Total Synthesis of (–)-Nakadomarin A

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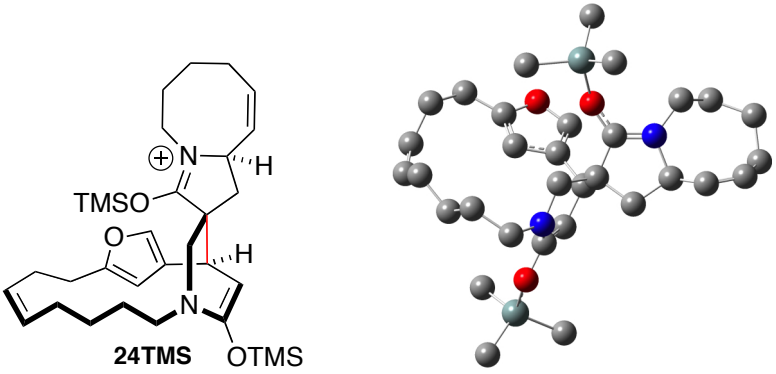
Supporting Information

Appendix III: Computational Methods

Molecular Mechanics. All molecular mechanics calculations were performed using Spartan 2008, v. 1.1.2 (Wavefunction, Inc., Irvine, CA, USA), using the molecular mechanics MM2 force field. To generate an initial subset of reasonable conformers, a conformer distribution calculation was performed, and the 100 structures of lowest energy were documented. A subset of these conformers was then optimized further via DFT.

Density Functional Theory. All DFT calculations were performed using Gaussian 09 (Revision A.02)[1] on the Odyssey Cluster at Harvard University. Each starting structure, already a local minimum with respect to the molecular mechanics potential energy surface, was re-optimized with the B3LYP hybrid functional[2] with the 6-31G* basis set. The SMD implicit solvation model[3] was used in all cases with dichloroethane as the specified solvent. DFT structures were verified to be true local minima by standard frequency analyses. Free energies are given at 298.15 K in all cases.

Computed geometries and energies.



Computed free energy: -1357640.693 kcal/mol; relative energy: 0 kcal/mol

1	C1	-4.4934	2.7599	-0.0336 C
2	H2	-5.4703	2.2975	-0.1900 H
3	C3	-3.9717	3.4491	-1.0597 C
4	H4	-4.5610	3.5034	-1.9775 H
5	C5	-2.6770	4.2238	-1.1144 C
6	H6	-2.1207	4.1406	-0.1751 H
7	H7	-2.9266	5.2881	-1.2320 H
8	C8	-1.7491	3.8564	-2.2952 C
9	H9	-2.3309	3.8447	-3.2287 H
10	C10	-1.0303	2.5548	-2.1288 C

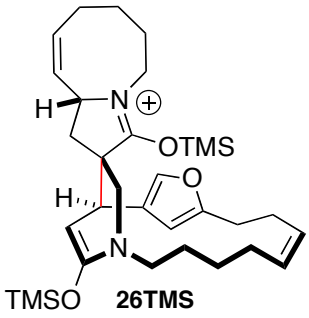
[1] Gaussian 09, Revision A.02: Frisch, M. J.; Trucks. G. W.; Schlegel, H. B.; Scuseria G. E.; Robb, M. A.; Cheeseman, J. R.; Scalmani, G.; Barone, V.; Mennucci, B.; Petersson, G. A.; Nakatsuji, H.; Caricato, M.; Li, X.; Hratchian, H. P.; Izmaylov, A. F.; Bloino, J.; Zheng, G.; Sonnenberg, J. L.; Hada, M.; Ehara, M.; Toyota, K.; Fukuda, R.; Hasegawa, J.; Ishida, M.; Nakajima, T.; Honda, Y.; Kitao, O.; Nakai, H.; Vreven, T.; Montgomery, Jr., J. A.; Peralta, J. E.; Ogliaro, F.; Bearpark, M.; Heyd, J. J.; Brothers, E.; Kudin, K. N.; Staroverov, V. N.; Kobayashi, R.; Normand, J.; Raghavachari, K.; Rendell, A.; Burant, J. C.; Iyengar, S. S.; Tomasi, J.; Cossi, M.; Rega, N.; Millam, J. M.; Klene, M.; Knox, J. E.; Cross, J. B.; Bakken, V.; Adamo, C.; Jaramillo, J.; Gomperts, R.; Stratmann. R. E.; Yazyev, O.; Austin, A. J.; Cammi, R.; Pomelli, C.; Ochterski, J. W.; Martin, R. L.; Morokuma, K.; Zakrzewski, V. G.; Voth G. A.; Salvador, P.; Dannenberg, J. J.; Dapprich, S.; Daniels, A. D.; Farkas, O.; Foresman, J. B.; Ortiz, J. V.; Cioslowski, J.; Fox, D. J. Gaussian Inc., Wallingford, CT, 2009.

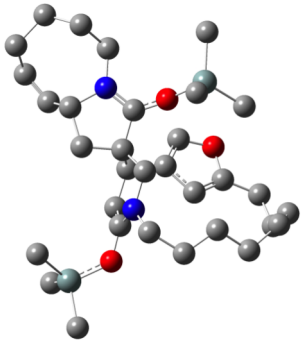
[2] (a) Becke, A. D. *J. Chem. Phys.* **1993,** *98*, 5648-5652. (b) Stephens, P. J.; Devlin, F. J.; Chablowski, C. F.; Frisch, M. J. *J. Chem. Phys.* **1994**, *98*, 11623-11627.

[3] Marenich, A. V.; Cramer. C. J.; Truhlar, D. G. *J. Phys. Chem. B.* **2009**, *113*, 6378-6396.

