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Towards Theory Driven Structure Elucidation of Complex Natural Products: Mandelalides and Coibamide A

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Table of Contents

Table S1 ^{1}H and ^{13}C data for Mandelalides A-D acquired in $CDCl_3$ (700 MHz, 298K) 3

Table S2 ^{1}H and ^{13}C data for Natural Product Coibamide A acquired in $CDCl_3$ (600 MHz, 298K) 5

Computational Methods - General Information 7

References for Computational Methods 7

Empirical Scaling 8

Conformational Averaging 8

Mandelalide A 9

Mandelalide B 10

Mandelalide C 11

Mandelalide D 11

Coibamide A 11

Computed Coordinates, Energies and NMR Data 12

Mandelalide A Revised Configuration (DFT Methodologies) 12

Mandelalide A Original Configuration (DFT Methodologies) 25

Mandelalide A Revised Configuration (MM Methodologies) 61

Mandelalide A Original Configuration (MM Methoudaligies) 75

Mandelalide A Revised Configuration (MD Methodologies) 90

Mandelalide A Original Configuration (MD Methodologies) 128

Mandelalide B Revised Configuration 166

Mandelalide B Original Configuration 178

Mandelalide C Revised Configuration 182

Mandelalide C Original Configuration 200

Mandelalide D Revised Configuration 203

Mandelalide D Original Configuration 208

Coibamide A - [D-N,O-diMe-Ser] Revised Configuration 211

Coibamide A - [D-Hiv], [D-MeAla] Revision 232

Coibamide A - Original Configuration 296

Comparison of Computational and Experimental NMR Data 311

Revised Mandelalide A (DFT Methodologies) 311

Original Mandelalide A (DFT Methodologies) 313

Revised Mandelalide A (MM Methodologies) 314

Original Mandelalide A (MM Methodologies) 316

Revised Mandelalide A (MD Methodologies) 317

Original Mandelalide A (MD Methodologies) 318

Revised Mandelalide B 320

Original Mandelalide B 322

Revised Mandelalide C 323

Original Mandelalide C 325

Revised Mandelalide D 326

Original Mandelalide D 327

Proposed Revised [D-N,O-diMe-Ser] Coibamide A 329

Coibamide A [D-HIV], [D-MeAla] Revision 332

Coibamide A- Original Configuration 335

Table S1 ^{1}H and ^{13}C data for Mandelalides A-D acquired in $CDCl_3$ (700 MHz, 298K)

	Mandelalide A		Mandelalide B		Mandelalide C		Mandelalide D	
No.	δ_C (mult)	δ_H (*J* in Hz)	δ_C (mult)	δ_H (J in Hz)	δ_C (mult)	δ_H (J in Hz)	δ_C (mult)	δ_H (J in Hz)
1	167.4 (s)		175.6 (s)	-	174.7 (s)	-	172.9 (s)	-
2	123.1 (d)	6.01 (dd, 15., 1.2)	79.3 (s)	-	82.0 (s)	-	81.3 (s)	-
3	147.1 (d)	6.97 (ddd, 15.2, 10.4, 4.6)	69.5 (d)	5.48 (dd, 6.0, 1.7)	68.3 (d)	5.51 (dd, 6.6, 0.9)	68.6 (d)	5.56 (dd, 6.6, 0.7)
4a	38.8 (t)	2.36 (m)	36.3 (t)	1.59 (m)	36.4 (t)	1.65 (m)	36.2 (t)	1.68 (m)
4b		2.39 (ddd, 14.1, 10.6, 10.6)		2.14 (ddd, 15.0, 11.7, 1.5)		2.14 (ddd, 15.6, 11.7, 1.0)		2.18 (ddd, 15.4, 11.5, 0.9)
5	73.9 (d)	3.36 (dddd, 11.4, 11.4, 2.3, 2.3)	72.7 (d)	3.30 (dddd, 11.4, 11.4, 1.5, 1.5)	72.3 (d)	3.25 (dddd, 11.4, 11.4, 1.8, 1.8)	72.2 (d)	3.21 (dddd, 11.2, 11.2, 1.3, 1.3)
6ax	37.6 (t)	1.20 (m)	37.4 (t)	1.10 (ddd, 11.7, 11.7, 11.7)	41.2 (t)	1.11 (ddd, 12.5, 11.4, 11.4)	41.2 (t)	1.12 (ddd, 11.3, 11.3, 11.3)
6eq		2.02 (dddd, 12.6, 4.4, 2.3, 1.6)[a]		1.89 (m)		1.86 (m)		1.85 (dddd, 12.2, 4.6, 1.5, 1.5)
7	73.1 (d)	3.82 (dddd, 11.1, 10.5, 4.4, 4.4)[a]	73.3 (d)	3.75 (m)	68.3 (d)	3.76 (dddd, 10.9, 10.9, 4.6, 4.1)	68.4 (d)	3.75 (m)
8ax	39.7 (t)	1.22 (m)	39.6 (t)	1.23 (m)	41.8 (t)	1.13 (ddd, 12.5, 11.2, 11.2)	41.8 (t)	1.12 (ddd, 11.3, 11.3, 11.3)
8eq		1.87 (m)		1.81 (dddd, 12.4, 4.8, 1.8, 1.8)		1.83 (m)		1.83 (dddd, 12.2, 4.6, 1.5, 1.5)
9	72.5 (d)	3.32 (dddd, 11.2, 11.2. 2.2, 2.2)[a]	72.4 (d)	3.39 (dddd, 11.0, 11.0, 2.2, 2.2)	72.3 (d)	3.37 (dddd, 10.9, 10.9, 2.1, 2.1)	72.2 (d)	3.36 (dddd, 11.0, 11.0, 2.2, 2.2)
10a	43.1 (t)	1.21 (ddd, 15.2, 9.6, 2.2)[a]	42.2 (t)	1.18 (ddd, 14.1, 12.3, 2.8)	42.1 (t)	1.19 (ddd, 14.2, 12.1, 2.8)	42.1 (t)	1.19 (ddd, 13.9, 11.5, 2.8)
10b		1.51 (ddd, 15.2, 11.2, 3.7)[a]		1.57 (m)		1.57 (m)		1.57 (ddd, 14.0, 11.5, 4.0)
11	34.2 (d)	2.37 (dqd, 9.6, 6.5, 3.7)[a]	33.9 (d)	2.50 (m)	34.0 (t)	2.49 (m)	34.2 (d)	2.48 (m)
12	141.5 (d)	5.45 (dd, 14.8, 9.7)	142.1 (d)	5.50 (dd, 15.1, 9.8)	142.2 (d)	5.50 (dd, 14.6, 9.6)	142.3 (d)	5.50 (dd, 14.8, 9.7)
13	123.9 (d)	6.28 (dd, 14.8, 11.0)	123.3 (d)	6.40 (dd, 14.7, 11.3)	123.2 (d)	6.39 (dd, 14.6, 11.4)	123.1 (d)	6.38 (dd, 15.0, 11.3)
14	131.3 (d)	6.05 (dd, 10.9, 10.9)	131.0 (d)	6.10 (dd, 11.1, 11.1)	131.1 (d)	6.10 (dd, 11.0, 11.0)	131.1 (d)	6.10 (dd, 11.0, 11.0)
15	126.9 (d)	5.28 (ddd, 10.8, 10.8, 5.6)	127.1 (d)	5.28 (ddd, 11.1, 11.1, 5.2)	127.1 (d)	5.28 (ddd, 11.0, 11.0, 5.4)	127.1 (d)	5.28 (ddd, 11.3, 11.3, 5.4)
16a	31.1 (t)	1.88 (m)	30.7 (t)	1.90 (m)	30.7 (t)	1.90 (ddd, 13.6, 5.2, 1.1)	30.6 (t)	1.90 (ddd, 13.6, 5.3, 1.0)
16b		2.28 (ddd, 13.1, 11.4, 11.4)		2.31 (ddd, 13.6, 11.6, 11.5,)		2.30 (ddd, 13.8, 11.9, 11.9)		2.29 (ddd, 13.1, 11.3, 11.3)
17	81.0 (d)	3.98 (ddd, 11.1, 8.1, 1.8)	81.5 (d)	3.95 (ddd, 11.6, 7.46, 1.6)	81.6 (d)	3.95 (ddd, 11.5, 7.5, 1.1)	81.6 (d)	3.94 (ddd, 12.0, 7.5, 1.1)
18	37.3 (d)	2.52 (dddq, 12.0, 7.0, 7.0, 7.0)[a]	38.3 (d)	2.52 (m)	38.3 (d)	2.53 (m)	38.3 (d)	2.54 (dddq, 12.3, 7.5, 7.02, 6.8)
19a	36.8 (t)	1.17 (ddd, 11.9, 11.9, 10.3)	35.6 (t)	1.33 (ddd, 12.2, 12.2, 8.2)	35.7 (t)	1.33 (ddd, 12.2, 12.2, 9.1)	35.7 (t)	1.34 (ddd, 12.3, 12.3, 9.2)
19b		2.01 (ddd, 12.2, 7.0, 5.6)[a]		2.05 (ddd, 12.8, 6.9, 6.9)		2.10 (ddd, 12.5, 7.0, 6.8)		2.08 (ddd, 12.2, 7.02, 7.02)

20	83.2 (d)	3.63 (m)	82.1 (t)	3.77 (m)	82.4 (d)	3.82 (ddd, 9.2, 9.2, 7.0)	82.2 (d)	3.79 (ddd, 9.3, 9.3, 7.0)
21	73.0 (d)	3.42 (ddd, 11.1, 8.8, 1.8)	74.5 (d)	3.76 (m)	74.4 (d)	3.73 (ddd, 10.8, 9.5, 1.2)	74.3 (d)	3.73 (ddd, 10.0, 10.0, 1.6)
22a	34.1 (t)	1.46 (ddd, 14.1, 11.1, 1.9)	37.9 (t)	1.51 (m)	32.1 (t)	1.59 (m)	32.5 (t)	1.47 (ddd, 14.2, 10.5, 1.0)
22b		1.76 (ddd, 13.9, 11.7, 1.8)		1.64 (m)		1.82 (ddd, 14.4, 11.0, 1.0)		1.65 (m)
23	72.3 (d)	5.23 (dddd, 11.7, 4.9, 2.9, 1.9)	74.9 (d)	4.84 (dddd, 10.4, 10.4, 4.9, 1.0)	78.9 (d)	5.01 (ddd, 11.2, 2.0, 2.0)	76.7 (d)	5.13 (ddd, 10.8, 3.3, 0.8)
24a	66.1 (t)	3.61 (m)	39.7 (t)	1.93 (dd, 12.7, 10.7)	72.2 (d)	3.98 (d, 2.8)	74.0 (d)	5.17 (d, 3.3)
24b		3.81 (dd, 12.2, 2.9)[a]		2.39 (dd, 12.8, 4.9)	-	-	-	-
25	18.3 (q)	0.85 (d, 6.6)	18.5 (q)	1.07 (d, 6.6)	18.4 (q)	1.06 (d, 6.2)	18.3 (q)	1.07 (d, 6.6)
26	14.5 (q)	1.03 (d, 6.9)	14.2 (q)	1.03 (d, 6.9)	14.2 (q)	1.03 (d, 6.9)	14.3 (q)	1.04 (d, 6.8)
	94.2 (d)	5.02 (d, 1.1)	OH-21	2.70 (br s)	OH	2.80 (br s)	OH	2.71 (br s)
	80.8 (d)	3.40 (dd, 3.8, 1.4)	OH-2	2.87 (s)	-	-	OH	2.78 (br s)
1′	71.7 (d)	3.68 (m)	94.8 (d)	5.04 (s)	173.4 (s)	-	173.6 (s)	-
2′a	74.3 (d)	3.34 (dd, 9.4, 9.4)	80.9 (d)	3.33 (ddd, 3.0, 1.5. 1.3)	36.3 (t)	2.34 (td, 7.5, 1.2)	36.3 (t)	2.40 (dt, 15.5, 7.3)
2′b	68.1 (d)	3.62 (m)	-	-	-	-		2.43 (dt, 15.5, 7.3)
3′	17.7 (q)	1.27 (d, 6.3)	66.6 (d)	3.74 (m)	18.7 (t)	1.65 (m)	18.6 (t)	1.70 (m)
4′	59.1 (q)	3.45 (s)	73.3 (d)	3.49 (ddt, 11.8, 3.3, 1.2, 1.2)	13.9 (q)	0.94 (t, 7.5)	13.9 (q)	0.96 (t, 7.4)
5′	OH-3′	2.24 (s)	67.4 (d)	3.85(br q, 6.6)	-	-	-	-
6′	OH-4′	1.54 (s)	16.6 (q)	1.23 (d, 6.5)	-	-	-	-
7′			59.6 (q)	3.45 (s)	-	-	-	-
			OH-3′	2.86 (d, 11.6)	-	-	-	-
			OH-4′	2.74 (d, 11.6)	-	-	-	-
1″			173.6 (s)	-	-	-	173.1 (s)	-
2″a			36.3 (t)	2.35 (t, 7.5)	-	-	36.0 (t)	2.31 (dt, 12.8, 7.5)
2″b			-	-	-	-		2.33 (dt, 12.8, 7.5)
3″			18.8 (t)	1.67 (tq, 7.4, 7.4)	-	-	18.6 (t)	1.63 (m)
4″			14.0 (q)	0.95 (t, 7.4)	-	-	13.8 (q)	0.93 (t, 7.3)

Table S2 ^{1}H and ^{13}C data for Natural Product Coibamide A acquired in $CDCl_3$ (600 MHz, 298K)

Unit	Atom #	Natural Product Coibamide A		Su Synthetic Coibamide A	
		δ_H	δ_C	δ_H	δ_C
N-Me-Alanine	1	-	170.4[b] C	-	170.4 C
	2	5.32 (m, ob)	51.1 CH	5.33 (m, ob)	51.1 CH
	3	1.11 (d, 7.2)	12.9 CH_3	1.12 (d, 7.2)	12.9 CH_3
	4	2.35 (s)	30.1 CH_3	2.35 (s)	30.3 CH_3
	*N	-	δ_N 115.1	-	-
O-Me-Tyrosine	5	-	171.4[a] C	-	172.2 C
	6	5.11 (m)	50.0 CH	5.12 (m)	50.4 CH
	7	2.99 (m)	38.9 CH_2	2.99 (m)	39.0 CH_2
		2.85 (ob)		2.86 (ob)	
	8	-	128.4 C	-	128.4 C
	9,13	7.09 (d, 8.3)	130.4 CH	7.09 (d, 8.3)	130.4 CH
	10,12	6.77 (d, 8.3)	113.7 CH	6.78 (d, 8.3)	113.7 CH
	11	-	158.6 C	-	158.6 C
	14	3.77 (s)	55.3 CH_3	3.77 (s)	55.4 CH_3
	NH	6.66 (br s)	δ_N 118.2	6.74 (br s)	-
N-Me-Leucine	15	-	171.2[a] C	-	
	16	3.62 (m, ob)	63.6 CH	3.63 (m, ob)	63.6 CH
	17	1.50 (m)	36.1 CH_2	1.49 (m)	
	18	1.60 (m)	24.9 CH	1.56	25.0 CH
	19	0.89 (d, 6.5)	21.4 CH_3	0.89	21.4 CH_3
	20	0.94 (d, 6.5)	23.2 CH_3	0.94	23.2 CH_3
	21	3.15 (s)	39.4 CH_3	3.15 (s)	39.4 CH_3
	N	-	δ_N 105.6	-	-
Alanine	22	-	171.5[a] C	-	171.5 C
	23	4.73 (br m)	47.0 CH	4.74 (br m)	47.4 CH
	24	1.28 (d, 6.5)	18.6 CH_3	1.28 (d, 6.5)	18.6 CH_3
	NH	6.63 (br s)	δ_N 122.4	6.63 (br s)	-
N-Me-Isoleucine	25	-	167.2 C		
	26	3.75 (m, ob)	64.8 CH	3.72 (m, ob)	64.7 CH
	27	2.05 (m)	32.0 CH	2.05 (m)	32.0 CH
	28	1.35 (m)	24.2 CH_2	1.35 (m)	24.3 CH_2
		1.11 (ob)		1.11 (ob)	

	29	0.93 (t, ob)	11.6 CH_3	0.95 (t, ob)	11.8 CH_3
	30	0.83 (d, 6.3)	15.7 CH_3	0.83 (d, 6.3)	15.9 CH_3
	31	2.75 (s)	28.9 CH_3	2.75 (s)	29.0 CH_3
	N	-	δ_N 120.5	-	-
N,*O*-diMe-Serine	32	-	168.7 C	-	168.7 C
	33	5.69 (m)	52.8 CH	5.70 (m)	52.9 CH
	34	3.83 (m)	68.6 CH_2	3.84 (m)	68.6 CH_2
		3.53 (m)		3.52 (m)	
	35	3.30 (s)	58.8 CH_3	3.31 (s)	58.8 CH_3
	36	2.85 (s)	30.0 CH_3	2.86 (s)	30.0 CH_3
	N	-	δ_N 113.4	-	-
N-Me-Threonine	37	-	169.7 C	-	
	38	6.35 (br s)	not observed	6.35 (br s)	not observed
	39	5.50 (br s)	68.0 CH	5.50 (br s)	68.0 CH
	40	1.07 (ob)	18.4 CH_3	1.06 (ob)	18.3 CH_3
	41	2.89 (br s, ob)	29.7 CH_3	2.89 (br s, ob)	
	N	-	δ_N 119.4	-	-
N-Me-Leucine	42	-	170.5[b] C	-	
	43	5.34 (m)	51.1 CH	5.34 (m)	51.1 CH
	44	1.68 (m)	37.9 CH_2	1.68 (m)	37.9 CH_2
		1.31 (m)		1.31 (m)	
	45	1.36 (m)	25.3 CH	1.36 (m)	25.3 CH
	46	0.89 (d, 6.5)	23.1 CH_3	0.90 (d, 6.5)	23.3 CH_3
	47	0.92 (d, 6.6)	21.2 CH_3	0.92 (d, 6.6)	21.2 CH_3
	48	3.13 (s)	31.2 CH_3	3.12 (s)	31.1 CH_3
	N	-	δ_N 117.5	-	-
N,*O*-diMe-Serine	49	-	170.5[b] C	-	
	50	6.02 (br s)	52.6 CH	6.02 / 6.18 (br s)	
	51	3.90 (m)	69.3 CH_2	3.89 (m)	69.3 CH_2
		3.64 (dd, 11.0, 4.0)		3.65 (dd, 11.0, 4.0)	
	52	3.35 (s)	58.6 CH_3	3.35 (s)	58.7 CH_3
	53	3.04 (s)	30.2 CH_3	3.04 (s)	30.2 CH_3
	N	-	δ_N 108.5	-	-
2-Hydroxyisovaleric acid	54	-	170.0 C	-	

	55	5.00 (d, 6.5)	74.7 CH	5.01 (br s)	74.7 CH
	56	2.21 (oct, 6.5)	29.9 CH	2.22 (m)	29.9 CH
	57	1.06 (ob)	18.0 CH_3	1.06 (ob)	18.0 CH_3
	58	1.06 (ob)	18.0 CH_3		
N,*N*-Dimethylvaline	59	-	172.4 C	-	
	60	2.84 (d, ob)	73.8 CH	2.86 / 2.84	
	61	2.02 (m)	27.6 CH		
	62	0.99 (d, 6.6)	19.5 CH_3		
	63	0.92 (d, 6.6)	19.6 CH_3		
	64	2.34 (s)	41.3 CH_3		
	65	2.34 (s)	41.3 CH_3		
	N	-	δ_N 24.6	-	-

^{15}N shifts referenced to formamide at δ_H 112.0 ppm.

ob = obscured

[a, b, c, d, e] carbonyl chemical shifts are exchangeable with others of the same superscript

Computational Methods - General Information

All molecular mechanics conformational searches were performed in Macromodel using Merck Molecular force fields (MMFFs) and were treated with chloroform solvation. Mixed torsional/Low-mode sampling was employed with a maximum number of steps set to 10,000. Interestingly conformational searches with no cutoff for handling Van der Waals and electrostatic interactions was necessary to capture all low energy conformations in the case of coibamide A. All conformations within 104 kJ/mol (~25 kcal/mol) were collected. Molecular Dynamics were performed using AMBER 12 package. Parameters were generated within the antechamber module using the general AMBER force field (gaff). Each diastereomer was immersed in a 12 Å buffer of CHCL3BOX chloroform molecules using the leap module. The systems were gently heated over for ten picoseconds from 0° to 300° kelvin under constant volume and periodic-boundary conditions. The total MD simulation, including initial minimization, heating and production, ran for 200 ps. Conformations were taken every 2 ps over the last 50 ps to generate 25 MD derived conformations. Solvent molecules were then removed in order to make a QM NMR prediction possible. Density functional theory calculations were performed using Gaussian 09. Each structure from MM within 3 kcal/mol of the global minima was subjected to further calculations. For all structures using DFT methodologies a geometry optimization was performed using B3LYP/6-13G**/PCM(Chloroform). For all structures, using all methods, computed chemical shifts were determined using the GIAO method in Gaussian 09 at the mPW1PW91/6-311+G(2d,p)/ PCM(Chloroform) level of theory and were empirically scaled (see below). The computed ^{1}H and ^{13}C chemical shifts were then submitted to a Boltzmann-weighed average (see below).

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Empirical Scaling

Empirical scaling is a common technique used to eliminate systematic errors that can occur as well as to standardize computed chemical shifts to be relevant TMS chemical shifts. In this work we used scaling factors for ^{1}H and ^{13}C obtained from a chemical database (http://cheshirenmr.info/ScalingFactors.htm) detailing scaling factors for many methods.

In order to find the scaled chemical shifts (δ) all ^{1}H and ^{13}C computed NMR isotropic shielding constants (σ) were scaled using the equation and parameters below (b = Intercept and m = Slope)

	^{1}H	^{13}C
Slope (m)	-1.008225	-1.04478
Intercept (b)	31.8426	186.060

$$\delta = \frac{b - \sigma}{-m}$$

Conformational Averaging

In order to account for each conformations influence on the total NMR shift from a particular ^{1}H or ^{13}C a Boltzmann average was employed using the formula:

$$\frac{P_i}{P_j} = e^{\frac{-(E_i - E_j}{RT}}$$

P_i = population of conformer I relative to the lowest energy conformer j
$E_{i \text{ and } j}$ = computed free energies (in J/mol)
R = molar gas constant (8.314510 J mol^{-1} K^{-1})

T = 298.15 K

Mandelalide A

For all configurations analyzed using DFT methodology a geometry optimization was conducted using B3LYP/6-31G**/PCM(Chloroform) for all conformations within 3 kcal/mol of the global MM minima. Energies for all relevant conformations were taken directly from the optimization geometry. Nine conformations were identified for the revised configuration and twenty-six conformations were located for the original configuration. Relative energies as well as Boltzmann averaged contribution percentages are reported below for all relevant conformations.

Mandelalide A – Revised Configuration DFT Structures

Conformer	*Relative Energy*	*% Contribution*
1	0.06	32.2
2	0.32	20.0
3	2.89	0.3
4	2.10	1.0
5	2.70	0.4
6	0.00	35.7
7	0.74	10.1
8	2.67	0.34

Mandelalide A – Original Configuration DFT Structures

Conformer	*Relative Energy*	*% Contribution*
1	1.09	6.0
2	0.16	29.3
3	1.67	2.2
4	0.00	38.6
5	3.39	0.1
6	1.58	2.6
7	2.19	0.9
8	3.79	0.1
9	2.23	0.9
10	1.12	5.7
11	1.67	2.2
12	1.65	2.3
13	1.86	1.6
14	1.50	3.0
15	2.25	0.8
16	3.34	0.1
17	1.90	1.5
18	2.64	0.4
19	3.89	0.1
20	2.46	0.6
21	2.32	0.7
22	3.94	0.1

For all configurations analyzed using MM methodologies NMR single points were conducted using mPW1PW91/6-311+G(2d,p)/PCM(Chloroform) for all conformations within 3 kcal/mol of the global MM minima. Ten relevant conformations were identified for both the revised configuration and the original configuration of mandelalide A. Relative energies as well as Boltzmann averaged contribution percentages are reported below for all relevant conformations.

Mandelalide A – Revised Configuration MMFF Structures

Conformer	*Relative Energy*	*% Contribution*
1	0.58	25.6
2	0.00	69.3
3	3.25	0.3
4	2.61	0.8
5	3.14	0.3
6	3.80	0.1
7	3.85	0.1

Mandelalide A – Original Configuration MMFF Structures

Conformer	*Relative Energy*	*% Contribution*
1	1.84	2.8
2	0.00	65.4
3	1.12	9.7
4	3.14	0.3
5	1.17	8.9
6	2.50	0.9
7	2.89	0.5

8	4.12	0.1	8	2.15	1.7
9	1.79	3.3	9	1.63	4.0
			10	1.45	5.5

For all configurations analyzed using MD methodologies NMR single points were conducted using mPW1PW91/6-311+G(2d,p)/PCM(Chloroform). Twenty-five conformations were identified for both the revised configuration and the original configuration of mandelalide A. Relative energies as well as Boltzmann averaged contribution percentages are reported below for all conformations.

Mandelalide A – Revised Configuration MD Structures			***Mandelalide A – Original Configuration MD Structures***		
Conformer	***Relative Energy***	***% Contribution***	***Conformer***	***Relative Energy***	***% Contribution***
1 (150ps)	26.27	0.0	1 (150ps)	18.76	0.0
2 (152ps)	12.16	0.0	2 (152ps)	36.45	0.0
3 (154ps)	13.71	0.0	3 (154ps)	18.92	0.0
4 (156ps)	17.92	0.0	4 (156ps)	1.18	11.6
5 (158ps)	22.22	0.0	5 (158ps)	8.35	0.0
6 (160ps)	24.92	0.0	6 (160ps)	23.42	0.0
7 (162ps)	22.54	0.0	7 (162ps)	0.00	87.1
8 (164ps)	29.69	0.0	8 (164ps)	18.16	0.0
9 (166ps)	24.16	0.0	9 (166ps)	15.78	0.0
10 (168ps)	8.38	0.0	10 (168ps)	16.68	0.0
11 (170ps)	16.73	0.0	11 (170ps)	7.17	0.0
12 (172ps)	10.25	0.0	12 (172ps)	2.60	1.0
13 (174ps)	24.76	0.0	13 (174ps)	17.79	0.0
14 (176ps)	18.99	0.0	14 (176ps)	5.06	0.0
15 (178ps)	18.91	0.0	15 (178ps)	9.99	0.0
16 (180ps)	8.21	0.0	16 (180ps)	13.33	0.0
17 (182ps)	25.73	0.0	17 (182ps)	10.42	0.0
18 (184ps)	9.54	0.0	18 (184ps)	26.59	0.0
19 (186ps)	22.64	0.0	19 (186ps)	17.45	0.0
20 (188ps)	24.12	0.0	20 (188ps)	5.62	0.0
21 (190ps)	0.00	100	21 (190ps)	22.89	0.0
22 (192ps)	15.78	0.0	22 (192ps)	3.55	0.2
23 (194ps)	21.91	0.0	23 (194ps)	21.60	0.0
24 (196ps)	15.40	0.0	24 (196ps)	6.58	0.0
25 (198ps)	10.63	0.0	25 (198ps)	23.66	0.0

For all configurations of mandelalide B geometries were optimized using B3LYP/6-31G**/PCM(Chloroform) for all conformations within 3 kcal/mol of the global MM minima. Seven relevant conformations were identified for the revised configuration and two relevant conformations were located for the original configuration. Relative energies as well as Boltzmann averaged contribution percentages are reported below for all relevant conformations.

Mandelalide B

Mandelalide B – Revised Configuration DFT Structures			***Mandelalide B – Original Configuration DFT Structures***		
Conformer	***Relative Energy***	***% Contribution***	***Conformer***	***Relative Energy***	***% Contribution***
1	2.74	0.3	1	0.00	59.2
2	2.09	0.9	2	0.22	40.8
3	1.52	2.3			

4	0.01	30.1
5	0.00	30.3
6	0.36	16.3
7	0.25	19.8

For all configurations of mandelalide C geometries were optimized using B3LYP/6-31G**/PCM(Chloroform) for all conformations within 3 kcal/mol of the global MM minima. Seven relevant conformations were identified for the revised configuration and two relevant conformations were located for the original configuration. Relative energies as well as Boltzmann averaged contribution percentages are reported below for all relevant conformations.

Mandelalide C

Mandelalide C – Revised Configuration
DFT Structures

Conformer	*Relative Energy*	*% Contribution*
1	0.10	17.0
2	0.40	10.2
3	0.00	20.1
4	0.04	18.8
5	0.21	14.1
6	0.23	13.5
7	2.46	0.3
8	3.00	0.1
9	1.36	2.0
10	1.36	2.0
11	1.45	1.7
12	2.85	0.2

Mandelalide C – Original Configuration
DFT Structures

Conformer	*Relative Energy*	*% Contribution*
1	0.0	94.4
2	1.66	5.6

For all configurations of mandelalide D geometries were optimized using B3LYP/6-31G**/PCM(Chloroform) for all conformations within 3 kcal/mol of the global MM minima. Three relevant conformations were identified for the revised configuration and two relevant conformations were located for the original configuration. Relative energies as well as Boltzmann averaged contribution percentages are reported below for all relevant conformations.

Mandelalide D

Mandelalide D – Revised Configuration
DFT Structures

Conformer	*Relative Energy*	*% Contribution*
1	0.00	42.3
2	0.23	28.8
3	0.22	28.9

Mandelalide D – Original Configuration
DFT Structures

Conformer	*Relative Energy*	*% Contribution*
1	0.00	50.5
2	0.01	49.5

Coibamide A

All configurations were analyzed using MM methodologies, NMR single points were conducted using mPW1PW91/6-311+G(2d,p)/PCM(Chloroform) for all conformations within 3 kcal/mol of the global MM minima. Twenty relevant conformations were identified for Wu Su's proposed revised configuration ([D-MeAla], [D-Hiv]), one relevant conformation was found for our proposed revision ([D-N,O-diMe-Ser] and five relevant conformations were located for the original configuration of coibamide A. Relative energies as well as Boltzmann averaged contribution percentages are reported below for all relevant conformations.

Coibamide A – [D-MeAla], [D-Hiv]

Coibamide A – [D-N,O-diMe-Ser]

Coibamide A – Original Configuration

(Wu Su's Proposed Revision)		
Conformer	Relative Energy	% Contribution
1	0.00	32.0
2	0.07	28.4
3	0.06	28.7
4	3.56	0.1
5	3.35	0.1
6	2.93	0.2
7	1.79	1.5
8	2.11	0.9
9	2.14	0.8
10	2.06	1.0
11	2.91	0.2
12	2.12	0.9
13	2.03	1.0
14	1.53	2.4
15	3.38	0.1
16	2.68	0.3
17	2.83	0.3
18	2.48	0.5
19	2.57	0.4
20	2.88	0.2
21	2.71	0.3
22	1.46	2.7

(Proposed Revision)		
Conformer	Relative Energy	% Contribution
1	1.15	4.2
2	2.87	0.2
3	0.00	29.9
4	0.11	25.0
5	0.10	25.2
6	0.78	8.2
7	0.83	7.3

Conformer	Relative Energy	% Contribution
1	0.00	64.9
2	1.26	7.6
3	0.51	27.4
4	3.86	0.1
5	4.18	0.1

Computed Coordinates, Energies and NMR Data

Mandelalide A Revised Configuration (DFT Methodologies)

Supporting Information: Revised-MandelalideA-0001.log

```
-----------------------------------------------------------------------
 Using  Gaussian 09:  AM64L-G09RevC.01 23-Sep-2011
=======================================================================
 #b3lyp/6-31G(d,p) scf=(maxcycle=300,direct,tight) density=current
 SCRF=(PCM,SOLVENT=Chloroform) opt=(maxcycle=250)
freq=noraman
 #N Geom=AllCheck Guess=TCheck SCRF=Check GenChk RB3LYP/6-
31G(d,p) Freq
-----------------------------------------------------------------------
 Pointgroup= C1   Stoichiometry= C33H52O11   C1[X(C33H52O11)]
#Atoms= 96
 Charge = 0                Multiplicity = 1
-----------------------------------------------------------------------
 SCF Energy= -2116.30621260      Predicted Change= -1.586709D-08
=======================================================================
 Optimization completed.          {Found       1       times}
 Item      Max Val.    Criteria    Pass?      RMS Val.    Criteria    Pass?
 Force      0.00001 ||  0.00045   [ YES ]      0.00000 ||  0.00030   [ YES ]
 Displ      0.00180 ||  0.00180   [ YES ]      0.00180 ||  0.00180   [ YES ]
-----------------------------------------------------------------------
     Atomic      Coordinates (Angstroms)
      Type      X                  Y                  Z
-----------------------------------------------------------------------
```

C	-6.849893	-0.712776	0.395619
C	-5.873327	0.324572	-0.167219
C	-6.247315	1.746903	0.244393
H	-6.300594	1.812815	1.337715
H	-7.240837	1.985322	-0.149996
C	-5.288523	2.814293	-0.267412
H	-5.101834	2.679512	-1.336245
C	-5.796488	4.240385	-0.010526
O	-7.024995	4.493751	-0.680867
H	-6.841439	4.515317	-1.630374
H	-5.019405	4.956776	-0.304663
H	-5.992941	4.371353	1.058791
O	-4.030114	2.637745	0.438385
C	-2.898040	3.044919	-0.188042
O	-2.887663	3.590382	-1.278835
C	-1.708170	2.720498	0.627242
H	-1.879292	2.233049	1.582205
C	-0.475651	2.992532	0.180762
H	-0.385632	3.475251	-0.792074
C	0.798761	2.662610	0.896245
H	0.589250	2.195644	1.864548
H	1.362390	3.586044	1.086163
C	1.692173	1.728492	0.067889
H	1.891878	2.203333	-0.909365
O	-5.876333	0.266346	-1.591542
H	-5.753511	-0.670477	-1.809560
H	-4.867889	0.084952	0.216334
H	-7.871974	-0.423552	0.106601
C	-6.760669	-0.966018	1.901650
H	-5.737159	-0.798896	2.262329
H	-7.428004	-0.319084	2.476982
C	-7.134739	-2.452600	2.014333
H	-8.222403	-2.529664	1.884681
C	-6.764790	-3.116168	3.340561
H	-7.012967	-4.183030	3.338332

H	-7.316815	-2.652119	4.164145
H	-5.697286	-3.017588	3.561089
C	-6.498999	-3.045929	0.732318
H	-7.119219	-3.865810	0.346139
O	-6.551966	-1.978568	-0.235166
O	0.948365	0.530766	-0.143967
C	1.606971	-0.405212	-1.004367
H	1.812171	0.092016	-1.967484
C	0.646138	-1.573859	-1.226313
C	-0.761576	-1.165484	-1.728625
H	-1.187999	-0.490158	-0.978780
C	-0.713514	-0.418850	-3.075226
H	-1.724132	-0.169292	-3.412025
H	-0.242849	-1.033656	-3.852160
H	-0.151165	0.515994	-2.995667
C	-1.648546	-2.378201	-1.836158
H	-1.415790	-3.072277	-2.647494
C	-2.684303	-2.657919	-1.025493
H	-2.911256	-1.966365	-0.215548
C	-3.534865	-3.829787	-1.180976
H	-3.308173	-4.454243	-2.045381
C	-4.554620	-4.213610	-0.390413
H	-5.096751	-5.114848	-0.677604
C	-5.052994	-3.560236	0.868988
H	-5.038525	-4.311174	1.670852
H	-4.400366	-2.742096	1.188206
H	0.535095	-2.118496	-0.280887
H	1.109913	-2.268427	-1.939430
C	2.943654	-0.835858	-0.385088
H	3.473136	-1.516520	-1.060633
H	2.751297	-1.375061	0.550507
C	3.813424	0.384793	-0.086444
O	4.984739	-0.066188	0.618424
C	6.145891	0.706184	0.407261
H	5.929544	1.777186	0.505300
H	4.129481	0.840926	-1.033990
C	3.031663	1.409305	0.745750
H	3.612450	2.329694	0.876065
H	2.842290	0.986319	1.739617
O	6.656115	0.580692	-0.907218
C	7.124610	-0.734251	-1.268248
C	7.615200	-0.646804	-2.704285
H	6.808088	-0.318071	-3.364451
H	7.958267	-1.627040	-3.047158
H	8.441472	0.066838	-2.787438
H	6.292767	-1.448908	-1.202453
C	8.210657	-1.183630	-0.277167
H	9.074111	-0.510154	-0.347631
O	8.605556	-2.541556	-0.506939
H	9.317896	-2.546398	-1.158505
C	7.666102	-1.134990	1.149092
O	8.644483	-1.538446	2.091644
H	9.031994	-2.344102	1.716419
H	6.789121	-1.799780	1.194857
C	7.179240	0.277480	1.470058
O	8.289009	1.163344	1.445911
C	8.159962	2.283153	2.306640
H	8.042355	1.972721	3.354527
H	7.310230	2.926261	2.036823
H	9.078831	2.865595	2.209916
H	6.700076	0.284575	2.458427

Statistical Thermodynamic Analysis
Temperature= 298.150 Kelvin Pressure= 1.00000 Atm
==========
==========

SCF Energy= -2116.30621260 Predicted Change= -1.586709D-08
Zero-point correction (ZPE)= -2115.4736 0.83256
Internal Energy (U)= -2115.4272 0.87891
Enthalpy (H)= -2115.4263
0.87986
Gibbs Free Energy (G)= -2115.5565
0.74964

Frequencies -- 12.6570 16.4575 17.3898

NMR-Shifts
Revised-MandelalideA-0001-NMR.txt

Atom	Type	Isotropic	Scaled Shift
Revised-MandelalideA-0001-NMR.txt			
1	C	98.9241	83.4011945098
2	C	110.6615	72.1668676659
3	C	151.6015	32.9815846398
6	C	112.4872	70.4194184422
8	C	120.9012	62.3660483547
14	C	11.9935	166.605888321
16	C	59.5738	121.064913187
18	C	25.5699	153.611382301
20	C	143.3965	40.8349126132
23	C	109.3466	73.4254101342
29	C	149.2812	35.2024349624
32	C	145.3101	39.0033308448
34	C	172.4289	13.0468615402
38	C	101.4948	80.9406765061
42	C	111.3636	71.4948601619
44	C	141.5266	42.6246673941
45	C	148.7467	35.7140259193
47	C	169.4889	15.8608510883
51	C	36.7161	142.942916212
53	C	56.9402	123.585635253
55	C	49.2410	130.954842168
57	C	50.7745	129.487069048
59	C	151.2796	33.2896877812
64	C	146.1164	38.2315894255
67	C	112.9167	70.0083271119
69	C	90.5595	91.4072819158
72	C	148.0257	36.4041233561
76	C	114.7889	68.2163709106
77	C	169.6891	15.6692318
82	C	109.2560	73.512126955
86	C	114.4187	68.5707038802
90	C	104.0905	78.4562300197
92	C	128.2936	55.2904917782
4	H	30.3997	1.33324093324
5	H	29.7288	1.95315315315
7	H	26.6086	4.83622083622
10	H	31.2453	0.551905751906
11	H	27.6211	3.90066990067
12	H	28.6841	2.91845691846
17	H	25.4855	5.87396627397
19	H	24.1563	7.10214830215
21	H	29.2879	2.36054516055
22	H	29.3093	2.34077154077
24	H	28.1440	3.41750981751
26	H	29.3283	2.32321552322
27	H	28.0006	3.55001155001
28	H	27.9284	3.61672441672
30	H	30.4185	1.31586971587
31	H	29.8924	1.80198660199
33	H	29.1024	2.53194733195
35	H	30.6911	1.06398706399
36	H	30.5027	1.23806883807
37	H	30.9949	0.783275583276
39	H	27.8040	3.73167013167
43	H	28.2976	3.27558327558
46	H	29.1026	2.53176253176
48	H	30.9560	0.819219219219
49	H	31.2388	0.557911757912

50	H	30.5670	1.17865557866
52	H	25.8533	5.53411873412
54	H	25.1895	6.14747054747
56	H	24.9664	6.35361515362
58	H	26.1478	5.262000462
60	H	29.9620	1.73767613768
61	H	29.2890	2.35952875953
62	H	30.3407	1.38775698776
63	H	30.6291	1.12127512128
65	H	30.0286	1.67613767614
66	H	30.6051	1.14345114345
70	H	26.6804	4.76987756988
71	H	27.5632	3.95416955417
73	H	29.6932	1.98604758605
74	H	30.6946	1.06075306075
78	H	30.5020	1.23871563872
79	H	30.4309	1.30441210441
80	H	30.8144	0.950057750058
81	H	27.9731	3.57542157542
83	H	28.1347	3.4261030261
85	H	30.4099	1.32381612382
88	H	29.5629	2.10644490644
89	H	27.8172	3.71947331947
93	H	28.5562	3.03663663664
94	H	28.2926	3.2802032802
95	H	28.2187	3.34848694849
96	H	28.2855	3.28676368676

Supporting Information: Revised-MandelalideA-0002.log

```
-----------------------------------------------------------------------------
 Using  Gaussian 09:  AM64L-G09RevC.01 23-Sep-2011
=============================================================
=====================
 #b3lyp/6-31G(d,p) scf=(maxcycle=300,direct,tight) density=current
 SCRF=(PCM,SOLVENT=Chloroform) opt=(maxcycle=250)
freq=noraman
 #N Geom=AllCheck Guess=TCheck SCRF=Check GenChk RB3LYP/6-
31G(d,p) Freq
-----------------------------------------------------------------------------
 Pointgroup= C1   Stoichiometry= C33H52O11   C1[X(C33H52O11)]
#Atoms= 96
 Charge = 0                Multiplicity = 1
-----------------------------------------------------------------------------
 SCF Energy= -2116.30681371      Predicted Change= -2.505671D-08
=============================================================
=====================
 Optimization completed.          {Found       1       times}
 Item      Max Val.    Criteria    Pass?      RMS Val.    Criteria    Pass?
 Force      0.00001 ||  0.00045   [ YES ]      0.00000 ||  0.00030   [ YES ]
 Displ      0.00259 ||  0.00180   [ NO ]       0.00259 ||  0.00180   [ YES ]
-----------------------------------------------------------------------------
     Atomic      Coordinates (Angstroms)
      Type      X                Y                Z
-----------------------------------------------------------------------------
      C       -6.680967      -0.956865       0.312597
      C       -5.829991       0.213625      -0.190812
      C       -6.350669       1.557893       0.310745
      H       -6.422165       1.552641       1.402742
      H       -7.364490       1.706337      -0.080622
      C       -5.505779       2.751495      -0.123289
      H       -5.349026       2.745501      -1.203852
      C       -6.098399       4.095528       0.300973
      O       -6.304667       4.183979       1.706129
      H       -5.441238       4.042987       2.120225
      H       -7.078825       4.220782      -0.169322
      H       -5.446350       4.902098      -0.060844
      O       -4.206604       2.605909       0.529034
      C       -3.120513       3.109478      -0.113564
      O       -3.179106       3.699846      -1.178068
      C       -1.888732       2.831711       0.655178
      H       -1.998673       2.291151       1.590458
      C       -0.692300       3.217216       0.194300
      H       -0.665404       3.747974      -0.757033
      C        0.621677       2.964002       0.867519
      H        0.477993       2.412729       1.802926
      H        1.095412       3.923468       1.116375
      C        1.585835       2.185224      -0.037328
      H        1.723854       2.750445      -0.976468
      O       -5.845082       0.244269      -1.615683
      H       -5.629727      -0.659491      -1.893567
      H       -4.800083       0.062278       0.171599
      H       -7.734796      -0.759165       0.062743
      C       -6.528513      -1.301586       1.794799
      H       -5.517392      -1.057552       2.146368
      H       -7.241437      -0.766065       2.427086
      C       -6.749416      -2.822484       1.810110
      H       -7.827341      -3.000177       1.699492
      C       -6.277694      -3.532185       3.078643
      H       -5.219848      -3.339249       3.283182
      H       -6.416846      -4.616357       3.007845
      H       -6.850646      -3.182838       3.943512
      C       -6.095738      -3.261866       0.475429
      H       -6.651344      -4.104842       0.043101
      O       -6.266409      -2.137304      -0.410467
      O        0.955014       0.942408      -0.336059
      C        1.688879       0.141535      -1.268749
      H        1.834066       0.726971      -2.192512
      C        0.839226      -1.093351      -1.571599
      C       -0.605485      -0.784288      -2.039388
      H       -1.074318      -0.178254      -1.256402
      C       -0.639651       0.017492      -3.354205
      H       -1.672293       0.202500      -3.664838
      H       -0.138362      -0.528170      -4.162922
      H       -0.148196       0.988785      -3.246063
      C       -1.391183      -2.061035      -2.186015
      H       -1.117203      -2.698859      -3.030050
      C       -2.384867      -2.459485      -1.372233
      H       -2.653661      -1.823152      -0.530098
      C       -3.138740      -3.690772      -1.562633
      H       -2.887977      -4.252974      -2.462382
      C       -4.096667      -4.197241      -0.763719
      H       -4.570198      -5.126815      -1.080335
      C       -4.606663      -3.652385       0.542364
      H       -4.498067      -4.438405       1.302411
      H       -4.017982      -2.795750       0.884074
      H        0.788268      -1.708658      -0.665058
      H        1.359181      -1.690894      -2.332076
      C        3.066655      -0.208720      -0.689379
      H        3.650513      -0.784017      -1.413439
      H        2.929783      -0.828784       0.205250
      C        3.824849       1.064758      -0.294303
      O        5.036605       0.786369       0.427601
      C        6.184897       0.521116      -0.343098
      H        6.212311       1.175584      -1.223670
      H        4.086417       1.624450      -1.206359
      C        2.958553       1.948990       0.604606
      H        3.463592       2.903083       0.790174
      H        2.823478       1.447263       1.570514
      O        6.214151      -0.786625      -0.888737
      C        6.293028      -1.865917       0.061897
      C        6.338635      -3.158489      -0.736338
      H        7.198397      -3.155043      -1.413481
      H        5.428822      -3.276975      -1.330925
      H        6.431558      -4.011594      -0.059913
      H        5.390611      -1.850550       0.693869
      C        7.516640      -1.677002       0.972584
      H        8.431655      -1.761939       0.379139
      O        7.614485      -2.696546       1.972131
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H	6.789723	-2.693084	2.481913
C	7.481240	-0.296230	1.630492
O	8.607837	-0.089710	2.464114
H	8.750265	-0.936429	2.915043
H	6.548905	-0.223141	2.216672
C	7.412314	0.787808	0.555795
O	8.599157	0.737821	-0.220308
C	8.975534	1.980374	-0.791644
H	9.909177	1.811083	-1.332343
H	9.143542	2.742882	-0.017873
H	8.226854	2.362419	-1.500157
H	7.300467	1.772421	1.029974

Statistical Thermodynamic Analysis
Temperature= 298.150 Kelvin Pressure= 1.00000 Atm
==========
SCF Energy= -2116.30681371 Predicted Change= -2.505671D-08
Zero-point correction (ZPE)= -2115.4741 0.83265
Internal Energy (U)= -2115.4280 0.87875
Enthalpy (H)= -2115.4271 0.87970
Gibbs Free Energy (G)= -2115.5561 0.75069

Frequencies -- 13.8125 18.7250 20.2588

NMR-Shifts
Revised-MandelalideA-0002-NMR.txt

Atom	Type	Isotropic	Scaled Shift
1	C	99.1092	83.224028025
2	C	109.9670	72.8316009112
3	C	151.5354	33.0448515477
6	C	111.4222	71.4387717988
8	C	119.4673	63.7384903999
14	C	12.5603	166.063381765
16	C	59.6756	120.967476407
18	C	25.0416	154.117038994
20	C	143.6702	40.5729435862
23	C	109.0596	73.7001091139
29	C	148.8964	35.5707421658
32	C	145.1005	39.2039472425
34	C	172.4971	12.9815846398
38	C	101.2407	81.1838856027
42	C	112.0405	70.8469725684
44	C	141.3072	42.834663757
45	C	148.7553	35.7057945213
47	C	169.2576	16.0822374088
51	C	36.0583	143.572522445
53	C	57.0240	123.50542698
55	C	49.3909	130.811366986
57	C	51.0710	129.203277245
59	C	150.9158	33.6378950592
64	C	144.0024	40.2549819101
67	C	103.9342	78.6058308926
69	C	83.6087	98.0601657765
72	C	145.8705	38.4669499799
76	C	113.1474	69.7875150749
77	C	169.0268	16.3031451597
82	C	109.3304	73.4409157909
86	C	112.2353	70.6605218323
90	C	103.6106	78.9155611708
92	C	128.2268	55.3544286836
4	H	29.6072	2.06551166551
5	H	30.4337	1.30182490182
7	H	26.2808	5.13910833911
10	H	30.9059	0.865511665512
11	H	28.3190	3.25580965581
12	H	27.5468	3.96932316932
17	H	25.4388	5.91711711712
19	H	24.1056	7.148995149
21	H	29.2899	2.3586971587
22	H	29.3277	2.32376992377
24	H	28.0294	3.5234003234
26	H	29.2973	2.35185955186
27	H	28.1073	3.45142065142
28	H	27.9549	3.59223839224
30	H	30.3599	1.37001617002
31	H	29.8483	1.84273504274
33	H	29.1259	2.51023331023
35	H	30.9996	0.778932778933
36	H	30.7354	1.02305382305
37	H	30.5719	1.17412797413
39	H	27.7966	3.73850773851
43	H	28.3802	3.19926079926
46	H	29.0843	2.54867174867
48	H	30.9480	0.826611226611
49	H	31.2386	0.558096558097
50	H	30.5582	1.18678678679
52	H	25.7850	5.59722799723
54	H	25.1623	6.1726033726
56	H	24.9776	6.34326634327
58	H	26.1035	5.30293370293
60	H	29.9456	1.75282975283
61	H	29.2945	2.35444675445
62	H	30.3472	1.38175098175
63	H	30.6482	1.10362670363
65	H	29.4855	2.17796257796
66	H	30.6159	1.13347193347
70	H	26.6211	4.82467082467
71	H	27.9627	3.58503118503
73	H	29.8841	1.80965580966
74	H	30.4937	1.24638484638
78	H	30.7748	0.986648186648
79	H	30.6260	1.12413952414
80	H	30.2303	1.48976668977
81	H	28.1634	3.39958419958
83	H	28.3653	3.21302841303
85	H	32.0763	-0.215939015939
88	H	29.6161	2.05728805729
89	H	28.0483	3.50593670594
93	H	28.2395	3.32926772927
94	H	28.5595	3.03358743359
95	H	28.2925	3.2802956803
96	H	28.1884	3.37648417648

Supporting Information: Revised-MandelalideA-0003.log

Using Gaussian 09: AM64L-G09RevC.01 23-Sep-2011
==========
#b3lyp/6-31G(d,p) scf=(maxcycle=300,direct,tight) density=current SCRF=(PCM,SOLVENT=Chloroform) opt=(maxcycle=250) freq=noraman
#N Geom=AllCheck Guess=TCheck SCRF=Check GenChk RB3LYP/6-31G(d,p) Freq

---

Pointgroup= C1 Stoichiometry= C33H52O11 C1[X(C33H52O11)]
#Atoms= 96
Charge = 0 Multiplicity = 1

SCF Energy= -2116.30116851 Predicted Change= -1.567169D-08
==========
Optimization completed. {Found 1 times}

Item	Max Val.	Criteria	Pass?	RMS Val.	Criteria	Pass?
Force	0.00000	0.00045	[YES]	0.00000	0.00030	[YES]
Displ	0.00410	0.00180	[NO]	0.00410	0.00180	[YES]

Atomic Type	Coordinates (Angstroms) X	Y	Z
C	-6.832248	-0.639527	0.081650
C	-5.859882	0.394083	-0.496760
C	-6.273466	1.824954	-0.118548
H	-6.372319	1.927791	0.966188
H	-7.263773	2.035463	-0.545491
C	-5.310820	2.891985	-0.627283
H	-5.121354	2.764296	-1.695228
C	-5.785672	4.319359	-0.354791
O	-6.027937	4.562318	1.026004
H	-5.196333	4.381008	1.486875
H	-6.733819	4.489193	-0.874925
H	-5.047697	5.023353	-0.762879
O	-4.053500	2.692019	0.088435
C	-2.903645	3.028507	-0.553700
O	-2.871723	3.507947	-1.673466
C	-1.730954	2.729233	0.294938
H	-1.924458	2.322465	1.282892
C	-0.487359	2.937042	-0.155134
H	-0.374692	3.337161	-1.162420
C	0.770147	2.652872	0.607018
H	0.540244	2.280439	1.610988
H	1.342136	3.583933	0.719837
C	1.667535	1.636444	-0.112460
H	1.865908	2.000244	-1.136426
O	-5.720272	0.257136	-1.910792
H	-6.602861	0.326080	-2.303281
H	-4.862027	0.184903	-0.095978
H	-7.834814	-0.443224	-0.341456
C	-6.917218	-0.667106	1.611018
H	-5.933090	-0.460806	2.052312
H	-7.625517	0.062793	2.011289
C	-7.337452	-2.117160	1.887703
H	-8.405802	-2.201590	1.647280
C	-7.139240	-2.585048	3.329319
H	-7.773942	-2.004815	4.006869
H	-6.103121	-2.460318	3.659348
H	-7.407984	-3.640068	3.450057
C	-6.574199	-2.892296	0.781596
H	-7.187298	-3.729975	0.421013
O	-6.422386	-1.959635	-0.306526
O	0.932226	0.417451	-0.187271
C	1.599326	-0.607468	-0.932877
H	1.792185	-0.228481	-1.950428
C	0.656298	-1.808559	-0.999436
C	-0.755830	-1.502603	-1.557879
H	-1.197115	-0.726567	-0.922651
C	-0.713937	-0.972821	-3.004301
H	-0.239100	-1.697378	-3.677191
H	-0.157260	-0.033320	-3.071241
H	-1.726744	-0.786084	-3.372960
C	-1.618725	-2.734286	-1.476190
H	-1.326619	-3.565423	-2.123013
C	-2.700896	-2.878295	-0.691612
H	-2.997009	-2.048104	-0.052555
C	-3.522970	-4.079640	-0.668716
H	-3.228824	-4.855702	-1.375747
C	-4.593017	-4.324706	0.110150
H	-5.106582	-5.275640	-0.033238
C	-5.190181	-3.446492	1.175619
H	-5.313469	-4.052650	2.082999
H	-4.527869	-2.614580	1.433910
H	0.551648	-2.220151	0.011912
H	1.135550	-2.586142	-1.609226
C	2.946037	-0.946942	-0.277095
H	3.481130	-1.691134	-0.876937
H	2.764812	-1.383201	0.712987
C	3.801860	0.308359	-0.116652
O	4.978351	-0.052938	0.630038
C	6.121284	0.733756	0.368449
H	5.877989	1.803048	0.397149
H	4.112746	0.663164	-1.108184
C	3.007625	1.407952	0.599187
H	3.576907	2.344016	0.629752
H	2.819165	1.093215	1.632700
O	6.641156	0.536815	-0.930868
C	7.139161	-0.786535	-1.213569
C	7.639105	-0.772932	-2.648396
H	6.826130	-0.517632	-3.333771
H	8.030352	-1.757265	-2.915724
H	8.438116	-0.034225	-2.767135
H	6.321676	-1.513062	-1.109921
C	8.229376	-1.157067	-0.200151
H	9.073825	-0.460757	-0.312314
O	8.638846	-2.496007	-0.449879
H	9.151049	-2.753192	0.332099
C	7.679752	-1.028316	1.218775
O	8.733891	-1.405991	2.102405
H	8.345822	-1.653135	2.952124
H	6.831568	-1.718993	1.315937
C	7.156111	0.392480	1.462123
O	8.248285	1.295386	1.407545
C	8.059813	2.486855	2.153537
H	7.217331	3.088032	1.783645
H	8.975135	3.073601	2.051097
H	7.890846	2.270844	3.218448
H	6.659384	0.446087	2.442428

Statistical Thermodynamic Analysis
Temperature= 298.150 Kelvin Pressure= 1.00000 Atm
==========
==========
SCF Energy= -2116.30116851 Predicted Change= -1.567169D-08
Zero-point correction (ZPE)= -2115.4691 0.83200
Internal Energy (U)= -2115.4226 0.87848
Enthalpy (H)= -2115.4217
0.87943
Gibbs Free Energy (G)= -2115.5520
0.74911

Frequencies -- 12.0282 15.6477 20.0175

NMR-Shifts
Revised-MandelalideA-0003-NMR.txt

Atom	Type	Isotropic	Scaled Shift
1	C	97.9355	84.3474224239
2	C	109.1679	73.5964509275
3	C	148.8808	35.5856735389
6	C	111.8989	70.9825034936
8	C	119.2649	63.9322153946
14	C	12.5611	166.062616053
16	C	60.1464	120.516855223
18	C	25.1321	154.030417887
20	C	143.1250	41.0947759337
23	C	109.4906	73.2875820747
29	C	147.1859	37.207928942
32	C	145.7530	38.5794138479
34	C	172.3574	13.1152970003
38	C	100.6361	81.7625720247
42	C	111.5298	71.3357836099
44	C	141.5580	42.59461322
45	C	148.6441	35.8122284117
47	C	168.9010	16.4235532839
51	C	38.1042	141.614311147
53	C	55.9626	124.521334635

55	C	49.2912	130.906793775
57	C	51.2752	129.007829399
59	C	152.4428	32.176343345
64	C	145.7677	38.5653439002
67	C	113.7884	69.1739887823
69	C	91.1603	90.8322326231
72	C	148.6217	35.8336683321
76	C	114.4025	68.5862095369
77	C	168.7666	16.5521928061
82	C	112.9344	69.9913857463
86	C	111.6244	71.245238232
90	C	102.6191	79.8645647888
92	C	128.4716	55.1201209824
4	H	29.4628	2.19893739894
5	H	30.6545	1.09780549781
7	H	26.2739	5.14548394548
10	H	30.9260	0.846939246939
11	H	28.3607	3.21727881728
12	H	27.5420	3.97375837376
17	H	25.4592	5.89826749827
19	H	24.1344	7.12238392238
21	H	29.2695	2.37754677755
22	H	29.2950	2.35398475398
24	H	28.1562	3.40623700624
26	H	32.1458	-0.280157080157
27	H	28.3310	3.24472164472
28	H	28.0143	3.53735273735
30	H	30.3819	1.34968814969
31	H	29.9248	1.77204897205
33	H	29.2070	2.4352968353
35	H	30.5433	1.20055440055
36	H	30.9742	0.802402402402
37	H	30.6952	1.0601986602
39	H	27.6448	3.87877107877
43	H	28.2912	3.2814968815
46	H	29.2923	2.35647955648
48	H	31.3044	0.497297297297
49	H	30.6711	1.08246708247
50	H	30.9100	0.861723261723
52	H	26.0326	5.36844536845
54	H	24.9679	6.35222915223
56	H	25.3965	5.9562023562
58	H	26.2949	5.12607992608
60	H	29.7559	1.92811272811
61	H	29.3994	2.25751905752
62	H	30.3857	1.34617694618
63	H	30.5782	1.16830676831
65	H	30.0011	1.70154770155
66	H	30.6628	1.09013629014
70	H	26.5569	4.88399168399
71	H	27.5542	3.96248556249
73	H	29.7089	1.97154077154
74	H	30.7785	0.983229383229
78	H	30.5660	1.17957957958
79	H	30.2035	1.51452991453
80	H	30.7626	0.997920997921
81	H	27.9559	3.59131439131
83	H	28.0984	3.45964425964
85	H	29.6046	2.06791406791
88	H	30.9045	0.866805266805
89	H	27.8335	3.70441210441
93	H	28.2765	3.29507969508
94	H	28.1521	3.41002541003
95	H	28.6423	2.95708015708
96	H	28.5291	3.06167706168

Using Gaussian 09: AM64L-G09RevC.01 23-Sep-2011

==========
==========
#b3lyp/6-31G(d,p) scf=(maxcycle=300,direct,tight) density=current SCRF=(PCM,SOLVENT=Chloroform) opt=(maxcycle=250) freq=noraman
#N Geom=AllCheck Guess=TCheck SCRF=Check GenChk RB3LYP/6-31G(d,p) Freq
---
Pointgroup= C1 Stoichiometry= C33H52O11 C1[X(C33H52O11)]
#Atoms= 96
Charge = 0 Multiplicity = 1

SCF Energy= -2116.30211021 Predicted Change= -9.211255D-09
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Optimization completed. {Found 1 times}

Item	Max Val.	Criteria	Pass?	RMS Val.	Criteria	Pass?
Force	0.00000	0.00045	[YES]	0.00000	0.00030	[YES]
Displ	0.00215	0.00180	[NO]	0.00215	0.00180	[YES]

Atomic Type	Coordinates (Angstroms) X	Y	Z
C	-6.791816	-0.673714	0.235704
C	-5.883180	0.430340	-0.316699
C	-6.318522	1.817162	0.184675
H	-6.352971	1.823883	1.280090
H	-7.339375	2.018477	-0.167884
C	-5.413962	2.955101	-0.286326
H	-5.286682	2.931420	-1.369981
C	-5.948295	4.313535	0.151541
O	-5.089833	5.330281	-0.343493
H	-5.363976	6.166367	0.054828
H	-6.005160	4.335244	1.250454
H	-6.972246	4.423861	-0.238500
O	-4.114553	2.757251	0.325843
C	-3.006328	2.942716	-0.438346
O	-3.025734	3.224593	-1.621771
C	-1.789388	2.727181	0.376413
H	-1.932944	2.453471	1.417453
C	-0.570204	2.855191	-0.160253
H	-0.507957	3.130060	-1.212839
C	0.723221	2.644245	0.566464
H	0.539008	2.308393	1.592759
H	1.268407	3.596740	0.624210
C	1.628458	1.632672	-0.147386
H	1.828586	1.999102	-1.170256
O	-5.816778	0.394586	-1.740618
H	-6.719243	0.481390	-2.080622
H	-4.860506	0.226992	0.018467
H	-7.816062	-0.496337	-0.143107
C	-6.825400	-0.798323	1.761523
H	-5.829129	-0.606265	2.181695
H	-7.529530	-0.106842	2.231656
C	-7.221735	-2.268416	1.957077
H	-8.299128	-2.346130	1.758917
C	-6.959003	-2.826881	3.355568
H	-5.908875	-2.721604	3.645447
H	-7.223614	-3.887679	3.421949
H	-7.561778	-2.291420	4.096288
C	-6.501556	-2.965619	0.769687
H	-7.148618	-3.751379	0.354677
O	-6.335383	-1.947799	-0.237600
O	0.900583	0.409474	-0.229969
C	1.577174	-0.603552	-0.982567
H	1.782066	-0.208744	-1.991845
C	0.636024	-1.803664	-1.082373
C	-0.769747	-1.481520	-1.648096
H	-1.218783	-0.726892	-0.992993

C	-0.712001	-0.905125	-3.075894
H	-0.161070	0.039515	-3.106089
H	-1.721045	-0.712179	-3.451577
H	-0.224158	-1.605147	-3.765430
C	-1.634180	-2.714255	-1.619855
H	-1.352703	-3.510861	-2.313169
C	-2.707039	-2.897007	-0.830691
H	-2.992577	-2.101836	-0.144189
C	-3.533804	-4.094856	-0.865711
H	-3.266566	-4.820075	-1.634713
C	-4.578739	-4.391159	-0.070805
H	-5.104377	-5.326358	-0.264655
C	-5.127332	-3.590197	1.079063
H	-5.246006	-4.267313	1.935320
H	-4.435447	-2.800955	1.388766
H	0.520299	-2.237387	-0.081536
H	1.120973	-2.568005	-1.704318
C	2.916507	-0.947133	-0.314786
H	3.458846	-1.687927	-0.912351
H	2.725089	-1.387980	0.671211
C	3.768386	0.309479	-0.141302
O	4.937422	-0.051233	0.618492
C	6.087841	0.721923	0.354972
H	5.855397	1.794247	0.367174
H	4.089915	0.666044	-1.128721
C	2.966629	1.407294	0.569335
H	3.534056	2.344522	0.603717
H	2.773904	1.091437	1.601650
O	6.613651	0.499867	-0.937690
C	7.089204	-0.838849	-1.192495
C	7.551947	-0.877799	-2.639026
H	7.929205	-1.873707	-2.882624
H	8.352888	-0.150062	-2.803848
H	6.723377	-0.639562	-3.311766
H	6.267639	-1.552190	-1.042878
C	8.200115	-1.164353	-0.189471
H	9.018404	-0.441205	-0.337552
O	8.653598	-2.492914	-0.410944
H	9.180677	-2.716192	0.371927
C	7.676419	-1.020109	1.243215
O	8.709553	-1.314166	2.179389
H	9.251977	-0.508869	2.215203
H	6.889032	-1.763996	1.400809
C	7.095177	0.377494	1.469908
O	8.204382	1.273701	1.467838
C	7.995679	2.477630	2.196335
H	8.929279	3.041544	2.149426
H	7.750511	2.270492	3.246942
H	7.194056	3.088720	1.762104
H	6.578381	0.417453	2.438099

Statistical Thermodynamic Analysis
Temperature= 298.150 Kelvin Pressure= 1.00000 Atm
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SCF Energy= -2116.30211021 Predicted Change= -9.211255D-09
Zero-point correction (ZPE)= -2115.4701 0.83200
Internal Energy (U)= -2115.4236 0.87844
Enthalpy (H)= -2115.4227
0.87939
Gibbs Free Energy (G)= -2115.5533
0.74879

Frequencies -- 11.2283 14.6165 17.1797

NMR-Shifts
Revised-MandelalideA-0004-NMR.txt

Atom	Type	Isotropic	Scaled Shift
1	C	97.7212	84.5525373763
2	C	109.9657	72.8328451923
3	C	148.6582	35.7987327476
6	C	116.2682	66.8004747411
8	C	116.6185	66.4651888436
14	C	12.8116	165.822852658
16	C	59.7050	120.939336511
18	C	26.3309	152.882999292
20	C	143.6275	40.6138134344
23	C	109.0982	73.6631635368
29	C	147.4727	36.9334213901
32	C	146.1920	38.1592296943
34	C	172.1776	13.2873906468
38	C	100.9734	81.4397289381
42	C	111.2811	71.5738241544
44	C	141.6719	42.4855950535
45	C	148.7443	35.7163230537
47	C	169.0933	16.2394953962
51	C	37.8952	141.814353261
53	C	55.9592	124.524588909
55	C	48.9297	131.252799632
57	C	51.5864	128.709967649
59	C	151.9054	32.6907100059
64	C	145.7665	38.5664924673
67	C	113.4890	69.4605562894
69	C	91.6289	90.3837171462
72	C	148.7744	35.6875131607
76	C	115.2466	67.7782882521
77	C	168.9333	16.3926376845
82	C	110.0355	72.766036869
86	C	112.5491	70.3601715194
90	C	102.7442	79.7448266621
92	C	128.0355	55.537529432
4	H	30.2523	1.46943866944
5	H	30.5937	1.15398475398
7	H	25.7178	5.65932085932
10	H	31.2744	0.525017325017
11	H	28.0199	3.53217833218
12	H	27.9024	3.64074844075
17	H	25.5127	5.84883344883
19	H	24.2655	7.00124740125
21	H	29.2529	2.39288519289
22	H	29.2819	2.36608916609
24	H	28.1144	3.44486024486
26	H	32.1269	-0.262693462693
27	H	28.3257	3.24961884962
28	H	28.1173	3.44218064218
30	H	30.5144	1.22725802726
31	H	30.1018	1.6085008085
33	H	29.2406	2.40425040425
35	H	30.9546	0.820512820513
36	H	30.7183	1.03885423885
37	H	30.5644	1.18105798106
39	H	27.6909	3.83617463617
43	H	28.2928	3.28001848002
46	H	29.2313	2.41284361284
48	H	30.6144	1.13485793486
49	H	30.8631	0.905058905059
50	H	31.2846	0.515592515593
52	H	25.9863	5.41122661123
54	H	25.0422	6.28357588358
56	H	25.2851	6.05913605914
58	H	26.2657	5.15306075306
60	H	29.8244	1.86481866482
61	H	29.3942	2.26232386232
62	H	30.3763	1.35486255486
63	H	30.6004	1.14779394779
65	H	29.9903	1.71152691153
66	H	30.6241	1.1258951259
70	H	26.5063	4.93074613075

71	H	27.5287	3.98604758605
73	H	29.7003	1.97948717949
74	H	30.7562	1.00383460383
78	H	30.2141	1.50473550474
79	H	30.7990	0.964287364287
80	H	30.5430	1.20083160083
81	H	27.9248	3.62005082005
83	H	28.3668	3.21164241164
85	H	29.7214	1.95999075999
88	H	29.8900	1.8042042042
89	H	28.1753	3.38858858859
93	H	28.1264	3.43377223377
94	H	28.5811	3.01362901363
95	H	28.1946	3.37075537076
96	H	28.3290	3.24656964657

Supporting Information: Revised-MandelalideA-0005.log

Using Gaussian 09: AM64L-G09RevC.01 23-Sep-2011

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#b3lyp/6-31G(d,p) scf=(maxcycle=300,direct,tight) density=current SCRF=(PCM,SOLVENT=Chloroform) opt=(maxcycle=250) freq=noraman

#N Geom=AllCheck Guess=TCheck SCRF=Check GenChk RB3LYP/6-31G(d,p) Freq

---

Pointgroup= C1 Stoichiometry= C33H52O11 C1[X(C33H52O11)]
#Atoms= 96
Charge = 0 Multiplicity = 1

SCF Energy= -2116.30158635 Predicted Change= -5.743462D-09

==========

Optimization completed. {Found 2 times}

Item	Max Val.	Criteria	Pass?	RMS Val.	Criteria	Pass?
Force	0.00000 ||	0.00045	[YES]	0.00000 ||	0.00030	[YES]
Displ	0.00088 ||	0.00180	[YES]	0.00088 ||	0.00180	[YES]

Atomic Type	Coordinates (Angstroms) X	Y	Z
C	6.651069	-0.952541	-0.238008
C	5.864066	0.286044	0.205476
C	6.377168	1.555002	-0.495038
H	6.354351	1.417457	-1.582030
H	7.427781	1.714619	-0.216062
C	5.587184	2.814935	-0.143344
H	5.501292	2.934236	0.938155
C	6.212192	4.059540	-0.762131
O	5.467097	5.200539	-0.363455
H	5.786613	5.953993	-0.876285
H	6.219238	3.946143	-1.856817
H	7.258825	4.123361	-0.425656
O	4.253179	2.654066	-0.689528
C	3.191440	3.012136	0.078992
O	3.276093	3.422200	1.221320
C	1.931567	2.806603	-0.670637
H	2.012804	2.402058	-1.675125
C	0.748313	3.101337	-0.119267
H	0.749703	3.501596	0.894262
C	-0.585722	2.922718	-0.778160
H	-0.472832	2.441068	-1.755570
H	-1.043640	3.907373	-0.947549
C	-1.550249	2.103259	0.087432
H	-1.673121	2.615342	1.058879
O	5.877673	0.439372	1.622924
H	6.802411	0.481632	1.907118
H	4.810849	0.129242	-0.051373
H	7.705458	-0.814433	0.066679
C	6.589690	-1.269358	-1.734968
H	5.591089	-1.043685	-2.131954
H	7.321159	-0.706601	-2.320873
C	6.850876	-2.781484	-1.755447
H	7.925495	-2.930511	-1.584839
C	6.477793	-3.483933	-3.060675
H	5.428737	-3.319320	-3.325658
H	6.645602	-4.564586	-2.998561
H	7.090635	-3.103265	-3.884193
C	6.128081	-3.254858	-0.465121
H	6.709216	-4.054631	0.015136
O	6.128320	-2.116044	0.419525
O	-0.934295	0.837262	0.310683
C	-1.673232	-0.000758	1.206211
H	-1.804976	0.539411	2.159198
C	-0.841467	-1.261234	1.442451
C	0.604888	-1.001341	1.932752
H	1.093044	-0.369923	1.182353
C	0.645621	-0.261212	3.283544
H	0.177206	0.725151	3.216921
H	1.679864	-0.114752	3.608364
H	0.125646	-0.831860	4.062836
C	1.364111	-2.298593	2.028408
H	1.044637	-2.983540	2.817930
C	2.391021	-2.657899	1.238630
H	2.711602	-1.971612	0.456600
C	3.126267	-3.905213	1.389917
H	2.834290	-4.514998	2.245259
C	4.117663	-4.370151	0.607359
H	4.578580	-5.315567	0.894203
C	4.681530	-3.755248	-0.644505
H	4.684983	-4.527474	-1.425259
H	4.057751	-2.933970	-1.010244
H	-0.796678	-1.826821	0.503685
H	-1.373407	-1.892070	2.167126
C	-3.060444	-0.301106	0.620239
H	-3.646105	-0.904182	1.319855
H	-2.939939	-0.876143	-0.306036
C	-3.803984	1.000908	0.300017
O	-5.023583	0.772727	-0.427816
C	-6.185608	0.557992	0.338048
H	-6.207541	1.241340	1.197265
H	-4.053938	1.513272	1.242435
C	-2.931344	1.921760	-0.554913
H	-3.423809	2.891855	-0.683306
H	-2.810628	1.472602	-1.548186
O	-6.253898	-0.728644	0.920878
C	-6.338041	-1.830473	-0.007787
C	-6.351926	-3.106752	0.816461
H	-6.430622	-3.973874	0.156687
H	-7.205595	-3.109048	1.501819
H	-5.434664	-3.194175	1.405383
H	-5.458971	-1.819306	-0.665847
C	-7.590394	-1.655999	-0.872147
H	-8.469770	-1.664651	-0.208248
O	-7.657355	-2.719416	-1.813044
H	-8.325596	-2.445547	-2.460239
C	-7.543962	-0.310216	-1.601868
O	-8.710373	-0.140250	-2.402656
H	-9.404047	0.132627	-1.779522
H	-6.690603	-0.316111	-2.287672
C	-7.375483	0.837657	-0.604524
O	-8.605187	0.919842	0.112823
C	-8.888238	2.200127	0.664375
H	-8.157831	2.490224	1.430355
H	-9.873673	2.132939	1.129393
H	-8.908106	2.974327	-0.114742
H	-7.186819	1.777671	-1.139910

Statistical Thermodynamic Analysis
Temperature= 298.150 Kelvin Pressure= 1.00000 Atm
==========
SCF Energy= -2116.30158635 Predicted Change= -5.743462D-09
Zero-point correction (ZPE)= -2115.4696 0.83197
Internal Energy (U)= -2115.4232 0.87837
Enthalpy (H)= -2115.4222
0.87931
Gibbs Free Energy (G)= -2115.5523
0.74922

Frequencies -- 11.3010 14.2108 19.5150

NMR-Shifts
Revised-MandelalideA-0005-NMR.txt

Atom	Type	Isotropic	Scaled Shift
1	C	98.4095	83.8937383947
2	C	110.5511	72.2725358449
3	C	148.5576	35.8950209614
6	C	115.6824	67.3611669442
8	C	116.7078	66.3797163039
14	C	12.8196	165.815195544
16	C	59.2213	121.402304791
18	C	26.2406	152.969428971
20	C	144.0473	40.2120063554
23	C	108.6917	74.0522406631
29	C	147.5521	36.8574245296
32	C	147.3230	37.0767051437
34	C	172.1409	13.3225176592
38	C	101.3331	81.0954459312
42	C	111.9450	70.9383793717
44	C	141.6016	42.5528819464
45	C	148.6281	35.8275426406
47	C	169.0531	16.2779723961
51	C	37.0209	142.651180153
53	C	56.3239	124.175520205
55	C	49.3460	130.854342541
57	C	51.6320	128.666322097
59	C	151.7079	32.8797450181
64	C	144.1111	40.1509408679
67	C	103.7737	78.7594517506
69	C	83.9842	97.7007599686
72	C	146.0279	38.3162962538
76	C	114.8030	68.2028752465
77	C	169.0021	16.3267865005
82	C	110.2835	72.5286663221
86	C	112.5692	70.3409330194
90	C	103.0728	79.4303106874
92	C	128.1838	55.3955856735
4	H	30.2716	1.45160545161
5	H	30.6810	1.07331947332
7	H	25.7746	5.60683760684
10	H	31.2303	0.565765765766
11	H	28.0440	3.50990990991
12	H	27.9417	3.60443520444
17	H	25.4396	5.91637791638
19	H	24.1815	7.07886347886
21	H	29.2952	2.3537999538
22	H	29.3131	2.33726033726
24	H	27.9933	3.55675675676
26	H	32.0700	-0.210117810118
27	H	28.3508	3.22642642643
28	H	28.1525	3.40965580966
30	H	30.3944	1.33813813814
31	H	30.1135	1.59768999769
33	H	29.2936	2.35527835528
35	H	31.0355	0.745761145761
36	H	30.7026	1.05336105336
37	H	30.5895	1.15786555787
39	H	27.7809	3.75301455301
43	H	28.3713	3.20748440748
46	H	29.1124	2.52270732271
48	H	30.5599	1.18521598522
49	H	30.8800	0.889443289443
50	H	31.3020	0.499514899515
52	H	25.8741	5.5148995149
54	H	25.1055	6.22508662509
56	H	25.1645	6.17057057057
58	H	26.1950	5.21838761839
60	H	29.8651	1.82721182721
61	H	29.3163	2.3343035343
62	H	30.3413	1.3872025872
63	H	30.6773	1.07673827674
65	H	29.5525	2.11605451605
66	H	30.5645	1.18096558097
70	H	26.5392	4.90034650035
71	H	27.9654	3.58253638254
73	H	29.8839	1.80984060984
74	H	30.4981	1.24231924232
78	H	30.2861	1.43820743821
79	H	30.8623	0.905798105798
80	H	30.6229	1.127003927
81	H	27.9365	3.60924000924
83	H	28.4172	3.16507276507
85	H	29.6768	2.0012012012
88	H	29.9593	1.74017094017
89	H	28.1965	3.368999769
93	H	28.2175	3.3495957496
94	H	28.1583	3.4042966043
95	H	28.5868	3.00836220836
96	H	28.3259	3.24943404943

Supporting Information: Revised-MandelalideA-0006.log

Using Gaussian 09: AM64L-G09RevC.01 23-Sep-2011
==========
#b3lyp/6-31G(d,p) scf=(maxcycle=300,direct,tight) density=current
SCRF=(PCM,SOLVENT=Chloroform) opt=(maxcycle=250)
freq=noraman
#N Geom=AllCheck Guess=TCheck SCRF=Check GenChk RB3LYP/6-
31G(d,p) Freq

Pointgroup= C1 Stoichiometry= C33H52O11 C1[X(C33H52O11)]
#Atoms= 96
Charge = 0 Multiplicity = 1

SCF Energy= -2116.30742873 Predicted Change= -3.359975D-09
==========
Optimization completed on the basis of negligible forces.
{Found 2 times}

Item	Max Val.	Criteria	Pass?	RMS Val.	Criteria	Pass?
Force	0.00000 ||	0.00045	[YES]	0.00000 ||	0.00030	[YES]
Displ	0.00237 ||	0.00180	[NO]	0.00237 ||	0.00180	[YES]

Atomic Type	Coordinates (Angstroms) X	Y	Z
C	6.683774	-1.014954	-0.381013
C	5.841848	0.178790	0.081181
C	6.352538	1.498956	-0.493542
H	6.388012	1.438231	-1.587140
H	7.377555	1.657970	-0.138183
C	5.515000	2.710193	-0.091861
H	5.330516	2.700559	0.985523

C	6.179444	4.026780	-0.496238
O	5.377826	5.173039	-0.268117
H	4.772861	4.967495	0.463251
H	6.418134	4.003324	-1.567147
H	7.133751	4.088563	0.051645
O	4.227159	2.571319	-0.761362
C	3.143805	3.107073	-0.160610
O	3.195214	3.778088	0.863485
C	1.909402	2.763035	-0.891970
H	2.016413	2.154126	-1.784290
C	0.714394	3.175956	-0.450435
H	0.692139	3.778174	0.457363
C	-0.603326	2.866823	-1.091058
H	-0.465032	2.252935	-1.987383
H	-1.084705	3.804538	-1.400620
C	-1.554742	2.147289	-0.125510
H	-1.679028	2.769531	0.778826
O	5.885503	0.279618	1.501567
H	5.673559	-0.608302	1.828739
H	4.805232	0.011965	-0.253935
H	7.741185	-0.806662	-0.155428
C	6.511138	-1.429069	-1.843094
H	5.493981	-1.205605	-2.190770
H	7.212925	-0.922011	-2.510381
C	6.739741	-2.947853	-1.788368
H	7.819797	-3.114325	-1.681356
C	6.258255	-3.719450	-3.016468
H	6.819691	-3.408543	-3.903282
H	5.197209	-3.542307	-3.218234
H	6.404891	-4.798144	-2.895828
C	6.102931	-3.326019	-0.427311
H	6.667038	-4.144570	0.039312
O	6.277863	-2.158641	0.402087
O	-0.921081	0.923784	0.239695
C	-1.645511	0.177493	1.224313
H	-1.776989	0.813078	2.116466
C	-0.794900	-1.041830	1.583024
C	0.654856	-0.712570	2.020431
H	1.116750	-0.147541	1.203435
C	0.702787	0.153452	3.293356
H	0.208469	-0.350764	4.132715
H	0.211007	1.118731	3.141488
H	1.738506	0.352060	3.584986
C	1.439758	-1.982200	2.222948
H	1.177267	-2.572990	3.104035
C	2.418466	-2.428338	1.415836
H	2.675427	-1.839966	0.535986
C	3.171126	-3.650669	1.660656
H	2.929621	-4.164765	2.591145
C	4.118588	-4.200452	0.878103
H	4.593517	-5.113845	1.236873
C	4.615053	-3.724482	-0.459662
H	4.502649	-4.550497	-1.175396
H	4.019963	-2.889478	-0.841697
H	-0.754269	-1.703420	0.709334
H	-1.308417	-1.597912	2.378471
C	-3.031751	-0.200961	0.684331
H	-3.605859	-0.734033	1.447404
H	-2.909806	-0.869564	-0.176724
C	-3.791850	1.051509	0.230992
O	-5.018248	0.742996	-0.451672
C	-6.149687	0.507596	0.355291
H	-6.154161	1.194403	1.211559
H	-4.032707	1.664733	1.114263
C	-2.936873	1.876318	-0.732523
H	-3.442192	2.819095	-0.968621
H	-2.817075	1.315591	-1.667481
O	-6.173668	-0.777916	0.945048
C	-6.266217	-1.887761	0.029195
C	-6.277325	-3.154415	0.868597
H	-5.358637	-3.232688	1.456556
H	-6.355842	-4.029651	0.219581
H	-7.129643	-3.149194	1.555476
H	-5.389225	-1.886299	-0.632296
C	-7.517010	-1.738035	-0.846058
H	-8.409853	-1.776500	-0.204522
O	-7.529220	-2.795755	-1.797052
H	-8.197399	-2.538834	-2.450840
C	-7.491030	-0.387559	-1.557610
O	-8.665258	-0.328717	-2.365261
H	-8.527190	0.330097	-3.058493
H	-6.590932	-0.352909	-2.185949
C	-7.391096	0.749091	-0.533761
O	-8.571497	0.756396	0.251632
C	-8.886931	2.015042	0.824413
H	-8.124635	2.357750	1.537998
H	-9.831225	1.892430	1.359089
H	-9.011379	2.787515	0.051649
H	-7.266528	1.712076	-1.051046

Statistical Thermodynamic Analysis
Temperature= 298.150 Kelvin Pressure= 1.00000 Atm
==========
SCF Energy= -2116.30742873 Predicted Change= -3.359975D-09
Zero-point correction (ZPE)= -2115.4747 0.83265
Internal Energy (U)= -2115.4286 0.87876
Enthalpy (H)= -2115.4277
0.87970
Gibbs Free Energy (G)= -2115.5566
0.75076

Frequencies -- 11.0386 16.4826 21.1544

NMR-Shifts
Revised-MandelalideA-0006-NMR.txt

Atom	Type	Isotropic	Scaled Shift
1	C	99.3012	83.040257279
2	C	110.9573	71.8837458604
3	C	151.9025	32.6934857099
6	C	111.7073	71.1658913838
8	C	116.0531	67.006355405
14	C	8.1554	170.279484676
16	C	58.9119	121.698443691
18	C	24.1759	154.945634488
20	C	143.4797	40.7552786233
23	C	109.0629	73.6969505542
29	C	149.1356	35.3417944448
32	C	145.1973	39.111296158
34	C	172.5342	12.9460747717
38	C	101.0939	81.3243936523
42	C	111.9797	70.905166638
44	C	141.3073	42.834568043
45	C	148.7633	35.6981374069
47	C	169.2154	16.1226286874
51	C	35.8735	143.749401788
53	C	57.0600	123.470969965
55	C	49.4736	130.732211566
57	C	51.4243	128.86511993
59	C	151.2219	33.3449147189
64	C	144.0489	40.2104749325
67	C	103.7657	78.767108865
69	C	83.8040	97.8732364708
72	C	145.6424	38.6852734547
76	C	113.9478	69.0214207776
77	C	168.7695	16.5494171022
82	C	112.8750	70.0482398208
86	C	111.7415	71.1331572197

90	C	102.2588	80.2094220793
92	C	128.2634	55.3193973851
4	H	30.3428	1.38581658582
5	H	30.4677	1.27040887041
7	H	25.9916	5.40632940633
10	H	29.4674	2.19468699469
11	H	28.2766	3.29498729499
12	H	27.9436	3.60267960268
17	H	25.3998	5.95315315315
19	H	23.9949	7.25128205128
21	H	29.2629	2.38364518365
22	H	29.3097	2.3404019404
24	H	28.0216	3.53060753061
26	H	29.3207	2.33023793024
27	H	27.9863	3.56322476322
28	H	28.0184	3.53356433356
30	H	30.3120	1.41427581428
31	H	29.9366	1.76114576115
33	H	29.1568	2.48168168168
35	H	30.5692	1.17662277662
36	H	31.0114	0.76802956803
37	H	30.6896	1.06537306537
39	H	27.7380	3.79265419265
43	H	28.3454	3.23141603142
46	H	29.1193	2.51633171633
48	H	31.2016	0.592284592285
49	H	30.5271	1.21552321552
50	H	30.9482	0.826426426426
52	H	25.8037	5.57994917995
54	H	25.1027	6.22767382767
56	H	25.0864	6.24273504274
58	H	26.1318	5.27678447678
60	H	29.8990	1.79588819589
61	H	29.3086	2.34141834142
62	H	30.3417	1.38683298683
63	H	30.6084	1.1404019404
65	H	29.4987	2.16576576577
66	H	30.5812	1.16553476553
70	H	26.6188	4.8267960268
71	H	28.0293	3.52349272349
73	H	29.9659	1.73407253407
74	H	30.5003	1.24028644029
78	H	30.6549	1.09743589744
79	H	30.2572	1.46491106491
80	H	30.8123	0.951998151998
81	H	27.9746	3.57403557404
83	H	28.1242	3.43580503581
85	H	29.5268	2.1398013398
88	H	30.9405	0.833541233541
89	H	27.8468	3.69212289212
93	H	28.2692	3.30182490182
94	H	28.1931	3.37214137214
95	H	28.6419	2.95744975745
96	H	28.4780	3.10889350889

Supporting Information: Revised-MandelalideA-0007.log

Using Gaussian 09: AM64L-G09RevC.01 23-Sep-2011

==========

#b3lyp/6-31G(d,p) scf=(maxcycle=300,direct,tight) density=current SCRF=(PCM,SOLVENT=Chloroform) opt=(maxcycle=250) freq=noraman

#N Geom=AllCheck Guess=TCheck SCRF=Check GenChk RB3LYP/6-31G(d,p) Freq

---

Pointgroup= C1 Stoichiometry= C33H52O11 C1[X(C33H52O11)] #Atoms= 96

Charge = 0 Multiplicity = 1

SCF Energy= -2116.30572945 Predicted Change= -1.459922D-08

==========

Optimization completed. {Found 1 times}

Item	Max Val.	Criteria	Pass?	RMS Val.	Criteria	Pass?
Force	0.00002 ||	0.00045	[YES]	0.00000 ||	0.00030	[YES]
Displ	0.00198 ||	0.00180	[NO]	0.00198 ||	0.00180	[YES]

Atomic Type	Coordinates (Angstroms) X	Y	Z
C	6.630758	-1.047055	-0.393948
C	5.794115	0.155867	0.052133
C	6.279675	1.460113	-0.576535
H	6.282205	1.365163	-1.668995
H	7.310155	1.651247	-0.258721
C	5.451779	2.679520	-0.190860
H	5.303757	2.714689	0.891870
C	6.077097	3.998144	-0.668522
O	7.359784	4.216689	-0.094375
H	7.233771	4.384573	0.849863
H	5.387934	4.822482	-0.446637
H	6.224441	3.960090	-1.752966
O	4.150057	2.532327	-0.820555
C	3.091232	3.128856	-0.218118
O	3.183166	3.817730	0.784085
C	1.839197	2.810448	-0.936630
H	1.921925	2.196415	-1.828256
C	0.657018	3.239352	-0.477615
H	0.656195	3.841589	0.430595
C	-0.673849	2.941804	-1.097314
H	-0.553132	2.330114	-1.997788
H	-1.156257	3.882300	-1.396627
C	-1.614460	2.223581	-0.120031
H	-1.733067	2.849400	0.782597
O	5.872613	0.297625	1.468590
H	5.667847	-0.580399	1.825319
H	4.750070	-0.028917	-0.249807
H	7.690395	-0.831611	-0.187423
C	6.438661	-1.494261	-1.843930
H	5.418718	-1.273224	-2.185051
H	7.134825	-1.005553	-2.530425
C	6.660573	-3.012531	-1.757862
H	7.740931	-3.182171	-1.658975
C	6.161234	-3.810085	-2.962102
H	6.302810	-4.886525	-2.817332
H	6.714727	-3.524017	-3.862198
H	5.099102	-3.631344	-3.156780
C	6.037767	-3.355672	-0.381551
H	6.597174	-4.172093	0.094544
O	6.239139	-2.174788	0.420923
O	-0.974610	1.003259	0.246496
C	-1.690373	0.261463	1.240174
H	-1.820127	0.903046	2.128355
C	-0.833788	-0.951929	1.605437
C	0.620933	-0.616758	2.021368
H	1.079123	-0.079232	1.184049
C	0.683504	0.287883	3.266421
H	1.722586	0.486282	3.545928
H	0.189482	-0.185147	4.123987
H	0.199436	1.252045	3.085921
C	1.400197	-1.884187	2.257317
H	1.141851	-2.444345	3.159452
C	2.368960	-2.363448	1.457211
H	2.622562	-1.806592	0.556246
C	3.115632	-3.582048	1.737296
H	2.877224	-4.063057	2.686132
C	4.054261	-4.164062	0.967409

H	4.525406	-5.068218	1.353635
C	4.544672	-3.736255	-0.388542
H	4.416236	-4.582359	-1.077761
H	3.955916	-2.906435	-0.791011
H	-0.802435	-1.626627	0.741386
H	-1.337809	-1.496689	2.414791
C	-3.077372	-0.127271	0.709814
H	-3.644456	-0.660191	1.478292
H	-2.955594	-0.799582	-0.148396
C	-3.847197	1.117976	0.252449
O	-5.069614	0.797746	-0.431580
C	-6.196352	0.530927	0.369585
H	-6.212743	1.200050	1.239588
H	-4.093581	1.732414	1.133400
C	-2.999858	1.945214	-0.715928
H	-3.511017	2.884852	-0.951669
H	-2.883902	1.382847	-1.650348
O	-6.198333	-0.768275	0.935185
C	-6.279142	-1.857183	-0.006301
C	-6.268474	-3.141964	0.806161
H	-5.355290	-3.209950	1.403436
H	-6.305655	-4.009798	0.141563
H	-7.127712	-3.176999	1.483883
H	-5.403861	-1.830189	-0.669714
C	-7.535740	-1.698773	-0.878622
H	-8.432161	-1.769740	-0.250327
O	-7.573330	-2.672725	-1.928835
H	-8.014932	-3.463955	-1.595798
C	-7.524774	-0.333818	-1.562860
O	-8.671432	-0.149857	-2.375311
H	-8.753678	-0.974792	-2.878069
H	-6.607935	-0.270877	-2.169928
C	-7.444916	0.768361	-0.508811
O	-8.616778	0.723610	0.292098
C	-8.987926	1.972757	0.851962
H	-9.176839	2.722466	0.070469
H	-8.226730	2.370177	1.538373
H	-9.908914	1.807267	1.415266
H	-7.352529	1.744601	-1.003612

Statistical Thermodynamic Analysis
Temperature= 298.150 Kelvin Pressure= 1.00000 Atm
==========
==========
SCF Energy= -2116.30572945 Predicted Change= -1.459922D-08
Zero-point correction (ZPE)= -2115.4732 0.83248
Internal Energy (U)= -2115.4269 0.87878
Enthalpy (H)= -2115.4259
0.87973
Gibbs Free Energy (G)= -2115.5554
0.75025

Frequencies -- 12.0577 18.2331 18.9764

NMR-Shifts
Revised-MandelalideA-0007-NMR.txt

Atom	Type	Isotropic	Scaled Shift
1	C	99.2971	83.0441815502
2	C	110.7279	72.1033136163
3	C	151.2511	33.3169662513
6	C	112.4434	70.4613411436
8	C	120.8654	62.4003139417
14	C	12.3546	166.260265319
16	C	58.8686	121.739887823
18	C	25.7780	153.412201612
20	C	143.5756	40.6634889642
23	C	109.0771	73.6833591761
29	C	149.4061	35.0828882636
32	C	144.9543	39.3438810084
34	C	172.5707	12.9111391872
38	C	101.0024	81.4119718984
42	C	112.0686	70.820076954
44	C	141.2985	42.8429908689
45	C	148.8358	35.6287448075
47	C	169.1957	16.1414843316
51	C	36.0657	143.565439614
53	C	57.0240	123.50542698
55	C	49.6226	130.58959781
57	C	51.3808	128.906755489
59	C	151.4205	33.1548268535
64	C	143.9360	40.3185359597
67	C	103.9627	78.5785524225
69	C	83.9561	97.727655583
72	C	145.7584	38.5742452957
76	C	114.1102	68.8659813549
77	C	169.6133	15.7417829591
82	C	109.7430	73.0460001149
86	C	114.5891	68.4076073432
90	C	103.6333	78.8938341086
92	C	128.3069	55.2777618255
4	H	30.3923	1.34007854008
5	H	29.6648	2.01228921229
7	H	26.5518	4.8887040887
10	H	31.2429	0.554123354123
11	H	27.6069	3.91379071379
12	H	28.6867	2.91605451605
17	H	25.4871	5.87248787249
19	H	24.1227	7.13319473319
21	H	29.2879	2.36054516055
22	H	29.3558	2.29780549781
24	H	28.0445	3.50944790945
26	H	29.4368	2.22296142296
27	H	27.9932	3.55684915685
28	H	27.9194	3.62504042504
30	H	30.3208	1.40614460614
31	H	29.8935	1.80097020097
33	H	29.1144	2.52085932086
35	H	30.6596	1.09309309309
36	H	30.5491	1.1951951952
37	H	30.9938	0.784291984292
39	H	27.6772	3.84883344883
43	H	28.3575	3.22023562024
46	H	29.1575	2.48103488103
48	H	30.9540	0.821067221067
49	H	31.2018	0.5920997921
50	H	30.5510	1.19343959344
52	H	25.8444	5.54234234234
54	H	25.0478	6.2784014784
56	H	25.1747	6.16114576115
58	H	26.1465	5.2632016632
60	H	29.8655	1.82684222684
61	H	29.3223	2.32875952876
62	H	30.3590	1.37084777085
63	H	30.6254	1.12469392469
65	H	29.5067	2.15837375837
66	H	30.5927	1.15490875491
70	H	26.6439	4.8036036036
71	H	28.0120	3.53947793948
73	H	29.9418	1.75634095634
74	H	30.4898	1.24998844999
78	H	30.5847	1.1623007623
79	H	30.4968	1.24352044352
80	H	30.8826	0.887040887041
81	H	28.0718	3.48422268422
83	H	28.1450	3.41658581659
85	H	30.4090	1.32464772465
88	H	29.4700	2.19228459228
89	H	27.8541	3.68537768538

93	H	28.5562	3.03663663664
94	H	28.2968	3.27632247632
95	H	28.2466	3.32270732271
96	H	28.2130	3.35375375375

Supporting Information: Revised-MandelalideA-0008.log

