Supporting Information

Verbenanone, an octahydro-5H-chromen-5-one from a Hawaiian-Plant Associated Fungus FT431

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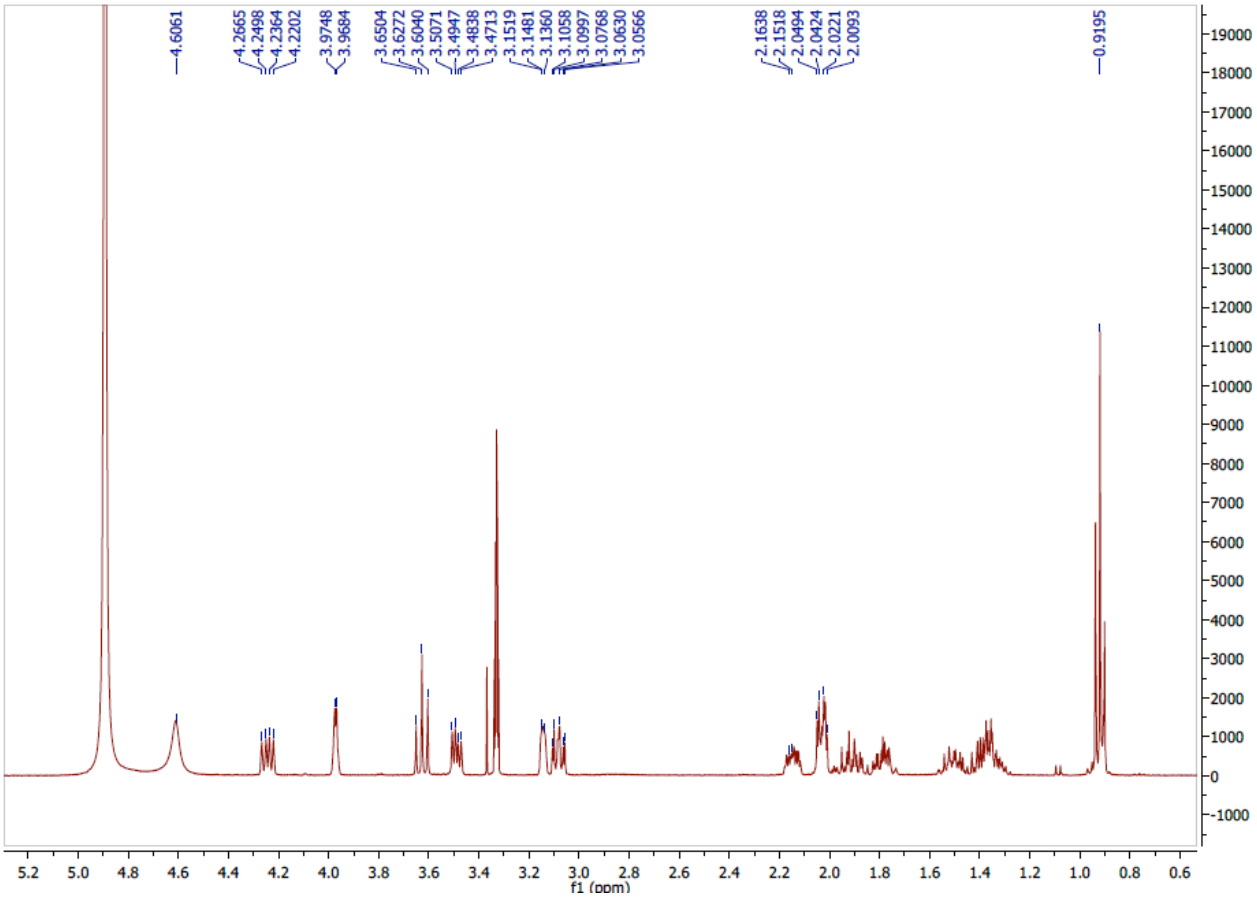
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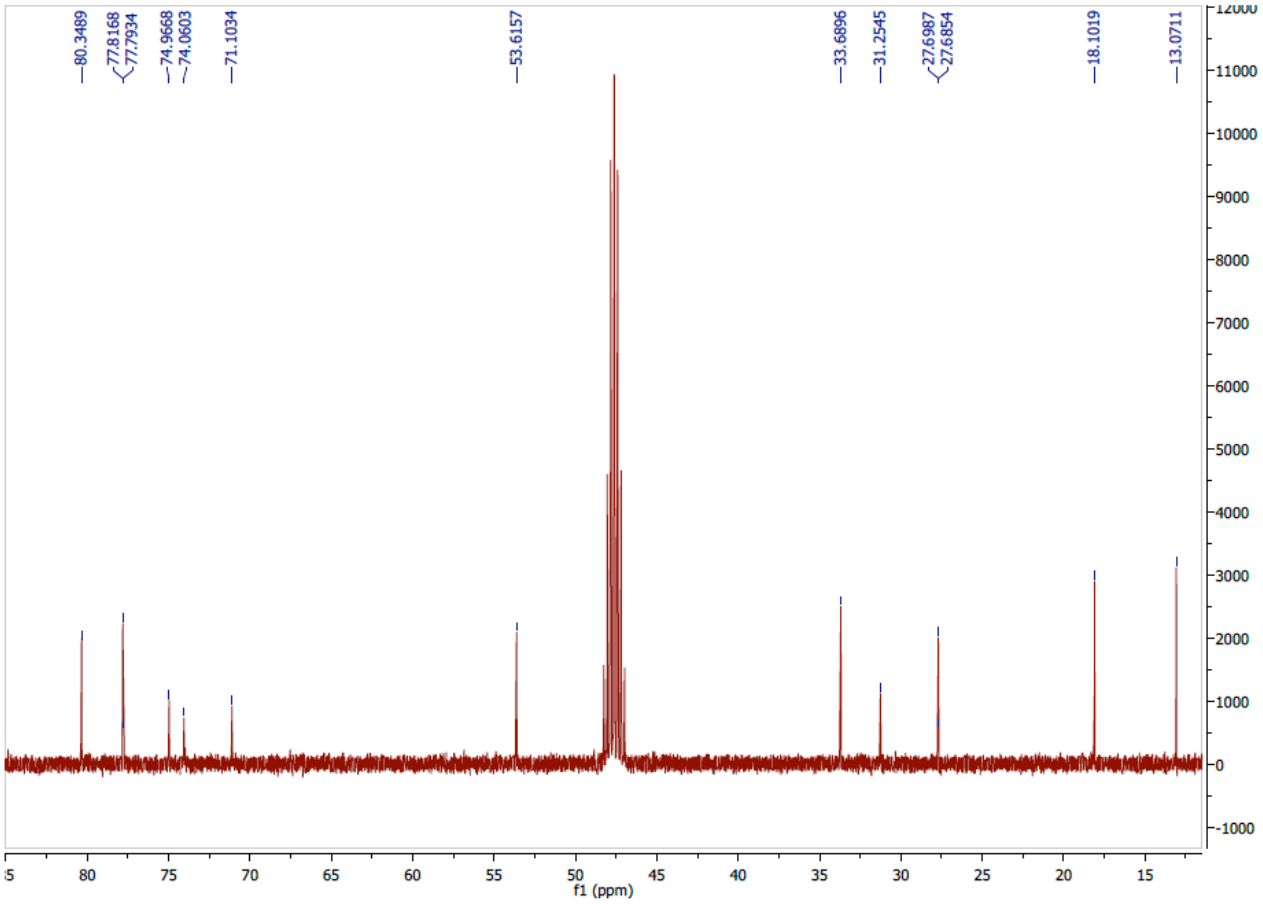
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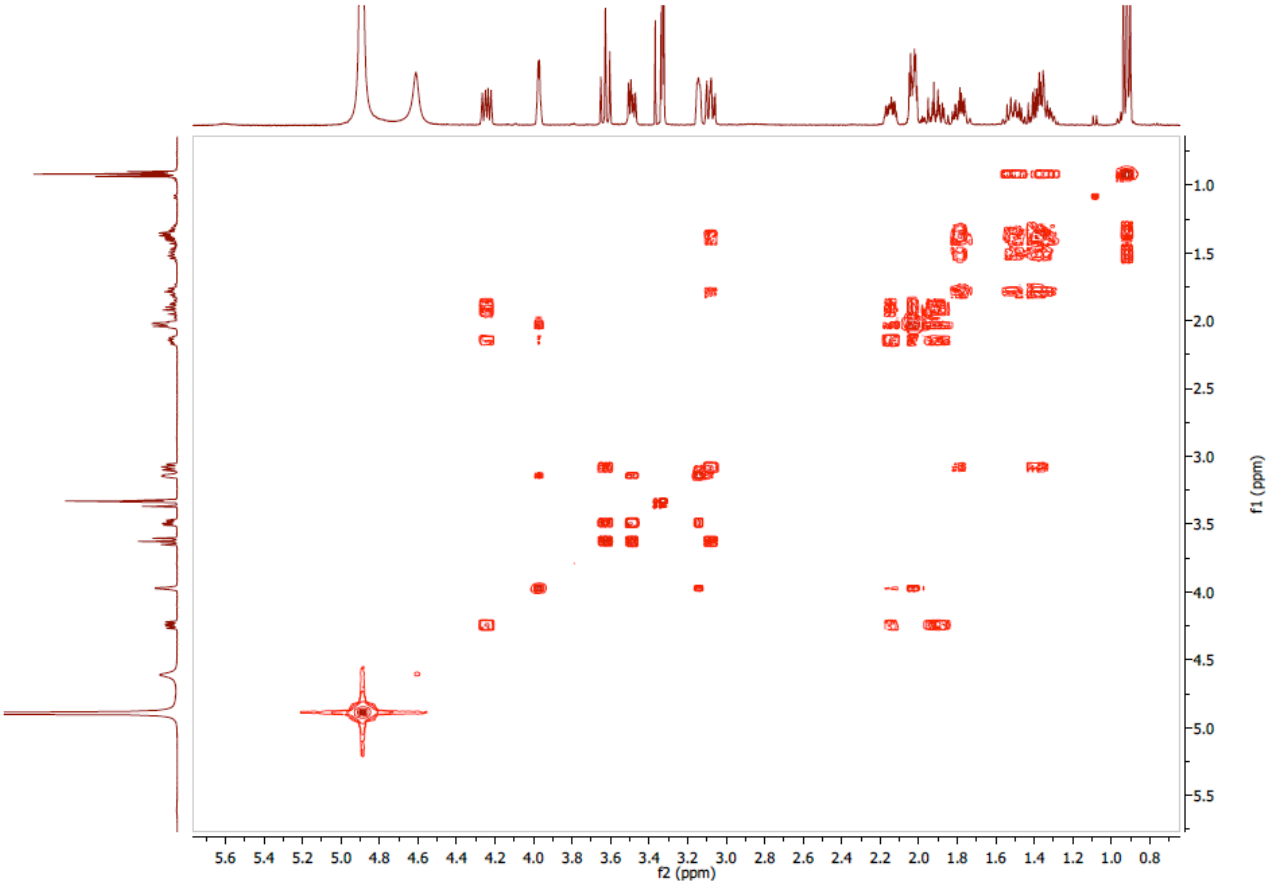
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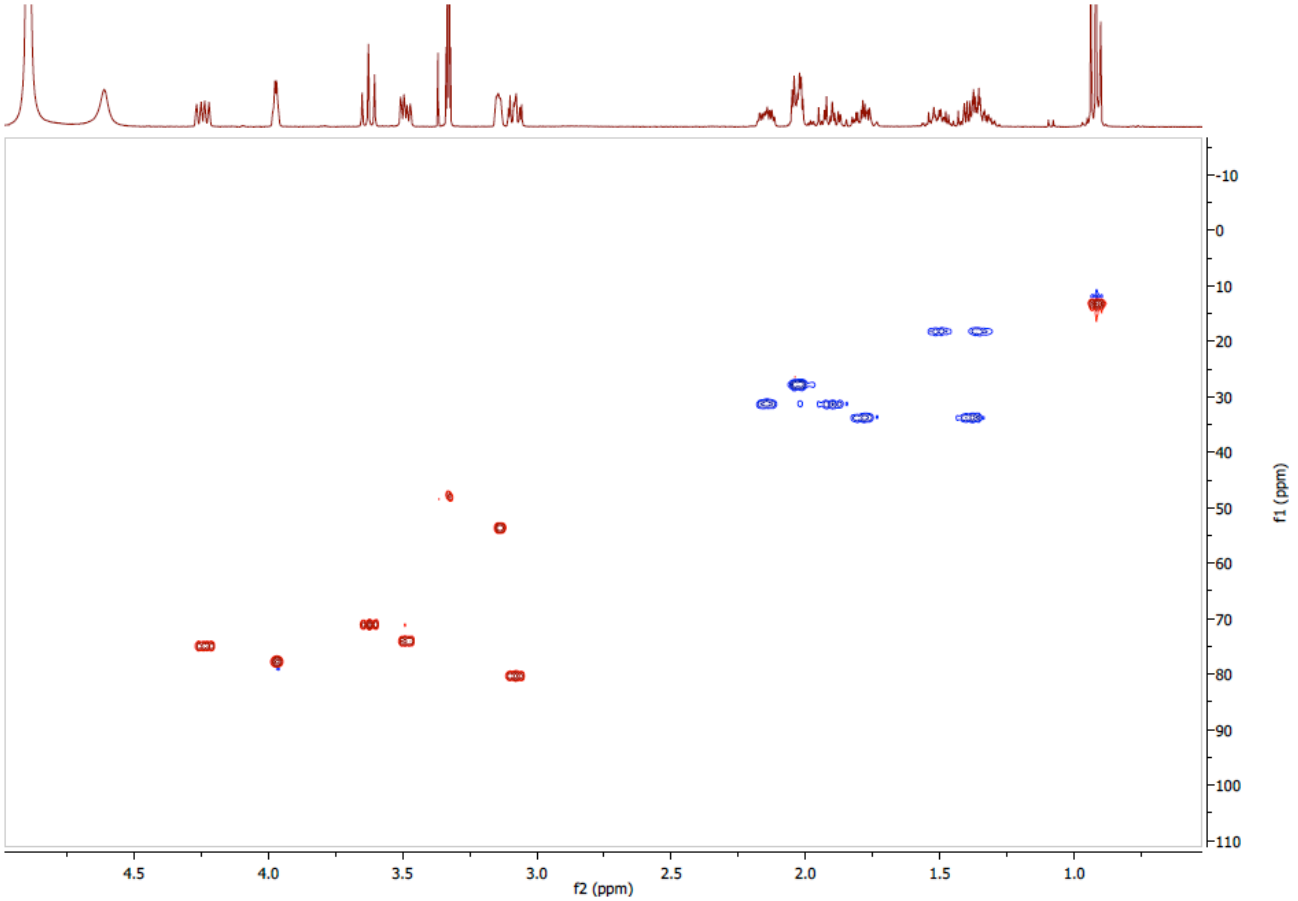
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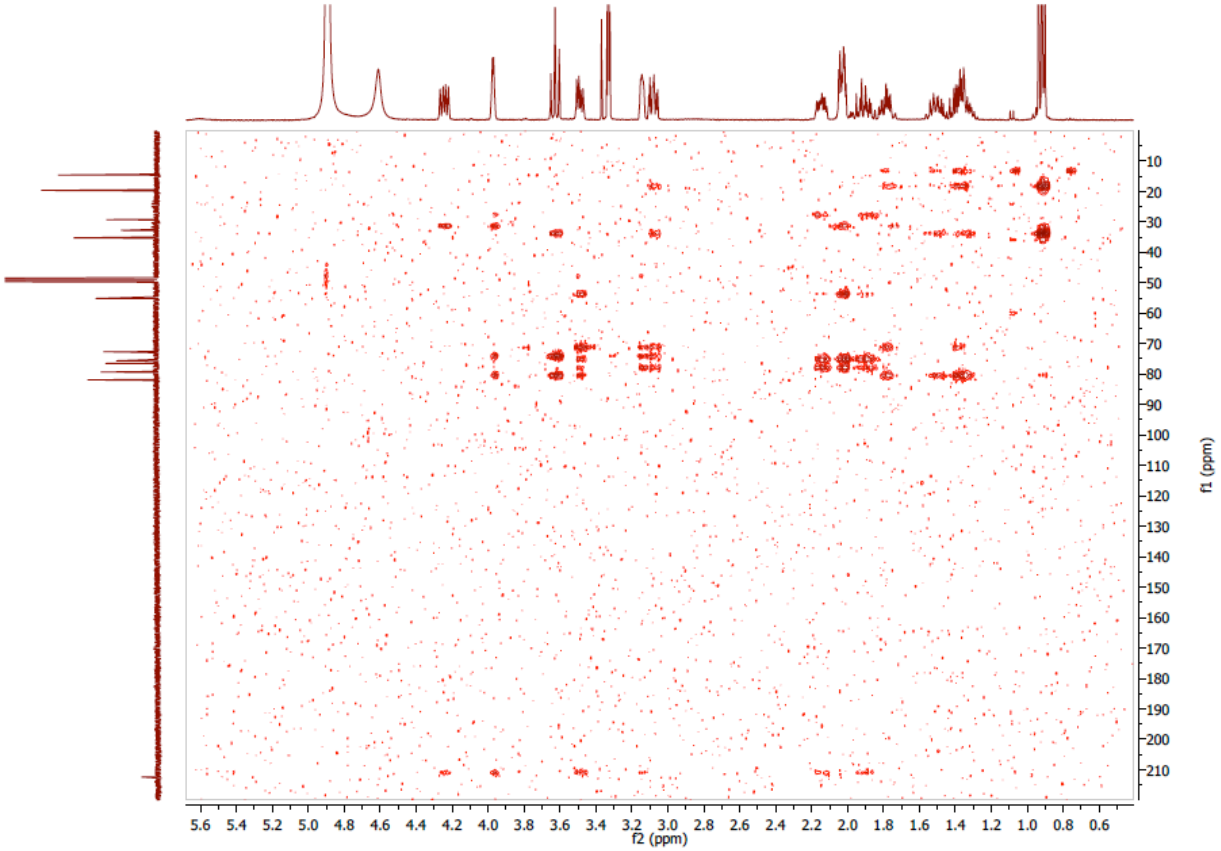
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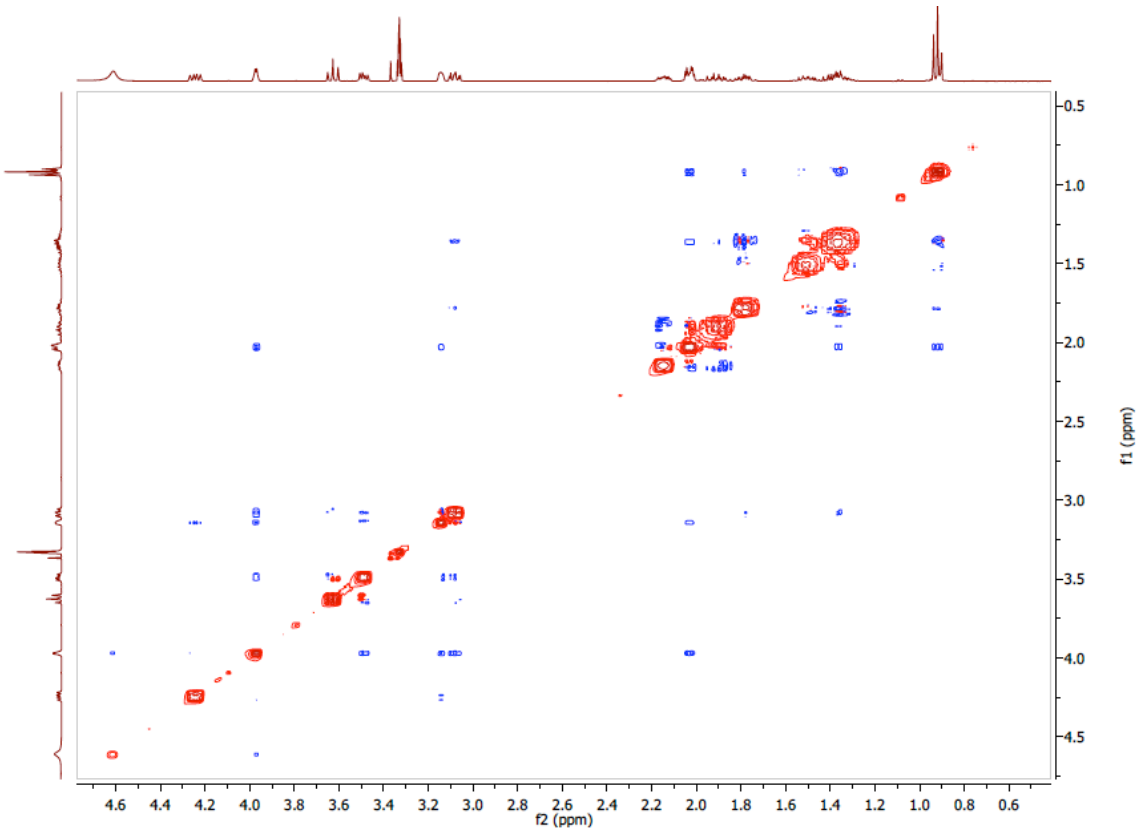
