Supporting Information

Pigments of the Moss *Paraleucobryum longifolium*: Isolation and Structure Elucidation of Prenyl-substituted 8,8'-linked 9,10-Phenanthrenequinone Dimers

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Content

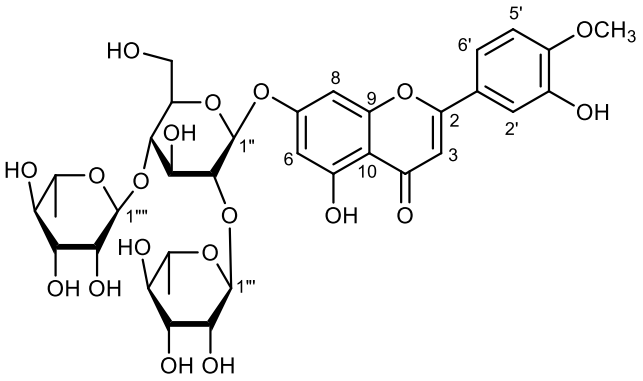
Table S1. ^{1}H,^{1}H-COSY correlations of compounds **1**-**5**.

position	**1**	**2**	**3**	**4**	**5**
3	4	4	4	4	4
4	3	3	3	3	3
11a	11b, 12a, 12b	12	12	12	12
11b	11a, 12a, 12b	12	12	12	12
12a	11a, 11b, 12b	11a, 11b, 16	11a, 11b, 16	11a, 11b, 16	11a, 11b, 16
12b	11a, 11b, 12a	-	-		
14a		14b, 15	14b, 15	14b, 15	14b, 15
14b		14a, 15	14a, 15	14a, 15	14a, 15
15		14a, 14b	14a, 14b	14a, 14b	14a, 14b
16		12, 17a, 17b	12, 17a, 17b	12, 17a, 17b	12, 17a, 17b
17a		16, 17b	16, 17b	16, 17b	16, 17b
17b		16, 17a	16, 17a	16, 17a	16, 17a
3’	4’	4’	4’	4’	4’
4’	3’	3’	3’	3’	3’
11’a	11’b, 12’a, 12’b	12’	12’	11’b, 12’a, 12’b	11’b, 12’a, 12’b
11’b	11’a, 12’a, 12’b	12’	12’	11’a, 12’a, 12’b	11’a, 12’a, 12’b
12’a	11’a, 11’b, 12’b	11’a, 11’b, 16’	11’a, 11’b, 16’	11’a, 11’b, 12’b	11’a, 11’b, 12’b
12’b	11’a, 11’b, 12’a	-	-	11’a, 11’b, 12’a	11’a, 11’b, 12’a
14’a		14’b, 15’	14’b, 15’		
14’b		14’a, 15’	14’a, 15’		
15’		14’a, 14’b	14’a, 14’b		
16’		12’, 17’a, 17’b	12’, 17’a, 17’b		
17’a		16’, 17’b	16’, 17’b		
17’b		16’, 17’a	16’, 17’a		

Table S2. HSQC and HMBC correlations of compounds **1**-**5.** (C No.)

H	**1**		**2**		**3**		**4**		**5**	
	HSQC	HMBC	HSQC	HMBC	HSQC	HMBC	HSQC	HMBC	HSQC	HMBC
3	C-3	1, 2, 4a	C-3	1, 2, 4a	C-3	1, 2, 4a	C-3	1, 2, 4a	C-3	1, 2, 4a
4	C-4	1a, 2, 5a, 10	C-4	1a, 2, 5a, 10	C-4	1a, 2, 5a, 10	C-4	1a, 2, 5a, 10	C-4	1a, 2, 5a, 10
6	C-6	5, 5a, 7, 8	C-6	5, 5a, 7, 8	C-6	5, 5a, 7, 8	C-6	5, 5a, 7, 8	C-6	5, 5a, 7, 8
11a	C-11	1, 1a, 2, 13	C-11	1, 1a, 2, 13	C-11	1, 1a, 2, 13	C-11	1, 1a, 2, 13	C-11	1, 1a, 2, 13
11b	C-11	1, 1a, 2, 13	C-11	1, 1a, 2, 13	C-11	1, 1a, 2, 13	C-11	1, 1a, 2, 13	C-11	1, 1a, 2, 13
12a	C-12	1, 11, 13	C-12	11, 13, 14, 15, 16, 17	C-12	11, 13, 14, 15, 16, 17	C-12	11, 13, 14, 15, 16, 17	C-12	11, 13, 14, 15, 16, 17
12b	C-12	1, 11, 13	-	-	-	-	C-12	-	C-12	-
14a	C-14	12, 13, 15	C-14	12, 13, 15	C-14	12, 13, 15	C-14	12, 13, 15	C-14	12, 13, 15
14b	C-14	-	C-14	12, 13, 15	C-14	12, 13, 15	C-14	12, 13, 15	C-14	12, 13, 15
15	C-15	12, 13, 14	C-15	12, 13, 14	C-15	12, 13, 14	C-15	12, 13, 14	C-15	12, 13, 14
16			C-16	11, 12, 17, 78	C-16	11, 12, 17, 78	C-16	11, 12, 17, 78	C-16	11, 12, 17, 78
17a			C-17	16, 18, 19, 20	C-17	16, 18, 19, 20	C-17	16, 18, 19, 20	C-17	16, 18, 19, 20
17b			C-17	16, 18, 19, 20	C-17	16, 18, 19, 20	C-17	16, 18, 19, 20	C-17	16, 18, 19, 20
19			C-19	17, 18	C-19	17, 18	C-19	17, 18	C-19	17, 18
20			C-20	17, 18	C-20	17, 18	C-20	17, 18	C-20	17, 18
3’	C-3’	1’, 2’, 4’a	C-3	1’, 2’, 4’a	C-3’	1’, 2’, 4’a	C-3’		C-3’	
4’	C-4’	1’a, 2’, 5’a, 10’	C-4	1’a, 2’, 5’a, 10’	C-4’	1’a, 2’, 5’a, 10’	C-4’	1’a, 2’, 5’a, 10’	C-4’	1’a, 2’, 5’a, 10’
6’	C-6’	5’, 5’a, 7’, 8’	C-6	5’, 5’a, 7’, 8’	C-6’	5’, 5’a, 7’, 8’	C-6’	5’, 5’a, 7’, 8’	C-6’	5’, 5’a, 7’, 8’
11’a	C-11’	1’, 1’a, 2’, 13’	C-11’	1’, 1’a, 2’, 13’	C-11’	1’, 1’a, 2’, 13’	C-11’	1’, 1’a, 2’, 13’	C-11’	1’, 1’a, 2’, 13’
11’b	C-11’	1’, 1’a, 2’, 13’	C-11’	1’, 1’a, 2’, 13’	C-11’	1’, 1’a, 2’, 13’	C-11’	1’, 1’a, 2’, 13’	C-11’	1’, 1’a, 2’, 13’
12’a	C-12’	1’, 11’, 13’	C-12’	11’, 13’, 14’, 15’, 16’, 17’	C-12’	11’, 13’, 14’, 15’, 16’, 17’	C-12’	1’, 11’, 13’	C-12’	1’, 11’, 13’
12’b	C-12”	1’, 11’, 13’	C-12’	-	C-12”	-	C-12’	1’, 11’, 13’	C-12’	1’, 11’, 13’
14’a	C-14’	12’, 13’, 15’	C-14’	12’, 13’, 15’	C-14’	12’, 13’, 15’	C-14’	12’, 13’, 15’	C-14’	12’, 13’, 15’
14’b	C-14’	-	C-14’	12’, 13’, 15’	C-14’	12’, 13’, 15’	C-14’		C-14’	
15’	C-15’	12’, 13’, 14’	C-15’	12’, 13’, 14	C-15’	12’, 13’, 14	C-15’	12’, 13’, 14’	C-15’	12’, 13’, 14’
16’			C-16’	11’, 12’, 17’, 18’	C-16’	11’, 12’, 17’, 18’				
17a’			C-17’	16’, 18’, 19’, 20’	C-17’	16’, 18’, 19’, 20’				
17b’			C-17’	16’, 18’, 19’, 20’	C-17’	16’, 18’, 19’, 20’				
19’			C-19’	17’, 18’	C-19’	17’, 18’				
20’			C-20’	17’, 18’	C-20’	17’, 18’				
7-OMe	OCH_3	7	7-OMe	7	7-OMe	7	7-OMe	7	7-OMe	7
7’-OMe	OCH_3	7’	7’-OMe	7’	7-OMe	7’	7-OMe	7’	7-OMe	7’

Table S3. NMR data of diosmetin 7-*O*-[2,4-di-*O*-(α-L-rhamnopyranosyl)]-β-D-glucopyranoside [CD_3OD, 700.25 (^1H), 176.08 (^{13}C) MHz]



Position	^1H	^{13}C	Position	^1H	^{13}C
2	-	165.2	7-*O*-glucose		
3	6.67 s	103.3	1”	5.26 d (7.3)	98.1
4	-	182.6	2”	3.75 m	78.0
5	-	161.5	3”	3.67 m	77.7
6	6.48 d (2.2)	99.5	4”	3.76 dd (9.4, 7.5)	76.1
7	-	162.9	5”	3.64 m	75.5
8	6.78 d (2.2)	94.6	6”	3.88 dd (12.4, 2.0)	60.2
9	-	157.6		3.72 dd (12.4, 3.8)	
10	-	105.6	2”-*O*-rhamnose		
1’	-	123.5	1”’	5.29 d (1.7)	101.3
2’	7.44 d (2.3)	112.6	2”’	3.96 dd (3.4, 1.7)	70.7
3’	-	146.7	3”’	3.60 dd (9.6, 3.4)	70.7
4’	-	151.3	4”’	3.41 t (9.6)	72.5
5’	7.09 d (8.6)	111.1	5”’	3.92 dd (9.6, 6.1)	68.5
6’	7.54 (8.6, 2.3)	118.8	6”’	1.33 d (6.1)	16.8
			4”-*O*-rhamnose		
			1””	4.89 d (1.8)	101.6
			2””	3.87 m	71.0
			3””	3.67 m	70.8
			4””	3.43 t (9.6)	72.2
			5””	3.99 dd (9.6, 6.2)	69.2
			6””	1.28 d (6.2)	16.4

Table S4. Boltzmann populations and specific optical rotations of the low-energy conformers of (*aS*,12*R*,12'*R*)-**2** computed at various levels for the CAM-B3LYP/TZVP PCM/acetone reoptimized AM1 conformers.

Conformer	Boltzmann population	B3LYP/TZVP PCM/acetone	BH&HLYP/TZVP PCM/acetone	CAM-B3LYP/TZVP PCM/acetone	PBE0/TZVP PCM/acetone
Conf. A	12.11 %	-34.26	-89.11	-75.70	-49.19
Conf. B	7.90 %	-41.34	-89.57	-74.49	-52.92
Conf. C	6.90 %	567.50	341.77	346.36	526.86
Conf. D	6.90 %	691.60	379.99	413.50	616.66
Conf. E	6.31 %	-17.83	-77.63	-64.02	-32.42
Conf. F	5.13 %	-104.40	-127.69	-120.91	-114.01
Conf. G	4.94 %	75.92	0.66	14.46	57.23
Conf. H	4.86 %	-98.71	-123.91	-115.72	-108.18
Conf. I	3.77 %	487.61	287.97	290.83	452.61
Conf. J	3.51 %	-45.07	-93.82	-80.28	-57.23
Conf. K	3.30 %	-26.93	-75.57	-61.86	-39.96
Conf. L	2.99 %	695.34	380.03	411.90	619.06
Conf. M	2.96 %	532.29	261.92	292.20	465.40
Conf. N	2.94 %	101.71	6.74	22.02	76.08
Conf. O	2.23 %	30.54	-40.45	-24.64	12.69
Conf. P	2.16 %	2.02	-40.17	-33.08	-11.06
Conf. Q	1.19 %	109.62	9.49	23.43	82.47
Average	N/A	161.59	46.49	61.14	134.52

Table S5. Boltzmann populations and specific optical rotations of the low-energy conformers of (*aR*,12*R*,12'*R*)-**3** computed at various levels for the CAM-B3LYP/TZVP PCM/acetone reoptimized AM1 conformers.

Conformer	Boltzmann population	B3LYP/TZVP PCM/acetone	BH&HLYP/TZVP PCM/acetone	CAM-B3LYP/TZVP PCM/acetone	PBE0/TZVP PCM/acetone
Conf. A	44.16 %	10.15	56.69	51.07	27.43
Conf. B	21.01 %	-374.06	-187.20	-198.28	-323.98
Conf. C	9.11 %	-444.49	-237.00	-249.11	-388.73
Conf. D	4.38 %	-715.30	-438.34	-450.84	-649.48
Conf. E	2.76 %	-700.44	-424.68	-439.66	-638.14
Conf. F	2.39 %	-535.51	-301.64	-311.88	-472.98
Conf. G	2.35 %	-564.30	-312.43	-327.87	-505.36
Conf. H	2.29 %	-630.46	-372.32	-377.55	-567.24
Conf. I	1.77 %	-189.88	-66.08	-73.96	-162.95
Conf. J	1.37 %	-298.69	-171.21	-174.47	-271.55
Conf. K	0.97 %	-348.09	-179.82	-200.74	-305.91
Average	N/A	-234.02	-102.81	-111.44	-197.91

Table S6. The antiproliferative action of leucobryns A (**1**), B (**2**) and C (**3**) against human cancer cell lines

Compound	conc.	Inhibition (%) ± SEM [calculated IC_{50} (μM)]			
		SiHa	HeLa	A2780	MDA-MB-231
1	30 μM	22.47 ± 1.56	25.69 ± 1.88	–*	–
	60 μM	69.34 ± 1.14	80.41 ± 2.20	86.43 ± 0.46	76.04 ± 0.61
		[45.56]	[40.40]	[46.34]	[50.81]
2	30 μM	–	10.72 ± 2.85	–	–
	60 μM	22.44 ± 0.69	37.48 ± 2.03	16.38 ± 2.44	59.80 ± 0.71
3	30 μM	–	–	–	–
	60 μM	–	31.63 ± 1.36	–	–
Cisplatin	10 μM	88.64 ± 0.50	42.61 ± 2.33	83.57 ± 1.21	67.51 ± 1.01
	30 μM	90.18 ± 7.78	99.93 ± 0.26	95.02 ± 0.28	87.75 ± 1.10
		[7.84]	[12.43]	[1.30]	[3.74]

*: inhibition values less than 10% are considered negligible and not presented numerically.

Antiproliferative assay. The antiproliferative properties of the isolated compounds were assayed by MTT (3-(4,5-dimethylthiazol-2-yl)-2,5-diphenyltetrazolium bromide) method against cervical (HeLa and SiHa), breast (MDA-MB-231), and ovarian (A2780) cancer cells.[i] Cell lines were purchased from the European Collection of Cell Cultures (Salisbury, UK). The cells were grown in Minimum Essential Medium (MEM) supplemented with 10% fetal calf serum (FCS), 1% nonessential amino acids, and 1% penicillin-streptomycin. All media and supplements were obtained from Lonza Group Ltd. (Basel, Switzerland). Experiments were performed as described earlier.[Error! Bookmark not defined.] Two independent experiments were carried out with five wells for each condition. Clinically available drug cisplatin (Ebewe Pharma GmbH, Unterach, Austria) was used as a reference agent. All the calculations were performed using GraphPad Prism 5 software (GraphPad Software; San Diego, CA, United States).

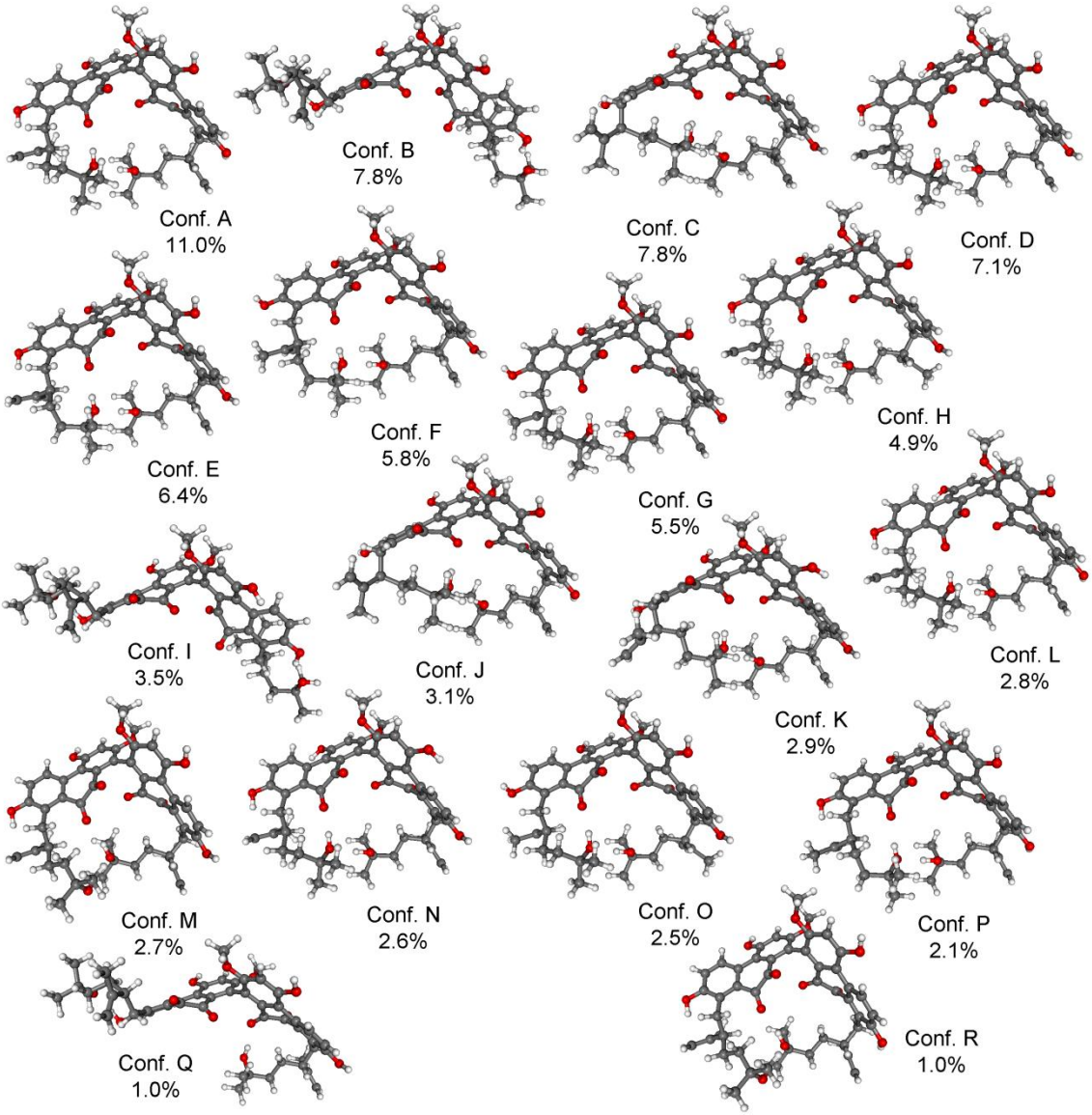


Figure S1. Low-energy (≥ 1%) CAM-B3LYP/TZVP PCM/MeCN conformers of (*aS*,12*R*,12'*R*)-**2**.

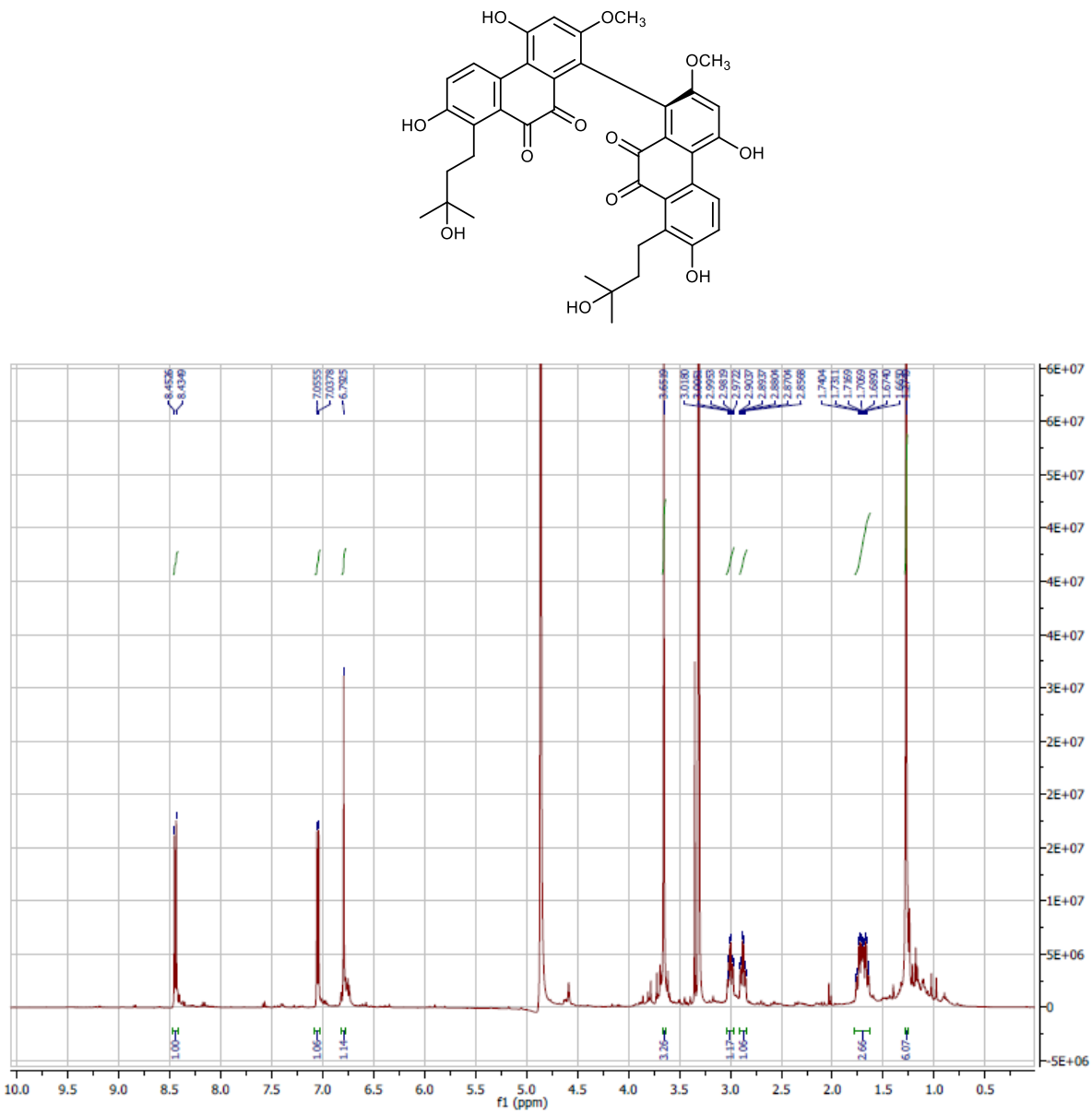


Figure S2. ^{1}H NMR spectrum of leucobryn A (**1**) (CD_3OD, 500 MHz)