```
-----------------------------------------------------------------------
 Using  Gaussian 09:  AM64L-G09RevC.01 23-Sep-2011
=======================================================================
 #b3lyp/6-31G(d,p) scf=(maxcycle=300,direct,tight) density=current
 SCRF=(PCM,SOLVENT=Chloroform) opt=(maxcycle=250)
freq=noraman
 #N Geom=AllCheck Guess=TCheck SCRF=Check GenChk RB3LYP/6-
31G(d,p) Freq
-----------------------------------------------------------------------
 Pointgroup= C1   Stoichiometry= C33H52O11   C1[X(C33H52O11)]
#Atoms= 96
 Charge = 0                Multiplicity = 1
-----------------------------------------------------------------------
 SCF Energy= -2116.30276511      Predicted Change= -1.252820D-08
=======================================================================
 Optimization completed.          {Found       1       times}
 Item     Max Val.    Criteria    Pass?     RMS Val.    Criteria    Pass?
 Force     0.00000 ||  0.00045   [ YES ]     0.00000 ||  0.00030   [ YES ]
 Displ     0.00199 ||  0.00180   [ NO ]      0.00199 ||  0.00180   [ YES ]
-----------------------------------------------------------------------
     Atomic      Coordinates (Angstroms)
      Type      X                Y                Z
-----------------------------------------------------------------------
      C       6.595782     -0.594921     -0.529161
      C       5.741445      0.481489      0.148522
      C       6.046485      1.878829     -0.412514
      H       5.948962      1.893001     -1.501996
      H       7.091553      2.133034     -0.187391
      C       5.161261      2.972717      0.174470
      H       5.145016      2.912370      1.264906
      C       5.564971      4.381916     -0.257884
      O       5.587772      4.536013     -1.672055
      H       4.697742      4.321758     -1.986423
      H       6.579116      4.590185      0.097625
      H       4.888114      5.106805      0.214679
      O       3.810690      2.718363     -0.319604
      C       2.768891      3.077737      0.476330
      O       2.902323      3.625926      1.556288
      C       1.485623      2.704531     -0.154999
      H       1.533238      2.234472     -1.132620
      C       0.321864      2.923543      0.469650
      H       0.355568      3.390206      1.453833
      C      -1.030435      2.569300     -0.068154
      H      -0.947051      2.118642     -1.062880
      H      -1.630470      3.484103     -0.167786
      C      -1.793068      1.610634      0.855864
      H      -1.848784      2.057208      1.864679
      O       5.889833      0.458567      1.568361
      H       6.831480      0.565527      1.767591
      H       4.687621      0.238348     -0.026452
      H       7.659195     -0.363781     -0.333755
      C       6.373665     -0.751852     -2.036523
      H       5.317000     -0.589257     -2.287076
      H       6.971789     -0.055881     -2.630256
      C       6.762152     -2.218383     -2.271939
      H       7.858638     -2.276410     -2.247824
      C       6.286582     -2.808109     -3.599493
      H       6.753044     -2.280222     -4.437553
      H       5.201818     -2.721997     -3.717488
      H       6.553874     -3.866646     -3.688600
      C       6.254982     -2.900837     -0.974174
      H       6.950361     -3.697016     -0.673405
      O       6.293409     -1.877807      0.039850
      O      -1.029673      0.407403      0.925368
      C      -1.559966     -0.550617      1.846741
      H      -1.621120     -0.081973      2.843406
      C      -0.586644     -1.728879      1.889596
      C       0.879557     -1.351878      2.219359
      H       1.204454     -0.624634      1.467070
      C       1.020531     -0.702531      3.609397
      H       0.668101     -1.378032      4.398529
      H       0.447054      0.226587      3.678266
      H       2.067626     -0.462828      3.816026
      C       1.760999     -2.569262      2.118443
      H       1.607171     -3.334899      2.883100
      C       2.704818     -2.773109      1.182996
      H       2.861188     -2.007832      0.424368
      C       3.555234     -3.954211      1.140273
      H       3.421334     -4.652235      1.966978
      C       4.477307     -4.264943      0.210150
      H       5.044495     -5.184253      0.357516
      C       4.836623     -3.501480     -1.035213
      H       4.800394     -4.199394     -1.882570
      H       4.115124     -2.706022     -1.244979
      H      -0.607844     -2.228822      0.913553
      H      -0.958653     -2.454334      2.625398
      C      -2.977718     -0.963367      1.418906
      H      -3.409078     -1.653138      2.152601
      H      -2.905533     -1.491606      0.460548
      C      -3.870170      0.276931      1.284146
      O      -5.231264     -0.052684      0.942216
      C      -5.509856     -0.549095     -0.348215
      H      -4.688386     -1.164632     -0.729284
      H      -3.977603      0.725483      2.279605
      C      -3.217430      1.315901      0.364175
      H      -3.812011      2.235559      0.355633
      H      -3.169776      0.941392     -0.663368
      O      -5.659231      0.470571     -1.316335
      C      -6.743253      1.392093     -1.081088
      C      -6.687361      2.435363     -2.184411
      H      -6.788576      1.959795     -3.165276
      H      -5.734619      2.971421     -2.156683
      H      -7.500591      3.154112     -2.059234
      H      -6.606557      1.873243     -0.103425
      C      -8.058721      0.608052     -1.055210
      H      -8.190880      0.128275     -2.038295
      O      -9.128785      1.503278     -0.782363
      H      -9.886587      0.937537     -0.567657
      C      -8.002638     -0.486999      0.015528
      O      -9.219283     -1.228604      0.027731
      H      -9.143409     -1.846032     -0.718571
      H      -7.916229     -0.009175      0.996593
      C      -6.791900     -1.397513     -0.204243
      O      -7.068774     -2.141292     -1.388874
      C      -6.393816     -3.390064     -1.479600
      H      -6.621134     -4.029861     -0.615992
      H      -5.305402     -3.267515     -1.549811
      H      -6.749324     -3.876214     -2.390184
      H      -6.672379     -2.078217      0.649282
-----------------------------------------------------------------------
 Statistical Thermodynamic Analysis
 Temperature= 298.150 Kelvin      Pressure= 1.00000 Atm
=======================================================================
 SCF Energy=     -2116.30276511   Predicted Change= -1.252820D-08
 Zero-point correction (ZPE)=          -2115.4703            0.83245
 Internal Energy (U)=                  -2115.4241            0.87865
 Enthalpy (H)=                                      -2115.4231
0.87960
```

Gibbs Free Energy (G)= -2115.5523
0.75036

Frequencies -- 13.0283 19.5031 20.3414

NMR-Shifts
Revised-MandelalideA-0008-NMR.txt

Atom	Type	Isotropic	Scaled Shift
1	C	97.3229	84.9337659603
2	C	109.3826	73.3909531193
3	C	148.3986	36.0472061104
6	C	111.7779	71.0983173491
8	C	119.2621	63.9348953847
14	C	12.6335	165.993319168
16	C	59.6926	120.951205038
18	C	25.2472	153.920251153
20	C	143.4049	40.826872643
23	C	108.4743	74.2603227474
29	C	146.8443	37.5348877276
32	C	144.6337	39.6507398687
34	C	172.5088	12.97038611
38	C	101.0800	81.3376978886
42	C	111.2910	71.5643484753
44	C	141.0814	43.0507858114
45	C	148.6156	35.8395068818
47	C	168.8203	16.5007944256
51	C	38.3935	141.337410747
53	C	55.5396	124.92620456
55	C	49.3723	130.829169777
57	C	50.5875	129.666054098
59	C	152.8508	31.7858305098
64	C	149.0825	35.3926185417
67	C	107.2304	75.4509083252
69	C	93.1816	88.8975669519
72	C	145.5810	38.7440418078
76	C	114.9741	68.0391087119
77	C	168.5614	16.7485977909
82	C	110.0301	72.7712054212
86	C	112.2062	70.688374586
90	C	101.8181	80.6312333697
92	C	128.1666	55.4120484695
4	H	29.4721	2.19034419034
5	H	30.6295	1.12090552091
7	H	26.2178	5.19732039732
10	H	30.9988	0.779671979672
11	H	28.4271	3.15592515593
12	H	27.5827	3.93615153615
17	H	25.3690	5.98161238161
19	H	24.1446	7.11295911296
21	H	29.2305	2.41358281358
22	H	29.2723	2.37495957496
24	H	28.1932	3.37204897205
26	H	32.1784	-0.31027951028
27	H	28.3424	3.23418803419
28	H	27.8377	3.70053130053
30	H	30.3981	1.33471933472
31	H	29.8374	1.85280665281
33	H	29.1104	2.52455532456
35	H	30.5302	1.21265881266
36	H	30.9026	0.868560868561
37	H	30.7300	1.02804342804
39	H	27.6847	3.8419034419
43	H	28.2791	3.29267729268
46	H	29.1785	2.46163086163
48	H	31.2566	0.541464541465
49	H	30.6920	1.06315546316
50	H	30.8368	0.92936012936
52	H	25.9151	5.47701547702
54	H	25.0246	6.29983829984
56	H	25.2862	6.05811965812
58	H	26.1580	5.25257565258
60	H	29.9349	1.76271656272
61	H	29.2572	2.38891198891
62	H	30.3169	1.40974820975
63	H	30.5623	1.182998383
65	H	30.2612	1.46121506122
66	H	30.2109	1.50769230769
70	H	26.3817	5.04587664588
71	H	27.7324	3.79782859783
73	H	29.8723	1.82055902056
74	H	29.9591	1.74035574036
78	H	30.8838	0.885932085932
79	H	30.6427	1.10870870871
80	H	30.1931	1.52413952414
81	H	27.8577	3.68205128205
83	H	28.4107	3.17107877108
85	H	29.7601	1.92423192423
88	H	29.9355	1.76216216216
89	H	28.0583	3.4966966967
93	H	28.5964	2.99949179949
94	H	28.1788	3.38535458535
95	H	28.1349	3.42591822592
96	H	28.3074	3.26652806653

Mandelalide A Original Configuration (DFT Methodologies)

Supporting Information: Original-MandelalideA-0001.log

Using Gaussian 09: AM64L-G09RevC.01 23-Sep-2011
==========
#b3lyp/6-31G(d,p) scf=(maxcycle=300,direct,tight) density=current SCRF=(PCM,SOLVENT=Chloroform) opt=(maxcycle=250) freq=noraman
#N Geom=AllCheck Guess=TCheck SCRF=Check GenChk RB3LYP/6-31G(d,p) Freq
---
Pointgroup= C1 Stoichiometry= C33H52O11 C1[X(C33H52O11)]
#Atoms= 96
Charge = 0 Multiplicity = 1

SCF Energy= -2116.30657338 Predicted Change= -1.690618D-08
==========
Optimization completed. {Found 1 times}

Item	Max Val.	Criteria	Pass?	RMS Val.	Criteria	Pass?
Force	0.00000 ||	0.00045	[YES]	0.00000 ||	0.00030	[YES]
Displ	0.00247 ||	0.00180	[NO]	0.00247 ||	0.00180	[YES]

Atomic Type	Coordinates (Angstroms) X	Y	Z
C	-6.903458	0.359796	0.960922
C	-5.551751	1.054907	0.769878
C	-5.681099	2.559114	0.539201
H	-6.260501	3.015987	1.348355
H	-6.228988	2.732252	-0.395138
C	-4.334650	3.275780	0.480960
H	-3.807176	3.164981	1.429397
C	-4.452228	4.759107	0.132971
O	-5.239994	5.377199	1.144195
H	-5.263400	6.325285	0.961973
H	-4.914094	4.859995	-0.861721
H	-3.443265	5.189232	0.087080
O	-3.545006	2.629295	-0.553031

C	-2.201225	2.584862	-0.374789
O	-1.616074	3.180768	0.513286
C	-1.570716	1.711709	-1.387608
H	-2.229827	1.218220	-2.095730
C	-0.245501	1.522132	-1.399162
H	0.340700	2.055278	-0.653517
C	0.483295	0.646744	-2.374279
H	0.994963	1.279736	-3.113785
H	-0.232560	0.029223	-2.926207
C	1.549981	-0.260267	-1.741017
H	1.924128	-0.932671	-2.532525
O	-4.749160	0.848172	1.929480
H	-4.755993	-0.110728	2.073512
H	-5.063130	0.602419	-0.107009
H	-7.407515	0.815064	1.824993
C	-7.823625	0.324020	-0.266639
H	-8.581016	1.111646	-0.241002
H	-7.246536	0.450654	-1.191748
C	-8.434508	-1.088415	-0.206729
H	-9.210958	-1.083767	0.569411
C	-9.058463	-1.581702	-1.511677
H	-9.910164	-0.952535	-1.789674
H	-9.425695	-2.609188	-1.415405
H	-8.343760	-1.554584	-2.340259
C	-7.256196	-1.910864	0.361697
H	-7.616854	-2.772026	0.938478
O	-6.634891	-1.021293	1.304991
O	0.906972	-1.043049	-0.733840
C	1.763825	-2.029302	-0.139977
H	2.118159	-2.706456	-0.938174
C	0.961917	-2.840536	0.878619
C	-0.082291	-3.837918	0.307222
H	0.386705	-4.303119	-0.576561
C	-0.353896	-4.959105	1.320591
H	-0.794117	-4.562997	2.242563
H	0.577438	-5.468819	1.586296
H	-1.040224	-5.708996	0.915977
C	-1.333874	-3.141211	-0.175837
H	-1.158539	-2.310171	-0.856364
C	-2.601289	-3.446192	0.154655
H	-2.806277	-4.264382	0.843221
C	-3.767573	-2.753539	-0.375597
H	-3.572297	-1.926750	-1.060265
C	-5.041126	-3.082980	-0.099186
H	-5.232210	-3.911389	0.585462
C	-6.249955	-2.417958	-0.690609
H	-5.937450	-1.596705	-1.345933
H	-6.784407	-3.141377	-1.324263
H	0.478896	-2.149027	1.579656
H	1.691866	-3.417642	1.459066
C	2.985092	-1.355346	0.505063
H	3.662503	-2.117238	0.904952
H	2.652699	-0.730648	1.343302
C	3.724616	-0.480764	-0.502027
O	4.771926	0.202813	0.210020
C	5.851851	0.653114	-0.579053
H	5.498151	1.220406	-1.448771
H	4.181444	-1.116244	-1.272649
C	2.749237	0.502545	-1.156133
H	3.239077	1.071807	-1.954321
H	2.412264	1.212706	-0.393173
O	6.601581	-0.404118	-1.141507
C	7.268833	-1.265934	-0.194618
C	7.966922	-2.350607	-0.997481
H	8.690024	-1.907674	-1.689709
H	7.239847	-2.926189	-1.577154
H	8.497418	-3.028178	-0.324498
H	6.524752	-1.716845	0.475915
C	8.229313	-0.421538	0.648020
H	8.971099	0.032103	-0.029193
O	8.864862	-1.257772	1.605544
H	9.279229	-0.651321	2.238882
C	7.464767	0.701857	1.355841
O	8.358343	1.493703	2.133075
H	8.785586	2.088295	1.494352
H	6.754294	0.250622	2.055620
C	6.695980	1.554628	0.343593
O	7.679857	2.281776	-0.388478
C	7.217263	3.500957	-0.957393
H	6.449635	3.333369	-1.723696
H	8.079993	3.978511	-1.425922
H	6.806943	4.169227	-0.188199
H	6.025018	2.248145	0.867697

Statistical Thermodynamic Analysis
Temperature= 298.150 Kelvin Pressure= 1.00000 Atm
==========
==========
SCF Energy= -2116.30657338 Predicted Change= -1.690618D-08
Zero-point correction (ZPE)= -2115.4740 0.83254
Internal Energy (U)= -2115.4277 0.87883
Enthalpy (H)= -2115.4267
0.87977
Gibbs Free Energy (G)= -2115.5568
0.74970

Frequencies -- 9.9722 13.2949 17.6112

NMR-Shifts
Original-MandelalideA-0001-NMR.txt

Atom	Type	Isotropic	Scaled Shift
1	C	99.0143	83.3148605448
2	C	110.3054	72.5077049714
3	C	152.0166	32.5842761155
6	C	114.2365	68.7450946611
8	C	120.4522	62.7958039013
14	C	12.4937	166.127127242
16	C	58.5471	122.047608109
18	C	28.4153	150.887938131
20	C	145.8079	38.5268669002
23	C	109.2769	73.4921227435
29	C	151.3424	33.229579433
32	C	144.1872	40.078102567
34	C	172.9192	12.5775761404
38	C	101.4182	81.0139933766
42	C	104.0077	78.5354811539
44	C	140.4893	43.6175079921
45	C	145.6787	38.650529298
47	C	167.6656	17.6060031777
51	C	41.9723	137.912000613
53	C	52.2915	128.035088727
55	C	46.2541	133.813721549
57	C	50.2869	129.953770172
59	C	147.0118	37.3745668945
64	C	146.0736	38.2725549877
67	C	114.3680	68.6192308429
69	C	92.3655	89.6786883363
72	C	151.4793	33.0985470625
76	C	115.2954	67.7315798541
77	C	168.8800	16.4436532093
82	C	111.0720	71.7739619824
86	C	112.8731	70.0500583855
90	C	103.1709	79.3364153219
92	C	127.7343	55.8258197898
4	H	29.7946	1.89235389235
5	H	30.3615	1.36853776854
7	H	26.4593	4.97417417417
10	H	31.2149	0.579995379995

11	H	28.3050	3.26874566875
12	H	27.5398	3.97579117579
17	H	25.3098	6.03631323631
19	H	23.7731	7.45622545623
21	H	29.3364	2.31573111573
22	H	28.7057	2.8984984985
24	H	27.9754	3.5732963733
26	H	29.4938	2.17029337029
27	H	28.1079	3.45086625087
28	H	27.9823	3.56692076692
30	H	29.8875	1.80651420651
31	H	30.4577	1.27964887965
33	H	29.1429	2.49452529453
35	H	30.5338	1.20933240933
36	H	30.6185	1.13106953107
37	H	30.9984	0.780041580042
39	H	27.6085	3.91231231231
43	H	28.0662	3.4893970894
46	H	29.4217	2.23691383691
48	H	30.8309	0.934811734812
49	H	30.9942	0.783922383922
50	H	30.5318	1.21118041118
52	H	24.7746	6.53083853084
54	H	25.4707	5.88764148764
56	H	25.1350	6.19782859783
58	H	25.8052	5.57856317856
60	H	29.8261	1.86324786325
61	H	29.5103	2.15504735505
62	H	30.3518	1.3775005775
63	H	30.3611	1.36890736891
65	H	30.0349	1.67031647032
66	H	30.5557	1.1890967891
70	H	26.3452	5.0796026796
71	H	27.4076	4.09794409794
73	H	29.7013	1.97856317856
74	H	30.2193	1.49993069993
78	H	30.8668	0.90164010164
79	H	30.5306	1.21228921229
80	H	30.3094	1.41667821668
81	H	28.0076	3.54354354354
83	H	28.3183	3.25645645646
85	H	29.6206	2.05313005313
88	H	29.9749	1.72575652576
89	H	28.2054	3.36077616078
93	H	28.1680	3.39533379533
94	H	28.1240	3.43598983599
95	H	28.5752	3.01908061908
96	H	28.3417	3.23483483483

Supporting Information: Original-MandelalideA-0002.log

Using Gaussian 09: AM64L-G09RevC.01 23-Sep-2011

==========

#b3lyp/6-31G(d,p) scf=(maxcycle=300,direct,tight) density=current SCRF=(PCM,SOLVENT=Chloroform) opt=(maxcycle=250) freq=noraman

#N Geom=AllCheck Guess=TCheck SCRF=Check GenChk RB3LYP/6-31G(d,p) Freq

---

Pointgroup= C1 Stoichiometry= C33H52O11 C1[X(C33H52O11)]

#Atoms= 96

Charge = 0 Multiplicity = 1

SCF Energy= -2116.30925954 Predicted Change= -9.573206D-10

==========

Optimization completed. {Found 2 times}

Item	Max Val.	Criteria	Pass?	RMS Val.	Criteria	Pass?
Force	0.00000	0.00045	YES	0.00000	0.00030	YES
Displ	0.00080	0.00180	YES	0.00080	0.00180	YES

Atomic Type	Coordinates (Angstroms) X	Y	Z
C	-6.770862	0.438953	1.159387
C	-5.419608	1.156831	1.106602
C	-5.550485	2.576655	0.562325
H	-6.221914	3.140892	1.221231
H	-6.009575	2.561517	-0.430743
C	-4.232863	3.341504	0.485331
H	-3.705228	3.305156	1.440383
C	-4.412428	4.797258	0.052135
O	-5.071351	4.916508	-1.203708
H	-4.535415	4.425203	-1.842655
H	-3.430638	5.289166	0.038762
H	-5.037476	5.315786	0.785924
O	-3.410507	2.670340	-0.519091
C	-2.061080	2.767961	-0.390521
O	-1.511806	3.385122	0.505651
C	-1.380467	2.035446	-1.479419
H	-2.009726	1.513466	-2.194084
C	-0.044455	2.019993	-1.568012
H	0.513877	2.567467	-0.811006
C	0.733225	1.310706	-2.635936
H	1.320214	2.042218	-3.208156
H	0.045369	0.825176	-3.335352
C	1.708266	0.249026	-2.094707
H	2.134737	-0.284075	-2.962391
O	-4.870429	1.245614	2.420350
H	-4.909733	0.345781	2.777901
H	-4.749927	0.570472	0.458117
H	-7.478757	1.062453	1.729849
C	-7.376076	0.035276	-0.184063
H	-7.977927	0.830630	-0.631822
H	-6.585109	-0.231518	-0.896085
C	-8.218796	-1.196278	0.189406
H	-9.149356	-0.825094	0.638335
C	-8.602383	-2.101990	-0.981604
H	-7.725097	-2.475968	-1.518259
H	-9.218183	-1.550445	-1.699271
H	-9.185650	-2.965929	-0.645657
C	-7.406111	-1.845753	1.349254
H	-8.106491	-2.146026	2.141233
O	-6.566299	-0.796496	1.870256
O	0.927931	-0.658462	-1.322578
C	1.653572	-1.784464	-0.813226
H	2.053059	-2.360167	-1.666585
C	0.641943	-2.624243	-0.033842
C	-0.467198	-3.255167	-0.913385
H	-0.735132	-2.518073	-1.679529
C	0.028955	-4.535834	-1.613226
H	-0.730171	-4.927473	-2.297064
H	0.255671	-5.318383	-0.879533
H	0.939619	-4.348659	-2.192773
C	-1.696750	-3.528248	-0.087144
H	-1.553687	-4.145672	0.802716
C	-2.925346	-3.057021	-0.359706
H	-3.068706	-2.447093	-1.253047
C	-4.100649	-3.281334	0.467988
H	-3.943030	-3.830503	1.397597
C	-5.338666	-2.851939	0.169082
H	-5.487484	-2.312864	-0.766084
C	-6.544395	-3.085317	1.035315
H	-7.206909	-3.835677	0.579219
H	-6.215141	-3.514384	1.988800
H	0.188520	-1.963130	0.713517
H	1.174321	-3.410874	0.516077

C	2.826804	-1.318998	0.059326
H	3.417074	-2.182942	0.383272
H	2.435840	-0.825833	0.957865
C	3.714611	-0.333682	-0.696691
O	4.704988	0.154826	0.226388
C	5.918080	0.579798	-0.355468
H	5.736883	1.245260	-1.208796
H	4.226783	-0.857193	-1.515201
C	2.868155	0.813799	-1.260246
H	3.476135	1.481263	-1.881814
H	2.478367	1.397062	-0.418982
O	6.666102	-0.485933	-0.905713
C	7.127410	-1.475481	0.038898
C	7.857110	-2.543708	-0.757635
H	8.703242	-2.106467	-1.297404
H	7.183825	-3.006125	-1.484834
H	8.234130	-3.316955	-0.084222
H	6.264372	-1.917221	0.555033
C	8.012508	-0.784991	1.081548
H	8.872945	-0.337460	0.558038
O	8.445518	-1.746271	2.034510
H	8.801290	-1.229471	2.774061
C	7.232047	0.332725	1.779788
O	8.054628	0.980548	2.745866
H	8.611046	1.589739	2.232711
H	6.398088	-0.116658	2.328330
C	6.678464	1.327812	0.757196
O	7.803927	2.034540	0.239722
C	7.511713	3.339255	-0.246581
H	8.459518	3.777692	-0.564834
H	7.067928	3.966923	0.538075
H	6.829188	3.315757	-1.105742
H	5.987344	2.025251	1.248654

Statistical Thermodynamic Analysis
Temperature= 298.150 Kelvin Pressure= 1.00000 Atm
==========
==========
SCF Energy= -2116.30925954 Predicted Change= -9.573206D-10
Zero-point correction (ZPE)= -2115.4762 0.83305
Internal Energy (U)= -2115.4301 0.87907
Enthalpy (H)= -2115.4292
0.88001
Gibbs Free Energy (G)= -2115.5583
0.75091

Frequencies -- 10.6695 14.6019 16.7102

NMR-Shifts
Original-MandelalideA-0002-NMR.txt

Atom	Type	Isotropic	Scaled Shift
1	C	99.4552	82.8928578265
2	C	112.2027	70.6917245736
3	C	151.0308	33.5278240395
6	C	111.4623	71.4003905128
8	C	119.3338	63.8662684967
14	C	12.8214	165.813472693
16	C	58.0945	122.480809357
18	C	27.9073	151.374164896
20	C	145.7888	38.5451482609
23	C	109.8949	72.9006106549
29	C	146.9275	37.4552537376
32	C	143.4558	40.7781542526
34	C	172.1138	13.3484561343
38	C	103.1169	79.3881008442
42	C	110.7479	72.0841708302
44	C	141.4880	42.6616129712
45	C	148.6304	35.8253412202
47	C	166.3212	18.8927812554
51	C	40.2872	139.52487605
53	C	52.5260	127.81063956
55	C	45.7252	134.319952526
57	C	50.5958	129.658109841
59	C	148.2907	36.1504814411
64	C	146.3265	38.0304944582
67	C	113.5969	69.3572809587
69	C	91.6913	90.3239916537
72	C	151.3468	33.2253680201
76	C	115.2497	67.7753211202
77	C	168.9349	16.3911062616
82	C	110.5178	72.3044085836
86	C	112.5282	70.3801757308
90	C	102.9866	79.5128160953
92	C	127.9308	55.637741917
4	H	30.4455	1.29092169092
5	H	29.6057	2.0668976669
7	H	26.3779	5.04938784939
10	H	31.0359	0.745391545392
11	H	27.5441	3.97181797182
12	H	28.3703	3.20840840841
17	H	25.4375	5.91831831832
19	H	23.9477	7.29489489489
21	H	29.3587	2.29512589513
22	H	28.9050	2.71434511435
24	H	28.0163	3.5355047355
26	H	29.6540	2.02226842227
27	H	28.3106	3.26357126357
28	H	27.9579	3.58946638947
30	H	29.8313	1.85844305844
31	H	30.5542	1.19048279048
33	H	28.9874	2.63820743821
35	H	30.8507	0.916516516517
36	H	30.4668	1.27124047124
37	H	30.6064	1.14224994225
39	H	27.3892	4.11494571495
43	H	28.1787	3.38544698545
46	H	29.1098	2.52510972511
48	H	30.9402	0.833818433818
49	H	31.1134	0.673781473781
50	H	30.5217	1.22051282051
52	H	25.9621	5.43358743359
54	H	25.6543	5.71799491799
56	H	25.2114	6.12723492723
58	H	25.9140	5.47803187803
60	H	29.3424	2.31018711019
61	H	29.3564	2.29725109725
62	H	30.3430	1.38563178563
63	H	30.5816	1.16516516517
65	H	30.0916	1.61792561793
66	H	30.5895	1.15786555787
70	H	26.4137	5.01630861631
71	H	27.6058	3.91480711481
73	H	29.7412	1.9416955417
74	H	30.3025	1.42305382305
78	H	30.8205	0.944421344421
79	H	30.5541	1.19057519058
80	H	30.2438	1.47729267729
81	H	27.9927	3.55731115731
83	H	28.3534	3.22402402402
85	H	29.6223	2.05155925156
88	H	29.9288	1.76835296835
89	H	28.2355	3.33296373296
93	H	28.1532	3.40900900901
94	H	28.5604	3.03275583276
95	H	28.2202	3.3471009471
96	H	28.2647	3.30598290598

Supporting Information: Original-MandelalideA-0003.log

```
---------------------------------------------------------------------------
 Using  Gaussian 09:  AM64L-G09RevC.01 23-Sep-2011
=============================================================
=====================
 #b3lyp/6-31G(d,p) scf=(maxcycle=300,direct,tight) density=current
 SCRF=(PCM,SOLVENT=Chloroform) opt=(maxcycle=250)
freq=noraman
 #N Geom=AllCheck Guess=TCheck SCRF=Check GenChk RB3LYP/6-
31G(d,p) Freq
---------------------------------------------------------------------------
 Pointgroup= C1   Stoichiometry= C33H52O11   C1[X(C33H52O11)]
#Atoms= 96
 Charge = 0                 Multiplicity = 1
---------------------------------------------------------------------------
 SCF Energy= -2116.30586769      Predicted Change= -1.396748D-09
=============================================================
=====================
 Optimization completed.          {Found       2       times}
 Item      Max Val.    Criteria    Pass?      RMS Val.    Criteria    Pass?
 Force      0.00000 ||  0.00045   [ YES ]      0.00000 ||  0.00030   [ YES ]
 Displ      0.00052 ||  0.00180   [ YES ]      0.00052 ||  0.00180   [ YES ]
---------------------------------------------------------------------------
     Atomic      Coordinates (Angstroms)
      Type      X                  Y                  Z
---------------------------------------------------------------------------
      C      -6.616818      0.492622      1.210884
      C      -5.291034      1.148354      0.814565
      C      -5.431759      2.638567      0.510767
      H      -5.910108      3.151011      1.352098
      H      -6.082427      2.765601     -0.363086
      C      -4.095368      3.330882      0.255584
      H      -3.466951      3.279862      1.146019
      C      -4.243818      4.788435     -0.179000
      O      -4.914230      5.481872      0.867537
      H      -4.948203      6.416756      0.628035
      H      -4.811668      4.826654     -1.121948
      H      -3.244512      5.203339     -0.363809
      O      -3.427579      2.604758     -0.811079
      C      -2.072452      2.559463     -0.777976
      O      -1.392997      3.208197     -0.001133
      C      -1.555743      1.616151     -1.792793
      H      -2.286803      1.081547     -2.392025
      C      -0.238724      1.420729     -1.932760
      H       0.419778      2.000843     -1.289420
      C       0.391300      0.481579     -2.917024
      H       0.845236      1.064768     -3.731342
      H      -0.375382     -0.155150     -3.370010
      C       1.498224     -0.405232     -2.324510
      H       1.806299     -1.119767     -3.107650
      O      -4.353177      0.995423      1.876970
      H      -4.350291      0.047120      2.079040
      H      -4.920011      0.635470     -0.086463
      H      -6.997936      0.998857      2.108954
      C      -7.688377      0.421583      0.115062
      H      -8.420268      1.229228      0.196913
      H      -7.234165      0.486733     -0.882155
      C      -8.313663     -0.969506      0.326389
      H      -8.979618     -0.908213      1.197142
      C      -9.116406     -1.507098     -0.857912
      H      -8.519877     -1.536096     -1.775212
      H      -9.985753     -0.869961     -1.049684
      H      -9.486887     -2.519335     -0.663038
      C      -7.085960     -1.793630      0.774858
      H      -7.382520     -2.618894      1.434594
      O      -6.329230     -0.877209      1.583812
      O       0.927699     -1.131637     -1.234682
      C       1.827297     -2.080148     -0.644173
      H       2.141371     -2.793934     -1.427966
      C       1.091010     -2.851202      0.452123
      C      -0.009203     -3.841904     -0.020366
      H       0.368367     -4.302281     -0.949083
      C      -0.186641     -4.969115      1.007172
      H       0.762095     -5.488973      1.172693
      H      -0.917954     -5.709404      0.669192
      H      -0.526482     -4.576548      1.972150
      C      -1.299151     -3.137104     -0.374212
      H      -1.188846     -2.307829     -1.070190
      C      -2.528432     -3.434023      0.083390
      H      -2.667140     -4.250243      0.790701
      C      -3.738126     -2.733994     -0.326402
      H      -3.608774     -1.913805     -1.034322
      C      -4.978467     -3.048285      0.085550
      H      -5.103760     -3.869167      0.794126
      C      -6.236253     -2.370797     -0.375263
      H      -5.989539     -1.582574     -1.096027
      H      -6.864970     -3.100237     -0.906989
      H       0.671547     -2.136882      1.171023
      H       1.853795     -3.427365      0.989612
      C       3.075938     -1.364471     -0.105243
      H       3.776090     -2.092690      0.312967
      H       2.778386     -0.681199      0.699669
      C       3.753680     -0.557256     -1.215548
      O       4.832409      0.265077     -0.740559
      C       6.075554     -0.368390     -0.544580
      H       6.242863     -1.128089     -1.319230
      H       4.156553     -1.251842     -1.970849
      C       2.741849      0.376178     -1.875050
      H       3.198073      0.879274     -2.734551
      H       2.463404      1.144789     -1.146197
      O       6.160707     -1.085807      0.671134
      C       6.048712     -0.287588      1.868988
      C       6.100525     -1.243349      3.048518
      H       6.025392     -0.683346      3.983503
      H       7.042697     -1.800921      3.048608
      H       5.274369     -1.958009      2.998895
      H       5.088344      0.244717      1.860946
      C       7.177045      0.749115      1.878436
      H       8.138166      0.210010      1.878658
      O       7.053561      1.561173      3.038206
      H       7.635198      2.321052      2.881014
      C       7.105309      1.616409      0.618102
      O       8.156895      2.578222      0.617202
      H       8.944967      2.087641      0.330626
      H       6.166135      2.178570      0.636233
      C       7.141371      0.744549     -0.638138
      O       8.460213      0.206753     -0.707351
      C       8.882960     -0.167105     -2.012850
      H       8.826495      0.680990     -2.708936
      H       8.287462     -0.995062     -2.418184
      H       9.921306     -0.493392     -1.927636
      H       6.936019      1.355310     -1.527391
---------------------------------------------------------------------------
 Statistical Thermodynamic Analysis
 Temperature= 298.150 Kelvin       Pressure= 1.00000 Atm
=============================================================
=====================
 SCF Energy=     -2116.30586769   Predicted Change= -1.396748D-09
 Zero-point correction (ZPE)=          -2115.4733            0.83255
 Internal Energy (U)=                  -2115.4270            0.87878
 Enthalpy (H)=                                   -2115.4261
0.87972
 Gibbs Free Energy (G)=                          -2115.5559
0.74993
---------------------------------------------------------------------------
 Frequencies --     7.7319            14.1111            18.5966
```

NMR-Shifts
Original-MandelalideA-0003-NMR.txt

Atom	Type	Isotropic	Scaled Shift
1	C	97.6568	84.6141771473
2	C	110.9151	71.9241371389
3	C	152.2266	32.3832768621
6	C	113.2169	69.7209938935
8	C	120.1565	63.0788299929
14	C	12.6893	165.939910795
16	C	58.7847	121.820191811
18	C	28.2709	151.026149046
20	C	145.8359	38.5000669998
23	C	109.0660	73.6939834223
29	C	150.8697	33.6820191811
32	C	143.6843	40.5594479221
34	C	173.0706	12.4326652501
38	C	101.9174	80.536189437
42	C	104.1987	78.3526675472
44	C	140.4396	43.6650778154
45	C	145.8271	38.5084898256
47	C	167.5459	17.7205727522
51	C	40.7866	139.046880683
53	C	52.7153	127.629453091
55	C	46.3064	133.763663164
57	C	50.2702	129.969754398
59	C	147.1709	37.2222860315
64	C	144.3934	39.880740443
67	C	103.7632	78.7695017133
69	C	84.6651	97.0490438178
72	C	149.1856	35.2939374797
76	C	114.8381	68.169279657
77	C	169.0676	16.2640938762
82	C	110.2569	72.5541262275
86	C	111.8356	71.0430904114
90	C	102.3000	80.16998794
92	C	128.0869	55.4883324719
4	H	29.8744	1.81861861862
5	H	30.3552	1.37435897436
7	H	26.3907	5.03756063756
10	H	31.2272	0.56863016863
11	H	28.2971	3.27604527605
12	H	27.4547	4.05442365442
17	H	25.3679	5.98262878263
19	H	23.8264	7.40697620698
21	H	29.3120	2.33827673828
22	H	28.7303	2.87576807577
24	H	27.9857	3.56377916378
26	H	29.5912	2.0802956803
27	H	28.1158	3.44356664357
28	H	27.8009	3.73453453453
30	H	29.7411	1.94178794179
31	H	30.4811	1.25802725803
33	H	29.1405	2.49674289674
35	H	31.0168	0.76303996304
36	H	30.5472	1.19695079695
37	H	30.6530	1.09919149919
39	H	27.6160	3.90538230538
43	H	28.2436	3.32547932548
46	H	29.4227	2.23598983599
48	H	30.8796	0.889812889813
49	H	30.5563	1.18854238854
50	H	30.7776	0.984060984061
52	H	24.8210	6.48796488796
54	H	25.4854	5.87405867406
56	H	25.2480	6.09341649342
58	H	25.8995	5.49142989143
60	H	29.8202	1.8686994687
61	H	29.6168	2.05664125664
62	H	30.2952	1.4297990298
63	H	30.4056	1.32778932779
65	H	29.4681	2.19404019404
66	H	30.4442	1.29212289212
70	H	26.5651	4.87641487641
71	H	28.0972	3.46075306075
73	H	30.1030	1.60739200739
74	H	29.9238	1.77297297297
78	H	30.2349	1.48551628552
79	H	30.8508	0.916424116424
80	H	30.5712	1.17477477477
81	H	27.8791	3.66227766228
83	H	28.3301	3.24555324555
85	H	29.6511	2.02494802495
88	H	29.8963	1.79838299838
89	H	28.0949	3.46287826288
93	H	28.5982	2.99782859783
94	H	28.1881	3.37676137676
95	H	28.1536	3.40863940864
96	H	28.1880	3.37685377685

Supporting Information: Original-MandelalideA-0004.log

```
-----------------------------------------------------------------------
 Using  Gaussian 09:  AM64L-G09RevC.01 23-Sep-2011
=======================================================================
 #b3lyp/6-31G(d,p) scf=(maxcycle=300,direct,tight) density=current
 SCRF=(PCM,SOLVENT=Chloroform) opt=(maxcycle=250)
freq=noraman
 #N Geom=AllCheck Guess=TCheck SCRF=Check GenChk RB3LYP/6-
31G(d,p) Freq
-----------------------------------------------------------------------
 Pointgroup= C1   Stoichiometry= C33H52O11   C1[X(C33H52O11)]
#Atoms= 96
 Charge = 0                Multiplicity = 1
-----------------------------------------------------------------------
 SCF Energy= -2116.31009321      Predicted Change= -3.427435D-08
=======================================================================
 Optimization completed.          {Found       1       times}
 Item     Max Val.    Criteria    Pass?      RMS Val.    Criteria    Pass?
 Force     0.00001 ||  0.00045   [ YES ]     0.00000 ||  0.00030   [ YES ]
 Displ     0.00188 ||  0.00180   [ NO ]      0.00188 ||  0.00180   [ YES ]
-----------------------------------------------------------------------
     Atomic      Coordinates (Angstroms)
      Type      X                Y                Z
-----------------------------------------------------------------------
      C      -6.820687      0.512826      1.044644
      C      -5.462121      1.216693      0.989246
      C      -5.567640      2.615297      0.383936
      H      -6.259915      3.205510      0.996395
      H      -5.992025      2.552589     -0.624251
      C      -4.240021      3.365911      0.316848
      H      -3.713733      3.287188      1.271318
      C      -4.440189      4.837218     -0.053016
      O      -3.235851      5.549166     -0.277088
      H      -2.542571      5.127245      0.256190
      H      -5.033611      5.294711      0.755357
      H      -5.033908      4.906249     -0.973392
      O      -3.424789      2.701201     -0.693005
      C      -2.082835      2.765860     -0.559345
      O      -1.516493      3.399424      0.323848
      C      -1.406839      1.976921     -1.607026
      H      -2.039936      1.440912     -2.307408
      C      -0.070025      1.933044     -1.679215
      H       0.490530      2.500873     -0.939181
      C       0.705898      1.169181     -2.709400
      H       1.299896      1.870362     -3.311607
      H       0.017636      0.657143     -3.389119
      C       1.671148      0.127665     -2.114815
      H       2.097439     -0.448785     -2.954337
      O      -4.940136      1.357530      2.308674
```

H	-4.995960	0.474620	2.704352
H	-4.784622	0.598536	0.379361
H	-7.532758	1.165109	1.576578
C	-7.406581	0.058510	-0.291058
H	-7.992291	0.839695	-0.783143
H	-6.606493	-0.246928	-0.976488
C	-8.268837	-1.147180	0.120885
H	-9.201056	-0.747009	0.540481
C	-8.645878	-2.097763	-1.016155
H	-9.244512	-2.939505	-0.652141
H	-7.765168	-2.504841	-1.522080
H	-9.244076	-1.570889	-1.766496
C	-7.479831	-1.756131	1.318307
H	-8.194336	-2.017162	2.111418
O	-6.638033	-0.693197	1.808926
O	0.880926	-0.737366	-1.304550
C	1.596781	-1.844701	-0.742781
H	1.995978	-2.459645	-1.568285
C	0.575941	-2.643408	0.066781
C	-0.526442	-3.312303	-0.793078
H	-0.781741	-2.613491	-1.598591
C	-0.028520	-4.628322	-1.422715
H	0.888197	-4.473061	-2.002248
H	-0.782530	-5.051357	-2.093371
H	0.188713	-5.373814	-0.648616
C	-1.767166	-3.537652	0.030600
H	-1.638373	-4.110709	0.951723
C	-2.989532	-3.074107	-0.280467
H	-3.118617	-2.508992	-1.204887
C	-4.176133	-3.250896	0.542556
H	-4.033161	-3.754031	1.500120
C	-5.407861	-2.830807	0.206639
H	-5.541657	-2.338450	-0.756232
C	-6.625623	-3.015224	1.067776
H	-7.290201	-3.778202	0.636369
H	-6.311583	-3.405657	2.042752
H	0.117558	-1.946502	0.777806
H	1.100719	-3.404708	0.658031
C	2.769706	-1.348128	0.112838
H	3.352608	-2.200348	0.478412
H	2.378567	-0.811593	0.986039
C	3.667568	-0.404805	-0.683776
O	4.658335	0.116160	0.220987
C	5.874074	0.514081	-0.374447
H	5.697413	1.152326	-1.249203
H	4.178354	-0.968413	-1.476038
C	2.831826	0.722136	-1.302155
H	3.446805	1.356103	-1.951233
H	2.444157	1.345870	-0.489442
O	6.615072	-0.573867	-0.889181
C	7.069900	-1.534362	0.087668
C	7.789083	-2.635332	-0.673158
H	7.111010	-3.115352	-1.384311
H	8.159478	-3.389333	0.025224
H	8.638852	-2.224126	-1.227440
H	6.204243	-1.950593	0.620322
C	7.962801	-0.815480	1.103823
H	8.823903	-0.390884	0.562701
O	8.393260	-1.747026	2.087058
H	8.755041	-1.208117	2.807689
C	7.191387	0.329820	1.766560
O	8.020914	1.004932	2.707536
H	8.578989	1.593036	2.172053
H	6.356724	-0.096101	2.332526
C	6.639951	1.293712	0.712871
O	7.767504	1.977680	0.169701
C	7.480827	3.269767	-0.352688
H	6.790999	3.226041	-1.205151
H	8.429140	3.691462	-0.691364
H	7.048061	3.923479	0.416687
H	5.953376	2.010180	1.182812

Statistical Thermodynamic Analysis
Temperature= 298.150 Kelvin Pressure= 1.00000 Atm
==========
SCF Energy= -2116.31009321 Predicted Change= -3.427435D-08
Zero-point correction (ZPE)= -2115.4769 0.83315
Internal Energy (U)= -2115.4310 0.87906
Enthalpy (H)= -2115.4300
0.88000
Gibbs Free Energy (G)= -2115.5586
0.75148

Frequencies -- 12.0460 13.5431 17.1472

NMR-Shifts
Original-MandelalideA-0004-NMR.txt

Atom	Type	Isotropic	Scaled Shift
1	C	99.5797	82.7736939834
2	C	112.7110	70.2052106664
3	C	151.7496	32.8398323092
6	C	112.1853	70.7083787975
8	C	115.7651	67.282011524
14	C	8.3252	170.116962423
16	C	58.0460	122.527230613
18	C	26.7042	152.52569919
20	C	146.0075	38.3358218955
23	C	109.8878	72.9074063439
29	C	147.3917	37.0109496736
32	C	143.1588	41.0624246253
34	C	172.1430	13.3205076667
38	C	103.0274	79.4737648117
42	C	110.6174	72.2090775091
44	C	141.5218	42.6292616627
45	C	148.6981	35.7605428894
47	C	166.4853	18.7357146959
51	C	39.7230	140.064894045
53	C	52.7343	127.611267444
55	C	45.2278	134.796033615
57	C	50.8218	129.441796359
59	C	148.4079	36.0383047149
64	C	146.3213	38.0354715825
67	C	113.8740	69.0920576581
69	C	91.7396	90.2777618255
72	C	151.5042	33.0747142939
76	C	115.3058	67.7216256054
77	C	168.9648	16.3624877965
82	C	110.5088	72.3130228373
86	C	112.5384	70.3704129099
90	C	102.8441	79.6492084458
92	C	127.9402	55.6287448075
4	H	30.4941	1.24601524602
5	H	30.2840	1.44014784015
7	H	26.0728	5.3313005313
10	H	29.4687	2.19348579349
11	H	27.8915	3.65082005082
12	H	28.2573	3.31282051282
17	H	25.3711	5.97967197967
19	H	23.8976	7.34118734119
21	H	29.3717	2.28311388311
22	H	28.8815	2.73605913606
24	H	27.9734	3.57514437514
26	H	29.6319	2.04268884269
27	H	28.2990	3.27428967429
28	H	28.0328	3.52025872026
30	H	29.9485	1.75015015015
31	H	30.5698	1.17606837607

33	H	28.9928	2.63321783322
35	H	30.6217	1.12811272811
36	H	30.8301	0.935550935551
37	H	30.4872	1.25239085239
39	H	27.3708	4.13194733195
43	H	28.1785	3.38563178563
46	H	29.1649	2.4741972742
48	H	30.4726	1.26588126588
49	H	30.9229	0.849803649804
50	H	31.1409	0.648371448371
52	H	25.9337	5.45982905983
54	H	25.5041	5.85677985678
56	H	25.1964	6.14109494109
58	H	25.9149	5.4772002772
60	H	29.3686	2.28597828598
61	H	29.3431	2.30954030954
62	H	30.3698	1.36086856087
63	H	30.5743	1.17191037191
65	H	30.1098	1.60110880111
66	H	30.5919	1.15564795565
70	H	26.3984	5.03044583045
71	H	27.6071	3.91360591361
73	H	29.7371	1.94548394548
74	H	30.2964	1.42869022869
78	H	30.5524	1.19214599215
79	H	30.2581	1.46407946408
80	H	30.8193	0.94553014553
81	H	28.0061	3.54492954493
83	H	28.3639	3.21432201432
85	H	29.6405	2.03474243474
88	H	29.9196	1.77685377685
89	H	28.2116	3.35504735505
93	H	28.2264	3.34137214137
94	H	28.1605	3.40226380226
95	H	28.5560	3.03682143682
96	H	28.2470	3.32233772234

Supporting Information: Original-MandelalideA-0005.log

```
-----------------------------------------------------------------------
 Using  Gaussian 09:  AM64L-G09RevC.01 23-Sep-2011
=======================================================================
 #b3lyp/6-31G(d,p) scf=(maxcycle=300,direct,tight) density=current
 SCRF=(PCM,SOLVENT=Chloroform) opt=(maxcycle=250)
freq=noraman
 #N Geom=AllCheck Guess=TCheck SCRF=Check GenChk RB3LYP/6-
31G(d,p) Freq
-----------------------------------------------------------------------
 Pointgroup= C1   Stoichiometry= C33H52O11   C1[X(C33H52O11)]
#Atoms= 96
 Charge = 0                Multiplicity = 1
-----------------------------------------------------------------------
 SCF Energy= -2116.30575612      Predicted Change= -6.422166D-09
=======================================================================
 Optimization completed.          {Found       2       times}
 Item     Max Val.    Criteria    Pass?      RMS Val.    Criteria    Pass?
 Force      0.00000 ||  0.00045   [ YES ]      0.00000 ||  0.00030   [ YES ]
 Displ      0.00091 ||  0.00180   [ YES ]      0.00091 ||  0.00180   [ YES ]
-----------------------------------------------------------------------
     Atomic      Coordinates (Angstroms)
      Type      X                Y              Z
-----------------------------------------------------------------------
      C       7.385821     -0.979225      0.708784
      C       7.301389      0.493186      0.264033
      C       5.973626      1.168708      0.603469
      H       5.943553      1.416825      1.670611
      H       5.180368      0.447122      0.401091
      C       5.688625      2.422193     -0.229908
      H       5.887206      2.225627     -1.287192
      C       6.443215      3.668290      0.217167
      O       6.158177      4.789474     -0.606743
      H       5.198229      4.909357     -0.577942
      H       7.515148      3.472295      0.150044
      H       6.206239      3.872735      1.273274
      O       4.276371      2.778308     -0.110552
      C       3.400023      2.129420     -0.920624
      O       3.735009      1.281471     -1.730720
      C       2.016708      2.585944     -0.670051
      H       1.880036      3.367897      0.071404
      C       0.984275      2.036045     -1.323340
      H       1.198231      1.251592     -2.045231
      C      -0.454315      2.397426     -1.117999
      H      -0.879575      2.767705     -2.060842
      H      -0.544361      3.198839     -0.377148
      C      -1.307745      1.201880     -0.665912
      H      -0.815600      0.725396      0.199561
      O       8.357152      1.244518      0.873662
      H       9.195671      0.943040      0.497452
      H       7.417075      0.495213     -0.830913
      H       8.375016     -1.349512      0.386748
      C       7.202383     -1.300028      2.192757
      H       8.124562     -1.174383      2.764915
      H       6.435918     -0.662105      2.647570
      C       6.723014     -2.761242      2.132304
      H       7.591516     -3.382605      1.875114
      C       6.115526     -3.306954      3.424662
      H       5.761967     -4.335773      3.297003
      H       5.271829     -2.700109      3.767164
      H       6.864369     -3.312717      4.223071
      C       5.805459     -2.741357      0.883504
      H       5.856704     -3.694416      0.341752
      O       6.370427     -1.728078      0.022608
      O      -1.351640      0.266128     -1.744651
      C      -2.007563     -0.958101     -1.383848
      H      -1.477944     -1.384894     -0.515630
      C      -1.926660     -1.950082     -2.545469
      C      -0.512438     -2.380573     -3.032910
      H      -0.690534     -3.291575     -3.627081
      C       0.126195     -1.356484     -3.980423
      H       1.076733     -1.726871     -4.377354
      H       0.303430     -0.403841     -3.478554
      H      -0.538911     -1.165639     -4.828913
      C       0.362494     -2.792434     -1.873285
      H      -0.052445     -3.576487     -1.235785
      C       1.564813     -2.284187     -1.552113
      H       1.999831     -1.498583     -2.167374
      C       2.350792     -2.683891     -0.393010
      H       1.933244     -3.466976      0.242462
      C       3.522877     -2.113693     -0.063906
      H       3.921192     -1.332997     -0.709541
      C       4.324813     -2.420797      1.167747
      H       4.283678     -1.550916      1.840541
      H       3.876870     -3.261054      1.711338
      H      -2.485977     -1.546396     -3.398777
      H      -2.468820     -2.845653     -2.216443
      C      -3.467610     -0.674624     -0.991449
      H      -3.958567     -1.596524     -0.667056
      H      -4.004042     -0.298087     -1.871279
      C      -3.546249      0.379254      0.117675
      O      -4.891794      0.820905      0.368232
      C      -5.649123      0.061088      1.280457
      H      -5.021630     -0.261841      2.121535
      H      -3.143368     -0.047232      1.050103
      C      -2.728175      1.613281     -0.260343
      H      -2.698553      2.314204      0.580877
      H      -3.212499      2.119641     -1.104098
      O      -6.148581     -1.146178      0.738580
```

C	-7.085374	-0.997670	-0.349719
C	-7.454572	-2.396474	-0.813945
H	-6.568374	-2.930757	-1.167521
H	-8.179151	-2.337455	-1.629432
H	-7.898547	-2.966725	0.008347
H	-6.604736	-0.446209	-1.168729
C	-8.289448	-0.186296	0.138335
H	-8.768588	-0.742938	0.959822
O	-9.194511	-0.002283	-0.942031
H	-9.809536	0.685901	-0.644337
C	-7.828234	1.172255	0.674598
O	-8.944872	1.926837	1.137924
H	-9.146066	1.563401	2.016184
H	-7.386915	1.739969	-0.150993
C	-6.779214	0.989880	1.772611
O	-7.469974	0.433261	2.888922
C	-6.859740	0.679642	4.149987
H	-6.740987	1.756474	4.332248
H	-5.877177	0.198076	4.234394
H	-7.521350	0.257694	4.909003
H	-6.344002	1.961073	2.043678

Statistical Thermodynamic Analysis
Temperature= 298.150 Kelvin Pressure= 1.00000 Atm
==========
==========
SCF Energy= -2116.30575612 Predicted Change= -6.422166D-09
Zero-point correction (ZPE)= -2115.4724 0.83332
Internal Energy (U)= -2115.4265 0.87918
Enthalpy (H)= -2115.4256
0.88012
Gibbs Free Energy (G)= -2115.5531
0.75256

Frequencies -- 12.0153 14.3067 18.3336

NMR-Shifts
Original-MandelalideA-0005-NMR.txt

Atom	Type	Isotropic	Scaled Shift
1	C	100.7645	81.6396753383
2	C	112.2127	70.6821531806
3	C	155.9001	28.867225636
6	C	104.2242	78.328260495
8	C	119.4929	63.7139876338
14	C	12.5241	166.098030207
16	C	60.1342	120.528532323
18	C	24.3552	154.774019411
20	C	144.1707	40.0938953655
23	C	107.1643	75.5141752331
29	C	152.6946	31.9353356688
32	C	145.4245	38.8938341086
34	C	173.5624	11.9619441414
38	C	101.1034	81.3153008289
42	C	108.5602	74.1781044813
44	C	143.2276	40.9965734413
45	C	148.1505	36.2846723712
47	C	167.5955	17.6730986428
51	C	43.9796	135.990734892
53	C	51.4946	128.797833037
55	C	48.4949	131.668963801
57	C	47.9581	132.182756178
59	C	147.6611	36.7530963456
64	C	143.3711	40.8592239515
67	C	103.4038	79.1134975784
69	C	84.3778	97.3240299393
72	C	145.6373	38.6901548651
76	C	114.8765	68.1325255078
77	C	169.0563	16.2749095503
82	C	110.5901	72.2352074121
86	C	112.5384	70.3704129099
90	C	102.5892	79.8931832539
92	C	128.2060	55.374337181
4	H	30.4962	1.24407484407
5	H	29.6674	2.00988680989
7	H	26.7154	4.73753753754
10	H	30.4265	1.30847770848
11	H	27.4123	4.0936012936
12	H	28.0178	3.53411873412
17	H	25.5578	5.80716100716
19	H	23.7153	7.50963270963
21	H	29.3021	2.34742434742
22	H	29.5192	2.14682374682
24	H	28.5910	3.00448140448
26	H	31.1576	0.632940632941
27	H	27.4120	4.09387849388
28	H	27.6678	3.85751905752
30	H	30.1012	1.60905520906
31	H	30.2479	1.4735042735
33	H	29.3434	2.30926310926
35	H	30.7622	0.998290598291
36	H	31.0792	0.705382305382
37	H	30.6900	1.065003465
39	H	27.7119	3.81677061677
43	H	28.3575	3.22023562024
46	H	29.1251	2.51097251097
48	H	30.4457	1.29073689074
49	H	29.9815	1.71965811966
50	H	30.7548	1.00512820513
52	H	25.7125	5.66421806422
54	H	25.2098	6.12871332871
56	H	25.1442	6.18932778933
58	H	25.3431	6.00554400554
60	H	29.7415	1.94141834142
61	H	30.0003	1.70228690229
62	H	30.0836	1.62531762532
63	H	30.0119	1.69156849157
65	H	29.6131	2.06006006006
66	H	30.4976	1.24278124278
70	H	26.5238	4.91457611458
71	H	28.1327	3.42795102795
73	H	30.0733	1.63483483483
74	H	30.5233	1.21903441903
78	H	30.5185	1.22346962347
79	H	30.2147	1.50418110418
80	H	30.8170	0.947655347655
81	H	27.8296	3.70801570802
83	H	28.4175	3.1647955648
85	H	29.6190	2.05460845461
88	H	29.9528	1.74617694618
89	H	28.1797	3.38452298452
93	H	28.5743	3.01991221991
94	H	28.1973	3.36826056826
95	H	28.1299	3.43053823054
96	H	28.2782	3.29350889351

Supporting Information: Original-MandelalideA-0006.log

Using Gaussian 09: AM64L-G09RevC.01 23-Sep-2011
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#b3lyp/6-31G(d,p) scf=(maxcycle=300,direct,tight) density=current
SCRF=(PCM,SOLVENT=Chloroform) opt=(maxcycle=250)
freq=noraman
#N Geom=AllCheck Guess=TCheck SCRF=Check GenChk RB3LYP/6-
31G(d,p) Freq

Pointgroup= C1 Stoichiometry= C33H52O11 C1[X(C33H52O11)]
#Atoms= 96

Charge = 0 Multiplicity = 1

SCF Energy= -2116.30797705 Predicted Change= -1.622199D-08

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Optimization completed. {Found 1 times}

Item	Max Val.	Criteria	Pass?	RMS Val.	Criteria	Pass?
Force	0.00001	0.00045	[YES]	0.00000	0.00030	[YES]
Displ	0.00224	0.00180	[NO]	0.00224	0.00180	[YES]

Atomic Type	Coordinates (Angstroms) X	Y	Z
C	7.026659	0.838068	-1.197704
C	6.062742	1.860534	-0.573510
C	4.852641	2.114803	-1.489832
H	4.415642	1.152644	-1.776740
H	5.208996	2.587014	-2.413183
C	3.739891	2.994137	-0.912845
H	3.024371	3.240385	-1.704901
C	4.227247	4.309162	-0.286692
O	3.276095	5.356105	-0.343759
H	2.423305	4.958893	-0.088281
H	5.101070	4.654670	-0.851094
H	4.563189	4.098628	0.740177
O	3.037598	2.147397	0.057448
C	1.822693	2.496418	0.504596
O	1.260522	3.552516	0.227914
C	1.265368	1.443542	1.375253
H	1.893453	0.577951	1.558836
C	0.039871	1.550993	1.903283
H	-0.534800	2.445074	1.668716
C	-0.596800	0.515373	2.782949
H	-1.117943	1.008277	3.612553
H	0.170599	-0.135353	3.213604
C	-1.614616	-0.386108	2.058196
H	-2.037947	-1.072263	2.811878
O	5.675704	1.452804	0.736245
H	5.094191	0.687545	0.619152
H	6.621926	2.793279	-0.430456
H	7.320399	1.192593	-2.198590
C	8.264470	0.541766	-0.349182
H	9.097313	1.211118	-0.582886
H	8.017844	0.653629	0.711811
C	8.566155	-0.925334	-0.685211
H	9.050089	-0.950790	-1.670859
C	9.480350	-1.640269	0.309628
H	9.084925	-1.593557	1.329174
H	10.470273	-1.172820	0.317811
H	9.616917	-2.694796	0.046340
C	7.146164	-1.518420	-0.882091
H	7.164094	-2.266356	-1.686595
O	6.332500	-0.417454	-1.335626
O	-0.886577	-1.150407	1.097732
C	-1.685650	-2.135496	0.430629
H	-2.108070	-2.814733	1.193608
C	-0.792569	-2.948136	-0.505408
C	0.284981	-3.841691	0.174997
H	-0.151287	-4.188823	1.126081
C	0.555984	-5.086324	-0.682563
H	1.288938	-5.747703	-0.210854
H	0.936595	-4.813893	-1.673425
H	-0.366498	-5.657117	-0.826745
C	1.534686	-3.063256	0.525851
H	1.370904	-2.209505	1.180773
C	2.781963	-3.328680	0.099384
H	2.954578	-4.170851	-0.569079
C	3.974245	-2.575812	0.469185
H	3.843109	-1.749634	1.169940
C	5.203210	-2.866198	0.008688
H	5.302778	-3.698008	-0.691894
C	6.486349	-2.165395	0.352398
H	6.325372	-1.404275	1.124527
H	7.186667	-2.905068	0.764422
H	-0.317750	-2.271742	-1.226337
H	-1.462204	-3.599245	-1.080382
C	-2.845227	-1.460000	-0.317400
H	-3.481338	-2.217945	-0.786455
H	-2.438986	-0.824273	-1.113536
C	-3.675340	-0.598660	0.630166
O	-4.649600	0.107303	-0.159790
C	-5.828343	0.475055	0.523033
H	-5.596389	0.941509	1.488497
H	-4.203403	-1.247240	1.342015
C	-2.766120	0.375553	1.386353
H	-3.328909	0.932122	2.144869
H	-2.362288	1.097398	0.668108
O	-6.634066	-0.635271	0.862186
C	-7.160978	-1.382533	-0.254789
C	-7.936433	-2.555708	0.319865
H	-8.363843	-3.150483	-0.490655
H	-8.750260	-2.199718	0.959628
H	-7.279144	-3.193345	0.917673
H	-6.330033	-1.749269	-0.872204
C	-8.020348	-0.445971	-1.108820
H	-8.844257	-0.069296	-0.481346
O	-8.524189	-1.164730	-2.226554
H	-8.860032	-0.487667	-2.834337
C	-7.184739	0.747138	-1.584382
O	-7.981261	1.625358	-2.374158
H	-8.491383	2.146129	-1.731824
H	-6.388004	0.374132	-2.235890
C	-6.555986	1.477222	-0.394625
O	-7.629574	2.123902	0.285442
C	-7.253266	3.275949	1.030520
H	-6.575739	3.028921	1.857880
H	-8.170935	3.697777	1.445022
H	-6.768167	4.024515	0.389574
H	-5.830654	2.221064	-0.750271

Statistical Thermodynamic Analysis

Temperature= 298.150 Kelvin Pressure= 1.00000 Atm

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SCF Energy= -2116.30797705 Predicted Change= -1.622199D-08

Zero-point correction (ZPE)= -2115.4745 0.83346

Internal Energy (U)= -2115.4287 0.87920

Enthalpy (H)= -2115.4278 0.88015

Gibbs Free Energy (G)= -2115.5560 0.75189

Frequencies -- 10.3668 14.7495 17.6105

NMR-Shifts

Original-MandelalideA-0006-NMR.txt

Atom	Type	Isotropic	Scaled Shift
1	C	101.1990	81.2237983116
2	C	115.4996	67.5361320087
3	C	147.5159	36.8920729723
6	C	101.3210	81.1070273168
8	C	117.4521	65.6673175214
14	C	9.4507	169.039702138
16	C	55.5730	124.894236107
18	C	28.5154	150.792128486
20	C	146.2207	38.1317597963
23	C	108.0787	74.6389670553
29	C	150.7620	33.7851030839

32	C	145.2539	39.0571220735
34	C	172.2552	13.213116637
38	C	101.0417	81.3743563238
42	C	104.6589	77.9121920404
44	C	141.3503	42.793411053
45	C	146.3971	37.9629204234
47	C	167.2047	18.047148682
51	C	41.1519	138.697237696
53	C	53.1335	127.229177434
55	C	49.0398	131.147418595
57	C	46.4433	133.632630793
59	C	148.1170	36.3167365378
64	C	146.7280	37.6462030284
67	C	113.3824	69.562587339
69	C	91.9028	90.1215566914
72	C	151.0590	33.5008327112
76	C	114.7830	68.2220180325
77	C	168.8086	16.5119929555
82	C	109.8470	72.9464576274
86	C	111.7538	71.1213844063
90	C	103.2257	79.2839640881
92	C	127.9620	55.6078791707
4	H	29.4822	2.18101178101
5	H	30.0764	1.63197043197
7	H	26.6641	4.78493878494
10	H	27.3706	4.13213213213
11	H	27.9786	3.57033957034
12	H	27.5707	3.94723954724
17	H	25.2564	6.08565488565
19	H	23.9691	7.27512127512
21	H	29.2526	2.39316239316
22	H	28.8709	2.74585354585
24	H	27.9717	3.57671517672
26	H	30.9844	0.792977592978
27	H	28.2820	3.28999769
28	H	27.7548	3.77713097713
30	H	30.0141	1.68953568954
31	H	29.7191	1.96211596212
33	H	29.1929	2.44832524833
35	H	31.0265	0.754077154077
36	H	30.5863	1.16082236082
37	H	30.6703	1.08320628321
39	H	27.6622	3.86269346269
43	H	28.1506	3.41141141141
46	H	29.2492	2.3963039963
48	H	30.4961	1.24416724417
49	H	30.7320	1.0261954262
50	H	30.8259	0.939431739432
52	H	24.8255	6.48380688381
54	H	25.5206	5.84153384153
56	H	25.2290	6.11097251097
58	H	25.8727	5.51619311619
60	H	29.7608	1.92358512359
61	H	29.5963	2.07558327558
62	H	30.3950	1.33758373758
63	H	30.4206	1.31392931393
65	H	30.1673	1.54797874798
66	H	30.7292	1.02878262878
70	H	26.5610	4.8802032802
71	H	27.6125	3.90861630862
73	H	29.7144	1.96645876646
74	H	30.7189	1.0382998383
78	H	30.2147	1.50418110418
79	H	30.7885	0.973989373989
80	H	30.6237	1.12626472626
81	H	27.9020	3.64111804112
83	H	28.3308	3.24490644491
85	H	29.7296	1.95241395241
88	H	29.8643	1.82795102795
89	H	27.9890	3.56072996073
93	H	28.1931	3.37214137214
94	H	28.1426	3.4188034188
95	H	28.5687	3.02508662509
96	H	28.3100	3.26412566413

Supporting Information: Original-MandelalideA-0007.log

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---------------------------------------------------------------------------
 Using  Gaussian 09:  AM64L-G09RevC.01 23-Sep-2011
=========================================================================
 #b3lyp/6-31G(d,p) scf=(maxcycle=300,direct,tight) density=current
 SCRF=(PCM,SOLVENT=Chloroform) opt=(maxcycle=250)
freq=noraman
 #N Geom=AllCheck Guess=TCheck SCRF=Check GenChk RB3LYP/6-
31G(d,p) Freq
---------------------------------------------------------------------------
 Pointgroup= C1   Stoichiometry= C33H52O11   C1[X(C33H52O11)]
#Atoms= 96
 Charge = 0                Multiplicity = 1
---------------------------------------------------------------------------
 SCF Energy= -2116.30451330      Predicted Change= -1.940529D-09
=========================================================================
 Optimization completed.          {Found       2       times}
 Item      Max Val.    Criteria    Pass?      RMS Val.    Criteria    Pass?
 Force      0.00000 ||  0.00045   [ YES ]      0.00000 ||  0.00030   [ YES ]
 Displ      0.00173 ||  0.00180   [ YES ]      0.00173 ||  0.00180   [ YES ]
---------------------------------------------------------------------------
     Atomic      Coordinates (Angstroms)
      Type      X                  Y                Z
---------------------------------------------------------------------------
      C      -5.548276     -1.030067     -0.351512
      C      -5.893294     -2.118583      0.673253
      C      -4.692608     -2.693993      1.444881
      H      -5.096791     -3.363698      2.209562
      H      -4.162787     -1.885240      1.962295
      C      -3.685273     -3.497503      0.624832
      H      -4.178455     -4.099424     -0.145146
      C      -2.830132     -4.428652      1.487980
      O      -3.699425     -5.407208      2.043921
      H      -3.177489     -5.969865      2.630066
      H      -2.326948     -3.837310      2.267749
      H      -2.060609     -4.887149      0.853197
      O      -2.796798     -2.552364     -0.025566
      C      -2.233579     -2.895648     -1.210125
      O      -2.368245     -3.988764     -1.733110
      C      -1.449266     -1.790740     -1.802547
      H      -0.953450     -2.043650     -2.735345
      C      -1.364220     -0.567455     -1.260695
      H      -1.896552     -0.381752     -0.329877
      C      -0.594113      0.591973     -1.812219
      H      -1.260630      1.461452     -1.861346
      H      -0.229728      0.388949     -2.824568
      C       0.572824      0.994195     -0.888999
      H       0.273100      0.811959      0.158117
      O      -6.855920     -1.606362      1.595308
      H      -6.510399     -0.735975      1.851234
      H      -6.388509     -2.938724      0.137798
      H      -4.714718     -1.360117     -0.982404
      C      -6.737926     -0.578163     -1.237868
      H      -6.571171     -0.874816     -2.276900
      H      -7.670400     -1.040279     -0.903309
      C      -6.797823      0.964729     -1.080419
      H      -6.870020      1.454103     -2.058067
      C      -7.989919      1.402255     -0.220047
      H      -8.926678      1.102737     -0.701078
      H      -8.022814      2.486857     -0.078353
      H      -7.962392      0.924069      0.764164
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C	-5.410084	1.267248	-0.462984
H	-4.664655	1.274937	-1.275910
O	-5.137184	0.139477	0.383551
O	0.788672	2.393459	-1.057119
C	1.746754	2.905103	-0.123670
H	1.430806	2.609840	0.893138
C	1.732116	4.430825	-0.213054
C	0.598770	5.109929	0.597557
H	0.691541	4.762164	1.636210
C	0.785229	6.639900	0.587994
H	0.024890	7.132035	1.201912
H	0.702251	7.037564	-0.430152
H	1.770884	6.917965	0.976505
C	-0.779147	4.750176	0.107143
H	-1.052456	5.152636	-0.870585
C	-1.678183	4.002068	0.768931
H	-1.409174	3.578567	1.737696
C	-3.013448	3.700826	0.270929
H	-3.319706	4.230323	-0.633251
C	-3.877906	2.842688	0.840975
H	-3.572932	2.298175	1.734156
C	-5.266290	2.570932	0.327034
H	-5.972052	2.551961	1.165819
H	-5.578331	3.385937	-0.337486
H	1.671443	4.717414	-1.270593
H	2.690070	4.811182	0.162533
C	3.117029	2.270359	-0.400444
H	3.860205	2.640038	0.314303
H	3.450836	2.549389	-1.407363
C	3.015489	0.747864	-0.302397
O	4.276098	0.188068	-0.716428
C	4.616881	-1.037996	-0.107144
H	3.771733	-1.737261	-0.127910
H	2.838699	0.471776	0.745631
C	1.869812	0.224837	-1.178091
H	1.709856	-0.847748	-1.018336
H	2.140233	0.371026	-2.230757
O	4.916499	-0.901272	1.267126
C	6.066371	-0.083994	1.571262
C	6.175582	-0.015953	3.085052
H	5.272081	0.426430	3.513948
H	7.036231	0.594075	3.368869
H	6.303681	-1.018879	3.504784
H	5.916093	0.923590	1.160995
C	7.297696	-0.699957	0.900241
H	7.438995	-1.713838	1.308329
O	8.430695	0.115076	1.168742
H	9.116012	-0.189850	0.554017
C	7.075133	-0.809728	-0.611991
O	8.214310	-1.391890	-1.238822
H	8.125449	-2.346732	-1.082589
H	6.973580	0.200441	-1.021387
C	5.801136	-1.601872	-0.916743
O	6.081277	-2.954293	-0.561865
C	5.309330	-3.924249	-1.260190
H	4.239368	-3.844338	-1.029479
H	5.664237	-4.904171	-0.935149
H	5.443131	-3.833171	-2.346700
H	5.562612	-1.533152	-1.986469

Statistical Thermodynamic Analysis
Temperature= 298.150 Kelvin Pressure= 1.00000 Atm
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==========

SCF Energy= -2116.30451330 Predicted Change= -1.940529D-09
Zero-point correction (ZPE)= -2115.4718 0.83265
Internal Energy (U)= -2115.4255 0.87894
Enthalpy (H)= -2115.4246
0.87988
Gibbs Free Energy (G)= -2115.5551
0.74940

Frequencies -- 7.9067 10.6840 15.3505

NMR-Shifts
Original-MandelalideA-0007-NMR.txt

Atom	Type	Isotropic	Scaled Shift
1	C	105.7418	76.8757058902
2	C	112.1056	70.7846627998
3	C	148.7654	35.6961274144
6	C	112.7216	70.1950649898
8	C	122.2042	61.1188958441
14	C	14.1949	164.498841861
16	C	58.4948	122.097666494
18	C	27.9544	151.329083635
20	C	143.2751	40.9511093245
23	C	109.6031	73.1799039032
29	C	148.5775	35.8759738892
32	C	145.9790	38.3631003656
34	C	170.3187	15.0666168954
38	C	97.4610	84.8015850227
42	C	104.9930	77.5924117996
44	C	141.6509	42.5056949788
45	C	141.3019	42.8397365953
47	C	163.6237	21.4746645227
51	C	37.8370	141.870058768
53	C	53.7934	126.597561209
55	C	47.6999	132.429889546
57	C	50.4879	129.761385172
59	C	149.4536	35.0374241467
64	C	145.5571	38.7669174372
67	C	112.9839	69.9440073508
69	C	91.0621	90.9262237026
72	C	149.5412	34.9535787439
76	C	115.2298	67.7943681923
77	C	168.9426	16.383736289
82	C	110.4539	72.365569785
86	C	112.4697	70.4361683799
90	C	102.9673	79.5312888838
92	C	127.9737	55.5966806409
4	H	29.2691	2.37791637792
5	H	29.8809	1.81261261261
7	H	26.8681	4.59644259644
10	H	31.1406	0.648648648649
11	H	28.3668	3.21164241164
12	H	27.7648	3.76789096789
17	H	25.9686	5.42758142758
19	H	24.1954	7.06601986602
21	H	29.1602	2.47854007854
22	H	29.4946	2.16955416955
24	H	28.5803	3.01436821437
26	H	29.7999	1.88745668746
27	H	28.4023	3.17884037884
28	H	27.8430	3.69563409563
30	H	29.6991	1.9805959806
31	H	30.2525	1.46925386925
33	H	29.5922	2.07937167937
35	H	31.0173	0.762577962578
36	H	30.8767	0.892492492492
37	H	30.7994	0.963917763918
39	H	28.0458	3.50824670825
43	H	28.4758	3.11092631093
46	H	29.4607	2.20087780088
48	H	30.6994	1.05631785632
49	H	30.8398	0.926588126588
50	H	30.5552	1.18955878956
52	H	25.8491	5.537999538
54	H	25.4014	5.95167475167

56	H	25.2755	6.06800646801
58	H	25.5642	5.80124740125
60	H	29.4612	2.20041580042
61	H	29.8054	1.88237468237
62	H	30.3304	1.39727419727
63	H	30.3555	1.37408177408
65	H	30.1293	1.58309078309
66	H	30.5556	1.18918918919
70	H	26.5846	4.8583968584
71	H	27.7760	3.75754215754
73	H	29.7342	1.94816354816
74	H	30.9065	0.864957264957
78	H	30.5927	1.15490875491
79	H	30.2711	1.45206745207
80	H	30.8433	0.923354123354
81	H	27.9225	3.62217602218
83	H	28.3948	3.18577038577
85	H	29.7025	1.97745437745
88	H	29.9849	1.71651651652
89	H	28.2528	3.31697851698
93	H	28.2625	3.30801570802
94	H	28.1611	3.40170940171
95	H	28.6030	2.99339339339
96	H	28.3155	3.25904365904

Supporting Information: Original-MandelalideA-0008.log

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-----------------------------------------------------------------------
 Using  Gaussian 09:  AM64L-G09RevC.01 23-Sep-2011
=======================================================================
 #b3lyp/6-31G(d,p) scf=(maxcycle=300,direct,tight) density=current
 SCRF=(PCM,SOLVENT=Chloroform) opt=(maxcycle=250)
freq=noraman
 #N Geom=AllCheck Guess=TCheck SCRF=Check GenChk RB3LYP/6-
31G(d,p) Freq
-----------------------------------------------------------------------
 Pointgroup= C1   Stoichiometry= C33H52O11   C1[X(C33H52O11)]
#Atoms= 96
 Charge = 0                Multiplicity = 1
-----------------------------------------------------------------------
 SCF Energy= -2116.30504501      Predicted Change= -2.197172D-09
=======================================================================
 Optimization completed.          {Found       2       times}
 Item      Max Val.    Criteria    Pass?      RMS Val.    Criteria    Pass?
 Force      0.00000 ||  0.00045   [ YES ]      0.00000 ||  0.00030   [ YES ]
 Displ      0.00106 ||  0.00180   [ YES ]      0.00106 ||  0.00180   [ YES ]
-----------------------------------------------------------------------
     Atomic      Coordinates (Angstroms)
      Type      X                Y                Z
-----------------------------------------------------------------------
      C       7.390875     -0.803817      0.815020
      C       7.277229      0.562505      0.111484
      C       5.865096      1.149328      0.151734
      H       5.625105      1.504182      1.159494
      H       5.165297      0.352138     -0.099396
      C       5.631067      2.292358     -0.842884
      H       5.783916      1.930657     -1.863734
      C       6.510265      3.517063     -0.630582
      O       6.648250      3.770870      0.773554
      H       7.151918      4.589156      0.880593
      H       6.061171      4.375498     -1.143710
      H       7.491295      3.316326     -1.078778
      O       4.243606      2.720451     -0.733488
      C       3.336540      2.001636     -1.441337
      O       3.636253      1.064827     -2.164362
      C       1.965027      2.499880     -1.207953
      H       1.852940      3.362094     -0.556981
      C       0.915838      1.882787     -1.767376
      H       1.113749      1.020384     -2.399137
      C      -0.518201      2.262363     -1.567334
      H      -0.978923      2.490528     -2.538026
      H      -0.593980      3.160102     -0.944863
      C      -1.340814      1.137479     -0.918644
      H      -0.824585      0.810061      0.000210
      O       8.267298      1.428287      0.675006
      H       7.811234      2.215607      1.021146
      H       7.539378      0.389293     -0.944324
      H       8.407233     -1.176114      0.612693
      C       7.143384     -0.855213      2.323307
      H       8.035782     -0.596664      2.897707
      H       6.341101     -0.171100      2.624411
      C       6.704181     -2.317646      2.513492
      H       7.597179     -2.947550      2.403938
      C       6.058265     -2.639434      3.861166
      H       5.191154     -2.002403      4.061400
      H       6.776361     -2.483594      4.672645
      H       5.729029     -3.683177      3.908709
      C       5.839472     -2.549687      1.248706
      H       5.914082     -3.588570      0.902519
      O       6.440389     -1.717449      0.233716
      O      -1.384691      0.043668     -1.837017
      C      -2.017299     -1.117413     -1.279088
      H      -1.468849     -1.396764     -0.363779
      C      -1.938410     -2.277314     -2.273200
      C      -0.525572     -2.776762     -2.693999
      H      -0.705278     -3.770748     -3.135529
      C       0.106729     -1.915823     -3.795328
      H       1.054952     -2.344182     -4.135129
      H       0.287114     -0.896127     -3.450853
      H      -0.563601     -1.861124     -4.659248
      C       0.356751     -2.998961     -1.488500
      H      -0.072416     -3.637788     -0.713159
      C       1.581548     -2.485551     -1.279023
      H       2.033800     -1.842396     -2.031990
      C       2.365922     -2.688255     -0.068664
      H       1.915475     -3.301409      0.714066
      C       3.569543     -2.126232      0.139474
      H       4.004747     -1.521086     -0.653833
      C       4.348948     -2.195341      1.421162
      H       4.286050     -1.215668      1.918753
      H       3.887288     -2.920718      2.101755
      H      -2.502737     -2.011744     -3.175869
      H      -2.476648     -3.112360     -1.806933
      C      -3.475343     -0.794824     -0.910059
      H      -3.947436     -1.662148     -0.439890
      H      -4.031778     -0.563703     -1.826905
      C      -3.550671      0.414640      0.026555
      O      -4.897560      0.871727      0.238321
      C      -5.627380      0.238986      1.263156
      H      -4.975919      0.028883      2.121632
      H      -3.121121      0.140944      1.003502
      C      -2.760838      1.586525     -0.553494
      H      -2.727910      2.409711      0.168351
      H      -3.268401      1.949189     -1.455566
      O      -6.137542     -1.028566      0.898246
      C      -7.109832     -1.023726     -0.168474
      C      -7.484977     -2.471440     -0.436456
      H      -8.239949     -2.518612     -1.224589
      H      -7.893686     -2.933532      0.467905
      H      -6.608393     -3.043802     -0.752349
      H      -6.660606     -0.580946     -1.067525
      C      -8.302509     -0.158810      0.251116
      H      -8.748814     -0.603351      1.155251
      O      -9.245594     -0.121863     -0.811878
      H      -9.855178      0.598071     -0.587132
      C      -7.833096      1.259514      0.587942
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O	-8.938223	2.065428	0.987464
H	-9.109209	1.815842	1.910719
H	-7.424709	1.715023	-0.320009
C	-6.745024	1.225235	1.663208
O	-7.393118	0.822879	2.868114
C	-6.750210	1.255475	4.060889
H	-6.653719	2.349453	4.087360
H	-5.753205	0.811488	4.177082
H	-7.376467	0.929638	4.893644
H	-6.305399	2.223888	1.786281

Statistical Thermodynamic Analysis
Temperature= 298.150 Kelvin Pressure= 1.00000 Atm
==========
SCF Energy= -2116.30504501 Predicted Change= -2.197172D-09
Zero-point correction (ZPE)= -2115.4714 0.83360
Internal Energy (U)= -2115.4258 0.87923
Enthalpy (H)= -2115.4248 0.88018
Gibbs Free Energy (G)= -2115.5525 0.75247

Frequencies -- 8.5383 13.1664 18.3722

NMR-Shifts
Original-MandelalideA-0008-NMR.txt

Atom	Type	Isotropic	Scaled Shift
1	C	101.6395	80.8021784491
2	C	114.7964	68.2091923659
3	C	157.4629	27.3714083348
6	C	109.3675	73.4054059228
8	C	119.7269	63.4900170371
14	C	12.6766	165.952066464
16	C	59.7912	120.856831103
18	C	24.8381	154.311816842
20	C	144.4225	39.8528876893
23	C	106.9317	75.7368058347
29	C	153.1362	31.512662953
32	C	146.2846	38.0705985949
34	C	173.2160	12.2934971956
38	C	101.6000	80.8399854515
42	C	108.9136	73.839851452
44	C	143.0289	41.1867570206
45	C	148.3859	36.0593617795
47	C	167.8750	17.4055782079
51	C	45.2855	134.740806677
53	C	50.2417	129.997032868
55	C	49.3108	130.888033844
57	C	47.8349	132.30067574
59	C	148.0020	36.4268075576
64	C	143.3985	40.8329983346
67	C	103.4541	79.0653534715
69	C	84.0842	97.6050460384
72	C	145.9602	38.3810945845
76	C	115.2363	67.7881467869
77	C	169.2199	16.1183215605
82	C	110.0287	72.7725454163
86	C	112.3751	70.5267137579
90	C	102.0175	80.4403797929
92	C	128.2188	55.362085798
4	H	30.0152	1.68851928852
5	H	29.2211	2.42226842227
7	H	26.5859	4.8571956572
10	H	30.7449	1.01427581428
11	H	27.6593	3.86537306537
12	H	27.4188	4.0875952876
17	H	25.5803	5.78637098637
19	H	23.6780	7.5440979441
21	H	29.3193	2.33153153153
22	H	29.5571	2.1118041118
24	H	28.6265	2.97167937168
26	H	28.1599	3.40281820282
27	H	27.6890	3.83793023793
28	H	27.4032	4.10200970201
30	H	29.9320	1.7653961654
31	H	30.2664	1.45641025641
33	H	29.2295	2.41450681451
35	H	31.0748	0.709447909448
36	H	30.5372	1.20619080619
37	H	30.7043	1.05179025179
39	H	27.8199	3.71697851698
43	H	28.3699	3.20877800878
46	H	29.0908	2.54266574267
48	H	30.5060	1.23501963502
49	H	30.0235	1.68085008085
50	H	30.7232	1.03432663433
52	H	25.6655	5.70764610765
54	H	25.0930	6.23663663664
56	H	25.2246	6.11503811504
58	H	25.3605	5.98946638947
60	H	29.6197	2.05396165396
61	H	29.8803	1.81316701317
62	H	30.0471	1.65904365904
63	H	29.9694	1.73083853084
65	H	29.5317	2.13527373527
66	H	30.4734	1.26514206514
70	H	26.6120	4.83307923308
71	H	28.1429	3.41852621853
73	H	30.0390	1.66652806653
74	H	30.5072	1.23391083391
78	H	30.2523	1.46943866944
79	H	30.8529	0.914483714484
80	H	30.6012	1.14705474705
81	H	27.8809	3.66061446061
83	H	28.3974	3.18336798337
85	H	29.6979	1.9817047817
88	H	29.9351	1.76253176253
89	H	28.1634	3.39958419958
93	H	28.5842	3.01076461076
94	H	28.2128	3.35393855394
95	H	28.1438	3.41769461769
96	H	28.2970	3.27613767614

Supporting Information: Original-MandelalideA-0009.log

Using Gaussian 09: AM64L-G09RevC.01 23-Sep-2011
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#b3lyp/6-31G(d,p) scf=(maxcycle=300,direct,tight) density=current SCRF=(PCM,SOLVENT=Chloroform) opt=(maxcycle=250) freq=noraman
#N Geom=AllCheck Guess=TCheck SCRF=Check GenChk RB3LYP/6-31G(d,p) Freq

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Pointgroup= C1 Stoichiometry= C33H52O11 C1[X(C33H52O11)]
#Atoms= 96
Charge = 0 Multiplicity = 1

SCF Energy= -2116.30413949 Predicted Change= -2.519932D-09
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Optimization completed. {Found 2 times}

Item	Max Val.	Criteria	Pass?	RMS Val.	Criteria	Pass?
Force	0.00000 ||	0.00045	[YES]	0.00000 ||	0.00030	[YES]
Displ	0.00148 ||	0.00180	[YES]	0.00148 ||	0.00180	[YES]

Atomic Coordinates (Angstroms)

Type	X	Y	Z
C	7.120838	0.670716	-1.129489
C	6.237753	1.720454	-0.436842
C	5.053921	2.131439	-1.325057
H	4.534105	1.232964	-1.676020
H	5.449983	2.637316	-2.211886
C	4.018184	3.056542	-0.683167
H	3.336683	3.426579	-1.453513
C	4.600445	4.247428	0.078391
O	5.423472	4.970621	-0.832796
H	5.787345	5.730601	-0.360792
H	5.170101	3.876171	0.940064
H	3.772121	4.864701	0.451607
O	3.242125	2.266725	0.257630
C	1.931993	2.568485	0.420422
O	1.362556	3.476024	-0.162000
C	1.317999	1.639306	1.392765
H	1.976741	0.914145	1.860940
C	0.009466	1.683801	1.668335
H	-0.587720	2.436473	1.156654
C	-0.684509	0.769819	2.632911
H	-1.212809	1.368420	3.387175
H	0.051633	0.154819	3.160097
C	-1.716400	-0.168485	1.982697
H	-2.130782	-0.806356	2.782769
O	5.820973	1.259198	0.848682
H	5.135979	0.594527	0.688707
H	6.861177	2.601137	-0.241954
H	7.431034	1.064148	-2.110360
C	8.342780	0.238289	-0.315985
H	9.221561	0.853060	-0.531026
H	8.120190	0.315267	0.753463
C	8.525027	-1.228713	-0.727099
H	8.978904	-1.242505	-1.727317
C	9.406816	-2.058560	0.205494
H	9.444040	-3.109096	-0.103178
H	9.050644	-2.021544	1.239757
H	10.432985	-1.677028	0.196435
C	7.059581	-1.698408	-0.911087
H	7.002205	-2.434178	-1.724725
O	6.341373	-0.525854	-1.343068
O	-1.010034	-0.992419	1.054518
C	-1.826152	-2.008739	0.458580
H	-2.232633	-2.645190	1.265678
C	-0.958171	-2.871443	-0.456230
C	0.112067	-3.759258	0.241507
H	-0.319290	-4.066801	1.208411
C	0.349142	-5.037040	-0.576953
H	0.724536	-4.804696	-1.579898
H	-0.586031	-5.593400	-0.693132
H	1.073841	-5.697268	-0.091160
C	1.381122	-2.995310	0.553716
H	1.244018	-2.117610	1.182886
C	2.616542	-3.306393	0.123466
H	2.757107	-4.171522	-0.522794
C	3.838223	-2.588362	0.465780
H	3.745725	-1.746170	1.153365
C	5.049719	-2.939780	0.000731
H	5.104150	-3.786573	-0.686963
C	6.369661	-2.303667	0.329499
H	6.256905	-1.530178	1.097100
H	7.030103	-3.079018	0.741873
H	-0.482516	-2.229851	-1.207619
H	-1.646115	-3.531828	-0.998046
C	-3.001227	-1.371694	-0.299239
H	-3.648669	-2.153132	-0.710781
H	-2.611809	-0.782796	-1.138603
C	-3.808363	-0.456771	0.616739
O	-4.802936	0.202763	-0.188328
C	-5.974016	0.591625	0.495571
H	-5.731553	1.115972	1.428363
H	-4.317786	-1.062675	1.378023
C	-2.880465	0.557730	1.291796
H	-3.424647	1.159207	2.029281
H	-2.495932	1.234839	0.521662
O	-6.756106	-0.508858	0.912710
C	-7.285060	-1.329277	-0.150145
C	-8.034319	-2.478005	0.503311
H	-7.359826	-3.069340	1.128833
H	-8.462490	-3.125723	-0.265063
H	-8.845714	-2.096845	1.131620
H	-6.456198	-1.718679	-0.756269
C	-8.171242	-0.460361	-1.047179
H	-8.995670	-0.063035	-0.433342
O	-8.672859	-1.254676	-2.113836
H	-9.032611	-0.623081	-2.755836
C	-7.365369	0.718880	-1.602294
O	-8.189231	1.535743	-2.429152
H	-8.702024	2.081738	-1.810359
H	-6.570021	0.324361	-2.242602
C	-6.734881	1.527180	-0.465032
O	-7.812062	2.189869	0.193223
C	-7.447892	3.384130	0.874981
H	-8.369012	3.814256	1.273017
H	-6.977097	4.104994	0.192855
H	-6.762166	3.190032	1.709739
H	-6.030145	2.263961	-0.873155

Statistical Thermodynamic Analysis
Temperature= 298.150 Kelvin Pressure= 1.00000 Atm
==========
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SCF Energy= -2116.30413949 Predicted Change= -2.519932D-09
Zero-point correction (ZPE)= -2115.4715 0.83259
Internal Energy (U)= -2115.4251 0.87894
Enthalpy (H)= -2115.4242
0.87988
Gibbs Free Energy (G)= -2115.5550
0.74908

Frequencies -- 6.3996 11.1995 16.0023

NMR-Shifts
Original-MandelalideA-0009-NMR.txt

Atom	Type	Isotropic	Scaled Shift
1	C	99.9952	82.3760026034
2	C	115.7085	67.3361856085
3	C	150.8675	33.6841248875
6	C	113.0909	69.8415934455
8	C	124.1166	59.2884626429
14	C	13.6296	165.039912709
16	C	55.9876	124.497406152
18	C	29.9693	149.400543655
20	C	145.5974	38.7283447233
23	C	108.6037	74.1364689217
29	C	150.3547	34.1749459216
32	C	145.7462	38.5859223951
34	C	172.3237	13.1475525948
38	C	101.2623	81.1632113938
42	C	104.2592	78.2947606195
44	C	141.1958	42.9412890752
45	C	146.2535	38.1003656272
47	C	167.0737	18.1725339306
51	C	41.4672	138.395451674
53	C	52.8405	127.50961925
55	C	49.3754	130.826202646
57	C	46.0530	134.006202263

59	C	148.5953	35.8589368097
64	C	146.5229	37.8425122992
67	C	113.3384	69.6047014683
69	C	91.9436	90.0825054078
72	C	151.1825	33.3826260074
76	C	115.2901	67.7366526924
77	C	168.9574	16.3695706273
82	C	110.1562	72.6505101552
86	C	112.0442	70.843431153
90	C	103.2195	79.2898983518
92	C	128.0323	55.5405922778
4	H	29.6725	2.00517440517
5	H	29.7218	1.95962115962
7	H	26.3834	5.04430584431
10	H	31.3048	0.496927696928
11	H	27.7033	3.82471702472
12	H	27.7326	3.79764379764
17	H	25.3593	5.99057519058
19	H	24.0176	7.23030723031
21	H	29.3572	2.29651189651
22	H	28.8976	2.72118272118
24	H	27.9596	3.5878955879
26	H	30.7532	1.00660660661
27	H	27.8023	3.73324093324
28	H	27.6340	3.88875028875
30	H	29.9870	1.71457611458
31	H	29.7443	1.93883113883
33	H	29.2467	2.39861399861
35	H	30.6925	1.06269346269
36	H	31.0162	0.763594363594
37	H	30.5946	1.15315315315
39	H	27.8022	3.73333333333
43	H	28.1574	3.40512820513
46	H	29.2825	2.36553476553
48	H	30.7341	1.02425502426
49	H	30.8257	0.939616539617
50	H	30.5355	1.20776160776
52	H	24.9648	6.35509355509
54	H	25.5403	5.82333102333
56	H	25.1981	6.13952413952
58	H	25.8798	5.50963270963
60	H	29.7584	1.9258027258
61	H	29.6183	2.05525525526
62	H	30.3797	1.35172095172
63	H	30.4366	1.29914529915
65	H	30.1317	1.58087318087
66	H	30.6729	1.0808038808
70	H	26.5267	4.9118965119
71	H	27.5710	3.94696234696
73	H	29.7625	1.92201432201
74	H	30.4505	1.2863016863
78	H	30.5866	1.16054516055
79	H	30.2562	1.46583506584
80	H	30.8159	0.948671748672
81	H	27.9873	3.5623007623
83	H	28.3508	3.22642642643
85	H	29.7217	1.95971355971
88	H	29.9076	1.78794178794
89	H	28.0327	3.52035112035
93	H	28.1546	3.40771540772
94	H	28.5738	3.02037422037
95	H	28.2017	3.36419496419
96	H	28.2888	3.28371448371

Supporting Information: Original-MandelalideA-0010.log

Using Gaussian 09: AM64L-G09RevC.01 23-Sep-2011

==========

#b3lyp/6-31G(d,p) scf=(maxcycle=300,direct,tight) density=current SCRF=(PCM,SOLVENT=Chloroform) opt=(maxcycle=250) freq=noraman

#N Geom=AllCheck Guess=TCheck SCRF=Check GenChk RB3LYP/6-31G(d,p) Freq

---

Pointgroup= C1 Stoichiometry= C33H52O11 C1[X(C33H52O11)] #Atoms= 96

Charge = 0 Multiplicity = 1

SCF Energy= -2116.30957470 Predicted Change= -7.752091D-09

==========

Optimization completed. {Found 1 times}

Item	Max Val.	Criteria	Pass?	RMS Val.	Criteria	Pass?
Force	0.00000	0.00045	[YES]	0.00000	0.00030	[YES]
Displ	0.00458	0.00180	[NO]	0.00458	0.00180	[YES]

Atomic Type	Coordinates (Angstroms) X	Y	Z
C	6.901107	1.711369	-0.263134
C	6.527021	1.465897	-1.735693
C	6.812441	0.032728	-2.231375
H	7.874383	-0.172764	-2.054660
H	6.660685	0.008279	-3.317145
C	6.019385	-1.116702	-1.601499
H	6.073817	-1.082466	-0.511623
C	6.499457	-2.493633	-2.093141
O	6.339162	-3.530013	-1.143758
H	5.432342	-3.439640	-0.800890
H	7.571989	-2.434684	-2.305826
H	5.993159	-2.714841	-3.047541
O	4.613694	-0.880044	-1.986998
C	3.630388	-1.612397	-1.424398
O	3.826422	-2.496141	-0.597121
C	2.307278	-1.213579	-1.941354
H	2.287883	-0.429497	-2.692449
C	1.189911	-1.816064	-1.509745
H	1.290402	-2.595493	-0.758887
C	-0.194720	-1.498582	-1.984269
H	-0.685504	-2.427717	-2.302734
H	-0.157758	-0.827890	-2.848997
C	-1.076564	-0.846842	-0.906327
H	-0.584311	0.081002	-0.568342
O	5.202133	1.897375	-2.026579
H	4.611132	1.199937	-1.709661
H	7.181913	2.126571	-2.319501
H	7.938172	1.368519	-0.113975
C	6.762573	3.165745	0.187894
H	7.656454	3.756745	-0.031830
H	5.909118	3.627535	-0.320193
C	6.495254	3.025763	1.693541
H	7.448982	2.785105	2.181815
C	5.916792	4.270881	2.366733
H	6.630666	5.098890	2.310400
H	5.702079	4.092542	3.425930
H	4.991215	4.598767	1.883578
C	5.631005	1.740834	1.752908
H	5.869363	1.156661	2.651041
O	6.035383	0.957230	0.606772
O	-1.166565	-1.746778	0.198405
C	-1.877217	-1.173373	1.306627
H	-1.383100	-0.223066	1.568357
C	-1.793594	-2.107494	2.513897
C	-0.366555	-2.430317	3.054666
H	-0.524213	-2.776442	4.088000
C	0.297346	-3.588265	2.296942
H	-0.322819	-4.487620	2.371028

H	1.280326	-3.822218	2.717813
H	0.416311	-3.356224	1.237434
C	0.469520	-1.175601	3.141243
H	0.085812	-0.407552	3.816510
C	1.584417	-0.904782	2.441086
H	1.983862	-1.649169	1.754584
C	2.308634	0.357210	2.499143
H	1.943573	1.105081	3.205463
C	3.358034	0.647333	1.711060
H	3.711087	-0.111293	1.015320
C	4.107773	1.948085	1.697442
H	3.877949	2.500234	0.774133
H	3.787018	2.572287	2.539159
H	-2.307697	-3.048485	2.281717
H	-2.372892	-1.625892	3.311560
C	-3.327321	-0.878030	0.896262
H	-3.873206	-0.424193	1.727981
H	-3.826863	-1.819529	0.636620
C	-3.355304	0.052490	-0.320579
O	-4.673687	0.226312	-0.867459
C	-5.491247	1.192090	-0.248429
H	-4.894174	2.065563	0.044735
H	-2.972994	1.041793	-0.021705
C	-2.475824	-0.506491	-1.438489
H	-2.407099	0.216796	-2.258211
H	-2.941397	-1.417848	-1.833092
O	-6.075668	0.749319	0.961269
C	-6.988484	-0.361943	0.836205
C	-7.448916	-0.722005	2.238547
H	-6.598348	-1.020586	2.857542
H	-8.160414	-1.549834	2.194203
H	-7.938594	0.135193	2.711629
H	-6.462918	-1.213514	0.384202
C	-8.136769	0.045018	-0.091882
H	-8.656033	0.904907	0.361032
O	-9.022383	-1.055828	-0.246844
H	-9.589238	-0.822849	-0.998418
C	-7.584932	0.471477	-1.455790
O	-8.648265	0.860415	-2.321003
H	-8.879540	1.762364	-2.043651
H	-7.103087	-0.394562	-1.920975
C	-6.554069	1.590401	-1.294936
O	-7.285001	2.744461	-0.885950
C	-6.666987	3.984643	-1.207264
H	-7.357464	4.771523	-0.897569
H	-6.481932	4.069960	-2.286750
H	-5.716808	4.122687	-0.675581
H	-6.052071	1.781275	-2.252804

Statistical Thermodynamic Analysis

Temperature= 298.150 Kelvin Pressure= 1.00000 Atm

==========

SCF Energy= -2116.30957470 Predicted Change= -7.752091D-09

Zero-point correction (ZPE)= -2115.4759 0.83358

Internal Energy (U)= -2115.4303 0.87925

Enthalpy (H)= -2115.4293 0.88019

Gibbs Free Energy (G)= -2115.5568 0.75275

Frequencies -- 9.4104 15.8168 19.5943

NMR-Shifts

Original-MandelalideA-0010-NMR.txt

Atom	Type	Isotropic	Scaled Shift
1	C	98.8948	83.4292386914
2	C	113.8956	69.0713834491
3	C	148.1926	36.2443768066
6	C	98.8576	83.4648442734
8	C	113.8326	69.1316832252
14	C	9.3527	169.13350179
16	C	59.8735	120.778058539
18	C	21.8449	157.176726201
20	C	144.1642	40.100116771
23	C	106.4795	76.1696242271
29	C	148.5583	35.8943509638
32	C	146.0628	38.2828920921
34	C	172.9516	12.546564827
38	C	100.1183	82.2581787553
42	C	108.5058	74.2301728594
44	C	144.8690	39.4255249909
45	C	148.4158	36.0307433144
47	C	167.5159	17.7492869312
51	C	44.6148	135.382760007
53	C	50.6480	129.60814717
55	C	50.2934	129.947548766
57	C	47.7057	132.424338138
59	C	148.4561	35.9921706005
64	C	144.0346	40.2241620245
67	C	103.3500	79.1649916729
69	C	84.0189	97.6675472348
72	C	145.7532	38.57922242
76	C	114.4552	68.5357682957
77	C	169.0599	16.2714638488
82	C	110.6540	72.1740462107
86	C	112.2841	70.6138134344
90	C	102.0802	80.3803671586
92	C	128.1659	55.412718467
4	H	30.0387	1.66680526681
5	H	29.4168	2.24144144144
7	H	25.7005	5.67530607531
10	H	27.4889	4.02282282282
11	H	28.1767	3.38729498729
12	H	27.8845	3.65728805729
17	H	25.4505	5.90630630631
19	H	23.5118	7.69766689767
21	H	29.2774	2.37024717025
22	H	29.5404	2.12723492723
24	H	28.5885	3.00679140679
26	H	29.3998	2.25714945715
27	H	28.2005	3.3653037653
28	H	27.5284	3.98632478632
30	H	30.0600	1.64712404712
31	H	29.9535	1.74553014553
33	H	29.2835	2.36461076461
35	H	30.5996	1.14853314853
36	H	30.7245	1.03312543313
37	H	31.0177	0.762208362208
39	H	27.8620	3.67807807808
43	H	28.5024	3.08634788635
46	H	29.0946	2.53915453915
48	H	30.7243	1.03331023331
49	H	30.6765	1.07747747748
50	H	29.9238	1.77297297297
52	H	25.6534	5.71882651883
54	H	25.2032	6.13481173481
56	H	25.3466	6.00231000231
58	H	25.8482	5.53883113883
60	H	29.6457	2.02993762994
61	H	29.8025	1.88505428505
62	H	30.0822	1.62661122661
63	H	30.0693	1.63853083853
65	H	29.5871	2.08408408408
66	H	30.4689	1.2693000693
70	H	26.5188	4.9191961192
71	H	28.0974	3.46056826057
73	H	30.0085	1.69471009471

74	H	30.5052	1.23575883576
78	H	30.5589	1.18613998614
79	H	30.2675	1.45539385539
80	H	30.8393	0.92705012705
81	H	27.8807	3.6607992608
83	H	28.4553	3.12986832987
85	H	29.6795	1.99870639871
88	H	29.9560	1.74322014322
89	H	28.1745	3.38932778933
93	H	28.1344	3.42638022638
94	H	28.5833	3.0115962116
95	H	28.1984	3.36724416724
96	H	28.2917	3.28103488103

Supporting Information: Original-MandelalideA-0011.log