11	O11	-0.0258	2.2840	-3.0261 O
12	C12	0.4925	1.0590	-2.6973 C
13	C13	-1.1402	1.5178	-1.2532 C
14	H14	-1.8620	1.4388	-0.4584 H
15	C15	-0.1475	0.5369	-1.6130 C
16	C16	-3.8764	2.4911	1.3157 C
17	H17	-4.5088	2.9182	2.1085 H
18	H18	-2.9042	2.9904	1.3959 H
19	C19	-3.6917	0.9776	1.5748 C
20	H20	-4.6718	0.5037	1.7203 H
21	H21	-3.2751	0.5236	0.6698 H
22	C22	-2.7736	0.6624	2.7670 C
23	H23	-3.3178	0.7877	3.7130 H
24	H24	-1.9518	1.3906	2.7963 H
25	C25	-2.1774	-0.7611	2.7556 C
26	H26	-1.5717	-0.8963	3.6610 H
27	H27	-1.0023	4.6519	-2.4195 H
28	H28	-2.9713	-1.5078	2.7806 H
29	N29	-1.3118	-1.0665	1.6069 N
30	C30	-1.8180	-1.6430	0.4443 C
31	C31	0.0922	-0.8143	-0.9719 C
32	C32	-1.1876	-1.5884	-0.7551 C
33	H33	-1.5892	-2.1385	-1.5965 H
34	H34	0.7339	-1.3814	-1.6589 H
35	C35	-0.1100	-0.2477	1.4967 C
36	H36	0.3904	-0.2544	2.4731 H
37	H37	-0.3513	0.7969	1.2623 H
38	C38	0.8466	-0.7819	0.4198 C
39	C39	1.4404	-2.1720	0.7409 C
40	H40	0.8408	-2.9823	0.3232 H
41	H41	1.4957	-2.3110	1.8263 H
42	N42	3.1782	-0.6837	0.1271 N
43	C43	2.8606	-2.1542	0.1520 C
44	H44	2.8571	-2.4831	-0.8915 H
45	H45	1.2881	0.6997	-3.3349 H
46	C46	2.1081	0.0505	0.3331 C
47	C47	3.8884	-2.9189	0.9371 C
48	H48	3.7042	-3.0123	2.0061 H
49	C49	5.0033	-3.4286	0.4003 C
50	H50	5.7014	-3.9345	1.0668 H
51	C51	5.4199	-3.3223	-1.0466 C
52	H52	6.1529	-4.1084	-1.2586 H
53	H53	4.5665	-3.5063	-1.7127 H
54	C54	4.5221	-0.1804	-0.2037 C
55	H55	4.4275	0.9000	-0.2991 H
56	H56	5.1841	-0.3886	0.6414 H
57	C57	5.1068	-0.7506	-1.5166 C
58	H58	5.6837	0.0676	-1.9634 H
59	H59	4.2901	-0.9588	-2.2196 H
60	C60	6.0538	-1.9608	-1.4145 C
61	H61	6.8568	-1.7294	-0.7018 H
62	H62	6.5363	-2.0731	-2.3936 H
63	O63	2.0893	1.3397	0.3898 O
64	O64	-2.9643	-2.3324	0.6700 O
65	Si65	2.7432	2.7450	1.2176 Si
66	Si66	-4.0650	-3.0862	-0.3985 Si

67	C67	3.6080	3.7358	-0.1111 C
68	H68	2.9376	3.9237	-0.9584 H
69	H69	4.5074	3.2377	-0.4905 H
70	H70	3.9134	4.7098	0.2927 H
71	C71	1.2323	3.6223	1.8803 C
72	H72	0.7376	3.0461	2.6703 H
73	H73	0.5019	3.8172	1.0868 H
74	H74	1.5228	4.5903	2.3093 H
75	C75	3.8608	2.1245	2.5856 C
76	H76	4.7572	1.6180	2.2122 H
77	H77	3.3305	1.4375	3.2564 H
78	H78	4.1920	2.9795	3.1899 H
79	C79	-5.4063	-3.7049	0.7585 C
80	H80	-6.1976	-4.2158	0.1948 H
81	H81	-5.8736	-2.8822	1.3133 H
82	H82	-5.0075	-4.4192	1.4893 H
83	C83	-4.7369	-1.8209	-1.6157 C
84	H84	-5.4310	-2.2994	-2.3192 H
85	H85	-3.9415	-1.3477	-2.2022 H
86	H86	-5.2876	-1.0263	-1.0978 H
87	C87	-3.2355	-4.5366	-1.2666 C
88	H88	-3.9892	-5.1332	-1.7977 H
89	H89	-2.7445	-5.1990	-0.5427 H
90	H90	-2.4838	-4.2273	-2.0012 H