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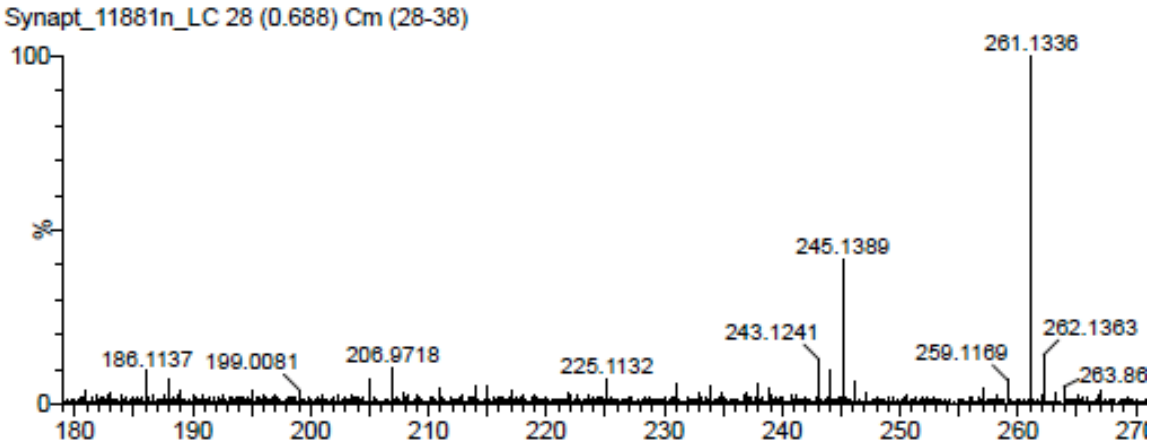
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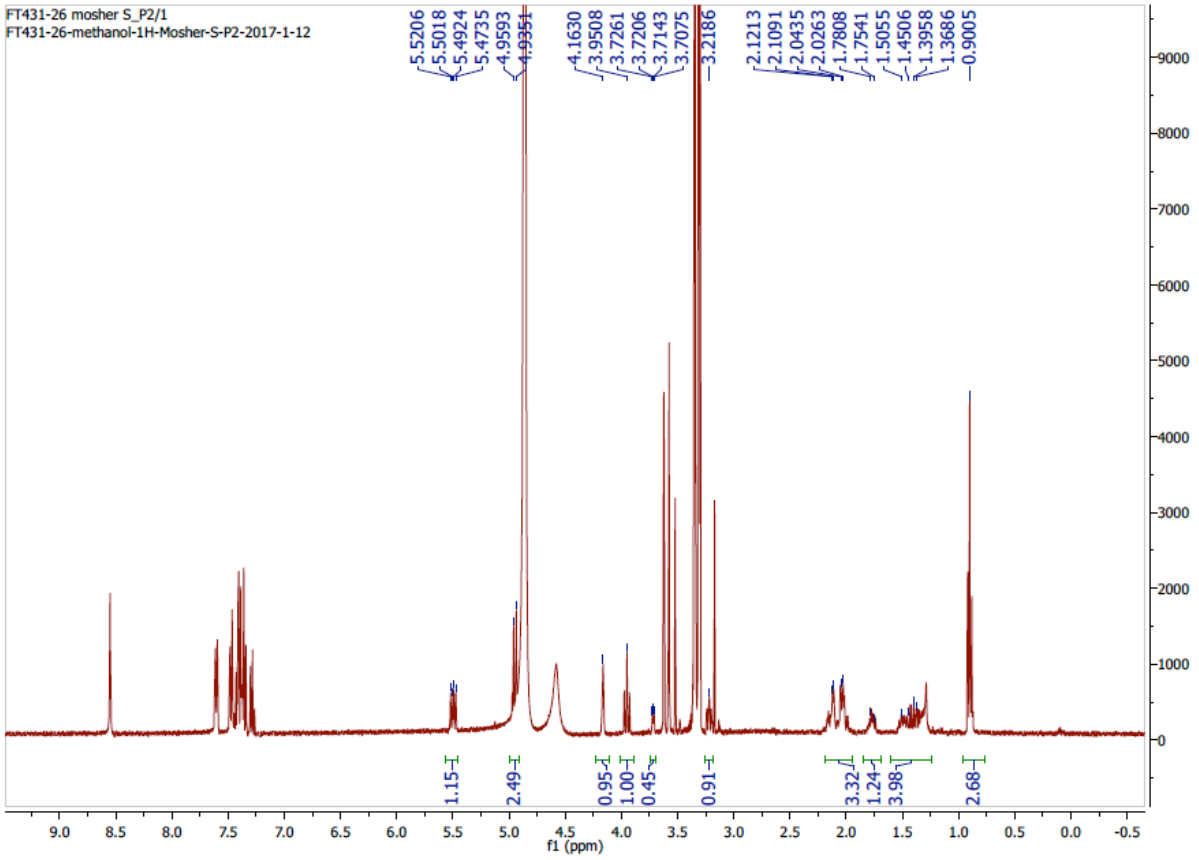
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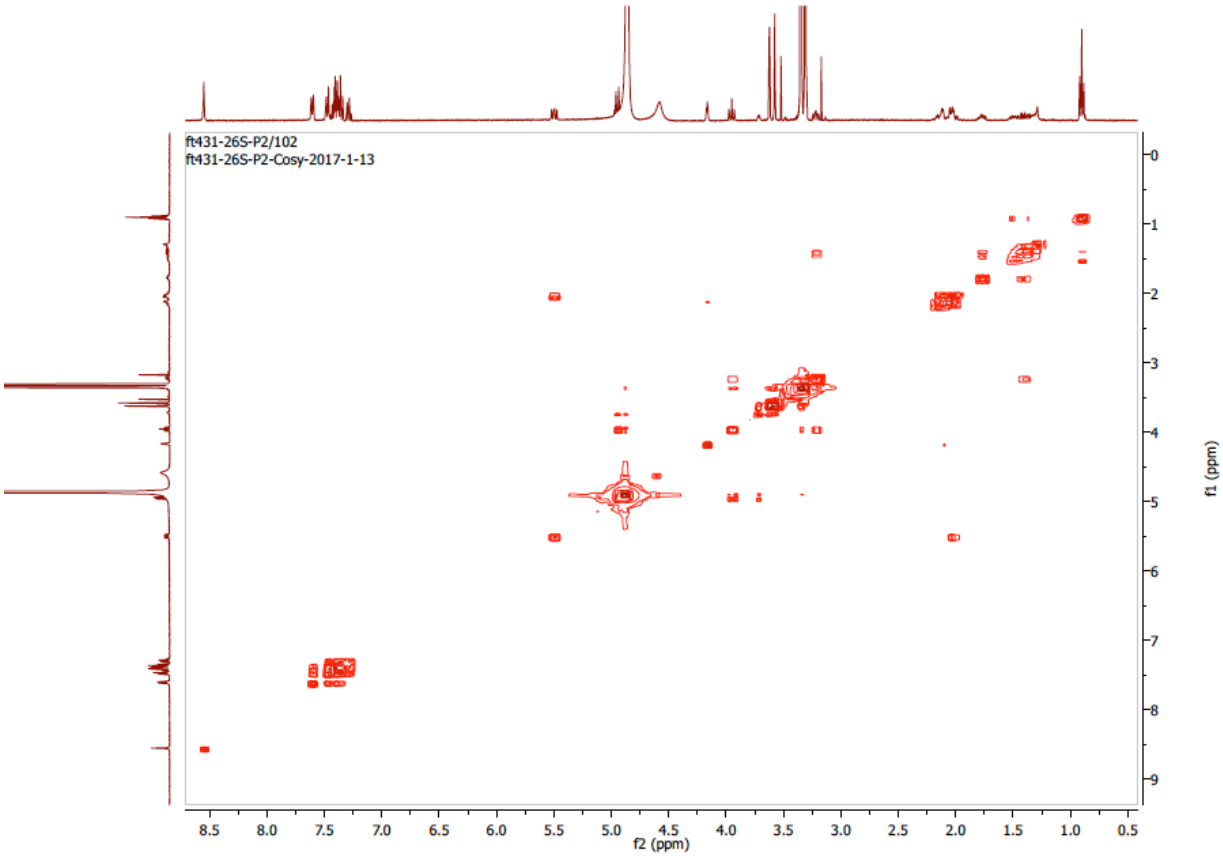
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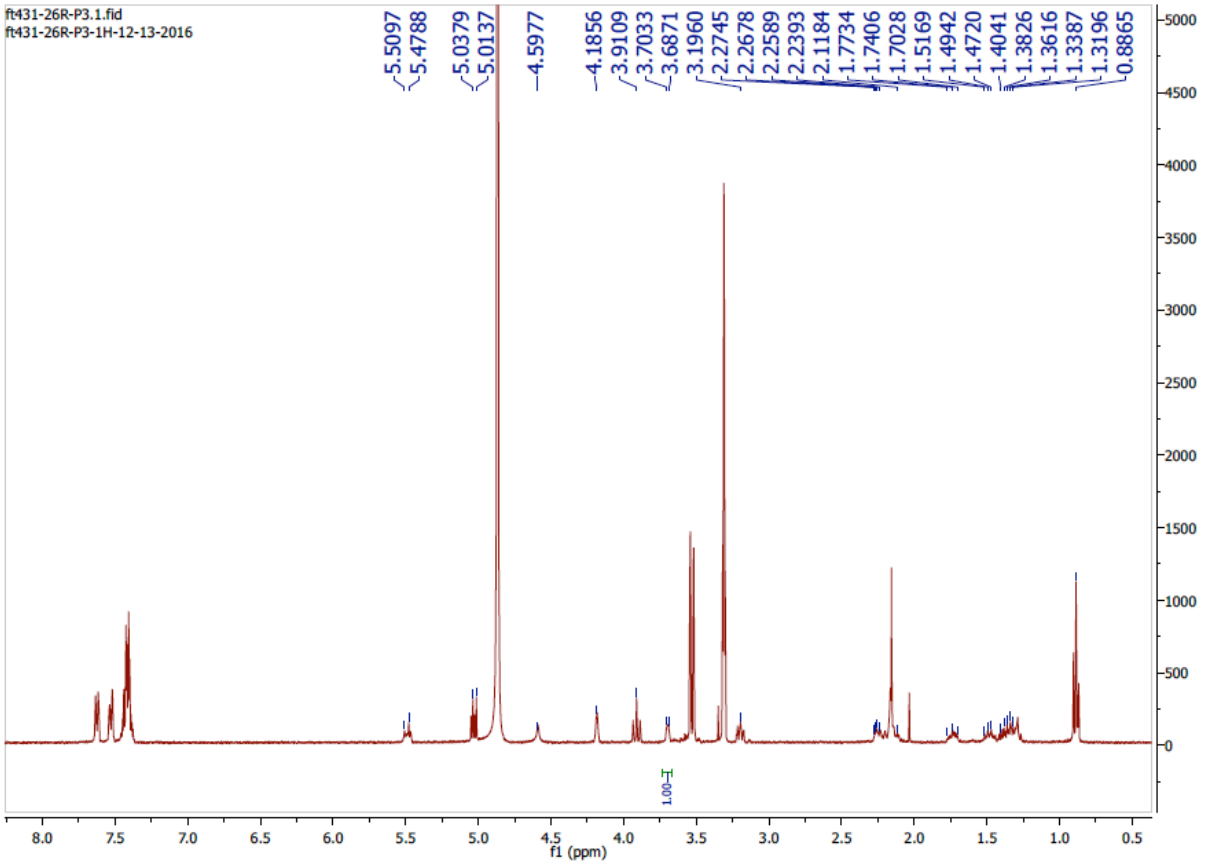
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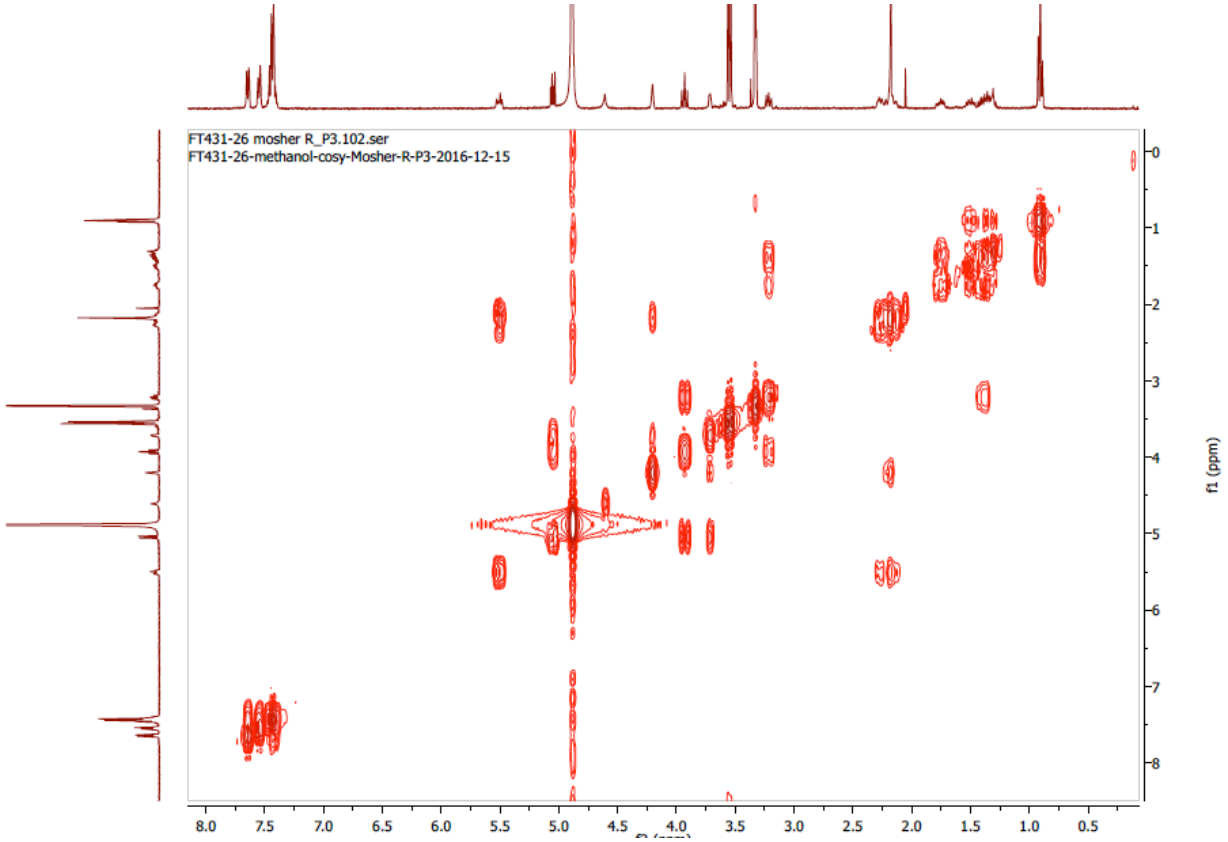
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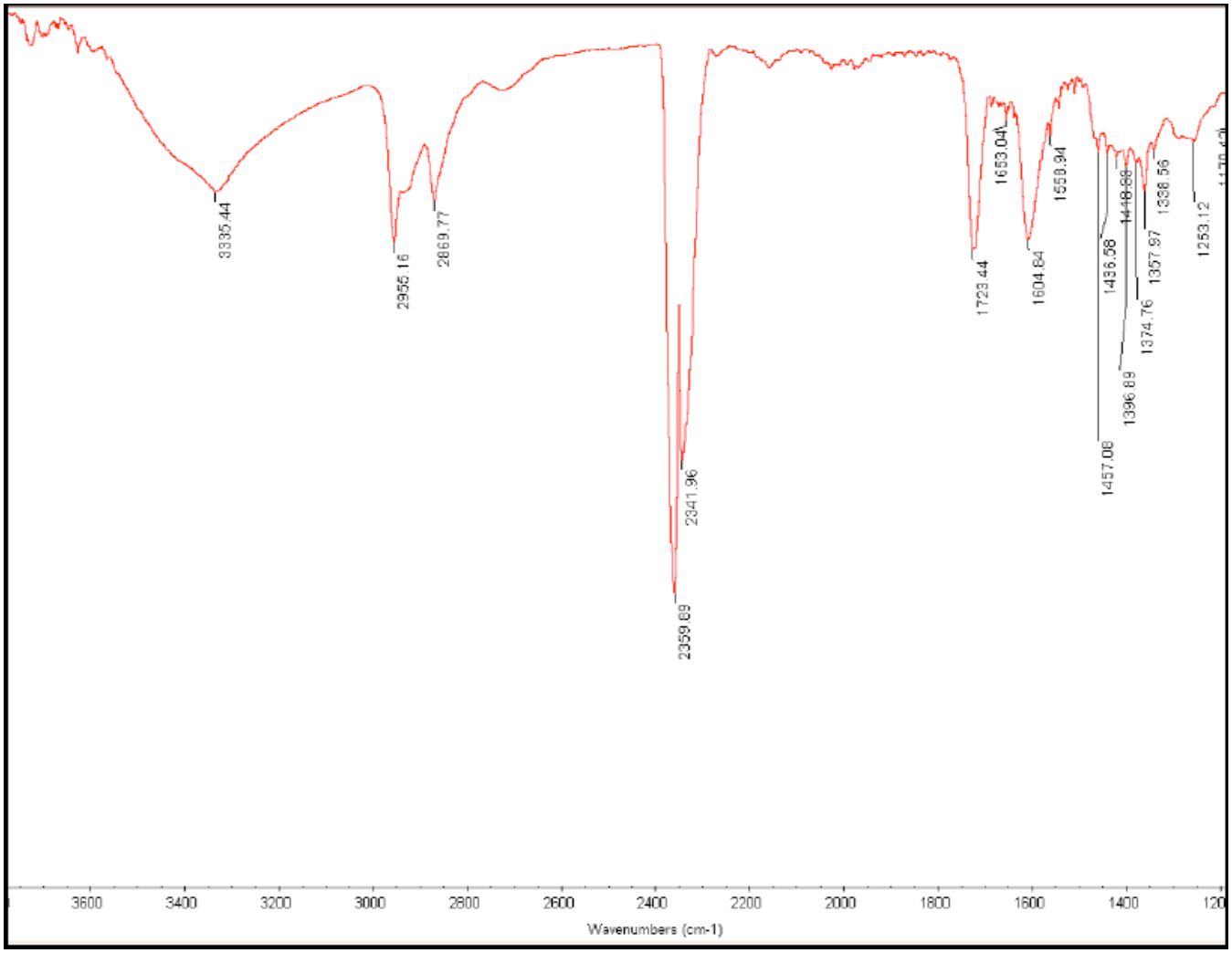
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Wavenumbers (cm-1)

