1.98700	61.01700	84.95300
H	-2.88300	60.53200	85.00000
C	0.11600	61.53000	85.25300
C	-1.75600	62.13200	84.28100
N	-0.48800	62.46500	84.44800
H	-0.03200	63.28300	84.04500
N	-3.53300	58.47400	86.41500
H	-3.18300	58.64400	87.35800
C	-4.96200	58.56600	86.15000
C	-5.54700	59.88400	86.63300
O	-6.57400	59.90700	87.31100
C	-5.68000	57.39300	86.81400
C	-5.10900	56.06300	86.37800

C	-6.02200	54.91000	86.71500
N	-5.88300	54.45700	88.09400
H	-6.00000	55.14100	88.84100
C	-5.61200	53.20000	88.42800
N	-5.44600	52.28400	87.48300
H	-5.51600	52.55200	86.50100
H	-5.23800	51.31900	87.73900
N	-5.52100	52.85200	89.70300
H	-5.64900	53.55600	90.43000
H	-5.31300	51.88700	89.95900
N	-4.88900	60.98000	86.27600
H	-4.04600	60.89300	85.70800
C	-5.34300	62.30400	86.67600
C	-6.17400	62.92900	85.55400
O	-6.93800	63.86900	85.77800
C	-4.13300	63.18400	87.00300
C	-3.08300	62.49200	87.88200
C	-1.90700	63.42000	88.13900
C	-3.72500	62.06500	89.18900
N	-6.02600	62.38300	84.35100
H	-5.38200	61.59900	84.24500
C	-6.75000	62.86200	83.17400
C	-7.89700	61.91300	82.82600
O	-8.31100	61.13400	83.71200
C	-5.79500	62.96800	81.98600
C	-4.64100	63.89100	82.22500
N	-3.49900	63.86900	81.45100
H	-3.33100	63.24200	80.66400
C	-4.45300	64.86400	83.14700
C	-2.65700	64.78700	81.89000
N	-3.21100	65.40500	82.91800
H	-2.78600	66.16100	83.45500
N	6.90000	12.12200	43.39200
H	7.21000	12.17600	42.42200
H	5.88900	12.00100	43.45100
H	7.19300	11.24600	43.82500
C	7.35000	13.29500	44.19000
C	6.88800	13.21500	45.63800
O	6.13200	12.31900	46.01700
C	6.83900	14.59400	43.56000
C	7.70600	15.20100	42.45300
C	9.00400	15.70600	43.06000
C	7.98600	14.16900	41.36700

N	7.35400	14.16200	46.44400
H	7.97800	14.87300	46.06200
C	7.00200	14.21700	47.85500
C	5.54700	14.61700	48.03500
O	4.92600	14.28800	49.04400
C	7.90500	15.21100	48.57300
N	5.00800	15.32600	47.04800
H	5.57600	15.55100	46.23200
C	3.62800	15.79000	47.10000
C	2.61200	14.65100	47.08700
O	1.42600	14.86800	47.33700
C	3.34500	16.72900	45.92400
C	4.24600	17.95400	45.75400
C	3.74600	18.78700	44.58100
C	4.24900	18.77800	47.03000
N	3.07300	13.43900	46.80200
H	4.06800	13.30900	46.61800
C	2.17500	12.29300	46.74900
C	2.26200	11.39300	47.97500
O	1.42400	10.51200	48.16200
C	2.45500	11.46800	45.49100
O	3.78500	10.98000	45.49100
H	3.95900	10.46800	44.71000
N	3.27300	11.61000	48.80800
H	3.93800	12.35500	48.60200
C	3.45200	10.80400	50.01200
C	2.27500	10.96500	50.96700
O	1.54600	11.95400	50.90800
C	4.74000	11.21100	50.73600
C	6.07400	11.03900	50.00600
C	7.18200	11.68800	50.81900
C	6.36100	9.56000	49.79100
N	2.09000	9.98500	51.84400
H	2.71400	9.17800	51.82700
C	1.01700	10.03300	52.83000
C	1.62500	10.54000	54.13500
O	2.84500	10.57500	54.28000
C	0.41600	8.63900	53.08700
O	1.41300	7.78800	53.66600
H	1.04200	6.92800	53.82500
C	-0.07600	8.01900	51.78700
N	0.77900	10.92700	55.08200
H	-0.22500	10.87200	54.91100

C	1.26200	11.42900	56.36300
C	2.24700	10.45900	57.01400
O	3.31300	10.86300	57.47500
C	0.09200	11.68700	57.29600
N	1.89200	9.17900	57.04400
H	1.00100	8.89500	56.63700
C	2.75900	8.17400	57.65100
C	4.04500	7.95100	56.86900
O	5.08400	7.63600	57.44800
C	2.01000	6.84800	57.80700
C	0.90400	6.92500	58.84200
O	1.19000	7.34600	59.98200
O	-0.24800	6.56300	58.51900
N	3.98000	8.11000	55.55300
H	3.09300	8.35900	55.11600
C	5.16600	7.93100	54.72800
C	6.13000	9.08200	54.98500
O	7.34500	8.88500	55.05300
C	4.78600	7.88000	53.24600
C	3.98600	6.64100	52.86400
C	3.66500	6.59000	51.38800
O	3.08500	7.52500	50.83500
N	4.03900	5.49100	50.73800
H	4.51900	4.71700	51.19600
H	3.82200	5.45700	49.74200
N	5.57400	10.28200	55.12700
H	4.56100	10.37000	55.04700
C	6.36900	11.47600	55.39300
C	7.13300	11.29300	56.70200
O	8.35800	11.38900	56.74000
C	5.45400	12.70200	55.49300
C	6.17400	14.00800	55.79100
S	7.35100	14.45600	54.51000
C	6.32000	15.45700	53.42400
N	6.40000	11.01700	57.77300
H	5.38700	10.94400	57.67800
C	7.00700	10.81600	59.08100
C	8.09500	9.75100	59.00500
O	9.18000	9.91300	59.56100
C	5.94900	10.38000	60.12300
C	6.61400	10.10700	61.46400
C	4.89200	11.46300	60.27600
N	7.80000	8.66300	58.30300

H	6.88600	8.59300	57.85600
C	8.74700	7.56700	58.15500
C	10.02300	8.02100	57.45600
O	11.12900	7.73700	57.91800
C	8.10300	6.42400	57.36300
O	9.02500	5.36700	57.17300
H	8.62600	4.65800	56.68200
N	9.86700	8.72700	56.34200
H	8.92500	8.92900	56.00800
C	11.01200	9.21900	55.58600
C	11.84600	10.18000	56.42400
O	13.07300	10.15000	56.37600
C	10.53800	9.91700	54.31400
N	11.17500	11.03500	57.19000
H	10.15500	11.01300	57.19000
C	11.87100	12.00300	58.03000
C	12.62300	11.32400	59.16900
O	13.79500	11.61800	59.40200
C	10.87700	13.02800	58.59300
C	10.21800	13.96000	57.57200
C	9.22000	14.87000	58.26900
C	11.28200	14.78300	56.86900
N	11.96100	10.41400	59.87900
H	10.99200	10.19700	59.64700
C	12.61400	9.72200	60.99100
C	13.86300	8.98600	60.51400
O	14.87700	8.94600	61.21300
C	11.65100	8.73200	61.66000
C	10.52400	9.33100	62.50500
C	9.59800	8.22600	62.99800
C	11.11800	10.10000	63.67900
N	13.78900	8.41600	59.31600
H	12.92500	8.49200	58.77900
C	14.91700	7.68500	58.75400
C	16.08700	8.57800	58.36400
O	17.24700	8.18900	58.51200
C	14.46700	6.87800	57.53600
C	13.69400	5.63100	57.91900
O	12.58000	5.75500	58.47100
O	14.21200	4.52000	57.67700
N	15.79000	9.77400	57.86900
H	14.81300	10.05100	57.77800
C	16.84000	10.69700	57.45300

C	17.59800	11.31500	58.62900
O	18.63200	11.95500	58.43800
C	16.24500	11.79500	56.58800
N	17.09200	11.11200	59.84000
H	16.24500	10.55200	59.93900
C	17.72000	11.67300	61.03500
C	19.22300	11.45100	61.11600
O	19.70500	10.32300	61.03300
C	17.05400	11.11800	62.29500
C	15.80200	11.86900	62.68200
C	16.11600	13.30800	63.04500
O	16.45900	13.56900	64.21700
O	16.04200	14.17100	62.14800
N	19.98800	12.53900	61.27600
C	21.44100	12.42100	61.36700
C	21.82000	11.82600	62.71400
O	20.98500	11.71400	63.61200
C	21.91000	13.86300	61.22000
C	20.81500	14.62500	61.91500
C	19.56600	13.94800	61.36800
N	23.08800	11.43100	62.86400
C	23.59800	10.84200	64.10100
C	23.98100	11.90300	65.12900
O	24.24800	13.05700	64.78200
C	24.80700	10.05800	63.61900
C	25.34900	10.94800	62.54400
C	24.09400	11.34300	61.78700
N	23.98800	11.50700	66.39800
H	23.71600	10.55100	66.62500
C	24.37600	12.41000	67.46800
C	25.88900	12.27000	67.62000
O	26.39200	11.21000	68.00600
C	23.67000	12.04000	68.78800
C	22.16400	12.25500	68.63900
C	24.20700	12.89000	69.93100
C	21.37600	11.96500	69.89900
N	26.61300	13.33500	67.29600
H	26.14000	14.18300	66.98300
C	28.06400	13.31900	67.37800
C	28.58800	13.64800	68.76400
O	27.86900	14.20100	69.60400
C	28.66600	14.30500	66.37000
C	28.18700	14.13600	64.92500

C	28.96300	15.07600	64.00800
C	28.36800	12.68800	64.49900
N	29.85300	13.30100	68.98800
H	30.37000	12.83100	68.24500
C	30.53000	13.56400	70.24900
C	31.55000	14.67700	70.04600
O	32.08300	14.85500	68.94700
C	31.26800	12.31500	70.74800
C	30.39700	11.32600	71.47500
C	29.46900	10.55600	70.79700
C	30.48300	11.18600	72.85200
C	28.64600	9.67700	71.46900
C	29.66600	10.30900	73.53100
C	28.74900	9.56100	72.84000
O	27.91900	8.70300	73.52800
H	27.99000	8.62300	74.47200
N	31.80800	15.43000	71.10700
H	31.30400	15.25800	71.97700
C	32.79600	16.49600	71.05300
C	34.16500	15.82000	71.05600
O	34.37000	14.83100	71.76400
C	32.66500	17.40800	72.27500
O	33.69500	18.38300	72.29300
H	33.61400	18.94900	73.05200
N	35.09300	16.34300	70.26000
H	34.86100	17.15800	69.69200
C	36.43600	15.77800	70.18100
C	37.36000	16.34700	71.25100
O	37.99800	17.37700	71.03800
C	37.03800	16.04000	68.79900
C	36.84000	14.90300	67.80600
C	37.41000	15.22700	66.43900
O	36.76700	15.99400	65.68900
O	38.51100	14.72400	66.11800
N	38.72300	27.86200	74.33200
H	39.68000	28.17800	74.49000
H	38.07600	28.25900	75.01300
H	38.32500	28.27000	73.48600
C	38.65800	26.40500	74.31100
C	37.22600	25.93200	74.07400
O	36.99100	24.98900	73.31600
C	39.17200	25.83600	75.63700
O	39.20800	24.41800	75.61100

H	39.52700	24.06500	76.43300
N	36.27000	26.59000	74.72300
H	36.51800	27.37100	75.33000
C	34.87100	26.20700	74.57700
C	34.35300	26.49300	73.17100
O	33.69800	25.64500	72.56400
C	34.00000	26.92700	75.60700
C	32.61900	26.29500	75.76500
S	31.61700	27.07000	77.04800
C	32.38300	26.39200	78.53300
N	34.63800	27.68600	72.65700
H	35.16200	28.36300	73.21200
C	34.21000	28.03600	71.31100
C	34.81100	27.02000	70.35800
O	34.14900	26.55500	69.42900
C	34.68200	29.44100	70.92900
C	33.79200	30.56000	71.44100
S	32.07800	30.36400	70.88700
C	32.26400	30.58500	69.11400
N	36.07100	26.67300	70.60400
H	36.57000	27.09400	71.38800
C	36.73800	25.70000	69.76500
C	35.95600	24.40300	69.69700
O	35.73700	23.84800	68.61600
N	35.52400	23.91400	70.85200
H	35.72100	24.41400	71.71900
C	34.77400	22.67400	70.89100
C	33.40400	22.80500	70.23100
O	32.95800	21.89200	69.54100
C	34.61000	22.19100	72.33600
C	35.87300	21.74300	73.09000
C	35.52800	21.49800	74.54400
C	36.44200	20.47900	72.46300
N	32.73800	23.93500	70.43500
H	33.15600	24.67400	71.00100
C	31.41100	24.12900	69.85600
C	31.43200	24.23300	68.33700
O	30.58800	23.63300	67.66300
C	30.73700	25.36800	70.46000
C	30.50100	25.28000	71.97000
C	29.73100	26.50400	72.45800
C	29.74300	24.00400	72.29200
N	32.39500	24.97700	67.79800

H	33.06800	25.44200	68.40700
C	32.50600	25.14100	66.35000
C	32.95300	23.85800	65.65600
O	32.44400	23.52300	64.58300
C	33.48800	26.28100	65.97400
O	34.80000	25.97600	66.46300
H	35.40200	26.67400	66.23300
C	33.02600	27.60200	66.57300
N	33.90500	23.13900	66.25300
H	34.31000	23.46300	67.13100
C	34.37000	21.89100	65.65500
C	33.20300	20.93300	65.55700
O	32.99100	20.30200	64.52500
C	35.48300	21.24400	66.48900
C	35.72900	19.78700	66.09900
O	35.08200	18.87400	66.61500
N	36.65000	19.56800	65.16500
H	37.18600	20.32400	64.73800
H	36.81400	18.59600	64.90500
N	32.44800	20.82900	66.64500
H	32.69100	21.37400	67.47200
C	31.28500	19.96000	66.68800
C	30.31300	20.37100	65.57900
O	29.83900	19.52700	64.81500
C	30.60400	20.07100	68.05900
C	29.27600	19.32700	68.22600
C	29.49900	17.83100	68.01500
C	28.69600	19.59600	69.61800
N	30.03000	21.67000	65.50200
H	30.45700	22.30900	66.17200
C	29.12500	22.21000	64.48600
C	29.62500	21.88200	63.07600
O	28.83700	21.50100	62.20800
C	28.99200	23.72000	64.65500
N	30.93100	22.03700	62.85200
H	31.52800	22.36900	63.60900
C	31.53100	21.74300	61.54600
C	31.26900	20.30800	61.09800
O	30.95100	20.06000	59.93300
C	33.04700	21.96100	61.57000
C	33.43300	23.42400	61.67100
O	32.75700	24.26600	61.04100
O	34.42900	23.73100	62.36700

N	31.41700	19.35700	62.01800
H	31.68700	19.61100	62.96800
C	31.19700	17.95600	61.68000
C	29.72100	17.63900	61.48800
O	29.35900	16.81200	60.65300
C	31.80000	17.04800	62.75500
C	33.31600	16.89800	62.65500
C	33.85800	15.97800	63.74400
N	33.81900	16.61700	65.05400
H	34.19500	17.56200	65.13400
C	33.32600	16.04900	66.15100
N	32.82600	14.82400	66.09700
H	32.81800	14.31700	65.21200
H	32.44800	14.38800	66.93800
N	33.33600	16.71000	67.30600
H	33.72100	17.65400	67.34800
H	32.95800	16.27400	68.14700
N	28.86200	18.29600	62.25700
H	29.20600	18.96300	62.94800
C	27.42700	18.06900	62.11900
C	26.92300	18.57300	60.77700
O	25.99300	18.00800	60.20700
C	26.65700	18.78200	63.22100
C	26.59800	18.02700	64.52400
C	25.76600	18.75600	65.55100
O	26.23900	19.78500	66.06700
O	24.63500	18.30500	65.82900
N	27.53000	19.64600	60.28400
H	28.29300	20.07600	60.80700
C	27.12300	20.22200	59.00300
C	27.19300	19.20100	57.87600
O	26.30000	19.12600	57.02800
C	27.99400	21.43400	58.66800
C	27.71700	22.70900	59.46600
C	28.73300	23.78100	59.08600
C	26.29400	23.19300	59.18000
N	28.26000	18.40900	57.86600
H	28.97500	18.52100	58.58500
C	28.42500	17.38600	56.84800
C	27.22000	16.46100	56.85100
O	26.67900	16.13100	55.79600
C	29.69700	16.54600	57.10300
C	29.79400	15.43300	56.07200

C	30.92300	17.44000	57.04800
N	26.79700	16.04800	58.04100
H	27.28900	16.36000	58.87800
C	25.65000	15.16200	58.18400
C	24.33800	15.86900	57.86000
O	23.36900	15.23600	57.42800
C	25.59300	14.59900	59.60600
C	26.66400	13.59300	59.89300
N	26.58900	12.28600	59.45900
H	25.80000	11.87300	58.96100
C	27.86400	13.72000	60.50600
C	27.70000	11.65300	59.79100
N	28.49000	12.50000	60.42600
H	29.41500	12.28300	60.79700
N	24.30500	17.18000	58.06900
H	25.13100	17.65500	58.43200
C	23.09600	17.94800	57.78300
C	22.81600	17.91800	56.28800
O	21.68100	17.73900	55.86000
C	23.26500	19.39600	58.22900
C	21.96400	20.18600	58.21300
S	22.25200	21.92200	58.59000
C	22.84400	21.82500	60.30200
N	23.86400	18.09800	55.49600
H	24.78400	18.24600	55.91100
C	23.73000	18.08900	54.04600
C	23.13100	16.77700	53.56900
O	22.23500	16.77500	52.73000
C	25.09000	18.31800	53.37200
C	25.64600	19.67100	53.81500
C	24.93700	18.27500	51.85400
C	27.02000	19.98000	53.27800
N	23.61200	15.65900	54.10600
H	24.36200	15.71100	54.79500
C	23.07700	14.36000	53.71800
C	21.64100	14.24200	54.17100
O	20.80000	13.68200	53.47000
C	23.87900	13.21700	54.33800
C	25.25500	13.10000	53.75300
O	25.42900	13.13400	52.53500
N	26.25000	12.95000	54.61700
H	26.10600	12.92200	55.62600
H	27.18600	12.87000	54.21900

N	21.36600	14.76200	55.36000
H	22.11400	15.19200	55.90400
C	20.01900	14.72900	55.89900
C	19.09600	15.53300	54.98100
O	18.01500	15.07300	54.62100
C	20.00200	15.33400	57.30500
C	18.65600	15.79000	57.73700
C	17.61300	15.01200	58.14300
C	18.17300	17.14200	57.73500
N	16.50900	15.79600	58.39000
H	15.60000	15.45700	58.70400
C	16.82900	17.10500	58.14600
C	18.75200	18.37600	57.42400
C	16.04900	18.25800	58.25500
C	17.97800	19.52100	57.53200
C	16.64300	19.45200	57.94300
N	19.53600	16.72700	54.60000
H	20.45600	17.04000	54.91100
C	18.73600	17.60600	53.74500
C	18.26300	16.89300	52.47900
O	17.06500	16.85900	52.17800
C	19.53800	18.84300	53.38200
N	19.20700	16.31700	51.74400
H	20.17900	16.37700	52.04800
C	18.89000	15.60200	50.51500
C	17.82400	14.52800	50.73000
O	17.12500	14.12500	49.79500
C	20.16300	14.97500	49.94500
C	21.15700	15.99000	49.40300
C	22.42000	15.31300	48.90200
C	23.24400	16.24200	48.01900
N	23.67000	17.49300	48.71600
H	24.22200	18.11500	48.12500
H	24.16900	17.27600	49.57900
H	22.86500	17.98300	49.10600
N	17.69000	14.07300	51.96800
H	18.28200	14.45000	52.70800
C	16.71200	13.04500	52.28700
C	15.34900	13.63700	52.63100
O	14.36300	12.90900	52.76300
C	17.22100	12.19900	53.45400
C	18.55900	11.52400	53.19100
C	18.38500	10.25000	52.39100

N	17.60200	9.26100	53.12900
H	16.70900	8.96900	52.73300
C	17.97800	8.71700	54.28300
N	19.13200	9.06100	54.83800
H	19.73400	9.74200	54.37400
H	19.42000	8.64400	55.72300
N	17.19600	7.83200	54.88600
H	16.30800	7.56700	54.45900
H	17.48400	7.41500	55.77100
N	15.29300	14.95600	52.79100
H	16.14200	15.51100	52.69000
C	14.03400	15.61900	53.10900
C	13.19500	15.68400	51.84000
O	13.59200	16.29500	50.84700
C	14.26400	17.05200	53.64100
C	12.93000	17.71600	53.92700
C	15.10900	17.00300	54.91400
N	12.02000	15.04800	51.86000
C	11.09400	15.00300	50.72400
C	10.89900	16.35200	50.04300
O	10.42200	17.30400	50.66300
C	9.80500	14.48400	51.35400
C	10.31000	13.58200	52.43600
C	11.42700	14.40400	53.04400
N	11.28000	16.42600	48.76900
H	11.68900	15.60800	48.31700
C	11.12000	17.65800	48.01600
C	12.36100	18.51900	47.87700
O	12.46400	19.30700	46.93900
N	13.30700	18.38000	48.80000
H	13.18200	17.70400	49.55300
C	14.52200	19.18400	48.74700
C	15.30700	18.99600	47.44800
O	15.63200	19.96800	46.77100
C	15.42900	18.86300	49.94700
C	16.55300	19.84700	50.14100
C	16.29500	21.13500	50.58000
C	17.86400	19.48800	49.87600
C	17.32300	22.04600	50.75000
C	18.89100	20.38900	50.04300
C	18.62000	21.67500	50.48300
N	15.60900	17.74800	47.09800
H	15.29800	16.97300	47.68400

C	16.38000	17.46900	45.88700
C	15.69700	17.88900	44.58900
O	16.30500	17.83100	43.52400
C	16.75700	15.96700	45.77900
C	17.75900	15.60200	46.86300
C	15.50900	15.10400	45.88600
N	14.44300	18.32000	44.67100
H	13.97800	18.35400	45.57800
C	13.72500	18.74600	43.47300
C	14.02400	20.19500	43.11900
O	13.61000	20.68000	42.06700
C	12.22100	18.57100	43.65700
C	11.83800	17.13900	43.93000
O	12.25300	16.25800	43.14700
O	11.12300	16.89100	44.92300
N	14.74600	20.88000	43.99800
H	15.06000	20.41500	44.85000
C	15.10400	22.27700	43.78100
C	16.44500	22.35000	43.06400
O	17.18500	21.36600	43.03000
C	15.21000	23.00400	45.12600
C	13.94900	23.03800	45.99200
C	14.29000	23.49800	47.41100
C	12.92100	23.95800	45.34500
N	16.75600	23.51000	42.49400
H	16.09300	24.28400	42.53700
C	18.03000	23.69300	41.80900
C	19.12600	23.61700	42.86100
O	18.86500	23.84600	44.04200
C	18.12400	25.07000	41.12600
O	19.41500	25.21300	40.51900
H	19.52600	24.51600	39.88300
C	17.94800	26.17700	42.13600
N	20.34600	23.29300	42.43700
H	20.49900	23.10300	41.44700
C	21.46900	23.20500	43.36600
C	21.61700	24.54000	44.08500
O	21.74400	24.59000	45.30900
C	22.76800	22.89500	42.61900
C	22.84000	21.59800	41.81200
C	24.19900	21.50800	41.12500
C	22.62000	20.40200	42.72900
N	21.59700	25.61400	43.30000

H	21.48500	25.48000	42.29500
C	21.72800	26.97300	43.81000
C	20.73600	27.22800	44.93900
O	21.09800	27.78200	45.97600
C	21.51000	27.97700	42.66700
C	21.54300	29.41400	43.09300
N	20.55800	29.98700	43.87100
H	19.74000	29.50100	44.23900
C	22.43300	30.40200	42.82900
C	20.83900	31.26400	44.06500
N	21.97100	31.54100	43.44300
H	22.42800	32.45300	43.42200
N	19.48800	26.81900	44.74000
H	19.23800	26.36100	43.86400
C	18.47500	27.02200	45.76700
C	18.68900	26.09100	46.94700
O	18.35900	26.43300	48.07900
C	17.06600	26.83200	45.20000
C	16.64500	27.98100	44.30000
O	17.06900	29.12100	44.56400
O	15.88100	27.75100	43.34100
N	19.22900	24.90600	46.68800
H	19.45600	24.64600	45.72800
C	19.49600	23.97800	47.77800
C	20.55400	24.59900	48.67800
O	20.43800	24.56900	49.90500
C	19.97900	22.62900	47.23300
C	18.84700	21.75800	46.71200
C	19.32800	20.48000	46.03800
O	20.11100	19.72200	46.60700
N	18.84700	20.23200	44.82000
H	18.19700	20.86100	44.34800
H	19.16900	19.37600	44.36900
N	21.58000	25.17600	48.06100
H	21.61400	25.17000	47.04200
C	22.65700	25.81700	48.80300
C	22.12200	27.01200	49.57900
O	22.52100	27.25600	50.72500
C	23.77100	26.30500	47.85700
C	24.82100	27.08600	48.64200
C	24.40300	25.11100	47.14500
N	21.21100	27.75200	48.95400
H	20.91200	27.49700	48.01300

C	20.63600	28.92300	49.60000
C	19.83500	28.57100	50.85200
O	19.97900	29.22600	51.88300
C	19.74900	29.70100	48.62300
C	19.16700	30.94800	49.21200
N	17.90400	30.99500	49.76300
H	17.24100	30.22000	49.78400
C	19.70100	32.18000	49.39300
C	17.68700	32.20000	50.26000
N	18.76200	32.93800	50.04900
H	18.87600	33.91200	50.32800
N	18.98600	27.55100	50.76300
H	18.89100	27.04700	49.88100
C	18.19000	27.14800	51.91500
C	19.09900	26.69400	53.05600
O	18.88300	27.04700	54.22200
C	17.22400	26.01800	51.53500
C	16.07900	26.38400	50.58600
C	15.20100	25.16800	50.35200
C	15.25000	27.52200	51.19400
N	20.11900	25.90700	52.72100
H	20.25200	25.64000	51.74600
C	21.05000	25.42200	53.73900
C	21.86200	26.54700	54.36500
O	22.05000	26.57600	55.57800
C	21.99700	24.37700	53.14700
C	21.43100	22.96400	53.00300
C	22.46300	22.09000	52.29900
C	21.08900	22.38600	54.37600
N	22.33800	27.48200	53.55000
H	22.15300	27.42800	52.54800
C	23.12500	28.58500	54.08700
C	22.26700	29.43100	55.01200
O	22.75400	30.01500	55.97100
C	23.68000	29.46400	52.96300
C	24.18600	30.81600	53.45600
C	24.95500	31.58900	52.39900
O	24.49200	31.63600	51.23500
O	26.01800	32.16100	52.73900
N	20.97600	29.47900	54.72400
H	20.62100	28.96000	53.92100
C	20.05400	30.26300	55.53700
C	19.55700	29.54600	56.79700

O	19.30200	30.18100	57.81900
C	18.85000	30.67300	54.68200
O	17.82100	31.21100	55.48900
H	17.07500	31.46500	54.95900
N	19.44800	28.22400	56.74400
H	19.74600	27.71900	55.90900
C	18.90200	27.49700	57.88200
C	19.81800	26.65600	58.76400
O	19.37500	26.16400	59.80400
C	17.76600	26.62500	57.39900
N	21.08200	26.50900	58.39600
H	21.44500	27.00600	57.58300
C	21.94700	25.62700	59.16900
C	22.00100	25.86200	60.68000
O	21.88300	24.90800	61.43600
C	23.36900	25.61300	58.59500
C	24.13500	26.85100	58.82600
C	24.10600	27.98100	58.07400
C	25.04100	27.10200	59.90100
N	24.94000	28.92900	58.61500
H	25.09700	29.86500	58.24100
C	25.52700	28.41100	59.74000
C	25.48800	26.34600	60.98800
C	26.43800	28.98200	60.62200
C	26.39000	26.91200	61.86300
C	26.85600	28.21800	61.67600
N	22.15400	27.10600	61.13000
H	22.21200	27.88800	60.47700
C	22.23900	27.33900	62.58000
C	20.92000	27.06500	63.28500
O	20.91300	26.53300	64.39600
C	22.74500	28.75500	62.88100
C	23.06100	29.05000	64.35500
C	23.90500	27.91600	64.95700
C	23.81000	30.37800	64.45300
N	19.80200	27.42800	62.65400
H	19.86900	27.90900	61.75700
C	18.48400	27.15100	63.22000
C	18.31900	25.63300	63.35300
O	17.73500	25.15000	64.31700
C	17.36300	27.66400	62.30100
C	17.20700	29.18200	62.23000
C	16.11600	29.58800	61.25400

O	14.91900	29.57500	61.62300
O	16.45900	29.89400	60.10100
N	18.81900	24.89200	62.36100
H	19.28200	25.35900	61.58100
C	18.72500	23.42900	62.35600
C	19.58900	22.80800	63.44900
O	19.16000	21.87000	64.13300
C	19.12300	22.86400	60.97700
C	18.03000	23.22100	59.96200
C	19.32900	21.34800	61.06400
C	18.46500	23.14800	58.52100
N	20.79200	23.33700	63.62700
H	21.10400	24.09900	63.02500
C	21.67600	22.83600	64.68100
C	21.06000	23.16200	66.03600
O	21.04200	22.33300	66.94400
C	23.05000	23.49900	64.60300
C	23.96900	23.09800	63.45300
C	25.24100	23.92000	63.54800
C	24.28900	21.61200	63.52000
N	20.54900	24.38200	66.17000
H	20.57600	25.03200	65.38500
C	19.95200	24.79400	67.43000
C	18.69200	24.03000	67.79100
O	18.50800	23.67700	68.95600
C	19.67800	26.30500	67.43400
C	20.92900	27.14700	67.60200
S	20.56600	28.92900	67.57600
C	22.09800	29.62000	68.16300
N	17.81400	23.75400	66.82800
H	17.96900	24.05000	65.86400
C	16.62400	23.01000	67.21400
C	17.02600	21.58300	67.59900
O	16.39100	20.96100	68.44700
C	15.52200	22.99300	66.12000
C	14.22600	22.45300	66.73500
C	15.95000	22.15300	64.92600
C	13.02000	22.48400	65.80800
N	18.09900	21.08000	67.00100
H	18.59200	21.62100	66.29100
C	18.56700	19.74900	67.36700
C	19.08500	19.78700	68.79800
O	18.76900	18.91300	69.61100

N	19.88000	20.81100	69.10800
H	20.10100	21.49900	68.38800
C	20.44700	20.98100	70.45000
C	19.33800	21.04600	71.49100
O	19.37700	20.35600	72.52400
C	21.28100	22.26800	70.52000
C	21.76100	22.70900	71.91300
C	22.68100	21.63800	72.52400
C	22.50600	24.02800	71.79800
N	18.34300	21.87600	71.21900
H	18.35800	22.41600	70.35400
C	17.23500	22.02400	72.13700
C	16.49100	20.70900	72.30900
O	16.07300	20.37400	73.41300
C	16.25100	23.11500	71.65900
C	15.00700	23.09800	72.52100
C	16.91800	24.48000	71.75300
N	16.34000	19.95200	71.22600
H	16.71500	20.26900	70.33200
C	15.64300	18.67200	71.30400
C	16.37900	17.64700	72.17600
O	15.76400	16.93700	72.97800
C	15.42900	18.09800	69.89900
C	15.01400	16.66300	69.89400
C	15.78100	15.58900	69.53500
C	13.74900	16.13400	70.30900
N	15.06900	14.42200	69.70700
H	15.41400	13.48200	69.51200
C	13.82100	14.73100	70.18400
C	12.56400	16.70900	70.78000
C	12.75200	13.89700	70.50900
C	11.50600	15.88300	71.10100
C	11.60700	14.49000	70.96700
N	17.69300	17.55200	72.04000
H	18.20100	18.14300	71.38200
C	18.38200	16.57400	72.86300
C	18.66000	17.06000	74.28300
O	19.11900	16.28600	75.12200
C	19.66000	16.08800	72.17400
C	20.60200	17.15100	71.71700
C	21.75000	16.52900	70.93000
N	22.79500	17.51400	70.70900
H	23.49900	17.63100	71.43800

C	22.89700	18.27100	69.62600
N	22.01700	18.14700	68.64400
H	21.27400	17.45100	68.70600
H	22.09600	18.73000	67.81000
N	23.86200	19.17400	69.54500
H	24.54000	19.26900	70.30100
H	23.94100	19.75700	68.71100
N	18.35600	18.33000	74.55400
H	17.97400	18.91500	73.81100
C	18.55200	18.91400	75.88400
C	17.25800	18.87200	76.68300
O	17.22700	19.26600	77.84500
C	18.99900	20.37700	75.79000
O	20.23800	20.50400	75.12600
H	20.51500	21.41100	75.06800
N	16.19000	18.39500	76.05700
H	16.28300	18.06300	75.09700
C	14.88400	18.33400	76.71000
C	14.82100	17.63500	78.06200
O	14.27600	18.18700	79.02100
C	13.86500	17.68400	75.78400
C	13.05700	18.67400	74.98300
S	11.80200	17.81600	74.04700
C	10.57900	17.53400	75.29100
N	15.35600	16.41900	78.12500
H	15.78500	16.02700	77.28700
C	15.35200	15.62300	79.35400
C	16.44500	16.05900	80.31200
O	16.73100	15.36700	81.28900
C	15.56500	14.14400	79.02800
C	14.54200	13.53300	78.08800
C	15.01000	12.19300	77.52600
O	16.05300	12.16800	76.82800
O	14.34100	11.16800	77.78300
N	17.06100	17.20100	80.03400
H	16.77200	17.74200	79.21900
C	18.14200	17.69300	80.87400
C	17.92200	19.12600	81.33900
O	18.65500	20.03300	80.95000
C	19.45600	17.58700	80.10300
C	19.78100	16.19300	79.66400
N	20.25300	15.23100	80.53200
H	20.45200	15.37700	81.52200

C	19.65800	15.58400	78.45900
C	20.40800	14.09100	79.88200
N	20.05300	14.27800	78.62200
H	20.07000	13.56800	77.89000
N	16.91200	19.34900	82.19500
C	16.64300	20.70400	82.68300
C	17.87500	21.43000	83.20700
O	18.68300	20.86700	83.95300
C	15.57100	20.48700	83.76000
C	15.70100	19.03400	84.12300
C	15.99800	18.37600	82.81300
N	18.01900	22.68100	82.78300
H	17.32800	23.07800	82.14600
C	19.14200	23.49100	83.21000
C	20.42700	23.30200	82.42200
O	21.39200	24.03500	82.64100
N	20.45300	22.34500	81.49800
H	19.62100	21.78000	81.32800
C	21.66900	22.10000	80.72600
C	21.43700	21.92300	79.23000
O	20.35000	21.56200	78.79100
C	22.38200	20.85800	81.26700
C	22.77800	20.97400	82.72700
C	23.18200	19.62800	83.30200
C	23.64300	19.76400	84.74900
N	24.00900	18.44800	85.34200
H	24.31700	18.53900	86.31000
H	24.70700	17.96700	84.77400
H	23.24400	17.77800	85.25800
N	22.47900	22.17900	78.45100
H	23.35400	22.48900	78.87400
C	22.40100	22.02700	77.00600
C	23.31200	20.87400	76.61400
O	24.52000	20.91200	76.85600
C	22.84800	23.31200	76.31100
C	21.92400	24.51100	76.56600
C	22.57300	25.79100	76.06000
C	20.57800	24.26600	75.88100
N	22.71800	19.84900	76.02300
H	21.71100	19.88500	75.86200
C	23.46200	18.67100	75.59600
C	24.03900	18.90500	74.20900
O	23.49700	18.43100	73.21200

C	22.53300	17.45300	75.58700
C	23.15800	16.05500	75.52600
C	24.13500	15.88900	76.67100
C	22.06400	15.00000	75.62600
N	25.12900	19.66100	74.13700
H	25.52400	20.06700	74.98600
C	25.76200	19.91200	72.85000
C	26.19600	18.57500	72.27200
O	26.10300	18.34200	71.07000
C	26.96300	20.84300	73.03200
C	26.57500	22.27500	73.28300
C	26.23900	23.10900	72.22700
C	26.50500	22.77500	74.57400
C	25.84400	24.41200	72.45200
C	26.11000	24.07800	74.80600
C	25.77900	24.89800	73.74300
N	26.65900	17.69500	73.15500
H	26.70100	17.96900	74.13600
C	27.11100	16.35200	72.78800
C	26.98300	15.48500	74.05200
O	27.04100	16.00100	75.15900
C	28.56000	16.40300	72.32000
N	26.81400	14.16000	73.90200
C	26.68200	13.30400	75.08900
C	27.81700	13.50400	76.08800
O	27.62700	13.35000	77.29700
C	26.65600	11.89400	74.50100
C	26.01500	12.11400	73.14500
C	26.72700	13.36100	72.66500
N	28.98800	13.87100	75.58400
H	29.07800	14.00500	74.57700
C	30.14700	14.08700	76.43800
C	30.39900	15.57500	76.64400
O	31.46200	15.97700	77.11000
C	31.38500	13.40600	75.82800
C	31.88800	14.10400	74.56600
O	31.11700	14.70000	73.81100
N	33.18900	14.01200	74.32500
H	33.82700	13.51900	74.95000
H	33.52500	14.47800	73.48200
N	29.41600	16.39900	76.29500
H	28.55400	16.01700	75.90700
C	29.55300	17.83700	76.45900

C	28.20300	18.43100	76.84600
O	27.48500	19.00500	76.02000
C	30.06700	18.48200	75.16700
C	30.50800	19.94500	75.28300
C	31.67100	20.04900	76.25100
C	30.91700	20.48000	73.91500
N	27.85800	18.26200	78.11400
H	28.49100	17.75800	78.73500
C	26.60900	18.77100	78.64800
C	26.98500	19.95800	79.52500
O	27.62800	19.79700	80.56300
C	25.91500	17.65100	79.42700
C	24.81700	17.91200	80.44700
C	23.91300	16.68600	80.57500
C	25.47100	18.23100	81.77500
N	26.59800	21.15300	79.08400
H	26.04500	21.20900	78.22900
C	26.94000	22.38300	79.78600
C	25.76600	23.11900	80.41700
O	24.64800	23.09700	79.89900
C	27.64900	23.33200	78.81700
C	28.77200	22.70800	77.98900
C	29.30900	23.72400	76.99700
C	29.87600	22.22000	78.92100
N	26.03500	23.77400	81.54300
H	26.97700	23.72900	81.93200
C	25.01900	24.55200	82.23300
C	25.25500	26.03200	81.96700
O	26.23600	26.42300	81.33000
C	25.05800	24.30200	83.74300
C	26.38800	24.68900	84.36900
O	26.97700	25.71600	83.96400
O	26.84100	23.97200	85.28100
N	24.34400	26.84800	82.47600
H	23.56700	26.44000	82.99600
C	24.39400	28.29400	82.33300
C	25.74200	28.91300	82.72000
O	26.33000	29.67300	81.94900
C	23.28500	28.90300	83.19000
C	23.22600	30.39500	83.15400
C	21.96100	30.89000	83.81700
N	21.60400	32.20200	83.29900
H	20.72500	32.29300	82.79000

C	22.35200	33.28700	83.44900
N	23.49900	33.21600	84.11100
H	24.07400	34.05000	84.22600
H	23.79900	32.32900	84.51500
N	21.96200	34.43900	82.92500
H	22.53700	35.27300	83.04000
H	21.08000	34.49400	82.41600
N	26.22300	28.59000	83.91800
H	25.69600	27.94700	84.50900
C	27.48700	29.13300	84.40700
C	28.65600	28.84700	83.47500
O	29.52000	29.70100	83.27200
C	27.79000	28.58700	85.80500
C	26.69200	28.90100	86.79500
O	26.24500	30.04600	86.89800
N	26.24800	27.88800	87.53200
H	26.61800	26.94100	87.44700
H	25.50700	28.10000	88.20000
N	28.68800	27.64500	82.91400
H	27.95500	26.96900	83.12900
C	29.75700	27.27900	81.99600
C	29.66600	28.16100	80.75500
O	30.65400	28.36500	80.05000
C	29.64300	25.79600	81.62500
C	29.98100	24.86300	82.78500
C	29.64200	23.40700	82.51100
O	28.47200	23.03700	82.40400
N	30.67100	22.57000	82.40300
H	31.64000	22.87600	82.49200
H	30.44300	21.59300	82.21900
N	28.47300	28.69300	80.50600
H	27.69100	28.48900	81.12800
C	28.27000	29.56100	79.35900
C	28.85700	30.94600	79.57000
O	29.30100	31.58900	78.61900
N	28.85900	31.40900	80.81800
H	28.46800	30.83300	81.56400
C	29.40800	32.72400	81.14500
C	30.86600	32.77800	80.71600
O	31.41800	33.85000	80.46500
C	29.32100	32.98100	82.64800
C	27.91900	32.96900	83.21000
C	27.95100	33.21600	84.70500

C	26.56400	33.14700	85.30700
N	26.60400	33.38800	86.77300
H	25.66900	33.34200	87.17900
H	27.06700	34.26900	86.99600
H	27.24900	32.75100	87.24100
N	31.47900	31.59900	80.64700
H	30.94900	30.76100	80.88800
C	32.87100	31.44800	80.24400
C	33.20500	32.36400	79.06500
O	34.10800	33.18900	79.15500
C	33.13800	29.98600	79.87300
O	34.46100	29.80100	79.41000
H	34.62700	28.89400	79.18000
N	32.47400	32.21900	77.96500
H	31.74000	31.51100	77.94800
C	32.69000	33.04400	76.77900
C	31.76000	34.25500	76.81200
O	30.64300	34.16900	77.32700
C	32.42400	32.22400	75.49100
C	32.59900	33.09600	74.27100
C	33.36800	31.02400	75.42900
N	32.20300	35.38800	76.28000
H	33.13200	35.41400	75.86000
C	31.38100	36.60500	76.28400
C	30.32700	36.59800	75.18900
O	30.61100	36.22500	74.05100
C	32.30000	37.81700	76.10900
C	31.79600	39.10200	76.68900
C	32.93200	40.03300	77.07900
O	34.06000	39.87400	76.56800
O	32.69100	40.94600	77.91100
N	29.12400	37.03100	75.55400
H	28.97800	37.33900	76.51500
C	28.01500	37.07700	74.62300
C	27.34600	35.72300	74.49200
O	26.31700	35.59300	73.82900
N	27.92100	34.72100	75.14900
H	28.74100	34.90900	75.72600
C	27.40900	33.36300	75.06500
C	26.29100	32.98900	76.02100
O	25.38900	32.23700	75.66100
C	28.56100	32.36400	75.22100
C	28.13100	30.90600	75.25000

S	29.54400	29.78900	75.34600
C	30.02600	29.69900	73.62500
N	26.33000	33.49600	77.24700
H	27.08400	34.12300	77.52800
C	25.26800	33.13600	78.18500
C	23.88100	33.62100	77.77600
O	22.89700	32.92700	78.02900
C	25.58800	33.58700	79.63900
C	25.44200	35.10100	79.78200
C	24.67400	32.88100	80.61700
N	23.78600	34.78200	77.13300
H	24.63000	35.31300	76.92000
C	22.47500	35.30400	76.72800
C	21.83600	34.29800	75.76400
O	20.64700	34.04600	75.81700
C	22.63600	36.67800	76.04600
C	24.08900	37.12200	75.95100
C	24.72400	37.34500	77.30800
O	25.95200	37.14500	77.42700
O	23.99600	37.72800	78.24800
N	22.65500	33.70800	74.90500
H	23.64800	33.94100	74.91900
C	22.16200	32.73300	73.94200
C	21.84700	31.41500	74.62300
O	20.85800	30.76800	74.29200
C	23.16000	32.53800	72.78300
C	23.32400	33.87000	72.02900
C	22.64700	31.44800	71.82700
C	24.48300	33.91400	71.09500
N	22.68000	31.04700	75.59400
H	23.48700	31.63600	75.79800
C	22.48100	29.83400	76.37500
C	21.11100	29.89500	77.04800
O	20.37300	28.90700	77.08200
C	23.55200	29.72800	77.46700
C	24.66300	28.75900	77.15700
C	25.36600	28.83100	75.96200
C	25.04200	27.80900	78.09400
C	26.43500	27.96900	75.71400
C	26.10100	26.95100	77.85800
C	26.80100	27.02800	76.67000
N	20.78200	31.06200	77.59700
H	21.43500	31.84400	77.53700

C	19.50600	31.24700	78.28300
C	18.30900	31.08200	77.35000
O	17.29200	30.50600	77.73300
C	19.46000	32.62100	78.96700
C	20.37400	32.69800	80.18300
O	20.48100	31.68200	80.90200
O	20.97200	33.77000	80.43200
N	18.42800	31.58600	76.12600
H	19.28700	32.06500	75.85600
C	17.33700	31.45800	75.16700
C	17.15300	29.99500	74.76200
O	16.02600	29.50800	74.62800
C	17.61300	32.30900	73.92900
C	17.70200	33.80800	74.21700
S	17.82600	34.82400	72.71600
C	19.52000	34.73300	72.37300
N	18.26500	29.29700	74.56400
H	19.17100	29.75200	74.68000
C	18.21100	27.88800	74.18300
C	17.59000	27.08500	75.32400
O	16.75100	26.22000	75.09500
C	19.62600	27.38400	73.84400
C	20.19200	27.97600	72.53900
C	21.69800	27.75400	72.43400
C	19.47800	27.34100	71.34700
N	17.99400	27.39100	76.55600
H	18.69200	28.12300	76.68300
C	17.46100	26.70300	77.73000
C	15.95500	26.92100	77.83500
O	15.19900	25.98100	78.07600
C	18.14900	27.20700	79.00500
C	19.59700	26.73900	79.21700
C	20.21900	27.48700	80.39600
C	19.60700	25.23100	79.46700
N	15.52000	28.16300	77.63900
H	16.19300	28.90200	77.43600
C	14.10200	28.48900	77.70900
C	13.31400	27.71200	76.65400
O	12.22100	27.20600	76.92700
C	13.90600	29.98900	77.52200
N	13.88500	27.59400	75.45700
H	14.80200	28.01200	75.29600
C	13.22200	26.87700	74.37000

C	13.09700	25.40500	74.71700
O	12.05700	24.78600	74.49200
C	14.00500	26.99400	73.05900
O	14.28900	28.37200	72.79600
H	14.77500	28.44500	71.98300
C	13.18600	26.42900	71.90100
N	14.17300	24.85000	75.25800
H	15.01100	25.41400	75.40100
C	14.17800	23.45500	75.64900
C	13.08200	23.25300	76.68900
O	12.35700	22.26300	76.64100
C	15.54600	23.06800	76.22600
O	15.69300	21.65700	76.26300
H	16.54000	21.41700	76.62000
N	12.95500	24.19800	77.62100
H	13.58600	24.99900	77.61400
C	11.92300	24.10200	78.65400
C	10.53600	24.12500	78.03100
O	9.65500	23.36300	78.44000
C	12.03400	25.25200	79.65500
O	13.21300	25.14800	80.42300
H	13.28200	25.86300	81.04500
N	10.33700	24.99700	77.04200
H	11.09800	25.60800	76.74600
C	9.03600	25.08600	76.37700
C	8.68600	23.74600	75.72800
O	7.55400	23.27000	75.84800
C	9.03000	26.18900	75.31200
C	7.64700	26.43000	74.71000
C	6.68800	26.95900	75.77300
N	5.28500	26.65100	75.50200
H	4.77400	26.11700	76.20500
C	4.62700	27.01600	74.40800
N	5.24700	27.70900	73.46300
H	6.22900	27.95900	73.57700
H	4.74200	27.98900	72.62300
N	3.34800	26.69100	74.26000
H	2.87100	26.15800	74.98700
H	2.84300	26.97100	73.42000
N	9.65600	23.13200	75.05000
H	10.57600	23.56700	74.98300
C	9.41700	21.84400	74.40200
C	9.05600	20.77500	75.42500

O	8.18400	19.94000	75.18200
C	10.64600	21.38600	73.61400
C	10.76400	22.01100	72.25500
C	9.69200	22.68300	71.69100
C	11.93400	21.89500	71.52600
C	9.78600	23.23000	70.41700
C	12.03700	22.43800	70.25500
C	10.95900	23.10700	69.70100
N	9.73700	20.80000	76.56400
H	10.45900	21.50800	76.69900
C	9.47400	19.83500	77.62700
C	8.05800	20.04400	78.14200
O	7.28700	19.09300	78.28400
C	10.47400	20.03500	78.76500
C	10.40200	19.00800	79.88500
C	11.34600	19.44000	80.98400
N	12.62200	19.85700	80.41000
H	13.04500	19.25300	79.70500
C	13.27200	20.96900	80.74100
N	12.77100	21.79200	81.65600
H	11.89000	21.56400	82.11600
H	13.27000	22.64500	81.91000
N	14.41600	21.26500	80.14400
H	14.80100	20.63300	79.44200
H	14.91500	22.11800	80.39800
N	7.72000	21.30000	78.41000
H	8.40700	22.03900	78.26200
C	6.39900	21.65500	78.90900
C	5.30400	21.20900	77.93800
O	4.23100	20.78000	78.36000
C	6.32500	23.16700	79.13100
C	5.07900	23.64000	79.85600
S	5.08400	25.43200	80.09100
C	5.88400	25.54800	81.69300
N	5.58300	21.31000	76.63800
H	6.49100	21.68000	76.35800
C	4.63400	20.90900	75.59800
C	4.70800	19.41700	75.31600
O	3.87200	18.87100	74.60200
C	4.92500	21.64400	74.29200
C	4.60000	23.11800	74.29800
S	4.90400	23.78800	72.66100
C	3.44500	23.26300	71.79400

N	5.72700	18.76600	75.86100
H	6.39300	19.27800	76.43900
C	5.91800	17.33800	75.65400
C	6.04200	17.02900	74.16300
O	5.39400	16.11900	73.63900
C	4.75300	16.55900	76.26600
C	5.04400	15.08000	76.37100
O	6.20200	14.67800	76.48600
N	3.99500	14.26100	76.35100
H	4.19100	13.26300	76.42200
H	3.03600	14.59400	76.25600
N	6.88900	17.79900	73.49000
H	7.39100	18.53000	73.99300
C	7.13000	17.64200	72.06400
C	7.52000	16.20700	71.73400
O	8.37400	15.62100	72.39600
C	8.24800	18.58800	71.61700
C	8.60000	18.56900	70.12800
C	7.39900	19.04100	69.31400
C	9.80300	19.46900	69.87600
N	6.89500	15.65000	70.70500
H	6.19900	16.19300	70.19400
C	7.17700	14.28200	70.28400
C	8.23700	14.26800	69.19000
O	8.38500	15.24100	68.44900
C	5.89700	13.62300	69.76500
C	4.78200	13.55500	70.79400
C	5.15000	12.67800	71.97200
O	5.33600	11.46700	71.82400
N	5.26900	13.28500	73.15000
H	5.11500	14.28600	73.27200
H	5.51700	12.69400	73.94400
N	8.97300	13.16300	69.10100
H	8.81000	12.39800	69.75600
C	10.00400	13.02700	68.08700
C	9.44200	13.17200	66.68200
O	10.11600	13.69100	65.78900
N	8.20800	12.71500	66.48000
H	7.70000	12.28800	67.25400
C	7.56500	12.81400	65.16600
C	7.32400	14.27800	64.80300
O	7.49400	14.68600	63.65300
C	6.22400	12.07700	65.16400

C	6.29900	10.55200	65.25400
C	6.72400	10.04100	66.62300
O	6.49800	10.74200	67.63900
O	7.27300	8.91600	66.68100
N	6.90800	15.05900	65.79300
H	6.76200	14.65600	66.71800
C	6.65500	16.48100	65.58700
C	7.99000	17.19000	65.34100
O	8.10300	18.01600	64.44100
C	5.94400	17.06200	66.81200
C	4.57200	16.43900	67.06300
C	3.89900	16.97600	68.31200
O	4.52200	16.93300	69.39800
O	2.74300	17.43600	68.21400
N	9.00000	16.84000	66.13400
H	8.83400	16.14500	66.86200
C	10.34100	17.41500	66.00200
C	10.90000	17.34100	64.57500
O	11.34800	18.35100	64.02400
C	11.32100	16.70100	66.94300
C	12.76600	17.03600	66.68200
C	13.26500	18.29900	66.96500
C	13.62000	16.09600	66.12400
C	14.58600	18.62100	66.69700
C	14.94400	16.41000	65.85400
C	15.42500	17.67200	66.13900
N	10.90900	16.14900	63.98100
H	10.54300	15.33200	64.46900
C	11.44500	16.01400	62.62800
C	10.65000	16.85700	61.63500
O	11.21600	17.43600	60.71600
C	11.49200	14.53400	62.16600
C	12.46400	13.75800	63.05400
C	10.10900	13.91500	62.21600
N	9.34100	16.94200	61.82700
H	8.90500	16.43000	62.59400
C	8.52400	17.76600	60.94400
C	9.00200	19.22400	61.04400
O	9.26700	19.86400	60.03100
C	7.05300	17.67200	61.34100
S	6.21800	16.12600	60.83800
N	9.12500	19.73200	62.26900
H	8.90900	19.14400	63.07400

C	9.56300	21.11700	62.49100
C	10.93100	21.42300	61.88700
O	11.14300	22.49600	61.32500
C	9.59700	21.43600	63.99000
C	8.29000	21.50300	64.77800
C	8.59200	21.86400	66.22400
C	7.35300	22.54200	64.16000
N	11.87000	20.48800	62.01200
H	11.65200	19.61600	62.49400
C	13.20400	20.69700	61.46900
C	13.14500	20.81900	59.94100
O	13.86100	21.63100	59.34000
C	14.13500	19.53900	61.87500
C	15.55300	19.98800	62.20400
C	16.56100	18.83400	62.18800
C	15.96900	17.53700	62.71100
N	17.01400	16.47000	62.75100
H	16.61600	15.59900	63.10200
H	17.83200	16.75800	63.28700
H	17.46500	16.34400	61.84500
N	12.28600	20.01800	59.31700
H	11.72700	19.36400	59.86600
C	12.12200	20.05000	57.86700
C	11.49100	21.37600	57.44300
O	11.84000	21.93700	56.40100
C	11.23300	18.89500	57.41400
O	11.86100	17.65900	57.70400
H	11.30800	16.94000	57.42200
N	10.56400	21.86600	58.26000
H	10.31300	21.34700	59.10200
C	9.89900	23.13500	57.97300
C	10.94300	24.24200	57.98100
O	10.96200	25.09900	57.09000
C	8.79800	23.43000	59.01100
C	7.60400	22.50400	58.75800
C	8.37300	24.91200	58.94200
C	6.48400	22.62700	59.78200
N	11.83300	24.20800	58.97300
H	11.77400	23.46800	59.67200
C	12.89200	25.21000	59.07900
C	13.74300	25.23000	57.81200
O	14.01700	26.29100	57.25300
C	13.80700	24.93800	60.31900

C	13.04200	25.26000	61.61200
C	15.07000	25.79500	60.24500
C	13.78400	24.88000	62.89300
N	14.15400	24.05200	57.35000
H	13.88700	23.20200	57.84600
C	14.97700	23.94800	56.15200
C	14.32000	24.58500	54.92400
O	14.95200	25.34000	54.18600
C	15.28500	22.47300	55.84700
C	16.02900	22.23800	54.52900
C	17.39700	22.89900	54.59700
C	16.16000	20.74000	54.25300
N	13.04500	24.28100	54.71900
H	12.56600	23.67000	55.38100
C	12.31100	24.80100	53.56800
C	11.83200	26.25500	53.69100
O	11.79100	26.97800	52.69300
C	11.10400	23.90200	53.28900
C	11.43100	22.42900	53.00300
C	10.15300	21.61900	52.86800
C	12.27400	22.33900	51.74500
N	11.47800	26.67400	54.90300
H	11.57500	26.03600	55.69300
C	10.95200	28.02600	55.14200
C	11.97200	29.14000	55.30300
O	11.76700	30.24700	54.81600
C	10.07400	28.03700	56.39900
C	9.36600	29.37800	56.61500
O	9.45800	29.99300	57.68500
N	8.65000	29.82300	55.60400
H	8.17900	30.71600	55.74800
H	8.57400	29.31600	54.72200
N	13.06300	28.84800	56.00000
H	13.19800	27.89600	56.34100
C	14.07300	29.86100	56.28800
C	14.55500	30.75100	55.14900
O	14.51400	31.98000	55.27000
C	15.27500	29.21300	56.97700
O	14.90000	28.72800	58.25700
H	15.64700	28.32600	58.68500
N	15.01000	30.14800	54.05600
H	15.00600	29.13000	53.99600
C	15.51300	30.93900	52.94700

C	14.56300	31.18300	51.78600
O	14.96000	31.76300	50.77500
N	13.30900	30.76800	51.92100
H	13.01500	30.32000	52.78900
C	12.34700	30.94800	50.83800
C	11.94500	32.41200	50.62200
O	11.65500	32.81900	49.49700
C	11.07100	30.10700	51.08200
C	10.18600	30.78200	52.12200
C	10.32100	29.91200	49.77600
N	11.93800	33.19700	51.69600
H	12.20400	32.80200	52.59800
C	11.56100	34.60700	51.62400
C	12.72300	35.48400	51.17500
O	12.64100	36.71100	51.24400
C	11.07500	35.10100	52.99100
C	9.96300	34.27600	53.59700
C	8.72400	34.17700	52.97300
C	10.15600	33.58700	54.79200
C	7.70700	33.41400	53.52000
C	9.14700	32.82300	55.34800
C	7.92400	32.73900	54.70600
O	6.92200	31.96600	55.24500
H	7.07100	31.50200	56.06000
N	13.80400	34.86200	50.71700
H	13.82200	33.84300	50.66800
C	14.96200	35.63000	50.28500
C	15.72400	35.02600	49.10500
O	16.94300	35.17800	49.00300
C	15.93700	35.84800	51.47100
O	17.08200	36.58500	51.02600
H	17.67900	36.71900	51.75300
C	16.38300	34.51800	52.05400
N	15.01300	34.34700	48.20900
H	14.00700	34.23900	48.33900
C	15.66000	33.75400	47.04100
C	16.23300	34.85100	46.15000
O	15.49500	35.69600	45.64100
C	14.67300	32.90800	46.22600
C	14.54100	31.49000	46.70700
C	15.60700	30.85300	47.32000
C	13.36600	30.78400	46.51600
C	15.50400	29.53800	47.73600