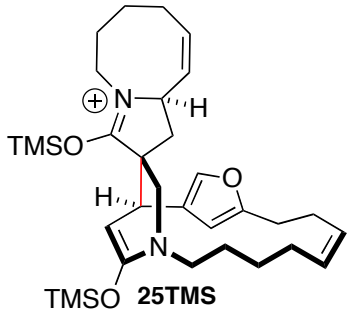


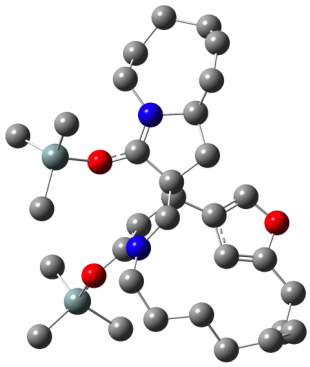


Computed free energy: -1357638.44 kcal/mol; relative energy: +2.25 kcal/mol

1	C1	3.9140	-3.6178	-0.8895 C
2	H2	3.7136	-4.2305	-1.7706 H
3	C3	3.6717	-4.1712	0.3083 C
4	H4	3.3038	-5.1994	0.3189 H
5	C5	3.8815	-3.5812	1.6807 C
6	H6	4.2678	-2.5582	1.6266 H
7	H7	4.6542	-4.1739	2.1907 H
8	C8	2.6272	-3.6192	2.5838 C
9	H9	2.1525	-4.6073	2.5172 H
10	C10	1.6083	-2.5649	2.2811 C
11	O11	0.3642	-2.7445	2.8372 O
12	C12	-0.3856	-1.6442	2.5250 C
13	C13	1.6351	-1.3697	1.6264 C
14	H14	2.4862	-0.9360	1.1241 H
15	C15	0.3336	-0.7634	1.7718 C
16	C16	4.3703	-2.2129	-1.1885 C
17	H17	5.2195	-2.2381	-1.8868 H
18	H18	4.7272	-1.7166	-0.2787 H
19	C19	3.2237	-1.3790	-1.7984 C
20	H20	2.9121	-1.8214	-2.7556 H
21	H21	2.3702	-1.4734	-1.1226 H
22	C22	3.5604	0.1052	-1.9945 C
23	H23	4.2791	0.2189	-2.8186 H
24	H24	4.0584	0.4941	-1.0979 H
25	C25	2.3493	1.0088	-2.3022 C
26	H26	2.7131	2.0053	-2.5677 H
27	H27	2.9461	-3.5112	3.6307 H
28	H28	1.8033	0.6275	-3.1723 H
29	N29	1.3606	1.1455	-1.2185 N
30	C30	1.7154	1.7445	-0.0143 C
31	C31	-0.1091	0.5933	1.2545 C
32	C32	1.0460	1.5614	1.1483 C
33	H33	1.3596	2.1064	2.0307 H
34	C34	0.2212	0.2309	-1.2358 C
35	H35	0.5287	-0.8075	-1.0676 H
36	H36	-0.2352	0.2801	-2.2315 H
37	C37	-0.8214	0.6027	-0.1692 C
38	C38	-1.5047	1.9712	-0.4184 C
39	H39	-1.3847	2.2620	-1.4657 H
40	H40	-1.0630	2.7552	0.1986 H
41	N41	-3.1580	0.2967	-0.1092 N

42	C42	-3.0030	1.7833	-0.0978 C
43	H43	-3.6195	2.1628	-0.9151 H
44	H44	-1.3963	-1.6431	2.9075 H
45	C45	-2.0100	-0.3349	-0.2078 C
46	C46	-3.4898	2.3505	1.2089 C
47	H47	-2.7703	2.3849	2.0250 H
48	C48	-4.7538	2.7451	1.4045 C
49	H49	-5.0284	3.0989	2.3978 H
50	C50	-5.8587	2.7218	0.3734 C
51	H51	-6.6540	3.3989	0.7035 H
52	H52	-5.4980	3.1167	-0.5859 H
53	C53	-4.4654	-0.3501	0.1116 C
54	H54	-4.3506	-1.3865	-0.1988 H
55	H55	-4.6517	-0.3501	1.1914 H
56	C56	-5.6483	0.2937	-0.6391 C
57	H57	-6.3217	-0.5329	-0.8942 H
58	H58	-5.3052	0.7034	-1.5976 H
59	C59	-6.4901	1.3312	0.1287 C
60	H60	-6.7986	0.8978	1.0896 H
61	H61	-7.4112	1.4870	-0.4468 H
62	O62	2.8059	2.5561	-0.1143 O
63	O63	-1.9099	-1.6224	-0.2305 O
64	H64	-0.8493	0.9879	1.9622 H
65	Si65	2.8744	4.2541	0.0499 Si
66	Si66	-1.9659	-3.0752	-1.2114 Si
67	C67	4.5857	4.6719	-0.5974 C
68	H68	4.7049	4.3650	-1.6437 H
69	H69	5.3669	4.1719	-0.0116 H
70	H70	4.7729	5.7520	-0.5447 H
71	C71	1.5185	5.0332	-0.9957 C
72	H72	1.6147	4.7611	-2.0539 H
73	H73	1.5698	6.1281	-0.9303 H
74	H74	0.5179	4.7340	-0.6608 H
75	C75	2.7021	4.7559	1.8548 C
76	H76	1.6971	4.5643	2.2486 H
77	H77	2.8984	5.8309	1.9665 H
78	H78	3.4217	4.2240	2.4893 H
79	C79	-3.6326	-3.8818	-0.9292 C
80	H80	-4.4592	-3.3408	-1.4035 H
81	H81	-3.8557	-3.9924	0.1385 H
82	H82	-3.6129	-4.8912	-1.3620 H
83	C83	-1.7223	-2.5264	-2.9844 C
84	H84	-2.4580	-1.7689	-3.2808 H
85	H85	-1.8512	-3.3873	-3.6534 H
86	H86	-0.7193	-2.1207	-3.1554 H
87	C87	-0.5839	-4.1299	-0.5313 C
88	H88	-0.5791	-5.1021	-1.0414 H
89	H89	-0.7198	-4.3183	0.5399 H
90	H90	0.4014	-3.6739	-0.6739 H