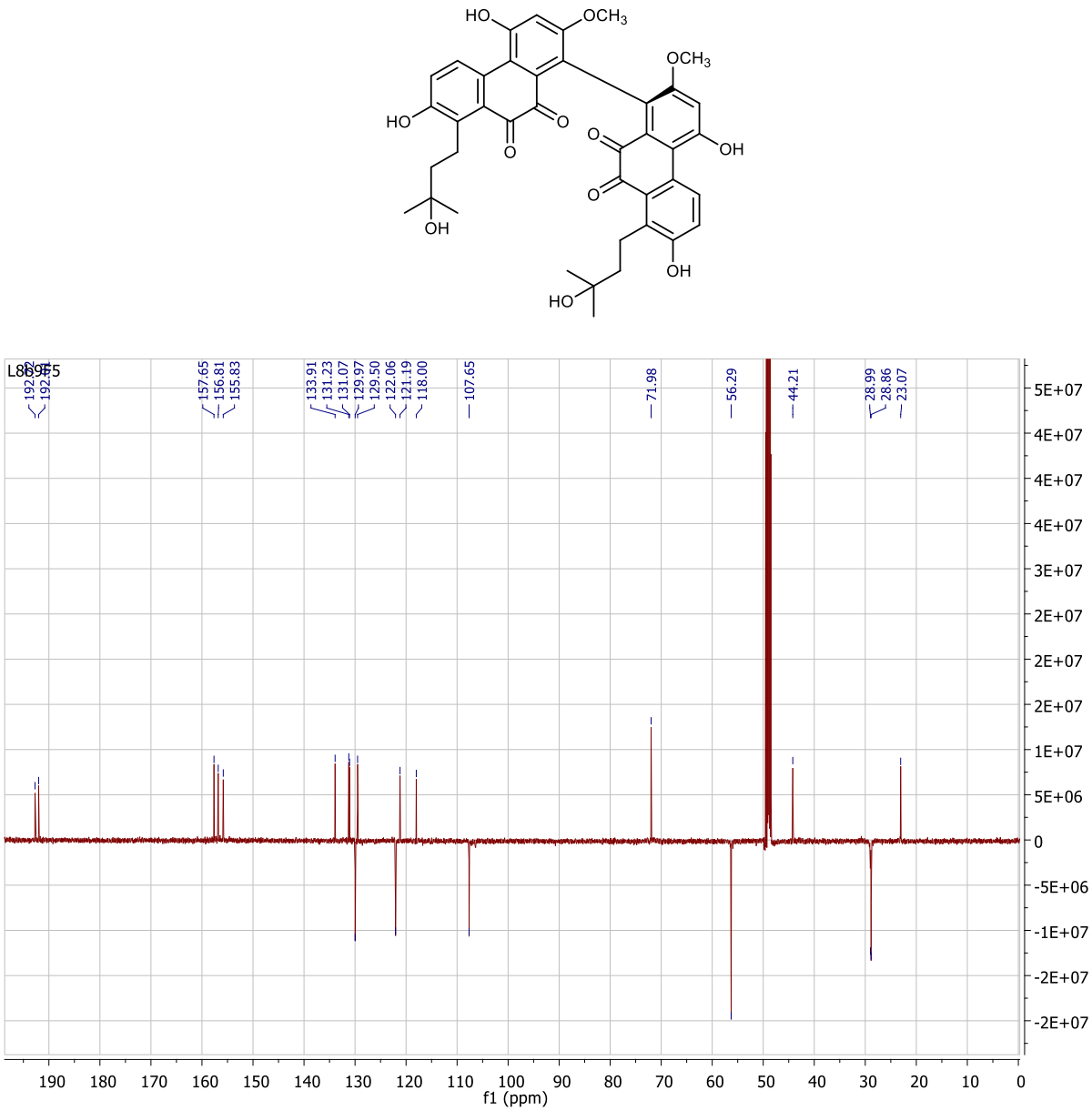


Figure S3. ^{13}C JMOD spectrum of leucobryn A (**1**) (CD_3OD, 125 MHz)

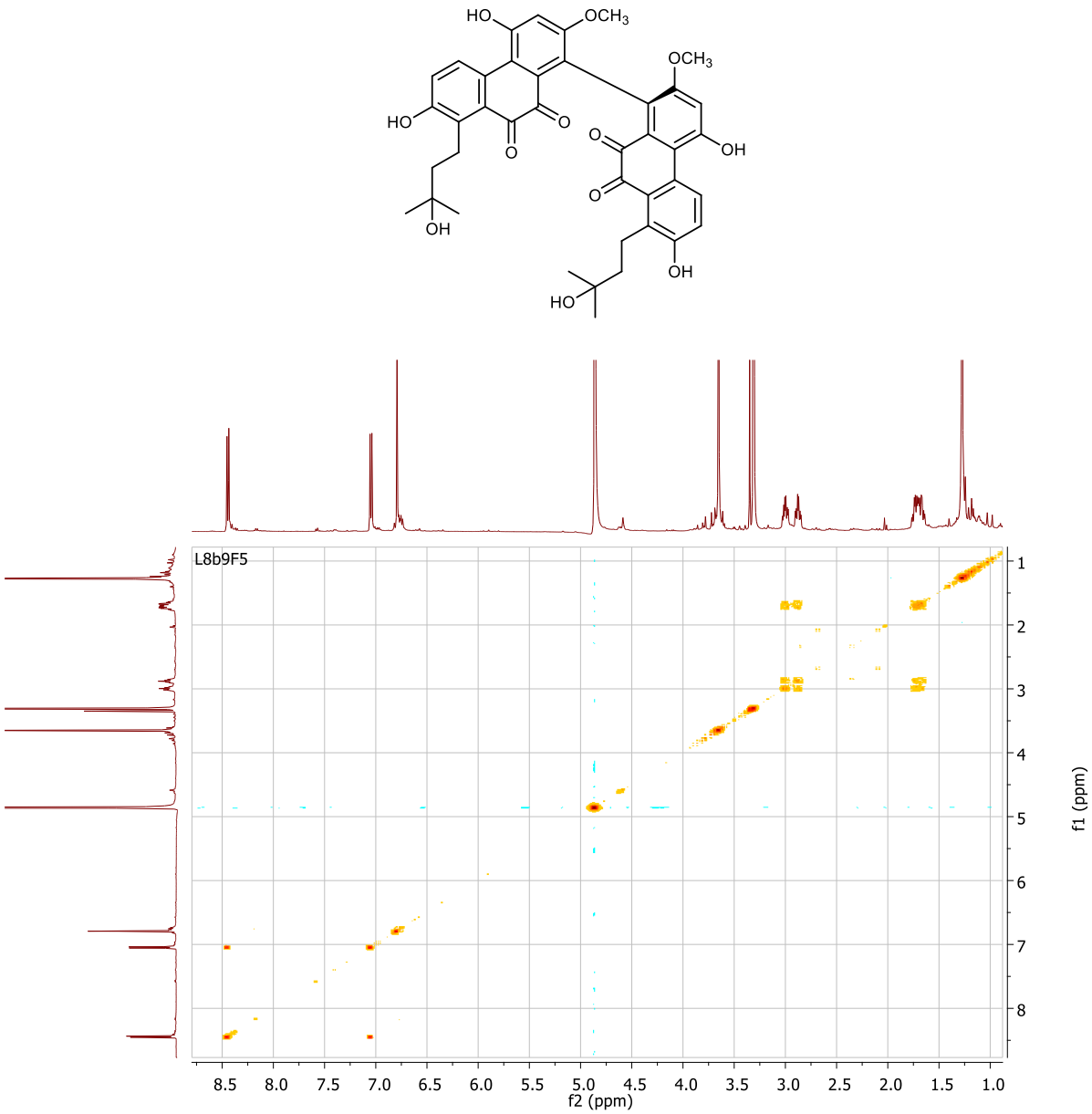


Figure S4. $^{1}H,^{1}H$ COSY spectrum of leucobryn A (**1**) (CD_3OD, 500 MHz)

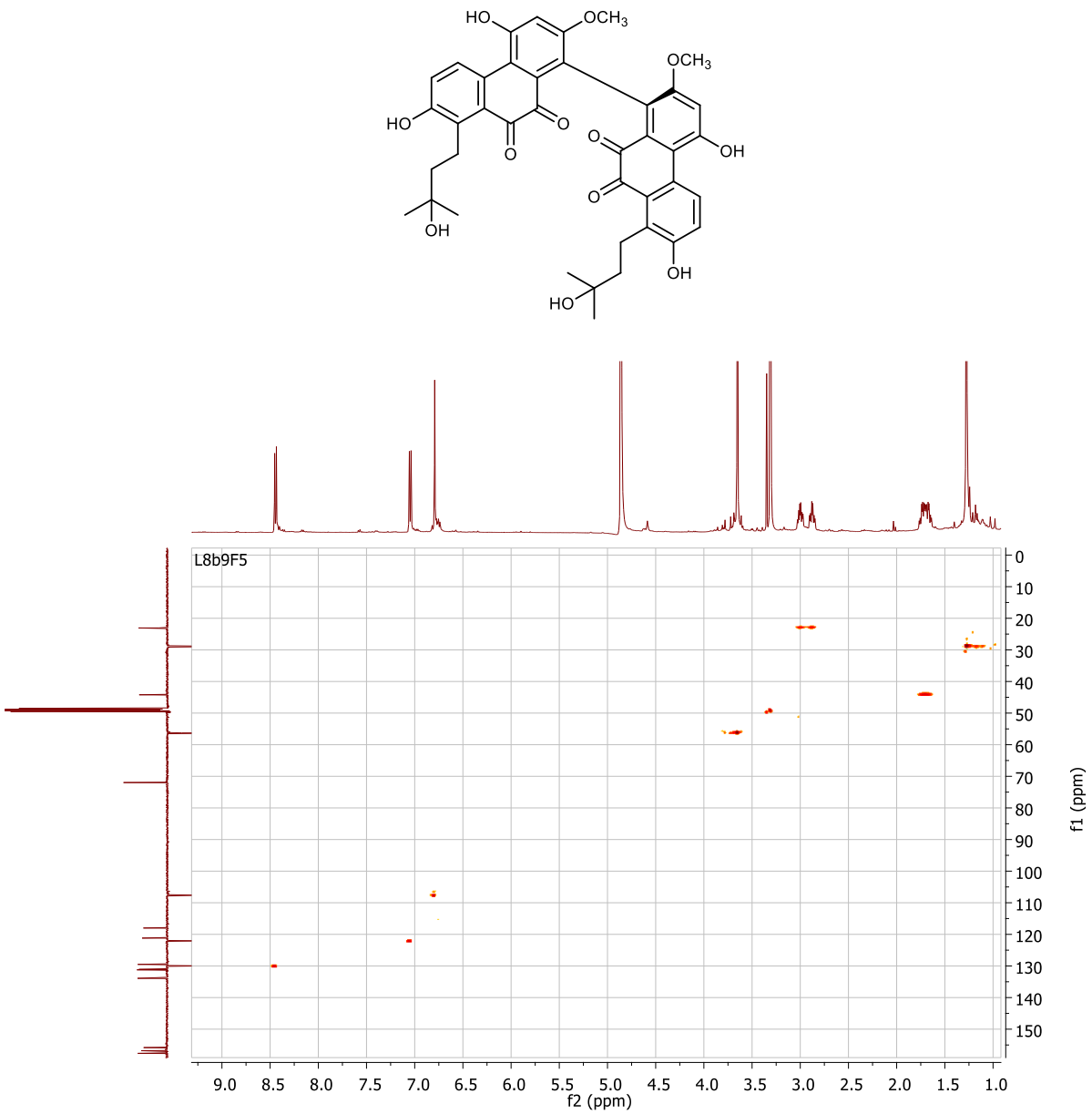


Figure S5. HSQC spectrum of leucobryn A (**1**) (CD_3OD)

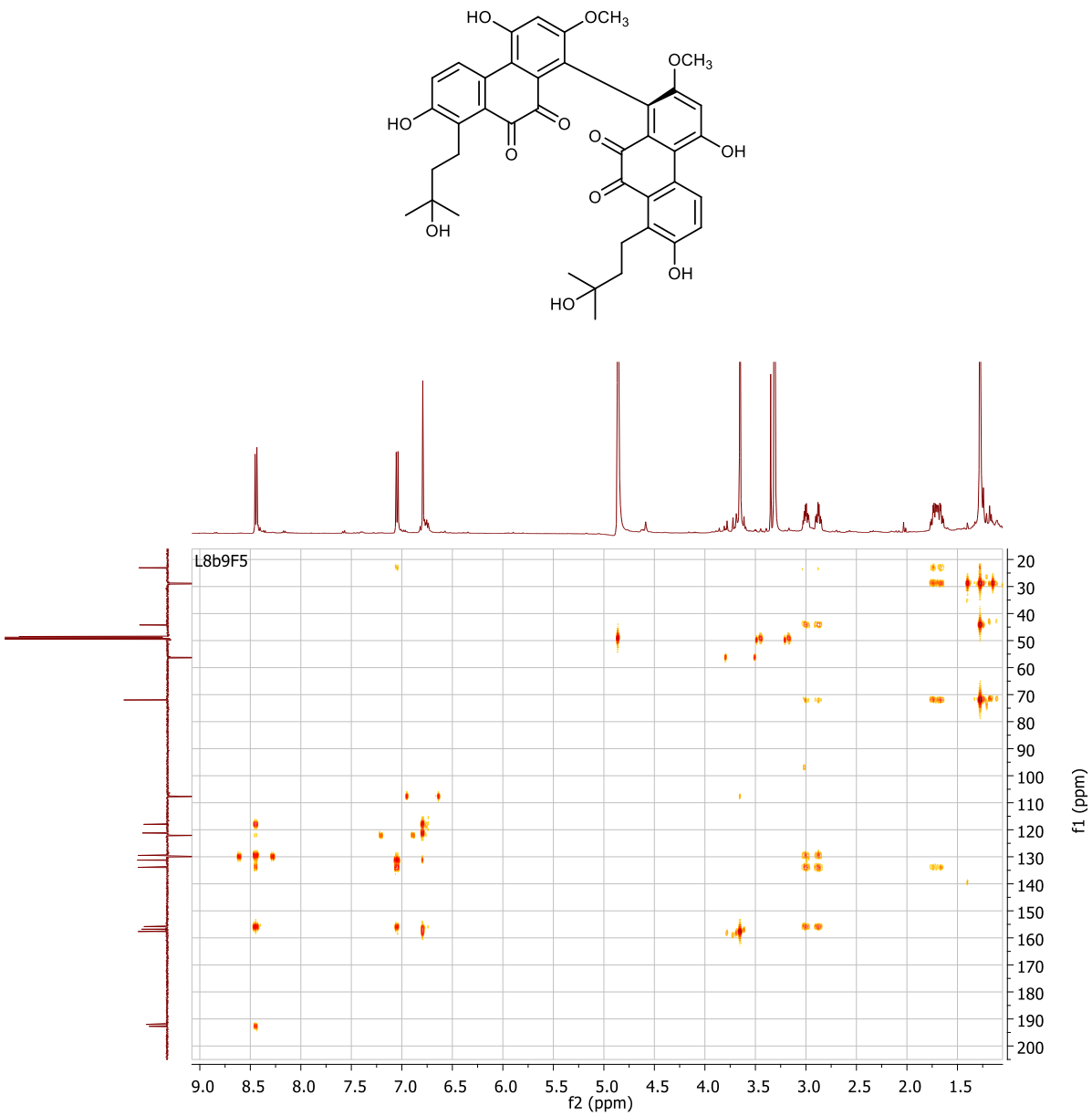


Figure S6. HMBC spectrum of leucobryn A (**1**) (CD_3OD)

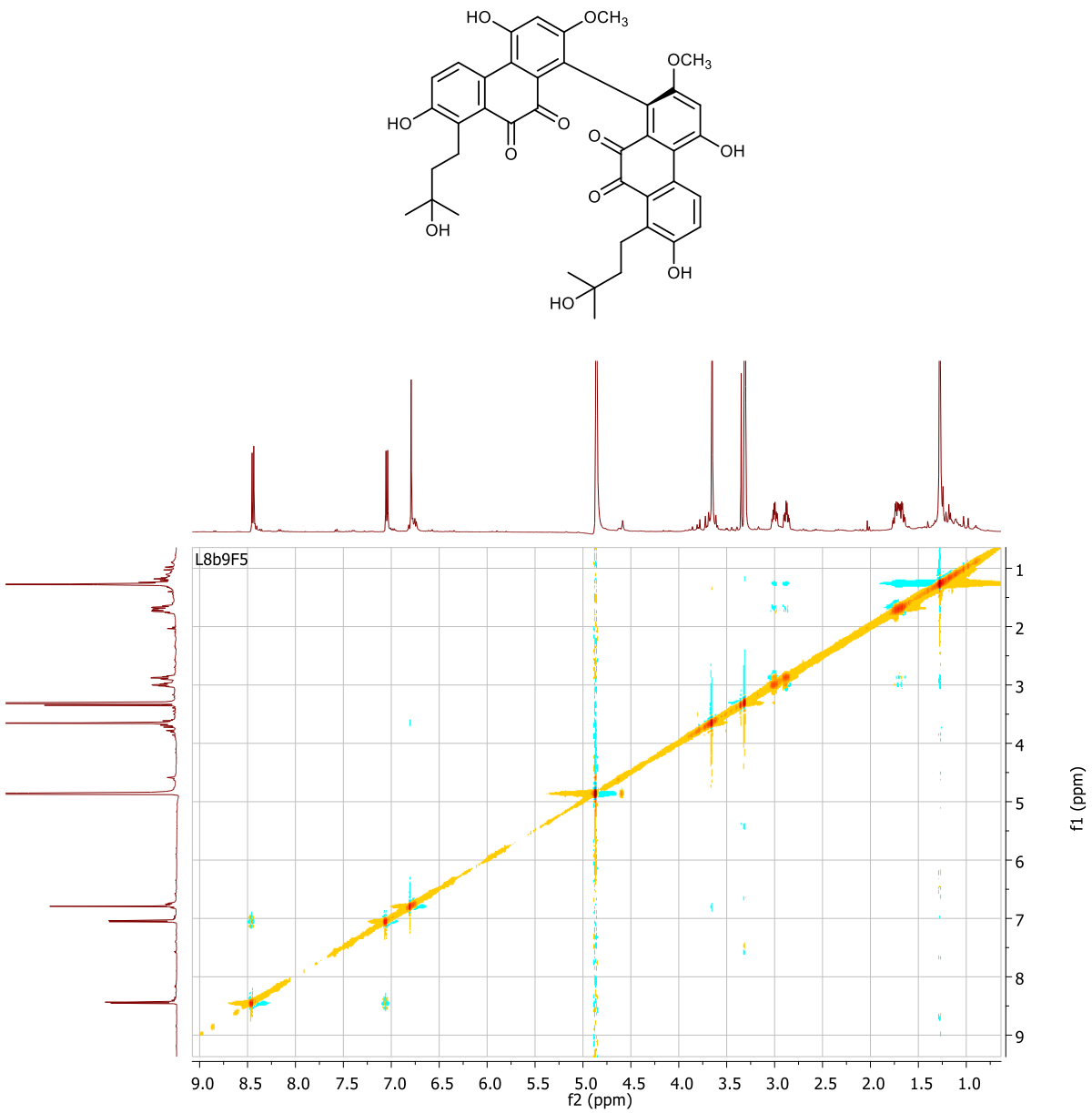


Figure S7. NOESY spectrum of leucobryn A (**1**) (CD_3OD)

Analysis Info

Analysis Name	D:\Data\20181129\kurtan_t_000005.d	Acquisition Date	11/29/2018 11:17:07 AM
Method	500-1500_pos.m	Operator	Demo User
Sample Name	sample	Instrument	maXis II 1828979.22359
Comment			

Acquisition Parameter

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	0.5 Bar
Focus	Active	Set Capillary	4500 V	Set Dry Heater	200 °C
Scan Begin	500 m/z	Set End Plate Offset	-500 V	Set Dry Gas	4.0 l/min
Scan End	1500 m/z	Set Charging Voltage	2000 V	Set Divert Valve	Source
		Set Corona	0 nA	Set APCI Heater	0 °C

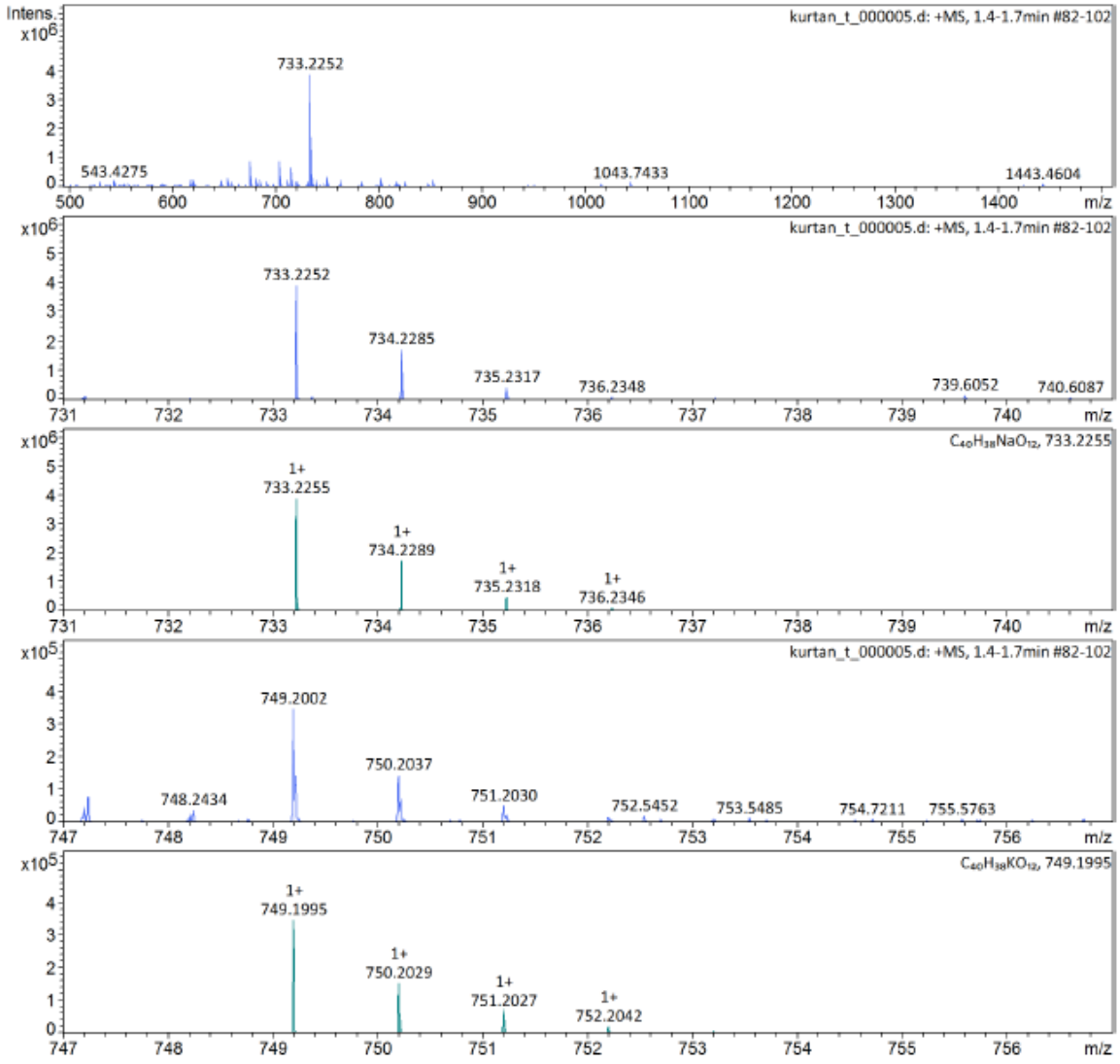


Figure S8. HRESIMS of leucobryn A (**1**)