```
-----------------------------------------------------------------------------
 Using  Gaussian 09:  AM64L-G09RevC.01 23-Sep-2011
=============================================================
=====================
 #b3lyp/6-31G(d,p) scf=(maxcycle=300,direct,tight) density=current
 SCRF=(PCM,SOLVENT=Chloroform) opt=(maxcycle=250)
freq=noraman
 #N Geom=AllCheck Guess=TCheck SCRF=Check GenChk RB3LYP/6-
31G(d,p) Freq
-----------------------------------------------------------------------------
 Pointgroup= C1   Stoichiometry= C33H52O11   C1[X(C33H52O11)]
#Atoms= 96
 Charge = 0                Multiplicity = 1
-----------------------------------------------------------------------------
 SCF Energy= -2116.30586770      Predicted Change= -2.853346D-08
=============================================================
=====================
 Optimization completed.          {Found       1       times}
 Item      Max Val.    Criteria    Pass?      RMS Val.    Criteria    Pass?
 Force      0.00001 ||  0.00045   [ YES ]      0.00000 ||  0.00030   [ YES ]
 Displ      0.00269 ||  0.00180   [ NO ]       0.00269 ||  0.00180   [ YES ]
-----------------------------------------------------------------------------
     Atomic      Coordinates (Angstroms)
      Type      X                Y                Z
-----------------------------------------------------------------------------
      C      -6.616832      0.492656      1.210987
      C      -5.291028      1.148197      0.814360
      C      -5.431661      2.638497      0.510862
      H      -5.909889      3.150813      1.352342
      H      -6.082413      2.765739     -0.362897
      C      -4.095270      3.330790      0.255672
      H      -3.466802      3.279653      1.146064
      C      -4.243706      4.788410     -0.178696
      O      -4.914038      5.481738      0.867969
      H      -4.947799      6.416687      0.628686
      H      -4.811603      4.826791     -1.121606
      H      -3.244391      5.203300     -0.363509
      O      -3.427559      2.604827     -0.811133
      C      -2.072436      2.559356     -0.777989
      O      -1.392932      3.207809     -0.000956
      C      -1.555793      1.616260     -1.793047
      H      -2.286879      1.082021     -2.392570
      C      -0.238785      1.420602     -1.932785
      H       0.419649      2.000383     -1.289071
      C       0.391364      0.481662     -2.917156
      H       0.845274      1.065011     -3.731373
      H      -0.375233     -0.155079     -3.370278
      C       1.498292     -0.405167     -2.324675
      H       1.806352     -1.119716     -3.107810
      O      -4.352900      0.994948      1.876461
      H      -4.350199      0.046633      2.078487
      H      -4.920328      0.635402     -0.086849
      H      -6.997642      0.999061      2.109080
      C      -7.688605      0.421671      0.115344
      H      -8.420540      1.229251      0.197452
      H      -7.234620      0.486991     -0.881962
      C      -8.313795     -0.969474      0.326615
      H      -8.979716     -0.908269      1.197400
      C      -9.116556     -1.507019     -0.857694
      H      -8.520079     -1.535835     -1.775033
      H      -9.985987     -0.869957     -1.049340
      H      -9.486912     -2.519322     -0.662924
      C      -7.086045     -1.793562      0.774984
      H      -7.382521     -2.618926      1.434629
      O      -6.329454     -0.877170      1.584104
      O       0.927720     -1.131539     -1.234845
      C       1.827294     -2.079922     -0.644136
      H       2.141617     -2.793714     -1.427827
      C       1.090896     -2.851047      0.452022
      C      -0.009235     -3.841732     -0.020791
      H       0.368415     -4.301824     -0.949611
      C      -0.186685     -4.969221      1.006424
      H       0.762034     -5.489170      1.171763
      H      -0.918056     -5.709373      0.668257
      H      -0.526467     -4.576939      1.971542
      C      -1.299193     -3.136913     -0.374533
      H      -1.188922     -2.307652     -1.070531
      C      -2.528432     -3.433801      0.083197
      H      -2.667077     -4.250046      0.790494
      C      -3.738145     -2.733736     -0.326473
      H      -3.608832     -1.913541     -1.034391
      C      -4.978460     -3.048021      0.085559
      H      -5.103726     -3.868922      0.794118
      C      -6.236279     -2.370554     -0.375190
      H      -5.989600     -1.582265     -1.095894
      H      -6.864936     -3.099994     -0.906989
      H       0.671276     -2.136827      1.170929
      H       1.853614     -3.427240      0.989574
      C       3.075777     -1.364069     -0.105051
      H       3.775904     -2.092167      0.313413
      H       2.778017     -0.680650      0.699658
      C       3.753662     -0.557117     -1.215442
      O       4.832335      0.265303     -0.740452
      C       6.075552     -0.368058     -0.544774
      H       6.242997     -1.127421     -1.319729
      H       4.156630     -1.251882     -1.970520
      C       2.741939      0.376224     -1.875269
      H       3.198269      0.879063     -2.734865
      H       2.463549      1.145063     -1.146633
      O       6.160792     -1.085982      0.670654
      C       6.048885     -0.288301      1.868823
      C       6.100798     -1.244565      3.047954
      H       6.025916     -0.684942      3.983185
      H       7.042899     -1.802261      3.047625
      H       5.274554     -1.959115      2.998202
      H       5.088498      0.244001      1.861136
      C       7.177199      0.748441      1.878674
      H       8.138330      0.209363      1.878547
      O       7.053823      1.559957      3.038835
      H       7.635219      2.320058      2.881814
      C       7.105267      1.616308      0.618743
      O       8.156722      2.578232      0.618147
      H       8.944797      2.087865      0.331220
      H       6.166027      2.178355      0.637219
      C       7.141268      0.745001     -0.637913
      O       8.460108      0.207322     -0.707534
      C       8.882760     -0.165920     -2.013226
      H       8.287187     -0.993634     -2.418946
      H       9.921086     -0.492328     -1.928231
      H       8.826325      0.682527     -2.708888
      H       6.935733      1.356175     -1.526846
-----------------------------------------------------------------------------
 Statistical Thermodynamic Analysis
```

Temperature= 298.150 Kelvin Pressure= 1.00000 Atm
==========
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SCF Energy= -2116.30586770 Predicted Change= -2.853346D-08
Zero-point correction (ZPE)= -2115.4733 0.83255
Internal Energy (U)= -2115.4270 0.87878
Enthalpy (H)= -2115.4261
0.87972
Gibbs Free Energy (G)= -2115.5559
0.74992

Frequencies -- 7.7167 14.0856 18.5841

NMR-Shifts
Original-MandelalideA-0011-NMR.txt

Atom	Type	Isotropic	Scaled Shift
1	C	97.6561	84.6148471449
2	C	110.9175	71.9218400046
3	C	152.2264	32.38346829
6	C	113.2201	69.7179310477
8	C	120.1557	63.0795957044
14	C	12.6889	165.94029365
16	C	58.7885	121.816554681
18	C	28.2687	151.028254752
20	C	145.8409	38.4952813032
23	C	109.0670	73.693026283
29	C	150.8702	33.6815406114
32	C	143.6845	40.5592564942
34	C	173.0697	12.4335266755
38	C	101.9134	80.5400179942
42	C	104.2008	78.3506575547
44	C	140.4397	43.6649821015
45	C	145.8270	38.5085855395
47	C	167.5476	17.7189456153
51	C	40.7819	139.051379238
53	C	52.7185	127.626390245
55	C	46.3070	133.76308888
57	C	50.2698	129.970137254
59	C	147.1737	37.2196060415
64	C	144.3919	39.8821761519
67	C	103.7598	78.7727559869
69	C	84.6637	97.0503838129
72	C	149.1859	35.2936503379
76	C	114.8412	68.1663125251
77	C	169.0668	16.2648595877
82	C	110.2598	72.5513505236
86	C	111.8379	71.040888991
90	C	102.3040	80.1661593828
92	C	128.0895	55.4858439097
4	H	29.8747	1.81834141834
5	H	30.3552	1.37435897436
7	H	26.3907	5.03756063756
10	H	31.2273	0.568537768538
11	H	28.2973	3.27586047586
12	H	27.4550	4.05414645415
17	H	25.3679	5.98262878263
19	H	23.8262	7.40716100716
21	H	29.3124	2.33790713791
22	H	28.7302	2.87586047586
24	H	27.9855	3.56396396396
26	H	29.5907	2.08075768076
27	H	28.1158	3.44356664357
28	H	27.8010	3.73444213444
30	H	29.7406	1.94224994225
31	H	30.4816	1.25756525757
33	H	29.1405	2.49674289674
35	H	31.0168	0.76303996304
36	H	30.5471	1.19704319704
37	H	30.6530	1.09919149919
39	H	27.6157	3.90565950566
43	H	28.2439	3.3252021252
46	H	29.4227	2.23598983599
48	H	30.8792	0.890182490182
49	H	30.5562	1.18863478863
50	H	30.7774	0.984245784246
52	H	24.8211	6.48787248787
54	H	25.4855	5.87396627397
56	H	25.2479	6.09350889351
58	H	25.8998	5.49115269115
60	H	29.8205	1.86842226842
61	H	29.6169	2.05654885655
62	H	30.2953	1.42970662971
63	H	30.4059	1.32751212751
65	H	29.4683	2.19385539386
66	H	30.4437	1.29258489258
70	H	26.5646	4.87687687688
71	H	28.0972	3.46075306075
73	H	30.1028	1.60757680758
74	H	29.9234	1.77334257334
78	H	30.2347	1.4857010857
79	H	30.8508	0.916424116424
80	H	30.5713	1.17468237468
81	H	27.8792	3.66218526219
83	H	28.3303	3.24536844537
85	H	29.6513	2.02476322476
88	H	29.8960	1.79866019866
89	H	28.0952	3.4626010626
93	H	28.1882	3.37666897667
94	H	28.1535	3.40873180873
95	H	28.5981	2.99792099792
96	H	28.1875	3.37731577732

Supporting Information: Original-MandelalideA-0012.log

Using Gaussian 09: AM64L-G09RevC.01 23-Sep-2011
==========
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#b3lyp/6-31G(d,p) scf=(maxcycle=300,direct,tight) density=current
SCRF=(PCM,SOLVENT=Chloroform) opt=(maxcycle=250)
freq=noraman
#N Geom=AllCheck Guess=TCheck SCRF=Check GenChk RB3LYP/6-
31G(d,p) Freq

Pointgroup= C1 Stoichiometry= C33H52O11 C1[X(C33H52O11)]
#Atoms= 96
Charge = 0 Multiplicity = 1

SCF Energy= -2116.30670580 Predicted Change= -1.889618D-08
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Optimization completed. {Found 2 times}

Item	Max Val.	Criteria	Pass?	RMS Val.	Criteria	Pass?
Force	0.00001 ||	0.00045	[YES]	0.00000 ||	0.00030	[YES]
Displ	0.00143 ||	0.00180	[YES]	0.00143 ||	0.00180	[YES]

Atomic Type	Coordinates (Angstroms) X	Y	Z
C	5.941559	1.130691	-1.266818
C	5.819496	-0.036120	-0.282711
C	5.962811	-1.393437	-0.967235
H	6.987594	-1.489105	-1.341000
H	5.285445	-1.460145	-1.826737
C	5.697975	-2.573777	-0.040583
H	6.150097	-2.401279	0.939829
C	6.202867	-3.906360	-0.612765
O	7.610610	-3.901819	-0.809594
H	8.029453	-3.877764	0.062052

H	5.752213	-4.075096	-1.596432
H	5.888682	-4.722943	0.049769
O	4.257936	-2.671472	0.129082
C	3.790462	-3.233538	1.271634
O	4.510416	-3.617157	2.178456
C	2.317535	-3.351739	1.298750
H	1.929249	-3.808592	2.204360
C	1.507469	-2.970890	0.302493
H	1.951187	-2.513973	-0.580375
C	0.019628	-3.147789	0.279116
H	-0.334574	-3.627029	1.197805
H	-0.235924	-3.811404	-0.558699
C	-0.745060	-1.832499	0.080003
H	-0.281962	-1.271127	-0.751678
O	6.847018	0.050090	0.703117
H	6.830738	0.967697	1.014774
H	4.829420	0.030906	0.198834
H	6.854870	0.995031	-1.868528
C	4.734501	1.388482	-2.167586
H	4.750663	0.789736	-3.082416
H	3.804269	1.168097	-1.629526
C	4.851459	2.896144	-2.450289
H	5.628923	3.022858	-3.215255
C	3.574976	3.563490	-2.963172
H	3.274066	3.121977	-3.918826
H	3.724665	4.635582	-3.130866
H	2.747737	3.441508	-2.258585
C	5.445191	3.454871	-1.126171
H	6.225053	4.190814	-1.365601
O	6.080627	2.330604	-0.480295
O	-0.601882	-1.079823	1.283435
C	-1.205648	0.220217	1.219940
H	-0.730680	0.784548	0.400033
C	-0.902345	0.911743	2.552539
C	-1.088079	2.440528	2.538364
H	-2.068238	2.662761	2.091671
C	-1.129724	2.996256	3.979860
H	-0.196451	2.770322	4.506672
H	-1.958607	2.554888	4.543582
H	-1.259540	4.083212	3.981510
C	-0.052783	3.200614	1.736701
H	-0.342572	4.218670	1.470145
C	1.183110	2.791729	1.399805
H	1.515226	1.787739	1.661315
C	2.161809	3.623818	0.713989
H	1.827881	4.614066	0.399694
C	3.436124	3.256516	0.490441
H	3.766242	2.276582	0.832677
C	4.496625	4.129227	-0.116694
H	4.051435	5.018316	-0.578495
H	5.144326	4.498525	0.692955
H	0.123763	0.660479	2.842079
H	-1.549909	0.479363	3.324873
C	-2.711081	0.093497	0.938605
H	-3.170573	1.081221	0.848320
H	-3.187347	-0.420587	1.782775
C	-2.959497	-0.722065	-0.333703
O	-4.348432	-1.016797	-0.556459
C	-5.140543	0.025280	-1.077745
H	-4.552793	0.643678	-1.768316
H	-2.584425	-0.157355	-1.203016
C	-2.225668	-2.058432	-0.251189
H	-2.323752	-2.600181	-1.198048
H	-2.685261	-2.669164	0.535372
O	-5.595227	0.934372	-0.094013
C	-6.465545	0.370142	0.909826
C	-6.784325	1.477840	1.899604
H	-5.869196	1.846157	2.371450
H	-7.453528	1.099838	2.675972
H	-7.274526	2.314943	1.392178
H	-5.944849	-0.450492	1.421081
C	-7.708293	-0.200806	0.219831
H	-8.221784	0.624847	-0.298721
O	-8.555654	-0.787875	1.198272
H	-9.197713	-1.314457	0.697379
C	-7.300218	-1.248740	-0.820578
O	-8.453206	-1.774861	-1.471830
H	-8.699840	-1.101743	-2.127484
H	-6.823735	-2.086690	-0.301534
C	-6.309901	-0.653069	-1.823185
O	-7.052676	0.283263	-2.600743
C	-6.520298	0.538550	-3.894724
H	-6.427726	-0.387906	-4.477777
H	-5.537507	1.024983	-3.848523
H	-7.218807	1.210709	-4.396876
H	-5.905158	-1.443450	-2.469387

Statistical Thermodynamic Analysis
Temperature= 298.150 Kelvin Pressure= 1.00000 Atm
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SCF Energy= -2116.30670580 Predicted Change= -1.889618D-08
Zero-point correction (ZPE)= -2115.4738 0.83286
Internal Energy (U)= -2115.4277 0.87896
Enthalpy (H)= -2115.4267
0.87991
Gibbs Free Energy (G)= -2115.5559
0.75073

Frequencies -- 11.6973 12.6850 16.7541

NMR-Shifts
Original-MandelalideA-0012-NMR.txt

Atom	Type	Isotropic	Scaled Shift
1	C	100.8282	81.5787055648
2	C	112.1105	70.7799728172
3	C	150.7329	33.8129558376
6	C	113.5160	69.4347135282
8	C	121.6495	61.649821015
14	C	14.0018	164.683665461
16	C	57.7974	122.765175444
18	C	28.0844	151.204655526
20	C	143.3017	40.925649419
23	C	108.5638	74.1746587798
29	C	147.4863	36.9204042956
32	C	144.2133	40.0531212313
34	C	173.1537	12.3531269741
38	C	102.5308	79.9490801891
42	C	110.7823	72.0512452382
44	C	146.8909	37.4902850361
45	C	151.0143	33.543616838
47	C	162.7439	22.3167556806
51	C	43.1735	136.762284883
53	C	52.3854	127.945213346
55	C	48.3722	131.786404793
57	C	50.3054	129.936063095
59	C	148.5941	35.8600853768
64	C	145.0525	39.249889929
67	C	103.7108	78.8196558127
69	C	85.0084	96.7204578954
72	C	144.8522	39.4416049312
76	C	114.8582	68.150041157
77	C	169.3905	15.9550335956
82	C	110.3638	72.4518080361
86	C	112.2570	70.6397519095
90	C	102.3887	80.085089684
92	C	128.2440	55.3379658876
4	H	29.5428	2.12501732502

5	H	30.3385	1.38978978979
7	H	26.4889	4.94682374682
10	H	31.1452	0.644398244398
11	H	28.7405	2.86634326634
12	H	27.7813	3.75264495264
17	H	25.6796	5.69461769462
19	H	24.3245	6.94673134673
21	H	29.3616	2.29244629245
22	H	29.4653	2.19662739663
24	H	28.2169	3.35015015015
26	H	29.3314	2.32035112035
27	H	28.0953	3.46250866251
28	H	27.9728	3.5756987757
30	H	29.9411	1.75698775699
31	H	30.5786	1.16793716794
33	H	29.1448	2.49276969277
35	H	30.7687	0.992284592285
36	H	30.7998	0.963548163548
37	H	30.7525	1.00725340725
39	H	27.3783	4.12501732502
43	H	28.4675	3.1185955186
46	H	29.4769	2.18590898591
48	H	31.2047	0.58942018942
49	H	30.6394	1.11175791176
50	H	30.5381	1.20535920536
52	H	25.7233	5.65423885424
54	H	25.2326	6.10764610765
56	H	25.3029	6.04268884269
58	H	25.5771	5.78932778933
60	H	29.4797	2.18332178332
61	H	29.0541	2.57657657658
62	H	29.7454	1.93781473781
63	H	30.4607	1.27687687688
65	H	29.2048	2.43732963733
66	H	30.6758	1.07812427812
70	H	26.7495	4.70602910603
71	H	28.0818	3.47498267498
73	H	29.9535	1.74553014553
74	H	30.3873	1.3446985447
78	H	30.5359	1.20739200739
79	H	30.3011	1.42434742435
80	H	30.8887	0.881404481404
81	H	27.8460	3.69286209286
83	H	28.3950	3.18558558559
85	H	29.6558	2.02060522061
88	H	29.9799	1.72113652114
89	H	28.2487	3.32076692077
93	H	28.6393	2.95985215985
94	H	28.2464	3.32289212289
95	H	28.1702	3.3933009933
96	H	28.3557	3.2218988219

Supporting Information: Original-MandelalideA-0013.log

Using Gaussian 09: AM64L-G09RevC.01 23-Sep-2011

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#b3lyp/6-31G(d,p) scf=(maxcycle=300,direct,tight) density=current SCRF=(PCM,SOLVENT=Chloroform) opt=(maxcycle=250) freq=noraman

#N Geom=AllCheck Guess=TCheck SCRF=Check GenChk RB3LYP/6-31G(d,p) Freq

---

Pointgroup= C1 Stoichiometry= C33H52O11 C1[X(C33H52O11)] #Atoms= 96

Charge = 0 Multiplicity = 1

SCF Energy= -2116.30609985 Predicted Change= -8.257719D-09

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Optimization completed. {Found 2 times}

Item	Max Val.	Criteria	Pass?	RMS Val.	Criteria	Pass?
Force	0.00000	0.00045	[YES]	0.00000	0.00030	[YES]
Displ	0.00179	0.00180	[YES]	0.00179	0.00180	[YES]

Atomic Type	Coordinates (Angstroms) X	Y	Z
C	-5.735022	-0.916145	-1.633082
C	-5.682846	0.263834	-0.658566
C	-5.613897	1.607512	-1.380131
H	-6.545329	1.736008	-1.945290
H	-4.789500	1.605264	-2.102106
C	-5.446031	2.803904	-0.445760
H	-6.091212	2.715616	0.429183
C	-5.697378	4.131111	-1.162926
O	-5.460931	5.255946	-0.332379
H	-4.518495	5.249313	-0.115253
H	-6.749265	4.175941	-1.461263
H	-5.086615	4.172982	-2.078582
O	-4.063475	2.837540	0.012676
C	-3.807394	2.825083	1.349136
O	-4.665434	2.737808	2.207648
C	-2.363134	2.941884	1.649364
H	-2.137317	3.039389	2.707151
C	-1.395354	2.917708	0.723819
H	-1.682145	2.793564	-0.318742
C	0.074380	3.034536	0.994859
H	0.263376	3.342732	2.028233
H	0.493061	3.804416	0.334009
C	0.833351	1.721319	0.740107
H	0.460493	1.262344	-0.193020
O	-6.858257	0.277789	0.146569
H	-6.951546	-0.624061	0.488674
H	-4.789473	0.139212	-0.024196
H	-6.545828	-0.738475	-2.358801
C	-4.437667	-1.272032	-2.357406
H	-4.282354	-0.683581	-3.265887
H	-3.576215	-1.117963	-1.695843
C	-4.635114	-2.769051	-2.652844
H	-5.316963	-2.841232	-3.510618
C	-3.363200	-3.542420	-3.001310
H	-2.913974	-3.140140	-3.915178
H	-3.577834	-4.601382	-3.181213
H	-2.620746	-3.476514	-2.201904
C	-5.436524	-3.264583	-1.415177
H	-6.236288	-3.938566	-1.752152
O	-6.056110	-2.085662	-0.856295
O	0.535185	0.858884	1.836277
C	1.097514	-0.455017	1.711986
H	0.681774	-0.929721	0.807706
C	0.650016	-1.235843	2.951664
C	0.779264	-2.765778	2.832522
H	1.771584	-2.996654	2.417386
C	0.727492	-3.426305	4.228981
H	-0.220239	-3.197873	4.728219
H	1.545351	-3.064647	4.861367
H	0.812373	-4.515192	4.155109
C	-0.243206	-3.424154	1.931367
H	0.001529	-4.448015	1.642577
C	-1.425281	-2.925617	1.528505
H	-1.713236	-1.912371	1.805150
C	-2.400229	-3.672539	0.746225
H	-2.108010	-4.675787	0.431605
C	-3.624723	-3.215202	0.429590
H	-3.917635	-2.221673	0.766569
C	-4.681680	-4.000678	-0.292139

H	-4.266888	-4.934321	-0.689718
H	-5.452318	-4.294639	0.436417
H	-0.387671	-0.961960	3.170281
H	1.240948	-0.891426	3.808792
C	2.626649	-0.370185	1.579595
H	3.051012	-1.365436	1.411464
H	3.044894	0.015239	2.517911
C	3.036395	0.563842	0.444200
O	4.470020	0.692457	0.481045
C	5.080438	0.994023	-0.754865
H	4.571006	1.827062	-1.255091
H	2.749492	0.118679	-0.517802
C	2.348748	1.922599	0.608753
H	2.560824	2.575477	-0.245559
H	2.732038	2.411724	1.512323
O	4.994458	-0.067772	-1.683116
C	5.676053	-1.281588	-1.302237
C	5.414775	-2.300679	-2.398335
H	4.341796	-2.485612	-2.500722
H	5.913684	-3.242241	-2.157392
H	5.797387	-1.937236	-3.357470
H	5.269108	-1.644941	-0.348913
C	7.162803	-0.969908	-1.104820
H	7.565893	-0.601604	-2.062150
O	7.835466	-2.153153	-0.695870
H	8.703246	-1.857335	-0.379690
C	7.337356	0.126170	-0.048170
O	8.718633	0.425149	0.131138
H	8.948772	1.004406	-0.614136
H	6.971746	-0.255466	0.910457
C	6.537152	1.375273	-0.425408
O	7.197953	1.944109	-1.553620
C	7.002867	3.344243	-1.713569
H	7.604008	3.651041	-2.571676
H	7.333772	3.897100	-0.823900
H	5.953060	3.594517	-1.913000
H	6.535361	2.087372	0.410524

Statistical Thermodynamic Analysis

Temperature= 298.150 Kelvin Pressure= 1.00000 Atm

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SCF Energy= -2116.30609985 Predicted Change= -8.257719D-09

Zero-point correction (ZPE)= -2115.4730 0.83303

Internal Energy (U)= -2115.4269 0.87915

Enthalpy (H)= -2115.4260 0.88009

Gibbs Free Energy (G)= -2115.5556 0.75046

Frequencies -- 10.7135 13.7598 18.7424

NMR-Shifts

Original-MandelalideA-0013-NMR.txt

Atom	Type	Isotropic	Scaled Shift
1	C	99.8564	82.5088535385
2	C	113.3463	69.5971400678
3	C	150.4012	34.1304389441
6	C	113.6843	69.2736269837
8	C	117.9139	65.2253105917
14	C	14.4875	164.218782902
16	C	56.7654	123.752943203
18	C	29.5487	149.803116446
20	C	143.9007	40.3523229771
23	C	110.0065	72.7937939088
29	C	147.8502	36.5721013036
32	C	144.7116	39.5761787171
34	C	173.7728	11.7605620322
38	C	102.5151	79.9641072762
42	C	110.3648	72.4508508968
44	C	145.9798	38.3623346542
45	C	151.1190	33.4434043531
47	C	162.7407	22.3198185264
51	C	43.0396	136.890445835
53	C	52.3323	127.996037443
55	C	48.9051	131.276345259
57	C	49.8379	130.383525718
59	C	148.2358	36.2030283888
64	C	147.0671	37.3216370911
67	C	113.8662	69.0995233446
69	C	91.8570	90.1653936714
72	C	146.9784	37.4065353472
76	C	115.1094	67.9096077643
77	C	169.0295	16.3005608836
82	C	109.8762	72.9185091598
86	C	111.9087	70.9731235284
90	C	103.1300	79.3755623193
92	C	127.9006	55.6666475239
4	H	30.3939	1.3386001386
5	H	30.3214	1.40559020559
7	H	25.7537	5.62614922615
10	H	30.8018	0.9617001617
11	H	28.1441	3.41741741742
12	H	28.1446	3.41695541696
17	H	25.5453	5.81871101871
19	H	24.2466	7.01871101871
21	H	29.3269	2.32450912451
22	H	29.4288	2.23035343035
24	H	28.3643	3.21395241395
26	H	29.3413	2.3112035112
27	H	28.0438	3.51009471009
28	H	28.0590	3.49604989605
30	H	30.1389	1.57422037422
31	H	30.7045	1.05160545161
33	H	29.2000	2.44176484176
35	H	30.8107	0.953476553477
36	H	30.9089	0.86273966274
37	H	30.7513	1.00836220836
39	H	27.4458	4.06264726265
43	H	28.4035	3.17773157773
46	H	29.5363	2.13102333102
48	H	31.2012	0.592654192654
49	H	30.5797	1.16692076692
50	H	30.5314	1.21155001155
52	H	25.7649	5.6158004158
54	H	25.2385	6.10219450219
56	H	25.4952	5.865003465
58	H	25.5517	5.8127974128
60	H	29.3910	2.26528066528
61	H	28.9677	2.65641025641
62	H	29.7133	1.96747516748
63	H	30.4642	1.27364287364
65	H	29.8201	1.86879186879
66	H	30.7979	0.965303765304
70	H	26.5402	4.89942249942
71	H	27.7463	3.78498498498
73	H	29.7836	1.90251790252
74	H	30.6644	1.08865788866
78	H	30.6227	1.12718872719
79	H	30.2900	1.4346038346
80	H	30.8284	0.937121737122
81	H	27.9715	3.5768999769
83	H	28.3763	3.20286440286
85	H	29.7127	1.96802956803
88	H	29.9095	1.78618618619
89	H	28.0797	3.47692307692
93	H	28.1672	3.39607299607
94	H	28.6064	2.99025179025

95	H	28.2738	3.29757449757
96	H	28.2834	3.2887040887

Supporting Information: Original-MandelalideA-0014.log

Using Gaussian 09: AM64L-G09RevC.01 23-Sep-2011

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#b3lyp/6-31G(d,p) scf=(maxcycle=300,direct,tight) density=current SCRF=(PCM,SOLVENT=Chloroform) opt=(maxcycle=250) freq=noraman

#N Geom=AllCheck Guess=TCheck SCRF=Check GenChk RB3LYP/6-31G(d,p) Freq

---

Pointgroup= C1 Stoichiometry= C33H52O11 C1[X(C33H52O11)] #Atoms= 96

Charge = 0 Multiplicity = 1

SCF Energy= -2116.30670502 Predicted Change= -5.769659D-09

==========

Optimization completed. {Found 2 times}

Item	Max Val.	Criteria	Pass?	RMS Val.	Criteria	Pass?
Force	0.00000	0.00045	[YES]	0.00000	0.00030	[YES]
Displ	0.00168	0.00180	[YES]	0.00168	0.00180	[YES]

Atomic Type	Coordinates (Angstroms) X	Y	Z
C	6.677810	-0.349979	1.331392
C	5.343835	-1.047272	1.049841
C	5.478678	-2.560483	0.907067
H	5.956400	-2.972739	1.804860
H	6.123597	-2.794013	0.055170
C	4.135734	-3.268885	0.733427
H	3.509031	-3.109426	1.613100
C	4.268472	-4.769720	0.508936
O	5.124843	-5.009408	-0.602781
H	5.157349	-5.963735	-0.746498
H	3.267873	-5.189837	0.346222
H	4.671981	-5.212829	1.433089
O	3.471263	-2.643691	-0.399896
C	2.118758	-2.622182	-0.387434
O	1.438963	-3.200602	0.444894
C	1.597546	-1.798134	-1.499759
H	2.327390	-1.315609	-2.143100
C	0.279803	-1.642248	-1.675670
H	-0.378908	-2.165179	-0.985086
C	-0.349562	-0.818659	-2.759457
H	-0.788111	-1.488380	-3.513320
H	0.415950	-0.223912	-3.268110
C	-1.471089	0.113207	-2.273519
H	-1.770006	0.746728	-3.126861
O	4.437409	-0.778998	2.117654
H	4.428622	0.186457	2.206528
H	4.943438	-0.638310	0.109759
H	7.089613	-0.753400	2.267355
C	7.713966	-0.396300	0.200529
H	8.455447	-1.185686	0.347974
H	7.228259	-0.576217	-0.766867
C	8.332881	1.013078	0.234694
H	9.026641	1.053008	1.084758
C	9.092829	1.418249	-1.027840
H	9.960118	0.766731	-1.175283
H	9.461952	2.447355	-0.959997
H	8.467120	1.341490	-1.922588
C	7.113078	1.875514	0.628675
H	7.423107	2.772039	1.180505
O	6.393754	1.051778	1.562073
O	-0.922164	0.944885	-1.250111
C	-1.831750	1.944321	-0.770061
H	-2.125960	2.583825	-1.622540
C	-1.117878	2.809166	0.269882
C	-0.013780	3.763447	-0.262651
H	-0.384266	4.157357	-1.224436
C	0.156170	4.961041	0.683404
H	0.885011	5.679136	0.295823
H	0.495841	4.638914	1.674190
H	-0.795019	5.487419	0.809868
C	1.278988	3.036375	-0.556842
H	1.170987	2.148257	-1.176331
C	2.508782	3.380555	-0.134908
H	2.646381	4.256858	0.496671
C	3.720486	2.655996	-0.492915
H	3.590632	1.773645	-1.121653
C	4.963168	3.017159	-0.129127
H	5.091189	3.900325	0.499604
C	6.220338	2.312939	-0.550185
H	5.967514	1.449532	-1.176626
H	6.819880	2.991613	-1.175130
H	-0.708654	2.158883	1.052694
H	-1.892188	3.423871	0.744640
C	-3.094890	1.284251	-0.194779
H	-3.806765	2.051063	0.122340
H	-2.820194	0.690548	0.685803
C	-3.746079	0.362937	-1.228860
O	-4.832044	-0.405945	-0.683858
C	-6.099614	0.207761	-0.676004
H	-6.256171	0.771218	-1.605358
H	-4.135991	0.972278	-2.060121
C	-2.718215	-0.628248	-1.769269
H	-3.156179	-1.218955	-2.581244
H	-2.448604	-1.317020	-0.961434
O	-6.257694	1.174120	0.344061
C	-6.188671	0.667716	1.693892
C	-6.313004	1.861733	2.625095
H	-6.285270	1.526324	3.664405
H	-7.258607	2.385306	2.451231
H	-5.492112	2.565066	2.459825
H	-5.220430	0.173039	1.847372
C	-7.298329	-0.369350	1.887461
H	-8.266750	0.129221	1.720190
O	-7.220565	-0.893688	3.205965
H	-7.780870	-1.685230	3.200084
C	-7.147327	-1.498102	0.862370
O	-8.182152	-2.462728	1.031057
H	-8.960819	-2.072645	0.600529
H	-6.201901	-2.015950	1.054164
C	-7.129752	-0.936334	-0.561394
O	-8.454102	-0.474264	-0.819457
C	-8.813235	-0.437046	-2.195203
H	-8.205940	0.281007	-2.761118
H	-9.857790	-0.122903	-2.240882
H	-8.712777	-1.427004	-2.660812
H	-6.860022	-1.726222	-1.274911

Statistical Thermodynamic Analysis

Temperature= 298.150 Kelvin Pressure= 1.00000 Atm

==========

SCF Energy= -2116.30670502 Predicted Change= -5.769659D-09

Zero-point correction (ZPE)= -2115.4739 0.83276

Internal Energy (U)= -2115.4278 0.87887

Enthalpy (H)= -2115.4268 0.87981

Gibbs Free Energy (G)= -2115.5562 0.75049

Frequencies -- 9.2268 13.5132 18.3966

NMR-Shifts
Original-MandelalideA-0014-NMR.txt

Atom	Type	Isotropic	Scaled Shift
1	C	98.4678	83.8379371734
2	C	109.9306	72.8664407818
3	C	154.0701	30.6187905588
6	C	112.3182	70.5811749842
8	C	120.2568	62.9828289209
14	C	12.3013	166.311280844
16	C	58.9132	121.69719941
18	C	28.7635	150.554662226
20	C	145.6702	38.6586649821
23	C	108.9926	73.7642374471
29	C	150.8850	33.6673749498
32	C	144.2261	40.0408698482
34	C	172.7799	12.7109056452
38	C	101.9917	80.4650739869
42	C	104.6820	77.8900821226
44	C	140.5723	43.53806543
45	C	146.1338	38.2149352017
47	C	167.6533	17.6177759911
51	C	40.2915	139.520760351
53	C	53.4847	126.893030112
55	C	46.4425	133.633396505
57	C	50.1074	130.125576676
59	C	146.9546	37.4293152625
64	C	144.2526	40.0155056567
67	C	103.1907	79.3174639637
69	C	84.4506	97.2543501981
72	C	149.1373	35.3401673079
76	C	115.1300	67.8898906947
77	C	169.1072	16.2261911599
82	C	110.3277	72.4863607649
86	C	112.3742	70.5275751833
90	C	102.5814	79.9006489404
92	C	127.9736	55.5967763548
4	H	30.5493	1.19501039501
5	H	29.4475	2.21307461307
7	H	26.5119	4.92557172557
10	H	31.3553	0.450265650266
11	H	27.3543	4.14719334719
12	H	27.9870	3.56257796258
17	H	25.3157	6.03086163086
19	H	23.8433	7.39136059136
21	H	29.2523	2.39343959344
22	H	28.7331	2.87318087318
24	H	27.9548	3.59233079233
26	H	29.5485	2.11975051975
27	H	28.1152	3.44412104412
28	H	27.8687	3.67188727189
30	H	29.8124	1.87590667591
31	H	30.3478	1.3811965812
33	H	29.1722	2.46745206745
35	H	30.6050	1.14354354354
36	H	30.6620	1.09087549088
37	H	30.9933	0.784753984754
39	H	27.6129	3.90824670825
43	H	28.2264	3.34137214137
46	H	29.3594	2.29447909448
48	H	30.4813	1.25784245784
49	H	30.8338	0.932132132132
50	H	30.8735	0.895449295449
52	H	24.8413	6.46920766921
54	H	25.5183	5.84365904366
56	H	25.2556	6.08639408639
58	H	25.9173	5.47498267498
60	H	29.7371	1.94548394548
61	H	29.6135	2.05969045969
62	H	30.3431	1.38553938554
63	H	30.4372	1.29859089859
65	H	29.4845	2.17888657889
66	H	30.4540	1.28306768307
70	H	26.5244	4.91402171402
71	H	28.0453	3.50870870871
73	H	30.0011	1.70154770155
74	H	29.8719	1.82092862093
78	H	30.2326	1.48764148764
79	H	30.9071	0.864402864403
80	H	30.6039	1.14455994456
81	H	27.8827	3.65895125895
83	H	28.4047	3.17662277662
85	H	29.7087	1.97172557173
88	H	29.8578	1.83395703396
89	H	28.0315	3.52145992146
93	H	28.1982	3.36742896743
94	H	28.1324	3.42822822823
95	H	28.5629	3.03044583045
96	H	28.1769	3.38711018711

Supporting Information: Original-MandelalideA-0015.log

```
-----------------------------------------------------------------------
 Using  Gaussian 09:  AM64L-G09RevC.01 23-Sep-2011
=======================================================================
 #b3lyp/6-31G(d,p) scf=(maxcycle=300,direct,tight) density=current
 SCRF=(PCM,SOLVENT=Chloroform) opt=(maxcycle=250)
freq=noraman
 #N Geom=AllCheck Guess=TCheck SCRF=Check GenChk RB3LYP/6-
31G(d,p) Freq
-----------------------------------------------------------------------
 Pointgroup= C1   Stoichiometry= C33H52O11   C1[X(C33H52O11)]
#Atoms= 96
 Charge = 0                Multiplicity = 1
-----------------------------------------------------------------------
 SCF Energy= -2116.30685058      Predicted Change= -5.940620D-09
=======================================================================
 Optimization completed.          {Found       1       times}
 Item     Max Val.    Criteria    Pass?     RMS Val.    Criteria    Pass?
 Force     0.00000 ||  0.00045   [ YES ]     0.00000 ||  0.00030   [ YES ]
 Displ     0.00223 ||  0.00180   [ NO ]      0.00223 ||  0.00180   [ YES ]
-----------------------------------------------------------------------
     Atomic     Coordinates (Angstroms)
      Type      X                Y              Z
-----------------------------------------------------------------------
      C       6.052223     -0.730633      1.654556
      C       6.114223      0.199610      0.438652
      C       6.266674      1.668578      0.833969
      H       7.305853      1.815015      1.148953
      H       5.633035      1.912340      1.691836
      C       5.939899      2.643777     -0.301774
      H       6.197030      2.210810     -1.271473
      C       6.601295      4.010075     -0.148333
      O       6.275022      4.637753      1.085071
      H       5.311140      4.724830      1.098933
      H       6.322045      4.641024     -1.004960
      H       7.688348      3.885878     -0.162524
      O       4.503569      2.911727     -0.276998
      C       3.696113      2.335617     -1.202194
      O       4.088350      1.582059     -2.075726
      C       2.293796      2.743030     -0.968975
      H       2.120821      3.470251     -0.180816
      C       1.284155      2.214300     -1.672315
      H       1.521775      1.484274     -2.442379
      C      -0.161487      2.536762     -1.446481
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H	-0.625465	2.850454	-2.390722
H	-0.256256	3.365667	-0.737058
C	-0.965558	1.340439	-0.910964
H	-0.438198	0.925106	-0.034787
O	7.238200	-0.123272	-0.378914
H	7.196517	-1.083018	-0.508244
H	5.186251	0.058153	-0.136824
H	6.866418	-0.474596	2.351550
C	4.706691	-0.770989	2.379913
H	4.613932	0.002473	3.147279
H	3.886338	-0.643112	1.662762
C	4.685259	-2.190305	2.968988
H	5.318347	-2.181933	3.866200
C	3.302965	-2.702634	3.373659
H	3.354318	-3.723193	3.768111
H	2.610712	-2.698826	2.527059
H	2.878775	-2.069026	4.159372
C	5.449696	-3.022576	1.901919
H	6.126047	-3.721992	2.412241
O	6.261889	-2.074690	1.176497
O	-1.005639	0.351304	-1.939544
C	-1.636215	-0.868115	-1.520736
H	-1.083269	-1.261924	-0.651077
C	-1.566020	-1.885277	-2.660252
C	-0.164300	-2.395694	-3.094427
H	-0.382962	-3.234488	-3.775859
C	0.635813	-1.369587	-3.906297
H	0.041190	-1.010289	-4.752074
H	1.552163	-1.816471	-4.304707
H	0.905059	-0.503358	-3.300564
C	0.591993	-2.998086	-1.934081
H	0.065391	-3.795726	-1.405165
C	1.832714	-2.679618	-1.524593
H	2.382162	-1.889192	-2.033666
C	2.543834	-3.358925	-0.450147
H	2.007486	-4.156510	0.066935
C	3.816622	-3.090094	-0.107851
H	4.344956	-2.303889	-0.645286
C	4.633277	-3.855818	0.892808
H	4.010581	-4.574315	1.438256
H	5.371666	-4.453720	0.337261
H	-2.075984	-1.463727	-3.535505
H	-2.161141	-2.750468	-2.341329
C	-3.093085	-0.592743	-1.110440
H	-3.560925	-1.509164	-0.739859
H	-3.652663	-0.261798	-1.994244
C	-3.170363	0.503987	-0.044260
O	-4.518538	0.931727	0.215188
C	-5.248549	0.193060	1.166316
H	-4.601075	-0.095149	2.004876
H	-2.740657	0.124243	0.896539
C	-2.386100	1.736421	-0.490994
H	-2.353464	2.472799	0.319177
H	-2.899960	2.196912	-1.343610
O	-5.743978	-1.036448	0.673098
C	-6.702181	-0.932823	-0.401818
C	-7.064565	-2.349310	-0.814796
H	-6.179436	-2.885267	-1.168499
H	-7.804970	-2.322980	-1.617650
H	-7.486899	-2.898086	0.033100
H	-6.242555	-0.402688	-1.246614
C	-7.906112	-0.118729	0.082236
H	-8.364385	-0.653406	0.929796
O	-8.832247	0.020896	-0.986878
H	-9.449945	0.711237	-0.699954
C	-7.450753	1.261057	0.566524
O	-8.567285	2.017896	1.026328
H	-8.749574	1.679336	1.918545
H	-7.031180	1.807071	-0.284602
C	-6.379817	1.124845	1.650145
O	-7.043381	0.596468	2.796220
C	-6.415746	0.895068	4.037250
H	-7.058012	0.490293	4.821787
H	-6.310018	1.979225	4.180028
H	-5.424751	0.430890	4.120999
H	-5.950657	2.108653	1.882462

Statistical Thermodynamic Analysis
Temperature= 298.150 Kelvin Pressure= 1.00000 Atm
==========
==========
SCF Energy= -2116.30685058 Predicted Change= -5.940620D-09
Zero-point correction (ZPE)= -2115.4735 0.83334
Internal Energy (U)= -2115.4276 0.87918
Enthalpy (H)= -2115.4267
0.88012
Gibbs Free Energy (G)= -2115.5550
0.75182

Frequencies -- 10.0887 15.5664 17.7655

NMR-Shifts
Original-MandelalideA-0015-NMR.txt

Atom	Type	Isotropic	Scaled Shift
1	C	100.9624	81.4502574705
2	C	110.3632	72.4523823197
3	C	145.9553	38.3857845671
6	C	111.1302	71.718256475
8	C	116.5425	66.5379314305
14	C	13.4814	165.181760753
16	C	59.2915	121.335113612
18	C	24.5218	154.614560003
20	C	144.0847	40.1762093455
23	C	106.6571	75.9996362871
29	C	147.7608	36.6576695572
32	C	143.7350	40.5109209594
34	C	172.9707	12.5282834664
38	C	101.0512	81.3652635004
42	C	109.1449	73.6184651314
44	C	142.9355	41.2761538314
45	C	147.3305	37.0695265989
47	C	168.1835	17.1103007332
51	C	43.5295	136.421543291
53	C	50.0410	130.189130726
55	C	49.9666	130.26034189
57	C	48.7587	131.416470453
59	C	148.3703	36.0742931526
64	C	143.2670	40.9588621528
67	C	103.7556	78.776775972
69	C	84.4160	97.287467218
72	C	145.9387	38.4016730795
76	C	115.0497	67.9667489806
77	C	169.1508	16.1844598863
82	C	110.4746	72.3457570015
86	C	112.5400	70.368881487
90	C	102.5361	79.9440073508
92	C	128.1852	55.3942456785
4	H	30.0811	1.62762762763
5	H	29.9614	1.73823053823
7	H	25.9856	5.41187341187
10	H	30.5902	1.15721875722
11	H	27.7497	3.78184338184
12	H	28.1970	3.36853776854
17	H	25.5222	5.84005544006
19	H	23.7539	7.47396627397
21	H	29.2764	2.37117117117
22	H	29.5413	2.1264033264
24	H	28.5579	3.03506583507

26	H	29.2697	2.37736197736
27	H	27.9850	3.56442596443
28	H	28.0746	3.48163548164
30	H	30.0780	1.63049203049
31	H	30.6844	1.07017787018
33	H	29.1451	2.49249249249
35	H	30.6801	1.07415107415
36	H	30.8021	0.961422961423
37	H	30.8244	0.940817740818
39	H	27.4594	4.05008085008
43	H	28.3266	3.24878724879
46	H	29.1005	2.5337029337
48	H	30.6605	1.09226149226
49	H	30.6101	1.13883113883
50	H	29.9598	1.73970893971
52	H	25.7047	5.67142527143
54	H	25.2195	6.11975051975
56	H	25.3919	5.96045276045
58	H	25.5164	5.84541464541
60	H	29.6183	2.05525525526
61	H	29.1520	2.48611688612
62	H	30.0165	1.68731808732
63	H	30.0684	1.63936243936
65	H	29.6106	2.06237006237
66	H	30.4803	1.25876645877
70	H	26.5602	4.88094248094
71	H	28.1610	3.4018018018
73	H	30.0633	1.64407484407
74	H	30.5350	1.20822360822
78	H	30.5423	1.20147840148
79	H	30.2255	1.4942018942
80	H	30.8293	0.93629013629
81	H	27.8488	3.69027489027
83	H	28.4086	3.17301917302
85	H	29.6200	2.05368445368
88	H	29.9706	1.72972972973
89	H	28.2092	3.35726495726
93	H	28.1323	3.42832062832
94	H	28.5778	3.01667821668
95	H	28.2165	3.35051975052
96	H	28.2851	3.28713328713

Supporting Information: Original-MandelalideA-0016.log

Using Gaussian 09: AM64L-G09RevC.01 23-Sep-2011

==========

#b3lyp/6-31G(d,p) scf=(maxcycle=300,direct,tight) density=current SCRF=(PCM,SOLVENT=Chloroform) opt=(maxcycle=250) freq=noraman

#N Geom=AllCheck Guess=TCheck SCRF=Check GenChk RB3LYP/6-31G(d,p) Freq

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Pointgroup= C1 Stoichiometry= C33H52O11 C1[X(C33H52O11)]

#Atoms= 96

Charge = 0 Multiplicity = 1

SCF Energy= -2116.30388307 Predicted Change= -1.174059D-08

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Optimization completed. {Found 1 times}

Item	Max Val.	Criteria	Pass?	RMS Val.	Criteria	Pass?
Force	0.00001	0.00045	[YES]	0.00000	0.00030	[YES]
Displ	0.00341	0.00180	[NO]	0.00341	0.00180	[YES]

Atomic Type	Coordinates (Angstroms) X	Y	Z
C	7.365958	-0.999695	0.205050
C	7.110461	0.501469	-0.023558
C	5.816317	1.022154	0.599241
H	5.857101	0.935921	1.691344
H	5.012209	0.371310	0.244852
C	5.478941	2.468039	0.214460
H	5.615842	2.620241	-0.859234
C	6.242302	3.534308	0.994893
O	5.871671	4.847727	0.600739
H	4.915329	4.910294	0.734939
H	7.308482	3.417969	0.797130
H	6.078560	3.376748	2.072958
O	4.073008	2.729603	0.518169
C	3.164997	2.506180	-0.467768
O	3.459355	2.096908	-1.576275
C	1.796943	2.820513	0.001266
H	1.695161	3.216023	1.007914
C	0.739525	2.597451	-0.790368
H	0.928831	2.188879	-1.779704
C	-0.692339	2.821651	-0.407516
H	-1.201295	3.386741	-1.198842
H	-0.760130	3.404078	0.517379
C	-1.447059	1.497883	-0.202545
H	-0.937868	0.933746	0.598182
O	8.210686	1.239776	0.522033
H	8.992985	1.052243	-0.014700
H	7.049253	0.660980	-1.110856
H	8.310615	-1.236943	-0.318439
C	7.475879	-1.492236	1.646670
H	8.449285	-1.275973	2.092697
H	6.704321	-1.037049	2.278100
C	7.209224	-2.995549	1.472132
H	8.120083	-3.444925	1.054687
C	6.863716	-3.745815	2.758780
H	5.990646	-3.315591	3.259278
H	7.703230	-3.700047	3.459997
H	6.655307	-4.803477	2.564761
C	6.141020	-3.014283	0.338127
H	6.356024	-3.833797	-0.362446
O	6.303664	-1.766326	-0.372716
O	-1.355200	0.750852	-1.416274
C	-1.889568	-0.573833	-1.282164
H	-1.367868	-1.065152	-0.442811
C	-1.606222	-1.369774	-2.557395
C	-0.128388	-1.401617	-3.053922
H	-0.006643	-2.335457	-3.618610
C	0.162518	-0.237700	-4.026020
H	-0.512430	-0.281397	-4.888482
H	1.191460	-0.286800	-4.395260
H	0.015904	0.726093	-3.533018
C	0.871028	-1.410946	-1.926590
H	0.866531	-0.528695	-1.287659
C	1.779847	-2.370018	-1.680889
H	1.819396	-3.253298	-2.320424
C	2.743713	-2.300644	-0.591566
H	2.661324	-1.434310	0.066423
C	3.701409	-3.209252	-0.344730
H	3.793783	-4.071072	-1.008282
C	4.677674	-3.144972	0.794789
H	4.427236	-2.311707	1.461525
H	4.595872	-4.068863	1.384330
H	-2.242987	-0.991226	-3.366835
H	-1.936902	-2.395298	-2.353932
C	-3.388839	-0.497047	-0.956157
H	-3.803369	-1.500721	-0.826378
H	-3.912501	-0.024862	-1.796327
C	-3.619173	0.343435	0.306297
O	-5.006295	0.616255	0.562819
C	-5.766536	-0.434126	1.114978
H	-5.147866	-1.040381	1.789023

H	-3.209294	-0.197853	1.174602
C	-2.916174	1.696518	0.186124
H	-2.993265	2.243163	1.132151
H	-3.416541	2.290343	-0.588188
O	-6.240164	-1.353518	0.150546
C	-7.147238	-0.803704	-0.828602
C	-7.481946	-1.919154	-1.804289
H	-8.180398	-1.553241	-2.560430
H	-7.944378	-2.760797	-1.278640
H	-6.577146	-2.276945	-2.303306
H	-6.651812	0.020972	-1.357996
C	-8.375475	-0.245010	-0.103320
H	-8.863106	-1.074740	0.433219
O	-9.258885	0.328627	-1.057557
H	-9.893227	0.847364	-0.538980
C	-7.949148	0.811399	0.921152
O	-9.088286	1.324089	1.606778
H	-9.303526	0.650665	2.273150
H	-7.500240	1.653987	0.385378
C	-6.920542	0.232307	1.894327
O	-7.626741	-0.710334	2.697819
C	-7.052877	-0.952433	3.976467
H	-7.727357	-1.631074	4.502205
H	-6.955144	-0.022047	4.552369
H	-6.065653	-1.426409	3.903411
H	-6.506009	1.030124	2.525013

Statistical Thermodynamic Analysis
Temperature= 298.150 Kelvin Pressure= 1.00000 Atm
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SCF Energy= -2116.30388307 Predicted Change= -1.174059D-08
Zero-point correction (ZPE)= -2115.4710 0.83280
Internal Energy (U)= -2115.4249 0.87896
Enthalpy (H)= -2115.4239 0.87990
Gibbs Free Energy (G)= -2115.5532 0.75059

Frequencies -- 11.5437 12.4492 17.8002

NMR-Shifts
Original-MandelalideA-0016-NMR.txt

Atom	Type	Isotropic	Scaled Shift
1	C	100.4706	81.9209785792
2	C	113.0406	69.8897375524
3	C	154.7434	29.9743486667
6	C	106.2527	76.3867034208
8	C	118.4661	64.6967782691
14	C	12.8446	165.791267061
16	C	60.1350	120.527766611
18	C	24.5458	154.59158866
20	C	144.8414	39.4519420356
23	C	104.7788	77.7974310381
29	C	151.5392	33.0412144183
32	C	145.6810	38.6483278776
34	C	172.3699	13.103332759
38	C	101.4481	80.9853749115
42	C	108.7875	73.960546718
44	C	143.7346	40.5113038152
45	C	146.2085	38.1434368958
47	C	161.6562	23.3578360995
51	C	42.0309	137.855912249
53	C	51.4171	128.872011333
55	C	46.7499	133.339171883
57	C	50.0666	130.16462796
59	C	146.5435	37.8227952296
64	C	143.8857	40.3666800666
67	C	103.9453	78.5952066464
69	C	85.2301	96.5082601122
72	C	145.2937	39.0190279293
76	C	114.8523	68.1556882789
77	C	169.4769	15.8723367599
82	C	110.1529	72.6536687149
86	C	112.1470	70.7450372327
90	C	102.4500	80.0264170447
92	C	128.2346	55.346962997
4	H	30.2739	1.44948024948
5	H	29.7299	1.95213675214
7	H	26.4988	4.93767613768
10	H	30.4754	1.26329406329
11	H	27.2943	4.20263340263
12	H	28.0887	3.46860706861
17	H	25.4668	5.89124509125
19	H	23.6005	7.61570801571
21	H	29.1938	2.44749364749
22	H	29.4893	2.17445137445
24	H	28.4259	3.15703395703
26	H	31.1396	0.649572649573
27	H	27.4371	4.07068607069
28	H	27.7123	3.8164010164
30	H	29.9501	1.74867174867
31	H	30.4435	1.29276969277
33	H	29.2577	2.38844998845
35	H	31.1599	0.630815430815
36	H	30.5050	1.23594363594
37	H	30.7117	1.04495264495
39	H	27.5784	3.94012474012
43	H	28.4016	3.17948717949
46	H	29.2485	2.39695079695
48	H	30.6716	1.08200508201
49	H	30.7880	0.974451374451
50	H	30.0280	1.67669207669
52	H	25.7121	5.66458766459
54	H	25.2467	6.09461769462
56	H	25.3613	5.98872718873
58	H	26.0279	5.37278817279
60	H	29.9966	1.70570570571
61	H	29.5705	2.09942249942
62	H	30.1316	1.58096558097
63	H	30.1566	1.55786555787
65	H	29.4094	2.24827904828
66	H	30.4477	1.28888888889
70	H	26.8045	4.65520905521
71	H	28.0067	3.54437514438
73	H	29.9152	1.78091938092
74	H	30.3276	1.39986139986
78	H	30.3114	1.41483021483
79	H	30.9189	0.8534996535
80	H	30.5761	1.17024717025
81	H	27.8297	3.70792330792
83	H	28.3788	3.20055440055
85	H	29.6715	2.0060984061
88	H	29.9616	1.73804573805
89	H	28.2129	3.35384615385
93	H	28.1758	3.38812658813
94	H	28.6404	2.95883575884
95	H	28.2501	3.31947331947
96	H	28.3460	3.23086163086

Supporting Information: Original-MandelalideA-0017.log

Using Gaussian 09: AM64L-G09RevC.01 23-Sep-2011
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#b3lyp/6-31G(d,p) scf=(maxcycle=300,direct,tight) density=current
SCRF=(PCM,SOLVENT=Chloroform) opt=(maxcycle=250)
freq=noraman

#N Geom=AllCheck Guess=TCheck SCRF=Check GenChk RB3LYP/6-31G(d,p) Freq

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Pointgroup= C1 Stoichiometry= C33H52O11 C1[X(C33H52O11)]
#Atoms= 96
Charge = 0 Multiplicity = 1

SCF Energy= -2116.30542761 Predicted Change= -1.642017D-08
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Optimization completed. {Found 2 times}

Item	Max Val.	Criteria	Pass?	RMS Val.	Criteria	Pass?
Force	0.00000	0.00045	[YES]	0.00000	0.00030	[YES]
Displ	0.00179	0.00180	[YES]	0.00179	0.00180	[YES]

Atomic Type	Coordinates (Angstroms) X	Y	Z
C	5.996420	-1.001872	1.360843
C	5.873463	0.150007	0.359569
C	5.967939	1.515437	1.036306
H	6.976682	1.615441	1.455605
H	5.259011	1.572361	1.870165
C	5.715250	2.692189	0.096452
H	6.224474	2.553158	-0.858122
C	6.118315	4.026096	0.727317
O	5.801277	5.138512	-0.093001
H	4.837282	5.166064	-0.165327
H	7.203848	4.036134	0.865517
H	5.652972	4.115434	1.721637
O	4.283631	2.772078	-0.161309
C	3.840346	2.752295	-1.447918
O	4.563969	2.616937	-2.416913
C	2.374434	2.926923	-1.545630
H	2.008751	3.023128	-2.563601
C	1.541651	2.953455	-0.497068
H	1.960392	2.827824	0.499709
C	0.054694	3.128870	-0.575548
H	-0.249961	3.468705	-1.570758
H	-0.249350	3.896334	0.147505
C	-0.718026	1.838275	-0.255567
H	-0.264006	1.352549	0.626847
O	6.928642	0.078713	-0.594849
H	6.928994	-0.835027	-0.917434
H	4.897688	0.054772	-0.145267
H	6.903912	-0.847744	1.967602
C	4.787710	-1.261408	2.258424
H	4.782819	-0.640073	3.158286
H	3.857728	-1.075950	1.707040
C	4.937761	-2.758478	2.578960
H	5.715326	-2.847535	3.349137
C	3.675986	-3.442531	3.105951
H	3.362790	-2.984346	4.049756
H	3.850593	-4.506183	3.300974
H	2.847857	-3.357909	2.397177
C	5.549710	-3.335262	1.270101
H	6.350681	-4.041002	1.530392
O	6.151855	-2.210460	0.593142
O	-0.570101	0.981196	-1.386056
C	-1.173708	-0.308829	-1.212304
H	-0.695197	-0.804357	-0.350985
C	-0.877692	-1.106681	-2.486167
C	-1.047917	-2.630586	-2.342747
H	-2.010861	-2.823960	-1.847182
C	-1.129000	-3.301515	-3.732681
H	-0.216130	-3.107891	-4.305974
H	-1.981351	-2.916037	-4.302326
H	-1.243710	-4.386434	-3.642841
C	0.020744	-3.316576	-1.518763
H	-0.242746	-4.320384	-1.180494
C	1.256759	-2.866338	-1.239522
H	1.564613	-1.875482	-1.570855
C	2.265045	-3.641500	-0.530264
H	1.956145	-4.619414	-0.157266
C	3.536455	-3.241208	-0.351181
H	3.843215	-2.274571	-0.748435
C	4.621937	-4.064685	0.280598
H	4.201624	-4.951499	0.769308
H	5.279426	-4.439492	-0.518456
H	0.142315	-0.870678	-2.808261
H	-1.538149	-0.745652	-3.283765
C	-2.678517	-0.159703	-0.938910
H	-3.132236	-1.136139	-0.750304
H	-3.158069	0.268466	-1.828012
C	-2.934420	0.773609	0.247771
O	-4.327422	1.082232	0.424895
C	-5.095968	0.150083	1.149259
H	-4.510477	-0.262514	1.981235
H	-2.565742	0.296846	1.170414
C	-2.200228	2.097122	0.042582
H	-2.303630	2.725889	0.933468
H	-2.653506	2.631176	-0.801369
O	-5.471953	-0.985441	0.393796
C	-6.337639	-0.723284	-0.731182
C	-6.574001	-2.050745	-1.431316
H	-5.629868	-2.469354	-1.790825
H	-7.242652	-1.906053	-2.283022
H	-7.032816	-2.768829	-0.744072
H	-5.840856	-0.022732	-1.415645
C	-7.626988	-0.070936	-0.222634
H	-8.118794	-0.775353	0.467491
O	-8.467909	0.221464	-1.330504
H	-9.148673	0.818681	-0.983529
C	-7.300632	1.213891	0.544594
O	-8.496488	1.820204	1.027001
H	-8.731191	1.313252	1.821913
H	-6.845314	1.927336	-0.149905
C	-6.318816	0.926824	1.681815
O	-7.044200	0.168038	2.646878
C	-6.546731	0.265125	3.975871
H	-7.225119	-0.308841	4.610053
H	-6.526914	1.308548	4.318889
H	-5.537480	-0.155593	4.070852
H	-5.970746	1.868763	2.126337

Statistical Thermodynamic Analysis
Temperature= 298.150 Kelvin Pressure= 1.00000 Atm
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SCF Energy= -2116.30542761 Predicted Change= -1.642017D-08
Zero-point correction (ZPE)= -2115.4726 0.83275
Internal Energy (U)= -2115.4265 0.87889
Enthalpy (H)= -2115.4255
0.87983
Gibbs Free Energy (G)= -2115.5555
0.74985

Frequencies -- 8.6437 11.2170 16.3279

NMR-Shifts
Original-MandelalideA-0017-NMR.txt

Atom	Type	Isotropic	Scaled Shift
1	C	100.6666	81.733379276
2	C	112.5560	70.3535672582
3	C	150.3855	34.1454660311
6	C	113.9057	69.0617163422
8	C	117.8477	65.2886732135
14	C	14.6443	164.068703459

16	C	56.2578	124.238787113
18	C	30.0841	149.290664063
20	C	144.1654	40.0989682038
23	C	109.6758	73.110319876
29	C	147.4281	36.976109803
32	C	144.3263	39.9449644901
34	C	173.2172	12.2923486284
38	C	102.8867	79.6084343115
42	C	110.7798	72.0536380865
44	C	146.0615	38.2841363732
45	C	151.0961	33.4653228431
47	C	162.7282	22.3317827677
51	C	42.9307	136.994678305
53	C	52.4421	127.890943548
55	C	48.4632	131.699305117
57	C	50.2994	129.94180593
59	C	148.1254	36.3086965677
64	C	145.1027	39.201841536
67	C	103.2426	79.2677884339
69	C	84.4020	97.3008671682
72	C	144.4753	39.8023507341
76	C	114.5722	68.4237829974
77	C	168.7274	16.5897126668
82	C	110.2517	72.5591033519
86	C	112.5274	70.3809414422
90	C	102.9516	79.5463159708
92	C	128.0560	55.5179080763
4	H	30.3844	1.34737814738
5	H	30.3732	1.35772695773
7	H	25.7507	5.62892122892
10	H	30.7598	1.00050820051
11	H	28.0934	3.46426426426
12	H	28.1471	3.41464541465
17	H	25.5144	5.84726264726
19	H	24.3002	6.96918456918
21	H	29.3566	2.29706629707
22	H	29.4361	2.22360822361
24	H	28.3500	3.22716562717
26	H	29.4150	2.2431046431
27	H	28.1245	3.43552783553
28	H	28.0623	3.493000693
30	H	30.0376	1.66782166782
31	H	30.6570	1.0954954955
33	H	29.1943	2.44703164703
35	H	30.7905	0.972141372141
36	H	30.8077	0.956248556249
37	H	30.7197	1.03756063756
39	H	27.4230	4.08371448371
43	H	28.5035	3.08533148533
46	H	29.4946	2.16955416955
48	H	31.1587	0.631924231924
49	H	30.6359	1.11499191499
50	H	30.5948	1.15296835297
52	H	25.7113	5.66532686533
54	H	25.2327	6.10755370755
56	H	25.3906	5.96165396165
58	H	25.5282	5.83451143451
60	H	29.4726	2.18988218988
61	H	28.9722	2.65225225225
62	H	29.6672	2.01007161007
63	H	30.4564	1.28085008085
65	H	29.3091	2.34095634096
66	H	30.6986	1.05705705706
70	H	26.5787	4.86384846385
71	H	28.1058	3.45280665281
73	H	30.0249	1.67955647956
74	H	30.3848	1.34700854701
78	H	30.6758	1.07812427812
79	H	30.1963	1.52118272118
80	H	30.8367	0.929452529453
81	H	27.8790	3.66237006237
83	H	28.4091	3.17255717256
85	H	29.7370	1.94557634558
88	H	29.9087	1.78692538693
89	H	28.1627	3.40023100023
93	H	28.1509	3.41113421113
94	H	28.6130	2.98415338415
95	H	28.2162	3.3507969508
96	H	28.3490	3.22808962809

Supporting Information: Original-MandelalideA-0018.log

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-----------------------------------------------------------------------
 Using  Gaussian 09:  AM64L-G09RevC.01 23-Sep-2011
=======================================================================
 #b3lyp/6-31G(d,p) scf=(maxcycle=300,direct,tight) density=current
 SCRF=(PCM,SOLVENT=Chloroform) opt=(maxcycle=250)
freq=noraman
 #N Geom=AllCheck Guess=TCheck SCRF=Check GenChk RB3LYP/6-
31G(d,p) Freq
-----------------------------------------------------------------------
 Pointgroup= C1   Stoichiometry= C33H52O11   C1[X(C33H52O11)]
#Atoms= 96
 Charge = 0                Multiplicity = 1
-----------------------------------------------------------------------
 SCF Energy= -2116.30681972      Predicted Change= -6.819954D-09
=======================================================================
 Optimization completed.          {Found       2       times}
 Item      Max Val.    Criteria    Pass?      RMS Val.    Criteria    Pass?
 Force      0.00000 ||  0.00045   [ YES ]      0.00000 ||  0.00030   [ YES ]
 Displ      0.00179 ||  0.00180   [ YES ]      0.00179 ||  0.00180   [ YES ]
-----------------------------------------------------------------------
     Atomic      Coordinates (Angstroms)
      Type      X                  Y                Z
-----------------------------------------------------------------------
      C      -6.583117     -0.866617     -0.504510
      C      -5.756428      0.342311     -0.057559
      C      -6.145766      1.615738     -0.831668
      H      -7.234698      1.742491     -0.770553
      H      -5.887855      1.522193     -1.890141
      C      -5.523606      2.900260     -0.282325
      H      -5.728673      2.981438      0.787873
      C      -6.040897      4.157958     -0.964733
      O      -5.866515      4.043636     -2.370581
      H      -6.205964      4.851780     -2.776113
      H      -5.499393      5.025302     -0.560742
      H      -7.102346      4.269787     -0.695889
      O      -4.072443      2.896575     -0.463820
      C      -3.286212      2.572666      0.579949
      O      -3.704788      2.153468      1.654094
      C      -1.861318      2.799867      0.262935
      H      -1.640072      3.249718     -0.700466
      C      -0.899206      2.471937      1.137026
      H      -1.199370      2.016983      2.077811
      C       0.568903      2.678360      0.915912
      H       0.989489      3.218286      1.774487
      H       0.739742      3.288588      0.022911
      C       1.348753      1.362827      0.757311
      H       0.930689      0.813155     -0.103567
      O      -5.980863      0.507174      1.338298
      H      -5.226317      1.019010      1.680465
      H      -4.699245      0.104475     -0.249451
      H      -7.613489     -0.702351     -0.151055
      C      -6.582959     -1.170709     -2.008409
      H      -7.380933     -0.648225     -2.542574
      H      -5.629713     -0.879707     -2.468183
      C      -6.745876     -2.699495     -2.037033
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H	-7.790179	-2.926876	-1.783780
C	-6.419395	-3.368007	-3.371886
H	-5.406690	-3.128816	-3.711198
H	-7.115205	-3.032021	-4.147534
H	-6.503854	-4.458053	-3.303563
C	-5.895572	-3.116021	-0.813941
H	-6.290265	-4.031247	-0.352879
O	-6.077252	-2.054645	0.133986
O	1.148235	0.585771	1.938879
C	1.720186	-0.727445	1.832983
H	1.293555	-1.210686	0.938126
C	1.333923	-1.555558	3.059012
C	-0.187593	-1.663058	3.383440
H	-0.332996	-2.618619	3.904252
C	-0.638270	-0.541887	4.344045
H	-1.699520	-0.643395	4.590823
H	-0.478625	0.441679	3.895284
H	-0.065338	-0.583225	5.277443
C	-1.042785	-1.674334	2.144187
H	-1.017096	-0.759162	1.553243
C	-1.845015	-2.671656	1.734387
H	-1.909890	-3.591403	2.317639
C	-2.665273	-2.581317	0.535734
H	-2.539402	-1.672120	-0.054496
C	-3.552526	-3.496608	0.113125
H	-3.703888	-4.404283	0.699235
C	-4.394956	-3.332283	-1.118404
H	-4.014884	-2.488408	-1.705998
H	-4.310475	-4.227078	-1.751002
H	1.860557	-1.164326	3.938512
H	1.730331	-2.562082	2.879703
C	3.241362	-0.619536	1.653588
H	3.679862	-1.616184	1.535202
H	3.679271	-0.166046	2.551264
C	3.581384	0.246820	0.442315
O	5.008833	0.432971	0.423037
C	5.572188	0.646848	-0.853366
H	5.024536	1.422965	-1.402896
H	3.285024	-0.281178	-0.473507
C	2.848196	1.591569	0.523750
H	2.997080	2.173223	-0.393097
H	3.258740	2.169148	1.360703
O	5.486316	-0.489145	-1.688463
C	6.215962	-1.649789	-1.237314
C	5.944362	-2.761652	-2.236284
H	6.483625	-3.664903	-1.941963
H	6.276065	-2.466209	-3.236836
H	4.874900	-2.986155	-2.277693
H	5.855330	-1.944065	-0.242463
C	7.698762	-1.283824	-1.123887
H	8.054632	-0.981083	-2.121951
O	8.421595	-2.412538	-0.651097
H	9.290527	-2.069085	-0.391292
C	7.877775	-0.103804	-0.163164
O	9.254856	0.246365	-0.059899
H	9.440429	0.770970	-0.856367
H	7.558052	-0.419182	0.835256
C	7.027447	1.090433	-0.605031
O	7.631556	1.589579	-1.796552
C	7.396793	2.970202	-2.046811
H	6.333044	3.184420	-2.211047
H	7.948659	3.225567	-2.953503
H	7.757115	3.592586	-1.216463
H	7.033519	1.863573	0.174722

Statistical Thermodynamic Analysis
Temperature= 298.150 Kelvin Pressure= 1.00000 Atm
==========
==========

SCF Energy= -2116.30681972 Predicted Change= -6.819954D-09
Zero-point correction (ZPE)= -2115.4735 0.83329
Internal Energy (U)= -2115.4277 0.87906
Enthalpy (H)= -2115.4268
0.88000
Gibbs Free Energy (G)= -2115.5543
0.75242

Frequencies -- 11.5787 13.5380 18.0607

NMR-Shifts
Original-MandelalideA-0018-NMR.txt

Atom	Type	Isotropic	Scaled Shift
1	C	100.2172	82.1635176784
2	C	111.6659	71.2055169509
3	C	150.3137	34.214188633
6	C	110.4815	72.3391527403
8	C	117.8865	65.2515362086
14	C	9.5226	168.970883822
16	C	60.0755	120.5847164
18	C	23.6183	155.479335362
20	C	144.1056	40.1562051341
23	C	106.8970	75.7700185685
29	C	149.8350	34.6723712169
32	C	146.3342	38.0231244855
34	C	173.4278	12.0907750914
38	C	103.0589	79.4436149237
42	C	108.5099	74.2262485882
44	C	143.5627	40.6758360612
45	C	146.6484	37.7223913168
47	C	161.8736	23.1497540152
51	C	42.3708	137.530580601
53	C	51.9094	128.400811654
55	C	45.1823	134.839583453
57	C	51.0280	129.244434235
59	C	145.7098	38.6207622657
64	C	145.5350	38.7880702157
67	C	114.2549	68.7274832979
69	C	91.9963	90.0320641666
72	C	147.1540	37.2384616857
76	C	115.1552	67.8657707843
77	C	169.1484	16.1867570206
82	C	109.6604	73.1250598212
86	C	112.0592	70.8290740634
90	C	102.9850	79.5143475181
92	C	127.8851	55.6814831831
4	H	30.5528	1.19177639178
5	H	29.6219	2.05192885193
7	H	26.5601	4.88103488103
10	H	31.1399	0.649295449295
11	H	27.6361	3.88680988681
12	H	27.8604	3.67955647956
17	H	25.4277	5.92737352737
19	H	23.5715	7.6425040425
21	H	29.1634	2.47558327558
22	H	29.4511	2.20974820975
24	H	28.3469	3.23003003003
26	H	27.6653	3.85982905983
27	H	28.4399	3.1440979441
28	H	27.8946	3.64795564796
30	H	30.1631	1.55185955186
31	H	30.3761	1.35504735505
33	H	29.2934	2.35546315546
35	H	31.1318	0.65677985678
36	H	30.6174	1.13208593209
37	H	30.7267	1.03109263109
39	H	27.7879	3.74654654655
43	H	28.2776	3.29406329406
46	H	29.2731	2.37422037422

48	H	30.7595	1.00078540079
49	H	30.0859	1.62319242319
50	H	30.6193	1.13033033033
52	H	25.6992	5.67650727651
54	H	25.2271	6.11272811273
56	H	25.4973	5.86306306306
58	H	25.7429	5.63612843613
60	H	29.9564	1.74285054285
61	H	29.7146	1.96627396627
62	H	30.1653	1.54982674983
63	H	30.1552	1.55915915916
65	H	30.0255	1.679002079
66	H	30.5291	1.21367521368
70	H	26.5457	4.89434049434
71	H	27.6204	3.90131670132
73	H	29.6680	2.00933240933
74	H	30.6623	1.0905982906
78	H	30.2827	1.44134904135
79	H	30.8283	0.937214137214
80	H	30.6140	1.13522753523
81	H	27.9699	3.57837837838
83	H	28.3792	3.20018480018
85	H	29.7177	1.96340956341
88	H	29.9037	1.79154539155
89	H	28.0770	3.47941787942
93	H	28.2612	3.30921690922
94	H	28.1540	3.40826980827
95	H	28.6032	2.99320859321
96	H	28.3114	3.26283206283

Supporting Information: Original-MandelalideA-0019.log

Using Gaussian 09: AM64L-G09RevC.01 23-Sep-2011

==========

#b3lyp/6-31G(d,p) scf=(maxcycle=300,direct,tight) density=current SCRF=(PCM,SOLVENT=Chloroform) opt=(maxcycle=250) freq=noraman

#N Geom=AllCheck Guess=TCheck SCRF=Check GenChk RB3LYP/6-31G(d,p) Freq

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Pointgroup= C1 Stoichiometry= C33H52O11 C1[X(C33H52O11)]

#Atoms= 96

Charge = 0 Multiplicity = 1

SCF Energy= -2116.30466911 Predicted Change= -7.317758D-09

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Optimization completed. {Found 2 times}

Item	Max Val.	Criteria	Pass?	RMS Val.	Criteria	Pass?
Force	0.00001	0.00045	[YES]	0.00000	0.00030	[YES]
Displ	0.00116	0.00180	[YES]	0.00116	0.00180	[YES]

Atomic Type	Coordinates (Angstroms) X	Y	Z
C	-7.020442	0.207404	0.875075
C	-5.654391	0.882279	0.700719
C	-5.752482	2.376638	0.404919
H	-6.352453	2.875844	1.173494
H	-6.264151	2.522061	-0.554386
C	-4.395708	3.072261	0.370792
H	-3.884379	2.939461	1.327067
C	-4.492176	4.566838	0.038376
O	-5.273443	5.274050	0.994184
H	-4.775285	5.292750	1.823057
H	-4.991902	4.695269	-0.927487
H	-3.479539	4.981577	-0.044318
O	-3.593119	2.422138	-0.652622
C	-2.251347	2.388409	-0.458316
O	-1.686564	2.958442	0.459940
C	-1.591275	1.570427	-1.498801
H	-2.230674	1.098087	-2.238775
C	-0.259831	1.423212	-1.511765
H	0.305690	1.937185	-0.737043
C	0.503503	0.637857	-2.535519
H	1.008908	1.340028	-3.214646
H	-0.188400	0.048385	-3.145479
C	1.586159	-0.293753	-1.969312
H	2.011265	-0.853117	-2.820951
O	-4.894724	0.712771	1.894422
H	-4.925411	-0.239763	2.075923
H	-5.140963	0.390635	-0.140002
H	-7.559571	0.719355	1.683949
C	-7.881484	0.091467	-0.392225
H	-8.663353	0.853983	-0.434006
H	-7.265807	0.201923	-1.294075
C	-8.453664	-1.337517	-0.306000
H	-9.278776	-1.324612	0.417930
C	-8.975446	-1.907608	-1.624351
H	-9.323244	-2.939185	-1.503183
H	-8.207512	-1.899188	-2.404236
H	-9.821474	-1.315608	-1.987901
C	-7.291359	-2.094511	0.374010
H	-7.656588	-2.948965	0.956868
O	-6.779138	-1.147933	1.325042
O	0.948048	-1.218830	-1.088088
C	1.832202	-2.238216	-0.603419
H	2.261325	-2.755741	-1.480367
C	1.026299	-3.295759	0.173915
C	-0.068992	-2.869523	1.196270
H	-0.316829	-3.793635	1.737074
C	0.393560	-1.841147	2.246651
H	0.563803	-0.860098	1.794599
H	1.318219	-2.160698	2.739519
H	-0.374803	-1.720610	3.016517
C	-1.334829	-2.404497	0.520100
H	-1.246821	-1.510803	-0.094180
C	-2.530963	-3.006054	0.639820
H	-2.622943	-3.899941	1.259526
C	-3.742285	-2.535953	-0.016509
H	-3.627396	-1.663742	-0.661829
C	-4.960308	-3.091476	0.105362
H	-5.083697	-3.960438	0.753914
C	-6.192160	-2.591400	-0.592005
H	-5.917314	-1.792580	-1.290406
H	-6.629891	-3.400372	-1.194442
H	1.760588	-3.921067	0.697798
H	0.538607	-3.949176	-0.558183
C	3.012722	-1.616985	0.163875
H	3.708185	-2.407127	0.467046
H	2.664773	-1.114983	1.069958
C	3.737422	-0.595225	-0.708996
O	4.743425	0.034597	0.105535
C	5.837444	0.581906	-0.597842
H	5.498594	1.203179	-1.436142
H	4.233150	-1.109760	-1.543184
C	2.737664	0.430072	-1.254901
H	3.224339	1.119328	-1.954444
H	2.353256	1.017651	-0.414146
O	6.647106	-0.403404	-1.206560
C	7.302421	-1.315511	-0.299423
C	8.070170	-2.313173	-1.149841
H	8.586974	-3.029599	-0.507111
H	8.812676	-1.797683	-1.767365
H	7.388707	-2.857886	-1.809224
H	6.545763	-1.839265	0.300032
C	8.196818	-0.509616	0.647688

H	8.949384	0.019303	0.040831
O	8.821014	-1.396774	1.566024
H	9.185295	-0.828050	2.262082
C	7.364013	0.529908	1.404250
O	8.194148	1.284683	2.282399
H	8.629645	1.941321	1.713950
H	6.638964	0.003035	2.032668
C	6.610853	1.435390	0.426868
O	7.598893	2.246999	-0.203950
C	7.121575	3.496812	-0.687794
H	6.670451	4.090576	0.118729
H	6.382543	3.374141	-1.489901
H	7.985271	4.031507	-1.087848
H	5.895532	2.065464	0.972079

Statistical Thermodynamic Analysis
Temperature= 298.150 Kelvin Pressure= 1.00000 Atm
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SCF Energy= -2116.30466911 Predicted Change= -7.317758D-09
Zero-point correction (ZPE)= -2115.4709 0.83374
Internal Energy (U)= -2115.4250 0.87959
Enthalpy (H)= -2115.4241
0.88053
Gibbs Free Energy (G)= -2115.5523
0.75227

Frequencies -- 11.8467 15.4437 18.3351

NMR-Shifts
Original-MandelalideA-0019-NMR.txt

Atom	Type	Isotropic	Scaled Shift
1	C	99.5627	82.7899653516
2	C	110.5937	72.2317617106
3	C	152.4462	32.1730890714
6	C	112.8309	70.090449664
8	C	120.3247	62.9178391623
14	C	12.3449	166.26954957
16	C	58.3423	122.243630238
18	C	27.9942	151.290989491
20	C	145.9559	38.3852102835
23	C	108.0677	74.6494955876
29	C	152.1091	32.4957407301
32	C	144.2752	39.9938743085
34	C	173.1806	12.3273799269
38	C	102.2964	80.1734336415
42	C	105.7775	76.8415360172
44	C	146.7320	37.6423744712
45	C	143.4234	40.809165566
47	C	165.5911	19.5915886598
51	C	36.0039	143.624590823
53	C	54.4696	125.950343613
55	C	45.2948	134.731905281
57	C	51.6123	128.685177741
59	C	146.8919	37.4893278968
64	C	147.0141	37.3723654741
67	C	112.2057	70.6888531557
69	C	91.8185	90.2022435345
72	C	151.8314	32.7615383143
76	C	115.1964	67.826336645
77	C	168.7156	16.6010069105
82	C	110.3444	72.4703765386
86	C	112.8362	70.0853768257
90	C	102.6056	79.8774861693
92	C	127.7429	55.8175883918
4	H	29.7898	1.89678909679
5	H	30.3780	1.35329175329
7	H	26.5488	4.89147609148
10	H	31.2517	0.545992145992
11	H	28.6222	2.97565257565
12	H	27.6570	3.8674982675
17	H	25.2678	6.07512127512
19	H	23.7466	7.48071148071
21	H	29.3886	2.2674982675
22	H	28.8135	2.79889119889
24	H	28.0555	3.49928389928
26	H	29.3959	2.26075306075
27	H	28.0799	3.47673827674
28	H	28.1104	3.44855624856
30	H	29.9111	1.78470778471
31	H	30.4699	1.26837606838
33	H	29.1945	2.44684684685
35	H	30.6490	1.10288750289
36	H	31.0549	0.727835527836
37	H	30.5771	1.16932316932
39	H	27.7345	3.79588819589
43	H	27.9006	3.64241164241
46	H	29.2770	2.37061677062
48	H	30.4583	1.27909447909
49	H	30.5713	1.17468237468
50	H	30.8579	0.909863709864
52	H	25.1595	6.17519057519
54	H	25.4772	5.88163548164
56	H	25.2270	6.11282051282
58	H	25.9307	5.4626010626
60	H	29.9243	1.77251097251
61	H	29.5343	2.13287133287
62	H	30.1614	1.55343035343
63	H	29.7260	1.95574035574
65	H	30.1644	1.55065835066
66	H	29.9471	1.75144375144
70	H	26.3483	5.07673827674
71	H	27.6062	3.91443751444
73	H	29.7800	1.90584430584
74	H	30.2164	1.50261030261
78	H	30.2773	1.44633864634
79	H	30.8553	0.912266112266
80	H	30.5688	1.17699237699
81	H	27.8982	3.64462924463
83	H	28.3395	3.23686763687
85	H	29.5016	2.16308616309
88	H	29.8723	1.82055902056
89	H	28.1243	3.43571263571
93	H	28.5574	3.03552783553
94	H	28.1762	3.38775698776
95	H	28.1434	3.41806421806
96	H	28.2858	3.28648648649

Supporting Information: Original-MandelalideA-0020.log

Using Gaussian 09: AM64L-G09RevC.01 23-Sep-2011
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#b3lyp/6-31G(d,p) scf=(maxcycle=300,direct,tight) density=current
SCRF=(PCM,SOLVENT=Chloroform) opt=(maxcycle=250)
freq=noraman
#N Geom=AllCheck Guess=TCheck SCRF=Check GenChk RB3LYP/6-
31G(d,p) Freq

Pointgroup= C1 Stoichiometry= C33H52O11 C1[X(C33H52O11)]
#Atoms= 96
Charge = 0 Multiplicity = 1

SCF Energy= -2116.30457310 Predicted Change= -5.400504D-09
==========
Optimization completed. {Found 2 times}
Item Max Val. Criteria Pass? RMS Val. Criteria Pass?

Force 0.00000 || 0.00045 [YES] 0.00000 || 0.00030 [YES]
Displ 0.00112 || 0.00180 [YES] 0.00112 || 0.00180 [YES]

Atomic Type	Coordinates (Angstroms) X	Y	Z
C	-6.654574	0.410461	1.280180
C	-5.362332	1.156813	0.936115
C	-5.581064	2.655791	0.747809
H	-6.062758	3.068987	1.642311
H	-6.268520	2.807269	-0.093396
C	-4.289364	3.442315	0.504500
H	-3.657686	3.434989	1.393415
C	-4.584803	4.877291	0.090600
O	-3.365450	5.600545	0.013990
H	-3.563568	6.472118	-0.352079
H	-5.269529	5.315693	0.833525
H	-5.107289	4.864919	-0.878271
O	-3.558807	2.790424	-0.565634
C	-2.230945	2.566244	-0.388078
O	-1.594474	2.933417	0.581674
C	-1.682147	1.802641	-1.531582
H	-2.383344	1.473810	-2.293263
C	-0.373220	1.531707	-1.602560
H	0.253804	1.908629	-0.797282
C	0.289000	0.773586	-2.716147
H	0.724894	1.487233	-3.430422
H	-0.459230	0.195044	-3.267816
C	1.419960	-0.158274	-2.256874
H	1.719986	-0.775374	-3.121727
O	-4.413693	0.973327	1.982237
H	-4.351038	0.013948	2.107043
H	-4.971766	0.735428	-0.002936
H	-7.058600	0.829022	2.213443
C	-7.724189	0.374190	0.182454
H	-8.475553	1.158415	0.306321
H	-7.271024	0.501626	-0.809072
C	-8.313980	-1.040327	0.321325
H	-8.971816	-1.042731	1.200498
C	-9.118506	-1.529559	-0.882565
H	-10.004702	-0.903418	-1.027659
H	-9.463099	-2.559661	-0.741433
H	-8.533141	-1.492309	-1.806677
C	-7.062799	-1.860221	0.710208
H	-7.334507	-2.719333	1.336919
O	-6.301925	-0.967961	1.543992
O	0.885124	-1.010853	-1.242928
C	1.808258	-2.003313	-0.774354
H	2.107430	-2.631976	-1.633141
C	1.108968	-2.884660	0.261458
C	0.009784	-3.844476	-0.270888
H	0.382582	-4.239017	-1.231438
C	-0.155886	-5.039872	0.678580
H	-0.491907	-4.715798	1.669968
H	0.796150	-5.565179	0.803087
H	-0.886036	-5.758923	0.295145
C	-1.285074	-3.122582	-0.566996
H	-1.183134	-2.250503	-1.209630
C	-2.508997	-3.450049	-0.116088
H	-2.639351	-4.308469	0.541104
C	-3.723379	-2.728742	-0.471174
H	-3.601942	-1.867850	-1.130514
C	-4.959080	-3.069037	-0.066474
H	-5.076839	-3.929851	0.594449
C	-6.222844	-2.370853	-0.477296
H	-5.984963	-1.543716	-1.156455
H	-6.852872	-3.073900	-1.042041
H	0.698434	-2.245389	1.052590
H	1.891927	-3.496556	0.725662
C	3.065135	-1.333752	-0.196289
H	3.786256	-2.095242	0.112615
H	2.785608	-0.750912	0.689976
C	3.703013	-0.396496	-1.223784
O	4.783661	0.378226	-0.676533
C	6.056228	-0.224914	-0.673854
H	6.214930	-0.784604	-1.605125
H	4.095379	-0.994235	-2.062388
C	2.663107	0.589068	-1.750612
H	3.091293	1.190357	-2.560030
H	2.391290	1.270205	-0.936807
O	6.225331	-1.192539	0.343344
C	6.154457	-0.689952	1.694547
C	6.291042	-1.884987	2.622704
H	6.261418	-1.552384	3.662870
H	7.241217	-2.399456	2.446493
H	5.476421	-2.595419	2.456736
H	5.182183	-0.204244	1.851025
C	7.255291	0.356508	1.888387
H	8.227786	-0.133057	1.718008
O	7.175640	0.876987	3.208263
H	7.727385	1.674524	3.202683
C	7.092266	1.486181	0.866212
O	8.118857	2.459602	1.035163
H	8.900148	2.077332	0.602409
H	6.142679	1.995205	1.060881
C	7.077005	0.927534	-0.558775
O	8.404866	0.477551	-0.820362
C	8.761723	0.446191	-2.196817
H	8.649055	1.435510	-2.660996
H	8.161677	-0.278090	-2.762558
H	9.809739	0.144122	-2.244902
H	6.799171	1.716673	-1.269993

Statistical Thermodynamic Analysis
Temperature= 298.150 Kelvin Pressure= 1.00000 Atm
==========
SCF Energy= -2116.30457310 Predicted Change= -5.400504D-09
Zero-point correction (ZPE)= -2115.4720 0.83249
Internal Energy (U)= -2115.4258 0.87869
Enthalpy (H)= -2115.4249 0.87963
Gibbs Free Energy (G)= -2115.5546 0.74988

Frequencies -- 7.6864 14.3748 17.3861

NMR-Shifts
Original-MandelalideA-0020-NMR.txt

Atom	Type	Isotropic	Scaled Shift
1	C	98.1053	84.1849001704
2	C	110.4222	72.3959111009
3	C	153.0396	31.6051226095
6	C	115.2953	67.7316755681
8	C	116.5819	66.500220142
14	C	13.3758	165.282834664
16	C	59.3505	121.278642394
18	C	28.1109	151.179291334
20	C	146.3123	38.0440858363
23	C	109.3282	73.4430214973
29	C	150.3834	34.1474760237
32	C	143.9704	40.2856103677
34	C	172.9149	12.5816918394
38	C	101.8561	80.5948620762
42	C	104.9224	77.6599858343
44	C	140.3033	43.7955359023
45	C	146.1409	38.2081395126
47	C	167.6802	17.5920289439

51	C	40.0539	139.74817665
53	C	53.4186	126.956297019
55	C	46.4368	133.638852199
57	C	50.1631	130.072264017
59	C	147.0463	37.3415455885
64	C	144.2615	40.0069871169
67	C	103.2086	79.3003311702
69	C	84.4458	97.2589444668
72	C	149.0051	35.4667011237
76	C	115.1086	67.9103734758
77	C	169.1113	16.2222668887
82	C	110.3443	72.4704722525
86	C	112.3864	70.5158980838
90	C	102.5624	79.9188345872
92	C	127.9721	55.5982120638
4	H	30.4857	1.25377685378
5	H	30.4452	1.2911988912
7	H	25.9153	5.47683067683
10	H	31.3128	0.489535689536
11	H	27.9063	3.63714483714
12	H	28.0277	3.52497112497
17	H	25.3777	5.97357357357
19	H	23.8098	7.42231462231
21	H	29.2459	2.39935319935
22	H	28.6900	2.91300531301
24	H	27.9470	3.59953799954
26	H	29.6753	2.00258720259
27	H	28.1856	3.37907137907
28	H	27.8926	3.6498036498
30	H	29.8829	1.81076461076
31	H	30.5204	1.22171402171
33	H	29.1794	2.4607992608
35	H	30.6170	1.13245553246
36	H	30.6821	1.0723030723
37	H	31.0413	0.740401940402
39	H	27.6126	3.90852390852
43	H	28.2232	3.34432894433
46	H	29.3654	2.28893508894
48	H	30.8144	0.950057750058
49	H	30.8623	0.905798105798
50	H	30.5178	1.22411642412
52	H	24.8593	6.45257565258
54	H	25.5561	5.80873180873
56	H	25.2610	6.0814044814
58	H	25.9717	5.42471702472
60	H	29.8628	1.82933702934
61	H	29.6613	2.01552321552
62	H	30.3308	1.3969045969
63	H	30.4182	1.31614691615
65	H	29.4715	2.1908985909
66	H	30.4139	1.32012012012
70	H	26.5215	4.9167013167
71	H	28.0299	3.52293832294
73	H	30.0246	1.67983367983
74	H	29.8170	1.87165627166
78	H	30.2228	1.4966966967
79	H	30.9050	0.866343266343
80	H	30.5919	1.15564795565
81	H	27.8632	3.67696927697
83	H	28.3988	3.18207438207
85	H	29.7024	1.97754677755
88	H	29.8679	1.82462462462
89	H	28.0308	3.52210672211
93	H	28.5658	3.02776622777
94	H	28.1975	3.36807576808
95	H	28.1313	3.42924462924
96	H	28.1822	3.38221298221

Supporting Information: Original-MandelalideA-0021.log

```
---------------------------------------------------------------------------
 Using  Gaussian 09:  AM64L-G09RevC.01 23-Sep-2011
=========================================================================
 #b3lyp/6-31G(d,p) scf=(maxcycle=300,direct,tight) density=current
 SCRF=(PCM,SOLVENT=Chloroform) opt=(maxcycle=250)
freq=noraman
 #N Geom=AllCheck Guess=TCheck SCRF=Check GenChk RB3LYP/6-
31G(d,p) Freq
---------------------------------------------------------------------------
 Pointgroup= C1   Stoichiometry= C33H52O11   C1[X(C33H52O11)]
#Atoms= 96
 Charge = 0                Multiplicity = 1
---------------------------------------------------------------------------
 SCF Energy= -2116.30378057      Predicted Change= -1.794406D-08
=========================================================================
 Optimization completed.          {Found       1       times}
 Item     Max Val.    Criteria    Pass?     RMS Val.    Criteria    Pass?
 Force     0.00000 ||  0.00045   [ YES ]     0.00000 ||  0.00030   [ YES ]
 Displ     0.00220 ||  0.00180   [ NO ]      0.00220 ||  0.00180   [ YES ]
---------------------------------------------------------------------------
     Atomic      Coordinates (Angstroms)
      Type      X                  Y                Z
---------------------------------------------------------------------------
      C      -6.518091     -1.549087     -0.479602
      C      -5.864756     -0.200510     -0.143550
      C      -6.645479      1.000941     -0.667868
      H      -7.650051      0.997411     -0.226785
      H      -6.762428      0.907718     -1.754355
      C      -5.992928      2.346145     -0.340611
      H      -5.902392      2.482317      0.737138
      C      -6.746738      3.519614     -0.963526
      O      -6.149288      4.772553     -0.671230
      H      -5.266049      4.758024     -1.065180
      H      -7.759376      3.549962     -0.549378
      H      -6.833607      3.360633     -2.049923
      O      -4.647422      2.366404     -0.903407
      C      -3.593899      2.508109     -0.049570
      O      -3.705914      2.691041      1.147717
      C      -2.311403      2.408107     -0.783929
      H      -2.357982      2.281975     -1.861766
      C      -1.153639      2.470582     -0.112496
      H      -1.204013      2.591510      0.966050
      C       0.221657      2.413240     -0.701841
      H       0.726774      3.360211     -0.463918
      H       0.184321      2.328162     -1.792904
      C       1.085399      1.267246     -0.138953
      H       0.718980      0.310511     -0.548079
      O      -5.748093     -0.074725      1.267835
      H      -5.344259     -0.906482      1.562822
      H      -4.865708     -0.192954     -0.608143
      H      -7.540454     -1.552476     -0.079360
      C      -6.482206     -1.953677     -1.962798
      H      -7.449610     -1.819358     -2.453193
      H      -5.748564     -1.352049     -2.514217
      C      -6.041669     -3.430472     -1.925870
      H      -6.919698     -4.036147     -1.666731
      C      -5.456007     -3.962696     -3.233230
      H      -6.212958     -3.949718     -4.023965
      H      -5.111281     -4.996682     -3.124400
      H      -4.610389     -3.358326     -3.576365
      C      -5.124098     -3.451899     -0.683134
      H      -5.110607     -4.442541     -0.213367
      O      -5.788942     -2.574566      0.240255
      O       0.912346      1.258424      1.275440
      C       1.634161      0.209260      1.941251
      H       1.341531     -0.752493      1.488287
      C       1.184987      0.240174      3.406098
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C	-0.015459	-0.687078	3.748333
H	0.374975	-1.711119	3.830008
C	-0.606384	-0.294971	5.115953
H	0.171434	-0.277285	5.887810
H	-1.380800	-1.002195	5.427367
H	-1.058394	0.702367	5.073085
C	-1.068066	-0.697724	2.669339
H	-1.496691	0.264731	2.390362
C	-1.470730	-1.807978	2.025485
H	-1.045150	-2.769053	2.319955
C	-2.403508	-1.835513	0.907798
H	-2.745903	-0.868423	0.538933
C	-2.802541	-2.957305	0.282032
H	-2.462640	-3.919096	0.669638
C	-3.668457	-3.004022	-0.945137
H	-3.671361	-2.023487	-1.433994
H	-3.228358	-3.711517	-1.660268
H	0.931884	1.281214	3.640834
H	2.022439	-0.032320	4.059123
C	3.138706	0.406421	1.723022
H	3.699819	-0.395449	2.215457
H	3.453830	1.359256	2.165786
C	3.445497	0.413666	0.226119
O	4.842056	0.723935	0.060395
C	5.439996	0.208693	-1.109774
H	4.811334	0.396486	-1.989101
H	3.258152	-0.588894	-0.180967
C	2.569666	1.445387	-0.495744
H	2.698314	1.377813	-1.582294
H	2.892446	2.445923	-0.183069
O	5.584452	-1.194798	-1.080997
C	6.452118	-1.699861	-0.046516
C	6.441785	-3.215139	-0.163962
H	7.107962	-3.649627	0.584375
H	6.785818	-3.521200	-1.157204
H	5.432060	-3.606258	-0.011630
H	6.051269	-1.400671	0.933642
C	7.863980	-1.097743	-0.192743
H	8.286971	-1.433947	-1.146312
O	8.739261	-1.592096	0.814440
H	8.503489	-1.164878	1.650532
C	7.795874	0.438847	-0.197400
O	9.062021	1.039762	-0.407832
H	9.228502	0.947009	-1.359616
H	7.446189	0.776386	0.786697
C	6.792008	0.926313	-1.252915
O	7.390041	0.647603	-2.517420
C	6.971656	1.502441	-3.574372
H	5.901571	1.394826	-3.793587
H	7.540193	1.211759	-4.459933
H	7.178902	2.555744	-3.341242
H	6.636858	2.007341	-1.137549

Statistical Thermodynamic Analysis

Temperature= 298.150 Kelvin Pressure= 1.00000 Atm

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SCF Energy= -2116.30378057 Predicted Change= -1.794406D-08

Zero-point correction (ZPE)= -2115.4716 0.83214

Internal Energy (U)= -2115.4252 0.87851

Enthalpy (H)= -2115.4243 0.87945

Gibbs Free Energy (G)= -2115.5549 0.74886

Frequencies -- 9.1592 10.8468 16.3502

NMR-Shifts

Original-MandelalideA-0021-NMR.txt

Atom	Type	Isotropic	Scaled Shift
1	C	100.0102	82.3616455139
2	C	110.5068	72.3149371159
3	C	152.6097	32.0165967955
6	C	112.8821	70.0414441318
8	C	117.8879	65.2501962136
14	C	13.1888	165.461819713
16	C	62.3550	118.402917361
18	C	24.0326	155.08279255
20	C	144.1437	40.1197381267
23	C	109.7852	73.0056088363
29	C	150.8531	33.6979076935
32	C	143.5096	40.7266601581
34	C	172.8356	12.6575929861
38	C	102.6548	79.8303949157
42	C	108.8760	73.8758398897
44	C	142.4025	41.7863090794
45	C	143.0455	41.1708685082
47	C	164.3526	20.7770056854
51	C	40.2532	139.557418787
53	C	50.4612	129.786940791
55	C	45.4076	134.623939968
57	C	50.5170	129.733532418
59	C	148.9255	35.5428894121
64	C	146.2312	38.1217098336
67	C	113.7264	69.2333314191
69	C	91.7012	90.3145159747
72	C	147.4087	36.9946783055
76	C	113.4118	69.5344474435
77	C	169.1741	16.1621585406
82	C	108.7464	73.9998851433
86	C	111.4184	71.4424089282
90	C	101.8620	80.5892149543
92	C	127.8916	55.6752617776
4	H	30.5364	1.20693000693
5	H	30.5089	1.23234003234
7	H	25.7180	5.65913605914
10	H	30.7606	0.999768999769
11	H	28.1622	3.40069300069
12	H	28.1557	3.4066990067
17	H	25.5139	5.84772464772
19	H	23.5990	7.61709401709
21	H	29.2840	2.36414876415
22	H	29.3362	2.31591591592
24	H	28.4243	3.15851235851
26	H	29.4573	2.20401940402
27	H	28.2727	3.29859089859
28	H	28.2156	3.35135135135
30	H	29.9277	1.76936936937
31	H	30.4984	1.24204204204
33	H	29.2968	2.35232155232
35	H	30.6251	1.12497112497
36	H	30.6894	1.06555786556
37	H	31.0983	0.687733887734
39	H	27.8300	3.70764610765
43	H	28.6259	2.97223377223
46	H	29.4600	2.20152460152
48	H	30.6878	1.06703626704
49	H	30.7338	1.02453222453
50	H	30.8024	0.961145761146
52	H	25.6991	5.6765996766
54	H	25.3508	5.99842919843
56	H	25.4049	5.94844074844
58	H	25.8686	5.51998151998
60	H	29.8592	1.83266343266
61	H	29.7155	1.96544236544
62	H	30.3281	1.3993993994
63	H	30.1448	1.56876876877
65	H	30.0664	1.64121044121

66	H	30.4505	1.2863016863
70	H	26.5173	4.92058212058
71	H	27.7165	3.81252021252
73	H	29.7234	1.95814275814
74	H	30.8176	0.947100947101
78	H	30.1675	1.54779394779
79	H	30.8430	0.923631323631
80	H	30.6247	1.12534072534
81	H	28.1156	3.44375144375
83	H	28.6188	2.97879417879
85	H	31.8704	-0.0256872256872
88	H	29.8399	1.8504966505
89	H	28.2721	3.29914529915
93	H	28.2733	3.29803649804
94	H	28.1571	3.40540540541
95	H	28.5938	3.00189420189
96	H	28.3511	3.22614922615

Supporting Information: Original-MandelalideA-0022.log

```
---------------------------------------------------------------------------
 Using  Gaussian 09:  AM64L-G09RevC.01 23-Sep-2011
=============================================================
=====================
 #b3lyp/6-31G(d,p) scf=(maxcycle=300,direct,tight) density=current
 SCRF=(PCM,SOLVENT=Chloroform) opt=(maxcycle=250)
freq=noraman
 #N Geom=AllCheck Guess=TCheck SCRF=Check GenChk RB3LYP/6-
31G(d,p) Freq
---------------------------------------------------------------------------
 Pointgroup= C1   Stoichiometry= C33H52O11   C1[X(C33H52O11)]
#Atoms= 96
 Charge = 0                Multiplicity = 1
---------------------------------------------------------------------------
 SCF Energy= -2116.30535977      Predicted Change= -6.531997D-09
=============================================================
=====================
 Optimization completed.          {Found       2       times}
 Item     Max Val.    Criteria    Pass?      RMS Val.    Criteria    Pass?
 Force      0.00000 ||  0.00045   [ YES ]      0.00000 ||  0.00030   [ YES ]
 Displ      0.00113 ||  0.00180   [ YES ]      0.00113 ||  0.00180   [ YES ]
---------------------------------------------------------------------------
     Atomic      Coordinates (Angstroms)
      Type      X                Y                Z
---------------------------------------------------------------------------
      C       6.690385      0.757390     -0.497771
      C       5.264634      1.300865     -0.629941
      C       5.172346      2.811567     -0.405691
      H       5.928507      3.320159     -1.016300
      H       5.391711      3.036496      0.644598
      C       3.808923      3.379023     -0.794894
      H       3.621817      3.167468     -1.849608
      C       3.675437      4.877045     -0.545085
      O       2.393351      5.384801     -0.881722
      H       2.001903      4.782831     -1.535577
      H       4.468569      5.382301     -1.119712
      H       3.849757      5.094869      0.516383
      O       2.799000      2.659367     -0.029385
      C       1.640421      2.372862     -0.660739
      O       1.336581      2.831502     -1.755631
      C       0.772551      1.434228      0.075235
      H       0.003980      0.979147     -0.535615
      C       0.893487      1.171935      1.383388
      H       1.690850      1.676168      1.926893
      C       0.072598      0.238585      2.230403
      H      -0.323660      0.802477      3.086531
      H       0.773562     -0.484293      2.671808
      C      -1.079398     -0.549197      1.596789
      H      -1.419205     -1.274510      2.357258
      O       4.786105      1.021473     -1.943445
      H       4.940579      0.072904     -2.072223
      H       4.633555      0.790309      0.113512
      H       7.329986      1.292621     -1.215452
      C       7.311561      0.768450      0.901526
      H       7.907021      1.666127      1.087475
      H       6.534349      0.717111      1.675028
      C       8.159866     -0.517562      0.904165
      H       9.054653     -0.325161      0.297631
      C       8.608266     -0.999430      2.283623
      H       9.266455     -0.259350      2.749869
      H       9.165563     -1.939914      2.216521
      H       7.759407     -1.156822      2.956204
      C       7.268306     -1.477847      0.082970
      H       7.875996     -2.206254     -0.468976
      O       6.649523     -0.630696     -0.902503
      O      -0.550353     -1.272623      0.484822
      C      -1.472316     -2.200142     -0.102112
      H      -1.778771     -2.925696      0.672944
      C      -0.755742     -2.942755     -1.233417
      C       0.306956     -3.998587     -0.818677
      H      -0.184093     -4.649071     -0.074986
      C       0.676745     -4.873321     -2.024081
      H       1.139674     -4.277491     -2.818666
      H      -0.214465     -5.352436     -2.441210
      H       1.380610     -5.662377     -1.742732
      C       1.499148     -3.374543     -0.133492
      H       1.249532     -2.735119      0.709116
      C       2.799073     -3.504200     -0.454040
      H       3.109233     -4.122415     -1.295049
      C       3.853772     -2.833516      0.294701
      H       3.516407     -2.189844      1.109086
      C       5.175381     -2.943097      0.077792
      H       5.534441     -3.583500     -0.729267
      C       6.216391     -2.245151      0.907592
      H       5.719252     -1.568827      1.612812
      H       6.762295     -2.984320      1.513411
      H      -0.300200     -2.201003     -1.901265
      H      -1.527269     -3.461335     -1.815855
      C      -2.720835     -1.451603     -0.594948
      H      -3.454762     -2.163795     -0.986750
      H      -2.438507     -0.779251     -1.414579
      C      -3.347795     -0.629767      0.530368
      O      -4.427435      0.135701     -0.035838
      C      -5.478008      0.442452      0.854778
      H      -5.090031      0.838249      1.801649
      H      -3.761721     -1.311759      1.285485
      C      -2.300990      0.284113      1.177976
      H      -2.715384      0.785296      2.060408
      H      -2.014812      1.058479      0.460399
      O      -6.221208     -0.696989      1.237599
      C      -6.924091     -1.366154      0.169206
      C      -7.600036     -2.584278      0.775338
      H      -8.149222     -3.127605      0.002946
      H      -8.303577     -2.281349      1.557521
      H      -6.857110     -3.253876      1.217689
      H      -6.205167     -1.679520     -0.599599
      C      -7.907682     -0.377928     -0.464401
      H      -8.619524     -0.057227      0.313341
      O      -8.585992     -1.018466     -1.536553
      H      -9.014839     -0.302839     -2.031048
      C      -7.157471      0.855120     -0.978734
      O      -8.069335      1.780715     -1.562978
      H      -8.469357      2.247584     -0.810653
      H      -6.477142      0.538873     -1.776047
      C      -6.342847      1.502232      0.144437
      O      -7.290441      2.086044      1.035972
      C      -6.797668      3.188797      1.787933
      H      -5.993483      2.894110      2.474212
      H      -7.635309      3.570360      2.375021
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H	-6.424639	3.985196	1.129851
H	-5.683976	2.277665	-0.268335

Statistical Thermodynamic Analysis
Temperature= 298.150 Kelvin Pressure= 1.00000 Atm
==========
SCF Energy= -2116.30535977 Predicted Change= -6.531997D-09
Zero-point correction (ZPE)= -2115.4718 0.83349
Internal Energy (U)= -2115.4261 0.87920
Enthalpy (H)= -2115.4252
0.88014
Gibbs Free Energy (G)= -2115.5523
0.75302

Frequencies -- 13.8918 16.7755 18.4599

NMR-Shifts
Original-MandelalideA-0022-NMR.txt

Atom	Type	Isotropic	Scaled Shift
1	C	98.9088	83.4158387412
2	C	111.5116	71.3532035452
3	C	154.3857	30.316717395
6	C	111.8328	71.0457704014
8	C	117.0038	66.0964030705
14	C	8.8720	169.593598652
16	C	57.3445	123.198663834
18	C	33.8591	145.677463198
20	C	147.8093	36.6112483011
23	C	110.6535	72.1745247803
29	C	150.8371	33.7132219223
32	C	143.8640	40.3874499895
34	C	173.4504	12.0691437432
38	C	102.5138	79.9653515573
42	C	105.0160	77.5703975957
44	C	139.9850	44.1001933421
45	C	145.7014	38.6288022359
47	C	167.8359	17.4430023546
51	C	38.0190	141.695859415
53	C	56.2425	124.253431344
55	C	45.6756	134.367426635
57	C	51.9460	128.365780356
59	C	146.1441	38.2050766669
64	C	145.8269	38.5086812535
67	C	113.2719	69.6683512318
69	C	91.7674	90.2511533529
72	C	152.7145	31.9162885966
76	C	115.0761	67.9414805031
77	C	169.0502	16.2807481001
82	C	109.9944	72.8053752943
86	C	111.5376	71.3283179234
90	C	103.0544	79.4479220506
92	C	128.0236	55.5489193897
4	H	30.6137	1.1355047355
5	H	30.3138	1.41261261261
7	H	26.1754	5.2364980365
10	H	29.6056	2.06699006699
11	H	27.9831	3.56618156618
12	H	28.2281	3.3398013398
17	H	25.1381	6.19496419496
19	H	24.4468	6.83372603373
21	H	29.2179	2.42522522523
22	H	28.6270	2.97121737122
24	H	27.9785	3.57043197043
26	H	29.4712	2.19117579118
27	H	28.3196	3.25525525526
28	H	27.9846	3.5647955648
30	H	30.0157	1.68805728806
31	H	30.5240	1.21838761839
33	H	29.1416	2.49572649573
35	H	30.6143	1.13495033495
36	H	30.6925	1.06269346269
37	H	31.0725	0.711573111573
39	H	27.5655	3.95204435204
43	H	28.1105	3.44846384846
46	H	29.2428	2.40221760222
48	H	30.8312	0.934534534535
49	H	30.8010	0.962439362439
50	H	30.4913	1.2486024486
52	H	24.8068	6.50108570109
54	H	25.4169	5.93735273735
56	H	25.1281	6.2042042042
58	H	25.8678	5.52072072072
60	H	29.9145	1.78156618157
61	H	29.5562	2.11263571264
62	H	30.3002	1.42517902518
63	H	30.2827	1.44134904135
65	H	29.9542	1.74488334488
66	H	30.3655	1.36484176484
70	H	26.5591	4.88195888196
71	H	27.5474	3.96876876877
73	H	29.8920	1.80235620236
74	H	30.0167	1.68713328713
78	H	30.1995	1.51822591823
79	H	30.7862	0.976114576115
80	H	30.5606	1.18456918457
81	H	27.8111	3.72510972511
83	H	28.3635	3.21469161469
85	H	29.7552	1.92875952876
88	H	29.9108	1.78498498498
89	H	27.9518	3.5951027951
93	H	28.2351	3.33333333333
94	H	28.1623	3.4006006006
95	H	28.5657	3.02785862786
96	H	28.2603	3.31004851005

Mandelalide A Revised Configuration (MM Methodologies)

Supporting Information: Revised-MandelalideA-0001.log

Using Gaussian 09: AM64L-G09RevC.01 23-Sep-2011
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#mPW1PW91/6-311G(2d,p) scf=(maxcycle=300,direct,tight) NMR density=current
SCRF=(PCM,SOLVENT=Chloroform)

Pointgroup= C1 Stoichiometry= C33H52O11 C1[X(C33H52O11)]
#Atoms= 96
Charge = 0 Multiplicity = 1

SCF Energy= -2116.32821269
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Optimization incomplete.