C	13.25500	29.46800	46.92700
C	14.32700	28.84400	47.53900
N	12.37800	37.20600	41.82000
H	12.33300	37.56400	42.77400
H	13.27900	37.40300	41.38400
H	12.41800	36.18700	41.80000
C	11.26800	37.72000	41.02500
C	11.33500	37.18400	39.59700
O	10.72700	37.73800	38.67800
C	11.29800	39.24900	41.00500
O	10.18200	39.77100	40.30000
H	10.20100	40.72100	40.28800
N	12.08800	36.10400	39.41800
H	12.57700	35.70100	40.21700
C	12.23200	35.48300	38.11200
C	11.13500	34.44200	37.96100
O	10.47000	34.08700	38.93600
C	13.58300	34.77300	37.98100
O	13.63400	33.67700	38.90200
H	14.47200	33.23700	38.82100
C	14.71700	35.73500	38.28000
N	10.94200	33.95500	36.74200
H	11.51200	34.29100	35.96600
C	9.92400	32.94600	36.50400
C	10.33800	31.65700	37.20200
O	9.51400	30.96600	37.79800
C	9.76300	32.71200	35.00200
C	9.36800	33.98800	34.25300
C	9.13100	33.68400	32.78200
C	8.12100	34.56300	34.88700
N	11.62800	31.34800	37.13300
H	12.26300	31.96800	36.63000
C	12.15600	30.14600	37.75900
C	11.89400	30.18400	39.26700
O	11.56000	29.16600	39.87100
C	13.65800	30.02700	37.47900
C	14.28300	28.73500	37.98100
C	13.53700	27.51900	37.44400
C	14.12200	26.22300	37.99100
N	13.42100	25.01400	37.46300
H	13.81300	24.14600	37.82900
H	13.41100	25.01100	36.44300
H	12.41700	25.06600	37.63600

N	12.03100	31.36200	39.86700
H	12.30300	32.17700	39.31800
C	11.79800	31.50600	41.29800
C	10.34900	31.16900	41.64300
O	10.08400	30.54200	42.66700
C	12.11800	32.93200	41.75700
O	11.14600	33.85200	41.29400
H	11.34400	34.73600	41.57900
N	9.41500	31.58300	40.78900
H	9.69400	32.10200	39.95600
C	7.99900	31.30900	41.02200
C	7.75100	29.82300	41.21400
O	7.10500	29.41200	42.17800
C	7.14000	31.78900	39.84900
C	6.90800	33.28200	39.61800
C	5.91600	33.45000	38.47200
C	6.36600	33.93300	40.88400
N	8.25500	29.02000	40.28300
H	8.77800	29.42300	39.50600
C	8.07600	27.57800	40.34900
C	8.71200	26.98900	41.60400
O	8.10100	26.16800	42.28900
C	8.67700	26.91300	39.10700
C	7.99400	27.28700	37.79800
C	6.53300	26.87100	37.75500
O	5.72700	27.42900	38.52700
O	6.18900	25.98100	36.94700
N	9.93900	27.40900	41.89300
H	10.39000	28.08900	41.28000
C	10.65800	26.92000	43.06800
C	9.82500	27.18900	44.31600
O	9.53100	26.27700	45.08700
C	12.02000	27.61500	43.18500
C	12.98200	27.30500	42.04100
C	13.59600	25.91900	42.14300
O	14.59200	25.75500	42.88000
O	13.07500	24.98600	41.49500
N	9.43800	28.44700	44.50000
H	9.71300	29.15700	43.82100
C	8.63100	28.83600	45.64700
C	7.30600	28.08000	45.71300
O	6.86400	27.70200	46.79200
C	8.36500	30.34200	45.61800

C	9.60300	31.20500	45.85500
C	9.20900	32.66300	46.06300
C	10.41300	33.54700	46.34700
N	10.00900	34.96600	46.60300
H	10.81700	35.55900	46.79400
H	9.31800	35.02700	47.35100
H	9.44700	35.33700	45.83700
N	6.67000	27.85800	44.56600
H	7.07200	28.19400	43.69100
C	5.40200	27.13800	44.55100
C	5.61700	25.72200	45.05800
O	4.80400	25.19100	45.82000
C	4.81300	27.08200	43.14000
C	3.45600	26.39700	43.10900
O	2.52000	26.90300	43.76500
O	3.32500	25.35000	42.44000
N	6.71200	25.11100	44.61900
H	7.33100	25.59900	43.97100
C	7.04800	23.75800	45.04300
C	7.22700	23.73800	46.56400
O	6.58500	22.95100	47.26400
C	8.34200	23.29500	44.37400
C	8.82200	21.96100	44.85800
N	8.12400	20.79500	44.63700
H	7.25100	20.72100	44.11400
C	9.91200	21.61400	45.58400
C	8.76000	19.78700	45.20700
N	9.84800	20.25700	45.78900
H	10.53000	19.70300	46.30700
N	8.09800	24.61000	47.06300
H	8.59600	25.23500	46.42900
C	8.35900	24.69400	48.49900
C	7.07800	24.82300	49.30700
O	6.88300	24.11500	50.29600
C	9.28000	25.89000	48.83800
C	10.69300	25.62700	48.30900
C	9.31600	26.10700	50.34500
C	11.66900	26.76500	48.56400
N	6.19200	25.72200	48.89200
H	6.37900	26.28300	48.06100
C	4.95500	25.89800	49.63200
C	4.05800	24.66500	49.63100
O	3.41600	24.37400	50.63400

C	4.20900	27.13400	49.12600
C	4.90300	28.41600	49.46700
N	5.33200	28.70600	50.74500
H	5.19200	28.11300	51.56300
C	5.28400	29.46100	48.69500
C	5.95300	29.87200	50.74400
N	5.93900	30.35100	49.51300
H	6.34800	31.23700	49.21700
N	4.01500	23.93000	48.52600
H	4.55200	24.20800	47.70500
C	3.19600	22.72200	48.49000
C	3.74400	21.69300	49.47500
O	2.98200	21.04000	50.19200
C	3.18700	22.10300	47.09400
C	2.54500	22.94600	46.01600
C	2.11000	22.01700	44.89800
N	2.00700	22.66300	43.59500
H	2.19900	23.66300	43.53300
C	1.67500	22.01200	42.48400
N	1.41800	20.70900	42.53800
H	1.16300	20.21000	41.68600
H	1.47000	20.21600	43.42900
N	1.60700	22.65400	41.32400
H	1.35200	22.15500	40.47200
H	1.80400	23.65400	41.28300
N	5.06500	21.54400	49.49100
H	5.63500	22.09900	48.85300
C	5.72000	20.60700	50.39700
C	5.43500	21.01300	51.84100
O	5.07600	20.17800	52.67300
C	7.24400	20.56800	50.16100
C	7.91100	19.64200	51.18000
C	7.53300	20.08300	48.74400
N	5.57900	22.30000	52.13500
H	5.88500	22.95300	51.41400
C	5.30200	22.78800	53.48400
C	3.87500	22.41200	53.89200
O	3.64300	21.97000	55.02200
C	5.51100	24.30900	53.55100
C	6.98000	24.74300	53.62600
C	7.11400	26.24900	53.40500
C	7.53700	24.34600	54.99800
N	2.92600	22.57300	52.96700

H	3.18400	22.94700	52.05400
C	1.52600	22.23000	53.22300
C	1.39100	20.75000	53.57100
O	0.58000	20.37300	54.41400
C	0.65000	22.53300	51.99900
C	0.35900	24.01500	51.83800
O	0.57600	24.77400	52.80700
O	-0.10300	24.41600	50.74600
N	2.18900	19.92100	52.90600
H	2.82700	20.30300	52.20800
C	2.18200	18.48300	53.14300
C	2.67100	18.22700	54.57300
O	2.09100	17.43200	55.30800
C	3.11500	17.78000	52.15100
C	2.71300	16.35100	51.81000
C	1.90600	16.31800	50.51100
C	1.27800	14.95300	50.26700
N	0.13800	14.69300	51.19000
H	-0.28300	13.77800	51.02700
H	-0.55900	15.43600	51.13800
H	0.41700	14.80400	52.16500
N	3.73900	18.91400	54.96800
H	4.18600	19.57000	54.32800
C	4.27400	18.73200	56.31500
C	3.26400	19.21400	57.35800
O	3.15900	18.63300	58.43500
C	5.63700	19.45700	56.48200
C	6.64700	18.86600	55.49500
C	6.15600	19.28200	57.91300
C	7.99900	19.55500	55.47100
N	2.51400	20.26800	57.04000
H	2.65200	20.73600	56.14400
C	1.49800	20.75800	57.96200
C	0.43100	19.66700	58.13000
O	0.00400	19.37600	59.24800
C	0.80800	22.04600	57.44300
O	1.76400	23.11300	57.36200
H	1.34100	23.90200	57.04400
C	-0.31800	22.46000	58.38700
N	0.00100	19.06200	57.02300
H	0.37700	19.33700	56.11600
C	-1.01000	18.00300	57.10200
C	-0.48200	16.86500	57.97000

O	-1.22800	16.25200	58.73400
C	-1.34800	17.44400	55.71300
C	-1.75900	18.52000	54.72500
O	-2.38200	19.52100	55.14300
O	-1.47100	18.35000	53.52000
N	0.81200	16.58600	57.84800
H	1.38200	17.13100	57.20100
C	1.43300	15.51600	58.62100
C	1.40800	15.82900	60.11400
O	1.08900	14.96200	60.93200
C	2.88400	15.27800	58.16700
O	2.89600	14.90900	56.77900
H	3.79200	14.76200	56.49900
C	3.52400	14.16700	58.99000
N	1.74600	17.06500	60.47400
H	2.02600	17.73800	59.76000
C	1.72200	17.46900	61.87200
C	0.31900	17.33100	62.43700
O	0.13000	16.81700	63.54300
C	2.17300	18.92300	62.02100
C	3.67300	19.14700	62.17000
C	3.98300	20.64100	62.08100
C	4.12600	18.56700	63.50800
N	-0.66200	17.81100	61.67800
H	-0.43500	18.24000	60.78100
C	-2.05000	17.73800	62.09900
C	-2.44900	16.27500	62.25900
O	-3.13000	15.90300	63.21400
C	-2.97800	18.41600	61.07000
C	-2.79000	19.93400	61.11700
C	-4.42200	18.06800	61.36700
C	-3.17000	20.55700	62.44600
N	-2.00700	15.44900	61.32000
H	-1.44800	15.82500	60.55400
C	-2.29500	14.02100	61.34900
C	-1.77500	13.40600	62.64900
O	-2.48600	12.65700	63.32300
C	-1.64400	13.34500	60.14100
C	-1.75000	11.85100	60.15000
N	-0.66100	11.03100	60.35600
H	0.29400	11.34900	60.52100
C	-2.81200	11.03000	59.97500
C	-1.04800	9.76900	60.30700

N	-2.34800	9.74100	60.07700
H	-2.91600	8.89800	59.98900
N	-0.53600	13.73100	63.00100
H	0.00400	14.35500	62.40100
C	0.07100	13.21800	64.22300
C	-0.73500	13.62800	65.45000
O	-0.93000	12.84000	66.38000
C	1.50200	13.73800	64.35100
C	2.47800	13.18100	63.31800
C	3.79700	13.94500	63.36600
C	2.69400	11.70100	63.59900
N	-1.20400	14.86800	65.44800
H	-1.01400	15.47400	64.65000
C	-1.98300	15.37900	66.56100
C	-3.34400	14.70000	66.65900
O	-3.86300	14.49800	67.75500
C	-2.13800	16.89300	66.41900
C	-0.82500	17.62200	66.66200
S	-0.89100	19.36400	66.29300
C	0.51500	19.52000	65.18900
N	-3.91400	14.34400	65.51300
H	-3.43500	14.54000	64.63400
C	-5.21300	13.67700	65.48700
C	-5.07700	12.28400	66.10200
O	-5.83200	11.92000	67.00300
C	-5.72300	13.57500	64.05200
N	-4.10800	11.51400	65.61600
H	-3.51700	11.87100	64.86500
C	-3.87100	10.16800	66.13300
C	-3.48800	10.19100	67.60700
O	-3.63200	9.19200	68.31000
C	-2.76400	9.47000	65.34100
C	-3.21900	8.86200	64.02400
C	-2.15600	7.93400	63.45500
C	-2.68500	7.15200	62.26100
N	-1.65800	6.22700	61.70600
H	-2.01200	5.70300	60.90600
H	-1.29200	5.60300	62.42600
H	-0.79800	6.72400	61.47300
N	-2.99400	11.33200	68.06700
H	-2.89400	12.12200	67.43000
C	-2.59000	11.48700	69.45600
C	-3.81200	11.67100	70.34600

O	-3.70800	11.61800	71.57200
C	-1.65000	12.67800	69.59700
N	-4.96600	11.89800	69.72500
H	-4.98800	11.95400	68.70700
C	-6.19500	12.06700	70.48000
C	-6.58800	13.50000	70.78500
O	-7.46000	13.73900	71.62400
N	-5.95600	14.46000	70.11600
H	-5.24200	14.21100	69.43200
C	-6.27300	15.86400	70.35000
C	-7.52600	16.27100	69.58500
O	-7.74300	15.82300	68.46400
C	-5.10900	16.75900	69.90800
C	-3.73100	16.47400	70.50800
C	-2.75000	17.57100	70.09100
C	-3.83800	16.41300	72.01400
N	-8.35000	17.12000	70.19100
H	-8.13700	17.44600	71.13400
C	-9.55600	17.59000	69.52000
C	-9.10400	18.54800	68.42400
O	-7.96300	19.01100	68.43400
C	-10.48300	18.35700	70.47700
O	-9.86400	19.59300	70.86000
H	-10.43700	20.06700	71.45100
C	-10.76600	17.52700	71.72200
N	-9.98900	18.84500	67.48200
H	-10.92100	18.43200	67.51500
C	-9.64100	19.75700	66.40000
C	-9.09700	21.08200	66.92500
O	-8.09600	21.58500	66.42200
C	-10.85600	20.01500	65.51000
C	-11.18400	18.89200	64.53000
C	-12.50100	19.19000	63.82500
C	-10.04600	18.75100	63.52300
N	-9.75600	21.64400	67.93400
H	-10.58300	21.18300	68.31500
C	-9.31200	22.90900	68.50200
C	-7.92300	22.76800	69.11100
O	-7.07200	23.64200	68.94700
C	-10.29100	23.39900	69.57000
C	-9.86300	24.70900	70.21700
C	-10.84100	25.19000	71.26300
O	-11.16200	24.46800	72.20300

N	-11.31700	26.41900	71.10900
H	-11.97700	26.74400	71.81500
H	-11.05000	27.01900	70.32800
N	-7.69500	21.66700	69.81700
H	-8.43900	20.97900	69.93100
C	-6.39600	21.43000	70.43000
C	-5.33700	21.30300	69.34400
O	-4.21600	21.79500	69.49600
C	-6.42300	20.15300	71.26700
C	-7.35200	20.21600	72.46100
C	-7.31100	18.94400	73.28900
O	-7.40100	17.83900	72.75600
N	-7.17700	19.09700	74.60200
H	-7.10200	20.01300	75.04400
H	-7.14900	18.24200	75.15800
N	-5.70800	20.63900	68.25100
H	-6.65500	20.26300	68.20600
C	-4.81600	20.42600	67.11200
C	-4.26700	21.72100	66.51200
O	-3.04900	21.87700	66.35400
C	-5.54600	19.65500	66.00800
C	-5.88700	18.21300	66.34800
C	-6.59600	17.51200	65.20200
O	-6.15900	17.58400	64.05300
N	-7.68800	16.82400	65.51100
H	-8.05000	16.76400	66.46300
H	-8.16400	16.35300	64.74100
N	-5.16100	22.64200	66.15900
H	-6.15500	22.47000	66.31000
C	-4.72500	23.89400	65.55900
C	-4.01000	24.79100	66.56300
O	-3.16000	25.59600	66.18700
C	-5.91300	24.62200	64.89200
C	-6.90200	25.22300	65.84600
N	-8.25900	25.21900	65.59700
H	-8.71100	24.77000	64.80000
C	-6.73600	25.92000	66.99600
C	-8.88300	25.88700	66.55200
N	-7.98100	26.32300	67.41400
H	-8.17700	26.86900	68.25300
N	-4.34400	24.64200	67.84200
H	-5.05900	23.96100	68.09900
C	-3.70200	25.43900	68.88300

C	-2.26100	24.95600	69.05700
O	-1.34800	25.76600	69.20200
C	-4.46900	25.32500	70.20900
C	-5.79900	26.08700	70.22900
C	-6.49700	26.03300	71.58100
O	-7.56100	26.62700	71.76800
N	-5.89700	25.32500	72.53100
H	-6.36500	25.28900	73.43700
H	-5.01700	24.83400	72.37600
N	-2.05700	23.64000	69.02400
H	-2.84900	23.01000	68.89600
C	-0.71100	23.08800	69.16900
C	0.11600	23.39800	67.92800
O	1.30300	23.71200	68.02600
C	-0.74800	21.56800	69.38300
C	0.63500	20.95800	69.65800
C	0.52600	19.46600	69.98500
N	1.80900	18.84700	70.32100
H	2.27500	18.30200	69.59500
C	2.41300	18.94200	71.50400
N	1.86200	19.64000	72.48900
H	2.32500	19.71300	73.39500
H	0.97800	20.12300	72.33000
N	3.56400	18.31300	71.71100
H	4.02700	18.38600	72.61700
H	3.98800	17.77600	70.95400
N	-0.50700	23.29600	66.75900
H	-1.48700	23.01300	66.73400
C	0.19200	23.58300	65.51200
C	0.75300	25.00000	65.56900
O	1.90900	25.22800	65.23100
C	-0.75600	23.45300	64.31900
C	-0.14200	23.86700	62.97700
C	1.04700	22.97600	62.65400
C	-1.19800	23.77600	61.88100
N	-0.07100	25.94600	66.01000
H	-1.02200	25.69500	66.28000
C	0.35800	27.33600	66.11500
C	1.43400	27.50600	67.18600
O	2.40700	28.22900	66.97900
C	-0.83300	28.23000	66.42900
N	1.24800	26.85700	68.33100
H	0.40800	26.29100	68.45000

C	2.21800	26.93300	69.42600
C	3.58400	26.49400	68.91800
O	4.59600	27.15200	69.17900
C	1.78600	26.03200	70.59400
C	0.55800	26.53500	71.33900
C	-0.10000	25.46300	72.20400
O	-1.16400	25.68900	72.78700
N	0.53000	24.29500	72.29200
H	0.09000	23.57900	72.87000
H	1.40900	24.10800	71.81000
N	3.61000	25.38800	68.18000
H	2.74000	24.89000	67.99400
C	4.86300	24.87300	67.63000
C	5.47400	25.79000	66.56500
O	6.67900	26.02300	66.56500
C	4.65700	23.48000	67.03000
C	4.25900	22.37100	68.01000
C	3.98600	21.10700	67.22400
C	5.36000	22.14500	69.04300
N	4.65700	26.31400	65.65300
H	3.65900	26.10500	65.67700
C	5.20000	27.18900	64.61800
C	5.68900	28.51100	65.20700
O	6.65200	29.09400	64.71000
C	4.15800	27.44200	63.51800
C	3.68300	26.17300	62.79700
C	2.70600	26.53600	61.67100
C	4.90400	25.43000	62.22800
N	5.04000	28.99300	66.26500
H	4.23900	28.49200	66.64900
C	5.48500	30.24500	66.87200
C	6.86500	30.08900	67.51300
O	7.62100	31.05500	67.61500
C	4.47400	30.75000	67.90300
C	3.21000	31.37100	67.28500
C	2.31500	31.94200	68.39000
C	3.62300	32.47200	66.31400
N	7.19700	28.87500	67.94200
H	6.52900	28.10800	67.86500
C	8.50900	28.63700	68.52100
C	9.57100	28.76700	67.42800
O	10.72100	29.12900	67.70000
C	8.58400	27.24700	69.19200

C	7.67700	27.22800	70.42500
C	10.02500	26.94000	69.61300
C	7.52300	25.84400	71.07200
N	9.19400	28.48700	66.18200
H	8.24000	28.17900	65.99400
C	10.15100	28.62200	65.08300
C	10.62000	30.07400	64.93600
O	11.71100	30.33400	64.44200
C	9.54700	28.14300	63.76000
C	9.19400	26.65800	63.64900
C	8.98400	26.30800	62.18000
C	10.31700	25.80200	64.21500
N	9.78400	31.02500	65.34800
H	8.86600	30.77100	65.71200
C	10.17500	32.42500	65.28100
C	11.27700	32.69400	66.29800
O	12.20700	33.47600	66.04200
C	8.97600	33.33900	65.56000
O	8.22900	33.52700	64.37100
H	7.48600	34.09300	64.54400
N	11.18600	32.04800	67.45500
H	10.40300	31.41800	67.62800
C	12.20800	32.24100	68.47900
C	13.51600	31.55600	68.05900
O	14.60700	32.02400	68.38900
C	11.74400	31.69000	69.83000
C	12.64800	32.06400	70.96500
N	13.24500	31.12900	71.78700
H	13.11100	30.12000	71.72700
C	13.09200	33.27300	71.38700
C	14.01800	31.74800	72.66400
N	13.94300	33.04800	72.44300
H	14.43600	33.76800	72.97000
N	13.40400	30.44800	67.33100
H	12.47800	30.08700	67.10200
C	14.59600	29.74100	66.85500
C	15.29800	30.62800	65.82500
O	16.51900	30.73400	65.81600
C	14.21700	28.36500	66.26900
C	13.77400	27.45800	67.42700
C	15.41200	27.73100	65.53100
C	13.10900	26.20000	67.00100
N	14.52100	31.28900	64.97100

H	13.51000	31.15800	65.00400
C	15.09800	32.19900	63.98800
C	15.85600	33.28900	64.73600
O	16.96800	33.65500	64.36600
C	13.99400	32.85100	63.14200
C	14.50000	33.95000	62.22700
C	15.61600	33.44700	61.32900
N	15.31200	33.65400	59.92100
H	15.89400	34.30600	59.39500
C	14.32100	33.04400	59.27900
N	13.54800	32.18500	59.92400
H	13.72400	31.98500	60.90900
H	12.78700	31.71700	59.43100
N	14.09300	33.30300	58.00200
H	14.68900	33.96500	57.50500
H	13.33200	32.83500	57.50900
N	15.23900	33.80200	65.79700
H	14.31700	33.44800	66.05100
C	15.84000	34.85500	66.60800
C	17.18000	34.39300	67.18200
O	18.19100	35.09600	67.09200
C	14.88800	35.23700	67.75200
C	15.39800	36.34500	68.62400
N	15.60600	37.62400	68.15700
H	15.43300	37.93700	67.20200
C	15.75100	36.36300	69.93300
C	16.06500	38.38300	69.13700
N	16.16200	37.64200	70.22500
H	16.48900	37.96600	71.13500
N	17.17800	33.20800	67.78300
H	16.31200	32.67100	67.83100
C	18.39400	32.66400	68.37500
C	19.48400	32.48100	67.33000
O	20.65500	32.76000	67.59700
C	18.09700	31.34400	69.08200
C	17.15800	31.50900	70.27100
S	17.05000	30.03600	71.32300
C	16.10600	28.94200	70.29400
N	19.10600	32.02700	66.13700
H	18.12700	31.79500	65.97100
C	20.08000	31.85800	65.06500
C	20.69400	33.21200	64.70400
O	21.91000	33.32600	64.53100

C	19.41700	31.25100	63.82700
O	20.33300	31.19600	62.74500
H	19.92100	30.81900	61.97600
N	19.85500	34.24300	64.59100
H	18.85700	34.10100	64.74400
C	20.35400	35.57300	64.25000
C	21.37300	36.02300	65.29000
O	22.44300	36.52700	64.94600
C	19.20500	36.59800	64.17600
C	18.32400	36.41000	62.94400
O	18.79800	36.01500	61.87800
N	17.04200	36.71200	63.08500
H	16.45300	36.58600	62.26200
H	16.64900	37.03900	63.96800
N	21.04000	35.84000	66.56200
H	20.13600	35.42600	66.78900
C	21.94400	36.22000	67.64000
C	23.19600	35.34300	67.61200
O	24.30100	35.81700	67.88400
C	21.24200	36.09100	68.99400
C	20.15300	37.13400	69.24300
C	20.74700	38.52700	69.46000
C	19.67100	39.53500	69.85900
N	20.24200	40.89400	70.12400
H	19.52300	41.56700	70.39000
H	20.78500	41.22900	69.32800
H	20.98600	40.85300	70.82000
N	23.01900	34.06900	67.27600
H	22.08200	33.72600	67.06700
C	24.15500	33.16100	67.20500
C	25.13300	33.60100	66.13000
O	26.35000	33.48200	66.28700
N	24.59600	34.10600	65.02500
H	23.58000	34.15900	64.94700
C	25.41500	34.58600	63.92300
C	26.13000	35.86100	64.36200
O	27.30900	36.04800	64.06800
C	24.54400	34.88000	62.70100
C	23.85600	33.66200	62.12300
S	25.01300	32.53400	61.34000
C	24.81100	33.04000	59.61700
N	25.41300	36.73400	65.06300
H	24.43400	36.52900	65.26400

C	25.99700	37.98100	65.55200
C	27.17900	37.68400	66.46800
O	28.19500	38.37600	66.43600
C	24.96200	38.79400	66.33500
C	23.87500	39.44000	65.49000
C	22.93700	40.30500	66.32100
O	23.43700	41.19000	67.04900
O	21.70500	40.10300	66.24300
N	27.02300	36.65200	67.29000
H	26.14800	36.12900	67.25500
C	28.04500	36.23300	68.23900
C	29.21500	35.56500	67.52600
O	30.37400	35.74700	67.89700
C	27.41900	35.27100	69.25400
C	28.36700	34.78800	70.30600
N	29.06600	33.60600	70.19400
H	29.01600	32.96400	69.40300
C	28.72400	35.32500	71.49700
C	29.81100	33.43400	71.27200
N	29.62200	34.46400	72.07800
H	30.07000	34.59800	72.98400
N	28.89600	34.79800	66.49200
H	27.91300	34.70300	66.23700
C	29.89300	34.08700	65.70700
C	30.68500	35.04700	64.81800
O	31.91500	34.97500	64.75300
C	29.19300	33.02900	64.85200
C	30.03500	32.00500	64.09600
C	30.98300	31.30100	65.05300
C	29.10800	30.99800	63.42600
N	29.97200	35.94800	64.14600
H	28.95800	35.95500	64.26000
C	30.58500	36.92900	63.25100
C	31.30200	38.03900	64.01300
O	32.06600	38.80800	63.42900
C	29.52000	37.55000	62.33800
C	29.00700	36.63000	61.24700
C	29.24100	35.25900	61.29500
C	28.27300	37.13200	60.17700
C	28.75800	34.41500	60.30900
C	27.78600	36.29700	59.18700
C	28.03100	34.93900	59.25700
O	27.54500	34.10500	58.27300

H	27.04500	34.46500	57.55000
N	31.05100	38.12500	65.31400
H	30.40400	37.46400	65.74400
C	31.68300	39.14600	66.13800
C	33.07500	38.69300	66.54600
O	33.75200	39.35500	67.33200
C	30.84400	39.41600	67.38800
O	31.41300	40.45100	68.17000
H	30.89200	40.61900	68.94600
N	33.49900	37.55800	66.00000
H	32.89000	37.06100	65.35000
C	34.81100	37.00500	66.30600
C	35.38600	36.23600	65.12000
O	35.81500	35.08100	65.32800
C	34.70400	36.07900	67.51500
C	33.63300	35.01400	67.36100
S	33.51800	33.93800	68.78900
C	34.76200	32.70800	68.36900
O	25.48900	27.29600	70.09700
O	27.04000	29.85900	67.33500
C	26.37400	29.49300	69.56800
C	25.68900	26.90600	68.78200
C	25.83800	28.57000	70.46400
C	26.19000	27.70200	67.81900
C	26.57800	29.09000	68.16800
C	26.71000	30.77900	69.99800
C	25.63300	28.92800	71.79600
C	25.96700	30.21100	72.22900
C	26.50600	31.13500	71.33100
C	25.27200	25.51800	68.52400
C	26.20900	24.48500	68.57900
C	25.81400	23.17000	68.33400
C	24.48200	22.88600	68.03400
C	23.54500	23.91800	67.97800
C	23.94000	25.23300	68.22300
O	26.73900	22.17100	68.39100
C	27.78300	22.19900	67.42000
O	24.08400	21.60600	67.79300
H	24.86600	21.07900	67.55200
O	26.34800	27.29400	66.51300
H	26.74300	28.03500	66.02100
O	27.23800	31.71800	69.16400
H	26.73700	31.75800	68.33500

O	25.76900	30.56300	73.52900
H	25.76200	31.53400	73.59500

Xyz Cartesian coordinates of the complex of Chrysophanol with Stromelysin-1

N	9.60700	-10.62500	1.62300
C	8.27000	-10.01500	1.36900
C	8.19800	-9.53000	-0.08100
O	8.66600	-8.45900	-0.41100
C	8.07300	-8.83000	2.31600
C	9.37000	-8.06800	2.44700
C	10.29800	-8.42900	3.43000
C	9.64400	-7.00000	1.58400
C	11.50100	-7.72300	3.55100
C	10.84600	-6.29300	1.70600
C	11.77500	-6.65400	2.69000
H	10.34700	-10.02700	1.20600
H	9.76100	-10.70500	2.65000
H	9.64400	-11.57100	1.19200
N	7.61400	-10.31000	-0.94800
C	7.51200	-9.89300	-2.37500
C	6.65100	-10.90000	-3.14100
O	5.91300	-11.67000	-2.56100
C	8.91500	-9.84800	-2.98400
C	9.56200	-11.23000	-2.87800
C	10.03700	-11.67800	-4.26200
N	11.05600	-12.75500	-4.10100
C	12.27600	-12.45600	-3.74300
N	12.61000	-11.21200	-3.52000
N	13.16400	-13.40200	-3.60500
H	7.24200	-11.17100	-0.66100
H	10.81100	-13.68800	-4.26600
H	11.93200	-10.48500	-3.62500
H	13.54500	-10.98800	-3.24600
H	12.91100	-14.35400	-3.77500
H	14.09900	-13.17400	-3.33000
N	6.74300	-10.90000	-4.44300
C	5.93100	-11.85800	-5.24500
C	6.11000	-13.27200	-4.68800
O	7.06500	-13.56000	-3.99400
C	6.40300	-11.81700	-6.70000
O	6.60900	-10.46700	-7.09100
C	5.34300	-12.45400	-7.60100
H	7.34400	-10.27200	-4.89300

H	7.45700	-10.41400	-7.53900
N	5.20000	-14.15700	-4.98900
C	5.32000	-15.55200	-4.47700
C	5.99600	-16.42800	-5.53500
O	5.39100	-16.77700	-6.52900
C	3.92100	-16.09600	-4.17800
C	3.31800	-15.33100	-3.02400
C	4.07500	-15.09200	-1.87100
C	2.00200	-14.86100	-3.10800
C	3.51600	-14.38300	-0.80100
C	1.44300	-14.15100	-2.03800
C	2.20000	-13.91300	-0.88500
H	4.43800	-13.90600	-5.55100
N	7.23500	-16.75200	-5.28200
C	8.01500	-17.59000	-6.21000
C	7.51700	-19.03800	-6.15600
O	8.00000	-19.84100	-5.38300
C	9.45300	-17.50500	-5.73000
C	9.32900	-17.14900	-4.27800
C	8.03600	-16.37300	-4.11000
N	6.55800	-19.37600	-6.97300
C	6.03200	-20.77000	-6.96800
C	4.50600	-20.74400	-6.85700
O	3.86100	-21.77300	-6.80900
H	6.18200	-18.71200	-7.58900
N	3.92200	-19.57700	-6.81600
C	2.43900	-19.49100	-6.70800
C	1.92900	-18.33100	-7.56500
O	1.79400	-17.22100	-7.09000
C	2.05900	-19.25500	-5.24600
C	2.92600	-20.13900	-4.34600
C	0.58500	-19.60500	-5.03600
C	2.52900	-21.60400	-4.53500
H	4.45800	-18.75800	-6.85500
N	1.66100	-18.63200	-8.80600
C	1.16100	-17.62000	-9.75300
C	-0.29000	-17.26400	-9.42000
O	-1.11600	-18.12600	-9.19500
C	1.25000	-18.26300	-11.12600
C	1.21200	-19.73500	-10.84100
C	1.79600	-19.94300	-9.45500
N	-0.60400	-15.99900	-9.38100
C	-1.99900	-15.58500	-9.05700

C	-2.97100	-16.18300	-10.07900
O	-3.68100	-17.12600	-9.79200
C	-2.08700	-14.05600	-9.08900
C	-3.00100	-13.57600	-7.96100
C	-2.32500	-12.42600	-7.21000
C	-1.35300	-12.99400	-6.17400
N	0.04200	-12.82500	-6.67200
H	0.07800	-15.31900	-9.56000
H	0.21600	-11.82000	-6.88300
H	0.71200	-13.14900	-5.94600
H	0.17300	-13.38800	-7.53700
N	-3.01800	-15.64000	-11.26700
C	-3.95500	-16.18100	-12.29300
C	-3.20500	-17.09800	-13.26300
O	-2.07100	-16.85000	-13.61900
C	-4.57400	-15.01300	-13.06300
C	-5.12900	-14.02300	-12.09100
C	-4.97100	-12.68200	-12.16700
C	-5.92600	-14.27200	-10.89700
N	-5.61900	-12.09300	-11.09600
C	-6.22300	-13.03300	-10.28600
C	-6.41300	-15.44400	-10.29300
C	-6.97800	-12.95800	-9.11600
C	-7.17200	-15.37300	-9.11600
C	-7.45500	-14.13200	-8.52700
H	-2.44400	-14.87500	-11.48100
H	-5.65800	-11.13100	-10.91600
N	-3.83800	-18.15600	-13.69500
C	-3.17300	-19.09300	-14.64600
C	-3.82500	-18.96500	-16.02500
O	-3.15600	-18.97900	-17.04000
C	-3.32500	-20.53000	-14.13700
C	-4.63100	-20.67000	-13.35000
C	-5.09400	-22.12800	-13.38200
N	-4.08800	-22.97600	-12.68400
C	-4.25600	-24.27000	-12.61700
N	-5.30700	-24.82500	-13.15900
N	-3.37200	-25.01000	-12.00600
H	-4.75500	-18.33200	-13.39500
H	-3.29800	-22.56300	-12.27600
H	-5.98700	-24.26100	-13.62700
H	-5.43300	-25.81500	-13.10500
H	-2.56600	-24.58800	-11.59100

H	-3.50000	-26.00100	-11.95400
N	-5.12600	-18.84600	-16.07000
C	-5.82200	-18.71800	-17.38600
C	-5.06300	-17.74800	-18.28600
O	-4.15300	-17.06600	-17.86000
C	-7.23500	-18.17100	-17.17500
C	-7.20100	-17.02200	-16.16600
C	-8.60600	-16.78500	-15.62000
C	-9.31800	-15.76700	-16.50600
N	-10.64800	-16.31000	-16.90400
H	-5.64300	-18.84700	-15.23800
H	-11.18000	-16.58100	-16.05200
H	-11.17900	-15.58300	-17.42400
H	-10.51300	-17.14500	-17.51100
N	-5.44400	-17.67500	-19.53000
C	-4.75800	-16.74400	-20.46400
C	-5.70100	-15.59400	-20.82700
O	-5.35000	-14.71600	-21.59300
C	-4.36300	-17.50300	-21.73700
O	-4.38100	-16.60800	-22.84000
C	-5.35000	-18.64500	-21.99100
H	-6.18800	-18.22800	-19.84700
H	-5.29200	-16.35100	-22.99700
N	-6.89100	-15.57700	-20.28200
C	-7.82900	-14.46500	-20.61600
C	-8.55300	-13.98500	-19.36000
O	-9.55600	-14.53800	-18.95700
C	-8.86000	-14.95100	-21.62700
C	-8.22400	-15.06500	-22.98400
N	-7.45200	-16.15700	-23.34900
C	-8.23200	-14.23200	-24.07500
C	-7.03300	-15.95400	-24.61000
N	-7.48000	-14.79500	-25.10200
H	-7.30800	-14.40700	-26.02900
H	-7.16500	-16.29000	-19.65600
H	-7.25000	-16.93500	-22.78800
N	-8.05400	-12.95200	-18.74800
C	-8.70400	-12.41900	-17.51800
C	-9.69800	-11.32300	-17.90000
O	-9.74200	-10.87900	-19.02700
C	-7.62900	-11.81400	-16.61000
C	-6.81800	-12.92600	-15.94500
C	-7.69700	-13.67000	-14.93900

C	-6.31600	-13.90400	-17.00800
H	-7.24900	-12.52200	-19.10000
N	-10.48900	-10.87400	-16.96500
C	-11.46400	-9.80000	-17.26400
C	-11.62000	-8.95400	-16.00500
O	-11.34300	-9.41100	-14.91700
C	-12.80200	-10.43700	-17.64700
O	-13.84100	-9.48800	-17.48400
C	-13.06900	-11.64800	-16.75200
H	-10.44100	-11.23900	-16.05600
H	-13.45700	-8.61800	-17.57100
N	-12.04500	-7.73200	-16.11800
C	-12.19300	-6.90500	-14.89400
C	-13.50300	-6.12100	-14.95600
O	-14.13400	-6.02000	-15.98900
C	-11.01800	-5.94100	-14.79800
C	-11.01800	-5.03700	-16.00400
C	-10.78200	-5.57400	-17.27200
C	-11.25900	-3.66800	-15.85800
C	-10.78900	-4.74500	-18.39500
C	-11.26500	-2.83500	-16.98400
C	-11.03100	-3.37500	-18.25300
O	-11.03600	-2.55600	-19.36300
H	-12.25900	-7.35600	-16.99600
H	-11.71800	-2.86900	-19.96000
N	-13.91300	-5.56500	-13.85100
C	-15.18200	-4.78300	-13.83400
C	-14.89700	-3.38100	-13.28700
O	-14.36600	-3.22300	-12.21000
C	-16.19100	-5.50300	-12.93700
C	-17.60700	-5.22200	-13.44100
C	-18.43500	-4.62600	-12.30300
N	-19.78500	-5.25900	-12.28600
C	-19.96200	-6.41200	-11.69800
N	-18.94900	-7.04700	-11.17400
N	-21.15600	-6.93700	-11.64200
H	-13.38100	-5.66200	-13.03000
H	-20.54500	-4.79800	-12.69900
H	-18.03200	-6.65500	-11.22300
H	-19.09200	-7.92700	-10.72100
H	-21.93200	-6.45500	-12.04600
H	-21.29300	-7.82000	-11.19400
N	-15.23300	-2.35900	-14.02400

C	-14.95800	-0.97300	-13.54100
C	-16.07500	-0.51300	-12.59300
O	-16.99700	0.17100	-12.99000
C	-14.89100	-0.01000	-14.73600
C	-13.61300	-0.25200	-15.55600
C	-14.89000	1.43300	-14.22800
C	-13.69800	-1.61300	-16.24700
H	-15.65200	-2.50500	-14.89300
N	-15.99000	-0.87400	-11.34400
C	-17.03500	-0.45100	-10.36100
C	-16.54600	0.77000	-9.56700
O	-17.17500	1.20000	-8.61700
C	-17.31600	-1.60200	-9.39800
C	-18.44200	-1.20600	-8.44200
C	-17.73700	-2.83600	-10.19300
H	-15.23400	-1.42100	-11.04600
N	-15.42600	1.33000	-9.93700
C	-14.91800	2.51900	-9.20200
C	-15.32700	3.79100	-9.94600
O	-15.64100	3.76500	-11.11900
C	-13.39400	2.46800	-9.12100
C	-12.96500	1.59000	-7.94700
O	-12.99000	2.01800	-6.81200
N	-12.56100	0.37500	-8.17700
H	-14.92300	0.97000	-10.68600
H	-12.53600	0.03700	-9.09500
H	-12.27800	-0.19700	-7.43400
N	-15.30700	4.90500	-9.27200
C	-15.67300	6.18900	-9.93100
C	-15.61100	7.32600	-8.90400
O	-15.50900	7.10100	-7.71400
C	-17.07700	6.06100	-10.53700
C	-17.75100	7.41400	-10.62400
C	-17.53600	8.23300	-11.73900
C	-18.59100	7.84500	-9.59000
C	-18.16100	9.48300	-11.82100
C	-19.21700	9.09500	-9.67200
C	-19.00200	9.91400	-10.78700
O	-19.61900	11.14600	-10.86800
H	-15.03500	4.89700	-8.33500
H	-19.94800	11.37000	-9.99500
N	-15.65800	8.54400	-9.36400
C	-15.58900	9.70900	-8.43500

C	-15.75300	10.99000	-9.24200
O	-15.51500	11.00200	-10.43100
C	-14.21600	9.72700	-7.75400
O	-13.88100	11.06300	-7.39900
C	-13.16100	9.18200	-8.71700
H	-15.72900	8.69600	-10.33000
H	-13.01400	11.26200	-7.76600
N	-16.12500	12.03800	-8.57200
C	-16.27700	13.33100	-9.24400
C	-14.90400	13.77800	-9.70400
O	-14.75200	14.49200	-10.67500
C	-16.84900	14.27100	-8.20900
C	-16.45200	13.64600	-6.90700
C	-16.43100	12.14900	-7.13900
N	-13.89700	13.31200	-9.02800
C	-12.51800	13.64900	-9.43500
C	-12.20100	12.83800	-10.69100
O	-11.21100	13.06400	-11.36100
C	-11.54900	13.27600	-8.31100
C	-10.71500	14.49800	-7.92600
O	-11.17900	15.60400	-8.15300
O	-9.62600	14.31000	-7.41000
H	-14.05200	12.71000	-8.27200
N	-13.05000	11.89100	-11.01600
C	-12.81900	11.05900	-12.22900
C	-14.14300	10.53700	-12.76900
O	-14.76200	9.68100	-12.16800
C	-11.94800	9.85600	-11.87600
C	-10.63100	10.33000	-11.28100
C	-9.82700	9.11700	-10.83200
C	-9.83600	11.11700	-12.32800
H	-13.84200	11.73400	-10.46100
N	-14.51900	11.03500	-13.90700
C	-15.75700	10.58500	-14.54900
C	-15.61300	9.11900	-14.95400
O	-14.58100	8.50800	-14.76100
C	-15.93700	11.47400	-15.77100
C	-14.54900	11.95700	-16.05800
C	-13.84600	12.05700	-14.71800
N	-16.64600	8.55900	-15.51100
C	-16.59900	7.13400	-15.93800
C	-15.23400	6.80500	-16.53400
O	-14.49400	5.99100	-16.02500

C	-17.65900	6.92700	-17.01600
C	-18.45800	5.65800	-16.71700
C	-18.36700	4.70500	-17.91100
C	-16.89700	4.42000	-18.23400
N	-16.75800	4.20000	-19.70200
H	-17.46400	9.08000	-15.65100
H	-17.28800	4.93400	-20.21400
H	-15.75300	4.24900	-19.96600
H	-17.13400	3.26300	-19.94900
N	-14.92600	7.41200	-17.63800
C	-13.63400	7.12800	-18.33000
C	-12.41500	7.41400	-17.44200
O	-11.36900	6.82700	-17.63200
C	-13.55400	7.98900	-19.59200
C	-14.06900	7.18900	-20.79000
O	-15.27600	7.13900	-20.96800
O	-13.25000	6.64100	-21.50800
H	-15.56900	8.03700	-18.03500
N	-12.50800	8.30200	-16.49200
C	-11.31900	8.58500	-15.64800
C	-11.09800	7.42900	-14.66700
O	-10.08300	6.76200	-14.70200
C	-11.54800	9.88900	-14.89700
H	-13.34200	8.78400	-16.33800
N	-12.05200	7.15600	-13.81300
C	-11.86800	6.01000	-12.88400
C	-11.64900	4.77600	-13.75000
O	-10.77300	3.96600	-13.51100
C	-13.11900	5.83600	-12.02200
C	-14.32200	5.52900	-12.91500
C	-12.90200	4.67900	-11.04700
H	-12.88700	7.68100	-13.80500
N	-12.42200	4.66900	-14.79500
C	-12.25200	3.53700	-15.73100
C	-10.83800	3.63900	-16.26900
O	-10.20200	2.65900	-16.58800
C	-13.25500	3.66800	-16.87800
C	-14.63400	3.19700	-16.41100
O	-15.18200	3.82400	-15.52000
O	-15.11800	2.21700	-16.95300
H	-13.09100	5.36300	-14.98000
N	-10.33800	4.84400	-16.34500
C	-8.95300	5.04500	-16.82800

C	-8.02000	4.24400	-15.92800
O	-7.39600	3.32400	-16.36700
C	-8.59500	6.53200	-16.77200
O	-7.80200	6.78800	-15.62100
H	-10.87300	5.61100	-16.06600
H	-6.92600	7.04900	-15.91600
N	-7.93300	4.57600	-14.66800
C	-7.04400	3.81600	-13.74400
C	-7.29000	2.32400	-13.89000
O	-6.39700	1.51900	-13.75800
C	-7.37400	4.22000	-12.32000
H	-8.45100	5.32000	-14.32400
N	-8.48800	1.95500	-14.17000
C	-8.80600	0.52100	-14.34500
C	-8.21500	0.07900	-15.67500
O	-7.92900	-1.07900	-15.90300
C	-10.32300	0.37000	-14.37500
C	-10.70100	-1.09900	-14.19900
C	-10.93600	1.19200	-13.23900
H	-9.17400	2.62100	-14.28500
N	-8.03700	1.02400	-16.55100
C	-7.47100	0.73500	-17.89300
C	-5.94600	0.87700	-17.84200
O	-5.22300	0.16200	-18.50700
C	-8.07200	1.75500	-18.86900
C	-7.07100	2.10600	-19.97100
C	-7.82300	2.46600	-21.25300
O	-8.67100	3.34100	-21.19300
O	-7.53800	1.86100	-22.27400
H	-8.28400	1.94900	-16.31900
N	-5.45600	1.78800	-17.05000
C	-3.99600	1.97000	-16.94800
C	-3.48100	0.87700	-16.03800
O	-2.46900	0.27400	-16.28600
C	-3.69400	3.33500	-16.35100
C	-2.69100	4.07400	-17.23700
C	-3.42800	5.11800	-18.08000
C	-3.77000	4.52200	-19.44600
N	-3.82600	5.61800	-20.45400
H	-6.05500	2.34600	-16.51000
H	-3.83300	6.53700	-19.96600
H	-2.99600	5.56000	-21.07600
H	-4.69100	5.52100	-21.02400

N	-4.21200	0.58700	-15.00900
C	-3.83000	-0.51700	-14.09100
C	-3.90200	-1.81700	-14.87600
O	-2.92800	-2.51700	-15.07200
C	-4.86700	-0.57300	-13.00000
H	-5.05500	1.08100	-14.85600
N	-5.09000	-2.12200	-15.32900
C	-5.29600	-3.36300	-16.11900
C	-4.24600	-3.44700	-17.21400
O	-3.64000	-4.47100	-17.43400
C	-6.67600	-3.31300	-16.77900
C	-6.72500	-4.32700	-17.92400
C	-6.49300	-5.72700	-17.36500
C	-8.08400	-4.26200	-18.60800
H	-5.85800	-1.51500	-15.14600
N	-4.06400	-2.38100	-17.92500
C	-3.08300	-2.40000	-19.04500
C	-1.67200	-2.46900	-18.49100
O	-0.79500	-3.07600	-19.06600
C	-3.23100	-1.13300	-19.88900
C	-2.05300	-1.03000	-20.86600
C	-2.56100	-1.20900	-22.29800
C	-2.84700	0.16100	-22.91300
N	-3.83100	0.00000	-24.02100
H	-4.59400	-1.57300	-17.73200
H	-4.58000	-0.65700	-23.72800
H	-4.25000	0.92500	-24.25000
H	-3.35000	-0.38000	-24.86000
N	-1.44700	-1.85400	-17.38300
C	-0.10100	-1.87700	-16.78600
C	0.32800	-3.33100	-16.65500
O	1.44000	-3.69300	-16.97700
C	-0.18100	-1.20500	-15.41500
C	0.93300	-1.72200	-14.51300
C	-0.03300	0.30800	-15.59000
H	-2.17600	-1.37200	-16.93200
N	-0.54600	-4.17500	-16.18600
C	-0.15900	-5.60400	-16.03500
C	-0.52400	-6.39900	-17.29000
O	0.04100	-7.44000	-17.55700
C	-0.87000	-6.18100	-14.81300
C	-0.76300	-5.19600	-13.69800
C	-1.76600	-4.39800	-13.27200

C	0.39500	-4.87500	-12.86900
N	-1.30000	-3.61400	-12.23500
C	0.02300	-3.86600	-11.95400
C	1.71600	-5.35600	-12.82000
C	0.92200	-3.34400	-11.02500
C	2.62800	-4.83900	-11.88300
C	2.23100	-3.83300	-10.98700
H	-1.45000	-3.86900	-15.93100
H	-1.82800	-2.95500	-11.74700
N	-1.43800	-5.91500	-18.07700
C	-1.80700	-6.65100	-19.30900
C	-0.66200	-6.50700	-20.28700
O	-0.43000	-7.34700	-21.13400
C	-3.07300	-6.04200	-19.90900
C	-3.37600	-6.71200	-21.25000
C	-4.84800	-6.49600	-21.60700
O	-5.39000	-5.47800	-21.20900
O	-5.40700	-7.35100	-22.27400
H	-1.86200	-5.06200	-17.87400
N	0.06000	-5.43700	-20.16500
C	1.20100	-5.21400	-21.06800
C	2.44600	-5.84600	-20.47400
O	3.20600	-6.50200	-21.15800
C	1.44100	-3.72000	-21.24200
C	1.81800	-3.09400	-19.89700
C	1.55500	-1.58800	-19.94300
O	2.42800	-0.86800	-20.39700
O	0.48500	-1.18000	-19.52300
H	-0.15100	-4.78100	-19.47200
N	2.67300	-5.66000	-19.20500
C	3.89300	-6.27500	-18.60900
C	3.84600	-7.78500	-18.86600
O	4.87000	-8.43200	-18.96200
C	3.95300	-5.99600	-17.10900
C	3.83200	-4.49400	-16.85700
C	2.80900	-6.72600	-16.44000
H	2.04300	-5.12500	-18.65300
N	2.66900	-8.35600	-19.01100
C	2.60300	-9.81900	-19.29700
C	1.92600	-10.00800	-20.66300
O	1.32500	-9.09200	-21.18700
C	1.79100	-10.57200	-18.21600
O	0.65800	-11.14400	-18.83000

C	1.29100	-9.64300	-17.12000
H	1.83400	-7.82300	-18.95700
H	0.15600	-10.41400	-19.21400
N	2.03800	-11.19800	-21.18600
C	1.43000	-11.52800	-22.48400
C	-0.05400	-11.87500	-22.29100
O	-0.80400	-12.00000	-23.23900
C	2.18700	-12.74500	-22.98100
C	2.71900	-13.39500	-21.73500
C	2.74700	-12.35200	-20.62800
N	-0.47000	-12.04200	-21.06400
C	-1.89300	-12.39500	-20.77800
C	-2.84800	-11.41600	-21.46800
O	-2.48500	-10.30600	-21.80500
C	-2.10700	-12.32900	-19.26400
C	-3.59500	-12.44500	-18.93700
C	-4.10200	-13.82700	-19.34400
C	-3.79900	-12.25200	-17.43300
H	0.16200	-11.94400	-20.32300
N	-4.07500	-11.82300	-21.66600
C	-5.07500	-10.92600	-22.31800
C	-6.08700	-10.46200	-21.26600
O	-6.10000	-10.95200	-20.15400
C	-5.80100	-11.69800	-23.42400
O	-6.90900	-12.39100	-22.86500
C	-4.84000	-12.70000	-24.06600
H	-4.34300	-12.72200	-21.37500
H	-7.55000	-11.73900	-22.57400
N	-6.93100	-9.51900	-21.59500
C	-7.91700	-9.03900	-20.58900
C	-9.19000	-8.52400	-21.27200
O	-9.14900	-7.95200	-22.34400
C	-7.28200	-7.90500	-19.78800
C	-6.26100	-8.47200	-18.83300
C	-4.94500	-8.68200	-19.26100
C	-6.62900	-8.79100	-17.52000
C	-3.99600	-9.20900	-18.37600
C	-5.68000	-9.31800	-16.63600
C	-4.36400	-9.52700	-17.06400
H	-6.90800	-9.12300	-22.48900
N	-10.31700	-8.70700	-20.63600
C	-11.60400	-8.21800	-21.20300
C	-12.27500	-7.33700	-20.14800

O	-11.69700	-7.06400	-19.11900
C	-12.50100	-9.41300	-21.53000
O	-13.85200	-8.97900	-21.60600
H	-10.31400	-9.15600	-19.76500
H	-14.41700	-9.73600	-21.43700
N	-13.47500	-6.88400	-20.37500
C	-14.12500	-6.02000	-19.34700
C	-15.63700	-6.21900	-19.34200
O	-16.21000	-6.77100	-20.26000
C	-13.81500	-4.55900	-19.65800
C	-14.11300	-4.27500	-21.13100
C	-14.97600	-3.01600	-21.24200
N	-14.22100	-1.85700	-20.69100
C	-14.81700	-0.70700	-20.52100
N	-16.07600	-0.56700	-20.83700
N	-14.15100	0.30500	-20.03500
H	-13.94300	-7.10400	-21.20800
H	-13.27600	-1.95700	-20.45300
H	-16.58900	-1.34000	-21.21000
H	-16.52800	0.31500	-20.70500
H	-13.18700	0.19900	-19.79300
H	-14.60600	1.18600	-19.90400
N	-16.28400	-5.76800	-18.30200
C	-17.75400	-5.91600	-18.21100
C	-18.28300	-4.98900	-17.11200
O	-17.60500	-4.08400	-16.66700
C	-18.07700	-7.37100	-17.86900
C	-17.11200	-7.87100	-16.79300
C	-17.89800	-8.24300	-15.53400
C	-16.37100	-9.10600	-17.31100
H	-15.79900	-5.33000	-17.57500
N	-19.48500	-5.21400	-16.66900
C	-20.07300	-4.36400	-15.59700
C	-21.23800	-5.12700	-14.97000
O	-22.18400	-4.55000	-14.47200
C	-20.58000	-3.05600	-16.20800
C	-21.22600	-2.21600	-15.13200
C	-20.53000	-1.93700	-13.95000
C	-22.52200	-1.71800	-15.31600
C	-21.12900	-1.16000	-12.95100
C	-23.12100	-0.94000	-14.31700
C	-22.42400	-0.66100	-13.13500
O	-23.01500	0.10500	-12.15200

H	-20.00500	-5.95000	-17.04000
H	-23.30800	0.92700	-12.55100
N	-21.16900	-6.42800	-15.00100
C	-22.26000	-7.25800	-14.42200
C	-21.66000	-8.51600	-13.79500
O	-20.46600	-8.73500	-13.85100
C	-23.22700	-7.66100	-15.53800
C	-22.51400	-8.58600	-16.52900
C	-21.92800	-7.75500	-17.67200
O	-21.12100	-6.88300	-17.39100
O	-22.29400	-8.00400	-18.80900
H	-20.39200	-6.86200	-15.41400
N	-22.47900	-9.34800	-13.21200
C	-21.96100	-10.59900	-12.58800
C	-20.64500	-10.30700	-11.86700
O	-20.63300	-9.84100	-10.74500
H	-23.43900	-9.15200	-13.18800
N	-19.53600	-10.57400	-12.50300
C	-18.22600	-10.30500	-11.84500
C	-17.07600	-10.72200	-12.76600
O	-16.96100	-11.86800	-13.15200
C	-18.15400	-11.10400	-10.54300
C	-18.60200	-12.54300	-10.80100
C	-18.88600	-13.23900	-9.46800
O	-19.44500	-12.59600	-8.59500
O	-18.54000	-14.40100	-9.34300
H	-19.56700	-10.94500	-13.41000
N	-16.21100	-9.80200	-13.10600
C	-15.05700	-10.15100	-13.98400
C	-13.99900	-10.86600	-13.15600
O	-14.29500	-11.51600	-12.17300
C	-14.46000	-8.86900	-14.56500
H	-16.31500	-8.88400	-12.77200
N	-12.76900	-10.74200	-13.54400
C	-11.67800	-11.40300	-12.78100
C	-11.18200	-10.44400	-11.70400
O	-10.85500	-10.85000	-10.61200
C	-10.53000	-11.74600	-13.73200
C	-9.50700	-12.61900	-13.00300
O	-8.61000	-12.06000	-12.39200
O	-9.63700	-13.83000	-13.06800
H	-12.56200	-10.20300	-14.33700
N	-11.14300	-9.17300	-12.02000

C	-10.68300	-8.13300	-11.04000
C	-11.79300	-7.09900	-10.87300
O	-11.79100	-6.06600	-11.51400
C	-9.44900	-7.43400	-11.60300
C	-8.42900	-8.48000	-12.05800
C	-8.83000	-6.55100	-10.52000
C	-8.70300	-8.85800	-13.51400
H	-11.43000	-8.89400	-12.91800
N	-12.74500	-7.36100	-10.02700
C	-13.84500	-6.37800	-9.84000
C	-13.27200	-5.09700	-9.23600
O	-13.06800	-5.00500	-8.04100
C	-14.89200	-6.96800	-8.89400
C	-16.22500	-6.24800	-9.09400
S	-17.11500	-6.18100	-7.51900
C	-17.69300	-7.89500	-7.51300
H	-12.73700	-8.20000	-9.51700
N	-13.00500	-4.10700	-10.04100
C	-12.45200	-2.83900	-9.49100
C	-13.61900	-2.00500	-8.97000
O	-14.43000	-1.54000	-9.73400
C	-11.73600	-2.06600	-10.60500
C	-10.99600	-3.03400	-11.53500
C	-10.73100	-1.09800	-9.98300
C	-9.91400	-3.77700	-10.75100
H	-13.17400	-4.19200	-11.00400
N	-13.73600	-1.81600	-7.68700
C	-14.89400	-1.01800	-7.18900
C	-14.46600	0.02000	-6.15400
O	-13.48800	-0.13100	-5.45900
C	-15.91200	-1.95600	-6.56100
O	-15.79900	-3.24300	-7.15400
H	-13.08500	-2.20500	-7.06200
H	-16.68200	-3.60900	-7.24000
N	-15.21500	1.07700	-6.04400
C	-14.87200	2.13700	-5.05200
C	-15.56200	1.84100	-3.71900
O	-16.69000	1.39100	-3.68100
C	-15.34400	3.49200	-5.58400
C	-16.85300	3.54300	-5.57500
C	-17.53900	3.78300	-4.37900
C	-17.56600	3.35300	-6.76500
C	-18.93800	3.83300	-4.37300

