

Supplementary Material

Mono-*endo*-6-*N,N*-diethylcarbamoyl and Bis-*endo,endo*-6,12-*N,N*-diethylcarbamoyl derivatives of Tröger's Base. Synthesis and *exo-endo* isomerization study

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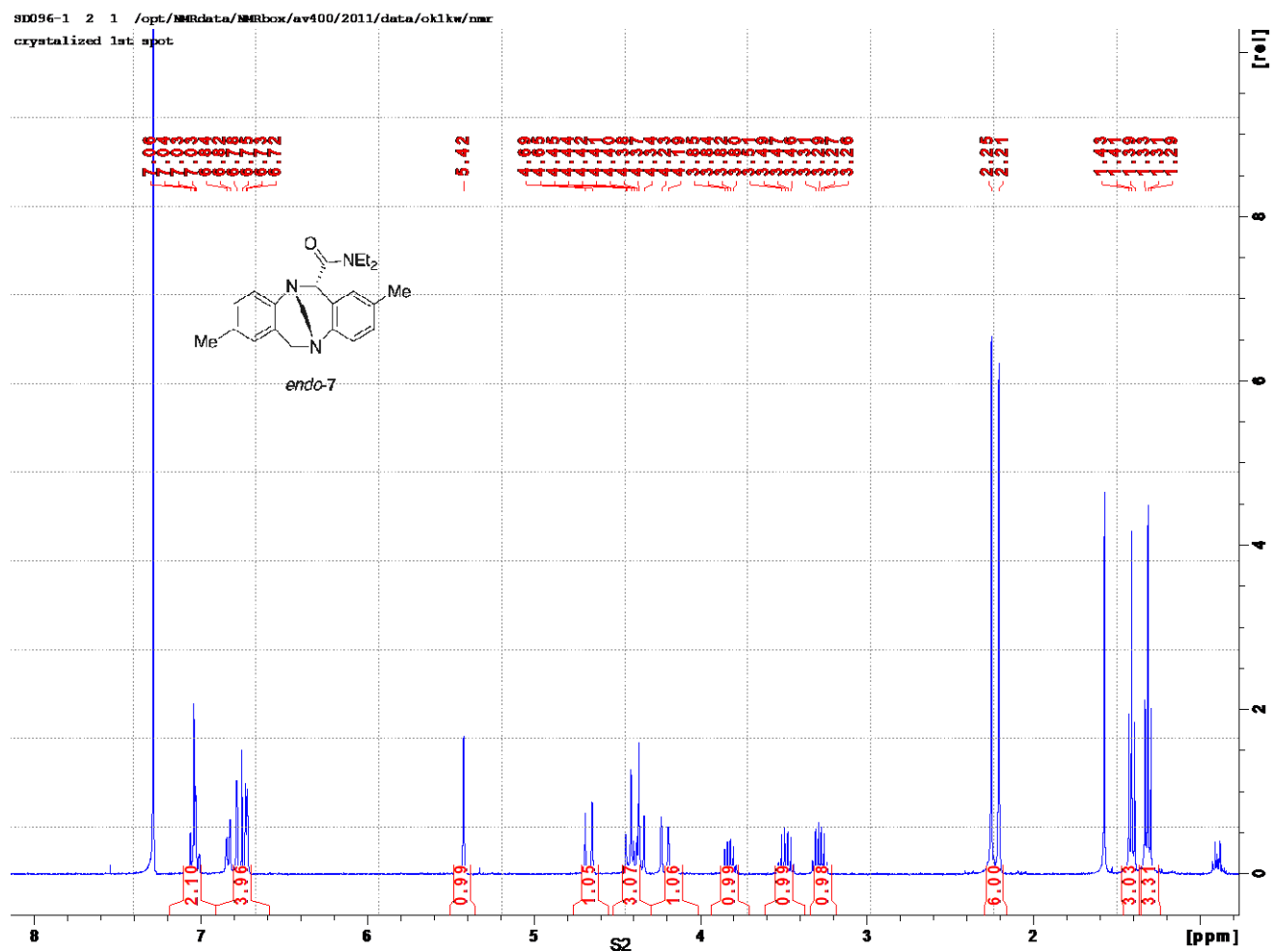
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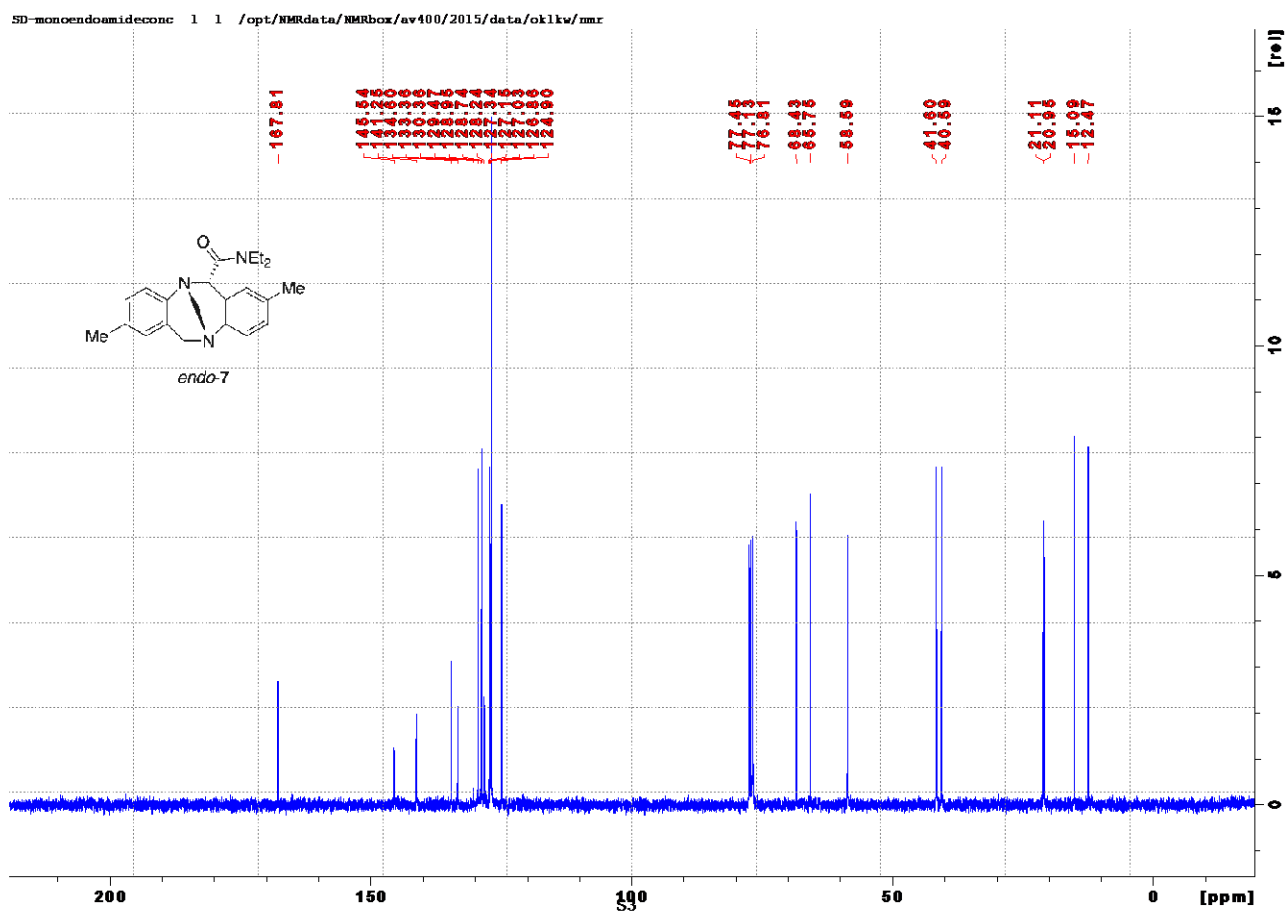
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Table of Contents