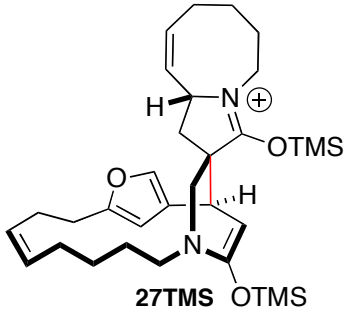


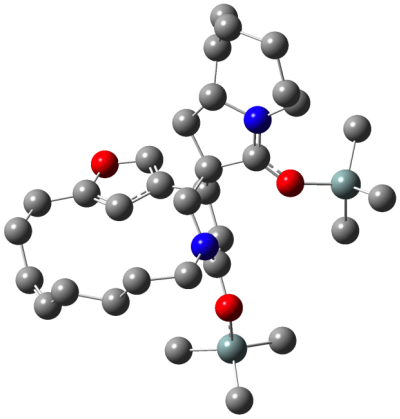


Computed free energy: -1357638.299 kcal/mol; relative energy: +2.39 kcal/mol

1	C1	-4.9536	-2.3418	2.1958 C
2	H2	-4.8913	-2.7246	3.2163 H
3	C3	-5.0301	-3.2426	1.2057 C
4	H4	-5.0385	-4.2980	1.4867 H
5	C5	-5.1493	-3.0020	-0.2789 C
6	H6	-5.1307	-1.9338	-0.5197 H
7	H7	-6.1309	-3.3727	-0.6073 H
8	C8	-4.0925	-3.7453	-1.1260 C
9	H9	-4.0119	-4.7870	-0.7866 H
10	C10	-2.7308	-3.1233	-1.1225 C
11	O11	-1.7227	-3.8872	-1.6583 O
12	C12	-0.5856	-3.1284	-1.6476 C
13	C13	-2.2320	-1.9014	-0.7795 C
14	H14	-2.7914	-1.0765	-0.3666 H
15	C15	-0.8284	-1.8956	-1.1148 C
16	C16	-4.8726	-0.8419	2.0735 C
17	H17	-5.6048	-0.3713	2.7455 H
18	H18	-5.1317	-0.5231	1.0575 H
19	C19	-3.4560	-0.3317	2.4132 C
20	H20	-3.2350	-0.5222	3.4730 H
21	H21	-2.7507	-0.9373	1.8386 H
22	C22	-3.2308	1.1516	2.0914 C
23	H23	-3.7937	1.7790	2.7973 H
24	H24	-3.6324	1.3760	1.0947 H
25	C25	-1.7568	1.6006	2.1328 C
26	H26	-1.7136	2.6880	2.0320 H
27	H27	-4.4491	-3.7976	-2.1649 H
28	H28	-1.3191	1.3505	3.1060 H
29	N29	-0.8827	0.9998	1.1153 N
30	C30	-0.9882	1.3430	-0.2229 C
31	C31	0.1562	-0.7470	-0.9714 C
32	C32	-0.4779	0.5971	-1.2323 C
33	H33	-0.4727	0.9875	-2.2421 H
34	C34	-0.1027	-0.1683	1.5131 C
35	H35	-0.7561	-1.0101	1.7754 H
36	H36	0.4582	0.0818	2.4234 H
37	C37	0.8702	-0.7023	0.4500 C
38	C38	1.4668	-2.0546	0.8968 C
39	H39	0.8559	-2.9030	0.5868 H
40	H40	1.5504	-2.0732	1.9900 H
41	N41	3.2076	-0.6459	0.1581 N

42	C42	2.8721	-2.1045	0.2841 C
43	H43	2.8404	-2.5020	-0.7350 H
44	H44	0.2941	-3.5986	-2.0641 H
45	C45	2.1443	0.1153	0.3049 C
46	C46	3.9002	-2.8360	1.0996 C
47	H47	3.7312	-2.8603	2.1749 H
48	C48	4.9982	-3.3969	0.5796 C
49	H49	5.6986	-3.8720	1.2659 H
50	C50	5.3938	-3.3869	-0.8769 C
51	H51	6.1084	-4.1987	-1.0519 H
52	H52	4.5260	-3.5934	-1.5176 H
53	C53	4.5563	-0.1874	-0.2158 C
54	H54	4.4810	0.8869	-0.3748 H
55	H55	5.2237	-0.3559	0.6339 H
56	C56	5.1185	-0.8439	-1.4987 C
57	H57	5.7056	-0.0632	-1.9964 H
58	H58	4.2931	-1.0775	-2.1833 H
59	C59	6.0460	-2.0625	-1.3358 C
60	H60	6.8633	-1.8027	-0.6497 H
61	H61	6.5120	-2.2424	-2.3129 H
62	O62	-1.5839	2.5539	-0.3952 O
63	O63	2.1516	1.4039	0.2527 O
64	H64	0.9472	-0.9189	-1.7135 H
65	Si65	-2.4537	3.2064	-1.7129 Si
66	Si66	2.8283	2.8515	0.9813 Si
67	C67	1.3604	3.7938	1.6487 C
68	H68	1.6905	4.7795	2.0032 H
69	H69	0.8974	3.2767	2.4959 H
70	H70	0.5944	3.9532	0.8822 H
71	C71	3.9815	2.3010	2.3501 C
72	H72	3.4809	1.6163	3.0458 H
73	H73	4.2909	3.1817	2.9287 H
74	H74	4.8897	1.8139	1.9806 H
75	C75	3.6614	3.7509	-0.4302 C
76	H76	4.5238	3.2043	-0.8286 H
77	H77	4.0189	4.7307	-0.0882 H
78	H78	2.9584	3.9253	-1.2538 H
79	C79	-3.8224	2.0249	-2.2292 C
80	H80	-4.5226	1.8380	-1.4059 H
81	H81	-3.4321	1.0583	-2.5671 H
82	H82	-4.3972	2.4572	-3.0590 H
83	C83	-1.3011	3.5936	-3.1505 C
84	H84	-0.9867	2.6968	-3.6965 H
85	H85	-0.3978	4.1154	-2.8102 H
86	H86	-1.8099	4.2516	-3.8675 H
87	C87	-3.1509	4.7934	-0.9910 C
88	H88	-2.3517	5.4731	-0.6704 H
89	H89	-3.7890	4.5928	-0.1218 H
90	H90	-3.7591	5.3251	-1.7338 H