Computational Methods. All the quantum mechanical calculations were performed using Gaussian 09.[1] Systematic conformational searches were done for each compound in the gas phase using the MMFF force field, implemented in Spartan 08.[2] All conformers within 10 kcal/mol of the lowest energy conformer were subjected to further reoptimization at the PCM/B3LYP/6-31G* level of theory using methanol as solvent. The choice for the 10 kcal/mol of cutoff was set as a balance between reducing the overall CPU calculation time and minimizing the possibility of losing further contributing conformers. Frequency calculations were done for all optimized geometries at the PCM/B3LYP/6-31G* level to determine the nature of the stationary point found, and to compute the thermochemical properties (at 1 atm and 298.15 K). All the PCM/B3LYP/6-31G* optimized geometries were next subjected to NMR calculations. The magnetic shielding constants (σ) were computed using the gauge including atomic orbitals (GIAO) method,[3] the method of choice to solve the gauge origin problem,[4] at PCM/mPW1PW91/6-31+G** level of theory, using the polarizable continuum model, PCM,[5] with methanol as the solvent. The unscaled chemical shifts (δ_u) were computed using TMS as reference standard according to $\delta_u = \sigma_0 - \sigma_x$, where σ_x is the Boltzmann averaged shielding tensor (over all significantly populated conformations) and σ_0 is the shielding tensor of TMS computed at the same level of theory employed for σ_x. The Boltzmann averaging was done according to eq 1:

$$\sigma^x = \frac{\sum_i \sigma_i^x e^{(-E_i/RT)}}{\sum_i e^{(-E_i/RT)}} \qquad \textit{(eq. 1)}$$

where σ_i^x is the shielding constant for nucleus *x* in conformer *i*, *R* is the molar gas constant (8.3145 J K^{-1} mol^{-1}), *T* is the temperature (298 K), and E_i is the SCF energy of conformer *i* (relative to the lowest energy conformer), obtained at the PCM/mPW1PW91/6-31+G** level of theory. The scaled chemical shifts (δ_s) were computed as $\delta_s = (\delta_u - b)/m$, where *m* and *b* are the slope and intercept, respectively, resulting from a linear regression calculation on a plot of δ_u against δ_{exp}.[4] The DP4+ calculations were carried out using the Excel spreadsheet available for free at sarotti-nmr.weebly.com, or as part of the Supporting Information of the original paper.[6]

References:

1) 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, J. A., Jr., 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 09*, Gaussian, Inc.: Wallingford, CT, 2009.

2) Spartan'08; Wavefunction: Irvine, CA.

3) a) Ditchfield, R. *J. Chem. Phys*. **1972**, *56*, 5688. b) Ditchfield, R. *Mol. Phys.* **1974**, *27*, 789. c) Rohlfing, C. M.; Allen, L. C.; Ditchfield, R. *Chem. Phys*. **1984**, *87*, 9. d) Wolinski, K.; Hinton, J. F.; Pulay, P. *J. Am. Chem. Soc*. **1990**, *112*, 8251.

4) a) Grimblat, N.; Sarotti, A. M. *Chem. Eur. J.* **2016**, *22*, 12246. b) Lodewyk, M. W.; Siebert, M. R.; Tantillo, D. J. *Chem. Rev.* **2012**, *112*, 1839.

5) For a review on continuum solvation models, see: Tomasi, J.; Mennucci, B.; Cammi, R. *Chem. Rev.* **2005**, *105*, 2999.

6) Grimblat, N.; Zanardi, M. M.; Sarotti, A. M. *J. Org. Chem.* **2015**, *80*, 12526.

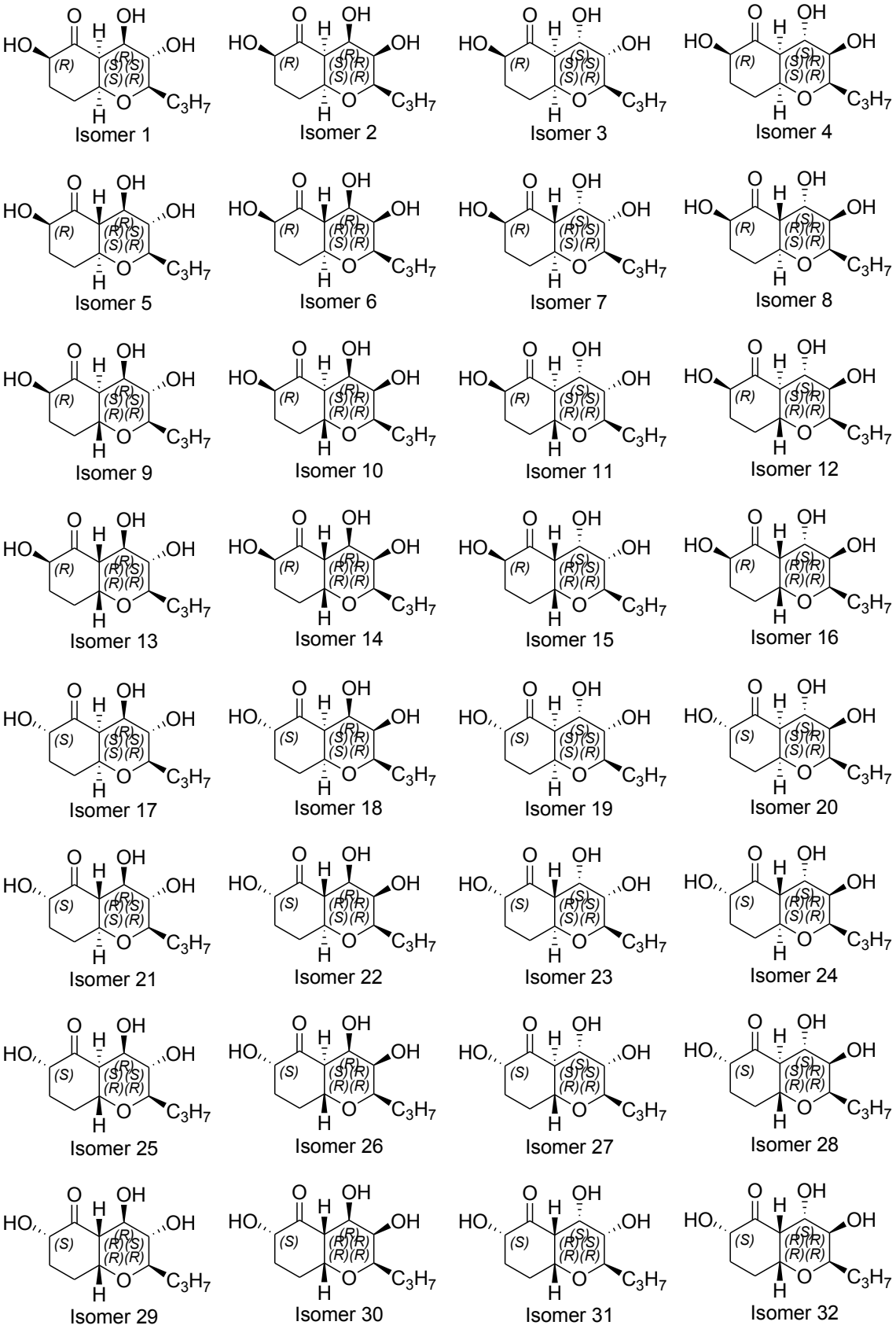
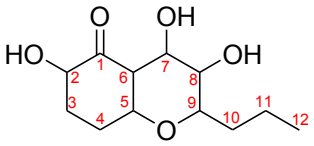


Figure S12. Structures of Isomers 1-32

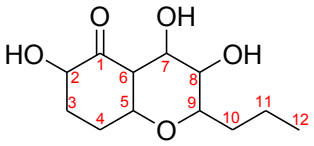
Table S1. NMR Boltzmann averaged isotropic magnetic shielding values (σ) calculated at the PCM/mPW1PW91/6-31+G**//PCM/B3LYP/6-31G* (solvent: MeOH) level of theory for all significantly populated conformers of Isomers 1-32.



	Shielding Tensors							
Atom	**Isomer 1**	**Isomer 2**	**Isomer 3**	**Isomer 4**	**Isomer 5**	**Isomer 6**	**Isomer 7**	**Isomer 8**
C-1	-23.4442	-24.6192	-18.1452	-23.9710	-23.1534	-22.2556	-21.2058	-22.7222
C-2	119.4385	118.8024	119.5161	119.0259	122.1023	121.0696	118.8367	118.5394
C-3	162.1287	157.2302	160.8190	157.1976	169.8284	167.2508	164.3656	164.5891
C-4	165.9719	165.7785	167.0149	166.0343	169.3953	169.3111	168.5223	168.1236
C-5	115.7863	113.1220	119.2641	115.7086	125.4721	120.5583	119.1846	117.4976
C-6	142.1111	139.1995	140.2048	139.6225	141.1619	143.3718	139.8175	143.6511
C-7	119.3329	124.9933	127.1662	126.1322	120.0491	123.6624	127.1969	125.7212
C-8	122.8219	125.1532	125.9619	123.3830	120.1596	124.9762	123.7546	124.4446
C-9	115.4249	114.6870	119.0739	116.2481	116.4438	117.2990	118.3535	119.4625
C-10	160.3435	161.0344	159.8731	160.7596	160.3975	160.8467	159.9180	161.4111
C-11	174.5795	174.1682	174.3952	174.1761	174.5200	174.0329	174.2480	174.1417
C-12	180.9368	181.0311	180.8977	180.7136	180.8874	180.9995	180.8472	180.7241
H-2	27.2294	27.0335	27.1988	26.9831	27.2606	27.5153	27.6704	27.6827
H-3a	29.5171	29.6681	29.6677	29.6561	29.8078	29.6264	29.8526	29.8649
H-3b	29.3022	29.2307	29.3281	29.2145	29.3852	29.5829	29.4268	29.4356
H-4	29.5346	29.5778	29.5416	29.5745	29.4789	29.5186	29.5785	29.5627
H-5	27.5345	27.6255	27.1548	27.1419	27.7911	28.0446	27.7223	27.6738
H-6	28.5513	28.3029	28.6304	28.5041	29.1735	28.4872	28.2811	28.0709
H-7	28.1722	27.8134	27.1270	27.0906	27.8379	27.6090	27.1173	27.2923
H-8	28.1201	28.0048	28.1017	28.4245	28.2974	27.8344	28.4120	28.0887
H-9a	28.3407	28.1534	28.0296	27.8406	28.2384	28.1131	28.0445	27.7013
H-9b	30.2278	30.0589	30.3234	30.1621	30.1915	30.0523	30.2625	30.1599
H-10a	29.7569	29.8874	29.8708	29.8739	29.7316	29.8037	29.7301	29.9341
H-10b	30.1916	30.1758	30.2685	30.2050	30.1888	30.1779	30.2072	30.1978
H-11	29.9715	30.0905	29.9734	30.0893	29.9451	30.0322	29.9477	30.0750
H-12	30.6475	30.6321	30.6583	30.6337	30.6361	30.6179	30.6286	30.6283

	Shielding Tensors							
Atom	**Isomer 9**	**Isomer 10**	**Isomer 11**	**Isomer 12**	**Isomer 13**	**Isomer 14**	**Isomer 15**	**Isomer 16**
C-1	-20.3719	-19.0143	-20.1516	-17.8470	-16.9325	-19.4722	-19.4885	-20.3978
C-2	119.5710	120.0040	119.7110	119.9951	121.8178	119.6876	118.8786	118.5517
C-3	161.6510	161.8052	163.7036	163.3626	163.7934	165.4403	165.0362	165.7570
C-4	165.4811	165.6225	165.6968	165.8957	170.5199	169.2306	168.2173	168.6221
C-5	125.7661	127.1782	124.0669	123.9390	119.2363	130.2194	121.4153	120.9284
C-6	142.3862	138.5096	141.3881	136.8842	135.7150	142.6571	141.0224	144.8673
C-7	125.6181	126.7401	126.6529	125.7311	120.1208	125.0675	125.3141	123.1271
C-8	124.6836	126.3962	123.6999	122.3611	123.2921	128.3932	123.8695	124.2186
C-9	115.2139	117.2527	116.3050	117.7753	120.4562	117.6440	128.3369	126.3598
C-10	163.6392	166.3957	163.7819	167.5624	163.3756	166.8808	161.4952	162.5753
C-11	173.3806	173.4439	173.5251	173.9524	175.1590	173.6196	176.2532	174.4525
C-12	181.2822	180.9829	181.2926	181.1465	180.0671	180.9470	181.7634	180.9004
H-2	27.1053	27.1817	27.2732	27.2927	27.0570	27.3226	26.8395	27.0292
H-3a	30.1436	30.1251	30.0146	30.0663	30.1591	29.7171	30.1271	30.0774
H-3b	29.1614	29.1351	29.1773	29.1722	29.2054	29.3574	29.2286	29.2463
H-4	29.6325	29.6620	29.5957	29.6432	29.4944	29.5360	29.2975	29.3649
H-5	27.4799	27.5989	27.8952	27.8921	27.3959	27.1051	27.5659	27.4494
H-6	28.7549	29.0696	28.6580	29.2010	28.7014	28.3454	28.7233	28.4953
H-7	27.2476	27.0329	27.3129	27.4681	27.6486	27.1194	27.5348	27.5815
H-8	27.9304	27.8329	27.7887	27.7798	28.0849	27.7451	28.0750	28.1506
H-9a	27.7503	27.6098	27.5013	27.4454	27.6041	27.6491	27.5324	27.2850
H-9b	30.1079	30.0696	30.3039	29.9888	30.0448	30.1405	29.9877	30.1607
H-10a	29.3064	29.4355	29.8086	29.9172	29.5080	29.3948	29.9875	30.0098
H-10b	30.2825	30.2997	30.2352	30.2530	30.1378	30.3612	30.1610	30.2040
H-11	30.0630	29.9700	30.0303	29.9999	29.8026	29.9855	29.9496	30.0626
H-12	30.6372	30.6159	30.6237	30.6071	30.5462	30.6305	30.6297	30.6182

Table S1 (cont). NMR Boltzmann averaged isotropic magnetic shielding values (σ) calculated at the PCM/mPW1PW91/6-31+G**//PCM/B3LYP/6-31G* (solvent: MeOH) level of theory for all significantly populated conformers of Isomers 1-32.