¹ H and ¹³ C NMR Spectra of <i>endo</i> -7	S2
¹ H and ¹³ C NMR Spectra of <i>endo</i> -8	S4
X-ray Diffraction Data for <i>endo</i> -8	S6
Calculated Pathway Energies	S7
xyz Files for Selected Calculated Structures	S8
References	S26

1. ^1H and ^{13}C NMR Spectra of *endo-7*.Figure S1. ^1H NMR (400 MHz) spectrum of *endo-7* in CDCl_3 .



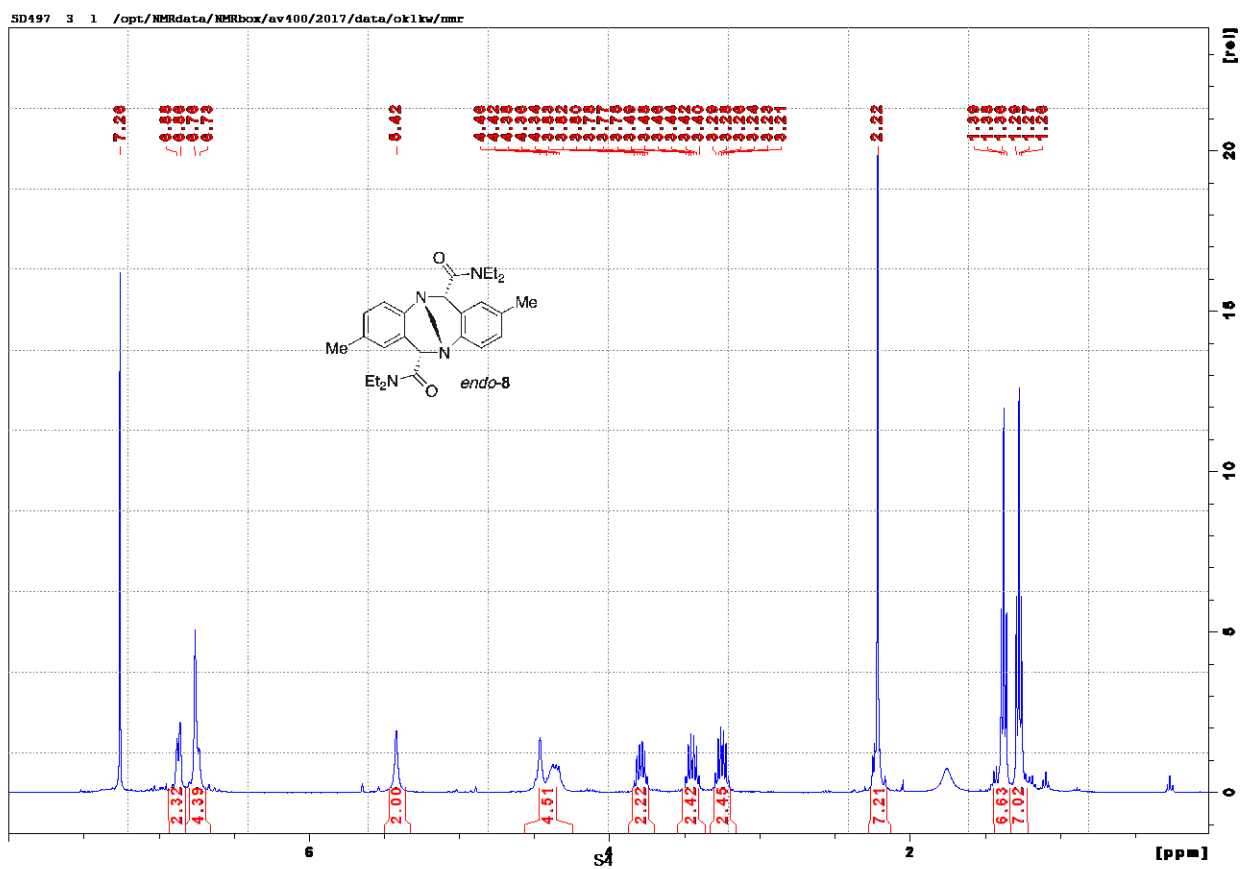


Figure S3. ^1H NMR (400 MHz) spectrum of *endo-8* in CDCl_3 .

