

SUPPLEMENTARY INFORMATION

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DFT investigation of the structural and spectral properties of cryptolepine: an antimalarial alkaloid

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1. Input file for cryptolepine

opt freq rb3lyp/6-311++g(d,p) geom=connectivity

0 1

C 3.45656200 -1.40870000 -0.02006800
C 4.53068700 -0.55474500 -0.07583900
C 4.30978500 0.83694000 -0.10576500
C 3.03095600 1.35138000 -0.06345300
C -0.45344500 0.13989700 0.02930400
C -2.74468800 1.43670700 -0.08504400
C -4.09937500 1.20155400 -0.11147100
C -4.61208900 -0.12511800 -0.06109100
C -3.78208400 -1.21901000 -0.00058800
C -2.37979200 -1.01972900 0.02263300
C 1.02205000 -1.81365600 0.05205000
C 2.12143500 -0.92604400 0.01543800
C 1.91127600 0.49129900 0.01102300
C -0.26092600 -1.31437600 0.04517800
C -1.85088600 0.33630400 0.00131600
H 1.18959200 -2.88483000 0.07313200
H 5.54099700 -0.94469100 -0.10639600
H 3.60732200 -2.48255600 -0.00752400
H 2.90058800 2.42286400 -0.11330200
H 5.15162000 1.51641600 -0.17078000
N 0.61577000 0.98376900 0.07000500
C 0.37578000 2.42507500 0.20118900
H -0.56393800 2.57016200 0.72479800
H 1.16459200 2.88067200 0.79449200
H 0.32796100 2.90842700 -0.77816500
N -1.43481200 -1.98457000 0.05086600
H -4.17167000 -2.22980900 0.02302200
H -5.68716300 -0.26951700 -0.08223900
H -4.78924800 2.03446200 -0.18090500
H -2.38884000 2.45734100 -0.15110300

1 2 2.0 12 1.5 18 1.0

2 3 1.5 17 1.0

3 4 2.0 20 1.0

4 13 1.5 19 1.0

5 14 1.0 15 1.5 21 1.5

6 7 2.0 15 1.5 30 1.0

7 8 1.5 29 1.0

8 9 2.0 28 1.0

9 10 1.5 27 1.0

10 15 1.0 26 1.5

11 12 1.5 14 2.0 16 1.0

12 13 1.5

13 21 1.0

14 26 1.5

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16
17
18
19
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21 22 1.0
22 23 1.0 24 1.0 25 1.0
23
24
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2. Optimized cartesian coordinates (Å) for the equilibrium structure of cryptolepine

C	-5.771328	-1.814551	-0.139184
C	-7.121113	-1.587157	-0.027530
C	-7.588734	-0.273517	0.177805
C	-6.710051	0.786812	0.251682
C	-3.071624	1.396203	0.163140
C	-1.672123	3.598968	0.528935
C	-0.368592	4.033563	0.584673
C	0.712700	3.127229	0.398017
C	0.502433	1.787871	0.172021
C	-0.825817	1.299031	0.113154
C	-3.439492	-1.003188	-0.155555
C	-4.827882	-0.756054	-0.059960
C	-5.317664	0.578040	0.122679
C	-2.548979	0.039738	-0.034527
C	-1.935891	2.226905	0.273800
H	-3.077342	-2.013356	-0.311558
H	-7.823197	-2.410131	-0.086774
H	-5.392979	-2.820162	-0.286325
H	-7.104467	1.776007	0.434675
H	-8.651051	-0.089083	0.287664
N	-4.414185	1.629228	0.178105
C	-4.891806	3.015343	0.230371
H	-4.144916	3.653247	-0.231712
H	-5.813860	3.112345	-0.337265
H	-5.060612	3.336482	1.261595
N	-1.197969	0.013517	-0.070305
H	1.325638	1.094979	0.044418
H	1.727085	3.508883	0.447467
H	-0.157130	5.077917	0.782390
H	-2.469513	4.311120	0.701255