Atomic Type	Coordinates (Angstroms) X	Y	Z
C	-6.751224	-0.649244	0.074825
C	-5.745643	0.422633	-0.358546
C	-6.151091	1.826730	0.114553
H	-6.223759	1.829376	1.207985
H	-7.142319	2.064553	-0.289601

C	-5.158726	2.921981	-0.318851
H	-5.068246	2.903223	-1.411877
C	-5.630656	4.306050	0.138127
O	-6.856152	4.663953	-0.484383
H	-6.709406	4.647033	-1.445820
H	-4.886690	5.074564	-0.095718
H	-5.772418	4.328959	1.224532
O	-3.885180	2.634403	0.296836
C	-2.777426	3.133700	-0.311752
O	-2.737075	3.807679	-1.328225
C	-1.605054	2.711479	0.483009
H	-1.771467	2.115484	1.373443
C	-0.369336	3.049023	0.087874
H	-0.222661	3.640646	-0.812063
C	0.878078	2.639502	0.826044
H	0.613861	2.209044	1.800451
H	1.473348	3.539784	1.017063
C	1.691665	1.627060	0.012383
H	1.844422	2.009112	-1.005527
O	-5.682255	0.426843	-1.787571
H	-5.490041	-0.485751	-2.066136
H	-4.743324	0.163726	0.003117
H	-7.719238	-0.473497	-0.412141
C	-6.925839	-0.786615	1.576834
H	-5.966709	-0.665041	2.094924
H	-7.631652	-0.057525	1.986820
C	-7.417373	-2.213075	1.692847
H	-8.467448	-2.232765	1.367958
C	-7.357096	-2.764697	3.106072
H	-7.655643	-3.818254	3.125444
H	-8.040070	-2.210591	3.759591
H	-6.354074	-2.681277	3.536642
C	-6.587958	-2.935762	0.624401
H	-7.194187	-3.722753	0.158819
O	-6.303145	-1.940490	-0.386147
O	0.938471	0.410876	-0.052764
C	1.556694	-0.577875	-0.877726
H	1.715040	-0.161881	-1.880026
C	0.615127	-1.787748	-0.972698
C	-0.815087	-1.442572	-1.444351
H	-1.256222	-0.726841	-0.737685
C	-0.839238	-0.799983	-2.832496
H	-1.869027	-0.652120	-3.178940
H	-0.322567	-1.421928	-3.571988
H	-0.360431	0.183764	-2.820918
C	-1.654763	-2.699369	-1.460189
H	-1.340749	-3.485873	-2.144911
C	-2.737320	-2.880559	-0.687935
H	-3.041089	-2.088831	-0.011321
C	-3.528763	-4.088596	-0.724629
H	-3.218910	-4.844603	-1.445151
C	-4.611884	-4.363963	0.022242
H	-5.097027	-5.323115	-0.151558
C	-5.249067	-3.520045	1.096449
H	-5.401473	-4.176437	1.960733
H	-4.577544	-2.719055	1.420586
H	0.537628	-2.251097	0.019838
H	1.061391	-2.537741	-1.638477
C	2.903535	-0.973249	-0.270094
H	3.410442	-1.720554	-0.893537
H	2.752546	-1.442785	0.710825
C	3.802141	0.254547	-0.093912
O	4.962589	-0.162027	0.627883
C	6.103536	0.679422	0.436704
H	5.813261	1.720841	0.597552
H	4.086185	0.623113	-1.088821
C	3.044775	1.346152	0.670734
H	3.640052	2.264254	0.723776
H	2.900467	1.012328	1.707209
O	6.637106	0.612101	-0.894022
C	7.110074	-0.685658	-1.269412
C	7.593864	-0.583459	-2.713632
H	6.798132	-0.187263	-3.352691
H	7.899322	-1.555877	-3.110146
H	8.437178	0.110742	-2.794367
H	6.269975	-1.392300	-1.256883
C	8.219422	-1.164520	-0.324517
H	9.125402	-0.555360	-0.433162
O	8.571056	-2.517237	-0.612119
H	9.031239	-2.528220	-1.467861
C	7.732930	-1.099335	1.124616
O	8.803538	-1.414931	2.014156
H	9.174409	-2.265893	1.720456
H	6.957779	-1.857982	1.290518
C	7.182513	0.291183	1.460568
O	8.268059	1.230193	1.406421
C	8.053356	2.382931	2.208897
H	7.944860	2.101635	3.261320
H	7.174497	2.939800	1.876034
H	8.928479	3.032121	2.113944
H	6.773363	0.261814	2.478601

NMR-Shifts

Revised-MandelalideA-0001-NMR.txt

Atom	Type	Isotropic	Scaled Shift
1	C	98.0111	84.2750626926
2	C	111.1986	71.6527881468
3	C	149.7114	34.7906736346
6	C	114.0434	68.9299182603
8	C	120.7300	62.5299106032
14	C	14.1450	164.546603113
16	C	56.4098	124.093301939
18	C	27.1658	152.083883688
20	C	142.8748	41.3342521871
23	C	110.9552	71.8857558529
29	C	148.9828	35.4880453301
32	C	147.8328	36.5887555275
34	C	171.5003	13.9356610961
38	C	101.8304	80.6194605563
42	C	113.0786	69.8533662589
44	C	141.2268	42.9116177568
45	C	147.9624	36.4647102739
47	C	168.3608	16.9405999349
51	C	37.6282	142.069909455
53	C	57.5966	122.957369015
55	C	50.6362	129.619441414
57	C	51.3842	128.903501216
59	C	153.4096	31.2509810678
64	C	145.1256	39.179923046
67	C	115.1726	67.8491165604
69	C	89.6190	92.3074714294
72	C	147.6886	36.7267750148
76	C	116.6704	66.4155133138
77	C	168.6938	16.6218725473
82	C	108.4025	74.3290453493
86	C	113.8618	69.1037347576
90	C	103.5687	78.9556653075
92	C	129.1631	54.458259155
4	H	30.3269	1.40050820051
5	H	29.6477	2.02808962809
7	H	26.8227	4.63839223839
10	H	31.5536	0.267036267036
11	H	27.6145	3.90676830677
12	H	28.6840	2.91854931855
17	H	25.4567	5.90057750058
19	H	24.1786	7.08154308154
21	H	29.3661	2.28828828829
22	H	29.4110	2.2468006468

24	H	28.4004	3.1805959806
26	H	29.9646	1.73527373527
27	H	27.7964	3.73869253869
28	H	27.8839	3.65784245784
30	H	30.5442	1.19972279972
31	H	29.9446	1.75375375375
33	H	29.2593	2.38697158697
35	H	30.7082	1.04818664819
36	H	30.5605	1.18466158466
37	H	31.0415	0.740217140217
39	H	27.7143	3.81455301455
43	H	28.4086	3.17301917302
46	H	29.1723	2.46735966736
48	H	30.9548	0.820328020328
49	H	31.3148	0.487687687688
50	H	30.5756	1.17070917071
52	H	25.9706	5.42573342573
54	H	25.0956	6.23423423423
56	H	25.4646	5.89327789328
58	H	26.1952	5.2182028182
60	H	29.8752	1.81787941788
61	H	29.4457	2.21473781474
62	H	30.2418	1.47914067914
63	H	30.6013	1.14696234696
65	H	30.0512	1.65525525526
66	H	30.6631	1.08985908986
70	H	26.3409	5.08357588358
71	H	27.6892	3.83774543775
73	H	29.6669	2.01034881035
74	H	30.7095	1.04698544699
78	H	30.5346	1.20859320859
79	H	30.5003	1.24028644029
80	H	30.8899	0.880295680296
81	H	28.0404	3.51323631324
83	H	28.0462	3.50787710788
85	H	30.6310	1.11951951952
88	H	29.8662	1.8261954262
89	H	27.6364	3.88653268653
93	H	28.7305	2.87558327558
94	H	28.4238	3.15897435897
95	H	28.3174	3.25728805729
96	H	28.1873	3.3775005775

Supporting Information: Revised-MandelalideA-0002.log

Using Gaussian 09: AM64L-G09RevC.01 23-Sep-2011

==========

#mPW1PW91/6-311G(2d,p) scf=(maxcycle=300,direct,tight) NMR density=current

SCRF=(PCM,SOLVENT=Chloroform)

Pointgroup= C1 Stoichiometry= C33H52O11 C1[X(C33H52O11)]

#Atoms= 96

Charge = 0 Multiplicity = 1

SCF Energy= -2116.32914323

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Optimization incomplete.

Atomic Type	Coordinates (Angstroms) X	Y	Z
C	-6.537159	-0.953119	0.012894
C	-5.690318	0.274098	-0.339404
C	-6.202999	1.552427	0.342304
H	-6.188579	1.403895	1.428203
H	-7.241961	1.729721	0.036930
C	-5.370302	2.797250	-0.010056
H	-5.315244	2.907238	-1.100572
C	-5.972444	4.071473	0.592963
O	-6.113833	3.956242	2.004299
H	-5.239238	3.728413	2.362970
H	-6.962968	4.266026	0.169552
H	-5.338856	4.940724	0.395574
O	-4.043478	2.601847	0.528591
C	-3.025417	3.285132	-0.058966
O	-3.106149	4.064259	-0.994229
C	-1.778377	2.913442	0.642492
H	-1.838489	2.207064	1.463498
C	-0.605826	3.427513	0.246142
H	-0.566330	4.128253	-0.585267
C	0.710470	3.077797	0.886881
H	0.540204	2.505708	1.807941
H	1.211826	4.010064	1.170412
C	1.593235	2.271767	-0.072468
H	1.665420	2.795008	-1.035887
O	-5.746116	0.462406	-1.756298
H	-5.477013	-0.379302	-2.165284
H	-4.640525	0.091928	-0.083324
H	-7.553052	-0.836402	-0.385061
C	-6.580843	-1.292992	1.493076
H	-5.604564	-1.124717	1.963415
H	-7.329061	-0.709494	2.036544
C	-6.902735	-2.772761	1.451395
H	-7.966380	-2.876268	1.191099
C	-6.677542	-3.481942	2.774786
H	-5.659834	-3.333597	3.150366
H	-6.856058	-4.557195	2.673282
H	-7.365289	-3.096874	3.534357
C	-6.082087	-3.254535	0.250332
H	-6.629057	-4.046170	-0.276167
O	-5.985708	-2.116007	-0.638446
O	0.972160	0.997690	-0.275435
C	1.657102	0.201112	-1.241613
H	1.727133	0.759907	-2.182731
C	0.847489	-1.083739	-1.474227
C	-0.628949	-0.842534	-1.857800
H	-1.114435	-0.275197	-1.052692
C	-0.777756	-0.035739	-3.148992
H	-1.831118	0.039583	-3.445737
H	-0.227693	-0.496907	-3.976098
H	-0.405885	0.986035	-3.022556
C	-1.329303	-2.172593	-2.014912
H	-0.969736	-2.822105	-2.812697
C	-2.344973	-2.574544	-1.234454
H	-2.693120	-1.917195	-0.445282
C	-3.005433	-3.848058	-1.404949
H	-2.662384	-4.459160	-2.237631
C	-4.003334	-4.340800	-0.651164
H	-4.394607	-5.317368	-0.934953
C	-4.654966	-3.727902	0.560896
H	-4.670095	-4.504752	1.334795
H	-4.057712	-2.900138	0.954607
H	0.861416	-1.677778	-0.549658
H	1.345109	-1.687329	-2.244802
C	3.065871	-0.120674	-0.735346
H	3.603365	-0.708633	-1.486901
H	3.010798	-0.740746	0.168098
C	3.836815	1.161860	-0.402730
O	5.061317	0.904657	0.287114
C	6.081975	0.288627	-0.503901
H	6.027011	0.671209	-1.527857
H	4.051941	1.717507	-1.324094
C	2.988706	2.054767	0.511414

H	3.498533	3.011476	0.673298
H	2.914406	1.576543	1.497788
O	5.942901	-1.136963	-0.596181
C	6.027095	-1.814025	0.659602
C	5.820508	-3.301692	0.392058
H	6.598179	-3.690411	-0.274485
H	4.863409	-3.466724	-0.114108
H	5.828062	-3.884374	1.317816
H	5.202734	-1.481420	1.303160
C	7.372153	-1.547107	1.344530
H	8.192760	-2.008153	0.781483
O	7.387660	-2.125590	2.648885
H	6.646840	-1.749464	3.154629
C	7.617435	-0.041219	1.457840
O	8.930025	0.205961	1.961238
H	9.039306	-0.340935	2.759054
H	6.919305	0.395652	2.182517
C	7.453252	0.646295	0.095650
O	8.500184	0.182214	-0.770374
C	8.822182	1.101839	-1.804806
H	9.628499	0.671389	-2.404469
H	9.174022	2.047163	-1.380082
H	7.963769	1.279379	-2.457741
H	7.552368	1.728639	0.244634

NMR-Shifts
Revised-MandelalideA-0002-NMR.txt

Atom	Type	Isotropic	Scaled Shift
1	C	98.0405	84.2469227971
2	C	110.4683	72.3517869791
3	C	150.8171	33.7323647084
6	C	113.6098	69.3449338617
8	C	119.4007	63.8022358774
14	C	14.5365	164.171883076
16	C	56.5091	123.998258006
18	C	26.7993	152.434675243
20	C	142.8654	41.3432492965
23	C	110.7912	72.0427266984
29	C	148.9774	35.4932138823
32	C	147.8962	36.5280728957
34	C	171.6058	13.8346828997
38	C	101.9942	80.4626811386
42	C	113.5908	69.3631195084
44	C	140.9496	43.1769367714
45	C	147.7753	36.6437910373
47	C	168.3786	16.9235628553
51	C	37.6596	142.039855281
53	C	57.4828	123.066291468
55	C	50.7292	129.530427458
57	C	51.2847	128.998736576
59	C	153.4108	31.2498325006
64	C	143.7344	40.511495243
67	C	106.5930	76.0609889163
69	C	82.8623	98.7745745516
72	C	145.3871	38.9296311185
76	C	115.0527	67.9638775627
77	C	168.0724	17.2166389096
82	C	108.4538	74.2799441031
86	C	110.2014	72.6072474588
90	C	103.3032	79.2097857922
92	C	129.0177	54.5974272096
4	H	29.5602	2.10893970894
5	H	30.4143	1.31975051975
7	H	26.4754	4.9592977593
10	H	31.0394	0.742157542158
11	H	28.3838	3.19593439593
12	H	27.5030	4.00979440979
17	H	25.4111	5.94271194271
19	H	24.1316	7.12497112497
21	H	29.3859	2.26999306999
22	H	29.4010	2.25604065604
24	H	28.3390	3.23732963733
26	H	29.9282	1.76890736891
27	H	27.9149	3.6291984292
28	H	27.8758	3.66532686533
30	H	30.5088	1.23243243243
31	H	29.9613	1.73832293832
33	H	29.2450	2.40018480018
35	H	31.0619	0.721367521368
36	H	30.6978	1.0577962578
37	H	30.5653	1.18022638023
39	H	27.7081	3.82028182028
43	H	28.4975	3.09087549088
46	H	29.2076	2.43474243474
48	H	30.9480	0.826611226611
49	H	31.3307	0.472996072996
50	H	30.5865	1.16063756064
52	H	25.9370	5.45677985678
54	H	25.1087	6.22212982213
56	H	25.4490	5.90769230769
58	H	26.2156	5.19935319935
60	H	29.8657	1.82665742666
61	H	29.4335	2.22601062601
62	H	30.2481	1.47331947332
63	H	30.5662	1.17939477939
65	H	29.3362	2.31591591592
66	H	30.6599	1.09281589282
70	H	26.5229	4.91540771541
71	H	28.0255	3.527003927
73	H	29.9692	1.73102333102
74	H	30.5425	1.20129360129
78	H	30.8563	0.911342111342
79	H	30.6875	1.06731346731
80	H	30.1365	1.57643797644
81	H	28.2388	3.32991452991
83	H	28.3333	3.2425964426
85	H	32.1019	-0.239593439593
88	H	29.7397	1.94308154308
89	H	27.9925	3.5574959575
93	H	28.3105	3.26366366366
94	H	28.7261	2.87964887965
95	H	28.3985	3.18235158235
96	H	28.1827	3.38175098175

Supporting Information: Revised-MandelalideA-0003.log

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 Using  Gaussian 09:  AM64L-G09RevC.01 23-Sep-2011
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 #mPW1PW91/6-311G(2d,p) scf=(maxcycle=300,direct,tight) NMR
density=current
 SCRF=(PCM,SOLVENT=Chloroform)
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 Pointgroup= C1   Stoichiometry= C33H52O11   C1[X(C33H52O11)]
#Atoms= 96
 Charge = 0                Multiplicity = 1
-----------------------------------------------------------------------
 SCF Energy= -2116.32397067
=======================================================================
 Optimization incomplete.


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      Atomic     Coordinates (Angstroms)
       Type      X                Y              Z
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       C       -6.791759     -0.614672      0.026324
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C	-5.800311	0.429727	-0.503847
C	-6.167478	1.860333	-0.077618
H	-6.200400	1.907230	1.016785
H	-7.167615	2.103349	-0.458764
C	-5.175246	2.915263	-0.599216
H	-5.069068	2.817079	-1.685615
C	-5.634191	4.338764	-0.266327
O	-5.840453	4.500368	1.133121
H	-5.014382	4.242794	1.577475
H	-6.576274	4.568502	-0.773773
H	-4.889398	5.078889	-0.575365
O	-3.901410	2.669259	0.040744
C	-2.786425	3.110399	-0.600039
O	-2.737129	3.705766	-1.663794
C	-1.621651	2.739156	0.229641
H	-1.796972	2.206746	1.157955
C	-0.382216	3.042767	-0.179170
H	-0.226204	3.570247	-1.117274
C	0.857894	2.677611	0.593445
H	0.584934	2.309709	1.590725
H	1.455299	3.587332	0.732888
C	1.677354	1.613770	-0.147050
H	1.845225	1.934362	-1.183916
O	-5.783929	0.360127	-1.932327
H	-6.690158	0.512300	-2.251305
H	-4.787928	0.175182	-0.169850
H	-7.774370	-0.470466	-0.440235
C	-6.926253	-0.653566	1.538928
H	-5.952980	-0.503371	2.023230
H	-7.618910	0.103146	1.918948
C	-7.418285	-2.068367	1.760530
H	-8.476357	-2.105026	1.464025
C	-7.324932	-2.525778	3.205417
H	-7.989126	-1.927222	3.837650
H	-6.311698	-2.417819	3.605313
H	-7.624449	-3.573681	3.300839
C	-6.617075	-2.861314	0.721954
H	-7.234215	-3.677086	0.326016
O	-6.358699	-1.935474	-0.358611
O	0.917126	0.399412	-0.149925
C	1.541855	-0.639868	-0.906152
H	1.717338	-0.284258	-1.928988
C	0.594439	-1.847619	-0.943055
C	-0.824237	-1.526088	-1.461433
H	-1.271423	-0.761359	-0.813936
C	-0.819564	-0.978783	-2.890285
H	-0.294369	-1.653156	-3.576476
H	-0.332109	0.000238	-2.937424
H	-1.841674	-0.847961	-3.264234
C	-1.674170	-2.775851	-1.407242
H	-1.361275	-3.605228	-2.038624
C	-2.764372	-2.898242	-0.633485
H	-3.065603	-2.062132	-0.010625
C	-3.567649	-4.098288	-0.600542
H	-3.269443	-4.895671	-1.280147
C	-4.647839	-4.322014	0.167528
H	-5.143261	-5.284719	0.049542
C	-5.267182	-3.414879	1.199903
H	-5.400953	-4.017964	2.105663
H	-4.591792	-2.594778	1.462128
H	0.496689	-2.248149	0.075238
H	1.048891	-2.641047	-1.552231
C	2.877376	-1.004412	-0.256754
H	3.388085	-1.790449	-0.825449
H	2.709351	-1.412965	0.749130
C	3.780035	0.227154	-0.140607
O	4.927423	-0.153307	0.622082
C	6.076026	0.672627	0.403514
H	5.787767	1.722266	0.506845
H	4.081231	0.532679	-1.151336
C	3.019298	1.366108	0.546339
H	3.618302	2.283126	0.552090
H	2.858845	1.095671	1.599188
O	6.628101	0.536095	-0.915134
C	7.098258	-0.781125	-1.215595
C	7.611775	-0.763862	-2.651279
H	6.821294	-0.430278	-3.333521
H	7.950652	-1.754066	-2.972114
H	8.440759	-0.055785	-2.762428
H	6.254243	-1.481734	-1.178149
C	8.190092	-1.215907	-0.232017
H	9.097851	-0.615238	-0.371714
O	8.536509	-2.576579	-0.482473
H	9.171086	-2.838425	0.207803
C	7.689581	-1.076538	1.205460
O	8.767091	-1.362510	2.099240
H	8.445255	-1.210685	3.004403
H	6.916825	-1.830965	1.397795
C	7.137405	0.331872	1.463233
O	8.229083	1.260238	1.387677
C	7.998337	2.461188	2.111874
H	7.141184	3.006289	1.711794
H	8.884864	3.093957	2.014125
H	7.845045	2.243486	3.173476
H	6.708354	0.352571	2.473376

NMR-Shifts

Revised-MandelalideA-0003-NMR.txt

Atom	Type	Isotropic	Scaled Shift
1	C	96.3197	85.8939681081
2	C	109.2545	73.5135626639
3	C	147.1813	37.2123317828
6	C	113.2809	69.6597369781
8	C	119.1759	64.0174007925
14	C	14.5085	164.198682976
16	C	56.7344	123.782614522
18	C	26.6857	152.543406267
20	C	142.6134	41.5844484006
23	C	110.8603	71.9765883727
29	C	148.2777	36.162924252
32	C	147.7057	36.7104079328
34	C	171.6249	13.8164015391
38	C	102.4379	80.0379984303
42	C	112.9835	69.9443902066
44	C	140.9985	43.1301326595
45	C	147.9703	36.4571488734
47	C	168.5279	16.7806619575
51	C	38.1069	141.611726871
53	C	57.2569	123.282509236
55	C	50.6197	129.635234212
57	C	51.7857	128.519209786
59	C	153.3174	31.3392293114
64	C	145.0809	39.2227071728
67	C	115.2113	67.8120752694
69	C	89.5310	92.391699688
72	C	147.6813	36.7337621317
76	C	118.0274	65.1166752809
77	C	167.7674	17.5085663968
82	C	111.5259	71.3395164532
86	C	110.4959	72.3253699343
90	C	100.9638	81.4489174754
92	C	128.8312	54.7759336894
4	H	29.4754	2.18729498729
5	H	30.7428	1.01621621622
7	H	26.4231	5.00762300762
10	H	31.0123	0.767197967198
11	H	28.4122	3.16969276969
12	H	27.4589	4.05054285054

17	H	25.4160	5.93818433818
19	H	24.1231	7.13282513283
21	H	29.3630	2.29115269115
22	H	29.3680	2.28653268653
24	H	28.3644	3.21386001386
26	H	32.2832	-0.407114807115
27	H	28.2364	3.33213213213
28	H	28.0777	3.47877107877
30	H	30.5093	1.23197043197
31	H	29.9130	1.78295218295
33	H	29.2835	2.36461076461
35	H	30.5817	1.16507276507
36	H	31.0520	0.730515130515
37	H	30.7252	1.03247863248
39	H	27.7433	3.78775698776
43	H	28.3841	3.19565719566
46	H	29.2115	2.43113883114
48	H	31.3285	0.475028875029
49	H	30.5958	1.15204435204
50	H	30.8728	0.896096096096
52	H	26.0006	5.39801339801
54	H	25.0876	6.24162624163
56	H	25.4594	5.89808269808
58	H	26.2168	5.19824439824
60	H	29.8976	1.79718179718
61	H	29.4583	2.2030954031
62	H	30.2502	1.47137907138
63	H	30.5685	1.17726957727
65	H	30.0378	1.66763686764
66	H	30.6700	1.08348348348
70	H	26.2993	5.12201432201
71	H	27.6675	3.8577962578
73	H	29.6631	2.01386001386
74	H	30.7316	1.02656502657
78	H	30.5927	1.15490875491
79	H	30.1268	1.5854007854
80	H	30.8171	0.947562947563
81	H	27.9273	3.61774081774
83	H	27.9723	3.57616077616
85	H	29.9772	1.72363132363
88	H	31.4875	0.328112728113
89	H	27.5716	3.94640794641
93	H	28.3923	3.18808038808
94	H	28.2545	3.31540771541
95	H	28.8105	2.80166320166
96	H	28.5239	3.06648186648

Supporting Information: Revised-MandelalideA-0004.log

Using Gaussian 09: AM64L-G09RevC.01 23-Sep-2011

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#mPW1PW91/6-311G(2d,p) scf=(maxcycle=300,direct,tight) NMR density=current

SCRF=(PCM,SOLVENT=Chloroform)

Pointgroup= C1 Stoichiometry= C33H52O11 C1[X(C33H52O11)]

#Atoms= 96

Charge = 0 Multiplicity = 1

SCF Energy= -2116.32498434

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Optimization incomplete.

Atomic Type	Coordinates (Angstroms) X	Y	Z
C	-6.783809	-0.626743	0.088669
C	-5.798762	0.463375	-0.352985
C	-6.197662	1.855040	0.163254
H	-6.225089	1.836034	1.259296
H	-7.208236	2.093279	-0.193526
C	-5.242927	2.971394	-0.289843
H	-5.179141	2.993924	-1.384282
C	-5.728532	4.324793	0.237258
O	-4.964914	5.372486	-0.350085
H	-5.298116	6.209621	0.014849
H	-5.606406	4.389712	1.323032
H	-6.778997	4.492372	-0.021252
O	-3.944886	2.695536	0.285625
C	-2.845197	3.036543	-0.438273
O	-2.815938	3.539039	-1.549030
C	-1.658938	2.685391	0.371667
H	-1.810670	2.179710	1.318460
C	-0.429763	2.976994	-0.076343
H	-0.298782	3.482319	-1.030768
C	0.830065	2.626284	0.671513
H	0.580327	2.244893	1.669732
H	1.414586	3.543541	0.807840
C	1.652690	1.583220	-0.094356
H	1.813501	1.926944	-1.124965
O	-5.757272	0.490348	-1.781927
H	-6.657869	0.662564	-2.105644
H	-4.788496	0.201990	-0.019445
H	-7.759686	-0.465410	-0.386377
C	-6.947254	-0.762645	1.593812
H	-5.983599	-0.643775	2.104995
H	-7.648868	-0.033278	2.008738
C	-7.441074	-2.187942	1.713755
H	-8.493314	-2.206295	1.394590
C	-7.376620	-2.737823	3.127607
H	-6.371547	-2.654026	3.554931
H	-7.675900	-3.789224	3.149510
H	-8.054823	-2.180869	3.783049
C	-6.618198	-2.912266	0.641178
H	-7.231700	-3.692841	0.174095
O	-6.326723	-1.915128	-0.366149
O	0.900306	0.364863	-0.119873
C	1.526282	-0.650988	-0.904993
H	1.698169	-0.268493	-1.917739
C	0.583923	-1.861140	-0.972656
C	-0.837548	-1.527854	-1.478560
H	-1.285288	-0.784902	-0.805658
C	-0.836646	-0.934165	-2.888459
H	-0.353966	0.048702	-2.903996
H	-1.859089	-0.795659	-3.257709
H	-0.308234	-1.582926	-3.596432
C	-1.684506	-2.779648	-1.464445
H	-1.370945	-3.587082	-2.123670
C	-2.775516	-2.928710	-0.697504
H	-3.079202	-2.114495	-0.046969
C	-3.581444	-4.127040	-0.711622
H	-3.282763	-4.898505	-1.419988
C	-4.664453	-4.375918	0.044647
H	-5.163077	-5.331649	-0.113273
C	-5.283327	-3.509520	1.110282
H	-5.437917	-4.153954	1.982748
H	-4.599237	-2.713377	1.420479
H	0.488792	-2.289586	0.035186
H	1.037937	-2.635782	-1.604010
C	2.865047	-1.025898	-0.266866
H	3.377811	-1.795427	-0.855897
H	2.702144	-1.457880	0.728873
C	3.762724	0.208128	-0.126521
O	4.914095	-0.183322	0.623847

C	6.058361	0.650211	0.417570
H	5.766993	1.696790	0.539611
H	4.058742	0.537566	-1.130751
C	2.999318	1.328612	0.587530
H	3.594311	2.248354	0.609970
H	2.845498	1.035664	1.635546
O	6.607604	0.538213	-0.903948
C	7.079627	-0.771477	-1.228966
C	7.583616	-0.730650	-2.667933
H	7.924086	-1.714112	-3.007014
H	8.409023	-0.017385	-2.772836
H	6.788309	-0.388968	-3.340227
H	6.237967	-1.476014	-1.198203
C	8.178831	-1.217807	-0.260686
H	9.083574	-0.613327	-0.396326
O	8.527742	-2.573872	-0.532207
H	9.148666	-2.854509	0.162747
C	7.687372	-1.101896	1.183276
O	8.763554	-1.383721	2.078720
H	9.382750	-0.634824	2.029438
H	6.922061	-1.864637	1.372633
C	7.123156	0.296101	1.468292
O	8.215521	1.226783	1.407247
C	7.979997	2.419922	2.143408
H	8.867970	3.052118	2.060850
H	7.815547	2.190765	3.200576
H	7.126723	2.971692	1.740254
H	6.699751	0.295580	2.480941

NMR-Shifts
Revised-MandelalideA-0004-NMR.txt

Atom	Type	Isotropic	Scaled Shift
1	C	96.4591	85.7605428894
2	C	110.4659	72.3540841134
3	C	147.4264	36.9777369398
6	C	115.0815	67.9363119508
8	C	115.1720	67.849690844
14	C	14.6430	164.06994774
16	C	56.0950	124.394609391
18	C	27.8501	151.428913264
20	C	142.6080	41.5896169529
23	C	110.6665	72.1620819694
29	C	148.2105	36.2272440131
32	C	147.7958	36.6241696817
34	C	171.4987	13.937192519
38	C	102.2001	80.2656061563
42	C	113.0329	69.897107525
44	C	141.0908	43.0417887019
45	C	147.9922	36.4361875227
47	C	168.5189	16.7892762113
51	C	38.0329	141.682555179
53	C	57.2682	123.271693562
55	C	50.4840	129.765118015
57	C	51.9911	128.322613373
59	C	153.4624	31.2004441126
64	C	145.1179	39.1872930186
67	C	115.0973	67.9211891499
69	C	89.7404	92.1912747181
72	C	147.7257	36.6912651467
76	C	118.0356	65.1088267386
77	C	167.5573	17.7096613641
82	C	108.9923	73.7645245889
86	C	111.3530	71.5050058385
90	C	102.1392	80.3238959398
92	C	128.8337	54.7735408411
4	H	30.1731	1.54261954262
5	H	30.7668	0.99404019404
7	H	25.9980	5.40041580042
10	H	31.3727	0.434188034188
11	H	27.8832	3.65848925849
12	H	27.8540	3.68547008547
17	H	25.4120	5.94188034188
19	H	24.1937	7.06759066759
21	H	29.3608	2.29318549319
22	H	29.3893	2.26685146685
24	H	28.3455	3.23132363132
26	H	32.2621	-0.387618387618
27	H	28.1631	3.39986139986
28	H	28.1347	3.4261030261
30	H	30.5404	1.20323400323
31	H	30.0374	1.66800646801
33	H	29.3188	2.33199353199
35	H	31.0331	0.747978747979
36	H	30.7532	1.00660660661
37	H	30.6039	1.14455994456
39	H	27.7583	3.7738969739
43	H	28.3960	3.18466158466
46	H	29.1787	2.46144606145
48	H	30.5493	1.19501039501
49	H	30.8616	0.906444906445
50	H	31.3336	0.470316470316
52	H	26.0000	5.39856779857
54	H	25.0924	6.23719103719
56	H	25.4693	5.88893508894
58	H	26.2235	5.19205359205
60	H	29.8943	1.80023100023
61	H	29.4598	2.20170940171
62	H	30.2301	1.48995148995
63	H	30.5924	1.15518595519
65	H	30.0340	1.67114807115
66	H	30.6614	1.09142989143
70	H	26.2716	5.14760914761
71	H	27.6559	3.86851466851
73	H	29.6500	2.02596442596
74	H	30.7039	1.05215985216
78	H	30.1451	1.56849156849
79	H	30.8583	0.909494109494
80	H	30.5976	1.15038115038
81	H	27.9264	3.61857241857
83	H	28.3361	3.24000924001
85	H	29.7861	1.90020790021
88	H	30.2838	1.44033264033
89	H	28.0309	3.52201432201
93	H	28.2512	3.31845691846
94	H	28.7266	2.87918687919
95	H	28.3186	3.25617925618
96	H	28.2599	3.31041811042

Supporting Information: Revised-MandelalideA-0005.log

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 Using  Gaussian 09:  AM64L-G09RevC.01 23-Sep-2011
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 #mPW1PW91/6-311G(2d,p) scf=(maxcycle=300,direct,tight) NMR
density=current
 SCRF=(PCM,SOLVENT=Chloroform)
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 Pointgroup= C1   Stoichiometry= C33H52O11   C1[X(C33H52O11)]
#Atoms= 96
 Charge = 0                Multiplicity = 1
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 SCF Energy= -2116.32413612
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 Optimization incomplete.


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Atomic Type	Coordinates (Angstroms) X	Y	Z
C	6.532358	-1.009064	-0.075340
C	5.711741	0.256241	0.211036
C	6.239425	1.479837	-0.554199
H	6.198329	1.274997	-1.630967
H	7.290720	1.645940	-0.284795
C	5.451829	2.767917	-0.265184
H	5.455866	2.981338	0.810181
C	6.059171	3.942152	-1.037281
O	5.459924	5.160005	-0.611850
H	5.865330	5.875613	-1.130384
H	5.881390	3.838239	-2.113013
H	7.135729	4.016466	-0.852650
O	4.097207	2.565284	-0.731644
C	3.090840	3.156738	-0.035890
O	3.186693	3.837821	0.971747
C	1.824960	2.827158	-0.726308
H	1.861878	2.158405	-1.578206
C	0.667255	3.338582	-0.286737
H	0.651887	4.006899	0.570580
C	-0.665728	3.029291	-0.915905
H	-0.521123	2.459388	-1.841738
H	-1.147426	3.976820	-1.186477
C	-1.560116	2.239278	0.047062
H	-1.624012	2.768584	1.007579
O	5.761998	0.526593	1.614241
H	6.694956	0.634291	1.866083
H	4.659208	0.072848	-0.031582
H	7.547772	-0.894719	0.325760
C	6.585465	-1.413025	-1.538467
H	5.613203	-1.260798	-2.022946
H	7.342025	-0.858056	-2.101221
C	6.899858	-2.890473	-1.429573
H	7.960164	-2.988261	-1.153919
C	6.683949	-3.655173	-2.723419
H	5.672465	-3.517194	-3.117103
H	6.855852	-4.725556	-2.574289
H	7.382806	-3.306571	-3.491787
C	6.064243	-3.315375	-0.215033
H	6.609032	-4.077601	0.354278
O	5.955364	-2.135277	0.614995
O	-0.954804	0.958921	0.256387
C	-1.648822	0.178543	1.230062
H	-1.713766	0.746084	2.166268
C	-0.852350	-1.111221	1.475046
C	0.624919	-0.878055	1.860713
H	1.116616	-0.320932	1.052727
C	0.776649	-0.061752	3.145440
H	0.414333	0.962165	3.009103
H	1.829322	0.007383	3.444752
H	0.220123	-0.511072	3.975215
C	1.316728	-2.211183	2.031277
H	0.952018	-2.850539	2.833085
C	2.334782	-2.622550	1.259971
H	2.691909	-1.973137	0.466247
C	2.994231	-3.893653	1.448692
H	2.651668	-4.492419	2.291536
C	3.992417	-4.399426	0.703969
H	4.384396	-5.370552	1.004849
C	4.642944	-3.807619	-0.520257
H	4.665581	-4.602492	-1.273648
H	4.038719	-2.994591	-0.934386
H	-0.867669	-1.713115	0.555774
H	-1.356945	-1.703940	2.249902
C	-3.060687	-0.131485	0.725754
H	-3.604537	-0.708290	1.481590
H	-3.011889	-0.757864	-0.175147
C	-3.815682	1.158498	0.384310
O	-5.044143	0.909957	-0.303549
C	-6.072444	0.314725	0.491831
H	-6.016368	0.711530	1.511543
H	-4.025646	1.722307	1.302925
C	-2.958553	2.036602	-0.534681
H	-3.456390	3.000306	-0.700473
H	-2.890189	1.553764	-1.518643
O	-5.948825	-1.109830	0.606332
C	-6.036095	-1.803804	-0.641474
C	-5.833056	-3.287472	-0.349707
H	-5.843140	-3.885073	-1.266936
H	-6.610029	-3.664170	0.324413
H	-4.874625	-3.446933	0.156529
H	-5.213103	-1.483670	-1.292597
C	-7.381297	-1.542301	-1.323799
H	-8.200370	-1.996904	-0.752574
O	-7.380213	-2.141230	-2.617867
H	-8.206165	-1.872706	-3.058328
C	-7.614714	-0.036578	-1.462178
O	-8.929558	0.198897	-1.969319
H	-9.555877	-0.028219	-1.259324
H	-6.920649	0.374760	-2.204235
C	-7.437051	0.678406	-0.117112
O	-8.501077	0.249123	0.748045
C	-8.794216	1.176939	1.783464
H	-7.936538	1.313134	2.447847
H	-9.624661	0.779514	2.371845
H	-9.099250	2.138379	1.360441
H	-7.521195	1.759927	-0.290310

NMR-Shifts

Revised-MandelalideA-0005-NMR.txt

Atom	Type	Isotropic	Scaled Shift
1	C	96.2768	85.9350293842
2	C	110.5692	72.2552116235
3	C	147.4458	36.9591684374
6	C	115.0240	67.9913474607
8	C	115.1516	67.8692164858
14	C	14.6332	164.079327705
16	C	56.0910	124.398437949
18	C	28.0996	151.190107008
20	C	142.6723	41.5280728957
23	C	110.5391	72.2840215165
29	C	148.2940	36.1473228814
32	C	147.6220	36.7905204924
34	C	171.5247	13.9123068971
38	C	102.5455	79.9350102414
42	C	113.4835	69.4658205555
44	C	140.9322	43.1935909952
45	C	147.8161	36.6047397538
47	C	168.5343	16.774536266
51	C	38.1074	141.611248301
53	C	57.1611	123.374203182
55	C	50.4829	129.766170869
57	C	51.7119	128.589846666
59	C	153.5351	31.1308600854
64	C	143.6351	40.6065391757
67	C	106.0699	76.5616684852
69	C	82.9863	98.6558892781
72	C	145.5061	38.8157315416
76	C	117.4692	65.6509504393
77	C	167.8467	17.4326652501
82	C	109.0010	73.756197477
86	C	111.5681	71.2991251747
90	C	101.6256	80.8154826854
92	C	128.9147	54.6960125577
4	H	30.1532	1.56100716101
5	H	30.7590	1.00124740125
7	H	25.9923	5.40568260568

10	H	31.3508	0.454423654424
11	H	27.8614	3.67863247863
12	H	27.8393	3.69905289905
17	H	25.4267	5.9282975283
19	H	24.2202	7.0431046431
21	H	29.3910	2.26528066528
22	H	29.3899	2.2662970663
24	H	28.3280	3.24749364749
26	H	32.2679	-0.392977592978
27	H	28.1774	3.38664818665
28	H	28.1131	3.44606144606
30	H	30.5129	1.22864402864
31	H	30.0286	1.67613767614
33	H	29.3150	2.3355047355
35	H	31.0661	0.717486717487
36	H	30.7164	1.04060984061
37	H	30.5842	1.16276276276
39	H	27.7753	3.75818895819
43	H	28.4982	3.09022869023
46	H	29.2068	2.43548163548
48	H	30.5846	1.16239316239
49	H	30.8675	0.900993300993
50	H	31.3667	0.439732039732
52	H	25.9895	5.40826980827
54	H	25.1031	6.2273042273
56	H	25.4572	5.90011550012
58	H	26.2425	5.1744975745
60	H	29.9068	1.78868098868
61	H	29.4523	2.20863940864
62	H	30.2376	1.48302148302
63	H	30.5839	1.16303996304
65	H	29.3320	2.3197967198
66	H	30.5561	1.18872718873
70	H	26.4759	4.95883575884
71	H	27.9958	3.55444675445
73	H	29.9428	1.75541695542
74	H	30.4871	1.25248325248
78	H	30.1925	1.52469392469
79	H	30.9316	0.841764841765
80	H	30.6587	1.09392469392
81	H	27.9202	3.6243012243
83	H	28.3457	3.23113883114
85	H	29.7751	1.91037191037
88	H	30.2593	1.46297066297
89	H	28.0686	3.48717948718
93	H	28.3139	3.26052206052
94	H	28.2807	3.2911988912
95	H	28.7479	2.85950565951
96	H	28.2447	3.32446292446

Supporting Information: Revised-MandelalideA-0006.log

Using Gaussian 09: AM64L-G09RevC.01 23-Sep-2011

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#mPW1PW91/6-311G(2d,p) scf=(maxcycle=300,direct,tight) NMR density=current

SCRF=(PCM,SOLVENT=Chloroform)

Pointgroup= C1 Stoichiometry= C33H52O11 C1[X(C33H52O11)]

#Atoms= 96

Charge = 0 Multiplicity = 1

SCF Energy= -2116.32308047

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Optimization incomplete.

Atomic Type	Coordinates (Angstroms) X	Y	Z
C	-6.590685	-0.272705	-0.255063
C	-5.430164	0.555556	-0.816503
C	-5.617452	2.059973	-0.578279
H	-5.670684	2.251315	0.498411
H	-6.578372	2.373300	-1.006499
C	-4.512686	2.923564	-1.211057
H	-4.508817	2.744792	-2.293433
C	-4.751775	4.421240	-1.000040
O	-3.785491	5.179575	-1.721655
H	-3.875855	4.951342	-2.662134
H	-4.673421	4.710257	0.051377
H	-5.745332	4.714017	-1.355849
O	-3.184253	2.529937	-0.779458
C	-2.805785	2.647353	0.518971
O	-3.478877	3.035300	1.459405
C	-1.395441	2.206446	0.603163
H	-0.930156	1.843428	-0.305758
C	-0.739391	2.253916	1.772278
H	-1.256373	2.635135	2.651767
C	0.680743	1.812988	2.036084
H	0.639318	1.111105	2.880103
H	1.242450	2.692456	2.375140
C	1.436835	1.145907	0.876604
H	1.438445	1.810415	0.003673
O	-5.359650	0.324392	-2.226542
H	-5.302782	-0.639409	-2.352900
H	-4.481301	0.210663	-0.390329
H	-7.518557	-0.025123	-0.785927
C	-6.790633	-0.161966	1.245813
H	-5.827250	-0.118867	1.768373
H	-7.373532	0.720439	1.528718
C	-7.504997	-1.464029	1.548933
H	-8.543735	-1.364876	1.201304
C	-7.539347	-1.810379	3.026474
H	-8.006718	-2.787212	3.185349
H	-8.120985	-1.065254	3.579707
H	-6.536941	-1.832249	3.465697
C	-6.795313	-2.453249	0.617305
H	-7.513057	-3.195057	0.246380
O	-6.346181	-1.670023	-0.512133
O	0.758837	-0.069976	0.548084
C	1.324146	-0.734177	-0.584889
H	1.342342	-0.043261	-1.435626
C	0.433331	-1.940140	-0.915535
C	-1.012209	-1.541790	-1.291550
H	-1.388439	-0.828503	-0.547991
C	-1.088182	-0.863719	-2.661229
H	-2.126790	-0.641003	-2.931184
H	-0.664928	-1.498616	-3.447505
H	-0.544822	0.085977	-2.664502
C	-1.902104	-2.763213	-1.286099
H	-1.632290	-3.577260	-1.955538
C	-2.988279	-2.863288	-0.504677
H	-3.237160	-2.030869	0.146046
C	-3.857007	-4.016588	-0.488775
H	-3.580411	-4.840886	-1.145140
C	-4.978266	-4.154567	0.239603
H	-5.535406	-5.082349	0.122876
C	-5.575676	-3.170757	1.214293
H	-5.867402	-3.737026	2.105634
H	-4.829474	-2.439636	1.540891
H	0.394783	-2.594016	-0.033464
H	0.884137	-2.522563	-1.728968
C	2.749860	-1.166233	-0.246503

H	3.218575	-1.675417	-1.097476
H	2.740575	-1.891158	0.579375
C	3.594423	0.042142	0.167928
O	4.857853	-0.452321	0.619443
C	5.914928	0.511231	0.570781
H	5.589376	1.427156	1.071207
H	3.732585	0.685991	-0.709971
C	2.879874	0.820277	1.279793
H	3.423230	1.741565	1.517284
H	2.890304	0.212182	2.193302
O	6.273259	0.890551	-0.766457
C	6.765051	-0.188373	-1.566339
C	7.059770	0.371854	-2.954236
H	6.160594	0.835469	-3.375377
H	7.400749	-0.408792	-3.641447
H	7.822358	1.156106	-2.906010
H	5.974848	-0.941490	-1.679008
C	8.011841	-0.818558	-0.938005
H	8.855628	-0.117150	-0.962506
O	8.390767	-1.968857	-1.691077
H	9.134112	-2.384599	-1.217876
C	7.721993	-1.232173	0.505699
O	8.932974	-1.694479	1.105851
H	8.740315	-1.895622	2.037144
H	7.027497	-2.081882	0.509884
C	7.137715	-0.061419	1.308144
O	8.155254	0.943205	1.434947
C	7.968947	1.793074	2.558989
H	7.988373	1.211062	3.485294
H	7.032549	2.351085	2.484245
H	8.795493	2.508931	2.584207
H	6.862026	-0.431654	2.303309

NMR-Shifts
Revised-MandelalideA-0006-NMR.txt

Atom	Type	Isotropic	Scaled Shift
1	C	98.2938	84.0044794119
2	C	112.0644	70.8240969391
3	C	153.5017	31.1628285381
6	C	103.6042	78.9216868623
8	C	119.9206	63.3046191543
14	C	13.6893	164.982771493
16	C	58.5699	122.025785333
18	C	29.5513	149.800627883
20	C	144.1439	40.1195466988
23	C	113.1067	69.8264706445
29	C	149.4455	35.0451769751
32	C	147.7802	36.6391010548
34	C	172.0292	13.4294301193
38	C	102.8741	79.6204942667
42	C	112.9891	69.9390302265
44	C	140.8443	43.2777235399
45	C	147.8868	36.5370700052
47	C	167.3096	17.9467447692
51	C	38.8906	140.8616168
53	C	57.0229	123.506479833
55	C	50.5876	129.665958384
57	C	52.2219	128.101705622
59	C	153.7965	30.8806638718
64	C	145.2447	39.0659277551
67	C	115.3164	67.7114799288
69	C	89.6455	92.2821072379
72	C	148.4968	35.9532150309
76	C	117.9741	65.1676908057
77	C	167.7980	17.4792779341
82	C	111.4826	71.380960585
86	C	110.3907	72.4260609889
90	C	100.9750	81.4381975153
92	C	128.6793	54.9213231494
4	H	29.1894	2.45155925156
5	H	30.5703	1.17560637561
7	H	27.3403	4.16012936013
10	H	31.6590	0.169646569647
11	H	27.1556	4.33079233079
12	H	27.9735	3.57505197505
17	H	25.3621	5.98798798799
19	H	24.2200	7.04328944329
21	H	29.2660	2.38078078078
22	H	29.3762	2.27895587896
24	H	28.0433	3.51055671056
26	H	29.8286	1.86093786094
27	H	27.8567	3.68297528298
28	H	27.9371	3.60868560869
30	H	30.5618	1.18346038346
31	H	30.0218	1.68242088242
33	H	29.2860	2.3623007623
35	H	30.7736	0.987756987757
36	H	30.6152	1.13411873412
37	H	31.0919	0.693647493647
39	H	27.7724	3.76086856087
43	H	28.2669	3.30395010395
46	H	29.0624	2.56890736891
48	H	30.7599	1.00041580042
49	H	31.2167	0.578332178332
50	H	30.3028	1.42277662278
52	H	25.9129	5.47904827905
54	H	25.0359	6.2893970894
56	H	25.4154	5.93873873874
58	H	26.1769	5.23511203511
60	H	29.9815	1.71965811966
61	H	29.4586	2.20281820282
62	H	30.2131	1.50565950566
63	H	30.5182	1.22374682375
65	H	30.0133	1.69027489027
66	H	30.6009	1.14733194733
70	H	26.2886	5.1319011319
71	H	27.6319	3.89069069069
73	H	29.7038	1.97625317625
74	H	30.7749	0.986555786556
78	H	30.5972	1.15075075075
79	H	30.1214	1.59039039039
80	H	30.8251	0.940170940171
81	H	27.8985	3.64435204435
83	H	27.9566	3.59066759067
85	H	29.9323	1.76511896512
88	H	31.5054	0.311573111573
89	H	27.5770	3.94141834142
93	H	28.8216	2.79140679141
94	H	28.3849	3.19491799492
95	H	28.2698	3.30127050127
96	H	28.5324	3.05862785863

Supporting Information: Revised-MandelalideA-0007.log

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 Using  Gaussian 09:  AM64L-G09RevC.01 23-Sep-2011
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density=current
 SCRF=(PCM,SOLVENT=Chloroform)
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#Atoms= 96
 Charge = 0                Multiplicity = 1
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 SCF Energy= -2116.32301083
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Optimization incomplete.

Atomic Type	Coordinates (Angstroms) X	Y	Z
C	6.765902	-0.553587	-0.047132
C	5.736867	0.531058	0.290049
C	6.111369	1.893787	-0.311656
H	6.179351	1.797811	-1.402138
H	7.099433	2.188174	0.062293
C	5.098917	3.004042	0.025207
H	5.013865	3.084488	1.116373
C	5.538440	4.349108	-0.560964
O	6.759568	4.788117	0.016504
H	6.618984	4.858535	0.976576
H	4.780412	5.121557	-0.393306
H	5.673738	4.274822	-1.645769
O	3.828274	2.635948	-0.552250
C	2.713058	3.167139	0.016426
O	2.665426	3.931821	0.966058
C	1.545246	2.649048	-0.727607
H	1.720351	1.979784	-1.562145
C	0.305072	2.992085	-0.353120
H	0.150192	3.658069	0.492103
C	-0.937694	2.488842	-1.039999
H	-0.670007	1.976515	-1.973337
H	-1.555224	3.354076	-1.307745
C	-1.722553	1.537429	-0.129173
H	-1.877191	2.008373	0.851125
O	5.676804	0.665083	1.712458
H	5.504880	-0.221978	2.073838
H	4.740505	0.218813	-0.042884
H	7.730603	-0.313699	0.417293
C	6.940732	-0.824582	-1.530800
H	5.978509	-0.774039	-2.054598
H	7.628970	-0.120676	-2.008654
C	7.466369	-2.244600	-1.517086
H	8.517326	-2.209322	-1.195923
C	7.417072	-2.924744	-2.872825
H	7.740168	-3.967568	-2.796236
H	8.084967	-2.416430	-3.578118
H	6.411695	-2.904756	-3.306163
C	6.655841	-2.884428	-0.383493
H	7.281215	-3.609648	0.150575
O	6.347035	-1.806785	0.530576
O	-0.941967	0.349253	0.039811
C	-1.530331	-0.573427	0.958501
H	-1.687556	-0.070388	1.920140
C	-0.560439	-1.747947	1.153127
C	0.865533	-1.331049	1.573214
H	1.284775	-0.675443	0.797385
C	0.890114	-0.559888	2.894556
H	1.918765	-0.359663	3.213777
H	0.392981	-1.119735	3.694392
H	0.389813	0.408704	2.796585
C	1.732532	-2.562765	1.698253
H	1.438190	-3.289471	2.453548
C	2.814437	-2.792223	0.937958
H	3.099408	-2.058891	0.189893
C	3.630428	-3.975628	1.079855
H	3.338308	-4.668609	1.868251
C	4.715545	-4.298173	0.355093
H	5.220604	-5.228018	0.613744
C	5.331630	-3.543221	-0.795219
H	5.498737	-4.273366	-1.594563
H	4.639661	-2.791930	-1.190267
H	-0.483773	-2.299313	0.205229
H	-0.983903	-2.443905	1.889932
C	-2.876750	-1.052122	0.408821
H	-3.349192	-1.750205	1.108996
H	-2.728903	-1.608543	-0.526561
C	-3.799885	0.138436	0.126773
O	-4.964339	-0.287773	-0.583428
C	-6.013054	-0.789688	0.248701
H	-5.582492	-1.336640	1.092450
H	-4.083723	0.622760	1.069546
C	-3.070245	1.162925	-0.747219
H	-3.699977	2.050527	-0.884766
H	-2.922274	0.733567	-1.747991
O	-6.805461	-1.766416	-0.448467
C	-7.498623	-1.252327	-1.588857
C	-8.244756	-2.422597	-2.224050
H	-7.550274	-3.240423	-2.444921
H	-8.741272	-2.132606	-3.154275
H	-8.995142	-2.826160	-1.535507
H	-6.766408	-0.894553	-2.324539
C	-8.448556	-0.114956	-1.191676
H	-9.274931	-0.484773	-0.571959
O	-9.018029	0.490915	-2.351588
H	-9.641462	-0.145180	-2.741706
C	-7.679339	0.960760	-0.423873
O	-8.581932	1.955853	0.059108
H	-9.105316	2.258078	-0.702509
H	-6.984140	1.474455	-1.098990
C	-6.908940	0.355635	0.755656
O	-7.861115	-0.154530	1.703028
C	-7.350186	-0.225486	3.027077
H	-7.074360	0.771742	3.382581
H	-6.491137	-0.897202	3.085554
H	-8.138981	-0.616969	3.676074
H	-6.325393	1.156234	1.225733

NMR-Shifts

Revised-MandelalideA-0007-NMR.txt

Atom	Type	Isotropic	Scaled Shift
1	C	98.0026	84.2831983767
2	C	111.4624	71.4002947989
3	C	149.6853	34.8156549704
6	C	114.0290	68.9437010663
8	C	120.6664	62.5907846628
14	C	14.1176	164.572828729
16	C	56.3610	124.140010337
18	C	27.3447	151.912651467
20	C	143.0310	41.1847470281
23	C	110.5640	72.2601887479
29	C	148.8569	35.6085491682
32	C	147.7454	36.6724095025
34	C	171.5970	13.8431057256
38	C	102.0082	80.4492811884
42	C	113.4376	69.5097532495
44	C	141.2046	42.9328662494
45	C	147.9784	36.4493960451
47	C	168.4121	16.8914986887
51	C	37.7862	141.918681445
53	C	57.3982	123.147265453
55	C	50.5681	129.6846226
57	C	51.1767	129.102107621
59	C	153.3370	31.3204693811
64	C	147.0560	37.3322613373
67	C	112.6293	70.2834089473
69	C	87.8173	94.0319493099
72	C	145.3096	39.0038094144
76	C	115.8269	67.2228603151
77	C	168.6555	16.6585309826
82	C	108.6543	74.088037673
86	C	113.6516	69.3049254388

90	C	106.2737	76.3666034955
92	C	129.4623	54.1718830759
4	H	30.3035	1.42212982213
5	H	29.6363	2.03862323862
7	H	26.7911	4.66759066759
10	H	31.5522	0.26832986833
11	H	27.6027	3.91767151767
12	H	28.6813	2.92104412104
17	H	25.4577	5.89965349965
19	H	24.1953	7.06611226611
21	H	29.3690	2.28560868561
22	H	29.4056	2.25179025179
24	H	28.3686	3.20997920998
26	H	29.9598	1.73970893971
27	H	27.8123	3.724000924
28	H	27.8898	3.65239085239
30	H	30.5303	1.21256641257
31	H	29.9415	1.75661815662
33	H	29.2818	2.36618156618
35	H	30.7535	1.00632940633
36	H	30.5610	1.1841995842
37	H	31.0351	0.746130746131
39	H	27.7441	3.78701778702
43	H	28.5028	3.08597828598
46	H	29.1662	2.472996073
48	H	30.9830	0.794271194271
49	H	31.3369	0.467267267267
50	H	30.5806	1.16608916609
52	H	25.9758	5.42092862093
54	H	25.0948	6.23497343497
56	H	25.4589	5.89854469854
58	H	26.1773	5.23474243474
60	H	29.8790	1.81436821437
61	H	29.4283	2.23081543082
62	H	30.1802	1.53605913606
63	H	30.5822	1.16461076461
65	H	29.6945	1.98484638485
66	H	30.6998	1.05594825595
70	H	26.6067	4.83797643798
71	H	28.2460	3.32326172326
73	H	29.9961	1.70616770617
74	H	30.4649	1.272996073
78	H	30.5277	1.21496881497
79	H	30.5302	1.21265881266
80	H	30.9503	0.824486024486
81	H	28.0297	3.52312312312
83	H	28.0963	3.46158466158
85	H	30.6282	1.12210672211
88	H	29.8549	1.83663663664
89	H	27.5834	3.9355047355
93	H	28.7339	2.87244167244
94	H	28.4543	3.13079233079
95	H	28.3141	3.26033726034
96	H	28.0598	3.49531069531

Supporting Information: Revised-MandelalideA-0008.log

Using Gaussian 09: AM64L-G09RevC.01 23-Sep-2011

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#mPW1PW91/6-311G(2d,p) scf=(maxcycle=300,direct,tight) NMR density=current

SCRF=(PCM,SOLVENT=Chloroform)

Pointgroup= C1 Stoichiometry= C33H52O11 C1[X(C33H52O11)] #Atoms= 96

Charge = 0 Multiplicity = 1

SCF Energy= -2116.32257114

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Optimization incomplete.

Atomic Type	Coordinates (Angstroms) X	Y	Z
C	-6.506534	-0.508738	0.348169
C	-5.538003	0.526763	-0.232926
C	-5.782711	1.935793	0.328829
H	-5.600057	1.925073	1.410553
H	-6.833974	2.205731	0.168916
C	-4.891521	3.010591	-0.319936
H	-5.078427	3.009326	-1.400155
C	-5.189364	4.403702	0.241330
O	-6.515518	4.810052	-0.062019
H	-6.609891	4.797427	-1.029750
H	-4.495196	5.144755	-0.170840
H	-5.058353	4.421839	1.328553
O	-3.514216	2.696762	-0.028278
C	-2.598505	2.971776	-0.991702
O	-2.817504	3.439789	-2.101084
C	-1.240030	2.575857	-0.564483
H	-0.560405	2.331986	-1.373110
C	-0.845366	2.563857	0.717977
H	-1.546636	2.867568	1.492846
C	0.515175	2.160191	1.238173
H	0.337730	1.543710	2.130171
H	1.033891	3.067318	1.571736
C	1.411473	1.368561	0.274144
H	1.561289	1.937932	-0.652485
O	-5.726201	0.561984	-1.650774
H	-5.625151	-0.351165	-1.972964
H	-4.502275	0.214459	-0.056955
H	-7.532380	-0.279097	0.030855
C	-6.442203	-0.675104	1.854685
H	-5.404954	-0.633210	2.209857
H	-7.019515	0.086142	2.388311
C	-7.008542	-2.070694	2.022716
H	-8.095163	-2.011625	1.872274
C	-6.760991	-2.664976	3.397840
H	-7.130525	-3.694499	3.447851
H	-7.285296	-2.083188	4.162989
H	-5.698037	-2.665939	3.659762
C	-6.412371	-2.814700	0.819931
H	-7.143328	-3.536268	0.434258
O	-6.203042	-1.808480	-0.197754
O	0.743390	0.139617	-0.021078
C	1.426123	-0.650238	-0.996281
H	1.564781	-0.056202	-1.908173
C	0.548584	-1.872414	-1.304460
C	-0.870195	-1.502858	-1.793065
H	-1.307338	-0.771821	-1.100031
C	-0.857102	-0.863228	-3.182939
H	-1.877326	-0.668424	-3.533235
H	-0.367485	-1.511564	-3.918272
H	-0.329621	0.095629	-3.172740
C	-1.745113	-2.734740	-1.808382
H	-1.501537	-3.507613	-2.533639
C	-2.781506	-2.900223	-0.970099
H	-3.002251	-2.117552	-0.251147
C	-3.631903	-4.066740	-0.980300
H	-3.448290	-4.791693	-1.772400
C	-4.633539	-4.328778	-0.123063
H	-5.193623	-5.248902	-0.285005
C	-5.072109	-3.519573	1.071465

H	-5.164049	-4.220725	1.909476
H	-4.308741	-2.788600	1.355187
H	0.450904	-2.466567	-0.385367
H	1.049847	-2.509788	-2.044505
C	2.788099	-1.064423	-0.438866
H	3.347263	-1.657167	-1.172856
H	2.656353	-1.708362	0.440655
C	3.604375	0.165903	-0.027578
O	4.784401	-0.302592	0.629080
C	5.864409	0.635383	0.630721
H	5.503136	1.598918	1.001688
H	3.872271	0.722117	-0.935342
C	2.772848	1.056615	0.903869
H	3.306445	1.985682	1.131290
H	2.639288	0.534778	1.860286
O	6.400725	0.885760	-0.677193
C	6.960359	-0.269712	-1.306619
C	7.443734	0.154934	-2.690537
H	6.619001	0.591859	-3.263259
H	7.848430	-0.689657	-3.255330
H	8.216218	0.928980	-2.613428
H	6.170668	-1.018595	-1.453869
C	8.099384	-0.858675	-0.469394
H	8.957835	-0.176275	-0.447347
O	8.539690	-2.080274	-1.061591
H	9.204807	-2.461991	-0.461631
C	7.617500	-1.133839	0.955695
O	8.728894	-1.557209	1.745917
H	8.414070	-1.668244	2.659117
H	6.905532	-1.967834	0.945554
C	6.967629	0.115236	1.567983
O	7.987935	1.110890	1.735355
C	7.682730	2.065952	2.743366
H	7.563518	1.573343	3.712623
H	6.781286	2.630680	2.494601
H	8.519542	2.765900	2.813442
H	6.558400	-0.157733	2.548755

NMR-Shifts

Revised-MandelalideA-0008-NMR.txt

Atom	Type	Isotropic	Scaled Shift
1	C	97.7587	84.5166446525
2	C	111.3889	71.4706445376
3	C	149.8851	34.6244185379
6	C	114.8485	68.1593254082
8	C	119.8100	63.4104787611
14	C	12.6964	165.933115106
16	C	57.6001	122.954019028
18	C	33.1440	146.361913513
20	C	145.1505	39.1560902774
23	C	114.0568	68.9170925937
29	C	149.1671	35.3116445567
32	C	147.7016	36.7143322039
34	C	171.7508	13.695897701
38	C	102.4850	79.9929171692
42	C	113.1999	69.7372652616
44	C	140.1508	43.9414996459
45	C	148.2902	36.1509600107
47	C	168.0333	17.2540630563
51	C	37.8896	141.819713241
53	C	56.9275	123.597790922
55	C	50.8866	129.379773732
57	C	51.8430	128.464365704
59	C	153.1724	31.4780145102
64	C	145.2599	39.0513792377
67	C	115.3238	67.704397098
69	C	89.6765	92.2524359195
72	C	148.7150	35.7443672352
76	C	117.9500	65.1907578629
77	C	167.8539	17.4257738471
82	C	111.5077	71.3569363885
86	C	110.4383	72.3805011581
90	C	100.9135	81.4970615823
92	C	128.8020	54.803882157
4	H	30.2847	1.4395010395
5	H	29.6698	2.00766920767
7	H	26.5758	4.86652806653
10	H	31.5594	0.261677061677
11	H	27.8367	3.70145530146
12	H	28.5736	3.02055902056
17	H	25.5580	5.80697620698
19	H	24.6074	6.68533148533
21	H	29.3156	2.33495033495
22	H	29.3713	2.28348348348
24	H	28.0016	3.54908754909
26	H	29.9842	1.71716331716
27	H	27.8701	3.67059367059
28	H	27.8894	3.65276045276
30	H	30.5738	1.17237237237
31	H	29.9699	1.73037653038
33	H	29.2651	2.38161238161
35	H	30.7324	1.02582582583
36	H	30.5948	1.15296835297
37	H	31.0558	0.727003927004
39	H	27.7096	3.8188958189
43	H	28.2819	3.29009009009
46	H	29.0613	2.56992376992
48	H	30.8533	0.914114114114
49	H	31.2506	0.547008547009
50	H	30.4185	1.31586971587
52	H	25.9213	5.47128667129
54	H	25.0632	6.26417186417
56	H	25.4333	5.9221991222
58	H	26.1721	5.23954723955
60	H	29.8994	1.79551859552
61	H	29.4693	2.19293139293
62	H	30.2864	1.43793023793
63	H	30.4993	1.24121044121
65	H	30.0141	1.68953568954
66	H	30.6642	1.08884268884
70	H	26.2842	5.13596673597
71	H	27.6215	3.9003003003
73	H	29.7012	1.97865557866
74	H	30.7834	0.978701778702
78	H	30.6085	1.14030954031
79	H	30.1418	1.57154077154
80	H	30.8032	0.960406560407
81	H	27.8900	3.65220605221
83	H	27.9545	3.59260799261
85	H	29.9542	1.74488334488
88	H	31.4714	0.342989142989
89	H	27.5685	3.94927234927
93	H	28.8431	2.77154077154
94	H	28.3815	3.19805959806
95	H	28.2756	3.29591129591
96	H	28.5599	3.03321783322

Supporting Information: Revised-MandelalideA-0009.log

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 Using  Gaussian 09:  AM64L-G09RevC.01 23-Sep-2011
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 #mPW1PW91/6-311G(2d,p) scf=(maxcycle=300,direct,tight) NMR
density=current
 SCRF=(PCM,SOLVENT=Chloroform)
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 Pointgroup= C1   Stoichiometry= C33H52O11   C1[X(C33H52O11)]
#Atoms= 96
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Charge = 0 Multiplicity = 1

SCF Energy= -2116.32628733

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Optimization incomplete.

Atomic Type	Coordinates (Angstroms) X	Y	Z
C	6.579007	-0.543511	-0.374115
C	5.647633	0.544362	0.176306
C	5.909329	1.920739	-0.458375
H	5.776965	1.841160	-1.543661
H	6.947779	2.214988	-0.264229
C	4.978619	3.019068	0.085945
H	5.041619	3.046131	1.180216
C	5.344165	4.398480	-0.472729
O	5.331852	4.398432	-1.895952
H	4.455009	4.084933	-2.176478
H	6.346196	4.694145	-0.145216
H	4.634705	5.163264	-0.138683
O	3.630293	2.688802	-0.319224
C	2.614441	3.192142	0.431942
O	2.711014	3.905912	1.416700
C	1.346309	2.718104	-0.162733
H	1.393092	2.084509	-1.041840
C	0.175618	3.056113	0.395567
H	0.150866	3.686141	1.281448
C	-1.156836	2.594714	-0.132648
H	-1.028128	2.118415	-1.112696
H	-1.791473	3.477515	-0.278589
C	-1.827081	1.616293	0.838709
H	-1.842290	2.050479	1.847282
O	5.843443	0.640419	1.590643
H	6.781715	0.838746	1.751261
H	4.604892	0.243451	0.028627
H	7.616016	-0.335995	-0.078651
C	6.491164	-0.754595	-1.875999
H	5.454773	-0.672797	-2.223646
H	7.099484	-0.039983	-2.437677
C	6.986427	-2.180056	-2.008374
H	8.077084	-2.170009	-1.869159
C	6.694968	-2.801751	-3.361883
H	7.242334	-2.273375	-4.148760
H	5.631691	-2.752753	-3.615741
H	7.007120	-3.850935	-3.381980
C	6.368077	-2.856647	-0.778757
H	7.059316	-3.614369	-0.389650
O	6.243950	-1.814676	0.216216
O	-1.048190	0.413140	0.856961
C	-1.513950	-0.534672	1.821245
H	-1.531086	-0.060602	2.810438
C	-0.538885	-1.721742	1.845306
C	0.935118	-1.327480	2.083877
H	1.251486	-0.645162	1.283775
C	1.145124	-0.607926	3.417253
H	0.754730	-1.196323	4.256030
H	0.645279	0.365965	3.424738
H	2.210040	-0.424166	3.601767
C	1.798943	-2.568525	2.043313
H	1.610810	-3.318355	2.808862
C	2.759145	-2.774326	1.129098
H	2.939017	-2.016059	0.373012
C	3.580276	-3.963145	1.112589
H	3.405835	-4.677346	1.914963
C	4.542014	-4.263341	0.222793
H	5.074389	-5.202061	0.374860
C	4.978927	-3.477867	-0.986489
H	4.996568	-4.180887	-1.827454
H	4.249828	-2.701208	-1.237764
H	-0.594950	-2.240449	0.878182
H	-0.866834	-2.438951	2.608604
C	-2.929122	-0.990312	1.449946
H	-3.324687	-1.688511	2.196340
H	-2.899657	-1.537290	0.501538
C	-3.859976	0.221100	1.317354
O	-5.195995	-0.164296	0.996062
C	-5.461706	-0.577042	-0.345318
H	-4.600098	-1.112532	-0.751704
H	-3.937869	0.673568	2.315035
C	-3.251971	1.279927	0.390000
H	-3.883393	2.175541	0.374390
H	-3.220390	0.895568	-0.636129
O	-5.698938	0.524995	-1.234882
C	-6.832515	1.323210	-0.885603
C	-6.907627	2.468957	-1.890284
H	-7.038673	2.087364	-2.909213
H	-5.971979	3.039209	-1.886643
H	-7.730118	3.153588	-1.662487
H	-6.670419	1.767154	0.104738
C	-8.115218	0.485576	-0.889797
H	-8.363874	0.162402	-1.907615
O	-9.202566	1.279506	-0.416778
H	-9.973170	0.690292	-0.338902
C	-7.946591	-0.733667	0.018270
O	-9.091847	-1.578961	-0.099816
H	-9.054206	-1.992905	-0.979952
H	-7.909525	-0.409266	1.065319
C	-6.678265	-1.520035	-0.336688
O	-6.872132	-2.095754	-1.639127
C	-6.068282	-3.243938	-1.872099
H	-6.299397	-4.026940	-1.143661
H	-5.004215	-2.998048	-1.835748
H	-6.298982	-3.624341	-2.870985
H	-6.553966	-2.322307	0.401342

NMR-Shifts

Revised-MandelalideA-0009-NMR.txt

Atom	Type	Isotropic	Scaled Shift
1	C	96.2249	85.984704914
2	C	109.2382	73.5291640345
3	C	147.2187	37.1765347729
6	C	113.4014	69.5444016922
8	C	119.0177	64.1688202301
14	C	14.4460	164.258504183
16	C	56.6284	123.884071288
18	C	26.5623	152.661517257
20	C	142.6757	41.5248186221
23	C	109.7722	73.0180516472
29	C	148.2723	36.1680928042
32	C	147.5605	36.8493845594
34	C	171.7418	13.7045119547
38	C	102.4470	80.0292884626
42	C	112.7809	70.1383066291
44	C	140.9254	43.2000995425
45	C	147.6812	36.7338578457
47	C	168.4559	16.8495759873
51	C	38.2916	141.434943242
53	C	57.3738	123.170619652
55	C	50.7851	129.476923371
57	C	51.8030	128.502651276
59	C	153.1716	31.4787802217
64	C	148.3729	36.0718045904
67	C	109.9825	72.816765252
69	C	90.7685	91.2072398017

72	C	144.9535	39.3446467199
76	C	118.1156	65.0322555945
77	C	167.6224	17.6473515956
82	C	108.9818	73.7745745516
86	C	111.6245	71.245142518
90	C	101.5703	80.8684124888
92	C	128.8671	54.7415723884
4	H	29.4770	2.18581658582
5	H	30.7553	1.00466620467
7	H	26.4017	5.0273966274
10	H	31.0188	0.761191961192
11	H	28.3950	3.18558558559
12	H	27.4491	4.0595980596
17	H	25.4000	5.95296835297
19	H	24.1284	7.12792792793
21	H	29.3333	2.3185955186
22	H	29.3262	2.32515592516
24	H	28.4542	3.13088473088
26	H	32.2926	-0.4158004158
27	H	28.2715	3.2996996997
28	H	28.0470	3.50713790714
30	H	30.5359	1.20739200739
31	H	29.9183	1.77805497805
33	H	29.2881	2.36036036036
35	H	30.5844	1.16257796258
36	H	31.0569	0.725987525988
37	H	30.7120	1.04467544468
39	H	27.7654	3.76733656734
43	H	28.4358	3.14788634789
46	H	29.1947	2.44666204666
48	H	31.3244	0.478817278817
49	H	30.6092	1.13966273966
50	H	30.8660	0.902379302379
52	H	26.0158	5.38396858397
54	H	25.0662	6.2613998614
56	H	25.4682	5.88995148995
58	H	26.1887	5.22420882421
60	H	29.8850	1.80882420882
61	H	29.4622	2.19949179949
62	H	30.2280	1.49189189189
63	H	30.5921	1.15546315546
65	H	30.2483	1.47313467313
66	H	30.4125	1.32141372141
70	H	26.2850	5.13522753523
71	H	27.7993	3.73601293601
73	H	29.7993	1.88801108801
74	H	29.9454	1.75301455301
78	H	30.9082	0.863386463386
79	H	30.6659	1.08727188727
80	H	30.1762	1.53975513976
81	H	27.8767	3.6644952645
83	H	28.3760	3.20314160314
85	H	29.7814	1.90455070455
88	H	30.3077	1.41824901825
89	H	28.0584	3.4966042966
93	H	28.7480	2.85941325941
94	H	28.3449	3.23187803188
95	H	28.2744	3.29702009702
96	H	28.3443	3.23243243243

Mandelalide A Original Configuration (MM Methoudaligies)

Supporting Information: Original-MandelalideA0001.log

Using Gaussian 09: AM64L-G09RevC.01 23-Sep-2011

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#mPW1PW91/6-311+G(2d,p) scf=(maxcycle=300,direct,tight) NMR density=current SCRF=(PCM,SOLVENT=Chloroform)

Pointgroup= C1 Stoichiometry= C33H52O11 C1[X(C33H52O11)]

#Atoms= 96

Charge = 0 Multiplicity = 1

SCF Energy= -2116.36754488

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Optimization incomplete.

Atomic Type	Coordinates (Angstroms) X	Y	Z
C	-6.594542	0.337561	1.298058
C	-5.303967	1.099484	0.980107
C	-5.534874	2.555681	0.552090
H	-6.107612	3.081091	1.326129
H	-6.132356	2.564826	-0.367545
C	-4.218527	3.316189	0.300115
H	-3.692086	3.416310	1.258788
C	-4.472303	4.703535	-0.291782
O	-5.214145	5.501603	0.618129
H	-5.333322	6.372798	0.203136
H	-5.024259	4.628882	-1.235713
H	-3.525619	5.208919	-0.508637
O	-3.429472	2.542533	-0.627715
C	-2.077582	2.655994	-0.541730
O	-1.447824	3.420584	0.170849
C	-1.489491	1.660979	-1.464527
H	-2.154952	0.966938	-1.965725
C	-0.164281	1.626904	-1.657210
H	0.475193	2.348224	-1.154779
C	0.513186	0.648305	-2.579374
H	1.012362	1.220605	-3.370924
H	-0.244894	0.022979	-3.069532
C	1.539203	-0.277383	-1.904600
H	1.959549	-0.913884	-2.696202
O	-4.484625	1.092546	2.152112
H	-4.369737	0.161930	2.413463
H	-4.747420	0.560726	0.204770
H	-7.023837	0.695645	2.241709
C	-7.647965	0.348866	0.199733
H	-8.359925	1.172213	0.317345
H	-7.189813	0.446025	-0.791683
C	-8.289253	-1.015951	0.361562
H	-8.941143	-0.979905	1.245616
C	-9.125632	-1.445802	-0.831014
H	-9.993170	-0.786247	-0.944370
H	-9.493607	-2.467300	-0.696816
H	-8.559755	-1.403835	-1.767265
C	-7.081384	-1.891010	0.701074
H	-7.388990	-2.752679	1.305390
O	-6.245255	-1.047677	1.518930
O	0.863329	-1.129167	-0.971643
C	1.721574	-2.135212	-0.424808
H	2.135170	-2.733357	-1.247008
C	0.919716	-3.062999	0.506063
C	-0.093117	-3.977007	-0.229080
H	0.347739	-4.285300	-1.188002
C	-0.291359	-5.265764	0.584282
H	-0.678099	-5.054784	1.586970
H	0.660353	-5.797378	0.700225
H	-0.981532	-5.951371	0.080414
C	-1.382898	-3.248173	-0.556980
H	-1.279399	-2.419291	-1.255090

C	-2.613822	-3.541465	-0.105162
H	-2.766488	-4.370175	0.579661
C	-3.793785	-2.801283	-0.490450
H	-3.650063	-1.932466	-1.129464
C	-5.035811	-3.141052	-0.104803
H	-5.190806	-4.014829	0.524761
C	-6.265537	-2.375623	-0.511913
H	-5.974255	-1.524213	-1.137614
H	-6.882377	-3.037712	-1.130001
H	0.389824	-2.465459	1.260441
H	1.638141	-3.693890	1.045222
C	2.862167	-1.465913	0.347318
H	3.541824	-2.216366	0.770614
H	2.461188	-0.899496	1.198209
C	3.646854	-0.514909	-0.557264
O	4.599395	0.168631	0.259980
C	5.724598	0.680467	-0.461164
H	5.369739	1.257061	-1.318985
H	4.161450	-1.106492	-1.325410
C	2.679845	0.474169	-1.212426
H	3.204977	1.114060	-1.928832
H	2.294858	1.137295	-0.427669
O	6.572150	-0.350028	-0.991168
C	7.157062	-1.192361	0.005762
C	7.982082	-2.250487	-0.719471
H	8.781141	-1.787990	-1.308813
H	7.353527	-2.804599	-1.425125
H	8.429515	-2.964528	-0.020473
H	6.359419	-1.716182	0.547824
C	8.015593	-0.380685	0.980705
H	8.904777	0.015892	0.475166
O	8.467195	-1.229697	2.033509
H	8.918838	-0.663760	2.683266
C	7.197186	0.768482	1.572380
O	8.047198	1.599822	2.365049
H	8.632140	2.080882	1.752511
H	6.438744	0.365573	2.254159
C	6.530878	1.602429	0.470501
O	7.572142	2.267371	-0.261980
C	7.126663	3.439043	-0.932719
H	6.372187	3.200406	-1.686438
H	7.985710	3.889735	-1.437799
H	6.728797	4.162563	-0.216254
H	5.884774	2.349681	0.948322

NMR-Shifts
Original-MandelalideA0001-NMR.txt

Atom	Type	Isotropic	Scaled Shift
1	C	97.3858	84.8735618982
2	C	109.6486	73.136354065
3	C	150.8218	33.7278661536
6	C	115.2913	67.7355041253
8	C	120.5362	62.7154041999
14	C	13.2431	165.409847049
16	C	55.2719	125.182430751
18	C	28.5027	150.804284156
20	C	144.4963	39.7822508088
23	C	108.8102	73.9388196558
29	C	150.0761	34.4416049312
32	C	146.6470	37.7237313119
34	C	172.4619	13.0152759433
38	C	102.3140	80.1565879898
42	C	104.2284	78.32424051
44	C	139.1390	44.9099331917
45	C	146.4367	37.9250177071
47	C	166.5037	18.7181033328
51	C	39.8986	139.896820383
53	C	54.0601	126.342292157
55	C	46.4240	133.651103582
57	C	48.0098	132.133272076
59	C	147.1316	37.2599016061
64	C	145.3252	38.9888780413
67	C	114.2248	68.7562931909
69	C	89.7049	92.2252531633
72	C	151.3492	33.2230708857
76	C	117.6336	65.4935967381
77	C	167.5375	17.7286127223
82	C	108.8061	73.942743927
86	C	110.8382	71.9977411512
90	C	102.8163	79.6758169184
92	C	128.6070	54.9905243209
4	H	29.7035	1.97653037653
5	H	30.2640	1.45862785863
7	H	26.4245	5.00632940633
10	H	31.0343	0.74686994687
11	H	28.2615	3.30893970894
12	H	27.5028	4.00997920998
17	H	25.1598	6.17491337491
19	H	23.9059	7.33351813352
21	H	29.2933	2.35555555556
22	H	28.8199	2.79297759298
24	H	28.0221	3.53014553015
26	H	29.7947	1.89226149226
27	H	27.7398	3.79099099099
28	H	27.7867	3.74765534766
30	H	29.8590	1.83284823285
31	H	30.4327	1.30274890275
33	H	29.3310	2.32072072072
35	H	30.6137	1.1355047355
36	H	30.7294	1.0285978286
37	H	31.1041	0.682374682375
39	H	27.6746	3.85123585124
43	H	28.3180	3.25673365673
46	H	29.4002	2.25677985678
48	H	30.6991	1.0565950566
49	H	30.8115	0.952737352737
50	H	30.6571	1.0954030954
52	H	24.9120	6.40388080388
54	H	25.5279	5.83478863479
56	H	25.0759	6.25243705244
58	H	25.9120	5.47987987988
60	H	29.8465	1.8443982444
61	H	29.6461	2.02956802957
62	H	30.2453	1.47590667591
63	H	30.3075	1.41843381843
65	H	30.0668	1.64084084084
66	H	30.5834	1.1635019635
70	H	26.4033	5.02591822592
71	H	27.6918	3.83534303534
73	H	29.6929	1.98632478632
74	H	30.3718	1.35902055902
78	H	30.8605	0.907461307461
79	H	30.5966	1.15130515131
80	H	30.1120	1.59907599908
81	H	27.9538	3.59325479325
83	H	28.3483	3.22873642874
85	H	29.6317	2.04287364287
88	H	30.0654	1.64213444213
89	H	27.8991	3.6437976438
93	H	28.2481	3.32132132132
94	H	28.1809	3.38341418341
95	H	28.6322	2.96641256641
96	H	28.2500	3.31956571957

Supporting Information: Original-MandelalideA0002.log

Using Gaussian 09: AM64L-G09RevC.01 23-Sep-2011

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#mPW1PW91/6-311+G(2d,p) scf=(maxcycle=300,direct,tight) NMR density=current SCRF=(PCM,SOLVENT=Chloroform)

Pointgroup= C1 Stoichiometry= C33H52O11 C1[X(C33H52O11)]
#Atoms= 96
Charge = 0 Multiplicity = 1

SCF Energy= -2116.37048834
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Optimization incomplete.

Atomic Type	Coordinates (Angstroms) X	Y	Z
C	-6.585181	0.394144	1.324485
C	-5.255976	1.151899	1.231466
C	-5.421118	2.531541	0.575090
H	-6.129234	3.124957	1.166743
H	-5.842999	2.398520	-0.428097
C	-4.100289	3.313946	0.465095
H	-3.610625	3.358086	1.446034
C	-4.337607	4.741075	-0.044069
O	-5.022124	4.735288	-1.291762
H	-4.493751	4.199011	-1.907861
H	-3.394053	5.276139	-0.190238
H	-4.944276	5.308017	0.669146
O	-3.249963	2.610709	-0.469932
C	-1.912448	2.850627	-0.397459
O	-1.339947	3.592207	0.383874
C	-1.259290	2.052176	-1.455991
H	-1.870448	1.376116	-2.043710
C	0.061056	2.161071	-1.663260
H	0.654096	2.847115	-1.064005
C	0.799501	1.370074	-2.711753
H	1.398721	2.061851	-3.315022
H	0.073591	0.906081	-3.392324
C	1.700876	0.264996	-2.137456
H	2.128460	-0.287086	-2.985901
O	-4.755512	1.341765	2.557754
H	-4.727265	0.463826	2.977675
H	-4.515138	0.551037	0.692793
H	-7.276927	0.928018	1.989129
C	-7.243566	0.104762	-0.013137
H	-7.807784	0.959792	-0.398040
H	-6.498575	-0.177015	-0.765764
C	-8.132450	-1.072289	0.331059
H	-9.017178	-0.669069	0.846418
C	-8.635633	-1.845918	-0.874961
H	-7.819251	-2.219866	-1.497940
H	-9.258316	-1.201831	-1.505569
H	-9.247693	-2.697234	-0.560871
C	-7.311104	-1.836274	1.376744
H	-7.987120	-2.119193	2.194299
O	-6.363399	-0.896864	1.929229
O	0.873111	-0.634597	-1.395850
C	1.571118	-1.775454	-0.887387
H	1.985031	-2.344579	-1.728858
C	0.548211	-2.629049	-0.122964
C	-0.551419	-3.215552	-1.036724
H	-0.830908	-2.469009	-1.791796
C	-0.059786	-4.463202	-1.773756
H	-0.849772	-4.877029	-2.411307
H	0.250374	-5.247440	-1.074768
H	0.792845	-4.229944	-2.418922
C	-1.768427	-3.554421	-0.209212
H	-1.617427	-4.208348	0.646367
C	-2.989820	-3.061271	-0.468775
H	-3.134079	-2.412264	-1.328755
C	-4.141396	-3.323847	0.360719
H	-3.976792	-3.884452	1.276880
C	-5.376203	-2.885554	0.060812
H	-5.541014	-2.339929	-0.863688
C	-6.567072	-3.112168	0.953074
H	-7.257444	-3.807815	0.462471
H	-6.228372	-3.615384	1.869265
H	0.075327	-1.991463	0.636426
H	1.059953	-3.439381	0.411994
C	2.699431	-1.325753	0.041661
H	3.261595	-2.188208	0.419448
H	2.283375	-0.821623	0.925002
C	3.646358	-0.360999	-0.673898
O	4.586928	0.113032	0.290568
C	5.811005	0.593239	-0.274884
H	5.582115	1.305305	-1.072525
H	4.163652	-0.906365	-1.474031
C	2.836592	0.798402	-1.260636
H	3.479983	1.468196	-1.841217
H	2.443376	1.393715	-0.427872
O	6.600215	-0.444221	-0.876323
C	7.022508	-1.459424	0.038282
C	7.803060	-2.496981	-0.761485
H	8.686300	-2.048130	-1.228573
H	7.185152	-2.892403	-1.575965
H	8.124719	-3.334044	-0.134214
H	6.138926	-1.962217	0.451303
C	7.870006	-0.865485	1.168115
H	8.829285	-0.500055	0.780299
O	8.156261	-1.881065	2.128144
H	8.603694	-1.448932	2.876815
C	7.114815	0.277200	1.848777
O	7.969360	0.913141	2.800678
H	8.643429	1.404346	2.298779
H	6.269620	-0.129384	2.417315
C	6.617375	1.304028	0.824726
O	7.770197	1.949894	0.260595
C	7.489185	3.235736	-0.275716
H	8.422804	3.657834	-0.656651
H	7.103477	3.898911	0.504738
H	6.776803	3.173540	-1.102006
H	6.004848	2.047316	1.351863

NMR-Shifts
Original-MandelalideA0002-NMR.txt

Atom	Type	Isotropic	Scaled Shift
1	C	98.1396	84.1520702923
2	C	111.4576	71.4048890676
3	C	149.8763	34.6328413637
6	C	113.3774	69.5673730355
8	C	118.4230	64.738030973
14	C	13.1325	165.515706656
16	C	54.8313	125.604146327
18	C	27.5855	151.682172323
20	C	145.7704	38.562759624
23	C	110.3934	72.4234767128
29	C	146.8738	37.5066521181
32	C	147.0538	37.3343670438
34	C	171.9605	13.4951855893
38	C	104.5674	77.9997702866
42	C	111.8789	71.0016462796
44	C	139.9837	44.1014376232
45	C	147.6656	36.7487892188
47	C	165.5084	19.6707440801
51	C	40.1850	139.622695687

53	C	51.6041	128.693026283
55	C	45.4281	134.604318613
57	C	49.6188	130.593234939
59	C	148.0626	36.3688049159
64	C	145.3455	38.9694481135
67	C	115.2016	67.8213595207
69	C	89.7302	92.201037539
72	C	150.9992	33.5580696415
76	C	117.5136	65.6084534543
77	C	167.8706	17.4097896208
82	C	108.7837	73.9641838473
86	C	111.1909	71.6601581194
90	C	102.6732	79.8127835525
92	C	128.7368	54.8662876395
4	H	30.3151	1.41141141141
5	H	29.5607	2.10847770848
7	H	26.5323	4.90672210672
10	H	31.0191	0.760914760915
11	H	27.4400	4.06800646801
12	H	28.3306	3.24509124509
17	H	25.2844	6.05978285978
19	H	23.9867	7.25885885886
21	H	29.3634	2.29078309078
22	H	28.9496	2.67313467313
24	H	28.1642	3.39884499884
26	H	29.8306	1.85908985909
27	H	28.1128	3.44633864634
28	H	27.9168	3.62744282744
30	H	29.9105	1.78526218526
31	H	30.6148	1.13448833449
33	H	29.1683	2.47105567106
35	H	30.9509	0.823931623932
36	H	30.5399	1.2036960037
37	H	30.6409	1.11037191037
39	H	27.3624	4.13970893971
43	H	28.2879	3.28454608455
46	H	29.0094	2.61787941788
48	H	30.9451	0.829290829291
49	H	31.1174	0.670085470085
50	H	30.4816	1.25756525757
52	H	25.9397	5.45428505429
54	H	25.6765	5.69748209748
56	H	25.1439	6.1896049896
58	H	25.9010	5.49004389004
60	H	29.3488	2.30427350427
61	H	29.4065	2.25095865096
62	H	30.1383	1.57477477477
63	H	30.5057	1.2352968353
65	H	30.0285	1.67623007623
66	H	30.5785	1.16802956803
70	H	26.2292	5.18678678679
71	H	27.7255	3.8042042042
73	H	29.6690	2.00840840841
74	H	30.4661	1.27188727189
78	H	30.8578	0.909956109956
79	H	30.5876	1.15962115962
80	H	30.1593	1.55537075537
81	H	27.8873	3.6547008547
83	H	28.2840	3.28814968815
85	H	29.5966	2.07530607531
88	H	30.0781	1.6303996304
89	H	28.0425	3.5112959113
93	H	28.1903	3.37472857473
94	H	28.6325	2.96613536614
95	H	28.2842	3.28796488796
96	H	28.2009	3.36493416493

Supporting Information: Original-MandelalideA0003.log

Using Gaussian 09: AM64L-G09RevC.01 23-Sep-2011

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#mPW1PW91/6-311+G(2d,p) scf=(maxcycle=300,direct,tight) NMR density=current SCRF=(PCM,SOLVENT=Chloroform)

Pointgroup= C1 Stoichiometry= C33H52O11 C1[X(C33H52O11)]

#Atoms= 96

Charge = 0 Multiplicity = 1

SCF Energy= -2116.36870147

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Optimization incomplete.