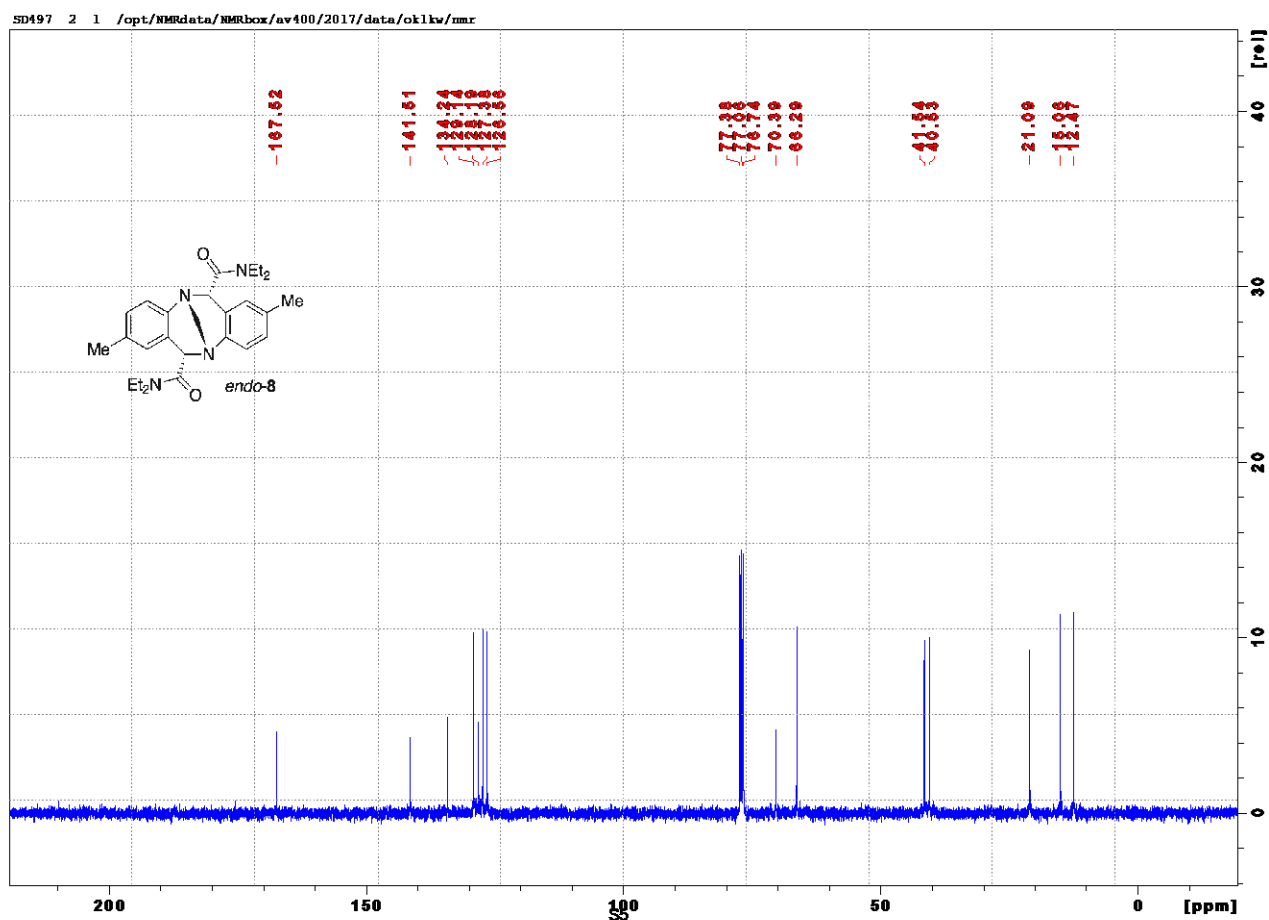


Figure S4. ¹³C NMR (100 MHz) spectrum of *endo-8* in CDCl₃.

3. X-ray Diffraction Data for *endo-8*.

A single crystal of *endo-8* grown from EtOAc/heptane was cut to size and mounted on a glass fiber. Data collection was performed at 293 K using an Agilent Xcalibur EOS diffractometer equipped with a Mo $K\alpha$ high-brilliance μ S radiation source ($\lambda = 0.71073 \text{ \AA}$). The structure was solved SUPERFLIP^{S1} and refined with SHELXL-2013.^{S2} Non-hydrogen atoms were refined anisotropically.

Table S1. Crystal data and structure refinement for *endo-8*.

Chemical formula	C ₂₇ H ₃₆ N ₄ O ₂	
Formula mass	448.61	
Crystal size	0.2 x 0.2 x 0.05 mm ³	
Crystal habit	Colorless, plate	
Temperature	293(2) K	
Wavelength	0.71073 Å	
Crystal system	Monoclinic	
Space group	C 2/c	
Unit cell dimensions	$a = 11.3586(13) \text{ \AA}$	$\beta = 90^\circ$.
	$b = 9.9446(14) \text{ \AA}$	$\gamma = 102.796(12)^\circ$.
	$c = 22.262(3) \text{ \AA}$	$\alpha = 90^\circ$.
Cell unit volume	2452.1(6) Å ³	
Number of formula units per cell, Z	4	
Density (calculated)	1.215 Mg/m ³	
Absorption coefficient	0.078 mm ⁻¹	
F(000)	968	
Reflections collected	8593	
Independent reflections	2829 [$R_{int} = 0.0568$]	
Data / restraints / parameters	2829/ 0 / 150	
Goodness-of-fit on F^2	0.946	
Final R indices [$I > 2\sigma(I)$]	$R_1 = 0.0735$, $wR2 = 0.1741$	
R indices (all data)	$R_1 = 0.1204$, $wR2 = 0.2061$	
Largest diff. peak and hole	0.224 and -0.195 e.Å ⁻³	
CCDC	1981491	

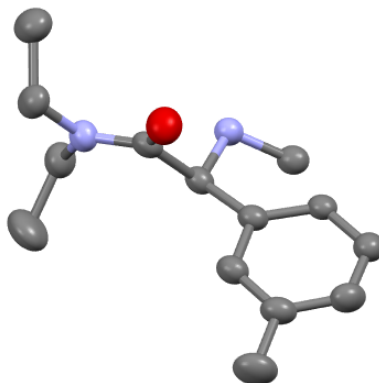


Figure S5. The asymmetric unit of *endo-8*. Gray = carbon atom, blue = nitrogen atom; red = oxygen atom. Thermal ellipsoids are shown at 30% probability. Hydrogen atoms are omitted for clarity.