	Shielding Tensors							
Atom	**Isomer 17**	**Isomer 18**	**Isomer 19**	**Isomer 20**	**Isomer 21**	**Isomer 22**	**Isomer 23**	**Isomer 24**
C-1	-25.0723	-26.4178	-19.0657	-24.1925	-17.6373	-19.9299	-18.5742	-20.1608
C-2	119.9050	121.1029	119.3970	118.1755	120.1330	119.8174	119.8968	119.7497
C-3	166.7454	165.3513	165.0465	161.8182	163.0819	163.4990	161.8484	161.7086
C-4	168.7934	168.7311	169.3488	168.6741	165.8069	166.0340	165.9676	165.5448
C-5	118.1246	119.1777	121.3267	117.6124	116.8894	117.0346	119.1202	117.7013
C-6	144.2042	146.0962	141.9913	141.9925	137.5984	141.2801	138.0446	141.7821
C-7	118.7231	121.2069	126.0219	124.6944	122.2404	124.4100	127.3606	125.9458
C-8	122.3197	124.8175	125.6813	124.2181	119.2261	124.9645	124.2152	124.7914
C-9	115.3262	116.4401	118.8752	117.3551	114.6884	116.9362	118.2638	119.5643
C-10	160.3865	160.6455	159.8577	160.9741	159.1014	161.0692	160.0334	161.6416
C-11	174.4917	174.0515	174.2873	174.2539	172.5959	174.0617	174.3761	174.1984
C-12	180.9950	180.7875	180.9675	180.8834	180.3551	181.0294	180.8397	180.8321
H-2	27.3469	26.5443	27.3944	27.1926	27.2681	27.2716	27.1461	27.1174
H-3a	29.6907	29.8744	29.7015	29.5946	30.0811	30.0416	30.1301	30.1803
H-3b	29.3321	29.3129	29.3898	29.3605	29.1811	29.1820	29.1466	29.1661
H-4	29.4475	29.4880	29.4827	29.5351	29.5774	29.5438	29.6086	29.5968
H-5	27.6298	27.7665	27.2149	27.1533	28.1130	28.1706	27.7305	27.6537
H-6	28.3112	28.5705	28.2659	28.1531	29.1267	28.7352	29.0511	28.8112
H-7	28.1239	27.6013	27.1530	27.2120	27.7055	27.5421	27.0978	27.2355
H-8	28.3187	28.0076	28.2338	28.3227	28.2796	27.7960	28.4308	28.0467
H-9a	28.3786	28.1848	28.0504	27.8523	28.2056	28.0956	28.0452	27.7149
H-9b	30.2499	30.0597	30.3454	30.1446	30.0889	30.0392	30.2648	30.1668
H-10a	29.7871	29.8468	29.8550	29.9410	29.7507	29.8034	29.7407	29.9270
H-10b	30.2091	30.1902	30.2606	30.2090	30.1832	30.1738	30.1964	30.1859
H-11	29.9726	30.0661	29.9556	30.0954	29.7309	30.0345	29.9577	30.0685
H-12	30.6490	30.6276	30.6535	30.6282	30.5974	30.6172	30.6368	30.6293

	Shielding Tensors							
Atom	**Isomer 25**	**Isomer 26**	**Isomer 27**	**Isomer 28**	**Isomer 29**	**Isomer 30**	**Isomer 31**	**Isomer 32**
C-1	-22.6756	-21.3430	-22.4888	-20.2869	-23.4424	-18.7333	-24.8156	-23.9652
C-2	118.2902	119.1319	121.0690	121.1261	119.1704	119.4857	118.7521	119.3893
C-3	164.1367	164.5764	167.2397	166.5760	159.4801	160.9931	157.6714	162.3498
C-4	168.1109	168.0213	169.1424	168.9854	166.1232	166.4849	165.7369	165.9726
C-5	125.9571	127.4995	127.5279	126.1496	124.6008	127.6062	120.4270	123.1163
C-6	144.3401	140.5734	143.5354	138.6685	139.8082	140.7067	139.4976	142.3623
C-7	125.1997	126.6742	126.0041	125.0874	125.3983	126.3660	127.6639	123.2653
C-8	124.3310	126.0504	123.8803	121.9201	123.5345	128.4393	124.4374	124.7753
C-9	115.6263	117.3334	116.5712	118.4719	113.6642	117.8608	113.1784	117.6876
C-10	163.5764	166.3465	163.7149	167.8711	161.9222	166.7182	162.8348	168.5431
C-11	173.4361	173.4869	173.5404	174.2511	173.6482	173.7253	173.7005	174.1939
C-12	181.1027	180.9315	181.1818	181.4040	181.0804	180.8726	181.1261	180.8041
H-2	27.6817	27.6988	27.5394	27.6730	27.0437	27.2022	27.0535	27.2629
H-3a	29.8433	29.8545	29.6202	29.7137	29.6223	29.6036	29.6314	29.4654
H-3b	29.4573	29.4326	29.5696	29.5193	29.2621	29.3243	29.2444	29.3444
H-4	29.5960	29.6515	29.5738	29.6101	29.5994	29.6057	29.6210	29.5896
H-5	27.4829	27.6172	27.7720	27.8085	27.0279	27.0105	27.3375	27.2615
H-6	28.0469	28.3518	28.4127	28.7672	28.6738	28.6266	28.3559	28.5909
H-7	27.2990	27.0824	27.3704	27.5286	27.2216	27.0690	27.6671	27.9127
H-8	27.9946	27.8316	27.8052	27.7287	28.3024	27.5415	28.0358	27.5990
H-9a	27.7246	27.6095	27.5247	27.4167	27.7494	27.6071	27.4392	27.3898
H-9b	30.1492	30.0985	30.3260	30.0072	30.1169	30.1035	30.2709	30.0759
H-10a	29.2142	29.3997	29.8291	29.8877	29.5860	29.3936	29.8880	29.9250
H-10b	30.2758	30.3293	30.2505	30.2478	30.2485	30.3521	30.2430	30.2703
H-11	30.0453	29.9410	30.0053	29.9874	30.0621	29.9895	30.0983	30.0117
H-12	30.6338	30.6252	30.6282	30.6148	30.6341	30.6323	30.6412	30.6385

Table S2. Experimental NMR shifts (δ_{exp}) of **1** and calculated (scaled) NMR chemical shifts (δ_{sc}) of Isomers 1-32, computed at the PCM/mPW1PW91/6-31+G**//PCM/B3LYP/6-31G* (solvent: MeOH) level of theory.

		δ_{sc}							
Atom	δ_{exp}	**Isomer 1**	**Isomer 2**	**Isomer 3**	**Isomer 4**	**Isomer 5**	**Isomer 6**	**Isomer 7**	**Isomer 8**
C-1	210.0	212.0	212.9	213.5	213.4	212.8	213.2	213.2	213.3
C-2	75.0	73.7	73.9	75.7	74.1	72.8	74.2	75.9	76.2
C-3	31.3	32.3	36.7	34.3	36.9	26.8	29.4	31.3	31.5
C-4	27.7	28.6	28.4	28.1	28.3	27.2	27.4	27.2	28.1
C-5	77.8	77.2	79.4	75.9	77.3	69.6	74.7	75.6	77.2
C-6	53.6	51.7	54.1	54.9	54.0	54.4	52.6	55.3	51.8
C-7	74.1	73.8	67.9	68.0	67.2	74.8	71.7	67.7	69.2
C-8	71.1	70.4	67.8	69.2	69.9	74.7	70.4	71.1	70.5
C-9	80.3	77.6	77.9	76.1	76.8	78.3	77.8	76.4	75.3
C-10	33.7	34.1	33.0	35.2	33.4	35.9	35.6	35.6	34.6
C-11	18.1	20.3	20.3	20.7	20.4	22.3	22.8	21.6	22.2
C-12	13.1	14.1	13.6	14.2	14.0	16.2	16.1	15.1	15.8
	CMAE	**1.3**	**2.3**	**2.4**	**2.2**	**2.9**	**2.1**	**2.2**	**2.1**
	CMAxErr	**2.7**	**6.2**	**6.1**	**6.9**	**8.2**	**4.7**	**6.4**	**5.0**
H-2	4.24	4.32	4.52	4.35	4.57	4.29	4.04	3.88	3.87
H-3a	1.90	2.03	1.88	1.88	1.89	1.74	1.92	1.70	1.69
H-3b	2.14	2.25	2.32	2.22	2.34	2.17	1.97	2.12	2.11
H-4	2.03	2.02	1.97	2.01	1.98	2.07	2.03	1.97	1.99
H-5	3.97	4.02	3.92	4.40	4.41	3.76	3.51	3.83	3.88
H-6	3.15	3.00	3.25	2.92	3.05	2.38	3.06	3.27	3.48
H-7	3.49	3.38	3.74	4.42	4.46	3.71	3.94	4.43	4.26
H-8	3.63	3.43	3.55	3.45	3.13	3.25	3.72	3.14	3.46
H-9a	3.08	3.21	3.40	3.52	3.71	3.31	3.44	3.51	3.85
H-9b	1.38	1.32	1.49	1.23	1.39	1.36	1.50	1.29	1.39
H-10a	1.78	1.79	1.66	1.68	1.68	1.82	1.75	1.82	1.62
H-10b	1.35	1.36	1.37	1.28	1.35	1.36	1.37	1.34	1.35
H-11	1.49	1.58	1.46	1.58	1.46	1.61	1.52	1.60	1.48
H-12	0.92	0.90	0.92	0.89	0.92	0.91	0.93	0.92	0.92
	CMAE	**0.09**	**0.10**	**0.17**	**0.19**	**0.18**	**0.15**	**0.22**	**0.22**
	CMAxErr	**0.19**	**0.21**	**0.63**	**0.69**	**0.72**	**0.49**	**0.92**	**0.65**

		δ_{sc}							
Atom	δ_{exp}	**Isomer 9**	**Isomer 10**	**Isomer 11**	**Isomer 12**	**Isomer 13**	**Isomer 14**	**Isomer 15**	**Isomer 16**
C-1	210.0	213.9	214.3	213.6	212.7	211.6	214.4	214.1	213.9
C-2	75.0	75.6	75.9	75.6	75.5	73.4	77.3	77.4	77.5
C-3	31.3	34.0	34.2	32.2	32.3	31.5	32.2	31.9	31.2
C-4	27.7	30.3	30.4	30.2	29.8	24.8	28.5	28.7	28.4
C-5	77.8	69.5	68.7	71.3	71.6	75.9	66.9	74.9	75.2
C-6	53.6	53.1	57.4	54.2	58.7	59.5	54.7	55.6	51.7
C-7	74.1	69.7	69.2	68.7	69.8	75.0	72.0	71.1	73.0
C-8	71.1	70.6	69.5	71.7	73.1	71.9	68.7	72.5	71.9
C-9	80.3	79.9	78.6	78.9	77.7	74.7	79.3	68.1	69.8
C-10	33.7	32.1	29.7	32.1	28.2	31.9	30.8	35.4	34.3
C-11	18.1	22.5	22.7	22.5	21.8	20.2	24.2	20.8	22.6
C-12	13.1	14.7	15.1	14.8	14.6	15.3	16.9	15.3	16.3
	CMAE	**2.6**	**3.6**	**2.5**	**3.1**	**2.3**	**3.2**	**3.0**	**2.7**
	CMAxErr	**8.3**	**9.1**	**6.5**	**6.2**	**5.9**	**10.9**	**12.2**	**10.5**
H-2	4.24	4.45	4.37	4.28	4.26	4.49	4.23	4.71	4.52
H-3a	1.90	1.41	1.43	1.54	1.48	1.39	1.83	1.42	1.47
H-3b	2.14	2.39	2.42	2.37	2.38	2.35	2.19	2.32	2.30
H-4	2.03	1.92	1.89	1.95	1.91	2.06	2.01	2.25	2.19
H-5	3.97	4.07	3.95	3.66	3.66	4.15	4.45	3.98	4.10
H-6	3.15	2.80	2.48	2.89	2.35	2.85	3.21	2.83	3.06
H-7	3.49	4.30	4.52	4.24	4.08	3.90	4.43	4.02	3.97
H-8	3.63	3.62	3.72	3.76	3.77	3.47	3.81	3.48	3.40
H-9a	3.08	3.80	3.94	4.05	4.11	3.95	3.90	4.02	4.27
H-9b	1.38	1.44	1.48	1.25	1.56	1.51	1.41	1.56	1.39
H-10a	1.78	2.24	2.12	1.74	1.63	2.04	2.16	1.56	1.54
H-10b	1.35	1.27	1.25	1.32	1.30	1.41	1.19	1.39	1.35
H-11	1.49	1.49	1.58	1.52	1.55	1.75	1.56	1.60	1.49
H-12	0.92	0.91	0.93	0.93	0.94	1.00	0.92	0.92	0.93
	CMAE	**0.24**	**0.29**	**0.23**	**0.29**	**0.21**	**0.19**	**0.25**	**0.21**
	CMAxErr	**0.55**	**0.77**	**0.79**	**0.95**	**0.68**	**0.52**	**0.70**	**0.90**

Table S2 (cont). Experimental NMR shifts (δ_{exp}) of **1** and calculated (scaled) NMR chemical shifts (δ_{sc}) of Isomers 1-32, computed at the PCM/mPW1PW91/6-31+G**//PCM/B3LYP/6-31G* (solvent: MeOH) level of theory.

		δ_{sc}							
Atom	δ_{exp}	**Isomer 17**	**Isomer 18**	**Isomer 19**	**Isomer 20**	**Isomer 21**	**Isomer 22**	**Isomer 23**	**Isomer 24**
C-1	210.0	212.0	213.6	213.3	213.2	211.2	212.6	213.2	213.5
C-2	75.0	73.8	73.2	76.3	75.7	73.2	74.7	74.9	75.1
C-3	31.3	29.2	31.1	31.1	33.6	30.2	31.6	32.9	33.5
C-4	27.7	27.2	27.9	26.8	27.0	27.5	29.1	28.8	29.7
C-5	77.8	75.5	75.1	74.4	76.3	76.5	77.4	75.6	77.1
C-6	53.6	50.7	49.5	53.9	52.8	55.7	53.5	56.7	53.3
C-7	74.1	75.0	73.1	69.7	69.5	71.1	70.2	67.4	68.9
C-8	71.1	71.5	69.7	70.0	69.9	74.1	69.6	70.5	70.1
C-9	80.3	78.2	77.7	76.8	76.5	78.7	77.5	76.5	75.2
C-10	33.7	35.2	35.6	36.2	34.4	34.2	34.0	34.8	33.6
C-11	18.1	21.8	22.9	22.0	21.6	20.7	21.2	20.4	21.2
C-12	13.1	15.6	16.4	15.3	15.2	12.9	14.3	14.0	14.6
	CMAE	**1.8**	**2.3**	**2.2**	**2.1**	**1.6**	**1.5**	**2.2**	**2.1**
	CMAxErr	**3.7**	**4.8**	**4.4**	**4.6**	**3.0**	**3.9**	**6.7**	**5.2**
H-2	4.24	4.20	5.01	4.16	4.36	4.28	4.28	4.40	4.43
H-3a	1.90	1.86	1.68	1.85	1.96	1.47	1.51	1.42	1.37
H-3b	2.14	2.22	2.24	2.16	2.19	2.37	2.37	2.40	2.38
H-4	2.03	2.10	2.06	2.07	2.02	1.97	2.01	1.94	1.95
H-5	3.97	3.92	3.78	4.34	4.40	3.44	3.38	3.82	3.90
H-6	3.15	3.24	2.98	3.28	3.40	2.42	2.82	2.50	2.74
H-7	3.49	3.43	3.95	4.40	4.34	3.84	4.01	4.45	4.32
H-8	3.63	3.23	3.54	3.32	3.23	3.27	3.75	3.12	3.50
H-9a	3.08	3.17	3.37	3.50	3.70	3.34	3.45	3.51	3.84
H-9b	1.38	1.30	1.49	1.21	1.41	1.46	1.51	1.29	1.38
H-10a	1.78	1.76	1.70	1.70	1.61	1.80	1.75	1.81	1.62
H-10b	1.35	1.34	1.36	1.29	1.34	1.37	1.38	1.35	1.36
H-11	1.49	1.58	1.48	1.59	1.46	1.82	1.52	1.59	1.48
H-12	0.92	0.90	0.92	0.90	0.92	0.95	0.93	0.91	0.92
	CMAE	**0.09**	**0.17**	**0.17**	**0.16**	**0.27**	**0.21**	**0.28**	**0.24**
	CMAxErr	**0.35**	**0.48**	**0.65**	**0.60**	**0.67**	**0.59**	**0.90**	**0.62**