C	-18.96500	3.40200	-6.75800
C	-19.65200	3.64300	-5.56200
H	-16.01000	1.16800	-6.61200
N	-14.89200	2.08700	-2.62400
C	-15.53400	1.80700	-1.29300
C	-14.71100	2.41200	-0.14700
O	-13.68200	3.01500	-0.36400
C	-15.63100	0.29200	-1.10200
H	-13.97500	2.45000	-2.68200
N	-15.15200	2.24700	1.07300
C	-14.39400	2.81000	2.23400
C	-14.64800	1.94000	3.47300
O	-15.11700	0.82500	3.36800
C	-14.87000	4.25300	2.47400
C	-16.12900	4.26200	3.34800
C	-13.76200	5.04900	3.16600
H	-15.98300	1.75100	1.22800
N	-14.33800	2.43600	4.64100
C	-14.55900	1.63500	5.87800
C	-16.02700	1.20500	5.96200
O	-16.83300	1.84000	6.61300
C	-14.20400	2.49300	7.09500
C	-14.99700	3.80100	7.04600
C	-14.05600	4.98100	7.29700
N	-14.86000	6.17100	7.69600
C	-15.35900	6.25300	8.90100
N	-15.16100	5.29000	9.76000
N	-16.05600	7.30100	9.24700
H	-13.95600	3.33500	4.70500
H	-15.01300	6.89500	7.05300
H	-14.62800	4.48500	9.49800
H	-15.54400	5.35600	10.68200
H	-16.20900	8.03900	8.58900
H	-16.43800	7.36500	10.16900
N	-16.37900	0.13200	5.30800
C	-17.79200	-0.33900	5.34900
C	-17.93500	-1.60600	4.50100
O	-18.96700	-1.85400	3.90800
C	-18.70100	0.75700	4.78800
C	-19.96000	0.86700	5.64900
C	-21.18600	0.51500	4.80500
O	-21.19100	-0.55600	4.22000
O	-22.10000	1.32200	4.75800

H	-15.71300	-0.36600	4.79000
N	-16.90800	-2.40800	4.43800
C	-16.98700	-3.65700	3.62700
C	-17.87300	-4.67600	4.34600
O	-18.66400	-5.36700	3.73500
C	-15.58000	-4.23500	3.45600
C	-14.72800	-3.27700	2.66700
N	-14.29200	-2.07100	3.19200
C	-14.21600	-3.34000	1.39400
C	-13.55100	-1.46300	2.24800
N	-13.47100	-2.19300	1.13100
H	-16.08600	-2.19100	4.92300
H	-14.48600	-1.72500	4.08800
N	-17.74600	-4.77700	5.64100
C	-18.57900	-5.75400	6.40000
C	-17.84100	-6.17400	7.67200
O	-18.25700	-5.86900	8.77200
H	-17.10100	-4.21200	6.11500
N	-16.74700	-6.87200	7.53100
C	-15.98100	-7.31000	8.73200
C	-14.54500	-7.64600	8.32500
O	-13.86900	-8.42000	8.97400
C	-16.65000	-8.55200	9.32600
C	-17.07400	-8.26400	10.76700
O	-16.33100	-7.58800	11.45800
O	-18.13500	-8.72500	11.15500
H	-16.42800	-7.10600	6.63500
N	-14.07400	-7.06900	7.25400
C	-12.68300	-7.35400	6.80200
C	-12.15000	-6.15800	6.00700
O	-12.74200	-5.09900	6.02300
C	-12.69700	-8.60000	5.91100
C	-12.81700	-9.83300	6.77400
C	-11.67000	-10.41700	7.32500
C	-14.07500	-10.39300	7.02300
C	-11.78200	-11.56100	8.12400
C	-14.18700	-11.53700	7.82200
C	-13.04000	-12.12100	8.37300
H	-14.63700	-6.44900	6.74500
N	-11.04100	-6.34400	5.32000
C	-10.40600	-5.25500	4.49200
C	-11.17900	-3.93700	4.58700
O	-11.79700	-3.50700	3.63300

C	-10.37100	-5.70900	3.02800
C	-11.53800	-6.63200	2.75300
C	-12.79300	-6.10000	2.43300
C	-11.36300	-8.01800	2.82600
C	-13.87200	-6.95700	2.18400
C	-12.44200	-8.87500	2.57700
C	-13.69800	-8.34300	2.25600
O	-14.76200	-9.18700	2.01100
H	-10.61200	-7.22400	5.34700
H	-14.45600	-10.09000	2.12300
N	-11.11200	-3.33600	5.74600
C	-11.79900	-2.06100	5.99100
C	-10.97200	-0.90700	5.41600
O	-9.81300	-0.74300	5.74100
C	-11.89100	-1.93100	7.49900
C	-10.75900	-2.77600	8.01700
C	-10.39500	-3.78900	6.94400
N	-11.55500	-0.10100	4.57200
C	-10.79500	1.03700	3.99400
C	-10.71300	2.16500	5.01300
O	-11.05200	2.00400	6.16900
C	-11.52400	1.54600	2.76600
C	-10.83800	1.08000	1.51300
C	-10.88500	-0.26200	1.13400
C	-10.17900	2.00700	0.71000
C	-10.27300	-0.66800	-0.05400
C	-9.57100	1.59800	-0.47600
C	-9.62500	0.25700	-0.85500
H	-12.49400	-0.23900	4.32000
N	-10.26500	3.31000	4.58800
C	-10.15500	4.45300	5.51800
C	-9.57500	5.66700	4.79200
O	-8.54300	6.17100	5.18400
C	-9.21800	4.06200	6.64600
C	-7.89600	3.56800	6.05500
O	-7.45000	4.15100	5.07800
O	-7.35300	2.61600	6.59000
H	-9.99900	3.41100	3.65900
N	-10.22300	6.13100	3.74200
C	-9.70200	7.32300	2.97300
C	-8.73000	8.14300	3.82200
O	-7.58000	8.30000	3.46200
H	-11.05600	5.68600	3.44700

N	-9.20800	8.61800	4.94000
C	-8.35900	9.39700	5.85700
C	-7.34700	8.46000	6.52200
O	-7.27100	8.36500	7.73000
C	-9.30300	9.98900	6.89000
C	-10.48300	9.06500	6.86800
C	-10.57400	8.48800	5.46800
N	-6.57600	7.76100	5.73300
C	-5.57400	6.81900	6.30000
C	-4.66800	6.31600	5.17400
O	-5.03300	6.33600	4.01400
H	-6.65800	7.85200	4.76300
N	-3.48800	5.87500	5.50600
C	-2.54700	5.38100	4.46100
C	-3.23000	4.33600	3.57100
O	-2.94500	4.23800	2.39600
C	-1.33500	4.75200	5.14700
C	-0.48900	5.84900	5.79500
O	-0.29400	6.90100	5.22100
N	0.02700	5.64600	6.97600
H	-3.21500	5.87500	6.44800
H	-0.13000	4.79800	7.44100
H	0.57100	6.34300	7.40000
N	-4.11700	3.54700	4.11900
C	-4.79900	2.50500	3.29100
C	-5.47200	3.15400	2.07700
O	-6.64500	3.47000	2.09400
C	-5.85000	1.79000	4.14200
C	-6.22200	0.46000	3.48400
C	-5.28100	1.52500	5.53800
H	-4.32800	3.63400	5.07200
N	-4.72500	3.36100	1.02700
C	-5.29700	4.00000	-0.20100
C	-6.20300	3.02400	-0.98600
O	-7.28100	3.38700	-1.40400
C	-4.14400	4.45200	-1.09800
C	-4.27400	5.95000	-1.37400
C	-3.66700	6.74000	-0.21400
C	-3.52900	6.29100	-2.66400
H	-3.78200	3.11200	1.05300
N	-5.78100	1.80000	-1.21200
C	-6.66200	0.86700	-1.98600
C	-6.15400	-0.58100	-1.92000

O	-5.15000	-0.87200	-1.31400
C	-6.70000	1.32300	-3.44200
H	-4.90400	1.50700	-0.88800
N	-6.83400	-1.50800	-2.55300
C	-6.33000	-2.91700	-2.50700
C	-7.25500	-3.86100	-3.27200
O	-8.36100	-3.51200	-3.63200
C	-6.20100	-3.38500	-1.04600
C	-7.51900	-3.27400	-0.31100
N	-7.66600	-2.48000	0.82000
C	-8.73800	-3.88400	-0.49800
C	-8.92900	-2.63100	1.26800
N	-9.62700	-3.48100	0.50000
H	-7.64900	-1.28000	-3.06300
H	-6.97500	-1.91100	1.22000
N	-6.80100	-5.06400	-3.52100
C	-7.64000	-6.03600	-4.26000
C	-7.65300	-7.38500	-3.52800
O	-7.21500	-7.48000	-2.39800
C	-7.08200	-6.20700	-5.67600
H	-5.91100	-5.32200	-3.22300
N	-8.16300	-8.43300	-4.14000
C	-8.19800	-9.73900	-3.42400
C	-7.21100	-10.72300	-4.05500
O	-6.35300	-10.35300	-4.83300
C	-9.61400	-10.30800	-3.49700
C	-10.53900	-9.48500	-2.63300
C	-10.99200	-8.24300	-3.08400
C	-10.94600	-9.96600	-1.38300
C	-11.85300	-7.47900	-2.28900
C	-11.80700	-9.20300	-0.58600
C	-12.26000	-7.95800	-1.03900
O	-13.11100	-7.20700	-0.25600
H	-8.53800	-8.35900	-5.06000
H	-14.01300	-7.43100	-0.49600
N	-7.32400	-11.97800	-3.71300
C	-6.39900	-13.00400	-4.27000
C	-7.21700	-14.06500	-5.01400
O	-8.39900	-13.88500	-5.22800
C	-5.63500	-13.64200	-3.11000
H	-8.02100	-12.24800	-3.08200
N	-6.57000	-15.14100	-5.39300
C	-7.26100	-16.21500	-6.12100

C	-8.14800	-17.02300	-5.17000
O	-7.67300	-17.71300	-4.29100
C	-6.16800	-17.08900	-6.70800
C	-4.98300	-16.84300	-5.82400
C	-5.14900	-15.46900	-5.19300
N	-9.43900	-16.93800	-5.34700
C	-10.37300	-17.69500	-4.46700
C	-11.70900	-17.87600	-5.19200
O	-11.74000	-18.11600	-6.38200
H	-9.79600	-16.37600	-6.06700
N	-12.77300	-17.75200	-4.44600
C	-14.12600	-17.89700	-5.01000
C	-14.47100	-16.67500	-5.87000
O	-14.14800	-16.61900	-7.04100
C	-15.06000	-17.99400	-3.81600
C	-14.30800	-17.31200	-2.71100
C	-12.82600	-17.46600	-3.00600
N	-15.11800	-15.69300	-5.30200
C	-15.47200	-14.47900	-6.09100
C	-14.36700	-13.44300	-5.93400
O	-14.12900	-12.62700	-6.80900
H	-15.36700	-15.75100	-4.35500
N	-13.66500	-13.48900	-4.83500
C	-12.55400	-12.52300	-4.63000
C	-11.37600	-12.92900	-5.52000
O	-10.29600	-12.38800	-5.40400
C	-12.13700	-12.49800	-3.14300
C	-10.93200	-13.41800	-2.90100
C	-13.30400	-12.95800	-2.26400
C	-10.62900	-13.47900	-1.40300
H	-13.85900	-14.16900	-4.15800
N	-11.58200	-13.87300	-6.40800
C	-10.48800	-14.30600	-7.32200
C	-10.10100	-13.11700	-8.20200
O	-10.26200	-13.14400	-9.40600
C	-11.01300	-15.44700	-8.19900
C	-9.86500	-16.37400	-8.59900
O	-9.29800	-17.05200	-7.76800
N	-9.50100	-16.43500	-9.85100
H	-12.46400	-14.29500	-6.48000
H	-9.96200	-15.89100	-10.52300
H	-8.76600	-17.02600	-10.11900
N	-9.62300	-12.06200	-7.60400

C	-9.25700	-10.85900	-8.38800
C	-10.34000	-9.79500	-8.18200
O	-11.41700	-9.85600	-8.73500
H	-9.52300	-12.05500	-6.62600
N	-10.06500	-8.81800	-7.38600
C	-11.06800	-7.75300	-7.14400
C	-10.33600	-6.57100	-6.53200
O	-9.77700	-6.68900	-5.47700
C	-12.11400	-8.27200	-6.15700
C	-13.05700	-9.25200	-6.85600
O	-12.72900	-10.42600	-6.90500
O	-14.09500	-8.81600	-7.32200
H	-9.19600	-8.77900	-6.94000
N	-10.32500	-5.43800	-7.16700
C	-9.60300	-4.28700	-6.57300
C	-10.61300	-3.25600	-6.12800
O	-11.76600	-3.30500	-6.50100
C	-8.68000	-3.66200	-7.61700
H	-10.79400	-5.33800	-8.02600
N	-10.19800	-2.30900	-5.35000
C	-11.15500	-1.27600	-4.91900
C	-10.38700	-0.02500	-4.48500
O	-9.39600	-0.08400	-3.78900
C	-12.05700	-1.85100	-3.80300
C	-12.39200	-0.81400	-2.76200
N	-12.59400	-1.14200	-1.42800
C	-12.55200	0.54600	-2.83900
C	-12.85400	0.00200	-0.76900
N	-12.82700	1.05300	-1.58300
H	-9.26200	-2.27100	-5.06600
H	-12.89300	1.99300	-1.33300
N	-10.85900	1.10500	-4.93800
C	-10.21000	2.41200	-4.61700
C	-10.87000	3.05600	-3.39600
O	-12.07900	3.09100	-3.28400
C	-10.42300	3.35800	-5.79700
C	-9.63200	2.89600	-6.99500
C	-8.29300	2.52000	-6.85500
C	-10.24600	2.84300	-8.25100
C	-7.56800	2.09000	-7.97300
C	-9.52300	2.41500	-9.36800
C	-8.18400	2.03800	-9.22900
H	-11.65800	1.09000	-5.51000

N	-10.09800	3.60700	-2.49500
C	-10.72600	4.27500	-1.32200
C	-11.79000	5.25000	-1.82700
O	-11.69500	5.76800	-2.91700
C	-9.65900	5.04800	-0.54700
C	-10.15800	5.32500	0.86700
O	-11.21100	5.92800	0.99800
O	-9.47600	4.92700	1.79700
H	-9.11700	3.60000	-2.59900
N	-12.80400	5.49900	-1.05200
C	-13.86800	6.43500	-1.50500
C	-14.03400	7.55400	-0.47800
O	-15.05100	8.21500	-0.42600
C	-15.18400	5.66800	-1.64400
C	-16.00500	6.26400	-2.78800
O	-15.50500	6.28900	-3.90000
O	-17.12200	6.68500	-2.53300
H	-12.87200	5.06600	-0.17500
N	-13.04100	7.77300	0.34000
C	-13.15400	8.85100	1.35800
C	-12.24900	10.02700	0.97100
O	-12.40600	11.12400	1.46900
C	-12.74500	8.30600	2.72500
C	-13.97400	8.22500	3.63200
O	-15.07400	8.19300	3.10400
O	-13.79600	8.19700	4.83800
H	-12.22600	7.23100	0.28500
N	-11.30800	9.82100	0.08000
C	-10.42300	10.94300	-0.32800
C	-10.72500	11.28600	-1.79000
O	-11.68000	11.97700	-2.08400
C	-8.94800	10.53200	-0.15700
C	-8.81500	9.00200	-0.12200
C	-7.44100	8.61600	0.43200
O	-6.47100	9.25500	0.05700
O	-7.38100	7.68500	1.22400
H	-11.18900	8.93600	-0.32900
N	-9.93900	10.80100	-2.70900
C	-10.20300	11.08700	-4.14500
C	-9.12000	10.43400	-4.98800
O	-8.08900	10.03900	-4.49200
C	-10.17900	12.59200	-4.38300
C	-11.60900	13.10800	-4.53800

C	-11.71400	14.50900	-3.93300
O	-11.21800	15.46500	-4.49500
N	-12.34400	14.67100	-2.80200
H	-9.18400	10.23500	-2.46000
H	-12.74400	13.90000	-2.34800
H	-12.41600	15.56400	-2.40500
N	-9.33700	10.32500	-6.26100
C	-8.30800	9.70600	-7.13400
C	-8.18200	10.52200	-8.42000
O	-9.15900	10.84100	-9.06600
C	-8.69900	8.26300	-7.48000
C	-9.66300	7.72000	-6.47300
C	-9.44900	7.67400	-5.13800
C	-10.97900	7.13500	-6.69600
N	-10.55700	7.11900	-4.52700
C	-11.52500	6.76600	-5.44500
C	-11.74500	6.89700	-7.85000
C	-12.78900	6.18100	-5.34300
C	-13.01500	6.30800	-7.75100
C	-13.53600	5.95100	-6.50000
H	-10.17000	10.65900	-6.64100
H	-10.66000	6.98000	-3.56200
N	-6.98200	10.85700	-8.79200
C	-6.77200	11.64600	-10.03600
C	-5.68100	10.98100	-10.85500
O	-4.76800	10.37800	-10.32700
C	-6.34200	13.06400	-9.67300
O	-5.19300	12.99900	-8.84700
C	-7.47700	13.77300	-8.93200
H	-6.21200	10.58600	-8.25200
H	-4.74400	12.17300	-9.04300
N	-5.75700	11.10400	-12.13900
C	-4.71400	10.50100	-12.99500
C	-3.48200	11.37000	-12.86300
O	-2.37100	10.90000	-12.78700
C	-5.19100	10.48200	-14.44800
C	-5.34100	11.91800	-14.95500
C	-5.78400	11.89800	-16.41900
C	-6.14000	13.31700	-16.86400
N	-6.05300	13.39700	-18.34900
H	-6.48500	11.61400	-12.53700
H	-6.09000	12.43800	-18.75100
H	-6.85000	13.95700	-18.71300

H	-5.16000	13.85500	-18.62100
N	-3.68500	12.64700	-12.78100
C	-2.54000	13.55800	-12.61400
C	-2.20400	13.59400	-11.13800
O	-2.42200	12.63800	-10.42300
C	-2.92800	14.95900	-13.09300
C	-1.67900	15.70300	-13.56700
O	-1.13200	15.31200	-14.58600
O	-1.29100	16.65100	-12.90500
H	-4.59700	13.00200	-12.78900
N	-1.70800	14.68200	-10.65300
C	-1.40900	14.73800	-9.21100
C	-2.39100	15.71900	-8.56600
O	-2.01200	16.59200	-7.81200
C	0.03000	15.21600	-8.99800
O	0.93100	14.22000	-9.46200
C	0.27300	15.47200	-7.51000
H	-1.55400	15.46200	-11.22800
H	0.75900	13.41400	-8.97100
N	-3.65300	15.60300	-8.89300
C	-4.65500	16.54800	-8.34000
C	-5.38900	15.94500	-7.14000
O	-5.78400	16.65500	-6.23600
C	-5.67300	16.88000	-9.43100
O	-4.99700	17.42500	-10.55600
C	-6.68200	17.89700	-8.89600
H	-3.93500	14.91200	-9.52300
H	-4.76500	16.70200	-11.14300
N	-5.59500	14.65700	-7.11300
C	-6.32500	14.07100	-5.95100
C	-5.42000	13.08500	-5.22800
O	-4.73900	13.42500	-4.28100
H	-5.28000	14.07700	-7.85200
N	-5.39500	11.87000	-5.68200
C	-4.52300	10.85700	-5.04400
C	-3.59400	10.30800	-6.12100
O	-2.59400	10.91200	-6.45500
C	-5.38400	9.72900	-4.45800
O	-6.12700	10.21800	-3.34900
C	-4.48600	8.58300	-3.99800
H	-5.94100	11.62700	-6.46100
H	-6.96000	9.73100	-3.31100
N	-3.92000	9.17900	-6.68300

C	-3.07800	8.60100	-7.74400
C	-3.93800	7.59700	-8.51600
O	-3.73300	6.40200	-8.43700
C	-1.88700	7.90000	-7.10100
C	-1.32700	8.74200	-5.95400
O	-1.75600	8.61400	-4.82600
N	-0.37900	9.60700	-6.19600
H	-4.72900	8.70900	-6.41700
H	-0.03400	9.71300	-7.10700
H	-0.01400	10.14900	-5.46600
N	-4.92100	8.09000	-9.23200
C	-5.84700	7.21100	-9.99800
C	-5.15800	5.91300	-10.45300
O	-5.08400	4.94700	-9.71600
C	-6.35400	8.01000	-11.20700
C	-7.40100	7.21700	-11.96300
C	-8.41700	6.65100	-10.96600
C	-8.10800	8.15300	-12.93900
H	-5.07000	9.06000	-9.25300
N	-4.68700	5.86800	-11.66600
C	-4.04600	4.62600	-12.17700
C	-2.88300	4.20000	-11.28400
O	-2.49700	3.04900	-11.28200
C	-3.61200	4.86600	-13.64000
C	-2.16200	4.46800	-13.87700
C	-1.74100	3.15400	-13.64200
C	-1.24500	5.41800	-14.34000
C	-0.40800	2.79100	-13.86600
C	0.08900	5.05600	-14.56500
C	0.50800	3.74300	-14.32700
H	-4.77800	6.64200	-12.25200
N	-2.33200	5.06700	-10.49300
C	-1.22900	4.59100	-9.63600
C	-1.78200	3.48600	-8.75000
O	-1.37800	2.34000	-8.82300
C	-0.72500	5.74200	-8.77800
C	0.71200	5.48600	-8.32600
C	1.63700	5.47100	-9.54200
C	1.14300	6.60500	-7.37400
H	-2.65100	5.99900	-10.43900
N	-2.73000	3.82400	-7.93100
C	-3.34600	2.80700	-7.05100
C	-4.20100	1.87600	-7.90000

O	-4.67000	0.85700	-7.43400
C	-4.22300	3.50200	-6.01600
C	-4.31800	2.62200	-4.77700
C	-3.60500	4.85000	-5.63600
H	-3.05000	4.75000	-7.90800
N	-4.39000	2.19000	-9.15400
C	-5.19300	1.28500	-10.00200
C	-4.30400	0.11200	-10.35400
O	-4.60300	-1.01400	-10.02300
C	-5.64800	2.01100	-11.26200
H	-3.98300	2.99800	-9.53600
N	-3.17900	0.35300	-10.97300
C	-2.29000	-0.77100	-11.25700
C	-1.82200	-1.29000	-9.92100
O	-1.34000	-2.39500	-9.81100
C	-1.10500	-0.30700	-12.10100
H	-2.90600	1.25900	-11.20400
N	-2.01100	-0.53700	-8.88100
C	-1.61100	-1.06900	-7.56000
C	-2.55300	-2.22500	-7.21300
O	-2.12100	-3.29500	-6.83400
C	-1.70400	0.02600	-6.50000
C	-0.94500	-0.41300	-5.27900
N	0.36900	-0.04200	-5.05500
C	-1.29900	-1.20700	-4.21900
C	0.75800	-0.61000	-3.89700
N	-0.22200	-1.33200	-3.34500
H	-2.44300	0.35200	-8.96600
H	0.91200	0.53800	-5.62700
N	-3.83800	-2.02200	-7.34300
C	-4.80100	-3.11100	-7.02700
C	-4.91200	-4.10800	-8.19400
O	-4.86600	-5.30500	-7.99300
C	-6.17100	-2.50100	-6.72500
C	-5.99900	-1.31900	-5.77100
C	-6.78700	-0.12000	-6.29800
O	-7.72800	-0.33600	-7.04400
O	-6.43700	0.99300	-5.94700
H	-4.16900	-1.15500	-7.64100
N	-5.03700	-3.63900	-9.41300
C	-5.11900	-4.59000	-10.55300
C	-3.81600	-5.35500	-10.57400
O	-3.74200	-6.51100	-10.93000

C	-5.30600	-3.78700	-11.83700
C	-6.58500	-2.96700	-11.67200
C	-5.39100	-4.73100	-13.04100
C	-7.19900	-2.61700	-13.03000
H	-5.04700	-2.66800	-9.58500
N	-2.79100	-4.69600	-10.14700
C	-1.45500	-5.33500	-10.07600
C	-1.44300	-6.25800	-8.87400
O	-0.79100	-7.28500	-8.85900
H	-2.91000	-3.75700	-9.84200
N	-2.17100	-5.89700	-7.87300
C	-2.22700	-6.73600	-6.64700
C	-2.78900	-8.12300	-6.95900
O	-2.24700	-9.13000	-6.54900
C	-3.15200	-6.06100	-5.65100
C	-2.38500	-5.69600	-4.41000
N	-2.89500	-5.89300	-3.13600
C	-1.14500	-5.13100	-4.23300
C	-1.97300	-5.45200	-2.25800
N	-0.88700	-4.97800	-2.87400
H	-2.69000	-5.05800	-7.92700
H	-3.76600	-6.28200	-2.91500
N	-3.90100	-8.18600	-7.63900
C	-4.52400	-9.51400	-7.92200
C	-3.95500	-10.16300	-9.19100
O	-3.53400	-11.30200	-9.17700
C	-6.02900	-9.31700	-8.09800
O	-6.61400	-9.01800	-6.83800
H	-4.34700	-7.35900	-7.93100
H	-7.23000	-8.29200	-6.96200
N	-3.96200	-9.46600	-10.29100
C	-3.44400	-10.07500	-11.56100
C	-2.06600	-9.51800	-11.90000
O	-1.66700	-9.48500	-13.04600
C	-4.41500	-9.78900	-12.71900
C	-4.68100	-8.28500	-12.84700
C	-3.43100	-7.57600	-13.37400
C	-5.83400	-8.06200	-13.82600
H	-4.30500	-8.55000	-10.27900
N	-1.34800	-9.05600	-10.92800
C	-0.01400	-8.47400	-11.21300
C	1.04500	-9.13600	-10.33800
O	1.77100	-10.00200	-10.77400

H	-1.69100	-9.06500	-10.00800
N	1.14700	-8.73600	-9.10700
C	2.18200	-9.35100	-8.23100
C	1.95400	-8.94200	-6.77600
O	0.88800	-8.49500	-6.40400
C	3.55800	-8.86000	-8.69100
C	3.60500	-7.33100	-8.60900
C	4.07500	-6.90800	-7.21700
C	4.58000	-6.79600	-9.65900
H	0.55200	-8.03400	-8.76400
N	2.95400	-9.09600	-5.95000
C	2.80100	-8.72100	-4.51500
C	3.42300	-7.34400	-4.27700
O	2.72800	-6.36600	-4.08300
C	3.51200	-9.76200	-3.64900
C	2.73000	-9.97500	-2.37500
C	1.42600	-10.48000	-2.43100
C	3.30900	-9.66900	-1.13800
C	0.70000	-10.67900	-1.25000
C	2.58500	-9.86700	0.04300
C	1.28000	-10.37200	-0.01200
H	3.80600	-9.46100	-6.27400
N	4.72600	-7.25700	-4.28800
C	5.38500	-5.94000	-4.06000
C	6.82800	-5.98800	-4.57300
O	7.70900	-6.52100	-3.92900
C	5.38000	-5.63300	-2.56000
C	3.98700	-5.25900	-2.13000
N	3.07500	-6.20000	-1.67900
C	3.33500	-4.05100	-2.07900
C	1.93400	-5.55000	-1.38000
N	2.03900	-4.23700	-1.60500
H	5.26900	-8.05700	-4.44600
H	3.23000	-7.16500	-1.59400
N	7.07300	-5.42900	-5.72800
C	8.45800	-5.43500	-6.28600
C	9.17100	-4.14500	-5.87900
O	8.62100	-3.31000	-5.19200
C	8.37800	-5.50300	-7.81800
O	8.19500	-6.85500	-8.21700
H	6.34500	-5.00200	-6.22700
H	8.96800	-7.35400	-7.94200
N	10.38500	-3.96300	-6.31300

C	11.10500	-2.70700	-5.96800
C	10.32500	-1.56200	-6.56400
O	10.57200	-1.13400	-7.67400
C	12.52200	-2.73700	-6.54200
H	10.80600	-4.63600	-6.87600
N	9.35300	-1.08200	-5.85100
C	8.54000	0.00400	-6.41200
C	9.11400	1.36100	-6.07200
O	8.51000	2.37400	-6.36600
C	7.09800	-0.08400	-5.95900
C	6.83900	-1.41200	-5.24800
O	6.92700	-1.49500	-4.04000
N	6.52000	-2.46100	-5.95200
H	9.14800	-1.45400	-4.97300
H	6.45000	-2.39500	-6.92700
H	6.34800	-3.31400	-5.50400
N	10.30600	1.41700	-5.53600
C	10.91400	2.75400	-5.29900
C	10.74900	3.49400	-6.62600
O	10.59600	4.69700	-6.69300
C	12.40000	2.59800	-4.95900
O	12.76100	1.22600	-5.04700
C	12.65600	3.10500	-3.53800
H	10.80900	0.59800	-5.35900
H	12.88700	1.01200	-5.97400
N	10.71400	2.71500	-7.68400
C	10.48600	3.24600	-9.04100
C	9.16400	2.66000	-9.55300
O	8.42700	3.30000	-10.27700
C	11.61700	2.78200	-9.96200
C	12.96000	2.93900	-9.24600
C	14.03600	3.33100	-10.26000
O	14.10800	2.69200	-11.29700
O	14.77000	4.26600	-9.98300
H	10.80200	1.74800	-7.56900
N	8.88000	1.42000	-9.20700
C	7.62700	0.76500	-9.70700
C	6.35800	1.45200	-9.20400
O	6.37700	2.54300	-8.66800
C	7.60600	-0.70600	-9.29300
H	9.51300	0.90700	-8.64500
N	5.24900	0.80900	-9.44200
C	3.91500	1.36700	-9.06800

C	3.48600	0.94400	-7.65600
O	2.56500	1.48900	-7.09900
C	2.89200	0.82100	-10.07000
C	1.69900	1.78700	-10.27900
C	1.37000	2.53200	-8.99000
C	2.05300	2.80000	-11.37000
H	5.29600	-0.04500	-9.91400
N	4.08200	-0.04000	-7.06900
C	3.57700	-0.43600	-5.72100
C	4.07200	0.51100	-4.61700
O	3.63900	0.41500	-3.48600
C	3.97100	-1.88400	-5.42500
C	2.72400	-2.67200	-5.02800
S	2.73400	-4.27900	-5.86000
C	1.40200	-3.93600	-7.03500
H	4.81300	-0.53400	-7.51200
N	4.95500	1.42400	-4.91300
C	5.42100	2.34900	-3.83100
C	5.53300	3.82800	-4.28400
O	6.14800	4.60700	-3.58300
C	6.78600	1.88100	-3.32400
C	6.94500	2.27500	-1.87500
C	6.04800	1.79300	-0.91600
C	7.99100	3.12500	-1.49300
C	6.19600	2.16000	0.42700
C	8.13900	3.49100	-0.15100
C	7.24100	3.00800	0.81000
O	7.38700	3.37100	2.13300
H	5.30600	1.49500	-5.82000
H	7.18200	4.30500	2.21000
N	4.94400	4.20700	-5.40200
C	5.01900	5.61500	-5.83300
C	4.01900	6.42100	-5.02100
O	4.25800	7.56000	-4.67000
C	4.57900	5.63700	-7.27700
C	3.69600	4.43800	-7.39300
C	4.17100	3.42000	-6.37400
N	2.88900	5.81300	-4.75100
C	1.79200	6.48300	-3.97500
C	2.33400	7.64100	-3.14000
O	1.92800	8.77400	-3.30200
C	1.14600	5.45300	-3.05600
C	-0.35000	5.73600	-2.94300

C	-0.56100	7.13700	-2.36600
C	-0.98900	5.65000	-4.33100
H	2.75600	4.89000	-5.08500
N	3.25100	7.37500	-2.25200
C	3.81500	8.47600	-1.42100
C	4.63900	9.41600	-2.31200
O	5.80800	9.64300	-2.07400
C	4.71400	7.87600	-0.33900
C	5.00900	8.92600	0.70600
C	4.01000	9.32100	1.60300
C	6.28300	9.50200	0.77900
C	4.28400	10.29400	2.57200
C	6.55700	10.47600	1.74800
C	5.55700	10.87100	2.64400
O	5.82700	11.83000	3.59900
H	3.56900	6.45600	-2.13200
H	5.08300	12.43700	3.62800
N	4.03700	9.96000	-3.33900
C	4.77700	10.87900	-4.24800
C	3.83000	11.34500	-5.36800
O	2.77300	11.88300	-5.10200
C	5.97700	10.13100	-4.83700
C	6.93500	11.11800	-5.44500
N	6.54900	12.40100	-5.80100
C	8.26800	11.02600	-5.76300
C	7.62800	13.02300	-6.30900
N	8.70400	12.23000	-6.30800
H	9.64200	12.45800	-6.63600
H	3.09400	9.76500	-3.51200
H	5.65200	12.78500	-5.70200
N	4.18700	11.14600	-6.61400
C	3.29000	11.58000	-7.72500
C	3.67500	10.84000	-9.00900
O	4.79600	10.92700	-9.47100
C	3.44700	13.08600	-7.93400
O	3.24700	13.75600	-6.69700
H	5.03700	10.71100	-6.82100
H	4.09700	13.82200	-6.25400
N	2.75800	10.11400	-9.59300
C	3.08500	9.37700	-10.84700
C	1.86400	8.59200	-11.32900
O	1.96900	7.45400	-11.74100
C	4.24000	8.41100	-10.57400

C	5.35400	8.64700	-11.59600
C	6.67500	8.88900	-10.86400
C	5.48900	7.41700	-12.49600
H	1.85900	10.05800	-9.21000
N	0.70900	9.19500	-11.30000
C	-0.50900	8.48300	-11.77900
C	-0.82400	8.94700	-13.20400
O	-1.64600	8.37700	-13.88800
C	-1.69000	8.79600	-10.85400
O	-2.90300	8.66900	-11.58300
C	-1.56700	10.22000	-10.31500
H	0.64700	10.11900	-10.97900
H	-3.56500	8.29900	-10.99400
N	-0.16100	9.97600	-13.65500
C	-0.39700	10.47700	-15.04100
C	0.49500	11.69100	-15.31600
O	0.80100	11.97200	-16.45500
C	-1.86300	10.87200	-15.22000
C	-2.18200	10.98600	-16.71200
O	-1.93400	10.02800	-17.42600
O	-2.66700	12.02900	-17.11600
H	0.50400	10.41100	-13.08700
N	0.90000	12.41600	-14.28600
C	1.77200	13.62400	-14.48800
C	2.59200	13.51400	-15.78600
O	2.10900	13.82300	-16.85700
C	2.72800	13.75500	-13.29200
C	1.95300	13.84200	-11.96300
C	0.56800	14.47500	-12.16200
C	1.78600	12.43600	-11.38200
H	0.61900	12.17100	-13.36800
N	3.83000	13.09700	-15.70600
C	4.65400	12.99100	-16.94400
C	5.42600	11.66700	-16.95600
O	6.07600	11.33100	-17.92500
C	5.64500	14.15800	-16.98100
O	6.02300	14.49600	-15.65300
C	4.99100	15.36700	-17.65100
H	4.21700	12.86600	-14.84100
H	6.62500	13.82000	-15.33400
N	5.36600	10.91200	-15.89100
C	6.10700	9.61500	-15.86000
C	5.10500	8.47100	-15.70900

O	5.26000	7.41900	-16.29300
C	7.06100	9.60800	-14.66100
C	7.73500	10.97500	-14.52200
C	7.76700	11.37700	-13.04600
N	9.15100	11.19700	-12.52400
C	10.11700	11.97000	-12.94600
N	9.87600	12.89900	-13.83200
N	11.32700	11.81300	-12.48100
H	4.83900	11.19500	-15.11300
H	9.33800	10.49900	-11.86200
H	8.95100	13.02200	-14.19000
H	10.61700	13.48900	-14.15100
H	11.51500	11.10200	-11.80500
H	12.06700	12.40500	-12.80400
N	4.09100	8.70300	-14.91800
C	3.01500	7.68800	-14.65400
C	3.25200	6.36000	-15.38700
O	2.98100	6.22000	-16.56300
C	1.67900	8.27800	-15.10000
C	1.63200	8.36800	-16.60700
C	2.41800	9.31500	-17.27700
C	0.80400	7.50500	-17.33500
C	2.37500	9.39800	-18.67400
C	0.76200	7.58800	-18.73300
C	1.54800	8.53500	-19.40100
H	4.03300	9.57700	-14.47500
N	3.73200	5.37500	-14.67900
C	3.96200	4.03400	-15.30300
C	4.56400	3.08200	-14.26900
O	4.87800	3.47200	-13.16200
C	4.88700	4.16800	-16.53000
C	6.37400	4.08700	-16.14200
C	6.93700	5.49800	-15.96700
N	8.40400	5.40600	-15.71400
C	9.17600	6.43700	-15.93700
N	8.67000	7.55800	-16.37700
N	10.46000	6.34700	-15.71600
H	3.91600	5.51000	-13.72600
H	8.79100	4.56900	-15.38200
H	7.68800	7.63200	-16.54500
H	9.26600	8.34200	-16.54700
H	10.85100	5.49100	-15.37800
H	11.05300	7.13500	-15.88700

N	4.72800	1.83600	-14.61900
C	5.31300	0.86500	-13.64700
C	6.82700	0.80000	-13.79600
O	7.39200	1.30400	-14.74600
C	4.76000	-0.51900	-13.92700
C	3.72900	-0.85300	-12.87200
C	2.56200	0.12100	-13.01000
C	3.24500	-2.28400	-13.07800
H	4.46300	1.53800	-15.52000
N	7.49100	0.16200	-12.86800
C	8.97800	0.05300	-12.98400
C	9.36600	-1.33100	-13.49100
O	8.53500	-2.11700	-13.91100
C	9.62600	0.27200	-11.62700
O	11.01900	0.00500	-11.71700
H	7.00800	-0.25200	-12.10000
H	11.34000	-0.19100	-10.83300
N	10.63000	-1.63700	-13.44800
C	11.09100	-2.96800	-13.92800
C	10.96600	-3.99600	-12.80800
O	11.05100	-5.18800	-13.03900
C	12.55300	-2.86100	-14.36700
C	13.01800	-4.20800	-14.92500
C	13.72900	-4.99900	-13.82600
O	14.53300	-4.45800	-13.09300
N	13.46600	-6.26900	-13.67900
H	11.27900	-0.98400	-13.09400
H	12.81700	-6.70600	-14.27000
H	13.91500	-6.78500	-12.97700
N	10.74700	-3.56500	-11.59800
C	10.61200	-4.52500	-10.50600
C	9.16300	-4.99700	-10.48000
O	8.90300	-6.18400	-10.44800
C	11.02500	-3.83400	-9.21000
C	12.24900	-4.55400	-8.63900
O	12.07400	-5.61800	-8.06900
O	13.34000	-4.02800	-8.78100
H	10.65600	-2.61700	-11.40600
N	8.20100	-4.10600	-10.53800
C	6.80700	-4.60800	-10.56500
C	6.63300	-5.34200	-11.89100
O	6.00300	-6.37800	-11.96300
C	5.79800	-3.45800	-10.44400

C	5.13000	-3.50800	-9.06800
O	5.50100	-4.36400	-8.28300
O	4.26200	-2.68700	-8.82300
H	8.39600	-3.13600	-10.60000
N	7.24000	-4.83600	-12.93900
C	7.16300	-5.54000	-14.24700
C	7.72600	-6.93700	-14.03000
O	7.28100	-7.90700	-14.60700
C	8.01900	-4.77400	-15.27400
C	7.16100	-3.72800	-15.99300
C	8.60000	-5.73800	-16.31400
C	6.13400	-3.14600	-15.02300
H	7.77800	-4.01700	-12.85200
N	8.70800	-7.02700	-13.18500
C	9.32800	-8.34900	-12.89300
C	8.31700	-9.22300	-12.14500
O	8.06600	-10.35300	-12.51300
C	10.56800	-8.14000	-12.02300
C	11.48200	-9.36300	-12.13200
O	11.18000	-10.29800	-12.84500
N	12.59300	-9.39300	-11.44900
H	9.03700	-6.21300	-12.73600
H	12.83600	-8.63900	-10.87300
H	13.18500	-10.17200	-11.51200
N	7.73600	-8.70600	-11.09700
C	6.74000	-9.50500	-10.32400
C	5.61700	-9.98500	-11.25000
O	5.32400	-11.16500	-11.33500
H	7.95600	-7.78800	-10.81500
N	4.97500	-9.08500	-11.94300
C	3.87200	-9.50900	-12.84000
C	4.42400	-10.40900	-13.93800
O	3.86500	-11.43900	-14.25400
C	3.21300	-8.28400	-13.45500
C	2.19300	-8.75500	-14.48600
C	4.27800	-7.41800	-14.13500
C	1.33200	-9.86700	-13.89000
H	5.21300	-8.13500	-11.87000
N	5.53500	-10.04500	-14.49700
C	6.14000	-10.90500	-15.54200
C	6.28600	-12.29900	-14.94400
O	6.17600	-13.30000	-15.62500
C	7.51300	-10.35300	-15.93200

C	7.35900	-9.37200	-17.09500
C	8.67500	-9.28800	-17.87000
O	9.35600	-8.28200	-17.82500
N	9.06400	-10.30700	-18.58700
H	5.97700	-9.22300	-14.21100
H	8.51400	-11.11800	-18.62400
H	9.90500	-10.26200	-19.08700
N	6.50000	-12.36300	-13.65700
C	6.61300	-13.68200	-12.98500
C	5.20700	-14.25900	-12.86500
O	5.01400	-15.45400	-12.76200
C	7.21900	-13.49500	-11.59300
O	6.17600	-13.26600	-10.65400
H	6.55600	-11.53900	-13.12800
H	6.54300	-12.77600	-9.91600
N	4.21700	-13.40400	-12.91000
C	2.81700	-13.87200	-12.83500
C	2.53100	-14.66500	-14.09900
O	2.29800	-15.85700	-14.06600
C	1.90200	-12.65000	-12.78500
C	0.92100	-12.77400	-11.62400
C	-0.21400	-11.77300	-11.82500
C	0.35000	-14.19200	-11.58900
H	4.39700	-12.44700	-13.01900
N	2.56900	-14.00400	-15.22000
C	2.32200	-14.71800	-16.50300
C	3.67500	-15.01200	-17.18200
O	4.47900	-15.75200	-16.65100
C	1.41500	-13.85700	-17.38900
C	0.64200	-14.75500	-18.32800
C	1.23300	-15.21300	-19.51000
C	-0.66900	-15.13300	-18.01200
C	0.51700	-16.04500	-20.37700
C	-1.38600	-15.96500	-18.87800
C	-0.79300	-16.42100	-20.06200
O	-1.50000	-17.24300	-20.91500
H	2.77500	-13.03800	-15.21400
H	-1.32200	-18.15300	-20.66600
N	3.95400	-14.45100	-18.33500
C	5.26800	-14.73000	-18.98700
C	5.04300	-15.34700	-20.37000
O	3.92300	-15.59200	-20.76900
H	3.31700	-13.85200	-18.76500

N	6.12800	-15.57800	-21.05700
C	6.07100	-16.16900	-22.40600
C	5.69100	-17.65000	-22.31900
O	6.05400	-18.33000	-21.38000
C	7.46900	-16.01400	-22.98000
C	8.34800	-15.91400	-21.77100
C	7.51500	-15.31500	-20.65300
N	4.96600	-18.09500	-23.30800
C	4.52100	-19.49800	-23.36600
C	5.70100	-20.41300	-23.70200
O	6.55800	-20.05900	-24.48600
C	3.47800	-19.55200	-24.46900
C	3.81800	-18.38400	-25.34600
C	4.49100	-17.33900	-24.47300
N	5.70200	-21.56600	-23.09100
C	6.77200	-22.55300	-23.31300
C	6.61400	-23.20000	-24.69100
O	7.49200	-23.12400	-25.52700
C	6.60300	-23.59300	-22.21900
C	5.15700	-23.48700	-21.83400
C	4.70800	-22.06800	-22.13300
N	5.49900	-23.83300	-24.93500
C	5.28500	-24.48300	-26.25800
C	3.79200	-24.74400	-26.46400
O	3.16900	-24.18300	-27.34400
C	6.04800	-25.80800	-26.29300
C	6.90000	-25.87400	-27.56100
O	7.41600	-24.84300	-27.95900
O	7.02400	-26.95500	-28.11300
H	4.80300	-23.88200	-24.24700
N	3.21100	-25.59300	-25.66100
C	1.75900	-25.88900	-25.81100
C	0.98700	-24.58300	-26.01200
O	0.78800	-23.82900	-25.07900
C	1.25900	-26.59100	-24.54800
O	-0.13900	-26.82300	-24.66300
H	3.73200	-26.03500	-24.95700
H	-0.30200	-27.24000	-25.51200
N	0.57500	-24.36000	-27.23000
C	-0.18200	-23.14300	-27.57600
C	-1.60200	-23.22800	-27.01100
O	-2.25000	-22.22600	-26.78200
C	-0.21700	-23.10100	-29.09400

C	-0.03100	-24.53200	-29.50100
C	0.77200	-25.21400	-28.40800
N	-2.09100	-24.41600	-26.78400
C	-3.46800	-24.56200	-26.23500
C	-3.52100	-25.77400	-25.30100
O	-2.59000	-26.54900	-25.22100
C	-4.45000	-24.76400	-27.39000
C	-3.80100	-25.63300	-28.46800
C	-4.83800	-25.97800	-29.53800
O	-5.81000	-26.63600	-29.20400
O	-4.64200	-25.57900	-30.67500
H	-1.55300	-25.21300	-26.97600
N	-4.60600	-25.94400	-24.59500
C	-4.71700	-27.10400	-23.66800
C	-4.33500	-28.38800	-24.40800
O	-4.18300	-29.40500	-23.75100
C	-6.16100	-27.21100	-23.17100
O	-6.34100	-28.45400	-22.50900
C	-7.12000	-27.11800	-24.35800
O	-4.19900	-28.33200	-25.61900
H	-5.34700	-25.30700	-24.67400
H	-7.24700	-28.49300	-22.19300
Zn	0.26300	-3.21400	-2.34100
Zn	-11.68300	-2.61000	-0.08200
Ca	-7.35400	5.77300	3.01700
Ca	-12.49400	-12.03200	-8.83700
O	-1.09900	4.36800	0.26300
H	-1.63500	3.93400	0.94900
C	-0.00900	3.60000	-0.02200
C	-0.05700	2.20200	-0.08600
C	1.10000	1.47900	-0.38200
C	-1.33500	1.50400	0.16200
C	1.06300	0.00300	-0.45300
C	2.30500	2.15200	-0.61700
O	2.07700	-0.63200	-0.71300
C	-0.21500	-0.69500	-0.20400
C	-1.37200	0.02900	0.09200
C	-0.26300	-2.09300	-0.26800
C	-2.57700	-0.64500	0.32500
C	-2.62000	-2.03800	0.26000
C	-1.46700	-2.76000	-0.03600
C	2.34800	3.54500	-0.55300
C	1.19300	4.26800	-0.25600

C	3.63100	4.26200	-0.80400
O	-2.34900	2.13900	0.42100
O	-3.74300	-0.00200	0.61900
H	-3.93400	0.68200	-0.03900

Xyz cartesian coordinates of the complex of Aloe-Emodin with Stromelysin-1

N	9.60700	-10.62500	1.62300
C	8.27000	-10.01500	1.36900
C	8.19800	-9.53000	-0.08100
O	8.66600	-8.45900	-0.41100
C	8.07300	-8.83000	2.31600
C	9.37000	-8.06800	2.44700
C	10.29800	-8.42900	3.43000
C	9.64400	-7.00000	1.58400
C	11.50100	-7.72300	3.55100
C	10.84600	-6.29300	1.70600
C	11.77500	-6.65400	2.69000
H	10.34700	-10.02700	1.20600
H	9.76100	-10.70500	2.65000
H	9.64400	-11.57100	1.19200
N	7.61400	-10.31000	-0.94800
C	7.51200	-9.89300	-2.37500
C	6.65100	-10.90000	-3.14100
O	5.91300	-11.67000	-2.56100
C	8.91500	-9.84800	-2.98400
C	9.56200	-11.23000	-2.87800
C	10.03700	-11.67800	-4.26200
N	11.05600	-12.75500	-4.10100
C	12.27600	-12.45600	-3.74300
N	12.61000	-11.21200	-3.52000
N	13.16400	-13.40200	-3.60500
H	7.24200	-11.17100	-0.66100
H	10.81100	-13.68800	-4.26600
H	11.93200	-10.48500	-3.62500
H	13.54500	-10.98800	-3.24600
H	12.91100	-14.35400	-3.77500
H	14.09900	-13.17400	-3.33000
N	6.74300	-10.90000	-4.44300
C	5.93100	-11.85800	-5.24500
C	6.11000	-13.27200	-4.68800
O	7.06500	-13.56000	-3.99400
C	6.40300	-11.81700	-6.70000
O	6.60900	-10.46700	-7.09100

C	5.34300	-12.45400	-7.60100
H	7.34400	-10.27200	-4.89300
H	7.45700	-10.41400	-7.53900
N	5.20000	-14.15700	-4.98900
C	5.32000	-15.55200	-4.47700
C	5.99600	-16.42800	-5.53500
O	5.39100	-16.77700	-6.52900
C	3.92100	-16.09600	-4.17800
C	3.31800	-15.33100	-3.02400
C	4.07500	-15.09200	-1.87100
C	2.00200	-14.86100	-3.10800
C	3.51600	-14.38300	-0.80100
C	1.44300	-14.15100	-2.03800
C	2.20000	-13.91300	-0.88500
H	4.43800	-13.90600	-5.55100
N	7.23500	-16.75200	-5.28200
C	8.01500	-17.59000	-6.21000
C	7.51700	-19.03800	-6.15600
O	8.00000	-19.84100	-5.38300
C	9.45300	-17.50500	-5.73000
C	9.32900	-17.14900	-4.27800
C	8.03600	-16.37300	-4.11000
N	6.55800	-19.37600	-6.97300
C	6.03200	-20.77000	-6.96800
C	4.50600	-20.74400	-6.85700
O	3.86100	-21.77300	-6.80900
H	6.18200	-18.71200	-7.58900
N	3.92200	-19.57700	-6.81600
C	2.43900	-19.49100	-6.70800
C	1.92900	-18.33100	-7.56500
O	1.79400	-17.22100	-7.09000
C	2.05900	-19.25500	-5.24600
C	2.92600	-20.13900	-4.34600
C	0.58500	-19.60500	-5.03600
C	2.52900	-21.60400	-4.53500
H	4.45800	-18.75800	-6.85500
N	1.66100	-18.63200	-8.80600
C	1.16100	-17.62000	-9.75300
C	-0.29000	-17.26400	-9.42000
O	-1.11600	-18.12600	-9.19500
C	1.25000	-18.26300	-11.12600
C	1.21200	-19.73500	-10.84100
C	1.79600	-19.94300	-9.45500

N	-0.60400	-15.99900	-9.38100
C	-1.99900	-15.58500	-9.05700
C	-2.97100	-16.18300	-10.07900
O	-3.68100	-17.12600	-9.79200
C	-2.08700	-14.05600	-9.08900
C	-3.00100	-13.57600	-7.96100
C	-2.32500	-12.42600	-7.21000
C	-1.35300	-12.99400	-6.17400
N	0.04200	-12.82500	-6.67200
H	0.07800	-15.31900	-9.56000
H	0.21600	-11.82000	-6.88300
H	0.71200	-13.14900	-5.94600
H	0.17300	-13.38800	-7.53700
N	-3.01800	-15.64000	-11.26700
C	-3.95500	-16.18100	-12.29300
C	-3.20500	-17.09800	-13.26300
O	-2.07100	-16.85000	-13.61900
C	-4.57400	-15.01300	-13.06300
C	-5.12900	-14.02300	-12.09100
C	-4.97100	-12.68200	-12.16700
C	-5.92600	-14.27200	-10.89700
N	-5.61900	-12.09300	-11.09600
C	-6.22300	-13.03300	-10.28600
C	-6.41300	-15.44400	-10.29300
C	-6.97800	-12.95800	-9.11600
C	-7.17200	-15.37300	-9.11600
C	-7.45500	-14.13200	-8.52700
H	-2.44400	-14.87500	-11.48100
H	-5.65800	-11.13100	-10.91600
N	-3.83800	-18.15600	-13.69500
C	-3.17300	-19.09300	-14.64600
C	-3.82500	-18.96500	-16.02500
O	-3.15600	-18.97900	-17.04000
C	-3.32500	-20.53000	-14.13700
C	-4.63100	-20.67000	-13.35000
C	-5.09400	-22.12800	-13.38200
N	-4.08800	-22.97600	-12.68400
C	-4.25600	-24.27000	-12.61700
N	-5.30700	-24.82500	-13.15900
N	-3.37200	-25.01000	-12.00600
H	-4.75500	-18.33200	-13.39500
H	-3.29800	-22.56300	-12.27600
H	-5.98700	-24.26100	-13.62700

H	-5.43300	-25.81500	-13.10500
H	-2.56600	-24.58800	-11.59100
H	-3.50000	-26.00100	-11.95400
N	-5.12600	-18.84600	-16.07000
C	-5.82200	-18.71800	-17.38600
C	-5.06300	-17.74800	-18.28600
O	-4.15300	-17.06600	-17.86000
C	-7.23500	-18.17100	-17.17500
C	-7.20100	-17.02200	-16.16600
C	-8.60600	-16.78500	-15.62000
C	-9.31800	-15.76700	-16.50600
N	-10.64800	-16.31000	-16.90400
H	-5.64300	-18.84700	-15.23800
H	-11.18000	-16.58100	-16.05200
H	-11.17900	-15.58300	-17.42400
H	-10.51300	-17.14500	-17.51100
N	-5.44400	-17.67500	-19.53000
C	-4.75800	-16.74400	-20.46400
C	-5.70100	-15.59400	-20.82700
O	-5.35000	-14.71600	-21.59300
C	-4.36300	-17.50300	-21.73700
O	-4.38100	-16.60800	-22.84000
C	-5.35000	-18.64500	-21.99100
H	-6.18800	-18.22800	-19.84700
H	-5.29200	-16.35100	-22.99700
N	-6.89100	-15.57700	-20.28200
C	-7.82900	-14.46500	-20.61600
C	-8.55300	-13.98500	-19.36000
O	-9.55600	-14.53800	-18.95700
C	-8.86000	-14.95100	-21.62700
C	-8.22400	-15.06500	-22.98400
N	-7.45200	-16.15700	-23.34900
C	-8.23200	-14.23200	-24.07500
C	-7.03300	-15.95400	-24.61000
N	-7.48000	-14.79500	-25.10200
H	-7.30800	-14.40700	-26.02900
H	-7.16500	-16.29000	-19.65600
H	-7.25000	-16.93500	-22.78800
N	-8.05400	-12.95200	-18.74800
C	-8.70400	-12.41900	-17.51800
C	-9.69800	-11.32300	-17.90000
O	-9.74200	-10.87900	-19.02700
C	-7.62900	-11.81400	-16.61000

C	-6.81800	-12.92600	-15.94500
C	-7.69700	-13.67000	-14.93900
C	-6.31600	-13.90400	-17.00800
H	-7.24900	-12.52200	-19.10000
N	-10.48900	-10.87400	-16.96500
C	-11.46400	-9.80000	-17.26400
C	-11.62000	-8.95400	-16.00500
O	-11.34300	-9.41100	-14.91700
C	-12.80200	-10.43700	-17.64700
O	-13.84100	-9.48800	-17.48400
C	-13.06900	-11.64800	-16.75200
H	-10.44100	-11.23900	-16.05600
H	-13.45700	-8.61800	-17.57100
N	-12.04500	-7.73200	-16.11800
C	-12.19300	-6.90500	-14.89400
C	-13.50300	-6.12100	-14.95600
O	-14.13400	-6.02000	-15.98900
C	-11.01800	-5.94100	-14.79800
C	-11.01800	-5.03700	-16.00400
C	-10.78200	-5.57400	-17.27200
C	-11.25900	-3.66800	-15.85800
C	-10.78900	-4.74500	-18.39500
C	-11.26500	-2.83500	-16.98400
C	-11.03100	-3.37500	-18.25300
O	-11.03600	-2.55600	-19.36300
H	-12.25900	-7.35600	-16.99600
H	-11.71800	-2.86900	-19.96000
N	-13.91300	-5.56500	-13.85100
C	-15.18200	-4.78300	-13.83400
C	-14.89700	-3.38100	-13.28700
O	-14.36600	-3.22300	-12.21000
C	-16.19100	-5.50300	-12.93700
C	-17.60700	-5.22200	-13.44100
C	-18.43500	-4.62600	-12.30300
N	-19.78500	-5.25900	-12.28600
C	-19.96200	-6.41200	-11.69800
N	-18.94900	-7.04700	-11.17400
N	-21.15600	-6.93700	-11.64200
H	-13.38100	-5.66200	-13.03000
H	-20.54500	-4.79800	-12.69900
H	-18.03200	-6.65500	-11.22300
H	-19.09200	-7.92700	-10.72100
H	-21.93200	-6.45500	-12.04600

H	-21.29300	-7.82000	-11.19400
N	-15.23300	-2.35900	-14.02400
C	-14.95800	-0.97300	-13.54100
C	-16.07500	-0.51300	-12.59300
O	-16.99700	0.17100	-12.99000
C	-14.89100	-0.01000	-14.73600
C	-13.61300	-0.25200	-15.55600
C	-14.89000	1.43300	-14.22800
C	-13.69800	-1.61300	-16.24700
H	-15.65200	-2.50500	-14.89300
N	-15.99000	-0.87400	-11.34400
C	-17.03500	-0.45100	-10.36100
C	-16.54600	0.77000	-9.56700
O	-17.17500	1.20000	-8.61700
C	-17.31600	-1.60200	-9.39800
C	-18.44200	-1.20600	-8.44200
C	-17.73700	-2.83600	-10.19300
H	-15.23400	-1.42100	-11.04600
N	-15.42600	1.33000	-9.93700
C	-14.91800	2.51900	-9.20200
C	-15.32700	3.79100	-9.94600
O	-15.64100	3.76500	-11.11900
C	-13.39400	2.46800	-9.12100
C	-12.96500	1.59000	-7.94700
O	-12.99000	2.01800	-6.81200
N	-12.56100	0.37500	-8.17700
H	-14.92300	0.97000	-10.68600
H	-12.53600	0.03700	-9.09500
H	-12.27800	-0.19700	-7.43400
N	-15.30700	4.90500	-9.27200
C	-15.67300	6.18900	-9.93100
C	-15.61100	7.32600	-8.90400
O	-15.50900	7.10100	-7.71400
C	-17.07700	6.06100	-10.53700
C	-17.75100	7.41400	-10.62400
C	-17.53600	8.23300	-11.73900
C	-18.59100	7.84500	-9.59000
C	-18.16100	9.48300	-11.82100
C	-19.21700	9.09500	-9.67200
C	-19.00200	9.91400	-10.78700
O	-19.61900	11.14600	-10.86800
H	-15.03500	4.89700	-8.33500
H	-19.94800	11.37000	-9.99500