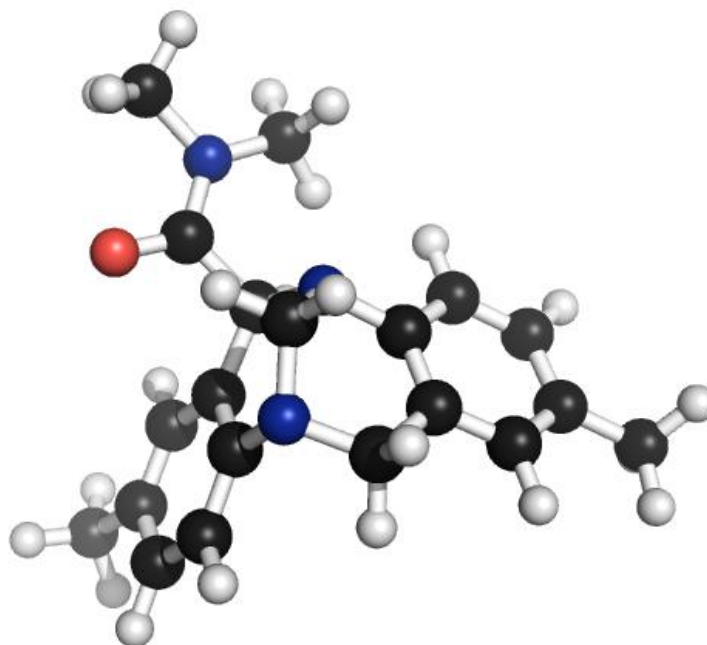
4. Calculated Pathway Energies

Table S2. Relative Energies of Species shown in Scheme 3 used to calculate the free energy surface in Figure 4.

Entry	Species	Relative Energy (kcal/mol)
1	<i>exo-9</i>	0.0
2	<i>endo-9</i>	2.0
3	<i>exo-10</i>	8.8
4	<i>endo-10</i>	10.3
5	<i>exo-11</i>	19.2
6	<i>endo-11</i>	14.2
7	<i>exo-12</i>	-13.8
8	<i>endo-12</i>	-15.0
9	13	-23.7

5. xyz Files for Selected Calculated Structures

Exo-9

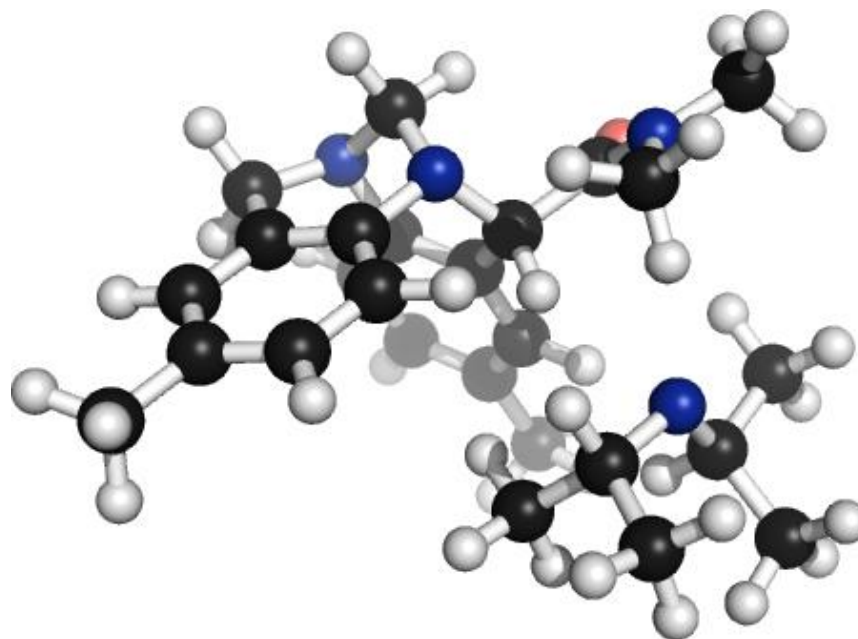


47

Exo-9

H	4.6424681	-0.1471754	0.6037628
C	3.8194090	0.4459524	0.2108416
C	1.7146147	1.8997595	-0.7879503
C	2.5450008	0.2328469	0.7264046
C	4.0678446	1.3586050	-0.8004870
C	2.9832787	2.0824558	-1.2966899
C	1.4762222	0.9794022	0.2292973
H	3.1426467	2.8069988	-2.0896859
H	0.8881197	2.4910676	-1.1673186
C	2.3179607	-0.8117196	1.7841862
H	2.7045535	-0.4694396	2.7506452
H	2.8647305	-1.7240361	1.5337366
N	0.8967811	-1.1191929	1.9363966
N	0.1545393	0.8257251	0.7488123
C	-0.7460587	0.0799873	-0.1445395
H	-0.5546077	0.4150908	-1.1674174
C	-0.4703907	-1.4012046	-0.0869081
C	0.3705192	-1.9288970	0.8906013
C	-1.0164480	-2.2478824	-1.0455172
H	-1.6846703	-1.8245048	-1.7930093
C	0.6918340	-3.2840392	0.8442598

