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Is nevirapine atropisomeric? Experimental and computational evidence for rapid conformational inversion

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SUPPORTING INFORMATION

Optimized structures (Å) of nevirapine with an explicit DMSO solvent molecule at the M06-2X/6-311G(2D,2P) level .

Minimum energy structure.

1	6	0	2.547342	-0.978103	3.729491
2	6	0	2.601787	-2.370431	4.263474
3	6	0	3.077912	-2.073382	2.865924
4	1	0	3.247133	-0.255249	4.121617
5	1	0	3.332893	-2.580841	5.028332
6	1	0	1.660669	-2.889431	4.365836
7	1	0	2.449373	-2.397774	2.050134
8	1	0	4.137802	-2.080532	2.665506
9	7	0	1.239201	-0.478654	3.384443
10	6	0	0.414285	-0.112725	4.464329
11	6	0	-0.976101	0.012040	4.312517
12	6	0	-1.740333	-0.374075	3.089838
13	7	0	-1.175281	-0.232765	1.865358
14	6	0	-0.012716	0.474420	1.515844
15	6	0	1.186150	0.338103	2.224548
16	1	0	-1.822850	-0.483258	1.109967

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17	8	0	-2.875348	-0.816608	3.202068
18	8	0	-3.196182	-0.989926	0.007416
19	16	0	-4.040878	-2.050283	0.673628
20	6	0	-5.420815	-1.163880	1.415615
21	1	0	-6.184180	-1.873359	1.728265
22	1	0	-5.005943	-0.641854	2.271716
23	1	0	-5.800521	-0.465856	0.672325
24	6	0	-4.960270	-2.782302	-0.696794
25	1	0	-5.720117	-3.459125	-0.312227
26	1	0	-4.241245	-3.327533	-1.301736
27	1	0	-5.399051	-1.972557	-1.275680
28	6	0	-0.026515	1.273803	0.371700
29	6	0	-1.283610	1.446996	-0.430387
30	1	0	-1.574134	0.517420	-0.921763
31	1	0	-1.146560	2.214156	-1.188781
32	1	0	-2.121727	1.723640	0.209734
33	6	0	1.167834	1.873383	-0.010105
34	1	0	1.205070	2.495773	-0.893365
35	6	0	2.304338	1.659891	0.745531
36	1	0	3.250919	2.102646	0.460096
37	7	0	2.314565	0.917927	1.849410
38	7	0	1.015727	0.052613	5.638701
39	6	0	0.276904	0.386223	6.691402
40	6	0	-1.094521	0.575834	6.641563
41	6	0	-1.722814	0.358304	5.429001

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42	1	0	-2.797187	0.414680	5.324086
43	1	0	-1.647685	0.851273	7.526650
44	1	0	0.815779	0.507873	7.624129

Transition structure.

1	6	0	0.286138	-0.299740	-0.141149
2	6	0	0.121994	-0.245330	1.249007
3	6	0	1.240291	0.061059	2.048630
4	7	0	2.376343	0.445791	1.483085
5	6	0	2.507467	0.467209	0.166461
6	6	0	1.506651	0.063088	-0.689800
7	7	0	-1.189987	-0.416157	1.720838
8	6	0	-1.612180	-1.229214	2.718909
9	8	0	-2.752478	-1.669180	2.707661
10	7	0	1.271490	0.015795	3.470990
11	6	0	2.371248	0.715359	4.127928
12	6	0	3.241316	0.032424	5.139076
13	6	0	3.809485	0.419727	3.819306
14	6	0	-0.852698	-0.712337	-1.031644
15	6	0	-0.738417	-1.447434	3.903039
16	6	0	-1.287260	-2.305953	4.850370
17	6	0	-0.854059	-2.311826	6.159959
18	6	0	0.046663	-1.315008	6.495164
19	7	0	0.628874	-0.526475	5.608163

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20	6	0	0.369125	-0.653520	4.302539
21	1	0	0.308458	-1.126429	7.530884
22	1	0	-1.268084	-2.976627	6.901906
23	1	0	-2.120814	-2.914617	4.531038
24	1	0	-0.491341	-0.869240	-2.045173
25	1	0	-1.644963	0.036514	-1.055427
26	1	0	-1.310912	-1.634974	-0.672961
27	1	0	1.656619	0.049245	-1.759829
28	1	0	3.460476	0.819822	-0.210425
29	1	0	-1.949354	-0.197620	1.070725
30	1	0	3.066104	-1.018745	5.300776
31	1	0	3.476291	0.591625	6.031853
32	1	0	4.468470	1.270511	3.732645
33	1	0	4.004967	-0.373654	3.119395
34	1	0	2.134879	1.750161	4.338009
35	8	0	-3.609534	0.194590	0.292321
36	16	0	-4.676810	-0.840294	0.552141
37	6	0	-5.466700	-0.340428	2.093431
38	1	0	-4.767115	-0.590077	2.884515
39	1	0	-5.631782	0.733592	2.036927
40	1	0	-6.400923	-0.884423	2.215983
41	6	0	-6.022787	-0.340651	-0.545020
42	1	0	-6.916597	-0.919571	-0.322762
43	1	0	-5.690742	-0.534461	-1.561186
44	1	0	-6.188679	0.724983	-0.402981