		δ_{sc}							
Atom	δ_{exp}	**Isomer 25**	**Isomer 26**	**Isomer 27**	**Isomer 28**	**Isomer 29**	**Isomer 30**	**Isomer 31**	**Isomer 32**
C-1	210.0	213.8	214.3	214.2	213.0	214.0	214.6	213.9	213.8
C-2	75.0	76.9	76.8	75.0	74.9	74.8	76.8	74.7	75.5
C-3	31.3	32.4	32.4	30.2	30.6	35.5	35.5	37.0	34.1
C-4	27.7	28.5	29.0	28.4	28.2	29.0	30.0	29.2	30.6
C-5	77.8	69.5	68.7	68.7	70.0	69.5	68.7	73.1	71.9
C-6	53.6	51.6	55.9	53.2	57.8	54.7	55.7	54.6	53.4
C-7	74.1	70.2	69.5	70.2	71.1	68.7	70.0	66.1	71.8
C-8	71.1	71.1	70.1	72.2	74.2	70.5	67.9	69.2	70.3
C-9	80.3	79.5	78.6	79.3	77.5	80.2	78.4	80.1	77.2
C-10	33.7	32.9	30.6	33.6	29.3	33.1	29.8	32.0	28.1
C-11	18.1	23.4	23.7	24.1	23.1	21.6	22.8	21.5	22.7
C-12	13.1	15.9	16.4	16.7	16.1	14.4	15.7	14.3	16.3
	CMAE	**2.6**	**3.3**	**2.6**	**3.1**	**2.5**	**3.7**	**2.8**	**3.0**
	CMAxErr	**8.3**	**9.1**	**9.1**	**7.8**	**8.3**	**9.1**	**8.0**	**5.9**
H-2	4.24	3.87	3.85	4.01	3.88	4.51	4.35	4.50	4.29
H-3a	1.90	1.71	1.70	1.93	1.84	1.93	1.95	1.92	2.09
H-3b	2.14	2.09	2.12	1.98	2.03	2.29	2.23	2.31	2.21
H-4	2.03	1.95	1.90	1.98	1.94	1.95	1.94	1.93	1.96
H-5	3.97	4.07	3.93	3.78	3.74	4.52	4.54	4.21	4.29
H-6	3.15	3.50	3.20	3.14	2.78	2.88	2.92	3.19	2.96
H-7	3.49	4.25	4.47	4.18	4.02	4.33	4.48	3.88	3.64
H-8	3.63	3.56	3.72	3.75	3.82	3.25	4.01	3.51	3.95
H-9a	3.08	3.83	3.94	4.03	4.13	3.80	3.94	4.11	4.16
H-9b	1.38	1.40	1.45	1.22	1.54	1.43	1.45	1.28	1.47
H-10a	1.78	2.34	2.15	1.72	1.66	1.96	2.16	1.66	1.63
H-10b	1.35	1.27	1.22	1.30	1.30	1.30	1.20	1.31	1.28
H-11	1.49	1.51	1.61	1.55	1.56	1.49	1.56	1.45	1.54
H-12	0.92	0.92	0.93	0.92	0.94	0.92	0.92	0.91	0.91
	CMAE	**0.25**	**0.25**	**0.20**	**0.25**	**0.20**	**0.19**	**0.14**	**0.16**
	CMAxErr	**0.57**	**0.77**	**0.79**	**0.99**	**0.59**	**0.51**	**0.74**	**0.81**

Table S3. DP4+ probability values (%) obtained after correlating the experimental NMR shifts of **1** with the calculated NMR data of Isomers 1-32.

Isomer Nº	**DP4+ (H data)**	**DP4+ (C data)**	**DP4+ (all data)**
1	*14.46*	*99.92*	***100.00***
2	0.05	0.00	**0.00**
3	0.00	0.00	**0.00**
4	0.00	0.00	**0.00**
5	0.00	0.00	**0.00**
6	0.00	0.00	**0.00**
7	0.00	0.00	**0.00**
8	0.00	0.00	**0.00**
9	0.00	0.00	**0.00**
10	0.00	0.00	**0.00**
11	0.00	0.00	**0.00**
12	0.00	0.00	**0.00**
13	0.00	0.00	**0.00**
14	0.00	0.00	**0.00**
15	0.00	0.00	**0.00**
16	0.00	0.00	**0.00**
17	85.49	0.00	**0.00**
18	0.00	0.00	**0.00**
19	0.00	0.00	**0.00**
20	0.00	0.00	**0.00**
21	0.00	0.05	**0.00**
22	0.00	0.02	**0.00**
23	0.00	0.00	**0.00**
24	0.00	0.00	**0.00**
25	0.00	0.00	**0.00**
26	0.00	0.00	**0.00**
27	0.00	0.00	**0.00**
28	0.00	0.00	**0.00**
29	0.00	0.00	**0.00**
30	0.00	0.00	**0.00**
31	0.00	0.00	**0.00**
32	0.00	0.00	**0.00**

Cartesian Coordinates of the global minima conformation found for each isomer at the PCM/B3LYP/6-31G* level of theory.

Isomer 1

B3LYP/6-31G* geometry

O 0	2.043347	2.847364	0.066811
C 0	1.332300	1.713488	0.560858
C 0	-0.660214	0.205353	0.209314
C 0	1.311034	-0.722567	1.220067
O 0	0.239338	-0.909009	0.295880
C 0	2.206728	0.460702	0.754670
C 0	0.112466	1.419989	-0.322768
C 0	3.007158	0.070370	-0.475029
C 0	3.745122	-1.261046	-0.432145
C 0	2.781273	-2.385501	-0.014397
C 0	2.079850	-2.041421	1.305246
O 0	-0.747407	2.553144	-0.335572
C 0	-1.828828	-0.200563	-0.682912
C 0	-2.685531	-1.335082	-0.106273
C 0	-3.847122	-1.724072	-1.026038
O 0	4.354729	-1.534867	-1.673780
O 0	3.102318	0.774398	-1.476895
H 0	2.473710	2.544252	-0.755655
H 0	0.954638	2.016740	1.544993
H 0	-1.032081	0.447560	1.219768
H 0	0.896863	-0.466460	2.207505
H 0	2.943444	0.658578	1.547397
H 0	0.456959	1.188524	-1.343208
H 0	4.515229	-1.156629	0.353621
H 0	2.043766	-2.525223	-0.812152
H 0	3.348049	-3.317761	0.077346
H 0	1.377886	-2.836055	1.578806
H 0	2.813125	-1.965769	2.118247
H 0	-0.155884	3.317761	-0.454658
H 0	-2.448012	0.689702	-0.846851
H 0	-1.428565	-0.494262	-1.663695
H 0	-3.080159	-1.026666	0.872253
H 0	-2.049674	-2.209178	0.078408
H 0	-4.445147	-2.532853	-0.590772
H 0	-3.481815	-2.067070	-2.001963
H 0	-4.515229	-0.872128	-1.203372
H 0	4.236883	-0.724496	-2.207505

Free Energy (PCM/B3LYP/6-31G*) = -845.158852

Number of imaginary frequencies = 0

Isomer 2

B3LYP/6-31G* geometry

O 0	-2.172568	3.046442	-0.380247
C 0	-1.429053	1.932695	-0.848705
C 0	0.633397	0.490823	-0.428745
C 0	-1.331062	-0.559734	-1.275542
O 0	-0.253958	-0.637848	-0.344872
C 0	-2.252595	0.620881	-0.847214
C 0	-0.088137	1.811753	-0.087156
C 0	-2.906099	0.213542	0.455269
C 0	-3.765346	-1.040336	0.401196
C 0	-2.812606	-2.197676	0.003612
C 0	-2.070196	-1.898006	-1.304614
O 0	-0.280582	2.035679	1.309383
C 0	1.833679	0.211259	0.471885
C 0	2.658201	-1.008055	0.041325
C 0	3.851993	-1.267335	0.965917
O 0	-4.396300	-1.277813	1.639138
O 0	-2.698482	0.732694	1.549760
H 0	-1.952060	3.116375	0.567037
H 0	-1.192362	2.131287	-1.901627
H 0	0.974848	0.576253	-1.475033
H 0	-0.930781	-0.339162	-2.277453
H 0	-3.055504	0.715156	-1.590528
H 0	0.559985	2.633350	-0.412053
H 0	-4.534660	-0.924070	-0.374760
H 0	-2.098697	-2.340819	0.823123
H 0	-3.401839	-3.116375	-0.082395
H 0	-1.348264	-2.692932	-1.520598
H 0	-2.778966	-1.872722	-2.141994
H 0	-0.983222	1.427127	1.616926
H 0	2.469748	1.106923	0.474514
H 0	1.475521	0.082796	1.500335
H 0	3.015884	-0.859154	-0.987412
H 0	2.008812	-1.891031	0.017946
H 0	4.425321	-2.142705	0.639949
H 0	3.522050	-1.449210	1.996314
H 0	4.534660	-0.408593	0.983937
H 0	-3.942779	-0.692795	2.277453

Free Energy (PCM/B3LYP/6-31G*) = -845.156190

Number of imaginary frequencies = 0

Isomer 3

B3LYP/6-31G* geometry

O 0	0.680519	2.578202	1.148958
C 0	1.098550	1.885105	-0.024369
C 0	-0.777877	0.159252	-0.005088
C 0	1.263464	-0.364185	1.134596
O 0	0.225865	-0.827327	0.268979
C 0	2.049169	0.766544	0.418486
C 0	-0.139902	1.333690	-0.762214
C 0	2.861123	0.185500	-0.723347
C 0	3.756573	-1.002727	-0.388193
C 0	2.902792	-2.105039	0.268962
C 0	2.147932	-1.559944	1.487843
O 0	-1.126650	2.372736	-0.840804
C 0	-1.897288	-0.518923	-0.789999
C 0	-2.641024	-1.600255	0.003983
C 0	-3.752928	-2.271721	-0.808359
O 0	4.413059	-1.466708	-1.547624
O 0	2.816427	0.597109	-1.875216
H 0	-0.139152	3.035915	0.881646
H 0	1.630212	2.571854	-0.699851
H 0	-1.172658	0.542752	0.949654
H 0	0.815382	0.057250	2.044887
H 0	2.764762	1.189845	1.138663
H 0	0.152984	0.997982	-1.763844
H 0	4.500937	-0.653525	0.347444
H 0	2.195471	-2.484643	-0.476940
H 0	3.557838	-2.935164	0.553791
H 0	1.519400	-2.342862	1.925632
H 0	2.857965	-1.246860	2.264186
H 0	-0.875075	2.971782	-1.562594
H 0	-2.599755	0.259120	-1.111724
H 0	-1.465181	-0.955884	-1.701638
H 0	-3.070013	-1.150066	0.910463
H 0	-1.922596	-2.355584	0.344018
H 0	-4.271044	-3.035915	-0.217712
H 0	-3.349354	-2.759485	-1.704371
H 0	-4.500937	-1.540031	-1.138207
H 0	4.110746	-0.872812	-2.264186

Free Energy (PCM/B3LYP/6-31G*) = -845.157209

Number of imaginary frequencies = 0

Isomer 4

B3LYP/6-31G* geometry

O 0	-1.033289	2.398468	-1.307525
C 0	-1.309094	1.757030	-0.060467
C 0	0.678280	0.161350	-0.028920
C 0	-1.313521	-0.561530	-1.111925
O 0	-0.259163	-0.914446	-0.219931
C 0	-2.179451	0.540084	-0.434725
C 0	0.007517	1.367136	0.661146
C 0	-2.933217	-0.091788	0.713170
C 0	-3.820196	-1.276493	0.366283
C 0	-2.897977	-2.360779	-0.243207
C 0	-2.119753	-1.816389	-1.447000
O 0	-0.187026	1.185333	2.057615
C 0	1.872110	-0.389809	0.744285
C 0	2.643274	-1.482535	-0.005888
C 0	3.832929	-2.022130	0.794523
O 0	-4.508335	-1.744030	1.504244
O 0	-2.806521	0.226783	1.893518
H 0	-0.549321	3.218573	-1.118001
H 0	-1.874618	2.426281	0.602631
H 0	1.009262	0.504132	-1.023418
H 0	-0.886770	-0.137164	-2.031415

H 0 -2.926435 0.879630 -1.165249
H 0 0.697858 2.216484 0.564483
H 0 -4.550681 -0.963839 -0.394269
H 0 -2.206490 -2.697580 0.537727
H 0 -3.515435 -3.218573 -0.528902
H 0 -1.433180 -2.578958 -1.830244
H 0 -2.811765 -1.569770 -2.262388
H 0 -1.070494 0.789797 2.187637
H 0 2.545420 0.448778 0.970665
H 0 1.514310 -0.769403 1.708638
H 0 2.998419 -1.081877 -0.966088
H 0 1.957413 -2.302732 -0.248667
H 0 4.367462 -2.800914 0.238451
H 0 3.504391 -2.457651 1.746392
H 0 4.550681 -1.225125 1.026146
H 0 -4.108918 -1.273962 2.262388
Free Energy (PCM/B3LYP/6-31G*) = -845.154496
Number of imaginary frequencies = 0

Isomer 5
B3LYP/6-31G* geometry
O 0 -1.426315 2.622491 0.471689
C 0 -0.913760 1.434452 -0.121333
C 0 1.179176 0.028274 -0.247461
C 0 -0.932108 -1.093326 -0.155630
O 0 0.425825 -1.076661 0.272927
C 0 -1.656162 0.171514 0.340508
C 0 0.563461 1.343074 0.259964
C 0 -3.116174 0.164065 -0.061314
C 0 -3.714053 -1.186071 -0.430794
C 0 -3.133987 -2.275985 0.482534
C 0 -1.589481 -2.380346 0.369048
O 0 1.283899 2.434571 -0.300431
C 0 2.631740 -0.152719 0.183256
C 0 3.303802 -1.395421 -0.414482
C 0 4.758955 -1.554139 0.037120
O 0 -5.121996 -1.148355 -0.358342
O 0 -3.812935 1.173592 -0.078904
H 0 -2.381850 2.630273 0.275423
H 0 -0.976216 1.502730 -1.220030
H 0 1.117334 0.021968 -1.349144
H 0 -0.949256 -1.090069 -1.258131
H 0 -1.647905 0.157490 1.442557
H 0 0.631998 1.357520 1.360239
H 0 -3.387904 -1.384384 -1.470220
H 0 -3.432171 -2.043503 1.511298
H 0 -3.603055 -3.230494 0.226975
H 0 -1.165347 -2.589882 1.356526
H 0 -1.304293 -3.211190 -0.283744
H 0 0.767001 3.230494 -0.087114
H 0 3.183178 0.748330 -0.110617
H 0 2.663710 -0.201576 1.280993
H 0 3.264617 -1.333384 -1.511298
H 0 2.729369 -2.286512 -0.134652
H 0 5.217806 -2.445626 -0.405607
H 0 4.826822 -1.650924 1.127830
H 0 5.362739 -0.686392 -0.256367
H 0 -5.362739 -0.203289 -0.411874
Free Energy (PCM/B3LYP/6-31G*) = -845.152813
Number of imaginary frequencies = 0

Isomer 6
B3LYP/6-31G* geometry
O 0 -1.853193 2.995577 -0.097796
C 0 -1.261905 1.790110 -0.578238
C 0 0.897991 0.479462 -0.471290
C 0 -1.163864 -0.720794 -0.463622
O 0 0.164822 -0.643769 0.036792
C 0 -1.948676 0.537476 -0.020544
C 0 0.205389 1.808750 -0.129482
C 0 -3.422019 0.443433 -0.366644
C 0 -4.109826 -0.883734 -0.016589
C 0 -3.273730 -2.088348 -0.452877
C 0 -1.819871 -2.002350 0.038170
O 0 0.270791 2.041120 1.274409
C 0 2.322524 0.389304 0.072930
C 0 3.078206 -0.865225 -0.382869
C 0 4.502846 -0.931727 0.176543
O 0 -4.231380 -0.931990 1.411660
O 0 -4.053785 1.387435 -0.826688
H 0 -2.800664 2.918961 -0.317981
H 0 -1.298815 1.760949 -1.678354
H 0 0.925506 0.411035 -1.573284
H 0 -1.130007 -0.742819 -1.567804
H 0 -1.890501 0.567438 1.076724
H 0 0.726128 2.614446 -0.672351
H 0 -5.097085 -0.895867 -0.494645
H 0 -3.755525 -2.995577 -0.072756
H 0 -3.296876 -2.146712 -1.548931
H 0 -1.788625 -2.016654 1.133497
H 0 -1.249009 -2.866231 -0.318904
H 0 -0.397225 2.729216 1.446838
H 0 2.866734 1.286667 -0.252096
H 0 2.278177 0.427180 1.167772
H 0 3.114031 -0.887531 -1.481464
H 0 2.516362 -1.754461 -0.073914
H 0 5.021038 -1.836653 -0.160960
H 0 4.496934 -0.939757 1.273592
H 0 5.097085 -0.067091 -0.144752
H 0 -4.884094 -0.263504 1.678354
Free Energy (PCM/B3LYP/6-31G*) = -845.152988
Number of imaginary frequencies = 0