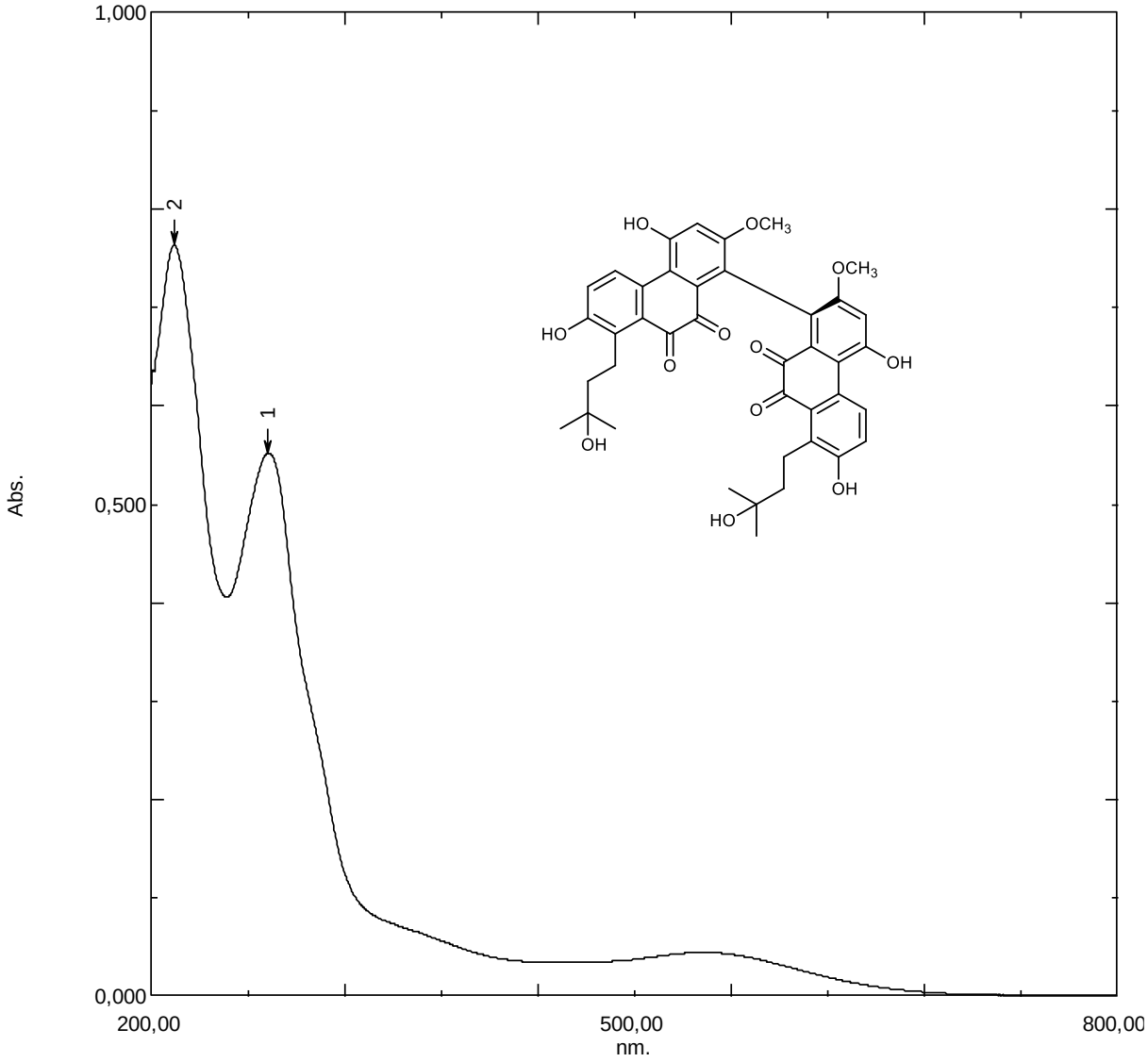


Figure S9. UV-VIS Spectrum of leucobryn A (**1**) in MeOH at 1.76×10^{-5} M concentration

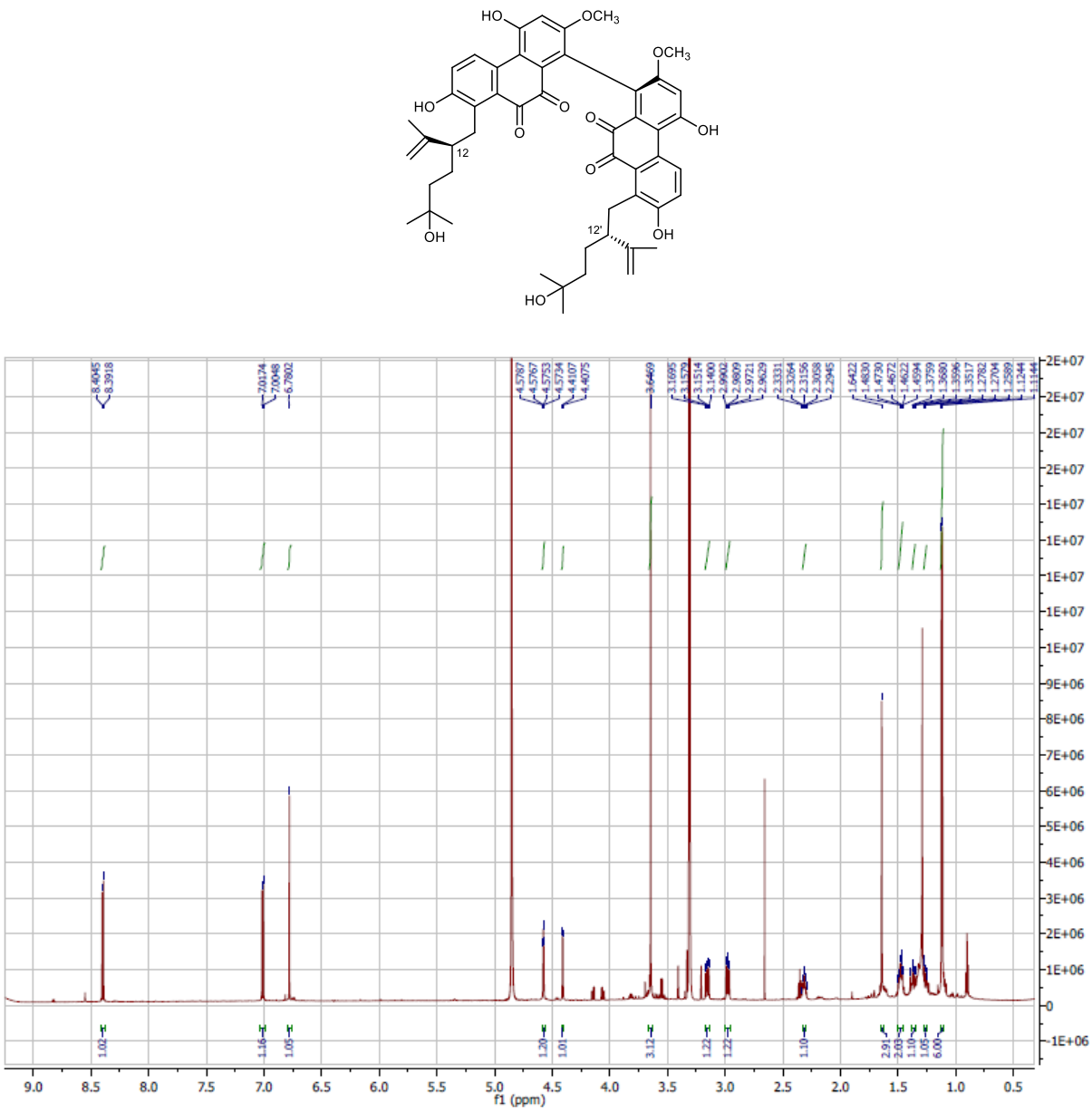


Figure S10. ^{1}H NMR spectrum of leucobryn B (**2**) (CD_3OD, 700 MHz)

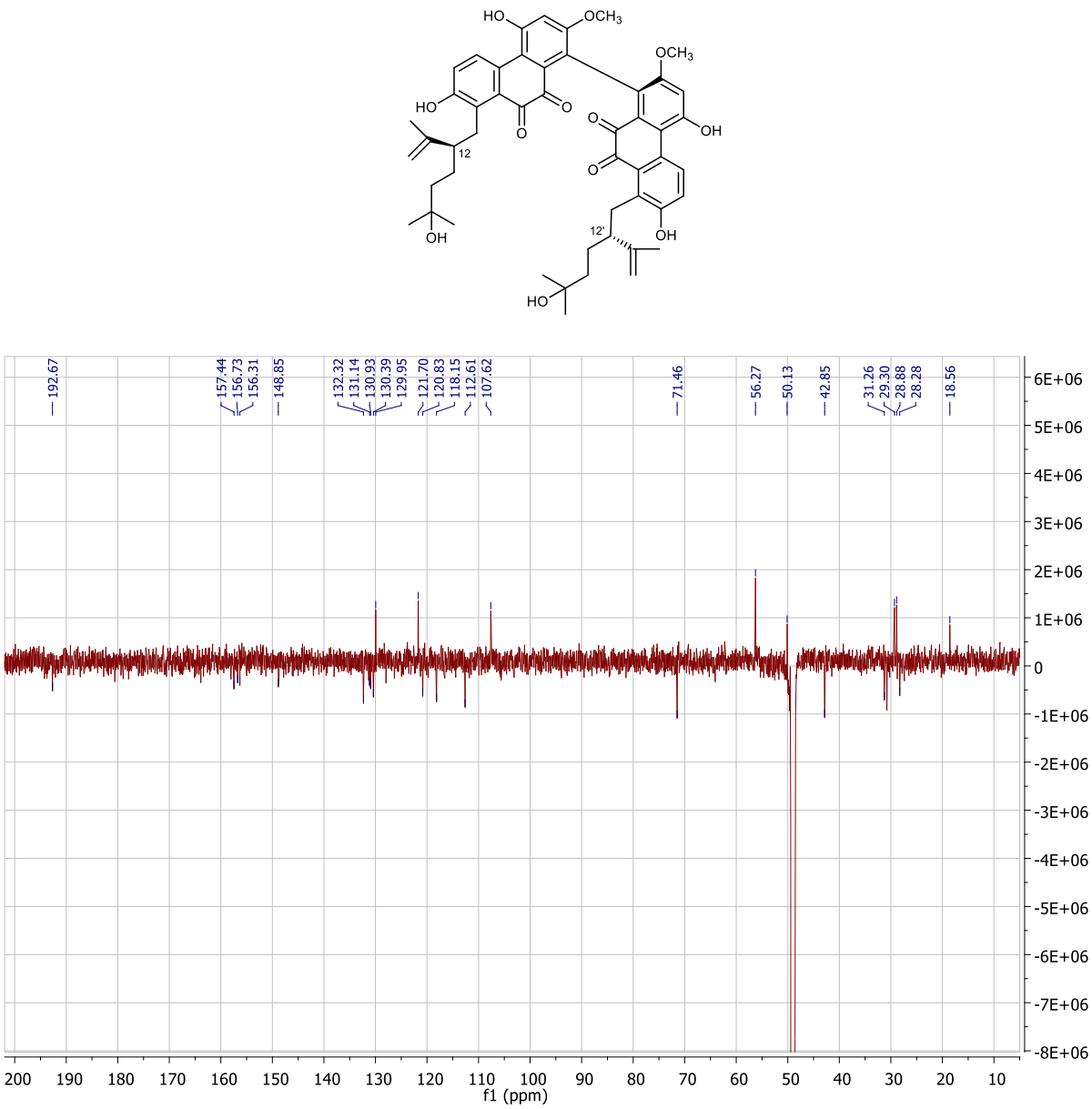


Figure S11. ^{13}C JMOD spectrum of leucobryn B (**2**) (CD_3OD, 175 MHz)

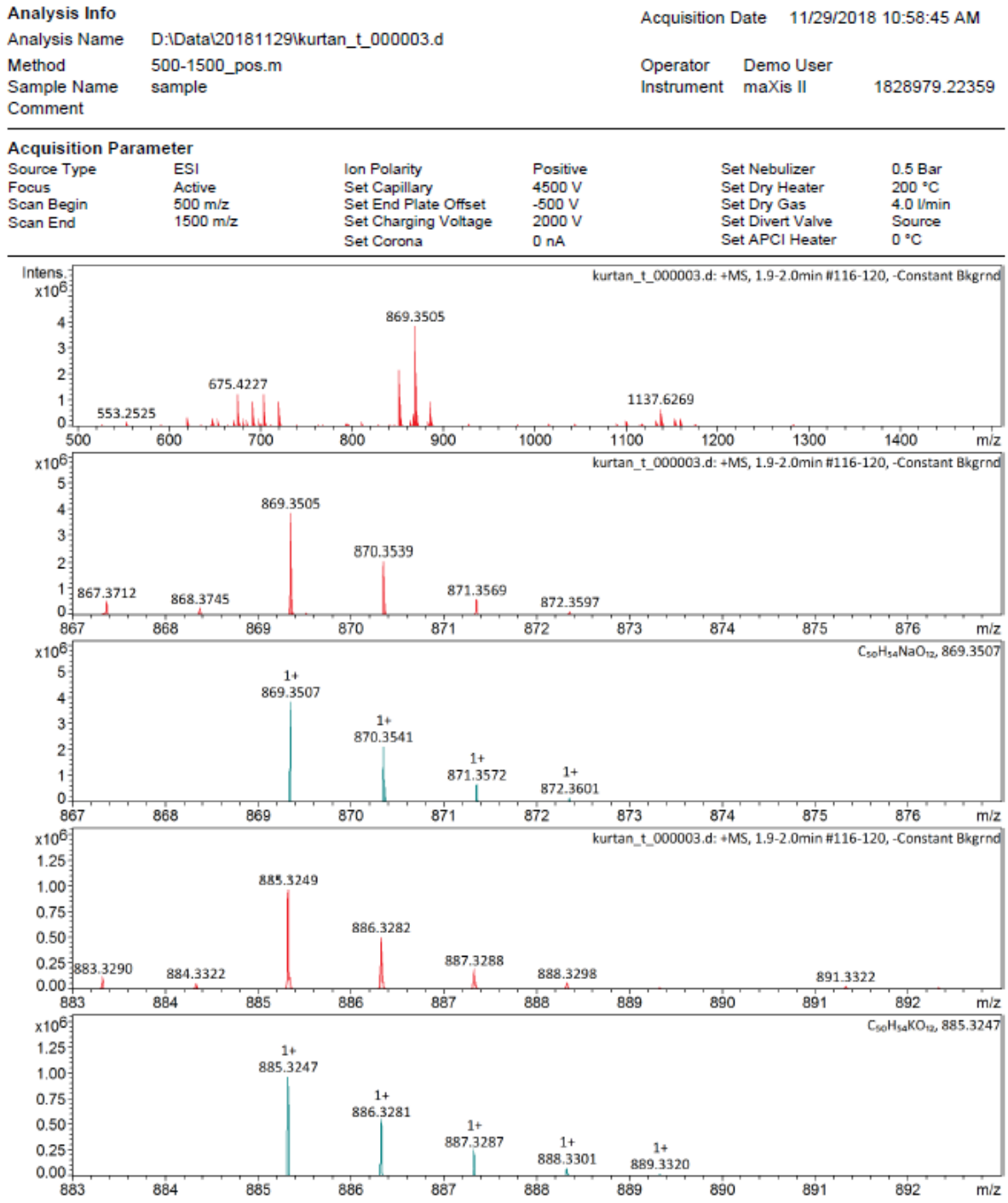


Figure S12. HRESIMS of leucobryn B (**2**)

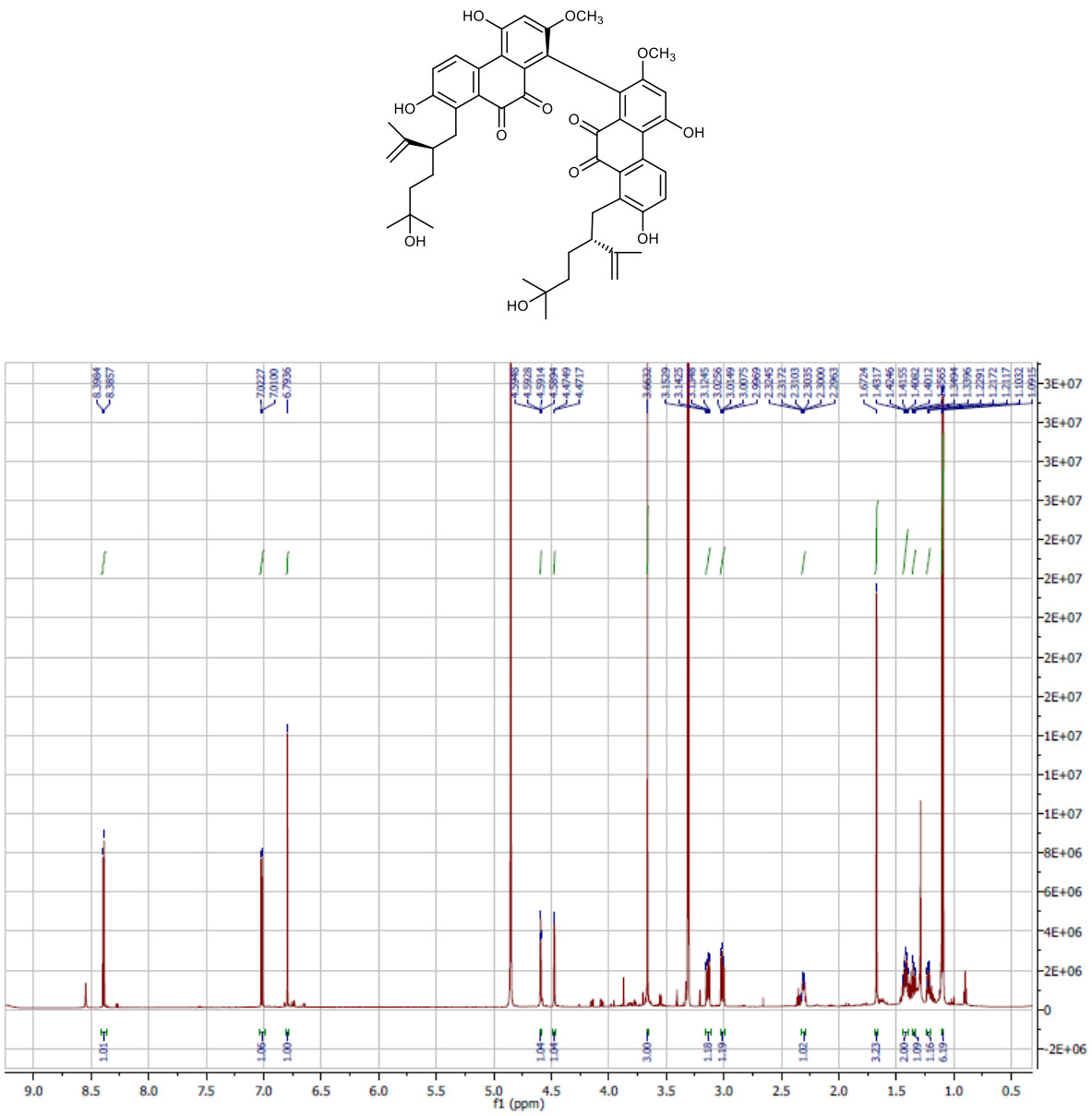


Figure S13. ^{1}H NMR spectrum of leucobryn C (**3**) (CD_3OD, 700 MHz)

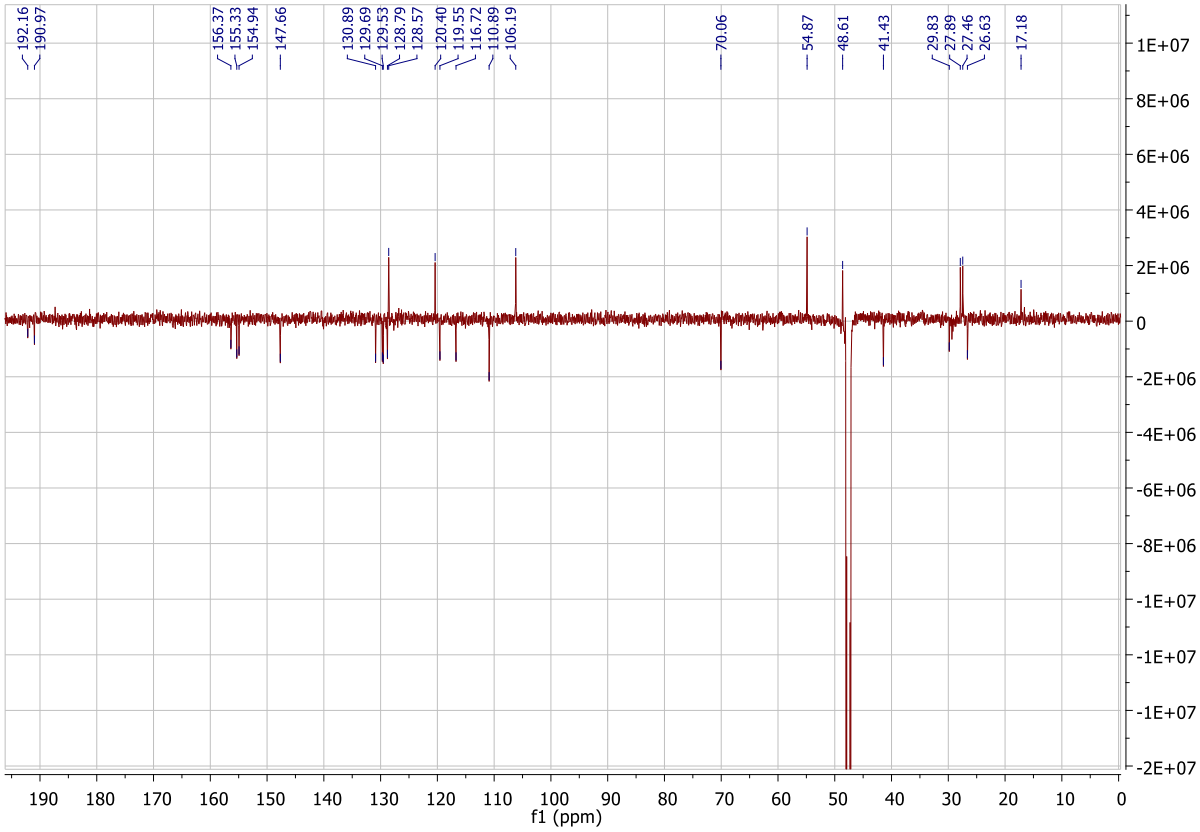


Figure S14. ^{13}C JMOD spectrum of leucobryn C (**3**) (CD_3OD, 175 MHz)

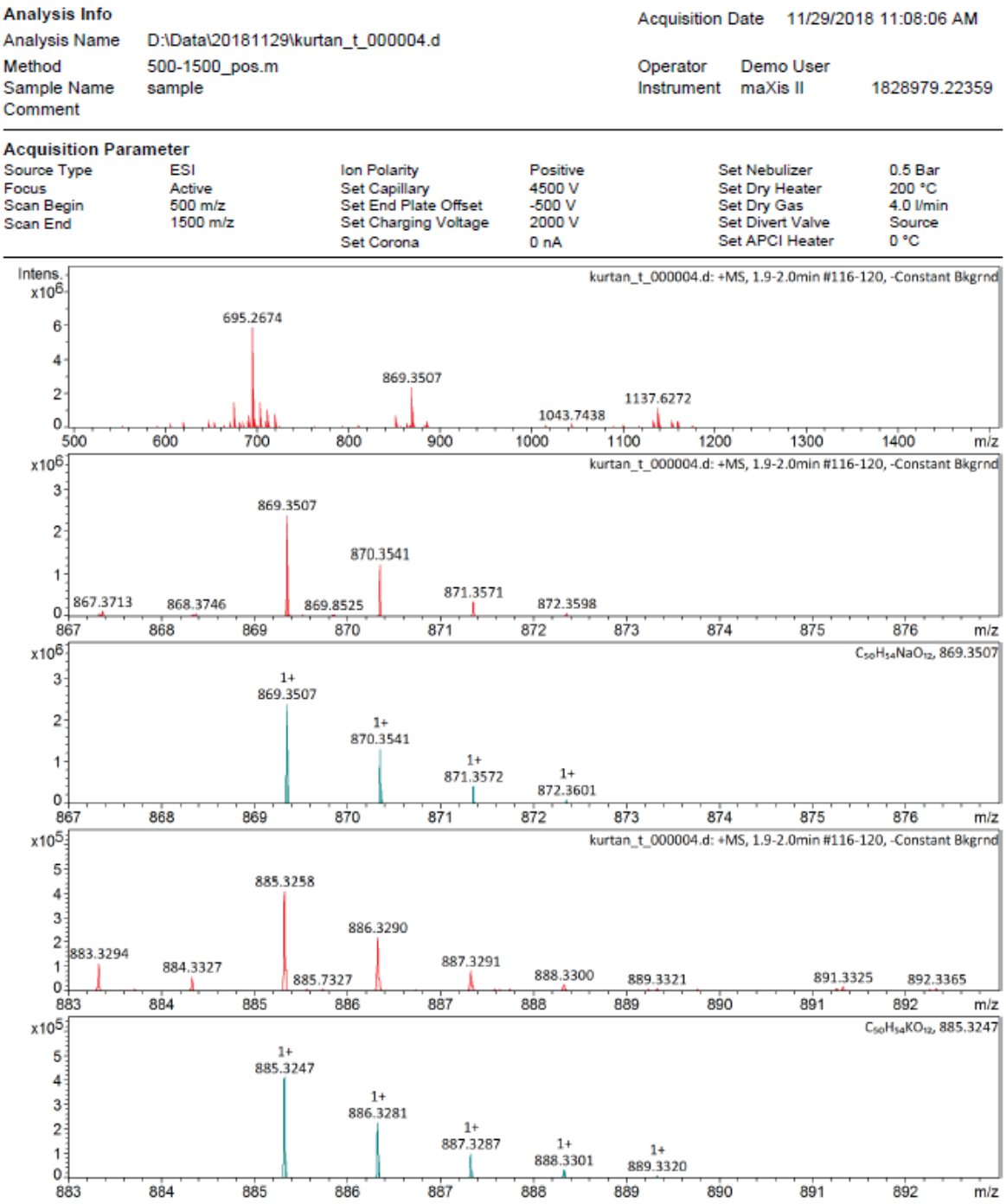
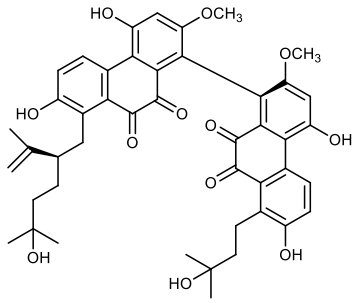