C	-0.7279220	-3.6004176	-1.0849914
H	1.3552481	-3.6889293	1.6017718
C	0.1562547	-4.1018397	-0.1274397
H	0.4125728	-5.1564316	-0.1415872
C	0.1784512	0.1367967	2.0316874
H	0.6704849	0.7667434	2.7748120
H	-0.8480013	-0.0483541	2.3530949
C	-2.1994031	0.4028717	0.2298732
N	-2.6753704	1.6286185	-0.0743529
C	-3.9976173	1.9783282	0.4073203
H	-4.1614687	1.5592868	1.3984513
H	-4.0779079	3.0632607	0.4610790
C	-1.9970671	2.6421150	-0.8497107
H	-2.7275446	3.1504761	-1.4812898
H	-1.2474909	2.2105079	-1.5066710
O	-2.8831598	-0.4164599	0.8259742
C	5.4432765	1.5630575	-1.3502900
H	5.8143098	2.5668114	-1.1267682
H	5.4556264	1.4536431	-2.4372183
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C	-1.3476138	-4.5048316	-2.1025391
H	-2.1071453	-5.1463260	-1.6470486
H	-0.6043229	-5.1644664	-2.5559833
H	-1.8321780	-3.9387320	-2.8988055
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H	-1.5131697	3.3857701	-0.2094030

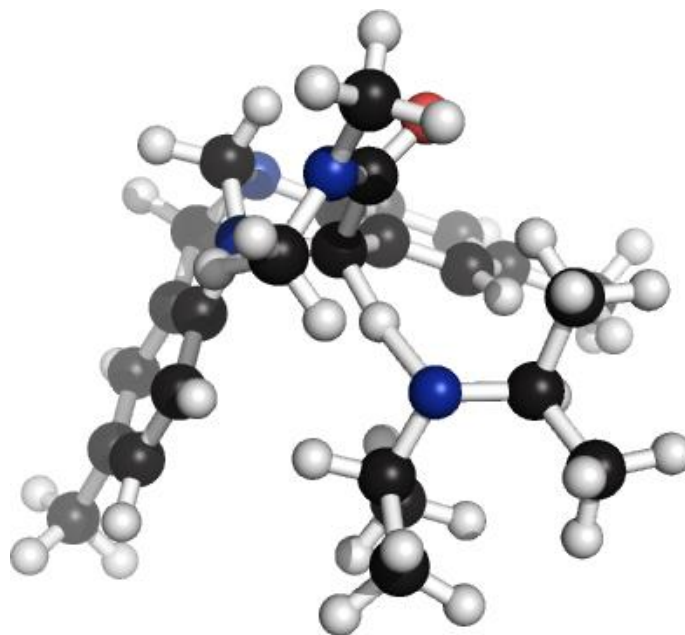
Exo-10

68

Exo-10

C	-1.9854512	-3.8540883	1.2359912
C	-0.5624825	-4.3460727	1.1843483
C	-0.6641736	-1.4258858	-0.7460028
C	0.4990024	-3.4387380	1.2164003
C	0.4804370	-1.2269284	0.2117071
H	-2.4447247	-4.0917848	2.2031301
H	-2.5803941	-4.3624113	0.4732716
H	1.4169804	-1.5055215	-0.2967217
C	-1.8540448	-2.0235455	-0.3296585
C	-0.5195168	-1.0590852	-2.0780086
H	0.4218121	-0.6125385	-2.3870366
C	-1.5126821	-1.2750358	-3.0170133
C	-2.6917740	-1.8853819	-2.5869431
C	-2.8599110	-2.2522594	-1.2669131
H	-3.7857915	-2.7131528	-0.9348904
C	1.7974634	-3.9165011	1.0593210
H	2.6197561	-3.2113596	1.0562771
C	2.0410254	-5.2653030	0.9114870
C	0.9987517	-6.1918745	0.9276702
C	-0.2913114	-5.7042642	1.0626453
H	-1.1278910	-6.4010895	1.0513063
N	-2.0614130	-2.4092571	1.0281418
N	0.2765111	-2.0462799	1.4197570
C	-1.0733456	-1.7976504	1.8997747
H	-1.1935157	-2.2126353	2.9034296

H	-1.2361247	-0.7199334	1.9501951
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N	1.7516003	0.5940578	1.2734948
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C	1.9575240	1.9962045	1.5588867
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H	2.4241466	2.5111411	0.7114039
H	1.0049051	2.4791332	1.7672228
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H	3.3353052	-0.4810277	0.4121222
H	3.6368991	0.2154521	2.0417912
H	2.6170204	-1.2152374	1.8978380
N	3.3377732	-0.8119615	-1.7142573
C	3.6895833	-2.1977942	-1.7541114
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C	2.9919849	-0.1722105	-2.9340971
H	2.1575500	-0.6840534	-3.4850637
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H	4.4096606	-0.9991450	-4.3906089
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H	2.1788857	1.7742541	-3.5128784
H	1.6402792	1.1976709	-1.9214410
C	5.1177801	-2.5487300	-2.2203901
H	5.8279413	-1.8443223	-1.7792872
H	5.3976751	-3.5650553	-1.9139922
H	5.2257921	-2.4934451	-3.3071283
C	2.7056933	-3.1133549	-2.4920180
H	2.6809700	-2.8840492	-3.5635965
H	2.9823894	-4.1682133	-2.3870865
H	1.6886219	-2.9913208	-2.1034211
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H	-1.6337798	-1.6594055	-5.1312007
H	-1.9278222	0.0146933	-4.6891029
H	-0.2818603	-0.6243699	-4.6490416
C	1.2693030	-7.6538357	0.7666829
H	1.3721291	-7.9254857	-0.2882070
H	2.2010846	-7.9419736	1.2590244
H	0.4622697	-8.2587480	1.1830219
H	3.0626102	-5.6142943	0.7912676
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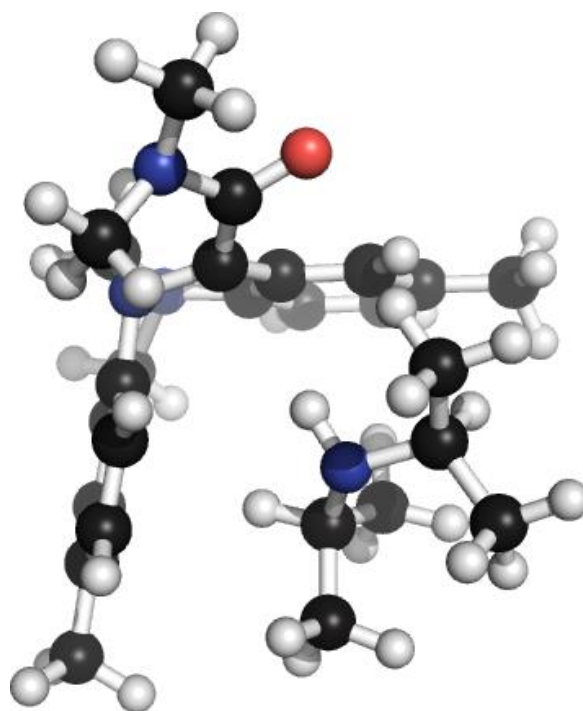
Exo-11