Isomer 7
B3LYP/6-31G* geometry
O 0 -1.097277 2.153571 -1.047327
C 0 -1.098544 1.622213 0.282275
C 0 0.967430 0.183382 -0.112830
C 0 -1.175113 -0.823856 -0.405075
O 0 0.143891 -0.976107 0.100871
C 0 -1.892717 0.314603 0.369904
C 0 0.376427 1.393401 0.644775
C 0 -3.315105 0.422419 -0.142420
C 0 -4.132696 -0.867412 -0.005227
C 0 -3.388306 -1.996096 -0.736064
C 0 -1.930193 -2.143148 -0.265477
O 0 1.120698 2.578960 0.386425
C 0 2.380290 -0.160614 0.347330
C 0 3.058414 -1.251380 -0.490999
C 0 4.467311 -1.590645 0.005593
O 0 -4.242354 -1.241902 1.369461
O 0 -3.764961 1.423419 -0.686241
H 0 -2.031996 2.346330 -1.247978
H 0 -1.522898 2.364130 0.974161
H 0 0.974429 0.422420 -1.188928
H 0 -1.122622 -0.537773 -1.467935
H 0 -1.947005 -0.010436 1.417290
H 0 0.448407 1.195868 1.721189
H 0 -5.120300 -0.700928 -0.453144
H 0 -3.939118 -2.928846 -0.573619
H 0 -3.417854 -1.786539 -1.813009
H 0 -1.902774 -2.459536 0.783415
H 0 -1.424117 -2.916257 -0.853872
H 0 0.753593 2.928846 -0.446395
H 0 2.974391 0.760664 0.315497
H 0 2.334359 -0.474131 1.400396
H 0 3.108366 -0.921369 -1.538429
H 0 2.433914 -2.152815 -0.480783
H 0 4.931120 -2.368227 -0.612166
H 0 4.445205 -1.955229 1.040132
H 0 5.120300 -0.709258 -0.020442
H 0 -4.814141 -0.594099 1.813009
Free Energy (PCM/B3LYP/6-31G*) = -845.153563
Number of imaginary frequencies = 0

Isomer 8
B3LYP/6-31G* geometry
O 0 -1.171750 2.374987 -1.550432
C 0 -1.186516 1.984479 -0.179794
C 0 0.919350 0.607633 -0.422695
C 0 -1.163092 -0.541771 -0.565405
O 0 0.165062 -0.563750 -0.043017

C 0 -1.942112 0.661786 0.035320
C 0 0.279076 1.820742 0.270239
C 0 -3.347792 0.635103 -0.528684
C 0 -4.120203 -0.654212 -0.224567
C 0 -3.311751 -1.847168 -0.759853
C 0 -1.861007 -1.859765 -0.244744
O 0 0.342838 1.687290 1.690333
C 0 2.379066 0.374262 -0.043329
C 0 3.032846 -0.790487 -0.797626
C 0 4.497780 -1.001626 -0.402622
O 0 -4.261203 -0.825721 1.187203
O 0 -3.817187 1.525650 -1.226465
H 0 -2.111844 2.428580 -1.806278
H 0 -1.648397 2.767597 0.439291
H 0 0.836011 0.746384 -1.510410
H 0 -1.106588 -0.408148 -1.657245
H 0 -2.030155 0.471970 1.113078
H 0 0.826110 2.732953 0.008341
H 0 -5.098179 -0.597153 -0.718547
H 0 -3.829612 -2.767597 -0.469644
H 0 -3.320191 -1.803145 -1.856473
H 0 -1.846906 -2.016552 0.839799
H 0 -1.308914 -2.687041 -0.703750
H 0 0.195304 0.743817 1.878714
H 0 2.929083 1.303235 -0.247885
H 0 2.446623 0.205251 1.038748
H 0 2.967134 -0.602966 -1.878714
H 0 2.461278 -1.706654 -0.607693
H 0 4.941982 -1.837697 -0.954757
H 0 4.591163 -1.221367 0.668165
H 0 5.098179 -0.107187 -0.610499
H 0 -4.869301 -0.142336 1.514087
Free Energy (PCM/B3LYP/6-31G*) = -845.151598
Number of imaginary frequencies = 0

Isomer 9
B3LYP/6-31G* geometry
O 0 0.676500 -0.108450 -1.285749
C 0 -1.274503 0.864750 -0.202024
C 0 0.940930 2.055831 -0.224520
C 0 -0.386153 1.879337 0.541627
C 0 1.627519 0.723192 -0.575862
C 0 -0.491301 -0.434583 -0.533692
C 0 -1.355134 -1.400292 -1.340283
C 0 -2.642850 -1.742315 -0.574009
C 0 -3.461866 -0.483620 -0.200449
C 0 -2.546326 0.495322 0.521909
O 0 -2.833815 0.882388 1.650772
C 0 2.337402 0.003242 0.577266
C 0 3.068986 -1.268903 0.129295
C 0 3.823156 -1.951093 1.274931
O 0 -0.092605 1.463187 1.871308
O 0 0.684669 2.787533 -1.428041
O 0 -4.578385 -0.809451 0.596695
H 0 -1.571151 1.304882 -1.165213
H 0 1.612408 2.672293 0.382124
H 0 -0.890148 2.856132 0.550207
H 0 2.377590 0.952876 -1.342026
H 0 -0.201165 -0.915601 0.410248
H 0 -0.786767 -2.314219 -1.543524
H 0 -1.592665 -0.944013 -2.310145
H 0 -2.402375 -2.272262 0.356550
H 0 -3.280232 -2.406252 -1.166384
H 0 -3.797596 0.005315 -1.129628
H 0 3.063584 0.713159 0.997714
H 0 1.637300 -0.222669 1.387140
H 0 3.773343 -1.016383 -0.676118
H 0 2.346417 -1.970090 -0.306435
H 0 4.336085 -2.856132 0.929918
H 0 3.138966 -2.241899 2.081646
H 0 4.578385 -1.282548 1.706491
H 0 -0.958488 1.374252 2.310145
H 0 0.439523 2.130794 -2.102199
H 0 -4.459056 -0.310454 1.428964
Free Energy (PCM/B3LYP/6-31G*) = -845.151615
Number of imaginary frequencies = 0

Isomer 10
B3LYP/6-31G* geometry
O 0 0.618004 -0.623314 -1.502989
C 0 -1.247189 0.725712 -0.736407
C 0 1.022995 1.754939 -1.093098
C 0 -0.300241 1.859505 -0.321654
C 0 1.630445 0.324300 -1.099053
C 0 -0.534735 -0.651096 -0.671618
C 0 -1.466875 -1.765234 -1.142235
C 0 -2.749876 -1.794222 -0.296629
C 0 -3.498804 -0.440273 -0.312241
C 0 -2.521590 0.662593 0.071652
O 0 -2.764156 1.391113 1.028838
C 0 2.369682 -0.089830 0.180917
C 0 3.045992 -1.461736 0.064901
C 0 3.821908 -1.847943 1.328183
O 0 0.021859 1.813788 1.070565
O 0 1.946239 2.724649 -0.613507
O 0 -4.609631 -0.451292 0.556239
H 0 -1.531071 0.873832 -1.788856
H 0 0.809975 2.014402 -2.136618
H 0 -0.760829 2.829259 -0.558126
H 0 2.353354 0.288707 -1.922632
H 0 -0.244507 -0.842874 0.370917
H 0 -0.948905 -2.727488 -1.069272
H 0 -1.706759 -1.606144 -2.201636
H 0 -2.512195 -2.033297 0.747833
H 0 -3.432517 -2.570587 -0.656275
H 0 -3.833938 -0.237200 -1.342719
H 0 3.130174 0.677256 0.373929
H 0 1.694235 -0.072713 1.043148
H 0 3.728283 -1.456630 -0.797321
H 0 2.287344 -2.224228 -0.151055
H 0 4.297945 -2.829259 1.218975
H 0 3.159611 -1.893875 2.201636
H 0 4.609631 -1.116791 1.548481
H 0 -0.813821 1.982574 1.541896
H 0 1.828138 2.735307 0.353526
H 0 -4.449907 0.273067 1.193205
Free Energy (PCM/B3LYP/6-31G*) = -845.152899
Number of imaginary frequencies = 0

Isomer 11
B3LYP/6-31G* geometry
O 0 -0.624843 -0.546955 1.190414
C 0 1.377474 0.398033 0.206845
C 0 -0.743567 1.712947 0.203232
C 0 0.548679 1.424909 -0.573103
C 0 -1.498390 0.426525 0.584914
C 0 0.528737 -0.878913 0.428121
C 0 1.318053 -1.959779 1.162053
C 0 2.598220 -2.310065 0.388878
C 0 3.498633 -1.076403 0.190858
C 0 2.708667 0.072120 -0.425806
O 0 3.174737 0.690409 -1.378239
C 0 -2.324839 -0.156746 -0.573175
C 0 -3.142285 -1.390891 -0.172038
C 0 -3.988717 -1.940874 -1.324237
O 0 1.220426 2.674055 -0.718169
O 0 -0.425745 2.413147 1.405165
O 0 4.628164 -1.384699 -0.595338
H 0 1.587688 0.810645 1.204458
H 0 -1.399503 2.332436 -0.427522
H 0 0.299341 1.012766 -1.561803
H 0 -2.184735 0.695013 1.395858
H 0 0.229949 -1.273672 -0.556330
H 0 0.691053 -2.850228 1.276937
H 0 1.562013 -1.602106 2.170872
H 0 2.349531 -2.717007 -0.599577
H 0 3.170489 -3.078895 0.917604
H 0 3.812857 -0.717911 1.188433
H 0 -3.002791 0.632247 -0.925981
H 0 -1.681014 -0.405190 -1.427548
H 0 -3.795508 -1.128969 0.672344
H 0 -2.464570 -2.170487 0.195925

H 0 -4.564786 -2.818524 -1.009505
H 0 -3.359064 -2.241522 -2.170872
H 0 -4.698685 -1.188860 -1.690232
H 0 2.066514 2.468967 -1.155823
H 0 0.236853 3.078895 1.146332
H 0 4.698685 -0.658952 -1.246349
Free Energy (PCM/B3LYP/6-31G*) = -845.154932
Number of imaginary frequencies = 0

Isomer 12
B3LYP/6-31G* geometry
O 0 0.609529 -0.899411 -1.417453
C 0 -1.296609 0.310779 -0.522265
C 0 0.902856 1.437428 -0.797923
C 0 -0.362427 1.373773 0.058066
C 0 1.579254 0.055708 -0.938361
C 0 -0.547744 -1.044447 -0.600606
C 0 -1.441243 -2.139168 -1.176759
C 0 -2.711678 -2.295399 -0.324763
C 0 -3.507962 -0.978523 -0.224537
C 0 -2.596934 0.154933 0.231395
O 0 -2.931826 0.876356 1.164230
C 0 2.333429 -0.418563 0.311673
C 0 3.046809 -1.761219 0.107714
C 0 3.842882 -2.201835 1.340097
O 0 -0.928419 2.683203 0.044586
O 0 1.834428 2.366797 -0.261003
O 0 -4.612771 -1.110227 0.642279
H 0 -1.556968 0.589509 -1.554877
H 0 0.589746 1.756949 -1.805550
H 0 -0.092705 1.098491 1.087952
H 0 2.301972 0.121482 -1.759366
H 0 -0.251816 -1.337872 0.418466
H 0 -0.887623 -3.083673 -1.201800
H 0 -1.698315 -1.885981 -2.213435
H 0 -2.450228 -2.613353 0.692550
H 0 -3.364939 -3.066721 -0.744611
H 0 -3.850708 -0.704414 -1.238491
H 0 3.064613 0.358934 0.561047
H 0 1.661098 -0.486818 1.176980
H 0 3.722067 -1.681935 -0.756233
H 0 2.309235 -2.530581 -0.151535
H 0 4.343553 -3.161456 1.167476
H 0 3.189292 -2.319154 2.213435
H 0 4.612771 -1.464596 1.599220
H 0 -1.660237 2.664384 0.685392
H 0 1.312955 3.161456 -0.051727
H 0 -4.560281 -0.345422 1.249030
Free Energy (PCM/B3LYP/6-31G*) = -845.153345
Number of imaginary frequencies = 0

Isomer 13
B3LYP/6-31G* geometry
O 0 -0.831171 2.568096 -0.193725
C 0 -0.473944 1.231281 -0.542505
C 0 1.404939 -0.358825 -1.034067
C 0 -0.604341 -1.249563 0.011862
O 0 0.816478 -1.296285 -0.119552
C 0 -1.081436 0.179265 0.410801
C 0 1.047705 1.066564 -0.591694
C 0 -2.595352 0.262152 0.448875
C 0 -3.368009 -0.334716 -0.724124
C 0 -2.872993 -1.771612 -0.978091
C 0 -1.355460 -1.807681 -1.209007
O 0 1.608392 1.989322 -1.514495
C 0 2.908631 -0.642012 -1.131553
C 0 3.792134 -0.297528 0.080696
C 0 3.573049 -1.159876 1.329688
O 0 -4.753249 -0.296101 -0.464442
O 0 -3.208219 0.747633 1.388660
H 0 -0.587536 2.714419 0.736996
H 0 -0.858842 1.106387 -1.559990
H 0 0.981240 -0.507460 -2.039102
H 0 -0.809382 -1.913440 0.858869
H 0 -0.721621 0.398858 1.423805
H 0 1.446383 1.239058 0.421826
H 0 -3.139390 0.274005 -1.616063
H 0 -3.145404 -2.389356 -0.112267
H 0 -3.405385 -2.177920 -1.843989
H 0 -1.022156 -2.837110 -1.377177
H 0 -1.108989 -1.243694 -2.116150
H 0 1.162647 2.837110 -1.338631
H 0 3.021622 -1.705410 -1.381381
H 0 3.273258 -0.078510 -1.998455
H 0 3.669395 0.763493 0.334625
H 0 4.836851 -0.403252 -0.241222
H 0 2.562341 -1.042088 1.729632
H 0 4.288477 -0.891449 2.116150
H 0 3.712996 -2.223585 1.099898
H 0 -4.836851 0.179756 0.386864
Free Energy (PCM/B3LYP/6-31G*) = -845.146401
Number of imaginary frequencies = 0

Isomer 14
B3LYP/6-31G* geometry
O 0 0.246950 1.395859 1.866370
C 0 -0.550244 1.413310 0.682914
C 0 0.976575 -0.029553 -0.818958
C 0 -0.759982 -1.105344 0.488385
O 0 -0.061249 -1.026493 -0.760468
C 0 -1.514960 0.225127 0.739745
C 0 0.343237 1.357014 -0.569878
C 0 -2.674400 0.358618 -0.240467
C 0 -3.631749 -0.839121 -0.284028
C 0 -2.838055 -2.112255 -0.591713
C 0 -1.696984 -2.311924 0.415453
O 0 1.400850 2.317759 -0.443891
C 0 2.197281 -0.373908 0.047701
C 0 2.831961 -1.720660 -0.322628
C 0 4.076860 -2.035544 0.512739
O 0 -4.254041 -1.013791 0.993855
O 0 -2.847229 1.334701 -0.953226
H 0 1.023526 1.943810 1.647396
H 0 -1.130997 2.347321 0.640896
H 0 1.300145 -0.055910 -1.866370
H 0 -0.045645 -1.251412 1.307049
H 0 -1.956047 0.175245 1.744740
H 0 -0.283943 1.593047 -1.436976
H 0 -4.380078 -0.643689 -1.062765
H 0 -3.525015 -2.966018 -0.576058
H 0 -2.433609 -2.033675 -1.607254
H 0 -2.112071 -2.485049 1.414281
H 0 -1.107851 -3.196637 0.149946
H 0 1.022774 3.196637 -0.612395
H 0 2.930944 0.428627 -0.094836
H 0 1.934345 -0.358932 1.110994
H 0 3.098223 -1.713477 -1.389509
H 0 2.091425 -2.520558 -0.198876
H 0 3.835024 -2.080537 1.581909
H 0 4.848115 -1.266537 0.380453
H 0 4.514092 -2.999786 0.228913
H 0 -4.848115 -0.259969 1.142356
Free Energy (PCM/B3LYP/6-31G*) = -845.144572
Number of imaginary frequencies = 0

Isomer 15
B3LYP/6-31G* geometry
O 0 0.727033 0.904948 1.404434
C 0 0.518483 1.250777 0.039373
C 0 -1.621366 -0.087523 -0.222673
C 0 0.452652 -1.128693 -0.955191
O 0 -0.941869 -0.916169 -1.174573
C 0 1.207393 0.226314 -0.889500
C 0 -0.996578 1.313390 -0.240975
C 0 2.671929 0.039594 -0.523980
C 0 3.026445 -0.976320 0.556675
C 0 2.277299 -2.299055 0.323157
C 0 0.762924 -2.066109 0.221184
O 0 -1.616662 2.073857 0.804013
C 0 -3.100226 -0.083893 -0.608080
C 0 -3.791554 -1.453404 -0.502671
C 0 -3.919052 -1.989691 0.928434