Figure S15. HRESIMS of leucobryn C (**3**)



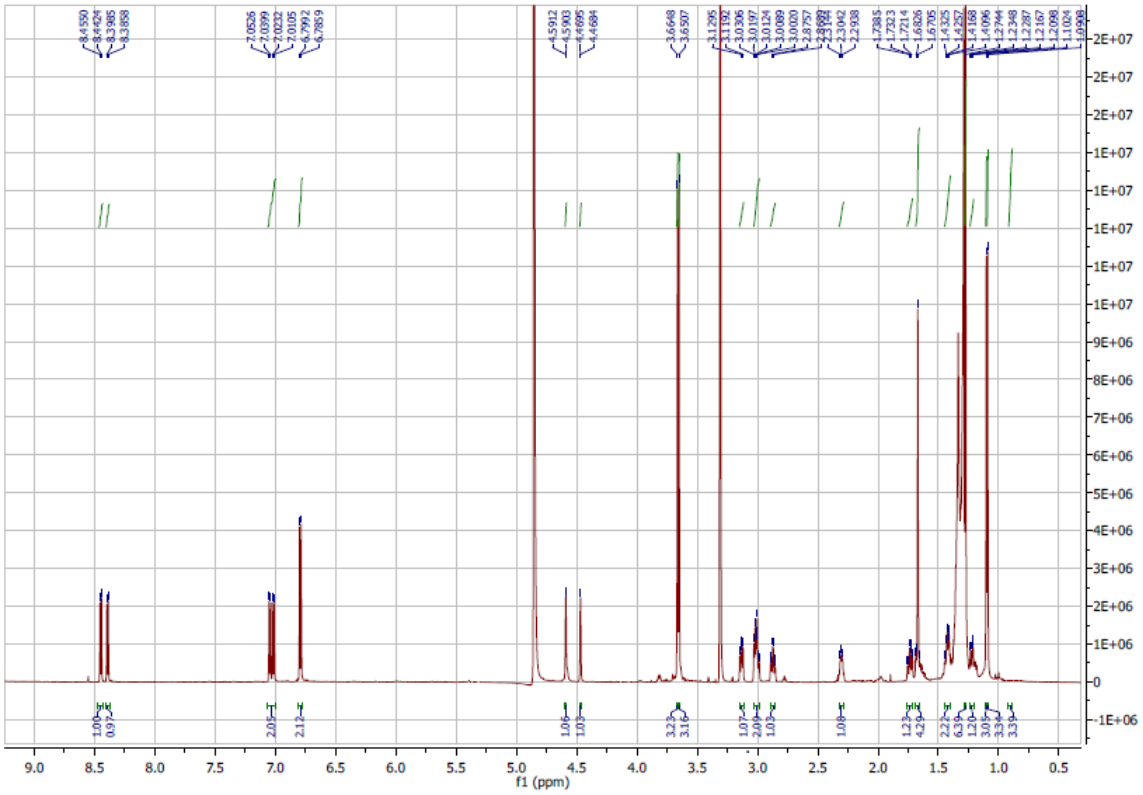
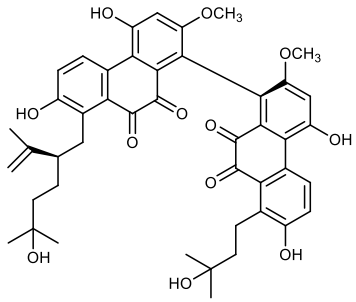


Figure S16. ^{1}H NMR spectrum of leucobryn D (**4**) (CD_3OD, 700 MHz)



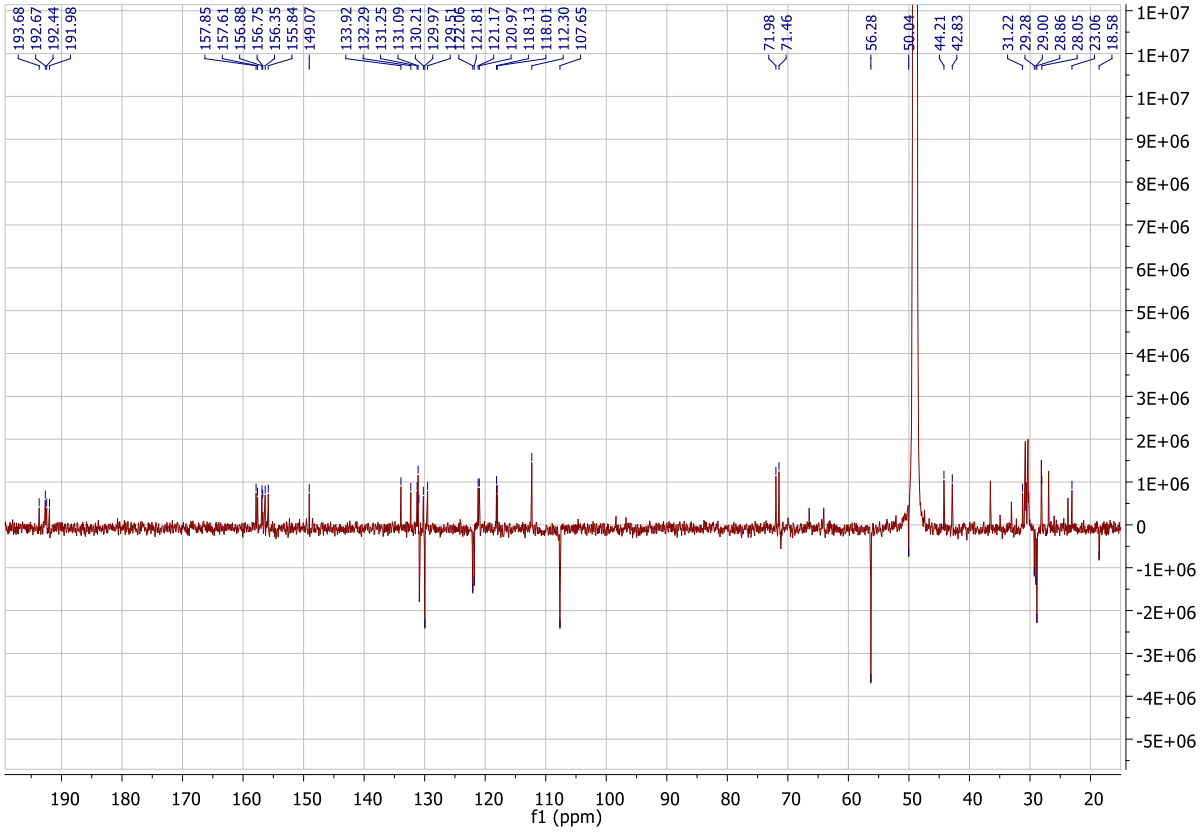


Figure S17. ^{13}C JMOD spectrum of leucobryn D (**4**) (CD_3OD, 175 MHz)

Analysis Info

Analysis Name	D:\Data\20181129\kurtan_t_000002.d	Acquisition Date	11/29/2018 10:46:07 AM
Method	500-1500_pos.m	Operator	Demo User
Sample Name	sample	Instrument	maXis II 1828979.22359
Comment			

Acquisition Parameter

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	0.5 Bar
Focus	Active	Set Capillary	4500 V	Set Dry Heater	200 °C
Scan Begin	500 m/z	Set End Plate Offset	-500 V	Set Dry Gas	4.0 l/min
Scan End	1500 m/z	Set Charging Voltage	2000 V	Set Divert Valve	Source
		Set Corona	0 nA	Set APCI Heater	0 °C

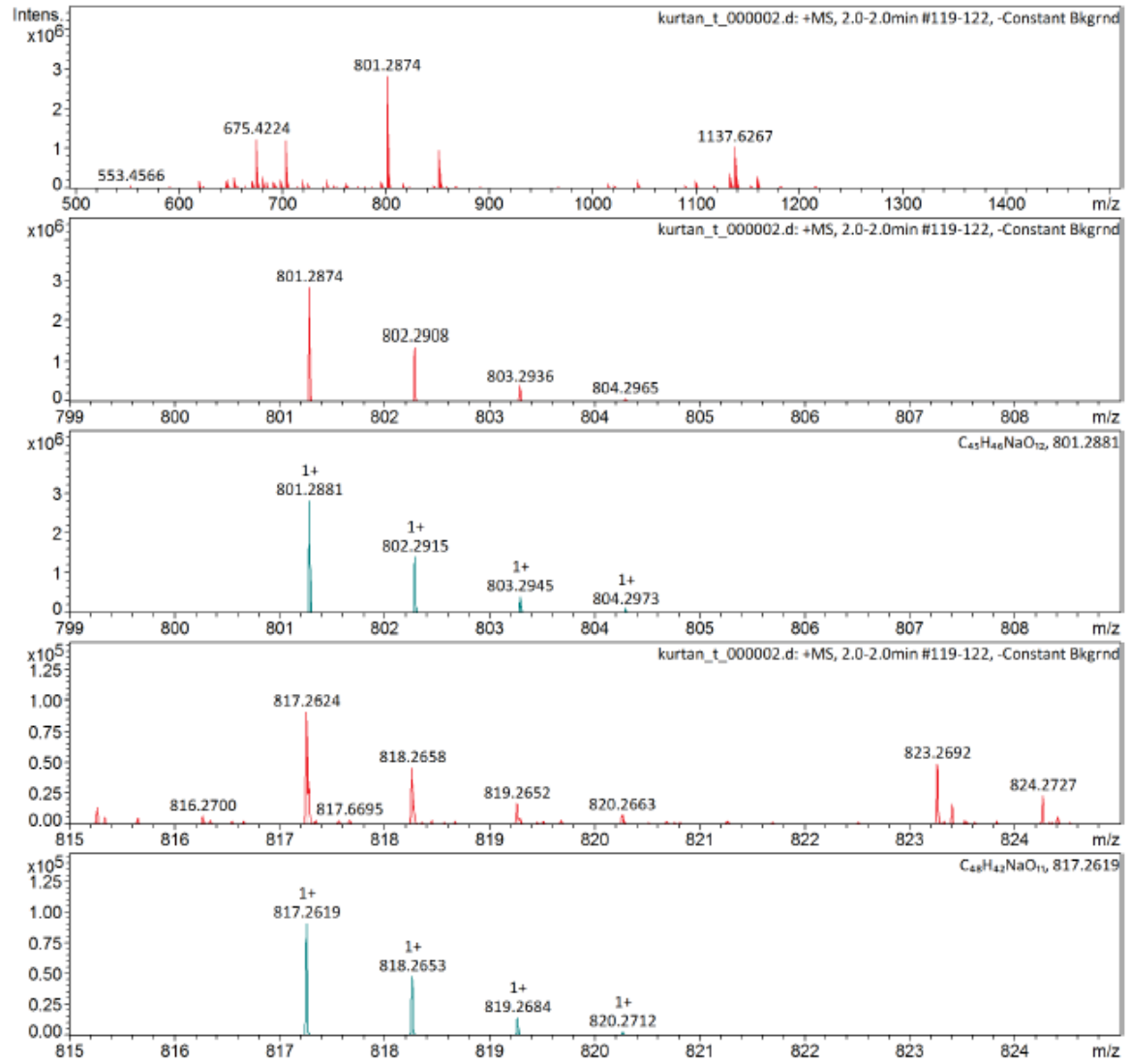
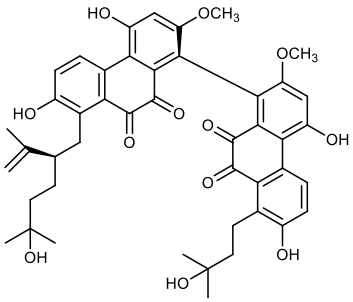


Figure S18. HRESIMS of leucobryn D (**4**)



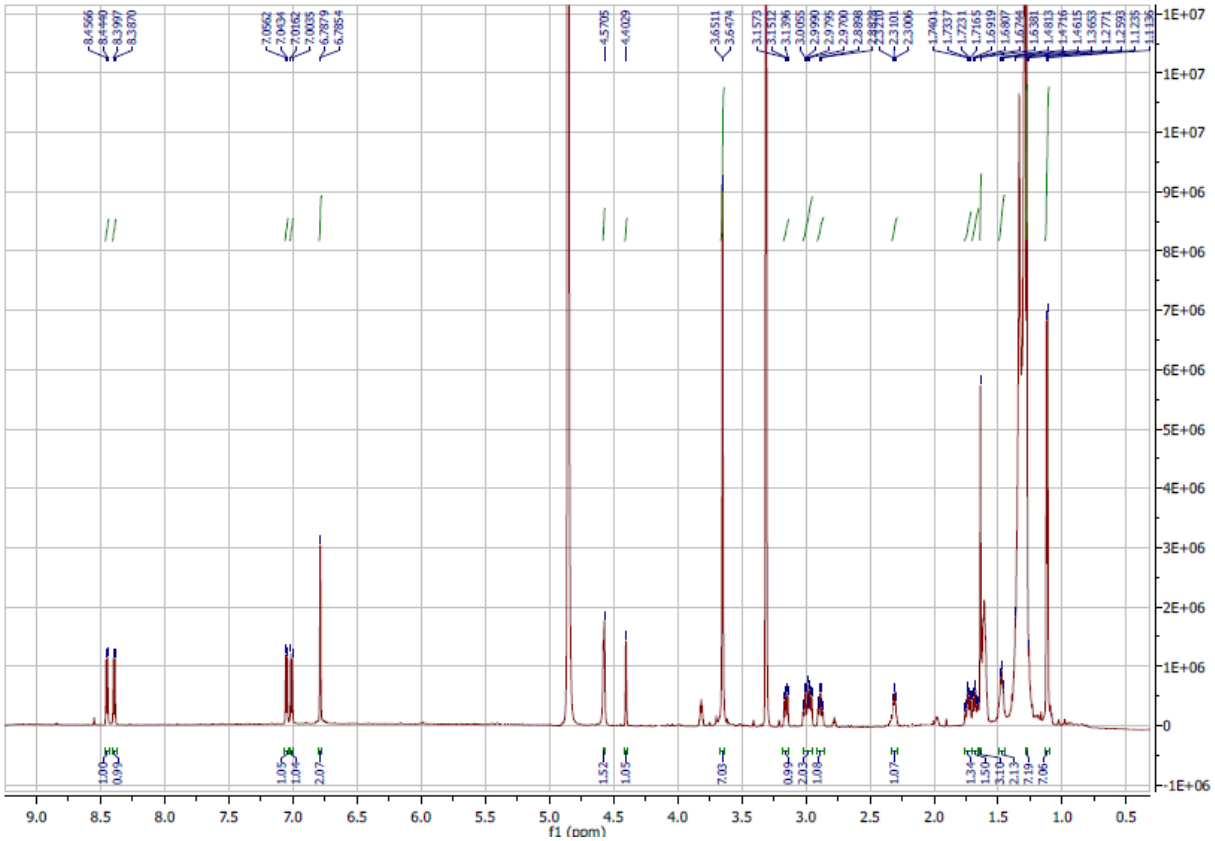


Figure S19. ^{1}H NMR spectrum of leucobryn E (**5**) (CD_3OD, 700 MHz)

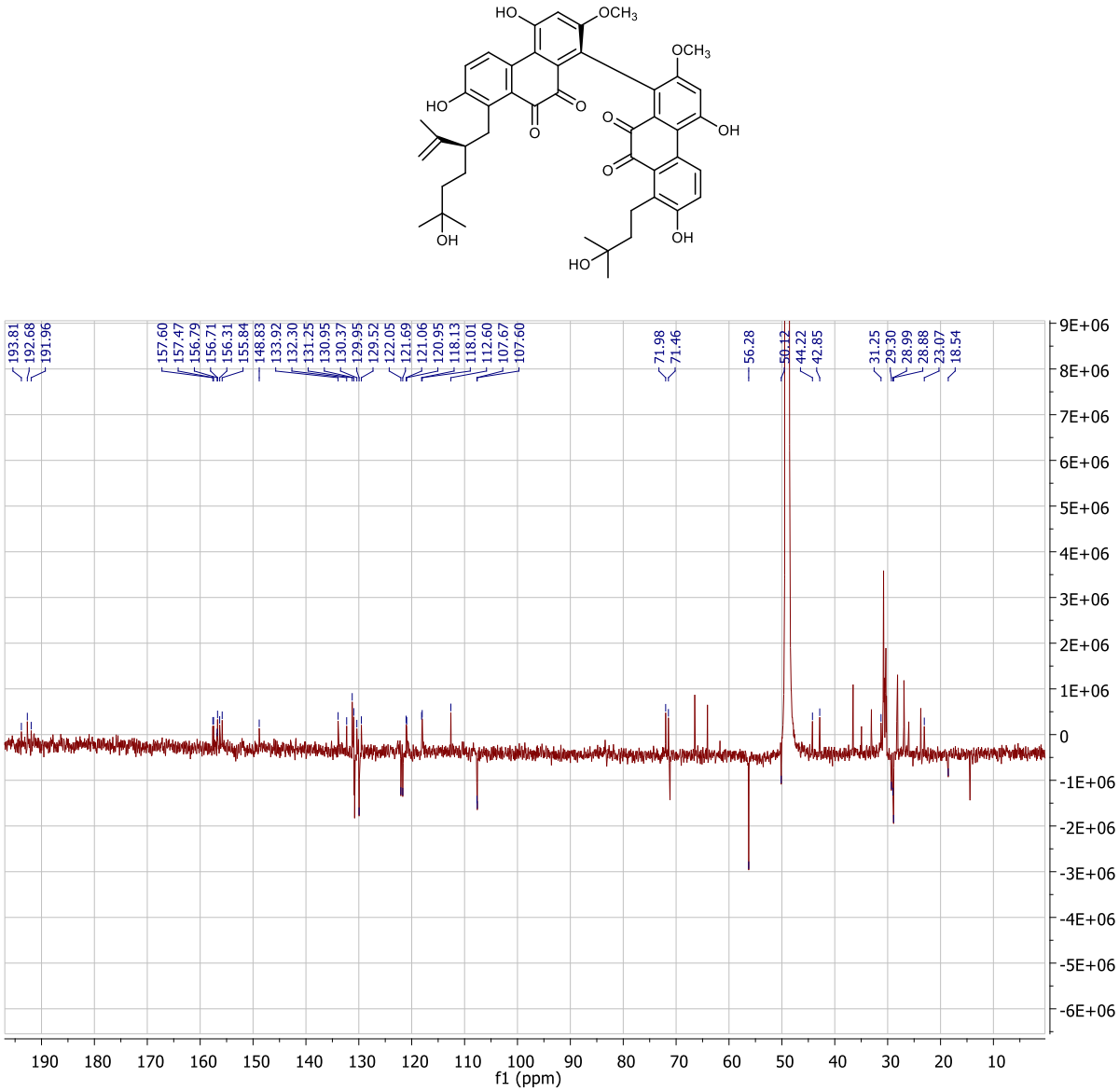


Figure S20. ^{13}C JMOD spectrum of leucobryn E (**5**) (CD_3OD, 175 MHz)

Analysis Info

Analysis Name	D:\Data\20181129\kurtan_t_000001.d	Acquisition Date	11/29/2018 10:28:53 AM
Method	500-1500_pos.m	Operator	Demo User
Sample Name	sample	Instrument	maXis II 1828979.22359
Comment			

Acquisition Parameter

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	0.5 Bar
Focus	Active	Set Capillary	4500 V	Set Dry Heater	200 °C
Scan Begin	500 m/z	Set End Plate Offset	-500 V	Set Dry Gas	4.0 l/min
Scan End	1500 m/z	Set Charging Voltage	2000 V	Set Divert Valve	Source
		Set Corona	0 nA	Set APCI Heater	0 °C

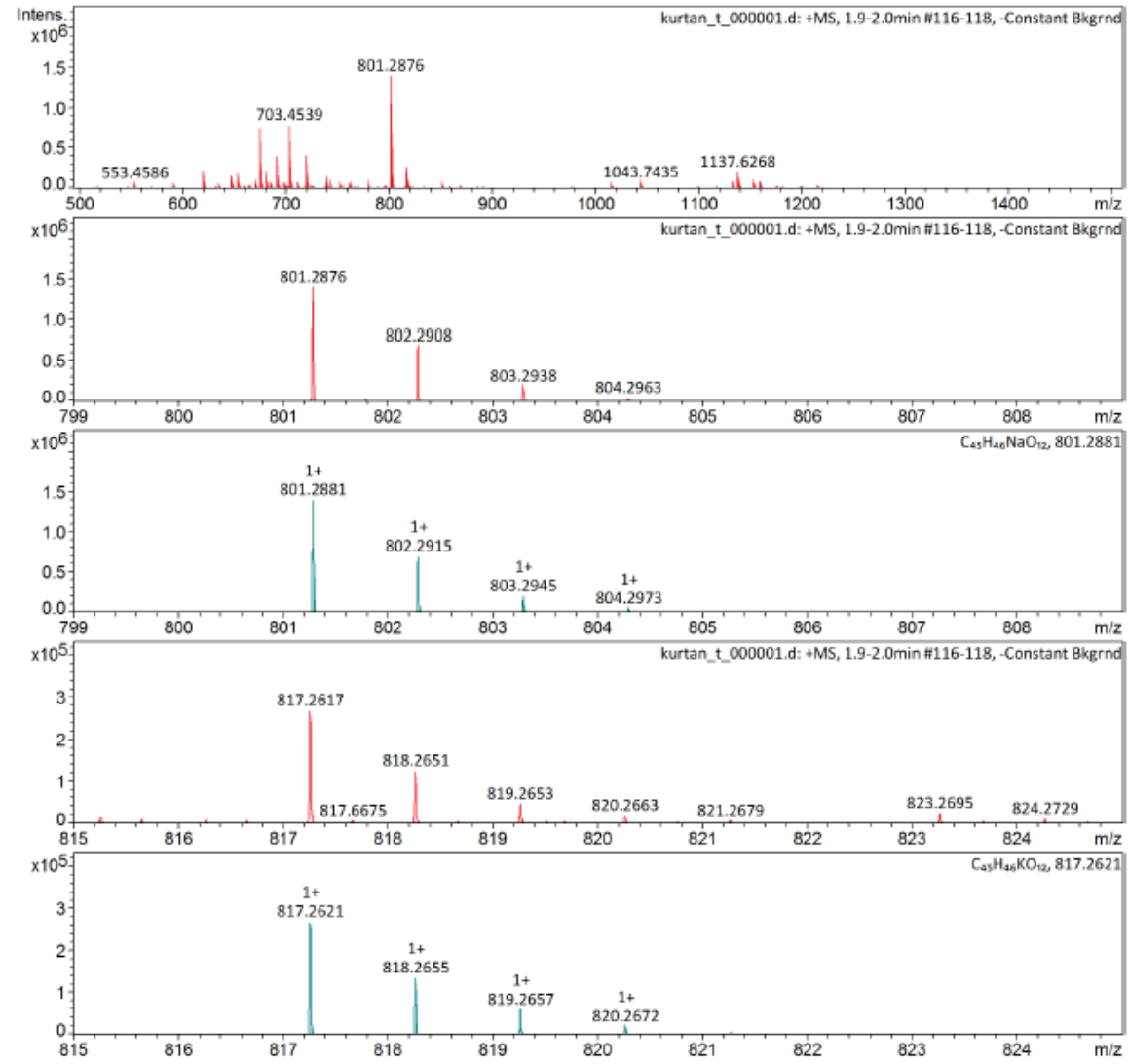


Figure S21. HRESIMS of leucobryn E (**5**)

Table S6. Cartesian coordinates and energies of the low-energy conformers calculated at the CAM-B3LYP/TZVP PCM/MeCN level.