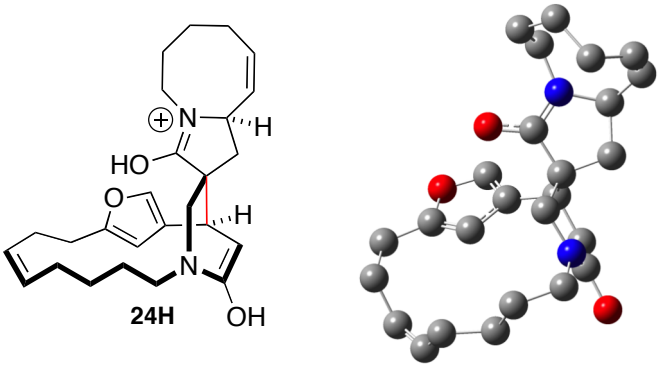




Computed free energy: -1357637.183 kcal/mol; relative energy: +3.51 kcal/mol

1	C1	5.1586	-1.8639	1.1732 C
2	H2	5.9236	-1.0910	1.2713 H
3	C3	5.2498	-2.6806	0.1127 C
4	H4	6.0833	-2.5164	-0.5736 H
5	C5	4.3785	-3.8576	-0.2533 C
6	H6	3.5547	-3.9842	0.4569 H
7	H7	4.9924	-4.7667	-0.1789 H
8	C8	3.8147	-3.8229	-1.6930 C
9	H9	4.6236	-3.5887	-2.4005 H
10	C10	2.6815	-2.8647	-1.8787 C
11	O11	2.0245	-2.9020	-3.0840 O
12	C12	1.0160	-1.9753	-3.0257 C
13	C13	2.1015	-1.9265	-1.0810 C
14	H14	2.4242	-1.6572	-0.0897 H
15	C15	1.0082	-1.3426	-1.8184 C
16	C16	4.0973	-1.8363	2.2434 C
17	H17	4.5564	-2.0099	3.2283 H
18	H18	3.3772	-2.6488	2.0913 H
19	C19	3.3412	-0.4878	2.2679 C
20	H20	4.0229	0.3115	2.5890 H
21	H21	3.0541	-0.2408	1.2408 H
22	C22	2.0873	-0.4958	3.1578 C
23	H23	2.3666	-0.3798	4.2139 H
24	H24	1.5964	-1.4754	3.0854 H
25	C25	1.0581	0.6061	2.8237 C
26	H26	0.2155	0.5201	3.5224 H
27	H27	3.4663	-4.8297	-1.9610 H
28	H28	1.4963	1.5944	2.9631 H
29	N29	0.4998	0.5550	1.4628 N
30	C30	1.0755	1.2713	0.4121 C
31	C31	0.0861	-0.2264	-1.3593 C
32	C32	0.8692	0.9788	-0.8931 C
33	H33	1.2808	1.6312	-1.6534 H
34	H34	-0.5271	0.0527	-2.2274 H
35	C35	-0.1711	-0.6944	1.1312 C
36	H36	-0.8799	-0.9217	1.9373 H
37	H37	0.5353	-1.5336	1.0904 H
38	C38	-0.8999	-0.6935	-0.2411 C
39	C39	-1.5295	-2.0815	-0.4953 C
40	H40	-0.9265	-2.8961	-0.0892 H

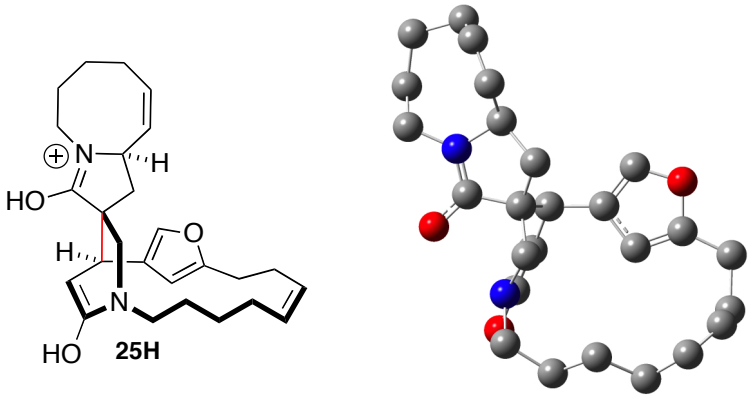
41	H41	-1.6293	-2.2426	-1.5737 H
42	N42	-3.2235	-0.5617	0.1336 N
43	C43	-2.9227	-2.0325	0.1477 C
44	H44	-2.8807	-2.3293	1.2002 H
45	H45	0.4155	-1.8792	-3.9192 H
46	C46	-2.1586	0.1606	-0.1419 C
47	C47	-3.9879	-2.8113	-0.5726 C
48	H48	-3.8498	-2.9335	-1.6458 H
49	C49	-5.0821	-3.2989	0.0240 C
50	H50	-5.8109	-3.8167	-0.5988 H
51	C51	-5.4345	-3.1536	1.4845 C
52	H52	-6.1689	-3.9232	1.7460 H
53	H53	-4.5556	-3.3370	2.1168 H
54	C54	-4.5447	-0.0401	0.5235 C
55	H55	-4.4345	1.0401	0.5956 H
56	H56	-5.2525	-0.2550	-0.2818 H
57	C57	-5.0648	-0.5765	1.8771 C
58	H58	-5.6073	0.2582	2.3360 H
59	H59	-4.2150	-0.7799	2.5412 H
60	C60	-6.0311	-1.7751	1.8501 C
61	H61	-6.8647	-1.5483	1.1718 H
62	H62	-6.4666	-1.8582	2.8538 H
63	O63	-2.1458	1.4466	-0.2374 O
64	O64	1.7807	2.3495	0.8442 O
65	Si65	-2.9113	2.8127	-1.0420 Si
66	Si66	3.0071	3.2814	0.1052 Si
67	C67	-4.0588	2.1242	-2.3521 C
68	H68	-4.9304	1.6074	-1.9370 H
69	H69	-3.5334	1.4333	-3.0227 H
70	H70	-4.4311	2.9543	-2.9674 H
71	C71	-1.4865	3.7660	-1.7795 C
72	H72	-1.8572	4.7073	-2.2065 H
73	H73	-0.9915	3.2096	-2.5823 H
74	H74	-0.7397	4.0150	-1.0189 H
75	C75	-3.7629	3.7882	0.3089 C
76	H76	-3.0766	3.9883	1.1406 H
77	H77	-4.6507	3.2872	0.7104 H
78	H78	-4.0850	4.7580	-0.0926 H
79	C79	2.2940	4.4014	-1.2291 C
80	H80	3.0773	5.0861	-1.5820 H
81	H81	1.4730	5.0170	-0.8426 H
82	H82	1.9245	3.8512	-2.1015 H
83	C83	3.6509	4.3208	1.5294 C
84	H84	4.4385	5.0035	1.1851 H
85	H85	4.0767	3.6991	2.3264 H
86	H86	2.8546	4.9329	1.9705 H
87	C87	4.3460	2.1627	-0.5947 C
88	H88	3.9470	1.4281	-1.3029 H
89	H89	4.8675	1.6150	0.1987 H
90	H90	5.0955	2.7639	-1.1267 H