O 0 4.425294 -1.174328 0.598043
O 0 3.565983 0.668645 -1.074355
H 0 0.027876 1.384958 1.889260
H 0 0.959289 2.240429 -0.162343
H 0 -1.499956 -0.494466 0.789989
H 0 0.780643 -1.635260 -1.871029
H 0 1.194164 0.675331 -1.889260
H 0 -1.173635 1.774601 -1.221382
H 0 2.668845 -0.540399 1.503757
H 0 2.659720 -2.759570 -0.597619
H 0 2.510345 -2.983896 1.145179
H 0 0.243816 -3.016485 0.054440
H 0 0.392383 -1.642959 1.159767
H 0 -1.468526 3.016485 0.622457
H 0 -3.612561 0.643438 0.032697
H 0 -3.178138 0.285852 -1.639651
H 0 -3.248903 -2.177674 -1.122119
H 0 -4.794497 -1.363037 -0.939876
H 0 -4.466141 -2.939369 0.942117
H 0 -4.461073 -1.282885 1.569314
H 0 -2.940145 -2.170060 1.387684
H 0 4.794497 -0.472940 0.024515
Free Energy (PCM/B3LYP/6-31G*) = -845.149673
Number of imaginary frequencies = 0

Isomer 16
B3LYP/6-31G* geometry
O 0 1.335207 1.089921 1.490433
C 0 1.012787 1.704569 0.242389
C 0 -1.132740 0.419274 -0.023363
C 0 0.822388 -0.459001 -1.173191
O 0 -0.591045 -0.214701 -1.199591
C 0 1.607499 0.856862 -0.908899
C 0 -0.518101 1.821256 0.064889
C 0 3.093166 0.605423 -0.703722
C 0 3.525368 -0.619121 0.095683
C 0 2.739620 -1.863523 -0.345721
C 0 1.226604 -1.617987 -0.250873
O 0 -0.826615 2.594909 -1.092046
C 0 -2.653571 0.414466 -0.156969
C 0 -3.264730 -0.992069 -0.190058
C 0 -4.791335 -0.969464 -0.315086
O 0 4.919053 -0.815790 -0.030143
O 0 3.945687 1.353931 -1.162578
H 0 1.075901 1.698720 2.201389
H 0 1.454833 2.708176 0.184703
H 0 -0.844166 -0.141526 0.874349
H 0 1.046130 -0.766642 -2.201389
H 0 1.529077 1.489029 -1.799781
H 0 -0.930850 2.360351 0.926443
H 0 3.257605 -0.395457 1.141768
H 0 3.027227 -2.115341 -1.375332
H 0 3.034512 -2.708176 0.285569
H 0 0.676298 -2.514195 -0.557344
H 0 0.956936 -1.402143 0.787662
H 0 -0.816859 1.970025 -1.839090
H 0 -3.064507 0.976580 0.693148
H 0 -2.935646 0.967082 -1.062200
H 0 -2.978770 -1.531766 0.723905
H 0 -2.831979 -1.551569 -1.027668
H 0 -5.203531 -1.984768 -0.336102
H 0 -5.105412 -0.462552 -1.235990
H 0 -5.251445 -0.439251 0.528058
H 0 5.251445 0.005595 -0.444783
Free Energy (PCM/B3LYP/6-31G*) = -845.149026
Number of imaginary frequencies = 0

Isomer 17
B3LYP/6-31G* geometry
O 0 2.248090 2.832816 0.009273
C 0 1.524868 1.705365 0.490926
C 0 -0.482931 0.218814 0.150367
C 0 1.484736 -0.710251 1.182188
O 0 0.396181 -0.910270 0.267472
C 0 2.376993 0.429950 0.654946
C 0 0.306980 1.418726 -0.396245
C 0 3.085043 0.024188 -0.630017
C 0 3.160105 -1.457086 -0.965346
C 0 3.385504 -2.256021 0.323200
C 0 2.229290 -2.050428 1.329323
O 0 -0.538546 2.559766 -0.433073
C 0 -1.650719 -0.185231 -0.744236
C 0 -2.528699 -1.298057 -0.157518
C 0 -3.692236 -1.678338 -1.078619
O 0 4.176396 -1.704766 -1.913166
O 0 3.615842 0.842897 -1.376788
H 0 2.814720 2.503451 -0.716554
H 0 1.151119 1.994069 1.481117
H 0 -0.859039 0.486047 1.152870
H 0 1.070734 -0.410849 2.156359
H 0 3.176326 0.639753 1.381711
H 0 0.657021 1.169332 -1.412856
H 0 2.168517 -1.719455 -1.373580
H 0 3.491272 -3.315090 0.069149
H 0 4.341374 -1.939036 0.757327
H 0 1.477406 -2.838784 1.221388
H 0 2.621675 -2.125242 2.348318
H 0 0.061705 3.315090 -0.567601
H 0 -2.256073 0.710999 -0.926312
H 0 -1.247897 -0.499580 -1.717564
H 0 -2.922873 -0.970804 0.815024
H 0 -1.908944 -2.180579 0.040931
H 0 -4.305791 -2.471888 -0.637018
H 0 -3.328029 -2.038767 -2.048659
H 0 -4.345138 -0.817497 -1.269143
H 0 4.345138 -0.847043 -2.348318
Free Energy (PCM/B3LYP/6-31G*) = -845.153429
Number of imaginary frequencies = 0

Isomer 18
B3LYP/6-31G* geometry
O 0 2.662521 3.097897 0.168556
C 0 1.802187 2.076742 0.666701
C 0 -0.348468 0.819870 0.230190
C 0 1.481986 -0.380796 1.205333
O 0 0.387274 -0.408138 0.284395
C 0 2.499245 0.696534 0.779894
C 0 0.552480 1.974417 -0.222863
C 0 3.235729 0.304002 -0.489634
C 0 3.015388 -1.088355 -1.046791
C 0 3.110993 -2.089092 0.120446
C 0 2.086703 -1.793474 1.245886
O 0 0.943413 1.763787 -1.577138
C 0 -1.560568 0.600884 -0.673961
C 0 -2.539468 -0.454746 -0.145598
C 0 -3.749555 -0.649857 -1.064571
O 0 3.959916 -1.379039 -2.055286
O 0 4.067429 1.046497 -1.012000
H 0 3.409300 2.656592 -0.284219
H 0 1.487010 2.371454 1.676202
H 0 -0.695619 1.065619 1.249348
H 0 1.094933 -0.121403 2.203029
H 0 3.278324 0.782257 1.551224
H 0 -0.014575 2.913796 -0.130948
H 0 1.994649 -1.107652 -1.454831
H 0 2.969442 -3.097897 -0.278893
H 0 4.135420 -2.046172 0.508565
H 0 1.247201 -2.494258 1.201721
H 0 2.566432 -1.936682 2.219422
H 0 1.571333 2.480455 -1.776555
H 0 -2.078390 1.563781 -0.782375
H 0 -1.204750 0.321316 -1.672648
H 0 -2.883167 -0.160830 0.856448
H 0 -2.009140 -1.406452 -0.023705
H 0 -4.432404 -1.409632 -0.667431
H 0 -3.438311 -0.971784 -2.066107
H 0 -4.316903 0.282381 -1.178258
H 0 4.432404 -0.539463 -2.219422
Free Energy (PCM/B3LYP/6-31G*) = -845.153135
Number of imaginary frequencies = 0

Isomer 19

B3LYP/6-31G* geometry
O 0 -0.510417 2.471863 -1.370480
C 0 -0.869321 1.863395 -0.117327
C 0 1.081615 0.231653 -0.187166
C 0 -1.032688 -0.493240 -1.040525
O 0 0.115572 -0.828931 -0.258434
C 0 -1.799351 0.661480 -0.344877
C 0 0.462856 1.449331 0.529543
C 0 -2.442718 0.154757 0.940381
C 0 -3.321080 -1.092794 0.778619
C 0 -2.503220 -2.212513 0.128308
C 0 -1.882470 -1.753499 -1.199326
O 0 1.355908 2.557707 0.534373
C 0 2.316203 -0.305014 0.529969
C 0 3.045416 -1.416205 -0.234715
C 0 4.278331 -1.938217 0.509795
O 0 -4.422467 -0.799331 -0.088829
O 0 -2.284920 0.686997 2.027521
H 0 -1.221084 3.078454 -1.630002
H 0 -1.356461 2.602402 0.528568
H 0 1.352637 0.534121 -1.212795
H 0 -0.703632 -0.136959 -2.027521
H 0 -2.623820 0.964063 -1.005888
H 0 0.271644 1.181198 1.573380
H 0 -3.672979 -1.390037 1.774836
H 0 -1.714487 -2.516668 0.825891
H 0 -3.156659 -3.078454 -0.026966
H 0 -1.255512 -2.548275 -1.618283
H 0 -2.675162 -1.546231 -1.926422
H 0 1.209642 2.991410 -0.327239
H 0 2.993864 0.540314 0.700428
H 0 2.010022 -0.672144 1.520360
H 0 3.346494 -1.036232 -1.221404
H 0 2.347513 -2.241220 -0.421587
H 0 4.782908 -2.728054 -0.058551
H 0 4.004003 -2.353984 1.487348
H 0 5.005839 -1.135617 0.684600
H 0 -5.005839 -0.173813 0.371261
Free Energy (PCM/B3LYP/6-31G*) = -845.151295
Number of imaginary frequencies = 0

Isomer 20
B3LYP/6-31G* geometry
O 0 -0.937302 2.304901 -1.709883
C 0 -1.032193 1.872555 -0.349883
C 0 1.015300 0.353431 -0.299521
C 0 -1.057181 -0.590610 -0.989079
O 0 0.111910 -0.761405 -0.188937
C 0 -1.884901 0.591997 -0.403926
C 0 0.378307 1.645923 0.254583
C 0 -2.459332 0.132462 0.919170
C 0 -3.373218 -1.090180 0.826466
C 0 -2.496048 -2.250373 0.325740
C 0 -1.838300 -1.905174 -1.018760
O 0 0.358663 1.705126 1.674296
C 0 2.315399 -0.027937 0.400896
C 0 3.041736 -1.213899 -0.246178
C 0 4.341604 -1.578935 0.477721
O 0 -4.426761 -0.903977 -0.116735
O 0 -2.160081 0.603341 2.011440
H 0 -0.450950 3.145203 -1.718816
H 0 -1.541823 2.631078 0.261375
H 0 1.211342 0.527204 -1.371079
H 0 -0.758324 -0.318546 -2.011440
H 0 -2.731923 0.771870 -1.077065
H 0 1.013482 2.481559 -0.071435
H 0 -3.764463 -1.301708 1.829362
H 0 -1.730939 -2.458397 1.082340
H 0 -3.121723 -3.145203 0.234827
H 0 -1.155666 -2.706622 -1.321817
H 0 -2.608424 -1.824820 -1.793279
H 0 -0.482061 1.302098 1.972555
H 0 2.972200 0.853232 0.400195
H 0 2.090196 -0.246256 1.451463
H 0 3.262017 -0.974859 -1.296460
H 0 2.370264 -2.080588 -0.261513
H 0 4.840940 -2.427884 -0.003460
H 0 4.149404 -1.853364 1.522435
H 0 5.044422 -0.736345 0.481075
H 0 -5.044422 -0.248626 0.246569
Free Energy (PCM/B3LYP/6-31G*) = -845.149134
Number of imaginary frequencies = 0

Isomer 21
B3LYP/6-31G* geometry
O 0 -1.096902 2.660432 0.413141
C 0 -0.559149 1.454562 -0.125279
C 0 1.572022 0.089747 -0.184136
C 0 -0.529005 -1.052529 -0.159617
O 0 0.812915 -1.026263 0.308956
C 0 -1.275399 0.198376 0.371958
C 0 0.913344 1.403527 0.280375
C 0 -2.740763 0.142993 0.006792
C 0 -3.470350 -1.151983 0.343189
C 0 -2.674465 -2.363376 -0.183546
C 0 -1.211117 -2.341853 0.286775
O 0 1.618513 2.496112 -0.297241
C 0 3.012384 -0.039125 0.310632
C 0 3.870215 -1.112444 -0.382153
C 0 3.516558 -2.565387 -0.042531
O 0 -4.782278 -1.134614 -0.174197
O 0 -3.341078 1.064582 -0.534590
H 0 -1.990901 2.743738 0.037771
H 0 -0.609671 1.482767 -1.224835
H 0 1.557216 0.076749 -1.287215
H 0 -0.525245 -1.013212 -1.262532
H 0 -1.217964 0.157996 1.470194
H 0 0.965196 1.449761 1.381146
H 0 -3.496578 -1.209320 1.446277
H 0 -3.172588 -3.279138 0.149880
H 0 -2.722263 -2.351520 -1.279884
H 0 -1.155971 -2.418093 1.380456
H 0 -0.671157 -3.200570 -0.125780
H 0 1.065104 3.279138 -0.131305
H 0 3.484685 0.938434 0.160839
H 0 2.987639 -0.214939 1.395263
H 0 4.918014 -0.931283 -0.107533
H 0 3.814962 -0.964559 -1.470194
H 0 4.211587 -3.257911 -0.532177
H 0 2.500896 -2.817016 -0.359044
H 0 3.578164 -2.740382 1.038997
H 0 -4.918014 -0.226161 -0.508989
Free Energy (PCM/B3LYP/6-31G*) = -845.156763
Number of imaginary frequencies = 0

Isomer 22
B3LYP/6-31G* geometry
O 0 -1.529197 2.976096 -0.031753
C 0 -0.991503 1.731596 -0.471434
C 0 1.152656 0.387713 -0.424136
C 0 -0.919484 -0.768973 -0.209777
O 0 0.437084 -0.688730 0.200606
C 0 -1.653446 0.529267 0.213719
C 0 0.503427 1.748817 -0.122763
C 0 -3.140815 0.428431 -0.024562
C 0 -3.829310 -0.843231 0.457405
C 0 -3.049660 -2.089215 -0.001603
C 0 -1.567898 -2.009944 0.396041
O 0 0.668497 2.064824 1.256063
C 0 2.608227 0.304671 0.030737
C 0 3.312539 -0.990952 -0.391481
C 0 4.772936 -1.045414 0.067876
O 0 -5.168407 -0.883887 0.016438
O 0 -3.801382 1.313790 -0.559644
H 0 -2.486450 2.927629 -0.206951
H 0 -1.103377 1.631341 -1.561621
H 0 1.105206 0.249444 -1.518561
H 0 -0.959046 -0.848174 -1.310605
H 0 -1.507785 0.628414 1.299522
H 0 0.997701 2.508675 -0.749332
H 0 -3.791238 -0.801732 1.561621
H 0 -3.519812 -2.976096 0.434825

H 0 -3.148874 -2.175113 -1.091181
H 0 -1.463270 -1.972846 1.488150
H 0 -1.035526 -2.902004 0.049633
H 0 0.043054 2.791641 1.427716
H 0 3.142847 1.168599 -0.387288
H 0 2.637935 0.413615 1.121247
H 0 3.268423 -1.087176 -1.485784
H 0 2.763244 -1.847592 0.016210
H 0 5.252903 -1.980301 -0.243357
H 0 4.846989 -0.979669 1.160502
H 0 5.353528 -0.215323 -0.353642
H 0 -5.353528 0.008110 -0.337858
Free Energy (PCM/B3LYP/6-31G*) = -845.158207
Number of imaginary frequencies = 0

Isomer 23
B3LYP/6-31G* geometry
O 0 1.021685 2.108023 1.086003
C 0 0.922412 1.680765 -0.276678
C 0 -1.141794 0.246955 0.155559
C 0 0.994838 -0.808821 0.230732
O 0 -0.355427 -0.905845 -0.195086
C 0 1.678968 0.368249 -0.516143
C 0 -0.578699 1.500326 -0.552048
C 0 3.137158 0.419514 -0.125584
C 0 3.930169 -0.860310 -0.352219
C 0 3.198767 -2.025082 0.357194
C 0 1.718721 -2.123543 -0.046112
O 0 -1.279658 2.674721 -0.160442
C 0 -2.587736 -0.043224 -0.232996
C 0 -3.226149 -1.190066 0.560580
C 0 -4.673405 -1.466804 0.141431
O 0 5.254097 -0.718682 0.112170
O 0 3.670934 1.384949 0.411533
H 0 1.959021 2.329127 1.229655
H 0 1.313597 2.465553 -0.938869
H 0 -1.073814 0.406489 1.244011
H 0 1.020885 -0.593609 1.310679
H 0 1.632164 0.121143 -1.586973
H 0 -0.725617 1.382431 -1.632376
H 0 3.935318 -1.057878 -1.436572
H 0 3.725282 -2.956078 0.124812
H 0 3.287845 -1.866262 1.439512
H 0 1.624679 -2.364642 -1.113007
H 0 1.232098 -2.931178 0.511060
H 0 -0.854733 2.956078 0.670803
H 0 -3.162022 0.879563 -0.087479
H 0 -2.618419 -0.271486 -1.308245
H 0 -3.194648 -0.947868 1.632376
H 0 -2.622686 -2.096446 0.430957
H 0 -5.106660 -2.287916 0.723980
H 0 -4.732763 -1.742295 -0.918858
H 0 -5.305405 -0.582238 0.289241
H 0 5.305405 0.185742 0.480043
Free Energy (PCM/B3LYP/6-31G*) = -845.159232
Number of imaginary frequencies = 0