Atomic Type	Coordinates (Angstroms) X	Y	Z
C	-6.624301	0.440968	1.232857
C	-5.307592	1.213637	1.094015
C	-5.501567	2.561991	0.384449
H	-6.219991	3.163562	0.955968
H	-5.925070	2.386287	-0.612307
C	-4.200745	3.367659	0.233293
H	-3.720236	3.500722	1.209845
C	-4.502980	4.731609	-0.400369
O	-3.344948	5.558968	-0.420989
H	-2.972958	5.571482	0.478254
H	-5.279602	5.261840	0.158598
H	-4.834913	4.614868	-1.436926
O	-3.327317	2.626923	-0.650643
C	-1.986049	2.780580	-0.486828
O	-1.418840	3.457432	0.355344
C	-1.314713	1.982009	-1.533816
H	-1.921723	1.325548	-2.148821
C	0.011872	2.071247	-1.701139
H	0.596505	2.742868	-1.077625
C	0.768136	1.278222	-2.734917
H	1.368916	1.969025	-3.337892
H	0.053406	0.802816	-3.419752
C	1.670852	0.183624	-2.141671
H	2.101303	-0.380644	-2.980604
O	-4.795043	1.466293	2.405112
H	-4.744856	0.607098	2.859546
H	-4.563521	0.600947	0.572492
H	-7.316988	0.993208	1.880732
C	-7.290496	0.085459	-0.084820
H	-7.865831	0.917794	-0.502877
H	-6.548199	-0.222363	-0.830598
C	-8.165351	-1.082536	0.318971
H	-9.050879	-0.666275	0.820792
C	-8.667566	-1.915019	-0.846850
H	-9.270653	-2.757002	-0.491908
H	-7.851119	-2.310035	-1.457361
H	-9.298973	-1.306256	-1.503739
C	-7.330283	-1.790656	1.393332
H	-7.996673	-2.033826	2.230358
O	-6.380164	-0.820885	1.888625
O	0.844350	-0.706460	-1.387237
C	1.544641	-1.835235	-0.857645
H	1.958350	-2.419531	-1.687883
C	0.522352	-2.674550	-0.076173
C	-0.577907	-3.279250	-0.976424
H	-0.854328	-2.551202	-1.749241
C	-0.090479	-4.546352	-1.682359
H	0.766231	-4.332633	-2.329563
H	-0.880450	-4.971765	-2.311801

H	0.214575	-5.315626	-0.963981
C	-1.796825	-3.592031	-0.140925
H	-1.646797	-4.222223	0.733672
C	-3.015678	-3.102286	-0.412668
H	-3.159145	-2.477400	-1.291111
C	-4.165770	-3.332827	0.427815
H	-4.001169	-3.864886	1.361923
C	-5.399920	-2.897925	0.120361
H	-5.565553	-2.380678	-0.821332
C	-6.585738	-3.084965	1.026307
H	-7.277397	-3.803023	0.572117
H	-6.242140	-3.542779	1.964172
H	0.050909	-2.022519	0.671835
H	1.035073	-3.474647	0.473740
C	2.671295	-1.367290	0.064679
H	3.235665	-2.221666	0.456737
H	2.254255	-0.849227	0.939281
C	3.615550	-0.410594	-0.666581
O	4.554701	0.080905	0.291820
C	5.775828	0.558201	-0.280409
H	5.545043	1.260908	-1.085493
H	4.135816	-0.967978	-1.456689
C	2.803694	0.735803	-1.272755
H	3.445271	1.398219	-1.863948
H	2.407610	1.343148	-0.449452
O	6.568816	-0.482097	-0.869255
C	6.995389	-1.484708	0.057542
C	7.779023	-2.529736	-0.730553
H	7.163311	-2.936277	-1.539615
H	8.103589	-3.357551	-0.093126
H	8.661375	-2.082221	-1.202607
H	6.113598	-1.986661	0.476699
C	7.840115	-0.874846	1.179590
H	8.798245	-0.510910	0.788588
O	8.130842	-1.877296	2.151586
H	8.575602	-1.435076	2.895384
C	7.081443	0.273016	1.847318
O	7.933437	0.922442	2.791442
H	8.605862	1.410377	2.284314
H	6.238226	-0.130470	2.420816
C	6.579841	1.286425	0.811159
O	7.731027	1.929000	0.239199
C	7.443520	3.208273	-0.311001
H	6.731102	3.133490	-1.136447
H	8.376007	3.629224	-0.697791
H	7.055862	3.878572	0.461915
H	5.965018	2.032057	1.329969

NMR-Shifts

Original-MandelalideA0003-NMR.txt

Atom	Type	Isotropic	Scaled Shift
1	C	98.3093	83.9896437528
2	C	112.1436	70.7482915063
3	C	150.6746	33.8687570589
6	C	112.2009	70.6934474243
8	C	113.6734	69.2840598021
14	C	11.7331	166.855127395
16	C	54.2352	126.174697065
18	C	28.8698	150.452918318
20	C	145.7216	38.609468022
23	C	110.3720	72.4439594939
29	C	146.9293	37.4535308869
32	C	147.2020	37.1925189992
34	C	171.9658	13.490112751
38	C	104.6778	77.8941021076
42	C	112.0026	70.8832481479
44	C	139.8882	44.1928444266
45	C	147.8994	36.52501005
47	C	165.6160	19.5677558912
51	C	39.9279	139.868776202
53	C	51.7877	128.517295507
55	C	44.7104	135.29125749
57	C	50.1441	130.090449664
59	C	148.2814	36.1593828366
64	C	145.3462	38.968778116
67	C	115.1296	67.8902735504
69	C	89.9529	91.9878826164
72	C	151.0975	33.4639828481
76	C	117.5365	65.5865349643
77	C	167.8447	17.4345795287
82	C	108.9212	73.8325771933
86	C	111.2466	71.6068454603
90	C	102.5539	79.9269702713
92	C	128.6403	54.9586515822
4	H	30.3336	1.39431739432
5	H	30.2522	1.46953106953
7	H	26.3135	5.10889350889
10	H	31.1420	0.647355047355
11	H	27.8016	3.73388773389
12	H	28.3264	3.24897204897
17	H	25.2447	6.09646569647
19	H	24.0513	7.19916839917
21	H	29.3754	2.2796950797
22	H	28.9467	2.67581427581
24	H	28.1442	3.41732501733
26	H	29.8867	1.80725340725
27	H	28.0425	3.5112959113
28	H	28.0906	3.46685146685
30	H	30.0128	1.69073689074
31	H	30.6704	1.08311388311
33	H	29.1531	2.4851004851
35	H	30.6657	1.08745668746
36	H	30.9630	0.812751212751
37	H	30.5630	1.18235158235
39	H	27.3975	4.10727650728
43	H	28.2998	3.27355047355
46	H	29.0305	2.59838299838
48	H	30.4721	1.26634326634
49	H	30.9753	0.801386001386
50	H	31.1434	0.646061446061
52	H	25.9514	5.44347424347
54	H	25.6338	5.73693693694
56	H	25.0831	6.24578424578
58	H	25.9225	5.47017787018
60	H	29.3734	2.28154308154
61	H	29.4072	2.25031185031
62	H	30.1429	1.57052437052
63	H	30.5126	1.22892122892
65	H	30.0493	1.65701085701
66	H	30.5801	1.16655116655
70	H	26.2242	5.19140679141
71	H	27.7391	3.79163779164
73	H	29.6691	2.00831600832
74	H	30.3941	1.33841533842
78	H	30.6107	1.13827673828
79	H	30.1686	1.54677754678
80	H	30.8449	0.921875721876
81	H	27.8840	3.65775005775
83	H	28.2868	3.28556248556
85	H	29.6267	2.04749364749
88	H	30.0816	1.62716562717
89	H	28.0457	3.50833910834
93	H	28.2769	3.29471009471
94	H	28.1795	3.38470778471
95	H	28.6347	2.9641025641
96	H	28.2238	3.34377454377

Supporting Information: Original-MandelalideA0004.log

Using Gaussian 09: AM64L-G09RevC.01 23-Sep-2011
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#mPW1PW91/6-311+G(2d,p) scf=(maxcycle=300,direct,tight) NMR density=current SCRF=(PCM,SOLVENT=Chloroform)

Pointgroup= C1 Stoichiometry= C33H52O11 C1[X(C33H52O11)]
#Atoms= 96
Charge = 0 Multiplicity = 1

SCF Energy= -2116.36548697
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Optimization incomplete.

Atomic Type	Coordinates (Angstroms) X	Y	Z
C	7.382807	-0.859032	0.596955
C	7.276801	0.630071	0.235745
C	5.897867	1.239661	0.528783
H	5.782710	1.436182	1.602567
H	5.118588	0.517838	0.269815
C	5.615406	2.539166	-0.247289
H	5.913385	2.449779	-1.299331
C	6.299241	3.761763	0.364350
O	6.057540	4.905336	-0.451292
H	5.092913	4.999324	-0.536089
H	7.381432	3.634771	0.425344
H	5.910423	3.980246	1.364463
O	4.185670	2.796184	-0.195983
C	3.405466	2.126710	-1.090885
O	3.779647	1.347457	-1.951211
C	1.997694	2.499206	-0.831607
H	1.796372	3.274674	-0.101153
C	1.007752	1.878480	-1.488478
H	1.233553	1.101429	-2.214772
C	-0.448012	2.209966	-1.296787
H	-0.864718	2.468482	-2.278377
H	-0.545584	3.096418	-0.656938
C	-1.233824	1.041013	-0.684363
H	-0.691667	0.651356	0.187508
O	8.275664	1.359487	0.939660
H	9.140808	0.992588	0.689870
H	7.474296	0.732760	-0.838707
H	8.355467	-1.228032	0.243776
C	7.257618	-1.207003	2.072789
H	8.202461	-1.084324	2.611017
H	6.503423	-0.590431	2.572675
C	6.801996	-2.653198	1.994013
H	7.669913	-3.265036	1.706566
C	6.257357	-3.194777	3.303957
H	5.874323	-4.211468	3.172573
H	5.451520	-2.571952	3.703365
H	7.050084	-3.228639	4.059184
C	5.836708	-2.620185	0.801930
H	5.845091	-3.582970	0.275384
O	6.378287	-1.621904	-0.092171
O	-1.355366	0.001761	-1.664441
C	-1.999947	-1.163441	-1.147728
H	-1.448855	-1.510018	-0.264443
C	-2.010065	-2.280588	-2.208044
C	-0.633005	-2.745573	-2.745840
H	-0.809921	-3.710626	-3.242041
C	-0.110454	-1.816942	-3.850152
H	0.794776	-2.231315	-4.308443
H	0.131389	-0.816246	-3.481561
H	-0.854765	-1.707458	-4.645621
C	0.335299	-3.034420	-1.619346
H	0.005495	-3.800491	-0.918575
C	1.514677	-2.430679	-1.404528
H	1.863433	-1.658421	-2.085136
C	2.361366	-2.718027	-0.268830
H	2.022132	-3.466743	0.441630
C	3.512702	-2.059256	-0.051482
H	3.830405	-1.297976	-0.761230
C	4.385892	-2.248082	1.158326
H	4.366954	-1.302632	1.713701
H	3.958519	-3.015576	1.814160
H	-2.623362	-1.963638	-3.062058
H	-2.516442	-3.154266	-1.775581
C	-3.437099	-0.820081	-0.736040
H	-3.923086	-1.705875	-0.314462
H	-4.022691	-0.528952	-1.618191
C	-3.461423	0.332381	0.270429
O	-4.781418	0.830002	0.504331
C	-5.634899	-0.049415	1.243388
H	-5.042515	-0.580381	1.995748
H	-3.023784	0.008059	1.223271
C	-2.633132	1.501562	-0.267824
H	-2.575420	2.293872	0.487852
H	-3.156739	1.937061	-1.129238
O	-6.252086	-1.057131	0.429774
C	-7.101091	-0.537635	-0.597224
C	-7.628586	-1.725769	-1.395252
H	-6.795276	-2.314949	-1.793509
H	-8.256492	-1.405596	-2.231067
H	-8.210681	-2.398711	-0.755518
H	-6.504415	0.076943	-1.282946
C	-8.241379	0.292204	-0.000331
H	-8.931739	-0.346216	0.563634
O	-8.987091	0.899140	-1.054733
H	-9.637015	1.492921	-0.639811
C	-7.675166	1.381458	0.911564
O	-8.747312	2.056840	1.571547
H	-9.121007	1.437345	2.222179
H	-7.162137	2.137849	0.304697
C	-6.712318	0.792301	1.949145
O	-7.482311	-0.029732	2.840894
C	-6.877858	-0.197264	4.115343
H	-6.752044	0.771077	4.609172
H	-5.914165	-0.706398	4.034190
H	-7.540580	-0.813590	4.729179
H	-6.264911	1.620988	2.512163

NMR-Shifts
Original-MandelalideA0004-NMR.txt

Atom	Type	Isotropic	Scaled Shift
1	C	101.2910	81.1357414958
2	C	113.6785	69.2791783916
3	C	154.6050	30.1068167461
6	C	104.0699	78.4759470893
8	C	118.4852	64.6784969084
14	C	12.7175	165.912919466
16	C	57.2303	123.307969142
18	C	23.3903	155.697563123
20	C	142.6667	41.5334328758
23	C	107.2877	75.3960642432
29	C	151.9325	32.6647715308
32	C	146.9992	37.3866268497
34	C	172.7671	12.7231570283
38	C	100.0401	82.3330270488
42	C	110.6166	72.2098432206
44	C	142.4287	41.7612320297
45	C	148.4740	35.975037807

47	C	167.0363	18.2083309405
51	C	44.5611	135.434158387
53	C	51.4489	128.841574303
55	C	48.4932	131.670590938
57	C	47.0326	133.068588602
59	C	147.6345	36.7785562511
64	C	142.4068	41.7821933804
67	C	106.1085	76.5247229082
69	C	83.5479	98.1183598461
72	C	145.3476	38.9674381209
76	C	116.9877	66.1118130133
77	C	167.8527	17.4269224143
82	C	108.1534	74.5674687494
86	C	110.9078	71.9311242558
90	C	102.1276	80.3349987557
92	C	128.9165	54.6942897069
4	H	30.4343	1.30127050127
5	H	29.6581	2.01848001848
7	H	26.7711	4.68607068607
10	H	30.3935	1.33896973897
11	H	27.4128	4.09313929314
12	H	27.9373	3.6085008085
17	H	25.3591	5.99075999076
19	H	23.5749	7.63936243936
21	H	29.2885	2.35999075999
22	H	29.4741	2.1884961885
24	H	28.6837	2.91882651883
26	H	31.0828	0.702055902056
27	H	27.4577	4.05165165165
28	H	27.6568	3.86768306768
30	H	29.9636	1.7361977362
31	H	30.3364	1.39173019173
33	H	29.4107	2.24707784708
35	H	30.7401	1.01871101871
36	H	31.1165	0.670917070917
37	H	30.6082	1.14058674059
39	H	27.7016	3.82628782629
43	H	28.5188	3.07119427119
46	H	29.2945	2.35444675445
48	H	30.7168	1.04024024024
49	H	29.8559	1.83571263571
50	H	30.7668	0.99404019404
52	H	25.7468	5.63252483252
54	H	25.1843	6.15227535228
56	H	25.1908	6.14626934627
58	H	25.3905	5.96174636175
60	H	29.8253	1.86398706399
61	H	29.9919	1.71004851005
62	H	30.0960	1.61386001386
63	H	29.8529	1.83848463848
65	H	29.3201	2.33079233079
66	H	30.3463	1.38258258258
70	H	26.7377	4.71693231693
71	H	28.2267	3.34109494109
73	H	30.0069	1.69618849619
74	H	30.4616	1.27604527605
78	H	30.6303	1.12016632017
79	H	30.1738	1.54197274197
80	H	30.9016	0.869484869485
81	H	27.8149	3.7215985216
83	H	28.3614	3.21663201663
85	H	29.6184	2.05516285516
88	H	30.1128	1.59833679834
89	H	28.0099	3.54141834142
93	H	28.6895	2.91346731347
94	H	28.3131	3.26126126126
95	H	28.1774	3.38664818665
96	H	28.2665	3.30431970432


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 Using  Gaussian 09:  AM64L-G09RevC.01 23-Sep-2011
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 #mPW1PW91/6-311+G(2d,p) scf=(maxcycle=300,direct,tight) NMR
 density=current SCRF=(PCM,SOLVENT=Chloroform)
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 Pointgroup= C1   Stoichiometry= C33H52O11   C1[X(C33H52O11)]
#Atoms= 96
 Charge = 0                 Multiplicity = 1
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 SCF Energy= -2116.36862016
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 Optimization incomplete.


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      Type      X                Y              Z
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      C       5.876555      1.235814     -1.179247
      C       5.848279      0.015772     -0.253600
      C       5.925772     -1.306712     -1.031646
      H       6.921768     -1.384541     -1.484773
      H       5.184565     -1.306770     -1.839329
      C       5.674542     -2.527023     -0.127107
      H       6.227476     -2.406816      0.812737
      C       6.095841     -3.828110     -0.815933
      O       7.499299     -3.867906     -1.023736
      H       7.926380     -3.784607     -0.152991
      H       5.595975     -3.934458     -1.785218
      H       5.809356     -4.699600     -0.218448
      O       4.251978     -2.588510      0.120011
      C       3.828342     -3.194286      1.257037
      O       4.533256     -3.616271      2.162410
      C       2.353251     -3.323067      1.286013
      H       1.935130     -3.715940      2.208104
      C       1.558610     -3.027493      0.247470
      H       1.979747     -2.655614     -0.683517
      C       0.063566     -3.213906      0.250340
      H      -0.260593     -3.692024      1.182892
      H      -0.182727     -3.895173     -0.572719
      C      -0.664780     -1.877610      0.063030
      H      -0.163943     -1.286122     -0.715102
      O       6.987370      0.075307      0.611563
      H       6.985617      0.958312      1.021359
      H       4.959861      0.046889      0.386027
      H       6.776946      1.219694     -1.805246
      C       4.625466      1.399230     -2.027381
      H       4.640352      0.775230     -2.926156
      H       3.726143      1.147994     -1.453406
      C       4.657437      2.880409     -2.344703
      H       5.393254      3.025859     -3.149589
      C       3.336638      3.438416     -2.841608
      H       3.068686      2.978765     -3.800233
      H       3.404179      4.519593     -2.997617
      H       2.515062      3.240362     -2.149158
      C       5.253726      3.497234     -1.074312
      H       6.014529      4.228733     -1.375872
      O       5.956011      2.437675     -0.387402
      O      -0.613411     -1.163595      1.304316
      C      -1.167950      0.155028      1.202796
      H      -0.611133      0.697097      0.429652
      C      -0.968869      0.830157      2.570640
      C      -1.177571      2.359881      2.559627
      H      -2.155536      2.565829      2.109509
      C      -1.223673      2.889364      3.997755
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H	-0.279870	2.705404	4.522662
H	-2.025021	2.402225	4.564324
H	-1.415522	3.967640	4.016830
C	-0.157689	3.164430	1.778727
H	-0.504785	4.143177	1.450385
C	1.104868	2.801725	1.500255
H	1.486937	1.844284	1.842667
C	2.033617	3.644835	0.782369
H	1.659657	4.586975	0.390236
C	3.326934	3.318962	0.615234
H	3.703826	2.390394	1.038946
C	4.330621	4.204489	-0.071345
H	3.836857	5.052794	-0.559848
H	4.961932	4.623278	0.723028
H	0.026216	0.583081	2.963440
H	-1.664548	0.371696	3.288132
C	-2.651124	0.067415	0.822417
H	-3.063640	1.071109	0.684939
H	-3.221021	-0.396155	1.637775
C	-2.859451	-0.761728	-0.447569
O	-4.236975	-1.062409	-0.687230
C	-5.036896	0.055858	-1.083675
H	-4.438379	0.724531	-1.711388
H	-2.451425	-0.227109	-1.315289
C	-2.126979	-2.099598	-0.316744
H	-2.207990	-2.658946	-1.256723
H	-2.629789	-2.707053	0.448039
O	-5.498213	0.843871	0.021954
C	-6.334377	0.130801	0.937241
C	-6.687726	1.089737	2.071112
H	-5.774702	1.471837	2.541625
H	-7.294522	0.602176	2.838962
H	-7.232728	1.960784	1.691307
H	-5.766500	-0.698611	1.376385
C	-7.588918	-0.400213	0.236553
H	-8.239084	0.426554	-0.072721
O	-8.332082	-1.211657	1.144061
H	-9.063035	-1.610065	0.639995
C	-7.191360	-1.236712	-0.981526
O	-8.363818	-1.609714	-1.706472
H	-8.708730	-0.804635	-2.131416
H	-6.724267	-2.170779	-0.648250
C	-6.235181	-0.463048	-1.898182
O	-6.967729	0.634960	-2.463969
C	-6.420921	1.104530	-3.688672
H	-6.415400	0.306191	-4.437619
H	-5.410163	1.495263	-3.547230
H	-7.054963	1.917096	-4.055184
H	-5.909517	-1.137345	-2.701157

NMR-Shifts

Original-MandelalideA0005-NMR.txt

Atom	Type	Isotropic	Scaled Shift
1	C	100.2989	82.0853193974
2	C	111.2047	71.646949597
3	C	148.8549	35.6104634469
6	C	113.1954	69.7415723884
8	C	122.3161	61.0117919562
14	C	13.3968	165.262734738
16	C	55.7867	124.689695438
18	C	27.5084	151.755967764
20	C	142.6116	41.5861712514
23	C	109.2088	73.55730393
29	C	147.1852	37.2085989395
32	C	147.8438	36.5782269952
34	C	173.0293	12.4721951033
38	C	104.6032	77.9655046996
42	C	111.5084	71.356266391
44	C	144.7907	39.5004689983
45	C	151.5869	32.9955588736
47	C	162.9641	22.1059936063
51	C	43.7053	136.253278202
53	C	52.2477	128.077011428
55	C	48.1347	132.013725378
57	C	48.3235	131.833017477
59	C	147.7549	36.6633166791
64	C	144.8479	39.4457206302
67	C	106.0043	76.6244568234
69	C	83.2419	98.4112444725
72	C	144.2686	40.0001914279
76	C	117.1831	65.9247879936
77	C	168.2861	17.0120982408
82	C	108.3692	74.360918088
86	C	110.5439	72.2794272478
90	C	101.8965	80.5561936484
92	C	128.7659	54.8384348858
4	H	29.4859	2.17759297759
5	H	30.2042	1.51388311388
7	H	26.6266	4.81958881959
10	H	31.1306	0.657888657889
11	H	28.7181	2.88704088704
12	H	27.8387	3.69960729961
17	H	25.7060	5.67022407022
19	H	24.3233	6.94784014784
21	H	29.3334	2.3185031185
22	H	29.5141	2.15153615154
24	H	28.5220	3.06823746824
26	H	29.5551	2.11365211365
27	H	27.9254	3.6194964195
28	H	27.9577	3.58965118965
30	H	29.9999	1.70265650266
31	H	30.6740	1.07978747979
33	H	29.2355	2.40896280896
35	H	30.7730	0.988311388311
36	H	30.7744	0.987017787018
37	H	30.8247	0.940540540541
39	H	27.4126	4.09332409332
43	H	28.5690	3.02480942481
46	H	29.5505	2.1179025179
48	H	31.2063	0.587941787942
49	H	30.6782	1.07590667591
50	H	30.4834	1.2559020559
52	H	25.7504	5.6291984292
54	H	25.3482	6.00083160083
56	H	25.3632	5.98697158697
58	H	25.4161	5.93809193809
60	H	29.4252	2.23367983368
61	H	29.0920	2.54155694156
62	H	29.7360	1.9465003465
63	H	30.3798	1.35162855163
65	H	29.1386	2.4984984985
66	H	30.7265	1.03127743128
70	H	26.6880	4.76285516286
71	H	28.2028	3.36317856318
73	H	30.0151	1.68861168861
74	H	30.3386	1.3896973897
78	H	30.5841	1.16285516286
79	H	30.2123	1.5063987064
80	H	30.8868	0.88316008316
81	H	27.7520	3.77971817972
83	H	28.3533	3.22411642412
85	H	29.6100	2.06292446292
88	H	30.0450	1.66098406098
89	H	27.9227	3.62199122199
93	H	28.6779	2.92418572419
94	H	28.3160	3.25858165858
95	H	28.1751	3.38877338877
96	H	28.2002	3.36558096558

Supporting Information: Original-MandelalideA0006.log

Using Gaussian 09: AM64L-G09RevC.01 23-Sep-2011

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#mPW1PW91/6-311+G(2d,p) scf=(maxcycle=300,direct,tight) NMR density=current SCRF=(PCM,SOLVENT=Chloroform)

Pointgroup= C1 Stoichiometry= C33H52O11 C1[X(C33H52O11)]

#Atoms= 96

Charge = 0 Multiplicity = 1

SCF Energy= -2116.36649706

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Optimization incomplete.

Atomic Type	Coordinates (Angstroms) X	Y	Z
C	6.054005	-0.626686	1.585773
C	6.142656	0.335283	0.397570
C	6.106200	1.806900	0.833492
H	7.071341	2.046338	1.296736
H	5.322557	1.960524	1.583834
C	5.861606	2.761931	-0.350955
H	6.258585	2.358813	-1.290025
C	6.491372	4.137725	-0.117210
O	6.080058	4.688608	1.129330
H	5.107095	4.704513	1.128304
H	6.195330	4.838863	-0.903700
H	7.583610	4.065940	-0.108925
O	4.431876	2.983455	-0.454142
C	3.719988	2.283344	-1.371882
O	4.145576	1.487905	-2.192138
C	2.298477	2.646899	-1.181325
H	2.063950	3.443913	-0.482712
C	1.330689	1.991331	-1.837385
H	1.582906	1.192479	-2.528673
C	-0.131657	2.308283	-1.671583
H	-0.551876	2.495724	-2.667473
H	-0.247216	3.231406	-1.090324
C	-0.889431	1.164155	-0.983258
H	-0.320607	0.817282	-0.109695
O	7.384153	0.119714	-0.280504
H	7.442582	-0.833784	-0.467141
H	5.346957	0.109232	-0.317386
H	6.854738	-0.423563	2.307797
C	4.691951	-0.632666	2.264156
H	4.580732	0.178344	2.990666
H	3.885723	-0.541592	1.527425
C	4.669158	-2.002142	2.910620
H	5.277700	-1.940658	3.824640
C	3.286235	-2.470373	3.323365
H	3.324541	-3.484371	3.732966
H	2.579136	-2.460265	2.489090
H	2.879048	-1.811415	4.098499
C	5.440948	-2.870883	1.912586
H	6.134198	-3.505241	2.479566
O	6.255895	-1.976630	1.123524
O	-1.027834	0.083082	-1.912857
C	-1.635771	-1.070405	-1.329499
H	-1.043872	-1.385111	-0.461401
C	-1.680466	-2.209579	-2.362790
C	-0.320965	-2.747940	-2.866566
H	-0.559848	-3.636656	-3.469727
C	0.370457	-1.784078	-3.836610
H	-0.317804	-1.470742	-4.629055
H	1.224256	-2.271536	-4.321579
H	0.743940	-0.885770	-3.341357
C	0.538546	-3.259204	-1.729639
H	0.086704	-4.063678	-1.150039
C	1.775849	-2.853473	-1.404525
H	2.260797	-2.061954	-1.967809
C	2.545955	-3.455847	-0.337617
H	2.071055	-4.244039	0.239914
C	3.818497	-3.113441	-0.072686
H	4.303237	-2.346767	-0.672558
C	4.667719	-3.797735	0.964291
H	4.076569	-4.513200	1.547867
H	5.406018	-4.389339	0.406112
H	-2.257900	-1.878445	-3.236713
H	-2.237526	-3.050675	-1.926797
C	-3.061008	-0.726312	-0.876554
H	-3.515991	-1.599854	-0.396531
H	-3.685445	-0.488385	-1.748416
C	-3.071747	0.471523	0.073269
O	-4.392592	0.959429	0.327827
C	-5.203113	0.105848	1.141120
H	-4.576546	-0.372900	1.899466
H	-2.598270	0.200534	1.026050
C	-2.281025	1.626026	-0.548274
H	-2.214161	2.454826	0.166406
H	-2.838516	2.010662	-1.413379
O	-5.828035	-0.954942	0.404831
C	-6.721966	-0.507629	-0.618344
C	-7.252100	-1.746254	-1.332368
H	-6.421113	-2.341097	-1.726688
H	-7.914708	-1.482759	-2.162011
H	-7.799278	-2.393778	-0.637528
H	-6.161268	0.080242	-1.356168
C	-7.857433	0.332887	-0.027692
H	-8.514824	-0.286867	0.594362
O	-8.650124	0.867849	-1.084829
H	-9.297421	1.472160	-0.680978
C	-7.282337	1.480685	0.804492
O	-8.343574	2.171208	1.463941
H	-8.682804	1.581571	2.160112
H	-6.804848	2.210862	0.140343
C	-6.272859	0.965040	1.837937
O	-6.995852	0.179662	2.798254
C	-6.345481	0.092933	4.058934
H	-6.975176	-0.501092	4.727041
H	-6.222498	1.089514	4.495652
H	-5.375186	-0.401961	3.971541
H	-5.822674	1.832176	2.339436

NMR-Shifts

Original-MandelalideA0006-NMR.txt

Atom	Type	Isotropic	Scaled Shift
1	C	100.0062	82.3654740711
2	C	109.8353	72.9576561573
3	C	145.1204	39.1849001704
6	C	111.8393	71.039548996
8	C	115.6620	67.380692586
14	C	13.7305	164.943337353
16	C	56.5921	123.918815444
18	C	24.0750	155.042209843
20	C	142.8440	41.3637320776
23	C	107.2528	75.4294684048
29	C	147.7454	36.6724095025
32	C	146.8679	37.51229924
34	C	173.0744	12.4290281208
38	C	102.8633	79.6308313712
42	C	110.9649	71.8764716017

44	C	141.8641	42.3016328796
45	C	148.2377	36.2012098241
47	C	167.4964	17.7679511476
51	C	43.6896	136.268305289
53	C	51.7378	128.565056758
55	C	50.0375	130.192480714
57	C	47.1294	132.975937518
59	C	147.0556	37.332644193
64	C	142.8660	41.3426750129
67	C	106.1553	76.4799287888
69	C	83.4539	98.2083309405
72	C	145.4048	38.9126897529
76	C	116.7625	66.3273607841
77	C	168.0036	17.2824900936
82	C	108.8775	73.8744041808
86	C	111.4528	71.4094833362
90	C	102.4783	79.9993300025
92	C	128.6955	54.9058174927
4	H	29.8766	1.81658581659
5	H	29.9739	1.72668052668
7	H	26.1414	5.26791406791
10	H	30.4921	1.24786324786
11	H	27.6812	3.84513744514
12	H	28.0846	3.4723954724
17	H	25.3628	5.98734118734
19	H	23.6394	7.57976437976
21	H	29.2763	2.37126357126
22	H	29.5246	2.14183414183
24	H	28.6591	2.94155694156
26	H	29.4900	2.1738045738
27	H	27.6853	3.84134904135
28	H	27.9734	3.57514437514
30	H	30.0844	1.62457842458
31	H	30.7063	1.04994224994
33	H	29.2069	2.43538923539
35	H	30.6988	1.05687225687
36	H	30.8060	0.957819357819
37	H	30.8184	0.946361746362
39	H	27.3926	4.1118041118
43	H	28.4735	3.11305151305
46	H	29.2225	2.42097482097
48	H	30.7654	0.995333795334
49	H	30.6557	1.0966966967
50	H	29.8978	1.796996997
52	H	25.7567	5.62337722338
54	H	25.3876	5.96442596443
56	H	25.4843	5.87507507508
58	H	25.3398	6.00859320859
60	H	29.5186	2.14737814738
61	H	29.1206	2.51513051513
62	H	30.0104	1.69295449295
63	H	29.8966	1.79810579811
65	H	29.3934	2.26306306306
66	H	30.3966	1.33610533611
70	H	26.6503	4.79768999769
71	H	28.1858	3.37888657889
73	H	29.9976	1.70478170478
74	H	30.4300	1.30524370524
78	H	30.5802	1.16645876646
79	H	30.1878	1.52903672904
80	H	30.9017	0.869392469392
81	H	27.8079	3.72806652807
83	H	28.3550	3.22254562255
85	H	29.5921	2.07946407946
88	H	30.1438	1.56969276969
89	H	28.0787	3.47784707785
93	H	28.1619	3.40097020097
94	H	28.6670	2.93425733426
95	H	28.2867	3.28565488565
96	H	28.2698	3.30127050127

Supporting Information: Original-MandelalideA0007.log

Using Gaussian 09: AM64L-G09RevC.01 23-Sep-2011

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#mPW1PW91/6-311+G(2d,p) scf=(maxcycle=300,direct,tight) NMR density=current SCRF=(PCM,SOLVENT=Chloroform)

Pointgroup= C1 Stoichiometry= C33H52O11 C1[X(C33H52O11)]

#Atoms= 96

Charge = 0 Multiplicity = 1

SCF Energy= -2116.36588332

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Optimization incomplete.

Atomic Type	Coordinates (Angstroms) X	Y	Z
C	-6.190243	0.488084	1.503266
C	-4.955397	1.204038	0.948086
C	-5.247215	2.612294	0.410997
H	-5.720854	3.215128	1.194748
H	-5.955050	2.535025	-0.422809
C	-3.976957	3.337082	-0.077782
H	-3.338250	3.531853	0.794397
C	-4.313322	4.657269	-0.773268
O	-4.945165	5.547650	0.134688
H	-5.121958	6.371879	-0.349544
H	-4.975501	4.489170	-1.629489
H	-3.403902	5.134758	-1.154227
O	-3.300761	2.468320	-1.011786
C	-1.950281	2.585700	-1.103494
O	-1.244896	3.417662	-0.557468
C	-1.469471	1.497123	-1.981223
H	-2.180685	0.751106	-2.317954
C	-0.176963	1.443365	-2.330933
H	0.505296	2.218932	-1.992375
C	0.403758	0.371684	-3.213711
H	0.812493	0.856819	-4.108351
H	-0.398130	-0.296626	-3.553070
C	1.503696	-0.483223	-2.559630
H	1.855263	-1.187760	-3.324494
O	-3.991704	1.306184	1.999405
H	-3.839639	0.404610	2.334028
H	-4.501225	0.586965	0.163825
H	-6.494685	0.940882	2.454919
C	-7.377819	0.400593	0.555419
H	-8.071203	1.237966	0.682316
H	-7.052318	0.394692	-0.491405
C	-7.987448	-0.935769	0.933812
H	-8.519020	-0.806012	1.886543
C	-8.970458	-1.472939	-0.090945
H	-8.531532	-1.530081	-1.091517
H	-9.847379	-0.819605	-0.155131
H	-9.314133	-2.473649	0.191489
C	-6.741481	-1.783981	1.199231
H	-6.965280	-2.577986	1.921047
O	-5.809282	-0.872115	1.813409
O	0.930926	-1.244299	-1.489281
C	1.850964	-2.193386	-0.942587
H	2.191423	-2.860644	-1.745868
C	1.155037	-3.039808	0.139149
C	0.075803	-4.005876	-0.409886

H	0.408525	-4.383400	-1.385852
C	-0.018836	-5.231081	0.513212
H	0.941887	-5.755421	0.555425
H	-0.761238	-5.948850	0.144868
H	-0.287575	-4.947070	1.536246
C	-1.248706	-3.302366	-0.641021
H	-1.235649	-2.540422	-1.417506
C	-2.412392	-3.547413	-0.016724
H	-2.473733	-4.308454	0.756040
C	-3.635946	-2.839265	-0.317240
H	-3.580780	-2.040931	-1.054322
C	-4.814477	-3.126585	0.261817
H	-4.881104	-3.930145	0.992093
C	-6.090626	-2.394246	-0.055539
H	-5.887232	-1.611560	-0.796157
H	-6.779254	-3.109261	-0.518153
H	0.705518	-2.379783	0.893618
H	1.929294	-3.626456	0.650690
C	3.056592	-1.459113	-0.346282
H	3.768846	-2.187534	0.056915
H	2.737401	-0.831200	0.496644
C	3.738454	-0.573797	-1.392769
O	4.736749	0.281497	-0.831902
C	5.893328	-0.388930	-0.324030
H	6.112469	-1.259127	-0.951759
H	4.197883	-1.196891	-2.170389
C	2.692010	0.332790	-2.047466
H	3.150758	0.908999	-2.860592
H	2.367565	1.064097	-1.296667
O	5.716681	-0.885660	1.009958
C	5.444165	0.131872	1.977303
C	5.228024	-0.562275	3.318977
H	4.969769	0.151093	4.106817
H	6.124643	-1.114317	3.622903
H	4.419325	-1.298131	3.239359
H	4.504395	0.636206	1.717286
C	6.587858	1.147140	2.046849
H	7.491906	0.685400	2.461682
O	6.216442	2.216411	2.915343
H	6.908479	2.897550	2.844382
C	6.881526	1.707169	0.653223
O	8.045626	2.532865	0.707316
H	8.810168	1.944851	0.841375
H	6.057133	2.357347	0.338628
C	7.086682	0.581310	-0.367432
O	8.300120	-0.104326	-0.021037
C	8.897312	-0.782627	-1.117943
H	9.150090	-0.075093	-1.913981
H	8.239859	-1.565294	-1.505156
H	9.820924	-1.251094	-0.768056
H	7.195084	1.034932	-1.361264

NMR-Shifts

Original-MandelalideA0007-NMR.txt

Atom	Type	Isotropic	Scaled Shift
1	C	98.2375	84.0583663546
2	C	109.6328	73.1514768659
3	C	150.9767	33.5796052758
6	C	115.9845	67.0720151611
8	C	120.5519	62.7003771129
14	C	13.7023	164.970328682
16	C	55.8309	124.647389881
18	C	27.9973	151.288022359
20	C	144.8347	39.458354869
23	C	109.2543	73.5137540918
29	C	149.9320	34.5795287046
32	C	146.7814	37.5950917897
34	C	172.5622	12.9192748713
38	C	101.8467	80.6038591857
42	C	105.2754	77.3221156607
44	C	137.8325	46.1604356898
45	C	146.9793	37.4056739218
47	C	166.2141	18.9952908746
51	C	39.3116	140.458661154
53	C	55.7019	124.770860851
55	C	47.0090	133.09117709
57	C	48.3248	131.831773196
59	C	146.5310	37.8347594709
64	C	143.8224	40.4272669844
67	C	106.7693	75.8922452574
69	C	83.6500	98.0206359234
72	C	149.3032	35.1813778977
76	C	117.2136	65.8955952449
77	C	167.8847	17.3962939566
82	C	108.5362	74.2010758246
86	C	111.1062	71.7412278183
90	C	101.8036	80.6451118896
92	C	128.8374	54.7699994257
4	H	29.7578	1.92635712636
5	H	30.2969	1.42822822823
7	H	26.4144	5.01566181566
10	H	31.0235	0.756849156849
11	H	28.2529	3.31688611689
12	H	27.5214	3.99279279279
17	H	25.2242	6.11540771541
19	H	23.8948	7.34377454377
21	H	29.2782	2.36950796951
22	H	28.8429	2.77172557173
24	H	28.1713	3.39228459228
26	H	29.8035	1.88413028413
27	H	27.7212	3.80817740818
28	H	27.8172	3.71947331947
30	H	29.9654	1.73453453453
31	H	30.4645	1.27336567337
33	H	29.3466	2.30630630631
35	H	31.1582	0.632386232386
36	H	30.5941	1.15361515362
37	H	30.7564	1.00364980365
39	H	27.6828	3.84365904366
43	H	28.5044	3.0844998845
46	H	29.5089	2.15634095634
48	H	30.8096	0.954492954493
49	H	30.6724	1.08126588127
50	H	30.6381	1.11295911296
52	H	24.9201	6.3963963964
54	H	25.5573	5.80762300762
56	H	25.3539	5.99556479556
58	H	25.9157	5.47646107646
60	H	29.7661	1.91868791869
61	H	29.7255	1.9562023562
62	H	30.2017	1.51619311619
63	H	30.3407	1.38775698776
65	H	29.4168	2.24144144144
66	H	30.5725	1.17357357357
70	H	26.5798	4.86283206283
71	H	28.1323	3.42832062832
73	H	29.9808	1.7203049203
74	H	30.0982	1.61182721183
78	H	30.2163	1.5027027027
79	H	30.9247	0.84814044814
80	H	30.6564	1.09604989605
81	H	27.8277	3.70977130977
83	H	28.3756	3.20351120351
85	H	29.6311	2.04342804343
88	H	29.9968	1.70552090552
89	H	27.9419	3.60425040425
93	H	28.6411	2.95818895819
94	H	28.2046	3.36151536152

95	H	28.1858	3.37888657889
96	H	28.1719	3.39173019173

Supporting Information: Original-MandelalideA0008.log

Using Gaussian 09: AM64L-G09RevC.01 23-Sep-2011

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#mPW1PW91/6-311+G(2d,p) scf=(maxcycle=300,direct,tight) NMR density=current SCRF=(PCM,SOLVENT=Chloroform)

Pointgroup= C1 Stoichiometry= C33H52O11 C1[X(C33H52O11)]

#Atoms= 96

Charge = 0 Multiplicity = 1

SCF Energy= -2116.36706108

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Optimization incomplete.

Atomic Type	Coordinates (Angstroms) X	Y	Z
C	5.942637	-1.176783	1.224371
C	5.889961	0.064353	0.328528
C	5.934454	1.366908	1.140130
H	6.918691	1.443877	1.619141
H	5.173087	1.340735	1.927823
C	5.704099	2.608218	0.264656
H	6.283449	2.548988	-0.664317
C	6.077713	3.880514	1.027777
O	6.039062	5.008298	0.159112
H	5.130364	5.091028	-0.174543
H	7.094299	3.815214	1.426650
H	5.385953	4.071871	1.855027
O	4.283845	2.670183	-0.017177
C	3.871377	2.968313	-1.273270
O	4.580024	3.136364	-2.254881
C	2.397624	3.116208	-1.335207
H	1.995035	3.378528	-2.308060
C	1.586391	2.961947	-0.278916
H	1.989600	2.702610	0.696714
C	0.093654	3.153292	-0.327484
H	-0.205169	3.589435	-1.288419
H	-0.169328	3.874562	0.455957
C	-0.641668	1.827622	-0.096075
H	-0.148615	1.261462	0.705565
O	7.031592	0.050486	-0.533393
H	7.045821	-0.818682	-0.971787
H	5.003120	0.029486	-0.315002
H	6.846773	-1.158939	1.845604
C	4.700913	-1.383423	2.076175
H	4.705670	-0.774053	2.984527
H	3.792579	-1.145988	1.509659
C	4.772714	-2.869194	2.368618
H	5.516851	-3.008276	3.166383
C	3.469590	-3.467726	2.866604
H	3.199627	-3.032691	3.835208
H	3.564782	-4.549670	3.002325
H	2.637145	-3.276508	2.185550
C	5.375486	-3.448798	1.083943
H	6.161430	-4.159839	1.368497
O	6.037736	-2.358625	0.406417
O	-0.584453	1.073412	-1.312709
C	-1.145768	-0.238097	-1.174574
H	-0.594317	-0.760926	-0.384981
C	-0.947285	-0.953094	-2.523528
C	-1.133654	-2.483841	-2.460725
H	-2.094641	-2.690020	-1.975190
C	-1.215453	-3.054781	-3.881726
H	-0.289731	-2.872818	-4.438871
H	-2.041014	-2.595892	-4.437079
H	-1.392336	-4.136276	-3.863643
C	-0.078820	-3.253184	-1.691456
H	-0.391985	-4.240192	-1.354913
C	1.176825	-2.853527	-1.430591
H	1.526844	-1.885929	-1.777910
C	2.140284	-3.671804	-0.729506
H	1.800909	-4.626301	-0.336350
C	3.426361	-3.309382	-0.583046
H	3.770109	-2.368710	-1.006972
C	4.465789	-4.170939	0.080613
H	4.004924	-5.041289	0.561700
H	5.101717	-4.558200	-0.726808
H	0.040333	-0.704667	-2.933294
H	-1.654728	-0.526961	-3.248260
C	-2.630017	-0.134368	-0.804018
H	-3.046244	-1.131989	-0.636857
H	-3.195725	0.304026	-1.636546
C	-2.843897	0.737559	0.436332
O	-4.221334	1.049851	0.656960
C	-5.028580	-0.051536	1.084017
H	-4.437875	-0.700691	1.738443
H	-2.442786	0.230323	1.323720
C	-2.106067	2.068018	0.265104
H	-2.192026	2.659205	1.185862
H	-2.601946	2.650521	-0.523579
O	-5.483772	-0.874239	0.001983
C	-6.310512	-0.190192	-0.943649
C	-6.656939	-1.185242	-2.047358
H	-5.742801	-1.586422	-2.497944
H	-7.256134	-0.721358	-2.836069
H	-7.208798	-2.040567	-1.643117
H	-5.735223	0.621918	-1.406426
C	-7.568033	0.368701	-0.272278
H	-8.224580	-0.445002	0.059486
O	-8.300381	1.151943	-1.212307
H	-9.034603	1.568792	-0.726882
C	-7.178064	1.243667	0.920460
O	-8.354588	1.645543	1.623249
H	-8.706518	0.856487	2.071558
H	-6.704127	2.165350	0.560613
C	-6.230864	0.498402	1.870412
O	-6.973516	-0.577758	2.467657
C	-6.437337	-1.008919	3.711234
H	-7.077775	-1.805399	4.100111
H	-6.433580	-0.186290	4.432504
H	-5.427867	-1.408799	3.589732
H	-5.909850	1.197926	2.652776

NMR-Shifts

Original-MandelalideA0008-NMR.txt

Atom	Type	Isotropic	Scaled Shift
1	C	100.4149	81.9742912383
2	C	111.3573	71.5008901396
3	C	149.1979	35.2821646662
6	C	111.3532	71.5048144107
8	C	114.9003	68.1097455924
14	C	13.6383	165.031585597
16	C	56.1127	124.377668026
18	C	27.5260	151.739122112
20	C	142.8352	41.3721549034
23	C	109.6218	73.1620053983
29	C	147.2023	37.1922318574
32	C	147.8027	36.6175654205
34	C	173.1352	12.3708340512

38	C	104.8050	77.7723539884
42	C	111.5718	71.2955837593
44	C	144.6603	39.6252799632
45	C	151.3745	33.1988552614
47	C	162.7804	22.2818200961
51	C	43.4874	136.461838856
53	C	52.3930	127.937939088
55	C	48.2068	131.944715634
57	C	48.6758	131.495817301
59	C	147.8513	36.5710484504
64	C	144.7321	39.5565573614
67	C	106.0172	76.6121097264
69	C	83.3303	98.3266333582
72	C	144.1405	40.1228009725
76	C	117.3370	65.7774842551
77	C	168.4903	16.8166503953
82	C	108.5113	74.2249085932
86	C	110.6102	72.2159689121
90	C	101.7288	80.7167059094
92	C	128.8516	54.7564080476
4	H	30.3176	1.4091014091
5	H	30.1097	1.6012012012
7	H	25.8908	5.49946869947
10	H	30.9564	0.81884961885
11	H	28.1067	3.45197505198
12	H	27.9571	3.59020559021
17	H	25.4861	5.87341187341
19	H	24.2616	7.00485100485
21	H	29.3081	2.34188034188
22	H	29.4680	2.19413259413
24	H	28.5462	3.04587664588
26	H	29.5288	2.13795333795
27	H	27.9345	3.61108801109
28	H	28.0162	3.5355971356
30	H	30.1008	1.60942480942
31	H	30.7328	1.02545622546
33	H	29.2807	2.3671979672
35	H	30.8323	0.933518133518
36	H	30.8120	0.952275352275
37	H	30.8497	0.917440517441
39	H	27.4280	4.07909447909
43	H	28.5920	3.00355740356
46	H	29.5427	2.12510972511
48	H	31.1800	0.612243012243
49	H	30.6533	1.09891429891
50	H	30.4819	1.25728805729
52	H	25.7442	5.63492723493
54	H	25.3345	6.01349041349
56	H	25.4025	5.95065835066
58	H	25.4231	5.93162393162
60	H	29.4324	2.22702702703
61	H	29.0334	2.5957033957
62	H	29.6949	1.98447678448
63	H	30.3628	1.36733656734
65	H	29.1263	2.50986370986
66	H	30.7085	1.04790944791
70	H	26.7478	4.7075999076
71	H	28.2018	3.3641025641
73	H	30.0194	1.68463848464
74	H	30.3121	1.41418341418
78	H	30.5467	1.19741279741
79	H	30.2228	1.4966966967
80	H	30.9062	0.865234465234
81	H	27.7409	3.78997458997
83	H	28.3285	3.24703164703
85	H	29.5669	2.10274890275
88	H	30.0575	1.64943404943
89	H	27.9284	3.61672441672
93	H	28.1883	3.37657657658
94	H	28.6892	2.91374451374
95	H	28.3388	3.23751443751
96	H	28.2091	3.35735735736

Supporting Information: Original-MandelalideA0009.log

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 Using  Gaussian 09:  AM64L-G09RevC.01 23-Sep-2011
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 density=current SCRF=(PCM,SOLVENT=Chloroform)
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 Pointgroup= C1   Stoichiometry= C33H52O11   C1[X(C33H52O11)]
#Atoms= 96
 Charge = 0                Multiplicity = 1
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 SCF Energy= -2116.36788288
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 Optimization incomplete.


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      Type      X                Y                Z
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      C      -6.531787     -0.829222     -0.569807
      C      -5.729340      0.383087     -0.076432
      C      -6.071694      1.677327     -0.829140
      H      -7.160366      1.820340     -0.808340
      H      -5.771181      1.557466     -1.875544
      C      -5.414501      2.945815     -0.253185
      H      -5.693368      3.075329      0.798810
      C      -5.873630      4.208587     -0.992393
      O      -5.644148      4.088864     -2.391643
      H      -5.949516      4.914763     -2.803113
      H      -5.315020      5.080411     -0.636530
      H      -6.942756      4.378879     -0.833597
      O      -3.975199      2.873769     -0.388940
      C      -3.245761      2.584898      0.721507
      O      -3.677494      2.267029      1.818762
      C      -1.812755      2.742357      0.386250
      H      -1.548609      3.131216     -0.590428
      C      -0.881368      2.428328      1.296842
      H      -1.178166      2.040211      2.268802
      C       0.599625      2.604669      1.089647
      H       1.000372      3.104202      1.981040
      H       0.786027      3.269845      0.237301
      C       1.320435      1.268405      0.867745
      H       0.871761      0.762639      0.001851
      O      -6.040700      0.540564      1.311692
      H      -5.319900      1.052385      1.720114
      H      -4.658133      0.163192     -0.148693
      H      -7.572632     -0.749775     -0.229315
      C      -6.495710     -1.090847     -2.067008
      H      -7.274014     -0.539603     -2.604640
      H      -5.526944     -0.808978     -2.495322
      C      -6.691178     -2.595619     -2.120206
      H      -7.745860     -2.807035     -1.896938
      C      -6.359465     -3.210540     -3.467420
      H      -5.348007     -2.954011     -3.800313
      H      -7.055404     -2.850442     -4.231919
      H      -6.439264     -4.301261     -3.424951
      C      -5.853587     -3.062566     -0.925310
      H      -6.263577     -3.986605     -0.503140
      O      -6.003363     -2.018183      0.058776
      O       1.150636      0.445255      2.029279
      C       1.670290     -0.870539      1.828042
      H       1.237613     -1.291116      0.909976
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C	1.282134	-1.781634	3.005410
C	-0.223940	-1.849261	3.370239
H	-0.383789	-2.814020	3.872117
C	-0.608530	-0.771991	4.389236
H	-1.656297	-0.879778	4.693500
H	-0.483176	0.239493	3.991010
H	0.005382	-0.855651	5.292477
C	-1.133724	-1.762465	2.171363
H	-1.165979	-0.798622	1.666092
C	-1.893728	-2.760506	1.695819
H	-1.897853	-3.730652	2.182901
C	-2.712800	-2.580971	0.520221
H	-2.640867	-1.617042	0.019416
C	-3.543716	-3.509520	0.016071
H	-3.650766	-4.478563	0.495861
C	-4.357306	-3.253243	-1.224192
H	-3.961516	-2.368141	-1.737353
H	-4.215666	-4.099539	-1.907142
H	1.843502	-1.482064	3.898905
H	1.619090	-2.798146	2.762542
C	3.187952	-0.778676	1.665352
H	3.629158	-1.770361	1.509900
H	3.642948	-0.377511	2.581681
C	3.547971	0.139343	0.491775
O	4.965664	0.323010	0.510191
C	5.523019	0.710561	-0.749266
H	4.965104	1.565414	-1.141058
H	3.243580	-0.355158	-0.439371
C	2.818703	1.482430	0.628936
H	2.976474	2.098456	-0.262532
H	3.260223	2.035590	1.469126
O	5.435934	-0.317520	-1.746657
C	6.147378	-1.512992	-1.415458
C	5.917453	-2.508495	-2.547822
H	6.398154	-3.470193	-2.346175
H	6.300663	-2.116487	-3.497245
H	4.844978	-2.680765	-2.690630
H	5.716157	-1.949133	-0.505686
C	7.638605	-1.228155	-1.210928
H	8.111691	-0.940790	-2.157876
O	8.287809	-2.412212	-0.752383
H	9.205382	-2.169986	-0.534352
C	7.825860	-0.116042	-0.176965
O	9.207225	0.237473	-0.099780
H	9.431568	0.705749	-0.923926
H	7.546827	-0.487961	0.815755
C	6.989735	1.120236	-0.532876
O	7.534680	1.682509	-1.737458
C	7.239456	3.064190	-1.896434
H	6.162562	3.232126	-1.978036
H	7.711753	3.408777	-2.820015
H	7.649298	3.641060	-1.062183
H	7.085434	1.845689	0.284805

NMR-Shifts
Original-MandelalideA0009-NMR.txt

Atom	Type	Isotropic	Scaled Shift
1	C	99.7637	82.5975803518
2	C	110.7624	72.0702923103
3	C	149.7062	34.795650759
6	C	113.5082	69.4421792148
8	C	117.2356	65.8745381803
14	C	10.3461	168.182679607
16	C	58.9191	121.691552289
18	C	22.0216	157.007599686
20	C	143.5528	40.6853117403
23	C	106.5550	76.0973602098
29	C	150.5811	33.9582495836
32	C	148.1530	36.282279523
34	C	173.0956	12.4087367675
38	C	104.0799	78.4663756963
42	C	109.9394	72.8580179559
44	C	142.4812	41.7109822164
45	C	146.8605	37.5193820709
47	C	162.1705	22.8655793564
51	C	41.0620	138.783284519
53	C	52.4286	127.903864929
55	C	43.0142	136.914757174
57	C	51.0007	129.270564138
59	C	146.4406	37.9212848638
64	C	144.9967	39.303298302
67	C	115.4807	67.5542219415
69	C	89.9815	91.9605084324
72	C	147.0005	37.3853825686
76	C	117.6912	65.4384655143
77	C	167.8393	17.4397480809
82	C	108.4018	74.3297153468
86	C	110.8739	71.9635712782
90	C	102.5059	79.9729129578
92	C	128.3738	55.2137292061
4	H	30.3995	1.33342573343
5	H	29.5866	2.08454608455
7	H	26.6085	4.83631323631
10	H	31.0048	0.774127974128
11	H	27.5707	3.94723954724
12	H	27.7920	3.74275814276
17	H	25.2821	6.06190806191
19	H	23.4969	7.71143451143
21	H	29.1644	2.47465927466
22	H	29.3729	2.28200508201
24	H	28.4171	3.16516516517
26	H	28.6414	2.95791175791
27	H	28.2283	3.33961653962
28	H	27.7900	3.74460614461
30	H	30.1969	1.52062832063
31	H	30.4277	1.30736890737
33	H	29.3750	2.28006468006
35	H	31.1147	0.67258027258
36	H	30.6250	1.12506352506
37	H	30.7907	0.971956571957
39	H	27.9257	3.61921921922
43	H	28.4386	3.1452991453
46	H	29.2578	2.38835758836
48	H	30.7089	1.04753984754
49	H	30.0249	1.67955647956
50	H	30.7086	1.04781704782
52	H	25.7596	5.6206976207
54	H	25.3443	6.00443520444
56	H	25.3969	5.95583275583
58	H	25.8477	5.53929313929
60	H	29.9483	1.75033495033
61	H	29.8616	1.83044583045
62	H	30.1377	1.57532917533
63	H	30.0143	1.68935088935
65	H	30.0086	1.69461769462
66	H	30.4960	1.24425964426
70	H	26.3997	5.02924462924
71	H	27.7079	3.82046662047
73	H	29.6022	2.07013167013
74	H	30.6154	1.13393393393
78	H	30.2131	1.50565950566
79	H	30.8374	0.928805728806
80	H	30.6054	1.14317394317
81	H	27.9617	3.58595518596
83	H	28.3047	3.26902286902
85	H	29.6085	2.06431046431
88	H	30.0377	1.66772926773
89	H	27.9682	3.57994917995

93	H	28.3173	3.25738045738
94	H	28.1934	3.37186417186
95	H	28.6734	2.92834372834
96	H	28.2697	3.30136290136

Supporting Information: Original-MandelalideA0010.log

Using Gaussian 09: AM64L-G09RevC.01 23-Sep-2011

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#mPW1PW91/6-311+G(2d,p) scf=(maxcycle=300,direct,tight) NMR density=current SCRF=(PCM,SOLVENT=Chloroform)

Pointgroup= C1 Stoichiometry= C33H52O11 C1[X(C33H52O11)]

#Atoms= 96

Charge = 0 Multiplicity = 1

SCF Energy= -2116.36817509

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Optimization incomplete.

Atomic Type	Coordinates (Angstroms) X	Y	Z
C	-5.646285	-1.018696	-1.643345
C	-5.691287	0.169280	-0.677516
C	-5.585118	1.515177	-1.408310
H	-6.489230	1.653190	-2.015144
H	-4.720517	1.506153	-2.081681
C	-5.448415	2.697598	-0.436071
H	-6.154573	2.606782	0.397562
C	-5.677173	4.022681	-1.167097
O	-5.733767	5.098107	-0.235726
H	-4.878957	5.131272	0.226369
H	-6.628350	4.013446	-1.708076
H	-4.871196	4.235636	-1.876428
O	-4.080861	2.695811	0.043380
C	-3.841659	2.913638	1.359352
O	-4.677140	3.054809	2.241255
C	-2.387829	3.004123	1.633617
H	-2.118078	3.200416	2.667137
C	-1.440825	2.877204	0.693503
H	-1.709103	2.683608	-0.342153
C	0.035404	3.011513	0.958947
H	0.208986	3.387915	1.974205
H	0.427009	3.761281	0.260457
C	0.758954	1.673792	0.761112
H	0.366071	1.164777	-0.129395
O	-6.945162	0.146944	0.011785
H	-7.044253	-0.743985	0.391905
H	-4.907124	0.069003	0.082036
H	-6.451019	-0.935542	-2.385787
C	-4.300667	-1.220676	-2.319876
H	-4.159216	-0.563323	-3.183554
H	-3.477684	-1.044436	-1.617079
C	-4.366504	-2.684754	-2.704843
H	-4.990918	-2.757160	-3.607397
C	-3.020216	-3.299134	-3.044188
H	-2.601620	-2.821364	-3.937375
H	-3.122023	-4.368611	-3.254889
H	-2.291565	-3.172912	-2.239678
C	-5.163888	-3.312409	-1.555535
H	-5.917414	-3.982556	-1.990211
O	-5.890403	-2.239179	-0.918650
O	0.505880	0.862367	1.915225
C	1.047169	-0.459936	1.791903
H	0.605442	-0.926305	0.903759
C	0.636038	-1.232429	3.057558
C	0.787120	-2.763580	2.938933
H	1.801022	-2.978187	2.581502
C	0.650854	-3.406272	4.323510
H	-0.339296	-3.220512	4.755973
H	1.401208	-3.005514	5.014336
H	0.798322	-4.491542	4.272806
C	-0.169994	-3.456544	1.989330
H	0.156422	-4.439792	1.654195
C	-1.359352	-2.996385	1.569604
H	-1.724896	-2.031757	1.908088
C	-2.235191	-3.745531	0.696449
H	-1.872876	-4.695129	0.312427
C	-3.471511	-3.325896	0.376740
H	-3.843473	-2.390795	0.788722
C	-4.426707	-4.115667	-0.475079
H	-3.925393	-4.976004	-0.932890
H	-5.182674	-4.521858	0.211114
H	-0.392596	-0.969121	3.335660
H	1.243511	-0.867500	3.897749
C	2.569876	-0.379196	1.648475
H	3.010479	-1.372341	1.505611
H	3.013669	0.020262	2.570628
C	2.974409	0.526822	0.484144
O	4.392561	0.689334	0.539530
C	4.989700	1.040950	-0.712972
H	4.443515	1.881137	-1.148527
H	2.684101	0.037703	-0.454721
C	2.267631	1.878528	0.613795
H	2.483708	2.509994	-0.254978
H	2.667857	2.406628	1.488977
O	4.934959	-0.017664	-1.681189
C	5.637749	-1.200247	-1.291345
C	5.444028	-2.231950	-2.398740
H	4.376845	-2.410479	-2.568026
H	5.919517	-3.184919	-2.152056
H	5.854606	-1.868755	-3.347553
H	5.180397	-1.608806	-0.381044
C	7.121480	-0.904694	-1.051260
H	7.621897	-0.643039	-1.991863
O	7.761235	-2.073156	-0.540006
H	8.671266	-1.820614	-0.302300
C	7.274143	0.236446	-0.044741
O	8.651444	0.595464	0.066712
H	8.901971	1.039448	-0.763564
H	6.964276	-0.107066	0.949236
C	6.447337	1.459509	-0.461997
O	7.029318	1.987838	-1.664764
C	6.738317	3.363648	-1.873052
H	7.238866	3.682272	-2.791261
H	7.122258	3.964815	-1.043750
H	5.664549	3.527725	-1.992151
H	6.516219	2.209594	0.336612

NMR-Shifts

Original-MandelalideA0010-NMR.txt

Atom	Type	Isotropic	Scaled Shift
1	C	99.0545	83.2763835449
2	C	112.2940	70.6043377553
3	C	148.8368	35.6277876682
6	C	111.3456	71.5120886694
8	C	114.7736	68.2310151419
14	C	13.2252	165.426979843
16	C	55.8300	124.648251306
18	C	27.7195	151.553915657
20	C	142.7295	41.4733245277
23	C	110.3270	72.4870307625
29	C	146.9651	37.4192652999

32	C	147.9296	36.496104443
34	C	173.2459	12.2648787305
38	C	104.2908	78.2645150175
42	C	110.6609	72.1674419495
44	C	144.1096	40.1523765769
45	C	151.4718	33.1057256073
47	C	162.7049	22.3540841134
51	C	43.6863	136.271463849
53	C	52.7444	127.601600337
55	C	49.6793	130.535328012
57	C	47.5125	132.609257451
59	C	147.6298	36.7830548058
64	C	146.1472	38.202109535
67	C	115.1192	67.9002277992
69	C	89.7036	92.2264974444
72	C	146.2413	38.1120427267
76	C	117.5317	65.5911292329
77	C	167.7880	17.4888493271
82	C	108.0792	74.6384884856
86	C	110.9420	71.8983900917
90	C	102.3980	80.0761882884
92	C	128.5407	55.0539826566
4	H	30.2516	1.47008547009
5	H	30.1562	1.55823515824
7	H	25.9065	5.48496188496
10	H	30.9201	0.852390852391
11	H	28.1486	3.41325941326
12	H	27.9568	3.59048279048
17	H	25.6176	5.75190575191
19	H	24.2323	7.03192423192
21	H	29.3033	2.34631554632
22	H	29.4059	2.25151305151
24	H	28.4878	3.09983829984
26	H	29.4895	2.17426657427
27	H	27.8862	3.65571725572
28	H	27.9303	3.61496881497
30	H	30.0600	1.64712404712
31	H	30.6931	1.06213906214
33	H	29.2442	2.40092400092
35	H	30.8023	0.961238161238
36	H	30.8059	0.957911757912
37	H	30.8388	0.927512127512
39	H	27.3888	4.11531531532
43	H	28.4364	3.14733194733
46	H	29.6174	2.05608685609
48	H	31.2386	0.558096558097
49	H	30.6100	1.13892353892
50	H	30.4075	1.32603372603
52	H	25.8341	5.55185955186
54	H	25.4677	5.89041349041
56	H	25.5703	5.79561099561
58	H	25.4080	5.94557634558
60	H	29.3518	2.3015015015
61	H	28.9758	2.64892584893
62	H	29.7655	1.91924231924
63	H	30.4077	1.32584892585
65	H	29.7477	1.93568953569
66	H	30.7682	0.992746592747
70	H	26.4285	5.00263340263
71	H	27.8036	3.73203973204
73	H	29.7297	1.95232155232
74	H	30.6373	1.1136983137
78	H	30.6789	1.07525987526
79	H	30.2188	1.50039270039
80	H	30.8527	0.914668514669
81	H	27.9613	3.58632478632
83	H	28.2917	3.28103488103
85	H	29.6091	2.06375606376
88	H	30.0132	1.69036729037
89	H	27.9428	3.60341880342
93	H	28.2031	3.3629013629
94	H	28.6836	2.91891891892
95	H	28.3501	3.22707322707
96	H	28.2482	3.32122892123

Mandelalide A Revised Configuration (MD Methodologies)

Supporting Information: Revised-MandelalideA150ps.log

Using Gaussian 09: AM64L-G09RevC.01 23-Sep-2011

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#mPW1PW91/6-311+G(2d,p) scf=(maxcycle=300,direct,tight) NMR density=current SCRF=(PCM,SOLVENT=Chloroform)

Pointgroup= C1 Stoichiometry= C33H52O11 C1[X(C33H52O11)]
#Atoms= 96
Charge = 0 Multiplicity = 1

SCF Energy= -2116.24418111

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Optimization incomplete.

Atomic Type	Coordinates (Angstroms) X	Y	Z
C	-6.831974	-0.900310	0.239814
C	-5.847823	0.141813	-0.435291
C	-6.365528	1.544830	-0.057530
H	-6.512501	1.761539	1.002140
H	-7.397494	1.762295	-0.342968
C	-5.369190	2.604980	-0.356296
H	-5.170865	2.641950	-1.430358
C	-5.863619	3.980015	0.082755
O	-5.551926	4.824948	-0.961243
H	-4.590576	4.789436	-1.111661
H	-5.411874	4.287611	1.029127
H	-6.955437	4.027795	0.116559
O	-4.075503	2.331574	0.237246
C	-3.027090	3.092415	-0.142282
O	-3.008999	4.096948	-0.860411
C	-1.802560	2.577292	0.374037
H	-1.878808	1.687105	0.996245
C	-0.615443	3.240622	0.341557
H	-0.538993	4.214408	-0.133767
C	0.652858	2.807559	1.113392
H	0.302830	2.200053	1.950431
H	1.133328	3.737879	1.423446
C	1.626483	1.993292	0.179382
H	1.724100	2.377857	-0.838963
O	-5.921883	-0.088094	-1.860050
H	-6.014803	-1.056259	-1.906405
H	-4.817568	0.094029	-0.073418
H	-7.871545	-0.720568	-0.045210
C	-6.595665	-0.896548	1.784902
H	-5.578330	-0.577394	2.020764
H	-7.256632	-0.192889	2.296928
C	-6.914741	-2.331619	2.106530
H	-7.997574	-2.466136	2.141886
C	-6.348249	-2.800330	3.455106
H	-5.270710	-2.647088	3.547344
H	-6.445845	-3.876209	3.618313
H	-6.736783	-2.196684	4.277427

C	-6.426583	-3.090113	0.862332
H	-7.021349	-3.960310	0.571033
O	-6.451990	-2.163270	-0.248679
O	0.933485	0.749133	0.013157
C	1.544731	-0.186209	-0.899614
H	1.546646	0.355278	-1.849070
C	0.595421	-1.375077	-1.066986
C	-0.919909	-1.111134	-1.486337
H	-1.259320	-0.637740	-0.562772
C	-1.051781	-0.231829	-2.705218
H	-2.123208	-0.236967	-2.916928
H	-0.599155	-0.717677	-3.573023
H	-0.723273	0.786707	-2.488665
C	-1.646660	-2.419936	-1.624044
H	-1.133422	-3.212276	-2.162078
C	-2.872318	-2.614027	-1.159719
H	-3.493885	-1.828348	-0.732487
C	-3.485678	-3.882403	-1.159785
H	-3.279367	-4.620605	-1.933022
C	-4.339768	-4.253374	-0.148988
H	-4.723394	-5.262859	-0.268767
C	-4.903089	-3.552821	1.032119
H	-4.932595	-4.268263	1.857097
H	-4.289536	-2.704759	1.344961
H	0.547554	-2.042306	-0.203481
H	1.069699	-1.895330	-1.901664
C	2.969015	-0.627705	-0.367715
H	3.479552	-1.189730	-1.152020
H	2.913815	-1.352740	0.446979
C	3.783024	0.601072	0.007571
O	4.923811	0.129481	0.774345
C	6.219565	0.693981	0.434521
H	6.122374	1.781405	0.574559
H	4.052246	1.101807	-0.926154
C	2.942780	1.600817	0.848111
H	3.476975	2.552149	0.882251
H	2.812133	1.219621	1.863862
O	6.608861	0.467372	-0.960592
C	6.713594	-0.903826	-1.320111
C	6.995123	-0.989692	-2.872261
H	7.036481	-2.006408	-3.267780
H	7.952766	-0.538800	-3.139727
H	6.224033	-0.451344	-3.425764
H	5.813405	-1.465984	-1.058266
C	7.947139	-1.401579	-0.511274
H	8.784694	-0.707643	-0.617838
O	8.337466	-2.815141	-0.791618
H	8.708081	-3.246430	-0.000627
C	7.598131	-1.294611	1.043146
O	8.727771	-1.602213	1.716900
H	9.012147	-0.746479	2.084993
H	6.791365	-1.983454	1.304009
C	7.269816	0.165816	1.444832
O	8.531745	0.912672	1.551331
C	8.402630	2.256409	1.890717
H	8.223251	2.806836	0.964049
H	9.297210	2.714845	2.320043
H	7.523043	2.398706	2.523925
H	6.858579	0.136465	2.457200

NMR-Shifts

Revised-MandelalideA150ps-NMR.txt

Atom	Type	Isotropic	Scaled Shift
1	C	97.2224	85.0299584602
2	C	106.9665	75.703497387
3	C	154.0217	30.665116101
6	C	100.4075	81.9813740692
8	C	116.5940	66.4886387565
14	C	8.8156	169.647581309
16	C	54.3834	126.032849021
18	C	15.1092	163.623729398
20	C	139.4497	44.6125500105
23	C	107.6850	75.0157927985
29	C	146.7830	37.5935603668
32	C	150.6425	33.8994812305
34	C	172.7184	12.7697697123
38	C	95.3936	86.7803748158
42	C	108.0790	74.6386799135
44	C	140.2390	43.8570799594
45	C	149.7472	34.7564080476
47	C	169.4322	15.9151208867
51	C	43.1969	136.739887823
53	C	55.8649	124.614847145
55	C	45.3244	134.703573958
57	C	47.1019	133.002258849
59	C	148.2128	36.2250425927
64	C	148.4948	35.9551293095
67	C	112.9888	69.9393173682
69	C	83.3602	98.2980148931
72	C	149.6398	34.8592048087
76	C	115.7662	67.2809586707
77	C	167.3246	17.9323876797
82	C	95.3253	86.8457474301
86	C	114.8973	68.1126170103
90	C	98.4869	83.8196558127
92	C	133.7651	50.053504087
4	H	30.0608	1.64638484638
5	H	29.8456	1.84522984523
7	H	26.9497	4.52104412104
10	H	25.7814	5.60055440055
11	H	28.0363	3.51702471702
12	H	28.2226	3.34488334488
17	H	25.3852	5.96664356664
19	H	23.6377	7.58133518134
21	H	29.0789	2.55366135366
22	H	29.1116	2.52344652345
24	H	28.2551	3.31485331485
26	H	28.6491	2.9507969508
27	H	27.6493	3.87461307461
28	H	27.6100	3.91092631093
30	H	30.3473	1.38165858166
31	H	29.6704	2.00711480711
33	H	29.1713	2.46828366828
35	H	31.1659	0.625271425271
36	H	30.7464	1.01288981289
37	H	30.6025	1.14585354585
39	H	27.5111	4.00231000231
43	H	28.1680	3.39533379533
46	H	29.0781	2.5544005544
48	H	30.9432	0.831046431046
49	H	31.1693	0.62212982213
50	H	30.4437	1.29258489258
52	H	26.0835	5.32141372141
54	H	24.5583	6.7306999307
56	H	24.6946	6.60475860476
58	H	26.3853	5.04255024255
60	H	29.8188	1.86999306999
61	H	29.2433	2.40175560176
62	H	30.1336	1.57911757912
63	H	30.8597	0.908200508201
65	H	30.0831	1.62577962578
66	H	30.5569	1.18798798799
70	H	26.0111	5.38831138831
71	H	27.5636	3.9537999538
73	H	29.9349	1.76271656272
74	H	30.5455	1.19852159852
78	H	30.3059	1.41991221991
79	H	30.7821	0.979902979903

80	H	30.7421	1.01686301686
81	H	27.6439	3.8796026796
83	H	28.1617	3.40115500116
85	H	29.6199	2.05377685378
88	H	28.0558	3.49900669901
89	H	27.9547	3.59242319242
93	H	28.2722	3.29905289905
94	H	28.0420	3.51175791176
95	H	28.6520	2.94811734812
96	H	27.8406	3.69785169785

Supporting Information: Revised-MandelalideA152ps.log

Using Gaussian 09: AM64L-G09RevC.01 23-Sep-2011

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Pointgroup= C1 Stoichiometry= C33H52O11 C1[X(C33H52O11)]

#Atoms= 96

Charge = 0 Multiplicity = 1

SCF Energy= -2116.25188029

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Optimization incomplete.

Atomic Type	Coordinates (Angstroms) X	Y	Z
C	-6.741122	-0.601468	0.213132
C	-5.650405	0.321962	-0.324017
C	-6.109185	1.816282	-0.100778
H	-6.355255	1.982381	0.949757
H	-7.017557	1.985722	-0.682127
C	-5.167530	2.916785	-0.492602
H	-5.102108	2.996599	-1.581036
C	-5.704447	4.273963	0.034882
O	-4.880922	5.394324	-0.464034
H	-4.033780	4.989245	-0.722891
H	-5.614769	4.232471	1.123956
H	-6.747973	4.463493	-0.228293
O	-3.948870	2.505142	0.211330
C	-2.773798	3.039104	-0.124395
O	-2.741225	3.884272	-1.003635
C	-1.552621	2.680442	0.625965
H	-1.759945	1.993256	1.444859
C	-0.335394	3.053043	0.216669
H	-0.207568	3.714510	-0.636482
C	0.975038	2.706697	0.986050
H	0.712448	2.198159	1.916015
H	1.596623	3.583561	1.179810
C	1.776147	1.720946	0.039290
H	1.886344	2.198132	-0.937579
O	-5.432986	0.070347	-1.714473
H	-4.843493	-0.697974	-1.816765
H	-4.700850	0.087388	0.163867
H	-7.772595	-0.370652	-0.067286
C	-6.829736	-0.712680	1.694861
H	-5.845425	-0.622816	2.159095
H	-7.541842	-0.015816	2.141405
C	-7.283924	-2.227435	1.894282
H	-8.363654	-2.253646	1.735020
C	-6.902279	-2.631909	3.351523
H	-5.839551	-2.580525	3.594250
H	-7.275756	-3.649116	3.488525
H	-7.453714	-1.996607	4.047974
C	-6.601328	-3.013214	0.760312
H	-7.367476	-3.684257	0.364469
O	-6.334304	-1.921268	-0.191973
O	0.826653	0.584518	-0.177804
C	1.423747	-0.449635	-1.112081
H	1.630625	-0.048305	-2.107193
C	0.354214	-1.571892	-1.184928
C	-1.086679	-1.159084	-1.518243
H	-1.403704	-0.502108	-0.705782
C	-1.245065	-0.237336	-2.766099
H	-2.313145	-0.095075	-2.945269
H	-0.782071	-0.650723	-3.665231
H	-0.729769	0.688558	-2.503834
C	-1.996147	-2.384177	-1.644311
H	-1.753546	-3.071447	-2.450482
C	-2.990278	-2.735659	-0.853136
H	-3.161396	-2.238880	0.100742
C	-3.770758	-3.982852	-1.030348
H	-3.552849	-4.619033	-1.887689
C	-4.747619	-4.454409	-0.257621
H	-5.047569	-5.480016	-0.454742
C	-5.250826	-3.803113	1.039162
H	-5.467794	-4.543711	1.811707
H	-4.529658	-3.107418	1.472394
H	0.299973	-1.959327	-0.164936
H	0.703144	-2.251890	-1.965438
C	2.795186	-1.008166	-0.409373
H	3.165598	-1.870665	-0.966433
H	2.488921	-1.365988	0.576434
C	3.762225	0.119608	-0.263539
O	4.829330	-0.367969	0.554913
C	6.034111	0.498146	0.489523
H	5.762458	1.545724	0.686866
H	4.121634	0.516443	-1.216752
C	3.085739	1.211548	0.669810
H	3.693800	2.118591	0.669013
H	2.963003	0.785790	1.668428
O	6.596959	0.520031	-0.866435
C	6.940138	-0.802384	-1.280985
C	7.338926	-0.534580	-2.760244
H	8.016536	0.320142	-2.707168
H	6.444915	-0.288435	-3.337721
H	7.754208	-1.370622	-3.327335
H	6.094701	-1.494431	-1.288630
C	8.081200	-1.458867	-0.366680
H	9.045698	-0.966707	-0.512623
O	8.259278	-2.838538	-0.736369
H	8.879540	-3.246425	-0.105611
C	7.694630	-1.338821	1.146702
O	8.804674	-1.418975	2.054437
H	9.231146	-0.544070	2.076543
H	6.885380	-2.047358	1.338908
C	7.172182	0.051026	1.499762
O	8.215369	1.054655	1.399339
C	8.081763	2.294000	2.181364
H	7.027532	2.584157	2.156481
H	8.659800	3.104286	1.732174
H	8.447774	2.111249	3.195123
H	6.864736	0.126637	2.545697

NMR-Shifts

Revised-MandelalideA152ps-NMR.txt

Atom	Type	Isotropic	Scaled Shift
1	C	107.4091	75.2798675319
2	C	107.6895	75.0114856716
3	C	150.3957	34.1357032102
6	C	107.1220	75.5546622255
8	C	108.9642	73.7914202033

14	C	7.7161	170.699955972
16	C	63.6387	117.174237639
18	C	21.9399	157.085797967
20	C	137.0697	46.8905415494
23	C	101.1260	81.2936694807
29	C	137.5811	46.4010605103
32	C	136.6866	47.257221616
34	C	171.7979	13.6508164398
38	C	101.1912	81.2312639982
42	C	96.7967	85.437412661
44	C	142.5730	41.6231168284
45	C	146.9630	37.4212752924
47	C	167.3836	17.8759164609
51	C	39.2941	140.475411091
53	C	60.8546	119.839009169
55	C	44.8669	135.141465189
57	C	53.6080	126.775014836
59	C	150.9806	33.5758724325
64	C	139.2339	44.8191006719
67	C	114.9359	68.0756714332
69	C	78.8458	102.618924558
72	C	142.7430	41.4604031471
76	C	114.7731	68.2314937116
77	C	165.7839	19.4070522024
82	C	102.4029	80.0714983059
86	C	112.6362	70.2768046862
90	C	99.7763	82.5855203966
92	C	125.0568	58.3885602711
4	H	30.3507	1.37851697852
5	H	30.3306	1.39708939709
7	H	26.1433	5.26615846616
10	H	26.7496	4.70593670594
11	H	28.0970	3.46093786094
12	H	27.9948	3.55537075537
17	H	25.5424	5.82139062139
19	H	23.7129	7.51185031185
21	H	29.2117	2.43095403095
22	H	29.1912	2.4498960499
24	H	27.8326	3.70524370524
26	H	29.6131	2.06006006006
27	H	27.5813	3.93744513745
28	H	28.2466	3.32270732271
30	H	30.4388	1.29711249711
31	H	29.7427	1.94030954031
33	H	28.9932	2.63284823285
35	H	30.8479	0.919103719104
36	H	30.8117	0.952552552553
37	H	30.7221	1.03534303534
39	H	27.7473	3.78406098406
43	H	27.8833	3.6583968584
46	H	29.2040	2.43806883807
48	H	30.9829	0.794363594364
49	H	31.1917	0.601432201432
50	H	30.4196	1.31485331485
52	H	25.9828	5.41446061446
54	H	25.0166	6.30723030723
56	H	25.2040	6.13407253407
58	H	25.8923	5.49808269808
60	H	30.0219	1.68232848233
61	H	29.2173	2.42577962578
62	H	29.7990	1.88828828829
63	H	30.3176	1.4091014091
65	H	29.7440	1.93910833911
66	H	30.4186	1.31577731578
70	H	26.2346	5.1817971818
71	H	27.4328	4.07465927466
73	H	29.2854	2.36285516286
74	H	30.4259	1.30903210903
78	H	30.6664	1.08680988681
79	H	30.5178	1.22411642412
80	H	30.2979	1.4273042273
81	H	27.9336	3.61191961192
83	H	27.9555	3.59168399168
85	H	30.0258	1.67872487872
88	H	28.4070	3.1744975745
89	H	27.9579	3.58946638947
93	H	28.2026	3.36336336336
94	H	28.0990	3.45908985909
95	H	28.0832	3.47368907369
96	H	27.8360	3.7021021021

Supporting Information: Revised-MandelalideA154ps.log

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 density=current SCRF=(PCM,SOLVENT=Chloroform)
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 Pointgroup= C1   Stoichiometry= C33H52O11   C1[X(C33H52O11)]
#Atoms= 96
 Charge = 0                Multiplicity = 1
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 SCF Energy= -2116.26099554
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 Optimization incomplete.


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     Atomic      Coordinates (Angstroms)
      Type      X                Y              Z
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      C      -6.885289     -0.603134      0.226195
      C      -5.718957      0.459053     -0.147562
      C      -6.259450      1.798311      0.068730
      H      -6.646659      1.812627      1.090014
      H      -7.127613      1.926665     -0.580922
      C      -5.256189      2.937562     -0.322611
      H      -5.037441      2.779841     -1.381917
      C      -5.834423      4.409528     -0.231599
      O      -5.313388      5.126453     -1.361884
      H      -4.473277      4.669971     -1.549547
      H      -5.420995      4.953187      0.622326
      H      -6.925427      4.441576     -0.275145
      O      -4.004272      2.691954      0.403169
      C      -2.891173      3.105051     -0.136915
      O      -2.844053      3.768666     -1.157709
      C      -1.747743      2.657658      0.696513
      H      -1.979146      2.120883      1.615960
      C      -0.491214      2.917094      0.423451
      H      -0.239770      3.414169     -0.509857
      C       0.695311      2.312221      1.195699
      H       0.368381      1.831829      2.120193
      H       1.278927      3.207523      1.422228
      C       1.578581      1.405795      0.361380
      H       1.813698      1.888574     -0.590879
      O      -5.498677      0.327918     -1.496386
      H      -5.638256     -0.633194     -1.572937
      H      -4.788663      0.314960      0.407973
      H      -7.804211     -0.366110     -0.314146
      C      -7.002996     -0.797188      1.738092
      H      -6.072339     -0.390385      2.138881
      H      -7.850167     -0.222495      2.119608
      C      -7.280672     -2.289050      1.966358
      H      -8.338590     -2.508276      1.808975
      C      -6.803916     -2.720829      3.422653
      H      -5.839269     -2.301294      3.715528
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H	-6.723570	-3.806212	3.512752
H	-7.461672	-2.340340	4.206603
C	-6.517605	-2.912037	0.774800
H	-7.066832	-3.804088	0.463678
O	-6.557756	-1.891929	-0.295247
O	0.845633	0.213357	-0.007012
C	1.569850	-0.702112	-0.958163
H	1.773955	-0.063752	-1.822433
C	0.575881	-1.855265	-1.134768
C	-0.752682	-1.470624	-1.749733
H	-1.189363	-0.675406	-1.141848
C	-0.471084	-0.891816	-3.221525
H	-1.348667	-1.008700	-3.860063
H	0.437817	-1.308620	-3.659298
H	-0.367879	0.192318	-3.143959
C	-1.778425	-2.606894	-1.800981
H	-1.503583	-3.460099	-2.415759
C	-2.931912	-2.668907	-1.141912
H	-3.300121	-1.834578	-0.546750
C	-3.692445	-3.885944	-1.050857
H	-3.384889	-4.607145	-1.807503
C	-4.615182	-4.235264	-0.152114
H	-4.833151	-5.296890	-0.234852
C	-5.045334	-3.370827	0.982600
H	-4.914167	-3.950364	1.898539
H	-4.409846	-2.482735	1.005853
H	0.398082	-2.454609	-0.239746
H	1.070183	-2.548491	-1.820272
C	2.934624	-1.173067	-0.342585
H	3.586750	-1.723555	-1.023300
H	2.722797	-1.758359	0.554746
C	3.758005	0.037488	0.123621
O	4.916322	-0.372719	0.809414
C	6.048119	0.574369	0.779593
H	5.811354	1.526022	1.278005
H	4.079218	0.588252	-0.763385
C	2.885969	0.935534	1.091372
H	3.483908	1.775071	1.453073
H	2.571562	0.327287	1.942208
O	6.556361	0.886249	-0.498922
C	6.824406	-0.258754	-1.309736
C	7.063776	0.236865	-2.731304
H	7.967502	0.846597	-2.798782
H	6.243787	0.853521	-3.104055
H	7.196635	-0.679403	-3.309159
H	5.938386	-0.876973	-1.478351
C	8.051023	-0.954645	-0.700581
H	8.831211	-0.189691	-0.677338
O	8.235599	-2.124023	-1.488478
H	8.989084	-2.493857	-0.994379
C	7.838847	-1.333476	0.798642
O	9.132059	-1.578306	1.473478
H	9.335231	-0.652785	1.698295
H	7.138934	-2.156042	0.969654
C	7.214284	-0.058884	1.592062
O	8.327242	0.900865	1.795638
C	8.035191	2.110079	2.467289
H	8.940815	2.555103	2.888415
H	7.471013	1.934899	3.386950
H	7.472673	2.857728	1.901578
H	6.820046	-0.459390	2.529430

NMR-Shifts
Revised-MandelalideA154ps-NMR.txt

Atom	Type	Isotropic	Scaled Shift
1	C	93.5305	88.5636210494
2	C	110.5750	72.2496602155
3	C	147.4218	36.9821397806
6	C	99.1960	83.1409483336
8	C	114.3829	68.6049694673
14	C	15.1164	163.616837995
16	C	59.8803	120.771549991
18	C	29.3186	150.023354199
20	C	144.0713	40.1890350122
23	C	107.3213	75.3639043626
29	C	147.7026	36.7133750646
32	C	145.0458	39.2563027623
34	C	170.0227	15.3499301288
38	C	93.4978	88.5949195046
42	C	101.6678	80.7750914068
44	C	143.0967	41.1218629759
45	C	148.6483	35.8082084267
47	C	164.0518	21.0649131875
51	C	38.7747	140.972549245
53	C	58.4235	122.165910527
55	C	45.1800	134.841784873
57	C	57.0606	123.470395681
59	C	154.6288	30.0840368307
64	C	144.6474	39.6376270602
67	C	115.2919	67.7349298417
69	C	86.2376	95.5439422654
72	C	142.4579	41.7332835621
76	C	117.1885	65.9196194414
77	C	165.7674	19.4228450009
82	C	105.0992	77.4907636057
86	C	102.5352	79.9448687762
90	C	94.6331	87.508279255
92	C	134.5770	49.2764026876
4	H	29.9568	1.74248094248
5	H	30.3405	1.38794178794
7	H	26.3436	5.08108108108
10	H	27.6835	3.84301224301
11	H	27.3547	4.14682374682
12	H	27.9281	3.617001617
17	H	25.3520	5.99732039732
19	H	24.4932	6.79085239085
21	H	29.3937	2.26278586279
22	H	29.3126	2.33772233772
24	H	28.1951	3.37029337029
26	H	28.2345	3.33388773389
27	H	28.1375	3.42351582352
28	H	27.9280	3.61709401709
30	H	30.1879	1.52894432894
31	H	29.4085	2.24911064911
33	H	29.2429	2.40212520213
35	H	31.0677	0.716008316008
36	H	30.7636	0.996996996997
37	H	30.5567	1.18817278817
39	H	27.6312	3.89133749134
43	H	27.8103	3.72584892585
46	H	29.0537	2.57694617695
48	H	30.9502	0.824578424578
49	H	31.2278	0.568075768076
50	H	30.2786	1.44513744514
52	H	25.9290	5.46417186417
54	H	24.9398	6.37819357819
56	H	25.3159	6.03067683068
58	H	26.1093	5.29757449757
60	H	29.7212	1.96017556018
61	H	28.9976	2.62878262878
62	H	30.1283	1.58401478401
63	H	30.5665	1.17911757912
65	H	29.7888	1.89771309771
66	H	30.5742	1.172002772
70	H	26.0504	5.351998152
71	H	27.8938	3.64869484869
73	H	29.8139	1.87452067452
74	H	30.7761	0.985446985447

78	H	30.8484	0.918641718642
79	H	30.4402	1.29581889582
80	H	30.0507	1.65571725572
81	H	27.7628	3.76973896974
83	H	28.3298	3.24583044583
85	H	29.9072	1.78831138831
88	H	28.2097	3.3568029568
89	H	27.6935	3.83377223377
93	H	28.1205	3.43922383922
94	H	28.8763	2.74086394086
95	H	28.3482	3.22882882883
96	H	27.9734	3.57514437514

Supporting Information: Revised-MandelalideA156ps.log

Using Gaussian 09: AM64L-G09RevC.01 23-Sep-2011

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#Atoms= 96

Charge = 0 Multiplicity = 1

SCF Energy= -2116.25407160

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Optimization incomplete.

Atomic Type	Coordinates (Angstroms) X	Y	Z
C	-7.052260	-0.497286	0.293487
C	-5.911131	0.394184	-0.156430
C	-6.064153	1.800101	0.325879
H	-6.019747	1.848150	1.416134
H	-7.030448	2.183809	-0.007296
C	-5.071183	2.821760	-0.168183
H	-5.107400	2.645193	-1.245950
C	-5.523241	4.306498	0.146467
O	-4.947553	5.170455	-0.709920
H	-4.174420	4.668877	-1.024777
H	-5.166102	4.591160	1.140051
H	-6.595755	4.516509	0.186803
O	-3.798187	2.423448	0.528379
C	-2.653960	3.063336	0.008916
O	-2.672355	3.895701	-0.839957
C	-1.371167	2.593278	0.566708
H	-1.429735	1.809634	1.319475
C	-0.180008	3.123568	0.140176
H	-0.081747	3.911313	-0.602166
C	1.057239	2.632056	0.853269
H	0.669727	2.129767	1.743157
H	1.631567	3.492002	1.202923
C	1.757297	1.543996	0.019746
H	2.027739	2.009540	-0.931495
O	-5.951538	0.343531	-1.625698
H	-5.829459	-0.585600	-1.890109
H	-4.959074	-0.045323	0.149786
H	-8.048065	-0.148068	0.008444
C	-7.027112	-0.712847	1.810296
H	-6.051267	-0.407159	2.193262
H	-7.757726	-0.073082	2.309285
C	-7.327530	-2.176588	2.111854
H	-8.399480	-2.337523	2.245537
C	-6.611764	-2.789273	3.328841
H	-5.590506	-2.402628	3.303000
H	-6.509403	-3.877089	3.350730
H	-7.109799	-2.439846	4.235551
C	-6.842716	-2.865032	0.800456
H	-7.489783	-3.714791	0.570656
O	-6.953902	-1.861722	-0.189245
O	0.953081	0.395912	-0.178649
C	1.467050	-0.578877	-1.092486
H	1.708250	-0.003447	-1.989913
C	0.508193	-1.711394	-1.305053
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H	-1.513036	-0.625455	-1.333702
C	-0.731909	-0.793420	-3.322758
H	-1.671731	-0.778673	-3.878133
H	-0.027946	-1.390951	-3.907257
H	-0.350745	0.228527	-3.279816
C	-1.813150	-2.548291	-2.020481
H	-1.390745	-3.349706	-2.622230
C	-2.931749	-2.750619	-1.320010
H	-3.230399	-1.930953	-0.667603
C	-3.787252	-3.964730	-1.339637
H	-3.629746	-4.619062	-2.195583
C	-4.821706	-4.128831	-0.488156
H	-5.406088	-5.020311	-0.704433
C	-5.285649	-3.224505	0.643851
H	-5.024715	-3.691006	1.596072
H	-4.676213	-2.319924	0.583935
H	0.231335	-2.015710	-0.293352
H	0.951889	-2.505644	-1.908873
C	2.793323	-1.108161	-0.441630
H	3.304543	-1.905010	-0.985927
H	2.513766	-1.591564	0.496085
C	3.802898	0.027227	-0.248619
O	4.846834	-0.564383	0.485153
C	5.914444	0.290192	0.940267
H	5.575806	1.000322	1.708605
H	4.119974	0.424063	-1.216846
C	3.118878	1.206105	0.621628
H	3.787016	2.070117	0.630523
H	3.004413	0.969153	1.681375
O	6.451032	1.128233	-0.085792
C	7.036233	0.342366	-1.181342
C	7.512355	1.307236	-2.321958
H	7.870655	2.292103	-2.015441
H	6.610957	1.318939	-2.938023
H	8.256415	0.762206	-2.906542
H	6.237888	-0.315524	-1.535312
C	8.157689	-0.643774	-0.570804
H	8.935083	-0.079246	-0.048136
O	8.771968	-1.459286	-1.624395
H	9.090752	-2.283575	-1.215090
C	7.610524	-1.545804	0.483009
O	8.675417	-2.325711	1.062482
H	8.995780	-1.788717	1.808821
H	6.890236	-2.216116	0.008329
C	6.978316	-0.618758	1.545340
O	8.033217	0.067893	2.215264
C	7.743144	0.682271	3.479939
H	8.657166	1.122260	3.885356
H	7.378348	-0.099208	4.150500
H	6.995966	1.474124	3.375313
H	6.510866	-1.283147	2.276175

NMR-Shifts

Revised-MandelalideA156ps-NMR.txt

Atom	Type	Isotropic	Scaled Shift
1	C	98.7874	83.5320354524
2	C	109.7412	73.0477229656
3	C	154.2142	30.4808667854

6	C	99.5530	82.7992496028
8	C	115.3807	67.6499358717
14	C	10.4379	168.094814219
16	C	50.9396	129.329045349
18	C	18.8435	160.049484102
20	C	142.3720	41.8155018281
23	C	116.7497	66.3396121672
29	C	149.0550	35.4189398725
32	C	144.4005	39.8739447539
34	C	169.5011	15.8491739888
38	C	97.5748	84.6926625701
42	C	111.5671	71.300082314
44	C	141.4051	42.7409598193
45	C	146.2942	38.0614100576
47	C	166.1342	19.0717663049
51	C	43.4671	136.481268784
53	C	55.7797	124.696395413
55	C	48.8969	131.284193802
57	C	47.5179	132.604088899
59	C	146.5521	37.8145638316
64	C	142.4401	41.7503206417
67	C	112.9218	70.0034457015
69	C	90.7061	91.2669652941
72	C	144.5420	39.7385095427
76	C	105.0842	77.5051206953
77	C	173.4635	12.0566052183
82	C	104.8895	77.6914757174
86	C	112.4180	70.4856524819
90	C	106.7643	75.8970309539
92	C	128.1146	55.4618197132
4	H	30.0106	1.69276969277
5	H	30.4412	1.29489489489
7	H	26.3352	5.08884268884
10	H	25.7709	5.61025641026
11	H	27.5596	3.9574959575
12	H	27.7912	3.7434973435
17	H	25.0634	6.26398706399
19	H	23.4465	7.758004158
21	H	29.3030	2.34659274659
22	H	29.1491	2.4887964888
24	H	28.4428	3.14141834142
26	H	29.2418	2.40314160314
27	H	27.7426	3.7884037884
28	H	27.5988	3.92127512128
30	H	30.7688	0.992192192192
31	H	29.8053	1.88246708247
33	H	29.0388	2.59071379071
35	H	31.0603	0.722845922846
36	H	30.6359	1.11499191499
37	H	30.3871	1.34488334488
39	H	27.4409	4.06717486717
43	H	28.2638	3.30681450681
46	H	29.3604	2.29355509356
48	H	31.0698	0.714067914068
49	H	31.2681	0.530838530839
50	H	30.4603	1.27724647725
52	H	26.2097	5.2048048048
54	H	24.9634	6.35638715639
56	H	24.6590	6.63765303765
58	H	25.9278	5.46528066528
60	H	29.5195	2.14654654655
61	H	28.9056	2.71379071379
62	H	29.8548	1.83672903673
63	H	30.3421	1.38646338646
65	H	30.0829	1.62596442596
66	H	30.6700	1.08348348348
70	H	26.2331	5.18318318318
71	H	27.8135	3.72289212289
73	H	29.5677	2.10200970201
74	H	30.7508	1.00882420882
78	H	30.4734	1.26514206514
79	H	30.0757	1.63261723262
80	H	30.1915	1.52561792562
81	H	27.7445	3.78664818665
83	H	27.9825	3.56673596674
85	H	29.7562	1.92783552784
88	H	29.3257	2.32561792562
89	H	27.9362	3.60951720952
93	H	28.0781	3.4784014784
94	H	28.6501	2.94987294987
95	H	28.1906	3.37445137445
96	H	28.3739	3.20508200508

Supporting Information: Revised-MandelalideA158ps.log

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 Using  Gaussian 09:  AM64L-G09RevC.01 23-Sep-2011
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 density=current SCRF=(PCM,SOLVENT=Chloroform)
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 Pointgroup= C1   Stoichiometry= C33H52O11   C1[X(C33H52O11)]
#Atoms= 96
 Charge = 0                Multiplicity = 1
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 SCF Energy= -2116.24972521
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 Optimization incomplete.


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     Atomic      Coordinates (Angstroms)
      Type      X                Y              Z
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      C      -6.527796     -0.712957      0.609140
      C      -5.909253      0.486955     -0.093732
      C      -5.991245      1.812005      0.772211
      H      -5.732013      1.680228      1.824696
      H      -7.013340      2.186848      0.686476
      C      -5.099061      2.854587      0.183010
      H      -5.213212      2.788292     -0.902647
      C      -5.488926      4.333511      0.557621
      O      -4.915058      5.329229     -0.329079
      H      -4.049179      4.989052     -0.617428
      H      -5.058174      4.609502      1.523772
      H      -6.572736      4.408895      0.673835
      O      -3.745198      2.564913      0.590832
      C      -2.686598      3.172295      0.097199
      O      -2.691594      4.079216     -0.744239
      C      -1.376074      2.698395      0.613376
      H      -1.345887      1.858919      1.305983
      C      -0.244446      3.089637      0.068908
      H      -0.257708      3.991180     -0.538514
      C       1.180634      2.670485      0.477891
      H       1.117803      2.457565      1.546834
      H       1.853902      3.502659      0.259696
      C       1.770342      1.496577     -0.316666
      H       2.038937      1.821302     -1.324292
      O      -6.536759      0.750172     -1.265144
      H      -6.545125     -0.056037     -1.811678
      H      -4.843050      0.323324     -0.268297
      H      -7.607764     -0.566614      0.696929
      C      -6.001170     -1.106578      2.062083
      H      -4.938501     -0.897099      2.201903
      H      -6.578464     -0.544916      2.799910
      C      -6.334150     -2.517300      2.213086
      H      -7.351848     -2.629049      2.592669
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C	-5.327521	-3.190347	3.221213
H	-4.353161	-2.880537	2.837688
H	-5.309990	-4.281106	3.253552
H	-5.461602	-2.723486	4.198958
C	-6.403566	-3.056241	0.694236
H	-7.325583	-3.621103	0.532013
O	-6.349149	-1.858462	-0.151439
O	0.806936	0.426812	-0.328623
C	1.195917	-0.634683	-1.165577
H	1.329598	-0.302199	-2.198414
C	0.012508	-1.624483	-1.233215
C	-1.348665	-1.042198	-1.750257
H	-1.778114	-0.389376	-0.986165
C	-1.246966	-0.161530	-3.028970
H	-2.173599	-0.148179	-3.605907
H	-0.538450	-0.682086	-3.678221
H	-0.910546	0.872075	-2.923680
C	-2.291356	-2.132210	-2.216452
H	-1.871035	-2.800600	-2.962316
C	-3.354477	-2.426193	-1.473369
H	-3.667182	-1.852895	-0.601567
C	-4.088377	-3.661984	-1.827598
H	-3.821069	-4.096460	-2.788711
C	-4.923065	-4.330946	-1.082334
H	-5.379236	-5.275604	-1.368116
C	-5.162036	-3.970977	0.416588
H	-5.272028	-4.868339	1.028243
H	-4.241977	-3.489194	0.756204
H	-0.023111	-1.968631	-0.196899
H	0.387582	-2.508430	-1.753562
C	2.525592	-1.279942	-0.656543
H	2.846239	-1.917227	-1.483842
H	2.179013	-1.874769	0.191325
C	3.633164	-0.246630	-0.372033
O	4.720110	-0.883776	0.354013
C	5.714249	-0.055947	0.969837
H	5.260897	0.475836	1.818484
H	4.073064	0.161691	-1.285024
C	3.033471	0.905169	0.405659
H	3.750586	1.727035	0.442213
H	2.803025	0.604407	1.429540
O	6.237251	0.890941	0.008995
C	6.952803	0.486456	-1.092215
C	7.429904	1.806269	-1.862843
H	8.177470	2.357312	-1.288985
H	6.503976	2.320622	-2.131103
H	7.906376	1.561011	-2.814624
H	6.372427	-0.113979	-1.797459
C	8.173049	-0.421451	-0.627292
H	8.848448	0.279095	-0.129685
O	8.687816	-1.094136	-1.731867
H	9.048082	-1.983113	-1.561731
C	7.604148	-1.490556	0.293626
O	8.728325	-2.296450	0.723079
H	8.981621	-1.852535	1.551851
H	6.905328	-2.128818	-0.253630
C	6.918667	-0.938583	1.525330
O	7.911516	-0.242749	2.327078
C	7.530501	0.680917	3.344835
H	8.462989	1.050136	3.780502
H	6.917744	0.255295	4.143603
H	6.978481	1.571465	3.035482
H	6.435300	-1.676157	2.170771

NMR-Shifts

Revised-MandelalideA158ps-NMR.txt

Atom	Type	Isotropic	Scaled Shift
1	C	99.8466	82.5182335037
2	C	116.2319	66.8352188978
3	C	147.7774	36.6417810448
6	C	105.0611	77.5272306131
8	C	110.2685	72.5430234116
14	C	8.8608	169.604318613
16	C	58.0351	122.537663432
18	C	27.8807	151.399624801
20	C	144.8093	39.4826662072
23	C	108.4569	74.2769769712
29	C	145.1972	39.111391872
32	C	147.2522	37.1444706063
34	C	165.9194	19.2773598269
38	C	91.4625	90.5429851261
42	C	111.5922	71.2760581175
44	C	143.3334	40.8953081031
45	C	148.8893	35.5775378549
47	C	168.3262	16.9737169548
51	C	36.0592	143.57166102
53	C	52.8788	127.472960815
55	C	49.8107	130.409559907
57	C	61.1930	119.51511323
59	C	147.8466	36.5755470051
64	C	150.0830	34.43500067
67	C	111.1983	71.6530752886
69	C	84.4406	97.2639215911
72	C	146.4918	37.8722793315
76	C	108.1515	74.5692873141
77	C	163.5544	21.5409942763
82	C	111.9398	70.9433564961
86	C	110.8116	72.0232010567
90	C	105.4214	77.1823733226
92	C	134.1009	49.7320967094
4	H	29.9916	1.71032571033
5	H	30.4986	1.24185724186
7	H	26.4214	5.00919380919
10	H	25.0612	6.26601986602
11	H	27.3842	4.11956571957
12	H	28.2058	3.36040656041
17	H	25.6469	5.72483252483
19	H	24.0196	7.22845922846
21	H	29.1111	2.52390852391
22	H	29.1716	2.46800646801
24	H	28.3757	3.20341880342
26	H	29.6258	2.04832524833
27	H	27.9951	3.55509355509
28	H	28.0050	3.54594594595
30	H	30.5844	1.16257796258
31	H	29.6131	2.06006006006
33	H	29.3400	2.3124047124
35	H	31.0371	0.744282744283
36	H	30.5709	1.17505197505
37	H	30.4465	1.28999769
39	H	27.2469	4.24643104643
43	H	28.3201	3.25479325479
46	H	29.2798	2.36802956803
48	H	31.1238	0.664171864172
49	H	31.1864	0.606329406329
50	H	30.6661	1.08708708709
52	H	25.6521	5.72002772003
54	H	24.4151	6.86301686302
56	H	25.5457	5.81834141834
58	H	26.2020	5.21191961192
60	H	30.2362	1.48431508432
61	H	29.1459	2.49175329175
62	H	30.6074	1.14132594133
63	H	31.0134	0.766181566182
65	H	30.1982	1.51942711943
66	H	30.6596	1.09309309309
70	H	25.7551	5.62485562486
71	H	27.4306	4.07669207669

73	H	29.5535	2.11513051513
74	H	30.7145	1.04236544237
78	H	30.5697	1.17616077616
79	H	30.2492	1.4723030723
80	H	30.2780	1.44569184569
81	H	28.2126	3.35412335412
83	H	28.1535	3.40873180873
85	H	29.1810	2.45932085932
88	H	29.4907	2.17315777316
89	H	27.9448	3.60157080157
93	H	28.2287	3.33924693925
94	H	28.6286	2.96973896974
95	H	28.4875	3.10011550012
96	H	27.9450	3.60138600139

Supporting Information: Revised-MandelalideA160ps.log

Using Gaussian 09: AM64L-G09RevC.01 23-Sep-2011

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#mPW1PW91/6-311+G(2d,p) scf=(maxcycle=300,direct,tight) NMR density=current SCRF=(PCM,SOLVENT=Chloroform)

Pointgroup= C1 Stoichiometry= C33H52O11 C1[X(C33H52O11)]

#Atoms= 96

Charge = 0 Multiplicity = 1

SCF Energy= -2116.24232132

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Optimization incomplete.