Computed free energy: -844810.5757 kcal/mol; relative energy: +2.66 kcal/mol

1	C1	-5.1979	0.2592	-0.8714 C
2	H2	-5.9241	0.8742	-0.3362 H
3	C3	-5.2256	-1.0616	-0.6374 C
4	H4	-5.9748	-1.4291	0.0669 H
5	C5	-4.3807	-2.1482	-1.2578 C
6	H6	-3.6377	-1.7359	-1.9485 H
7	H7	-5.0391	-2.7884	-1.8621 H
8	C8	-3.6782	-3.0770	-0.2418 C
9	H9	-4.4074	-3.4360	0.4984 H
10	C10	-2.5246	-2.4429	0.4671 C
11	O11	-1.8267	-3.2266	1.3487 O
12	C12	-0.8275	-2.4589	1.8811 C
13	C13	-1.9739	-1.1949	0.4437 C
14	H14	-2.3452	-0.3573	-0.1223 H
15	C15	-0.8640	-1.1941	1.3704 C
16	C16	-4.2508	1.0289	-1.7568 C
17	H17	-4.8165	1.5473	-2.5453 H
18	H18	-3.5666	0.3442	-2.2712 H
19	C19	-3.4246	2.0653	-0.9603 C
20	H20	-4.0755	2.8820	-0.6213 H
21	H21	-3.0575	1.5819	-0.0488 H
22	C22	-2.2335	2.6330	-1.7512 C
23	H23	-2.5749	3.3966	-2.4631 H
24	H24	-1.7872	1.8350	-2.3597 H
25	C25	-1.1290	3.2670	-0.8810 C
26	H26	-0.3310	3.6411	-1.5342 H
27	H27	-3.3198	-3.9728	-0.7671 H
28	H28	-1.5197	4.1190	-0.3245 H
29	N29	-0.5017	2.3488	0.0847 N
30	C30	-0.9738	2.2279	1.3805 C
31	C31	0.0423	-0.0356	1.7401 C
32	C32	-0.7188	1.1816	2.2015 C
33	H33	-1.0626	1.2171	3.2306 H
34	H34	0.6897	-0.3862	2.5540 H
35	C35	0.2043	1.2147	-0.4903 C
36	H36	0.8929	1.5964	-1.2536 H
37	H37	-0.4873	0.5320	-1.0027 H
38	C38	1.0063	0.4378	0.5795 C
39	C39	2.2068	1.2519	1.1309 C

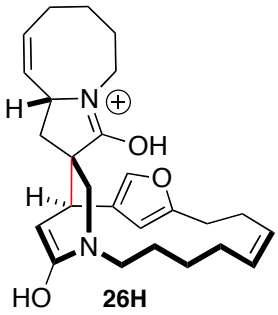
40	H40	1.9855	1.6852	2.1073 H
41	H41	2.4502	2.0664	0.4438 H
42	N42	2.9872	-0.8045	0.2399 N
43	C43	3.3951	0.2616	1.2057 C
44	H44	3.4159	-0.2282	2.1863 H
45	H45	-0.1958	-2.9463	2.6101 H
46	C46	1.7176	-0.7352	-0.0412 C
47	C47	4.7533	0.8587	0.9583 C
48	H48	5.2475	1.1814	1.8727 H
49	C49	5.3953	1.0302	-0.2037 C
50	H50	6.3923	1.4661	-0.1396 H
51	C51	4.9635	0.6528	-1.6012 C
52	H52	3.8865	0.7975	-1.7448 H
53	H53	5.4595	1.3399	-2.2958 H
54	C54	3.8604	-1.9306	-0.1566 C
55	H55	4.7121	-1.9183	0.5261 H
56	H56	3.2934	-2.8493	0.0174 H
57	C57	4.3107	-1.8683	-1.6236 C
58	H58	3.4227	-1.7508	-2.2563 H
59	H59	4.7253	-2.8562	-1.8589 H
60	C60	5.3500	-0.7989	-1.9867 C
61	H61	5.5015	-0.8487	-3.0716 H
62	H62	6.3160	-1.0479	-1.5287 H
63	O63	1.1673	-1.6648	-0.7886 O
64	O64	-1.6764	3.3278	1.7744 O
65	H65	-1.9848	3.1811	2.6864 H
66	H66	0.1876	-1.5796	-0.7803 H



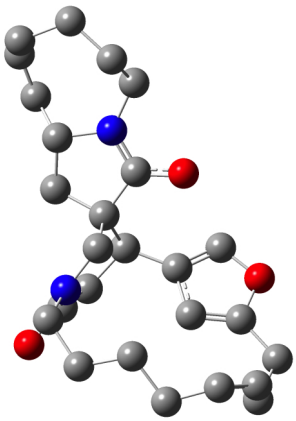
Computed free energy: -844813.2344 kcal/mol; relative energy: 0 kcal/mol