Isomer 24
B3LYP/6-31G* geometry
O 0 1.056365 -2.196153 -1.561823
C 0 0.960363 -1.953361 -0.161532
C 0 -1.127495 -0.548712 -0.425560
C 0 0.955985 0.597127 -0.299166
O 0 -0.405186 0.575551 0.123908
C 0 1.688436 -0.659556 0.249053
C 0 -0.537296 -1.829159 0.186480
C 0 3.136419 -0.592699 -0.171655
C 0 3.891399 0.660677 0.249875
C 0 3.107969 1.899891 -0.246046
C 0 1.631882 1.876405 0.183729
O 0 -0.709409 -1.842367 1.603516
C 0 -2.611290 -0.346255 -0.131566
C 0 -3.210600 0.891246 -0.811853
C 0 -4.699794 1.072080 -0.501637
O 0 5.209023 0.646023 -0.252194
O 0 3.690462 -1.435952 -0.870288
H 0 2.009990 -2.272720 -1.746962
H 0 1.374901 -2.797719 0.407260
H 0 -0.964379 -0.577156 -1.512596
H 0 0.982489 0.559384 -1.399228
H 0 1.668558 -0.580814 1.345763
H 0 -1.058277 -2.707285 -0.209832
H 0 3.913127 0.677183 1.351713
H 0 3.606178 2.797719 0.132783
H 0 3.183673 1.926712 -1.340478
H 0 1.547600 1.936574 1.276649
H 0 1.107772 2.744469 -0.230076
H 0 -0.595795 -0.921963 1.898793
H 0 -3.143474 -1.247265 -0.466340
H 0 -2.757515 -0.284480 0.954148
H 0 -3.068932 0.810120 -1.898793
H 0 -2.654650 1.780804 -0.493000
H 0 -5.104461 1.960281 -1.000128
H 0 -4.868303 1.188311 0.576173
H 0 -5.283624 0.205680 -0.836503
H 0 5.283624 -0.183981 -0.763559
Free Energy (PCM/B3LYP/6-31G*) = -845.156619
Number of imaginary frequencies = 0

Isomer 25
B3LYP/6-31G* geometry
O 0 0.442401 -0.259354 -1.349633
C 0 -1.425209 0.677678 -0.093879
C 0 0.677046 2.000951 -0.503817
C 0 -0.527798 1.807147 0.439780
C 0 1.409558 0.687101 -0.835484
C 0 -0.599141 -0.593417 -0.430459
C 0 -1.482208 -1.671478 -1.053825
C 0 -2.658798 -2.019688 -0.124934
C 0 -3.494454 -0.787889 0.256184
C 0 -2.556748 0.279980 0.831364
O 0 -2.691800 0.717531 1.967682
C 0 2.305451 0.116061 0.271336
C 0 3.031749 -1.168750 -0.147323
C 0 3.978148 -1.692504 0.937677
O 0 -0.040718 1.535845 1.750714
O 0 0.222419 2.607604 -1.718425
O 0 -4.122411 -0.306040 -0.933933
H 0 -1.889065 1.005101 -1.033724
H 0 1.372181 2.709186 -0.040812
H 0 -1.098724 2.747306 0.434126
H 0 2.041569 0.895015 -1.707242
H 0 -0.158405 -0.979161 0.499350
H 0 -0.882210 -2.567145 -1.248059
H 0 -1.856384 -1.311330 -2.018913
H 0 -2.285793 -2.481375 0.798273
H 0 -3.322761 -2.747306 -0.603944
H 0 -4.236943 -1.044706 1.021821
H 0 3.045383 0.891987 0.513660
H 0 1.733069 -0.049035 1.189038
H 0 3.598651 -0.981092 -1.070385
H 0 2.292050 -1.939838 -0.395642
H 0 4.480446 -2.612437 0.617132
H 0 3.434284 -1.914557 1.864206
H 0 4.753365 -0.954364 1.177822
H 0 -0.842111 1.394958 2.289840
H 0 -0.079958 1.880961 -2.289840
H 0 -4.753365 0.387931 -0.681312
Free Energy (PCM/B3LYP/6-31G*) = -845.146263
Number of imaginary frequencies = 0

Isomer 26
B3LYP/6-31G* geometry
O 0 0.406090 -0.679282 -1.341369
C 0 -1.376930 0.673870 -0.395103
C 0 0.812517 1.717610 -1.078326
C 0 -0.406753 1.835736 -0.154147
C 0 1.441355 0.296680 -1.098777
C 0 -0.639277 -0.690871 -0.375132
C 0 -1.599325 -1.834499 -0.696017
C 0 -2.787004 -1.843675 0.282420
C 0 -3.537232 -0.503290 0.314082

C 0 -2.528940 0.618639 0.588291
O 0 -2.628720 1.361533 1.556979
C 0 2.332679 -0.053364 0.101416
C 0 3.002255 -1.427245 -0.029896
C 0 3.915490 -1.757143 1.154950
O 0 0.086660 1.862812 1.188127
O 0 1.770242 2.719684 -0.756550
O 0 -4.143089 -0.316005 -0.967060
H 0 -1.813240 0.772467 -1.398193
H 0 0.468510 1.928217 -2.097706
H 0 -0.913007 2.787371 -0.374161
H 0 2.063595 0.235650 -1.999770
H 0 -0.220005 -0.844802 0.629417
H 0 -1.061917 -2.787371 -0.639165
H 0 -1.957180 -1.720963 -1.725571
H 0 -2.435172 -2.064809 1.298352
H 0 -3.501796 -2.628011 0.010927
H 0 -4.287915 -0.497543 1.114146
H 0 3.104335 0.724200 0.167263
H 0 1.763606 0.002647 1.035700
H 0 3.584290 -1.459011 -0.962260
H 0 2.229500 -2.199939 -0.126980
H 0 4.380691 -2.742737 1.037393
H 0 3.354329 -1.763639 2.097706
H 0 4.720009 -1.017754 1.254512
H 0 -0.701680 1.991557 1.748172
H 0 1.771129 2.768414 0.216519
H 0 -4.720009 0.463780 -0.915625
Free Energy (PCM/B3LYP/6-31G*) = -845.147626
Number of imaginary frequencies = 0

Isomer 27
B3LYP/6-31G* geometry
O 0 0.456328 -0.420609 -1.255437
C 0 -1.492962 0.479519 -0.129579
C 0 0.528756 1.912806 -0.455436
C 0 -0.656343 1.614022 0.472256
C 0 1.321653 0.645274 -0.820703
C 0 -0.590765 -0.757465 -0.350042
C 0 -1.374953 -1.936290 -0.917965
C 0 -2.546091 -2.295890 0.010029
C 0 -3.494229 -1.116513 0.234759
C 0 -2.734938 0.143486 0.672416
O 0 -3.157909 0.864482 1.568707
C 0 2.298763 0.203833 0.281549
C 0 3.137635 -1.019210 -0.108604
C 0 4.126082 -1.434028 0.985611
O 0 -1.391650 2.830488 0.592935
O 0 0.044401 2.498446 -1.663107
O 0 -4.122677 -0.819062 -1.019334
H 0 -1.840464 0.793110 -1.124062
H 0 1.204382 2.616638 0.055101
H 0 -0.281073 1.302004 1.458392
H 0 1.903049 0.886621 -1.717972
H 0 -0.164305 -1.057685 0.621156
H 0 -0.705858 -2.796082 -1.031049
H 0 -1.746646 -1.674587 -1.914972
H 0 -2.164550 -2.623492 0.986046
H 0 -3.125107 -3.127963 -0.404736
H 0 -4.241611 -1.352172 1.002421
H 0 2.964386 1.051505 0.494180
H 0 1.764229 -0.001911 1.218627
H 0 3.685765 -0.797235 -1.035273
H 0 2.468931 -1.856280 -0.342238
H 0 4.713308 -2.307520 0.679908
H 0 3.603385 -1.692446 1.914972
H 0 4.828502 -0.623211 1.215476
H 0 -2.187860 2.595305 1.105738
H 0 -0.643842 3.127963 -1.380610
H 0 -4.828502 -0.172352 -0.853808
Free Energy (PCM/B3LYP/6-31G*) = -845.149360
Number of imaginary frequencies = 0

Isomer 28
B3LYP/6-31G* geometry
O 0 0.466218 -0.951686 -1.401880
C 0 -1.381082 0.236712 -0.357324
C 0 0.724752 1.423923 -0.941905
C 0 -0.431166 1.361191 0.054684
C 0 1.440770 0.062763 -1.081908
C 0 -0.594360 -1.092283 -0.458742
C 0 -1.499385 -2.240347 -0.893206
C 0 -2.669025 -2.400515 0.093234
C 0 -3.488940 -1.115856 0.249628
C 0 -2.583154 0.085635 0.556512
O 0 -2.842855 0.882775 1.447858
C 0 2.341754 -0.314446 0.102235
C 0 3.106383 -1.625401 -0.121871
C 0 4.021700 -1.985964 1.052180
O 0 -1.051192 2.646863 0.045649
O 0 1.666949 2.420878 -0.567200
O 0 -4.141820 -0.864078 -1.001225
H 0 -1.778840 0.448325 -1.360759
H 0 0.287307 1.669622 -1.923688
H 0 -0.034064 1.152841 1.059407
H 0 2.069513 0.108833 -1.978517
H 0 -0.180288 -1.330454 0.533758
H 0 -0.916440 -3.166633 -0.937723
H 0 -1.876976 -2.039808 -1.902247
H 0 -2.287845 -2.688907 1.081578
H 0 -3.343252 -3.198277 -0.236496
H 0 -4.219530 -1.214151 1.062245
H 0 3.049133 0.510029 0.248631
H 0 1.761656 -0.381977 1.031806
H 0 3.703881 -1.539952 -1.040803
H 0 2.391113 -2.438367 -0.297553
H 0 4.559092 -2.922673 0.864515
H 0 3.447206 -2.110838 1.978517
H 0 4.768389 -1.201861 1.229070
H 0 -1.727639 2.609953 0.745325
H 0 1.133409 3.198277 -0.325577
H 0 -4.768389 -0.133275 -0.870259
Free Energy (PCM/B3LYP/6-31G*) = -845.147853
Number of imaginary frequencies = 0

Isomer 29
B3LYP/6-31G* geometry
O 0 0.143530 1.845877 1.980472
C 0 -0.715712 1.893787 0.839109
C 0 0.737762 0.665101 -0.911064
C 0 -0.690771 -0.630578 0.546942
O 0 -0.185296 -0.437234 -0.773401
C 0 -1.553567 0.604268 0.929168
C 0 0.094342 2.005653 -0.479019
C 0 -2.806309 0.590159 0.083932
C 0 -3.665155 -0.661173 0.171158
C 0 -2.777530 -1.848467 -0.273883
C 0 -1.496875 -1.930778 0.565704
O 0 -0.690142 2.573499 -1.523517
C 0 2.096008 0.390417 -0.244964
C 0 2.752889 -0.918785 -0.699151
C 0 4.130984 -1.138529 -0.067025
O 0 -4.821726 -0.537031 -0.625150
O 0 -3.124012 1.470902 -0.712283
H 0 0.665912 2.664268 1.993553
H 0 -1.377164 2.769469 0.894546
H 0 0.891186 0.733207 -1.993553
H 0 0.133209 -0.703301 1.266252
H 0 -1.867642 0.485286 1.975192
H 0 0.907183 2.722183 -0.302780
H 0 -3.961316 -0.813288 1.219841
H 0 -3.363275 -2.769469 -0.187716
H 0 -2.532279 -1.711655 -1.333220
H 0 -1.745983 -2.162559 1.609286
H 0 -0.857582 -2.742402 0.201764
H 0 -1.606474 2.251581 -1.419619
H 0 2.753878 1.233224 -0.500608
H 0 1.999879 0.407727 0.847156
H 0 2.846672 -0.913922 -1.794552
H 0 2.095499 -1.761721 -0.453672
H 0 4.578539 -2.080008 -0.405707
H 0 4.062938 -1.175873 1.027368

H 0 4.821726 -0.327120 -0.328052
H 0 -4.697309 0.285318 -1.138592
Free Energy (PCM/B3LYP/6-31G*) = -845.149562
Number of imaginary frequencies = 0

Isomer 30
B3LYP/6-31G* geometry
O 0 0.348078 1.510550 1.771323
C 0 -0.580912 1.450892 0.691149
C 0 0.798201 -0.037757 -0.905951
C 0 -0.744667 -1.082339 0.646981
O 0 -0.201023 -1.049967 -0.676380
C 0 -1.498061 0.244150 0.924107
C 0 0.162045 1.347258 -0.654704
C 0 -2.771369 0.301655 0.099309
C 0 -3.695744 -0.908406 0.184035
C 0 -2.895221 -2.177957 -0.163606
C 0 -1.658667 -2.305671 0.734820
O 0 1.201522 2.333397 -0.698973
C 0 2.117592 -0.311259 -0.169039
C 0 2.731927 -1.671068 -0.525999
C 0 4.071618 -1.915056 0.175665
O 0 -4.808008 -0.738568 -0.667185
O 0 -3.076502 1.238394 -0.627099
H 0 1.078103 2.064315 1.436942
H 0 -1.189425 2.367628 0.673315
H 0 0.998951 -0.114778 -1.980927
H 0 0.061245 -1.175653 1.384034
H 0 -1.803527 0.244247 1.980927
H 0 -0.566544 1.525858 -1.453878
H 0 -4.035214 -0.986318 1.231107
H 0 -3.550088 -3.048892 -0.053943
H 0 -2.596584 -2.120942 -1.216331
H 0 -1.963740 -2.433514 1.781594
H 0 -1.079684 -3.193779 0.459668
H 0 0.786752 3.193779 -0.876114
H 0 2.813270 0.490071 -0.445505
H 0 1.978421 -0.231673 0.914469
H 0 2.871687 -1.730803 -1.615034
H 0 2.027328 -2.470355 -0.265051
H 0 4.490046 -2.891807 -0.093249
H 0 3.957339 -1.889745 1.266509
H 0 4.808008 -1.149045 -0.097438
H 0 -4.685436 0.144570 -1.070461
Free Energy (PCM/B3LYP/6-31G*) = -845.150845
Number of imaginary frequencies = 0

Isomer 31
B3LYP/6-31G* geometry
O 0 -1.684670 2.799837 1.142738
C 0 -0.875716 1.660186 0.898502
C 0 0.671985 0.562638 -0.844246
C 0 -0.723822 -0.833778 0.555150
O 0 -0.186979 -0.593362 -0.745849
C 0 -1.682647 0.340173 0.905287
C 0 -0.040562 1.858602 -0.388005
C 0 -2.866982 0.238508 -0.031213
C 0 -3.668664 -1.052097 0.053077
C 0 -2.692697 -2.193429 -0.333531
C 0 -1.437105 -2.186980 0.546619
O 0 -0.840363 2.448063 -1.415697
C 0 2.029955 0.351857 -0.153627
C 0 2.762804 -0.914365 -0.614637
C 0 4.144138 -1.065352 0.030182
O 0 -4.792186 -1.007561 -0.796943
O 0 -3.151718 1.044972 -0.913753
H 0 -1.903041 3.146461 0.257462
H 0 -0.178196 1.583303 1.741707
H 0 0.846777 0.662114 -1.920922
H 0 0.080640 -0.857446 1.302649
H 0 -2.067134 0.175641 1.920922
H 0 0.725340 2.612427 -0.178367
H 0 -4.008253 -1.204185 1.087215
H 0 -3.224878 -3.146461 -0.249096
H 0 -2.421273 -2.060316 -1.387043
H 0 -1.701839 -2.433512 1.582687
H 0 -0.732604 -2.953386 0.205942
H 0 -1.636810 1.890791 -1.533051
H 0 2.646934 1.232089 -0.379841
H 0 1.919263 0.337671 0.939259
H 0 2.867453 -0.889197 -1.708515
H 0 2.150189 -1.794919 -0.387100
H 0 4.644686 -1.977167 -0.314924
H 0 4.067522 -1.119842 1.123193
H 0 4.792186 -0.214847 -0.214804
H 0 -4.648229 -0.232825 -1.375356
Free Energy (PCM/B3LYP/6-31G*) = -845.151440
Number of imaginary frequencies = 0

Isomer 32
B3LYP/6-31G* geometry
O 0 -1.402948 2.630259 0.922231
C 0 -0.713858 1.395121 0.729854
C 0 0.734578 0.070630 -0.896129
C 0 -0.764492 -1.126273 0.597760
O 0 -0.183131 -1.024322 -0.704467
C 0 -1.599639 0.147525 0.912691
C 0 -0.028530 1.384369 -0.643890
C 0 -2.876760 0.170747 0.090146
C 0 -3.706915 -1.105930 0.052002
C 0 -2.818154 -2.302781 -0.327617
C 0 -1.611400 -2.399794 0.613029
O 0 0.858142 2.489820 -0.754837
C 0 2.044515 -0.082127 -0.111039
C 0 2.802593 -1.370867 -0.454056
C 0 4.136463 -1.488949 0.290226
O 0 -4.796620 -0.966807 -0.831891
O 0 -3.278344 1.160238 -0.517069
H 0 -2.171418 2.594981 0.320240
H 0 0.061465 1.379473 1.503573
H 0 0.977790 0.019226 -1.963606
H 0 0.024745 -1.208344 1.356895
H 0 -1.919207 0.085848 1.963606
H 0 -0.813817 1.454992 -1.412307
H 0 -4.072372 -1.262056 1.083342
H 0 -3.421071 -3.215752 -0.284782
H 0 -2.484522 -2.175495 -1.363118
H 0 -1.945594 -2.581986 1.642511
H 0 -0.974502 -3.243601 0.327723
H 0 0.364141 3.243601 -0.384440
H 0 2.664260 0.790294 -0.348581
H 0 1.866811 -0.037991 0.971478
H 0 2.982726 -1.403687 -1.538005
H 0 2.172637 -2.238862 -0.223331
H 0 4.658377 -2.415973 0.026448
H 0 3.985638 -1.489009 1.376959
H 0 4.801077 -0.650343 0.048383
H 0 -4.801077 -0.025693 -1.095882
Free Energy (PCM/B3LYP/6-31G*) = -845.152982
Number of imaginary frequencies = 0