Atomic Type	Coordinates (Angstroms) X	Y	Z
C	-6.679529	-0.702963	0.428213
C	-5.883678	0.533995	-0.045214
C	-6.256225	1.936453	0.522289
H	-6.155169	1.885997	1.609175
H	-7.334554	2.022727	0.374213
C	-5.278292	2.957154	-0.073656
H	-5.166381	2.834621	-1.154146
C	-5.795702	4.350322	0.303034
O	-5.387589	5.255651	-0.708664
H	-4.596431	4.908344	-1.158497
H	-5.317847	4.544888	1.266800
H	-6.858475	4.401145	0.553488
O	-3.929332	2.758223	0.503560
C	-2.843555	3.185047	-0.219953
O	-2.956506	3.778737	-1.293330
C	-1.594297	2.737152	0.446275
H	-1.884776	2.156138	1.320274
C	-0.350776	3.084641	0.051928
H	-0.393971	3.842530	-0.725299
C	0.929292	2.619458	0.702769
H	0.681053	2.098449	1.630336
H	1.576092	3.474129	0.915558
C	1.660212	1.618612	-0.210875
H	1.882013	2.028490	-1.199762
O	-5.927858	0.607967	-1.431248
H	-5.699684	-0.268369	-1.790808
H	-4.832800	0.360874	0.201219
H	-7.737723	-0.608967	0.171209
C	-6.400514	-0.931630	1.884366
H	-5.312985	-0.859744	1.948436
H	-6.838893	-0.349045	2.697095
C	-6.703062	-2.375167	2.082878
H	-7.778209	-2.561683	2.141644
C	-6.010173	-2.836227	3.387269
H	-4.929354	-2.689023	3.336460
H	-6.234873	-3.900231	3.482181
H	-6.382982	-2.281069	4.250854
C	-6.271912	-3.049896	0.738220
H	-7.086292	-3.653660	0.328840
O	-6.268523	-1.928518	-0.185633
O	0.871289	0.429493	-0.485709
C	1.519715	-0.664797	-1.200454
H	1.768806	-0.290409	-2.197637
C	0.546862	-1.841658	-1.354682
C	-0.962289	-1.475216	-1.653588
H	-1.365593	-0.934372	-0.794370
C	-1.162559	-0.577212	-2.909201
H	-2.162081	-0.626213	-3.344875
H	-0.498344	-0.779118	-3.752348
H	-0.997942	0.465930	-2.631502
C	-1.920993	-2.686984	-1.797457
H	-1.403910	-3.455739	-2.364900
C	-3.147931	-2.883228	-1.254451
H	-3.667461	-2.064286	-0.757521
C	-3.899727	-4.104450	-1.389496
H	-3.599526	-4.668882	-2.270493
C	-4.752407	-4.521768	-0.506243
H	-5.351426	-5.418302	-0.646378
C	-5.023106	-3.845684	0.847682
H	-5.122560	-4.625590	1.605297
H	-4.215752	-3.123327	0.989001
H	0.589336	-2.403274	-0.418693
H	0.891033	-2.505605	-2.149172
C	2.812993	-1.089302	-0.518040
H	3.362633	-1.694193	-1.240700
H	2.614871	-1.657920	0.393300
C	3.722936	0.081729	-0.362221
O	4.897990	-0.499982	0.313742
C	5.861509	0.510145	0.702631
H	5.315985	1.287608	1.257861
H	4.027655	0.494949	-1.326734
C	2.963849	1.179215	0.419848
H	3.629360	2.025421	0.600462
H	2.620663	0.703305	1.340717
O	6.472057	0.993180	-0.505559
C	7.222477	0.002474	-1.314270
C	7.758135	0.600205	-2.643873
H	8.521650	1.341753	-2.398082
H	6.918194	1.045161	-3.183060
H	8.200799	-0.252108	-3.163520
H	6.446571	-0.673075	-1.682351
C	8.217095	-0.824525	-0.458965
H	9.024264	-0.199628	-0.068727
O	8.688219	-1.912521	-1.240384
H	9.032183	-2.584522	-0.624805
C	7.447950	-1.353307	0.810248
O	8.403614	-1.984806	1.693777
H	8.543814	-1.357055	2.425247
H	6.703574	-2.038679	0.398909
C	6.859544	-0.179410	1.678448
O	7.964667	0.730394	2.174725
C	7.603635	1.580588	3.260749
H	8.507055	2.079104	3.621894
H	7.167335	0.902954	3.999646
H	6.819344	2.230228	2.864181
H	6.320634	-0.635801	2.512605

NMR-Shifts

Revised-MandelalideA160ps-NMR.txt

Atom	Type	Isotropic	Scaled Shift
1	C	103.3535	79.1616416853

2	C	109.4179	73.357166102
3	C	152.5355	32.0876165317
6	C	103.2022	79.3064568617
8	C	113.4770	69.472041961
14	C	3.6034	174.636382779
16	C	52.7498	127.596431785
18	C	28.6630	150.650854725
20	C	144.6421	39.6426998985
23	C	111.1227	71.7254350198
29	C	146.0192	38.3246233657
32	C	144.7778	39.5128160953
34	C	168.6478	16.6659009552
38	C	103.2590	79.2520913494
42	C	110.8000	72.0343038726
44	C	143.9748	40.2813989548
45	C	147.4580	36.9474913379
47	C	169.3815	15.9636478493
51	C	32.3920	147.081682268
53	C	56.2463	124.249794215
55	C	60.0472	120.611803442
57	C	58.1728	122.40586535
59	C	152.5972	32.0285610368
64	C	148.3636	36.0807059859
67	C	109.6588	73.1265912441
69	C	89.1322	92.7734068416
72	C	146.8347	37.5440762649
76	C	109.6038	73.1792339057
77	C	168.9699	16.357606386
82	C	108.7591	73.9877294741
86	C	105.5270	77.0812994123
90	C	91.2419	90.7541300561
92	C	126.4446	57.0602423477
4	H	30.1921	1.52506352506
5	H	29.9462	1.75227535228
7	H	25.8539	5.53356433356
10	H	28.5083	3.0808962809
11	H	28.1875	3.37731577732
12	H	28.0571	3.49780549781
17	H	25.2603	6.08205128205
19	H	23.8824	7.35523215523
21	H	29.1240	2.51198891199
22	H	29.0890	2.54432894433
24	H	28.1392	3.42194502195
26	H	29.5091	2.15615615616
27	H	28.2536	3.31623931624
28	H	28.0301	3.52275352275
30	H	30.8785	0.890829290829
31	H	29.6998	1.97994917995
33	H	29.3360	2.3161007161
35	H	31.0339	0.74723954724
36	H	30.6507	1.10131670132
37	H	30.6036	1.14483714484
39	H	27.4957	4.01653961654
43	H	28.1795	3.38470778471
46	H	29.1879	2.45294525295
48	H	31.2884	0.512081312081
49	H	31.0166	0.763224763225
50	H	30.4665	1.27151767152
52	H	25.7316	5.64656964657
54	H	24.7054	6.59477939478
56	H	25.3671	5.98336798337
58	H	26.3391	5.08523908524
60	H	29.7356	1.94686994687
61	H	28.9798	2.64522984523
62	H	30.3032	1.42240702241
63	H	30.3286	1.39893739894
65	H	29.8593	1.83257103257
66	H	30.5406	1.20304920305
70	H	25.5271	5.83552783553
71	H	27.5660	3.95158235158
73	H	29.4482	2.21242781243
74	H	30.8695	0.899145299145
78	H	30.7250	1.03266343266
79	H	30.2678	1.45511665512
80	H	30.1963	1.52118272118
81	H	27.7442	3.78692538693
83	H	27.9925	3.5574959575
85	H	29.7708	1.91434511435
88	H	29.4314	2.22795102795
89	H	27.4050	4.10034650035
93	H	27.7175	3.8115962116
94	H	28.1790	3.38516978517
95	H	27.7129	3.81584661585
96	H	28.0110	3.5404019404

Supporting Information: Revised-MandelalideA162ps.log

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 Using  Gaussian 09:  AM64L-G09RevC.01 23-Sep-2011
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 density=current SCRF=(PCM,SOLVENT=Chloroform)
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#Atoms= 96
 Charge = 0                Multiplicity = 1
-----------------------------------------------------------------------
 SCF Energy= -2116.23982118
=======================================================================
 Optimization incomplete.


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     Atomic      Coordinates (Angstroms)
      Type      X                Y              Z
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      C      -6.540508     -0.863128      0.328982
      C      -5.693522      0.371400     -0.172845
      C      -5.952244      1.668702      0.685810
      H      -5.776287      1.617291      1.762436
      H      -7.012381      1.908535      0.584193
      C      -5.083801      2.803314      0.142343
      H      -5.062516      2.834337     -0.950090
      C      -5.698790      4.168796      0.575767
      O      -4.976570      5.276387     -0.100387
      H      -4.103986      4.988897     -0.423116
      H      -5.543874      4.342051      1.644204
      H      -6.761155      4.380247      0.431350
      O      -3.742177      2.619169      0.666020
      C      -2.741690      3.294502      0.054056
      O      -2.827804      3.947700     -0.985722
      C      -1.465793      2.994309      0.752974
      H      -1.597918      2.478607      1.703955
      C      -0.326673      3.394222      0.180289
      H      -0.357058      4.003386     -0.719514
      C       1.093420      3.153339      0.688974
      H       1.188524      2.962458      1.760044
      H       1.703137      4.054186      0.591975
      C       1.699382      1.917999     -0.048545
      H       2.173819      2.199196     -0.992349
      O      -6.024130      0.619197     -1.560524
      H      -6.065206     -0.264920     -1.967484
      H      -4.611820      0.217309     -0.165518
      H      -7.620314     -0.719576      0.239707
      C      -6.246613     -1.189144      1.783970
      H      -5.184497     -1.002605      1.953605
      H      -6.849985     -0.513914      2.394950
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C	-6.665137	-2.659742	1.833236
H	-7.748341	-2.524960	1.886529
C	-6.256301	-3.269069	3.162178
H	-5.220257	-3.199519	3.501504
H	-6.306605	-4.340010	2.953658
H	-6.989529	-3.001952	3.925286
C	-6.163764	-3.293128	0.532454
H	-6.881496	-3.992880	0.097717
O	-6.042523	-2.129653	-0.378686
O	0.756598	0.816135	-0.224212
C	1.316601	-0.246228	-1.045498
H	1.750140	0.130980	-1.974528
C	0.343460	-1.368777	-1.446354
C	-1.014612	-0.923733	-2.068654
H	-1.526904	-0.209693	-1.420388
C	-0.839091	-0.199991	-3.393724
H	-1.828018	0.072091	-3.767811
H	-0.270859	-0.833535	-4.078654
H	-0.305531	0.747493	-3.304052
C	-1.916275	-2.180215	-2.274590
H	-1.998301	-2.579590	-3.283046
C	-2.642846	-2.791054	-1.256511
H	-2.649073	-2.316730	-0.275757
C	-3.462611	-3.948995	-1.581896
H	-3.221464	-4.465568	-2.509561
C	-4.300189	-4.580292	-0.749065
H	-4.772561	-5.527235	-0.999813
C	-4.804973	-4.010640	0.587500
H	-4.882974	-4.878424	1.247288
H	-4.042949	-3.381556	1.052985
H	0.144772	-1.896313	-0.510886
H	0.868996	-1.984584	-2.179495
C	2.426615	-0.888429	-0.292562
H	2.825390	-1.752134	-0.828847
H	2.056934	-1.283996	0.655464
C	3.495749	0.189023	-0.019445
O	4.462092	-0.493134	0.830527
C	5.748356	0.089627	1.214381
H	5.525789	0.647645	2.135863
H	4.034756	0.502782	-0.918266
C	2.938731	1.444647	0.724860
H	3.704301	2.213556	0.847232
H	2.703107	1.100430	1.733641
O	6.220613	1.045588	0.159088
C	6.705480	0.469412	-1.124822
C	7.224277	1.641783	-1.945971
H	8.059090	2.053125	-1.374039
H	6.499516	2.450917	-2.061818
H	7.640859	1.400895	-2.926370
H	5.922938	-0.004179	-1.723548
C	7.816704	-0.510570	-0.739019
H	8.644635	-0.078484	-0.171488
O	8.281830	-1.212881	-1.891476
H	8.391009	-2.147475	-1.640027
C	7.268461	-1.627816	0.131227
O	8.339517	-2.492614	0.437218
H	8.591774	-2.055366	1.270688
H	6.479944	-2.172207	-0.394442
C	6.709510	-1.108268	1.459743
O	7.889695	-0.716815	2.263921
C	7.750612	0.121888	3.384323
H	8.733258	0.360575	3.799956
H	7.093345	-0.386318	4.095395
H	7.306072	1.105456	3.211077
H	6.121089	-1.873832	1.972662

NMR-Shifts
Revised-MandelalideA162ps-NMR.txt

Atom	Type	Isotropic	Scaled Shift
1	C	88.5969	93.28576351
2	C	105.1009	77.4891364689
3	C	150.2864	34.240318536
6	C	110.6431	72.1844790291
8	C	108.0288	74.6867283064
14	C	3.7640	174.482666207
16	C	57.7415	122.818679531
18	C	28.3218	150.977430655
20	C	145.1730	39.1345546431
23	C	111.3266	71.5302743161
29	C	144.5877	39.6947682766
32	C	147.6079	36.8040161565
34	C	175.7273	9.88983326633
38	C	102.6796	79.806657861
42	C	111.1121	71.7355806964
44	C	134.7915	49.0710963074
45	C	148.7156	35.7437929516
47	C	169.6548	15.7020616781
51	C	21.6092	157.402323934
53	C	44.0922	135.882961006
55	C	47.3787	132.73732269
57	C	53.7848	126.605792607
59	C	153.7354	30.9391450832
64	C	143.5504	40.6876088746
67	C	107.3680	75.3192059572
69	C	78.3224	103.119891269
72	C	140.7293	43.3877945596
76	C	106.1654	76.4702616819
77	C	168.7150	16.6015811941
82	C	112.6092	70.3026474473
86	C	114.1441	68.8335343326
90	C	102.9560	79.5421045579
92	C	133.8103	50.0102413905
4	H	29.9437	1.75458535459
5	H	30.4329	1.30256410256
7	H	25.9554	5.43977823978
10	H	27.5594	3.95768075768
11	H	27.7224	3.80706860707
12	H	27.6854	3.84125664126
17	H	25.2246	6.11503811504
19	H	23.8863	7.35162855163
21	H	29.3701	2.28459228459
22	H	29.1111	2.52390852391
24	H	28.1427	3.41871101871
26	H	29.7725	1.91277431277
27	H	27.4761	4.03465003465
28	H	27.9133	3.63067683068
30	H	30.4731	1.26541926542
31	H	30.1245	1.58752598753
33	H	29.2898	2.35878955879
35	H	30.9511	0.823746823747
36	H	30.8815	0.888057288057
37	H	30.6438	1.10769230769
39	H	27.7706	3.76253176253
43	H	28.5241	3.0662970663
46	H	29.1398	2.49738969739
48	H	30.6759	1.07803187803
49	H	31.1318	0.65677985678
50	H	30.8037	0.959944559945
52	H	25.1998	6.13795333795
54	H	24.4290	6.85017325017
56	H	25.1290	6.20337260337
58	H	25.9124	5.47951027951
60	H	30.1645	1.55056595057
61	H	29.4290	2.23016863017
62	H	30.0799	1.62873642874
63	H	30.4514	1.28547008547
65	H	30.1286	1.58373758374
66	H	30.5798	1.16682836683

70	H	25.3848	5.96701316701
71	H	27.5505	3.9659043659
73	H	29.2846	2.36359436359
74	H	30.6721	1.08154308154
78	H	30.9477	0.826888426888
79	H	30.5289	1.21386001386
80	H	30.1886	1.5282975283
81	H	27.7695	3.76354816355
83	H	28.3190	3.25580965581
85	H	29.4505	2.2103026103
88	H	28.1198	3.43987063987
89	H	28.2314	3.33675213675
93	H	28.0042	3.54668514669
94	H	28.3620	3.21607761608
95	H	28.4022	3.17893277893
96	H	27.8870	3.65497805498

Supporting Information: Revised-MandelalideA164ps.log

Using Gaussian 09: AM64L-G09RevC.01 23-Sep-2011

==========

#mPWPW91/6-311+G(2d,p) scf=(maxcycle=300,direct,tight) NMR density=current

SCRF=(PCM,SOLVENT=Chloroform)

Pointgroup= C1 Stoichiometry= C33H52O11 C1[X(C33H52O11)]

#Atoms= 96

Charge = 0 Multiplicity = 1

SCF Energy= -2116.45813272

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Optimization incomplete.

Atomic Type	Coordinates (Angstroms) X	Y	Z
C	-6.399374	-0.715015	0.370803
C	-5.420825	0.301568	-0.327924
C	-5.923646	1.678927	0.072542
H	-6.150261	1.700472	1.141008
H	-6.885487	1.921682	-0.383604
C	-4.970138	2.847613	-0.304528
H	-4.748124	2.743067	-1.368995
C	-5.640713	4.248253	-0.077855
O	-4.993085	5.242503	-0.882654
H	-4.078079	4.910297	-0.844303
H	-5.511388	4.603806	0.947834
H	-6.704391	4.181595	-0.318970
O	-3.905028	2.663554	0.623656
C	-2.742855	3.242054	0.261890
O	-2.566142	4.173574	-0.467987
C	-1.564760	2.756513	1.050429
H	-1.622302	1.974084	1.805974
C	-0.293044	3.140731	0.761120
H	-0.185343	3.925032	0.015840
C	0.963598	2.657989	1.416634
H	0.587764	2.126341	2.293646
H	1.566105	3.497489	1.770979
C	1.577793	1.713535	0.364719
H	1.761923	2.312167	-0.530717
O	-5.540672	0.171709	-1.745520
H	-5.353383	-0.765208	-1.932761
H	-4.428227	0.238556	0.122954
H	-7.445566	-0.541899	0.104288
C	-6.330459	-0.875547	1.902185
H	-5.406754	-0.443300	2.291629
H	-7.164905	-0.396812	2.417204
C	-6.461976	-2.414375	2.166284
H	-7.497769	-2.668316	2.402222
C	-5.593340	-2.910830	3.348249
H	-4.545603	-2.813993	3.057730
H	-5.943636	-3.914633	3.597081
H	-5.731803	-2.271007	4.222505
C	-6.222393	-3.093396	0.805489
H	-7.095862	-3.619806	0.413245
O	-6.118232	-2.066671	-0.199036
O	0.680485	0.597969	0.080913
C	1.094438	-0.289489	-1.018947
H	1.210018	0.320235	-1.918023
C	0.134793	-1.457150	-1.348605
C	-1.247490	-1.017957	-1.848365
H	-1.698964	-0.355896	-1.107151
C	-1.076386	-0.164628	-3.168895
H	-2.034137	-0.022709	-3.673414
H	-0.477470	-0.857998	-3.763705
H	-0.573116	0.795783	-3.036510
C	-2.036132	-2.283899	-2.131639
H	-1.801945	-2.762900	-3.078234
C	-3.019696	-2.764196	-1.345396
H	-3.270109	-2.148438	-0.483259
C	-3.782544	-3.942218	-1.591481
H	-3.799364	-4.264164	-2.631405
C	-4.683533	-4.441908	-0.676215
H	-5.214618	-5.336874	-0.988550
C	-4.926396	-3.999476	0.718410
H	-5.028112	-4.769448	1.486380
H	-4.075518	-3.390487	1.028682
H	-0.019732	-2.044083	-0.440689
H	0.715972	-1.972036	-2.116760
C	2.454210	-0.849635	-0.656521
H	2.820000	-1.452422	-1.490565
H	2.358725	-1.466633	0.239205
C	3.447226	0.114983	-0.267828
O	4.547362	-0.655061	0.350474
C	5.681013	0.097048	0.960628
H	5.293094	0.601076	1.858469
H	3.762404	0.670668	-1.154328
C	2.886448	1.071735	0.825250
H	3.592727	1.903069	0.876107
H	2.926149	0.507519	1.759951
O	6.287215	1.025372	-0.028188
C	6.896093	0.487675	-1.219827
C	7.441786	1.613922	-2.113173
H	8.312519	2.160034	-1.744283
H	6.657437	2.365476	-2.228335
H	7.666524	1.110080	-3.055339
H	6.093284	0.065373	-1.829730
C	7.989122	-0.602152	-0.811018
H	8.865718	-0.172599	-0.320447
O	8.486233	-1.352430	-1.964267
H	8.168174	-2.264864	-1.840427
C	7.264930	-1.634065	0.146362
O	8.333487	-2.421518	0.627444
H	8.870215	-1.890430	1.242554
H	6.508300	-2.270416	-0.319931
C	6.779156	-0.886673	1.434710
O	7.915789	-0.271553	2.111279
C	7.568111	0.505590	3.362827
H	8.483291	0.998553	3.700049
H	7.136780	-0.139291	4.133217
H	6.817441	1.272714	3.156230
H	6.240002	-1.561265	2.104668

NMR-Shifts

Revised-MandelalideA164ps-NMR.txt

Atom	Type	Isotropic	Scaled Shift
1	C	83.1927	98.4583357262
2	C	106.1096	76.5236700549
3	C	138.7627	45.270104711
6	C	101.4734	80.9611592871
8	C	104.3769	78.1821053236
14	C	11.8982	166.697103696
16	C	49.5896	130.621183407
18	C	17.5955	161.243993951
20	C	140.5339	43.5748195792
23	C	102.9790	79.520090354
29	C	141.1324	43.001971707
32	C	137.1724	46.7922433431
34	C	166.2477	18.9631309941
38	C	93.2981	88.7860602232
42	C	100.5784	81.8177989625
44	C	129.4433	54.1900687226
45	C	139.9740	44.1107218745
47	C	159.7550	25.1775493405
51	C	35.3266	144.272861272
53	C	53.1681	127.196060415
55	C	45.2638	134.7615766
57	C	45.0842	134.933478819
59	C	145.7309	38.6005666265
64	C	142.2592	41.9234671414
67	C	104.4415	78.1202741247
69	C	69.1260	111.922127146
72	C	141.3653	42.7790539635
76	C	99.1745	83.1615268286
77	C	163.8979	21.2122169261
82	C	91.2720	90.7253201631
86	C	102.2514	80.2165049101
90	C	95.1521	87.0115239572
92	C	117.9319	65.2080820843
4	H	30.2114	1.50723030723
5	H	30.2894	1.43515823516
7	H	26.7130	4.73975513976
10	H	25.9746	5.42203742204
11	H	27.3773	4.12594132594
12	H	28.0031	3.5477015477
17	H	25.3896	5.96257796258
19	H	24.0030	7.2437976438
21	H	29.2172	2.42587202587
22	H	28.8479	2.76710556711
24	H	28.1028	3.45557865558
26	H	29.3171	2.33356433356
27	H	27.8229	3.71420651421
28	H	27.2161	4.27489027489
30	H	30.3860	1.3458997459
31	H	29.0794	2.5531993532
33	H	28.5154	3.07433587434
35	H	30.2666	1.45622545623
36	H	30.5129	1.22864402864
37	H	30.7992	0.964102564103
39	H	27.1192	4.36442596443
43	H	28.0197	3.53236313236
46	H	29.1932	2.44804804805
48	H	30.6449	1.10667590668
49	H	31.2739	0.525479325479
50	H	30.1766	1.53938553939
52	H	26.1405	5.26874566875
54	H	24.4436	6.83668283668
56	H	24.8102	6.49794409794
58	H	25.7930	5.58983598984
60	H	29.6465	2.0291984292
61	H	28.8047	2.80702240702
62	H	29.8000	1.88736428736
63	H	30.4692	1.26902286902
65	H	30.1070	1.6036960037
66	H	30.4999	1.24065604066
70	H	24.7668	6.53804573805
71	H	27.6650	3.86010626011
73	H	29.4772	2.18563178563
74	H	30.4088	1.32483252483
78	H	30.6739	1.07987987988
79	H	30.5008	1.23982443982
80	H	30.0921	1.61746361746
81	H	27.3477	4.15329175329
83	H	27.7553	3.77666897667
85	H	30.4062	1.32723492723
88	H	29.3429	2.30972510973
89	H	27.5260	3.98854238854
93	H	27.8956	3.64703164703
94	H	28.2981	3.27512127512
95	H	27.8310	3.70672210672
96	H	27.8736	3.66735966736

Supporting Information: Revised-MandelalideA166ps.log

Using Gaussian 09: AM64L-G09RevC.01 23-Sep-2011

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#mPWPW91/6-311+G(2d,p) scf=(maxcycle=300,direct,tight) NMR density=current

SCRF=(PCM,SOLVENT=Chloroform)

Pointgroup= C1 Stoichiometry= C33H52O11 C1[X(C33H52O11)]

#Atoms= 96

Charge = 0 Multiplicity = 1

SCF Energy= -2116.46287816

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Optimization incomplete.

Atomic Type	Coordinates (Angstroms) X	Y	Z
C	-6.652977	-1.042038	0.226749
C	-5.556528	0.081587	-0.219008
C	-6.096908	1.535720	0.262750
H	-6.171672	1.461463	1.349024
H	-7.041683	1.790817	-0.222219
C	-5.111356	2.666467	-0.098647
H	-4.682152	2.491335	-1.088886
C	-5.873719	3.993367	0.046174
O	-5.413812	5.069994	-0.770971
H	-4.441966	5.124123	-0.783993
H	-5.857455	4.304563	1.093983
H	-6.862550	3.781841	-0.370394
O	-4.028868	2.674550	0.889855
C	-2.840661	3.289062	0.527500
O	-2.716404	4.007842	-0.465221
C	-1.731862	2.857078	1.351043
H	-1.872724	2.102736	2.123282
C	-0.456461	3.158842	0.964288
H	-0.389339	3.670309	0.007758
C	0.797229	2.585199	1.638958
H	0.496019	1.858300	2.397012
H	1.410644	3.388424	2.051729
C	1.611138	1.870404	0.515189
H	1.861435	2.567521	-0.288374
O	-5.371229	0.011570	-1.659775
H	-5.603216	-0.927292	-1.775635
H	-4.606747	-0.104111	0.288821

H	-7.685722	-0.752294	0.014000
C	-6.439583	-1.389648	1.694096
H	-5.371250	-1.419078	1.920242
H	-7.011355	-0.744848	2.364814
C	-6.928307	-2.852967	1.682662
H	-8.012163	-2.968103	1.609978
C	-6.501052	-3.669491	2.888288
H	-5.466150	-3.518638	3.204354
H	-6.533258	-4.751282	2.739427
H	-7.157274	-3.314039	3.684314
C	-6.238249	-3.420628	0.339190
H	-6.773663	-4.228362	-0.165147
O	-6.113557	-2.203704	-0.486228
O	0.767705	0.772007	0.073092
C	1.247587	0.241394	-1.226095
H	1.377449	1.105684	-1.882295
C	0.283453	-0.826444	-1.816053
C	-1.211771	-0.404423	-1.722089
H	-1.256675	-0.219458	-0.646892
C	-1.527595	0.882821	-2.448734
H	-2.518226	1.295398	-2.244529
H	-1.285321	0.752576	-3.505611
H	-0.862522	1.652665	-2.052576
C	-2.024210	-1.581312	-2.174149
H	-1.885316	-1.998241	-3.168617
C	-2.770787	-2.264749	-1.272167
H	-2.888527	-1.842025	-0.274904
C	-3.275698	-3.629676	-1.596737
H	-3.082116	-3.985730	-2.607584
C	-4.092833	-4.331937	-0.823553
H	-4.408484	-5.273425	-1.265056
C	-4.754836	-3.908969	0.514904
H	-4.871813	-4.823740	1.099938
H	-4.140455	-3.184858	1.053189
H	0.469316	-1.787734	-1.332368
H	0.428545	-0.977551	-2.887981
C	2.615833	-0.410467	-1.015631
H	3.039742	-0.847372	-1.922182
H	2.440919	-1.327244	-0.449795
C	3.631247	0.443093	-0.132173
O	4.673568	-0.499133	0.337567
C	5.865139	0.137226	0.919229
H	5.538136	0.722049	1.791302
H	4.082027	1.201220	-0.778072
C	2.970815	1.217317	1.009685
H	3.675697	1.995660	1.308786
H	2.765956	0.545184	1.844683
O	6.614847	1.012351	-0.019250
C	7.241102	0.420694	-1.294823
C	8.148307	1.466062	-1.908890
H	8.651542	1.989142	-1.093315
H	7.480772	2.173527	-2.404583
H	8.785589	1.028097	-2.680295
H	6.465491	0.155560	-2.018994
C	8.094774	-0.830088	-0.932958
H	9.097079	-0.476576	-0.679754
O	8.242388	-1.653396	-2.083805
H	8.151078	-2.591846	-1.839099
C	7.380831	-1.741153	0.157001
O	8.358838	-2.561391	0.611964
H	8.742020	-2.184021	1.424433
H	6.692418	-2.413100	-0.362723
C	6.799217	-0.966422	1.336240
O	7.919219	-0.586596	2.205315
C	7.585713	0.087141	3.461150
H	8.472762	0.140092	4.098091
H	6.747941	-0.389661	3.977617
H	7.131823	1.061231	3.261107
H	6.151884	-1.640029	1.903319

NMR-Shifts

Revised-MandelalideA166ps-NMR.txt

Atom	Type	Isotropic	Scaled Shift
1	C	87.7864	94.0615249143
2	C	86.4634	95.327820211
3	C	135.6001	48.2971534677
6	C	97.4797	84.7836865177
8	C	100.9689	81.444036065
14	C	5.7368	172.594421792
16	C	51.0354	129.237351404
18	C	9.7866	168.718199047
20	C	135.2188	48.6621106836
23	C	95.1904	86.9748655219
29	C	141.0584	43.0728000153
32	C	133.0447	50.7430272402
34	C	167.5256	17.74000268
38	C	85.6503	96.1060701775
42	C	98.1168	84.1738930684
44	C	131.0892	52.6147131454
45	C	142.6243	41.5740155822
47	C	166.0900	19.114071862
51	C	31.9462	147.508374969
53	C	44.4073	135.581366412
55	C	41.7702	138.105438466
57	C	51.1535	129.124313253
59	C	142.9258	41.2854380827
64	C	139.4781	44.5853672544
67	C	103.2117	79.2973640384
69	C	74.0492	107.209938935
72	C	141.4756	42.6734814985
76	C	90.1782	91.7722391317
77	C	163.0374	22.0358352955
82	C	94.2182	87.9053963514
86	C	103.5998	78.9258982752
90	C	99.4625	82.8858707096
92	C	122.8296	60.5203009246
4	H	29.6674	2.00988680989
5	H	29.9165	1.77971817972
7	H	26.3614	5.06463386463
10	H	28.9615	2.66213906214
11	H	27.1968	4.29272349272
12	H	27.5790	3.93957033957
17	H	25.0628	6.26454146454
19	H	23.3389	7.85742665743
21	H	28.9452	2.6772002772
22	H	29.0547	2.57602217602
24	H	27.8330	3.70487410487
26	H	28.1637	3.39930699931
27	H	27.6741	3.8516978517
28	H	27.6786	3.84753984754
30	H	29.8008	1.88662508663
31	H	29.6085	2.06431046431
33	H	28.9464	2.67609147609
35	H	31.2558	0.542203742204
36	H	30.5905	1.15694155694
37	H	30.3173	1.40937860938
39	H	27.3992	4.10570570571
43	H	27.9342	3.61136521137
46	H	28.8992	2.7197043197
48	H	30.6742	1.0796026796
49	H	31.3827	0.424948024948
50	H	31.0173	0.762577962578
52	H	25.7653	5.61543081543
54	H	24.5590	6.73005313005
56	H	24.9189	6.39750519751
58	H	26.2119	5.20277200277
60	H	29.9119	1.78396858397
61	H	28.9966	2.62970662971

62	H	30.3238	1.40337260337
63	H	30.1937	1.52358512359
65	H	29.6808	1.99750519751
66	H	30.6832	1.07128667129
70	H	25.2102	6.12834372834
71	H	26.9600	4.51152691153
73	H	29.2859	2.36239316239
74	H	30.4437	1.29258489258
78	H	30.4482	1.28842688843
79	H	30.4138	1.32021252021
80	H	30.1300	1.58244398244
81	H	27.4977	4.01469161469
83	H	28.1342	3.42656502657
85	H	30.0622	1.64509124509
88	H	28.6892	2.91374451374
89	H	27.7664	3.76641256641
93	H	27.8356	3.70247170247
94	H	28.6385	2.96059136059
95	H	27.9192	3.62522522523
96	H	28.0214	3.53079233079

Supporting Information: Revised-MandelalideA168ps.log

Using Gaussian 09: AM64L-G09RevC.01 23-Sep-2011

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#mPWPW91/6-311+G(2d,p) scf=(maxcycle=300,direct,tight) NMR density=current

SCRF=(PCM,SOLVENT=Chloroform)

Pointgroup= C1 Stoichiometry= C33H52O11 C1[X(C33H52O11)]

#Atoms= 96

Charge = 0 Multiplicity = 1

SCF Energy= -2116.48672355

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Optimization incomplete.

Atomic Type	Coordinates (Angstroms) X	Y	Z
C	-6.178959	-0.883537	0.155777
C	-5.369647	0.277644	-0.383591
C	-6.140314	1.569635	-0.112304
H	-6.503301	1.553987	0.917341
H	-7.060208	1.602179	-0.700633
C	-5.202207	2.758265	-0.219323
H	-5.031689	2.998678	-1.271875
C	-5.873254	4.043564	0.236577
O	-5.527383	5.192039	-0.625391
H	-4.563399	5.316894	-0.567466
H	-5.585127	4.269879	1.266945
H	-6.952478	3.889540	0.310886
O	-3.877477	2.496876	0.472124
C	-2.835647	3.322545	0.331017
O	-2.882481	4.442702	-0.195660
C	-1.647736	2.657158	0.851843
H	-1.769922	1.741900	1.430633
C	-0.414983	3.159844	0.983979
H	-0.166762	4.108583	0.514259
C	0.751790	2.393530	1.557984
H	0.461405	1.590946	2.239400
H	1.470119	3.073377	2.020041
C	1.543110	1.706228	0.434422
H	1.743133	2.475935	-0.315747
O	-5.139753	0.055555	-1.794502
H	-5.026298	-0.906679	-1.892586
H	-4.365553	0.295956	0.048520
H	-7.150766	-0.732768	-0.321722
C	-6.304478	-1.044490	1.677201
H	-5.387170	-0.763239	2.198451
H	-7.148750	-0.428560	1.995095
C	-6.660595	-2.489239	1.807433
H	-7.738252	-2.618639	1.690755
C	-6.107135	-2.944153	3.164062
H	-5.039696	-2.740953	3.271630
H	-6.237521	-4.021251	3.280159
H	-6.635446	-2.418998	3.962484
C	-6.093286	-3.184264	0.535266
H	-6.893904	-3.740275	0.041468
O	-5.524834	-2.085597	-0.256411
O	0.733923	0.575776	-0.130096
C	1.328575	-0.110698	-1.239585
H	1.549327	0.497992	-2.119311
C	0.387738	-1.367889	-1.543302
C	-1.063349	-0.874719	-1.646544
H	-1.305214	-0.528835	-0.639814
C	-1.310193	0.326644	-2.722781
H	-2.371357	0.576788	-2.662096
H	-1.022357	-0.049406	-3.707000
H	-0.684261	1.128118	-2.325162
C	-1.917982	-2.126943	-1.976822
H	-1.898862	-2.497986	-2.998625
C	-2.602913	-2.836386	-1.032415
H	-2.700835	-2.552108	0.014049
C	-3.429764	-3.995375	-1.401990
H	-3.173304	-4.263001	-2.426230
C	-4.418687	-4.659704	-0.708782
H	-5.027301	-5.457590	-1.128698
C	-4.920961	-4.245976	0.628230
H	-5.166918	-5.133834	1.214317
H	-4.072183	-3.833017	1.177183
H	0.520242	-2.210031	-0.861073
H	0.664218	-1.795888	-2.508513
C	2.639910	-0.772753	-0.713037
H	3.096211	-1.407092	-1.476251
H	2.328754	-1.407698	0.118481
C	3.592394	0.249073	-0.103267
O	4.631034	-0.483433	0.649378
C	5.789470	0.281102	1.039866
H	5.600416	0.905510	1.925378
H	4.043910	0.877628	-0.874550
C	2.905596	1.124772	0.946130
H	3.577623	1.898600	1.324515
H	2.695153	0.462452	1.789039
O	6.298272	1.179614	0.058775
C	6.572361	0.607610	-1.282632
C	6.992373	1.759138	-2.196845
H	6.331950	2.593009	-1.950522
H	6.798025	1.485848	-3.236333
H	8.036259	1.980084	-1.965866
H	5.638043	0.141459	-1.606281
C	7.751783	-0.420491	-0.991592
H	8.654123	0.033334	-0.572866
O	8.186779	-1.058613	-2.215562
H	8.607509	-1.893283	-1.941963
C	7.342785	-1.477445	0.047711
O	8.400071	-2.425593	0.389948
H	8.928053	-2.093700	1.137767
H	6.516995	-2.040533	-0.393723
C	6.838096	-0.815782	1.358436
O	7.982603	-0.284737	2.029358
C	7.893081	-0.148441	3.485310
H	8.853350	0.121346	3.933675
H	7.593308	-1.066700	3.996314

H	7.242153	0.690537	3.745481
H	6.460682	-1.576022	2.046340

NMR-Shifts
Revised-MandelalideA168ps-NMR.txt

Atom	Type	Isotropic	Scaled Shift
1	C	94.3273	87.8009724535
2	C	106.4684	76.1802484734
3	C	146.0258	38.3183062463
6	C	88.8853	93.0097245353
8	C	107.3215	75.3637129348
14	C	12.8009	165.833094049
16	C	53.8189	126.573154157
18	C	26.3258	152.887880702
20	C	136.5459	47.3918911158
23	C	96.1322	86.0734317273
29	C	139.7702	44.3057868642
32	C	144.5006	39.7781351098
34	C	164.8863	20.2661804399
38	C	88.2772	93.5917609449
42	C	103.9924	78.5501253852
44	C	127.8359	55.7285744367
45	C	134.0725	49.7592794655
47	C	161.2897	23.7086276537
51	C	29.8690	149.496544727
53	C	48.1968	131.954287027
55	C	37.1712	142.507322116
57	C	52.0617	128.255039338
59	C	149.2752	35.2081777982
64	C	135.9145	47.9962288711
67	C	107.6249	75.0733168705
69	C	80.6686	100.874251038
72	C	139.2388	44.8144106893
76	C	100.5166	81.8769501713
77	C	163.5192	21.5746855797
82	C	95.2660	86.9025057907
86	C	101.3739	81.0563946477
90	C	92.2415	89.7973736098
92	C	119.8593	63.3632917935
4	H	30.2141	1.50473550474
5	H	29.9351	1.76253176253
7	H	26.4233	5.00743820744
10	H	26.9582	4.51319011319
11	H	27.6730	3.85271425271
12	H	28.2203	3.34700854701
17	H	25.4054	5.94797874798
19	H	24.5629	6.72644952645
21	H	29.2065	2.43575883576
22	H	29.0660	2.56558096558
24	H	27.9926	3.5574035574
26	H	29.1866	2.45414645415
27	H	27.2576	4.23654423654
28	H	28.4159	3.16627396627
30	H	30.4688	1.26939246939
31	H	29.4357	2.22397782398
33	H	29.2623	2.3841995842
35	H	30.8561	0.911526911527
36	H	30.5877	1.15952875953
37	H	30.5713	1.17468237468
39	H	27.4171	4.08916608917
43	H	27.9252	3.61968121968
46	H	28.5652	3.02832062832
48	H	30.3710	1.35975975976
49	H	31.0344	0.746777546778
50	H	30.2589	1.46334026334
52	H	25.5453	5.81871101871
54	H	24.5652	6.72432432432
56	H	25.1558	6.17860937861
58	H	25.7204	5.65691845692
60	H	29.6262	2.04795564796
61	H	29.0872	2.54599214599
62	H	30.1110	1.6
63	H	30.1547	1.55962115962
65	H	29.7460	1.93726033726
66	H	30.4869	1.25266805267
70	H	25.7889	5.59362439362
71	H	27.6123	3.9088011088
73	H	29.2617	2.38475398475
74	H	30.5208	1.22134442134
78	H	30.3835	1.34820974821
79	H	30.0352	1.67003927004
80	H	30.1542	1.56008316008
81	H	27.4224	4.08426888427
83	H	27.4443	4.06403326403
85	H	29.9410	1.75708015708
88	H	29.4414	2.21871101871
89	H	27.6508	3.87322707323
93	H	27.9947	3.55546315546
94	H	28.5736	3.02055902056
95	H	27.9642	3.58364518365
96	H	27.8747	3.66634326634

Supporting Information: Revised-MandelalideA170ps.log

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 Using  Gaussian 09:  AM64L-G09RevC.01 23-Sep-2011
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 #mPWPW91/6-311+G(2d,p) scf=(maxcycle=300,direct,tight) NMR
density=current
 SCRF=(PCM,SOLVENT=Chloroform)
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 Pointgroup= C1   Stoichiometry= C33H52O11   C1[X(C33H52O11)]
#Atoms= 96
 Charge = 0                 Multiplicity = 1
-----------------------------------------------------------------------
 SCF Energy= -2116.47290439
=======================================================================
 Optimization incomplete.


-----------------------------------------------------------------------
     Atomic      Coordinates (Angstroms)
      Type      X                Y              Z
-----------------------------------------------------------------------
      C      -6.992477     -0.655706      0.194227
      C      -5.959318      0.362783     -0.336862
      C      -6.155056      1.752163      0.344904
      H      -6.041397      1.661373      1.426732
      H      -7.163347      2.094955      0.105326
      C      -5.079506      2.802645      0.007652
      H      -5.122769      2.878431     -1.082224
      C      -5.424431      4.107832      0.678937
      O      -5.114054      5.050749     -0.283961
      H      -4.178241      4.797070     -0.373664
      H      -4.822524      4.326552      1.564427
      H      -6.463299      4.177806      1.012286
      O      -3.806545      2.292277      0.388610
      C      -2.650520      2.872686      0.205563
      O      -2.599031      3.906938     -0.464380
      C      -1.446581      2.413430      0.928285
      H      -1.556982      1.614742      1.660270
      C      -0.226313      2.964773      0.741097
      H      -0.161674      3.780211      0.024155
      C       1.061658      2.466739      1.402667
      H       0.985216      1.973239      2.373162
      H       1.713562      3.326023      1.576410
      C       1.796037      1.577511      0.348320
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H	1.945937	2.235462	-0.512237
O	-6.253388	0.520823	-1.713733
H	-5.986446	-0.361501	-2.030351
H	-4.967660	-0.062133	-0.163729
H	-8.019254	-0.310466	0.050045
C	-6.852180	-0.971352	1.648743
H	-5.778316	-1.056656	1.827207
H	-7.272997	-0.299250	2.398232
C	-7.370660	-2.421394	1.686733
H	-8.448979	-2.491581	1.525065
C	-7.038666	-3.242584	2.946976
H	-5.979837	-3.110867	3.179664
H	-7.149104	-4.311294	2.749250
H	-7.627264	-3.066543	3.849515
C	-6.808624	-3.025271	0.368115
H	-7.452920	-3.779988	-0.089178
O	-6.758524	-1.878954	-0.543118
O	0.912810	0.547826	-0.089496
C	1.427593	-0.169472	-1.204604
H	1.493237	0.619007	-1.958667
C	0.324764	-1.244983	-1.601720
C	-1.144208	-0.717495	-1.684227
H	-1.371662	-0.395297	-0.665470
C	-1.212173	0.470053	-2.662104
H	-2.228281	0.733382	-2.962818
H	-0.637948	0.200229	-3.551208
H	-0.795837	1.377648	-2.219345
C	-2.071913	-1.851629	-1.947408
H	-1.891664	-2.328899	-2.907977
C	-3.042361	-2.361024	-1.110988
H	-3.190331	-1.914058	-0.128752
C	-3.949378	-3.467353	-1.505910
H	-3.588229	-3.950050	-2.412500
C	-4.886149	-4.057099	-0.775917
H	-5.401128	-4.885111	-1.256376
C	-5.400841	-3.624356	0.510332
H	-5.465041	-4.541461	1.099708
H	-4.715020	-2.933291	1.003093
H	0.427436	-2.061896	-0.883306
H	0.567805	-1.765784	-2.530408
C	2.787792	-0.898901	-0.938550
H	3.156451	-1.158165	-1.933276
H	2.640071	-1.743822	-0.263431
C	3.793297	0.015660	-0.295921
O	4.930534	-0.695751	0.320991
C	6.062511	0.023304	0.856889
H	5.675150	0.502649	1.767437
H	4.153772	0.719279	-1.051957
C	3.157240	0.903941	0.794338
H	3.736881	1.794556	1.045817
H	2.887024	0.357383	1.700906
O	6.598005	0.992262	-0.060243
C	7.312039	0.514344	-1.238606
C	8.007349	1.774292	-1.764250
H	7.310991	2.557371	-2.071263
H	8.732352	1.552361	-2.549344
H	8.498479	2.433317	-1.045323
H	6.685144	0.049871	-2.003846
C	8.352268	-0.498073	-0.806575
H	9.206807	-0.028235	-0.311862
O	8.769504	-1.252060	-1.959793
H	8.940788	-2.157962	-1.646721
C	7.743519	-1.553489	0.099251
O	8.850956	-2.415886	0.458797
H	9.363655	-2.023662	1.188833
H	6.986503	-2.075607	-0.490890
C	7.104773	-0.984126	1.389465
O	8.129342	-0.409086	2.232621
C	7.901592	-0.444595	3.692071
H	8.673899	0.186828	4.137416
H	8.053247	-1.498414	3.938234
H	6.908358	-0.030029	3.884242
H	6.732076	-1.880331	1.892798

NMR-Shifts
Revised-MandelalideA170ps-NMR.txt

Atom	Type	Isotropic	Scaled Shift
1	C	93.1270	88.9498267578
2	C	101.2019	81.2210226076
3	C	140.1052	43.985145198
6	C	98.5384	83.7703631387
8	C	111.8687	71.0114091005
14	C	9.4743	169.017113651
16	C	52.4491	127.884243573
18	C	21.9004	157.123604969
20	C	139.0047	45.0384769999
23	C	98.8495	83.4725971018
29	C	146.4931	37.8710350504
32	C	142.4935	41.6992094029
34	C	168.4294	16.8749401788
38	C	92.4381	89.609200023
42	C	100.8283	81.5786098509
44	C	130.2026	53.4633128506
45	C	145.3312	38.9831352055
47	C	165.3383	19.8335534754
51	C	31.6582	147.784031088
53	C	48.7596	131.415609028
55	C	48.9443	131.238825399
57	C	53.0699	127.290051494
59	C	148.6677	35.7896399242
64	C	145.9255	38.4143073183
67	C	106.0546	76.5763127166
69	C	81.3600	100.212484925
72	C	145.2614	39.0499435288
76	C	104.8454	77.7336855606
77	C	165.9786	19.2206971803
82	C	102.4414	80.0346484427
86	C	101.8187	80.6306590861
90	C	97.0070	85.2361262658
92	C	116.0187	67.039280997
4	H	30.0676	1.6401016401
5	H	29.9916	1.71032571033
7	H	26.2156	5.19935319935
10	H	26.2885	5.13199353199
11	H	27.4193	4.08713328713
12	H	28.0828	3.47405867406
17	H	25.4146	5.93947793948
19	H	23.7521	7.47562947563
21	H	29.1692	2.47022407022
22	H	29.0438	2.58609378609
24	H	28.2298	3.33823053823
26	H	29.4395	2.22046662047
27	H	28.2709	3.30025410025
28	H	27.9102	3.63354123354
30	H	30.5342	1.20896280896
31	H	29.8652	1.82711942712
33	H	29.0242	2.6042042042
35	H	31.2348	0.561607761608
36	H	30.7854	0.976853776854
37	H	30.5257	1.21681681682
39	H	27.8312	3.70653730654
43	H	27.9073	3.63622083622
46	H	29.0566	2.57426657427
48	H	31.0499	0.732455532456
49	H	31.0935	0.692169092169
50	H	30.4694	1.26883806884
52	H	25.8381	5.54816354816
54	H	24.7035	6.59653499653

56	H	25.3194	6.02744282744
58	H	26.2466	5.17070917071
60	H	29.7835	1.90261030261
61	H	29.0183	2.60965580966
62	H	30.2632	1.45936705937
63	H	30.2793	1.44449064449
65	H	29.6550	2.02134442134
66	H	30.4798	1.25922845923
70	H	25.3630	5.98715638716
71	H	27.2844	4.21178101178
73	H	29.5343	2.13287133287
74	H	30.8114	0.95282975283
78	H	30.4996	1.24093324093
79	H	30.5045	1.23640563641
80	H	30.7230	1.03451143451
81	H	27.7343	3.79607299607
83	H	28.1191	3.44051744052
85	H	28.9421	2.68006468006
88	H	29.5820	2.0887964888
89	H	27.8296	3.70801570802
93	H	27.7939	3.741002541
94	H	27.6541	3.87017787018
95	H	27.6219	3.89993069993
96	H	27.7783	3.75541695542

Supporting Information: Revised-MandelalideA172ps.log

Using Gaussian 09: AM64L-G09RevC.01 23-Sep-2011

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#mPWPW91/6-311+G(2d,p) scf=(maxcycle=300,direct,tight) NMR density=current

SCRF=(PCM,SOLVENT=Chloroform)

Pointgroup= C1 Stoichiometry= C33H52O11 C1[X(C33H52O11)]

#Atoms= 96

Charge = 0 Multiplicity = 1

SCF Energy= -2116.48230668

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Optimization incomplete.

Atomic Type	Coordinates (Angstroms) X	Y	Z
C	-6.764182	-0.602989	0.109354
C	-5.729183	0.407086	-0.466194
C	-6.025532	1.887516	0.083885
H	-6.033824	1.715810	1.162840
H	-6.900733	2.314470	-0.410147
C	-4.922795	2.895656	-0.156668
H	-4.570278	2.727623	-1.177573
C	-5.307408	4.378076	0.133893
O	-4.642812	5.229392	-0.861723
H	-3.714400	4.938621	-0.900971
H	-5.040857	4.540300	1.181467
H	-6.376843	4.573051	0.013742
O	-3.855378	2.551374	0.751402
C	-2.654294	3.119250	0.557442
O	-2.401802	4.114073	-0.129572
C	-1.593113	2.373029	1.320106
H	-1.831875	1.550817	1.993476
C	-0.317276	2.755004	1.174366
H	-0.118791	3.575449	0.489871
C	0.834886	1.988122	1.663638
H	0.659726	1.187164	2.385093
H	1.424365	2.713469	2.229287
C	1.677746	1.495219	0.465205
H	1.807396	2.350399	-0.203281
O	-5.755135	0.341443	-1.888746
H	-5.471776	-0.579407	-2.031702
H	-4.766729	0.046591	-0.093416
H	-7.788625	-0.294859	-0.113818
C	-6.604222	-0.967753	1.617895
H	-5.547471	-0.821214	1.849441
H	-7.125690	-0.363295	2.363091
C	-7.199841	-2.395569	1.734119
H	-8.284874	-2.348267	1.613770
C	-6.785703	-3.084714	3.103963
H	-5.728532	-3.308085	3.262601
H	-7.305306	-4.035162	3.234893
H	-7.100709	-2.505297	3.974997
C	-6.623072	-3.081802	0.440059
H	-7.361618	-3.812067	0.100651
O	-6.493344	-1.959496	-0.491726
O	0.802897	0.501958	-0.144630
C	1.325267	-0.148307	-1.356657
H	1.402204	0.570697	-2.175776
C	0.350456	-1.191820	-1.764760
C	-1.152787	-0.859219	-1.603776
H	-1.482857	-0.608929	-0.592874
C	-1.628029	0.313576	-2.569387
H	-2.691262	0.470237	-2.375609
H	-1.483977	0.084803	-3.626942
H	-1.055061	1.205997	-2.308682
C	-1.929900	-2.083537	-1.841995
H	-1.580133	-2.703850	-2.663294
C	-3.054409	-2.427447	-1.171038
H	-3.421402	-1.896139	-0.294721
C	-3.719903	-3.676523	-1.493753
H	-3.401451	-4.202312	-2.391803
C	-4.691889	-4.281332	-0.754514
H	-5.025637	-5.260439	-1.086587
C	-5.240902	-3.816165	0.544247
H	-5.342895	-4.653620	1.238417
H	-4.419946	-3.313414	1.060264
H	0.474411	-2.127561	-1.214691
H	0.524015	-1.564334	-2.776345
C	2.640034	-0.787604	-0.920721
H	3.102150	-1.123984	-1.851006
H	2.484943	-1.640701	-0.257194
C	3.702383	0.165125	-0.290316
O	4.779050	-0.620945	0.213565
C	5.949667	-0.055205	0.922143
H	5.451032	0.500094	1.730013
H	4.067787	0.790239	-1.108950
C	3.075126	0.924708	0.865192
H	3.745929	1.718508	1.199676
H	3.005551	0.234696	1.707531
O	6.593301	0.996358	0.199722
C	7.117960	0.699279	-1.059557
C	7.602675	2.012238	-1.734123
H	7.007150	2.891555	-1.482999
H	7.470008	1.888918	-2.811274
H	8.648458	2.271478	-1.555458
H	6.312602	0.331343	-1.700200
C	8.164894	-0.463214	-0.867101
H	9.088935	-0.110685	-0.402570
O	8.544254	-1.046414	-2.121961
H	9.332050	-1.607303	-2.005468
C	7.609981	-1.690056	0.002948
O	8.678222	-2.625965	0.301118
H	9.091730	-2.265481	1.105600
H	6.861027	-2.134395	-0.657462
C	6.998009	-1.132922	1.339057

O	8.066552	-0.610797	2.175851
C	7.533789	-0.151798	3.493530
H	8.383431	0.079969	4.141796
H	6.797647	-0.836314	3.920247
H	6.940298	0.741800	3.281546
H	6.533668	-1.960287	1.881216

NMR-Shifts
Revised-MandelalideA172ps-NMR.txt

Atom	Type	Isotropic	Scaled Shift
1	C	83.6777	97.9941231647
2	C	96.9555	85.2854189399
3	C	140.2563	43.8405214495
6	C	98.0005	84.2852083692
8	C	102.5392	79.941040219
14	C	6.4218	171.93878137
16	C	52.2251	128.098642776
18	C	22.6191	156.435708953
20	C	140.1498	43.9424567852
23	C	99.6890	82.6690786577
29	C	140.0160	44.0705220238
32	C	130.9984	52.701621394
34	C	169.4600	15.8885124141
38	C	92.8421	89.2225157449
42	C	107.1056	75.5703593101
44	C	140.8160	43.3048105821
45	C	140.8015	43.318689102
47	C	157.7340	27.11192787
51	C	28.6855	150.629319091
53	C	54.9262	125.513313808
55	C	39.4587	140.317865962
57	C	51.2100	129.070234882
59	C	149.7677	34.7367866919
64	C	138.1613	45.8457282873
67	C	107.9105	74.7999578859
69	C	78.0678	103.363578935
72	C	145.2166	39.0928233695
76	C	110.2864	72.5258906181
77	C	164.6689	20.4742625242
82	C	94.0799	88.0377687169
86	C	94.4920	87.6433316105
90	C	94.8553	87.295602902
92	C	117.1236	65.9817377821
4	H	29.8844	1.80937860938
5	H	29.8509	1.84033264033
7	H	26.9354	4.53425733426
10	H	25.6146	5.75467775468
11	H	27.9912	3.5586971587
12	H	27.8397	3.69868329868
17	H	25.2017	6.1361977362
19	H	23.9237	7.31707091707
21	H	29.2839	2.36424116424
22	H	29.2876	2.36082236082
24	H	27.8953	3.64730884731
26	H	29.5381	2.12936012936
27	H	27.7265	3.80328020328
28	H	27.4770	4.03381843382
30	H	30.2572	1.46491106491
31	H	29.7184	1.96276276276
33	H	28.8033	2.80831600832
35	H	30.8341	0.931854931855
36	H	30.8810	0.888519288519
37	H	30.6281	1.1221991222
39	H	27.4572	4.05211365211
43	H	27.8729	3.66800646801
46	H	28.7997	2.81164241164
48	H	30.9107	0.861076461076
49	H	31.2398	0.556987756988
50	H	30.3320	1.3957957958
52	H	25.6703	5.70321090321
54	H	24.5635	6.7258951259
56	H	25.0362	6.28911988912
58	H	25.8430	5.54363594364
60	H	30.1586	1.55601755602
61	H	28.9751	2.64957264957
62	H	30.2234	1.49614229614
63	H	30.3201	1.40679140679
65	H	29.6814	1.99695079695
66	H	30.7197	1.03756063756
70	H	24.8823	6.43132363132
71	H	27.5178	3.99611919612
73	H	29.3104	2.33975513976
74	H	30.6900	1.065003465
78	H	30.5582	1.18678678679
79	H	30.2104	1.50815430815
80	H	30.5666	1.17902517903
81	H	27.5011	4.01155001155
83	H	27.7014	3.82647262647
85	H	29.3531	2.3003003003
88	H	29.5468	2.12132132132
89	H	27.5092	4.00406560407
93	H	27.8708	3.66994686995
94	H	28.6284	2.96992376992
95	H	27.6894	3.83756063756
96	H	27.6778	3.84827904828

Supporting Information: Revised-MandelalideA174ps.log

Using Gaussian 09: AM64L-G09RevC.01 23-Sep-2011
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#mPWPW91/6-311+G(2d,p) scf=(maxcycle=300,direct,tight) NMR density=current
SCRF=(PCM,SOLVENT=Chloroform)

Pointgroup= C1 Stoichiometry= C33H52O11 C1[X(C33H52O11)]
#Atoms= 96
Charge = 0 Multiplicity = 1

SCF Energy= -2116.46828773
==========
Optimization incomplete.

Atomic Type	Coordinates (Angstroms) X	Y	Z
C	-6.571886	-0.787129	0.142204
C	-5.545748	0.317124	-0.300639
C	-5.999227	1.606156	0.267736
H	-6.160912	1.511565	1.343869
H	-6.997607	1.810095	-0.126355
C	-5.069806	2.799970	0.020573
H	-5.056201	2.934053	-1.063744
C	-5.641327	4.127435	0.590070
O	-5.167491	5.174907	-0.223838
H	-4.266896	4.900714	-0.472749
H	-5.393270	4.297642	1.640436
H	-6.728881	4.028477	0.559505
O	-3.746584	2.583624	0.580065
C	-2.719985	3.344903	0.256850
O	-2.707246	4.268352	-0.493917
C	-1.483545	2.835976	0.883534
H	-1.545738	1.956034	1.522294
C	-0.228871	3.316000	0.697619
H	-0.125447	4.144622	0.001169

C	1.035249	2.738239	1.265812
H	0.837314	1.994022	2.040953
H	1.729035	3.476766	1.671823
C	1.796708	1.910186	0.266567
H	1.960493	2.608056	-0.558050
O	-5.670783	0.375376	-1.671095
H	-5.893810	-0.561928	-1.814321
H	-4.502629	0.063679	-0.095916
H	-7.578538	-0.404054	-0.047787
C	-6.380510	-1.182479	1.606319
H	-5.305107	-1.246585	1.785806
H	-6.735953	-0.502273	2.382982
C	-6.884287	-2.546367	1.762288
H	-7.966016	-2.398843	1.767772
C	-6.444008	-3.282804	3.019215
H	-5.366630	-3.445448	2.950942
H	-7.009767	-4.201958	3.186740
H	-6.639677	-2.604998	3.851448
C	-6.586043	-3.215935	0.378159
H	-7.430138	-3.817824	0.032839
O	-6.416711	-2.097750	-0.578266
O	0.861488	0.854297	-0.137143
C	1.291459	-0.000844	-1.252290
H	1.416348	0.656903	-2.115817
C	0.329095	-1.112187	-1.462211
C	-1.213982	-0.758080	-1.551073
H	-1.473410	-0.293239	-0.596957
C	-1.620911	0.276423	-2.569951
H	-1.559950	-0.084479	-3.599197
H	-1.039829	1.200859	-2.553916
H	-2.678038	0.442112	-2.353947
C	-1.939250	-1.987602	-1.872440
H	-1.942528	-2.154936	-2.946605
C	-2.716295	-2.768923	-1.078512
H	-2.741475	-2.659757	0.004802
C	-3.496412	-3.869353	-1.580127
H	-3.129878	-4.318559	-2.502282
C	-4.627542	-4.426844	-0.977863
H	-5.136835	-5.248315	-1.475282
C	-5.244566	-3.992038	0.368486
H	-5.479003	-4.891009	0.940804
H	-4.467922	-3.465309	0.926808
H	0.434297	-1.846977	-0.660577
H	0.692955	-1.516842	-2.409342
C	2.646311	-0.662834	-0.807638
H	3.033030	-1.334134	-1.577847
H	2.472275	-1.369140	0.006549
C	3.702633	0.313459	-0.255864
O	4.669376	-0.625466	0.319993
C	5.853337	-0.183421	1.132251
H	5.485462	-0.006622	2.153727
H	4.259981	0.749440	-1.089561
C	3.072806	1.248687	0.779783
H	3.802320	1.996935	1.096410
H	2.762850	0.563136	1.571157
O	6.505494	1.056856	0.649307
C	7.071070	0.927304	-0.712175
C	7.861978	2.207790	-0.895999
H	7.185970	3.066286	-0.892096
H	8.368448	2.351153	-1.852515
H	8.558685	2.313781	-0.062517
H	6.221781	0.834051	-1.394399
C	8.003480	-0.338948	-0.880926
H	8.878416	-0.008910	-0.313805
O	8.437736	-0.562586	-2.188066
H	8.693185	-1.501926	-2.217020
C	7.305038	-1.617361	-0.289044
O	8.382086	-2.567736	-0.283892
H	8.959167	-2.295927	0.451721
H	6.436360	-1.915059	-0.881381
C	6.787851	-1.373061	1.050863
O	7.983133	-1.201837	1.915632
C	7.670287	-1.406234	3.351400
H	8.413704	-0.890310	3.964156
H	7.664767	-2.448051	3.680809
H	6.665344	-0.998464	3.486854
H	6.297331	-2.276051	1.423523

NMR-Shifts

Revised-MandelalideA174ps-NMR.txt

Atom	Type	Isotropic	Scaled Shift
1	C	79.9083	101.60196405
2	C	108.8566	73.8944083922
3	C	143.9556	40.2997760294
6	C	97.0147	85.2287562932
8	C	107.8705	74.838243458
14	C	18.6063	160.276517544
16	C	47.5429	132.580160417
18	C	26.4738	152.746224085
20	C	139.3897	44.6699783687
23	C	104.5911	77.9770860851
29	C	145.5051	38.8166886809
32	C	142.4864	41.706005092
34	C	169.4543	15.8939681081
38	C	88.2843	93.5849652558
42	C	101.9186	80.5350408698
44	C	134.2394	49.599532916
45	C	145.6266	38.7003962557
47	C	164.1955	20.9273722698
51	C	34.9380	144.644805605
53	C	55.7114	124.761768028
55	C	38.0567	141.659775264
57	C	42.9752	136.952085607
59	C	144.4084	39.8663833534
64	C	133.4146	50.3889814124
67	C	103.9558	78.5851566837
69	C	69.4996	111.564539903
72	C	142.6120	41.5857883956
76	C	97.2261	85.0264170447
77	C	165.0373	20.1216524053
82	C	98.3659	83.9354696683
86	C	107.2504	75.4317655392
90	C	97.7366	84.537797431
92	C	119.9472	63.2791592488
4	H	29.9749	1.72575652576
5	H	30.2079	1.51046431046
7	H	26.3645	5.06176946177
10	H	25.5125	5.84901824902
11	H	27.6319	3.89069069069
12	H	28.3156	3.25895125895
17	H	25.5438	5.8200970201
19	H	24.4356	6.84407484407
21	H	29.4181	2.24024024024
22	H	29.2268	2.417001617
24	H	28.1166	3.44282744283
26	H	28.6632	2.93776853777
27	H	27.6646	3.86047586048
28	H	27.6276	3.89466389466
30	H	30.5314	1.21155001155
31	H	30.0091	1.69415569416
33	H	28.9612	2.66241626242
35	H	30.7209	1.03645183645
36	H	30.4769	1.26190806191
37	H	30.7120	1.04467544468
39	H	26.9723	4.50016170016
43	H	27.9107	3.63307923308
46	H	29.1513	2.48676368676
48	H	31.5167	0.301131901132

49	H	30.4978	1.2425964426
50	H	30.5775	1.16895356895
52	H	26.0164	5.38341418341
54	H	24.6977	6.60189420189
56	H	24.6890	6.60993300993
58	H	25.6084	5.76040656041
60	H	29.9425	1.75569415569
61	H	28.6330	2.96567336567
62	H	30.1140	1.59722799723
63	H	30.2951	1.42989142989
65	H	29.6863	1.99242319242
66	H	30.8424	0.924185724186
70	H	25.1344	6.19838299838
71	H	26.8093	4.65077385077
73	H	29.2607	2.38567798568
74	H	30.5280	1.21469161469
78	H	30.3598	1.37010857011
79	H	30.1459	1.56775236775
80	H	30.7602	1.00013860014
81	H	27.6084	3.9124047124
83	H	27.9376	3.60822360822
85	H	29.1032	2.53120813121
88	H	29.2813	2.36664356664
89	H	27.5405	3.97514437514
93	H	28.1280	3.43229383229
94	H	28.3127	3.26163086163
95	H	28.0210	3.53116193116
96	H	27.7675	3.7653961654

Supporting Information: Revised-MandelalideA176ps.log

Using Gaussian 09: AM64L-G09RevC.01 23-Sep-2011

==========

#mPWPW91/6-311+G(2d,p) scf=(maxcycle=300,direct,tight) NMR density=current

SCRF=(PCM,SOLVENT=Chloroform)

Pointgroup= C1 Stoichiometry= C33H52O11 C1[X(C33H52O11)]

#Atoms= 96

Charge = 0 Multiplicity = 1

SCF Energy= -2116.47317828

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Optimization incomplete.

Atomic Type	Coordinates (Angstroms) X	Y	Z
C	-6.088352	-0.981481	0.463946
C	-5.343576	0.313502	-0.091000
C	-6.018750	1.640686	0.341805
H	-6.202455	1.729729	1.414065
H	-7.037616	1.652031	-0.049779
C	-5.238021	2.835213	-0.133128
H	-5.207179	2.848979	-1.225574
C	-5.818823	4.178342	0.424965
O	-5.281303	5.251255	-0.322307
H	-4.321072	5.129066	-0.213600
H	-5.689896	4.309486	1.501762
H	-6.886420	4.056558	0.227270
O	-3.905520	2.607731	0.331890
C	-2.871467	3.328299	-0.069140
O	-2.850230	4.292391	-0.796128
C	-1.676460	2.743977	0.529790
H	-1.774005	1.795458	1.056647
C	-0.543382	3.387377	0.290159
H	-0.483281	4.337915	-0.234060
C	0.796688	2.970028	0.905999
H	0.684210	2.416634	1.840413
H	1.491275	3.774720	1.153079
C	1.501143	1.941219	-0.076337
H	1.746790	2.455474	-1.009126
O	-5.399742	0.084117	-1.504726
H	-5.184153	-0.864440	-1.552276
H	-4.327150	0.202098	0.294739
H	-7.060105	-1.070572	-0.030509
C	-6.203831	-1.136572	2.001034
H	-5.350010	-0.639493	2.466203
H	-7.144225	-0.699577	2.341610
C	-6.085497	-2.639750	2.261433
H	-6.990796	-3.112945	2.646026
C	-4.946720	-2.859474	3.310158
H	-4.001212	-2.662434	2.800676
H	-4.987214	-3.906160	3.618993
H	-5.083611	-2.209335	4.176974
C	-5.802035	-3.229077	0.849235
H	-6.749544	-3.572637	0.424338
O	-5.368884	-2.171677	-0.037103
O	0.563550	0.846422	-0.275389
C	1.109433	-0.147336	-1.229350
H	1.364583	0.502638	-2.070013
C	0.102209	-1.365071	-1.622235
C	-1.436514	-1.047671	-1.717802
H	-1.770614	-0.628719	-0.766569
C	-1.622762	0.006673	-2.832122
H	-1.112868	-0.290560	-3.750893
H	-1.207369	0.926034	-2.414442
H	-2.665974	0.191198	-3.096263
C	-2.159128	-2.264468	-2.141161
H	-2.104488	-2.584705	-3.178539
C	-2.848257	-3.023611	-1.230366
H	-2.856828	-2.768093	-0.171538
C	-3.736142	-4.158878	-1.529984
H	-3.508908	-4.525430	-2.530195
C	-4.543102	-4.818130	-0.689579
H	-5.207913	-5.603488	-1.039113
C	-4.836496	-4.352004	0.649704
H	-5.214411	-5.186577	1.243394
H	-4.002478	-4.190010	1.336347
H	0.273921	-2.177015	-0.911748
H	0.390146	-1.777359	-2.591648
C	2.375629	-0.712991	-0.660829
H	2.771951	-1.296271	-1.493948
H	2.145666	-1.350847	0.194517
C	3.433637	0.346447	-0.315330
O	4.458146	-0.424404	0.414257
C	5.669728	0.312454	0.724968
H	5.357055	1.176947	1.329164
H	3.793489	0.716845	-1.278302
C	2.832001	1.405470	0.576689
H	3.550824	2.208988	0.751628
H	2.644156	0.918037	1.535348
O	6.247795	0.875844	-0.456809
C	6.776938	-0.077332	-1.415212
C	7.292893	0.855111	-2.657488
H	6.512272	1.460062	-3.122809
H	7.646443	0.165102	-3.427678
H	8.101657	1.480820	-2.274865
H	6.017013	-0.820832	-1.668344
C	7.914938	-0.839727	-0.664604
H	8.795351	-0.218030	-0.482696
O	8.453169	-1.813056	-1.531587
H	8.918781	-2.434992	-0.945122
C	7.405479	-1.520952	0.603937

O	8.607156	-1.992722	1.301336
H	8.863970	-1.218577	1.834833
H	6.765945	-2.358273	0.315222
C	6.711369	-0.573507	1.538700
O	7.700504	0.347381	2.145457
C	7.546718	0.899321	3.457859
H	8.433348	1.447025	3.786611
H	7.390569	0.091604	4.179134
H	6.635237	1.502629	3.439588
H	6.143094	-1.051500	2.341636

NMR-Shifts
Revised-MandelalideA176ps-NMR.txt

Atom	Type	Isotropic	Scaled Shift
1	C	80.5812	100.957905013
2	C	101.0660	81.3510978388
3	C	149.8493	34.6586841249
6	C	101.6670	80.7758571182
8	C	107.2947	75.3893642681
14	C	14.5204	164.187293019
16	C	52.2993	128.02762304
18	C	30.2276	149.153314573
20	C	134.9889	48.8821570091
23	C	98.7026	83.6132008653
29	C	143.3366	40.8922452574
32	C	141.1231	43.0108731025
34	C	162.5272	22.5241677674
38	C	97.0057	85.2373705469
42	C	94.4322	87.7005685407
44	C	125.3122	58.1441068933
45	C	141.3402	42.80307816
47	C	160.6665	24.3051168667
51	C	39.6613	140.12394954
53	C	41.1456	138.703267674
55	C	40.7942	139.039606424
57	C	60.2403	120.426979843
59	C	162.6653	22.3919868298
64	C	140.1135	43.9772009418
67	C	103.9470	78.5935795096
69	C	76.3692	104.989375754
72	C	141.2026	42.934780528
76	C	100.5394	81.8551273952
77	C	158.3740	26.4993587167
82	C	100.7969	81.608664025
86	C	106.2024	76.4348475277
90	C	92.0778	89.9540573135
92	C	122.4872	60.8480254216
4	H	30.1795	1.53670593671
5	H	30.2672	1.45567105567
7	H	26.5805	4.86218526219
10	H	27.2799	4.21593901594
11	H	27.7013	3.82656502657
12	H	28.3038	3.26985446985
17	H	24.8878	6.42624162624
19	H	23.7121	7.51258951259
21	H	29.2565	2.38955878956
22	H	29.2510	2.39464079464
24	H	28.1734	3.39034419034
26	H	28.9642	2.65964425964
27	H	27.5556	3.96119196119
28	H	27.6598	3.86491106491
30	H	30.6237	1.12626472626
31	H	29.5381	2.12936012936
33	H	29.3522	2.30113190113
35	H	30.3181	1.40863940864
36	H	30.7582	1.00198660199
37	H	30.7827	0.979348579349
39	H	27.5710	3.94696234696
43	H	27.5928	3.92681912682
46	H	28.9076	2.71194271194
48	H	31.1236	0.664356664357
49	H	30.2293	1.49069069069
50	H	30.7150	1.0419034419
52	H	25.8245	5.56072996073
54	H	24.5971	6.69484869485
56	H	25.1639	6.17112497112
58	H	25.7942	5.58872718873
60	H	30.1876	1.52922152922
61	H	29.2347	2.4097020097
62	H	30.0978	1.6121968122
63	H	30.0956	1.61422961423
65	H	29.8082	1.87978747979
66	H	30.3429	1.38572418572
70	H	25.7316	5.64656964657
71	H	27.3620	4.14007854008
73	H	29.3263	2.32506352506
74	H	30.7057	1.0504966505
78	H	30.3377	1.39052899053
79	H	30.1006	1.60960960961
80	H	30.4903	1.24952644953
81	H	27.5721	3.94594594595
83	H	27.5259	3.98863478863
85	H	29.7053	1.97486717487
88	H	28.5404	3.05123585124
89	H	27.9983	3.55213675214
93	H	27.7866	3.74774774775
94	H	28.3008	3.27262647263
95	H	27.8388	3.69951489951
96	H	27.8421	3.69646569647

Supporting Information: Revised-MandelalideA178ps.log

Using Gaussian 09: AM64L-G09RevC.01 23-Sep-2011

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#mPWPW91/6-311+G(2d,p) scf=(maxcycle=300,direct,tight) NMR density=current

SCRF=(PCM,SOLVENT=Chloroform)

Pointgroup= C1 Stoichiometry= C33H52O11 C1[X(C33H52O11)] #Atoms= 96

Charge = 0 Multiplicity = 1

SCF Energy= -2116.47317828

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Optimization incomplete.

Atomic Type	Coordinates (Angstroms) X	Y	Z
C	-6.088352	-0.981481	0.463946
C	-5.343576	0.313502	-0.091000
C	-6.018750	1.640686	0.341805
H	-6.202455	1.729729	1.414065
H	-7.037616	1.652031	-0.049779
C	-5.238021	2.835213	-0.133128
H	-5.207179	2.848979	-1.225574
C	-5.818823	4.178342	0.424965
O	-5.281303	5.251255	-0.322307
H	-4.321072	5.129066	-0.213600
H	-5.689896	4.309486	1.501762
H	-6.886420	4.056558	0.227270
O	-3.905520	2.607731	0.331890
C	-2.871467	3.328299	-0.069140
O	-2.850230	4.292391	-0.796128

C	-1.676460	2.743977	0.529790
H	-1.774005	1.795458	1.056647
C	-0.543382	3.387377	0.290159
H	-0.483281	4.337915	-0.234060
C	0.796688	2.970028	0.905999
H	0.684210	2.416634	1.840413
H	1.491275	3.774720	1.153079
C	1.501143	1.941219	-0.076337
H	1.746790	2.455474	-1.009126
O	-5.399742	0.084117	-1.504726
H	-5.184153	-0.864440	-1.552276
H	-4.327150	0.202098	0.294739
H	-7.060105	-1.070572	-0.030509
C	-6.203831	-1.136572	2.001034
H	-5.350010	-0.639493	2.466203
H	-7.144225	-0.699577	2.341610
C	-6.085497	-2.639750	2.261433
H	-6.990796	-3.112945	2.646026
C	-4.946720	-2.859474	3.310158
H	-4.001212	-2.662434	2.800676
H	-4.987214	-3.906160	3.618993
H	-5.083611	-2.209335	4.176974
C	-5.802035	-3.229077	0.849235
H	-6.749544	-3.572637	0.424338
O	-5.368884	-2.171677	-0.037103
O	0.563550	0.846422	-0.275389
C	1.109433	-0.147336	-1.229350
H	1.364583	0.502638	-2.070013
C	0.102209	-1.365071	-1.622235
C	-1.436514	-1.047671	-1.717802
H	-1.770614	-0.628719	-0.766569
C	-1.622762	0.006673	-2.832122
H	-1.112868	-0.290560	-3.750893
H	-1.207369	0.926034	-2.414442
H	-2.665974	0.191198	-3.096263
C	-2.159128	-2.264468	-2.141161
H	-2.104488	-2.584705	-3.178539
C	-2.848257	-3.023611	-1.230366
H	-2.856828	-2.768093	-0.171538
C	-3.736142	-4.158878	-1.529984
H	-3.508908	-4.525430	-2.530195
C	-4.543102	-4.818130	-0.689579
H	-5.207913	-5.603488	-1.039113
C	-4.836496	-4.352004	0.649704
H	-5.214411	-5.186577	1.243394
H	-4.002478	-4.190010	1.336347
H	0.273921	-2.177015	-0.911748
H	0.390146	-1.777359	-2.591648
C	2.375629	-0.712991	-0.660829
H	2.771951	-1.296271	-1.493948
H	2.145666	-1.350847	0.194517
C	3.433637	0.346447	-0.315330
O	4.458146	-0.424404	0.414257
C	5.669728	0.312454	0.724968
H	5.357055	1.176947	1.329164
H	3.793489	0.716845	-1.278302
C	2.832001	1.405470	0.576689
H	3.550824	2.208988	0.751628
H	2.644156	0.918037	1.535348
O	6.247795	0.875844	-0.456809
C	6.776938	-0.077332	-1.415212
C	7.292893	0.855111	-2.657488
H	6.512272	1.460062	-3.122809
H	7.646443	0.165102	-3.427678
H	8.101657	1.480820	-2.274865
H	6.017013	-0.820832	-1.668344
C	7.914938	-0.839727	-0.664604
H	8.795351	-0.218030	-0.482696
O	8.453169	-1.813056	-1.531587
H	8.918781	-2.434992	-0.945122
C	7.405479	-1.520952	0.603937
O	8.607156	-1.992722	1.301336
H	8.863970	-1.218577	1.834833
H	6.765945	-2.358273	0.315222
C	6.711369	-0.573507	1.538700
O	7.700504	0.347381	2.145457
C	7.546718	0.899321	3.457859
H	8.433348	1.447025	3.786611
H	7.390569	0.091604	4.179134
H	6.635237	1.502629	3.439588
H	6.143094	-1.051500	2.341636

NMR-Shifts

Revised-MandelalideA178ps-NMR.txt

Atom	Type	Isotropic	Scaled Shift
1	C	80.5812	100.957905013
2	C	101.0660	81.3510978388
3	C	149.8493	34.6586841249
6	C	101.6670	80.7758571182
8	C	107.2947	75.3893642681
14	C	14.5204	164.187293019
16	C	52.2993	128.02762304
18	C	30.2276	149.153314573
20	C	134.9889	48.8821570091
23	C	98.7026	83.6132008653
29	C	143.3366	40.8922452574
32	C	141.1231	43.0108731025
34	C	162.5272	22.5241677674
38	C	97.0057	85.2373705469
42	C	94.4322	87.7005685407
44	C	125.3122	58.1441068933
45	C	141.3402	42.80307816
47	C	160.6665	24.3051168667
51	C	39.6613	140.12394954
53	C	41.1456	138.703267674
55	C	40.7942	139.039606424
57	C	60.2403	120.426979843
59	C	162.6653	22.3919868298
64	C	140.1135	43.9772009418
67	C	103.9470	78.5935795096
69	C	76.3692	104.989375754
72	C	141.2026	42.934780528
76	C	100.5394	81.8551273952
77	C	158.3740	26.4993587167
82	C	100.7969	81.608664025
86	C	106.2024	76.4348475277
90	C	92.0778	89.9540573135
92	C	122.4872	60.8480254216
4	H	30.1795	1.53670593671
5	H	30.2672	1.45567105567
7	H	26.5805	4.86218526219
10	H	27.2799	4.21593901594
11	H	27.7013	3.82656502657
12	H	28.3038	3.26985446985
17	H	24.8878	6.42624162624
19	H	23.7121	7.51258951259
21	H	29.2565	2.38955878956
22	H	29.2510	2.39464079464
24	H	28.1734	3.39034419034
26	H	28.9642	2.65964425964
27	H	27.5556	3.96119196119
28	H	27.6598	3.86491106491
30	H	30.6237	1.12626472626
31	H	29.5381	2.12936012936
33	H	29.3522	2.30113190113
35	H	30.3181	1.40863940864
36	H	30.7582	1.00198660199
37	H	30.7827	0.979348579349

39	H	27.5710	3.94696234696
43	H	27.5928	3.92681912682
46	H	28.9076	2.71194271194
48	H	31.1236	0.664356664357
49	H	30.2293	1.49069069069
50	H	30.7150	1.0419034419
52	H	25.8245	5.56072996073
54	H	24.5971	6.69484869485
56	H	25.1639	6.17112497112
58	H	25.7942	5.58872718873
60	H	30.1876	1.52922152922
61	H	29.2347	2.4097020097
62	H	30.0978	1.6121968122
63	H	30.0956	1.61422961423
65	H	29.8082	1.87978747979
66	H	30.3429	1.38572418572
70	H	25.7316	5.64656964657
71	H	27.3620	4.14007854008
73	H	29.3263	2.32506352506
74	H	30.7057	1.0504966505
78	H	30.3377	1.39052899053
79	H	30.1006	1.60960960961
80	H	30.4903	1.24952644953
81	H	27.5721	3.94594594595
83	H	27.5259	3.98863478863
85	H	29.7053	1.97486717487
88	H	28.5404	3.05123585124
89	H	27.9983	3.55213675214
93	H	27.7866	3.74774774775
94	H	28.3008	3.27262647263
95	H	27.8388	3.69951489951
96	H	27.8421	3.69646569647

Supporting Information: Revised-MandelalideA180ps.log

Using Gaussian 09: AM64L-G09RevC.01 23-Sep-2011

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#mPWPW91/6-311+G(2d,p) scf=(maxcycle=300,direct,tight) NMR density=current

SCRF=(PCM,SOLVENT=Chloroform)

Pointgroup= C1 Stoichiometry= C33H52O11 C1[X(C33H52O11)]

#Atoms= 96

Charge = 0 Multiplicity = 1

SCF Energy= -2116.49369485

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Optimization incomplete.

Atomic Type	Coordinates (Angstroms) X	Y	Z
C	-6.522741	-0.870503	0.300471
C	-5.579387	0.319464	-0.084573
C	-6.026136	1.689811	0.547162
H	-5.996895	1.575127	1.632687
H	-7.053386	1.919467	0.256062
C	-5.185932	2.845039	0.036188
H	-5.269844	2.919121	-1.051009
C	-5.668639	4.193475	0.756061
O	-5.467218	5.339809	-0.081420
H	-4.646529	5.162533	-0.574528
H	-5.097048	4.298985	1.682453
H	-6.721450	4.170702	1.048238
O	-3.780206	2.562326	0.391623
C	-2.791295	3.389585	-0.043477
O	-3.042325	4.412424	-0.691277
C	-1.450286	2.956110	0.409681
H	-1.531943	2.048295	1.005529
C	-0.286721	3.551188	0.112911
H	-0.246170	4.452665	-0.492227
C	1.008564	2.981266	0.680861
H	0.809372	2.403587	1.586056
H	1.722040	3.796507	0.818758
C	1.670318	1.976001	-0.303491
H	1.952363	2.364582	-1.285191
O	-5.589811	0.506726	-1.536012
H	-5.616875	-0.390833	-1.912655
H	-4.561602	0.063439	0.218610
H	-7.508308	-0.767425	-0.162495
C	-6.497842	-1.256014	1.827470
H	-5.518506	-1.095008	2.282253
H	-7.187112	-0.627107	2.393651
C	-6.827734	-2.684861	1.787688
H	-7.895035	-2.859392	1.635727
C	-6.539815	-3.523001	3.098609
H	-5.477479	-3.480329	3.349376
H	-6.776766	-4.586538	3.019622
H	-7.148694	-3.204966	3.946856
C	-6.216628	-3.201866	0.451617
H	-6.959076	-3.841146	-0.033812
O	-5.866766	-1.996337	-0.296385
O	0.790131	0.822643	-0.440098
C	1.296037	-0.089082	-1.404120
H	1.313615	0.413456	-2.374413
C	0.439042	-1.342596	-1.412250
C	-1.074276	-1.178800	-1.704147
H	-1.651377	-0.715587	-0.901157
C	-1.373355	-0.439823	-3.045916
H	-1.376019	-0.988861	-3.990279
H	-0.666254	0.364976	-3.254788
H	-2.367371	0.009594	-2.987335
C	-1.703180	-2.515204	-1.848508
H	-1.163254	-3.244050	-2.446973
C	-2.796817	-2.868149	-1.191519
H	-3.301866	-2.068314	-0.651141
C	-3.528531	-4.077754	-1.455585
H	-3.249161	-4.570921	-2.384968
C	-4.506140	-4.477231	-0.648779
H	-5.070309	-5.363894	-0.927063
C	-4.940254	-3.835676	0.655578
H	-5.138706	-4.638867	1.369330
H	-4.197901	-3.099888	0.972668
H	0.505631	-1.957373	-0.511493
H	0.762345	-1.931427	-2.273095
C	2.681578	-0.579410	-0.995308
H	3.215424	-1.104255	-1.789174
H	2.587983	-1.307314	-0.186548
C	3.684861	0.427095	-0.506150
O	4.597299	-0.421343	0.223478
C	5.663856	0.243215	0.796926
H	5.305598	1.096432	1.392192
H	4.198600	0.941506	-1.322215
C	2.986774	1.448030	0.345384
H	3.697770	2.209398	0.671810
H	2.789872	0.944189	1.294261
O	6.538006	0.903703	-0.231209
C	7.266631	0.081568	-1.136085
C	8.111706	0.969835	-2.077353
H	7.383884	1.542508	-2.656078
H	8.643057	0.314789	-2.771333
H	8.784270	1.606244	-1.497996
H	6.537447	-0.560010	-1.638152
C	8.133782	-0.876901	-0.392568

H	9.062789	-0.378466	-0.105975
O	8.641010	-1.859198	-1.274455
H	9.020208	-2.586137	-0.749364
C	7.308101	-1.645386	0.682977
O	8.232271	-2.402017	1.447874
H	8.700278	-1.699883	1.932874
H	6.562478	-2.232822	0.142846
C	6.572772	-0.708135	1.636040
O	7.638112	-0.020753	2.350636
C	7.212333	0.801400	3.439336
H	8.062019	1.169778	4.020951
H	6.569899	0.214892	4.101580
H	6.587093	1.602109	3.036038
H	5.973008	-1.304067	2.328191

NMR-Shifts
Revised-MandelalideA180ps-NMR.txt

Atom	Type	Isotropic	Scaled Shift
1	C	87.9023	93.9505924692
2	C	95.0833	87.0773751412
3	C	143.2747	40.9514921802
6	C	91.7082	90.3078159995
8	C	101.8418	80.6085491682
14	C	5.4542	172.864909359
16	C	51.3188	128.966098126
18	C	30.7986	148.606788032
20	C	135.3760	48.5116483853
23	C	100.6201	81.7778862536
29	C	146.2176	38.1347269282
32	C	148.9879	35.4831639197
34	C	165.6173	19.5665116101
38	C	93.3928	88.6954191313
42	C	109.1994	73.5663010395
44	C	133.8738	49.9494630449
45	C	140.2517	43.8449242903
47	C	167.2001	18.0515515228
51	C	34.7546	144.820344953
53	C	53.4581	126.918490017
55	C	51.4329	128.856888532
57	C	47.1854	132.922337717
59	C	144.3611	39.9116560424
64	C	141.6046	42.5500105285
67	C	111.8879	70.9930320259
69	C	81.0572	100.502306706
72	C	143.0764	41.1412929038
76	C	109.6730	73.112999866
77	C	164.1460	20.9747506652
82	C	101.9131	80.540305136
86	C	103.6413	78.8861769942
90	C	93.8021	88.303662015
92	C	124.7391	58.6926434273
4	H	29.9951	1.70709170709
5	H	30.0230	1.68131208131
7	H	26.2586	5.15962115962
10	H	26.3735	5.05345345345
11	H	27.7163	3.81270501271
12	H	27.9440	3.60231000231
17	H	25.1699	6.16558096558
19	H	24.2068	7.05548625549
21	H	28.8885	2.72959112959
22	H	28.8795	2.73790713791
24	H	28.2511	3.31854931855
26	H	29.3597	2.2942018942
27	H	27.3100	4.18812658813
28	H	27.5181	3.99584199584
30	H	30.1937	1.52358512359
31	H	29.9383	1.75957495957
33	H	29.3772	2.27803187803
35	H	31.3101	0.49203049203
36	H	30.5726	1.17348117348
37	H	30.5262	1.21635481635
39	H	27.5877	3.93153153153
43	H	27.8401	3.69831369831
46	H	29.0858	2.54728574729
48	H	31.5507	0.269715869716
49	H	31.0390	0.742527142527
50	H	30.8365	0.929637329637
52	H	26.3623	5.0638022638
54	H	24.5675	6.7221991222
56	H	25.0567	6.27017787018
58	H	26.2101	5.20443520444
60	H	29.4206	2.23793023793
61	H	28.6365	2.96243936244
62	H	29.9784	1.72252252252
63	H	30.1507	1.56331716332
65	H	29.5863	2.08482328482
66	H	30.6212	1.12857472857
70	H	25.3472	6.00175560176
71	H	27.3612	4.14081774082
73	H	29.3239	2.32728112728
74	H	31.0063	0.772741972742
78	H	30.5186	1.22337722338
79	H	30.1652	1.54991914992
80	H	30.8155	0.949041349041
81	H	28.1412	3.4200970201
83	H	27.6003	3.91988911989
85	H	29.1366	2.50034650035
88	H	29.3120	2.33827673828
89	H	28.3000	3.27336567337
93	H	27.9168	3.62744282744
94	H	28.5849	3.01011781012
95	H	27.8984	3.64444444444
96	H	28.1912	3.3738969739

Supporting Information: Revised-MandelalideA182ps.log

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 Using  Gaussian 09:  AM64L-G09RevC.01 23-Sep-2011
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density=current
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#Atoms= 96
 Charge = 0                 Multiplicity = 1
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 SCF Energy= -2116.46244187
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 Optimization incomplete.


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     Atomic     Coordinates (Angstroms)
      Type      X              Y              Z
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      C      -6.252087     -1.057120      0.655021
      C      -5.613680      0.166912     -0.139503
      C      -6.179638      1.468716      0.422963
      H      -6.121877      1.287682      1.498860
      H      -7.251434      1.588381      0.255340
      C      -5.329199      2.673930      0.069807
      H      -5.565099      2.972151     -0.954938
      C      -5.636680      3.878755      1.016555
      O      -5.251522      5.086689      0.326462
      H      -4.440618      4.754396     -0.100547
      H      -5.201510      3.696894      2.002135
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H	-6.716191	3.942841	1.170328
O	-3.902556	2.340985	0.242630
C	-2.898259	3.210365	-0.089148
O	-3.065989	4.132101	-0.839445
C	-1.628161	2.881271	0.539534
H	-1.743196	2.041056	1.222847
C	-0.469768	3.479445	0.280674
H	-0.397456	4.273902	-0.457748
C	0.853589	2.998095	0.894431
H	0.551561	2.468948	1.800425
H	1.427337	3.895560	1.132757
C	1.671001	2.111671	-0.080566
H	2.019086	2.745674	-0.899529
O	-5.921097	0.067846	-1.510944
H	-5.254982	-0.502831	-1.932646
H	-4.527197	0.185628	-0.025624
H	-7.339547	-0.950588	0.683822
C	-5.660333	-1.398049	2.018832
H	-4.577635	-1.314913	1.907434
H	-6.143994	-0.704975	2.710012
C	-6.063135	-2.844858	2.227353
H	-7.145047	-2.855132	2.375162
C	-5.305489	-3.623760	3.340545
H	-4.256759	-3.764509	3.069167
H	-5.755066	-4.610626	3.464102
H	-5.458094	-3.061202	4.263135
C	-5.849982	-3.416527	0.740942
H	-6.677094	-4.093351	0.515984
O	-5.986545	-2.249760	-0.119690
O	0.737339	1.083724	-0.461453
C	1.188027	-0.004902	-1.334229
H	1.463351	0.391826	-2.314187
C	0.024204	-1.018619	-1.596533
C	-1.387865	-0.484216	-1.820521
H	-1.861283	-0.048551	-0.937868
C	-1.449849	0.642612	-2.894863
H	-0.921946	0.420719	-3.823714
H	-1.007897	1.568244	-2.519490
H	-2.483225	0.953796	-3.063345
C	-2.296479	-1.632173	-2.244352
H	-2.642069	-1.578200	-3.273578
C	-2.703314	-2.614627	-1.509281
H	-2.402389	-2.637500	-0.462178
C	-3.651980	-3.632987	-1.929903
H	-3.676157	-3.815324	-3.003937
C	-4.462551	-4.410616	-1.153262
H	-5.085258	-5.208651	-1.548375
C	-4.535351	-4.182026	0.339655
H	-4.538588	-5.148810	0.848742
H	-3.730673	-3.649657	0.850694
H	-0.038177	-1.735913	-0.775746
H	0.400431	-1.471160	-2.516517
C	2.422052	-0.616352	-0.597180
H	2.862617	-1.388120	-1.232790
H	2.116201	-1.161014	0.298058
C	3.464210	0.369167	-0.239417
O	4.509287	-0.356810	0.439371
C	5.721213	0.287598	0.901728
H	5.424032	1.097536	1.584613
H	3.819482	0.732994	-1.207221
C	2.821095	1.399231	0.689930
H	3.542365	2.189813	0.908364
H	2.500973	0.913629	1.613464
O	6.318810	0.892922	-0.327465
C	6.898665	-0.074736	-1.249675
C	7.656492	0.744597	-2.306485
H	7.016026	1.583435	-2.586613
H	7.770569	0.212802	-3.253057
H	8.563760	1.206856	-1.911353
H	6.141180	-0.719280	-1.703174
C	7.945960	-0.986162	-0.577616
H	8.849011	-0.466564	-0.246681
O	8.287643	-2.046987	-1.413897
H	8.397943	-2.799179	-0.804902
C	7.226595	-1.715109	0.590267
O	8.171211	-2.576248	1.271759
H	8.552338	-1.864243	1.815504
H	6.273518	-2.186350	0.337153
C	6.757185	-0.606243	1.611951
O	8.012932	0.038305	1.971222
C	7.811592	1.088211	2.879718
H	8.716699	1.402224	3.405691
H	7.135271	0.691276	3.640498
H	7.272273	1.872267	2.342618
H	6.339840	-1.144970	2.466215

NMR-Shifts

Revised-MandelalideA182ps-NMR.txt

Atom	Type	Isotropic	Scaled Shift
1	C	85.5329	96.2184383315
2	C	102.5495	79.9311816842
3	C	147.8420	36.5799498459
6	C	95.2503	86.9175328777
8	C	102.2148	80.2515362086
14	C	9.8397	168.66737495
16	C	55.7582	124.716973908
18	C	24.2529	154.871934761
20	C	133.1536	50.6387947702
23	C	103.1473	79.3590038094
29	C	143.3569	40.8728153295
32	C	131.5205	52.2018989644
34	C	170.1691	15.209804935
38	C	89.0192	92.8815635828
42	C	97.8970	84.384272287
44	C	136.9863	46.9703669672
45	C	146.0195	38.3243362239
47	C	164.3561	20.7736556979
51	C	42.8333	137.087903674
53	C	57.4746	123.07414001
55	C	43.2453	136.693562281
57	C	47.5251	132.597197496
59	C	147.4905	36.9163843106
64	C	141.0195	43.1100327342
67	C	106.7666	75.8948295335
69	C	75.7479	105.584046402
72	C	141.5726	42.5806389862
76	C	104.0833	78.4631214227
77	C	163.4998	21.5932540822
82	C	101.9208	80.5329351634
86	C	98.4740	83.8320029097
90	C	90.9445	91.0387832845
92	C	126.6975	56.8181818182
4	H	30.5196	1.22245322245
5	H	29.8490	1.84208824209
7	H	26.0114	5.38803418803
10	H	26.3235	5.09965349965
11	H	27.9398	3.60619080619
12	H	28.2611	3.30930930931
17	H	25.3970	5.95574035574
19	H	24.1210	7.13476553477
21	H	29.1781	2.462000462
22	H	28.9207	2.69983829984
24	H	27.8037	3.73194733195
26	H	30.2554	1.46657426657
27	H	27.5462	3.96987756988
28	H	27.8082	3.72778932779
30	H	30.4745	1.26412566413
31	H	29.7850	1.90122430122

33	H	28.9074	2.71212751213
35	H	30.6445	1.10704550705
36	H	30.6656	1.08754908755
37	H	30.3411	1.38738738739
39	H	27.3267	4.1726957727
43	H	27.6362	3.88671748672
46	H	29.0784	2.55412335412
48	H	30.9317	0.841672441672
49	H	30.6687	1.08468468468
50	H	30.8741	0.894894894895
52	H	26.0809	5.32381612382
54	H	25.1286	6.20374220374
56	H	25.3395	6.00887040887
58	H	25.4737	5.88486948487
60	H	30.0213	1.68288288288
61	H	29.0726	2.55948255948
62	H	29.8274	1.86204666205
63	H	30.2385	1.48218988219
65	H	29.9364	1.76133056133
66	H	30.7382	1.02046662047
70	H	24.9973	6.32506352506
71	H	27.2540	4.23987063987
73	H	29.3548	2.29872949873
74	H	30.8363	0.929822129822
78	H	30.8036	0.960036960037
79	H	30.0281	1.6765996766
80	H	30.6398	1.11138831139
81	H	28.0354	3.51785631786
83	H	27.7765	3.75708015708
85	H	29.1202	2.5155001155
88	H	28.8501	2.76507276507
89	H	27.5418	3.97394317394
93	H	28.0882	3.46906906907
94	H	28.6782	2.92390852391
95	H	27.6615	3.86334026334
96	H	27.7174	3.81168861169

Supporting Information: Revised-MandelalideA184ps.log

Using Gaussian 09: AM64L-G09RevC.01 23-Sep-2011

==========

#mPWPW91/6-311+G(2d,p) scf=(maxcycle=300,direct,tight) NMR density=current

SCRF=(PCM,SOLVENT=Chloroform)

Pointgroup= C1 Stoichiometry= C33H52O11 C1[X(C33H52O11)]

#Atoms= 96

Charge = 0 Multiplicity = 1

SCF Energy= -2116.47926342

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Optimization incomplete.