(*aR*,12*R*,12'*R*)-**2**/**3**, Conf A

C	5.622542	0.279488	-2.445312
C	5.872721	0.922723	-1.245950
C	5.168300	0.584729	-0.089919
C	4.221566	-0.449421	-0.188794
C	3.975715	-1.135456	-1.396593
C	4.689792	-0.731689	-2.521428
C	3.373389	-0.833974	0.954334
C	1.968287	-1.319590	0.579121
C	1.912107	-2.284503	-0.534806
C	2.977290	-2.236056	-1.460442
C	0.902174	-3.236889	-0.579528
C	0.976535	-4.227375	-1.565579
C	2.024950	-4.232007	-2.461671
C	3.015651	-3.256223	-2.410246
O	1.028703	-0.922520	1.226539
O	3.664172	-0.786549	2.127800
O	4.048133	-3.317882	-3.290979
O	6.817680	1.903402	-1.273720
C	5.428694	1.381046	1.165657
C	4.807596	2.800755	1.150606
C	3.275179	2.734532	1.188308
C	-0.199843	-3.311893	0.418878
C	-1.420327	-2.666599	0.271563
C	-2.451641	-2.721810	1.229526
C	-2.179108	-3.450574	2.389460
C	-0.971604	-4.119784	2.551798
C	0.009918	-4.059479	1.582267
C	-1.637960	-1.780568	-0.883798
C	-2.602607	-0.610657	-0.657249
C	-3.813547	-0.915872	0.109284
C	-3.740231	-2.021485	0.985876
C	-5.006678	-0.196178	-0.105002
C	-6.143845	-0.623676	0.584723
C	-6.096721	-1.743316	1.397782
C	-4.919058	-2.429431	1.600483
O	-3.098527	-3.493641	3.387967
O	-7.358850	-0.021305	0.456771
C	-5.129315	0.927347	-1.108565
C	-4.829797	2.349600	-0.581474
C	-4.809195	3.365870	-1.738414
O	-2.317131	0.453653	-1.164910
O	-1.104006	-1.881338	-1.961908
C	5.389725	3.629695	2.277357
C	6.147661	4.689225	2.022403
C	5.086294	3.202276	3.685169
C	2.613710	4.106054	1.145723
C	1.103437	4.099363	0.900663
C	0.577258	5.531799	0.947164
C	0.359790	3.238497	1.919026
O	0.912678	3.565927	-0.414786
C	-5.820110	2.761924	0.497329
C	-5.299473	2.743705	1.903369
C	-7.070839	3.122147	0.219545
C	-3.654933	3.254851	-2.738262
C	-2.295314	3.855316	-2.346860
C	-2.380691	5.344151	-2.054858
C	-1.295684	3.597031	-3.471450
O	-1.795133	3.248961	-1.136627
O	1.207895	-4.671785	1.692505
C	1.489601	-5.428291	2.863313
O	-0.010570	-5.146596	-1.564393
C	0.018405	-6.187104	-2.533058
H	6.173907	0.586123	-3.324520
H	4.521124	-1.212674	-3.469434
H	2.098638	-5.000326	-3.218458
H	3.961013	-4.095668	-3.854045
H	7.006121	2.231807	-0.387737
H	5.070577	0.837269	2.030896
H	6.510831	1.470524	1.310184
H	5.085618	3.294472	0.215359
H	2.959674	2.189571	2.080462
H	2.931407	2.155809	0.329905
H	-0.810560	-4.678984	3.462805
H	-7.008688	-2.065338	1.883285
H	-4.921276	-3.284851	2.253522
H	-2.751584	-3.981519	4.143720
H	-7.259382	0.928973	0.278421
H	-6.142446	0.918396	-1.516435
H	-4.463913	0.724242	-1.942547
H	-3.844152	2.332223	-0.121505
H	-5.743236	3.263758	-2.296543
H	-4.830389	4.370370	-1.314143
H	6.578263	5.282986	2.820042
H	6.361615	5.002171	1.007062
H	5.565253	3.863805	4.405559
H	4.011480	3.211060	3.877957
H	5.432069	2.184557	3.877372
H	3.068383	4.699342	0.346868
H	2.807229	4.642819	2.077527
H	-0.487243	5.553454	0.707976
H	1.104849	6.153926	0.222624
H	0.710523	5.967097	1.938973
H	-0.716204	3.295629	1.744694
H	0.659408	2.194136	1.840226
H	0.555775	3.580180	2.937018
H	-0.041882	3.515851	-0.613934
H	-4.895778	1.760646	2.156377
H	-6.070909	3.002546	2.627413
H	-4.474454	3.453540	2.003866
H	-7.757956	3.413981	1.004481
H	-7.446506	3.166429	-0.795733
H	-3.493974	2.210437	-3.015262
H	-3.957498	3.756955	-3.660066
H	-1.389594	5.735645	-1.824204
H	-3.028809	5.544039	-1.202834
H	-2.768216	5.881791	-2.920639
H	-0.316416	3.992688	-3.200699
H	-1.194462	2.526237	-3.657298
H	-1.617269	4.074657	-4.397999
H	-1.905117	2.287666	-1.197733

H	0.788253	-6.257109	2.974013
H	2.492958	-5.820196	2.728655
H	1.462860	-4.798179	3.753982
H	-0.860262	-6.795318	-2.341861
H	-0.033374	-5.783117	-3.545573
H	0.914769	-6.800499	-2.424940

CAM-B3LYP Energy = -2840.09714581 a.u.

(*aR*,12*R*,12'*R*)-**2**/**3**, Conf B

C	-6.289478	1.825947	-2.019864
C	-6.504159	0.515133	-1.623692
C	-5.477328	-0.221699	-1.025376
C	-4.227946	0.408153	-0.880988
C	-3.989784	1.731649	-1.310550
C	-5.059277	2.425451	-1.867717
C	-3.092902	-0.261405	-0.221562
C	-2.145280	0.668321	0.546390
C	-1.763156	1.904161	-0.158944
C	-2.651048	2.361614	-1.153024
C	-0.525698	2.483842	0.091553
C	-0.140208	3.571845	-0.697282
C	-0.969315	4.023159	-1.705352
C	-2.200937	3.423743	-1.940442
O	-1.745045	0.318831	1.631340
O	-2.847786	-1.446783	-0.217139
O	-2.969267	3.872326	-2.967753
O	-7.746903	0.029597	-1.848210
C	-5.785674	-1.616560	-0.538402
C	-6.709924	-1.677541	0.703247
C	-7.083546	-3.132334	1.030016
C	0.410896	2.018842	1.151739
C	1.433236	1.104578	0.933175
C	2.345948	0.706706	1.932825
C	2.218722	1.332749	3.172517
C	1.214121	2.265457	3.408910
C	0.316495	2.606822	2.418697
C	1.660247	0.560949	-0.418330
C	3.107674	0.166828	-0.750471
C	3.829503	-0.538125	0.318695
C	3.373923	-0.325938	1.639324
C	4.842755	-1.469249	0.016848
C	5.336583	-2.251333	1.064700
C	4.859170	-2.081389	2.352133
C	3.908097	-1.124021	2.643631
O	3.103374	1.049881	4.164044
O	6.245560	-3.244652	0.815552
C	5.391649	-1.680798	-1.369999
C	6.448643	-0.636983	-1.780096
C	7.690260	-0.641517	-0.865593
O	3.512986	0.406775	-1.865588
O	0.819372	0.436207	-1.276704
C	-6.089196	-1.000753	1.910003
C	-6.541335	0.174047	2.332391
C	-4.968295	-1.705035	2.623208
C	-7.824549	-3.940857	-0.036048
C	-9.203511	-3.463721	-0.492397
C	-10.110334	-3.074819	0.667124
C	-9.859057	-4.544848	-1.343782
O	-8.983562	-2.304514	-1.335529
C	6.838356	-0.719319	-3.242206
C	7.647541	0.440558	-3.754328
C	6.503103	-1.720605	-4.046877
C	8.620122	-1.838034	-1.053413
C	9.585945	-2.094019	0.103475
C	10.454456	-0.885173	0.421827
C	10.445923	-3.315291	-0.190853
O	8.747099	-2.380767	1.253302
O	-0.673630	3.507483	2.587236
C	-0.811715	4.148693	3.848527
O	1.068523	4.111838	-0.426714
C	1.516030	5.217254	-1.200769
H	-7.115311	2.372571	-2.456450
H	-4.933593	3.443876	-2.192330
H	-0.668413	4.847797	-2.336296
H	-2.514120	4.575224	-3.445404
H	-7.903134	-0.889854	-1.555238
H	-6.273799	-2.155170	-1.353194
H	-4.870843	-2.160101	-0.334823
H	-7.625978	-1.130853	0.481572
H	-7.669071	-3.133232	1.952469
H	-6.168466	-3.683186	1.260151
H	1.156991	2.723129	4.386694
H	5.245187	-2.721075	3.135597
H	3.574345	-1.010506	3.660740
H	2.911806	1.582540	4.944378
H	7.160742	-2.961179	1.046096
H	4.580443	-1.636126	-2.093123
H	5.817144	-2.681080	-1.410208
H	5.981136	0.342403	-1.650949
H	8.246249	0.282038	-1.031529
H	7.349484	-0.598134	0.169421
H	-6.105044	0.675136	3.188510
H	-7.363086	0.676427	1.835848
H	-4.503884	-1.049211	3.358309
H	-5.335307	-2.589637	3.147789
H	-4.194915	-2.044746	1.933037
H	-7.957297	-4.948346	0.364252
H	-7.207619	-4.056869	-0.929486
H	-11.097471	-2.790576	0.297618
H	-9.700911	-2.233805	1.224366
H	-10.238165	-3.913987	1.352141
H	-10.802604	-4.186133	-1.760536
H	-9.204940	-4.831690	-2.167786
H	-10.073325	-5.430885	-0.745633
H	-9.832597	-2.015080	-1.690148
H	7.142852	1.387153	-3.546060
H	7.809056	0.365099	-4.828864
H	8.625371	0.491341	-3.270387
H	6.805720	-1.721763	-5.087309
H	5.922203	-2.569071	-3.712534
H	8.035017	-2.748175	-1.195833

H	9.213840	-1.712145	-1.960924
H	11.137679	-1.112004	1.242638
H	9.845392	-0.030337	0.711354
H	11.053458	-0.606769	-0.446171
H	11.093780	-3.546099	0.657437
H	9.819362	-4.184180	-0.394302
H	11.081772	-3.135981	-1.058374
H	9.297488	-2.612914	2.009517
H	-1.014946	3.423356	4.638324
H	0.081226	4.725268	4.096685
H	-1.658846	4.820311	3.749107
H	1.617821	4.945578	-2.252906
H	0.838098	6.066983	-1.101800
H	2.489790	5.484074	-0.801746

CAM-B3LYP Energy = -2840.09682590 a.u.

(*aR*,12*R*,12'*R*)-**2**/**3**, Conf C

C	5.579180	-0.376167	2.727994
C	6.026793	-0.820445	1.497578
C	5.439899	-0.363867	0.316697
C	4.405378	0.574803	0.430460
C	3.917544	1.024394	1.676821
C	4.535041	0.522691	2.817953
C	3.721552	1.104358	-0.761982
C	2.227085	1.382913	-0.586015
C	1.841328	2.037575	0.677464
C	2.748995	1.943897	1.754967
C	0.659763	2.766670	0.732886
C	0.375908	3.471578	1.906801
C	1.268704	3.446906	2.959729
C	2.442839	2.708132	2.884320
O	1.478752	1.090328	-1.488295
O	4.222814	1.329273	-1.839638
O	3.311122	2.743387	3.928587
O	7.034551	-1.729907	1.389033
C	5.874294	-1.001560	-0.978440
C	5.245483	-2.404941	-1.176817
C	3.718406	-2.323543	-1.292426
C	-0.273791	2.932863	-0.415994
C	-1.451705	2.213934	-0.565446
C	-2.382758	2.439293	-1.602813
C	-2.083500	3.485483	-2.477557
C	-0.909983	4.219712	-2.348135
C	-0.010582	3.953607	-1.335679
C	-1.817012	1.187811	0.420398
C	-3.318036	0.983746	0.626910
C	-4.101115	0.873432	-0.614218
C	-3.591530	1.579595	-1.729479
C	-5.246002	0.067235	-0.688978
C	-5.891735	-0.013194	-1.925925
C	-5.390274	0.642370	-3.034091
C	-4.257416	1.426745	-2.938986
O	-2.957652	3.811397	-3.464900
O	-7.023637	-0.766703	-1.995129
C	-5.816851	-0.741860	0.450149
C	-5.588568	-2.258236	0.295904
C	-4.105390	-2.668026	0.420981
O	-3.728538	0.918402	1.763341
O	-1.043293	0.523749	1.075793
C	5.888282	-3.103117	-2.357170
C	6.657901	-4.170513	-2.181020
C	5.630586	-2.543098	-3.727375
C	3.031526	-3.681075	-1.366179
C	1.521928	-3.650848	-1.108276
C	0.957202	-5.063350	-1.236674
C	0.795164	-2.709967	-2.065159
O	1.360408	-3.194718	0.240409
C	-6.472575	-3.093070	1.201931
C	-6.469475	-4.569200	0.913227
C	-7.213085	-2.596846	2.185753
C	-3.530572	-2.597345	1.831465
C	-2.078667	-3.076537	1.977501
C	-1.925140	-4.550182	1.636716
C	-1.594572	-2.812149	3.399110
O	-1.223796	-2.374143	1.052421
O	1.139086	4.638856	-1.157950
C	1.455281	5.696315	-2.054922
O	-0.781703	4.167434	1.925556
C	-1.121979	4.906663	3.091835
H	6.040036	-0.752683	3.633888
H	4.199875	0.826409	3.793915
H	1.073126	4.013502	3.859296
H	2.977215	3.320804	4.624740
H	7.351745	-1.981319	2.263944
H	5.629627	-0.362064	-1.818058
H	6.958176	-1.115956	-0.960121
H	5.481313	-2.996147	-0.289260
H	3.450121	-1.714761	-2.159012
H	3.333845	-1.805500	-0.414180
H	-0.722528	5.017896	-3.052589
H	-5.893923	0.542561	-3.988725
H	-3.899261	1.926000	-3.822185
H	-2.631526	4.569724	-3.963059
H	-7.388157	-0.739115	-2.887120
H	-6.892760	-0.565089	0.456878
H	-5.433502	-0.389124	1.399501
H	-5.884458	-2.520611	-0.723356
H	-4.005033	-3.683312	0.036015
H	-3.513830	-2.041587	-0.248745
H	7.132444	-4.672343	-3.016241
H	6.840270	-4.578760	-1.193935
H	6.179667	-3.098845	-4.486335
H	4.568554	-2.586255	-3.978219
H	5.926512	-1.494172	-3.793706
H	3.473644	-4.346196	-0.618322
H	3.208155	-4.147219	-2.338702
H	-0.108211	-5.071176	-1.001335
H	1.465625	-5.738752	-0.547034
H	1.083207	-5.445268	-2.251285
H	-0.280473	-2.744340	-1.882052
H	1.126844	-1.680930	-1.932838

H	0.970072	-3.000740	-3.102517
H	0.426086	-2.984845	0.424103
H	-6.677600	-4.759931	-0.142402
H	-7.215790	-5.089592	1.511978
H	-5.496100	-5.015324	1.128865
H	-7.832623	-3.244336	2.794764
H	-7.233425	-1.543106	2.427555
H	-3.585478	-1.571504	2.203308
H	-4.142482	-3.196255	2.510157
H	-0.893228	-4.865827	1.791669
H	-2.186273	-4.744523	0.597547
H	-2.569688	-5.156132	2.273848
H	-0.559907	-3.137201	3.513393
H	-1.650639	-1.747315	3.633838
H	-2.208092	-3.349822	4.123367
H	-1.219525	-1.426165	1.260539
H	1.550064	5.328373	-3.077975
H	0.702641	6.485656	-2.013133
H	2.410743	6.090682	-1.723205
H	-2.081787	5.367819	2.880686
H	-1.217563	4.250518	3.958607
H	-0.383140	5.683854	3.294638

CAM-B3LYP Energy = -2840.09682330 a.u.

(*aR*,12*R*,12'*R*)-**2**/**3**, Conf D

C	-5.607546	-0.249223	-2.500518
C	-5.865582	-0.909317	-1.313369
C	-5.183314	-0.574130	-0.141784
C	-4.243425	0.463836	-0.217230
C	-3.985697	1.166970	-1.415321
C	-4.683284	0.775470	-2.551317
C	-3.408500	0.837122	0.939723
C	-1.997275	1.318903	0.582392
C	-1.928448	2.298002	-0.518982
C	-2.986654	2.268136	-1.452639
C	-0.912200	3.244776	-0.545162
C	-0.974995	4.249956	-1.516180
C	-2.019189	4.274685	-2.417557
C	-3.014036	3.302631	-2.387517
O	-1.064370	0.910793	1.232725
O	-3.713397	0.786051	2.109047
O	-4.040012	3.379265	-3.274855
O	-6.784042	-1.912250	-1.239354
C	-5.481855	-1.377619	1.098464
C	-4.842512	-2.787534	1.100940
C	-3.310803	-2.715642	1.161993
C	0.192776	3.287898	0.451119
C	1.408198	2.644106	0.274304
C	2.441738	2.675052	1.230684
C	2.163946	3.321494	2.433773
C	0.963400	3.994721	2.624459
C	-0.007072	3.997571	1.643519
C	1.619541	1.765900	-0.888578
C	2.593256	0.594984	-0.669582
C	3.816789	0.909620	0.078782
C	3.742773	2.024388	0.940647
C	5.021286	0.222923	-0.161424
C	6.169332	0.696471	0.484750
C	6.122823	1.842233	1.259546
C	4.930741	2.500191	1.482965
O	3.003840	3.342607	3.502795
O	7.392194	0.119685	0.333809
C	5.140180	-0.918115	-1.144125
C	4.868709	-2.329549	-0.575748
C	4.838476	-3.377332	-1.704021
O	2.309569	-0.469469	-1.175139
O	1.072810	1.860264	-1.960329
C	-5.433859	-3.613150	2.225412
C	-6.193299	-4.671430	1.969199
C	-5.140491	-3.184888	3.635500
C	-2.643795	-4.085249	1.138123
C	-1.127702	-4.080297	0.931977
C	-0.603708	-5.512763	1.001522
C	-0.409899	-3.213252	1.963465
O	-0.900723	-3.555567	-0.381635
C	5.887211	-2.701452	0.491802
C	5.388945	-2.683726	1.905668
C	7.143043	-3.028277	0.196277
C	3.671503	-3.301031	-2.692119
C	2.321668	-3.903347	-2.270896
C	2.423054	-5.384426	-1.946381
C	1.307642	-3.678959	-3.389959
O	1.829799	-3.273508	-1.068942
O	-1.198005	4.620212	1.772175
C	-1.471504	5.335550	2.970601
O	0.019170	5.161769	-1.497490
C	0.000259	6.218782	-2.448316
H	-6.135662	-0.539351	-3.401461
H	-4.509367	1.270616	-3.491161
H	-2.084164	5.054948	-3.162818
H	-3.946564	4.164019	-3.827114
H	-7.197234	-2.049603	-2.099398
H	-5.171174	-0.831659	1.980864
H	-6.563982	-1.502379	1.157031
H	-5.117289	-3.279131	0.165588
H	-3.009074	-2.164414	2.055258
H	-2.955550	-2.140387	0.305686
H	0.812532	4.485205	3.574045
H	7.043684	2.212418	1.690186
H	4.946898	3.410986	2.064292
H	3.686341	2.665965	3.418105
H	7.309100	-0.837539	0.186042
H	6.143951	-0.906083	-1.573360
H	4.453394	-0.740884	-1.966828
H	3.892156	-2.312199	-0.096293
H	5.765156	-3.286014	-2.275969
H	4.871002	-4.369012	-1.251238
H	-6.630663	-5.262148	2.765707
H	-6.403806	-4.983393	0.953003
H	-5.629561	-3.841914	4.353484
H	-4.067510	-3.199049	3.838323

H	-5.481885	-2.164605	3.821755
H	-3.078422	-4.681731	0.330447
H	-2.859311	-4.620239	2.066208
H	0.466975	-5.537169	0.791712
H	-1.112041	-6.139273	0.267035
H	-0.764341	-5.941468	1.992130
H	0.670362	-3.273354	1.818237
H	-0.706064	-2.169263	1.869088
H	-0.633411	-3.547212	2.978364
H	0.058293	-3.519143	-0.559616
H	4.964237	-1.708973	2.156779
H	6.178423	-2.915998	2.619124
H	4.584072	-3.413362	2.025876
H	7.851292	-3.292901	0.971941
H	7.502356	-3.073059	-0.825019
H	3.498553	-2.265293	-2.993452
H	3.967908	-3.823222	-3.604667
H	1.438004	-5.778833	-1.695723
H	3.082396	-5.560162	-1.097611
H	2.805264	-5.938176	-2.804338
H	0.335182	-4.078010	-3.100645
H	1.193990	-2.613412	-3.597424
H	1.624531	-4.173046	-4.309426
H	1.930916	-2.313229	-1.154391
H	-0.749256	6.139676	3.121256
H	-2.463241	5.758504	2.843748
H	-1.468612	4.669231	3.834834
H	-0.892004	6.836654	-2.332003
H	0.882700	6.817346	-2.244428
H	0.052009	5.831921	-3.467503

CAM-B3LYP Energy = -2840.09673009 a.u.