N	-15.65800	8.54400	-9.36400
C	-15.58900	9.70900	-8.43500
C	-15.75300	10.99000	-9.24200
O	-15.51500	11.00200	-10.43100
C	-14.21600	9.72700	-7.75400
O	-13.88100	11.06300	-7.39900
C	-13.16100	9.18200	-8.71700
H	-15.72900	8.69600	-10.33000
H	-13.01400	11.26200	-7.76600
N	-16.12500	12.03800	-8.57200
C	-16.27700	13.33100	-9.24400
C	-14.90400	13.77800	-9.70400
O	-14.75200	14.49200	-10.67500
C	-16.84900	14.27100	-8.20900
C	-16.45200	13.64600	-6.90700
C	-16.43100	12.14900	-7.13900
N	-13.89700	13.31200	-9.02800
C	-12.51800	13.64900	-9.43500
C	-12.20100	12.83800	-10.69100
O	-11.21100	13.06400	-11.36100
C	-11.54900	13.27600	-8.31100
C	-10.71500	14.49800	-7.92600
O	-11.17900	15.60400	-8.15300
O	-9.62600	14.31000	-7.41000
H	-14.05200	12.71000	-8.27200
N	-13.05000	11.89100	-11.01600
C	-12.81900	11.05900	-12.22900
C	-14.14300	10.53700	-12.76900
O	-14.76200	9.68100	-12.16800
C	-11.94800	9.85600	-11.87600
C	-10.63100	10.33000	-11.28100
C	-9.82700	9.11700	-10.83200
C	-9.83600	11.11700	-12.32800
H	-13.84200	11.73400	-10.46100
N	-14.51900	11.03500	-13.90700
C	-15.75700	10.58500	-14.54900
C	-15.61300	9.11900	-14.95400
O	-14.58100	8.50800	-14.76100
C	-15.93700	11.47400	-15.77100
C	-14.54900	11.95700	-16.05800
C	-13.84600	12.05700	-14.71800
N	-16.64600	8.55900	-15.51100
C	-16.59900	7.13400	-15.93800

C	-15.23400	6.80500	-16.53400
O	-14.49400	5.99100	-16.02500
C	-17.65900	6.92700	-17.01600
C	-18.45800	5.65800	-16.71700
C	-18.36700	4.70500	-17.91100
C	-16.89700	4.42000	-18.23400
N	-16.75800	4.20000	-19.70200
H	-17.46400	9.08000	-15.65100
H	-17.28800	4.93400	-20.21400
H	-15.75300	4.24900	-19.96600
H	-17.13400	3.26300	-19.94900
N	-14.92600	7.41200	-17.63800
C	-13.63400	7.12800	-18.33000
C	-12.41500	7.41400	-17.44200
O	-11.36900	6.82700	-17.63200
C	-13.55400	7.98900	-19.59200
C	-14.06900	7.18900	-20.79000
O	-15.27600	7.13900	-20.96800
O	-13.25000	6.64100	-21.50800
H	-15.56900	8.03700	-18.03500
N	-12.50800	8.30200	-16.49200
C	-11.31900	8.58500	-15.64800
C	-11.09800	7.42900	-14.66700
O	-10.08300	6.76200	-14.70200
C	-11.54800	9.88900	-14.89700
H	-13.34200	8.78400	-16.33800
N	-12.05200	7.15600	-13.81300
C	-11.86800	6.01000	-12.88400
C	-11.64900	4.77600	-13.75000
O	-10.77300	3.96600	-13.51100
C	-13.11900	5.83600	-12.02200
C	-14.32200	5.52900	-12.91500
C	-12.90200	4.67900	-11.04700
H	-12.88700	7.68100	-13.80500
N	-12.42200	4.66900	-14.79500
C	-12.25200	3.53700	-15.73100
C	-10.83800	3.63900	-16.26900
O	-10.20200	2.65900	-16.58800
C	-13.25500	3.66800	-16.87800
C	-14.63400	3.19700	-16.41100
O	-15.18200	3.82400	-15.52000
O	-15.11800	2.21700	-16.95300
H	-13.09100	5.36300	-14.98000

N	-10.33800	4.84400	-16.34500
C	-8.95300	5.04500	-16.82800
C	-8.02000	4.24400	-15.92800
O	-7.39600	3.32400	-16.36700
C	-8.59500	6.53200	-16.77200
O	-7.80200	6.78800	-15.62100
H	-10.87300	5.61100	-16.06600
H	-6.92600	7.04900	-15.91600
N	-7.93300	4.57600	-14.66800
C	-7.04400	3.81600	-13.74400
C	-7.29000	2.32400	-13.89000
O	-6.39700	1.51900	-13.75800
C	-7.37400	4.22000	-12.32000
H	-8.45100	5.32000	-14.32400
N	-8.48800	1.95500	-14.17000
C	-8.80600	0.52100	-14.34500
C	-8.21500	0.07900	-15.67500
O	-7.92900	-1.07900	-15.90300
C	-10.32300	0.37000	-14.37500
C	-10.70100	-1.09900	-14.19900
C	-10.93600	1.19200	-13.23900
H	-9.17400	2.62100	-14.28500
N	-8.03700	1.02400	-16.55100
C	-7.47100	0.73500	-17.89300
C	-5.94600	0.87700	-17.84200
O	-5.22300	0.16200	-18.50700
C	-8.07200	1.75500	-18.86900
C	-7.07100	2.10600	-19.97100
C	-7.82300	2.46600	-21.25300
O	-8.67100	3.34100	-21.19300
O	-7.53800	1.86100	-22.27400
H	-8.28400	1.94900	-16.31900
N	-5.45600	1.78800	-17.05000
C	-3.99600	1.97000	-16.94800
C	-3.48100	0.87700	-16.03800
O	-2.46900	0.27400	-16.28600
C	-3.69400	3.33500	-16.35100
C	-2.69100	4.07400	-17.23700
C	-3.42800	5.11800	-18.08000
C	-3.77000	4.52200	-19.44600
N	-3.82600	5.61800	-20.45400
H	-6.05500	2.34600	-16.51000
H	-3.83300	6.53700	-19.96600

H	-2.99600	5.56000	-21.07600
H	-4.69100	5.52100	-21.02400
N	-4.21200	0.58700	-15.00900
C	-3.83000	-0.51700	-14.09100
C	-3.90200	-1.81700	-14.87600
O	-2.92800	-2.51700	-15.07200
C	-4.86700	-0.57300	-13.00000
H	-5.05500	1.08100	-14.85600
N	-5.09000	-2.12200	-15.32900
C	-5.29600	-3.36300	-16.11900
C	-4.24600	-3.44700	-17.21400
O	-3.64000	-4.47100	-17.43400
C	-6.67600	-3.31300	-16.77900
C	-6.72500	-4.32700	-17.92400
C	-6.49300	-5.72700	-17.36500
C	-8.08400	-4.26200	-18.60800
H	-5.85800	-1.51500	-15.14600
N	-4.06400	-2.38100	-17.92500
C	-3.08300	-2.40000	-19.04500
C	-1.67200	-2.46900	-18.49100
O	-0.79500	-3.07600	-19.06600
C	-3.23100	-1.13300	-19.88900
C	-2.05300	-1.03000	-20.86600
C	-2.56100	-1.20900	-22.29800
C	-2.84700	0.16100	-22.91300
N	-3.83100	0.00000	-24.02100
H	-4.59400	-1.57300	-17.73200
H	-4.58000	-0.65700	-23.72800
H	-4.25000	0.92500	-24.25000
H	-3.35000	-0.38000	-24.86000
N	-1.44700	-1.85400	-17.38300
C	-0.10100	-1.87700	-16.78600
C	0.32800	-3.33100	-16.65500
O	1.44000	-3.69300	-16.97700
C	-0.18100	-1.20500	-15.41500
C	0.93300	-1.72200	-14.51300
C	-0.03300	0.30800	-15.59000
H	-2.17600	-1.37200	-16.93200
N	-0.54600	-4.17500	-16.18600
C	-0.15900	-5.60400	-16.03500
C	-0.52400	-6.39900	-17.29000
O	0.04100	-7.44000	-17.55700
C	-0.87000	-6.18100	-14.81300

C	-0.76300	-5.19600	-13.69800
C	-1.76600	-4.39800	-13.27200
C	0.39500	-4.87500	-12.86900
N	-1.30000	-3.61400	-12.23500
C	0.02300	-3.86600	-11.95400
C	1.71600	-5.35600	-12.82000
C	0.92200	-3.34400	-11.02500
C	2.62800	-4.83900	-11.88300
C	2.23100	-3.83300	-10.98700
H	-1.45000	-3.86900	-15.93100
H	-1.82800	-2.95500	-11.74700
N	-1.43800	-5.91500	-18.07700
C	-1.80700	-6.65100	-19.30900
C	-0.66200	-6.50700	-20.28700
O	-0.43000	-7.34700	-21.13400
C	-3.07300	-6.04200	-19.90900
C	-3.37600	-6.71200	-21.25000
C	-4.84800	-6.49600	-21.60700
O	-5.39000	-5.47800	-21.20900
O	-5.40700	-7.35100	-22.27400
H	-1.86200	-5.06200	-17.87400
N	0.06000	-5.43700	-20.16500
C	1.20100	-5.21400	-21.06800
C	2.44600	-5.84600	-20.47400
O	3.20600	-6.50200	-21.15800
C	1.44100	-3.72000	-21.24200
C	1.81800	-3.09400	-19.89700
C	1.55500	-1.58800	-19.94300
O	2.42800	-0.86800	-20.39700
O	0.48500	-1.18000	-19.52300
H	-0.15100	-4.78100	-19.47200
N	2.67300	-5.66000	-19.20500
C	3.89300	-6.27500	-18.60900
C	3.84600	-7.78500	-18.86600
O	4.87000	-8.43200	-18.96200
C	3.95300	-5.99600	-17.10900
C	3.83200	-4.49400	-16.85700
C	2.80900	-6.72600	-16.44000
H	2.04300	-5.12500	-18.65300
N	2.66900	-8.35600	-19.01100
C	2.60300	-9.81900	-19.29700
C	1.92600	-10.00800	-20.66300
O	1.32500	-9.09200	-21.18700

C	1.79100	-10.57200	-18.21600
O	0.65800	-11.14400	-18.83000
C	1.29100	-9.64300	-17.12000
H	1.83400	-7.82300	-18.95700
H	0.15600	-10.41400	-19.21400
N	2.03800	-11.19800	-21.18600
C	1.43000	-11.52800	-22.48400
C	-0.05400	-11.87500	-22.29100
O	-0.80400	-12.00000	-23.23900
C	2.18700	-12.74500	-22.98100
C	2.71900	-13.39500	-21.73500
C	2.74700	-12.35200	-20.62800
N	-0.47000	-12.04200	-21.06400
C	-1.89300	-12.39500	-20.77800
C	-2.84800	-11.41600	-21.46800
O	-2.48500	-10.30600	-21.80500
C	-2.10700	-12.32900	-19.26400
C	-3.59500	-12.44500	-18.93700
C	-4.10200	-13.82700	-19.34400
C	-3.79900	-12.25200	-17.43300
H	0.16200	-11.94400	-20.32300
N	-4.07500	-11.82300	-21.66600
C	-5.07500	-10.92600	-22.31800
C	-6.08700	-10.46200	-21.26600
O	-6.10000	-10.95200	-20.15400
C	-5.80100	-11.69800	-23.42400
O	-6.90900	-12.39100	-22.86500
C	-4.84000	-12.70000	-24.06600
H	-4.34300	-12.72200	-21.37500
H	-7.55000	-11.73900	-22.57400
N	-6.93100	-9.51900	-21.59500
C	-7.91700	-9.03900	-20.58900
C	-9.19000	-8.52400	-21.27200
O	-9.14900	-7.95200	-22.34400
C	-7.28200	-7.90500	-19.78800
C	-6.26100	-8.47200	-18.83300
C	-4.94500	-8.68200	-19.26100
C	-6.62900	-8.79100	-17.52000
C	-3.99600	-9.20900	-18.37600
C	-5.68000	-9.31800	-16.63600
C	-4.36400	-9.52700	-17.06400
H	-6.90800	-9.12300	-22.48900
N	-10.31700	-8.70700	-20.63600

C	-11.60400	-8.21800	-21.20300
C	-12.27500	-7.33700	-20.14800
O	-11.69700	-7.06400	-19.11900
C	-12.50100	-9.41300	-21.53000
O	-13.85200	-8.97900	-21.60600
H	-10.31400	-9.15600	-19.76500
H	-14.41700	-9.73600	-21.43700
N	-13.47500	-6.88400	-20.37500
C	-14.12500	-6.02000	-19.34700
C	-15.63700	-6.21900	-19.34200
O	-16.21000	-6.77100	-20.26000
C	-13.81500	-4.55900	-19.65800
C	-14.11300	-4.27500	-21.13100
C	-14.97600	-3.01600	-21.24200
N	-14.22100	-1.85700	-20.69100
C	-14.81700	-0.70700	-20.52100
N	-16.07600	-0.56700	-20.83700
N	-14.15100	0.30500	-20.03500
H	-13.94300	-7.10400	-21.20800
H	-13.27600	-1.95700	-20.45300
H	-16.58900	-1.34000	-21.21000
H	-16.52800	0.31500	-20.70500
H	-13.18700	0.19900	-19.79300
H	-14.60600	1.18600	-19.90400
N	-16.28400	-5.76800	-18.30200
C	-17.75400	-5.91600	-18.21100
C	-18.28300	-4.98900	-17.11200
O	-17.60500	-4.08400	-16.66700
C	-18.07700	-7.37100	-17.86900
C	-17.11200	-7.87100	-16.79300
C	-17.89800	-8.24300	-15.53400
C	-16.37100	-9.10600	-17.31100
H	-15.79900	-5.33000	-17.57500
N	-19.48500	-5.21400	-16.66900
C	-20.07300	-4.36400	-15.59700
C	-21.23800	-5.12700	-14.97000
O	-22.18400	-4.55000	-14.47200
C	-20.58000	-3.05600	-16.20800
C	-21.22600	-2.21600	-15.13200
C	-20.53000	-1.93700	-13.95000
C	-22.52200	-1.71800	-15.31600
C	-21.12900	-1.16000	-12.95100
C	-23.12100	-0.94000	-14.31700

C	-22.42400	-0.66100	-13.13500
O	-23.01500	0.10500	-12.15200
H	-20.00500	-5.95000	-17.04000
H	-23.30800	0.92700	-12.55100
N	-21.16900	-6.42800	-15.00100
C	-22.26000	-7.25800	-14.42200
C	-21.66000	-8.51600	-13.79500
O	-20.46600	-8.73500	-13.85100
C	-23.22700	-7.66100	-15.53800
C	-22.51400	-8.58600	-16.52900
C	-21.92800	-7.75500	-17.67200
O	-21.12100	-6.88300	-17.39100
O	-22.29400	-8.00400	-18.80900
H	-20.39200	-6.86200	-15.41400
N	-22.47900	-9.34800	-13.21200
C	-21.96100	-10.59900	-12.58800
C	-20.64500	-10.30700	-11.86700
O	-20.63300	-9.84100	-10.74500
H	-23.43900	-9.15200	-13.18800
N	-19.53600	-10.57400	-12.50300
C	-18.22600	-10.30500	-11.84500
C	-17.07600	-10.72200	-12.76600
O	-16.96100	-11.86800	-13.15200
C	-18.15400	-11.10400	-10.54300
C	-18.60200	-12.54300	-10.80100
C	-18.88600	-13.23900	-9.46800
O	-19.44500	-12.59600	-8.59500
O	-18.54000	-14.40100	-9.34300
H	-19.56700	-10.94500	-13.41000
N	-16.21100	-9.80200	-13.10600
C	-15.05700	-10.15100	-13.98400
C	-13.99900	-10.86600	-13.15600
O	-14.29500	-11.51600	-12.17300
C	-14.46000	-8.86900	-14.56500
H	-16.31500	-8.88400	-12.77200
N	-12.76900	-10.74200	-13.54400
C	-11.67800	-11.40300	-12.78100
C	-11.18200	-10.44400	-11.70400
O	-10.85500	-10.85000	-10.61200
C	-10.53000	-11.74600	-13.73200
C	-9.50700	-12.61900	-13.00300
O	-8.61000	-12.06000	-12.39200
O	-9.63700	-13.83000	-13.06800

H	-12.56200	-10.20300	-14.33700
N	-11.14300	-9.17300	-12.02000
C	-10.68300	-8.13300	-11.04000
C	-11.79300	-7.09900	-10.87300
O	-11.79100	-6.06600	-11.51400
C	-9.44900	-7.43400	-11.60300
C	-8.42900	-8.48000	-12.05800
C	-8.83000	-6.55100	-10.52000
C	-8.70300	-8.85800	-13.51400
H	-11.43000	-8.89400	-12.91800
N	-12.74500	-7.36100	-10.02700
C	-13.84500	-6.37800	-9.84000
C	-13.27200	-5.09700	-9.23600
O	-13.06800	-5.00500	-8.04100
C	-14.89200	-6.96800	-8.89400
C	-16.22500	-6.24800	-9.09400
S	-17.11500	-6.18100	-7.51900
C	-17.69300	-7.89500	-7.51300
H	-12.73700	-8.20000	-9.51700
N	-13.00500	-4.10700	-10.04100
C	-12.45200	-2.83900	-9.49100
C	-13.61900	-2.00500	-8.97000
O	-14.43000	-1.54000	-9.73400
C	-11.73600	-2.06600	-10.60500
C	-10.99600	-3.03400	-11.53500
C	-10.73100	-1.09800	-9.98300
C	-9.91400	-3.77700	-10.75100
H	-13.17400	-4.19200	-11.00400
N	-13.73600	-1.81600	-7.68700
C	-14.89400	-1.01800	-7.18900
C	-14.46600	0.02000	-6.15400
O	-13.48800	-0.13100	-5.45900
C	-15.91200	-1.95600	-6.56100
O	-15.79900	-3.24300	-7.15400
H	-13.08500	-2.20500	-7.06200
H	-16.68200	-3.60900	-7.24000
N	-15.21500	1.07700	-6.04400
C	-14.87200	2.13700	-5.05200
C	-15.56200	1.84100	-3.71900
O	-16.69000	1.39100	-3.68100
C	-15.34400	3.49200	-5.58400
C	-16.85300	3.54300	-5.57500
C	-17.53900	3.78300	-4.37900

C	-17.56600	3.35300	-6.76500
C	-18.93800	3.83300	-4.37300
C	-18.96500	3.40200	-6.75800
C	-19.65200	3.64300	-5.56200
H	-16.01000	1.16800	-6.61200
N	-14.89200	2.08700	-2.62400
C	-15.53400	1.80700	-1.29300
C	-14.71100	2.41200	-0.14700
O	-13.68200	3.01500	-0.36400
C	-15.63100	0.29200	-1.10200
H	-13.97500	2.45000	-2.68200
N	-15.15200	2.24700	1.07300
C	-14.39400	2.81000	2.23400
C	-14.64800	1.94000	3.47300
O	-15.11700	0.82500	3.36800
C	-14.87000	4.25300	2.47400
C	-16.12900	4.26200	3.34800
C	-13.76200	5.04900	3.16600
H	-15.98300	1.75100	1.22800
N	-14.33800	2.43600	4.64100
C	-14.55900	1.63500	5.87800
C	-16.02700	1.20500	5.96200
O	-16.83300	1.84000	6.61300
C	-14.20400	2.49300	7.09500
C	-14.99700	3.80100	7.04600
C	-14.05600	4.98100	7.29700
N	-14.86000	6.17100	7.69600
C	-15.35900	6.25300	8.90100
N	-15.16100	5.29000	9.76000
N	-16.05600	7.30100	9.24700
H	-13.95600	3.33500	4.70500
H	-15.01300	6.89500	7.05300
H	-14.62800	4.48500	9.49800
H	-15.54400	5.35600	10.68200
H	-16.20900	8.03900	8.58900
H	-16.43800	7.36500	10.16900
N	-16.37900	0.13200	5.30800
C	-17.79200	-0.33900	5.34900
C	-17.93500	-1.60600	4.50100
O	-18.96700	-1.85400	3.90800
C	-18.70100	0.75700	4.78800
C	-19.96000	0.86700	5.64900
C	-21.18600	0.51500	4.80500

O	-21.19100	-0.55600	4.22000
O	-22.10000	1.32200	4.75800
H	-15.71300	-0.36600	4.79000
N	-16.90800	-2.40800	4.43800
C	-16.98700	-3.65700	3.62700
C	-17.87300	-4.67600	4.34600
O	-18.66400	-5.36700	3.73500
C	-15.58000	-4.23500	3.45600
C	-14.72800	-3.27700	2.66700
N	-14.29200	-2.07100	3.19200
C	-14.21600	-3.34000	1.39400
C	-13.55100	-1.46300	2.24800
N	-13.47100	-2.19300	1.13100
H	-16.08600	-2.19100	4.92300
H	-14.48600	-1.72500	4.08800
N	-17.74600	-4.77700	5.64100
C	-18.57900	-5.75400	6.40000
C	-17.84100	-6.17400	7.67200
O	-18.25700	-5.86900	8.77200
H	-17.10100	-4.21200	6.11500
N	-16.74700	-6.87200	7.53100
C	-15.98100	-7.31000	8.73200
C	-14.54500	-7.64600	8.32500
O	-13.86900	-8.42000	8.97400
C	-16.65000	-8.55200	9.32600
C	-17.07400	-8.26400	10.76700
O	-16.33100	-7.58800	11.45800
O	-18.13500	-8.72500	11.15500
H	-16.42800	-7.10600	6.63500
N	-14.07400	-7.06900	7.25400
C	-12.68300	-7.35400	6.80200
C	-12.15000	-6.15800	6.00700
O	-12.74200	-5.09900	6.02300
C	-12.69700	-8.60000	5.91100
C	-12.81700	-9.83300	6.77400
C	-11.67000	-10.41700	7.32500
C	-14.07500	-10.39300	7.02300
C	-11.78200	-11.56100	8.12400
C	-14.18700	-11.53700	7.82200
C	-13.04000	-12.12100	8.37300
H	-14.63700	-6.44900	6.74500
N	-11.04100	-6.34400	5.32000
C	-10.40600	-5.25500	4.49200

C	-11.17900	-3.93700	4.58700
O	-11.79700	-3.50700	3.63300
C	-10.37100	-5.70900	3.02800
C	-11.53800	-6.63200	2.75300
C	-12.79300	-6.10000	2.43300
C	-11.36300	-8.01800	2.82600
C	-13.87200	-6.95700	2.18400
C	-12.44200	-8.87500	2.57700
C	-13.69800	-8.34300	2.25600
O	-14.76200	-9.18700	2.01100
H	-10.61200	-7.22400	5.34700
H	-14.45600	-10.09000	2.12300
N	-11.11200	-3.33600	5.74600
C	-11.79900	-2.06100	5.99100
C	-10.97200	-0.90700	5.41600
O	-9.81300	-0.74300	5.74100
C	-11.89100	-1.93100	7.49900
C	-10.75900	-2.77600	8.01700
C	-10.39500	-3.78900	6.94400
N	-11.55500	-0.10100	4.57200
C	-10.79500	1.03700	3.99400
C	-10.71300	2.16500	5.01300
O	-11.05200	2.00400	6.16900
C	-11.52400	1.54600	2.76600
C	-10.83800	1.08000	1.51300
C	-10.88500	-0.26200	1.13400
C	-10.17900	2.00700	0.71000
C	-10.27300	-0.66800	-0.05400
C	-9.57100	1.59800	-0.47600
C	-9.62500	0.25700	-0.85500
H	-12.49400	-0.23900	4.32000
N	-10.26500	3.31000	4.58800
C	-10.15500	4.45300	5.51800
C	-9.57500	5.66700	4.79200
O	-8.54300	6.17100	5.18400
C	-9.21800	4.06200	6.64600
C	-7.89600	3.56800	6.05500
O	-7.45000	4.15100	5.07800
O	-7.35300	2.61600	6.59000
H	-9.99900	3.41100	3.65900
N	-10.22300	6.13100	3.74200
C	-9.70200	7.32300	2.97300
C	-8.73000	8.14300	3.82200

O	-7.58000	8.30000	3.46200
H	-11.05600	5.68600	3.44700
N	-9.20800	8.61800	4.94000
C	-8.35900	9.39700	5.85700
C	-7.34700	8.46000	6.52200
O	-7.27100	8.36500	7.73000
C	-9.30300	9.98900	6.89000
C	-10.48300	9.06500	6.86800
C	-10.57400	8.48800	5.46800
N	-6.57600	7.76100	5.73300
C	-5.57400	6.81900	6.30000
C	-4.66800	6.31600	5.17400
O	-5.03300	6.33600	4.01400
H	-6.65800	7.85200	4.76300
N	-3.48800	5.87500	5.50600
C	-2.54700	5.38100	4.46100
C	-3.23000	4.33600	3.57100
O	-2.94500	4.23800	2.39600
C	-1.33500	4.75200	5.14700
C	-0.48900	5.84900	5.79500
O	-0.29400	6.90100	5.22100
N	0.02700	5.64600	6.97600
H	-3.21500	5.87500	6.44800
H	-0.13000	4.79800	7.44100
H	0.57100	6.34300	7.40000
N	-4.11700	3.54700	4.11900
C	-4.79900	2.50500	3.29100
C	-5.47200	3.15400	2.07700
O	-6.64500	3.47000	2.09400
C	-5.85000	1.79000	4.14200
C	-6.22200	0.46000	3.48400
C	-5.28100	1.52500	5.53800
H	-4.32800	3.63400	5.07200
N	-4.72500	3.36100	1.02700
C	-5.29700	4.00000	-0.20100
C	-6.20300	3.02400	-0.98600
O	-7.28100	3.38700	-1.40400
C	-4.14400	4.45200	-1.09800
C	-4.27400	5.95000	-1.37400
C	-3.66700	6.74000	-0.21400
C	-3.52900	6.29100	-2.66400
H	-3.78200	3.11200	1.05300
N	-5.78100	1.80000	-1.21200

C	-6.66200	0.86700	-1.98600
C	-6.15400	-0.58100	-1.92000
O	-5.15000	-0.87200	-1.31400
C	-6.70000	1.32300	-3.44200
H	-4.90400	1.50700	-0.88800
N	-6.83400	-1.50800	-2.55300
C	-6.33000	-2.91700	-2.50700
C	-7.25500	-3.86100	-3.27200
O	-8.36100	-3.51200	-3.63200
C	-6.20100	-3.38500	-1.04600
C	-7.51900	-3.27400	-0.31100
N	-7.66600	-2.48000	0.82000
C	-8.73800	-3.88400	-0.49800
C	-8.92900	-2.63100	1.26800
N	-9.62700	-3.48100	0.50000
H	-7.64900	-1.28000	-3.06300
H	-6.97500	-1.91100	1.22000
N	-6.80100	-5.06400	-3.52100
C	-7.64000	-6.03600	-4.26000
C	-7.65300	-7.38500	-3.52800
O	-7.21500	-7.48000	-2.39800
C	-7.08200	-6.20700	-5.67600
H	-5.91100	-5.32200	-3.22300
N	-8.16300	-8.43300	-4.14000
C	-8.19800	-9.73900	-3.42400
C	-7.21100	-10.72300	-4.05500
O	-6.35300	-10.35300	-4.83300
C	-9.61400	-10.30800	-3.49700
C	-10.53900	-9.48500	-2.63300
C	-10.99200	-8.24300	-3.08400
C	-10.94600	-9.96600	-1.38300
C	-11.85300	-7.47900	-2.28900
C	-11.80700	-9.20300	-0.58600
C	-12.26000	-7.95800	-1.03900
O	-13.11100	-7.20700	-0.25600
H	-8.53800	-8.35900	-5.06000
H	-14.01300	-7.43100	-0.49600
N	-7.32400	-11.97800	-3.71300
C	-6.39900	-13.00400	-4.27000
C	-7.21700	-14.06500	-5.01400
O	-8.39900	-13.88500	-5.22800
C	-5.63500	-13.64200	-3.11000
H	-8.02100	-12.24800	-3.08200

N	-6.57000	-15.14100	-5.39300
C	-7.26100	-16.21500	-6.12100
C	-8.14800	-17.02300	-5.17000
O	-7.67300	-17.71300	-4.29100
C	-6.16800	-17.08900	-6.70800
C	-4.98300	-16.84300	-5.82400
C	-5.14900	-15.46900	-5.19300
N	-9.43900	-16.93800	-5.34700
C	-10.37300	-17.69500	-4.46700
C	-11.70900	-17.87600	-5.19200
O	-11.74000	-18.11600	-6.38200
H	-9.79600	-16.37600	-6.06700
N	-12.77300	-17.75200	-4.44600
C	-14.12600	-17.89700	-5.01000
C	-14.47100	-16.67500	-5.87000
O	-14.14800	-16.61900	-7.04100
C	-15.06000	-17.99400	-3.81600
C	-14.30800	-17.31200	-2.71100
C	-12.82600	-17.46600	-3.00600
N	-15.11800	-15.69300	-5.30200
C	-15.47200	-14.47900	-6.09100
C	-14.36700	-13.44300	-5.93400
O	-14.12900	-12.62700	-6.80900
H	-15.36700	-15.75100	-4.35500
N	-13.66500	-13.48900	-4.83500
C	-12.55400	-12.52300	-4.63000
C	-11.37600	-12.92900	-5.52000
O	-10.29600	-12.38800	-5.40400
C	-12.13700	-12.49800	-3.14300
C	-10.93200	-13.41800	-2.90100
C	-13.30400	-12.95800	-2.26400
C	-10.62900	-13.47900	-1.40300
H	-13.85900	-14.16900	-4.15800
N	-11.58200	-13.87300	-6.40800
C	-10.48800	-14.30600	-7.32200
C	-10.10100	-13.11700	-8.20200
O	-10.26200	-13.14400	-9.40600
C	-11.01300	-15.44700	-8.19900
C	-9.86500	-16.37400	-8.59900
O	-9.29800	-17.05200	-7.76800
N	-9.50100	-16.43500	-9.85100
H	-12.46400	-14.29500	-6.48000
H	-9.96200	-15.89100	-10.52300

H	-8.76600	-17.02600	-10.11900
N	-9.62300	-12.06200	-7.60400
C	-9.25700	-10.85900	-8.38800
C	-10.34000	-9.79500	-8.18200
O	-11.41700	-9.85600	-8.73500
H	-9.52300	-12.05500	-6.62600
N	-10.06500	-8.81800	-7.38600
C	-11.06800	-7.75300	-7.14400
C	-10.33600	-6.57100	-6.53200
O	-9.77700	-6.68900	-5.47700
C	-12.11400	-8.27200	-6.15700
C	-13.05700	-9.25200	-6.85600
O	-12.72900	-10.42600	-6.90500
O	-14.09500	-8.81600	-7.32200
H	-9.19600	-8.77900	-6.94000
N	-10.32500	-5.43800	-7.16700
C	-9.60300	-4.28700	-6.57300
C	-10.61300	-3.25600	-6.12800
O	-11.76600	-3.30500	-6.50100
C	-8.68000	-3.66200	-7.61700
H	-10.79400	-5.33800	-8.02600
N	-10.19800	-2.30900	-5.35000
C	-11.15500	-1.27600	-4.91900
C	-10.38700	-0.02500	-4.48500
O	-9.39600	-0.08400	-3.78900
C	-12.05700	-1.85100	-3.80300
C	-12.39200	-0.81400	-2.76200
N	-12.59400	-1.14200	-1.42800
C	-12.55200	0.54600	-2.83900
C	-12.85400	0.00200	-0.76900
N	-12.82700	1.05300	-1.58300
H	-9.26200	-2.27100	-5.06600
H	-12.89300	1.99300	-1.33300
N	-10.85900	1.10500	-4.93800
C	-10.21000	2.41200	-4.61700
C	-10.87000	3.05600	-3.39600
O	-12.07900	3.09100	-3.28400
C	-10.42300	3.35800	-5.79700
C	-9.63200	2.89600	-6.99500
C	-8.29300	2.52000	-6.85500
C	-10.24600	2.84300	-8.25100
C	-7.56800	2.09000	-7.97300
C	-9.52300	2.41500	-9.36800

C	-8.18400	2.03800	-9.22900
H	-11.65800	1.09000	-5.51000
N	-10.09800	3.60700	-2.49500
C	-10.72600	4.27500	-1.32200
C	-11.79000	5.25000	-1.82700
O	-11.69500	5.76800	-2.91700
C	-9.65900	5.04800	-0.54700
C	-10.15800	5.32500	0.86700
O	-11.21100	5.92800	0.99800
O	-9.47600	4.92700	1.79700
H	-9.11700	3.60000	-2.59900
N	-12.80400	5.49900	-1.05200
C	-13.86800	6.43500	-1.50500
C	-14.03400	7.55400	-0.47800
O	-15.05100	8.21500	-0.42600
C	-15.18400	5.66800	-1.64400
C	-16.00500	6.26400	-2.78800
O	-15.50500	6.28900	-3.90000
O	-17.12200	6.68500	-2.53300
H	-12.87200	5.06600	-0.17500
N	-13.04100	7.77300	0.34000
C	-13.15400	8.85100	1.35800
C	-12.24900	10.02700	0.97100
O	-12.40600	11.12400	1.46900
C	-12.74500	8.30600	2.72500
C	-13.97400	8.22500	3.63200
O	-15.07400	8.19300	3.10400
O	-13.79600	8.19700	4.83800
H	-12.22600	7.23100	0.28500
N	-11.30800	9.82100	0.08000
C	-10.42300	10.94300	-0.32800
C	-10.72500	11.28600	-1.79000
O	-11.68000	11.97700	-2.08400
C	-8.94800	10.53200	-0.15700
C	-8.81500	9.00200	-0.12200
C	-7.44100	8.61600	0.43200
O	-6.47100	9.25500	0.05700
O	-7.38100	7.68500	1.22400
H	-11.18900	8.93600	-0.32900
N	-9.93900	10.80100	-2.70900
C	-10.20300	11.08700	-4.14500
C	-9.12000	10.43400	-4.98800
O	-8.08900	10.03900	-4.49200

C	-10.17900	12.59200	-4.38300
C	-11.60900	13.10800	-4.53800
C	-11.71400	14.50900	-3.93300
O	-11.21800	15.46500	-4.49500
N	-12.34400	14.67100	-2.80200
H	-9.18400	10.23500	-2.46000
H	-12.74400	13.90000	-2.34800
H	-12.41600	15.56400	-2.40500
N	-9.33700	10.32500	-6.26100
C	-8.30800	9.70600	-7.13400
C	-8.18200	10.52200	-8.42000
O	-9.15900	10.84100	-9.06600
C	-8.69900	8.26300	-7.48000
C	-9.66300	7.72000	-6.47300
C	-9.44900	7.67400	-5.13800
C	-10.97900	7.13500	-6.69600
N	-10.55700	7.11900	-4.52700
C	-11.52500	6.76600	-5.44500
C	-11.74500	6.89700	-7.85000
C	-12.78900	6.18100	-5.34300
C	-13.01500	6.30800	-7.75100
C	-13.53600	5.95100	-6.50000
H	-10.17000	10.65900	-6.64100
H	-10.66000	6.98000	-3.56200
N	-6.98200	10.85700	-8.79200
C	-6.77200	11.64600	-10.03600
C	-5.68100	10.98100	-10.85500
O	-4.76800	10.37800	-10.32700
C	-6.34200	13.06400	-9.67300
O	-5.19300	12.99900	-8.84700
C	-7.47700	13.77300	-8.93200
H	-6.21200	10.58600	-8.25200
H	-4.74400	12.17300	-9.04300
N	-5.75700	11.10400	-12.13900
C	-4.71400	10.50100	-12.99500
C	-3.48200	11.37000	-12.86300
O	-2.37100	10.90000	-12.78700
C	-5.19100	10.48200	-14.44800
C	-5.34100	11.91800	-14.95500
C	-5.78400	11.89800	-16.41900
C	-6.14000	13.31700	-16.86400
N	-6.05300	13.39700	-18.34900
H	-6.48500	11.61400	-12.53700

H	-6.09000	12.43800	-18.75100
H	-6.85000	13.95700	-18.71300
H	-5.16000	13.85500	-18.62100
N	-3.68500	12.64700	-12.78100
C	-2.54000	13.55800	-12.61400
C	-2.20400	13.59400	-11.13800
O	-2.42200	12.63800	-10.42300
C	-2.92800	14.95900	-13.09300
C	-1.67900	15.70300	-13.56700
O	-1.13200	15.31200	-14.58600
O	-1.29100	16.65100	-12.90500
H	-4.59700	13.00200	-12.78900
N	-1.70800	14.68200	-10.65300
C	-1.40900	14.73800	-9.21100
C	-2.39100	15.71900	-8.56600
O	-2.01200	16.59200	-7.81200
C	0.03000	15.21600	-8.99800
O	0.93100	14.22000	-9.46200
C	0.27300	15.47200	-7.51000
H	-1.55400	15.46200	-11.22800
H	0.75900	13.41400	-8.97100
N	-3.65300	15.60300	-8.89300
C	-4.65500	16.54800	-8.34000
C	-5.38900	15.94500	-7.14000
O	-5.78400	16.65500	-6.23600
C	-5.67300	16.88000	-9.43100
O	-4.99700	17.42500	-10.55600
C	-6.68200	17.89700	-8.89600
H	-3.93500	14.91200	-9.52300
H	-4.76500	16.70200	-11.14300
N	-5.59500	14.65700	-7.11300
C	-6.32500	14.07100	-5.95100
C	-5.42000	13.08500	-5.22800
O	-4.73900	13.42500	-4.28100
H	-5.28000	14.07700	-7.85200
N	-5.39500	11.87000	-5.68200
C	-4.52300	10.85700	-5.04400
C	-3.59400	10.30800	-6.12100
O	-2.59400	10.91200	-6.45500
C	-5.38400	9.72900	-4.45800
O	-6.12700	10.21800	-3.34900
C	-4.48600	8.58300	-3.99800
H	-5.94100	11.62700	-6.46100

H	-6.96000	9.73100	-3.31100
N	-3.92000	9.17900	-6.68300
C	-3.07800	8.60100	-7.74400
C	-3.93800	7.59700	-8.51600
O	-3.73300	6.40200	-8.43700
C	-1.88700	7.90000	-7.10100
C	-1.32700	8.74200	-5.95400
O	-1.75600	8.61400	-4.82600
N	-0.37900	9.60700	-6.19600
H	-4.72900	8.70900	-6.41700
H	-0.03400	9.71300	-7.10700
H	-0.01400	10.14900	-5.46600
N	-4.92100	8.09000	-9.23200
C	-5.84700	7.21100	-9.99800
C	-5.15800	5.91300	-10.45300
O	-5.08400	4.94700	-9.71600
C	-6.35400	8.01000	-11.20700
C	-7.40100	7.21700	-11.96300
C	-8.41700	6.65100	-10.96600
C	-8.10800	8.15300	-12.93900
H	-5.07000	9.06000	-9.25300
N	-4.68700	5.86800	-11.66600
C	-4.04600	4.62600	-12.17700
C	-2.88300	4.20000	-11.28400
O	-2.49700	3.04900	-11.28200
C	-3.61200	4.86600	-13.64000
C	-2.16200	4.46800	-13.87700
C	-1.74100	3.15400	-13.64200
C	-1.24500	5.41800	-14.34000
C	-0.40800	2.79100	-13.86600
C	0.08900	5.05600	-14.56500
C	0.50800	3.74300	-14.32700
H	-4.77800	6.64200	-12.25200
N	-2.33200	5.06700	-10.49300
C	-1.22900	4.59100	-9.63600
C	-1.78200	3.48600	-8.75000
O	-1.37800	2.34000	-8.82300
C	-0.72500	5.74200	-8.77800
C	0.71200	5.48600	-8.32600
C	1.63700	5.47100	-9.54200
C	1.14300	6.60500	-7.37400
H	-2.65100	5.99900	-10.43900
N	-2.73000	3.82400	-7.93100

C	-3.34600	2.80700	-7.05100
C	-4.20100	1.87600	-7.90000
O	-4.67000	0.85700	-7.43400
C	-4.22300	3.50200	-6.01600
C	-4.31800	2.62200	-4.77700
C	-3.60500	4.85000	-5.63600
H	-3.05000	4.75000	-7.90800
N	-4.39000	2.19000	-9.15400
C	-5.19300	1.28500	-10.00200
C	-4.30400	0.11200	-10.35400
O	-4.60300	-1.01400	-10.02300
C	-5.64800	2.01100	-11.26200
H	-3.98300	2.99800	-9.53600
N	-3.17900	0.35300	-10.97300
C	-2.29000	-0.77100	-11.25700
C	-1.82200	-1.29000	-9.92100
O	-1.34000	-2.39500	-9.81100
C	-1.10500	-0.30700	-12.10100
H	-2.90600	1.25900	-11.20400
N	-2.01100	-0.53700	-8.88100
C	-1.61100	-1.06900	-7.56000
C	-2.55300	-2.22500	-7.21300
O	-2.12100	-3.29500	-6.83400
C	-1.70400	0.02600	-6.50000
C	-0.94500	-0.41300	-5.27900
N	0.36900	-0.04200	-5.05500
C	-1.29900	-1.20700	-4.21900
C	0.75800	-0.61000	-3.89700
N	-0.22200	-1.33200	-3.34500
H	-2.44300	0.35200	-8.96600
H	0.91200	0.53800	-5.62700
N	-3.83800	-2.02200	-7.34300
C	-4.80100	-3.11100	-7.02700
C	-4.91200	-4.10800	-8.19400
O	-4.86600	-5.30500	-7.99300
C	-6.17100	-2.50100	-6.72500
C	-5.99900	-1.31900	-5.77100
C	-6.78700	-0.12000	-6.29800
O	-7.72800	-0.33600	-7.04400
O	-6.43700	0.99300	-5.94700
H	-4.16900	-1.15500	-7.64100
N	-5.03700	-3.63900	-9.41300
C	-5.11900	-4.59000	-10.55300

C	-3.81600	-5.35500	-10.57400
O	-3.74200	-6.51100	-10.93000
C	-5.30600	-3.78700	-11.83700
C	-6.58500	-2.96700	-11.67200
C	-5.39100	-4.73100	-13.04100
C	-7.19900	-2.61700	-13.03000
H	-5.04700	-2.66800	-9.58500
N	-2.79100	-4.69600	-10.14700
C	-1.45500	-5.33500	-10.07600
C	-1.44300	-6.25800	-8.87400
O	-0.79100	-7.28500	-8.85900
H	-2.91000	-3.75700	-9.84200
N	-2.17100	-5.89700	-7.87300
C	-2.22700	-6.73600	-6.64700
C	-2.78900	-8.12300	-6.95900
O	-2.24700	-9.13000	-6.54900
C	-3.15200	-6.06100	-5.65100
C	-2.38500	-5.69600	-4.41000
N	-2.89500	-5.89300	-3.13600
C	-1.14500	-5.13100	-4.23300
C	-1.97300	-5.45200	-2.25800
N	-0.88700	-4.97800	-2.87400
H	-2.69000	-5.05800	-7.92700
H	-3.76600	-6.28200	-2.91500
N	-3.90100	-8.18600	-7.63900
C	-4.52400	-9.51400	-7.92200
C	-3.95500	-10.16300	-9.19100
O	-3.53400	-11.30200	-9.17700
C	-6.02900	-9.31700	-8.09800
O	-6.61400	-9.01800	-6.83800
H	-4.34700	-7.35900	-7.93100
H	-7.23000	-8.29200	-6.96200
N	-3.96200	-9.46600	-10.29100
C	-3.44400	-10.07500	-11.56100
C	-2.06600	-9.51800	-11.90000
O	-1.66700	-9.48500	-13.04600
C	-4.41500	-9.78900	-12.71900
C	-4.68100	-8.28500	-12.84700
C	-3.43100	-7.57600	-13.37400
C	-5.83400	-8.06200	-13.82600
H	-4.30500	-8.55000	-10.27900
N	-1.34800	-9.05600	-10.92800
C	-0.01400	-8.47400	-11.21300

C	1.04500	-9.13600	-10.33800
O	1.77100	-10.00200	-10.77400
H	-1.69100	-9.06500	-10.00800
N	1.14700	-8.73600	-9.10700
C	2.18200	-9.35100	-8.23100
C	1.95400	-8.94200	-6.77600
O	0.88800	-8.49500	-6.40400
C	3.55800	-8.86000	-8.69100
C	3.60500	-7.33100	-8.60900
C	4.07500	-6.90800	-7.21700
C	4.58000	-6.79600	-9.65900
H	0.55200	-8.03400	-8.76400
N	2.95400	-9.09600	-5.95000
C	2.80100	-8.72100	-4.51500
C	3.42300	-7.34400	-4.27700
O	2.72800	-6.36600	-4.08300
C	3.51200	-9.76200	-3.64900
C	2.73000	-9.97500	-2.37500
C	1.42600	-10.48000	-2.43100
C	3.30900	-9.66900	-1.13800
C	0.70000	-10.67900	-1.25000
C	2.58500	-9.86700	0.04300
C	1.28000	-10.37200	-0.01200
H	3.80600	-9.46100	-6.27400
N	4.72600	-7.25700	-4.28800
C	5.38500	-5.94000	-4.06000
C	6.82800	-5.98800	-4.57300
O	7.70900	-6.52100	-3.92900
C	5.38000	-5.63300	-2.56000
C	3.98700	-5.25900	-2.13000
N	3.07500	-6.20000	-1.67900
C	3.33500	-4.05100	-2.07900
C	1.93400	-5.55000	-1.38000
N	2.03900	-4.23700	-1.60500
H	5.26900	-8.05700	-4.44600
H	3.23000	-7.16500	-1.59400
N	7.07300	-5.42900	-5.72800
C	8.45800	-5.43500	-6.28600
C	9.17100	-4.14500	-5.87900
O	8.62100	-3.31000	-5.19200
C	8.37800	-5.50300	-7.81800
O	8.19500	-6.85500	-8.21700
H	6.34500	-5.00200	-6.22700

H	8.96800	-7.35400	-7.94200
N	10.38500	-3.96300	-6.31300
C	11.10500	-2.70700	-5.96800
C	10.32500	-1.56200	-6.56400
O	10.57200	-1.13400	-7.67400
C	12.52200	-2.73700	-6.54200
H	10.80600	-4.63600	-6.87600
N	9.35300	-1.08200	-5.85100
C	8.54000	0.00400	-6.41200
C	9.11400	1.36100	-6.07200
O	8.51000	2.37400	-6.36600
C	7.09800	-0.08400	-5.95900
C	6.83900	-1.41200	-5.24800
O	6.92700	-1.49500	-4.04000
N	6.52000	-2.46100	-5.95200
H	9.14800	-1.45400	-4.97300
H	6.45000	-2.39500	-6.92700
H	6.34800	-3.31400	-5.50400
N	10.30600	1.41700	-5.53600
C	10.91400	2.75400	-5.29900
C	10.74900	3.49400	-6.62600
O	10.59600	4.69700	-6.69300
C	12.40000	2.59800	-4.95900
O	12.76100	1.22600	-5.04700
C	12.65600	3.10500	-3.53800
H	10.80900	0.59800	-5.35900
H	12.88700	1.01200	-5.97400
N	10.71400	2.71500	-7.68400
C	10.48600	3.24600	-9.04100
C	9.16400	2.66000	-9.55300
O	8.42700	3.30000	-10.27700
C	11.61700	2.78200	-9.96200
C	12.96000	2.93900	-9.24600
C	14.03600	3.33100	-10.26000
O	14.10800	2.69200	-11.29700
O	14.77000	4.26600	-9.98300
H	10.80200	1.74800	-7.56900
N	8.88000	1.42000	-9.20700
C	7.62700	0.76500	-9.70700
C	6.35800	1.45200	-9.20400
O	6.37700	2.54300	-8.66800
C	7.60600	-0.70600	-9.29300
H	9.51300	0.90700	-8.64500

N	5.24900	0.80900	-9.44200
C	3.91500	1.36700	-9.06800
C	3.48600	0.94400	-7.65600
O	2.56500	1.48900	-7.09900
C	2.89200	0.82100	-10.07000
C	1.69900	1.78700	-10.27900
C	1.37000	2.53200	-8.99000
C	2.05300	2.80000	-11.37000
H	5.29600	-0.04500	-9.91400
N	4.08200	-0.04000	-7.06900
C	3.57700	-0.43600	-5.72100
C	4.07200	0.51100	-4.61700
O	3.63900	0.41500	-3.48600
C	3.97100	-1.88400	-5.42500
C	2.72400	-2.67200	-5.02800
S	2.73400	-4.27900	-5.86000
C	1.40200	-3.93600	-7.03500
H	4.81300	-0.53400	-7.51200
N	4.95500	1.42400	-4.91300
C	5.42100	2.34900	-3.83100
C	5.53300	3.82800	-4.28400
O	6.14800	4.60700	-3.58300
C	6.78600	1.88100	-3.32400
C	6.94500	2.27500	-1.87500
C	6.04800	1.79300	-0.91600
C	7.99100	3.12500	-1.49300
C	6.19600	2.16000	0.42700
C	8.13900	3.49100	-0.15100
C	7.24100	3.00800	0.81000
O	7.38700	3.37100	2.13300
H	5.30600	1.49500	-5.82000
H	7.18200	4.30500	2.21000
N	4.94400	4.20700	-5.40200
C	5.01900	5.61500	-5.83300
C	4.01900	6.42100	-5.02100
O	4.25800	7.56000	-4.67000
C	4.57900	5.63700	-7.27700
C	3.69600	4.43800	-7.39300
C	4.17100	3.42000	-6.37400
N	2.88900	5.81300	-4.75100
C	1.79200	6.48300	-3.97500
C	2.33400	7.64100	-3.14000
O	1.92800	8.77400	-3.30200

C	1.14600	5.45300	-3.05600
C	-0.35000	5.73600	-2.94300
C	-0.56100	7.13700	-2.36600
C	-0.98900	5.65000	-4.33100
H	2.75600	4.89000	-5.08500
N	3.25100	7.37500	-2.25200
C	3.81500	8.47600	-1.42100
C	4.63900	9.41600	-2.31200
O	5.80800	9.64300	-2.07400
C	4.71400	7.87600	-0.33900
C	5.00900	8.92600	0.70600
C	4.01000	9.32100	1.60300
C	6.28300	9.50200	0.77900
C	4.28400	10.29400	2.57200
C	6.55700	10.47600	1.74800
C	5.55700	10.87100	2.64400
O	5.82700	11.83000	3.59900
H	3.56900	6.45600	-2.13200
H	5.08300	12.43700	3.62800
N	4.03700	9.96000	-3.33900
C	4.77700	10.87900	-4.24800
C	3.83000	11.34500	-5.36800
O	2.77300	11.88300	-5.10200
C	5.97700	10.13100	-4.83700
C	6.93500	11.11800	-5.44500
N	6.54900	12.40100	-5.80100
C	8.26800	11.02600	-5.76300
C	7.62800	13.02300	-6.30900
N	8.70400	12.23000	-6.30800
H	9.64200	12.45800	-6.63600
H	3.09400	9.76500	-3.51200
H	5.65200	12.78500	-5.70200
N	4.18700	11.14600	-6.61400
C	3.29000	11.58000	-7.72500
C	3.67500	10.84000	-9.00900
O	4.79600	10.92700	-9.47100
C	3.44700	13.08600	-7.93400
O	3.24700	13.75600	-6.69700
H	5.03700	10.71100	-6.82100
H	4.09700	13.82200	-6.25400
N	2.75800	10.11400	-9.59300
C	3.08500	9.37700	-10.84700
C	1.86400	8.59200	-11.32900

O	1.96900	7.45400	-11.74100
C	4.24000	8.41100	-10.57400
C	5.35400	8.64700	-11.59600
C	6.67500	8.88900	-10.86400
C	5.48900	7.41700	-12.49600
H	1.85900	10.05800	-9.21000
N	0.70900	9.19500	-11.30000
C	-0.50900	8.48300	-11.77900
C	-0.82400	8.94700	-13.20400
O	-1.64600	8.37700	-13.88800
C	-1.69000	8.79600	-10.85400
O	-2.90300	8.66900	-11.58300
C	-1.56700	10.22000	-10.31500
H	0.64700	10.11900	-10.97900
H	-3.56500	8.29900	-10.99400
N	-0.16100	9.97600	-13.65500
C	-0.39700	10.47700	-15.04100
C	0.49500	11.69100	-15.31600
O	0.80100	11.97200	-16.45500
C	-1.86300	10.87200	-15.22000
C	-2.18200	10.98600	-16.71200
O	-1.93400	10.02800	-17.42600
O	-2.66700	12.02900	-17.11600
H	0.50400	10.41100	-13.08700
N	0.90000	12.41600	-14.28600
C	1.77200	13.62400	-14.48800
C	2.59200	13.51400	-15.78600
O	2.10900	13.82300	-16.85700
C	2.72800	13.75500	-13.29200
C	1.95300	13.84200	-11.96300
C	0.56800	14.47500	-12.16200
C	1.78600	12.43600	-11.38200
H	0.61900	12.17100	-13.36800
N	3.83000	13.09700	-15.70600
C	4.65400	12.99100	-16.94400
C	5.42600	11.66700	-16.95600
O	6.07600	11.33100	-17.92500
C	5.64500	14.15800	-16.98100
O	6.02300	14.49600	-15.65300
C	4.99100	15.36700	-17.65100
H	4.21700	12.86600	-14.84100
H	6.62500	13.82000	-15.33400
N	5.36600	10.91200	-15.89100

C	6.10700	9.61500	-15.86000
C	5.10500	8.47100	-15.70900
O	5.26000	7.41900	-16.29300
C	7.06100	9.60800	-14.66100
C	7.73500	10.97500	-14.52200
C	7.76700	11.37700	-13.04600
N	9.15100	11.19700	-12.52400
C	10.11700	11.97000	-12.94600
N	9.87600	12.89900	-13.83200
N	11.32700	11.81300	-12.48100
H	4.83900	11.19500	-15.11300
H	9.33800	10.49900	-11.86200
H	8.95100	13.02200	-14.19000
H	10.61700	13.48900	-14.15100
H	11.51500	11.10200	-11.80500
H	12.06700	12.40500	-12.80400
N	4.09100	8.70300	-14.91800
C	3.01500	7.68800	-14.65400
C	3.25200	6.36000	-15.38700
O	2.98100	6.22000	-16.56300
C	1.67900	8.27800	-15.10000
C	1.63200	8.36800	-16.60700
C	2.41800	9.31500	-17.27700
C	0.80400	7.50500	-17.33500
C	2.37500	9.39800	-18.67400
C	0.76200	7.58800	-18.73300
C	1.54800	8.53500	-19.40100
H	4.03300	9.57700	-14.47500
N	3.73200	5.37500	-14.67900
C	3.96200	4.03400	-15.30300
C	4.56400	3.08200	-14.26900
O	4.87800	3.47200	-13.16200
C	4.88700	4.16800	-16.53000
C	6.37400	4.08700	-16.14200
C	6.93700	5.49800	-15.96700
N	8.40400	5.40600	-15.71400
C	9.17600	6.43700	-15.93700
N	8.67000	7.55800	-16.37700
N	10.46000	6.34700	-15.71600
H	3.91600	5.51000	-13.72600
H	8.79100	4.56900	-15.38200
H	7.68800	7.63200	-16.54500
H	9.26600	8.34200	-16.54700

H	10.85100	5.49100	-15.37800
H	11.05300	7.13500	-15.88700
N	4.72800	1.83600	-14.61900
C	5.31300	0.86500	-13.64700
C	6.82700	0.80000	-13.79600
O	7.39200	1.30400	-14.74600
C	4.76000	-0.51900	-13.92700
C	3.72900	-0.85300	-12.87200
C	2.56200	0.12100	-13.01000
C	3.24500	-2.28400	-13.07800
H	4.46300	1.53800	-15.52000
N	7.49100	0.16200	-12.86800
C	8.97800	0.05300	-12.98400
C	9.36600	-1.33100	-13.49100
O	8.53500	-2.11700	-13.91100
C	9.62600	0.27200	-11.62700
O	11.01900	0.00500	-11.71700
H	7.00800	-0.25200	-12.10000
H	11.34000	-0.19100	-10.83300
N	10.63000	-1.63700	-13.44800
C	11.09100	-2.96800	-13.92800
C	10.96600	-3.99600	-12.80800
O	11.05100	-5.18800	-13.03900
C	12.55300	-2.86100	-14.36700
C	13.01800	-4.20800	-14.92500
C	13.72900	-4.99900	-13.82600
O	14.53300	-4.45800	-13.09300
N	13.46600	-6.26900	-13.67900
H	11.27900	-0.98400	-13.09400
H	12.81700	-6.70600	-14.27000
H	13.91500	-6.78500	-12.97700
N	10.74700	-3.56500	-11.59800
C	10.61200	-4.52500	-10.50600
C	9.16300	-4.99700	-10.48000
O	8.90300	-6.18400	-10.44800
C	11.02500	-3.83400	-9.21000
C	12.24900	-4.55400	-8.63900
O	12.07400	-5.61800	-8.06900
O	13.34000	-4.02800	-8.78100
H	10.65600	-2.61700	-11.40600
N	8.20100	-4.10600	-10.53800
C	6.80700	-4.60800	-10.56500
C	6.63300	-5.34200	-11.89100

O	6.00300	-6.37800	-11.96300
C	5.79800	-3.45800	-10.44400
C	5.13000	-3.50800	-9.06800
O	5.50100	-4.36400	-8.28300
O	4.26200	-2.68700	-8.82300
H	8.39600	-3.13600	-10.60000
N	7.24000	-4.83600	-12.93900
C	7.16300	-5.54000	-14.24700
C	7.72600	-6.93700	-14.03000
O	7.28100	-7.90700	-14.60700
C	8.01900	-4.77400	-15.27400
C	7.16100	-3.72800	-15.99300
C	8.60000	-5.73800	-16.31400
C	6.13400	-3.14600	-15.02300
H	7.77800	-4.01700	-12.85200
N	8.70800	-7.02700	-13.18500
C	9.32800	-8.34900	-12.89300
C	8.31700	-9.22300	-12.14500
O	8.06600	-10.35300	-12.51300
C	10.56800	-8.14000	-12.02300
C	11.48200	-9.36300	-12.13200
O	11.18000	-10.29800	-12.84500
N	12.59300	-9.39300	-11.44900
H	9.03700	-6.21300	-12.73600
H	12.83600	-8.63900	-10.87300
H	13.18500	-10.17200	-11.51200
N	7.73600	-8.70600	-11.09700
C	6.74000	-9.50500	-10.32400
C	5.61700	-9.98500	-11.25000
O	5.32400	-11.16500	-11.33500
H	7.95600	-7.78800	-10.81500
N	4.97500	-9.08500	-11.94300
C	3.87200	-9.50900	-12.84000
C	4.42400	-10.40900	-13.93800
O	3.86500	-11.43900	-14.25400
C	3.21300	-8.28400	-13.45500
C	2.19300	-8.75500	-14.48600
C	4.27800	-7.41800	-14.13500
C	1.33200	-9.86700	-13.89000
H	5.21300	-8.13500	-11.87000
N	5.53500	-10.04500	-14.49700
C	6.14000	-10.90500	-15.54200
C	6.28600	-12.29900	-14.94400