Atomic Type	Coordinates (Angstroms) X	Y	Z
C	6.101202	-1.579312	-0.820285
C	5.755117	-0.216870	-0.054768
C	6.261973	1.051150	-0.789291
H	5.991985	1.041112	-1.847099
H	7.353401	1.029261	-0.776061
C	5.585768	2.363272	-0.178300
H	5.704030	2.410495	0.906356
C	6.180945	3.612385	-0.849364
O	5.917908	4.830098	-0.159301
H	4.972391	4.902870	0.061417
H	5.866447	3.680017	-1.893596
H	7.259077	3.436908	-0.809983
O	4.204315	2.374870	-0.720178
C	3.199126	3.138368	-0.231149
O	3.330951	4.115500	0.514145
C	1.972045	2.698198	-0.909378
H	1.946164	1.754036	-1.451562
C	0.784529	3.199482	-0.614908
H	0.621091	4.003980	0.098603
C	-0.487056	2.801561	-1.289472
H	-0.273815	2.075997	-2.077807
H	-1.009880	3.669373	-1.696694
C	-1.402241	2.044055	-0.259326
H	-1.750143	2.850941	0.390994
O	6.420355	-0.240359	1.167394
H	6.088403	-1.046431	1.600982
H	4.691187	-0.168298	0.187616
H	7.173954	-1.569835	-1.029600
C	5.412714	-1.733833	-2.190495
H	4.429193	-1.270792	-2.298142
H	6.021891	-1.378678	-3.024677
C	5.232628	-3.242361	-2.228079
H	6.127160	-3.666431	-2.688934
C	4.077808	-3.718248	-3.193445
H	3.140034	-3.263818	-2.867222
H	3.942460	-4.801200	-3.154428
H	4.369659	-3.417617	-4.201841
C	5.133564	-3.747718	-0.743711
H	5.589960	-4.724159	-0.562184
O	5.708237	-2.700335	-0.027513
O	-0.679329	0.986421	0.454328
C	-1.318704	0.334465	1.543932
H	-1.666732	1.005925	2.332555
C	-0.316903	-0.768778	2.015461
C	0.908136	-0.084050	2.742338
H	1.345336	0.667219	2.082369
C	0.497516	0.580184	4.080479
H	0.085373	-0.116323	4.813210
H	-0.202623	1.407769	3.949665
H	1.421006	0.963434	4.519929
C	1.886688	-1.306475	3.019647
H	1.944627	-1.631435	4.055706
C	2.501072	-1.945354	2.013753
H	2.353145	-1.656572	0.974269
C	3.228090	-3.190602	2.255182
H	3.187132	-3.449470	3.312373
C	3.652431	-4.054662	1.315725
H	4.122513	-4.965414	1.678938
C	3.685349	-3.839661	-0.188958
H	3.215613	-4.723586	-0.625803
H	3.161138	-2.915711	-0.440485
H	0.089553	-1.386653	1.212541
H	-0.848232	-1.327638	2.788111
C	-2.546231	-0.375350	0.952993
H	-3.049070	-0.956396	1.728779
H	-2.156205	-1.238389	0.409731
C	-3.448978	0.577064	0.093016
O	-4.380862	-0.289588	-0.561595
C	-5.555089	0.425377	-1.168810
H	-5.195298	0.969591	-2.053822
H	-3.886730	1.321335	0.763363
C	-2.561823	1.338052	-0.949589
H	-3.079522	2.012073	-1.635169
H	-2.046489	0.576054	-1.537600
O	-6.197656	1.237868	-0.148170
C	-6.645055	0.545385	1.052029
C	-7.323185	1.628620	1.978809
H	-6.587034	2.369233	2.296783

H	-7.889678	1.293829	2.850199
H	-8.040604	2.246528	1.434335
H	-5.789729	0.224293	1.652470
C	-7.573151	-0.727012	0.675867
H	-8.470467	-0.355963	0.173599
O	-7.928806	-1.494939	1.854362
H	-8.346947	-2.353870	1.661622
C	-6.871208	-1.618193	-0.401801
O	-7.716236	-2.657117	-0.850472
H	-8.155213	-2.267827	-1.627831
H	-5.950576	-2.104862	-0.071665
C	-6.414991	-0.773816	-1.607388
O	-7.637337	-0.373078	-2.260569
C	-7.550622	0.516643	-3.433554
H	-8.510606	0.541004	-3.955879
H	-6.732044	0.193199	-4.082300
H	-7.328827	1.535693	-3.106812
H	-5.828558	-1.331339	-2.341724

NMR-Shifts
Revised-MandelalideA184ps-NMR.txt

Atom	Type	Isotropic	Scaled Shift
1	C	88.6334	93.2508279255
2	C	100.5444	81.8503416987
3	C	139.7787	44.2976511802
6	C	90.8177	91.160148548
8	C	104.7509	77.8241352246
14	C	8.2155	170.221960604
16	C	56.6486	123.864737074
18	C	24.7074	154.436914949
20	C	132.5990	51.1696242271
23	C	100.5689	81.8268917858
29	C	146.7774	37.5989203469
32	C	138.0701	45.9330193916
34	C	164.7339	20.4120484695
38	C	98.3328	83.9671509792
42	C	104.8989	77.6824786079
44	C	122.3144	61.013419093
45	C	138.3771	45.6391776259
47	C	164.0960	21.0226076303
51	C	27.2687	151.985394054
53	C	49.3727	130.828786922
55	C	43.0728	136.858668811
57	C	51.0446	129.228545723
59	C	142.2959	41.888340129
64	C	137.1090	46.8529259748
67	C	108.6907	74.0531978024
69	C	72.3615	108.825302935
72	C	137.8814	46.1136315779
76	C	100.6355	81.7631463083
77	C	165.3475	19.8247477938
82	C	96.9450	85.2954689025
86	C	106.3861	76.2590210379
90	C	95.0064	87.1509791535
92	C	120.9311	62.3374298895
4	H	30.0601	1.64703164703
5	H	30.0308	1.6741048741
7	H	26.2848	5.13541233541
10	H	27.7473	3.78406098406
11	H	27.6349	3.88791868792
12	H	28.0288	3.52395472395
17	H	25.1922	6.14497574498
19	H	24.2445	7.02065142065
21	H	29.5384	2.12908292908
22	H	29.1111	2.52390852391
24	H	27.7889	3.74562254562
26	H	29.5745	2.09572649573
27	H	27.6708	3.85474705475
28	H	27.8384	3.69988449988
30	H	30.4748	1.26384846385
31	H	29.8603	1.83164703165
33	H	28.7929	2.81792561793
35	H	30.7816	0.980364980365
36	H	30.7386	1.0200970201
37	H	30.4353	1.30034650035
39	H	27.6132	3.90796950797
43	H	27.7725	3.76077616078
46	H	29.1120	2.52307692308
48	H	31.3503	0.454885654886
49	H	30.9146	0.857472857473
50	H	30.4405	1.29554169554
52	H	25.1840	6.15255255255
54	H	24.7101	6.59043659044
56	H	24.9999	6.32266112266
58	H	26.2040	5.21007161007
60	H	29.7994	1.88791868792
61	H	29.1061	2.52852852853
62	H	29.8665	1.82591822592
63	H	30.3735	1.35744975745
65	H	30.1078	1.60295680296
66	H	30.5120	1.22947562948
70	H	25.3701	5.9805959806
71	H	27.4895	4.02226842227
73	H	29.4492	2.2115038115
74	H	30.7509	1.00873180873
78	H	30.6087	1.14012474012
79	H	30.0776	1.63086163086
80	H	30.9491	0.825594825595
81	H	27.2764	4.21917301917
83	H	27.6290	3.89337029337
85	H	29.6179	2.05562485562
88	H	29.3173	2.33337953338
89	H	27.4242	4.08260568261
93	H	27.8164	3.72021252021
94	H	28.4859	3.10159390159
95	H	28.0025	3.54825594826
96	H	27.9649	3.582998383

Supporting Information: Revised-MandelalideA186ps.log

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 Using  Gaussian 09:  AM64L-G09RevC.01 23-Sep-2011
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 #mPWPW91/6-311+G(2d,p) scf=(maxcycle=300,direct,tight) NMR
density=current
 SCRF=(PCM,SOLVENT=Chloroform)
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 Pointgroup= C1   Stoichiometry= C33H52O11   C1[X(C33H52O11)]
#Atoms= 96
 Charge = 0                 Multiplicity = 1
-----------------------------------------------------------------------
 SCF Energy= -2116.46572193
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 Optimization incomplete.


-----------------------------------------------------------------------
     Atomic     Coordinates (Angstroms)
      Type      X              Y              Z
-----------------------------------------------------------------------
      C       6.317014     -1.222113     -1.090721
      C       5.933372      0.073660     -0.231735
      C       6.089470      1.423447     -0.967612
      H       5.864876      1.388016     -2.034880
      H       7.120687      1.738366     -0.795910
      C       5.284843      2.612362     -0.303212
      H       5.580238      2.592567      0.748450
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C	5.711538	3.971606	-0.957053
O	5.322837	5.026032	-0.122138
H	4.476076	4.766480	0.283814
H	5.124838	4.049465	-1.875565
H	6.780541	4.046593	-1.168381
O	3.862382	2.395423	-0.444517
C	2.883444	3.144431	0.011102
O	3.105624	3.997053	0.871982
C	1.572923	2.790665	-0.622064
H	1.592708	1.962026	-1.328673
C	0.436044	3.489937	-0.367523
H	0.465787	4.355856	0.289425
C	-0.924864	3.047913	-0.943274
H	-0.947123	2.779277	-2.000956
H	-1.553423	3.935368	-0.846125
C	-1.547278	1.936811	-0.146677
H	-1.846053	2.443207	0.775097
O	6.837338	0.159566	0.938682
H	6.773021	-0.784655	1.169884
H	4.897297	-0.069577	0.085707
H	7.371483	-1.118274	-1.358741
C	5.349160	-1.604901	-2.215517
H	4.330642	-1.299939	-1.967836
H	5.727070	-1.131132	-3.124846
C	5.447358	-3.187953	-2.181308
H	6.298435	-3.452949	-2.811791
C	4.264087	-3.846456	-2.913652
H	3.298761	-3.841640	-2.401888
H	4.574080	-4.862051	-3.169173
H	4.068910	-3.410417	-3.896099
C	5.686299	-3.521620	-0.696038
H	6.462672	-4.277168	-0.554118
O	6.241396	-2.278994	-0.157527
O	-0.668188	0.862826	0.153573
C	-1.064507	-0.006091	1.223712
H	-1.298791	0.609428	2.095267
C	0.097583	-0.984584	1.559171
C	1.230507	-0.365581	2.525597
H	1.869665	0.363943	2.022409
C	0.765636	0.208903	3.877236
H	-0.012894	-0.419266	4.312311
H	0.233379	1.160742	3.817678
H	1.531432	0.340858	4.645149
C	1.969611	-1.581232	2.868107
H	1.673610	-2.089675	3.781631
C	2.730378	-2.171661	1.974191
H	3.054832	-1.732739	1.031783
C	3.546746	-3.332849	2.310861
H	3.592324	-3.529032	3.381782
C	4.284320	-4.001949	1.439812
H	4.883248	-4.808856	1.854312
C	4.287598	-3.811520	-0.067502
H	3.935774	-4.785928	-0.413254
H	3.469028	-3.148004	-0.355447
H	0.484536	-1.465394	0.658039
H	-0.411195	-1.821114	2.044108
C	-2.377121	-0.681426	0.701983
H	-2.786284	-1.327609	1.480680
H	-2.016044	-1.396581	-0.039680
C	-3.460167	0.281818	0.253586
O	-4.462729	-0.495060	-0.348238
C	-5.521302	0.180600	-1.008998
H	-5.147914	0.633978	-1.939416
H	-3.857770	0.908944	1.055965
C	-2.844534	1.240558	-0.758078
H	-3.519536	2.081097	-0.932514
H	-2.519055	0.740360	-1.673032
O	-6.263822	1.152974	-0.213112
C	-6.921538	0.637459	1.057333
C	-7.686834	1.845375	1.559254
H	-8.408600	1.486657	2.295853
H	-8.218742	2.411999	0.792308
H	-6.977436	2.566164	1.971636
H	-6.186822	0.337229	1.809206
C	-7.855727	-0.569101	0.759700
H	-8.690064	-0.145902	0.194812
O	-8.202261	-1.249062	1.992095
H	-8.655009	-2.084506	1.777404
C	-7.114108	-1.632723	-0.185381
O	-8.067492	-2.594565	-0.647870
H	-8.440281	-2.106237	-1.403635
H	-6.257188	-2.109816	0.296940
C	-6.527347	-0.975872	-1.418322
O	-7.535250	-0.517307	-2.346640
C	-7.062061	-0.112670	-3.693818
H	-7.937043	0.300002	-4.202155
H	-6.721155	-1.017187	-4.203749
H	-6.311302	0.681120	-3.692465
H	-6.058156	-1.766636	-2.010624

NMR-Shifts

Revised-MandelalideA186ps-NMR.txt

Atom	Type	Isotropic	Scaled Shift
1	C	93.5771	88.5190183579
2	C	91.6828	90.3321273378
3	C	139.4172	44.6436570378
6	C	93.3541	88.7324604223
8	C	104.3972	78.1626753958
14	C	8.7047	169.753728058
16	C	43.0758	136.855797393
18	C	25.4005	153.773521698
20	C	143.6104	40.6301805165
23	C	105.4278	77.1762476311
29	C	139.9568	44.1271846705
32	C	137.9970	46.0029862746
34	C	168.4822	16.8244032236
38	C	95.3439	86.8279446391
42	C	97.8544	84.4250464213
44	C	123.8380	59.5551216524
45	C	145.1886	39.11962327
47	C	166.1879	19.0203679243
51	C	34.1053	145.441815502
53	C	53.4518	126.924519995
55	C	45.3544	134.674859779
57	C	52.6624	127.68008576
59	C	142.4642	41.7272535845
64	C	143.8895	40.3630429373
67	C	112.2633	70.6337219319
69	C	80.1577	101.363253508
72	C	139.5570	44.5098489634
76	C	94.8387	87.3114914145
77	C	164.4896	20.645877601
82	C	95.4396	86.7363464079
86	C	103.0048	79.49539616
90	C	91.9107	90.1139952909
92	C	118.8242	64.354026685
4	H	29.8252	1.86407946408
5	H	30.0900	1.6194040194
7	H	26.0277	5.37297297297
10	H	26.1449	5.26468006468
11	H	27.2881	4.20836220836
12	H	27.8130	3.72335412335
17	H	24.9851	6.33633633634
19	H	24.0407	7.20896280896
21	H	29.2125	2.43021483021
22	H	28.8903	2.72792792793
24	H	28.5010	3.08764148764
26	H	29.0310	2.59792099792

27	H	28.0371	3.51628551629
28	H	27.8606	3.67937167937
30	H	29.9485	1.75015015015
31	H	29.4612	2.20041580042
33	H	28.6978	2.9057981058
35	H	30.5098	1.23150843151
36	H	30.4835	1.25580965581
37	H	30.5876	1.15962115962
39	H	26.8614	4.60263340263
43	H	28.2677	3.30321090321
46	H	29.1465	2.4911988912
48	H	31.4120	0.397874797875
49	H	30.9375	0.836313236313
50	H	30.6465	1.1051975052
52	H	25.7035	5.67253407253
54	H	24.6999	6.59986139986
56	H	25.3275	6.01995841996
58	H	26.3958	5.03284823285
60	H	29.4532	2.20780780781
61	H	28.7297	2.87632247632
62	H	29.9166	1.77962577963
63	H	30.3597	1.3702009702
65	H	30.3138	1.41261261261
66	H	30.6665	1.08671748672
70	H	25.3561	5.99353199353
71	H	27.6357	3.88717948718
73	H	29.5536	2.11503811504
74	H	30.8461	0.920766920767
78	H	30.2391	1.48163548164
79	H	30.6500	1.10196350196
80	H	30.3723	1.35855855856
81	H	27.4942	4.01792561793
83	H	28.0693	3.48653268653
85	H	29.4041	2.25317625318
88	H	29.1955	2.44592284592
89	H	27.4877	4.02393162393
93	H	27.9228	3.6218988219
94	H	28.3330	3.24287364287
95	H	27.8908	3.65146685147
96	H	27.6464	3.87729267729

Supporting Information: Revised-MandelalideA188ps.log

Using Gaussian 09: AM64L-G09RevC.01 23-Sep-2011

==========

#mPWPW91/6-311+G(2d,p) scf=(maxcycle=300,direct,tight) NMR density=current

SCRF=(PCM,SOLVENT=Chloroform)

Pointgroup= C1 Stoichiometry= C33H52O11 C1[X(C33H52O11)]

#Atoms= 96

Charge = 0 Multiplicity = 1

SCF Energy= -2116.46642325

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Optimization incomplete.

Atomic Type	Coordinates (Angstroms) X	Y	Z
C	-6.683020	-1.035188	0.685814
C	-5.974709	0.121998	0.000952
C	-6.143934	1.490632	0.701854
H	-5.881361	1.346370	1.751517
H	-7.178602	1.838788	0.731726
C	-5.320852	2.686372	0.253020
H	-5.371476	2.764241	-0.836190
C	-5.922166	4.051443	0.612657
O	-5.200532	5.054093	-0.053950
H	-4.428878	4.673636	-0.510857
H	-5.676808	4.194725	1.667972
H	-7.001682	4.095535	0.450188
O	-3.916764	2.543546	0.704806
C	-2.955647	3.059658	0.027777
O	-3.017880	3.750602	-0.978677
C	-1.669971	2.837777	0.740796
H	-1.805825	2.358256	1.708676
C	-0.477100	3.125675	0.137351
H	-0.457061	3.564883	-0.856108
C	1.004342	2.943220	0.664901
H	1.088935	2.607431	1.700849
H	1.477715	3.913532	0.504232
C	1.786118	1.876464	-0.200223
H	2.249920	2.298471	-1.095746
O	-6.441827	0.263638	-1.346044
H	-6.859448	-0.595062	-1.534036
H	-4.955750	-0.245327	-0.140289
H	-7.745729	-0.792958	0.768180
C	-6.009360	-1.414703	2.105015
H	-4.933847	-1.280597	1.966829
H	-6.436987	-0.763385	2.869686
C	-6.271732	-2.906276	2.204960
H	-7.290426	-2.996977	2.586646
C	-5.473616	-3.602847	3.344666
H	-4.419183	-3.849341	3.202774
H	-6.020277	-4.468120	3.723502
H	-5.440176	-2.819425	4.104501
C	-6.064010	-3.410464	0.742466
H	-6.587838	-4.329410	0.467448
O	-6.682420	-2.326962	-0.089679
O	0.852485	0.853439	-0.568389
C	1.395052	-0.224034	-1.351625
H	1.852976	0.270046	-2.211763
C	0.339442	-1.218398	-1.768639
C	-1.038822	-0.602456	-1.969913
H	-1.371893	-0.122037	-1.047156
C	-0.985210	0.529580	-2.997913
H	-0.900842	0.153620	-4.019590
H	-0.186955	1.256501	-2.830958
H	-1.933873	1.069339	-3.012857
C	-1.944960	-1.706322	-2.463585
H	-2.190099	-1.694462	-3.522180
C	-2.634694	-2.517480	-1.649537
H	-2.527555	-2.466659	-0.567107
C	-3.726304	-3.435625	-2.057647
H	-3.827372	-3.544665	-3.136130
C	-4.567218	-3.968242	-1.161965
H	-5.355074	-4.524927	-1.663783
C	-4.587026	-3.682098	0.365537
H	-4.148859	-4.499225	0.942529
H	-4.156005	-2.698963	0.565750
H	0.202542	-1.980037	-0.998477
H	0.744159	-1.545527	-2.728750
C	2.552642	-0.779481	-0.565071
H	3.102508	-1.546430	-1.115191
H	2.170092	-1.193902	0.370320
C	3.598589	0.280794	-0.198223
O	4.621805	-0.388750	0.585067
C	5.798417	0.353081	0.898467
H	5.631026	1.199606	1.580806
H	4.012492	0.684759	-1.126017
C	2.938082	1.299845	0.646773
H	3.630970	2.108719	0.885406
H	2.595624	0.858824	1.585182

O	6.346477	0.814676	-0.341999
C	6.964157	-0.144136	-1.327007
C	7.392691	0.742567	-2.460704
H	7.842114	1.672994	-2.107374
H	6.459965	1.134805	-2.871694
H	7.984782	0.179663	-3.184842
H	6.325156	-0.915177	-1.765104
C	8.101602	-0.911434	-0.576822
H	8.977657	-0.301289	-0.342735
O	8.520574	-2.028121	-1.431676
H	9.140718	-2.502637	-0.849373
C	7.437201	-1.529931	0.662498
O	8.422369	-2.266995	1.305693
H	8.827080	-1.661104	1.951836
H	6.635683	-2.191672	0.323417
C	6.850661	-0.515483	1.620159
O	7.931967	0.340485	2.106225
C	7.776892	0.898698	3.449594
H	8.676050	1.471388	3.694090
H	7.493174	0.139195	4.182963
H	7.057332	1.720978	3.469228
H	6.507958	-1.083441	2.488737

NMR-Shifts
Revised-MandelalideA188ps-NMR.txt

Atom	Type	Isotropic	Scaled Shift
1	C	81.3580	100.214399204
2	C	103.8787	78.6589521239
3	C	148.1479	36.2871609334
6	C	99.7929	82.5696318842
8	C	109.0216	73.7364804074
14	C	12.6565	165.971304964
16	C	54.1917	126.216332625
18	C	15.6599	163.096632784
20	C	131.7684	51.9646241314
23	C	100.6271	81.7711862785
29	C	136.2767	47.6495530159
32	C	138.5108	45.5112081012
34	C	169.5602	15.792607056
38	C	83.3480	98.3096919926
42	C	105.4799	77.1263806734
44	C	139.0548	44.9905243209
45	C	146.7250	37.6490744463
47	C	163.5063	21.5870326767
51	C	38.0080	141.706387948
53	C	43.3096	136.632018224
55	C	40.7328	139.098374777
57	C	48.5719	131.595264075
59	C	146.4447	37.9173605927
64	C	139.2250	44.8276192117
67	C	105.6914	76.9239457111
69	C	81.9966	99.6031700454
72	C	140.8718	43.2514022091
76	C	96.2777	85.9341679588
77	C	165.6008	19.5823044086
82	C	97.3214	84.9352016693
86	C	107.5835	75.1129424376
90	C	90.7250	91.2488753613
92	C	120.1495	63.085529968
4	H	30.1902	1.52681912682
5	H	30.3530	1.37639177639
7	H	25.8067	5.57717717718
10	H	27.1663	4.32090552091
11	H	27.5174	3.99648879649
12	H	27.9161	3.62808962809
17	H	25.2838	6.06033726034
19	H	24.0834	7.16950796951
21	H	28.9197	2.70076230076
22	H	28.5929	3.00272580273
24	H	28.0526	3.50196350196
26	H	29.8175	1.87119427119
27	H	27.6164	3.90501270501
28	H	27.4497	4.05904365904
30	H	29.8092	1.87886347886
31	H	29.3655	2.28884268884
33	H	28.6335	2.96521136521
35	H	30.7456	1.01362901363
36	H	30.6168	1.13264033264
37	H	30.4557	1.2814968815
39	H	26.7916	4.66712866713
43	H	28.1432	3.41824901825
46	H	29.1481	2.48972048972
48	H	31.4474	0.365165165165
49	H	30.5812	1.16553476553
50	H	30.7643	0.99635019635
52	H	25.8280	5.5574959575
54	H	24.6731	6.62462462462
56	H	25.0957	6.23414183414
58	H	26.1234	5.28454608455
60	H	29.2410	2.40388080388
61	H	28.7106	2.89397089397
62	H	30.0676	1.6401016401
63	H	29.9960	1.70626010626
65	H	29.7428	1.94021714022
66	H	30.8787	0.890644490644
70	H	25.6362	5.73471933472
71	H	27.5056	4.00739200739
73	H	29.2911	2.35758835759
74	H	30.9017	0.869392469392
78	H	30.7012	1.05465465465
79	H	30.4689	1.2693000693
80	H	30.1278	1.58447678448
81	H	27.6263	3.89586509587
83	H	27.8936	3.64887964888
85	H	29.2274	2.41644721645
88	H	29.8120	1.87627627628
89	H	27.9161	3.62808962809
93	H	27.7910	3.74368214368
94	H	28.3978	3.182998383
95	H	28.0018	3.5489027489
96	H	27.8828	3.65885885886

Supporting Information: Revised-MandelalideA190ps.log

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 Using  Gaussian 09:  AM64L-G09RevC.01 23-Sep-2011
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 #mPWPW91/6-311+G(2d,p) scf=(maxcycle=300,direct,tight) NMR
density=current
 SCRF=(PCM,SOLVENT=Chloroform)
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 Pointgroup= C1   Stoichiometry= C33H52O11   C1[X(C33H52O11)]
#Atoms= 96
 Charge = 0                Multiplicity = 1
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 SCF Energy= -2116.49599266
=========================================================================
 Optimization incomplete.


---------------------------------------------------------------------------
     Atomic     Coordinates (Angstroms)
      Type     X                Y              Z
---------------------------------------------------------------------------
      C      -6.480670     -0.936504      0.442446
      C      -5.591971      0.168599     -0.116425
      C      -5.954076      1.513371      0.613417
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H	-5.897936	1.456336	1.702648
H	-7.002899	1.669797	0.351084
C	-5.103795	2.646289	0.109503
H	-5.080989	2.589878	-0.981902
C	-5.777090	4.031552	0.489605
O	-5.242475	5.095325	-0.294916
H	-4.319365	4.865084	-0.500905
H	-5.715400	4.277207	1.552490
H	-6.831529	4.049280	0.203090
O	-3.799593	2.381283	0.684455
C	-2.743182	3.067230	0.285433
O	-2.786969	4.037041	-0.507195
C	-1.554383	2.539288	0.976649
H	-1.733982	1.577532	1.455043
C	-0.359092	3.162192	0.871312
H	-0.230927	4.048109	0.254450
C	0.886530	2.610790	1.482423
H	0.502719	1.916164	2.232799
H	1.460371	3.375883	2.010074
C	1.669584	1.839044	0.398710
H	2.179025	2.611724	-0.182486
O	-5.836473	0.214641	-1.547544
H	-6.170335	-0.686519	-1.708571
H	-4.536646	-0.048741	0.067465
H	-7.541984	-0.700918	0.550822
C	-6.038842	-1.448753	1.779220
H	-4.947172	-1.432731	1.800325
H	-6.465371	-0.818322	2.562081
C	-6.596140	-2.897751	1.761162
H	-7.685089	-2.822808	1.762208
C	-6.160651	-3.789974	2.958448
H	-5.104205	-3.628902	3.183605
H	-6.327522	-4.850121	2.756839
H	-6.706132	-3.534635	3.869806
C	-6.159999	-3.404090	0.346094
H	-6.835146	-4.226696	0.095597
O	-6.310686	-2.105433	-0.415247
O	0.779562	0.986020	-0.340519
C	1.397787	0.204558	-1.391705
H	1.609709	0.936001	-2.175503
C	0.338077	-0.764272	-1.964390
C	-1.148791	-0.295970	-1.867975
H	-1.436101	0.136018	-0.907079
C	-1.326098	0.871651	-2.960921
H	-1.147935	0.494334	-3.970891
H	-0.672091	1.745319	-2.912006
H	-2.356577	1.221272	-2.876929
C	-1.918934	-1.512366	-2.176114
H	-1.693557	-1.949855	-3.145953
C	-2.678900	-2.246376	-1.309528
H	-2.981394	-1.811271	-0.357894
C	-3.304581	-3.519556	-1.766807
H	-2.993167	-3.815484	-2.767757
C	-4.199638	-4.255775	-1.084194
H	-4.645156	-5.133873	-1.544514
C	-4.643749	-3.843722	0.352385
H	-4.509318	-4.714283	0.997207
H	-3.954844	-3.095615	0.751339
H	0.251764	-1.716420	-1.435617
H	0.527604	-1.016298	-3.009138
C	2.672736	-0.603104	-0.909066
H	3.231295	-1.065343	-1.724255
H	2.274024	-1.423427	-0.308395
C	3.570142	0.327031	-0.133429
O	4.661720	-0.508281	0.358377
C	5.650619	0.078132	1.107966
H	5.185047	0.561801	1.979300
H	4.057730	1.039757	-0.803276
C	2.739857	0.952137	1.020374
H	3.355643	1.559337	1.687645
H	2.276564	0.123163	1.558913
O	6.353444	1.017597	0.288328
C	6.911551	0.541682	-0.969204
C	7.678137	1.592745	-1.699472
H	8.600015	1.853427	-1.175821
H	7.075640	2.500284	-1.772822
H	7.928830	1.253039	-2.706632
H	6.091288	0.164885	-1.586753
C	7.887057	-0.671309	-0.749782
H	8.806594	-0.314235	-0.279045
O	8.233241	-1.281735	-2.015587
H	8.640734	-2.149853	-1.844788
C	7.178100	-1.733545	0.149705
O	8.143558	-2.798441	0.370106
H	8.703945	-2.513150	1.113385
H	6.266775	-2.036114	-0.372518
C	6.678858	-1.046600	1.452251
O	7.865336	-0.642454	2.059122
C	7.652705	0.044930	3.264800
H	8.628151	0.195458	3.735698
H	6.995551	-0.501999	3.944813
H	7.218633	1.030223	3.072159
H	6.142838	-1.737531	2.108197

NMR-Shifts

Revised-MandelalideA190ps-NMR.txt

Atom	Type	Isotropic	Scaled Shift
1	C	96.3851	85.8313711978
2	C	100.6779	81.7225636019
3	C	141.4217	42.7250713069
6	C	99.0331	83.2968663259
8	C	104.5773	77.9902946075
14	C	6.6496	171.720745037
16	C	51.7101	128.591569517
18	C	22.0253	157.004058271
20	C	138.0182	45.9826949214
23	C	106.4490	76.1988169758
29	C	140.6330	43.4799670744
32	C	132.0137	51.7298378606
34	C	168.2671	17.0302838875
38	C	84.6135	97.0984322058
42	C	103.3165	79.1970558395
44	C	130.2402	53.4273244128
45	C	139.5645	44.5026704187
47	C	160.4133	24.547464538
51	C	27.6676	151.603591187
53	C	49.2150	130.97972779
55	C	40.7087	139.121441835
57	C	50.3125	129.929267406
59	C	141.9527	42.2168303375
64	C	137.1190	46.8433545818
67	C	105.3571	77.2439173797
69	C	86.1067	95.6692318
72	C	140.1500	43.9422653573
76	C	107.4136	75.2755604051
77	C	165.5826	19.5997243439
82	C	93.2873	88.7963973277
86	C	99.2851	83.0556672218
90	C	97.3673	84.8912689753
92	C	126.9874	56.5407071345
4	H	29.9038	1.79145299145
5	H	30.3607	1.36927696928
7	H	26.3779	5.04938784939
10	H	26.3930	5.03543543544
11	H	27.4654	4.04453684454
12	H	27.6393	3.88385308385
17	H	24.9388	6.37911757912
19	H	23.8720	7.36484176484

21	H	29.0961	2.53776853777
22	H	29.0700	2.56188496188
24	H	28.0735	3.48265188265
26	H	28.2850	3.28722568723
27	H	27.7584	3.7738045738
28	H	27.9392	3.60674520675
30	H	29.8479	1.8431046431
31	H	29.8484	1.84264264264
33	H	29.1281	2.5082005082
35	H	30.9858	0.791683991684
36	H	30.7700	0.991083391083
37	H	30.5858	1.16128436128
39	H	27.1362	4.34871794872
43	H	27.6308	3.89170709171
46	H	29.0591	2.57195657196
48	H	31.4152	0.394917994918
49	H	30.4171	1.31716331716
50	H	30.7968	0.96632016632
52	H	25.6478	5.724000924
54	H	24.3853	6.89055209055
56	H	25.1972	6.14035574036
58	H	25.8026	5.58096558097
60	H	29.6229	2.051004851
61	H	28.5304	3.06047586048
62	H	29.9847	1.7167013167
63	H	30.1104	1.60055440055
65	H	29.5716	2.09840609841
66	H	30.4606	1.27696927697
70	H	25.3006	6.04481404481
71	H	27.3162	4.1823977824
73	H	29.3346	2.31739431739
74	H	30.8928	0.877616077616
78	H	30.7901	0.972510972511
79	H	30.6604	1.09235389235
80	H	29.9708	1.72954492954
81	H	27.9230	3.62171402171
83	H	27.9941	3.55601755602
85	H	29.4125	2.24541464541
88	H	29.9218	1.77482097482
89	H	27.5048	4.00813120813
93	H	28.1258	3.43432663433
94	H	28.8054	2.80637560638
95	H	28.1004	3.4577962578
96	H	28.3013	3.27216447216

Supporting Information: Revised-MandelalideA192ps.log

Using Gaussian 09: AM64L-G09RevC.01 23-Sep-2011

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#mPWPW91/6-311+G(2d,p) scf=(maxcycle=300,direct,tight) NMR density=current

SCRF=(PCM,SOLVENT=Chloroform)

Pointgroup= C1 Stoichiometry= C33H52O11 C1[X(C33H52O11)]

#Atoms= 96

Charge = 0 Multiplicity = 1

SCF Energy= -2116.47747787

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Optimization incomplete.

Atomic Type	Coordinates (Angstroms) X	Y	Z
C	-6.683800	-0.982149	0.676038
C	-5.869612	0.087139	-0.053075
C	-6.129900	1.519545	0.410461
H	-6.077018	1.524995	1.501283
H	-7.147206	1.809317	0.139324
C	-5.205493	2.628651	-0.127352
H	-5.262902	2.575971	-1.218126
C	-5.680311	3.909742	0.489529
O	-5.293876	5.086651	-0.208248
H	-4.386031	4.906114	-0.513631
H	-5.420400	3.929663	1.550539
H	-6.769758	3.885585	0.403923
O	-3.827361	2.345643	0.381324
C	-2.803855	3.159720	-0.078233
O	-2.985656	4.093861	-0.808539
C	-1.522712	2.694135	0.475937
H	-1.429493	1.744427	1.000462
C	-0.431274	3.448202	0.386035
H	-0.483403	4.438732	-0.058731
C	0.900707	2.968334	0.891982
H	0.698412	2.518090	1.865596
H	1.697920	3.686638	1.090280
C	1.577136	2.022112	-0.134496
H	1.698008	2.503665	-1.107937
O	-6.285632	0.076378	-1.438391
H	-6.370830	-0.883834	-1.575855
H	-4.831490	-0.240292	0.049449
H	-7.746056	-0.737549	0.752495
C	-6.106102	-1.208771	2.136291
H	-5.088756	-0.832931	2.262826
H	-6.715260	-0.757197	2.921063
C	-6.235298	-2.728956	2.268257
H	-7.271508	-2.978719	2.505711
C	-5.356450	-3.330189	3.420197
H	-4.371642	-2.858448	3.426292
H	-5.056105	-4.377097	3.336958
H	-5.889938	-3.227593	4.366765
C	-6.021973	-3.316704	0.833861
H	-6.740142	-4.126173	0.681297
O	-6.395301	-2.229748	-0.053399
O	0.755797	0.862640	-0.349361
C	1.388511	-0.238042	-1.085111
H	1.869520	0.085452	-2.011737
C	0.338223	-1.249728	-1.436329
C	-0.974109	-0.764902	-2.018960
H	-1.543897	-0.081044	-1.386375
C	-0.622811	0.098384	-3.263067
H	-0.022453	-0.526163	-3.927917
H	-0.044053	0.959819	-2.922769
H	-1.524869	0.446123	-3.771375
C	-1.814778	-1.998668	-2.361499
H	-1.671832	-2.504000	-3.313233
C	-2.777134	-2.375192	-1.503911
H	-2.770839	-1.873625	-0.537140
C	-3.698707	-3.461766	-1.878828
H	-3.632975	-3.722047	-2.933986
C	-4.498622	-4.096999	-1.021816
H	-4.952583	-5.019783	-1.373070
C	-4.662826	-3.827608	0.490761
H	-4.346897	-4.703120	1.061899
H	-3.825780	-3.165218	0.722957
H	0.204453	-1.871870	-0.548760
H	0.899757	-1.893628	-2.115705
C	2.506098	-0.771017	-0.250192
H	2.933173	-1.659685	-0.717386
H	2.055153	-1.077277	0.695932
C	3.514259	0.311487	-0.184366
O	4.496383	-0.177866	0.814548
C	5.785032	0.477845	0.938965
H	5.666108	1.344577	1.605809

H	3.955227	0.564478	-1.151670
C	2.907754	1.610868	0.467479
H	3.739029	2.311226	0.354341
H	2.698789	1.428667	1.523268
O	6.416431	0.894300	-0.288556
C	6.751796	-0.020297	-1.278956
C	7.131766	0.598010	-2.626824
H	8.058671	1.172975	-2.662888
H	6.246016	1.048227	-3.079607
H	7.453152	-0.188396	-3.313308
H	5.871998	-0.651864	-1.424733
C	7.727389	-1.114798	-0.717406
H	8.711800	-0.673115	-0.538793
O	7.961132	-2.079450	-1.687203
H	8.668555	-2.640345	-1.321941
C	7.312012	-1.702715	0.691428
O	8.514940	-2.216372	1.317746
H	8.961605	-1.511729	1.821598
H	6.593018	-2.517273	0.576274
C	6.777019	-0.496929	1.574001
O	7.968895	0.160564	2.066208
C	7.860548	1.009976	3.239045
H	7.152892	1.840265	3.176233
H	8.842725	1.452134	3.424783
H	7.496199	0.401638	4.070257
H	6.321014	-0.963887	2.450963

NMR-Shifts
Revised-MandelalideA192ps-NMR.txt

Atom	Type	Isotropic	Scaled Shift
1	C	85.4318	96.315205115
2	C	100.7948	81.6106740175
3	C	141.7033	42.4555408794
6	C	98.2622	84.0347250139
8	C	107.8937	74.8160378261
14	C	10.3699	168.159899692
16	C	53.4016	126.972568388
18	C	29.7912	149.571010165
20	C	136.8490	47.1017821934
23	C	105.4651	77.1405463351
29	C	138.9462	45.0944696491
32	C	136.9064	47.0468423974
34	C	168.0711	17.2178831907
38	C	94.4123	87.7196156129
42	C	104.1732	78.3770745994
44	C	137.7135	46.2743352668
45	C	142.3455	41.8408660196
47	C	161.4090	23.5944409349
51	C	30.5430	148.851432838
53	C	46.9681	133.130324087
55	C	43.0325	136.897241525
57	C	52.1525	128.16813109
59	C	151.3264	33.2448936618
64	C	143.5821	40.6572675587
67	C	99.7408	82.6194988419
69	C	78.7411	102.719137043
72	C	137.4763	46.5013687092
76	C	112.9851	69.9428587837
77	C	171.2512	14.1740844963
82	C	97.4652	84.7975650376
86	C	98.5008	83.8063515764
90	C	98.3773	83.9245582802
92	C	122.3061	61.0213633492
4	H	30.2562	1.46583506584
5	H	30.2570	1.4650958651
7	H	26.2089	5.20554400554
10	H	25.9297	5.46352506353
11	H	27.8848	3.65701085701
12	H	27.9832	3.56608916609
17	H	24.8878	6.42624162624
19	H	24.1655	7.09364749365
21	H	29.2775	2.37015477015
22	H	29.3273	2.32413952414
24	H	27.9631	3.58466158466
26	H	28.8209	2.79205359205
27	H	28.0078	3.54335874336
28	H	27.5662	3.9513975514
30	H	30.4482	1.28842688843
31	H	29.4830	2.18027258027
33	H	28.8384	2.77588357588
35	H	30.9638	0.812012012012
36	H	30.6401	1.11111111111
37	H	30.4571	1.2802032802
39	H	27.0561	4.42273042273
43	H	28.4769	3.10990990991
46	H	28.9355	2.68616308616
48	H	31.3551	0.45045045045
49	H	30.3991	1.3337953338
50	H	30.7227	1.03478863479
52	H	25.5526	5.81196581197
54	H	24.3058	6.96401016401
56	H	24.8387	6.47161007161
58	H	26.3754	5.0516978517
60	H	29.7863	1.90002310002
61	H	29.0664	2.56521136521
62	H	30.3106	1.41556941557
63	H	30.6706	1.08292908293
65	H	30.0716	1.63640563641
66	H	30.5351	1.20813120813
70	H	25.3804	5.97107877108
71	H	27.5106	4.00277200277
73	H	28.7247	2.88094248094
74	H	30.5038	1.23705243705
78	H	30.5696	1.17625317625
79	H	30.3928	1.33961653962
80	H	30.2068	1.51148071148
81	H	28.0032	3.54760914761
83	H	27.9850	3.56442596443
85	H	29.7002	1.97957957958
88	H	28.2961	3.27696927697
89	H	27.6442	3.87932547933
93	H	28.2978	3.2753984754
94	H	27.9692	3.57902517903
95	H	28.5248	3.06565026565
96	H	28.0306	3.52229152229

Supporting Information: Revised-MandelalideA194ps.log

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 Using  Gaussian 09:  AM64L-G09RevC.01 23-Sep-2011
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 #mPWPW91/6-311+G(2d,p) scf=(maxcycle=300,direct,tight) NMR
density=current
 SCRF=(PCM,SOLVENT=Chloroform)
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#Atoms= 96
 Charge = 0                Multiplicity = 1
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 SCF Energy= -2116.47105680
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 Optimization incomplete.


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     Atomic     Coordinates (Angstroms)
      Type     X                Y              Z
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C	-6.281598	-0.895809	0.740020
C	-5.479042	0.274533	-0.024156
C	-5.941519	1.577364	0.576843
H	-5.673533	1.560859	1.634701
H	-7.023824	1.656133	0.460269
C	-5.203036	2.776361	0.038946
H	-5.412035	2.811153	-1.032844
C	-5.733557	4.065133	0.691134
O	-5.486701	5.191271	-0.213418
H	-4.552648	5.235432	-0.485236
H	-5.166477	4.102325	1.624717
H	-6.803437	4.036777	0.916652
O	-3.777017	2.593211	0.300948
C	-2.822544	3.352496	-0.287755
O	-2.989155	4.416576	-0.882955
C	-1.518689	2.788261	0.134127
H	-1.490177	1.747630	0.453464
C	-0.373679	3.465855	0.082849
H	-0.325111	4.515354	-0.194493
C	0.976201	2.956105	0.661011
H	0.845604	2.669673	1.707576
H	1.758025	3.715010	0.737036
C	1.658783	1.819205	-0.133242
H	2.158873	2.172361	-1.038724
O	-5.770970	0.152894	-1.384797
H	-5.661651	-0.788279	-1.608729
H	-4.404899	0.135275	0.124031
H	-7.365566	-0.790874	0.650027
C	-5.975925	-1.171470	2.232719
H	-4.932524	-0.894044	2.392394
H	-6.545748	-0.597565	2.966991
C	-6.303034	-2.620648	2.357687
H	-7.379489	-2.767614	2.465587
C	-5.564184	-3.172353	3.623160
H	-4.501440	-3.115365	3.379883
H	-5.899034	-4.203936	3.752972
H	-5.785631	-2.657137	4.559898
C	-5.893856	-3.225668	0.973033
H	-6.642524	-3.965072	0.678685
O	-5.880292	-2.116030	0.038550
O	0.740892	0.783590	-0.547632
C	1.158513	-0.305656	-1.364569
H	1.604643	0.177833	-2.238155
C	0.055097	-1.425896	-1.686157
C	-1.182503	-1.009962	-2.494461
H	-1.720528	-0.273997	-1.893024
C	-0.864457	-0.422811	-3.864013
H	-0.154931	-0.982951	-4.475811
H	-0.485821	0.598947	-3.799659
H	-1.800573	-0.380666	-4.425632
C	-2.115513	-2.245646	-2.665545
H	-2.015615	-2.800861	-3.594331
C	-2.878442	-2.706525	-1.683111
H	-2.903321	-2.094739	-0.783199
C	-3.702380	-3.886394	-1.755964
H	-3.813152	-4.404498	-2.708180
C	-4.434257	-4.346539	-0.727955
H	-5.104656	-5.192026	-0.863157
C	-4.563177	-3.882300	0.722551
H	-4.270518	-4.685782	1.402349
H	-3.864997	-3.081047	0.973882
H	-0.368384	-1.725665	-0.725164
H	0.569110	-2.297703	-2.097541
C	2.407282	-0.941307	-0.614615
H	2.889038	-1.743078	-1.178459
H	1.976020	-1.491949	0.224471
C	3.478381	0.091870	-0.154224
O	4.441668	-0.585083	0.724269
C	5.658351	0.207474	0.988826
H	5.424925	0.957831	1.758977
H	4.043622	0.524548	-0.983537
C	2.778059	1.207431	0.634378
H	3.519607	1.949428	0.938299
H	2.450235	0.726364	1.558138
O	6.218745	0.832508	-0.205438
C	6.863086	0.074398	-1.219988
C	7.477069	1.026148	-2.193944
H	8.201413	1.676445	-1.698496
H	6.686947	1.691541	-2.546224
H	7.980580	0.491339	-3.002346
H	6.095586	-0.580348	-1.640286
C	7.961655	-0.736242	-0.595771
H	8.801090	-0.142235	-0.224531
O	8.486042	-1.619096	-1.552965
H	9.148626	-2.095454	-1.021557
C	7.402661	-1.532964	0.645371
O	8.427701	-2.124769	1.271330
H	8.885419	-1.459040	1.815628
H	6.639098	-2.229626	0.289084
C	6.755346	-0.605009	1.680186
O	7.618976	0.343377	2.392326
C	7.064759	0.995380	3.568369
H	6.177168	1.610760	3.400984
H	7.915023	1.534270	3.994662
H	6.650051	0.210974	4.207178
H	6.225318	-1.283187	2.354597

NMR-Shifts

Revised-MandelalideA194ps-NMR.txt

Atom	Type	Isotropic	Scaled Shift
1	C	81.9509	99.6469113115
2	C	102.7768	79.7136239208
3	C	147.2019	37.1926147131
6	C	98.3585	83.9425524991
8	C	104.2664	78.2878692165
14	C	9.5719	168.923696855
16	C	48.6059	131.562721338
18	C	31.9720	147.483680775
20	C	141.0077	43.1213269779
23	C	104.6796	77.8923792569
29	C	141.9822	42.1885947281
32	C	139.0909	44.9559715921
34	C	166.6831	18.546392542
38	C	96.6424	85.5850992553
42	C	100.8180	81.5884683857
44	C	130.5605	53.1207526943
45	C	140.7947	43.3251976493
47	C	166.9271	18.3128505523
51	C	34.6224	144.946878769
53	C	51.6288	128.669384942
55	C	51.3892	128.898715519
57	C	46.3916	133.682114895
59	C	148.4414	36.0062405482
64	C	139.9919	44.093589081
67	C	103.7011	78.8289400639
69	C	74.8696	106.424701851
72	C	142.9339	41.2776852543
76	C	110.7278	72.1034093302
77	C	162.9588	22.1110664446
82	C	95.6380	86.5464499703
86	C	107.9414	74.7703822814
90	C	94.4242	87.7082256552
92	C	120.7835	62.4787036505
4	H	30.2228	1.4966966967
5	H	30.1140	1.59722799723
7	H	26.7394	4.71536151536
10	H	26.7671	4.68976668977

11	H	28.0111	3.54030954031
12	H	27.9650	3.58290598291
17	H	24.7983	6.50893970894
19	H	24.3091	6.96096096096
21	H	29.3264	2.32497112497
22	H	29.3003	2.34908754909
24	H	28.1744	3.38942018942
26	H	29.0988	2.53527373527
27	H	27.4772	4.03363363363
28	H	27.7761	3.75744975745
30	H	30.2956	1.42942942943
31	H	29.8181	1.87063987064
33	H	29.0316	2.59736659737
35	H	30.8652	0.903118503119
36	H	30.5672	1.17847077847
37	H	30.5660	1.17957957958
39	H	27.5102	4.00314160314
43	H	27.6755	3.8504042504
46	H	29.1368	2.50016170016
48	H	31.1894	0.603557403557
49	H	30.6676	1.0857010857
50	H	30.6847	1.0699006699
52	H	25.9855	5.41196581197
54	H	24.5123	6.7732039732
56	H	25.2610	6.0814044814
58	H	26.2720	5.14723954724
60	H	29.7191	1.96211596212
61	H	29.4144	2.24365904366
62	H	29.6615	2.01533841534
63	H	30.1640	1.55102795103
65	H	30.1777	1.53836913837
66	H	30.6686	1.08477708478
70	H	25.3350	6.01302841303
71	H	27.2832	4.21288981289
73	H	29.5032	2.16160776161
74	H	30.9609	0.814691614692
78	H	30.7407	1.01815661816
79	H	30.6516	1.10048510049
80	H	29.7072	1.97311157311
81	H	27.7600	3.77232617233
83	H	28.4288	3.15435435435
85	H	29.4178	2.24051744052
88	H	29.8961	1.79856779857
89	H	27.9707	3.57763917764
93	H	27.8185	3.71827211827
94	H	27.6288	3.89355509356
95	H	28.5267	3.06389466389
96	H	28.1705	3.39302379302

Supporting Information: Revised-MandelalideA196ps.log

Using Gaussian 09: AM64L-G09RevC.01 23-Sep-2011

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#mPWPW91/6-311+G(2d,p) scf=(maxcycle=300,direct,tight) NMR density=current

SCRF=(PCM,SOLVENT=Chloroform)

Pointgroup= C1 Stoichiometry= C33H52O11 C1[X(C33H52O11)]

#Atoms= 96

Charge = 0 Multiplicity = 1

SCF Energy= -2116.47245763

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Optimization incomplete.

Atomic Type	Coordinates (Angstroms) X	Y	Z
C	-6.221004	-1.012797	0.209865
C	-5.371456	0.237893	-0.290264
C	-6.122682	1.537487	0.010400
H	-6.395219	1.521728	1.067354
H	-6.939992	1.641223	-0.706513
C	-5.278521	2.809053	-0.204939
H	-5.033268	2.945937	-1.261462
C	-6.035252	4.080577	0.276930
O	-5.391046	5.325489	-0.029396
H	-4.554127	5.082020	-0.464411
H	-6.053649	4.039131	1.369030
H	-7.025052	4.137478	-0.183790
O	-3.976636	2.617154	0.405672
C	-2.903516	3.287068	0.051672
O	-2.914315	4.287861	-0.650316
C	-1.655197	2.817381	0.675824
H	-1.878385	1.926360	1.260456
C	-0.469350	3.458420	0.482688
H	-0.310585	4.302096	-0.184091
C	0.829989	3.004989	1.132155
H	0.640231	2.557170	2.110126
H	1.460637	3.846080	1.427154
C	1.602496	1.951759	0.198549
H	1.828429	2.507309	-0.714599
O	-4.942627	0.118804	-1.691267
H	-4.736513	-0.812837	-1.888549
H	-4.402638	0.235271	0.214303
H	-7.265823	-1.023207	-0.111040
C	-6.150530	-1.280798	1.711965
H	-5.106979	-1.152387	2.006422
H	-6.720044	-0.599637	2.347413
C	-6.489254	-2.785386	1.898450
H	-7.556358	-2.947166	1.737282
C	-6.093000	-3.424150	3.190499
H	-5.029780	-3.300703	3.405681
H	-6.398496	-4.466492	3.072110
H	-6.644578	-3.053725	4.056501
C	-5.939761	-3.460920	0.618083
H	-6.694260	-4.108086	0.163809
O	-5.705433	-2.320100	-0.308685
O	0.656575	0.884134	-0.080995
C	1.094203	-0.040894	-1.068759
H	1.328883	0.529188	-1.971261
C	-0.020904	-1.089857	-1.256173
C	-1.461779	-0.638956	-1.458151
H	-1.846417	-0.252940	-0.511815
C	-1.525902	0.470378	-2.527590
H	-1.073180	0.119984	-3.457595
H	-1.067275	1.432005	-2.286202
H	-2.565578	0.776515	-2.661828
C	-2.196481	-1.851639	-1.994766
H	-2.280439	-1.988176	-3.069433
C	-2.733969	-2.792263	-1.166271
H	-2.608852	-2.532896	-0.116206
C	-3.335840	-4.061936	-1.454036
H	-3.238221	-4.295186	-2.513672
C	-4.191778	-4.767655	-0.666385
H	-4.594607	-5.748265	-0.907700
C	-4.584926	-4.267277	0.692477
H	-4.721186	-5.148766	1.322301
H	-3.796429	-3.627664	1.096903
H	0.114278	-1.745958	-0.394568
H	0.373937	-1.597025	-2.139737
C	2.440595	-0.698327	-0.563878
H	2.837210	-1.334253	-1.358537
H	2.303137	-1.434378	0.230622

C	3.536919	0.393944	-0.251158
O	4.627248	-0.300439	0.441384
C	5.866499	0.387311	0.780584
H	5.723426	1.135239	1.573895
H	3.845326	0.796640	-1.218536
C	2.937977	1.429241	0.760445
H	3.565214	2.321508	0.809823
H	2.766955	1.048030	1.768965
O	6.630804	0.970872	-0.228880
C	6.927730	0.090518	-1.282533
C	7.490095	0.907506	-2.431446
H	8.278079	1.500080	-1.962670
H	6.752411	1.575082	-2.880713
H	7.937538	0.217940	-3.151250
H	5.951931	-0.264377	-1.624104
C	7.860732	-1.090547	-0.838050
H	8.846583	-0.667844	-0.628385
O	7.878180	-2.143079	-1.770840
H	8.521952	-2.822313	-1.502783
C	7.321208	-1.742985	0.454874
O	8.355173	-2.549103	1.087925
H	8.852492	-1.854452	1.555037
H	6.515747	-2.438430	0.207944
C	6.844664	-0.648116	1.470862
O	8.018940	0.071111	2.085759
C	7.819624	1.157411	2.994519
H	7.230101	1.935017	2.500547
H	8.715898	1.570563	3.465825
H	7.197119	0.778968	3.809357
H	6.305717	-1.161642	2.271043

NMR-Shifts
Revised-MandelalideA196ps-NMR.txt

Atom	Type	Isotropic	Scaled Shift
1	C	88.5572	93.3237619403
2	C	98.8336	83.4878156167
3	C	146.6720	37.6998028293
6	C	100.5185	81.8751316067
8	C	107.4982	75.1945864201
14	C	11.4023	167.171749076
16	C	50.4844	129.76473516
18	C	26.3705	152.845096575
20	C	137.0968	46.8646030743
23	C	99.0856	83.2466165126
29	C	139.6280	44.441892073
32	C	139.1670	44.8831332912
34	C	170.6294	14.7692337143
38	C	85.5564	96.1959455579
42	C	100.2866	82.0970922108
44	C	135.0290	48.8437757231
45	C	145.2711	39.0406592776
47	C	165.1604	20.0038285572
51	C	37.1931	142.486360765
53	C	45.8064	134.242232815
55	C	48.3895	131.769846283
57	C	45.0634	134.953387316
59	C	146.5872	37.7809682421
64	C	139.5065	44.5581844982
67	C	99.3646	82.9795746473
69	C	81.7606	99.8290549207
72	C	143.1254	41.094393078
76	C	112.2504	70.6460690289
77	C	164.2638	20.8619996554
82	C	101.9703	80.4855567679
86	C	94.7639	87.3830854343
90	C	86.8243	94.9823886368
92	C	126.8772	56.6461838856
4	H	29.9383	1.75957495957
5	H	29.8686	1.82397782398
7	H	26.2996	5.12173712174
10	H	27.3209	4.17805497805
11	H	27.6128	3.90833910834
12	H	27.5139	3.99972279972
17	H	25.0736	6.25456225456
19	H	23.7322	7.49401709402
21	H	29.4043	2.25299145299
22	H	29.3306	2.32109032109
24	H	28.2654	3.30533610534
26	H	29.4361	2.22360822361
27	H	26.9180	4.55033495033
28	H	27.4163	4.08990528991
30	H	30.5039	1.23696003696
31	H	29.7914	1.89531069531
33	H	28.8939	2.7246015246
35	H	30.7981	0.965118965119
36	H	30.6026	1.14576114576
37	H	30.7250	1.03266343266
39	H	27.4363	4.07142527143
43	H	28.0526	3.50196350196
46	H	29.0944	2.53933933934
48	H	31.2366	0.559944559945
49	H	30.8358	0.930284130284
50	H	30.2502	1.47137907138
52	H	25.8721	5.51674751675
54	H	24.8243	6.48491568492
56	H	25.2386	6.1021021021
58	H	25.3308	6.01690921691
60	H	29.5879	2.08334488334
61	H	28.6678	2.93351813352
62	H	30.0160	1.68778008778
63	H	30.4870	1.25257565258
65	H	29.9613	1.73832293832
66	H	30.7179	1.03922383922
70	H	25.3155	6.03104643105
71	H	27.2685	4.22647262647
73	H	29.6097	2.0632016632
74	H	30.4059	1.32751212751
78	H	30.7761	0.985446985447
79	H	30.3955	1.33712173712
80	H	30.1672	1.54807114807
81	H	27.5145	3.99916839917
83	H	28.4239	3.15888195888
85	H	29.3474	2.30556710557
88	H	29.5866	2.08454608455
89	H	27.3968	4.10792330792
93	H	27.7983	3.73693693694
94	H	27.9231	3.62162162162
95	H	28.5567	3.03617463617
96	H	27.7754	3.7580965581

Supporting Information: Revised-MandelalideA198ps.log

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 Using  Gaussian 09:  AM64L-G09RevC.01 23-Sep-2011
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 #mPWPW91/6-311+G(2d,p) scf=(maxcycle=300,direct,tight) NMR
density=current
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#Atoms= 96
 Charge = 0                Multiplicity = 1
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 SCF Energy= -2116.48148130
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 Optimization incomplete.
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Atomic Type	Coordinates (Angstroms) X	Y	Z
C	-6.590549	-0.791769	0.117805
C	-5.619666	0.320096	-0.417884
C	-6.153252	1.719075	0.044989
H	-6.347854	1.727156	1.120000
H	-7.128790	1.969127	-0.374927
C	-5.139011	2.822119	-0.348099
H	-5.003123	2.826710	-1.431672
C	-5.717526	4.223003	0.122244
O	-5.105544	5.299732	-0.584885
H	-4.217546	5.037208	-0.884821
H	-5.498106	4.263564	1.192668
H	-6.794469	4.242420	-0.065908
O	-3.978636	2.446456	0.359144
C	-2.877929	3.067186	0.065057
O	-2.878536	4.100033	-0.581476
C	-1.680546	2.492534	0.730949
H	-1.786707	1.473118	1.099015
C	-0.530471	3.155294	0.838911
H	-0.389341	4.159995	0.449177
C	0.741397	2.584918	1.443649
H	0.489282	2.036339	2.352577
H	1.251407	3.416492	1.935724
C	1.646538	1.729925	0.533211
H	1.791821	2.329917	-0.368168
O	-5.531794	0.165627	-1.810503
H	-5.023793	-0.648877	-1.974774
H	-4.595375	0.178150	-0.062006
H	-7.612409	-0.592571	-0.215802
C	-6.614048	-1.014637	1.609927
H	-5.588534	-0.950645	1.979639
H	-7.176732	-0.313297	2.229434
C	-7.152392	-2.404879	1.759406
H	-8.219864	-2.500498	1.552274
C	-6.994279	-3.105796	3.152167
H	-6.053184	-2.858368	3.648173
H	-7.002852	-4.193039	3.044888
H	-7.840962	-2.708533	3.714838
C	-6.397833	-3.207467	0.583386
H	-7.122129	-3.900327	0.147206
O	-6.200581	-2.146309	-0.352052
O	0.807148	0.627237	0.054118
C	1.389205	-0.387087	-0.933021
H	1.618897	-0.007624	-1.931520
C	0.208707	-1.407611	-1.099817
C	-1.006909	-0.851970	-1.856110
H	-1.367686	-0.019568	-1.248484
C	-0.608244	-0.342724	-3.222609
H	0.035408	-1.007930	-3.803126
H	-0.143059	0.645169	-3.189499
H	-1.510006	-0.249405	-3.830300
C	-2.030546	-1.946994	-2.052173
H	-1.984273	-2.379165	-3.048510
C	-2.755000	-2.456896	-1.043663
H	-2.741997	-1.997597	-0.055553
C	-3.571946	-3.627189	-1.311969
H	-3.434155	-4.093348	-2.286685
C	-4.366191	-4.304264	-0.468387
H	-4.861230	-5.193373	-0.851185
C	-4.997264	-3.801227	0.845423
H	-5.026535	-4.591476	1.598314
H	-4.354311	-3.082080	1.356896
H	-0.065873	-1.726369	-0.091998
H	0.561226	-2.314973	-1.594459
C	2.619725	-0.930591	-0.242697
H	3.092119	-1.702302	-0.852932
H	2.365844	-1.391999	0.713888
C	3.587771	0.194537	0.068836
O	4.805485	-0.437714	0.541479
C	5.988104	0.341231	0.836273
H	5.796258	1.058221	1.647903
H	3.862522	0.667986	-0.877332
C	2.899698	1.097119	1.098878
H	3.563150	1.857266	1.515547
H	2.629309	0.407403	1.900720
O	6.370947	1.032546	-0.390037
C	6.930655	0.157282	-1.403651
C	7.429390	1.048530	-2.526632
H	8.214459	1.770919	-2.295313
H	6.578326	1.593674	-2.940363
H	7.859489	0.391469	-3.285833
H	6.111398	-0.430979	-1.825286
C	8.089657	-0.691781	-0.837052
H	8.910206	-0.062827	-0.484435
O	8.439008	-1.604796	-1.833033
H	9.021892	-2.239871	-1.379396
C	7.605820	-1.567582	0.327030
O	8.825855	-2.265306	0.827112
H	9.227882	-1.790612	1.577282
H	6.766478	-2.212533	0.055041
C	6.989535	-0.622393	1.447782
O	8.102106	0.186869	2.030782
C	7.932831	0.651087	3.335621
H	7.073661	1.327207	3.332166
H	8.898780	1.127326	3.524358
H	7.799809	-0.168609	4.047213
H	6.594996	-1.259524	2.243473

NMR-Shifts

Revised-MandelalideA198ps-NMR.txt

Atom	Type	Isotropic	Scaled Shift
1	C	84.5933	97.1177664197
2	C	102.4702	80.0070828308
3	C	142.7911	41.4143647466
6	C	101.9967	80.4602882904
8	C	104.9269	77.6556787075
14	C	14.0418	164.645379889
16	C	51.9775	128.335630468
18	C	30.3512	149.035012156
20	C	144.9500	39.3479967074
23	C	104.2837	78.2713107066
29	C	149.0674	35.4070713452
32	C	131.3418	52.3729397577
34	C	166.9966	18.2463293708
38	C	96.4750	85.7453243745
42	C	92.1913	89.8454220027
44	C	127.8736	55.692490285
45	C	148.9475	35.5218323475
47	C	165.9919	19.2079672276
51	C	27.9188	151.363157794
53	C	51.8439	128.463504278
55	C	40.8774	138.959972434
57	C	51.5604	128.734853271
59	C	150.1719	34.349910986
64	C	137.6108	46.3726334731
67	C	106.2751	76.3652635004
69	C	79.6706	101.829476062
72	C	144.3618	39.9109860449
76	C	103.5238	78.9986408622
77	C	165.3768	19.7967036122
82	C	104.0010	78.5418939873
86	C	95.5499	86.6307739428
90	C	87.0470	94.7692337143
92	C	123.7830	59.607764314

4	H	30.1004	1.60979440979
5	H	30.2536	1.46823746824
7	H	26.7462	4.70907830908
10	H	25.4663	5.89170709171
11	H	27.9465	3.6
12	H	27.8770	3.66421806422
17	H	25.0866	6.24255024255
19	H	24.1758	7.08413028413
21	H	29.6373	2.0376992377
22	H	29.2816	2.36636636637
24	H	27.5390	3.97653037653
26	H	29.7712	1.91397551398
27	H	27.0248	4.45165165165
28	H	27.8363	3.70182490182
30	H	30.6485	1.10334950335
31	H	30.1423	1.57107877108
33	H	28.9676	2.6565026565
35	H	31.0639	0.71951951952
36	H	30.4593	1.27817047817
37	H	30.1106	1.60036960037
39	H	27.6928	3.83441903442
43	H	27.5354	3.97985677986
46	H	28.9700	2.65428505429
48	H	31.2928	0.508015708016
49	H	30.5540	1.19066759067
50	H	30.9478	0.826796026796
52	H	25.5749	5.79136059136
54	H	24.5988	6.69327789328
56	H	25.0655	6.26204666205
58	H	26.2818	5.13818433818
60	H	29.7826	1.90344190344
61	H	29.4843	2.17907137907
62	H	30.0880	1.62125202125
63	H	30.5862	1.16091476091
65	H	29.9918	1.71014091014
66	H	30.3377	1.39052899053
70	H	25.5365	5.82684222684
71	H	27.3364	4.16373296373
73	H	29.4587	2.20272580273
74	H	30.6557	1.0966966967
78	H	30.7287	1.02924462924
79	H	30.6598	1.09290829291
80	H	29.9893	1.71245091245
81	H	27.5003	4.01228921229
83	H	28.0883	3.46897666898
85	H	29.2153	2.42762762763
88	H	29.3478	2.3051975052
89	H	27.3003	4.19708939709
93	H	27.7035	3.82453222453
94	H	27.5738	3.94437514438
95	H	28.3221	3.25294525295
96	H	27.6946	3.83275583276

Mandelalide A Original Configuration (MD Methodologies)

Supporting Information: Original-MandelalideA150ps.log

Using Gaussian 09: AM64L-G09RevC.01 23-Sep-2011

==========

#mPW1PW91/6-311+G(2d,p) scf=(maxcycle=300,direct,tight) NMR density=current SCRF=(PCM,SOLVENT=Chloroform)

Pointgroup= C1 Stoichiometry= C33H52O11 C1[X(C33H52O11)]
#Atoms= 96
Charge = 0 Multiplicity = 1

SCF Energy= -2116.24112075

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Optimization incomplete.

Atomic Type	Coordinates (Angstroms) X	Y	Z
C	6.901669	0.156785	-1.037524
C	5.711532	1.119033	-1.161894
C	5.609749	2.130244	0.079657
H	6.430972	2.844467	0.165708
H	5.619927	1.612494	1.041596
C	4.302448	2.977694	-0.048629
H	3.797326	2.729650	-0.985595
C	4.526065	4.499026	0.095720
O	3.497551	5.183198	-0.486676
H	2.655536	4.704473	-0.383517
H	5.505777	4.748333	-0.320043
H	4.611946	4.698459	1.166126
O	3.393915	2.556382	1.025486
C	2.041850	2.933584	0.772852
O	1.652049	3.465965	-0.195718
C	1.146736	2.548748	1.909282
H	1.624341	2.088921	2.773400
C	-0.235618	2.651019	1.866513
H	-0.637841	3.104729	0.963650
C	-1.163742	2.065296	2.959053
H	-1.878933	2.834111	3.259196
H	-0.552630	1.769519	3.813915
C	-1.927454	0.849421	2.438189
H	-2.361473	0.300776	3.277449
O	5.770735	1.735493	-2.423572
H	6.094283	1.011329	-2.989181
H	4.757565	0.586890	-1.201955
H	7.815964	0.732026	-1.205409
C	6.903976	-0.677049	0.179796
H	7.425395	-0.221319	1.023874
H	5.855808	-0.856404	0.431430
C	7.553699	-1.968212	-0.296108
H	8.620884	-1.784930	-0.153083
C	7.239407	-3.164467	0.646530
H	7.444074	-2.832071	1.665421
H	7.829131	-3.992082	0.246216
H	6.177379	-3.408485	0.577300
C	7.094403	-2.126921	-1.799660
H	7.943536	-2.483866	-2.389061
O	6.876580	-0.790355	-2.174826
O	-0.972602	-0.116792	1.930239
C	-1.533850	-1.392609	1.544194
H	-1.988028	-1.954687	2.364318
C	-0.389975	-2.269838	0.847230
C	0.874725	-2.573739	1.785845
H	1.286764	-1.637332	2.167414
C	0.538507	-3.369036	3.057491
H	1.427465	-3.432882	3.689589
H	0.154300	-4.377173	2.885561
H	-0.242608	-2.792120	3.554799
C	1.938699	-3.268343	0.937663
H	2.034283	-4.349382	0.882707
C	2.796811	-2.567547	0.254808
H	2.821680	-1.479002	0.242505
C	3.833502	-3.160289	-0.597728
H	4.069913	-4.218754	-0.501350
C	4.555388	-2.494876	-1.494143
H	4.292518	-1.450996	-1.644857
C	5.875298	-3.067379	-1.963473
H	6.020680	-4.117974	-1.704240

H	5.681829	-3.082484	-3.037922
H	-0.010128	-1.894591	-0.105305
H	-0.749175	-3.243595	0.508335
C	-2.507178	-1.142190	0.393814
H	-2.867889	-2.145145	0.156602
H	-1.923355	-0.759426	-0.445469
C	-3.586354	-0.217354	0.801273
O	-4.370898	0.151754	-0.405864
C	-5.663483	0.773378	-0.261669
H	-5.560922	1.799976	0.118703
H	-4.246799	-0.683667	1.536089
C	-2.982803	1.164257	1.355384
H	-3.730684	1.873605	1.716504
H	-2.609457	1.664766	0.459465
O	-6.502526	0.064948	0.648935
C	-6.884960	-1.291720	0.333987
C	-7.600219	-1.914919	1.537387
H	-6.949843	-2.018766	2.408040
H	-7.806966	-2.964945	1.318704
H	-8.509548	-1.364064	1.788489
H	-5.953049	-1.855011	0.239709
C	-7.625561	-1.426907	-0.993624
H	-8.569998	-0.903929	-0.823511
O	-7.697262	-2.768077	-1.451509
H	-7.794569	-2.733357	-2.419339
C	-6.917385	-0.588802	-2.058231
O	-7.740400	-0.619059	-3.294975
H	-8.342367	0.146452	-3.267264
H	-5.956719	-1.077746	-2.239177
C	-6.455850	0.834032	-1.598236
O	-7.677544	1.658321	-1.503354
C	-7.418086	3.115819	-1.606973
H	-6.975447	3.382003	-2.570365
H	-6.703159	3.464528	-0.858122
H	-8.313998	3.707805	-1.402801
H	-5.912164	1.319797	-2.413247

NMR-Shifts
Original-MandelalideA150ps-NMR.txt

Atom	Type	Isotropic	Scaled Shift
1	C	95.8442	86.3490878462
2	C	104.2473	78.3061505772
3	C	147.8506	36.5717184479
6	C	102.5165	79.9627672812
8	C	113.3697	69.5747430081
14	C	9.5063	168.986485193
16	C	46.7185	133.369226057
18	C	15.9542	162.814946687
20	C	144.7622	39.5277474684
23	C	109.3691	73.4038744999
29	C	152.5779	32.0470338253
32	C	137.1832	46.7819062386
34	C	170.6120	14.7858879381
38	C	108.8341	73.9159440265
42	C	110.2341	72.5759490036
44	C	130.4193	53.2559007638
45	C	145.4905	38.8306629147
47	C	169.3029	16.0388789984
51	C	44.2365	135.744845805
53	C	51.2507	129.031279312
55	C	41.1653	138.684412029
57	C	48.2092	131.9424185
59	C	151.0393	33.5196883554
64	C	147.2215	37.1738547828
67	C	109.0260	73.7322689944
69	C	87.9043	93.9486781906
72	C	148.0558	36.3753134631
76	C	116.2679	66.8007618829
77	C	169.9728	15.39769138
82	C	114.7054	68.2962920423
86	C	104.1641	78.3857845671
90	C	97.4632	84.7994793162
92	C	125.6864	57.7859453665
4	H	30.3378	1.39043659044
5	H	30.1321	1.5805035805
7	H	26.0650	5.33850773851
10	H	26.0795	5.32510972511
11	H	28.1892	3.37574497574
12	H	27.9650	3.58290598291
17	H	25.1983	6.13933933934
19	H	23.5838	7.63113883114
21	H	29.2066	2.43566643567
22	H	28.8219	2.79112959113
24	H	27.7891	3.74543774544
26	H	29.0494	2.58091938092
27	H	27.3615	4.14054054054
28	H	27.7614	3.77103257103
30	H	30.1401	1.57311157311
31	H	30.6164	1.13300993301
33	H	29.1158	2.51956571957
35	H	30.7220	1.03543543544
36	H	30.6282	1.12210672211
37	H	30.4653	1.27262647263
39	H	27.4113	4.09452529453
43	H	27.9677	3.58041118041
46	H	29.0617	2.56955416955
48	H	30.6549	1.09743589744
49	H	31.0414	0.74030954031
50	H	30.5585	1.18650958651
52	H	25.8380	5.54825594826
54	H	25.5249	5.83756063756
56	H	25.4431	5.91314391314
58	H	25.4381	5.91776391776
60	H	29.6650	2.0121044121
61	H	29.1410	2.49628089628
62	H	30.1804	1.53587433587
63	H	30.2908	1.43386463386
65	H	29.9932	1.70884730885
66	H	30.3030	1.42259182259
70	H	26.0457	5.35634095634
71	H	27.4297	4.07752367752
73	H	29.4784	2.18452298452
74	H	30.4158	1.31836451836
78	H	30.5114	1.23003003003
79	H	30.3766	1.35458535459
80	H	30.7342	1.02416262416
81	H	28.1139	3.44532224532
83	H	28.4596	3.1258951259
85	H	29.3586	2.29521829522
88	H	29.6574	2.01912681913
89	H	28.0837	3.47322707323
93	H	28.6790	2.92316932317
94	H	28.5132	3.07636867637
95	H	28.2032	3.36280896281
96	H	27.8457	3.69313929314

Supporting Information: Original-MandelalideA152ps.log

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 Using  Gaussian 09:  AM64L-G09RevC.01 23-Sep-2011
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 #mPW1PW91/6-311+G(2d,p) scf=(maxcycle=300,direct,tight) NMR
 density=current SCRF=(PCM,SOLVENT=Chloroform)
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 Pointgroup= C1   Stoichiometry= C33H52O11   C1[X(C33H52O11)]
#Atoms= 96
 Charge = 0                Multiplicity = 1
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SCF Energy= -2116.21291985
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Optimization incomplete.

Atomic Type	Coordinates (Angstroms) X	Y	Z
C	-6.679914	0.130369	1.253837
C	-5.513649	1.145918	1.101910
C	-5.736990	2.379710	0.181530
H	-6.565130	2.948502	0.608812
H	-5.962992	2.039212	-0.830389
C	-4.478077	3.239224	0.104119
H	-4.151774	3.413579	1.132818
C	-4.769616	4.623234	-0.559108
O	-3.738364	5.549563	-0.210483
H	-2.958029	4.975547	-0.111409
H	-5.608521	5.081032	-0.028027
H	-4.860306	4.508588	-1.642544
O	-3.417374	2.526347	-0.655122
C	-2.113570	2.867088	-0.509936
O	-1.613137	3.726977	0.175660
C	-1.253656	2.260224	-1.508678
H	-1.680088	1.455611	-2.105207
C	0.045671	2.624566	-1.853057
H	0.624664	3.264586	-1.192079
C	0.794706	1.956570	-2.946149
H	1.372264	2.718741	-3.473018
H	0.105772	1.479510	-3.646398
C	1.752559	0.773960	-2.483338
H	2.170028	0.295939	-3.374019
O	-5.530133	1.588268	2.464961
H	-5.800994	0.743633	2.867497
H	-4.596827	0.640165	0.790627
H	-7.511824	0.824364	1.399651
C	-7.069912	-0.737816	-0.068194
H	-7.843714	-0.272575	-0.683430
H	-6.205475	-0.855732	-0.724718
C	-7.643449	-1.986653	0.550414
H	-8.626669	-1.717743	0.940442
C	-7.846253	-3.111911	-0.426404
H	-8.673448	-2.871315	-1.098117
H	-8.182577	-3.966921	0.163370
H	-6.945544	-3.325111	-1.004994
C	-6.832565	-2.232719	1.819314
H	-7.355916	-2.629652	2.692100
O	-6.516419	-0.899131	2.291859
O	0.927760	-0.161394	-1.690106
C	1.637267	-1.356508	-1.461719
H	2.030802	-1.672373	-2.431231
C	0.642360	-2.381054	-0.969912
C	-0.350136	-2.977373	-1.986497
H	-0.553536	-2.156300	-2.677143
C	0.340936	-4.119569	-2.734162
H	-0.297164	-4.565893	-3.498528
H	0.481736	-4.975664	-2.072006
H	1.303123	-3.879017	-3.191723
C	-1.594399	-3.420826	-1.270594
H	-1.648882	-4.506794	-1.299515
C	-2.383912	-2.631047	-0.533851
H	-2.299952	-1.546079	-0.489591
C	-3.585585	-3.178557	0.129412
H	-3.877516	-4.181572	-0.178631
C	-4.394021	-2.551508	0.993984
H	-4.163705	-1.546074	1.338370
C	-5.535799	-3.187129	1.726440
H	-5.845483	-4.092097	1.198790
H	-5.200929	-3.435175	2.735872
H	0.108713	-1.640667	-0.369473
H	1.036545	-3.151634	-0.304278
C	2.664596	-1.081906	-0.340227
H	3.339053	-1.882260	-0.029995
H	2.188844	-0.866463	0.618117
C	3.607746	0.096708	-0.825009
O	4.402166	0.620237	0.331624
C	5.794505	0.890178	0.039534
H	5.773734	1.812190	-0.560927
H	4.232606	-0.291058	-1.633362
C	2.819441	1.286509	-1.398650
H	3.576328	1.820032	-1.977510
H	2.511182	1.933581	-0.574696
O	6.525229	-0.107775	-0.650776
C	6.692050	-1.407527	-0.119999
C	7.556538	-2.180653	-1.059440
H	7.336770	-1.789323	-2.055379
H	7.339169	-3.250763	-1.048479
H	8.622162	-2.008115	-0.896218
H	5.709047	-1.884473	-0.125582
C	7.116439	-1.388172	1.305971
H	8.192387	-1.197967	1.320120
O	6.699865	-2.629652	1.897458
H	6.705706	-2.420981	2.848555
C	6.418604	-0.294913	2.087166
O	6.876660	-0.236629	3.463442
H	7.783914	0.116575	3.483997
H	5.350080	-0.524696	2.078329
C	6.518675	1.152317	1.424851
O	7.944105	1.540068	1.179289
C	8.132098	2.998632	1.152018
H	8.191728	3.275075	2.208101
H	7.282816	3.264972	0.518495
H	9.031979	3.307677	0.613291
H	6.016831	1.854142	2.095372

NMR-Shifts
Original-MandelalideA152ps-NMR.txt

Atom	Type	Isotropic	Scaled Shift
1	C	92.0607	89.9704243956
2	C	112.1574	70.735082984
3	C	149.4388	35.0515898084
6	C	101.2176	81.2059955206
8	C	111.0286	71.8155018281
14	C	10.6578	167.884339287
16	C	46.9588	133.139225483
18	C	17.9198	160.933593675
20	C	145.8557	38.4811156416
23	C	97.2373	85.0156970846
29	C	145.8138	38.5212197783
32	C	147.5955	36.8158846839
34	C	174.6218	10.9479507648
38	C	95.2290	86.9379199449
42	C	112.5739	70.3364344647
44	C	133.7413	50.0762840024
45	C	156.0393	28.7339918452
47	C	169.2762	16.0644346178
51	C	38.1539	141.566741324
53	C	52.2232	128.100461341
55	C	48.9994	131.186087023
57	C	50.9062	129.361013802
59	C	145.7773	38.5561553629
64	C	146.4713	37.8919006872
67	C	104.5353	78.0304944582
69	C	85.9267	95.8415168744
72	C	148.7355	35.7247458795
76	C	119.9812	63.2466165126

77	C	168.0538	17.2344417006
82	C	111.6452	71.2253297345
86	C	104.3103	78.2458508011
90	C	90.6262	91.3434407244
92	C	122.8800	60.4720611038
4	H	30.2255	1.4942018942
5	H	30.0550	1.65174405174
7	H	26.1335	5.27521367521
10	H	28.0094	3.54188034188
11	H	27.5861	3.93300993301
12	H	27.6776	3.84846384846
17	H	25.5108	5.85058905059
19	H	23.9010	7.33804573805
21	H	29.1349	2.50191730192
22	H	28.8622	2.75389235389
24	H	27.6921	3.83506583507
26	H	28.2168	3.35024255024
27	H	27.9615	3.58613998614
28	H	27.3447	4.15606375606
30	H	29.9642	1.73564333564
31	H	30.4734	1.26514206514
33	H	29.2332	2.41108801109
35	H	30.6976	1.05798105798
36	H	30.6670	1.08625548626
37	H	30.9354	0.838253638254
39	H	26.8303	4.63136983137
43	H	28.4085	3.17311157311
46	H	29.3822	2.27341187341
48	H	30.8839	0.88583968584
49	H	31.3862	0.421714021714
50	H	30.7939	0.968999769
52	H	25.5527	5.81187341187
54	H	25.1360	6.1969045969
56	H	25.5657	5.79986139986
58	H	25.7333	5.644998845
60	H	29.5818	2.08898128898
61	H	29.1841	2.45645645646
62	H	30.1503	1.56368676369
63	H	30.4511	1.28574728575
65	H	29.9457	1.75273735274
66	H	30.5770	1.16941556942
70	H	25.9624	5.43331023331
71	H	27.3172	4.18147378147
73	H	29.7156	1.96534996535
74	H	29.8929	1.80152460152
78	H	30.6618	1.09106029106
79	H	30.2126	1.50612150612
80	H	30.8244	0.940817740818
81	H	28.2882	3.28426888427
83	H	28.5445	3.04744744745
85	H	29.3230	2.32811272811
88	H	30.3726	1.35828135828
89	H	27.4915	4.02042042042
93	H	27.4588	4.05063525064
94	H	27.5327	3.98235158235
95	H	28.1475	3.41427581428
96	H	27.7878	3.74663894664

Supporting Information: Original-MandelalideA154ps.log

Using Gaussian 09: AM64L-G09RevC.01 23-Sep-2011

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#mPW1PW91/6-311+G(2d,p) scf=(maxcycle=300,direct,tight) NMR density=current SCRF=(PCM,SOLVENT=Chloroform)

Pointgroup= C1 Stoichiometry= C33H52O11 C1[X(C33H52O11)]

#Atoms= 96

Charge = 0 Multiplicity = 1

SCF Energy= -2116.24086192

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Optimization incomplete.

Atomic Type	Coordinates (Angstroms) X	Y	Z
C	-6.822145	-0.145902	1.120526
C	-5.914579	1.026076	1.311195
C	-6.017851	2.008860	0.121624
H	-7.035795	2.401326	0.179515
H	-5.898427	1.426523	-0.794080
C	-4.838725	3.061325	0.113601
H	-4.602477	3.303924	1.152777
C	-5.335501	4.270668	-0.756838
O	-4.501187	5.383259	-0.466662
H	-3.605253	5.013691	-0.375038
H	-6.368011	4.495057	-0.479097
H	-5.289640	4.093494	-1.834599
O	-3.634750	2.426920	-0.451703
C	-2.429520	3.036156	-0.415755
O	-2.131630	4.002288	0.224543
C	-1.492728	2.471022	-1.333411
H	-2.015807	1.791399	-2.004528
C	-0.180812	2.747984	-1.357826
H	0.135470	3.322762	-0.491790
C	0.687999	2.292883	-2.503241
H	1.382278	3.076992	-2.812489
H	0.054127	1.953035	-3.324953
C	1.565829	0.980386	-2.148901
H	2.099134	0.674302	-3.053266
O	-6.390402	1.753918	2.428567
H	-6.437090	1.101186	3.150383
H	-4.912723	0.604151	1.421991
H	-7.874004	0.151881	1.109080
C	-6.612730	-0.971688	-0.194537
H	-7.156684	-0.644610	-1.083121
H	-5.571721	-0.886644	-0.513224
C	-7.038886	-2.334656	0.308595
H	-8.127305	-2.399077	0.361548
C	-6.746917	-3.476508	-0.600991
H	-7.240844	-3.248877	-1.547762
H	-7.191921	-4.409556	-0.247983
H	-5.695044	-3.670134	-0.821567
C	-6.556018	-2.371588	1.812561
H	-7.294049	-2.916927	2.405650
O	-6.603387	-1.062928	2.263183
O	0.771531	-0.126689	-1.656430
C	1.611533	-1.334220	-1.477752
H	2.045980	-1.612089	-2.442083
C	0.725445	-2.454409	-0.793437
C	-0.379941	-2.979109	-1.815521
H	-0.814414	-2.160066	-2.392304
C	0.206065	-3.760709	-2.947036
H	-0.598385	-4.112150	-3.596590
H	0.623280	-4.664146	-2.498195
H	1.013831	-3.299099	-3.519072
C	-1.584184	-3.592474	-1.188735
H	-1.567317	-4.676361	-1.116430
C	-2.407657	-2.805066	-0.476343
H	-2.266454	-1.732362	-0.351190
C	-3.495567	-3.457638	0.274432
H	-3.743233	-4.502313	0.097322
C	-4.147966	-2.623972	1.086845
H	-3.782508	-1.603275	1.163595

C	-5.174547	-2.993666	2.024720
H	-5.265229	-4.080187	2.067169
H	-4.951468	-2.720540	3.057596
H	0.314898	-2.182886	0.180821
H	1.309241	-3.340145	-0.532138
C	2.812089	-1.028886	-0.518982
H	3.468010	-1.895416	-0.409372
H	2.397159	-0.857324	0.476268
C	3.645693	0.221673	-0.857721
O	4.465623	0.524772	0.378919
C	5.800660	0.943968	0.029943
H	5.682569	1.850770	-0.582339
H	4.278744	0.010003	-1.723280
C	2.743345	1.359983	-1.156096
H	3.397428	2.170369	-1.483537
H	2.354064	1.726520	-0.203524
O	6.412156	-0.062416	-0.841644
C	6.711314	-1.319525	-0.233528
C	7.495529	-2.234193	-1.255902
H	6.898885	-2.442018	-2.146209
H	7.729653	-3.190863	-0.783698
H	8.426823	-1.738703	-1.535638
H	5.746722	-1.768137	0.015815
C	7.522561	-1.196788	1.116534
H	8.521937	-0.777019	0.978061
O	7.555343	-2.473255	1.811818
H	7.481360	-2.371832	2.778614
C	6.840565	-0.192300	2.037265
O	7.580417	-0.059718	3.307933
H	8.315238	0.569201	3.192114
H	5.881962	-0.674625	2.244697
C	6.625650	1.234330	1.370965
O	7.948565	1.811953	1.243107
C	7.894284	3.178883	0.770326
H	7.140892	3.732916	1.336970
H	7.740821	3.207831	-0.311698
H	8.843301	3.676338	0.985467
H	5.970036	1.913483	1.922822

NMR-Shifts

Original-MandelalideA154ps-NMR.txt

Atom	Type	Isotropic	Scaled Shift
1	C	91.0517	90.9361779513
2	C	112.4670	70.4387526561
3	C	144.9415	39.3561323915
6	C	100.2396	82.142077758
8	C	109.9768	72.822220946
14	C	11.9441	166.653171003
16	C	53.8011	126.590191236
18	C	28.9853	150.342368728
20	C	141.9859	42.1850533127
23	C	104.0970	78.4500086143
29	C	151.5313	33.0487758188
32	C	142.5616	41.6340282165
34	C	174.7580	10.8175883918
38	C	109.7907	73.0003445701
42	C	103.1117	79.3930779686
44	C	132.7188	51.0549589387
45	C	154.6324	30.0805911292
47	C	168.8609	16.46193457
51	C	42.9358	136.989796895
53	C	35.5055	144.101629051
55	C	40.2242	139.585175826
57	C	51.2989	128.985145198
59	C	149.7431	34.7603323188
64	C	144.4404	39.8357548958
67	C	107.7928	74.9126131817
69	C	80.5402	100.997147725
72	C	150.3531	34.1764773445
76	C	110.7372	72.0944122208
77	C	167.1884	18.0627500526
82	C	108.5670	74.1715959341
86	C	103.1365	79.3693409139
90	C	95.5655	86.6158425697
92	C	126.9246	56.6008154827
4	H	30.1420	1.57135597136
5	H	30.2695	1.45354585355
7	H	26.0529	5.34968814969
10	H	28.5013	3.08736428736
11	H	28.1742	3.3896049896
12	H	27.4053	4.10006930007
17	H	25.6415	5.72982212982
19	H	23.6731	7.54862554863
21	H	29.2262	2.41755601756
22	H	28.5215	3.0686994687
24	H	28.2189	3.3483021483
26	H	29.5318	2.13518133518
27	H	28.2148	3.35209055209
28	H	27.6538	3.87045507046
30	H	30.3831	1.34857934858
31	H	30.6079	1.14086394086
33	H	29.0221	2.60614460614
35	H	31.1249	0.663155463155
36	H	31.0486	0.733656733657
37	H	30.2087	1.50972510973
39	H	27.8956	3.64703164703
43	H	27.8879	3.65414645415
46	H	28.7035	2.90053130053
48	H	30.8175	0.947193347193
49	H	31.4289	0.382259182259
50	H	30.5376	1.20582120582
52	H	25.7131	5.66366366366
54	H	24.6210	6.67276507277
56	H	24.8553	6.45627165627
58	H	25.4091	5.94455994456
60	H	29.7148	1.96608916609
61	H	29.6964	1.98309078309
62	H	30.1894	1.52755832756
63	H	30.4615	1.27613767614
65	H	30.0130	1.69055209055
66	H	30.7093	1.04717024717
70	H	25.9331	5.46038346038
71	H	27.0770	4.40341880342
73	H	29.7993	1.88801108801
74	H	30.4497	1.28704088704
78	H	30.5129	1.22864402864
79	H	30.2122	1.50649110649
80	H	30.7236	1.03395703396
81	H	27.7781	3.7556017556
83	H	28.2122	3.35449295449
85	H	29.5455	2.12252252252
88	H	29.7097	1.9708015708
89	H	27.8750	3.66606606607
93	H	28.6177	2.97981057981
94	H	28.0762	3.48015708016
95	H	28.1422	3.41917301917
96	H	27.9123	3.6316008316

Supporting Information: Original-MandelalideA156ps.log

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 Using  Gaussian 09:  AM64L-G09RevC.01 23-Sep-2011
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 #mPW1PW91/6-311+G(2d,p) scf=(maxcycle=300,direct,tight) NMR
 density=current SCRF=(PCM,SOLVENT=Chloroform)
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 Pointgroup= C1   Stoichiometry= C33H52O11   C1[X(C33H52O11)]
#Atoms= 96
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Charge = 0 Multiplicity = 1

SCF Energy= -2116.26913210

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Optimization incomplete.

Atomic Type	Coordinates (Angstroms) X	Y	Z
C	-6.768796	0.047731	1.147174
C	-5.616057	1.072301	1.228311
C	-5.943858	2.229949	0.268864
H	-6.780933	2.819660	0.648890
H	-6.216693	1.819906	-0.706212
C	-4.692950	3.123064	0.157715
H	-4.409929	3.453209	1.160674
C	-5.013060	4.404532	-0.712095
O	-4.282221	5.566733	-0.234385
H	-3.368376	5.274771	-0.069266
H	-6.067975	4.670638	-0.606269
H	-4.812486	4.125732	-1.750382
O	-3.599282	2.396990	-0.556722
C	-2.382052	2.950743	-0.661286
O	-2.099170	4.080167	-0.236629
C	-1.304997	2.174831	-1.323136
H	-1.545121	1.126474	-1.495278
C	-0.195887	2.794159	-1.704738
H	-0.119640	3.836089	-1.402998
C	0.928876	2.224880	-2.610105
H	1.639794	2.986712	-2.937120
H	0.528887	1.907875	-3.575973
C	1.749319	1.061251	-2.030204
H	2.504759	0.736517	-2.748738
O	-5.719834	1.551496	2.543777
H	-5.902384	0.741213	3.052467
H	-4.643605	0.638738	0.981746
H	-7.759011	0.489093	1.287084
C	-6.923051	-0.789607	-0.180991
H	-7.507337	-0.332893	-0.982222
H	-5.953586	-0.970195	-0.648796
C	-7.487090	-2.148937	0.314421
H	-8.553643	-1.983234	0.480983
C	-7.302630	-3.325359	-0.714282
H	-7.867246	-3.187100	-1.638994
H	-7.668967	-4.266754	-0.298486
H	-6.266887	-3.646993	-0.841997
C	-6.873416	-2.355276	1.731249
H	-7.644222	-2.807410	2.360509
O	-6.532905	-0.972823	2.170337
O	0.909776	-0.016951	-1.553435
C	1.531550	-1.253638	-1.078006
H	2.212808	-1.439575	-1.912184
C	0.548649	-2.374338	-0.674789
C	-0.433149	-2.874502	-1.771725
H	-0.788494	-1.994235	-2.310210
C	0.190275	-3.805001	-2.840820
H	-0.445186	-3.868576	-3.726164
H	0.300128	-4.793121	-2.388951
H	1.207328	-3.467383	-3.050966
C	-1.705399	-3.542955	-1.165168
H	-1.890910	-4.602452	-1.323441
C	-2.554962	-2.943773	-0.405439
H	-2.368155	-1.923621	-0.071723
C	-3.729002	-3.459081	0.215475
H	-4.102736	-4.443174	-0.061390
C	-4.381716	-2.727850	1.104448
H	-3.975547	-1.759774	1.383855
C	-5.600906	-3.152888	1.850641
H	-5.820553	-4.187949	1.580409
H	-5.367711	-3.228117	2.915470
H	-0.049990	-1.992782	0.155259
H	1.128888	-3.234432	-0.331973
C	2.503033	-0.856571	0.091832
H	3.192888	-1.653545	0.376284
H	1.874401	-0.532116	0.924333
C	3.502477	0.209702	-0.455943
O	4.462579	0.431692	0.625303
C	5.781099	0.977728	0.289350
H	5.666212	2.019562	-0.044605
H	4.016983	-0.135845	-1.356243
C	2.652645	1.443583	-0.835335
H	3.254038	2.273317	-1.212335
H	2.100018	1.745816	0.056558
O	6.412422	0.252150	-0.778944
C	6.609735	-1.180208	-0.523115
C	7.180491	-1.771647	-1.793332
H	6.415579	-1.759425	-2.573325
H	7.558785	-2.763030	-1.533909
H	8.004042	-1.172266	-2.186179
H	5.625159	-1.573630	-0.257181
C	7.555828	-1.354101	0.642536
H	8.492737	-0.847069	0.400870
O	7.830363	-2.705363	0.950425
H	8.305391	-2.573286	1.790387
C	7.004516	-0.553007	1.854652
O	8.000609	-0.733059	2.914281
H	8.617376	0.003690	2.756113
H	6.060307	-0.987545	2.191510
C	6.776072	0.928971	1.518339
O	8.047981	1.571682	1.296994
C	7.987799	2.952694	1.572042
H	7.486983	3.111721	2.529578
H	7.398923	3.424614	0.780846
H	8.959647	3.451286	1.622281
H	6.342383	1.324901	2.440158

NMR-Shifts

Original-MandelalideA156ps-NMR.txt

Atom	Type	Isotropic	Scaled Shift
1	C	94.7903	87.3578169567
2	C	115.8731	67.1786404793
3	C	146.2407	38.1126170103
6	C	93.4136	88.6755106338
8	C	107.3993	75.2892474971
14	C	4.0528	174.206244377
16	C	56.2965	124.201745822
18	C	31.5226	147.913819177
20	C	150.4667	34.0677463198
23	C	105.9819	76.6458967438
29	C	145.4748	38.8456900017
32	C	143.3307	40.8978923793
34	C	175.6238	9.9888971841
38	C	95.7198	86.4681559754
42	C	104.5795	77.988188901
44	C	142.2842	41.8995386589
45	C	152.6737	31.9553398802
47	C	167.8068	17.4708551083
51	C	48.2868	131.86814449
53	C	51.6676	128.632247937
55	C	52.0323	128.283179234
57	C	47.5046	132.616818852
59	C	151.0864	33.4746070943
64	C	141.6015	42.5529776604
67	C	104.7339	77.8404065928
69	C	85.1001	96.6326882214

72	C	143.3188	40.909282337
76	C	113.7423	69.2181129042
77	C	170.5474	14.847719137
82	C	110.0192	72.7816382396
86	C	107.3534	75.333180191
90	C	98.2997	83.9988322901
92	C	127.7473	55.8133769789
4	H	30.1777	1.53836913837
5	H	30.0366	1.66874566875
7	H	26.4370	4.99477939478
10	H	26.1676	5.24370524371
11	H	27.9876	3.56202356202
12	H	27.9891	3.56063756064
17	H	25.2324	6.10783090783
19	H	23.6357	7.58318318318
21	H	29.3804	2.27507507508
22	H	28.9701	2.65419265419
24	H	28.1720	3.39163779164
26	H	28.5792	3.01538461538
27	H	27.8761	3.66504966505
28	H	27.5379	3.97754677755
30	H	30.0198	1.68426888427
31	H	30.4604	1.27715407715
33	H	29.2964	2.35269115269
35	H	30.7354	1.02305382305
36	H	31.0578	0.725155925156
37	H	30.5094	1.23187803188
39	H	27.2413	4.25160545161
43	H	27.8170	3.71965811966
46	H	29.1070	2.5276969277
48	H	30.4622	1.27549087549
49	H	31.0735	0.710649110649
50	H	30.6853	1.06934626935
52	H	26.2894	5.13116193116
54	H	25.5080	5.85317625318
56	H	25.4137	5.94030954031
58	H	25.5511	5.81335181335
60	H	29.8710	1.82176022176
61	H	29.2827	2.36534996535
62	H	29.7967	1.89041349041
63	H	30.2117	1.50695310695
65	H	29.9432	1.75504735505
66	H	30.3249	1.40235620236
70	H	26.0143	5.38535458535
71	H	27.7268	3.803003003
73	H	30.0426	1.6632016632
74	H	30.4364	1.29933009933
78	H	30.5523	1.19223839224
79	H	30.0625	1.64481404481
80	H	30.8982	0.872626472626
81	H	27.8630	3.67715407715
83	H	28.5807	3.013998614
85	H	29.0769	2.55550935551
88	H	29.8135	1.87489027489
89	H	27.9665	3.58151998152
93	H	28.8082	2.80378840379
94	H	28.1496	3.41233541234
95	H	28.0888	3.46851466851
96	H	28.0436	3.51027951028

Supporting Information: Original-MandelalideA158ps.log

Using Gaussian 09: AM64L-G09RevC.01 23-Sep-2011

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#mPW1PW91/6-311+G(2d,p) scf=(maxcycle=300,direct,tight) NMR density=current SCRF=(PCM,SOLVENT=Chloroform)

Pointgroup= C1 Stoichiometry= C33H52O11 C1[X(C33H52O11)]

#Atoms= 96

Charge = 0 Multiplicity = 1

SCF Energy= -2116.25771087

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Optimization incomplete.