(*aR*,12*R*,12'*R*)-**2**/**3**, Conf E

C	5.508894	0.539155	-2.656376
C	5.789326	1.180044	-1.463328
C	5.186371	0.773987	-0.271223
C	4.296109	-0.306752	-0.335075
C	4.008905	-0.983297	-1.540719
C	4.633263	-0.528109	-2.695516
C	3.539557	-0.755912	0.848342
C	2.125643	-1.264182	0.544451
C	2.031980	-2.205926	-0.587407
C	3.048461	-2.118401	-1.563755
C	1.042953	-3.180763	-0.599582
C	1.098709	-4.160976	-1.596753
C	2.104774	-4.129962	-2.540042
C	3.068111	-3.125830	-2.526629
O	1.216642	-0.906640	1.255523
O	3.909691	-0.745920	1.999607
O	4.056343	-3.143996	-3.459107
O	6.652105	2.232221	-1.402879
C	5.499837	1.554277	0.979763
C	4.749072	2.904942	1.079324
C	3.232387	2.702170	1.198304
C	-0.018679	-3.277552	0.439758
C	-1.270255	-2.686814	0.319771
C	-2.262819	-2.756894	1.320250
C	-1.909919	-3.431537	2.491406
C	-0.670948	-4.047988	2.624320
C	0.266805	-3.981878	1.613925
C	-1.562930	-1.848446	-0.856012
C	-2.606054	-0.745371	-0.655154
C	-3.777997	-1.115759	0.146294
C	-3.598844	-2.142106	1.098418
C	-5.027811	-0.511147	-0.087750
C	-6.105703	-0.929659	0.691499
C	-5.953021	-1.964088	1.599390
C	-4.727309	-2.562899	1.797673
O	-2.782424	-3.478362	3.531288
O	-7.355234	-0.402373	0.570440
C	-5.248337	0.479568	-1.202283
C	-4.993895	1.956648	-0.835363
C	-4.803531	2.779817	-2.118102
O	-2.409918	0.323781	-1.194856
O	-1.035619	-1.942426	-1.938547
C	5.322474	3.721929	2.219275
C	5.982503	4.849838	1.985762
C	5.129058	3.204802	3.616798
C	2.454620	4.007330	1.310732
C	0.937503	3.893184	1.145464
C	0.300860	5.255720	1.407864
C	0.331430	2.848110	2.078816
O	0.710089	3.512408	-0.217586
C	-6.078790	2.512275	0.078030
C	-5.665124	2.791649	1.492219
C	-7.324317	2.719055	-0.340261
C	-4.137802	4.142690	-1.911423
C	-2.600925	4.171269	-1.968311
C	-2.115640	5.564341	-1.601687
C	-2.068742	3.778342	-3.342437
O	-2.030849	3.290051	-0.974533
O	1.491573	-4.544316	1.691500
C	1.846710	-5.261020	2.867399
O	0.136472	-5.105728	-1.560137
C	0.143243	-6.131115	-2.544955
H	5.978100	0.880598	-3.571845
H	4.436901	-1.004110	-3.641017
H	2.163455	-4.889183	-3.307278
H	3.963428	-3.915691	-4.029566
H	7.010895	2.419629	-2.277763
H	5.289654	0.952933	1.856057
H	6.569574	1.766421	0.978722
H	4.941084	3.460877	0.159079
H	3.018108	2.064123	2.058245
H	2.885789	2.163243	0.315023
H	-0.451902	-4.569403	3.545617
H	-6.819446	-2.294529	2.157352
H	-4.651644	-3.360443	2.515834
H	-2.383583	-3.929412	4.284293
H	-7.323956	0.501479	0.216396
H	-6.265461	0.370443	-1.583915

H	-4.589227	0.223169	-2.027627
H	-4.062741	1.987592	-0.274703
H	-4.215868	2.188809	-2.822841
H	-5.774662	2.919804	-2.595288
H	6.406639	5.436614	2.792277
H	6.121696	5.224931	0.978700
H	5.586306	3.871484	4.346762
H	4.069004	3.109447	3.861306
H	5.569892	2.213511	3.740580
H	2.809719	4.706987	0.548473
H	2.656918	4.476084	2.276651
H	-0.775728	5.214054	1.237059
H	0.724871	6.009137	0.742423
H	0.468146	5.571072	2.438991
H	-0.754936	2.834254	1.970942
H	0.706683	1.852016	1.847672
H	0.563580	3.073679	3.121460
H	-0.247573	3.464158	-0.393681
H	-5.256126	1.892723	1.960506
H	-6.496164	3.152691	2.096710
H	-4.868309	3.539247	1.510559
H	-8.084759	3.105302	0.327232
H	-7.626042	2.535005	-1.364917
H	-4.490653	4.834378	-2.679334
H	-4.452154	4.566161	-0.954223
H	-1.026869	5.607229	-1.619822
H	-2.456141	5.836956	-0.602464
H	-2.502344	6.298303	-2.308822
H	-0.981374	3.856273	-3.353783
H	-2.333642	2.752843	-3.602261
H	-2.470438	4.436310	-4.113938
H	-2.202146	2.365886	-1.208002
H	2.856186	-5.623509	2.700031
H	1.835988	-4.609523	3.742842
H	1.178510	-6.108943	3.027469
H	0.033114	-5.713922	-3.547451
H	1.058093	-6.723880	-2.489649
H	-0.710409	-6.763465	-2.321370

CAM-B3LYP Energy = -2840.09663205 a.u.

(*aR*,12*R*,12'*R*)-**2**/**3**, Conf F

C	5.517442	0.411688	-2.706536
C	5.828731	1.049396	-1.519372
C	5.229540	0.663722	-0.318676
C	4.308609	-0.391661	-0.368359
C	3.989085	-1.064552	-1.567832
C	4.612949	-0.631736	-2.731420
C	3.551054	-0.812637	0.824891
C	2.119171	-1.277592	0.536339
C	1.987299	-2.223004	-0.588501
C	2.996517	-2.171987	-1.574713
C	0.971043	-3.169248	-0.583010
C	0.991374	-4.160061	-1.571176
C	1.988202	-4.164351	-2.524829
C	2.978494	-3.186580	-2.529950
O	1.227656	-0.888184	1.252605
O	3.933082	-0.809824	1.972261
O	3.956380	-3.237707	-3.472144
O	6.719300	2.078946	-1.473490
C	5.579417	1.437906	0.926446
C	4.856711	2.802832	1.038726
C	3.338006	2.629804	1.176961
C	-0.083082	-3.226409	0.466890
C	-1.332179	-2.630897	0.337910
C	-2.319172	-2.670572	1.344836
C	-1.962952	-3.311848	2.533330
C	-0.726127	-3.929657	2.677185
C	0.205301	-3.898068	1.659006
C	-1.629804	-1.821327	-0.856525
C	-2.669424	-0.708060	-0.678709
C	-3.840089	-1.056954	0.136603
C	-3.657694	-2.067878	1.107642
C	-5.092580	-0.470442	-0.115848
C	-6.183332	-0.935602	0.618654
C	-6.024170	-1.936326	1.560243
C	-4.783603	-2.491130	1.803925
O	-2.832152	-3.324570	3.577440
O	-7.404380	-0.394606	0.355651
C	-5.315027	0.569302	-1.179314
C	-4.944784	2.011104	-0.761250
C	-4.730808	2.856064	-2.027869
O	-2.471896	0.341138	-1.254640
O	-1.106401	-1.941508	-1.938341
C	5.460344	3.605530	2.173217
C	6.140155	4.720433	1.933986
C	5.272672	3.089981	3.572149
C	2.586302	3.948666	1.303712
C	1.065366	3.861475	1.156606
C	0.456159	5.233912	1.431992
C	0.452310	2.823912	2.093680
O	0.815966	3.489374	-0.204844
C	-5.950154	2.621158	0.192916
C	-7.314998	2.961532	-0.333578
C	-5.623063	2.854729	1.458678
C	-4.043467	4.204391	-1.799900
C	-2.509547	4.213270	-1.901385
C	-1.990971	5.587147	-1.509602
C	-2.021374	3.851940	-3.300357
O	-1.928080	3.293825	-0.949452
O	1.427666	-4.465624	1.745466
C	1.786177	-5.149284	2.939686
O	0.006114	-5.079647	-1.515294
C	-0.024289	-6.113985	-2.490059
H	5.985106	0.737221	-3.628577
H	4.393122	-1.106321	-3.672532
H	2.017586	-4.931352	-3.285955
H	3.837469	-4.010018	-4.036859
H	7.072999	2.252762	-2.353239
H	5.372558	0.840413	1.806225
H	6.652785	1.629359	0.907233
H	5.048080	3.357185	0.117303

H	3.122623	1.993063	2.037489
H	2.968932	2.101314	0.296573
H	-0.503452	-4.425502	3.611650
H	-6.886686	-2.297084	2.108560
H	-4.702729	-3.267897	2.544097
H	-2.431548	-3.752131	4.343039
H	-8.078897	-0.815797	0.900394
H	-6.356313	0.531840	-1.493775
H	-4.711936	0.314827	-2.049065
H	-4.000210	1.957515	-0.225895
H	-4.149441	2.261377	-2.734482
H	-5.694698	3.016035	-2.514769
H	6.585275	5.296933	2.736590
H	6.274986	5.094840	0.926073
H	5.752991	3.745312	4.297564
H	4.213858	3.017179	3.829426
H	5.693364	2.089171	3.689097
H	2.944239	4.644425	0.539215
H	2.808852	4.410420	2.268535
H	-0.623090	5.211861	1.275452
H	0.884546	5.982451	0.763847
H	0.642552	5.542268	2.461996
H	-0.635429	2.830366	1.999459
H	0.806314	1.822058	1.854347
H	0.701405	3.041571	3.134118
H	-0.144001	3.447087	-0.369963
H	-7.264666	3.766516	-1.070090
H	-7.972229	3.286223	0.472167
H	-7.777673	2.103835	-0.823762
H	-6.332312	3.280259	2.159201
H	-4.634123	2.626988	1.838409
H	-4.409807	4.926770	-2.532658
H	-4.320612	4.594952	-0.817698
H	-0.902260	5.612123	-1.551594
H	-2.304357	5.839468	-0.496349
H	-2.380544	6.345654	-2.188696
H	-0.933475	3.912140	-3.339599
H	-2.311364	2.838998	-3.581527
H	-2.432511	4.538591	-4.041447
H	-2.146673	2.382138	-1.191949
H	1.114346	-5.988318	3.128961
H	2.792548	-5.522426	2.776967
H	1.784657	-4.472321	3.795678
H	-0.135025	-5.703674	-3.495340
H	0.875631	-6.729665	-2.439139
H	-0.891255	-6.722145	-2.251053

CAM-B3LYP Energy = -2840.09653645 a.u.

(*aR*,12*R*,12'*R*)-**2**/**3**, Conf G

C	5.624547	0.209059	-2.486550
C	5.897757	0.850544	-1.291113
C	5.203257	0.523144	-0.126112
C	4.238923	-0.495478	-0.213409
C	3.967747	-1.178302	-1.417366
C	4.675847	-0.788084	-2.550688
C	3.395480	-0.863194	0.938939
C	1.976192	-1.315921	0.576811
C	1.890678	-2.283461	-0.533003
C	2.948668	-2.260566	-1.467663
C	0.862262	-3.216019	-0.563675
C	0.911270	-4.215349	-1.542543
C	1.951466	-4.244761	-2.447830
C	2.959533	-3.286021	-2.412183
O	1.050939	-0.894911	1.229570
O	3.700386	-0.825103	2.109095
O	3.982437	-3.369746	-3.302326
O	6.854974	1.818788	-1.331858
C	5.489749	1.314412	1.126987
C	4.874352	2.736670	1.128214
C	3.342054	2.675572	1.174729
C	-0.233672	-3.260710	0.443168
C	-1.455289	-2.618869	0.283697
C	-2.482630	-2.651155	1.246803
C	-2.203929	-3.346523	2.425503
C	-0.995171	-4.009563	2.601103
C	-0.018470	-3.975890	1.625285
C	-1.679495	-1.763691	-0.893432
C	-2.652868	-0.592593	-0.699911
C	-3.857914	-0.881408	0.083153
C	-3.776498	-1.967504	0.986134
C	-5.055528	-0.180227	-0.150161
C	-6.201488	-0.641528	0.501412
C	-6.144877	-1.727839	1.355464
C	-4.950929	-2.374220	1.604508
O	-3.120337	-3.363531	3.428145
O	-7.377933	-0.006905	0.246598
C	-5.181893	0.988861	-1.093312
C	-4.765184	2.356182	-0.497856
C	-4.741444	3.436626	-1.596496
O	-2.380285	0.451218	-1.254358
O	-1.142148	-1.886551	-1.967651
C	5.465873	3.553555	2.258982
C	6.226479	4.612482	2.009457
C	5.167152	3.116129	3.664793
C	2.682637	4.048302	1.147026
C	1.172029	4.043337	0.903197
C	0.645735	5.475269	0.961453
C	0.429396	3.174582	1.915695
O	0.981227	3.519583	-0.416062
C	-5.660411	2.782685	0.648551
C	-7.051457	3.248563	0.323350
C	-5.213063	2.763648	1.898698
C	-3.647349	3.322479	-2.662289
C	-2.249344	3.863849	-2.324385
C	-2.263888	5.350401	-2.008832
C	-1.311081	3.584849	-3.495908
O	-1.721555	3.219795	-1.146253
O	1.180237	-4.585830	1.746547
C	1.465366	-5.313171	2.934744
O	-0.090910	-5.117939	-1.525409
C	-0.089269	-6.164939	-2.487331

H	6.170172	0.506561	-3.372460
H	4.488952	-1.268030	-3.495897
H	2.004502	-5.019514	-3.199755
H	3.874840	-4.146352	-3.863420
H	7.055651	2.148070	-0.448959
H	5.144407	0.768851	1.996349
H	6.574449	1.399204	1.253281
H	5.149149	3.237178	0.195496
H	3.030065	2.123977	2.063984
H	2.991275	2.105609	0.313434
H	-0.829328	-4.543237	3.526443
H	-7.051697	-2.079104	1.834406
H	-4.945452	-3.207791	2.285266
H	-2.768452	-3.826808	4.196944
H	-8.093574	-0.420880	0.741917
H	-6.216027	1.050088	-1.428489
H	-4.570956	0.802744	-1.973309
H	-3.761792	2.249103	-0.093579
H	-5.706883	3.420608	-2.108818
H	-4.679389	4.415536	-1.117202
H	6.662777	5.198057	2.810046
H	6.437051	4.932935	0.995748
H	5.652415	3.769882	4.388070
H	4.093330	3.128201	3.862786
H	5.509272	2.095450	3.847543
H	3.136459	4.648998	0.353233
H	2.877308	4.575927	2.083830
H	-0.419443	5.498624	0.725811
H	1.171127	6.102712	0.239863
H	0.782141	5.903194	1.956059
H	-0.646712	3.232446	1.742204
H	0.729466	2.130907	1.829639
H	0.625485	3.509465	2.935962
H	0.026873	3.470894	-0.617392
H	-7.030456	4.177284	-0.250581
H	-7.623451	3.428826	1.232968
H	-7.585715	2.508728	-0.273136
H	-5.839585	3.065164	2.730217
H	-4.204355	2.444978	2.133761
H	-3.537662	2.282910	-2.978549
H	-3.978490	3.864932	-3.550938
H	-1.249864	5.699959	-1.813174
H	-2.869304	5.562501	-1.128847
H	-2.664308	5.915305	-2.851093
H	-0.307065	3.943252	-3.266995
H	-1.256560	2.513352	-3.696927
H	-1.657689	4.083994	-4.401912
H	-1.867921	2.264543	-1.221942
H	0.762194	-6.136893	3.069707
H	2.467005	-5.711300	2.805450
H	1.444629	-4.660811	3.809422
H	0.796845	-6.793775	-2.383153
H	-0.976978	-6.756016	-2.284426
H	-0.142846	-5.766686	-3.502030

CAM-B3LYP Energy = -2840.09649361 a.u.

(*aR*,12*R*,12'*R*)-**2**/**3**, Conf H

C	5.579791	0.213458	-2.437144
C	5.844658	0.839767	-1.233429
C	5.145676	0.495205	-0.074551
C	4.185945	-0.522005	-0.178435
C	3.924415	-1.195056	-1.393051
C	4.635618	-0.791174	-2.516156
C	3.335221	-0.903725	0.964238
C	1.920135	-1.357816	0.586495
C	1.847674	-2.318323	-0.530898
C	2.911141	-2.281753	-1.458781
C	0.824926	-3.257187	-0.576276
C	0.885384	-4.247191	-1.563285
C	1.931491	-4.263146	-2.462280
C	2.933543	-3.299200	-2.412004
O	0.987300	-0.946070	1.234624
O	3.630453	-0.879231	2.136854
O	3.961967	-3.369024	-3.297244
O	6.786177	1.818583	-1.129300
C	5.449579	1.268008	1.183628
C	4.852962	2.698304	1.213069
C	3.324400	2.673822	1.262244
C	-0.279438	-3.315309	0.420541
C	-1.488247	-2.648950	0.270998
C	-2.521770	-2.684994	1.227523
C	-2.264413	-3.419117	2.387538
C	-1.069003	-4.109269	2.552067
C	-0.084515	-4.065679	1.584676
C	-1.688595	-1.759544	-0.884986
C	-2.628035	-0.569773	-0.657313
C	-3.845291	-0.850218	0.108492
C	-3.795712	-1.958501	0.983404
C	-5.022477	-0.104481	-0.104577
C	-6.168393	-0.507915	0.585025
C	-6.145686	-1.630052	1.395704
C	-4.983196	-2.342030	1.597069
O	-3.186346	-3.446723	3.384281
O	-7.369537	0.122091	0.459183
C	-5.120587	1.022916	-1.106496
C	-4.790269	2.437491	-0.576862
C	-4.745130	3.454930	-1.731933
O	-2.319825	0.488809	-1.163648
O	-1.158885	-1.872131	-1.964033
C	5.517848	3.456270	2.349121
C	5.056934	3.455633	3.593005
C	6.778885	4.181302	1.977267
C	2.691111	4.057587	1.168255
C	1.182154	4.077259	0.917006
C	0.687163	5.521626	0.924990
C	0.415664	3.259780	1.954104
O	0.981889	3.514741	-0.385645
C	-5.772812	2.870040	0.501233
C	-5.254631	2.838196	1.907959
C	-7.014858	3.258400	0.222516
C	-3.592470	3.319573	-2.730743

C	-2.220088	3.889212	-2.337415
C	-2.273489	5.379074	-2.043059
C	-1.226222	3.611242	-3.462429
O	-1.733644	3.270065	-1.128215
O	1.102912	-4.697647	1.697821
C	1.370903	-5.454834	2.871413
O	-0.113119	-5.154371	-1.561411
C	-0.098319	-6.194204	-2.530963
H	6.119838	0.512545	-3.327999
H	4.458027	-1.261912	-3.467761
H	1.993388	-5.030762	-3.220832
H	3.863889	-4.143756	-3.862678
H	7.212580	1.962547	-1.981778
H	5.104585	0.729661	2.058369
H	6.534449	1.348926	1.263009
H	5.144768	3.195012	0.284000
H	2.994064	2.165855	2.170705
H	2.963341	2.074684	0.424499
H	-0.919355	-4.671173	3.463326
H	-7.064394	-1.933042	1.880757
H	-5.004013	-3.198352	2.248577
H	-2.848641	-3.939697	4.140920
H	-7.248630	1.070317	0.282602
H	-6.133587	1.036281	-1.514682
H	-4.459438	0.806719	-1.940520
H	-3.806024	2.397124	-0.115273
H	-5.680545	3.375015	-2.291406
H	-4.744005	4.458967	-1.305990
H	5.581883	3.975299	4.385663
H	4.142846	2.945397	3.869424
H	7.268583	4.615556	2.848319
H	7.484829	3.511354	1.480657
H	6.559613	4.983866	1.268055
H	3.159564	4.610547	0.348242
H	2.893954	4.620774	2.080828
H	-0.375647	5.561434	0.680584
H	1.231437	6.113816	0.187739
H	0.826316	5.978599	1.906182
H	-0.658096	3.333325	1.771927
H	0.695188	2.208037	1.906342
H	0.613174	3.625625	2.963401
H	0.027738	3.492026	-0.590653
H	-4.873437	1.845994	2.160159
H	-6.021037	3.113349	2.631334
H	-4.413986	3.529131	2.010563
H	-7.696190	3.564372	1.007121
H	-7.388356	3.312502	-0.793067
H	-3.454564	2.272345	-3.009565
H	-3.882870	3.829876	-3.651967
H	-1.273953	5.749653	-1.814461
H	-2.915082	5.590732	-1.188949
H	-2.652203	5.925985	-2.906938
H	-0.238542	3.984952	-3.191040
H	-1.148538	2.538799	-3.650238
H	-1.537277	4.097471	-4.388121
H	-1.865063	2.311603	-1.191025
H	1.352643	-4.821551	3.760050
H	0.656486	-6.272212	2.983699
H	2.368192	-5.862861	2.739585
H	0.790669	-6.818635	-2.424818
H	-0.984026	-6.791897	-2.338989
H	-0.146731	-5.788866	-3.543118

CAM-B3LYP Energy = -2840.09639060 a.u.

(*aR*,12*R*,12'*R*)-**2**/**3**, Conf I

C	-6.344143	2.230316	-1.590216
C	-6.609146	0.877654	-1.444802
C	-5.597611	-0.007857	-1.050609
C	-4.311581	0.522754	-0.861061
C	-4.019985	1.886498	-1.063296
C	-5.074134	2.730048	-1.396734
C	-3.190251	-0.288591	-0.346339
C	-2.190602	0.470919	0.545972
C	-1.770714	1.788945	0.037707
C	-2.641816	2.406643	-0.881809
C	-0.517543	2.296232	0.350357
C	-0.097959	3.460349	-0.308494
C	-0.896210	4.039398	-1.273756
C	-2.145432	3.509772	-1.572670
O	-1.779931	-0.072817	1.542952
O	-2.996779	-1.466887	-0.536249
O	-2.808833	4.143176	-2.577518
O	-7.883329	0.500399	-1.690028
C	-5.956102	-1.454266	-0.818186
C	-6.796231	-1.715690	0.456962
C	-7.248842	-3.183209	0.516533
C	0.395199	1.684287	1.354490
C	1.454244	0.847900	1.026709
C	2.350388	0.318504	1.978376
C	2.164012	0.728077	3.298933
C	1.117044	1.573810	3.649340
C	0.237794	2.047291	2.697310
C	1.735650	0.536650	-0.386728
C	3.204100	0.246406	-0.731695
C	3.922116	-0.599110	0.233089
C	3.423792	-0.618543	1.555353
C	4.977232	-1.435562	-0.181742
C	5.473537	-2.358824	0.743061
C	4.956351	-2.414783	2.025037
C	3.961284	-1.550074	2.435233
O	3.030611	0.316180	4.260540
O	6.425461	-3.268776	0.367837
C	5.565401	-1.406482	-1.568314
C	6.592107	-0.277993	-1.781739
C	7.813539	-0.389126	-0.846391
O	3.630552	0.677241	-1.779436
O	0.920811	0.524744	-1.278463
C	-6.046031	-1.333550	1.718958
C	-6.349897	-0.218498	2.372610
C	-4.968529	-2.257739	2.214453
C	-8.122397	-3.713767	-0.621074

C	-9.497617	-3.083962	-0.842731
C	-10.283786	-2.903734	0.448396
C	-10.288353	-3.926055	-1.837008
O	-9.266280	-1.784812	-1.443775
C	7.015912	-0.117659	-3.227794
C	7.802408	1.128779	-3.528185
C	6.728429	-0.987305	-4.188879
C	8.786695	-1.511791	-1.197905
C	9.738229	-1.920421	-0.073271
C	10.563410	-0.753508	0.450096
C	10.639426	-3.056986	-0.534704
O	8.886827	-2.406575	0.997649
O	-0.789979	2.874538	2.977827
C	-0.995799	3.284134	4.323630
O	1.123478	3.929523	0.030097
C	1.614806	5.093579	-0.622198
H	-7.160764	2.890492	-1.850902
H	-4.925387	3.797833	-1.471790
H	-0.572524	4.902711	-1.834964
H	-3.539593	3.601674	-2.899747
H	-8.088522	-0.442701	-1.532372
H	-6.528984	-1.798624	-1.681535
H	-5.061609	-2.066039	-0.794598
H	-7.683564	-1.083969	0.422190
H	-7.764328	-3.340952	1.466698
H	-6.361385	-3.819221	0.552735
H	1.011507	1.860553	4.686236
H	5.346215	-3.158946	2.707847
H	3.596787	-1.613670	3.446079
H	2.803573	0.714647	5.108605
H	7.324676	-2.992430	0.661504
H	4.769592	-1.275701	-2.298116
H	6.028532	-2.373145	-1.753002
H	6.087835	0.653702	-1.513381
H	8.341123	0.565469	-0.848204
H	7.449581	-0.522315	0.172995
H	-5.818111	0.075844	3.269745
H	-7.140543	0.439794	2.032369
H	-4.400153	-1.794025	3.019448
H	-5.397515	-3.185583	2.598286
H	-4.272323	-2.533816	1.421386
H	-8.289769	-4.775118	-0.425091
H	-7.586675	-3.670217	-1.571584
H	-11.274661	-2.498115	0.234888
H	-9.776973	-2.221220	1.128728
H	-10.415794	-3.861090	0.954170
H	-11.232949	-3.438439	-2.086721
H	-9.719184	-4.066179	-2.756491
H	-10.517850	-4.905753	-1.417183
H	-10.119468	-1.379587	-1.639444
H	7.264336	2.017490	-3.189294
H	7.993256	1.227429	-4.595980
H	8.765354	1.127630	-3.012879
H	7.054151	-0.816252	-5.208055
H	6.165640	-1.892946	-4.007954
H	8.234925	-2.404591	-1.497537
H	9.393313	-1.225414	-2.059347
H	11.236124	-1.086626	1.242843
H	9.923188	0.029757	0.852911
H	11.172144	-0.327940	-0.348809
H	11.276141	-3.401738	0.282658
H	10.042643	-3.898670	-0.887171
H	11.287353	-2.727049	-1.347393
H	9.429254	-2.741909	1.720264
H	-1.194545	2.426963	4.969315
H	-0.136357	3.840780	4.701666
H	-1.866314	3.932572	4.306624
H	2.589201	5.289483	-0.185348
H	1.724972	4.926156	-1.694984
H	0.959200	5.948399	-0.447431

CAM-B3LYP Energy = -2840.09606076 a.u.