O	6.17600	-13.30000	-15.62500
C	7.51300	-10.35300	-15.93200
C	7.35900	-9.37200	-17.09500
C	8.67500	-9.28800	-17.87000
O	9.35600	-8.28200	-17.82500
N	9.06400	-10.30700	-18.58700
H	5.97700	-9.22300	-14.21100
H	8.51400	-11.11800	-18.62400
H	9.90500	-10.26200	-19.08700
N	6.50000	-12.36300	-13.65700
C	6.61300	-13.68200	-12.98500
C	5.20700	-14.25900	-12.86500
O	5.01400	-15.45400	-12.76200
C	7.21900	-13.49500	-11.59300
O	6.17600	-13.26600	-10.65400
H	6.55600	-11.53900	-13.12800
H	6.54300	-12.77600	-9.91600
N	4.21700	-13.40400	-12.91000
C	2.81700	-13.87200	-12.83500
C	2.53100	-14.66500	-14.09900
O	2.29800	-15.85700	-14.06600
C	1.90200	-12.65000	-12.78500
C	0.92100	-12.77400	-11.62400
C	-0.21400	-11.77300	-11.82500
C	0.35000	-14.19200	-11.58900
H	4.39700	-12.44700	-13.01900
N	2.56900	-14.00400	-15.22000
C	2.32200	-14.71800	-16.50300
C	3.67500	-15.01200	-17.18200
O	4.47900	-15.75200	-16.65100
C	1.41500	-13.85700	-17.38900
C	0.64200	-14.75500	-18.32800
C	1.23300	-15.21300	-19.51000
C	-0.66900	-15.13300	-18.01200
C	0.51700	-16.04500	-20.37700
C	-1.38600	-15.96500	-18.87800
C	-0.79300	-16.42100	-20.06200
O	-1.50000	-17.24300	-20.91500
H	2.77500	-13.03800	-15.21400
H	-1.32200	-18.15300	-20.66600
N	3.95400	-14.45100	-18.33500
C	5.26800	-14.73000	-18.98700
C	5.04300	-15.34700	-20.37000

O	3.92300	-15.59200	-20.76900
H	3.31700	-13.85200	-18.76500
N	6.12800	-15.57800	-21.05700
C	6.07100	-16.16900	-22.40600
C	5.69100	-17.65000	-22.31900
O	6.05400	-18.33000	-21.38000
C	7.46900	-16.01400	-22.98000
C	8.34800	-15.91400	-21.77100
C	7.51500	-15.31500	-20.65300
N	4.96600	-18.09500	-23.30800
C	4.52100	-19.49800	-23.36600
C	5.70100	-20.41300	-23.70200
O	6.55800	-20.05900	-24.48600
C	3.47800	-19.55200	-24.46900
C	3.81800	-18.38400	-25.34600
C	4.49100	-17.33900	-24.47300
N	5.70200	-21.56600	-23.09100
C	6.77200	-22.55300	-23.31300
C	6.61400	-23.20000	-24.69100
O	7.49200	-23.12400	-25.52700
C	6.60300	-23.59300	-22.21900
C	5.15700	-23.48700	-21.83400
C	4.70800	-22.06800	-22.13300
N	5.49900	-23.83300	-24.93500
C	5.28500	-24.48300	-26.25800
C	3.79200	-24.74400	-26.46400
O	3.16900	-24.18300	-27.34400
C	6.04800	-25.80800	-26.29300
C	6.90000	-25.87400	-27.56100
O	7.41600	-24.84300	-27.95900
O	7.02400	-26.95500	-28.11300
H	4.80300	-23.88200	-24.24700
N	3.21100	-25.59300	-25.66100
C	1.75900	-25.88900	-25.81100
C	0.98700	-24.58300	-26.01200
O	0.78800	-23.82900	-25.07900
C	1.25900	-26.59100	-24.54800
O	-0.13900	-26.82300	-24.66300
H	3.73200	-26.03500	-24.95700
H	-0.30200	-27.24000	-25.51200
N	0.57500	-24.36000	-27.23000
C	-0.18200	-23.14300	-27.57600
C	-1.60200	-23.22800	-27.01100

O	-2.25000	-22.22600	-26.78200
C	-0.21700	-23.10100	-29.09400
C	-0.03100	-24.53200	-29.50100
C	0.77200	-25.21400	-28.40800
N	-2.09100	-24.41600	-26.78400
C	-3.46800	-24.56200	-26.23500
C	-3.52100	-25.77400	-25.30100
O	-2.59000	-26.54900	-25.22100
C	-4.45000	-24.76400	-27.39000
C	-3.80100	-25.63300	-28.46800
C	-4.83800	-25.97800	-29.53800
O	-5.81000	-26.63600	-29.20400
O	-4.64200	-25.57900	-30.67500
H	-1.55300	-25.21300	-26.97600
N	-4.60600	-25.94400	-24.59500
C	-4.71700	-27.10400	-23.66800
C	-4.33500	-28.38800	-24.40800
O	-4.18300	-29.40500	-23.75100
C	-6.16100	-27.21100	-23.17100
O	-6.34100	-28.45400	-22.50900
C	-7.12000	-27.11800	-24.35800
O	-4.19900	-28.33200	-25.61900
H	-5.34700	-25.30700	-24.67400
H	-7.24700	-28.49300	-22.19300
Zn	0.26300	-3.21400	-2.34100
Zn	-11.68300	-2.61000	-0.08200
Ca	-7.35400	5.77300	3.01700
Ca	-12.49400	-12.03200	-8.83700
O	-3.12700	1.78800	-1.75300
H	-3.29600	1.74600	-0.79700
C	-1.80900	2.06400	-1.97500
C	-0.86000	2.12900	-0.94900
C	0.47300	2.41700	-1.24900
C	-1.27800	1.89200	0.44900
C	1.48500	2.49000	-0.17600
C	0.85700	2.64000	-2.57700
O	2.65400	2.74000	-0.43900
C	1.06700	2.25200	1.22100
C	-0.26600	1.96400	1.52200
C	2.01600	2.31800	2.24700
C	-0.65000	1.74200	2.85000
C	0.29900	1.80800	3.87100
C	1.63000	2.09500	3.56900

C	-0.09300	2.57400	-3.59800
C	-1.42300	2.28600	-3.29700
O	-2.44600	1.63900	0.71200
O	-1.93100	1.45500	3.21500
H	-2.55600	2.04900	2.77500
C	0.31600	2.81200	-5.01200
O	1.73400	2.89800	-5.08500
H	2.07600	2.05000	-5.41500

Xyz cartesian coordinates of the complex of 6-Hydroxymusicin with Carbonic anhydrase II

N	13.28300	-1.99700	7.43000
H	13.43600	-1.80800	8.42100
H	14.08500	-2.46300	7.00600
H	12.58700	-2.72900	7.28800
C	12.92400	-0.74700	6.70300
C	11.67900	-0.11700	7.32700
O	11.40000	1.06100	7.11200
C	12.69400	-1.03200	5.21100
C	12.56700	0.20200	4.36300
N	12.80800	1.47300	4.84600
H	13.07500	1.69900	5.80400
C	12.23900	0.35300	3.05700
C	12.63900	2.35100	3.87300
N	12.29400	1.69800	2.77800
H	12.10000	2.12300	1.87100
N	10.93200	-0.91900	8.08300
H	11.21600	-1.89400	8.18300
C	9.71900	-0.47000	8.78100
C	9.13000	-1.66400	9.55800
O	9.46700	-2.81200	9.27200
C	8.70200	0.08000	7.78200
C	7.77200	1.07900	8.37900
N	8.20600	2.29500	8.86100
H	9.16700	2.63400	8.82600
C	6.44000	1.03000	8.61800
C	7.18200	2.95300	9.37600
N	6.09900	2.20700	9.24100
H	5.16100	2.46300	9.54900
N	8.25900	-1.40400	10.53200
H	7.99900	-0.43600	10.72200
C	7.66300	-2.47900	11.34100
C	6.71400	-3.38100	10.55900

O	6.19900	-3.00200	9.49600
C	6.94900	-1.92000	12.59200
C	5.69500	-1.13800	12.30000
C	5.60200	0.20700	12.01300
C	4.35500	-1.64900	12.26300
N	4.28200	0.55500	11.80200
H	3.94500	1.49000	11.57400
C	3.49700	-0.56200	11.94900
C	3.79200	-2.91500	12.46800
C	2.11500	-0.70800	11.84200
C	2.41400	-3.05700	12.35900
C	1.59400	-1.95900	12.05100
N	6.46100	-4.55700	11.12400
H	6.89600	-4.78500	12.01800
C	5.58000	-5.52300	10.49800
C	5.21400	-6.60700	11.49100
O	5.21600	-6.37800	12.70600
N	4.90300	-7.79100	10.98000
H	4.92000	-7.91900	9.96800
C	4.53700	-8.91200	11.83600
C	5.38700	-10.13800	11.51400
O	5.08600	-11.23900	11.96800
C	3.05300	-9.25600	11.67900
C	2.10500	-8.20500	12.19500
C	1.68100	-8.22700	13.52000
C	1.59800	-7.21600	11.34700
C	0.77400	-7.29800	13.99400
C	0.68400	-6.27900	11.80800
C	0.27600	-6.32400	13.13700
O	-0.60500	-5.39300	13.63100
H	-0.94500	-4.72700	13.04500
N	6.44500	-9.94500	10.72900
H	6.64700	-9.01100	10.37300
C	7.31600	-11.05800	10.37400
C	8.34500	-11.40200	11.45400
O	8.46300	-10.70300	12.47500
N	9.13600	-12.44800	11.20200
H	9.03100	-12.94600	10.31800
C	10.14700	-12.90000	12.15400
C	11.10600	-11.77500	12.50500
O	11.39200	-11.53500	13.69000
C	10.94800	-14.08100	11.57000
C	11.42900	-15.11800	12.61500

C	12.33500	-14.51300	13.71300
C	12.29700	-15.36700	14.99100
N	10.95600	-15.26800	15.69800
H	10.93100	-15.83500	16.54600
H	10.18700	-15.50500	15.07100
H	10.71000	-14.29700	15.89300
N	11.51700	-11.02800	11.48200
H	11.14000	-11.20500	10.55100
C	12.49400	-9.96200	11.66600
C	12.09400	-8.53700	12.02700
O	12.96500	-7.75400	12.43100
C	13.49100	-9.98200	10.50800
C	14.35000	-11.20600	10.51600
N	14.04400	-12.33900	9.78500
H	13.27100	-12.42400	9.12500
C	15.44800	-11.51600	11.25100
C	14.91200	-13.29600	10.07500
N	15.77400	-12.82100	10.96100
H	16.55500	-13.33900	11.36400
N	10.79600	-8.22900	11.98400
H	10.12400	-8.95200	11.72600
C	10.30500	-6.87500	12.29800
C	8.97800	-6.96800	13.06200
O	8.21200	-5.99700	13.13800
C	10.10200	-6.04700	11.00800
C	9.10600	-6.69700	10.02500
O	8.77500	-7.90000	10.13300
N	8.62900	-5.90600	9.06000
H	8.89900	-4.92600	8.97200
H	7.97100	-6.33600	8.41000
N	8.74600	-8.14800	13.62900
H	9.44500	-8.88500	13.53400
C	7.53600	-8.42400	14.37700
C	7.41600	-7.74000	15.72200
O	8.27000	-6.96100	16.11900
N	6.35100	-8.05500	16.46800
C	6.09400	-7.47400	17.78300
C	7.26700	-7.48700	18.78300
O	7.45400	-6.52900	19.54800
C	4.88600	-8.28600	18.25500
C	4.12100	-8.46300	16.99400
C	5.22900	-8.92300	16.06400
N	8.05600	-8.55700	18.76900

H	7.85500	-9.30500	18.10500
C	9.19600	-8.70500	19.66400
C	10.35200	-7.72000	19.38800
O	11.33000	-7.69800	20.12500
C	9.70900	-10.15800	19.63200
C	10.14100	-10.67100	18.24400
C	9.02600	-11.38500	17.46800
O	8.13500	-10.70700	16.90700
O	9.06000	-12.63400	17.39400
N	10.24700	-6.92000	18.32800
H	9.41700	-6.98500	17.73900
C	11.28700	-5.95100	17.98400
C	10.77100	-4.50900	18.10300
O	11.56400	-3.57000	18.08500
C	11.74900	-6.11600	16.51600
C	12.43700	-7.41600	16.19000
N	13.79400	-7.50100	15.95300
H	14.45700	-6.73300	16.05800
C	11.94100	-8.65200	15.93700
C	14.10400	-8.72600	15.57000
N	12.99800	-9.44400	15.55200
H	12.93600	-10.42900	15.29400
N	9.45600	-4.31300	18.20200
H	8.82500	-5.11200	18.26800
C	8.91400	-2.94500	18.21600
C	9.48400	-2.03100	19.28900
O	9.61500	-0.82000	19.07500
C	7.38100	-2.92400	18.26800
C	6.68600	-3.63600	17.13100
C	7.24900	-4.10400	15.97600
C	5.29200	-3.98000	17.06600
N	6.29100	-4.72400	15.19800
H	6.45600	-5.16100	14.29100
C	5.08300	-4.65700	15.84000
C	4.20100	-3.78400	17.92700
C	3.81400	-5.14000	15.44800
C	2.94400	-4.26300	17.54300
C	2.76000	-4.93200	16.31500
N	9.88700	-2.61400	20.41000
H	9.82000	-3.62700	20.50600
C	10.42500	-1.81700	21.50500
C	11.68500	-1.05500	21.13300
O	11.98800	-0.04100	21.76600

C	10.68400	-2.67700	22.75600
C	11.90500	-3.53800	22.66300
N	13.15300	-3.10900	23.07300
H	13.35600	-2.19700	23.48300
C	12.07800	-4.79500	22.18800
C	14.04200	-4.06100	22.85300
N	13.41800	-5.09400	22.31900
H	13.85700	-5.97400	22.04700
N	12.42900	-1.54800	20.13500
H	12.13100	-2.40400	19.66800
C	13.67100	-0.88200	19.69400
C	13.45100	0.52600	19.12400
O	14.26900	1.41100	19.32400
C	14.44200	-1.76000	18.70300
C	15.39500	-2.75400	19.38900
C	16.06300	-3.67400	18.39800
C	15.06600	-4.66600	17.86100
N	15.65700	-5.65800	16.92600
H	14.98200	-6.33000	16.56200
H	16.44500	-6.13800	17.36100
H	16.14400	-5.18800	16.16300
N	12.34200	0.74300	18.42700
H	11.68200	-0.01600	18.25800
C	12.07900	2.07300	17.90800
C	10.92600	2.76100	18.61100
O	10.74400	3.96600	18.46600
C	11.85300	2.04500	16.40100
C	13.15700	1.97200	15.63200
O	13.76300	3.04300	15.42300
O	13.57000	0.84900	15.25200
N	10.12100	1.98500	19.33300
H	10.31100	0.98400	19.37500
C	8.97700	2.51500	20.06600
C	9.13900	2.07300	21.52800
O	8.60700	1.05000	21.96000
C	7.66400	2.01700	19.42700
C	7.52400	2.38300	17.95000
C	7.11400	3.65800	17.56600
C	7.87900	1.47000	16.95000
C	7.06700	4.02500	16.19800
C	7.83700	1.82600	15.59100
C	7.43300	3.10400	15.21600
N	9.94500	2.82800	22.29400

C	10.21100	2.53600	23.70500
C	8.94100	2.32000	24.54400
O	8.94300	1.54600	25.51200
C	11.00300	3.76800	24.15800
C	11.76400	4.14900	22.92500
C	10.72400	4.00200	21.84300
N	7.83400	2.93200	24.11900
H	7.87400	3.48900	23.26500
C	6.56200	2.82800	24.84200
C	6.04400	1.37000	24.95200
O	5.26700	1.04200	25.86800
C	5.49700	3.76100	24.20100
C	4.36800	4.06100	25.19600
C	4.96600	3.15300	22.88400
C	4.78600	4.98400	26.38000
N	6.54100	0.49600	24.07300
H	7.21400	0.82900	23.38200
C	6.16300	-0.92100	24.05600
C	6.28800	-1.63400	25.41000
O	5.58900	-2.60000	25.66600
C	6.98200	-1.68100	22.98200
N	7.21800	-1.20000	26.25000
H	7.81000	-0.41400	25.98100
C	7.40900	-1.83200	27.55800
C	6.76100	-0.98000	28.65100
O	7.10900	-1.09800	29.83000
C	8.90600	-2.02200	27.85500
C	9.58100	-3.16500	27.08500
C	11.10600	-3.20200	27.36500
C	11.82800	-4.30500	26.55800
N	11.08600	-5.64600	26.56200
H	11.56200	-6.37400	26.02900
H	10.12600	-5.52900	26.23700
H	10.90400	-5.95600	27.51700
N	5.79400	-0.15800	28.23700
H	5.53700	-0.16000	27.25000
C	5.09300	0.74000	29.14100
C	4.14000	0.08400	30.12400
O	4.02800	-1.12900	30.16800
N	3.40400	0.91400	30.85700
H	3.50000	1.91700	30.69600
C	2.46400	0.46200	31.88300
C	1.00400	0.20000	31.43900

O	0.26500	-0.49100	32.14500
C	2.47200	1.47800	33.05200
C	2.44100	0.85300	34.47400
C	3.72600	0.08900	34.87100
O	3.71700	-0.58500	35.95200
O	4.75000	0.18300	34.12800
N	0.54600	0.81300	30.34600
H	1.14900	1.44200	29.81500
C	-0.83700	0.57000	29.91700
C	-0.92300	0.18900	28.43100
O	-1.50000	0.89700	27.59300
C	-1.77700	1.73900	30.29600
C	-1.38300	3.08700	29.76100
C	-2.44200	4.17400	30.02000
N	-3.61200	4.11800	29.12900
H	-3.76200	3.26200	28.59500
C	-4.49500	5.11500	28.97100
N	-4.36700	6.26700	29.63400
H	-5.03900	7.02500	29.51400
H	-3.58900	6.37200	30.28500
N	-5.50800	4.97800	28.12300
H	-6.18000	5.73600	28.00300
H	-5.60600	4.09800	27.61700
N	-0.30200	-0.94800	28.13100
H	0.15600	-1.46600	28.88100
C	-0.24700	-1.48600	26.78000
C	-1.38100	-2.48100	26.53300
O	-1.95000	-3.04500	27.48300
C	1.11000	-2.15200	26.53200
C	2.24100	-1.15900	26.39100
C	2.17600	-0.37100	25.08800
O	2.43000	-0.91200	24.00600
N	1.83900	0.90800	25.18500
H	1.79500	1.43500	24.31300
H	1.62900	1.35400	26.07800
N	-1.72800	-2.63400	25.25600
H	-1.23500	-2.08400	24.55200
C	-2.76500	-3.53700	24.81600
C	-2.14700	-4.40600	23.73000
O	-1.23700	-3.97300	23.04000
C	-3.94000	-2.74700	24.22700
O	-4.49400	-1.86300	25.17900
H	-5.22200	-1.37400	24.81400

N	-2.74300	-5.57300	23.46800
C	-3.94400	-6.03400	24.17000
C	-3.54100	-6.80800	25.42600
O	-2.35500	-6.97000	25.68500
C	-4.58900	-6.93700	23.13800
C	-3.38400	-7.62100	22.54200
C	-2.35400	-6.52100	22.40800
N	-4.54000	-7.22000	26.21200
H	-5.49400	-6.97600	25.94700
C	-4.34000	-8.00200	27.43300
C	-5.31800	-9.18200	27.43600
O	-6.26400	-9.22700	26.63500
C	-4.57200	-7.17300	28.73700
C	-3.71500	-5.92100	28.73800
C	-6.04200	-6.84000	28.92700
N	-5.05900	-10.15400	28.30600
H	-4.23000	-10.08900	28.89700
C	-5.93500	-11.30900	28.43200
C	-7.03000	-10.96000	29.43800
O	-6.71900	-10.51900	30.54600
C	-5.16000	-12.52700	28.94400
C	-6.07900	-13.67200	29.33900
O	-6.91300	-14.09400	28.51000
O	-5.99300	-14.13300	30.48600
N	-8.29300	-11.16900	29.07600
H	-8.49000	-11.53500	28.14500
C	-9.40700	-10.88500	29.98400
C	-9.71200	-12.08900	30.88900
O	-10.31100	-13.08500	30.44300
C	-10.71700	-10.53600	29.21800
C	-10.46100	-9.46500	28.15300
C	-11.77600	-10.03300	30.19800
C	-10.32800	-8.06600	28.69700
N	-9.26200	-12.01300	32.14300
H	-8.71200	-11.20200	32.42600
C	-9.54000	-13.07100	33.12900
C	-10.96300	-12.79900	33.69300
O	-11.13800	-11.93700	34.56400
C	-8.49400	-13.03700	34.25700
C	-8.64800	-14.19500	35.24000
O	-7.74900	-15.05000	35.30500
O	-9.66500	-14.26500	35.95100
N	-11.96600	-13.52200	33.19200

H	-11.75700	-14.22300	32.48100
C	-13.37000	-13.34600	33.62700
C	-13.63900	-13.43600	35.13500
O	-14.59100	-12.83700	35.61700
C	-14.35400	-14.33700	32.93100
O	-13.95200	-15.69400	33.18300
H	-14.55100	-16.29700	32.75900
C	-14.41700	-14.07500	31.43000
N	-12.82300	-14.19300	35.87000
H	-12.05300	-14.68500	35.41600
C	-13.01200	-14.33200	37.32200
C	-12.39700	-13.20300	38.14800
O	-12.66500	-13.09600	39.33400
C	-12.46400	-15.68300	37.81100
C	-13.09300	-16.85700	37.13900
N	-14.43700	-17.14800	37.26200
H	-15.10300	-16.62800	37.83300
C	-12.58000	-17.78600	36.30000
C	-14.72500	-18.20500	36.52400
N	-13.61500	-18.61000	35.93000
H	-13.53900	-19.40700	35.29800
N	-11.61100	-12.33900	37.52200
H	-11.45100	-12.43500	36.51900
C	-10.97200	-11.24900	38.25700
C	-11.47500	-9.84400	37.87400
O	-11.08000	-8.84400	38.49800
C	-9.43700	-11.36900	38.13000
O	-9.08200	-12.74600	38.29900
H	-8.13800	-12.82000	38.22100
C	-8.73200	-10.56800	39.21100
N	-12.34400	-9.77400	36.85900
H	-12.60900	-10.63400	36.38000
C	-12.93000	-8.50800	36.41000
C	-13.97500	-8.08500	37.43000
O	-14.80600	-8.89400	37.83900
C	-13.58300	-8.68300	35.07200
N	-13.94700	-6.81800	37.83400
H	-13.25500	-6.18000	37.44000
C	-14.88900	-6.32800	38.83000
C	-16.18900	-5.80000	38.23200
O	-16.18200	-4.89500	37.37500
C	-14.23800	-5.26000	39.72200
C	-15.14600	-4.79200	40.88000

C	-14.40000	-4.00300	41.97000
C	-15.37500	-3.32400	42.96900
N	-16.34200	-4.30900	43.60900
H	-16.98300	-3.86300	44.26500
H	-15.84000	-5.07800	44.05300
H	-16.85300	-4.83400	42.89900
N	-17.30500	-6.40100	38.65800
H	-17.23500	-7.17700	39.31600
C	-18.62400	-5.96600	38.19800
C	-18.79000	-4.53900	38.70200
O	-18.69200	-4.29500	39.90900
C	-19.74600	-6.82800	38.78900
C	-21.11200	-6.26400	38.46800
C	-21.59900	-6.28200	37.15700
C	-21.90300	-5.65800	39.45400
C	-22.85600	-5.70100	36.81800
C	-23.17000	-5.07200	39.12000
C	-23.62300	-5.10400	37.79200
O	-24.81600	-4.52200	37.42600
H	-25.34600	-4.11000	38.09800
N	-19.03900	-3.59900	37.80000
H	-19.12900	-3.84900	36.81500
C	-19.18300	-2.21900	38.21300
C	-20.57500	-1.74600	37.82700
O	-20.78400	-1.19000	36.74100
C	-18.10000	-1.37300	37.56400
C	-18.12200	0.06300	38.03600
O	-19.15400	0.45000	38.64100
O	-17.11800	0.80200	37.79000
N	-21.51600	-1.83000	38.78200
C	-22.92700	-1.44200	38.60200
C	-23.16100	0.02200	38.20900
O	-24.25900	0.37300	37.75800
C	-23.54200	-1.77000	39.97000
C	-22.41900	-1.38700	40.92300
C	-21.19100	-1.99300	40.21800
N	-22.14900	0.87200	38.40900
H	-21.27400	0.52500	38.80200
C	-22.27200	2.28700	38.07600
C	-21.92200	2.58300	36.61000
O	-22.01600	3.72900	36.16100
C	-21.41000	3.14100	39.01800
O	-20.03700	2.79200	38.93400

H	-19.50400	3.32000	39.51700
N	-21.45700	1.57100	35.88100
H	-21.32600	0.65500	36.31100
C	-21.13400	1.76300	34.47100
C	-22.50000	1.88100	33.77500
O	-23.42800	1.14200	34.12800
C	-20.39700	0.53500	33.93300
C	-18.90800	0.34100	34.20800
C	-18.51000	-1.10500	33.86800
C	-18.10300	1.32000	33.36900
N	-22.65700	2.82900	32.84900
H	-21.88800	3.46600	32.64000
C	-23.93300	2.96100	32.12700
C	-23.91500	2.19100	30.81700
O	-22.85400	1.67500	30.38800
C	-24.29300	4.41300	31.83800
C	-24.62100	5.19400	33.09600
C	-23.32700	5.64700	33.73000
C	-22.60300	6.57100	32.75200
N	-23.45800	7.77500	32.51600
H	-22.97500	8.39200	31.86300
H	-23.71700	8.24700	33.38200
H	-24.39800	7.53300	32.20300
N	-25.10500	2.02700	30.19600
C	-25.12800	1.29500	28.92500
C	-24.51700	2.13500	27.80500
O	-24.47300	3.36400	27.88500
C	-26.62500	1.01500	28.70500
C	-27.33000	2.09400	29.51100
C	-26.46900	2.26100	30.72300
N	-23.93500	1.44900	26.83000
H	-23.91100	0.43100	26.88700
C	-23.33000	2.10800	25.68100
C	-24.43400	2.71400	24.82900
O	-25.55100	2.20500	24.81400
C	-22.59500	1.08300	24.81800
C	-21.26200	0.59800	25.35700
C	-20.72600	-0.42800	24.37700
C	-20.29700	1.79300	25.52000
N	-24.11200	3.78800	24.12200
H	-23.17100	4.17200	24.20800
C	-25.05800	4.43600	23.22800
C	-24.35200	4.51700	21.87300

O	-23.47000	5.35100	21.66600
C	-25.42100	5.83900	23.72700
O	-26.54400	6.36000	23.01900
H	-26.76900	7.23000	23.32800
N	-24.67000	3.57100	20.99900
H	-25.35800	2.86800	21.26800
C	-24.07500	3.49600	19.66900
C	-25.06600	4.09000	18.65100
O	-26.13100	3.51700	18.41500
C	-23.78600	2.02300	19.31600
C	-23.03900	1.92900	18.01700
C	-22.99400	1.35100	20.43800
N	-24.76300	5.27000	18.11900
H	-23.89800	5.73200	18.40000
C	-25.63300	5.92400	17.14400
C	-24.92700	6.04000	15.80500
O	-24.20800	7.00900	15.53900
C	-26.07200	7.30400	17.64900
O	-26.94000	7.15800	18.76500
H	-27.21200	8.01300	19.07800
N	-25.15400	5.03900	14.95900
H	-25.79200	4.29500	15.24200
C	-24.52700	4.95900	13.63800
C	-25.53000	5.12100	12.47700
O	-25.22400	4.73200	11.34700
C	-23.83000	3.58700	13.47200
C	-22.55400	3.32500	14.27800
C	-21.86500	4.35700	14.92200
C	-22.02300	2.03400	14.34800
C	-20.66800	4.10100	15.61800
C	-20.85300	1.76400	15.02600
C	-20.17400	2.80000	15.66200
O	-19.00300	2.52600	16.32900
H	-18.54000	3.23300	16.76300
N	-26.70700	5.69700	12.72200
H	-26.93000	6.05600	13.65000
C	-27.67300	5.80200	11.62500
C	-27.37900	6.78200	10.46700
O	-27.83800	6.55400	9.34600
C	-29.11400	5.96300	12.14400
C	-29.31600	7.22800	12.95100
O	-29.02300	7.21300	14.17400
O	-29.80000	8.22800	12.37100

N	-26.61300	7.84300	10.70400
H	-26.23200	7.99800	11.63700
C	-26.31600	8.78800	9.62900
C	-24.86200	8.61800	9.16100
O	-24.27500	9.54300	8.58300
C	-26.59800	10.25100	10.06000
C	-28.10800	10.63100	10.37000
C	-29.07200	10.54200	9.14300
O	-28.63400	10.53600	7.97200
N	-30.39400	10.48000	9.41900
H	-30.75100	10.48500	10.37400
H	-31.02300	10.42200	8.61800
N	-24.32000	7.41100	9.36800
H	-24.90200	6.69200	9.79900
C	-22.92500	7.05600	9.00900
C	-22.56300	7.11300	7.51200
O	-23.23900	6.52800	6.67100
C	-22.55800	5.66300	9.58700
N	-21.42300	7.72000	7.21100
H	-20.83800	8.08900	7.96000
C	-20.99500	7.86700	5.83200
C	-19.65400	7.22600	5.57100
O	-18.62200	7.77400	5.97400
C	-20.87700	9.34700	5.44600
O	-22.04800	10.04000	5.87800
H	-22.12900	9.94700	6.82000
C	-20.74600	9.49800	3.92100
N	-19.65800	6.08200	4.89500
H	-20.54300	5.66300	4.60800
C	-18.41400	5.43100	4.56600
C	-17.94900	6.10000	3.26600
O	-18.78400	6.56000	2.45200
C	-18.63600	3.93800	4.39500
O	-19.70300	3.70400	3.50700
H	-19.84200	2.77000	3.40000
N	-16.63300	6.20100	3.09100
H	-16.00500	5.81500	3.79600
C	-16.06800	6.85300	1.91100
C	-15.28000	5.89200	1.04800
O	-15.47800	5.82200	-0.17600
C	-15.14400	7.98700	2.33500
C	-15.67200	9.03400	3.32300
C	-14.57900	10.00700	3.68300

C	-16.88500	9.74700	2.71100
N	-14.33500	5.19300	1.67500
H	-14.19000	5.32100	2.67600
C	-13.51000	4.24900	0.93900
C	-12.86200	3.18500	1.78800
O	-12.91900	3.21700	3.02200
C	-12.44500	4.96100	0.11100
C	-11.43000	5.67600	0.89700
C	-10.23900	6.11500	0.03600
N	-9.25800	6.70600	0.94900
H	-9.62100	7.16200	1.78600
C	-7.93600	6.70300	0.78800
N	-7.36500	6.16200	-0.29300
H	-7.94400	5.86100	-1.07700
H	-6.35200	6.16000	-0.41600
N	-7.18500	7.09300	1.80600
H	-7.62100	7.50600	2.63100
H	-6.17200	7.09100	1.68300
N	-12.26800	2.22800	1.09100
H	-12.28400	2.28300	0.07300
C	-11.60100	1.11300	1.71300
C	-10.20800	1.04300	1.09400
O	-10.04500	1.30000	-0.10900
C	-12.42400	-0.21300	1.51900
C	-11.76900	-1.36900	2.29000
C	-12.62800	-0.53000	0.02000
C	-12.60000	-2.65000	2.34800
N	-9.19900	0.80400	1.93200
H	-9.39200	0.68300	2.92600
C	-7.81300	0.71100	1.45100
C	-6.97800	-0.34100	2.18400
O	-7.25500	-0.71800	3.33300
C	-7.08700	2.06700	1.53400
C	-6.38700	2.40300	2.85900
C	-5.39300	3.54300	2.68800
C	-7.41300	2.70500	3.91600
N	-5.94200	-0.79200	1.50100
H	-5.79000	-0.44800	0.55300
C	-5.01000	-1.76100	2.05300
C	-3.76800	-0.92700	2.37900
O	-3.22200	-0.27200	1.49100
C	-4.69600	-2.83800	1.00300
C	-3.60000	-3.77200	1.43800

O	-2.76600	-3.42700	2.28400
N	-3.57800	-4.96600	0.85500
H	-2.83500	-5.59900	1.15000
H	-4.26600	-5.25000	0.15700
N	-3.35900	-0.91000	3.65100
H	-3.87500	-1.45100	4.34400
C	-2.18900	-0.13500	4.07900
C	-0.95200	-0.97500	4.47500
O	-0.08000	-0.50400	5.22100
C	-2.57200	0.80500	5.22800
C	-2.88900	0.05800	6.52500
O	-2.64000	-1.14200	6.66900
N	-3.43100	0.78100	7.47900
H	-3.63700	1.77300	7.36000
H	-3.64200	0.28300	8.34400
N	-0.90300	-2.22800	4.03100
H	-1.67200	-2.59500	3.47000
C	0.23400	-3.07900	4.33700
C	0.25600	-3.75600	5.69700
O	1.12800	-4.58900	5.95200
N	-0.66000	-3.37100	6.58300
H	-1.31400	-2.63500	6.31900
C	-0.77000	-3.95700	7.91900
C	-2.14600	-4.63600	8.05100
O	-2.28100	-5.68500	8.69300
C	-0.59000	-2.86200	8.97000
C	0.66600	-2.06300	8.78800
N	0.66000	-0.70400	8.55700
H	-0.17300	-0.11700	8.51600
C	1.97000	-2.44100	8.76300
C	1.90400	-0.28000	8.39600
N	2.71800	-1.31400	8.51600
H	3.73500	-1.28100	8.43800
N	-3.14900	-4.04700	7.39500
H	-2.93500	-3.20400	6.86200
C	-4.53300	-4.52400	7.38500
C	-5.30400	-3.68500	6.35000
O	-4.68600	-2.98500	5.52700
C	-5.16000	-4.32600	8.78200
N	-6.63500	-3.80700	6.34700
H	-7.07100	-4.48600	6.97100
C	-7.49000	-2.99100	5.47100
C	-8.45000	-2.16300	6.34900

O	-8.99400	-2.65600	7.35500
C	-8.23800	-3.80900	4.38900
C	-9.22200	-4.83000	4.92500
C	-8.84300	-6.16200	5.09000
C	-10.53400	-4.46800	5.23200
C	-9.73100	-7.12000	5.54500
C	-11.45000	-5.44200	5.69700
C	-11.03900	-6.76700	5.85000
N	-8.55200	-0.88000	6.02900
H	-8.01200	-0.52200	5.24100
C	-9.41300	0.03400	6.77000
C	-10.57100	0.58300	5.92200
O	-10.37800	0.93200	4.75200
C	-8.62000	1.26700	7.24800
C	-7.39900	0.92600	8.11600
O	-6.57500	1.80300	8.38300
N	-7.28000	-0.31800	8.55900
H	-6.46900	-0.54400	9.13500
H	-7.96200	-1.04400	8.33800
N	-11.76100	0.65100	6.51200
H	-11.87100	0.26200	7.44800
C	-12.91900	1.26700	5.86000
C	-12.96000	2.63200	6.57900
O	-12.99200	2.68400	7.81200
C	-14.24400	0.48700	6.11300
C	-15.45500	1.34100	5.71100
C	-14.24200	-0.81500	5.34600
N	-12.89000	3.71500	5.81700
H	-12.84400	3.59900	4.80500
C	-12.87600	5.06400	6.36800
C	-14.24200	5.73600	6.28800
O	-15.00300	5.48000	5.35700
C	-11.84800	5.90500	5.62500
C	-10.44700	5.30900	5.70100
C	-9.41000	6.02400	4.84900
O	-9.76300	6.59500	3.79100
O	-8.21700	5.96900	5.22800
N	-14.53200	6.61000	7.24900
H	-13.83700	6.78700	7.97500
C	-15.80500	7.32800	7.30800
C	-15.56100	8.82300	7.34700
O	-14.46500	9.27400	7.69900
C	-16.59700	6.92100	8.55600

C	-17.06400	5.50200	8.53200
C	-16.17800	4.46400	8.77300
C	-18.38300	5.19700	8.22200
C	-16.59100	3.14500	8.70400
C	-18.80200	3.88100	8.14800
C	-17.90400	2.85300	8.39000
N	-16.57500	9.58300	6.95500
H	-17.43000	9.13100	6.63000
C	-16.51600	11.03900	6.97000
C	-16.73200	11.47800	8.42400
O	-17.83700	11.43400	8.92400
C	-17.63500	11.59500	6.08100
C	-17.81500	13.10500	6.21700
O	-16.91800	13.79000	6.78000
O	-18.87000	13.60400	5.76300
N	-15.68500	11.94500	9.08000
H	-14.78400	12.01500	8.60700
C	-15.80300	12.36200	10.47500
C	-15.72400	13.88700	10.66700
O	-15.21400	14.37000	11.68900
C	-14.72800	11.64200	11.32300
C	-13.29800	12.15200	11.05500
O	-13.00300	12.68100	9.95300
O	-12.45600	12.02700	11.96000
N	-16.21500	14.64900	9.69000
H	-16.63000	14.21600	8.86500
C	-16.15900	16.10400	9.80000
C	-17.35500	16.61400	10.59200
O	-17.44700	17.81300	10.88400
C	-16.14200	16.75300	8.41800
O	-17.26100	16.33000	7.65400
H	-17.25000	16.73400	6.79400
N	-18.26600	15.70000	10.93500
H	-18.10300	14.73100	10.66200
C	-19.48800	16.01300	11.68200
C	-19.91700	14.85500	12.59800
O	-19.58400	13.69600	12.34000
C	-20.62500	16.27400	10.70500
C	-20.58500	17.61900	10.00300
C	-21.90400	17.87200	9.30400
O	-22.34100	17.06200	8.47100
N	-22.59800	18.94000	9.70100
H	-22.23900	19.60600	10.38500

H	-23.48700	19.11000	9.23000
N	-20.69400	15.17100	13.63400
H	-20.95900	16.14700	13.77000
C	-21.18100	14.16900	14.58300
C	-22.23400	13.22100	13.97200
O	-23.29400	13.01300	14.56000
C	-21.76800	14.86400	15.83200
C	-20.70900	15.20200	16.90100
O	-19.52300	14.85600	16.73000
O	-21.07700	15.78600	17.94900
N	-21.90100	12.57100	12.86000
H	-20.97100	12.70300	12.46200
C	-22.84400	11.67100	12.19900
C	-22.89700	10.22800	12.73300
O	-23.95100	9.58100	12.67400
C	-22.59700	11.65200	10.68400
C	-21.28600	11.00300	10.31000
C	-21.23000	10.59100	8.84600
C	-19.92100	9.84700	8.51700
N	-19.59800	8.67900	9.36500
H	-18.73200	8.18700	9.14700
H	-20.37800	8.02200	9.35700
H	-19.59900	8.95600	10.34700
N	-21.76400	9.67900	13.15600
H	-20.89800	10.21600	13.11200
C	-21.74000	8.31400	13.68400
C	-20.96500	8.42700	14.97400
O	-19.74400	8.66100	14.93500
C	-21.02500	7.36800	12.70500
N	-21.65500	8.29300	16.10800
H	-22.65300	8.08500	16.06900
C	-20.99500	8.44200	17.41100
C	-21.15900	7.34300	18.45900
O	-22.08700	6.53100	18.41600
C	-21.39200	9.77100	18.09800
C	-20.95000	10.96900	17.26000
C	-22.90900	9.80100	18.36900
N	-20.22900	7.35800	19.41200
H	-19.48400	8.05200	19.34800
C	-20.21700	6.43400	20.54500
C	-20.21400	7.29500	21.81100
O	-19.45700	8.26900	21.92400
C	-18.96800	5.55300	20.51000

C	-18.82400	4.47100	21.57800
C	-20.00100	3.52200	21.54000
C	-17.51200	3.71500	21.34400
N	-21.11300	6.98200	22.72700
H	-21.76600	6.21900	22.55000
C	-21.18500	7.70900	23.98300
C	-21.70200	6.78200	25.08900
O	-22.03900	5.62300	24.83000
C	-22.03900	8.98300	23.82600
C	-23.43500	8.74800	23.28000
C	-24.02500	10.00300	22.64100
C	-24.56000	10.99600	23.66800
N	-23.50200	11.68800	24.45900
H	-23.86000	12.35200	25.14600
H	-22.83200	12.14300	23.83800
H	-22.88900	11.00700	24.90700
N	-21.72100	7.27100	26.32200
H	-21.39500	8.22200	26.49300
C	-22.20100	6.46700	27.42800
C	-21.15600	5.46700	27.87200
O	-19.96600	5.67200	27.60600
N	-21.59300	4.37800	28.50700
H	-22.59300	4.24900	28.65900
C	-20.65700	3.37600	28.98300
C	-19.67900	3.97900	29.97700
O	-20.10600	4.64400	30.91900
N	-18.36000	3.78000	29.78900
C	-17.30900	4.30700	30.67000
C	-16.79000	5.66400	30.18500
O	-15.82100	6.19200	30.73900
C	-16.20300	3.27400	30.49600
C	-16.27300	3.01300	28.99400
C	-17.78100	2.89500	28.75200
N	-17.44600	6.22800	29.17100
H	-18.28900	5.77700	28.81700
C	-16.99900	7.46500	28.55300
C	-17.63200	8.76900	29.03800
O	-18.77000	8.80300	29.50700
C	-17.18100	7.35100	27.02500
C	-16.81800	6.03400	26.30900
C	-17.39500	6.02400	24.88700
C	-15.29700	5.82700	26.29500
N	-16.87200	9.84700	28.92000

H	-15.92100	9.75200	28.56300
C	-17.36400	11.15700	29.28800
C	-17.12400	11.93400	28.00500
O	-15.98300	12.02700	27.53300
C	-16.56200	11.76700	30.46400
C	-16.60400	10.89100	31.74300
O	-17.70700	10.70700	32.33300
O	-15.51900	10.39100	32.16800
N	-18.20300	12.38600	27.38000
H	-19.13000	12.21300	27.76900
C	-18.06200	13.12600	26.14400
C	-18.49600	12.31400	24.93200
O	-19.00900	11.20000	25.06100
N	-18.26700	12.86000	23.74800
H	-17.80100	13.76600	23.69400
C	-18.66800	12.19000	22.52900
C	-17.45700	11.81700	21.68600
O	-16.53400	12.61300	21.52000
C	-19.62600	13.09100	21.73500
O	-20.78600	13.35500	22.54100
H	-21.37800	13.91200	22.05000
C	-20.03700	12.43300	20.42100
N	-17.48000	10.59600	21.16700
H	-18.28900	10.00400	21.35900
C	-16.41300	10.05700	20.33900
C	-16.94600	9.77200	18.93100
O	-17.92600	9.03700	18.75500
C	-15.85100	8.78700	20.98800
C	-15.08600	9.02300	22.29300
C	-15.74400	9.41600	23.46900
C	-13.70600	8.82800	22.35200
C	-15.04100	9.60300	24.66100
C	-12.99600	9.01200	23.53100
C	-13.66300	9.39600	24.68400
O	-12.94100	9.55500	25.85300
H	-13.39800	9.81800	26.64300
N	-16.28100	10.35400	17.93700
H	-15.46200	10.91400	18.17300
C	-16.65200	10.24100	16.52100
C	-15.92700	9.09100	15.77400
O	-14.70100	8.95600	15.85300
C	-16.34300	11.58200	15.85300
C	-17.07500	11.84800	14.60100

C	-16.76100	13.25400	14.11700
N	-17.32000	14.29600	14.97300
H	-18.04200	14.02800	15.64200
C	-16.94700	15.57800	14.93600
N	-15.99700	15.98300	14.08600
H	-15.71200	16.96200	14.05800
H	-15.53900	15.29800	13.48500
N	-17.54500	16.47200	15.72000
H	-17.26000	17.45100	15.69200
H	-18.26900	16.16300	16.36800
N	-16.69300	8.27400	15.05400
H	-17.69800	8.44700	15.02000
C	-16.14900	7.13500	14.30800
C	-15.29400	7.56600	13.11500
O	-15.76800	8.25700	12.20700
C	-17.29400	6.22700	13.82300
C	-16.94800	5.06400	12.88000
C	-16.06400	4.04500	13.60700
C	-18.22700	4.40600	12.35300
N	-14.03400	7.14600	13.11300
H	-13.68800	6.57300	13.88300
C	-13.14600	7.50000	12.01700
C	-12.89700	6.34200	11.05000
O	-12.83000	6.54700	9.83500
C	-11.80700	8.14600	12.50800
C	-10.95300	8.51600	11.29100
C	-11.03600	7.21500	13.46600
C	-10.09200	9.72500	11.50900
N	-12.78800	5.12700	11.58100
H	-12.85900	5.01400	12.59200
C	-12.56900	3.95300	10.74200
C	-12.62800	2.64500	11.51900
O	-12.68200	2.64500	12.74700
C	-11.21500	4.04400	10.01800
C	-10.00600	4.13700	10.93400
C	-9.23600	2.82200	11.09500
O	-9.81600	1.73200	11.26500
N	-7.90800	2.92600	11.06600
H	-7.43300	3.81800	10.92700
H	-7.39500	2.05100	11.17300
N	-12.71600	1.54100	10.78100
H	-12.80600	1.62400	9.76800
C	-12.68700	0.22000	11.38500

C	-11.79300	-0.68800	10.54800
O	-11.57700	-0.42400	9.36200
C	-14.08700	-0.36800	11.64200
C	-14.86400	-0.73600	10.40600
C	-14.58400	-1.91600	9.70300
C	-15.94300	0.04700	9.99600
C	-15.36500	-2.31100	8.61900
C	-16.73300	-0.34000	8.91600
C	-16.44400	-1.52300	8.22500
N	-11.23000	-1.70700	11.19700
H	-11.44100	-1.81200	12.18900
C	-10.33000	-2.68600	10.58400
C	-10.40300	-3.99000	11.36600
O	-11.02600	-4.05100	12.43100
C	-8.88800	-2.18000	10.60100
C	-8.36900	-1.87100	11.97800
N	-8.54500	-0.66400	12.61800
H	-9.02100	0.15000	12.23000
C	-7.68600	-2.65000	12.85500
C	-7.98700	-0.73700	13.83400
N	-7.44500	-1.92200	14.03800
N	-9.75100	-5.02300	10.83900
H	-9.25100	-4.89200	9.96000
C	-9.72500	-6.33700	11.47300
C	-8.27700	-6.81200	11.72000
O	-7.32400	-6.29000	11.14300
C	-10.42400	-7.40700	10.60300
C	-11.87600	-7.11200	10.26300
C	-12.21100	-6.13300	9.31200
C	-12.90300	-7.85200	10.84600
C	-13.55800	-5.90200	8.95000
C	-14.24600	-7.62900	10.49000
C	-14.57200	-6.65500	9.54400
N	-8.14600	-7.79100	12.60500
H	-8.98600	-8.10500	13.09200
C	-6.88900	-8.45000	12.93200
C	-7.33400	-9.91500	12.79400
O	-8.41900	-10.27700	13.25700
C	-6.45600	-8.14000	14.37700
C	-6.12300	-6.69400	14.62300
N	-4.86400	-6.15100	14.47600
H	-4.02800	-6.65300	14.17800
C	-6.91500	-5.66600	15.03000

C	-4.92800	-4.83500	14.79600
N	-6.15300	-4.47300	15.14400
N	-6.57100	-10.73100	12.08100
H	-5.70600	-10.38400	11.66700
C	-6.95900	-12.11600	11.88500
C	-5.76600	-13.05800	11.80100
O	-4.61200	-12.62200	11.76500
C	-7.84100	-12.25400	10.63200
C	-7.15500	-11.86900	9.33400
C	-6.44900	-12.68800	8.50400
C	-7.13500	-10.57300	8.72300
N	-5.99000	-11.98400	7.41300
H	-5.43600	-12.37000	6.64900
C	-6.39800	-10.68500	7.52100
C	-7.67100	-9.33000	9.06800
C	-6.18600	-9.60000	6.66800
C	-7.45700	-8.24500	8.21100
C	-6.72300	-8.39200	7.02900
N	-6.05500	-14.35300	11.76600
H	-7.02800	-14.65700	11.77100
C	-4.99200	-15.33400	11.72100
C	-4.91900	-16.18400	10.47200
O	-5.71900	-16.06100	9.53600
N	-3.90000	-17.03300	10.44600
H	-3.24900	-17.05500	11.23100
C	-3.69200	-17.93200	9.32400
C	-4.50200	-19.20900	9.55400
O	-4.64100	-20.03300	8.65300
C	-2.20300	-18.26500	9.18300
O	-1.65600	-18.71000	10.40800
H	-0.73300	-18.91600	10.32100
N	-5.00100	-19.36800	10.77800
H	-4.81800	-18.64500	11.47400
C	-5.79600	-20.52300	11.17400
C	-6.97800	-20.04600	12.01400
O	-6.87400	-19.03100	12.70000
C	-4.94500	-21.47400	12.00400
C	-3.70800	-22.04400	11.32100
C	-2.89400	-22.84300	12.33100
C	-4.12400	-22.88300	10.12800
N	-8.07800	-20.79800	11.98300
H	-8.07500	-21.64700	11.41800
C	-9.29800	-20.45300	12.73200

C	-9.10800	-20.26500	14.24500
O	-9.86800	-19.53000	14.87100
C	-10.41200	-21.50300	12.51200
C	-10.98700	-21.49900	11.07300
O	-10.66500	-20.59000	10.26600
O	-11.79300	-22.40800	10.76200
N	-8.09700	-20.92200	14.81700
H	-7.48500	-21.50000	14.24100
C	-7.85300	-20.82800	16.25200
C	-6.93200	-19.72500	16.77100
O	-6.37500	-19.84600	17.86200
N	-6.75200	-18.66500	15.98900
H	-7.22000	-18.63800	15.08300
C	-5.91700	-17.54700	16.37500
C	-6.23900	-16.41600	15.41000
O	-6.68500	-16.65200	14.28900
C	-4.42600	-17.92700	16.30900
C	-3.85300	-18.07700	14.89000
C	-2.52600	-18.82700	14.85200
O	-2.42400	-19.96000	15.32000
N	-1.51100	-18.20300	14.26400
H	-0.62300	-18.70500	14.23900
H	-1.59600	-17.26400	13.87600
N	-6.07500	-15.19500	15.87800
H	-5.76400	-15.06300	16.84000
C	-6.33000	-14.04300	15.04800
C	-6.69800	-12.84300	15.87800
O	-6.44700	-11.70000	15.49300
N	-7.34600	-13.09200	17.01000
H	-7.56500	-14.05400	17.26800
C	-7.74500	-11.99900	17.88500
C	-6.51900	-11.52400	18.67000
O	-5.51700	-12.24900	18.78300
C	-8.90100	-12.41500	18.82100
O	-8.54300	-13.46000	19.71200
H	-9.25400	-13.71600	20.28800
N	-6.58700	-10.27900	19.13100
H	-7.41800	-9.72700	18.91800
C	-5.53000	-9.66300	19.92800
C	-5.89500	-9.86800	21.41000
O	-5.08300	-10.34300	22.18500
C	-5.38300	-8.18400	19.54500
C	-5.11200	-7.98800	18.05000

C	-4.38300	-6.70900	17.75200
O	-4.98900	-5.62600	17.91100
O	-3.19900	-6.78300	17.36900
N	-7.11600	-9.50300	21.80200
H	-7.74800	-9.05600	21.13800
C	-7.55600	-9.73800	23.17600
C	-7.94700	-11.21000	23.23700
O	-8.25100	-11.80900	22.20700
C	-8.76100	-8.87900	23.53800
C	-8.43700	-7.43300	23.70500
N	-8.39000	-6.55300	22.64500
H	-8.58100	-6.79100	21.67200
C	-8.11900	-6.71200	24.80800
C	-8.05800	-5.35300	23.08800
N	-7.88800	-5.42300	24.39700
H	-7.62700	-4.64500	25.00300
N	-7.88300	-11.79400	24.42500
H	-7.57100	-11.23800	25.22100
C	-8.24000	-13.20600	24.65500
C	-9.21900	-13.25900	25.84800
O	-9.25400	-12.33000	26.65400
C	-6.98900	-14.04300	25.03200
O	-6.15700	-13.27600	25.91000
H	-6.66300	-13.03200	26.67600
C	-6.18500	-14.43000	23.81600
N	-10.05700	-14.28300	25.93300
H	-10.07200	-14.99500	25.20300
C	-10.96400	-14.38700	27.08300
C	-10.58400	-15.66800	27.79600
O	-10.71200	-16.75700	27.23700
C	-12.44100	-14.47500	26.68300
C	-13.29800	-14.57200	27.94100
C	-12.85000	-13.26100	25.83500
N	-10.09400	-15.54500	29.02200
H	-10.02100	-14.62000	29.44500
C	-9.65500	-16.72400	29.77800
C	-8.67000	-17.55200	28.92000
O	-8.76400	-18.78000	28.84100
C	-10.85300	-17.57400	30.22700
C	-11.67500	-16.91300	31.33700
O	-11.12700	-16.11100	32.11900
O	-12.88500	-17.20500	31.43400
N	-7.77600	-16.84300	28.22800

H	-7.81900	-15.82600	28.29300
C	-6.73400	-17.43500	27.37800
C	-7.20700	-17.88800	26.00000
O	-6.39800	-18.28800	25.14900
C	-6.03200	-18.59600	28.09900
C	-4.63600	-18.27300	28.60300
C	-4.64500	-17.07900	29.52100
C	-3.26100	-16.42400	29.59200
N	-2.22500	-17.27200	30.26900
H	-1.30400	-16.83600	30.31600
H	-2.16600	-18.18900	29.82700
H	-2.53900	-17.55000	31.19900
N	-8.51300	-17.77600	25.77500
H	-9.10300	-17.39300	26.51400
C	-9.14500	-18.17900	24.51200
C	-8.97100	-17.15500	23.38100
O	-9.31700	-15.98100	23.55300
C	-10.64600	-18.43000	24.73600
C	-11.37500	-19.00100	23.53300
C	-12.83800	-19.27700	23.86400
C	-13.50600	-20.13700	22.78300
N	-13.45900	-19.46400	21.45200
H	-13.90300	-20.03600	20.73300
H	-12.50500	-19.21100	21.19300
H	-13.86400	-18.52900	21.49000
N	-8.42900	-17.61600	22.25000
H	-8.13400	-18.59200	22.21700
C	-8.23700	-16.79200	21.05500
C	-9.35400	-17.10600	20.04900
O	-9.69800	-18.27400	19.84200
C	-6.91400	-17.13700	20.36600
C	-5.64400	-16.67000	21.01800
C	-4.47100	-17.15600	20.17300
C	-3.13100	-16.82300	20.80500
N	-2.92100	-17.64000	22.02500
H	-2.02100	-17.41600	22.45000
H	-3.01500	-18.63800	21.83600
H	-3.69000	-17.53900	22.68800
N	-9.92700	-16.06900	19.44300
H	-9.63200	-15.12700	19.69800
C	-10.97000	-16.23100	18.41900
C	-10.29000	-16.15600	17.03100
O	-9.10100	-15.85700	16.95200

C	-12.02800	-15.12400	18.56200
C	-13.04200	-15.35300	19.67300
C	-14.31800	-15.83200	19.38600
C	-12.74100	-15.05300	21.00700
C	-15.27900	-16.00200	20.39800
C	-13.70200	-15.22000	22.03100
C	-14.96800	-15.69200	21.71500
O	-15.93800	-15.82400	22.69900
H	-15.72500	-15.61200	23.60000
N	-11.01800	-16.39600	15.94600
H	-12.00800	-16.62200	16.04200
C	-10.40900	-16.33900	14.60300
C	-10.01500	-14.92700	14.12400
O	-9.12100	-14.77100	13.28600
C	-11.31300	-17.01500	13.56700
N	-10.67400	-13.89600	14.64700
H	-11.41400	-14.06100	15.32900
C	-10.34300	-12.52200	14.24800
C	-10.92000	-11.53500	15.24200
O	-11.64500	-11.93800	16.17200
C	-10.88500	-12.21900	12.83000
N	-10.62700	-10.25000	15.02900
H	-10.02100	-9.99800	14.24800
C	-11.15100	-9.20700	15.88400
C	-11.37400	-7.89000	15.14800
O	-10.50000	-7.40400	14.43300
C	-10.23900	-9.01600	17.10000
C	-10.74200	-8.00200	18.14300
C	-9.85000	-7.94200	19.38300
O	-9.28900	-8.99600	19.77400
O	-9.71500	-6.84200	19.95700
N	-12.58500	-7.36100	15.27500
H	-13.27800	-7.86200	15.83100
C	-12.97100	-6.10000	14.65900
C	-12.70900	-4.91400	15.60200
O	-13.01700	-4.97900	16.78700
C	-14.45900	-6.15300	14.30000
C	-15.18500	-4.89300	13.84700
C	-14.52700	-4.29100	12.63400
C	-16.60900	-5.26600	13.52600
N	-12.15000	-3.83800	15.06500
H	-11.90900	-3.85400	14.07400
C	-11.86700	-2.63900	15.83200