1	C1	-5.2698	0.3508	-1.5474 C
2	H2	-5.4335	0.2598	-2.6230 H
3	C3	-5.2650	1.5902	-1.0349 C
4	H4	-5.4352	2.4161	-1.7288 H
5	C5	-5.1077	2.0261	0.4014 C
6	H6	-4.9590	1.1738	1.0723 H
7	H7	-6.0497	2.4989	0.7130 H
8	C8	-3.9931	3.0730	0.6326 C
9	H9	-4.0329	3.8368	-0.1563 H
10	C10	-2.6103	2.5052	0.7070 C
11	O11	-1.5844	3.4143	0.8039 O
12	C12	-0.4224	2.7090	0.9417 C
13	C13	-2.0985	1.2450	0.7819 C
14	H14	-2.6655	0.3270	0.7677 H
15	C15	-0.6678	1.3664	0.9309 C
16	C16	-5.0028	-0.9532	-0.8404 C
17	H17	-5.8233	-1.6603	-1.0307 H
18	H18	-4.9634	-0.8054	0.2450 H
19	C19	-3.6667	-1.5675	-1.3145 C
20	H20	-3.7462	-1.8686	-2.3681 H
21	H21	-2.9288	-0.7644	-1.2843 H
22	C22	-3.1933	-2.7575	-0.4637 C
23	H23	-3.8113	-3.6366	-0.6932 H
24	H24	-3.3626	-2.5442	0.5982 H
25	C25	-1.7231	-3.1879	-0.6441 C
26	H26	-1.5817	-4.1662	-0.1804 H
27	H27	-4.1979	3.6053	1.5724 H
28	H28	-1.4731	-3.2925	-1.7046 H
29	N29	-0.6879	-2.2796	-0.0669 N
30	C30	-0.7798	-1.9951	1.3183 C
31	C31	0.3301	0.2332	1.0936 C
32	C32	-0.2639	-0.8971	1.8974 C
33	H33	-0.2966	-0.8027	2.9789 H
34	C34	-0.2964	-1.1412	-0.9357 C
35	H35	-1.1242	-0.4572	-1.1309 H
36	H36	0.0225	-1.5638	-1.8938 H
37	C37	0.8413	-0.3376	-0.2961 C
38	C38	1.4681	0.7440	-1.2009 C
39	H39	0.9653	1.7078	-1.1156 H

40	H40	1.4269	0.4212	-2.2477 H
41	N41	3.1831	-0.6053	-0.2969 N
42	C42	2.9380	0.8156	-0.7482 C
43	H43	3.0402	1.4436	0.1426 H
44	H44	0.4765	3.2992	1.0508 H
45	C45	2.0531	-1.2257	-0.0960 C
46	C46	3.9200	1.2441	-1.7996 C
47	H47	3.6142	1.1067	-2.8351 H
48	C48	5.1365	1.7253	-1.5151 C
49	H49	5.7920	1.9731	-2.3496 H
50	C50	5.7209	1.9025	-0.1354 C
51	H51	6.4978	2.6738	-0.1816 H
52	H52	4.9603	2.2668	0.5681 H
53	C53	4.5186	-1.1990	-0.1097 C
54	H54	4.3448	-2.2310	0.1975 H
55	H55	5.0141	-1.2182	-1.0842 H
56	C56	5.3861	-0.4736	0.9410 C
57	H57	5.9951	-1.2497	1.4194 H
58	H58	4.7363	-0.0727	1.7293 H
59	C59	6.3542	0.6128	0.4379 C
60	H60	7.0279	0.1756	-0.3112 H
61	H61	6.9856	0.8992	1.2882 H
62	O62	-1.3147	-3.0477	1.9953 O
63	O63	1.9956	-2.4955	0.2011 O
64	H64	1.0227	-2.7735	0.1386 H
65	H65	-1.3202	-2.8315	2.9457 H
66	H66	1.2041	0.6311	1.6241 H



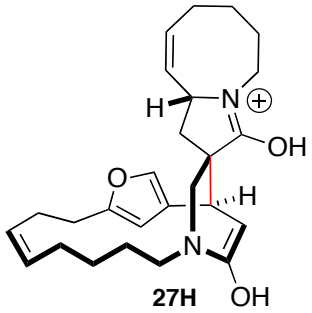
26H



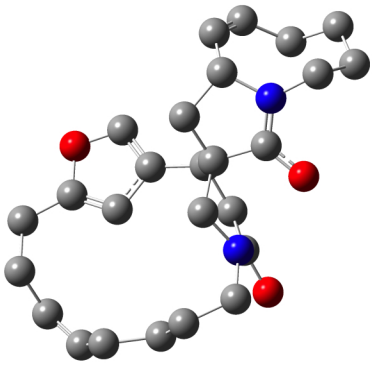
Computed free energy: -844812.5498 kcal/mol; relative energy: +0.68 kcal/mol

1	C1	-4.7028	0.0812	2.3366 C
2	H2	-4.5407	0.0521	3.4159 H
3	C3	-5.0463	-1.0684	1.7381 C
4	H4	-5.1534	-1.9516	2.3715 H
5	C5	-5.3566	-1.3166	0.2827 C
6	H6	-5.2479	-0.4058	-0.3150 H
7	H7	-6.4131	-1.6094	0.2043 H
8	C8	-4.5364	-2.4629	-0.3512 C
9	H9	-4.5192	-3.3268	0.3265 H
10	C10	-3.1307	-2.1051	-0.7196 C
11	O11	-2.3082	-3.1562	-1.0419 O
12	C12	-1.1044	-2.6352	-1.4224 C
13	C13	-2.4531	-0.9354	-0.8919 C
14	H14	-2.8485	0.0580	-0.7512 H
15	C15	-1.1252	-1.2646	-1.3517 C
16	C16	-4.4373	1.4183	1.6943 C
17	H17	-4.9984	2.2037	2.2213 H
18	H18	-4.7858	1.4282	0.6551 H
19	C19	-2.9307	1.7514	1.7219 C
20	H20	-2.5871	1.8347	2.7627 H
21	H21	-2.4079	0.8918	1.2943 H
22	C22	-2.5511	3.0190	0.9443 C
23	H23	-2.8795	3.9117	1.4950 H
24	H24	-3.0804	3.0389	-0.0164 H
25	C25	-1.0427	3.1660	0.6670 C
26	H26	-0.8525	4.1464	0.2210 H
27	H27	-5.0517	-2.8061	-1.2596 H
28	H28	-0.4785	3.1234	1.6046 H
29	N29	-0.4665	2.1329	-0.2115 N
30	C30	-0.8102	2.0620	-1.5472 C
31	C31	-0.0285	-0.2907	-1.7753 C
32	C32	-0.5920	0.9877	-2.3442 C
33	H33	-0.8164	1.0482	-3.4041 H
34	C34	0.1812	0.9843	0.4097 C
35	H35	-0.5397	0.3226	0.9062 H
36	H36	0.8636	1.3556	1.1833 H
37	C37	0.9682	0.1530	-0.6385 C
38	C38	2.1862	0.9252	-1.2099 C