(*aR*,12*R*,12'*R*)-**2**/**3**, Conf J

C	5.579481	-0.367394	2.725232
C	6.032133	-0.808246	1.494074
C	5.442612	-0.356642	0.313872
C	4.402412	0.580498	0.427698
C	3.914350	1.027213	1.672254
C	4.532644	0.523669	2.815361
C	3.717726	1.109079	-0.764417
C	2.223723	1.390500	-0.588391
C	1.837636	2.042540	0.675994
C	2.745979	1.946861	1.752721
C	0.656061	2.770882	0.733381
C	0.372786	3.473604	1.909087
C	1.266623	3.447874	2.960888
C	2.441233	2.709632	2.883277
O	1.476277	1.099641	-1.491836
O	4.218196	1.328066	-1.843940
O	3.311078	2.745119	3.925927
O	7.044133	-1.719299	1.513144
C	5.856757	-0.995740	-0.989325
C	5.243314	-2.408639	-1.174138
C	3.715968	-2.331265	-1.287119
C	-0.278220	2.938159	-0.414711
C	-1.454422	2.216794	-0.565958
C	-2.384779	2.441129	-1.604094
C	-2.087329	3.489259	-2.477126
C	-0.916021	4.226572	-2.345262
C	-0.016837	3.961119	-1.332412
C	-1.818869	1.189372	0.418871
C	-3.319827	0.982030	0.623000
C	-4.100569	0.870172	-0.619495
C	-3.590910	1.578180	-1.733501
C	-5.243020	0.060817	-0.696691
C	-5.885691	-0.021612	-1.935113
C	-5.383945	0.635731	-3.042113
C	-4.253841	1.423771	-2.944407
O	-2.961263	3.813834	-3.465040
O	-7.014925	-0.778857	-2.006837
C	-5.814480	-0.749364	0.441332

C	-5.580008	-2.265057	0.289521
C	-4.095990	-2.669327	0.422173
O	-3.732031	0.915629	1.758717
O	-1.044611	0.527011	1.075336
C	5.890119	-3.113448	-2.348407
C	6.657462	-4.180406	-2.161351
C	5.637489	-2.559842	-3.721826
C	3.032553	-3.690820	-1.349986
C	1.523322	-3.659636	-1.089797
C	0.960523	-5.073993	-1.204644
C	0.794004	-2.728231	-2.054044
O	1.364519	-3.191132	0.254674
C	-6.465359	-3.102242	1.192095
C	-6.456530	-4.578473	0.904022
C	-7.211492	-2.607853	2.172574
C	-3.528049	-2.594106	1.835265
C	-2.075826	-3.069794	1.989227
C	-1.918623	-4.544967	1.656862
C	-1.597431	-2.797134	3.411189
O	-1.218768	-2.370729	1.063611
O	1.131026	4.648838	-1.152573
C	1.444782	5.709464	-2.046694
O	-0.785163	4.168364	1.929821
C	-1.125347	4.905381	3.097640
H	6.049924	-0.752748	3.620370
H	4.193290	0.824682	3.790714
H	1.071754	4.013144	3.861432
H	2.977117	3.320232	4.623972
H	7.360463	-1.906408	0.622396
H	5.581225	-0.362226	-1.823513
H	6.947607	-1.072698	-1.036472
H	5.472807	-2.999367	-0.282970
H	3.446939	-1.729574	-2.158221
H	3.332116	-1.807361	-0.412125
H	-0.729995	5.026429	-3.048200
H	-5.885174	0.534423	-3.997862
H	-3.895455	1.924533	-3.826680
H	-2.636707	4.573531	-3.962139
H	-7.378266	-0.751467	-2.899313
H	-6.891053	-0.576696	0.444145
H	-5.435750	-0.394090	1.391606
H	-5.870119	-2.529358	-0.730932
H	-3.990014	-3.684882	0.039402
H	-3.503570	-2.041920	-0.245901
H	7.134888	-4.688051	-2.991169
H	6.833524	-4.584655	-1.171375
H	6.184869	-3.123350	-4.476054
H	4.575693	-2.599065	-3.973951
H	5.939569	-1.513068	-3.794821
H	3.476388	-4.349366	-0.597454
H	3.208644	-4.163571	-2.319297
H	-0.104563	-5.081017	-0.968124
H	1.470581	-5.742322	-0.509379
H	1.085915	-5.464984	-2.215868
H	-0.281229	-2.762407	-1.868823
H	1.124240	-1.697508	-1.931148
H	0.967644	-3.027796	-3.089083
H	0.430149	-2.981616	0.439173
H	-6.660189	-4.770283	-0.152284
H	-7.203368	-5.101004	1.500246
H	-5.482542	-5.021407	1.123389
H	-7.831568	-3.256973	2.779299
H	-7.236082	-1.554069	2.413788
H	-3.587155	-1.567546	2.204411
H	-4.141787	-3.192897	2.512400
H	-0.886333	-4.857636	1.815272
H	-2.177820	-4.745747	0.618423
H	-2.562951	-5.148620	2.296397
H	-0.562885	-3.120460	3.531246
H	-1.655549	-1.731088	3.639831
H	-2.213242	-3.331468	4.135965
H	-1.216957	-1.421628	1.266712
H	1.541622	5.344313	-3.070553
H	0.689661	6.496354	-2.003644
H	2.398711	6.105970	-1.713127
H	-1.219761	4.247613	3.963287
H	-0.386992	5.682818	3.301184
H	-2.085676	5.366038	2.887845

CAM-B3LYP Energy = -2840.09594292 a.u.

(*aR*,12*R*,12'*R*)-**2**/**3**, Conf K

C	5.260976	-0.329935	3.009857
C	5.883640	-0.634975	1.814172
C	5.408515	-0.119414	0.604093
C	4.317347	0.754850	0.659028
C	3.681739	1.095001	1.870995
C	4.164678	0.511705	3.036257
C	3.686414	1.289480	-0.564329
C	2.158964	1.439890	-0.490677
C	1.642686	2.039316	0.754276
C	2.489681	1.980482	1.880780
C	0.425874	2.706649	0.758002
C	0.048606	3.379040	1.929248
C	0.901671	3.417201	3.013827
C	2.118008	2.748395	2.983013
O	1.501404	1.108334	-1.447596
O	4.244220	1.591971	-1.592605
O	2.887886	2.912902	4.092476
O	6.954697	-1.471373	1.758260
C	6.029297	-0.625030	-0.672143
C	5.529028	-2.043668	-1.049019
C	4.017675	-2.055540	-1.307221
C	-0.452344	2.834599	-0.437755
C	-1.620624	2.108074	-0.609421
C	-2.505789	2.289779	-1.693325
C	-2.166879	3.290697	-2.603210
C	-1.001626	4.035053	-2.452756
C	-0.150346	3.817245	-1.388037
C	-2.038556	1.122838	0.402883
C	-3.552425	1.010718	0.579074
C	-4.272180	0.800701	-0.691346

C	-3.706662	1.420717	-1.827536
C	-5.384647	-0.046214	-0.766618
C	-5.933998	-0.270928	-2.030996
C	-5.395477	0.326801	-3.155809
C	-4.299062	1.161873	-3.057107
O	-2.996659	3.557851	-3.644754
O	-7.002731	-1.110569	-2.109817
C	-5.977038	-0.788795	0.404292
C	-5.428159	-2.232316	0.543700
C	-3.974408	-2.216454	1.033272
O	-4.022425	1.080172	1.690463
O	-1.307414	0.422684	1.067280
C	6.330121	-2.584993	-2.214761
C	7.152761	-3.614922	-2.056126
C	6.166116	-1.914246	-3.549289
C	3.444915	-3.444043	-1.561976
C	1.923044	-3.540536	-1.419966
C	1.474660	-4.970770	-1.709340
C	1.196240	-2.569446	-2.346241
O	1.636069	-3.218438	-0.053400
C	-6.334853	-3.054650	1.435204
C	-6.442888	-2.653962	2.878982
C	-7.015958	-4.085096	0.949338
C	-3.315355	-3.585486	1.092419
C	-1.849039	-3.578854	1.548813
C	-1.264830	-4.973452	1.398350
C	-1.692156	-3.091462	2.984308
O	-1.065617	-2.733301	0.674432
O	0.988516	4.513983	-1.187099
C	1.346019	5.530691	-2.115219
O	-1.151410	3.998475	1.902375
C	-1.582092	4.709999	3.056356
H	5.618989	-0.772333	3.931923
H	3.665483	0.665843	3.981720
H	0.664336	3.980952	3.903167
H	3.802068	2.659641	3.916814
H	7.187508	-1.779019	2.641755
H	5.834839	0.065640	-1.483982
H	7.109458	-0.673033	-0.534082
H	5.725331	-2.696463	-0.195788
H	3.783256	-1.389323	-2.140443
H	3.516146	-1.649114	-0.429149
H	-0.781307	4.800079	-3.183894
H	-5.832770	0.129725	-4.127885
H	-3.903226	1.607268	-3.953766
H	-2.652769	4.290823	-4.168286
H	-7.300623	-1.185329	-3.023523
H	-7.053780	-0.848397	0.250349
H	-5.808382	-0.239931	1.324358
H	-5.448255	-2.692568	-0.447139
H	-3.398919	-1.593979	0.346501
H	-3.932322	-1.728471	2.008308
H	7.738891	-4.005254	-2.879909
H	7.268530	-4.102963	-1.095553
H	6.819285	-2.364605	-4.295508
H	5.137589	-1.993213	-3.907834
H	6.398469	-0.848826	-3.493711
H	3.881140	-4.147845	-0.846840
H	3.725488	-3.798720	-2.556649
H	0.397785	-5.070915	-1.563417
H	1.977890	-5.669201	-1.039249
H	1.703787	-5.252662	-2.738555
H	0.115910	-2.685638	-2.238811
H	1.449092	-1.536086	-2.112693
H	1.453338	-2.763008	-3.389209
H	0.676868	-3.117815	0.082892
H	-5.478638	-2.732674	3.385923
H	-7.154348	-3.286593	3.407868
H	-6.768307	-1.616647	2.981408
H	-7.677892	-4.672765	1.574556
H	-6.935690	-4.375675	-0.091452
H	-3.873216	-4.243438	1.763042
H	-3.356626	-4.044409	0.100366
H	-0.217838	-4.984975	1.701058
H	-1.329473	-5.304735	0.361528
H	-1.813070	-5.682190	2.019199
H	-0.646821	-3.154265	3.287957
H	-2.013701	-2.055205	3.094984
H	-2.286135	-3.703332	3.664070
H	-1.202691	-1.804347	0.906514
H	1.491112	5.116755	-3.114537
H	0.590605	6.317849	-2.146388
H	2.283348	5.943885	-1.755869
H	-1.656676	4.047905	3.920506
H	-0.907656	5.537739	3.281835
H	-2.565392	5.100669	2.813504

CAM-B3LYP Energy = -2840.09588209 a.u.

(*aR*,12*R*,12'*R*)-**2**/**3**, Conf L

C	-5.626139	-0.213255	-2.490173
C	-5.885533	-0.874787	-1.302768
C	-5.190709	-0.553891	-0.135979
C	-4.241688	0.479780	-0.212421
C	-3.985514	1.183301	-1.407847
C	-4.692286	0.798473	-2.543784
C	-3.400751	0.844754	0.942461
C	-1.990376	1.327442	0.583841
C	-1.921262	2.306643	-0.516922
C	-2.981853	2.280272	-1.448033
C	-0.902249	3.249983	-0.544807
C	-0.963558	4.255372	-1.516141
C	-2.009744	4.283780	-2.414822
C	-3.008285	3.315309	-2.382320
O	-1.057608	0.917703	1.233200
O	-3.701203	0.784309	2.112805
O	-4.036745	3.397267	-3.265929
O	-6.830382	-1.854586	-1.352425
C	-5.466116	-1.364119	1.107342
C	-4.846879	-2.784638	1.086103
C	-3.315228	-2.722214	1.156786
C	0.203553	3.291108	0.450601

C	1.417164	2.643862	0.274159
C	2.451036	2.673378	1.230156
C	2.175304	3.321910	2.432648
C	0.976634	3.998562	2.622873
C	0.005942	4.002830	1.642151
C	1.625425	1.763419	-0.887562
C	2.596825	0.590617	-0.667732
C	3.821347	0.903290	0.079849
C	3.750338	2.019166	0.940527
C	5.024110	0.213356	-0.159717
C	6.173369	0.684463	0.486074
C	6.129937	1.831254	1.259523
C	4.939569	2.492586	1.482157
O	3.015481	3.341875	3.501424
O	7.394597	0.104046	0.335944
C	5.140283	-0.928664	-1.141527
C	4.865336	-2.339096	-0.572393
C	4.833543	-3.387304	-1.700186
O	2.310497	-0.473840	-1.171773
O	1.077169	1.857093	-1.958588
C	-5.454108	-3.626119	2.190138
C	-6.210139	-4.679749	1.906562
C	-5.178568	-3.217090	3.609116
C	-2.656486	-4.095324	1.119981
C	-1.139491	-4.093790	0.920290
C	-0.621721	-5.528984	0.977337
C	-0.422835	-3.240391	1.963964
O	-0.906209	-3.555910	-0.386516
C	5.882396	-2.712477	0.496001
C	5.383474	-2.692061	1.909616
C	7.137519	-3.042853	0.201445
C	3.667840	-3.308158	-2.689566
C	2.316223	-3.907633	-2.270087
C	2.414000	-5.389250	-1.946785
C	1.303773	-3.679995	-3.389890
O	1.824602	-3.277625	-1.067963
O	-1.183291	4.628857	1.770341
C	-1.454348	5.346830	2.967768
O	0.033615	5.163585	-1.499412
C	0.016174	6.221164	-2.449767
H	-6.171242	-0.505814	-3.378039
H	-4.516409	1.294258	-3.482888
H	-2.074024	5.064495	-3.159668
H	-3.940510	4.180657	-3.819648
H	-7.023667	-2.197807	-0.473118
H	-5.118697	-0.829731	1.982817
H	-6.550080	-1.453871	1.237169
H	-5.106730	-3.265972	0.139225
H	-3.018266	-2.184377	2.059519
H	-2.951857	-2.137759	0.310273
H	0.827305	4.490653	3.571874
H	7.051770	2.199507	1.689748
H	4.958077	3.404014	2.062428
H	3.696566	2.663765	3.416958
H	7.308794	-0.853099	0.189329
H	6.144148	-0.919361	-1.570623
H	4.454020	-0.750268	-1.964414
H	3.888515	-2.319310	-0.093522
H	5.761115	-3.298667	-2.271129
H	4.862917	-4.378870	-1.246949
H	-6.659018	-5.281575	2.687915
H	-6.404201	-4.979702	0.883314
H	-5.675580	-3.885007	4.311147
H	-4.108125	-3.233353	3.824451
H	-5.523730	-2.200141	3.806395
H	-3.090016	-4.680129	0.303371
H	-2.878625	-4.639391	2.041076
H	0.449744	-5.555492	0.772099
H	-1.129196	-6.145938	0.234257
H	-0.788412	-5.967127	1.962799
H	0.657727	-3.303531	1.822677
H	-0.713860	-2.194106	1.878999
H	-0.652140	-3.583784	2.974403
H	0.053488	-3.521094	-0.561668
H	4.960556	-1.716194	2.159388
H	6.172156	-2.925024	2.623739
H	4.577139	-3.420009	2.030340
H	7.844666	-3.308532	0.977768
H	7.497241	-3.089749	-0.819610
H	3.497535	-2.271983	-2.990864
H	3.964003	-3.830782	-3.601936
H	1.427704	-5.782070	-1.698593
H	3.071288	-5.567083	-1.096855
H	2.796840	-5.942838	-2.804559
H	0.330096	-4.076967	-3.101830
H	1.192834	-2.614044	-3.596754
H	1.620383	-4.174223	-4.309385
H	1.928086	-2.317512	-1.152434
H	-0.729735	6.149099	3.116950
H	-2.444915	5.772417	2.840547
H	-1.453086	4.681827	3.833024
H	-0.873651	6.842053	-2.330985
H	0.901208	6.816473	-2.247630
H	0.064164	5.834501	-3.469201

CAM-B3LYP Energy = -2840.09586660 a.u.

(*aR*,12*R*,12'*R*)-**2**/**3**, Conf M

C	5.052483	-2.188006	2.220387
C	4.957291	-2.851896	1.010807
C	4.448734	-2.211672	-0.120794
C	4.044998	-0.877765	0.021308
C	4.136047	-0.182324	1.245616
C	4.649044	-0.872401	2.337361
C	3.418427	-0.136583	-1.088339
C	2.306027	0.822973	-0.653805
C	2.637601	1.689304	0.493416
C	3.647288	1.217610	1.361522
C	2.030031	2.931634	0.634502
C	2.492476	3.776635	1.650705
C	3.524108	3.370914	2.472392
C	4.095748	2.110576	2.332964

O	1.271823	0.824661	-1.280188
O	3.675408	-0.229042	-2.266136
O	5.118482	1.751144	3.151862
O	5.343651	-4.150669	0.875775
C	4.322603	-3.013435	-1.390222
C	3.092500	-3.954299	-1.416864
C	1.777536	-3.161505	-1.454738
C	0.941147	3.428528	-0.250657
C	-0.384610	3.041471	-0.113735
C	-1.421858	3.487238	-0.954941
C	-1.048951	4.351072	-1.986982
C	0.269628	4.764542	-2.138313
C	1.259570	4.313942	-1.285426
C	-0.739560	2.006667	0.874978
C	-1.907495	1.109566	0.470435
C	-3.082810	1.828744	-0.037772
C	-2.820668	3.036328	-0.719061
C	-4.385428	1.362049	0.216592
C	-5.443822	2.133720	-0.267510
C	-5.202833	3.335600	-0.912940
C	-3.918070	3.783580	-1.134817
O	-1.985789	4.778339	-2.871984
O	-6.749958	1.795612	-0.083235
C	-4.667217	0.159763	1.090735
C	-4.755369	-1.205552	0.377696
C	-4.803255	-2.369017	1.381379
O	-1.801328	-0.089333	0.614298
O	-0.190662	1.809020	1.932042
C	3.224103	-4.925053	-2.572914
C	3.383083	-6.225089	-2.357074
C	3.185203	-4.362242	-3.965582
C	0.537311	-4.041231	-1.534425
C	-0.804686	-3.318527	-1.378361
C	-1.939105	-4.293271	-1.672130
C	-0.917739	-2.094396	-2.276059
O	-0.924424	-2.914190	0.009355
C	-5.914071	-1.259716	-0.605493
C	-5.545389	-1.204311	-2.057783
C	-7.181847	-1.347954	-0.210435
C	-3.629026	-2.392498	2.363837
C	-3.154826	-3.789507	2.786063
C	-4.274814	-4.617268	3.395257
C	-2.000176	-3.653797	3.775818
O	-2.705934	-4.514781	1.634204
O	2.558621	4.658585	-1.402179
C	2.944733	5.547399	-2.442878
O	1.876387	4.971566	1.760952
C	2.312678	5.879721	2.763855
H	5.440939	-2.708646	3.088028
H	4.731264	-0.387446	3.295044
H	3.902482	4.024258	3.246119
H	5.333968	2.471920	3.754817
H	5.681557	-4.486619	1.713792
H	4.295346	-2.351603	-2.247986
H	5.216763	-3.630324	-1.483488
H	3.103112	-4.546545	-0.499165
H	1.798453	-2.472598	-2.301557
H	1.717164	-2.547792	-0.553295
H	0.509179	5.436455	-2.950476
H	-6.050994	3.921490	-1.242337
H	-3.773423	4.721388	-1.643219
H	-1.578657	5.318484	-3.559042
H	-6.854387	0.831428	-0.022397
H	-5.599548	0.334139	1.632979
H	-3.887670	0.095624	1.845091
H	-3.834517	-1.317202	-0.195273
H	-5.747222	-2.345950	1.928957
H	-4.803069	-3.294406	0.802514
H	3.491050	-6.926958	-3.175782
H	3.411015	-6.632075	-1.353204
H	3.291571	-5.151224	-4.708900
H	2.245259	-3.840220	-4.157029
H	3.985240	-3.636413	-4.124932
H	0.583477	-4.810611	-0.758268
H	0.524251	-4.571209	-2.489605
H	-2.904733	-3.817095	-1.500319
H	-1.870303	-5.168922	-1.025666
H	-1.898792	-4.627853	-2.709421
H	-1.914984	-1.657580	-2.198398
H	-0.186991	-1.330946	-2.009480
H	-0.754109	-2.373345	-3.317556
H	-1.133391	-1.972537	0.071403
H	-4.952092	-0.312679	-2.273999
H	-6.423683	-1.205133	-2.701964
H	-4.922094	-2.063500	-2.318295
H	-7.992009	-1.383151	-0.928630
H	-7.456993	-1.414588	0.835422
H	-2.770782	-1.887291	1.917861
H	-3.876603	-1.827715	3.265586
H	-3.899911	-5.600665	3.682189
H	-5.088073	-4.758381	2.684017
H	-4.674091	-4.128898	4.285168
H	-1.627340	-4.640136	4.054805
H	-1.178241	-3.089441	3.331040
H	-2.316917	-3.135264	4.682355
H	-2.077985	-3.962274	1.133129
H	2.446030	6.512849	-2.340936
H	4.016613	5.681807	-2.335539
H	2.729456	5.121203	-3.424333
H	3.354653	6.165567	2.609215
H	1.679839	6.756398	2.666296
H	2.190080	5.453369	3.761087

CAM-B3LYP Energy = -2840.09583211 a.u.