C	-12.54700	-1.41700	15.21200
O	-12.27700	-1.07600	14.05900
C	-10.34600	-2.37200	15.89900
C	-9.58900	-3.31400	16.78900
N	-8.21300	-3.47100	16.68700
C	-10.05900	-4.11800	17.77500
C	-7.89200	-4.36300	17.60600
N	-8.97300	-4.78100	18.28700
H	-8.98400	-5.46400	19.04400
N	-13.48400	-0.81900	15.94200
H	-13.74500	-1.22100	16.84200
C	-14.15100	0.40200	15.48600
C	-13.52500	1.55300	16.27500
O	-13.74800	1.72100	17.48000
C	-15.66800	0.34500	15.67600
C	-16.41000	-0.67700	14.80100
C	-16.68100	-1.94300	15.56100
C	-17.73200	-0.06900	14.31300
N	-12.71100	2.32300	15.57600
H	-12.60700	2.13900	14.57800
C	-11.95700	3.41900	16.15900
C	-12.68800	4.76000	16.18400
O	-13.20500	5.21300	15.15100
C	-10.62200	3.55400	15.39500
C	-9.73600	4.62600	16.01400
C	-9.93600	2.21000	15.33100
N	-12.71000	5.38800	17.36400
H	-12.24400	4.94600	18.15600
C	-13.37500	6.69000	17.58100
C	-12.43300	7.67300	18.27600
O	-11.55700	7.25400	19.03200
C	-14.59000	6.55200	18.51100
C	-15.58700	5.51600	18.09300
N	-15.31200	4.16700	18.11100
H	-14.41600	3.75100	18.36400
C	-16.87800	5.63200	17.70100
C	-16.39200	3.49500	17.74900
N	-17.35700	4.36100	17.49400
H	-18.30200	4.12500	17.19300
N	-12.62600	8.97200	18.05700
H	-13.35700	9.27200	17.41200
C	-11.80000	9.97600	18.73300
C	-12.65600	10.98100	19.50000

O	-13.76600	11.31100	19.08700
C	-10.81000	10.68200	17.77700
C	-11.43100	11.37500	16.59600
C	-11.76500	10.80900	15.39000
C	-11.82100	12.75400	16.51600
N	-12.35100	11.75100	14.57400
H	-12.69800	11.58100	13.63000
C	-12.39400	12.95300	15.23100
C	-11.74500	13.84100	17.40300
C	-12.89000	14.19900	14.80900
C	-12.24200	15.08300	16.98100
C	-12.80600	15.24700	15.69400
N	-12.13700	11.44100	20.63500
H	-11.20800	11.11900	20.90600
C	-12.82700	12.38400	21.51500
C	-13.00100	13.76100	20.85600
O	-12.03100	14.50000	20.68700
C	-12.06000	12.49500	22.83800
C	-12.90900	13.04500	23.96400
O	-13.73100	13.94800	23.76100
N	-12.72700	12.49300	25.16200
H	-12.05000	11.74900	25.32900
H	-13.29900	12.86400	25.92100
N	-14.25300	14.12200	20.56400
H	-15.02000	13.50100	20.82200
C	-14.55900	15.38100	19.88500
C	-14.05200	16.64200	20.57400
O	-13.78700	17.64200	19.90500
C	-16.06300	15.52000	19.56200
O	-16.82200	15.39000	20.76800
H	-16.55600	16.06300	21.38400
C	-16.49400	14.43200	18.56600
N	-13.86800	16.58900	21.89300
H	-14.07800	15.73300	22.40600
C	-13.36500	17.76100	22.59800
C	-11.95500	18.14700	22.11400
O	-11.53100	19.29300	22.28600
C	-13.42700	17.57700	24.13000
C	-12.48500	16.54000	24.75500
C	-12.87100	16.18900	26.23400
C	-14.23800	15.45000	26.32000
N	-14.54700	14.73200	27.63100
H	-15.44300	14.24800	27.68700

H	-14.46300	15.38700	28.40800
H	-13.79200	14.08200	27.85200
N	-11.25300	17.22500	21.45400
H	-11.65700	16.30300	21.29200
C	-9.90800	17.52400	20.96000
C	-9.79800	18.11200	19.55100
O	-8.69900	18.45000	19.11600
C	-8.95400	16.33600	21.16600
C	-8.87400	15.94400	22.62200
C	-8.58800	16.90000	23.60900
C	-9.17200	14.64700	23.03500
C	-8.61400	16.56800	24.97800
C	-9.20200	14.30800	24.38700
C	-8.92500	15.27200	25.35100
O	-8.97100	14.93300	26.68200
H	-9.18400	14.04300	26.93800
N	-10.92200	18.25500	18.85100
H	-11.80400	17.93100	19.24800
C	-10.91300	18.86700	17.52600
C	-10.64700	17.98000	16.33300
O	-11.36900	18.04700	15.34600
N	-9.54800	17.23300	16.37200
H	-8.93000	17.29700	17.18100
C	-9.20600	16.32200	15.28000
C	-8.47600	15.10200	15.83100
O	-8.02900	15.10400	16.98500
C	-8.39300	17.02200	14.16600
C	-7.06800	17.61200	14.65400
O	-6.27500	16.91800	15.32200
O	-6.78100	18.77700	14.32300
N	-8.32300	14.08400	14.99000
H	-8.67100	14.18700	14.03700
C	-7.68000	12.82400	15.36300
C	-6.25200	12.97300	15.88700
O	-5.83200	12.27800	16.81600
C	-7.72000	11.85500	14.16700
C	-7.18700	10.49300	14.47800
C	-8.02000	9.52200	15.00800
C	-5.84100	10.19200	14.28700
C	-7.52000	8.26900	15.35300
C	-5.33300	8.94700	14.62800
C	-6.17500	7.98400	15.16600
N	-5.50900	13.88100	15.27300

H	-5.91100	14.42700	14.51000
C	-4.12800	14.11200	15.67000
C	-3.95100	14.67000	17.07000
O	-2.95100	14.38700	17.72100
N	-4.89700	15.47400	17.53900
H	-5.70800	15.69700	16.96200
C	-4.78000	16.03600	18.87100
C	-5.15200	14.96600	19.90800
O	-4.47800	14.81500	20.93200
C	-5.68100	17.25800	19.02200
C	-5.35500	18.40200	18.08800
C	-3.86300	18.75400	18.15000
C	-3.57500	20.04700	17.39000
N	-4.12500	19.98400	15.98900
H	-3.93300	20.84800	15.48100
H	-5.12000	19.75900	15.98500
H	-3.77900	19.16700	15.48600
N	-6.19100	14.19100	19.59700
H	-6.66400	14.34200	18.70600
C	-6.68100	13.13400	20.47900
C	-5.61600	12.11200	20.89000
O	-5.61200	11.67200	22.04900
C	-7.90100	12.42900	19.85000
N	-4.72200	11.74000	19.96600
H	-4.78400	12.13500	19.02800
C	-3.64900	10.77400	20.26900
C	-2.55800	11.31700	21.22000
O	-1.60500	10.60600	21.55600
C	-2.95800	10.17000	18.98200
C	-3.96500	9.34900	18.14800
C	-2.29500	11.26600	18.14800
N	-2.68600	12.56600	21.64900
H	-3.47500	13.12500	21.32500
C	-1.72100	13.16100	22.57700
C	-2.33900	13.25200	23.98400
O	-1.76600	13.85100	24.88000
C	-1.33300	14.57000	22.08100
C	-0.65200	14.57900	20.70200
C	-0.46600	15.97500	20.11800
O	-0.21900	16.94300	20.83500
N	-0.57900	16.07600	18.80200
H	-0.45500	17.01000	18.41100
H	-0.78400	15.27300	18.20700

N	-3.52900	12.68400	24.15300
H	-3.95600	12.19200	23.36800
C	-4.24900	12.74100	25.43200
C	-4.57200	11.34200	25.97700
O	-4.90800	10.43200	25.20300
C	-5.55600	13.53100	25.25500
C	-5.42200	14.91000	24.56300
C	-4.56700	15.90500	25.35400
O	-4.94700	16.33400	26.45700
N	-3.39700	16.25900	24.80800
H	-3.08500	15.90700	23.90300
H	-2.82800	16.92200	25.33500
N	-4.54700	11.17000	27.32300
C	-4.84100	9.87800	27.97000
C	-6.25900	9.33300	27.66300
O	-6.50000	8.12300	27.71300
C	-4.66500	10.18800	29.45300
C	-5.05200	11.65700	29.54700
C	-4.35700	12.23200	28.33000
N	-7.20000	10.22100	27.35200
H	-6.97500	11.21600	27.33900
C	-8.55700	9.77500	27.02900
C	-8.99700	10.27900	25.64100
O	-10.16800	10.64200	25.42900
C	-9.52300	10.26300	28.08400
C	-9.51700	11.76700	28.21500
O	-8.54900	12.41600	27.73900
O	-10.48900	12.29700	28.78700
N	-8.04600	10.29200	24.70600
H	-7.10800	9.96600	24.94000
C	-8.32100	10.76000	23.36900
C	-9.03600	9.77100	22.48100
O	-9.80200	10.19700	21.62100
N	-8.83600	8.47400	22.70000
H	-8.23400	8.18000	23.46900
C	-9.46800	7.46700	21.85200
C	-10.35700	6.43500	22.52700
O	-10.16900	6.09800	23.69500
C	-8.41200	6.71000	21.03800
C	-7.58600	7.44500	19.98200
C	-6.83800	6.41700	19.12900
C	-8.46400	8.33700	19.10300
N	-11.31500	5.92000	21.76500

H	-11.43300	6.27700	20.81700
C	-12.20800	4.85900	22.23500
C	-12.31300	3.85100	21.09100
O	-12.65600	4.21300	19.95900
C	-13.59400	5.40500	22.59600
N	-11.91600	2.61600	21.35000
H	-11.54900	2.38500	22.27300
C	-12.00000	1.58500	20.32700
C	-12.97300	0.50800	20.80200
O	-12.83800	-0.00200	21.91300
C	-10.62200	0.93600	20.03600
C	-10.73500	-0.05900	18.86100
C	-9.58300	2.00300	19.77600
N	-13.97600	0.20600	19.98400
H	-14.06300	0.70600	19.09900
C	-14.95500	-0.82000	20.31800
C	-14.42600	-2.09800	19.67600
O	-14.18700	-2.12000	18.47800
C	-16.30600	-0.45600	19.72300
C	-17.54500	-1.06600	20.34600
C	-17.76900	-0.44200	21.70500
C	-18.75200	-0.80800	19.42700
N	-14.21700	-3.14400	20.46600
H	-14.42700	-3.07700	21.46200
C	-13.69100	-4.38400	19.92100
C	-14.70600	-5.50600	19.90300
O	-15.38500	-5.75700	20.90100
N	-14.77700	-6.22200	18.79200
H	-14.14700	-6.00700	18.01900
C	-15.73800	-7.31300	18.64800
C	-15.02600	-8.56500	18.16700
O	-14.24000	-8.51900	17.22700
C	-16.86400	-6.93000	17.63100
C	-17.48000	-5.58700	18.02900
C	-17.93300	-8.02400	17.55400
C	-18.53800	-5.07700	17.09800
N	-15.28700	-9.68100	18.81800
H	-15.93100	-9.66600	19.60800
C	-14.66200	-10.93900	18.41800
C	-15.44100	-11.58200	17.27000
O	-16.67800	-11.44600	17.19200
C	-14.63800	-11.92600	19.59300
C	-13.81200	-11.47500	20.76900

C	-12.43800	-11.30000	20.64800
C	-14.40700	-11.29200	22.01500
C	-11.66700	-10.96000	21.74100
C	-13.64100	-10.94700	23.13500
C	-12.26900	-10.78300	22.99800
N	-14.72300	-12.25000	16.37200
H	-13.70600	-12.26100	16.45500
C	-15.35800	-12.96900	15.26700
C	-15.03200	-14.44200	15.42700
O	-13.86500	-14.81600	15.64000
C	-14.86000	-12.48900	13.90200
C	-15.38400	-11.14500	13.38300
C	-14.89900	-9.97300	14.23600
C	-14.95200	-10.99300	11.92800
N	-16.06200	-15.27200	15.30100
H	-16.98200	-14.87300	15.11300
C	-15.94900	-16.73300	15.41700
C	-16.41400	-17.41200	14.11600
O	-17.31900	-16.91200	13.45400
C	-16.82000	-17.20300	16.59600
C	-16.93000	-18.70400	16.76800
C	-18.02000	-19.04400	17.74900
C	-19.30500	-18.37000	17.34800
N	-20.42800	-18.74800	18.25000
H	-21.29900	-18.29100	17.97800
H	-20.20000	-18.56300	19.22700
H	-20.53900	-19.76100	18.30200
N	-15.81500	-18.54900	13.75800
H	-15.07400	-18.93200	14.34500
C	-16.20800	-19.26200	12.52600
C	-17.48500	-20.09800	12.75000
O	-17.55800	-20.94700	13.65400
C	-15.04300	-20.14600	11.93500
C	-15.51100	-20.95600	10.73800
C	-13.87400	-19.26900	11.50300
N	-18.52100	-19.74300	11.99700
H	-18.41200	-18.96500	11.34600
C	-19.80000	-20.42100	12.06700
C	-20.62800	-20.04300	10.85100
O	-20.24600	-20.30000	9.69300
N	-21.76400	-19.40500	11.11300
H	-22.00900	-19.20400	12.08300
C	-22.66700	-18.98600	10.05200

C	-22.23000	-17.68000	9.41800
O	-21.53200	-16.87700	10.04400
C	-24.08100	-18.85400	10.60300
O	-24.49700	-20.10900	11.13700
H	-25.37900	-20.02700	11.48100
N	-22.62500	-17.49200	8.15900
H	-23.17500	-18.22200	7.70700
C	-22.30700	-16.29100	7.40100
C	-23.02400	-15.07600	7.97000
O	-24.19200	-15.15900	8.38500
C	-22.69100	-16.48300	5.93300
N	-22.30100	-13.95600	7.99400
H	-21.34100	-13.99200	7.65100
C	-22.81300	-12.68200	8.48600
C	-23.14500	-11.83900	7.24800
O	-22.24700	-11.39200	6.51300
C	-21.75300	-11.97700	9.33900
C	-22.19500	-10.67600	9.99200
C	-23.07700	-10.93400	11.22800
C	-23.13100	-9.70700	12.14700
N	-24.21500	-9.84900	13.15600
H	-24.25100	-9.03300	13.76700
H	-24.12400	-10.71500	13.68800
H	-25.11700	-10.03200	12.71700
N	-24.45100	-11.61700	7.00500
C	-24.97700	-10.84900	5.87800
C	-24.27700	-9.53500	5.65400
O	-23.77400	-9.28300	4.55700
C	-26.44200	-10.64300	6.26500
C	-26.76900	-11.94700	6.95300
C	-25.54900	-12.12500	7.85100
N	-24.19900	-8.74000	6.72000
H	-24.58900	-9.06700	7.60400
C	-23.57700	-7.41900	6.67300
C	-22.07900	-7.34500	6.41700
O	-21.53200	-6.25300	6.23800
N	-21.40800	-8.49100	6.43500
H	-21.90200	-9.36200	6.62800
C	-19.98600	-8.51600	6.18400
C	-19.70200	-8.74900	4.70100
O	-18.67000	-8.31200	4.19900
C	-19.29200	-9.59300	7.03300
C	-17.75900	-9.54500	6.93200

C	-17.24900	-8.28700	7.63800
C	-17.12300	-10.78700	7.53800
N	-20.65200	-9.36200	3.99300
H	-21.52200	-9.62500	4.45600
C	-20.48200	-9.66800	2.57000
C	-20.11000	-8.49800	1.62900
O	-19.34200	-8.69800	0.70600
C	-21.68600	-10.45100	2.03800
C	-21.38900	-11.24300	0.75100
C	-20.29900	-12.31100	0.92100
O	-20.21100	-12.99000	1.94700
N	-19.48100	-12.47300	-0.10300
H	-19.55400	-11.91200	-0.95100
H	-18.75700	-13.18200	0.01000
N	-20.60500	-7.28600	1.86400
H	-21.24400	-7.14100	2.64500
C	-20.23400	-6.15800	1.00300
C	-18.71900	-5.94200	1.08400
O	-18.03200	-5.68900	0.08100
C	-20.92400	-4.85600	1.43500
C	-22.42500	-4.84200	1.26800
C	-22.83300	-5.21600	-0.15400
C	-24.35700	-5.11100	-0.35400
N	-24.87100	-3.69800	-0.29500
H	-25.88000	-3.62800	-0.42700
H	-24.37700	-3.10500	-0.96200
H	-24.58800	-3.24600	0.57500
N	-18.21300	-6.04200	2.30700
H	-18.84200	-6.24400	3.08400
C	-16.79600	-5.87400	2.57900
C	-16.00800	-6.96000	1.84400
O	-15.04500	-6.65500	1.14500
C	-16.53100	-5.95200	4.09100
C	-15.02600	-5.89600	4.37700
C	-17.29700	-4.82800	4.79700
N	-16.46800	-8.20700	1.96200
H	-17.30500	-8.36300	2.52400
C	-15.83400	-9.36300	1.32700
C	-15.81200	-9.29100	-0.22300
O	-14.81600	-9.68200	-0.84800
C	-16.52200	-10.68700	1.81200
C	-16.09300	-11.87700	0.97200
C	-16.18800	-10.95200	3.27700

N	-16.87900	-8.76100	-0.83300
H	-17.65000	-8.41700	-0.26000
C	-16.98600	-8.65400	-2.30900
C	-15.96300	-7.70600	-2.94300
O	-15.50600	-7.93400	-4.06200
C	-18.40500	-8.19500	-2.76200
C	-19.47200	-9.29500	-2.64600
O	-19.11300	-10.49900	-2.67500
O	-20.68800	-8.95100	-2.54200
N	-15.61300	-6.63700	-2.23700
H	-16.00600	-6.50800	-1.30500
C	-14.67800	-5.63700	-2.75900
C	-13.16900	-5.89700	-2.53900
O	-12.34500	-5.31600	-3.23900
C	-15.07400	-4.21800	-2.22100
C	-14.79700	-4.11000	-0.74500
C	-14.37400	-3.11000	-3.00100
N	-12.81600	-6.77900	-1.60000
H	-13.55000	-7.26500	-1.08500
C	-11.40900	-7.08000	-1.27600
C	-10.50600	-7.30700	-2.48400
O	-9.34000	-6.87300	-2.50700
C	-11.32100	-8.28400	-0.33500
C	-11.93600	-8.08000	1.06100
C	-11.48100	-9.17000	2.01200
C	-11.51800	-6.73200	1.62400
N	-11.05100	-7.96400	-3.50100
H	-12.01800	-8.28100	-3.43400
C	-10.28800	-8.24000	-4.71300
C	-9.77400	-6.99800	-5.43900
O	-8.83400	-7.09700	-6.23400
C	-11.09000	-9.13300	-5.67200
C	-10.67700	-10.59500	-5.58100
O	-9.48500	-10.85200	-5.27900
O	-11.53200	-11.48800	-5.81400
N	-10.38100	-5.83800	-5.18100
H	-11.16000	-5.81900	-4.52300
C	-9.95400	-4.58600	-5.82300
C	-8.87300	-3.84300	-5.03700
O	-8.39100	-2.81300	-5.49700
C	-11.13500	-3.65000	-6.03200
O	-11.62400	-3.18800	-4.78600
H	-12.36100	-2.60400	-4.91700

N	-8.52300	-4.34500	-3.84800
H	-8.99500	-5.18300	-3.50900
C	-7.47900	-3.72900	-3.01100
C	-6.51200	-4.81500	-2.50400
O	-6.10200	-4.81400	-1.33400
C	-8.10000	-2.97900	-1.77900
C	-8.97900	-3.92900	-0.95800
C	-8.90100	-1.77000	-2.23400
C	-9.29200	-3.41800	0.41600
N	-6.12100	-5.71600	-3.39600
H	-6.42400	-5.62600	-4.36600
C	-5.26300	-6.83500	-3.01100
C	-3.88500	-6.52600	-2.46000
O	-3.40600	-7.22800	-1.56400
C	-5.09900	-7.83600	-4.16600
C	-4.35400	-9.12400	-3.76800
C	-4.22300	-10.09000	-4.95400
C	-3.57300	-11.42900	-4.53200
N	-2.98700	-12.20500	-5.66900
H	-2.55800	-13.08800	-5.39100
H	-2.32200	-11.63200	-6.18900
H	-3.68600	-12.35900	-6.39500
N	-3.24500	-5.49200	-2.99000
H	-3.70600	-4.92000	-3.69800
C	-1.88500	-5.16600	-2.56800
C	-1.77800	-3.81600	-1.86200
O	-2.68000	-2.97800	-1.96600
C	-0.91400	-5.27700	-3.79200
O	-1.41800	-4.49300	-4.89100
H	-1.49100	-3.58600	-4.61700
C	-0.79600	-6.74400	-4.23600
N	-0.67200	-3.59000	-1.16400
H	0.07400	-4.28600	-1.15500
C	-0.51900	-2.35100	-0.41000
C	-0.69000	-1.10400	-1.25400
O	-0.24300	-1.05300	-2.39200
C	0.82200	-2.31900	0.33800
C	1.01800	-1.04000	1.19300
C	2.18400	-1.15200	2.16400
C	3.50400	-1.49500	1.47200
N	3.96900	-0.40700	0.54200
H	4.84900	-0.63600	0.08000
H	4.03100	0.48800	1.02700

H	3.24700	-0.17400	-0.14000
N	-1.38700	-0.11800	-0.70000
H	-1.78300	-0.24900	0.23100
C	-1.59800	1.14300	-1.39200
C	-2.85200	1.23000	-2.23800
O	-3.22800	2.32800	-2.66900
N	-3.47500	0.09200	-2.53200
H	-3.09800	-0.79500	-2.19800
C	-4.69300	0.11000	-3.32900
C	-5.86400	0.54500	-2.45400
O	-5.89900	0.28200	-1.24000
C	-5.00100	-1.26200	-3.92500
C	-3.93700	-1.83600	-4.82900
C	-3.85900	-1.09400	-6.16200
C	-3.31200	-2.01800	-7.29100
N	-3.37500	-1.35500	-8.65100
H	-3.01700	-1.96000	-9.39000
H	-2.89600	-0.45500	-8.64600
H	-4.32000	-1.03400	-8.86200
N	-6.78700	1.27000	-3.07200
H	-6.64400	1.51000	-4.05300
C	-7.99300	1.73700	-2.41100
C	-9.12500	1.64700	-3.42900
O	-8.90000	1.37600	-4.61700
C	-7.81800	3.17000	-1.87400
O	-7.79500	4.15800	-2.89700
H	-7.68700	5.04200	-2.56600
N	-10.34800	1.80700	-2.95200
H	-10.47000	1.97000	-1.95300
C	-11.52400	1.75800	-3.80300
C	-12.61100	2.50600	-3.06400
O	-12.61700	2.54100	-1.83300
C	-11.93700	0.33100	-4.03300
N	-13.49300	3.16200	-3.80900
H	-13.40300	3.14700	-4.82500
C	-14.59000	3.90400	-3.19400
C	-15.51000	2.88600	-2.54200
O	-15.77000	1.83100	-3.12300
C	-15.32500	4.73800	-4.25400
C	-14.39400	5.75300	-4.93800
O	-13.43200	6.22800	-4.28100
O	-14.60500	6.05800	-6.13600
N	-15.95900	3.17200	-1.32600

H	-15.69000	4.05400	-0.88900
C	-16.82800	2.25400	-0.60200
C	-17.90300	3.05900	0.10900
O	-17.79800	3.33400	1.30900
C	-15.99400	1.44000	0.39500
C	-16.65600	0.17100	0.85700
C	-16.92500	-0.85300	-0.03300
C	-17.01700	0.00600	2.19000
C	-17.54700	-2.02400	0.39900
C	-17.64000	-1.16800	2.63000
C	-17.90400	-2.18000	1.73700
N	-18.92700	3.46200	-0.64500
H	-18.95600	3.19600	-1.62900
C	-20.00800	4.27600	-0.09200
C	-21.27100	3.51300	0.28500
O	-21.53000	2.40100	-0.18400
C	-20.42800	5.44600	-1.05400
O	-20.78600	4.91400	-2.33700
H	-21.04000	5.62100	-2.91800
C	-19.31200	6.46400	-1.21400
N	-22.03700	4.14500	1.16600
H	-21.70900	5.03800	1.53300
C	-23.31000	3.64100	1.63600
C	-23.21600	2.32900	2.40100
O	-24.10000	1.49100	2.30900
C	-24.30600	3.55600	0.46100
C	-24.50900	4.91000	-0.23900
O	-23.85900	5.20700	-1.25100
N	-25.36900	5.75000	0.32700
H	-25.50400	6.64800	-0.13700
H	-25.90400	5.50500	1.16000
N	-22.12500	2.14800	3.14100
H	-21.38800	2.85300	3.12600
C	-21.96100	0.95800	3.97600
C	-22.52100	1.29100	5.35900
O	-22.15500	2.30900	5.96000
C	-20.49200	0.51900	4.12400
C	-20.33600	-0.73000	4.95500
C	-20.66000	-1.97900	4.42200
C	-19.97800	-0.65400	6.30600
C	-20.64000	-3.12700	5.22400
C	-19.95500	-1.79900	7.11200
C	-20.29000	-3.03500	6.56800

N	-23.38300	0.41900	5.87000
H	-23.61500	-0.41200	5.32600
C	-24.01900	0.59800	7.18600
C	-23.24000	-0.24100	8.21700
O	-23.27800	-1.47700	8.15900
C	-25.46900	0.10900	7.07900
C	-26.29400	0.39200	8.31400
O	-25.76400	0.91100	9.32700
O	-27.50400	0.07600	8.27000
N	-22.51000	0.40300	9.15500
C	-21.74000	-0.33900	10.16800
C	-22.58400	-1.12500	11.18900
O	-22.11300	-2.08400	11.79000
C	-20.90500	0.76300	10.82900
C	-21.76100	1.95300	10.69300
C	-22.25000	1.84200	9.27700
N	-23.85500	-0.75600	11.31700
H	-24.20300	0.01600	10.74900
C	-24.76900	-1.41900	12.24300
C	-24.97800	-2.89400	11.93300
O	-25.48500	-3.63700	12.77100
C	-26.12200	-0.71200	12.26200
C	-26.03800	0.71300	12.75900
C	-27.40300	1.37500	12.72300
N	-27.91100	1.48400	11.35600
H	-27.29600	1.20900	10.59000
C	-29.12900	1.92100	11.05700
N	-29.96800	2.28400	12.02000
H	-29.68100	2.20900	12.99600
H	-30.90300	2.62000	11.79000
N	-29.50200	2.01800	9.79000
H	-28.85700	1.73900	9.05000
H	-30.43700	2.35400	9.56000
N	-24.60100	-3.31600	10.73000
H	-24.19100	-2.66100	10.06400
C	-24.77300	-4.70700	10.36700
C	-23.69300	-5.60600	10.93100
O	-23.79700	-6.81500	10.78100
N	-22.68900	-5.03100	11.60200
H	-22.70100	-4.01900	11.72700
C	-21.56600	-5.80100	12.16800
C	-21.61300	-5.99000	13.68300
O	-20.67800	-6.55300	14.25900

C	-20.21900	-5.13100	11.82100
C	-19.75100	-4.91300	10.37100
C	-18.43600	-4.14500	10.36400
C	-19.59100	-6.23000	9.63700
N	-22.65400	-5.46800	14.33100
H	-23.37300	-4.98000	13.79700
C	-22.80100	-5.57200	15.79000
C	-23.55100	-6.84200	16.22500
O	-24.38000	-7.37500	15.47300
C	-23.54200	-4.33000	16.33300
C	-22.92400	-2.96400	15.99200
C	-23.86800	-1.79600	16.21800
C	-21.66900	-2.77600	16.80100
N	-23.21300	-7.39100	17.40900
C	-23.89500	-8.59800	17.90900
C	-25.22900	-8.10600	18.49200
O	-25.49900	-6.90900	18.45500
C	-22.95600	-9.08900	19.00600
C	-22.38100	-7.80000	19.55700
C	-22.11100	-6.98500	18.30900
N	-26.05300	-8.99200	19.04300
H	-25.79700	-9.97900	19.06900
C	-27.33400	-8.55000	19.61600
C	-27.20100	-7.75200	20.91000
O	-27.86700	-6.72000	21.07800
C	-28.24800	-9.73700	19.87000
C	-28.54000	-10.57600	18.63600
C	-29.68000	-11.55800	18.87500
O	-30.18600	-12.14200	17.87900
O	-30.07500	-11.72700	20.05800
N	-26.36900	-8.25700	21.82500
H	-25.88300	-9.12700	21.60800
C	-26.11600	-7.62500	23.12800
C	-24.93800	-6.64800	23.08300
O	-24.01900	-6.82400	22.29200
C	-25.82100	-8.69100	24.19600
O	-25.59400	-8.09200	25.46800
H	-25.41200	-8.75100	26.12800
N	-24.98800	-5.63800	23.95200
H	-25.80200	-5.56200	24.56200
C	-23.93800	-4.64100	24.07100
C	-23.23500	-4.69800	25.43800
O	-22.73100	-3.68200	25.92600

C	-24.46200	-3.23200	23.80900
C	-24.84600	-2.89000	22.36400
C	-24.67100	-1.38900	22.17700
C	-23.98400	-3.65600	21.34200
N	-23.26700	-5.87400	26.07400
H	-23.78400	-6.64700	25.65500
C	-22.58200	-6.09100	27.35700
C	-21.07100	-6.00400	27.04100
O	-20.61800	-6.53700	26.01000
C	-22.93400	-7.47000	27.94100
C	-24.29300	-7.48900	28.65300
O	-24.81300	-6.40400	29.00200
O	-24.82100	-8.59800	28.90700
N	-20.28800	-5.42500	27.95500
H	-20.68400	-5.12300	28.84500
C	-18.86800	-5.22300	27.68600
C	-17.92800	-5.25700	28.90700
O	-18.38500	-5.30200	30.04100
C	-18.72700	-3.85100	26.98200
C	-19.14000	-2.65400	27.84800
C	-18.21300	-2.02100	28.70600
C	-20.44900	-2.16700	27.84000
C	-18.58800	-0.93900	29.53100
C	-20.83500	-1.07800	28.66600
C	-19.90000	-0.47400	29.50500
O	-20.26200	0.58500	30.30700
H	-19.62500	0.99700	30.87900
N	-16.62100	-5.30100	28.64600
H	-16.33000	-5.40000	27.67300
C	-15.57500	-5.21600	29.67400
C	-14.83700	-3.94700	29.21900
O	-14.82000	-3.64400	28.01600
C	-14.56300	-6.36700	29.60700
C	-15.07300	-7.73700	29.91900
C	-15.35100	-8.25600	31.15800
C	-15.28300	-8.80300	28.98400
N	-15.71400	-9.57600	31.04800
H	-15.96600	-10.18800	31.82400
C	-15.68300	-9.93800	29.72500
C	-15.16600	-8.91300	27.58400
C	-15.96700	-11.17300	29.10900
C	-15.44700	-10.14200	26.97500
C	-15.84100	-11.25000	27.73700

N	-14.20600	-3.23300	30.14300
H	-14.24000	-3.54400	31.11400
C	-13.46200	-2.01300	29.81800
C	-12.19800	-1.86800	30.69800
O	-12.16400	-2.31900	31.86200
C	-14.37500	-0.73200	29.95000
O	-13.68300	0.42900	29.48600
H	-13.42000	0.27700	28.58600
C	-14.79800	-0.48800	31.39900
N	-11.16500	-1.25300	30.12600
H	-11.26100	-0.93200	29.16200
C	-9.90000	-1.01700	30.81700
C	-9.11700	0.04200	30.02100
O	-9.42300	0.28400	28.83700
C	-9.06900	-2.32300	30.92900
C	-8.31400	-2.73600	29.65900
C	-8.96300	-3.40400	28.62700
C	-6.94700	-2.44800	29.49700
C	-8.28800	-3.77700	27.46800
C	-6.26000	-2.81500	28.32500
C	-6.94500	-3.48200	27.31500
O	-6.29800	-3.85600	26.14600
H	-6.76600	-4.31200	25.45600
N	-8.17600	0.75100	30.68400
C	-7.32600	1.78500	30.07700
C	-6.14200	1.09900	29.37300
O	-5.42500	0.30900	29.98300
C	-6.88100	2.60300	31.28800
C	-6.75700	1.57500	32.35000
C	-7.99100	0.72100	32.14800
N	-5.96700	1.38000	28.08300
H	-6.59000	2.04600	27.62600
C	-4.90400	0.75400	27.31600
C	-4.22700	1.61000	26.25600
O	-4.05800	2.82300	26.43600
N	-3.88600	0.99800	25.12500
H	-4.13400	0.01800	24.99200
C	-3.16300	1.70400	24.07000
C	-3.48600	1.17100	22.66800
O	-4.29500	0.24900	22.50300
C	-1.68000	1.45900	24.27800
O	-1.41900	0.07600	24.05800
H	-0.49100	-0.07700	24.18800

N	-2.80600	1.74100	21.67200
H	-2.18200	2.52000	21.88100
C	-2.92900	1.28100	20.28700
C	-2.18500	-0.06200	20.28200
O	-1.22000	-0.23700	21.04100
C	-2.22200	2.25300	19.34800
C	-2.84200	3.64200	19.28800
C	-1.92200	4.57100	18.52700
C	-4.22700	3.57700	18.63500
N	-2.62100	-1.01100	19.46100
H	-3.42000	-0.82800	18.85400
C	-1.96800	-2.30600	19.42200
C	-0.91800	-2.42300	18.32000
O	-0.33900	-3.50200	18.11000
C	-2.98800	-3.44700	19.31600
O	-3.66600	-3.37200	18.05900
H	-3.03900	-3.41600	17.34600
C	-4.00000	-3.37600	20.46700
N	-0.73100	-1.33700	17.57000
H	-1.31500	-0.51700	17.73600
C	0.28300	-1.28000	16.51600
C	1.07800	0.02700	16.75500
O	0.57800	0.96000	17.42100
C	-0.37100	-1.26400	15.08100
O	-0.90200	0.03400	14.80000
H	-0.18900	0.65900	14.86200
C	-1.52600	-2.27600	14.98100
N	2.34000	0.09600	16.29300
C	3.10200	1.33500	16.49600
C	2.25000	2.49300	15.97300
O	1.52800	2.32900	14.97900
C	4.32600	1.12500	15.59800
C	4.57000	-0.31800	15.71500
C	3.16300	-0.91200	15.60500
N	2.39600	3.69600	16.55000
C	3.27000	4.14300	17.64300
C	2.96000	3.69700	19.09700
O	3.60300	4.17600	20.03900
C	3.24600	5.66700	17.48100
C	1.87400	5.92600	16.97000
C	1.66800	4.83700	15.96000
N	1.98400	2.79500	19.26300
H	1.47600	2.48200	18.43500

C	1.59600	2.22400	20.57000
C	1.26500	3.23100	21.68500
O	1.47400	2.95100	22.87200
C	2.67400	1.24500	21.06400
C	3.07200	0.06500	20.16900
C	4.42000	-0.49000	20.63400
C	1.99700	-1.02400	20.18400
N	0.67200	4.35700	21.29700
H	0.46700	4.48300	20.30600
C	0.29900	5.42900	22.23400
C	-0.76600	4.97700	23.25500
O	-1.70000	4.25800	22.93000
C	-0.14800	6.66400	21.43500
C	0.84200	7.02500	20.30900
C	0.39200	8.26600	19.56600
C	2.23800	7.25700	20.88600
N	-0.58100	5.35800	24.50900
H	0.21900	5.94800	24.73800
C	-1.49100	4.95500	25.56500
C	-2.53300	6.03500	25.74600
O	-2.52100	6.77000	26.73200
C	-0.68100	4.69000	26.84600
C	0.39300	3.57900	26.63700
C	1.43900	3.44500	27.75500
O	1.81800	4.45700	28.37700
O	1.88900	2.30600	28.00600
N	-3.41400	6.13000	24.75300
H	-3.33700	5.47400	23.97500
C	-4.49000	7.12600	24.71600
C	-5.88300	6.46900	24.57900
O	-6.87900	7.15500	24.35500
C	-4.27700	8.05100	23.50200
S	-2.53200	8.56200	23.16600
N	-5.95000	5.15800	24.79200
H	-5.11800	4.66200	25.11100
C	-7.18700	4.41400	24.58000
C	-8.00400	3.79200	25.72500
O	-7.46000	3.14900	26.62500
C	-6.94500	3.28200	23.52800
C	-8.27400	2.62000	23.12300
C	-6.24100	3.83900	22.30400
N	-9.32600	3.97700	25.64200
H	-9.68900	4.56100	24.88900

C	-10.26700	3.38500	26.57400
C	-10.85100	2.26200	25.72600
O	-11.53400	2.48900	24.72200
C	-11.37400	4.35400	27.00000
O	-10.81300	5.36000	27.84600
H	-11.50000	5.96100	28.11000
C	-12.50700	3.60900	27.73900
N	-10.46000	1.05100	26.06800
H	-9.82600	0.93700	26.85900
C	-10.90700	-0.11700	25.35100
C	-12.27100	-0.57300	25.85400
O	-12.53000	-0.56400	27.06400
C	-9.88300	-1.23800	25.52600
C	-8.72700	-1.11200	24.60500
C	-7.49000	-0.58400	24.88100
C	-8.68500	-1.54900	23.24100
N	-6.68800	-0.66900	23.77100
H	-5.72200	-0.34700	23.71300
C	-7.39400	-1.25700	22.75100
C	-9.61900	-2.16500	22.38600
C	-7.01000	-1.55900	21.44600
C	-9.23300	-2.46600	21.07900
C	-7.94300	-2.16200	20.62600
N	-13.14000	-0.95100	24.92100
H	-12.86100	-0.89800	23.94100
C	-14.47500	-1.43800	25.24200
C	-14.62500	-2.73600	24.45800
O	-14.84700	-2.71900	23.25300
C	-15.55600	-0.40300	24.84500
C	-15.35100	0.87500	25.65400
C	-16.94700	-0.96300	25.06500
C	-16.15400	2.01900	25.17600
N	-14.40700	-3.85700	25.13600
H	-14.16400	-3.80000	26.12500
C	-14.50600	-5.16700	24.50300
C	-15.87000	-5.81300	24.73400
O	-16.27000	-6.01900	25.86900
C	-13.39600	-6.11400	24.99800
C	-13.49500	-7.44600	24.28000
C	-12.02100	-5.47700	24.77400
N	-16.57400	-6.13200	23.65100
H	-16.17900	-5.94300	22.73000
C	-17.90100	-6.74700	23.74300

C	-17.86900	-8.22100	24.13300
O	-17.04000	-8.98700	23.64600
C	-18.69100	-6.54100	22.43900
C	-19.42800	-5.20500	22.36600
C	-18.50700	-4.05400	22.77200
C	-19.98300	-4.98000	20.96900
N	-18.76800	-8.60400	25.03500
H	-19.42100	-7.91800	25.41300
C	-18.83800	-9.99300	25.49600
C	-19.25500	-11.00600	24.40900
O	-18.61800	-12.04500	24.23300
C	-19.79600	-10.11300	26.68800
C	-19.90400	-11.52800	27.21500
C	-20.96400	-11.67300	28.29200
C	-22.39000	-11.58200	27.72800
N	-22.73100	-12.69200	26.75800
H	-23.67800	-12.63200	26.38400
H	-22.57000	-13.60500	27.18400
H	-22.04700	-12.73300	26.00300
N	-20.33600	-10.68800	23.70600
H	-20.79300	-9.79700	23.90100
C	-20.91000	-11.54900	22.66300
C	-20.20300	-11.37300	21.31100
O	-20.13400	-10.26200	20.79500
C	-22.42100	-11.24400	22.52000
C	-23.19000	-12.04100	21.43600
C	-24.67900	-11.61100	21.28600
O	-25.18900	-10.83100	22.10700
O	-25.36000	-12.03800	20.32100
N	-19.60500	-12.45600	20.76300
C	-18.91700	-12.33500	19.46300
C	-19.88500	-12.46100	18.27800
O	-21.05100	-12.79300	18.47800
C	-17.90900	-13.49300	19.50800
C	-18.60800	-14.54400	20.32200
C	-19.29700	-13.74700	21.42000
N	-19.46300	-12.08400	17.07500
H	-18.54100	-11.66300	16.96300
C	-20.33700	-12.27800	15.90400
C	-19.78500	-13.50100	15.16000
O	-18.59400	-13.82400	15.29100
C	-20.38600	-11.05800	14.91100
C	-18.97500	-10.67100	14.44700

C	-21.09100	-9.88100	15.55900
C	-18.93500	-9.63800	13.33600
N	-20.64100	-14.22500	14.44700
H	-21.62800	-13.97000	14.41900
C	-20.16500	-15.38500	13.70500
C	-20.10700	-15.01400	12.21800
O	-20.90300	-14.20200	11.74100
C	-21.05300	-16.62300	13.95700
O	-22.38000	-16.43400	13.48900
H	-22.92600	-17.19600	13.64400
N	-19.07500	-15.51100	11.54300
H	-18.40100	-16.08600	12.04900
C	-18.85100	-15.28000	10.11300
C	-18.51700	-16.63400	9.48300
O	-17.98400	-17.53600	10.16500
C	-17.68700	-14.27300	9.86900
C	-17.94600	-12.97800	10.65900
C	-16.34300	-14.89500	10.25600
N	-18.82400	-16.80600	8.20000
H	-19.24300	-16.04700	7.66200
C	-18.55300	-18.09800	7.57100
C	-17.07800	-18.33300	7.26200
O	-16.28600	-17.39900	7.11700
C	-19.40800	-18.28500	6.31300
O	-19.04700	-17.34800	5.31200
H	-19.57700	-17.46400	4.53200
N	-16.72100	-19.60500	7.17500
H	-17.42800	-20.32200	7.34000
C	-15.36900	-20.02500	6.85500
C	-14.91700	-19.36100	5.54800
O	-13.77600	-18.88800	5.45100
C	-15.34000	-21.54900	6.70900
O	-14.05700	-22.01100	6.31100
H	-14.03900	-22.95700	6.22000
N	-15.81900	-19.31800	4.55900
H	-16.73900	-19.73100	4.71400
C	-15.53300	-18.70000	3.26300
C	-15.29800	-17.18600	3.37300
O	-14.50400	-16.63300	2.60000
C	-16.65900	-18.96000	2.25800
C	-16.83500	-20.42300	1.84300
C	-17.61100	-21.27300	2.86600
O	-17.67800	-22.51800	2.66400

O	-18.17600	-20.71800	3.84600
N	-16.01900	-16.50800	4.27800
H	-16.70800	-17.00300	4.84500
C	-15.83200	-15.06700	4.46400
C	-14.42000	-14.77000	5.00500
O	-13.71000	-13.90800	4.46000
C	-16.92000	-14.47700	5.37000
C	-18.34700	-14.55900	4.78000
C	-19.43700	-13.91100	5.65000
O	-19.63100	-14.27100	6.81500
N	-20.18800	-12.99900	5.05600
H	-20.02800	-12.70200	4.09400
H	-20.91100	-12.56900	5.63300
N	-13.97400	-15.54000	6.00400
H	-14.57600	-16.27500	6.37700
C	-12.62700	-15.34600	6.57700
C	-11.53100	-15.76800	5.59500
O	-10.41800	-15.22300	5.61500
C	-12.39400	-16.12000	7.90400
C	-11.04300	-15.71700	8.49400
C	-13.51600	-15.84500	8.90200
N	-11.84800	-16.74100	4.74000
H	-12.77200	-17.16900	4.79700
C	-10.90600	-17.21300	3.72100
C	-10.42700	-16.06000	2.82300
O	-9.23500	-15.97300	2.50700
C	-11.56900	-18.29400	2.86000
C	-11.11300	-19.75600	3.02400
C	-12.04700	-20.70000	2.23400
C	-9.66200	-19.89400	2.55100
N	-11.36000	-15.18600	2.42100
H	-12.32400	-15.33500	2.71900
C	-11.06200	-14.02200	1.57100
C	-10.14000	-12.97200	2.22200
O	-9.46100	-12.22300	1.51500
C	-12.35900	-13.35400	1.06200
C	-13.12700	-14.18800	0.00100
C	-13.68000	-13.33900	-1.15600
C	-14.79500	-14.11200	-1.92800
N	-15.62400	-13.27100	-2.89200
H	-16.35300	-13.77600	-3.39600
H	-15.01200	-12.78800	-3.55000
H	-16.02700	-12.47200	-2.40200

N	-10.14300	-12.88400	3.55400
H	-10.77200	-13.48000	4.09200
C	-9.25400	-11.94000	4.26700
C	-7.79600	-12.40000	4.05500
O	-6.90300	-11.59100	3.79800
C	-9.49900	-11.96500	5.78900
C	-10.73700	-11.21800	6.26600
C	-11.74600	-10.81800	5.39100
C	-10.87200	-10.90700	7.62400
C	-12.87100	-10.11700	5.86600
C	-11.98100	-10.21300	8.10600
C	-12.98100	-9.81700	7.23200
N	-7.58500	-13.71200	4.19200
H	-8.39000	-14.30600	4.39100
C	-6.27000	-14.35600	4.07500
C	-5.62200	-14.29500	2.68100
O	-4.44000	-14.65200	2.52800
C	-6.36600	-15.82300	4.53800
C	-6.94900	-15.99600	5.94200
C	-7.00900	-17.44600	6.39800
N	-7.47700	-17.52800	7.78800
H	-7.14700	-16.81300	8.43700
C	-8.30000	-18.46300	8.27100
N	-8.76000	-19.44100	7.49100
H	-9.38800	-20.15500	7.86000
H	-8.41800	-19.51400	6.53300
N	-8.74400	-18.36800	9.51600
H	-9.37200	-19.08200	9.88500
H	-8.39200	-17.62000	10.11300
N	-6.39500	-13.86300	1.68000
H	-7.35900	-13.60300	1.88700
C	-5.91900	-13.74500	0.29600
C	-5.39100	-12.35000	-0.05800
O	-4.99400	-12.11400	-1.20400
C	-7.00100	-14.16400	-0.71200
C	-7.28500	-15.68100	-0.78800
C	-8.40800	-15.98200	-1.79900
C	-8.42100	-17.44800	-2.27200
N	-9.57500	-18.24600	-1.71200
H	-9.58400	-19.21700	-2.02500
H	-10.46400	-17.79100	-1.91800
H	-9.59100	-18.19400	-0.69300
N	-5.37400	-11.44000	0.91900

H	-5.73100	-11.69500	1.84000
C	-4.85600	-10.08300	0.70700
C	-3.33600	-10.13400	0.82000
O	-2.77200	-11.13500	1.26700
C	-5.41000	-9.10800	1.74300
C	-6.92000	-8.85000	1.74800
C	-7.23400	-7.88600	2.87800
C	-7.36300	-8.28900	0.39200
N	-2.66600	-9.05100	0.46200
H	-3.16700	-8.21600	0.15900
C	-1.21100	-9.05500	0.50200
C	-0.60100	-7.93400	1.35800
O	-1.12700	-6.82900	1.39200
C	-0.65600	-8.89500	-0.92500
C	-0.77400	-10.15300	-1.78700
O	-0.30700	-10.14500	-2.91700
N	-1.34300	-11.23000	-1.26000
H	-1.73300	-11.23700	-0.31700
H	-1.42200	-12.06900	-1.83500
N	0.51900	-8.23900	2.02200
H	0.87600	-9.19300	1.97200
C	1.25200	-7.25200	2.81800
C	2.01700	-6.36400	1.81600
O	2.18000	-5.15600	2.01100
C	2.29900	-7.92900	3.72700
C	1.74600	-8.52900	5.00100
C	1.00300	-7.76200	5.89300
C	2.04700	-9.84500	5.34900
C	0.57300	-8.30800	7.12300
C	1.62600	-10.39300	6.56400
C	0.89100	-9.62800	7.45300
N	2.50500	-6.99900	0.75600
H	2.32500	-7.99800	0.65900
C	3.28900	-6.32400	-0.27700
C	2.48800	-5.47600	-1.25800
O	1.30500	-5.72900	-1.49700
C	4.09600	-7.35100	-1.08200
C	3.21200	-8.44300	-1.66600
O	2.62200	-9.23000	-0.93000
N	3.10500	-8.48300	-2.99000
H	3.59500	-7.83000	-3.60100
H	2.51200	-9.21500	-3.38200
N	3.14800	-4.45400	-1.80100

H	4.10700	-4.26500	-1.50900
C	2.52700	-3.60500	-2.80000
C	2.63400	-4.31800	-4.14100
O	3.20900	-5.41800	-4.22800
N	2.10600	-3.72000	-5.20200
H	1.66300	-2.80600	-5.11500
C	2.17100	-4.39200	-6.49100
C	3.61400	-4.56700	-6.98400
O	4.50600	-3.78500	-6.61800
C	1.33200	-3.65200	-7.53000
C	0.64300	-4.61300	-8.49500
C	0.05100	-3.91600	-9.70800
O	-0.63100	-2.86700	-9.54400
O	0.27800	-4.42900	-10.83100
N	3.85300	-5.64800	-7.73100
H	3.09400	-6.30300	-7.91800
C	5.17800	-5.91200	-8.28500
C	6.30100	-6.37800	-7.34200
O	7.47400	-6.42300	-7.75900
N	5.97500	-6.66900	-6.07800
H	5.00900	-6.55000	-5.77300
C	6.97200	-7.15400	-5.12000
C	6.62200	-8.61800	-4.86800
O	5.53800	-9.07200	-5.24100
C	6.88000	-6.40000	-3.79000
C	6.97500	-4.88100	-3.83100
C	7.03200	-4.28500	-2.41100
O	8.03600	-3.59600	-2.09600
O	6.09100	-4.50600	-1.60500
N	7.54900	-9.39800	-4.29100
C	7.21300	-10.80700	-4.03900
C	6.03400	-10.88500	-3.06600
O	5.90000	-10.07800	-2.12900
C	8.49600	-11.36800	-3.40800
C	9.57500	-10.52900	-4.01400
C	8.95900	-9.12600	-3.94600
N	5.20000	-11.88700	-3.27600
H	5.39700	-12.54800	-4.02700
C	4.00900	-12.07300	-2.46500
C	4.21200	-12.57200	-1.05700
O	4.83300	-13.61600	-0.82900
C	3.04500	-13.01800	-3.16400
C	1.65400	-12.98900	-2.55500

C	0.58700	-13.49500	-3.50600
O	0.87200	-13.58800	-4.73500
O	-0.54800	-13.77700	-3.02800
N	3.55800	-11.87900	-0.13300
H	3.01700	-11.06300	-0.42100
C	3.58400	-12.24000	1.27500
C	2.12100	-12.11500	1.76600
O	1.59300	-10.99900	1.91900
C	4.53500	-11.30300	2.02900
C	4.93000	-11.78900	3.42500
C	5.77300	-13.06600	3.41600
O	6.53600	-13.29600	2.44500
O	5.69500	-13.84300	4.40800
N	1.44600	-13.25500	1.93100
H	1.91400	-14.14400	1.75500
C	0.05200	-13.25100	2.35800
C	-0.18400	-12.50300	3.67200
O	0.61000	-12.62000	4.60700
C	-0.48900	-14.67400	2.45100
C	-0.63000	-15.44100	1.13500
C	-1.19600	-16.80200	1.45200
C	-1.56000	-14.69500	0.15400
N	-1.24800	-11.69500	3.70800
H	-1.83400	-11.61400	2.87700
C	-1.60300	-10.91600	4.90900
C	-2.38500	-11.77600	5.91100
O	-3.60400	-11.93300	5.80000
C	-2.41100	-9.65600	4.53900
C	-2.67500	-8.68900	5.70800
S	-3.64000	-7.21200	5.24000
C	-2.34500	-6.06000	4.74800
N	-1.65500	-12.37400	6.84500
H	-0.64400	-12.23700	6.83800
C	-2.24100	-13.22300	7.88600
C	-1.48600	-12.99200	9.19400
O	-0.37800	-12.44800	9.18800
C	-2.19800	-14.74500	7.53000
C	-2.99300	-15.02500	6.26600
C	-0.75900	-15.23500	7.40700
N	-2.11900	-13.34400	10.31200
H	-3.05200	-13.74900	10.24100
C	-1.52800	-13.17200	11.63300
C	-1.03800	-11.73700	11.93800

O	0.05600	-11.53700	12.48000
C	-0.41600	-14.20300	11.85200
C	-0.94800	-15.64100	11.89000
O	-1.97600	-15.90200	12.54900
O	-0.33800	-16.51300	11.24500
N	-1.85900	-10.74200	11.60100
H	-2.74800	-10.95900	11.15100
C	-1.51000	-9.34600	11.86400
C	-2.03900	-8.96100	13.24200
O	-2.78800	-7.99300	13.38200
C	-2.09500	-8.41900	10.79300
C	-3.57100	-8.68000	10.52900
O	-4.16100	-9.60300	11.09600
N	-4.16400	-7.88300	9.65400
H	-3.67600	-7.12000	9.18500
H	-5.15300	-8.05800	9.47700
N	-1.62700	-9.71800	14.25800
H	-0.98500	-10.48800	14.06700
C	-2.06100	-9.48700	15.64200
C	-0.89000	-9.45800	16.65600
O	0.12400	-10.14300	16.48300
C	-3.12300	-10.53400	16.06300
C	-2.72500	-11.96100	15.81800
C	-2.89500	-12.66300	14.66300
C	-2.05600	-12.85500	16.73300
N	-2.37100	-13.92500	14.79000
H	-2.37000	-14.63900	14.06200
C	-1.85000	-14.07600	16.04600
C	-1.61400	-12.74300	18.06400
C	-1.21900	-15.18100	16.63800
C	-0.97900	-13.86000	18.66300
C	-0.79200	-15.05700	17.94000
N	-1.04800	-8.63900	17.69700
H	-1.90700	-8.09200	17.75600
C	-0.05500	-8.48600	18.75500
C	-0.42500	-9.37700	19.92900
O	-1.58300	-9.41200	20.34200
C	-0.00500	-7.03800	19.23600
C	1.07500	-6.79000	20.25700
C	1.11600	-5.34300	20.67700
N	2.31600	-5.08300	21.46700
H	3.13200	-5.67100	21.29600
C	2.42300	-4.13600	22.39300

N	1.39600	-3.33400	22.67900
H	1.47800	-2.60700	23.39000
H	0.49700	-3.48000	22.22000
N	3.59200	-3.94600	22.99000
H	3.67400	-3.21900	23.70100
H	4.37700	-4.55900	22.77100
N	0.55300	-10.11800	20.47600
C	0.26400	-11.00200	21.61800
C	-0.10800	-10.20900	22.89500
O	0.24000	-9.02300	23.02500
C	1.57100	-11.78700	21.77900
C	2.61700	-10.81800	21.27900
C	1.97300	-10.20200	20.07000
N	-0.85000	-10.85200	23.79800
H	-1.14000	-11.81300	23.61400
C	-1.25600	-10.20800	25.04400
C	-0.07500	-9.63900	25.90500
O	0.99800	-10.25000	26.05100
C	-2.13300	-11.16400	25.86200
N	-0.29700	-8.44700	26.45400
H	-1.20200	-8.00600	26.28900
C	0.66700	-7.73400	27.27300
C	0.27400	-7.82600	28.75900
O	-0.88200	-8.11600	29.08300
C	0.72500	-6.27700	26.82000
C	1.12400	-6.10800	25.36100
C	2.45200	-6.79900	25.02000
O	3.49500	-6.46000	25.57400
N	2.41500	-7.75600	24.09400
H	1.54900	-8.03700	23.63400
H	3.29700	-8.21500	23.86700
N	1.25200	-7.65600	29.67800
C	1.03500	-7.71200	31.13100
C	0.02900	-6.65700	31.59500
O	0.15200	-5.47700	31.24300
C	2.42200	-7.35900	31.69900
C	3.33900	-7.84700	30.69200
C	2.67500	-7.42600	29.39100
N	-0.90500	-7.07300	32.44200
H	-0.91400	-8.05400	32.72200
C	-1.92200	-6.17300	32.98800
C	-1.34300	-5.08400	33.91100
O	-1.87500	-3.98700	33.97000

C	-2.98500	-6.99200	33.72800
C	-4.31000	-6.31800	34.10900
C	-4.96200	-5.69300	32.89700
C	-5.24400	-7.32600	34.76100
N	-0.25000	-5.38100	34.61400
H	0.16200	-6.30700	34.50100
C	0.39600	-4.43200	35.55200
C	-0.58300	-3.90500	36.60400
O	-1.38500	-4.66700	37.15900
C	1.04100	-3.24700	34.81700
C	2.09900	-3.61100	33.77400
C	3.42800	-3.97800	34.42000
C	4.59300	-4.05500	33.39300
N	4.81600	-2.76800	32.62400
H	5.58000	-2.81900	31.95000
H	4.95200	-1.98600	33.26400
H	3.95400	-2.46800	32.16800
N	-0.53300	-2.60300	36.86700
H	0.13800	-2.02200	36.36600
C	-1.41700	-1.97800	37.85900
C	-2.74500	-1.48600	37.28300
O	-3.07000	-0.28500	37.40000
C	-0.70000	-0.79700	38.54000
C	0.04800	-1.21900	39.80100
O	0.64800	-0.36800	40.50300
N	0.01200	-2.53800	40.11800
H	0.51200	-2.82000	40.96100
H	-0.47500	-3.22900	39.54800
N	-3.51000	-2.38500	36.67000
H	-3.20000	-3.35500	36.61500
C	-4.78800	-2.00400	36.07400
C	-5.89400	-2.95000	36.50000
O	-5.64000	-4.06900	36.94000
C	-4.70300	-2.00300	34.52200
C	-3.91600	-0.84700	33.88500
C	-3.83700	-1.01300	32.36500
N	-2.89900	-2.05700	31.93500
H	-2.36000	-2.53700	32.65600
C	-2.70200	-2.42300	30.66000
N	-3.39300	-1.84800	29.67100
H	-4.12400	-1.17500	29.90200
H	-3.24300	-2.12600	28.70100
N	-1.74800	-3.30100	30.35800

H	-1.22100	-3.74000	31.11300
H	-1.59800	-3.57900	29.38800
N	-7.13000	-2.51000	36.31900
H	-7.28200	-1.57700	35.93600
C	-8.26600	-3.33800	36.65800
C	-9.27400	-3.31400	35.51100
O	-9.58300	-2.24500	34.95100
C	-8.92500	-2.87200	37.97600
C	-9.96600	-3.87200	38.51200
C	-10.42600	-3.58500	39.94000
O	-10.81000	-4.51300	40.67300
N	-10.40600	-2.30000	40.34500
H	-10.09100	-1.53900	39.74400
H	-10.71300	-2.10800	41.29900
N	-9.73800	-4.50400	35.14200
H	-9.38200	-5.33800	35.60900
C	-10.73700	-4.65700	34.09500
C	-12.11000	-4.70800	34.76300
O	-12.35700	-5.54600	35.64400
C	-10.55200	-5.97700	33.29400
C	-9.19500	-6.00000	32.56700
C	-11.70100	-6.13800	32.27500
C	-8.87900	-7.35800	31.92500
N	-13.00000	-3.81600	34.35200
H	-12.73300	-3.14000	33.63700
C	-14.36100	-3.77800	34.90200
C	-15.33400	-4.42700	33.90900
O	-15.05600	-4.45600	32.70500
C	-14.78700	-2.32600	35.16200
C	-13.94400	-1.61000	36.19800
C	-14.29100	-0.12800	36.29200
C	-13.55700	0.54600	37.47600
N	-13.85600	-0.10600	38.82000
H	-13.37200	0.33800	39.60000
H	-13.65500	-1.10600	38.79100
H	-14.86100	-0.14200	38.99000
N	-16.43900	-4.97900	34.41200
H	-16.57300	-4.98000	35.42300
C	-17.46900	-5.58500	33.56100
C	-18.80400	-4.85700	33.77100
O	-19.14000	-4.46100	34.89600
C	-17.62000	-7.05800	33.85100
N	-19.54600	-4.64100	32.68600