68

Exo-11

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C	-0.5576750	-1.3753429	-0.8532736
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C	-0.5008043	-1.0244651	-2.1997171
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C	-2.7810476	-2.2259740	-1.2903515
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C	2.1138966	-5.2978017	0.8886012
C	1.0455229	-6.1938787	0.9115675
C	-0.2290646	-5.6643413	1.0339160
H	-1.0860962	-6.3364549	1.0520139
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H	-0.9711661	-2.1550650	2.8065133

H	-1.0293013	-0.6605160	1.8598892
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H	2.4298996	2.5395815	0.7499602
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H	2.0107927	-0.6733579	-3.4974188
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H	3.7726946	0.6047133	-4.5859465
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H	4.2920819	-1.0408029	-4.2458705
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H	2.0773489	1.7377639	-3.4061205
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H	5.3365282	-3.4731976	-1.7828386
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H	0.4588151	-8.2415118	1.2181115
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Exo-12

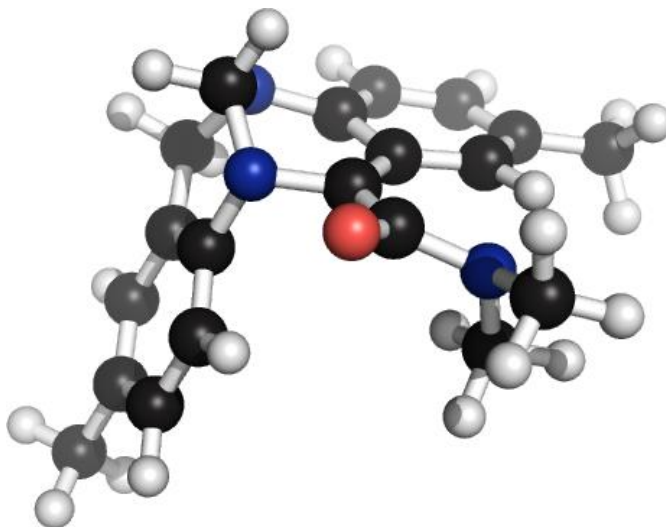
68

Exo-12

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C	0.7954556	-2.8936836	1.2520334
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C	-0.4422070	-0.3815286	-1.9643996
H	0.2916318	0.4089319	-2.0634566
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C	-2.2895162	-2.3973370	-1.7421121
H	-3.0446164	-3.1714637	-1.6281757
C	2.1911517	-2.9447750	1.2761444
H	2.7475692	-2.0255079	1.4029470
C	2.8624791	-4.1385716	1.1206273
C	2.1765364	-5.3358610	0.9157786
C	0.7947233	-5.2704455	0.8326701
H	0.2304117	-6.1773787	0.6184162
N	-1.8768964	-2.6582774	0.6296286
N	0.1106092	-1.6759147	1.4998249

C	-1.3000809	-1.9202132	1.7391429
H	-1.4500300	-2.5079940	2.6515923
H	-1.7912937	-0.9522832	1.8587308
C	0.5606754	0.6673420	0.7587830
N	1.0761708	1.0174941	2.0385061
O	0.3684807	1.6093637	-0.0370727
C	1.3283693	2.4326058	2.2025386
H	1.5275136	2.6324979	3.2584462
H	2.1928752	2.7829746	1.6181227
H	0.4669301	3.0191305	1.8907423
C	2.1153514	0.2161632	2.6453048
H	3.0172674	0.1651382	2.0129186
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N	2.7678479	-1.9332661	-1.9228294
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C	4.0295543	-1.3040773	-3.9460783
H	4.1923368	-0.4848316	-4.6506770
H	4.9568260	-1.4668409	-3.3875158
H	3.8226918	-2.2020698	-4.5305142
C	3.1660760	0.3967253	-2.3525539
H	4.1009924	0.3650334	-1.7844619
H	3.2608773	1.1738155	-3.1161846
H	2.3653688	0.6831405	-1.6644710
C	3.5460766	-4.2189033	-2.4949483
H	4.3020236	-4.0995738	-1.7145019
H	3.2238259	-5.2645308	-2.5057421
H	4.0190383	-4.0116535	-3.4581779
C	1.2954648	-3.4556197	-3.3018204
H	1.6625261	-3.1533741	-4.2878472
H	0.9860235	-4.5023742	-3.3756832
H	0.4127117	-2.8561096	-3.0681285
C	-0.9404566	-0.0857504	-4.4031016
H	-0.6473246	-0.8171321	-5.1627819
H	-1.8448818	0.4058790	-4.7740874
H	-0.1524277	0.6678989	-4.3384937
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H	3.3469828	-6.6812158	-0.2837092
H	3.7551178	-6.7051379	1.4232388
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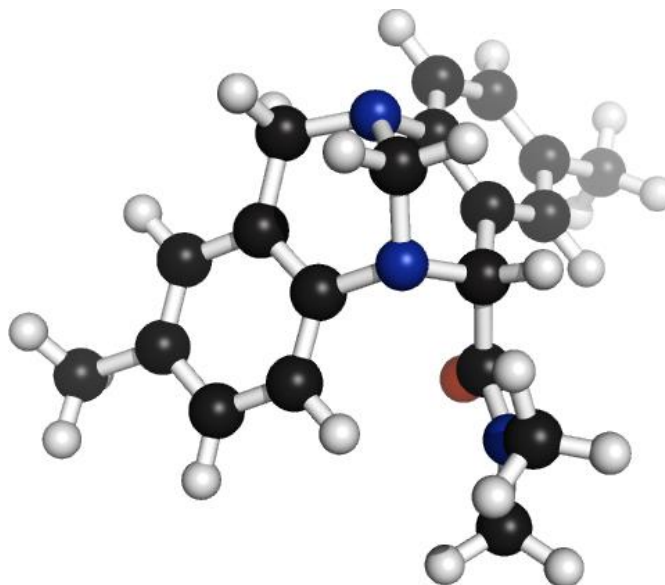