(*aR*,12*R*,12'*R*)-**2**/**3**, Conf N

C	-5.462343	-0.303215	-2.582252
C	-5.788061	-0.924899	-1.391974
C	-5.163530	-0.562011	-0.193244
C	-4.232706	0.482595	-0.241360
C	-3.930428	1.166303	-1.438427
C	-4.540122	0.726746	-2.606099

C	-3.419970	0.866114	0.931619
C	-1.994356	1.342208	0.598813
C	-1.902748	2.311504	-0.509866
C	-2.960802	2.289592	-1.443524
C	-0.888370	3.257565	-0.542666
C	-0.961297	4.268465	-1.511854
C	-2.029275	4.319738	-2.382344
C	-3.026017	3.350753	-2.341882
O	-1.079810	0.945437	1.280569
O	-3.747572	0.818166	2.093685
O	-4.042592	3.542057	-3.224776
O	-6.707319	-1.925933	-1.337386
C	-5.511063	-1.344943	1.046331
C	-4.875432	-2.755815	1.093688
C	-3.344958	-2.687486	1.180928
C	0.224414	3.296468	0.444458
C	1.431949	2.639545	0.262703
C	2.473048	2.667175	1.210973
C	2.210228	3.322964	2.412310
C	1.017349	4.008455	2.607959
C	0.039979	4.015133	1.634053
C	1.627732	1.754011	-0.897456
C	2.593059	0.575843	-0.678826
C	3.824956	0.884642	0.058248
C	3.766562	2.005002	0.914022
C	5.022125	0.187086	-0.187196
C	6.179234	0.656646	0.445676
C	6.147780	1.807557	1.213566
C	4.962424	2.475347	1.443434
O	3.058293	3.342539	3.474718
O	7.396576	0.070171	0.287826
C	5.123460	-0.963094	-1.161110
C	4.846621	-2.366852	-0.576541
C	4.795534	-3.425504	-1.693787
O	2.295700	-0.489284	-1.175034
O	1.074125	1.848225	-1.965651
C	-5.491062	-3.553929	2.225064
C	-6.254993	-4.610891	1.977043
C	-5.214833	-3.101867	3.631186
C	-2.682947	-4.059792	1.188759
C	-1.165829	-4.062224	0.990323
C	-0.646424	-5.495175	1.080829
C	-0.450437	-3.183934	2.013887
O	-0.932170	-3.554953	-0.328735
C	5.873825	-2.737568	0.483180
C	5.390940	-2.705296	1.902135
C	7.123986	-3.075845	0.176757
C	3.619271	-3.349163	-2.670629
C	2.268621	-3.934980	-2.229488
C	2.360053	-5.413571	-1.890875
C	1.245350	-3.712726	-3.340563
O	1.794782	-3.288570	-1.028946
O	-1.143993	4.649648	1.767362
C	-1.402566	5.373869	2.963830
O	0.042849	5.169557	-1.505365
C	0.015412	6.232302	-2.449691
H	-5.925733	-0.630606	-3.505299
H	-4.274586	1.153013	-3.562993
H	-2.134156	5.113295	-3.106423
H	-4.802309	2.992544	-2.997146
H	-7.075752	-2.091160	-2.212884
H	-5.231891	-0.784558	1.930394
H	-6.594961	-1.466755	1.065829
H	-5.134184	-3.267380	0.164731
H	-3.056128	-2.123178	2.070293
H	-2.972433	-2.128127	0.321420
H	0.877956	4.505772	3.555731
H	7.075018	2.173691	1.633863
H	4.990018	3.389296	2.019368
H	3.735058	2.660364	3.388085
H	7.305547	-0.887512	0.147918
H	6.123201	-0.962627	-1.599753
H	4.430119	-0.788302	-1.978819
H	3.875656	-2.336537	-0.086382
H	5.717095	-3.348169	-2.275985
H	4.824168	-4.412756	-1.231182
H	-6.709464	-5.182824	2.777637
H	-6.452158	-4.940591	0.963793
H	-5.725612	-3.737459	4.353298
H	-4.145760	-3.128406	3.852494
H	-5.543454	-2.073179	3.792448
H	-3.114509	-4.669933	0.389736
H	-2.905418	-4.576427	2.125553
H	0.425597	-5.525339	0.878571
H	-1.151653	-6.129096	0.350581
H	-0.815031	-5.911163	2.075521
H	0.630276	-3.247602	1.873337
H	-0.744360	-2.140619	1.905961
H	-0.678214	-3.505269	3.031880
H	0.027348	-3.523306	-0.505042
H	4.975919	-1.725588	2.150144
H	6.186378	-2.937691	2.608903
H	4.582228	-3.428159	2.036678
H	7.838617	-3.339740	0.946789
H	7.472006	-3.130973	-0.847949
H	3.452459	-2.315215	-2.981379
H	3.901711	-3.883645	-3.580495
H	1.374066	-5.796698	-1.626709
H	3.026039	-5.586580	-1.046739
H	2.729026	-5.979315	-2.746790
H	0.272307	-4.100081	-3.037731
H	1.139245	-2.648321	-3.557685
H	1.548827	-4.218764	-4.258049
H	1.902355	-2.330093	-1.126082
H	-0.671920	6.172053	3.105204
H	-2.391205	5.805308	2.841533
H	-1.399740	4.712054	3.831522
H	-0.862341	6.864558	-2.304649
H	0.913800	6.814145	-2.268125
H	0.029916	5.850089	-3.471779

CAM-B3LYP Energy = -2840.09577193 a.u.

(*aR*,12*R*,12'*R*)-**2**/**3**, Conf O

C	5.585610	0.146864	-2.473490
C	5.871602	0.771469	-1.273596
C	5.180873	0.437417	-0.106799
C	4.204609	-0.564678	-0.199819
C	3.919196	-1.234252	-1.410783
C	4.625694	-0.843683	-2.541517
C	3.358335	-0.929974	0.951619
C	1.930227	-1.351655	0.586398
C	1.829070	-2.313761	-0.527416
C	2.885398	-2.302196	-1.463936
C	0.787967	-3.232356	-0.559729
C	0.822880	-4.230045	-1.540407
C	1.860759	-4.270221	-2.448299
C	2.880199	-3.323803	-2.412673
O	1.011744	-0.916823	1.239770
O	3.666662	-0.914632	2.120978
O	3.898859	-3.414820	-3.307332
O	6.826294	1.738675	-1.181158
C	5.507541	1.206626	1.147790
C	4.911568	2.636962	1.190387
C	3.383683	2.611523	1.256564
C	-0.310073	-3.261173	0.445255
C	-1.520952	-2.600061	0.282902
C	-2.550554	-2.614630	1.244025
C	-2.286085	-3.315087	2.422981
C	-1.088253	-3.996977	2.601582
C	-0.108598	-3.978626	1.628376
C	-1.729142	-1.742325	-0.895330
C	-2.679510	-0.552555	-0.702293
C	-3.889847	-0.817231	0.080990
C	-3.830854	-1.906353	0.982148
C	-5.072585	-0.090640	-0.150741
C	-6.228098	-0.529925	0.499138
C	-6.194061	-1.619176	1.350620
C	-5.013677	-2.290314	1.598998
O	-3.205153	-3.318443	3.423346
O	-7.391247	0.129439	0.245579
C	-5.173751	1.083926	-1.090126
C	-4.721585	2.438893	-0.492585
C	-4.674621	3.521246	-1.588608
O	-2.386663	0.485223	-1.257735
O	-1.195231	-1.876685	-1.969911
C	5.589129	3.390515	2.321830
C	5.141502	3.384935	3.570547
C	6.846051	4.117148	1.939394
C	2.745983	3.994336	1.181710
C	1.237653	4.009778	0.925670
C	0.733782	5.450643	0.959619
C	0.472533	3.167588	1.943907
O	1.046483	3.470727	-0.388130
C	-5.601898	2.884466	0.658230
C	-6.984150	3.380688	0.340415
C	-5.148961	2.855349	1.906180
C	-3.586816	3.382515	-2.658071
C	-2.175390	3.890826	-2.324111
C	-2.154290	5.377716	-2.010510
C	-1.247404	3.588548	-3.498073
O	-1.659932	3.235750	-1.146768
O	1.080467	-4.606430	1.753193
C	1.353006	-5.333467	2.944535
O	-0.190942	-5.119888	-1.523706
C	-0.204529	-6.164285	-2.488162
H	6.120899	0.436894	-3.370190
H	4.431201	-1.313237	-3.490488
H	1.902012	-5.043345	-3.202674
H	3.780579	-4.187838	-3.871165
H	7.245314	1.876050	-2.038384
H	5.176686	0.666304	2.026866
H	6.593497	1.287001	1.208946
H	5.192532	3.137432	0.259802
H	3.063507	2.094969	2.163806
H	3.014313	2.019751	0.417312
H	-0.933080	-4.532986	3.527405
H	-7.108007	-1.952902	1.828460
H	-5.025640	-3.125073	2.278180
H	-2.862134	-3.787493	4.192666
H	-8.115751	-0.272012	0.738369
H	-6.207149	1.171330	-1.421632
H	-4.570505	0.885351	-1.972725
H	-3.719929	2.306121	-0.091790
H	-5.641687	3.530363	-2.098043
H	-4.586867	4.497168	-1.107162
H	5.674827	3.901354	4.359728
H	4.230378	2.873520	3.854471
H	7.344275	4.548957	2.806823
H	7.547473	3.449083	1.433875
H	6.619386	4.921801	1.234901
H	3.213814	4.561630	0.371183
H	2.943757	4.544823	2.103088
H	-0.328474	5.488677	0.712831
H	1.276697	6.060192	0.235571
H	0.867367	5.889296	1.949910
H	-0.601084	3.239375	1.759971
H	0.757577	2.118395	1.875747
H	0.665045	3.514301	2.960926
H	0.093547	3.445729	-0.599232
H	-6.946096	4.304797	-0.239958
H	-7.544581	3.580172	1.253217
H	-7.540161	2.649413	-0.246658
H	-5.764484	3.170900	2.740696
H	-4.146472	2.514354	2.136474
H	-3.502431	2.341066	-2.975858
H	-3.907885	3.933560	-3.545143
H	-1.131807	5.704032	-1.818876
H	-2.751336	5.605032	-1.128593
H	-2.544676	5.950669	-2.852044
H	-0.234650	3.924182	-3.273204
H	-1.218186	2.515738	-3.697288
H	-1.585525	4.093877	-4.403877
H	-1.828041	2.284082	-1.222028

H	0.637912	-6.146576	3.081283
H	2.349096	-5.746319	2.818593
H	1.339936	-4.677637	3.816768
H	0.673396	-6.805035	-2.387109
H	-1.099546	-6.744295	-2.285331
H	-0.254579	-5.762921	-3.501837

CAM-B3LYP Energy = -2840.09576564 a.u.

(*aR*,12*R*,12'*R*)-**2**/**3**, Conf P

C	5.449667	0.555215	-2.755937
C	5.767357	1.184376	-1.564550
C	5.195265	0.772212	-0.360778
C	4.296392	-0.306262	-0.409781
C	3.975348	-0.969916	-1.611115
C	4.569535	-0.504737	-2.780958
C	3.569119	-0.762196	0.789079
C	2.147178	-1.267886	0.518954
C	2.021128	-2.197568	-0.619230
C	3.013254	-2.103819	-1.619544
C	1.029387	-3.169288	-0.615768
C	1.059521	-4.142319	-1.621339
C	2.043113	-4.106457	-2.587699
C	3.008350	-3.103727	-2.590185
O	1.259410	-0.917370	1.259487
O	3.967466	-0.755932	1.931139
O	3.974412	-3.116600	-3.545338
O	6.643234	2.224152	-1.646350
C	5.532094	1.534917	0.897242
C	4.797370	2.892749	1.033407
C	3.286749	2.689092	1.213164
C	-0.008503	-3.269637	0.446936
C	-1.262370	-2.678402	0.357317
C	-2.230988	-2.748934	1.382028
C	-1.849329	-3.425444	2.543326
C	-0.608138	-4.043519	2.644867
C	0.304889	-3.976422	1.612649
C	-1.580953	-1.839458	-0.811892
C	-2.624296	-0.743033	-0.588051
C	-3.778003	-1.119161	0.233921
C	-3.572667	-2.134100	1.193844
C	-5.033713	-0.520073	0.022282
C	-6.082290	-0.914402	0.851332
C	-5.907651	-1.934844	1.768678
C	-4.680217	-2.542758	1.932168
O	-2.694325	-3.474261	3.605283
O	-7.332936	-0.372694	0.748817
C	-5.300139	0.421661	-1.125615
C	-5.056573	1.921441	-0.827749
C	-4.638049	2.644398	-2.115100
O	-2.443819	0.332923	-1.119741
O	-1.074967	-1.930249	-1.904941
C	5.420846	3.702260	2.152352
C	6.056658	4.839203	1.897385
C	5.302039	3.166721	3.550954
C	2.516500	3.993853	1.371169
C	0.993775	3.879232	1.269773
C	0.368398	5.242000	1.556875
C	0.427285	2.835478	2.229219
O	0.711452	3.496504	-0.081651
C	-6.268249	2.547546	-0.162965
C	-7.436073	2.920902	-1.033637
C	-6.300243	2.741083	1.152751
C	-4.072651	4.051528	-1.897999
C	-2.541787	4.146560	-1.803140
C	-2.148089	5.551559	-1.379397
C	-1.863883	3.788383	-3.121921
O	-2.043284	3.273137	-0.764886
O	1.530703	-4.539243	1.659877
C	1.913757	-5.257779	2.826022
O	0.096455	-5.085031	-1.568573
C	0.076207	-6.102399	-2.561565
H	5.903710	0.914391	-3.670206
H	4.343352	-0.971898	-3.724254
H	2.081938	-4.860323	-3.361458
H	3.865340	-3.881951	-4.121450
H	6.873151	2.554781	-0.771125
H	5.323457	0.922536	1.765916
H	6.612001	1.714792	0.925642
H	4.939810	3.462202	0.110464
H	3.110428	2.043286	2.075673
H	2.903143	2.158669	0.340219
H	-0.367615	-4.566720	3.559744
H	-6.756655	-2.248614	2.361893
H	-4.586237	-3.332338	2.656599
H	-2.276201	-3.927966	4.346185
H	-7.259908	0.582145	0.598636
H	-6.327631	0.271946	-1.461943
H	-4.666609	0.133985	-1.961031
H	-4.231223	1.983883	-0.120621
H	-3.899267	2.021677	-2.620811
H	-5.490141	2.686800	-2.795261
H	6.514694	5.421954	2.687834
H	6.138641	5.228670	0.889385
H	5.785241	3.832031	4.265029
H	4.256450	3.054227	3.845248
H	5.762263	2.180769	3.642480
H	2.838399	4.700036	0.600310
H	2.760739	4.453400	2.331687
H	-0.714086	5.200399	1.428019
H	0.766318	5.995334	0.875450
H	0.575683	5.557518	2.580688
H	-0.662629	2.821684	2.166344
H	0.792518	1.838872	1.984431
H	0.702052	3.062810	3.261054
H	-0.252478	3.442739	-0.219983
H	-7.191842	3.783432	-1.656917
H	-8.307168	3.177339	-0.432578
H	-7.713069	2.112355	-1.713526
H	-7.171288	3.158607	1.643956
H	-5.450452	2.498256	1.779531
H	-4.381064	4.704253	-2.717182

H	-4.496518	4.481295	-0.986630
H	-1.064320	5.641773	-1.309608
H	-2.579646	5.791423	-0.407240
H	-2.508839	6.280213	-2.105591
H	-0.782710	3.886242	-3.020768
H	-2.081324	2.763422	-3.423899
H	-2.197894	4.453556	-3.919166
H	-2.212902	2.348760	-1.000712
H	1.249329	-6.105727	3.000809
H	2.918817	-5.620239	2.633910
H	1.924103	-4.607490	3.702359
H	-0.056994	-5.676611	-3.557630
H	0.990381	-6.698089	-2.533203
H	-0.773641	-6.734143	-2.322367

CAM-B3LYP Energy = -2840.09557315 a.u.

(*aR*,12*R*,12'*R*)-**2**/**3**, Conf Q

C	-6.445785	2.576325	-2.159530
C	-7.102996	1.502026	-1.586506
C	-6.532333	0.797537	-0.524916
C	-5.275078	1.220054	-0.076439
C	-4.580331	2.303059	-0.656350
C	-5.202592	2.971291	-1.703856
C	-4.545726	0.479942	0.970755
C	-3.042884	0.394660	0.711752
C	-2.403510	1.694584	0.440198
C	-3.218389	2.667161	-0.177594
C	-1.097395	1.926852	0.847000
C	-0.575268	3.212478	0.653618
C	-1.352719	4.196472	0.076172
C	-2.656759	3.934310	-0.329646
O	-2.493260	-0.684015	0.736303
O	-5.007110	-0.049680	1.954094
O	-3.401038	4.934830	-0.867277
O	-8.315030	1.079394	-2.039973
C	-7.259291	-0.413143	0.003215
C	-6.983381	-1.698992	-0.818615
C	-5.507293	-2.104591	-0.718354
C	-0.274524	0.919971	1.571267
C	0.874616	0.346101	1.041920
C	1.706275	-0.538177	1.755479
C	1.340736	-0.797830	3.078754
C	0.191779	-0.242991	3.628781
C	-0.612550	0.603571	2.892232
C	1.311506	0.701594	-0.321496
C	2.824354	0.660753	-0.573881
C	3.527167	-0.492178	0.008236
C	2.902924	-1.133504	1.102988
C	4.699643	-0.998961	-0.586589
C	5.196432	-2.215140	-0.108615
C	4.558669	-2.873440	0.927381
C	3.441445	-2.338410	1.537479
O	2.127964	-1.587060	3.853989
O	6.273085	-2.808778	-0.711461
C	5.413788	-0.318039	-1.725149
C	6.320522	0.845000	-1.280049
C	7.460068	0.395551	-0.343651
O	3.301510	1.528949	-1.269653
O	0.582002	1.030292	-1.225721
C	-7.926584	-2.802241	-0.386706
C	-8.849754	-3.271762	-1.216899
C	-7.785737	-3.334307	1.011317
C	-5.129413	-3.373407	-1.467743
C	-3.614852	-3.646155	-1.516206
C	-2.894102	-2.676147	-2.448057
C	-3.369569	-5.077554	-1.964988
O	-3.048301	-3.557254	-0.197566
C	6.845674	1.672646	-2.435699
C	7.503894	2.967902	-2.046803
C	6.745943	1.317996	-3.711162
C	8.579420	-0.385671	-1.027580
C	9.459898	-1.210656	-0.089075
C	10.100265	-0.368916	1.005552
C	10.518943	-1.959037	-0.886236
O	8.569633	-2.177515	0.527480
O	-1.736302	1.172883	3.378931
C	-2.138931	0.875318	4.710394
O	0.694863	3.412268	1.065637
C	1.282895	4.695775	0.892808
H	-6.905569	3.107256	-2.985091
H	-4.715484	3.804681	-2.180681
H	-0.962002	5.195011	-0.061395
H	-2.894176	5.754568	-0.892554
H	-8.609001	1.632608	-2.772606
H	-6.998377	-0.580717	1.042271
H	-8.328752	-0.210172	-0.037144
H	-7.203696	-1.478031	-1.865966
H	-5.237699	-2.219180	0.332510
H	-4.914640	-1.274815	-1.106846
H	-0.051203	-0.477211	4.655677
H	4.952511	-3.827425	1.254088
H	2.985083	-2.873365	2.352200
H	1.768056	-1.644007	4.746700
H	7.108969	-2.628814	-0.221394
H	4.682366	0.077256	-2.426476
H	6.000153	-1.070470	-2.247845
H	5.693117	1.519498	-0.692315
H	7.875842	1.277265	0.145671
H	7.024724	-0.207200	0.454233
H	-9.537249	-4.054075	-0.917263
H	-8.950287	-2.888468	-2.225470
H	-8.513206	-4.121538	1.204286
H	-6.788053	-3.744728	1.181063
H	-7.932680	-2.547873	1.754351
H	-5.504020	-3.326765	-2.494318
H	-5.615637	-4.231768	-0.998208
H	-1.827238	-2.901115	-2.465721
H	-3.013034	-1.640960	-2.126097
H	-3.280725	-2.758632	-3.464642
H	-2.299866	-5.279307	-2.030111
H	-3.811368	-5.776840	-1.254157

H	-3.815810	-5.254775	-2.944226
H	-2.986422	-2.630021	0.072122
H	6.842545	3.564061	-1.413305
H	7.764193	3.557438	-2.924899
H	8.418116	2.796019	-1.474394
H	7.135656	1.954562	-4.496634
H	6.279613	0.394312	-4.025350
H	8.160444	-1.071649	-1.766103
H	9.229074	0.296301	-1.579499
H	10.726503	-0.990570	1.648534
H	9.343202	0.108784	1.625419
H	10.731807	0.406373	0.569887
H	11.112656	-2.601500	-0.232805
H	10.053205	-2.579698	-1.652273
H	11.197773	-1.258391	-1.373479
H	9.074968	-2.776205	1.088809
H	-2.327770	-0.192360	4.833230
H	-1.388099	1.205046	5.430334
H	-3.060236	1.426309	4.871360
H	1.324329	4.969730	-0.162685
H	0.736634	5.456698	1.452809
H	2.291952	4.614268	1.284680

CAM-B3LYP Energy = -2840.09491065 a.u.

(*aR*,12*R*,12'*R*)-**2**/**3**, Conf R

C	5.050516	-2.183646	2.231063
C	4.956869	-2.852595	1.022622
C	4.450884	-2.216117	-0.110881
C	4.047031	-0.878454	0.026874
C	4.136358	-0.181478	1.247466
C	4.647358	-0.870851	2.344041
C	3.423387	-0.139541	-1.085714
C	2.313262	0.825737	-0.657315
C	2.641027	1.691071	0.491310
C	3.649331	1.219270	1.360998
C	2.032282	2.932537	0.632344
C	2.493085	3.777485	1.649752
C	3.524668	3.372483	2.471622
C	4.097347	2.112373	2.332311
O	1.283071	0.830409	-1.290082
O	3.679484	-0.240475	-2.263263
O	5.120732	1.754150	3.150547
O	5.364361	-4.151874	1.019230
C	4.309986	-3.011175	-1.385009
C	3.084252	-3.960042	-1.407780
C	1.771454	-3.164541	-1.454015
C	0.943408	3.428858	-0.253113
C	-0.382287	3.041521	-0.116084
C	-1.419657	3.487470	-0.957120
C	-1.046838	4.351150	-1.989310
C	0.271722	4.764761	-2.140722
C	1.261690	4.314443	-1.287769
C	-0.736992	2.006662	0.872590
C	-1.905898	1.110430	0.468715
C	-3.081104	1.830183	-0.038718
C	-2.818623	3.037355	-0.720574
C	-4.383809	1.364199	0.216471
C	-5.442048	2.136249	-0.267368
C	-5.200728	3.337779	-0.913371
C	-3.915853	3.785010	-1.136087
O	-1.983739	4.778154	-2.874331
O	-6.748253	1.798948	-0.082408
C	-4.665683	0.162456	1.091335
C	-4.755387	-1.203105	0.378965
C	-4.803044	-2.366098	1.383206
O	-1.800021	-0.088632	0.611673
O	-0.186958	1.808043	1.928874
C	3.221863	-4.940161	-2.555153
C	3.376216	-6.238239	-2.325549
C	3.193750	-4.387161	-3.951644
C	0.530769	-4.043220	-1.534351
C	-0.809214	-3.316142	-1.381344
C	-1.945848	-4.288156	-1.675434
C	-0.917176	-2.093021	-2.281087
O	-0.927882	-2.909936	0.005474
C	-5.914956	-1.256957	-0.603213
C	-5.547541	-1.200947	-2.055816
C	-7.182390	-1.345234	-0.207080
C	-3.627891	-2.390006	2.364599
C	-3.153510	-3.787240	2.785891
C	-4.272933	-4.614932	3.396205
C	-1.997550	-3.652159	3.774166
O	-2.706238	-4.512277	1.633186
O	2.560690	4.659377	-1.404284
C	2.946592	5.549091	-2.444330
O	1.875579	4.971461	1.759956
C	2.309808	5.879783	2.763725
H	5.438449	-2.715050	3.090200
H	4.726635	-0.382377	3.300191
H	3.902250	4.025905	3.245652
H	5.334361	2.474118	3.755146
H	5.337103	-4.524301	0.131034
H	4.264763	-2.341138	-2.235277
H	5.217157	-3.605208	-1.537297
H	3.077958	-4.547276	-0.485068
H	1.798351	-2.480811	-2.304664
H	1.709276	-2.546496	-0.555827
H	0.511181	5.436676	-2.952914
H	-6.048755	3.924003	-1.242521
H	-3.771007	4.722573	-1.644890
H	-1.576886	5.318830	-3.561139
H	-6.853191	0.834902	-0.020385
H	-5.597437	0.337689	1.634293
H	-3.885573	0.098087	1.845097
H	-3.835125	-1.315527	-0.194787
H	-5.746458	-2.342163	1.931693
H	-4.804036	-3.291738	0.804751
H	3.489114	-6.947575	-3.136862
H	3.392286	-6.637451	-1.318170
H	3.995658	-3.663525	-4.111641
H	3.304450	-5.182023	-4.687784

H	2.255524	-3.866039	-4.153343
H	0.573988	-4.810715	-0.756308
H	0.518411	-4.574707	-2.488606
H	-2.910242	-3.808854	-1.505577
H	-1.880567	-5.163064	-1.027639
H	-1.905155	-4.624167	-2.712242
H	-1.913258	-1.653287	-2.205496
H	-0.184903	-1.330979	-2.014489
H	-0.752937	-2.373918	-3.321952
H	-1.139444	-1.968753	0.066796
H	-4.954535	-0.309165	-2.272217
H	-6.426397	-1.201595	-2.699230
H	-4.924382	-2.059945	-2.317268
H	-7.993179	-1.380095	-0.924584
H	-7.456625	-1.412198	0.838992
H	-2.769941	-1.884742	1.918088
H	-3.874513	-1.825522	3.266788
H	-3.897880	-5.598496	3.682374
H	-5.087131	-4.755642	2.685960
H	-4.670953	-4.126747	4.286771
H	-1.624681	-4.638681	4.052445
H	-1.175948	-3.087972	3.328556
H	-2.312991	-3.133770	4.681236
H	-2.078877	-3.959620	1.131632
H	2.447282	6.514170	-2.341883
H	4.018363	5.684045	-2.336606
H	2.731810	5.123384	-3.426106
H	1.675741	6.755550	2.666098
H	2.187091	5.452566	3.760559
H	3.351461	6.167210	2.609914

CAM-B3LYP Energy = -2840.09488810 a.u.

(i) Mosmann, T. *J. Immunol. Methods* **1983**, *65*, 55–63.