H	-19.20300	-4.96000	31.78000
C	-20.83800	-3.96000	32.75500
C	-21.98200	-4.93900	33.07700
O	-23.13400	-4.55000	33.14500
C	-21.12200	-3.23600	31.43200
O	-21.50600	-4.15400	30.41800
H	-21.68200	-3.70600	29.59900
N	-21.65400	-6.21000	33.28800
H	-20.67200	-6.48300	33.24600
C	-22.66600	-7.22800	33.57900
C	-22.18900	-8.12200	34.70800
O	-20.97700	-8.24800	34.94200
C	-22.93800	-8.08800	32.33600
C	-21.71600	-8.79400	31.80200
C	-20.82400	-8.13200	30.95200
C	-21.45100	-10.11400	32.15500
C	-19.69800	-8.76700	30.46600
C	-20.31600	-10.76700	31.67200
C	-19.43500	-10.08700	30.82200
N	-23.14800	-8.71200	35.41500
H	-24.11900	-8.53100	35.16100
C	-22.87600	-9.61000	36.54200
C	-22.68000	-11.03000	36.00200
O	-23.59700	-11.49200	35.27400
C	-24.04800	-9.57200	37.54500
C	-23.94100	-10.58700	38.70700
C	-25.12800	-10.51200	39.69600
C	-25.15900	-9.21700	40.56100
N	-26.27600	-9.22900	41.60900
H	-26.29600	-8.38100	42.17500
H	-26.21600	-10.06000	42.19800
H	-27.18300	-9.39900	41.17400
Zn	-6.90800	-2.89700	15.47900
O	-26.98100	-4.56900	31.44000
H	-27.72000	-4.32400	30.86200
C	-26.03400	-3.58400	31.48000
C	-25.44600	-3.07600	30.31000
C	-24.47000	-2.05600	30.41200
C	-25.80500	-3.55900	29.04100
C	-24.11100	-1.57400	31.68000
C	-23.88200	-1.54800	29.24100
C	-24.70500	-2.08900	32.83300
C	-25.66500	-3.09200	32.73200

C	-24.29100	-1.54300	34.16100
C	-24.25100	-2.04000	27.98900
C	-25.21100	-3.04300	27.88900
C	-26.28500	-3.62800	33.94100
O	-27.07500	-2.94600	34.61700
C	-25.97000	-5.04600	34.39500
O	-23.67400	-1.53700	26.86400
H	-22.84300	-2.01400	26.69500
O	-26.73600	-4.54100	28.85900
H	-26.52300	-5.30400	29.42500

Xyz Cartesian coordinates of the complex of Kaempferol with Carbonic anhydrase II

N	10.90600	-0.53700	7.85400
H	11.40600	0.23800	7.41800
H	10.42700	-1.10800	7.15700
H	11.55200	-1.23700	8.21900
C	9.98300	-0.07900	8.88800
C	9.23500	-1.23700	9.54000
O	9.48300	-2.41700	9.27100
C	8.99400	0.93800	8.30200
C	9.34900	2.34500	8.68600
N	8.97900	2.90400	9.89000
H	8.44100	2.43300	10.61700
C	10.04500	3.30100	8.02800
C	9.42800	4.14500	9.95700
N	10.08000	4.41200	8.83800
H	10.53400	5.29700	8.61300
N	8.29600	-0.90900	10.42700
H	8.04000	0.07200	10.53500
C	7.62300	-1.90800	11.24700
C	6.60100	-2.73100	10.47600
O	6.03900	-2.28100	9.47400
C	6.93900	-1.20200	12.41600
C	5.74100	-0.38400	12.06900
C	5.69600	0.94900	11.76300
C	4.38300	-0.84400	12.00700
N	4.40900	1.34500	11.50800
H	4.11500	2.28900	11.25500
C	3.58000	0.25700	11.65000
C	3.79700	-2.09800	12.22100
C	2.19400	0.13700	11.49900
C	2.42600	-2.21200	12.07000
C	1.64700	-1.10000	11.71400
N	6.34300	-3.93400	10.99000
H	6.86400	-4.26100	11.80400
C	5.31600	-4.78600	10.39100
C	5.07000	-5.96000	11.31700
O	5.16000	-5.81500	12.54400
N	4.76300	-7.12700	10.77200

H	4.76300	-7.23600	9.75800
C	4.42500	-8.25500	11.63100
C	5.30000	-9.47000	11.37300
O	4.99600	-10.57100	11.85000
C	2.94800	-8.60400	11.42000
C	2.02700	-7.54300	11.96200
C	1.51600	-6.53700	11.15200
C	1.66000	-7.53900	13.30000
C	0.67300	-5.56200	11.64500
C	0.82000	-6.56700	13.80500
C	0.31900	-5.58200	12.98000
O	-0.51400	-4.61100	13.48400
H	-0.85900	-3.93200	12.91600
N	6.40300	-9.32500	10.64200
H	6.65300	-8.42100	10.24100
C	7.24500	-10.50300	10.43200
C	8.29900	-10.71700	11.49400
O	8.40000	-9.93900	12.44900
N	9.11600	-11.76700	11.34500
H	8.99300	-12.36500	10.52800
C	10.17400	-12.09900	12.29300
C	11.19600	-10.99100	12.48300
O	11.79400	-10.87500	13.55400
C	10.93800	-13.35700	11.84300
C	10.02600	-14.43700	11.27800
C	8.81700	-14.63600	12.18200
C	7.99500	-15.83900	11.75300
N	8.75500	-17.11700	11.86900
H	8.20300	-17.92500	11.58100
H	9.12400	-17.24100	12.81200
H	9.63400	-17.07000	11.35400
N	11.44600	-10.16500	11.47300
H	10.90300	-10.21500	10.61100
C	12.51900	-9.18200	11.62600
C	12.04000	-7.78300	11.94900
O	12.82900	-6.89600	12.30400
C	13.35600	-9.21500	10.32200
C	14.02200	-10.56800	10.22100
N	15.05900	-10.95200	11.04800
H	15.47000	-10.37200	11.77900
C	13.78600	-11.62400	9.41400
C	15.44200	-12.18400	10.75200
N	14.67800	-12.61300	9.75700
H	14.74200	-13.53100	9.31600
N	10.73500	-7.52800	11.84200
H	10.08500	-8.27300	11.59000
C	10.24200	-6.17400	12.08900
C	8.93600	-6.18700	12.87900
O	8.20200	-5.20100	12.89000
C	10.00700	-5.46900	10.75900
C	8.96900	-6.17100	9.90700
O	8.38100	-7.19800	10.26900

N	8.71100	-5.60000	8.73100
H	9.19600	-4.75400	8.43300
H	8.01200	-6.07300	8.15700
N	8.64600	-7.30200	13.53600
H	9.34100	-8.04500	13.60600
C	7.33200	-7.47200	14.16100
C	7.31700	-6.92800	15.57700
O	8.27200	-6.30100	16.04100
N	6.20200	-7.16000	16.26300
C	5.95900	-6.53700	17.56500
C	7.10700	-6.65800	18.55500
O	7.28500	-5.74500	19.37400
C	4.71100	-7.31200	18.05800
C	3.98500	-7.54800	16.75400
C	5.07800	-8.01400	15.81600
N	7.89500	-7.73200	18.53600
H	7.77100	-8.48200	17.85500
C	8.95500	-7.77100	19.55700
C	10.06700	-6.78400	19.23300
O	10.99000	-6.51400	20.01300
C	9.48600	-9.19700	19.71300
C	10.99400	-9.29300	19.75300
C	11.67700	-9.12700	21.09100
O	11.31000	-8.26500	21.92900
O	12.65600	-9.87700	21.34900
N	10.04100	-6.17300	18.04900
H	9.29000	-6.38800	17.39300
C	11.05600	-5.21000	17.67400
C	10.58400	-3.76600	17.79900
O	11.38500	-2.84600	17.65000
C	11.45400	-5.43600	16.20600
C	12.24100	-6.68900	15.96300
N	13.62000	-6.72000	15.97800
H	14.22600	-5.91800	16.15300
C	11.84100	-7.96300	15.69200
C	14.03700	-7.95800	15.72900
N	12.97700	-8.73400	15.55100
H	12.99800	-9.73300	15.34500
N	9.27800	-3.54400	17.98500
H	8.65500	-4.32100	18.20400
C	8.74700	-2.19300	17.87400
C	9.36800	-1.24900	18.89800
O	9.51900	-0.06000	18.64600
C	7.21800	-2.22400	18.05100
C	6.51800	-2.92700	16.90800
C	7.07000	-3.38600	15.73400
C	5.11800	-3.25600	16.83500
N	6.09100	-3.97000	14.95900
H	6.24100	-4.38800	14.04100
C	4.89000	-3.90400	15.60500
C	4.05600	-3.04300	17.72900
C	3.62800	-4.36200	15.20400

C	2.80400	-3.49300	17.33700
C	2.59800	-4.13800	16.10400
N	9.70300	-1.80000	20.06400
H	9.64300	-2.80900	20.19900
C	10.15900	-0.92600	21.14800
C	11.42100	-0.15600	20.78400
O	11.67600	0.92100	21.31200
C	10.38000	-1.75400	22.41800
C	11.58100	-2.63400	22.28600
N	12.80200	-2.31700	22.84200
H	13.00800	-1.47800	23.38400
C	11.73200	-3.82000	21.66300
C	13.65900	-3.27600	22.55800
N	13.04300	-4.20400	21.83500
H	13.46800	-5.05600	21.46900
N	12.26800	-0.64700	19.88300
H	12.08300	-1.55100	19.44800
C	13.46700	0.11300	19.51700
C	13.15100	1.42100	18.80500
O	13.85400	2.43000	18.92200
C	14.36400	-0.77600	18.63100
C	14.91900	-2.02800	19.30600
C	15.66700	-2.92100	18.34100
C	14.79300	-3.92100	17.61700
N	15.54000	-4.70000	16.58700
H	14.95100	-5.37400	16.09900
H	16.35700	-5.15500	16.99400
H	16.00900	-4.07900	15.92700
N	12.09000	1.50200	18.00000
H	11.54300	0.66700	17.79000
C	11.71400	2.78600	17.42100
C	10.57900	3.46100	18.19000
O	10.44400	4.67900	18.06400
C	11.25400	2.65100	15.96800
C	12.37500	2.31100	14.99800
O	13.33800	3.10200	14.88600
O	12.28200	1.24200	14.35500
N	9.78200	2.70700	18.93100
H	9.95500	1.70300	18.97500
C	8.66100	3.26500	19.68900
C	8.78800	2.83200	21.13000
O	8.20300	1.83400	21.53600
C	7.31900	2.80900	19.08700
C	7.22500	3.19700	17.61400
C	6.88800	4.49300	17.25600
C	7.47600	2.25700	16.63000
C	6.82200	4.84100	15.91000
C	7.42700	2.60000	15.28300
C	7.09900	3.89400	14.94100
N	9.58700	3.52700	21.94100
C	9.88700	3.03400	23.27900
C	8.64600	2.96600	24.17100

O	8.64700	2.20700	25.14600
C	10.87800	4.05200	23.84700
C	11.16700	5.02800	22.77400
C	10.25100	4.79100	21.62700
N	7.59800	3.70000	23.82000
H	7.66300	4.33800	23.02700
C	6.34000	3.59100	24.58000
C	5.75500	2.18900	24.48900
O	4.87600	1.81100	25.26700
C	5.32900	4.64800	24.10600
C	4.16600	4.90900	25.05500
C	4.81400	4.28900	22.71100
C	4.55300	5.57400	26.35300
N	6.22900	1.32600	23.58600
H	6.91800	1.65900	22.91100
C	5.81200	-0.06200	23.51800
C	5.93800	-0.79500	24.84700
O	5.22200	-1.76600	25.08200
C	6.63700	-0.80500	22.45700
N	6.85800	-0.33200	25.70700
H	7.45300	0.45300	25.44300
C	7.00800	-0.95200	27.02200
C	6.36200	-0.08000	28.08700
O	6.77500	-0.09300	29.25200
C	8.50100	-1.15200	27.29100
C	9.23100	-2.02000	26.27600
C	10.65700	-2.27700	26.73400
C	11.52400	-2.95000	25.68600
N	10.85900	-4.09700	25.00400
H	11.44200	-4.54900	24.30000
H	9.96700	-3.80800	24.60200
H	10.52600	-4.77800	25.68700
N	5.36000	0.69700	27.69600
H	5.00800	0.57200	26.74700
C	4.72800	1.71300	28.52000
C	3.84800	1.06800	29.57300
O	3.79200	-0.16300	29.55900
N	3.19100	1.85800	30.41000
H	3.29100	2.86700	30.30400
C	2.32800	1.35300	31.48000
C	0.87800	1.12100	31.07700
O	0.09000	0.57600	31.87200
C	2.33400	2.36600	32.63500
C	3.73000	2.66000	33.17100
C	3.86700	2.19500	34.61500
O	4.28700	1.04100	34.83900
O	3.53700	2.99100	35.52600
N	0.48200	1.55100	29.87500
H	1.13000	1.97400	29.21100
C	-0.95600	1.37500	29.56700
C	-1.07000	0.91100	28.10600
O	-1.77500	1.44000	27.25900

C	-1.77800	2.59700	29.89800
C	-1.65000	3.86700	29.11300
C	-2.69800	4.90000	29.50100
N	-3.88000	4.87900	28.63600
H	-4.01000	4.05100	28.05500
C	-4.79400	5.82700	28.53400
N	-4.76800	6.96300	29.22900
H	-5.47400	7.69500	29.15000
H	-3.98500	7.09200	29.87000
N	-5.80900	5.66000	27.70300
H	-6.51500	6.39200	27.62400
H	-5.82900	4.79000	27.17100
N	-0.33400	-0.17700	27.85500
H	0.19700	-0.63200	28.59800
C	-0.31000	-0.70100	26.48300
C	-1.44400	-1.69400	26.25800
O	-1.95700	-2.31000	27.21900
C	1.04900	-1.34900	26.23000
C	2.16200	-0.30900	26.05700
C	1.96200	0.45800	24.76400
O	2.15800	-0.15000	23.69500
N	1.58200	1.74000	24.84300
H	1.42100	2.23800	25.71900
H	1.44700	2.25600	23.97300
N	-1.77400	-1.81500	24.97100
H	-1.27000	-1.25800	24.28100
C	-2.83100	-2.71600	24.51100
C	-2.30700	-3.64200	23.41200
O	-1.33700	-3.26100	22.74500
C	-4.05400	-1.96500	23.95200
O	-4.74600	-1.22400	24.94300
H	-5.50000	-0.76100	24.59800
N	-2.90600	-4.80900	23.17700
C	-4.07200	-5.30700	23.88200
C	-3.72600	-6.02800	25.17600
O	-2.57000	-6.10000	25.57500
C	-4.60700	-6.32900	22.85600
C	-3.34800	-6.91900	22.25600
C	-2.44700	-5.72100	22.10800
N	-4.75000	-6.54600	25.83500
H	-5.68800	-6.44300	25.44800
C	-4.58100	-7.25700	27.09300
C	-5.50800	-8.46200	27.12300
O	-6.49700	-8.54800	26.38900
C	-4.90100	-6.38500	28.32300
C	-3.98300	-5.15900	28.36000
C	-6.35600	-5.99900	28.28900
N	-5.17800	-9.41300	28.00000
H	-4.29700	-9.37400	28.51300
C	-6.12000	-10.51100	28.20100
C	-7.15000	-10.08300	29.22500
O	-6.86800	-9.49100	30.28300

C	-5.38600	-11.76200	28.69300
C	-6.34900	-12.88500	29.02600
O	-7.02800	-13.37800	28.10700
O	-6.42800	-13.28900	30.21000
N	-8.41100	-10.36800	28.90300
H	-8.62000	-10.82700	28.01600
C	-9.48800	-10.02500	29.81500
C	-9.83000	-11.26800	30.64200
O	-10.40100	-12.23600	30.13800
C	-10.70700	-9.52300	29.04200
C	-10.36600	-8.26800	28.23200
C	-11.88500	-9.29900	29.98200
C	-11.35000	-7.99700	27.10100
N	-9.42500	-11.19500	31.89600
H	-8.86600	-10.39600	32.19500
C	-9.76400	-12.24500	32.87200
C	-11.15700	-11.95700	33.40700
O	-11.34200	-10.98600	34.14700
C	-8.72600	-12.26600	33.98800
C	-8.92600	-13.41400	34.96900
O	-10.07800	-13.71600	35.35600
O	-7.90500	-14.02100	35.35900
N	-12.11900	-12.77000	32.99900
H	-11.88100	-13.63600	32.51500
C	-13.50800	-12.43500	33.23700
C	-13.85200	-12.60900	34.72300
O	-14.87400	-12.06000	35.14800
C	-14.50100	-13.26900	32.42300
O	-14.33100	-14.65200	32.75600
H	-14.49200	-14.74600	33.68800
C	-14.24400	-13.11800	30.93300
N	-12.99200	-13.33700	35.43300
H	-12.18400	-13.77600	34.99200
C	-13.24500	-13.48800	36.87300
C	-12.56700	-12.41700	37.70100
O	-12.84600	-12.31700	38.90700
C	-12.81700	-14.88000	37.34000
C	-13.58100	-15.96300	36.64700
N	-13.00300	-16.81100	35.73300
H	-12.02400	-16.78700	35.44700
C	-14.87800	-16.32500	36.74100
C	-13.90600	-17.66200	35.28100
N	-15.04900	-17.38500	35.87800
H	-15.92700	-17.88100	35.72400
N	-11.69700	-11.56200	37.15800
H	-11.37800	-11.66100	36.19400
C	-11.22500	-10.47500	38.01900
C	-11.66900	-9.10600	37.52500
O	-11.36600	-8.08200	38.15000
C	-9.69600	-10.51000	38.16300
O	-9.14000	-10.67300	36.86900
H	-8.19400	-10.69500	36.95800

C	-9.28200	-11.70200	39.01800
N	-12.41900	-9.06700	36.41800
H	-12.58900	-9.91200	35.87300
C	-12.99000	-7.78500	36.00700
C	-14.07300	-7.38100	37.00700
O	-14.78100	-8.25400	37.50300
C	-13.55900	-7.86600	34.60500
N	-14.17500	-6.09400	37.29800
H	-13.58700	-5.45200	36.76600
C	-15.04400	-5.50900	38.30300
C	-16.32300	-5.01800	37.65000
O	-16.29000	-4.08800	36.84700
C	-14.42100	-4.30100	38.97100
C	-14.81000	-3.92600	40.37400
C	-15.89700	-4.77300	41.00600
C	-16.21100	-4.28700	42.41900
N	-15.97000	-5.36500	43.42700
H	-16.18000	-5.04000	44.37100
H	-15.02200	-5.73600	43.36000
H	-16.48700	-6.21400	43.19900
N	-17.42600	-5.62600	38.02500
H	-17.39000	-6.46900	38.59900
C	-18.69900	-5.06600	37.60100
C	-18.85600	-3.65700	38.14900
O	-18.62300	-3.39300	39.34000
C	-19.84000	-5.96700	38.08600
C	-21.17000	-5.28700	37.84700
C	-21.57100	-4.93800	36.56700
C	-21.99000	-5.00500	38.93000
C	-22.78800	-4.31300	36.35900
C	-23.20600	-4.38200	38.72900
C	-23.59500	-4.04300	37.44700
O	-24.81600	-3.42100	37.28500
H	-25.08300	-3.18800	36.40400
N	-19.25600	-2.70600	37.30900
H	-19.46900	-2.92100	36.33500
C	-19.38200	-1.33400	37.82700
C	-20.77100	-0.80100	37.51200
O	-21.08700	-0.35500	36.41100
C	-18.29100	-0.43600	37.26400
C	-18.36600	1.01600	37.67200
O	-19.31800	1.42200	38.36800
O	-17.45000	1.77800	37.29000
N	-21.66100	-0.80700	38.50500
C	-22.98000	-0.19300	38.32600
C	-22.87800	1.26900	37.93600
O	-23.80800	1.85300	37.37100
C	-23.64100	-0.30000	39.71200
C	-22.91300	-1.39900	40.40600
C	-21.51400	-1.40000	39.84000
N	-21.75800	1.93700	38.20100
H	-20.96800	1.49900	38.67500

C	-21.72400	3.33400	37.77500
C	-21.74100	3.45100	36.25100
O	-21.98700	4.55200	35.74000
C	-20.51100	4.04400	38.36400
O	-19.32100	3.81300	37.63300
H	-18.56500	4.25600	38.00000
N	-21.48500	2.36100	35.52100
H	-21.40000	1.44600	35.96400
C	-21.32900	2.50800	34.07400
C	-22.66900	2.60500	33.35500
O	-23.63300	1.88600	33.60400
C	-20.51400	1.35600	33.48200
C	-19.02700	1.38600	33.82900
C	-18.35700	0.07900	33.44400
C	-18.36000	2.56300	33.13900
N	-22.69200	3.54900	32.41800
H	-21.86700	4.13100	32.27100
C	-23.88100	3.76400	31.59700
C	-23.90900	2.86100	30.37900
O	-22.90100	2.34200	29.90700
C	-23.91600	5.23200	31.16700
C	-24.22000	6.17900	32.32800
C	-23.26100	7.36000	32.30500
C	-22.08800	7.14900	33.25100
N	-21.40600	5.84200	33.02300
H	-20.62000	5.70100	33.65700
H	-21.11700	5.74200	32.05000
H	-22.06700	5.06700	33.07700
N	-25.08600	2.62700	29.81600
C	-25.14000	1.90200	28.54500
C	-24.38400	2.71300	27.49100
O	-24.26500	3.94300	27.60400
C	-26.62200	1.87600	28.22700
C	-27.31000	2.08300	29.54100
C	-26.41700	3.01000	30.32300
N	-23.88200	2.02600	26.47700
H	-23.90500	1.00600	26.48700
C	-23.30100	2.73100	25.35500
C	-24.44300	3.34000	24.52700
O	-25.50200	2.72500	24.53100
C	-22.56800	1.82600	24.37500
C	-21.31400	1.11500	24.83400
C	-20.75000	0.29300	23.69100
C	-20.32900	2.14900	25.36400
N	-24.18300	4.43000	23.85800
H	-23.29200	4.88500	24.05900
C	-25.02000	5.06200	22.86400
C	-24.26200	5.13900	21.53400
O	-23.35600	5.95400	21.44200
C	-25.41100	6.48100	23.26600
O	-26.28200	7.06200	22.31100
H	-26.52500	7.94600	22.56100

N	-24.67300	4.31700	20.59700
H	-25.41100	3.64800	20.81700
C	-24.11000	4.32800	19.25100
C	-25.11500	4.98200	18.32500
O	-26.22400	4.48200	18.12100
C	-23.78200	2.90800	18.75800
C	-23.05500	2.95600	17.42800
C	-22.94300	2.16200	19.78900
N	-24.75100	6.12800	17.76500
H	-23.86100	6.56300	18.00600
C	-25.65000	6.75800	16.79400
C	-24.96600	6.81600	15.43000
O	-24.26500	7.78100	15.13100
C	-26.07700	8.16200	17.22400
O	-26.28900	8.15300	18.63200
H	-26.55400	9.02500	18.89900
N	-25.18800	5.75900	14.66500
H	-25.81100	5.02600	15.00500
C	-24.57300	5.60700	13.35400
C	-25.56400	5.83300	12.21100
O	-25.20300	5.53900	11.05500
C	-23.95000	4.21400	13.23600
C	-22.67000	3.96100	14.00600
C	-21.97800	4.96600	14.66600
C	-22.16500	2.66900	14.05400
C	-20.80900	4.65400	15.35300
C	-21.00200	2.35000	14.73100
C	-20.32100	3.36500	15.38900
O	-19.15300	3.06000	16.07100
H	-18.68700	3.75500	16.52100
N	-26.75700	6.34300	12.50100
C	-27.73200	6.47400	11.41300
C	-27.76700	6.58600	11.48500
C	-27.25400	7.43600	10.33100
O	-27.56700	7.22300	9.15600
C	-29.10300	6.88900	11.94800
C	-28.97100	7.27500	12.14400
C	-29.06900	8.16300	12.76200
C	-30.21300	7.20100	11.28300
O	-28.63700	8.11300	13.93300
O	-30.81100	6.11000	11.18500
O	-29.48100	9.21000	12.22100
O	-30.58200	8.24100	10.69800
N	-26.47100	8.46200	10.64400
H	-26.17900	8.62900	11.60700
C	-26.04200	9.34400	9.56000
C	-24.60200	9.14300	9.11100
O	-23.99900	10.07700	8.58300
C	-26.24100	10.79900	10.01300
C	-27.49600	10.94400	10.86700
C	-28.76800	10.97600	10.04600
O	-29.86400	10.77600	10.58400

N	-28.65000	11.23100	8.74400
H	-27.74600	11.39600	8.30000
H	-29.50700	11.25300	8.19100
N	-24.01700	7.96100	9.29200
H	-24.54700	7.19700	9.71000
C	-22.63800	7.74400	8.90400
C	-22.44000	8.00300	7.41400
O	-23.27000	7.65800	6.56100
C	-22.19500	6.33900	9.27400
N	-21.31000	8.63800	7.12200
H	-20.71500	8.98800	7.87300
C	-20.91900	8.83600	5.73300
C	-19.58400	8.18000	5.41800
O	-18.52500	8.74900	5.66400
C	-20.80800	10.34500	5.43000
O	-22.13900	10.87700	5.44400
H	-22.49900	10.71800	6.30800
C	-20.23100	10.60000	4.04600
N	-19.64000	6.96800	4.85400
H	-20.53300	6.51200	4.67000
C	-18.36600	6.31700	4.50800
C	-17.81000	6.96700	3.23900
O	-18.61300	7.42300	2.41200
C	-18.56500	4.81800	4.37900
O	-19.46900	4.46800	3.34500
H	-19.59400	3.53000	3.26400
N	-16.49700	7.03400	3.07700
H	-15.90600	6.68100	3.83000
C	-15.84200	7.57700	1.89900
C	-15.08300	6.57800	1.03900
O	-15.19800	6.50900	-0.19400
C	-14.81300	8.63900	2.34800
C	-15.42400	9.78600	3.16300
C	-14.32300	10.71800	3.65200
C	-16.47000	10.50700	2.33800
N	-14.23100	5.77800	1.69000
H	-14.33000	5.62800	2.69400
C	-13.15800	5.12200	0.95000
C	-12.67300	3.89300	1.68300
O	-12.83900	3.84300	2.91600
C	-12.02300	6.13700	0.86000
C	-10.89600	5.83200	-0.10400
C	-10.08800	7.14600	-0.24900
N	-9.20500	7.21300	0.92200
H	-9.60000	7.07500	1.85200
C	-7.89600	7.45000	0.79700
N	-7.18300	7.48500	1.90000
H	-6.18400	7.66600	1.80500
H	-7.59900	7.33400	2.81900
N	-7.35700	7.64500	-0.39300
H	-6.35800	7.82600	-0.48800
H	-7.91100	7.61800	-1.24900

N	-12.09100	2.96300	0.96500
H	-12.07500	3.01200	-0.05400
C	-11.45800	1.84000	1.69200
C	-10.02900	1.79900	1.20600
O	-9.77700	2.04600	0.00800
C	-12.16400	0.50300	1.48500
C	-11.57200	-0.68900	2.25000
C	-12.21900	0.16100	-0.00600
C	-12.48100	-1.89100	2.28900
N	-9.09500	1.52900	2.10800
H	-9.37300	1.19900	3.03200
C	-7.68200	1.69400	1.80500
C	-6.92400	0.45900	2.26000
O	-7.23500	-0.12000	3.30100
C	-7.12600	2.93800	2.50100
C	-5.60300	3.02600	2.61600
C	-4.96900	3.20500	1.24400
C	-5.19900	4.15800	3.54900
N	-5.92700	0.05500	1.48200
H	-5.85400	0.40400	0.52600
C	-4.92800	-0.89300	1.99300
C	-3.70400	-0.07200	2.37900
O	-3.09200	0.53300	1.50600
C	-4.57600	-1.94600	0.95300
C	-3.54800	-2.95700	1.40100
O	-2.75400	-2.69200	2.30800
N	-3.55000	-4.12200	0.74600
H	-2.85600	-4.80500	1.04900
H	-4.20600	-4.34100	-0.00400
N	-3.40200	-0.03800	3.68500
H	-3.92800	-0.59000	4.36200
C	-2.29000	0.82000	4.10600
C	-1.00300	0.03900	4.36700
O	-0.06800	0.64000	4.89900
C	-2.64500	1.63600	5.35400
C	-2.93400	0.77500	6.56100
O	-2.57400	-0.39000	6.62200
N	-3.58900	1.39700	7.53900
H	-3.89000	2.37000	7.48800
H	-3.78400	0.81600	8.35400
N	-0.96300	-1.24600	4.02600
H	-1.79400	-1.68600	3.63000
C	0.24200	-2.03100	4.20800
C	0.21700	-2.80000	5.50900
O	1.06800	-3.67900	5.70300
N	-0.73900	-2.49600	6.39400
H	-1.39900	-1.73700	6.22400
N	-0.74500	-2.49100	6.37800
H	-1.40700	-1.73800	6.18900
C	-0.79800	-3.30400	7.62300
C	-0.81700	-3.27800	7.62100
C	-2.22500	-3.67600	8.01700

C	-2.20300	-3.88500	7.80100
O	-2.42300	-4.41600	8.98600
O	-2.37800	-4.96600	8.37400
C	-0.11200	-2.59800	8.79100
C	-0.41800	-2.39500	8.81000
C	-0.65400	-1.25500	9.16400
C	0.81900	-1.57700	8.55500
N	-0.04200	-0.07200	8.80300
H	0.81800	0.00500	8.26000
N	0.78000	-0.23600	8.24100
H	-0.06800	0.32500	8.15600
C	-1.75500	-0.89600	9.87000
C	2.13000	-1.91600	8.55800
C	-0.74400	0.94700	9.27000
C	2.01800	0.21200	8.06600
N	-1.79500	0.47300	9.92800
H	-2.50900	1.03100	10.39600
N	2.86000	-0.79100	8.25600
H	3.87600	-0.73800	8.19000
N	-3.22400	-3.20700	7.28900
C	-4.60600	-3.60800	7.41800
C	-5.36600	-2.89800	6.29000
O	-4.69400	-2.24300	5.48500
C	-5.19300	-3.27000	8.77000
N	-6.68600	-3.03200	6.24600
H	-7.15900	-3.73000	6.81900
C	-7.44300	-2.15700	5.35800
C	-8.34900	-1.28900	6.24100
O	-8.92600	-1.76300	7.21600
C	-8.27400	-2.85800	4.29300
C	-9.30000	-3.83600	4.81500
C	-10.59000	-3.43100	5.11000
C	-8.95400	-5.16400	5.00300
C	-11.51700	-4.33400	5.61100
C	-9.86900	-6.06900	5.52000
C	-11.15300	-5.65600	5.82700
N	-8.43300	-0.01200	5.88200
H	-7.93800	0.31700	5.05300
C	-9.22300	0.91100	6.66200
C	-10.46100	1.33600	5.86300
O	-10.24800	1.69400	4.69900
C	-8.46000	2.19100	6.98300
C	-7.39200	1.99500	8.04100
O	-7.23400	0.89800	8.56700
N	-6.67100	3.06200	8.33500
H	-5.95200	2.93000	9.04700
H	-6.80200	3.97400	7.89800
N	-11.61400	1.32600	6.48600
H	-11.70800	0.85200	7.38400
C	-12.77600	2.00400	5.88000
C	-12.86900	3.39000	6.50500
O	-12.98500	3.43900	7.74100

C	-14.07600	1.21600	6.09500
C	-15.29400	2.02200	5.65200
C	-13.93600	-0.11900	5.36300
N	-12.81100	4.47400	5.75200
H	-12.81700	4.33900	4.74100
C	-12.74000	5.83700	6.23500
C	-14.06100	6.58900	6.13900
O	-14.75700	6.39100	5.13400
C	-11.70100	6.61000	5.40000
C	-10.37800	5.85100	5.45600
C	-9.31200	6.55400	4.63700
O	-8.16000	6.41100	5.08000
O	-9.67000	7.23800	3.66300
N	-14.35200	7.42100	7.13800
H	-13.65900	7.56900	7.87200
C	-15.62400	8.12700	7.22000
C	-15.41700	9.63700	7.18500
O	-14.35900	10.11900	7.55800
C	-16.37800	7.75800	8.51700
C	-16.91900	6.33100	8.44400
C	-16.08700	5.26500	8.74800
C	-18.21700	6.06500	8.08100
C	-16.54800	3.95300	8.67800
C	-18.69700	4.76400	7.99800
C	-17.85600	3.70700	8.30000
N	-16.43700	10.36400	6.78000
H	-17.25000	9.89900	6.37700
C	-16.43200	11.81900	6.89400
C	-16.65800	12.16700	8.35900
O	-17.70900	11.77100	8.87400
C	-17.55300	12.38300	6.02300
C	-17.81700	13.86000	6.20100
O	-16.99200	14.58300	6.79600
O	-18.88600	14.33200	5.75000
N	-15.71300	12.82000	9.00900
H	-14.87500	13.09900	8.49900
C	-15.81300	13.16200	10.42600
C	-15.78100	14.68300	10.60000
O	-15.30000	15.19700	11.61200
C	-14.67400	12.50800	11.20900
C	-13.32200	13.08600	10.82500
O	-13.20800	13.76900	9.77000
O	-12.33200	12.86700	11.54900
N	-16.28300	15.43700	9.62400
H	-16.66600	14.98100	8.79600
C	-16.30300	16.89800	9.70100
C	-17.51900	17.39700	10.46600
O	-17.65700	18.58900	10.76300
C	-16.28400	17.52000	8.29600
O	-17.45100	17.13800	7.56800
H	-17.43900	17.52300	6.69900
N	-18.42700	16.49800	10.82200

H	-18.30800	15.52600	10.53700
C	-19.58800	16.87300	11.61100
C	-20.00800	15.68600	12.47900
O	-19.54600	14.58800	12.18000
C	-20.77600	17.22900	10.73300
C	-20.65500	18.41400	9.79800
C	-21.88900	18.50100	8.90200
O	-22.89500	19.11100	9.26300
N	-21.82000	17.88000	7.73600
H	-20.98600	17.37400	7.43700
H	-22.64400	17.93800	7.13800
N	-20.87300	15.90000	13.45300
H	-21.20900	16.84900	13.61900
C	-21.36100	14.81600	14.29800
C	-22.40700	13.92100	13.63100
O	-23.56500	13.91700	14.04300
C	-21.95500	15.39200	15.58100
C	-20.90000	15.74200	16.61200
O	-21.30900	16.37300	17.60400
O	-19.70000	15.42100	16.45300
N	-22.00500	13.14600	12.63800
H	-21.02000	13.19300	12.37900
C	-22.84700	12.23400	11.88600
C	-22.94900	10.85700	12.53300
O	-24.00300	10.24700	12.69400
C	-22.25900	12.02500	10.48700
C	-22.47000	13.13900	9.48300
C	-21.52400	12.94900	8.29700
C	-22.21200	13.37300	7.00700
N	-21.34200	14.28000	6.20800
H	-21.80300	14.56400	5.34400
H	-20.42900	13.86200	6.02700
H	-21.03800	15.08600	6.75400
N	-21.78700	10.31700	12.89000
H	-20.92300	10.84300	12.75800
C	-21.73700	8.98200	13.46800
C	-20.93000	9.11700	14.76500
O	-19.71900	9.35400	14.70300
C	-21.08600	7.97300	12.54900
N	-21.62100	8.98500	15.87900
H	-22.60300	8.71300	15.84900
C	-20.96100	9.23400	17.15600
C	-21.26200	8.13900	18.17900
O	-22.26000	7.42800	18.19000
C	-21.36900	10.59900	17.77300
C	-21.03600	11.73600	16.80500
C	-22.84000	10.59300	18.14400
N	-20.30500	8.08000	19.08800
H	-19.49500	8.68700	18.96300
C	-20.32500	7.21400	20.24900
C	-20.37300	8.11000	21.48400
O	-19.63300	9.09800	21.59100

C	-19.08600	6.32100	20.16700
C	-18.89600	5.37700	21.35200
C	-20.08600	4.42600	21.38600
C	-17.55700	4.65900	21.28900
N	-21.25300	7.76900	22.40200
H	-21.85900	6.96900	22.21900
C	-21.40500	8.47200	23.65900
C	-21.74700	7.44800	24.75000
O	-22.03100	6.29100	24.45000
C	-22.52600	9.50400	23.64000
C	-22.55200	10.57900	22.58000
C	-23.78400	11.46800	22.76500
C	-24.21400	12.13600	21.46800
N	-25.25800	11.34900	20.74200
H	-25.54600	11.79700	19.87200
H	-26.06100	11.16000	21.34300
H	-24.94900	10.39100	20.57800
N	-21.74000	7.94600	25.98400
H	-21.43000	8.90400	26.14500
C	-22.17300	7.12700	27.10100
C	-21.10600	6.13300	27.50900
O	-19.90200	6.35700	27.30400
N	-21.57900	5.03100	28.11600
H	-22.58200	4.86200	28.19700
C	-20.60400	4.08000	28.65700
C	-19.67900	4.78600	29.63600
O	-20.18900	5.51300	30.49200
N	-18.37300	4.57400	29.53600
C	-17.41700	5.23800	30.42200
C	-16.93200	6.58700	29.91900
O	-16.03900	7.22900	30.48100
C	-16.23700	4.27300	30.35100
C	-16.27200	3.70800	28.97500
C	-17.71800	3.66100	28.58000
N	-17.51900	7.03500	28.81300
H	-18.33200	6.55300	28.43100
C	-16.99300	8.21400	28.15600
C	-17.60700	9.49300	28.70300
O	-18.72600	9.50900	29.18200
C	-17.27300	8.11000	26.64700
C	-16.73400	6.80200	26.03600
C	-17.27900	6.62000	24.62900
C	-15.21100	6.80700	26.01800
N	-16.83200	10.54100	28.58000
H	-15.85500	10.37000	28.34300
C	-17.23300	11.91000	28.74900
C	-17.34400	12.59600	27.40100
O	-16.35800	12.69000	26.67200
C	-16.19200	12.67000	29.59100
C	-16.90100	13.06400	30.87700
O	-17.71400	12.21700	31.31300
O	-16.64700	14.17300	31.38100

N	-18.52600	13.08900	27.05200
H	-19.35700	12.97200	27.63200
C	-18.55800	13.81000	25.78400
C	-18.76300	12.89300	24.59000
O	-19.03200	11.70600	24.70700
N	-18.62000	13.50600	23.42600
H	-18.25600	14.45800	23.45000
C	-18.92700	12.96300	22.13100
C	-17.67700	12.58600	21.35300
O	-16.74900	13.37700	21.25100
C	-19.70600	14.02500	21.31800
O	-20.80800	14.44400	22.13500
H	-20.47100	14.82400	22.93800
C	-20.24200	13.42100	20.04000
N	-17.70500	11.35500	20.84700
H	-18.51900	10.76700	21.02800
C	-16.62200	10.82100	20.04900
C	-17.09400	10.48600	18.64200
O	-18.03000	9.72300	18.38400
C	-16.06100	9.56600	20.72500
C	-15.28000	9.78100	22.00000
C	-15.89800	10.24600	23.16500
C	-13.92400	9.51200	22.05000
C	-15.14900	10.43000	24.30900
C	-13.14400	9.68000	23.17900
C	-13.79200	10.14600	24.31800
O	-13.09000	10.33700	25.48200
H	-13.53300	10.65500	26.26000
N	-16.42600	11.07200	17.66300
H	-15.65100	11.69500	17.89100
C	-16.76900	10.84900	16.27500
C	-16.03300	9.66900	15.64100
O	-14.81800	9.51000	15.80200
C	-16.35600	12.11100	15.49300
C	-17.46400	13.12700	15.37400
C	-17.00000	14.29400	14.49000
N	-17.64700	15.51500	14.97800
H	-18.41200	15.43000	15.64700
C	-17.27700	16.72900	14.58400
N	-16.28600	16.88500	13.70900
H	-16.00200	17.81700	13.40700
H	-15.79000	16.08000	13.32600
N	-17.92200	17.77600	15.08200
H	-17.63800	18.70800	14.78000
H	-18.68100	17.65600	15.75200
N	-16.77200	8.88900	14.85900
H	-17.77300	9.07200	14.78900
C	-16.21300	7.79200	14.10400
C	-15.33900	8.31800	12.96600
O	-15.82200	9.17900	12.20800
C	-17.35300	6.95400	13.50900
C	-16.96400	5.76700	12.63000

C	-16.19100	4.71200	13.40000
C	-18.24400	5.16100	12.03600
N	-14.12500	7.83300	12.83400
H	-13.76600	7.15100	13.50200
C	-13.29600	8.28200	11.71800
C	-12.92700	7.10800	10.81600
O	-12.84700	7.23000	9.59300
C	-12.03100	9.00600	12.19600
C	-11.15000	9.48800	11.03700
C	-11.24800	8.12100	13.15000
C	-10.05800	10.43100	11.54900
N	-12.73900	5.90600	11.36600
H	-12.84300	5.78500	12.37300
C	-12.38400	4.76400	10.52600
C	-12.65100	3.45100	11.27300
O	-12.73300	3.46100	12.49100
C	-10.91700	4.78900	10.09600
C	-9.89300	4.82700	11.22800
C	-9.08000	3.56700	11.38300
O	-9.58200	2.46000	11.32900
N	-7.77400	3.71700	11.57900
H	-7.35300	4.64500	11.62400
H	-7.22400	2.86400	11.68400
N	-12.80400	2.35700	10.52500
H	-12.98700	2.42500	9.52400
C	-12.70100	1.05100	11.18900
C	-11.71300	0.18400	10.41500
O	-11.47700	0.36100	9.22300
C	-14.04300	0.33600	11.37900
C	-14.79200	-0.16500	10.15100
C	-14.46200	-1.30800	9.45800
C	-15.90800	0.53900	9.69600
C	-15.15000	-1.78400	8.37100
C	-16.62200	0.09200	8.60000
C	-16.25700	-1.06400	7.91900
N	-11.15700	-0.82300	11.08700
H	-11.35000	-0.91200	12.08500
C	-10.29200	-1.79400	10.46000
C	-10.38300	-3.09900	11.25800
O	-10.99800	-3.15400	12.31600
C	-8.82700	-1.31400	10.37600
C	-8.31700	-1.01300	11.76200
N	-8.40500	0.23400	12.32800
H	-8.80700	1.05900	11.88300
C	-7.71900	-1.82300	12.68900
C	-7.88000	0.19200	13.55400
N	-7.46400	-1.03200	13.78100
N	-9.72500	-4.13000	10.72900
H	-9.24900	-4.01400	9.83400
C	-9.67200	-5.41500	11.40100
C	-8.21700	-5.86100	11.60500
O	-7.30800	-5.37200	10.96300

C	-10.39600	-6.49600	10.58800
C	-11.85500	-6.26900	10.23700
C	-12.21200	-5.39200	9.21200
C	-12.83800	-6.96400	10.92600
C	-13.53600	-5.21100	8.85300
C	-14.17200	-6.75800	10.59300
C	-14.51300	-5.89000	9.55700
N	-8.05000	-6.80400	12.51600
H	-8.83100	-6.98100	13.14700
C	-6.85600	-7.61200	12.70200
C	-7.28400	-9.07600	12.56800
O	-8.37000	-9.46200	13.05000
C	-6.20600	-7.36300	14.05400
C	-5.91100	-5.91900	14.33300
N	-4.66800	-5.34300	14.18000
H	-3.81700	-5.81100	13.86800
C	-6.77600	-4.95400	14.74800
C	-4.78900	-4.05600	14.51700
N	-6.05500	-3.79800	14.85900
N	-6.50800	-9.90200	11.89500
H	-5.61900	-9.57800	11.51300
C	-6.93400	-11.28700	11.70200
C	-5.73600	-12.22100	11.60400
O	-4.57700	-11.80000	11.52100
C	-7.83800	-11.41000	10.47200
C	-7.15900	-11.01500	9.19300
C	-6.49100	-11.83600	8.33200
C	-7.07700	-9.70000	8.61400
N	-5.98800	-11.12100	7.24700
H	-5.45000	-11.50500	6.47000
C	-6.34900	-9.80300	7.41300
C	-7.56900	-8.45500	9.02600
C	-6.07400	-8.71300	6.57800
C	-7.29500	-7.38300	8.20300
C	-6.56500	-7.51000	7.01200
N	-6.06600	-13.51200	11.62700
H	-7.05300	-13.76800	11.58900
C	-5.07900	-14.55900	11.70400
C	-4.89800	-15.32700	10.39800
O	-5.66800	-15.15300	9.45300
N	-3.84700	-16.15600	10.39800
H	-3.20100	-16.16800	11.18700
C	-3.63500	-17.04200	9.25900
C	-4.47300	-18.30100	9.39000
O	-4.60000	-19.04200	8.43100
C	-2.15800	-17.43300	9.17000
O	-1.70800	-17.82300	10.45800
H	-0.79100	-18.06600	10.40300
N	-5.02700	-18.56100	10.55500
H	-4.88900	-17.87100	11.29300
C	-5.81400	-19.73000	10.89500
C	-7.00200	-19.31300	11.74500

O	-6.89400	-18.28600	12.43600
C	-4.93600	-20.73000	11.66300
C	-3.87700	-21.43000	10.79900
C	-2.63600	-21.76300	11.60800
C	-4.44800	-22.69000	10.18000
N	-8.10800	-20.05200	11.73900
H	-8.15000	-20.92700	11.21700
C	-9.26200	-19.57600	12.50100
C	-8.99400	-19.52300	14.01300
O	-9.74100	-18.81400	14.69300
C	-10.50300	-20.42800	12.23300
C	-10.93400	-20.48700	10.78300
O	-10.59200	-19.61900	9.94800
O	-11.66000	-21.45800	10.47800
N	-7.98500	-20.21600	14.53400
H	-7.36200	-20.74400	13.92300
C	-7.76600	-20.22400	15.97500
C	-6.97700	-19.05900	16.52200
O	-6.59500	-18.98800	17.69800
N	-6.68900	-18.07200	15.67500
H	-6.96700	-18.13200	14.69500
C	-5.97000	-16.90500	16.17100
C	-6.27600	-15.72600	15.27500
O	-6.79600	-15.87500	14.16500
C	-4.46700	-17.22100	16.20000
C	-3.91700	-17.27100	14.77700
C	-2.55500	-17.92800	14.63700
O	-2.33600	-19.01200	15.17800
N	-1.65000	-17.28200	13.90200
H	-1.83100	-16.38400	13.45400
H	-0.73500	-17.72300	13.80800
N	-5.95800	-14.51600	15.73600
H	-5.52100	-14.40000	16.65000
C	-6.25600	-13.35600	14.88800
C	-6.74000	-12.18700	15.74100
O	-6.46800	-11.03800	15.36800
N	-7.44900	-12.43000	16.85600
H	-7.69400	-13.37800	17.14100
C	-7.85200	-11.26000	17.64100
C	-6.65300	-10.70800	18.41100
O	-5.62800	-11.35000	18.61600
C	-8.98400	-11.57800	18.62100
O	-8.59800	-12.54300	19.58800
H	-9.30100	-12.74000	20.19600
N	-6.79900	-9.47400	18.87700
H	-7.65100	-8.95500	18.66300
C	-5.75900	-8.84600	19.69200
C	-6.09300	-9.00100	21.17200
O	-5.27300	-9.54900	21.91500
C	-5.68500	-7.37500	19.28900
C	-5.24200	-7.23500	17.84300
C	-4.51500	-5.94500	17.57400

O	-5.06700	-4.84400	17.79100
O	-3.35800	-6.01900	17.12800
N	-7.29400	-8.55300	21.57700
H	-7.89700	-8.01000	20.95900
C	-7.69900	-8.88100	22.94900
C	-8.00900	-10.36600	23.05000
O	-8.36900	-10.98300	22.04500
C	-8.92800	-8.06700	23.36900
C	-8.53800	-6.63300	23.53400
N	-8.57100	-5.75300	22.46400
H	-8.85600	-5.97100	21.50900
C	-8.10000	-5.94400	24.61900
C	-8.16200	-4.57100	22.91500
N	-7.87300	-4.65000	24.20500
H	-7.54000	-3.88500	24.79100
N	-7.86900	-10.92000	24.25500
H	-7.48700	-10.38100	25.03200
C	-8.27400	-12.31900	24.44400
C	-9.21500	-12.33300	25.63800
O	-9.20700	-11.37900	26.41400
C	-7.08800	-13.27600	24.64300
O	-6.22000	-12.81300	25.68600
H	-5.48700	-13.40500	25.80900
C	-6.21400	-13.29500	23.38900
N	-10.01300	-13.37900	25.76800
H	-9.98000	-14.13300	25.08200
C	-10.94400	-13.45600	26.89600
C	-10.63800	-14.75400	27.63600
O	-10.84200	-15.81100	27.02300
C	-12.40800	-13.44900	26.44700
C	-13.32000	-13.53200	27.66400
C	-12.73900	-12.21000	25.62600
N	-10.15300	-14.66900	28.85700
H	-10.10200	-13.76000	29.31800
C	-9.68700	-15.86500	29.56000
C	-8.77400	-16.70200	28.65400
O	-8.96900	-17.90400	28.53700
C	-10.87600	-16.67900	30.08300
C	-11.59100	-15.90500	31.18900
O	-10.95400	-15.06600	31.84700
O	-12.80400	-16.14700	31.36900
N	-7.83400	-16.01800	28.02700
H	-7.81000	-15.01500	28.20900
C	-6.83500	-16.52500	27.11200
C	-7.44000	-17.11200	25.83900
O	-6.72000	-17.64900	24.99600
C	-5.96300	-17.55700	27.83900
C	-5.20400	-17.03500	29.04300
C	-3.96700	-16.25800	28.63900
C	-2.92800	-16.16700	29.74600
N	-3.48200	-16.00100	31.12000
H	-2.78500	-15.94000	31.86200

H	-4.14800	-16.74600	31.32300
H	-4.10300	-15.19300	31.15300
N	-8.74400	-17.00400	25.61200
H	-9.34000	-16.61600	26.34300
C	-9.35400	-17.42100	24.35200
C	-9.07700	-16.41500	23.22800
O	-9.30700	-15.22100	23.40400
C	-10.87200	-17.57800	24.50200
C	-11.56100	-18.08700	23.23200
C	-13.07400	-18.02100	23.37400
C	-13.81300	-18.44000	22.11200
N	-12.93600	-19.19800	21.17800
H	-13.43100	-19.47900	20.33200
H	-12.50900	-20.00000	21.64000
H	-12.09100	-18.67200	20.95500
N	-8.58800	-16.91100	22.10100
H	-8.37000	-17.90700	22.06200
C	-8.34600	-16.09500	20.90700
C	-9.52500	-16.22200	19.94600
O	-10.07400	-17.32800	19.80300
C	-7.05000	-16.53900	20.22700
C	-5.75700	-16.13100	20.91100
C	-4.54200	-16.67400	20.17400
C	-3.25500	-16.16600	20.82900
N	-2.82000	-17.03100	21.96000
H	-1.96200	-16.69300	22.39600
H	-2.72500	-18.00300	21.66600
H	-3.56500	-17.14200	22.64800
N	-9.96200	-15.15900	19.28200
H	-9.57500	-14.24500	19.51900
C	-10.96600	-15.23500	18.23400
C	-10.31400	-15.12400	16.86000
O	-9.14100	-14.82500	16.75300
C	-11.99100	-14.09700	18.37900
C	-12.94900	-14.39900	19.51600
C	-14.12800	-15.09000	19.28400
C	-12.63100	-13.98100	20.80600
C	-14.99500	-15.36100	20.34200
C	-13.49900	-14.25400	21.85300
C	-14.66800	-14.93900	21.60900
O	-15.53400	-15.21000	22.64300
H	-15.30800	-14.91800	23.51800
N	-11.06200	-15.34800	15.78400
H	-12.06700	-15.48300	15.89100
C	-10.46800	-15.40400	14.45400
C	-10.07100	-14.03000	13.94100
O	-9.23800	-13.87600	13.04000
C	-11.44800	-16.04600	13.46900
N	-10.70300	-13.00000	14.50500
H	-11.40000	-13.15900	15.23200
C	-10.38500	-11.64000	14.06900
C	-10.95700	-10.65000	15.07000

O	-11.78100	-11.06500	15.91200
C	-10.93700	-11.39000	12.66500
N	-10.54800	-9.40500	14.94200
H	-9.84300	-9.16800	14.24400
C	-11.11100	-8.35300	15.80900
C	-11.32400	-7.09700	14.98200
O	-10.43600	-6.67800	14.25500
C	-10.17300	-8.07800	16.98400
C	-10.69100	-7.12100	18.05400
C	-9.72400	-7.07700	19.24800
O	-9.14600	-8.13300	19.58600
O	-9.56800	-5.98800	19.82800
N	-12.50200	-6.51600	15.09300
H	-13.20300	-7.00300	15.65200
C	-12.90300	-5.25200	14.50000
C	-12.64700	-4.08900	15.47100
O	-13.06100	-4.20900	16.61700
C	-14.39600	-5.33400	14.18500
C	-15.11700	-4.06300	13.73800
C	-14.48000	-3.45400	12.48300
C	-16.59300	-4.37500	13.47700
N	-12.01900	-3.02500	14.97900
H	-11.69300	-3.06300	14.01300
C	-11.77000	-1.81100	15.73800
C	-12.48500	-0.64200	15.07300
O	-12.13300	-0.32200	13.93000
C	-10.25700	-1.53300	15.79700
C	-9.56000	-2.51900	16.69100
N	-8.20200	-2.70000	16.75100
C	-10.10200	-3.37300	17.59700
C	-7.93000	-3.63500	17.65200
N	-9.07100	-4.07000	18.18900
H	-9.16400	-4.78800	18.90700
N	-13.45800	-0.07800	15.77700
H	-13.73200	-0.49600	16.66600
C	-14.15100	1.12900	15.31400
C	-13.55400	2.30700	16.09700
O	-13.75000	2.39900	17.31100
C	-15.65200	1.08100	15.50400
C	-16.37000	0.00600	14.66900
C	-17.28400	-0.87800	15.49300
C	-17.16400	0.67500	13.55100
N	-12.83600	3.14100	15.37600
H	-12.83400	3.04700	14.36000
C	-12.03900	4.20200	15.99900
C	-12.76900	5.54100	16.02100
O	-13.18300	6.02900	14.96500
C	-10.71900	4.36500	15.22600
C	-9.81000	5.41500	15.86300
C	-10.00000	3.03300	15.10300
N	-12.90700	6.13800	17.20000
H	-12.51500	5.67400	18.02000

C	-13.58100	7.40900	17.39400
C	-12.68600	8.39700	18.15600
O	-11.87800	7.95800	18.98300
C	-14.85400	7.23400	18.20100
C	-15.73800	6.10400	17.81800
N	-15.43200	4.79100	18.02600
H	-14.56900	4.45400	18.45300
C	-16.97200	6.12500	17.23800
C	-16.41100	4.02000	17.59700
N	-17.36300	4.81100	17.10500
H	-18.24200	4.49400	16.69500
N	-12.84700	9.68500	17.88600
H	-13.53900	9.99000	17.20100
C	-12.01000	10.66500	18.59200
C	-12.87900	11.73000	19.24000
O	-13.95600	12.04400	18.72300
C	-10.99100	11.32100	17.66300
C	-11.56400	11.99600	16.45200
C	-11.85000	11.42800	15.24600
C	-11.91900	13.38700	16.33600
N	-12.36500	12.37400	14.36000
H	-12.65400	12.20500	13.39700
C	-12.41100	13.59000	15.03200
C	-11.86000	14.47400	17.21700
C	-12.84800	14.84100	14.58900
C	-12.29000	15.71700	16.77500
C	-12.77600	15.89300	15.47000
N	-12.37100	12.20600	20.36800
H	-11.43400	11.91300	20.64500
C	-13.09900	13.13300	21.23000
C	-13.18300	14.53300	20.63100
O	-12.17700	15.23800	20.40100
C	-12.35400	13.10300	22.57600
C	-13.09900	13.87800	23.64200
O	-13.89400	14.76500	23.33600
N	-12.81500	13.47800	24.87700
H	-12.15600	12.74200	25.13100
H	-13.31700	14.00000	25.59500
N	-14.42600	14.95300	20.33200
H	-15.24200	14.42500	20.64300
C	-14.58600	16.18600	19.54900
C	-14.09000	17.39700	20.33200
O	-13.85600	18.46200	19.76000
C	-16.06100	16.35700	19.15700
O	-16.87700	16.43500	20.32100
H	-16.60200	17.20900	20.79900
C	-16.50000	15.12000	18.39200
N	-13.74900	17.16500	21.45300
H	-13.70600	16.22900	21.85600
C	-13.40100	18.38300	22.17600
C	-12.03300	18.90500	21.75000
O	-11.69000	20.05800	22.01000

C	-13.42400	18.13600	23.68500
C	-12.05300	18.17400	24.34100
C	-12.16600	18.35100	25.84700
C	-12.42400	17.02400	26.54100
N	-11.34100	16.68000	27.50300
H	-11.51400	15.78900	27.96900
H	-11.19400	17.42900	28.17900
H	-10.42700	16.69000	27.05100
N	-11.25600	18.04800	21.09600
H	-11.62400	17.12700	20.85700
C	-9.89200	18.39000	20.71200
C	-9.81600	18.78200	19.24000
O	-8.73200	19.01100	18.70300
C	-8.94600	17.22100	20.99400
C	-8.86300	16.84000	22.45500
C	-8.40200	17.74200	23.40300
C	-9.24700	15.57600	22.88500
C	-8.32500	17.39800	24.74000
C	-9.17300	15.22300	24.21900
C	-8.71200	16.13700	25.14200
O	-8.63600	15.79100	26.47100
H	-8.31800	16.42100	27.10700
N	-10.97400	18.85700	18.59200
H	-11.80500	18.43900	19.01000
C	-11.08700	19.52000	17.30300
C	-10.69600	18.68500	16.10600
O	-11.29900	18.79100	15.02300
N	-9.65700	17.84400	16.22300
H	-9.09200	17.83800	17.07200
C	-9.34300	16.93700	15.12000
C	-8.60000	15.72500	15.69800
O	-8.14000	15.73400	16.83200
C	-8.53800	17.57200	13.99400
C	-7.16900	18.06700	14.40300
O	-6.34100	17.25600	14.86500
O	-6.86400	19.27200	14.28500
N	-8.51300	14.68800	14.88000
H	-8.88200	14.78500	13.93400
C	-7.92000	13.42300	15.26100
C	-6.46600	13.57800	15.71500
O	-6.07800	12.97800	16.72100
C	-8.01100	12.44700	14.07400
C	-7.40000	11.08700	14.40000
C	-8.17800	10.16200	15.07700
C	-6.09100	10.77700	14.02700
C	-7.62900	8.93400	15.37400
C	-5.54100	9.54800	14.33800
C	-6.33000	8.63700	15.01900
N	-5.70200	14.35400	14.93500
H	-6.12200	14.77800	14.10800
C	-4.30500	14.61800	15.21500
C	-4.06400	15.17000	16.61100