46

13

H -1.2931327 -3.9977444 0.7103050
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C -2.2905664 -0.2899618 0.7538784
C -1.0071456 -2.0839129 -0.1990515
C -2.5134969 -2.5204336 1.6592040
C -2.8483148 -1.1642935 1.6628990
C -1.3736173 -0.7381341 -0.1969779
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H -2.5522244 0.7630023 0.7501556
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C 3.9843635 -0.8971252 -0.1092285
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H	-4.2061745	-3.4764198	2.5847775
H	-2.8663589	-3.1706085	3.6789112
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H	4.6158307	2.0065932	1.5769930
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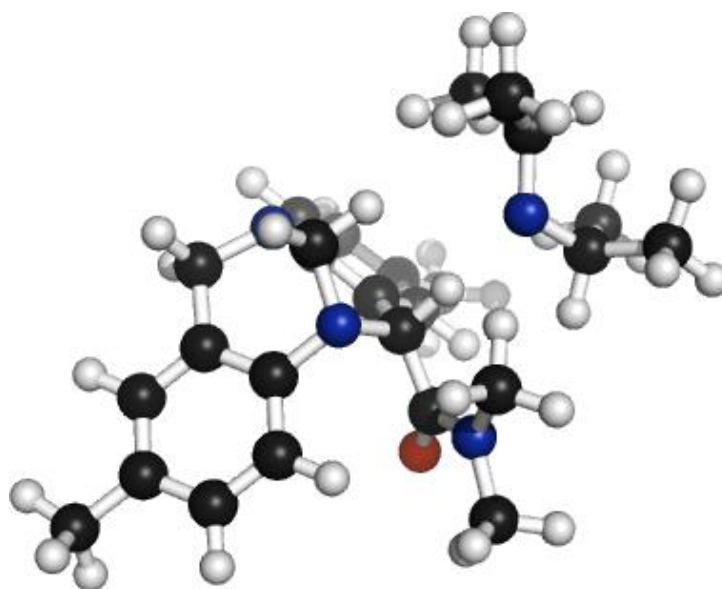
Endo-9

47

Endo-9

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C	0.82582830	-3.46822750	1.75004430
C	1.31683270	-1.85111680	-0.05814660
H	-2.06258880	-2.75683970	2.85733010
H	-2.45230820	-3.49050440	1.31276010
H	1.74400790	-0.84212830	-0.11659850
C	-1.19926790	-1.86357380	-0.21662130
C	0.05093020	-1.83453850	-2.25358960
H	1.00213390	-1.79312710	-2.77509290
C	-1.11691610	-1.88574070	-2.98413790
C	-2.35610750	-1.96379980	-2.34496180
C	-2.37491720	-1.93665300	-0.96210130
H	-3.32269910	-1.93991770	-0.42934950
C	1.89538180	-4.34150940	1.91777280
H	2.90338930	-3.97325230	1.74907240
C	1.71361580	-5.65789720	2.31275510
C	0.41823080	-6.09227760	2.57731430
C	-0.65086440	-5.22771200	2.43617690
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N	-1.29273160	-1.75078420	1.19772780
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C	-0.05116950	-1.26803170	1.76590180
H	-0.14204580	-1.26068390	2.85397860

H	0.14328270	-0.24831290	1.42595020
C	2.36012100	-2.83034410	-0.60524220
N	3.65078640	-2.60460310	-0.26278950
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C	4.13206240	-1.56445120	0.62050690
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H	4.70596750	-0.81604760	0.06643840
H	3.32032450	-1.08172420	1.15562860
C	4.65994950	-3.55883350	-0.66715990
H	5.55026250	-3.02831730	-1.01244220
H	4.94541070	-4.19698520	0.17787660
H	4.27887420	-4.18711870	-1.46715140
H	2.55443384	-6.31322230	2.40480966
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C	0.18049146	-7.54257138	3.03745335
H	-0.55455149	-7.55413300	3.81493531
H	-0.16568408	-8.12688209	2.21062598
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H	-0.86066259	-2.85386615	-4.88469035
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H	-0.28045654	-1.20624641	-4.84253958

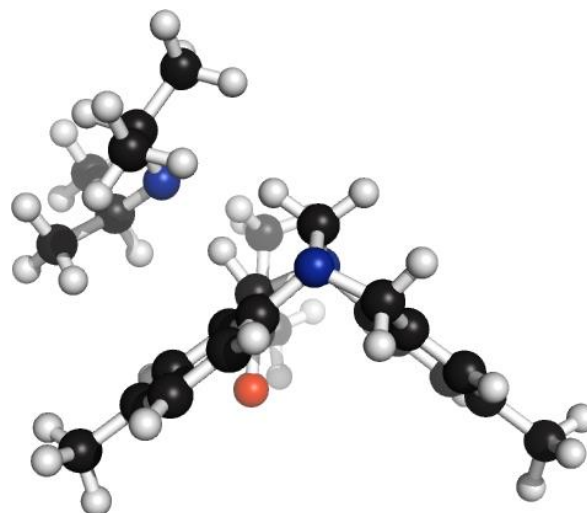
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68