39 H39	2.0423	2.0053	-1.1630 H
40 H40	2.3379	0.6466	-2.2572 H
41 N41	2.9496	-0.8271	0.1939 N
42 C42	3.4040	0.4900	-0.3731 C
43 H43	3.5416	1.1515	0.4880 H
44 H44	-0.3705	-3.3491	-1.7712 H
45 C45	1.6612	-0.9820	0.0743 C
46 C46	4.6930	0.3459	-1.1307 C
47 H47	4.6075	0.1318	-2.1947 H
48 C48	5.8991	0.4104	-0.5538 C
49 H49	6.7720	0.2473	-1.1853 H
50 C50	6.1729	0.6349	0.9132 C
51 H51	7.1899	1.0276	1.0221 H
52 H52	5.4986	1.3986	1.3226 H
53 C53	3.8542	-1.7749	0.8705 C
54 H54	3.2263	-2.5963	1.2154 H
55 H55	4.5375	-2.1700	0.1133 H
56 C56	4.6355	-1.1684	2.0565 C
57 H57	4.7310	-1.9714	2.7966 H
58 H58	4.0268	-0.3909	2.5357 H
59 C59	6.0558	-0.6447	1.7743 C
60 H60	6.6490	-1.4473	1.3160 H
61 H61	6.5206	-0.4358	2.7459 H
62 O62	-1.3418	3.2351	-1.9959 O
63 O63	1.0677	-2.0318	0.5874 O
64 H64	0.1358	-2.0877	0.2503 H
65 H65	-1.5905	3.1183	-2.9303 H
66 H66	0.5779	-0.7953	-2.5368 H



27H



Computed free energy: -844811.6575 kcal/mol; relative energy: +1.58 kcal/mol

1	C1	5.2986	-0.3760	0.4669 C
2	H2	5.7129	-0.8775	1.3439 H
3	C3	5.3506	0.9648	0.4500 C
4	H4	5.8081	1.4569	1.3109 H
5	C5	4.9030	1.9163	-0.6338 C
6	H6	4.4464	1.3821	-1.4734 H
7	H7	5.7972	2.4147	-1.0347 H
8	C8	3.9494	3.0391	-0.1604 C
9	H9	4.3657	3.5221	0.7359 H
10	C10	2.5537	2.5751	0.1106 C
11	O11	1.5938	3.5403	0.2966 O
12	C12	0.4037	2.8982	0.5069 C
13	C13	1.9764	1.3472	0.2084 C
14	H14	2.4929	0.4056	0.1384 H
15	C15	0.5712	1.5447	0.4610 C
16	C16	4.6908	-1.3028	-0.5561 C
17	H17	5.4632	-1.9769	-0.9557 H
18	H18	4.3067	-0.7338	-1.4106 H
19	C19	3.5442	-2.1464	0.0481 C
20	H20	3.9493	-2.8649	0.7724 H
21	H21	2.9008	-1.4764	0.6258 H
22	C22	2.7003	-2.8804	-1.0085 C
23	H23	3.2292	-3.7757	-1.3615 H
24	H24	2.5832	-2.2384	-1.8911 H
25	C25	1.3083	-3.3408	-0.5365 C
26	H26	0.7989	-3.8462	-1.3636 H
27	H27	3.9121	3.8202	-0.9313 H
28	H28	1.3882	-4.0533	0.2843 H
29	N29	0.3877	-2.2543	-0.0924 N
30	C30	0.4912	-1.7792	1.2433 C
31	C31	-0.4733	0.4673	0.6798 C
32	C32	0.0359	-0.5792	1.6421 C
33	H33	0.0783	-0.3265	2.6977 H
34	H34	-1.3599	0.9521	1.1037 H
35	C35	0.1880	-1.1979	-1.1146 C
36	H36	-0.0934	-1.7017	-2.0448 H
37	H37	1.1043	-0.6320	-1.3039 H
38	C38	-0.9218	-0.2285	-0.6698 C
39	C39	-1.3803	0.7733	-1.7548 C
40	H40	-1.1542	0.3727	-2.7479 H

41	H41	-0.8897	1.7416	-1.6554 H
42	N42	-3.2675	-0.3959	-0.9170 N
43	C43	-2.9255	0.8829	-1.5882 C
44	H44	-3.3995	0.8473	-2.5759 H
45	H45	-0.4509	3.5349	0.6852 H
46	C46	-2.2035	-1.0175	-0.4872 C
47	C47	-3.4216	2.1227	-0.8914 C
48	H48	-3.2817	3.0079	-1.5116 H
49	C49	-4.0164	2.2889	0.2978 C
50	H50	-4.3113	3.3136	0.5233 H
51	C51	-4.3793	1.2895	1.3776 C
52	H52	-3.5317	0.6377	1.6204 H
53	H53	-4.5818	1.8652	2.2866 H
54	C54	-4.6319	-0.9621	-0.9130 C
55	H55	-5.2068	-0.3790	-1.6360 H
56	H56	-4.5537	-1.9871	-1.2882 H
57	C57	-5.3094	-0.9628	0.4607 C
58	H58	-4.6985	-1.5480	1.1593 H
59	H59	-6.2478	-1.5168	0.3326 H
60	C60	-5.6211	0.4075	1.0745 C
61	H61	-6.1526	0.2231	2.0157 H
62	H62	-6.3177	0.9589	0.4299 H
63	O63	-2.2642	-2.2301	-0.0165 O
64	O64	0.9592	-2.7443	2.0782 O
65	H65	0.9540	-2.3931	2.9876 H
66	H66	-1.2995	-2.5665	0.0497 H