O	-3.10300	14.74200	17.25800
N	-4.88000	16.09700	17.10600
H	-5.61100	16.46300	16.49600
C	-4.79900	16.62400	18.46000
C	-5.28300	15.59500	19.47900
O	-4.70600	15.43900	20.54900
C	-5.68200	17.86200	18.64300
C	-5.22100	19.02600	17.76900
C	-3.76400	19.35200	18.08800
C	-3.42200	20.78800	17.70800
N	-2.93500	21.56300	18.89100
H	-2.70600	22.52400	18.63700
H	-2.14800	21.09800	19.34400
H	-3.60300	21.52900	19.66100
N	-6.36700	14.89300	19.12700
H	-6.80000	15.05300	18.21700
C	-6.93300	13.90400	20.03100
C	-5.93500	12.81300	20.40100
O	-5.93700	12.42300	21.57500
C	-8.22000	13.28100	19.45800
N	-5.10100	12.28500	19.50900
H	-5.08200	12.65600	18.55900
C	-4.20800	11.17700	19.86900
C	-3.10000	11.59400	20.83500
O	-2.36300	10.74400	21.35400
C	-3.52300	10.50400	18.65700
C	-4.53000	9.86500	17.72800
C	-2.65400	11.50000	17.89400
N	-2.95600	12.88500	21.10700
H	-3.54100	13.56700	20.62500
C	-1.98000	13.34200	22.07800
C	-2.63000	13.48300	23.44800
O	-2.04200	14.06900	24.35000
C	-1.38600	14.69500	21.66000
C	-0.56600	14.62200	20.37400
C	-0.36800	16.01200	19.78000
O	-0.22100	17.00300	20.50800
N	-0.36700	16.10900	18.45100
H	-0.48800	15.29300	17.85100
H	-0.23500	17.03900	18.05400
N	-3.84200	12.98700	23.65900
H	-4.30100	12.45400	22.92000
C	-4.53300	13.19000	24.93200
C	-4.93700	11.85600	25.53800
O	-5.23200	10.90300	24.80800
C	-5.75200	14.07200	24.72200
C	-5.47500	15.39700	24.03600
C	-4.59700	16.29500	24.90200
O	-4.65200	16.22000	26.12500
N	-3.78500	17.13100	24.26900
H	-3.19800	17.73100	24.84800
H	-3.73900	17.19300	23.25200

N	-4.91000	11.75000	26.86700
C	-5.16300	10.46500	27.50600
C	-6.60600	10.00900	27.31600
O	-6.87300	8.80800	27.41500
C	-4.89200	10.72300	28.99400
C	-4.98800	12.20000	29.15200
C	-4.59900	12.80800	27.82800
N	-7.49400	10.94700	27.01900
H	-7.19100	11.91900	26.96100
C	-8.90300	10.62000	26.77100
C	-9.27000	11.01300	25.33600
O	-10.40700	11.37000	25.02500
C	-9.82500	11.33900	27.75000
C	-9.65700	12.83900	27.66700
O	-8.66500	13.31000	27.06800
O	-10.51600	13.57100	28.20100
N	-8.28600	10.92400	24.43600
H	-7.37600	10.54300	24.69500
C	-8.53900	11.38000	23.08300
C	-9.29900	10.40800	22.19900
O	-10.07100	10.89600	21.36400
N	-9.10000	9.10200	22.33500
H	-8.48600	8.77000	23.07900
C	-9.73200	8.12800	21.45300
C	-10.62300	7.17900	22.24000
O	-10.35000	6.89100	23.40600
C	-8.71300	7.28300	20.70500
C	-7.82900	7.96500	19.64800
C	-7.18800	6.91600	18.73500
C	-8.59100	9.00500	18.85000
N	-11.66900	6.69600	21.57600
H	-11.90400	7.09800	20.66800
C	-12.49700	5.60600	22.10300
C	-12.60000	4.57700	20.97700
O	-12.93300	4.91500	19.84200
C	-13.84500	6.11400	22.57600
N	-12.24300	3.33900	21.26300
H	-12.01500	3.09200	22.22600
C	-12.17000	2.31600	20.22000
C	-13.10300	1.19900	20.69100
O	-12.93200	0.70700	21.80300
C	-10.77100	1.76200	19.94000
C	-10.86100	0.69100	18.84500
C	-9.82600	2.88800	19.53500
N	-14.06500	0.90800	19.83800
H	-14.16500	1.47300	18.99500
C	-14.98800	-0.19300	20.06100
C	-14.34000	-1.43300	19.44800
O	-14.06300	-1.39600	18.23900
C	-16.29400	0.09900	19.36400
C	-17.63700	-0.42400	19.80500
C	-17.88100	-0.13000	21.27700

C	-18.75300	0.18600	18.96000
N	-14.12300	-2.44200	20.27400
H	-14.37700	-2.35500	21.25800
C	-13.52200	-3.68100	19.78600
C	-14.57200	-4.77600	19.76000
O	-15.27200	-4.99100	20.73700
N	-14.70400	-5.47700	18.65200
H	-14.07700	-5.26800	17.87500
C	-15.68900	-6.53000	18.46900
C	-14.97800	-7.76700	17.94600
O	-14.21900	-7.71400	16.97100
C	-16.74300	-6.05600	17.45100
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C	-17.67400	-7.19300	17.07200
C	-18.57500	-4.27800	17.02900
N	-15.22400	-8.87200	18.63400
H	-15.81000	-8.82900	19.46800
C	-14.66400	-10.14800	18.20800
C	-15.44000	-10.79400	17.06300
O	-16.66900	-10.65700	16.98700
C	-14.68000	-11.13600	19.38900
C	-13.80400	-10.67500	20.55300
C	-12.44100	-10.47900	20.36300
C	-14.36800	-10.45000	21.78800
C	-11.61100	-10.08400	21.41100
C	-13.56500	-10.06000	22.84200
C	-12.21500	-9.87400	22.65000
N	-14.71200	-11.48600	16.20300
H	-13.69700	-11.46800	16.30300
C	-15.28400	-12.27100	15.12300
C	-14.99800	-13.75200	15.36700
O	-13.85400	-14.12500	15.57400
C	-14.71100	-11.92300	13.73600
C	-15.30300	-10.68500	13.05700
C	-15.03300	-9.42100	13.85500
C	-14.75400	-10.55400	11.63700
N	-16.05000	-14.57400	15.32800
H	-17.00300	-14.21100	15.29700
C	-15.78800	-16.00900	15.33200
C	-16.30700	-16.63300	14.03700
O	-17.16500	-16.09500	13.35000
C	-16.40400	-16.71300	16.53400
C	-17.88000	-17.00100	16.43300
C	-18.48300	-17.31200	17.80500
C	-19.98200	-17.53600	17.64100
N	-20.62100	-17.97200	18.91500
H	-21.62400	-18.12200	18.80500
H	-20.42400	-17.31700	19.67200
H	-20.16200	-18.79900	19.29600
N	-15.76700	-17.80100	13.71500
H	-15.08900	-18.26700	14.31800
C	-16.20500	-18.38700	12.43100

C	-17.43000	-19.25900	12.64200
O	-17.53900	-20.12000	13.51000
C	-15.01400	-19.12200	11.78900
C	-15.43800	-20.03000	10.64700
C	-14.00600	-18.07400	11.31400
N	-18.42500	-19.00400	11.81200
H	-18.29300	-18.29200	11.09400
C	-19.69700	-19.69500	11.88000
C	-20.52100	-19.28800	10.66100
O	-20.10600	-19.52300	9.52800
N	-21.66500	-18.67700	10.93200
H	-21.92900	-18.48200	11.89800
C	-22.54400	-18.28600	9.83400
C	-22.08200	-16.95000	9.28700
O	-21.40000	-16.23000	10.01600
C	-23.98900	-18.17900	10.31700
O	-24.00200	-17.42300	11.52200
H	-24.90100	-17.35600	11.82200
N	-22.45500	-16.68000	8.04800
H	-23.02500	-17.35900	7.54300
C	-22.07700	-15.44500	7.38400
C	-22.78900	-14.23600	7.98800
O	-23.90400	-14.35200	8.49800
C	-22.42000	-15.53100	5.90700
N	-22.11200	-13.10000	7.90000
H	-21.18200	-13.12800	7.48300
C	-22.61700	-11.81400	8.36300
C	-22.92500	-10.97700	7.13200
O	-22.03200	-10.51300	6.41900
C	-21.59500	-11.13900	9.28200
C	-22.11200	-9.85500	9.93500
C	-23.10800	-10.23100	11.02000
C	-23.08100	-9.26500	12.19200
N	-24.29100	-9.41200	13.05200
H	-24.27300	-8.76300	13.83900
H	-24.41100	-10.37500	13.36600
H	-25.14900	-9.31500	12.50800
N	-24.22200	-10.81600	6.88400
C	-24.67800	-10.10200	5.68800
C	-24.08500	-8.70500	5.64800
O	-23.62000	-8.23800	4.59800
C	-26.19600	-10.01400	5.87100
C	-26.55100	-11.03200	6.89100
C	-25.32900	-11.27800	7.73700
N	-24.06500	-8.00700	6.78700
H	-24.39100	-8.41200	7.66400
C	-23.56000	-6.64900	6.72300
C	-22.08000	-6.53500	6.43500
O	-21.52100	-5.45400	6.22500
N	-21.36000	-7.65800	6.42300
H	-21.81300	-8.55500	6.59900
C	-19.93300	-7.60800	6.16000

C	-19.58400	-7.82000	4.69900
O	-18.47500	-7.50800	4.27500
C	-19.26900	-8.71100	6.99600
C	-17.74500	-8.84800	6.83200
C	-17.03300	-7.55300	7.18700
C	-17.23100	-10.00900	7.67400
N	-20.51600	-8.35900	3.91000
H	-21.47200	-8.44500	4.25500
C	-20.19700	-8.83000	2.56000
C	-19.82400	-7.71300	1.60700
O	-18.99900	-7.90800	0.70800
C	-21.40200	-9.61900	2.00100
C	-21.11300	-10.41400	0.73700
C	-20.05300	-11.48100	0.89600
O	-19.90100	-12.14600	1.92900
N	-19.27000	-11.65800	-0.16000
H	-19.39500	-11.11000	-1.01100
H	-18.55500	-12.37800	-0.05300
N	-20.39400	-6.51900	1.78300
H	-21.07900	-6.37600	2.52500
C	-20.02000	-5.41800	0.89200
C	-18.54300	-5.10200	1.05800
O	-17.86400	-4.76600	0.10000
C	-20.82700	-4.15300	1.16200
C	-22.33600	-4.27800	0.99600
C	-22.85300	-3.01000	0.32800
C	-24.36900	-2.92200	0.31500
N	-24.80600	-1.49100	0.33400
H	-25.82400	-1.43200	0.32500
H	-24.38700	-0.95500	-0.42600
H	-24.40200	-0.98000	1.11900
N	-18.03700	-5.20600	2.29700
H	-18.64900	-5.41400	3.08600
C	-16.61100	-5.02000	2.50500
C	-15.82600	-6.11500	1.81200
O	-14.85400	-5.91500	1.08300
C	-16.27900	-5.01900	4.01400
C	-14.77500	-4.88900	4.20400
C	-17.01600	-3.90800	4.75200
N	-16.21200	-7.38100	2.03800
H	-17.05100	-7.59200	2.57800
C	-15.38500	-8.44000	1.48100
C	-15.42100	-8.40000	-0.05900
O	-14.41900	-8.70500	-0.70500
C	-15.73800	-9.86200	1.96800
C	-15.95400	-9.93400	3.47600
C	-16.96300	-10.40700	1.28600
N	-16.54300	-8.00800	-0.65700
H	-17.35900	-7.73400	-0.11000
C	-16.57600	-7.98000	-2.11500
C	-15.58900	-6.98100	-2.69400
O	-15.15000	-7.23200	-3.81900

C	-18.00600	-7.68600	-2.58200
C	-18.80800	-8.98400	-2.55300
O	-18.19700	-10.07200	-2.47400
O	-20.04200	-8.90400	-2.59900
N	-15.23400	-5.89400	-2.00200
H	-15.56900	-5.74800	-1.05000
C	-14.34700	-4.91200	-2.64800
C	-12.87300	-5.18000	-2.40600
O	-12.01200	-4.45800	-2.91700
C	-14.73800	-3.49400	-2.18200
C	-16.23500	-3.26800	-2.37300
C	-14.36200	-3.27000	-0.73000
N	-12.49800	-6.20200	-1.62500
H	-13.19300	-6.87100	-1.29400
C	-11.09600	-6.35900	-1.24700
C	-10.20600	-6.62400	-2.46200
O	-9.03900	-6.26200	-2.45700
C	-10.94500	-7.47500	-0.21300
C	-11.61800	-7.15000	1.13700
C	-11.36200	-8.26800	2.12700
C	-11.15700	-5.81400	1.68800
N	-10.79000	-7.25400	-3.47200
H	-11.75500	-7.56300	-3.35500
C	-10.13100	-7.52600	-4.73200
C	-9.48000	-6.29200	-5.31200
O	-8.44500	-6.35300	-5.97200
C	-11.17400	-8.00500	-5.76500
C	-10.95200	-9.46300	-6.10300
O	-9.76900	-9.83100	-6.24400
O	-11.96100	-10.18900	-6.21200
N	-10.14100	-5.15800	-5.07600
H	-10.94200	-5.14100	-4.44500
C	-9.68900	-3.94200	-5.74400
C	-8.63400	-3.18800	-4.94900
O	-8.07100	-2.20700	-5.42600
C	-10.91000	-3.05900	-6.03600
O	-11.26700	-2.35100	-4.87000
H	-12.02300	-1.80400	-5.05100
N	-8.33500	-3.62200	-3.72500
H	-8.83800	-4.41600	-3.32900
C	-7.28700	-2.96100	-2.94800
C	-6.31900	-3.98000	-2.38500
O	-5.92500	-3.99600	-1.22300
C	-7.91500	-2.16300	-1.78700
C	-8.68300	-3.06800	-0.82200
C	-8.76600	-1.03500	-2.34800
C	-8.80100	-2.53200	0.59200
N	-5.89900	-4.90200	-3.25100
H	-6.10700	-4.80700	-4.24500
C	-5.14400	-6.04100	-2.76900
C	-3.77500	-5.67400	-2.22600
O	-3.32700	-6.35500	-1.30800

C	-4.99700	-7.04200	-3.93700
C	-4.24700	-8.30100	-3.51200
C	-3.74600	-9.07000	-4.72700
C	-3.84100	-10.57300	-4.49700
N	-2.48600	-11.19500	-4.51400
H	-2.55000	-12.20100	-4.36000
H	-1.85700	-10.74900	-3.84600
H	-1.98000	-10.97500	-5.37200
N	-3.13000	-4.65900	-2.80000
H	-3.61000	-4.11200	-3.51400
C	-1.77200	-4.30600	-2.44600
C	-1.72600	-2.92400	-1.79400
O	-2.63700	-2.11400	-1.91000
C	-0.76700	-4.30900	-3.63200
O	-1.25500	-3.47600	-4.67600
H	-0.64100	-3.47800	-5.40100
C	-0.59900	-5.69000	-4.25000
N	-0.62400	-2.70300	-1.10400
H	0.10100	-3.41900	-1.14300
C	-0.35500	-1.53300	-0.29700
C	-0.47800	-0.25000	-1.09800
O	0.07600	-0.14500	-2.18300
C	1.06900	-1.64300	0.30000
C	1.50200	-0.38300	1.04300
C	2.85100	-0.62100	1.70300
C	3.34700	0.64400	2.39400
N	3.37600	1.81900	1.47700
H	3.70800	2.66500	1.93900
H	2.46500	1.97000	1.04400
H	3.92400	1.61900	0.64000
N	-1.19300	0.72800	-0.54900
H	-1.62600	0.57100	0.36100
C	-1.37800	2.01000	-1.20000
C	-2.59600	2.05800	-2.10800
O	-3.00000	3.13100	-2.58700
N	-3.23100	0.93600	-2.41600
H	-2.87600	0.03900	-2.08400
C	-4.44600	0.98900	-3.23700
C	-5.64600	1.45700	-2.42300
O	-5.84600	1.04600	-1.27500
C	-4.77800	-0.37600	-3.83400
C	-3.77000	-0.75900	-4.91700
C	-3.94700	0.19000	-6.09600
C	-2.79700	0.12600	-7.09100
N	-2.29000	1.49200	-7.43400
H	-1.51900	1.44900	-8.10100
H	-2.03000	2.01400	-6.59700
H	-3.04100	2.09500	-7.77000
N	-6.47700	2.29300	-3.03900
H	-6.22300	2.66300	-3.95500
C	-7.75100	2.69600	-2.43200
C	-8.89800	2.56400	-3.42200

O	-8.75300	2.45700	-4.63700
C	-7.64400	4.11800	-1.89600
O	-7.57300	5.11000	-2.90000
H	-7.50600	5.99700	-2.56600
N	-10.11100	2.56600	-2.90200
H	-10.21700	2.58200	-1.88800
C	-11.30100	2.54600	-3.73900
C	-12.39600	3.36600	-3.05600
O	-12.43600	3.43000	-1.82300
C	-11.75100	1.11400	-3.97300
N	-13.26000	3.96000	-3.86200
H	-13.08100	3.94900	-4.86600
C	-14.46000	4.63100	-3.37100
C	-15.26800	3.61800	-2.58700
O	-15.41300	2.47400	-3.02400
C	-15.25700	5.18700	-4.56400
C	-14.30900	5.86800	-5.54600
O	-14.21800	5.42800	-6.71500
O	-13.62200	6.85000	-5.17500
N	-15.79300	4.01700	-1.43100
H	-15.63900	4.97100	-1.10500
C	-16.59100	3.09100	-0.62700
C	-17.71500	3.84300	0.07800
O	-17.74000	3.94000	1.30400
C	-15.68500	2.37200	0.37600
C	-16.29700	1.10500	0.94600
C	-16.60600	0.04300	0.10800
C	-16.56900	1.00400	2.29000
C	-17.18100	-1.11500	0.61300
C	-17.13600	-0.14800	2.82000
C	-17.44600	-1.20100	1.96900
N	-18.64800	4.39000	-0.69400
H	-18.58700	4.25300	-1.70300
C	-19.75400	5.17600	-0.16600
C	-20.94000	4.30500	0.24100
O	-21.08400	3.15500	-0.18000
C	-20.25000	6.18800	-1.22200
O	-20.58500	5.44800	-2.41000
H	-20.89000	6.07000	-3.06000
C	-19.17900	7.19100	-1.60600
N	-21.82200	4.87600	1.05600
H	-21.56600	5.79600	1.41500
C	-23.09500	4.36100	1.49700
C	-22.96100	3.02400	2.21900
O	-23.85000	2.17800	2.17500
C	-24.05000	4.25100	0.27800
C	-24.18800	5.64300	-0.32300
O	-23.69600	5.94300	-1.40800
N	-24.81000	6.56400	0.39600
H	-24.90200	7.49700	-0.00700
H	-25.21800	6.31500	1.29700
N	-21.84500	2.80400	2.90600

H	-21.06700	3.45900	2.83500
C	-21.72900	1.62500	3.76400
C	-22.26700	1.94000	5.17000
O	-21.89800	2.96600	5.75200
C	-20.27500	1.15800	3.90200
C	-20.19100	-0.06600	4.81100
C	-20.58600	-1.29500	4.33400
C	-19.73800	0.05000	6.11400
C	-20.55100	-2.44000	5.11600
C	-19.67800	-1.09600	6.89900
C	-20.07100	-2.33200	6.40800
N	-23.11100	1.07800	5.72300
H	-23.32800	0.21600	5.22200
C	-23.74800	1.31500	7.03200
C	-23.07200	0.45700	8.07700
O	-23.19300	-0.77000	8.09700
C	-25.23200	1.00500	6.93600
C	-26.02500	1.22600	8.20900
O	-25.43300	1.53500	9.25100
O	-27.26800	1.10400	8.16100
N	-22.31100	1.06400	8.97000
C	-21.58000	0.20700	9.92300
C	-22.50400	-0.45900	10.94100
O	-22.03900	-1.30800	11.72200
C	-20.60600	1.19100	10.56800
C	-21.23100	2.52600	10.39700
C	-22.06800	2.48700	9.14700
N	-23.79300	-0.13800	10.95600
H	-24.15900	0.53300	10.28000
C	-24.68700	-0.74600	11.94100
C	-24.80600	-2.24700	11.71000
O	-25.10800	-3.00700	12.64000
C	-26.08600	-0.10500	11.91900
C	-26.06300	1.26500	12.59800
C	-27.39200	1.97500	12.44300
N	-27.72800	2.17500	11.02700
H	-27.06300	1.89800	10.30500
C	-28.89500	2.71600	10.68000
N	-29.75400	3.06500	11.63500
H	-29.53200	2.92600	12.62100
H	-30.64700	3.47900	11.36900
N	-29.18200	2.89600	9.40300
H	-28.52400	2.62900	8.67100
H	-30.07500	3.31000	9.13700
N	-24.53400	-2.66100	10.47000
H	-24.27600	-1.98800	9.74800
C	-24.60900	-4.08900	10.15600
C	-23.42700	-4.85700	10.70400
O	-23.38900	-6.06800	10.48500
N	-22.49000	-4.23400	11.42500
H	-22.55700	-3.22600	11.56900
C	-21.37300	-4.96700	12.01000

C	-21.52000	-5.14600	13.51800
O	-20.61200	-5.72600	14.13000
C	-20.03100	-4.24800	11.77700
C	-19.72600	-3.88900	10.31900
C	-18.53200	-2.95500	10.23400
C	-19.51300	-5.16000	9.51900
N	-22.58800	-4.64200	14.11600
H	-23.30200	-4.18100	13.55200
C	-22.77200	-4.72900	15.57000
C	-23.46600	-6.00800	16.01900
O	-24.33200	-6.53500	15.30500
C	-23.57400	-3.52100	16.09700
C	-22.94100	-2.17000	15.72400
C	-23.69100	-0.97600	16.29500
C	-21.47200	-2.13200	16.16000
N	-23.10900	-6.50600	17.20900
C	-23.79100	-7.69500	17.73800
C	-25.13700	-7.22800	18.30500
O	-25.41800	-6.02600	18.30300
C	-22.83000	-8.20300	18.80400
C	-22.13300	-6.98500	19.28000
C	-22.08700	-6.00600	18.12700
N	-26.00200	-8.11700	18.77500
H	-25.77200	-9.11000	18.74400
C	-27.27800	-7.69000	19.33500
C	-27.13200	-6.96200	20.66600
O	-27.81900	-5.98300	20.96900
C	-28.16500	-8.92700	19.55700
C	-28.17700	-9.87600	18.37200
C	-29.22800	-10.97200	18.48900
O	-29.62600	-11.32100	19.63300
O	-29.67500	-11.47200	17.43100
N	-26.22500	-7.45500	21.51000
H	-25.64800	-8.25000	21.23600
C	-26.06300	-6.84900	22.82800
C	-24.88800	-5.88700	22.86000
O	-23.88300	-6.19700	22.19700
C	-25.82900	-7.94400	23.87000
O	-25.10400	-7.46700	24.99400
H	-24.95900	-8.14700	25.64100
N	-25.00500	-4.80400	23.61500
H	-25.88400	-4.62200	24.09900
C	-23.89500	-3.86800	23.76400
C	-23.23200	-3.97700	25.13700
O	-22.58300	-3.00600	25.54500
C	-24.36700	-2.42200	23.53400
C	-24.90100	-2.10500	22.12500
C	-25.36800	-0.65900	22.01100
C	-23.86700	-2.39600	21.05300
N	-23.33500	-5.09200	25.86000
H	-23.94000	-5.84700	25.53700
C	-22.59500	-5.24500	27.10500

C	-21.08900	-5.20200	26.80000
O	-20.67400	-5.69400	25.74600
C	-22.89300	-6.57700	27.79500
C	-24.31900	-6.67200	28.32700
O	-24.96800	-5.62000	28.44100
O	-24.74400	-7.81500	28.59900
N	-20.28200	-4.64300	27.71200
H	-20.64500	-4.35900	28.62200
C	-18.88100	-4.44800	27.38200
C	-17.95300	-4.52700	28.59100
O	-18.38200	-4.42500	29.73100
C	-18.70600	-3.07300	26.69700
C	-19.12700	-1.90100	27.55000
C	-18.22700	-1.25400	28.39900
C	-20.44800	-1.45500	27.50600
C	-18.60400	-0.18100	29.19300
C	-20.82700	-0.37200	28.29600
C	-19.91600	0.24400	29.12100
O	-20.30800	1.31300	29.90000
H	-19.67800	1.73900	30.47000
N	-16.67400	-4.68400	28.29200
H	-16.42800	-4.98600	27.34900
C	-15.59500	-4.44400	29.25500
C	-14.89400	-3.14500	28.87500
O	-14.87500	-2.77400	27.70100
C	-14.55900	-5.54400	29.25800
C	-15.03200	-6.89100	29.68400
C	-15.27900	-7.32500	30.96000
C	-15.31600	-7.99400	28.81200
N	-15.70000	-8.63600	30.92400
H	-15.95100	-9.19700	31.73800
C	-15.72900	-9.07200	29.61300
C	-15.24700	-8.16000	27.42000
C	-16.08000	-10.30700	29.07400
C	-15.60100	-9.39500	26.90600
C	-16.01500	-10.46600	27.71300
N	-14.28900	-2.44700	29.84300
H	-14.30800	-2.76100	30.81300
C	-13.59400	-1.20600	29.45300
C	-12.33900	-1.03600	30.30900
O	-12.35100	-1.36100	31.49600
C	-14.52300	0.01500	29.54200
O	-13.82800	1.17900	29.07800
H	-13.56600	1.01200	28.18000
C	-14.94400	0.28400	30.98500
N	-11.26100	-0.54300	29.72200
H	-11.30700	-0.32800	28.72600
C	-10.01500	-0.29200	30.42600
C	-9.25700	0.79900	29.65500
O	-9.53000	0.98800	28.45900
C	-9.20000	-1.57900	30.57400
C	-8.48700	-1.97500	29.28000

C	-9.17800	-2.68300	28.30200
C	-7.16500	-1.66000	29.04000
C	-8.52700	-3.04700	27.12900
C	-6.47900	-1.99900	27.87100
C	-7.19900	-2.70500	26.92400
O	-6.57100	-3.05100	25.76100
H	-7.06500	-3.53600	25.11100
N	-8.34800	1.52200	30.28000
C	-7.55500	2.52700	29.56200
C	-6.33900	1.89200	28.89500
O	-5.60700	1.12200	29.53700
C	-7.08800	3.49900	30.65900
C	-6.98600	2.60400	31.86200
C	-8.04800	1.52900	31.72200
N	-6.11400	2.23200	27.62100
H	-6.66400	2.94600	27.14300
C	-5.01800	1.50600	26.95500
C	-4.45300	2.30400	25.80800
O	-4.37400	3.53800	25.91300
N	-4.04500	1.60300	24.74300
H	-4.26000	0.61000	24.64900
C	-3.27000	2.32200	23.70700
C	-3.61600	1.89900	22.29000
O	-4.38200	0.94400	22.14200
C	-1.78000	2.00900	23.92600
O	-1.53900	0.66200	23.50400
H	-0.61900	0.46900	23.63900
N	-3.06900	2.55000	21.26400
H	-2.59700	3.44200	21.41000
C	-3.15500	1.96600	19.92200
C	-2.41000	0.62800	19.96800
O	-1.44400	0.49700	20.73300
C	-2.50900	2.83300	18.84600
C	-3.00000	4.26800	18.64400
C	-2.39600	4.85300	17.35900
C	-4.50000	4.36600	18.55700
N	-2.82400	-0.35200	19.16900
H	-3.64000	-0.22400	18.57100
C	-2.09000	-1.61300	19.16300
C	-1.10500	-1.68600	17.99600
O	-0.53600	-2.75500	17.78600
C	-3.03300	-2.81700	19.10300
O	-3.75100	-2.80900	17.86200
H	-3.13100	-2.87300	17.14500
C	-4.03900	-2.71300	20.26600
N	-0.94700	-0.59800	17.25100
H	-1.57100	0.19200	17.41500
C	0.06600	-0.46800	16.21300
C	0.90500	0.78200	16.46200
O	0.38500	1.70600	17.10200
C	-0.56200	-0.30300	14.80800
O	-1.38500	0.87600	14.85100

H	-0.83500	1.62300	15.05700
C	-1.44200	-1.49900	14.47900
N	2.15000	0.83400	15.99000
C	2.90300	2.07800	16.13800
C	2.10300	3.24100	15.59800
O	1.38100	3.07000	14.59900
C	4.12900	1.81800	15.24200
C	4.34800	0.34700	15.44100
C	2.94100	-0.22200	15.32700
N	2.12200	4.41100	16.18800
C	3.00700	4.78100	17.27500
C	2.58100	4.40100	18.69300
O	3.21100	4.89300	19.62900
C	3.01900	6.31400	17.12900
C	1.72400	6.68400	16.52200
C	1.26700	5.52100	15.70200
N	1.58100	3.54700	18.88800
H	0.97800	3.31100	18.10000
C	1.31100	2.93100	20.19000
C	0.96700	3.94300	21.27300
O	1.21300	3.68500	22.46100
C	2.53900	2.09700	20.59100
C	2.84200	0.90300	19.68100
C	4.21800	0.33000	20.00200
C	1.79900	-0.21000	19.79200
N	0.40900	5.07600	20.87100
H	0.17500	5.19500	19.88500
C	0.12200	6.15600	21.80800
C	-0.89400	5.70500	22.84400
O	-1.85100	4.99200	22.51100
C	-0.41000	7.39300	21.05100
C	0.62500	7.92600	20.03500
C	0.00100	8.90000	19.05300
C	1.77900	8.57200	20.78100
N	-0.70500	6.13300	24.08200
H	0.09200	6.74200	24.26600
C	-1.57700	5.78000	25.20000
C	-2.71200	6.76700	25.38100
O	-2.80300	7.51800	26.36000
C	-0.70200	5.66600	26.47100
C	0.26800	4.50400	26.30700
C	1.20500	4.23200	27.48100
O	1.51900	5.14400	28.26700
O	1.62900	3.06800	27.62000
N	-3.63100	6.75300	24.40800
H	-3.59200	6.00200	23.71900
C	-4.68300	7.75000	24.28000
C	-6.05800	7.11500	24.12900
O	-6.97600	7.82800	23.75300
C	-4.37500	8.61900	23.04600
S	-4.31100	7.67400	21.48800
N	-6.17900	5.81000	24.40100

H	-5.41400	5.31100	24.85500
C	-7.41300	5.09400	24.04600
C	-8.20500	4.62000	25.24800
O	-7.65100	4.00800	26.15500
C	-7.09100	3.84800	23.19300
C	-8.36900	3.06400	22.88800
C	-6.39200	4.24300	21.89700
N	-9.49800	4.89600	25.26400
H	-9.85700	5.60500	24.62400
C	-10.43200	4.22300	26.16500
C	-10.95500	3.01600	25.39100
O	-11.67600	3.19800	24.40400
C	-11.57500	5.12500	26.62200
O	-11.00800	6.21300	27.38100
H	-11.72000	6.77500	27.66500
C	-12.55100	4.37900	27.51800
N	-10.56700	1.81600	25.81800
H	-9.92300	1.72200	26.60300
C	-11.09100	0.63600	25.12800
C	-12.46800	0.22400	25.60200
O	-12.72000	0.17900	26.82300
C	-10.10200	-0.54200	25.31500
C	-8.92500	-0.40100	24.37800
C	-7.68300	0.10800	24.62300
C	-8.94400	-0.81300	22.99400
N	-6.91600	0.04100	23.46600
H	-5.95100	0.35600	23.37300
C	-7.67400	-0.52000	22.47100
C	-9.94900	-1.40200	22.20400
C	-7.34500	-0.79200	21.14300
C	-9.61800	-1.67300	20.88000
C	-8.34300	-1.36600	20.39300
N	-13.32600	-0.08000	24.62000
H	-13.05700	0.07100	23.64800
C	-14.65300	-0.63000	24.93200
C	-14.76500	-1.93300	24.15700
O	-14.88700	-1.85100	22.92700
C	-15.74400	0.38000	24.59800
C	-15.55200	1.67400	25.40700
C	-17.12800	-0.18500	24.83200
C	-16.19400	2.88000	24.76100
N	-14.65800	-3.05900	24.86100
H	-14.60200	-3.02700	25.87900
C	-14.62100	-4.34700	24.15600
C	-15.93800	-5.05200	24.41600
O	-16.31600	-5.24100	25.58200
C	-13.43800	-5.22500	24.60400
C	-13.44300	-6.56300	23.88000
C	-12.12600	-4.48400	24.36200
N	-16.64900	-5.38800	23.32900
H	-16.25000	-5.25100	22.40000
C	-17.99300	-5.94900	23.46600

C	-17.90700	-7.42500	23.83600
O	-17.04600	-8.13600	23.31100
C	-18.85000	-5.80500	22.19400
C	-19.14400	-4.36500	21.76500
C	-20.16100	-4.29100	20.63200
C	-19.65900	-3.52500	22.93700
N	-18.81800	-7.81600	24.72100
H	-19.51000	-7.14900	25.06300
C	-18.83700	-9.18700	25.20700
C	-19.21700	-10.18900	24.13100
O	-18.66200	-11.27900	24.02100
C	-19.85000	-9.29400	26.36700
C	-20.06500	-10.72900	26.82900
C	-20.80600	-10.84400	28.15000
C	-22.14100	-10.12800	28.14400
N	-23.19500	-10.78100	28.96700
H	-24.09400	-10.29900	28.96300
H	-22.86700	-10.91300	29.92400
H	-23.31300	-11.75400	28.68600
N	-20.21000	-9.80800	23.33900
H	-20.58600	-8.86400	23.43100
C	-20.77800	-10.71000	22.33700
C	-20.04900	-10.65500	20.99900
O	-20.04000	-9.57900	20.39100
C	-22.23700	-10.30700	22.05400
C	-22.94900	-11.24900	21.08400
C	-24.36700	-10.80900	20.77700
O	-25.05400	-10.27300	21.66800
O	-24.81500	-10.97900	19.62100
N	-19.50700	-11.74400	20.49300
C	-18.87200	-11.68900	19.17600
C	-19.91800	-11.66000	18.06200
O	-21.10200	-11.95900	18.22500
C	-18.07800	-12.99100	19.07900
C	-18.32300	-13.73700	20.34300
C	-19.46300	-13.08600	21.07600
N	-19.45300	-11.31100	16.86300
H	-18.51500	-10.92400	16.76100
C	-20.31600	-11.49500	15.69700
C	-19.80800	-12.72900	14.97200
O	-18.61500	-13.03300	15.11700
C	-20.29700	-10.27000	14.78600
C	-18.91400	-9.84700	14.29500
C	-20.94200	-9.09200	15.51500
C	-18.96500	-8.93800	13.07600
N	-20.67000	-13.43200	14.23600
H	-21.65800	-13.18200	14.18900
C	-20.13600	-14.57700	13.50000
C	-19.93400	-14.18500	12.03500
O	-20.78300	-13.42200	11.56400
C	-21.06400	-15.79100	13.53900
O	-22.39200	-15.32200	13.71300

H	-22.96900	-16.07700	13.73700
N	-18.87100	-14.69000	11.43100
H	-18.20000	-15.22500	11.98100
C	-18.62600	-14.50700	10.00300
C	-18.37000	-15.87600	9.39500
O	-18.02700	-16.84800	10.08200
C	-17.45100	-13.55400	9.71100
C	-17.81700	-12.16100	10.20800
C	-16.19400	-14.09900	10.36700
N	-18.54400	-15.99700	8.07400
H	-18.81600	-15.22400	7.46700
C	-18.30000	-17.37200	7.58800
C	-16.83800	-17.58300	7.28600
O	-16.04100	-16.65200	7.16000
C	-19.17800	-17.56500	6.35100
O	-18.73800	-16.61700	5.38400
H	-19.28300	-16.73700	4.61600
N	-16.41300	-18.83800	7.15500
H	-17.05600	-19.61000	7.32900
C	-15.04400	-19.11700	6.76700
C	-14.66300	-18.44900	5.44600
O	-13.53100	-17.95400	5.30400
C	-14.85300	-20.63600	6.65800
O	-13.51300	-20.89500	6.23900
H	-13.39500	-21.83500	6.17200
N	-15.60400	-18.45900	4.48100
H	-16.51500	-18.88200	4.65600
C	-15.30800	-17.86000	3.18700
C	-15.11800	-16.35200	3.32000
O	-14.34700	-15.75800	2.57800
C	-16.39400	-18.08200	2.13500
C	-16.64600	-19.56300	1.83200
C	-17.78400	-20.04500	2.72900
O	-17.62000	-20.01800	3.96300
O	-18.85300	-20.42200	2.20000
N	-15.84500	-15.72900	4.25700
H	-16.50900	-16.24000	4.83900
C	-15.65000	-14.28800	4.41300
C	-14.24200	-14.02400	4.93800
O	-13.46500	-13.24600	4.39100
C	-16.74100	-13.71300	5.31200
C	-18.09700	-13.59700	4.63000
C	-19.17700	-12.99000	5.51400
O	-19.37500	-13.36600	6.67300
N	-19.90200	-12.03000	4.95300
H	-20.62600	-11.62300	5.54500
H	-19.73800	-11.71900	3.99500
N	-13.83500	-14.67600	6.02600
H	-14.42200	-15.36200	6.50000
C	-12.46800	-14.33700	6.50300
C	-11.38800	-14.85700	5.57500
O	-10.25700	-14.36500	5.53500

C	-12.30100	-14.85900	7.93900
C	-12.52200	-16.36100	7.93700
C	-10.92600	-14.50800	8.48600
N	-11.67600	-15.86400	4.74500
H	-12.58900	-16.31700	4.79300
C	-10.69400	-16.31600	3.77400
C	-10.31200	-15.19100	2.82800
O	-9.15100	-15.03400	2.46400
C	-11.22100	-17.50800	2.96400
C	-11.10400	-18.86200	3.68300
C	-11.82300	-19.96200	2.92000
C	-9.63300	-19.20700	3.89000
N	-11.28500	-14.37600	2.43300
H	-12.24200	-14.52400	2.75200
C	-10.96900	-13.26500	1.53600
C	-10.07600	-12.22900	2.17800
O	-9.27800	-11.55200	1.51800
C	-12.30000	-12.64600	1.08300
C	-12.72200	-13.13300	-0.29900
C	-13.88800	-14.09600	-0.25200
C	-14.32400	-14.49500	-1.65400
N	-15.70400	-15.02900	-1.71000
H	-15.99600	-15.29600	-2.65000
H	-16.36400	-14.36900	-1.30000
H	-15.81800	-15.80700	-1.06000
N	-10.16200	-12.08300	3.50900
H	-10.86900	-12.59300	4.03800
C	-9.23400	-11.18700	4.19300
C	-7.77600	-11.59800	4.00400
O	-6.86000	-10.79000	3.87800
C	-9.42500	-11.16900	5.71500
C	-10.61500	-10.43600	6.28600
C	-11.69100	-10.04600	5.50300
C	-10.62500	-10.14500	7.64200
C	-12.77000	-9.36800	6.03600
C	-11.70200	-9.47000	8.17900
C	-12.75700	-9.06700	7.38800
N	-7.58500	-12.91500	4.06000
H	-8.39200	-13.53400	4.13200
C	-6.24600	-13.49000	4.02000
C	-5.64400	-13.45100	2.62000
O	-4.48800	-13.87100	2.51800
C	-6.26700	-14.94100	4.52400
C	-6.89000	-15.07200	5.91400
C	-6.84500	-16.51700	6.40500
N	-7.35100	-16.63500	7.77800
H	-6.96200	-16.01000	8.48400
C	-8.28100	-17.50000	8.16300
N	-8.80700	-18.33600	7.26600
H	-9.52200	-19.00100	7.56200
H	-8.49000	-18.29800	6.29700
N	-8.69300	-17.55000	9.42200

H	-9.40800	-18.21500	9.71800
H	-8.29100	-16.91100	10.10800
N	-6.38000	-12.96900	1.61900
H	-7.33800	-12.66700	1.79600
C	-5.82500	-12.87000	0.26800
C	-5.17500	-11.51900	0.02900
O	-4.49700	-11.28100	-0.98100
C	-6.91400	-13.12700	-0.78900
C	-7.24600	-14.61000	-0.89800
C	-8.38000	-14.89400	-1.86800
C	-8.32000	-14.04800	-3.13000
N	-9.13600	-14.62700	-4.23900
H	-9.09600	-14.05900	-5.08600
H	-10.10000	-14.78200	-3.94500
H	-8.86700	-15.59200	-4.42900
N	-5.34700	-10.58200	0.96100
H	-5.90600	-10.78100	1.79100
C	-4.73100	-9.26800	0.78900
C	-3.22000	-9.37300	0.94000
O	-2.70100	-10.40300	1.36900
C	-5.29700	-8.25400	1.76800
C	-6.77400	-7.85900	1.59900
C	-7.29200	-7.17900	2.86400
C	-6.97200	-6.94400	0.40500
N	-2.51700	-8.31100	0.55700
H	-3.00700	-7.46600	0.26400
C	-1.06600	-8.33300	0.54900
C	-0.49900	-7.20700	1.40700
O	-1.04900	-6.10300	1.42100
C	-0.56000	-8.14500	-0.87800
C	-0.60500	-9.30500	-1.84000
O	-0.14200	-9.15900	-2.99300
N	-1.12800	-10.46100	-1.43900
H	-1.50500	-10.58000	-0.49900
H	-1.15800	-11.24600	-2.09000
N	0.61300	-7.46300	2.08300
H	0.99600	-8.40800	2.06500
C	1.30200	-6.43900	2.84700
C	2.12000	-5.54500	1.90400
O	2.28600	-4.34900	2.15200
C	2.27700	-7.02500	3.86000
C	1.75800	-7.60700	5.16500
C	0.93000	-6.88000	6.01000
C	2.12000	-8.90100	5.53700
C	0.49600	-7.44600	7.20100
C	1.71700	-9.45900	6.74200
C	0.91800	-8.70700	7.58700
N	2.61700	-6.18100	0.84200
H	2.38100	-7.16300	0.70000
C	3.48100	-5.52300	-0.11500
C	2.74500	-4.60200	-1.08000
O	1.53900	-4.72200	-1.27300

C	4.17500	-6.63300	-0.93600
C	3.17400	-7.60500	-1.54500
O	2.65000	-8.50600	-0.89200
N	2.86800	-7.43300	-2.84400
H	3.30300	-6.68600	-3.38600
H	2.19700	-8.08400	-3.25200
N	3.48400	-3.70000	-1.72400
H	4.44600	-3.54500	-1.42300
C	2.96400	-2.93000	-2.84100
C	2.98300	-3.71300	-4.14000
O	3.70100	-4.70200	-4.30200
N	2.18500	-3.28800	-5.11400
H	1.55300	-2.50800	-4.93300
C	2.18900	-3.90700	-6.43400
C	3.59600	-3.97800	-7.00400
O	4.40100	-3.06700	-6.78200
C	1.32000	-3.08700	-7.39100
C	0.91300	-3.90100	-8.60900
C	0.16300	-3.05100	-9.61700
O	-0.12700	-1.87700	-9.30700
O	-0.11300	-3.59300	-10.70600
N	3.94300	-5.03800	-7.73400
H	3.27900	-5.79100	-7.91300
C	5.30000	-5.09100	-8.27000
C	6.36100	-5.42700	-7.24100
O	7.56500	-5.26100	-7.50100
N	5.94400	-5.90700	-6.06700
H	4.94700	-5.91800	-5.85000
C	6.90000	-6.41500	-5.09300
C	6.63200	-7.90000	-4.86300
O	5.55800	-8.37500	-5.24600
C	6.83200	-5.65800	-3.76900
C	6.42600	-4.19500	-3.89800
C	6.96800	-3.39100	-2.73100
O	6.24800	-3.22800	-1.72500
O	8.12700	-2.93200	-2.82300
N	7.58500	-8.62000	-4.28300
C	7.31400	-9.99200	-3.87300
C	6.05000	-10.05100	-3.00600
O	5.85900	-9.22200	-2.12700
C	8.53000	-10.36000	-3.01100
C	9.62800	-9.48300	-3.52000
C	8.97500	-8.21100	-3.97800
N	5.20800	-11.04100	-3.22900
H	5.44700	-11.75100	-3.92100
C	3.94000	-11.14700	-2.50900
C	4.10400	-11.70800	-1.10400
O	4.63400	-12.80300	-0.89100
C	2.99000	-12.02900	-3.32600
C	1.65400	-12.26300	-2.64000
C	0.60700	-12.90700	-3.53300
O	0.97300	-13.47400	-4.58600

O	-0.59100	-12.84600	-3.17500
N	3.60000	-10.95000	-0.12500
H	3.23800	-10.02300	-0.34800
C	3.55600	-11.42000	1.25500
C	2.10800	-11.29600	1.72200
O	1.57900	-10.18200	1.72500
C	4.49200	-10.62100	2.15500
C	4.56500	-9.15400	1.74200
C	5.98300	-8.67300	1.49400
O	6.17100	-7.73800	0.68500
O	6.92200	-9.22500	2.11700
N	1.47600	-12.41100	2.05700
H	1.96600	-13.30400	2.10200
C	0.05200	-12.31300	2.35900
C	-0.15500	-11.54400	3.66700
O	0.62900	-11.71800	4.59700
C	-0.57900	-13.70400	2.44500
C	-0.51900	-14.52400	1.15200
C	-1.22100	-15.85900	1.33900
C	-1.11300	-13.74500	-0.00900
N	-1.22900	-10.76200	3.68400
H	-1.78800	-10.67500	2.83500
C	-1.63400	-10.02700	4.86900
C	-2.38300	-10.94900	5.83300
O	-3.61600	-11.10700	5.73000
C	-2.54400	-8.84000	4.51700
C	-2.61300	-7.84000	5.68300
S	-3.66700	-6.45000	5.21100
C	-2.43100	-5.41100	4.42400
N	-1.59900	-11.54400	6.72900
H	-0.58900	-11.40700	6.68900
C	-2.18000	-12.39600	7.77400
C	-1.41800	-12.16600	9.08700
O	-0.28600	-11.70500	9.09000
C	-2.15900	-13.88900	7.40800
C	-2.95800	-14.17500	6.14400
C	-0.72700	-14.38500	7.19400
N	-2.07500	-12.51500	10.19600
H	-3.01600	-12.89700	10.10600
C	-1.50400	-12.37300	11.52900
C	-1.02600	-10.95600	11.80700
O	0.08900	-10.75000	12.31600
C	-0.37500	-13.41100	11.70600
C	-0.94400	-14.82300	11.77300
O	-2.01000	-15.04300	12.39800
O	-0.33200	-15.74800	11.18300
N	-1.87700	-9.98600	11.48700
H	-2.76300	-10.22400	11.04200
C	-1.56600	-8.58600	11.76100
C	-2.12100	-8.17200	13.12900
O	-2.81200	-7.17000	13.28600
C	-2.13600	-7.66600	10.69000

C	-3.61200	-7.87900	10.43500
O	-4.29600	-8.72400	11.02100
N	-4.13100	-7.05700	9.51100
H	-3.56600	-6.35900	9.02700
H	-5.12600	-7.20100	9.33900
N	-1.80200	-8.98900	14.12800
H	-1.27000	-9.83200	13.91000
C	-2.16800	-8.74900	15.51300
C	-0.96800	-8.67700	16.44500
O	0.04800	-9.32600	16.23500
C	-3.11200	-9.86800	15.95400
C	-2.68100	-11.28000	15.73700
C	-2.87800	-12.04200	14.61600
C	-1.98000	-12.12100	16.66500
N	-2.34200	-13.29700	14.79900
H	-2.35600	-14.05100	14.11200
C	-1.78700	-13.37400	16.04700
C	-1.50200	-11.94100	17.97200
C	-1.13300	-14.43600	16.68400
C	-0.84700	-12.99500	18.60700
C	-0.67100	-14.22700	17.95600
N	-1.09100	-7.86900	17.49400
H	-1.93500	-7.30300	17.58100
C	-0.06400	-7.76300	18.52400
C	-0.42700	-8.64800	19.70300
O	-1.59100	-8.69900	20.09600
C	0.03100	-6.30400	18.98200
C	1.11600	-6.07100	20.03300
C	0.99600	-4.66000	20.61300
N	2.22800	-4.24400	21.25200
H	3.06400	-4.78100	21.02100
C	2.38600	-3.24000	22.10500
N	1.34600	-2.49100	22.48100
H	0.40100	-2.65200	22.13200
H	1.46700	-1.71900	23.13700
N	3.62400	-3.02900	22.56200
H	4.41800	-3.60100	22.27500
H	3.74500	-2.25700	23.21800
N	0.49800	-9.35800	20.30300
C	0.13600	-10.17700	21.46000
C	-0.21500	-9.30300	22.67500
O	0.12400	-8.11900	22.74900
C	1.38600	-11.00300	21.72500
C	2.47400	-10.45800	20.88400
C	1.91600	-9.44200	19.93300
N	-0.93200	-9.96200	23.59300
H	-1.18100	-10.93200	23.39800
C	-1.37900	-9.38400	24.85000
C	-0.20400	-8.80900	25.63100
O	0.88600	-9.37900	25.63800
C	-2.12100	-10.41700	25.69700
N	-0.43200	-7.66800	26.26300

H	-1.37700	-7.28600	26.23800
C	0.58700	-6.92800	26.99100
C	0.25900	-6.99000	28.47400
O	-0.91300	-7.22500	28.82200
C	0.59600	-5.47200	26.51800
C	0.97600	-5.29200	25.04600
C	2.32800	-5.91300	24.74400
O	3.35800	-5.54800	25.31800
N	2.28500	-6.87400	23.82900
H	1.43400	-7.17600	23.35500
H	3.19300	-7.29100	23.62600
N	1.25600	-6.78700	29.32900
C	1.05100	-6.84200	30.78000
C	0.05900	-5.78400	31.25200
O	0.24200	-4.60000	30.97100
C	2.44400	-6.54400	31.33700
C	3.09200	-5.71200	30.28800
C	2.57300	-6.22800	28.97600
N	-0.97800	-6.21400	31.96200
H	-1.03400	-7.20100	32.21200
C	-2.03900	-5.31100	32.39300
C	-1.52200	-4.29700	33.40800
O	-1.94700	-3.14200	33.41600
C	-3.20700	-6.10200	32.98700
C	-4.34600	-5.27700	33.59000
C	-5.15200	-4.59400	32.49600
C	-5.24200	-6.15000	34.45500
N	-0.60400	-4.73700	34.26100
H	-0.31200	-5.71300	34.21700
C	-0.00300	-3.86000	35.25900
C	-1.14600	-3.15100	35.97800
O	-2.21700	-3.72500	36.17600
C	0.84200	-2.77800	34.58300
C	1.89000	-3.31900	33.62300
C	3.02100	-2.32300	33.42300
C	4.23000	-2.98300	32.77900
N	4.97800	-2.03900	31.90400
H	5.78900	-2.48200	31.47200
H	5.24300	-1.19400	32.41100
H	4.36700	-1.62000	31.20300
N	-0.84800	-1.91900	36.44300
H	-0.01200	-1.44800	36.09700
C	-1.68700	-1.24200	37.42500
C	-3.02100	-0.70900	36.91300
O	-3.31700	0.47900	37.04500
C	-0.86600	-0.10600	38.03600
C	-1.60400	0.61500	39.14700
O	-2.15000	-0.01300	40.05400
N	-1.62600	1.94100	39.08000
H	-1.17400	2.46100	38.32800
H	-2.12200	2.42600	39.82700
N	-3.82100	-1.59400	36.32800

H	-3.48900	-2.54800	36.18800
C	-5.16200	-1.23600	35.88100
C	-6.19200	-2.25500	36.35900
O	-5.85000	-3.39100	36.68600
C	-5.20600	-1.12000	34.35600
C	-4.28500	-0.05200	33.78900
C	-4.12300	-0.11100	32.27900
N	-3.22300	-1.18500	31.86700
H	-2.80400	-1.76200	32.59600
C	-2.91600	-1.45800	30.60600
N	-3.43600	-0.73500	29.62400
H	-4.07300	0.03100	29.84100
H	-3.20000	-0.94500	28.65400
N	-2.08800	-2.45400	30.32400
H	-1.68800	-3.01000	31.08000
H	-1.85200	-2.66400	29.35400
N	-7.45400	-1.83900	36.39700
H	-7.65400	-0.84500	36.28200
C	-8.56000	-2.76700	36.59900
C	-9.54600	-2.71100	35.43700
O	-10.10400	-1.65600	35.13500
C	-9.28000	-2.46500	37.91500
C	-10.75900	-2.81500	37.90800
C	-11.53300	-2.09500	38.99400
O	-12.50100	-1.38900	38.70800
N	-11.11000	-2.26900	40.24000
H	-10.30800	-2.85400	40.47700
H	-11.63100	-1.78400	40.97100
N	-9.75600	-3.85200	34.78900
H	-9.21400	-4.67700	35.04700
C	-10.74500	-3.95600	33.71400
C	-12.12000	-3.86100	34.33000
O	-12.34900	-4.57100	35.32700
C	-10.53900	-5.26500	32.93400
C	-9.17500	-5.25600	32.24300
C	-11.67500	-5.49700	31.96600
C	-8.77700	-6.49400	31.48900
N	-12.99700	-3.00600	33.80700
H	-12.74400	-2.43200	33.00300
C	-14.33700	-2.90300	34.40800
C	-15.38300	-3.48500	33.45500
O	-15.21600	-3.40200	32.22700
C	-14.65000	-1.44700	34.76400
C	-13.77100	-0.91500	35.90400
C	-14.40300	0.29800	36.56000
C	-13.41800	1.45800	36.66500
N	-13.96100	2.69100	36.03200
H	-13.30200	3.46700	36.10200
H	-14.87200	2.93900	36.41700
H	-14.23900	2.52300	35.06500
N	-16.42500	-4.06500	34.03200
H	-16.49200	-4.08100	35.05000

C	-17.48400	-4.68500	33.22800
C	-18.79600	-3.94000	33.38900
O	-19.10000	-3.42400	34.46600
C	-17.63400	-6.14300	33.59900
N	-19.56500	-3.87700	32.29700
H	-19.27000	-4.32000	31.42700
C	-20.82400	-3.16900	32.37400
C	-21.94000	-4.11000	32.77800
O	-23.08800	-3.66900	32.78300
C	-21.19000	-2.56300	31.00100
O	-21.60500	-3.61900	30.14300
H	-21.83000	-3.24600	29.29900
N	-21.63400	-5.35600	33.06500
H	-20.64700	-5.59800	33.15400
C	-22.61900	-6.41500	33.26400
C	-22.12400	-7.33700	34.37200
O	-20.91500	-7.47800	34.57600
C	-22.88000	-7.20100	31.97200
C	-21.63800	-7.93000	31.47900
C	-20.69700	-7.24900	30.71600
C	-21.41700	-9.25800	31.78700
C	-19.54000	-7.88800	30.30400
C	-20.26900	-9.90500	31.37900
C	-19.33600	-9.21800	30.62100
N	-23.04800	-7.95600	35.10300
H	-24.04000	-7.80400	34.92300
C	-22.61400	-8.86000	36.17100
C	-22.95800	-10.30300	35.80200
O	-23.46700	-10.55800	34.70600
C	-23.22100	-8.47100	37.51500
C	-24.72600	-8.60300	37.64700
C	-25.22500	-8.29400	39.05300
C	-26.17100	-9.36300	39.57200
N	-27.50100	-8.81800	39.97600
H	-28.13600	-9.53600	40.32500
H	-27.92700	-8.29400	39.21200
H	-27.39500	-8.06500	40.65500
Zn	-6.68400	-2.00900	15.48500
C	-6.47200	3.13800	16.21500
C	-6.28200	1.81500	16.62100
O	-6.78200	1.19500	17.71900
H	-6.65300	0.29500	17.99500
S	-5.38000	-0.65000	16.57800
C	-5.49100	0.95800	15.86600
C	-4.88100	1.42700	14.69400
C	-5.08200	2.74200	14.28400
C	-5.87300	3.59500	15.03800
O	-6.02400	4.89700	14.67000
H	-5.61700	5.20800	13.87000
C	-8.46100	11.31000	7.72200
C	-10.35600	12.66200	8.37000
C	-11.22800	11.66600	8.09800

C	-10.74000	10.47300	7.64900
C	-8.85600	7.75800	8.12100
O	-8.00200	7.41100	8.89000
O	-11.62400	9.51600	7.34300
H	-11.28400	8.68600	7.03000
O	-9.81400	7.16600	8.18400
S	-8.73800	8.90100	6.85100
C	-9.38400	10.31400	7.43600
O	-10.80800	13.80100	8.91100
H	-10.19500	14.50100	9.10200
C	-8.99700	12.47500	8.21000
O	-5.64500	-8.99600	33.23800
O	-4.82400	-12.82700	34.35900
C	-4.42600	-11.05900	32.85000
C	-4.75100	-9.74500	32.51900
C	-6.24100	-9.56700	34.35100
C	-5.06600	-11.67500	34.02200
C	-6.02100	-10.82600	34.77300
C	-3.50700	-11.77500	32.07800
C	-4.15800	-9.13800	31.41000
C	-3.24100	-9.85000	30.63700
C	-2.91600	-11.16500	30.97100
C	-7.17900	-8.65700	35.03200
C	-8.35400	-8.26100	34.39400
C	-9.24200	-7.39900	35.03900
C	-8.95500	-6.93400	36.32100
C	-7.77900	-7.33000	36.96000
C	-6.89200	-8.19200	36.31600
O	-9.82200	-6.09300	36.95000
H	-10.25400	-6.57400	37.67600
O	-6.65700	-11.37600	35.86600
H	-6.52900	-12.33800	35.87200
O	-3.15600	-13.06100	32.35900
H	-3.49300	-13.32300	33.22900
O	-2.66200	-9.26000	29.55500
H	-2.24700	-8.42700	29.83400