Endo-10

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C	-1.0095410	-2.2248517	-0.3386336
C	-2.7935717	-2.6513073	1.2558322
C	-3.1141477	-1.2942246	1.2068096
C	-1.3511477	-0.8715954	-0.3909643
H	-3.9419435	-0.9225806	1.8037785
H	-2.6992233	0.6207477	0.3459478
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H	-0.2539240	-3.3941996	-1.9659922
H	0.7763351	-3.3906803	-0.5456233
N	0.9296032	-1.6867683	-1.7521017
N	-0.6809911	0.0208873	-1.2750902
C	1.5585341	0.1777791	-0.2623673
C	1.8249609	-1.0759740	-0.8227610
C	2.5316673	0.7615079	0.5407998
H	2.3531500	1.7555317	0.9397250
C	3.0017019	-1.7388437	-0.4942362
C	3.7168519	0.1171436	0.8625907
H	3.1880336	-2.7125333	-0.9372440
C	3.9312557	-1.1579473	0.3464639
H	4.8507180	-1.6849646	0.5842023
C	0.0131764	-0.7090447	-2.3181019
H	-0.7048877	-1.2384923	-2.9500029
H	0.5628599	0.0177505	-2.9211941

C	-3.5704207	-3.5906708	2.1217087
H	-4.6279491	-3.6003870	1.8452664
H	-3.5213307	-3.2977443	3.1735475
H	-3.1923387	-4.6108792	2.0405314
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H	4.4503908	0.6794381	2.8082037
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H	0.6791462	1.5790867	-1.5183337
C	-0.3174082	1.7722585	0.4050690
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H	-1.9033029	2.9380261	1.9248037
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H	-2.3971847	2.4170871	-1.7459455
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O	-0.0785373	1.6110612	1.5957517
H	-1.7497395	4.0476223	-1.4907573
H	-3.1162293	3.2221963	0.6548333
N	1.4410849	2.6311639	-2.9134665
C	1.8864681	3.7426725	-2.1335395
H	1.2820454	3.7443081	-1.2026951
C	2.2263390	2.3420974	-4.0697198
H	2.8659933	3.2008827	-4.3767514
C	3.1825786	1.1505290	-3.8915110
H	2.6013531	0.2437754	-3.6808954
H	3.7964932	0.9614527	-4.7824257
H	3.8484508	1.3040268	-3.0385181
C	1.3186061	2.0550493	-5.2622159
H	0.6512984	1.2227555	-5.0125953
H	0.6897728	2.9254142	-5.4666225
H	1.8734669	1.7892300	-6.1714459
C	1.6124864	5.1025972	-2.8009131
H	0.5555540	5.1616538	-3.0728718
H	1.8595049	5.9555215	-2.1557707
H	2.1977176	5.2004571	-3.7224995
C	3.3469524	3.7079765	-1.6593452
H	3.5939687	4.5682850	-1.0255770
H	3.5407446	2.7931777	-1.0898126
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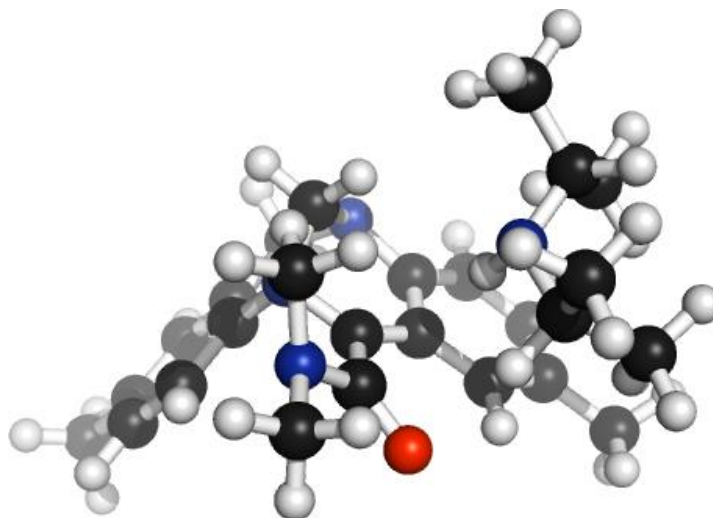
Endo 11

68

Endo-11

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C	2.34627760	0.63353490	0.29710750
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C	2.74746380	-1.81344670	-0.88618120
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C	3.78043650	-1.23012980	-0.17406930
H	4.74285610	-1.72650310	-0.08701910
C	-0.45102000	-0.86340780	-2.29047960
H	-1.22239730	-1.38719250	-2.86436840
H	0.02234660	-0.11453990	-2.93293740

C	-3.33155070	-3.82904920	2.61666480
H	-4.42269460	-3.84701880	2.55362730
H	-3.07704960	-3.53348640	3.63813230
H	-2.97105690	-4.84796920	2.46684840
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H	4.41929670	1.68274390	1.49306770
H	5.58706960	0.78470610	0.51520690
H	5.00583170	0.10390480	2.02363640
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H	-2.78945150	2.91790340	-2.23192910
H	-1.61156130	1.62002230	-2.44741550
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H	-1.07238810	3.30933970	-2.50886270
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C	2.59430210	2.46575020	-3.62061270
H	3.20557630	3.34047490	-3.87639850
C	3.52099380	1.32749630	-3.22417330
H	2.92998450	0.44875770	-2.93563830
H	4.17588540	1.03671680	-4.05063940
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H	1.12013780	2.91404400	-5.12939130
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C	1.65268430	5.29109580	-2.60651800
H	0.64339930	5.21683090	-3.01795170
H	1.72650360	6.19987570	-2.00441130
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C	3.37056280	4.13505950	-1.18909470
H	3.48026940	5.02768460	-0.56834620
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H	4.13513280	4.18817850	-1.97300350

Endo-12

68

Endo-12

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H	2.1889893	1.6016984	0.7564749
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C	3.5794614	0.0219443	0.4108215
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H	-1.2223973	-1.3871925	-2.8643684
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C	-3.3315507	-3.8290492	2.6166648
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H	-3.0770496	-3.5334864	3.6381323
H	-2.9710569	-4.8479692	2.4668484
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H	3.5787086	3.2584797	-0.5699374
H	4.1351328	4.1881785	-1.9730035

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- S2. Sheldrick, G. M. *Acta Cryst A.* **2008**, *64*, 112–122.