Atomic Type	Coordinates (Angstroms) X	Y	Z
C	-6.523376	0.337177	1.326335
C	-5.286521	1.214225	1.253988
C	-5.448050	2.402401	0.284012
H	-6.230592	3.080048	0.633429
H	-5.828478	2.149317	-0.707448
C	-4.090560	3.138230	0.112415
H	-3.731359	3.303687	1.130731
C	-4.336282	4.566497	-0.571558
O	-3.376391	5.592539	-0.045027
H	-2.523741	5.121920	-0.020516
H	-5.369474	4.906947	-0.460389
H	-4.277682	4.469188	-1.659271
O	-3.142039	2.300530	-0.672557
C	-1.865226	2.690835	-0.749628
O	-1.438265	3.706117	-0.232264
C	-1.092462	1.963591	-1.790817
H	-1.622876	1.170649	-2.313966
C	0.176868	2.329367	-2.058500
H	0.682158	3.061060	-1.433779
C	1.025322	1.748832	-3.162657
H	1.714090	2.499676	-3.555001
H	0.380978	1.382857	-3.965309
C	1.819838	0.606085	-2.523887
H	2.337527	0.040221	-3.302037
O	-5.052384	1.603537	2.618498
H	-5.062956	0.861335	3.250018
H	-4.399543	0.724049	0.845038
H	-7.299354	1.043126	1.634314
C	-6.980684	-0.285090	-0.031777
H	-7.745366	0.308674	-0.536139
H	-6.060286	-0.440913	-0.598084
C	-7.619138	-1.618920	0.308018
H	-8.702545	-1.563233	0.434328
C	-7.372839	-2.724578	-0.733061
H	-7.967072	-2.492987	-1.620289
H	-7.754459	-3.690212	-0.394084
H	-6.334883	-2.870010	-1.038346
C	-7.093109	-1.887694	1.770390
H	-7.807437	-2.369688	2.443541
O	-6.589198	-0.669916	2.326482
O	0.831386	-0.368897	-1.944719
C	1.484191	-1.469991	-1.336273
H	2.059073	-1.987699	-2.107799
C	0.441558	-2.431803	-0.687067
C	-0.488544	-3.148628	-1.679696
H	-0.889960	-2.419802	-2.387333
C	0.319179	-4.266986	-2.476711
H	-0.266911	-4.660156	-3.310209
H	0.611030	-5.083539	-1.813938
H	1.268306	-3.852940	-2.823862
C	-1.741762	-3.670681	-1.005318
H	-1.796024	-4.755845	-0.974134
C	-2.653605	-2.871101	-0.421258
H	-2.525497	-1.802370	-0.261217
C	-3.784096	-3.285915	0.360912

H	-4.089463	-4.330691	0.369378
C	-4.579617	-2.460928	1.009112
H	-4.303286	-1.428411	1.205645
C	-5.869741	-2.880914	1.753383
H	-6.160004	-3.846875	1.334900
H	-5.769047	-3.054175	2.826749
H	-0.234797	-1.859706	-0.049474
H	0.983377	-3.137769	-0.054519
C	2.386511	-0.950859	-0.216247
H	2.888841	-1.836675	0.179649
H	1.845493	-0.453411	0.590899
C	3.502106	-0.019665	-0.754646
O	4.225837	0.476796	0.405536
C	5.581770	0.852126	0.027517
H	5.541855	1.723228	-0.642797
H	4.049947	-0.583812	-1.514414
C	2.781782	1.122048	-1.451825
H	3.466403	1.824335	-1.931852
H	2.225582	1.740933	-0.744782
O	6.250435	-0.241491	-0.682516
C	6.215209	-1.459960	0.002569
C	6.857700	-2.429652	-0.925572
H	6.301818	-2.494085	-1.863671
H	6.935333	-3.421263	-0.473953
H	7.840087	-2.047302	-1.209848
H	5.203459	-1.850382	0.145178
C	7.088986	-1.315148	1.273888
H	8.112657	-0.996056	1.060004
O	7.220156	-2.541978	2.031002
H	7.272295	-2.282629	2.967638
C	6.432737	-0.174888	2.132811
O	7.143826	-0.032213	3.352837
H	7.422659	0.891202	3.495718
H	5.412157	-0.403379	2.450789
C	6.380536	1.161949	1.371440
O	7.698234	1.707671	1.075815
C	7.782993	3.087326	0.729846
H	7.071330	3.657949	1.331103
H	7.613340	3.331458	-0.322213
H	8.784770	3.385910	1.050077
H	5.845706	1.872939	2.006032

NMR-Shifts
Original-MandelalideA158ps-NMR.txt

Atom	Type	Isotropic	Scaled Shift
1	C	101.3058	81.1215758341
2	C	113.9388	69.0300350313
3	C	148.5627	35.8901395509
6	C	98.5743	83.7360018377
8	C	106.4820	76.1672313789
14	C	10.2221	168.301364881
16	C	55.3135	125.142613756
18	C	25.1185	154.043434982
20	C	147.8914	36.5326671644
23	C	103.3363	79.1781044813
29	C	149.7295	34.7733494133
32	C	146.4380	37.923773426
34	C	170.8420	14.5657458987
38	C	94.8985	87.2542544842
42	C	111.7986	71.0785045656
44	C	135.6216	48.2765749727
45	C	151.3367	33.235035127
47	C	167.0571	18.188422443
51	C	40.2472	139.563161623
53	C	52.2599	128.065334329
55	C	50.2168	130.020865637
57	C	51.7264	128.575968146
59	C	143.0528	41.1638813913
64	C	143.6386	40.6031891882
67	C	113.8573	69.1080418844
69	C	82.1933	99.4149007447
72	C	151.0054	33.5521353778
76	C	121.8628	61.4456632018
77	C	167.4486	17.8137024062
82	C	104.4885	78.0752885775
86	C	111.2169	71.6352724976
90	C	95.1347	87.0281781811
92	C	127.3938	56.1517257222
4	H	30.3126	1.41372141372
5	H	29.8527	1.83866943867
7	H	26.1225	5.28537768538
10	H	26.8837	4.58202818203
11	H	28.0679	3.48782628783
12	H	27.9210	3.62356202356
17	H	25.2874	6.05701085701
19	H	23.6152	7.60212520213
21	H	29.2964	2.35269115269
22	H	28.9929	2.63312543313
24	H	28.0544	3.5003003003
26	H	29.0636	2.5677985678
27	H	27.6817	3.84467544468
28	H	27.5521	3.96442596443
30	H	29.3113	2.33892353892
31	H	30.5443	1.19963039963
33	H	29.2423	2.40267960268
35	H	30.8767	0.892492492492
36	H	30.9707	0.805636405636
37	H	30.7940	0.968907368907
39	H	27.3178	4.18091938092
43	H	28.0923	3.46528066528
46	H	29.0411	2.58858858859
48	H	30.4794	1.2595980596
49	H	31.2227	0.572788172788
50	H	30.7292	1.02878262878
52	H	25.3755	5.97560637561
54	H	25.0585	6.26851466851
56	H	25.2373	6.1033033033
58	H	25.7814	5.60055440055
60	H	29.8228	1.8662970663
61	H	29.1979	2.44370524371
62	H	29.9419	1.75624855625
63	H	30.4780	1.26089166089
65	H	30.3599	1.37001617002
66	H	30.5943	1.15343035343
70	H	26.1674	5.24389004389
71	H	27.8339	3.70404250404
73	H	29.8011	1.88634788635
74	H	30.2860	1.4382998383
78	H	30.7605	0.999861399861
79	H	30.1780	1.53809193809
80	H	30.9645	0.811365211365
81	H	27.9729	3.57560637561
83	H	27.8699	3.67077847078
85	H	29.8290	1.86056826057
88	H	30.3648	1.36548856549
89	H	27.3877	4.11633171633
93	H	28.7254	2.8802956803
94	H	28.0871	3.47008547009
95	H	27.8393	3.69905289905
96	H	28.0294	3.5234003234

Supporting Information: Original-MandelalideA160ps.log

Using Gaussian 09: AM64L-G09RevC.01 23-Sep-2011

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#mPW1PW91/6-311+G(2d,p) scf=(maxcycle=300,direct,tight) NMR density=current SCRF=(PCM,SOLVENT=Chloroform)

Pointgroup= C1 Stoichiometry= C33H52O11 C1[X(C33H52O11)]
#Atoms= 96
Charge = 0 Multiplicity = 1

SCF Energy= -2116.23369499
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Optimization incomplete.

Atomic Type	Coordinates (Angstroms) X	Y	Z
C	-6.743555	0.146344	1.351344
C	-5.630799	1.200718	1.239617
C	-5.796651	2.246223	0.092796
H	-6.733850	2.776672	0.273175
H	-5.947517	1.808650	-0.896048
C	-4.602509	3.247596	0.001082
H	-4.303674	3.347060	1.047749
C	-4.951797	4.561793	-0.678865
O	-4.077548	5.759812	-0.356293
H	-3.258387	5.238908	-0.280117
H	-6.001821	4.762809	-0.450850
H	-4.975538	4.469752	-1.767786
O	-3.578059	2.537778	-0.765261
C	-2.346608	3.110803	-0.978792
O	-2.031645	4.173737	-0.452344
C	-1.474873	2.290961	-1.787749
H	-1.914943	1.380533	-2.193049
C	-0.160288	2.524446	-1.865813
H	0.382078	3.357796	-1.426612
C	0.804844	1.668619	-2.698431
H	1.554620	2.384271	-3.041802
H	0.261943	1.345555	-3.588677
C	1.580467	0.512973	-2.013895
H	2.111105	0.046496	-2.846773
O	-5.732553	1.878139	2.506552
H	-5.518988	1.090551	3.038593
H	-4.707196	0.629315	1.116847
H	-7.692921	0.621289	1.611856
C	-6.978284	-0.734997	0.108088
H	-7.745475	-0.331608	-0.556123
H	-6.119934	-0.743751	-0.566947
C	-7.421673	-2.141750	0.670452
H	-8.457574	-1.861189	0.873345
C	-7.314533	-3.328814	-0.246962
H	-7.806184	-3.087878	-1.190889
H	-7.780726	-4.190233	0.237173
H	-6.258902	-3.502513	-0.467808
C	-6.654520	-2.146229	2.015362
H	-7.294190	-2.622280	2.762550
O	-6.401514	-0.776665	2.444478
O	0.749828	-0.520685	-1.492503
C	1.450958	-1.707279	-1.265951
H	1.908139	-1.884311	-2.242631
C	0.601456	-2.890555	-0.780303
C	-0.386774	-3.298609	-1.905731
H	-0.629592	-2.464926	-2.567400
C	0.143063	-4.466336	-2.752680
H	-0.652124	-4.819929	-3.412983
H	0.454282	-5.295122	-2.113363
H	1.000381	-4.018896	-3.261261
C	-1.529089	-3.746865	-1.185103
H	-1.552044	-4.810791	-0.966308
C	-2.459588	-2.874870	-0.661739
H	-2.408791	-1.812093	-0.892764
C	-3.517955	-3.307918	0.186251
H	-3.523459	-4.354024	0.488802
C	-4.317584	-2.456698	0.844632
H	-4.315007	-1.401533	0.581418
C	-5.294349	-2.989249	1.921493
H	-5.507687	-4.059004	1.882277
H	-4.787746	-2.907239	2.885288
H	0.077940	-2.572480	0.124267
H	1.294139	-3.687050	-0.504337
C	2.648651	-1.430589	-0.228534
H	3.229513	-2.341108	-0.066875
H	2.242407	-1.086589	0.724775
C	3.550112	-0.264818	-0.709872
O	4.421494	0.262676	0.317817
C	5.760214	0.858317	0.018059
H	5.619357	1.735187	-0.631097
H	4.108360	-0.564196	-1.600831
C	2.627324	0.987940	-1.060963
H	3.292675	1.753389	-1.463339
H	2.069777	1.212562	-0.149610
O	6.425565	-0.138569	-0.750692
C	6.721553	-1.346865	-0.018712
C	7.586872	-2.167961	-1.014019
H	7.013348	-2.865384	-1.627928
H	8.159681	-2.909273	-0.453095
H	8.163644	-1.501558	-1.659247
H	5.802344	-1.917835	0.137955
C	7.515097	-0.950092	1.295408
H	8.538314	-0.636324	1.073842
O	7.632090	-2.107562	2.204010
H	7.867381	-1.811749	3.102051
C	6.812768	0.166439	2.121637
O	7.573669	0.503345	3.292677
H	8.154902	1.268412	3.133591
H	5.909121	-0.320594	2.494797
C	6.504487	1.358599	1.282332
O	7.768726	2.002664	0.982967
C	7.615806	3.312686	0.296625
H	6.990816	3.939545	0.936685
H	7.209033	3.107033	-0.697472
H	8.579959	3.820850	0.212598
H	5.845110	2.023681	1.846742

NMR-Shifts
Original-MandelalideA160ps-NMR.txt

Atom	Type	Isotropic	Scaled Shift
1	C	95.8907	86.3045808687
2	C	108.4510	74.2826240931
3	C	147.4258	36.9783112234
6	C	107.1640	75.5144623749
8	C	111.5137	71.3511935527
14	C	6.5340	171.831390341
16	C	61.5003	119.220984322
18	C	21.6069	157.404525355
20	C	142.7208	41.4816516396
23	C	107.4343	75.2557476215
29	C	147.3903	37.0122896686
32	C	145.7041	38.6262179598
34	C	176.3778	9.26721415035
38	C	99.6645	82.6925285706
42	C	106.0880	76.5443442639
44	C	131.3835	52.3330270488
45	C	152.8534	31.7833419476
47	C	164.4059	20.7259901606
51	C	29.5517	149.800245028
53	C	49.1458	131.045961829
55	C	45.4730	134.561343058
57	C	50.1964	130.040391279
59	C	142.1020	42.0739294397

64	C	141.9531	42.2164474818
67	C	107.2187	75.462106855
69	C	83.7004	97.9723961025
72	C	144.0906	40.1705622236
76	C	111.8295	71.0489289611
77	C	167.6988	17.5742261529
82	C	103.0262	79.4749133789
86	C	110.6384	72.1889775838
90	C	106.3326	76.3102279906
92	C	124.2142	59.195045847
4	H	30.4379	1.29794409794
5	H	29.9556	1.74358974359
7	H	26.2567	5.16137676138
10	H	25.2919	6.05285285285
11	H	28.2610	3.3094017094
12	H	27.8676	3.6729036729
17	H	25.0819	6.24689304689
19	H	23.3953	7.80531300531
21	H	29.5098	2.15550935551
22	H	28.9393	2.68265188265
24	H	28.5592	3.03386463386
26	H	29.1858	2.45488565489
27	H	27.9343	3.61127281127
28	H	27.6956	3.83183183183
30	H	30.3173	1.40937860938
31	H	30.5365	1.20683760684
33	H	29.3657	2.28865788866
35	H	30.8445	0.922245322245
36	H	30.7999	0.963455763456
37	H	30.3061	1.41972741973
39	H	27.5578	3.95915915916
43	H	28.2988	3.27447447447
46	H	29.0391	2.59043659044
48	H	30.4462	1.29027489027
49	H	31.1299	0.658535458535
50	H	30.1873	1.5294987295
52	H	25.3897	5.96248556249
54	H	25.3146	6.03187803188
56	H	25.1518	6.18230538231
58	H	25.5646	5.80087780088
60	H	29.5885	2.08279048279
61	H	29.3331	2.31878031878
62	H	29.9531	1.7458997459
63	H	30.1359	1.57699237699
65	H	29.9890	1.71272811273
66	H	30.6643	1.08875028875
70	H	25.9010	5.49004389004
71	H	27.7153	3.81362901363
73	H	29.3823	2.27331947332
74	H	30.3760	1.35513975514
78	H	30.3787	1.35264495264
79	H	30.3124	1.41390621391
80	H	30.5684	1.17736197736
81	H	27.3381	4.16216216216
83	H	27.8235	3.71365211365
85	H	29.4134	2.24458304458
88	H	29.5831	2.08778008778
89	H	27.8602	3.67974127974
93	H	28.3175	3.2571956572
94	H	27.5962	3.92367752368
95	H	27.9624	3.58530838531
96	H	28.0220	3.53023793024

Supporting Information: Original-MandelalideA162.log

Using Gaussian 09: AM64L-G09RevC.01 23-Sep-2011

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#mPW1PW91/6-311+G(2d,p) scf=(maxcycle=300,direct,tight) NMR density=current SCRF=(PCM,SOLVENT=Chloroform)

Pointgroup= C1 Stoichiometry= C33H52O11 C1[X(C33H52O11)]

#Atoms= 96

Charge = 0 Multiplicity = 1

SCF Energy= -2116.27101321

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Optimization incomplete.

Atomic Type	Coordinates (Angstroms) X	Y	Z
C	-7.084358	0.138725	0.823451
C	-5.983282	1.182799	1.093269
C	-5.831156	2.258955	0.053129
H	-6.731041	2.861768	0.192973
H	-5.852456	1.878459	-0.971073
C	-4.562204	3.095578	0.229795
H	-4.274178	3.046420	1.283463
C	-4.789615	4.522699	-0.373254
O	-3.678685	5.374518	-0.123096
H	-3.108617	4.928739	0.528305
H	-5.636954	4.951375	0.166822
H	-4.977896	4.595661	-1.447657
O	-3.581061	2.464761	-0.642288
C	-2.226096	2.686528	-0.404673
O	-1.853492	3.403646	0.517707
C	-1.386093	2.178566	-1.479627
H	-1.919979	1.712954	-2.305746
C	-0.087933	2.293280	-1.496914
H	0.403200	2.851285	-0.702807
C	0.713764	1.694249	-2.586469
H	1.254437	2.524183	-3.046497
H	0.066599	1.345727	-3.394692
C	1.720975	0.608190	-2.090041
H	2.080592	0.096575	-2.985961
O	-6.359288	1.855216	2.231393
H	-6.777795	1.290659	2.905409
H	-5.078664	0.570295	1.135735
H	-8.029296	0.686681	0.803006
C	-6.892088	-0.666879	-0.516674
H	-7.471562	-0.238967	-1.337870
H	-5.825411	-0.642971	-0.746940
C	-7.442247	-2.007861	-0.047367
H	-8.530038	-2.072865	-0.109278
C	-7.016157	-3.099416	-1.069369
H	-7.524678	-2.981280	-2.028778
H	-7.304491	-4.086900	-0.703596
H	-5.952116	-3.134195	-1.311588
C	-7.225152	-2.183376	1.416940
H	-8.095989	-2.696950	1.832184
O	-7.160062	-0.842681	1.924663
O	0.897553	-0.299050	-1.364583
C	1.591091	-1.503816	-0.972734
H	2.061651	-1.966632	-1.844321
C	0.543523	-2.377605	-0.243305
C	-0.515104	-2.870396	-1.293492
H	-0.782999	-1.950752	-1.817726
C	0.101097	-3.841641	-2.386234
H	-0.658698	-4.224659	-3.071132
H	0.592719	-4.659063	-1.855436
H	0.791089	-3.327825	-3.059201
C	-1.706863	-3.471800	-0.685080
H	-1.879312	-4.539266	-0.788834
C	-2.573893	-2.669567	-0.067877

H	-2.417791	-1.605390	0.101380
C	-3.824549	-3.103236	0.373492
H	-4.139588	-4.106605	0.088120
C	-4.593300	-2.427780	1.247123
H	-4.347348	-1.406868	1.528852
C	-5.922301	-2.947883	1.781939
H	-5.976761	-4.010653	1.538946
H	-5.856696	-2.962435	2.871683
H	0.093740	-1.757083	0.534750
H	1.036097	-3.212616	0.259355
C	2.728313	-1.091451	0.010516
H	3.289585	-1.932059	0.423620
H	2.360913	-0.668349	0.947847
C	3.634800	-0.066222	-0.702002
O	4.583329	0.360803	0.211879
C	5.926258	0.667190	-0.227264
H	5.811468	1.288112	-1.127642
H	4.137863	-0.648980	-1.479110
C	2.828575	1.168450	-1.186980
H	3.531779	1.782189	-1.756134
H	2.319349	1.714320	-0.389373
O	6.650053	-0.430891	-0.849245
C	6.870420	-1.516771	0.046522
C	7.370625	-2.729882	-0.726972
H	6.875362	-2.786204	-1.699141
H	7.123077	-3.620416	-0.145380
H	8.448728	-2.657186	-0.883821
H	5.897969	-1.844609	0.422650
C	7.801639	-1.110263	1.158898
H	8.698520	-0.730355	0.662578
O	8.053151	-2.113267	2.142024
H	8.259671	-1.633818	2.964916
C	7.045710	0.086692	1.905703
O	7.858959	0.563029	2.964853
H	8.305724	1.356799	2.619164
H	6.065052	-0.250479	2.251991
C	6.721806	1.245682	0.968369
O	8.002635	1.848142	0.537595
C	7.857432	3.094769	-0.203557
H	7.256995	3.654535	0.519155
H	7.331927	2.871136	-1.134759
H	8.893606	3.418291	-0.328756
H	6.096087	2.037436	1.387572

NMR-Shifts

Original-MandelalideA162ps-NMR.txt

Atom	Type	Isotropic	Scaled Shift
1	C	91.7055	90.3104002757
2	C	116.6689	66.4169490228
3	C	147.9630	36.4641359904
6	C	106.6317	76.0239476253
8	C	110.8149	72.020042497
14	C	4.7582	173.531078313
16	C	63.2923	117.505790693
18	C	33.2694	146.241888244
20	C	144.0014	40.2559390494
23	C	109.7855	73.0053216945
29	C	147.8584	36.5642527613
32	C	150.7843	33.7637588775
34	C	172.0419	13.4172744501
38	C	103.4381	79.0806677004
42	C	108.0262	74.6892168686
44	C	136.9389	47.0157353701
45	C	151.5596	33.0216887766
47	C	165.7900	19.4012136526
51	C	45.6850	134.358429526
53	C	50.7605	129.500468998
55	C	44.8706	135.137923773
57	C	49.3789	130.822852658
59	C	146.5337	37.8321751948
64	C	142.9104	41.3001780279
67	C	116.6350	66.4493960451
69	C	84.1596	97.532877735
72	C	150.3904	34.1407760485
76	C	120.7105	62.5485748196
77	C	167.4357	17.8260495032
82	C	107.9694	74.743582381
86	C	109.5901	73.1923467141
90	C	98.9574	83.3693217711
92	C	124.1800	59.2277800111
4	H	30.4798	1.25922845923
5	H	30.2734	1.44994224994
7	H	25.9501	5.44467544468
10	H	29.2142	2.42864402864
11	H	27.8598	3.68011088011
12	H	27.6875	3.83931623932
17	H	25.5235	5.83885423885
19	H	24.0070	7.2401016401
21	H	29.4419	2.21824901825
22	H	29.1205	2.51522291522
24	H	28.1098	3.44911064911
26	H	29.3912	2.2650958651
27	H	28.2541	3.31577731578
28	H	28.1193	3.44033264033
30	H	29.9178	1.77851697852
31	H	30.4039	1.32936012936
33	H	29.2432	2.40184800185
35	H	30.9393	0.83465003465
36	H	30.8174	0.947285747286
37	H	30.6177	1.13180873181
39	H	27.5483	3.96793716794
43	H	28.3314	3.24435204435
46	H	28.7880	2.82245322245
48	H	30.5817	1.16507276507
49	H	31.0845	0.700485100485
50	H	30.7918	0.97094017094
52	H	25.7962	5.58687918688
54	H	24.9645	6.35537075537
56	H	25.3371	6.01108801109
58	H	25.6552	5.71716331716
60	H	29.6150	2.0583044583
61	H	29.5703	2.09960729961
62	H	30.1200	1.59168399168
63	H	30.4309	1.30441210441
65	H	30.1445	1.56904596905
66	H	30.5528	1.19177639178
70	H	26.0040	5.39487179487
71	H	27.5709	3.94705474705
73	H	29.5551	2.11365211365
74	H	29.8783	1.81501501502
78	H	30.6718	1.08182028182
79	H	30.3314	1.39635019635
80	H	30.7494	1.01011781012
81	H	28.1316	3.42896742897
83	H	28.3526	3.22476322476
85	H	29.1349	2.50191730192
88	H	29.3330	2.31887271887
89	H	27.9457	3.60073920074
93	H	27.8912	3.6510972511
94	H	27.7862	3.74811734812
95	H	27.5606	3.95657195657
96	H	28.0913	3.4662046662

Supporting Information: Original-MandelalideA164pss.log

Using Gaussian 09: AM64L-G09RevC.01 23-Sep-2011

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#mPW1PW91/6-311+G(2d,p) scf=(maxcycle=300,direct,tight) NMR density=current SCRF=(PCM,SOLVENT=Chloroform)

Pointgroup= C1 Stoichiometry= C33H52O11 C1[X(C33H52O11)]
#Atoms= 96
Charge = 0 Multiplicity = 1

SCF Energy= -2116.24206838
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Optimization incomplete.

Atomic Type	Coordinates (Angstroms) X	Y	Z
C	-7.052865	0.170941	0.757158
C	-6.004176	1.323954	0.978250
C	-5.821594	2.216598	-0.297900
H	-6.696957	2.866370	-0.363965
H	-5.644799	1.665659	-1.224227
C	-4.596176	3.192501	-0.024561
H	-4.762986	3.634930	0.960066
C	-4.574173	4.288272	-1.099902
O	-3.754164	5.309675	-0.507551
H	-3.054909	4.819733	-0.038188
H	-5.615525	4.591895	-1.234034
H	-4.198186	3.945168	-2.066647
O	-3.347592	2.441284	-0.260772
C	-2.109210	2.887480	0.062640
O	-1.848362	3.767709	0.870214
C	-1.092364	2.215273	-0.859866
H	-1.483392	1.527791	-1.608844
C	0.152535	2.574225	-1.096071
H	0.496073	3.405092	-0.484434
C	0.939730	2.008241	-2.296451
H	1.645543	2.810060	-2.523039
H	0.269763	1.782346	-3.129187
C	1.692756	0.752244	-1.953535
H	2.176756	0.327568	-2.837178
O	-6.526846	2.113187	2.084990
H	-6.332088	1.519901	2.832587
H	-5.066500	0.845558	1.273240
H	-8.057556	0.592743	0.849097
C	-7.081513	-0.726513	-0.467468
H	-7.755345	-0.370121	-1.250168
H	-6.036739	-0.868953	-0.749984
C	-7.640045	-2.023964	0.017512
H	-8.708956	-1.859907	-0.134374
C	-7.175512	-3.257153	-0.794477
H	-7.831352	-3.338499	-1.663681
H	-7.416731	-4.203252	-0.305933
H	-6.200630	-3.193485	-1.283100
C	-7.151539	-2.094502	1.456776
H	-7.984154	-2.494541	2.041193
O	-6.840391	-0.756288	1.893448
O	0.780890	-0.246574	-1.373188
C	1.455860	-1.469168	-1.059342
H	1.801900	-1.941212	-1.981423
C	0.353926	-2.401469	-0.411486
C	-0.603035	-2.993466	-1.456394
H	-0.753471	-2.302338	-2.288088
C	0.055951	-4.252426	-2.138855
H	-0.611258	-4.847672	-2.764744
H	0.437938	-4.872447	-1.324620
H	0.871685	-3.907282	-2.778216
C	-1.898617	-3.426289	-0.881593
H	-2.199518	-4.468867	-0.931178
C	-2.724239	-2.630629	-0.211616
H	-2.553802	-1.598495	0.089672
C	-3.861610	-3.193472	0.444855
H	-4.166072	-4.185338	0.113225
C	-4.688740	-2.494383	1.282465
H	-4.504933	-1.458647	1.559009
C	-5.946982	-2.996252	1.840231
H	-6.129477	-4.051656	1.627732
H	-5.868802	-2.821478	2.914952
H	-0.175793	-1.773148	0.307768
H	0.906576	-3.164476	0.140893
C	2.589892	-1.156298	-0.025190
H	3.120729	-2.099367	0.118511
H	2.025733	-0.959395	0.888267
C	3.533800	-0.201390	-0.633576
O	4.584603	0.082029	0.307104
C	5.846576	0.478198	-0.297174
H	5.731740	1.242642	-1.080208
H	3.907804	-0.630220	-1.566912
C	2.780482	1.099931	-0.918158
H	3.517591	1.741646	-1.405433
H	2.353269	1.565368	-0.028531
O	6.523430	-0.675062	-0.928163
C	6.968723	-1.666304	0.025058
C	7.756828	-2.624847	-0.836657
H	7.170528	-3.034880	-1.661744
H	8.172006	-3.458869	-0.268185
H	8.562079	-2.030407	-1.273060
H	6.186225	-2.298733	0.453512
C	7.811766	-1.049658	1.112955
H	8.660831	-0.602008	0.591400
O	8.418259	-1.990589	2.013900
H	8.698526	-1.490225	2.801151
C	7.061955	0.111948	1.876930
O	7.924507	0.685248	2.886127
H	8.407232	1.301384	2.307469
H	6.126288	-0.197783	2.350193
C	6.717230	1.117478	0.848138
O	7.873220	1.846321	0.427155
C	7.592666	3.148221	-0.196303
H	7.000592	3.704883	0.533953
H	6.987462	3.040485	-1.100910
H	8.506845	3.621302	-0.564681
H	6.038076	1.791726	1.376538

NMR-Shifts
Original-MandelalideA164ps-NMR.txt

Atom	Type	Isotropic	Scaled Shift
Original-MandelalideA164pss-NMR.txt			
1	C	90.8384	91.1403357645
2	C	103.9264	78.6132965792
3	C	145.1790	39.1288118073
6	C	96.1463	86.0599360631
8	C	109.3596	73.4129673233
14	C	5.9199	172.419169586
16	C	45.0273	134.987940045
18	C	33.4766	146.043568981
20	C	145.8312	38.5045655545
23	C	106.4776	76.1714427918
29	C	148.8714	35.5946706484
32	C	148.6326	35.8232355137
34	C	174.4607	11.1021459063
38	C	103.1113	79.3934608243
42	C	103.7296	78.8016615938
44	C	133.2520	50.5446122629
45	C	156.2750	28.5083941117
47	C	161.6286	23.3842531442

51	C	41.7756	138.100269913
53	C	47.1623	132.944447635
55	C	41.1751	138.675032064
57	C	46.0942	133.966768123
59	C	147.3928	37.0098968204
64	C	148.2329	36.2058040927
67	C	110.4817	72.3389613124
69	C	81.9663	99.6321713662
72	C	145.9088	38.4302915446
76	C	117.5407	65.5825149792
77	C	165.4478	19.7287467218
82	C	107.9844	74.7292252914
86	C	114.3510	68.635502211
90	C	105.1956	77.398495377
92	C	124.4978	58.9236011409
4	H	30.2622	1.46029106029
5	H	29.7709	1.91425271425
7	H	25.8418	5.54474474474
10	H	27.9330	3.61247401247
11	H	28.3676	3.2109032109
12	H	27.9229	3.62180642181
17	H	25.3827	5.96895356895
19	H	24.4407	6.83936243936
21	H	28.9772	2.64763224763
22	H	28.8776	2.73966273966
24	H	28.3486	3.22845922846
26	H	29.3007	2.34871794872
27	H	27.7714	3.76179256179
28	H	27.7432	3.78784938785
30	H	29.6339	2.04084084084
31	H	30.6250	1.12506352506
33	H	29.2445	2.40064680065
35	H	31.0500	0.732363132363
36	H	30.7271	1.03072303072
37	H	30.7598	1.00050820051
39	H	27.5682	3.94954954955
43	H	28.1032	3.45520905521
46	H	29.2353	2.40914760915
48	H	30.7139	1.04291984292
49	H	31.0590	0.724047124047
50	H	30.4264	1.30857010857
52	H	25.5756	5.79071379071
54	H	24.9187	6.39768999769
56	H	25.2662	6.0765996766
58	H	25.1932	6.14405174405
60	H	29.3709	2.28385308385
61	H	29.2093	2.43317163317
62	H	29.9690	1.73120813121
63	H	30.5508	1.19362439362
65	H	30.3184	1.40836220836
66	H	30.4080	1.32557172557
70	H	26.1458	5.26384846385
71	H	27.8957	3.64693924694
73	H	29.9794	1.7215985216
74	H	30.4640	1.27382767383
78	H	30.5720	1.17403557404
79	H	30.3706	1.36012936013
80	H	31.0695	0.714345114345
81	H	27.8733	3.66763686764
83	H	28.1779	3.38618618619
85	H	29.4094	2.24827904828
88	H	29.4130	2.24495264495
89	H	28.0174	3.53448833449
93	H	28.3901	3.19011319011
94	H	28.1962	3.36927696928
95	H	27.8205	3.71642411642
96	H	28.2068	3.35948255948

Supporting Information: Original-MandelalideA166.log

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 Using  Gaussian 09:  AM64L-G09RevC.01 23-Sep-2011
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 #mPW1pw91/6-311+G(2d,p) scf=(maxcycle=300,direct,tight) NMR
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 Pointgroup= C1   Stoichiometry= C33H52O11   C1[X(C33H52O11)]
#Atoms= 96
 Charge = 0                 Multiplicity = 1
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 SCF Energy= -2116.24586760
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 Optimization incomplete.


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      Type      X                Y              Z
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      C      -6.916909      0.233098      1.276084
      C      -5.677095      1.197785      1.309684
      C      -5.840517      2.414192      0.358659
      H      -6.668793      3.021455      0.730841
      H      -6.242372      2.188371     -0.631989
      C      -4.532329      3.248986      0.210100
      H      -4.060806      3.388695      1.185743
      C      -4.773763      4.579580     -0.546502
      O      -3.763751      5.571493     -0.122938
      H      -2.947649      5.048257     -0.028059
      H      -5.766398      4.939370     -0.262456
      H      -4.740641      4.239697     -1.584855
      O      -3.619614      2.409496     -0.657127
      C      -2.326679      2.763776     -0.826075
      O      -1.848781      3.745874     -0.340691
      C      -1.617937      1.959113     -1.753226
      H      -2.191716      1.195285     -2.276518
      C      -0.320446      2.227241     -1.975919
      H       0.158191      3.030586     -1.420450
      C       0.621719      1.573495     -2.993485
      H       1.139525      2.451546     -3.383915
      H       0.125610      0.972011     -3.757761
      C       1.598817      0.457757     -2.365542
      H       2.185626     -0.024614     -3.150272
      O      -5.562477      1.642615      2.604647
      H      -5.679104      0.850764      3.159494
      H      -4.781463      0.627757      1.048633
      H      -7.834436      0.674899      1.674279
      C      -7.062049     -0.447099     -0.103097
      H      -7.740262      0.158750     -0.708021
      H      -6.077965     -0.594214     -0.551281
      C      -7.661387     -1.818076      0.260442
      H      -8.746744     -1.701706      0.265646
      C      -7.427785     -2.890003     -0.827673
      H      -7.765572     -2.558967     -1.811750
      H      -7.941657     -3.816673     -0.561561
      H      -6.411717     -3.247210     -1.006260
      C      -6.982991     -2.097768      1.624413
      H      -7.692673     -2.640555      2.253606
      O      -6.601039     -0.847582      2.166127
      O       0.855986     -0.570981     -1.680656
      C       1.607033     -1.667553     -1.231413
      H       2.091563     -2.196647     -2.055412
      C       0.752608     -2.643364     -0.485475
      C      -0.205838     -3.318067     -1.473329
      H      -0.604898     -2.565283     -2.156421
      C       0.430914     -4.402451     -2.313987
      H      -0.187539     -4.443951     -3.212877
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H	0.484532	-5.385477	-1.840250
H	1.459931	-4.217314	-2.628088
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H	-1.071594	-4.734224	-0.101477
C	-2.344284	-3.021854	-0.326734
H	-2.418644	-2.017640	-0.740388
C	-3.475335	-3.396449	0.588113
H	-3.509362	-4.437996	0.902703
C	-4.449537	-2.535180	0.879495
H	-4.450578	-1.521588	0.485730
C	-5.649927	-3.004957	1.671935
H	-5.979530	-3.981380	1.311907
H	-5.450659	-3.110577	2.739778
H	0.185143	-2.007863	0.196887
H	1.390865	-3.359254	0.036410
C	2.670242	-1.142479	-0.242937
H	3.321477	-1.958248	0.078647
H	2.239208	-0.758224	0.683532
C	3.543222	-0.054844	-0.846742
O	4.460412	0.363056	0.242782
C	5.736784	0.926318	-0.146905
H	5.514279	1.740791	-0.851719
H	4.114234	-0.496199	-1.667352
C	2.642715	1.051359	-1.363029
H	3.370255	1.678262	-1.883271
H	2.147741	1.563855	-0.534984
O	6.419459	-0.228781	-0.836074
C	6.841897	-1.355857	0.011685
C	7.876349	-2.190444	-0.804391
H	8.516506	-2.883105	-0.252244
H	8.497005	-1.564074	-1.448041
H	7.289964	-2.849290	-1.448815
H	6.012343	-2.050404	0.167250
C	7.548171	-0.903576	1.352514
H	8.498051	-0.457642	1.046682
O	7.774177	-1.926844	2.395161
H	7.907335	-1.428581	3.221369
C	6.647393	0.056287	2.057296
O	7.380327	0.575279	3.180813
H	7.825844	1.407284	2.941066
H	5.713454	-0.413565	2.374870
C	6.431430	1.320762	1.139421
O	7.658730	1.991147	0.919938
C	7.532583	3.298280	0.284876
H	6.696450	3.869776	0.694690
H	7.243693	3.106539	-0.752076
H	8.447210	3.897905	0.271680
H	5.756071	1.983081	1.686134

NMR-Shifts
Original-MandelalideA166ps-NMR.txt

Atom	Type	Isotropic	Scaled Shift
1	C	95.6290	86.555064224
2	C	110.0802	72.7232527422
3	C	149.3691	35.1183024177
6	C	93.5475	88.5473496813
8	C	109.4775	73.3001205996
14	C	15.0285	163.700970539
16	C	62.8310	117.947319053
18	C	20.9958	157.989433182
20	C	143.4030	40.8286912077
23	C	102.6869	79.7996707441
29	C	146.1182	38.2298665748
32	C	145.3469	38.9681081185
34	C	173.0096	12.4910507475
38	C	101.0455	81.3707191945
42	C	115.7692	67.2780872528
44	C	134.4932	49.3566109612
45	C	150.5405	33.9971094393
47	C	172.7010	12.7864239361
51	C	36.9303	142.737896974
53	C	47.5547	132.568866173
55	C	44.8789	135.129979517
57	C	52.9552	127.399835372
59	C	145.3211	38.9928023124
64	C	143.8832	40.3690729149
67	C	108.0182	74.696873983
69	C	81.6128	99.9705201095
72	C	150.6769	33.8665556385
76	C	110.0313	72.7700568541
77	C	167.6688	17.6029403319
82	C	105.5730	77.0372710044
86	C	112.7909	70.1287352361
90	C	104.2515	78.3021305921
92	C	126.9050	56.619575413
4	H	30.3700	1.36068376068
5	H	29.9041	1.79117579118
7	H	26.2711	5.14807114807
10	H	26.1772	5.23483483483
11	H	28.1345	3.42628782629
12	H	28.0051	3.54585354585
17	H	25.3832	5.96849156849
19	H	23.4785	7.72843612844
21	H	28.9075	2.71203511204
22	H	28.6212	2.97657657658
24	H	28.0838	3.47313467313
26	H	29.0648	2.56668976669
27	H	27.8441	3.69461769462
28	H	27.7976	3.73758373758
30	H	29.9018	1.7933009933
31	H	30.3013	1.42416262416
33	H	29.0812	2.55153615154
35	H	30.8795	0.889905289905
36	H	30.9778	0.799075999076
37	H	31.1611	0.629706629707
39	H	27.3661	4.13629013629
43	H	28.5189	3.0711018711
46	H	29.2723	2.37495957496
48	H	30.5631	1.18225918226
49	H	31.0280	0.752691152691
50	H	30.9107	0.861076461076
52	H	25.8518	5.5355047355
54	H	25.3144	6.03206283206
56	H	25.1031	6.2273042273
58	H	25.5855	5.78156618157
60	H	29.7036	1.97643797644
61	H	29.1717	2.46791406791
62	H	30.5655	1.18004158004
63	H	30.3520	1.37731577732
65	H	30.4417	1.29443289443
66	H	30.9655	0.810441210441
70	H	25.4149	5.9392007392
71	H	27.5725	3.94557634558
73	H	29.6158	2.05756525757
74	H	30.4463	1.29018249018
78	H	30.3088	1.41723261723
79	H	30.8509	0.916331716332
80	H	30.4953	1.24490644491
81	H	27.6129	3.90824670825
83	H	28.0393	3.51425271425
85	H	28.3442	3.23252483252
88	H	29.1103	2.52464772465
89	H	27.5893	3.93005313005
93	H	28.8191	2.79371679372
94	H	28.1180	3.44153384153
95	H	27.8557	3.6838992839
96	H	28.2238	3.34377454377

Supporting Information: Original-MandelalideA168.log

Using Gaussian 09: AM64L-G09RevC.01 23-Sep-2011

==========

#mPW1pw91/6-311+G(2d,p) scf=(maxcycle=300,direct,tight) NMR density=current SCRF=(PCM,SOLVENT=Chloroform)

Pointgroup= C1 Stoichiometry= C33H52O11 C1[X(C33H52O11)]

#Atoms= 96

Charge = 0 Multiplicity = 1

SCF Energy= -2116.24442355

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Optimization incomplete.

Atomic Type	Coordinates (Angstroms) X	Y	Z
C	-6.531238	0.464422	1.120835
C	-5.284594	1.339109	1.025597
C	-5.474603	2.598253	0.190572
H	-6.357339	3.143003	0.531366
H	-5.726607	2.178986	-0.786719
C	-4.184115	3.418068	0.140909
H	-3.684855	3.618803	1.092757
C	-4.514676	4.853967	-0.527355
O	-3.401621	5.754042	-0.311011
H	-2.637642	5.154364	-0.382833
H	-5.455039	5.206578	-0.095439
H	-4.596059	4.756079	-1.613169
O	-3.345567	2.684464	-0.852096
C	-2.039033	2.984431	-0.828042
O	-1.514314	3.884248	-0.235172
C	-1.348671	2.119299	-1.762938
H	-2.011278	1.432784	-2.289082
C	0.019025	2.114991	-1.852006
H	0.604915	2.814142	-1.260984
C	0.697933	1.321385	-2.934291
H	1.266714	1.999683	-3.574716
H	-0.106435	0.825885	-3.482366
C	1.578287	0.148394	-2.358309
H	2.031491	-0.290061	-3.251149
O	-5.009799	1.730317	2.360200
H	-5.393299	0.937383	2.776119
H	-4.441985	0.762951	0.634381
H	-7.446028	1.038176	1.292646
C	-6.695431	-0.506363	-0.119252
H	-7.142350	-0.017141	-0.987063
H	-5.746292	-0.889710	-0.499525
C	-7.566969	-1.641249	0.505753
H	-8.548035	-1.184446	0.655222
C	-7.742875	-2.952211	-0.328333
H	-8.375222	-2.926182	-1.217541
H	-8.243880	-3.701255	0.288716
H	-6.765837	-3.407134	-0.505910
C	-6.938552	-1.807576	1.899138
H	-7.728775	-2.076635	2.604489
O	-6.369610	-0.513470	2.175115
O	0.741699	-0.747642	-1.615818
C	1.487308	-1.899256	-1.207349
H	1.904211	-2.430399	-2.067431
C	0.401648	-2.802006	-0.620714
C	-0.619149	-3.396204	-1.648344
H	-1.043192	-2.576579	-2.231980
C	-0.069051	-4.553710	-2.504767
H	-0.839600	-5.195047	-2.938783
H	0.717674	-5.187741	-2.090419
H	0.423735	-4.171819	-3.401234
C	-1.774563	-3.860585	-0.819675
H	-1.795403	-4.931693	-0.631580
C	-2.724306	-2.930984	-0.387065
H	-2.621628	-1.847824	-0.403879
C	-3.901777	-3.315665	0.402573
H	-4.330366	-4.286871	0.161675
C	-4.470780	-2.470773	1.239002
H	-3.963995	-1.523491	1.403556
C	-5.777940	-2.779256	2.022586
H	-6.297815	-3.724948	1.855995
H	-5.582737	-2.949916	3.082936
H	-0.058840	-2.212722	0.174555
H	1.041711	-3.567041	-0.175796
C	2.618489	-1.511756	-0.297770
H	3.217258	-2.397207	-0.071743
H	2.200947	-1.135235	0.638605
C	3.582977	-0.476339	-0.861825
O	4.368800	0.088606	0.141280
C	5.642162	0.677659	-0.275899
H	5.525406	1.449048	-1.051295
H	4.153465	-0.980028	-1.647598
C	2.824541	0.672558	-1.487912
H	3.463039	1.340808	-2.070165
H	2.467945	1.299257	-0.668245
O	6.595943	-0.283626	-0.686554
C	6.706581	-1.409631	0.205219
C	7.577213	-2.519913	-0.444255
H	7.351713	-3.508861	-0.039516
H	8.642174	-2.291433	-0.356789
H	7.331870	-2.513902	-1.508334
H	5.718371	-1.858065	0.334960
C	7.348815	-0.898101	1.510372
H	8.370511	-0.523924	1.414296
O	7.490100	-1.948872	2.531456
H	8.084398	-1.765601	3.279765
C	6.519258	0.306890	2.096054
O	7.213796	0.769792	3.194129
H	7.941811	1.258616	2.769883
H	5.570364	-0.091577	2.462771
C	6.201981	1.374333	1.051930
O	7.472333	2.170977	0.876959
C	7.378678	3.270221	-0.033374
H	6.634322	4.005054	0.282419
H	7.029084	2.888852	-0.996135
H	8.359840	3.736493	-0.152019
H	5.394032	2.012440	1.418028

NMR-Shifts

Original-MandelalideA154ps-NMR.txt

Atom	Type	Isotropic	Scaled Shift
1	C	99.5113	82.8391623117
2	C	113.8958	69.0711920213
3	C	150.1675	34.354122399
6	C	98.8768	83.4464671988
8	C	104.1590	78.3906659775
14	C	13.4558	165.20626352
16	C	51.4883	128.803863014
18	C	18.8037	160.087578246
20	C	141.3063	42.8355251823
23	C	107.0165	75.6556404219
29	C	144.8385	39.4547177396
32	C	141.9999	42.1716533624
34	C	175.6098	10.0022971343
38	C	101.6031	80.8370183196
42	C	112.1035	70.7866727924
44	C	133.9358	49.8901204081

45	C	152.6552	31.9730469573
47	C	173.8417	11.6946151343
51	C	25.3396	153.831811482
53	C	40.9170	138.922069718
55	C	46.8664	133.227665154
57	C	54.9944	125.448036907
59	C	152.4289	32.1896475813
64	C	151.9453	32.6525201478
67	C	123.0368	60.3219816612
69	C	86.5446	95.2501004996
72	C	148.2656	36.1745056376
76	C	116.2153	66.8511074102
77	C	164.8086	20.3405501637
82	C	97.9763	84.3083711403
86	C	113.7691	69.1924615709
90	C	94.3126	87.8150424013
92	C	130.9068	52.789295354
4	H	30.3051	1.42065142065
5	H	30.1204	1.59131439131
7	H	25.9566	5.43866943867
10	H	26.5248	4.91365211365
11	H	28.0902	3.46722106722
12	H	27.4489	4.05978285978
17	H	24.9976	6.32478632479
19	H	23.4818	7.72538692539
21	H	29.2046	2.43751443751
22	H	28.8004	2.810995611
24	H	28.2026	3.36336336336
26	H	27.9255	3.6194040194
27	H	27.9353	3.61034881035
28	H	27.8349	3.70311850312
30	H	30.1224	1.58946638947
31	H	30.2883	1.43617463617
33	H	29.2946	2.35435435435
35	H	30.6468	1.10492030492
36	H	31.0734	0.710741510742
37	H	30.8385	0.927789327789
39	H	27.4498	4.05895125895
43	H	28.6116	2.98544698545
46	H	28.6721	2.92954492954
48	H	30.8724	0.896465696466
49	H	31.0858	0.699283899284
50	H	30.8086	0.955416955417
52	H	24.9833	6.337999538
54	H	24.7348	6.56761376761
56	H	25.2692	6.07382767383
58	H	25.7398	5.63899283899
60	H	30.0114	1.69203049203
61	H	29.4223	2.23635943636
62	H	30.2729	1.4504042504
63	H	30.5368	1.20656040656
65	H	30.1797	1.53652113652
66	H	30.9783	0.798613998614
70	H	25.6178	5.75172095172
71	H	27.9565	3.59075999076
73	H	29.7393	1.94345114345
74	H	30.5629	1.18244398244
78	H	30.1029	1.60748440748
79	H	30.5745	1.17172557173
80	H	30.7139	1.04291984292
81	H	27.4089	4.09674289674
83	H	27.9666	3.58142758143
85	H	29.3527	2.30066990067
88	H	30.1550	1.55934395934
89	H	28.1072	3.45151305151
93	H	28.5636	3.0297990298
94	H	28.2140	3.35282975283
95	H	28.1652	3.39792099792
96	H	27.8586	3.68121968122

Supporting Information: Original-MandelalideA170.log

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 Using  Gaussian 09:  AM64L-G09RevC.01 23-Sep-2011
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 #mPW1pw91/6-311+G(2d,p) scf=(maxcycle=300,direct,tight) NMR
 density=current SCRF=(PCM,SOLVENT=Chloroform)
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 Pointgroup= C1   Stoichiometry= C33H52O11   C1[X(C33H52O11)]
#Atoms= 96
 Charge = 0                Multiplicity = 1
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 SCF Energy= -2116.25959095
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 Optimization incomplete.


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     Atomic      Coordinates (Angstroms)
      Type      X                Y              Z
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      C      -6.734118      0.598361      0.922782
      C      -5.395783      1.366511      0.998858
      C      -5.595187      2.647289      0.206367
      H      -6.401630      3.183030      0.710734
      H      -6.024996      2.288032     -0.731504
      C      -4.296125      3.462779      0.052160
      H      -3.874007      3.481348      1.060946
      C      -4.480221      4.947998     -0.514345
      O      -3.356434      5.765333     -0.184495
      H      -2.721556      5.169240      0.252709
      H      -5.359192      5.417391     -0.065528
      H      -4.611346      4.951499     -1.599296
      O      -3.465640      2.705885     -0.863087
      C      -2.130636      2.803884     -0.810193
      O      -1.564931      3.482165      0.016671
      C      -1.416715      1.976046     -1.806789
      H      -1.999275      1.403616     -2.525870
      C      -0.062553      1.857135     -1.876020
      H       0.578993      2.489668     -1.267789
      C       0.636577      1.070617     -2.859850
      H       1.140393      1.829833     -3.461313
      H      -0.115630      0.624539     -3.512955
      C       1.570664     -0.014801     -2.260442
      H       2.079048     -0.560002     -3.060122
      O      -5.214308      1.603064      2.339454
      H      -5.440680      0.746709      2.745005
      H      -4.477776      0.841203      0.721714
      H      -7.520243      1.355795      0.979660
      C      -6.852664     -0.255449     -0.401813
      H      -7.332147      0.203719     -1.268601
      H      -5.843418     -0.557126     -0.687249
      C      -7.703707     -1.490214     -0.039865
      H      -8.729089     -1.145270      0.112064
      C      -7.644447     -2.679119     -0.970643
      H      -8.059147     -2.402566     -1.942032
      H      -8.276895     -3.460587     -0.542756
      H      -6.614913     -3.025861     -1.077713
      C      -7.293722     -1.694076      1.479506
      H      -8.127590     -2.086903      2.066694
      O      -6.811793     -0.430426      1.998988
      O       0.785124     -0.984295     -1.479826
      C       1.549552     -2.097726     -0.864408
      H       2.034435     -2.639154     -1.681045
      C       0.561176     -2.941441     -0.012582
      C      -0.415159     -3.773917     -0.888373
      H      -0.700355     -3.216736     -1.782773
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C	0.266552	-5.128470	-1.341722
H	-0.302983	-5.731257	-2.052815
H	0.462776	-5.763300	-0.474452
H	1.199781	-4.854545	-1.837701
C	-1.754149	-4.081616	-0.146067
H	-1.962614	-5.042663	0.317650
C	-2.710394	-3.145093	-0.091917
H	-2.503498	-2.145028	-0.470758
C	-3.950573	-3.381711	0.625500
H	-4.224221	-4.402156	0.889732
C	-4.771473	-2.408134	1.014716
H	-4.447796	-1.371352	1.047503
C	-6.094014	-2.687968	1.666228
H	-6.525895	-3.663218	1.429255
H	-5.984567	-2.899394	2.731657
H	0.003260	-2.243126	0.613744
H	1.133660	-3.563390	0.680582
C	2.707192	-1.599722	0.038058
H	3.425869	-2.384521	0.283086
H	2.314513	-1.212668	0.980361
C	3.507031	-0.532480	-0.667785
O	4.364760	0.139345	0.277794
C	5.578078	0.873051	-0.189801
H	5.299629	1.650870	-0.916645
H	4.127009	-0.970819	-1.453454
C	2.611944	0.553871	-1.297805
H	3.278085	1.199915	-1.873425
H	2.232374	1.206934	-0.508757
O	6.500529	0.004166	-0.918189
C	6.990114	-1.186219	-0.159816
C	7.938956	-1.947179	-1.120465
H	8.289854	-2.866097	-0.645879
H	8.739955	-1.347179	-1.557366
H	7.266063	-2.317068	-1.896871
H	6.222458	-1.912174	0.121092
C	7.830882	-0.792554	1.049473
H	8.762448	-0.354900	0.681582
O	8.038153	-1.962361	1.855046
H	8.636453	-1.628588	2.547568
C	6.983014	0.246097	1.839772
O	7.814574	0.784849	2.800743
H	8.339984	1.440840	2.309456
H	6.172478	-0.340579	2.279762
C	6.273467	1.409937	1.108011
O	7.318437	2.389740	0.769161
C	6.868097	3.781251	0.327246
H	6.232190	4.193438	1.114723
H	6.314080	3.677507	-0.608323
H	7.743475	4.416300	0.171462
H	5.454474	1.815461	1.708319

NMR-Shifts
Original-MandelalideA170ps-NMR.txt

Atom	Type	Isotropic	Scaled Shift
1	C	90.9423	91.040888991
2	C	115.5164	67.5200520684
3	C	147.1515	37.240854534
6	C	106.2131	76.4246061372
8	C	110.8591	71.9777369398
14	C	13.4450	165.216600624
16	C	59.4573	121.176419916
18	C	21.5240	157.483872203
20	C	148.0781	36.3539692567
23	C	107.5952	75.1017439078
29	C	146.5279	37.8377266027
32	C	141.6339	42.521966347
34	C	174.7800	10.7965313272
38	C	96.2108	85.9982005781
42	C	105.9794	76.6482895921
44	C	136.8386	47.1117364421
45	C	146.2461	38.107448458
47	C	166.7518	18.4806370719
51	C	33.4763	146.043856123
53	C	45.4196	134.612454297
55	C	47.2468	132.863569364
57	C	55.0762	125.369742912
59	C	150.5203	34.0164436532
64	C	149.7588	34.7453052317
67	C	115.1000	67.9186048738
69	C	78.0618	103.369321771
72	C	152.5651	32.0592852084
76	C	108.2253	74.4986504336
77	C	165.6676	19.5183675032
82	C	104.4845	78.0791171347
86	C	113.0269	69.9028503608
90	C	99.1940	83.1428626122
92	C	120.0245	63.2051723808
4	H	30.4439	1.2924000924
5	H	30.1879	1.52894432894
7	H	26.0940	5.31171171171
10	H	28.9886	2.6370986371
11	H	27.9137	3.63030723031
12	H	27.8363	3.70182490182
17	H	25.5326	5.83044583045
19	H	23.9563	7.28694848695
21	H	29.1709	2.46865326865
22	H	28.9410	2.68108108108
24	H	27.8778	3.66347886348
26	H	28.4390	3.14492954493
27	H	27.3825	4.12113652114
28	H	27.9098	3.63391083391
30	H	29.8529	1.83848463848
31	H	30.3431	1.38553938554
33	H	29.3018	2.3477015477
35	H	30.6985	1.05714945715
36	H	30.7160	1.04097944098
37	H	30.6827	1.07174867175
39	H	27.5229	3.99140679141
43	H	28.0476	3.50658350658
46	H	29.1148	2.52048972049
48	H	30.7640	0.996627396627
49	H	31.1662	0.624994224994
50	H	30.7948	0.968168168168
52	H	25.4127	5.94123354123
54	H	24.8604	6.45155925156
56	H	25.1551	6.17925617926
58	H	25.7860	5.5963039963
60	H	30.0699	1.63797643798
61	H	29.3441	2.30861630862
62	H	30.1301	1.58235158235
63	H	30.3569	1.37278817279
65	H	30.0643	1.64315084315
66	H	30.7476	1.01178101178
70	H	25.6910	5.68408408408
71	H	27.6978	3.8297990298
73	H	29.9762	1.72455532456
74	H	30.2515	1.47017787018
78	H	30.1276	1.58466158466
79	H	30.6802	1.07405867406
80	H	30.5977	1.15028875029
81	H	27.9946	3.55555555556
83	H	28.6248	2.97325017325
85	H	29.2537	2.39214599215
88	H	29.4865	2.17703857704
89	H	28.2438	3.32529452529
93	H	28.2697	3.30136290136
94	H	27.9092	3.63446523447
95	H	27.9653	3.58262878263

96 H 27.8647 3.67558327558

Supporting Information: Original-MandelalideA172.log

Using Gaussian 09: AM64L-G09RevC.01 23-Sep-2011

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#mPW1pw91/6-311+G(2d,p) scf=(maxcycle=300,direct,tight) NMR density=current SCRF=(PCM,SOLVENT=Chloroform)

Pointgroup= C1 Stoichiometry= C33H52O11 C1[X(C33H52O11)]

#Atoms= 96

Charge = 0 Multiplicity = 1

SCF Energy= -2116.26687627

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Optimization incomplete.

Atomic Type	Coordinates (Angstroms) X	Y	Z
C	-6.354694	0.656996	1.436987
C	-5.046042	1.424056	1.133001
C	-5.276379	2.743950	0.328838
H	-5.866892	3.404473	0.966966
H	-5.806445	2.562300	-0.608350
C	-3.976244	3.482045	-0.019740
H	-3.425386	3.660208	0.907220
C	-4.362570	4.739440	-0.887572
O	-3.200248	5.563757	-1.093381
H	-2.400411	5.011863	-1.036002
H	-5.189216	5.266634	-0.405814
H	-4.795926	4.404652	-1.833779
O	-3.189707	2.583866	-0.806370
C	-1.878881	2.805203	-1.034423
O	-1.278710	3.800106	-0.584857
C	-1.265053	1.695647	-1.845150
H	-1.854743	0.823755	-2.122542
C	0.012166	1.857490	-2.251674
H	0.570368	2.750275	-1.982155
C	0.678681	0.840274	-3.153299
H	1.288216	1.445471	-3.826831
H	-0.028526	0.235649	-3.724554
C	1.663882	-0.110224	-2.444906
H	2.336893	-0.541781	-3.191314
O	-4.402374	1.818036	2.360424
H	-4.627295	1.128277	3.010801
H	-4.401879	0.779812	0.528275
H	-7.089483	1.345360	1.861503
C	-6.801857	-0.106009	0.210300
H	-7.316146	0.450942	-0.576314
H	-5.973476	-0.655943	-0.239932
C	-7.684467	-1.164984	0.783932
H	-8.655541	-0.800583	1.125968
C	-7.955365	-2.203857	-0.317912
H	-8.558702	-1.694291	-1.072169
H	-8.612248	-3.041651	-0.073546
H	-6.990350	-2.570312	-0.675082
C	-6.853865	-1.586427	2.035844
H	-7.448177	-1.939521	2.882955
O	-6.135299	-0.439326	2.384078
O	0.717230	-1.077558	-1.843800
C	1.411523	-2.173852	-1.128620
H	1.963781	-2.731074	-1.889329
C	0.415738	-3.080971	-0.444262
C	-0.655727	-3.695216	-1.365323
H	-0.906308	-2.956319	-2.129153
C	-0.002925	-4.963751	-1.959585
H	-0.593519	-5.216773	-2.842847
H	0.075809	-5.780897	-1.239841
H	1.023743	-4.777197	-2.281069
C	-1.970977	-4.063362	-0.740571
H	-2.378393	-5.070457	-0.753266
C	-2.694333	-3.099405	-0.119963
H	-2.296550	-2.096565	0.030361
C	-4.028854	-3.341928	0.390411
H	-4.455824	-4.335966	0.266630
C	-4.680884	-2.416421	1.087582
H	-4.344301	-1.387399	1.193839
C	-5.936163	-2.783920	1.753652
H	-6.458866	-3.495674	1.109994
H	-5.684111	-3.244858	2.711291
H	-0.156878	-2.462065	0.249234
H	0.990068	-3.790120	0.154631
C	2.452768	-1.715724	-0.138012
H	3.157261	-2.467283	0.224647
H	2.059245	-1.397251	0.828407
C	3.371602	-0.662922	-0.664456
O	4.208939	-0.160173	0.388634
C	5.353874	0.659518	0.014998
H	4.887335	1.400134	-0.651921
H	4.119408	-0.996742	-1.389247
C	2.524819	0.550752	-1.291708
H	3.183488	1.251473	-1.807977
H	1.943416	1.002797	-0.485640
O	6.256849	-0.173116	-0.762711
C	6.741221	-1.256689	0.097996
C	7.475955	-2.316424	-0.724276
H	7.378105	-3.285442	-0.228402
H	8.529268	-2.041722	-0.798815
H	6.992238	-2.469814	-1.691184
H	5.897081	-1.819942	0.501380
C	7.630594	-0.655136	1.279785
H	8.446415	-0.171257	0.737955
O	7.993407	-1.691078	2.146811
H	8.274109	-1.306778	2.996367
C	6.779484	0.379879	2.064185
O	7.684566	1.127739	2.888037
H	7.824334	1.992962	2.463595
H	6.072410	-0.104221	2.742096
C	6.005407	1.343191	1.208698
O	6.988629	2.308523	0.697484
C	6.502451	3.655725	0.491311
H	6.186334	4.015111	1.474318
H	5.733459	3.634338	-0.284572
H	7.307138	4.267179	0.074784
H	5.360099	1.908374	1.887240

NMR-Shifts

Original-MandelalideA172ps-NMR.txt

Atom	Type	Isotropic	Scaled Shift
1	C	97.2736	84.9809529279
2	C	108.9381	73.8164015391
3	C	147.2044	37.1902218649
6	C	109.8846	72.9104691897
8	C	109.6253	73.1586554107
14	C	1.8613	176.303815157
16	C	52.6708	127.67204579
18	C	19.7851	159.148241735
20	C	144.2437	40.0240241965
23	C	101.6715	80.7715499914
29	C	147.3303	37.0697180268
32	C	141.9055	42.2620073125
34	C	168.6264	16.6863837363
38	C	111.4283	71.4329332491

42	C	113.9173	69.0506135263
44	C	138.1717	45.8357740386
45	C	155.5236	29.2275885832
47	C	167.1580	18.0918470874
51	C	39.2991	140.470625395
53	C	40.0278	139.773157985
55	C	48.6926	131.479737361
57	C	51.1048	129.170925937
59	C	149.7219	34.780623672
64	C	153.3810	31.2783552518
67	C	111.1999	71.6515438657
69	C	86.6391	95.1596508356
72	C	146.4968	37.867493635
76	C	112.6226	70.2898217807
77	C	168.3325	16.9676869772
82	C	106.2984	76.3429621547
86	C	111.3284	71.5285514654
90	C	103.9397	78.6005666265
92	C	125.6229	57.8467237122
4	H	30.3123	1.413998614
5	H	30.2888	1.43571263571
7	H	26.0825	5.32233772234
10	H	26.5425	4.8972972973
11	H	28.2745	3.29692769693
12	H	28.0574	3.49752829753
17	H	24.9112	6.40462000462
19	H	23.5047	7.70422730423
21	H	29.2620	2.38447678448
22	H	28.9387	2.68320628321
24	H	27.9626	3.58512358512
26	H	29.2659	2.38087318087
27	H	27.6892	3.83774543775
28	H	27.8552	3.68436128436
30	H	30.0814	1.62735042735
31	H	30.7289	1.02905982906
33	H	29.1996	2.44213444213
35	H	30.6378	1.11323631324
36	H	30.7756	0.985908985909
37	H	30.9426	0.831600831601
39	H	27.4975	4.01487641488
43	H	27.9576	3.58974358974
46	H	29.0268	2.6018018018
48	H	30.5028	1.23797643798
49	H	31.1235	0.664449064449
50	H	30.8778	0.891476091476
52	H	25.3766	5.97458997459
54	H	24.6516	6.64449064449
56	H	25.0743	6.25391545392
58	H	25.0414	6.28431508432
60	H	29.0469	2.58322938323
61	H	29.2660	2.38078078078
62	H	30.0127	1.69082929083
63	H	30.5357	1.20757680758
65	H	29.9681	1.73203973204
66	H	30.7376	1.02102102102
70	H	25.7401	5.63871563872
71	H	26.9878	4.48583968584
73	H	29.3773	2.27793947794
74	H	30.6935	1.06176946177
78	H	30.2934	1.43146223146
79	H	30.5503	1.19408639409
80	H	30.4778	1.26107646108
81	H	27.6137	3.90750750751
83	H	28.2670	3.30385770386
85	H	29.7555	1.92848232848
88	H	28.6405	2.95874335874
89	H	28.0800	3.47664587665
93	H	28.1769	3.38711018711
94	H	27.9934	3.55666435666
95	H	28.0251	3.52737352737
96	H	27.9825	3.56673596674

Supporting Information: Original-MandelalideA174.log

Using Gaussian 09: AM64L-G09RevC.01 23-Sep-2011

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#mPW1pw91/6-311+G(2d,p) scf=(maxcycle=300,direct,tight) NMR density=current SCRF=(PCM,SOLVENT=Chloroform)

Pointgroup= C1 Stoichiometry= C33H52O11 C1[X(C33H52O11)]

#Atoms= 96

Charge = 0 Multiplicity = 1

SCF Energy= -2116.24265698

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Optimization incomplete.

Atomic Type	Coordinates (Angstroms) X	Y	Z
C	-6.709628	0.660667	1.174378
C	-5.340082	1.449674	1.153810
C	-5.321902	2.758332	0.347240
H	-6.058434	3.423293	0.801526
H	-5.653047	2.562952	-0.675149
C	-3.946471	3.385813	0.182008
H	-3.505643	3.561290	1.167111
C	-4.125137	4.740594	-0.598980
O	-2.990952	5.640672	-0.420239
H	-2.129794	5.191136	-0.345355
H	-4.947269	5.336122	-0.194235
H	-4.400171	4.484904	-1.625156
O	-3.062590	2.464951	-0.464133
C	-1.790949	2.749741	-0.725578
O	-1.172226	3.706364	-0.344473
C	-1.172001	1.858015	-1.680705
H	-1.728548	0.925554	-1.758936
C	-0.012371	2.107766	-2.256685
H	0.426313	3.095880	-2.145152
C	0.726516	1.055387	-3.109779
H	1.424020	1.570436	-3.775034
H	-0.031829	0.580251	-3.734844
C	1.647265	0.039958	-2.445762
H	2.239847	-0.484982	-3.199241
O	-4.994422	1.747404	2.503978
H	-5.381248	0.993940	2.985280
H	-4.563307	0.817778	0.714333
H	-7.462277	1.347349	1.571024
C	-7.071810	0.082879	-0.216143
H	-7.533440	0.808773	-0.888782
H	-6.123291	-0.286636	-0.611101
C	-7.842705	-1.165840	0.142183
H	-8.820178	-0.771241	0.429083
C	-7.935151	-2.248908	-0.971673
H	-8.437274	-1.744418	-1.799370
H	-8.637058	-3.049207	-0.726559
H	-7.076450	-2.848130	-1.282800
C	-7.323527	-1.637140	1.514464
H	-8.214310	-1.803221	2.125045
O	-6.560894	-0.503895	1.961807
O	0.813098	-0.933613	-1.804555
C	1.415085	-1.929895	-0.980277
H	1.862121	-2.622343	-1.697992
C	0.367264	-2.753370	-0.096392

C	-0.475514	-3.734865	-0.946215
H	-0.793462	-3.107364	-1.782491
C	0.273468	-4.920633	-1.539854
H	-0.417201	-5.267484	-2.311524
H	0.323504	-5.708215	-0.785521
H	1.257958	-4.590068	-1.880682
C	-1.729110	-4.147016	-0.233612
H	-1.808257	-5.119116	0.247183
C	-2.796373	-3.297082	-0.128049
H	-2.630261	-2.262297	-0.425327
C	-4.070328	-3.671330	0.542282
H	-4.085465	-4.652464	1.013677
C	-4.986113	-2.712130	0.745451
H	-4.816406	-1.659616	0.535907
C	-6.240398	-2.786920	1.533921
H	-6.739004	-3.741390	1.351823
H	-5.942984	-2.846900	2.582676
H	-0.301904	-2.163257	0.534672
H	0.955221	-3.383014	0.572994
C	2.451071	-1.278759	-0.048932
H	2.986321	-2.122097	0.391966
H	1.859103	-0.766424	0.712653
C	3.393607	-0.367035	-0.757020
O	4.273286	0.237020	0.256917
C	5.511684	0.897991	-0.083799
H	5.344679	1.866275	-0.578758
H	4.017241	-0.865985	-1.503402
C	2.547586	0.700981	-1.378362
H	3.128184	1.526876	-1.795158
H	1.987250	1.187669	-0.577273
O	6.464966	0.139483	-0.908684
C	6.934008	-1.149434	-0.337542
C	7.843093	-1.845920	-1.232248
H	8.304402	-2.756909	-0.843324
H	8.636981	-1.219636	-1.645255
H	7.223930	-2.217725	-2.051099
H	6.066076	-1.809834	-0.259504
C	7.584280	-0.931165	1.099238
H	8.588196	-0.506406	1.019477
O	7.638548	-2.210991	1.751240
H	7.936282	-2.120432	2.674108
C	6.700338	-0.020380	2.018854
O	7.439102	0.264375	3.257121
H	7.828304	1.133195	3.052458
H	5.816955	-0.547978	2.387203
C	6.235176	1.212812	1.315372
O	7.401913	2.035754	1.065051
C	7.148468	3.401273	0.607282
H	6.414097	3.777933	1.324611
H	6.773533	3.279296	-0.412987
H	7.992701	4.088003	0.708283
H	5.510605	1.761314	1.923431

NMR-Shifts

Original-MandelalideA174ps-NMR.txt

Atom	Type	Isotropic	Scaled Shift
1	C	101.0743	81.3431535826
2	C	107.7258	74.976741515
3	C	152.5402	32.083117977
6	C	109.6884	73.0982599207
8	C	108.5597	74.178583051
14	C	13.9815	164.703095389
16	C	58.1000	122.475545091
18	C	33.1289	146.376366316
20	C	149.2504	35.2319148529
23	C	107.6067	75.0907368058
29	C	146.3044	38.0516472367
32	C	145.9615	38.3798503034
34	C	177.4283	8.26173931354
38	C	99.4164	82.9299948314
42	C	108.4931	74.2423285285
44	C	132.9883	50.7970098968
45	C	151.8278	32.7649840158
47	C	170.3876	15.0006699975
51	C	34.8582	144.721185321
53	C	36.5405	143.110989873
55	C	53.3973	126.976684087
57	C	51.3101	128.974425238
59	C	153.1517	31.4978272938
64	C	147.1029	37.287371504
67	C	113.5043	69.445912058
69	C	81.4239	100.151323724
72	C	150.3979	34.1335975038
76	C	108.1640	74.5573230728
77	C	173.8465	11.6900208656
82	C	104.5756	77.9919217443
86	C	105.8497	76.7724305595
90	C	97.9327	84.3501024139
92	C	125.3054	58.1506154406
4	H	30.1904	1.52663432663
5	H	30.3924	1.33998613999
7	H	26.3459	5.07895587896
10	H	26.8710	4.59376299376
11	H	27.8913	3.651004851
12	H	27.9968	3.55352275352
17	H	25.5946	5.77315777316
19	H	23.9942	7.25192885193
21	H	29.4490	2.21168861169
22	H	29.1062	2.52843612844
24	H	28.0291	3.52367752368
26	H	29.2374	2.40720720721
27	H	27.8875	3.65451605452
28	H	28.1338	3.42693462693
30	H	29.8546	1.83691383691
31	H	30.3961	1.33656733657
33	H	29.2283	2.41561561562
35	H	30.8200	0.944883344883
36	H	31.1079	0.678863478863
37	H	30.7513	1.00836220836
39	H	26.9657	4.50626010626
43	H	27.7778	3.75587895588
46	H	29.1352	2.50164010164
48	H	30.4258	1.30912450912
49	H	31.1848	0.607807807808
50	H	30.4277	1.30736890737
52	H	25.5527	5.81187341187
54	H	24.6681	6.62924462924
56	H	25.2021	6.13582813583
58	H	25.3754	5.9756987757
60	H	29.7802	1.90565950566
61	H	29.3850	2.27082467082
62	H	30.0262	1.67835527836
63	H	30.4750	1.26366366366
65	H	30.1826	1.53384153384
66	H	30.5082	1.23298683299
70	H	25.4649	5.893000693
71	H	27.8348	3.70321090321
73	H	29.8791	1.81427581428
74	H	30.8465	0.920397320397
78	H	29.9987	1.70376530377
79	H	30.8062	0.957634557635
80	H	30.4651	1.27281127281
81	H	27.5988	3.92127512128
83	H	28.1772	3.38683298683
85	H	29.5802	2.09045969046
88	H	29.5242	2.1422037422
89	H	27.5995	3.92062832063
93	H	28.4731	3.11342111342

94	H	27.5215	3.9927003927
95	H	27.8591	3.68075768076
96	H	28.1894	3.37556017556

Supporting Information: Original-MandelalideA176.log

Using Gaussian 09: AM64L-G09RevC.01 23-Sep-2011

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#mPW1pw91/6-311+G(2d,p) scf=(maxcycle=300,direct,tight) NMR density=current SCRF=(PCM,SOLVENT=Chloroform)

Pointgroup= C1 Stoichiometry= C33H52O11 C1[X(C33H52O11)]

#Atoms= 96

Charge = 0 Multiplicity = 1

SCF Energy= -2116.26295177

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Optimization incomplete.

Atomic Type	Coordinates (Angstroms) X	Y	Z
C	-6.506405	0.468704	1.120073
C	-5.231676	1.349303	1.028222
C	-5.485152	2.721027	0.285556
H	-6.307454	3.290506	0.724720
H	-5.845192	2.484975	-0.717694
C	-4.186950	3.517812	0.151334
H	-3.762274	3.624532	1.152458
C	-4.501486	4.944045	-0.357514
O	-3.442737	5.857965	-0.014676
H	-2.637327	5.340960	0.168766
H	-5.502438	5.307300	-0.113466
H	-4.552137	4.914071	-1.449425
O	-3.326545	2.666681	-0.619010
C	-2.045665	2.978425	-0.851918
O	-1.463362	3.970398	-0.533308
C	-1.366511	1.841401	-1.509285
H	-1.968806	0.951219	-1.683378
C	-0.089590	1.891216	-1.886300
H	0.551358	2.751542	-1.714027
C	0.618484	0.938858	-2.875763
H	1.252476	1.447842	-3.604222
H	-0.147826	0.394039	-3.431013
C	1.435782	-0.022759	-2.114822
H	1.954753	-0.567846	-2.907116
O	-4.841897	1.625569	2.320574
H	-4.743985	0.755218	2.746602
H	-4.450091	0.740920	0.566376
H	-7.296442	1.012196	1.645084
C	-7.011062	-0.088615	-0.257725
H	-7.776640	0.550506	-0.703204
H	-6.141769	-0.132604	-0.917064
C	-7.653219	-1.457859	0.179421
H	-8.702898	-1.322820	0.444919
C	-7.696686	-2.434127	-1.012379
H	-8.294405	-2.059027	-1.846713
H	-8.122251	-3.365392	-0.631150
H	-6.658452	-2.602293	-1.304385
C	-6.981842	-1.823921	1.518683
H	-7.787961	-2.034366	2.225952
O	-6.227236	-0.641911	1.961481
O	0.716347	-0.824266	-1.195627
C	1.533608	-1.918464	-0.646192
H	2.021431	-2.397079	-1.498299
C	0.571370	-2.916068	0.065202
C	-0.311271	-3.656674	-0.976466
H	-0.504349	-2.952844	-1.788065
C	0.389260	-4.864117	-1.534236
H	-0.089636	-5.226706	-2.445595
H	0.361967	-5.790694	-0.957409
H	1.389865	-4.627705	-1.902055
C	-1.642381	-4.090705	-0.333388
H	-1.711074	-5.031502	0.207330
C	-2.691135	-3.302461	-0.418422
H	-2.634144	-2.358659	-0.959202
C	-3.845785	-3.578300	0.278690
H	-3.944357	-4.605141	0.626005
C	-4.784357	-2.690513	0.594310
H	-4.719874	-1.648435	0.291714
C	-5.905364	-2.988847	1.496612
H	-6.382507	-3.943828	1.267190
H	-5.469682	-3.095244	2.492225
H	-0.004214	-2.371014	0.816071
H	1.219984	-3.638165	0.566519
C	2.448561	-1.186791	0.362886
H	2.894368	-1.972957	0.976293
H	1.920402	-0.518052	1.044459
C	3.431378	-0.319312	-0.477221
O	4.336024	0.428671	0.331983
C	5.548658	0.972704	-0.292467
H	5.254029	1.746379	-1.016072
H	3.970695	-0.937146	-1.200440
C	2.618463	0.674961	-1.337524
H	3.236106	1.314894	-1.970308
H	2.154641	1.393868	-0.658748
O	6.296132	-0.038346	-0.997964
C	6.641532	-1.249301	-0.167499
C	7.355917	-2.175813	-1.078777
H	7.813823	-2.978387	-0.496376
H	8.110398	-1.609894	-1.628382
H	6.704734	-2.623443	-1.832494
H	5.676898	-1.724818	0.027693
C	7.411612	-0.897027	1.120214
H	8.446880	-0.607296	0.924345
O	7.413659	-2.041168	1.968367
H	7.464601	-1.627125	2.848148
C	6.624429	0.241181	1.856612
O	7.323342	0.693667	3.064492
H	7.871540	1.383746	2.649663
H	5.705834	-0.290299	2.116993
C	6.358850	1.441587	0.931195
O	7.632769	1.927334	0.575816
C	7.619577	3.231401	-0.027708
H	7.173903	4.077452	0.500981
H	7.188622	3.147802	-1.028908
H	8.672901	3.520460	0.014487
H	5.788349	2.207890	1.462760

NMR-Shifts

Original-MandelalideA176ps-NMR.txt

Atom	Type	Isotropic	Scaled Shift
1	C	100.5862	81.8103332759
2	C	111.6087	71.260265319
3	C	148.6881	35.7701142824
6	C	110.0868	72.7169356228
8	C	117.1012	66.0031777025
14	C	19.2863	159.625662819
16	C	58.6396	121.959072723
18	C	27.5333	151.732134995
20	C	144.4167	39.8584390972
23	C	114.1886	68.7909416336
29	C	142.1723	42.0066425468
32	C	146.7480	37.6270602423

34	C	170.9654	14.4476349088
38	C	97.7052	84.5678516051
42	C	100.5972	81.7998047436
44	C	137.6163	46.3673692069
45	C	149.3294	35.156300848
47	C	172.2492	13.2188594728
51	C	42.3761	137.525507762
53	C	52.6304	127.710714217
55	C	52.6727	127.670227225
57	C	54.9023	125.536189437
59	C	150.3576	34.1721702177
64	C	144.7641	39.5259289037
67	C	115.7805	67.2672715787
69	C	85.5687	96.1841727445
72	C	146.2326	38.1203698386
76	C	108.5371	74.2002143992
77	C	171.0754	14.3423495856
82	C	109.8851	72.90999062
86	C	103.0589	79.4436149237
90	C	104.6046	77.9641647045
92	C	129.5246	54.1122532973
4	H	30.2127	1.50602910603
5	H	30.3539	1.37556017556
7	H	26.8677	4.59681219681
10	H	27.7156	3.81335181335
11	H	28.0425	3.5112959113
12	H	28.0108	3.54058674059
17	H	25.4048	5.94853314853
19	H	23.8987	7.34017094017
21	H	29.2835	2.36461076461
22	H	29.0092	2.61806421806
24	H	28.1820	3.3823977824
26	H	29.4090	2.24864864865
27	H	27.6753	3.85058905059
28	H	28.0897	3.46768306768
30	H	29.7690	1.91600831601
31	H	30.2551	1.46685146685
33	H	29.1643	2.47475167475
35	H	30.6227	1.12718872719
36	H	30.6378	1.11323631324
37	H	30.6731	1.08061908062
39	H	27.2318	4.26038346038
43	H	28.2540	3.31586971587
46	H	29.3058	2.34400554401
48	H	31.0405	0.741141141141
49	H	30.9932	0.784846384846
50	H	31.0139	0.76571956572
52	H	25.7699	5.61118041118
54	H	25.1768	6.15920535921
56	H	25.3792	5.97218757219
58	H	25.7344	5.64398244398
60	H	29.4005	2.2565026565
61	H	29.1267	2.50949410949
62	H	30.2425	1.47849387849
63	H	30.5703	1.17560637561
65	H	30.1062	1.60443520444
66	H	30.3243	1.40291060291
70	H	25.6962	5.67927927928
71	H	27.6797	3.84652344652
73	H	29.8320	1.8577962578
74	H	30.6034	1.14502194502
78	H	30.2992	1.4261030261
79	H	30.7562	1.00383460383
80	H	30.5659	1.17967197967
81	H	27.6560	3.86842226842
83	H	28.0908	3.46666666667
85	H	29.8126	1.87572187572
88	H	29.4124	2.24550704551
89	H	27.6272	3.89503349503
93	H	28.6735	2.92825132825
94	H	28.0665	3.48911988912
95	H	27.9974	3.55296835297
96	H	28.1733	3.39043659044

Supporting Information: Original-MandelalideA178.log

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 Using  Gaussian 09:  AM64L-G09RevC.01 23-Sep-2011
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 density=current SCRF=(PCM,SOLVENT=Chloroform)
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 Pointgroup= C1   Stoichiometry= C33H52O11   C1[X(C33H52O11)]
#Atoms= 96
 Charge = 0                Multiplicity = 1
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 SCF Energy= -2116.25508569
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 Optimization incomplete.


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     Atomic      Coordinates (Angstroms)
      Type      X                Y                Z
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      C      -6.358183      0.590335      1.056922
      C      -5.158488      1.566704      1.037330
      C      -5.329440      2.852987      0.212161
      H      -6.015471      3.519896      0.739356
      H      -5.671046      2.590616     -0.790849
      C      -3.938649      3.521901      0.002802
      H      -3.368603      3.658948      0.925218
      C      -4.069418      4.983635     -0.525834
      O      -2.862748      5.730039     -0.428497
      H      -2.180747      5.091049     -0.704601
      H      -4.771413      5.550469      0.092656
      H      -4.441862      4.986248     -1.553726
      O      -3.247301      2.604340     -0.912148
      C      -1.869381      2.711162     -1.071380
      O      -1.210917      3.623938     -0.670362
      C      -1.226906      1.595559     -1.882973
      H      -1.944857      0.835620     -2.188040
      C      -0.022477      1.799841     -2.385747
      H       0.594401      2.640262     -2.076664
      C       0.763642      0.811552     -3.238335
      H       1.377265      1.432854     -3.892429
      H       0.030208      0.217845     -3.787557
      C       1.615829     -0.186479     -2.435653
      H       2.328240     -0.727330     -3.064412
      O      -4.970210      2.058213      2.370596
      H      -5.476186      1.438898      2.926617
      H      -4.332833      0.961874      0.655263
      H      -7.269582      1.192295      1.096050
      C      -6.407082     -0.210969     -0.251240
      H      -6.946550      0.377856     -0.996818
      H      -5.447709     -0.648645     -0.536249
      C      -7.387509     -1.326043      0.219809
      H      -8.362686     -0.837552      0.172230
      C      -7.285960     -2.473763     -0.781846
      H      -7.191550     -2.020953     -1.770814
      H      -8.073587     -3.227862     -0.714823
      H      -6.351675     -3.013417     -0.618115
      C      -7.050575     -1.572664      1.748559
      H      -7.980327     -1.765745      2.289905
      O      -6.393866     -0.313442      2.160584
      O       0.845215     -1.173185     -1.759655
      C       1.533293     -2.144095     -0.856453
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H	2.027374	-2.903145	-1.467713
C	0.414908	-2.946227	-0.117428
C	-0.586075	-3.633795	-1.147366
H	-0.913763	-2.881690	-1.868966
C	0.144973	-4.895614	-1.853726
H	-0.463817	-5.520513	-2.510565
H	0.555073	-5.544326	-1.076744
H	1.013440	-4.658434	-2.471375
C	-1.831972	-4.083106	-0.379251
H	-1.895019	-5.162543	-0.269448
C	-2.785585	-3.228862	0.030905
H	-2.651606	-2.156321	-0.105232
C	-4.069757	-3.489162	0.727752
H	-4.523888	-4.458508	0.527096
C	-4.676132	-2.535003	1.408408
H	-4.222775	-1.552104	1.307588
C	-6.058734	-2.699450	2.073624
H	-6.522855	-3.655274	1.820412
H	-5.962287	-2.756775	3.160109
H	-0.196430	-2.161668	0.333295
H	0.820586	-3.640898	0.621173
C	2.426534	-1.418160	0.117551
H	3.058135	-2.133503	0.648845
H	1.789541	-1.000290	0.899807
C	3.246811	-0.402439	-0.630593
O	4.075986	0.249256	0.351079
C	5.287012	0.958114	-0.030410
H	5.011058	1.832190	-0.637309
H	3.803226	-0.930106	-1.409057
C	2.328869	0.616469	-1.331266
H	2.947081	1.375954	-1.813385
H	1.669882	1.148883	-0.643275
O	6.109959	0.105595	-0.833412
C	6.425679	-1.181901	-0.155638
C	7.124325	-2.112003	-1.224926
H	7.244685	-3.094436	-0.763900
H	8.126861	-1.742886	-1.447851
H	6.594138	-2.272967	-2.165864
H	5.506147	-1.684091	0.156204
C	7.238951	-0.882009	1.095084
H	8.206877	-0.486367	0.777374
O	7.543802	-2.041419	1.928928
H	7.819690	-1.587414	2.745117
C	6.589888	0.068711	1.990076
O	7.521286	0.432013	3.006300
H	7.910933	1.230154	2.606723
H	5.652215	-0.353989	2.359991
C	6.097261	1.399576	1.247168
O	7.288783	2.126739	0.925316
C	7.246094	3.554608	0.821011
H	7.108255	3.885164	1.853210
H	6.456522	3.835822	0.119711
H	8.192660	3.974842	0.469854
H	5.504270	1.928847	1.997552

NMR-Shifts

Original-MandelalideA178ps-NMR.txt

Atom	Type	Isotropic	Scaled Shift
1	C	102.9272	79.5696701698
2	C	110.9362	71.9039414996
3	C	144.0769	40.1836750321
6	C	100.2923	82.0916365168
8	C	113.2177	69.720228182
14	C	8.3364	170.106242463
16	C	60.9584	119.73965811
18	C	29.9049	149.462183426
20	C	147.3707	37.031049599
23	C	109.1882	73.5770209996
29	C	140.7597	43.3586975248
32	C	139.4461	44.615995712
34	C	173.3186	12.1952947032
38	C	97.9616	84.3224410881
42	C	104.6035	77.9652175578
44	C	131.6016	52.124274967
45	C	144.8300	39.4628534237
47	C	168.0502	17.2378874021
51	C	41.2544	138.599130918
53	C	46.9119	133.184115316
55	C	48.3535	131.804303298
57	C	48.8559	131.323436513
59	C	146.3734	37.9856046249
64	C	149.9450	34.5670858937
67	C	110.8772	71.9604127185
69	C	85.5671	96.1857041674
72	C	148.7963	35.66655181
76	C	111.9372	70.9458450583
77	C	167.8847	17.3962939566
82	C	111.4769	71.386416279
86	C	114.3532	68.6333965045
90	C	100.4803	81.911694328
92	C	127.5823	55.9713049637
4	H	29.9956	1.70662970663
5	H	30.1605	1.55426195426
7	H	26.4946	4.94155694156
10	H	27.0995	4.38262878263
11	H	28.1156	3.44375144375
12	H	27.9862	3.56331716332
17	H	25.4887	5.87100947101
19	H	23.9050	7.33434973435
21	H	29.1178	2.51771771772
22	H	29.2518	2.3939015939
24	H	27.9027	3.64047124047
26	H	29.1616	2.47724647725
27	H	27.9645	3.58336798337
28	H	28.1197	3.43996303996
30	H	29.5859	2.08519288519
31	H	30.2270	1.49281589282
33	H	29.2311	2.41302841303
35	H	30.8247	0.940540540541
36	H	30.8599	0.908015708016
37	H	30.3313	1.39644259644
39	H	27.2340	4.25835065835
43	H	27.7672	3.76567336567
46	H	28.6165	2.98091938092
48	H	30.8012	0.962254562255
49	H	31.2438	0.553291753292
50	H	30.6249	1.12515592516
52	H	25.6886	5.6863016863
54	H	25.1035	6.22693462693
56	H	25.2146	6.12427812428
58	H	25.4151	5.93901593902
60	H	29.7268	1.955001155
61	H	29.2712	2.37597597598
62	H	29.9812	1.71993531994
63	H	30.0775	1.63095403095
65	H	30.0459	1.66015246015
66	H	30.4385	1.29738969739
70	H	26.0817	5.32307692308
71	H	27.9913	3.5586047586
73	H	29.9717	1.72871332871
74	H	30.3419	1.38664818665
78	H	30.5804	1.16627396627
79	H	30.7774	0.984245784246
80	H	30.4390	1.29692769693
81	H	27.7962	3.73887733888
83	H	28.3257	3.24961884962
85	H	28.9139	2.70612150612
88	H	28.8237	2.78946638947

89	H	27.9668	3.58124278124
93	H	28.0420	3.51175791176
94	H	28.0565	3.49835989836
95	H	28.0116	3.53984753985
96	H	27.9776	3.57126357126

Supporting Information: Original-MandelalideA180.log

Using Gaussian 09: AM64L-G09RevC.01 23-Sep-2011

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#mPW1pw91/6-311+G(2d,p) scf=(maxcycle=300,direct,tight) NMR density=current SCRF=(PCM,SOLVENT=Chloroform)

Pointgroup= C1 Stoichiometry= C33H52O11 C1[X(C33H52O11)]

#Atoms= 96

Charge = 0 Multiplicity = 1

SCF Energy= -2116.24976844

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Optimization incomplete.

Atomic Type	Coordinates (Angstroms) X	Y	Z
C	-6.570060	0.720158	1.039683
C	-5.233148	1.431793	1.032418
C	-5.256911	2.599438	0.068675
H	-5.971619	3.351598	0.407652
H	-5.771180	2.271157	-0.836990
C	-3.906300	3.244998	-0.127059
H	-3.464511	3.508263	0.838336
C	-4.121691	4.633057	-0.838406
O	-2.967165	5.479829	-0.670876
H	-2.251616	4.824019	-0.584686
H	-4.956417	5.123217	-0.331756
H	-4.496248	4.639884	-1.865659
O	-3.035028	2.374144	-0.885016
C	-1.678491	2.654552	-1.030977
O	-1.096095	3.552764	-0.422946
C	-0.975608	1.752746	-1.991164
H	-1.658258	0.986505	-2.353092
C	0.291708	1.868604	-2.338084
H	0.900454	2.661145	-1.909833
C	1.046436	0.916392	-3.261160
H	1.672174	1.583631	-3.856701
H	0.330486	0.352489	-3.863976
C	1.877251	-0.206378	-2.585746
H	2.455837	-0.750271	-3.336601
O	-4.931138	1.842474	2.423081
H	-4.960828	1.060077	3.002248
H	-4.470491	0.786208	0.587968
H	-7.438107	1.315812	1.331465
C	-7.077027	-0.059865	-0.206135
H	-7.737500	0.524729	-0.849669
H	-6.297530	-0.617991	-0.729827
C	-7.940512	-1.152338	0.447021
H	-8.947672	-0.750052	0.575519
C	-8.069254	-2.441155	-0.467649
H	-8.573335	-2.143441	-1.389781
H	-8.637670	-3.298721	-0.100631
H	-7.050599	-2.719968	-0.743362
C	-7.323395	-1.448531	1.836016
H	-8.115871	-1.610053	2.572136
O	-6.609751	-0.226642	2.152522
O	0.951590	-1.112528	-1.920243
C	1.488073	-2.226612	-1.198128
H	1.986539	-2.984708	-1.808544
C	0.325571	-2.855122	-0.364281
C	-0.747986	-3.498129	-1.169375
H	-0.997715	-2.799383	-1.970516
C	-0.222891	-4.814668	-1.780961
H	-0.957885	-5.432665	-2.299954
H	0.153304	-5.498459	-1.017681
H	0.604627	-4.473903	-2.405090
C	-2.039791	-3.745215	-0.359486
H	-2.257657	-4.799748	-0.208883
C	-2.826959	-2.763191	0.146095
H	-2.553639	-1.713454	0.054484
C	-4.019986	-3.204968	0.829635
H	-4.231773	-4.271734	0.771186
C	-4.918808	-2.323850	1.307206
H	-4.676382	-1.269930	1.421568
C	-6.290803	-2.690332	1.816862
H	-6.711096	-3.563179	1.313603
H	-6.076901	-3.215644	2.750223
H	-0.087507	-2.106096	0.313761
H	0.870417	-3.562754	0.264488
C	2.543692	-1.635968	-0.207976
H	3.067109	-2.464088	0.275759
H	2.057680	-0.940089	0.479350
C	3.617551	-0.771464	-0.918690
O	4.291765	-0.158700	0.205703
C	5.427725	0.671465	0.042261
H	5.149214	1.556567	-0.549271
H	4.300640	-1.300097	-1.588972
C	2.885327	0.366884	-1.627205
H	3.658950	0.875781	-2.204902
H	2.379403	0.977295	-0.875526
O	6.441656	0.053223	-0.732711
C	7.123378	-1.085553	-0.138377
C	8.255443	-1.508703	-1.108521
H	9.249731	-1.079672	-0.971650
H	7.992401	-1.214902	-2.127052
H	8.383916	-2.591742	-1.160544
H	6.483275	-1.971951	-0.158035
C	7.734743	-0.550315	1.211370
H	8.339134	0.358116	1.134132
O	8.465039	-1.561386	1.856626
H	8.522721	-1.351974	2.806667
C	6.602690	-0.090558	2.124672
O	7.216306	0.174636	3.375907
H	7.370913	1.133020	3.454904
H	5.858234	-0.882472	2.242088
C	5.882087	1.159429	1.407393
O	6.737759	2.279895	1.301565
C	6.022073	3.547833	1.176410
H	5.039596	3.531472	1.655618
H	5.837240	3.720360	0.113232
H	6.573829	4.338043	1.691410
H	4.967919	1.351463	1.974469

NMR-Shifts

Original-MandelalideA180ps-NMR.txt

Atom	Type	Isotropic	Scaled Shift
1	C	97.4698	84.7931621968
2	C	114.3138	68.671107793
3	C	153.4125	31.2482053638
6	C	107.7371	74.9659258408
8	C	110.1008	72.7035356726
14	C	0.3682	177.732919849
16	C	59.9760	120.67995176
18	C	31.7425	147.703344245
20	C	145.7484	38.5838166887

23	C	108.8564	73.8945998201
29	C	145.2929	39.0197936408
32	C	141.2463	42.8929535405
34	C	167.0962	18.1509982963
38	C	101.4979	80.9377093742
42	C	111.2170	71.6351767836
44	C	136.0481	47.8683550604
45	C	155.4717	29.277264113
47	C	167.4377	17.8241352246
51	C	31.1354	148.284423515
53	C	46.5141	133.564865331
55	C	49.1096	131.080610272
57	C	50.2747	129.965447271
59	C	152.6942	31.9357185245
64	C	139.4274	44.633894217
67	C	113.6745	69.2830069488
69	C	92.1845	89.85193055
72	C	149.2493	35.2329677061
76	C	112.2110	70.6837803174
77	C	167.3639	17.8947721051
82	C	108.8870	73.8653113574
86	C	108.6875	74.0562606482
90	C	99.8595	82.5058864067
92	C	122.6554	60.687034591
4	H	30.1578	1.55675675676
5	H	30.0278	1.67687687688
7	H	25.9342	5.45936705937
10	H	26.6870	4.76377916378
11	H	28.3598	3.21811041811
12	H	27.7056	3.82259182259
17	H	25.5842	5.78276738277
19	H	24.1162	7.1392007392
21	H	29.1346	2.50219450219
22	H	28.9825	2.64273504274
24	H	28.3475	3.22947562948
26	H	28.9259	2.69503349503
27	H	27.3725	4.13037653038
28	H	26.9233	4.54543774544
30	H	29.4929	2.17112497112
31	H	30.6109	1.13809193809
33	H	28.9854	2.64005544006
35	H	30.8163	0.948302148302
36	H	30.7222	1.03525063525
37	H	31.1189	0.668699468699
39	H	27.1388	4.34631554632
43	H	27.9518	3.5951027951
46	H	29.2015	2.44037884038
48	H	30.7471	1.01224301224
49	H	31.3846	0.423192423192
50	H	30.2407	1.48015708016
52	H	25.4158	5.93836913837
54	H	24.7740	6.53139293139
56	H	25.1546	6.17971817972
58	H	25.0330	6.29207669208
60	H	29.5679	2.10182490182
61	H	28.9359	2.68579348579
62	H	30.2713	1.45188265188
63	H	30.6371	1.11388311388
65	H	29.8555	1.83608223608
66	H	30.6116	1.13744513745
70	H	26.1246	5.28343728344
71	H	27.7107	3.81787941788
73	H	29.2965	2.3525987526
74	H	30.4802	1.25885885886
78	H	30.4933	1.24675444675
79	H	30.8462	0.920674520675
80	H	30.4607	1.27687687688
81	H	27.3165	4.18212058212
83	H	27.9746	3.57403557404
85	H	28.8754	2.7416955417
88	H	30.1988	1.51887271887
89	H	28.1279	3.43238623239
93	H	28.7822	2.82781242781
94	H	27.6568	3.86768306768
95	H	27.7729	3.76040656041
96	H	28.2866	3.28574728575

Supporting Information: Original-MandelalideA182.log

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 Using  Gaussian 09:  AM64L-G09RevC.01 23-Sep-2011
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 density=current SCRF=(PCM,SOLVENT=Chloroform)
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#Atoms= 96
 Charge = 0                Multiplicity = 1
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 SCF Energy= -2116.25440502
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 Optimization incomplete.


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     Atomic      Coordinates (Angstroms)
      Type      X                Y              Z
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      C      -6.521689      0.348901      1.352375
      C      -5.128973      0.984390      0.943742
      C      -5.362411      2.321308      0.188263
      H      -6.059300      2.969188      0.723516
      H      -5.793015      2.058199     -0.780130
      C      -4.060410      3.178091     -0.007162
      H      -3.685768      3.287808      1.012913
      C      -4.350050      4.645075     -0.487405
      O      -3.422193      5.532935      0.199245
      H      -2.507833      5.220637      0.080634
      H      -5.377644      4.866699     -0.189641
      H      -4.249717      4.688528     -1.575410
      O      -3.069073      2.523936     -0.811675
      C      -1.864108      3.060153     -1.008742
      O      -1.438583      4.050293     -0.470197
      C      -0.992808      2.233808     -1.833536
      H      -1.409118      1.431363     -2.440682
      C       0.234681      2.605926     -2.063800
      H       0.591029      3.411196     -1.426166
      C       1.170650      1.843832     -2.927551
      H       2.020538      2.476815     -3.191438
      H       0.715753      1.641276     -3.898983
      C       1.834810      0.545165     -2.355451
      H       2.524305      0.121301     -3.090380
      O      -4.494268      1.304921      2.145532
      H      -4.872962      0.745135      2.846589
      H      -4.506748      0.355655      0.301795
      H      -7.163473      1.136198      1.754185
      C      -7.201081     -0.318952      0.170407
      H      -7.895085      0.344832     -0.350050
      H      -6.471135     -0.663214     -0.565023
      C      -7.921565     -1.554743      0.743642
      H      -8.927528     -1.294843      1.080992
      C      -8.019369     -2.545075     -0.400515
      H      -8.422940     -1.996569     -1.254023
      H      -8.783010     -3.300633     -0.206856
      H      -7.082811     -2.953088     -0.786810
      C      -6.991295     -1.937110      1.991374
      H      -7.691269     -2.131436      2.808415
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O	-6.332615	-0.693281	2.349462
O	0.858814	-0.369295	-1.948290
C	1.396249	-1.631168	-1.436593
H	1.955844	-2.184238	-2.194678
C	0.324113	-2.543243	-0.854007
C	-0.793529	-2.959428	-1.879529
H	-0.996512	-2.111490	-2.536905
C	-0.248212	-3.940344	-2.894849
H	-0.978366	-4.168921	-3.674393
H	0.167696	-4.846185	-2.449054
H	0.627742	-3.535742	-3.406760
C	-2.118959	-3.496127	-1.291963
H	-2.495523	-4.450160	-1.651433
C	-2.805390	-2.838542	-0.362121
H	-2.366475	-1.937254	0.062377
C	-4.043918	-3.343212	0.261174
H	-4.377021	-4.339203	-0.026356
C	-4.747430	-2.666016	1.234941
H	-4.296965	-1.716527	1.511992
C	-5.946085	-3.113259	1.930216
H	-6.416405	-3.890235	1.322500
H	-5.799004	-3.474772	2.950876
H	-0.184700	-2.028622	-0.036631
H	0.767934	-3.418468	-0.375968
C	2.449942	-1.312680	-0.310463
H	2.893794	-2.248254	0.038523
H	1.927441	-0.925933	0.567305
C	3.447338	-0.255015	-0.677917
O	4.251693	0.039520	0.524461
C	5.464276	0.853124	0.370339
H	5.184922	1.846036	-0.011914
H	4.113087	-0.423299	-1.528415
C	2.601296	0.937801	-1.114820
H	3.256970	1.806240	-1.206401
H	1.973377	1.163066	-0.250008
O	6.363422	0.202192	-0.638672
C	6.880830	-1.159271	-0.405481
C	7.855487	-1.610191	-1.540575
H	8.091393	-2.659739	-1.357845
H	8.739226	-0.984806	-1.686422
H	7.318628	-1.582385	-2.490897
H	6.027795	-1.837686	-0.320524
C	7.557173	-1.140517	1.024119
H	8.518710	-0.621988	0.994705
O	7.838585	-2.590131	1.286639
H	8.301778	-2.563878	2.143452
C	6.565039	-0.618655	2.052019
O	7.105655	-0.609600	3.433148
H	7.299487	0.325598	3.625227
H	5.604843	-1.129768	1.950911
C	6.208660	0.808952	1.697144
O	7.404239	1.581008	1.818323
C	7.232382	3.020890	1.487766
H	6.360696	3.352687	2.058068
H	7.053544	3.180265	0.421180
H	8.160834	3.573865	1.655070
H	5.453686	1.213570	2.374906

NMR-Shifts
Original-MandelalideA182ps-NMR.txt

Atom	Type	Isotropic	Scaled Shift
1	C	95.8910	86.3042937269
2	C	111.6914	71.1811098987
3	C	143.5627	40.6758360612
6	C	102.6516	79.8334577614
8	C	110.8517	71.9848197707
14	C	15.3348	163.407798771
16	C	56.4413	124.063152051
18	C	35.4533	144.151591723
20	C	150.6171	33.9237925688
23	C	112.1807	70.7127816382
29	C	142.4261	41.7637205919
32	C	138.1961	45.8124198396
34	C	172.9138	12.5827446927
38	C	99.0861	83.2461379429
42	C	109.7965	72.9947931622
44	C	143.5308	40.7063688049
45	C	155.2722	29.4682134038
47	C	168.1703	17.122934972
51	C	43.4504	136.49725301
53	C	46.8788	133.215796627
55	C	42.6618	137.252053064
57	C	42.9898	136.938111373
59	C	154.1202	30.5708378797
64	C	143.9241	40.3299259174
67	C	110.4638	72.3560941059
69	C	78.7150	102.744118379
72	C	145.6364	38.6910162905
76	C	104.8340	77.7445969486
77	C	169.4185	15.9282336951
82	C	101.3321	81.0964030705
86	C	109.7056	73.0817971248
90	C	105.2086	77.3860525661
92	C	125.5308	57.9348762419
4	H	30.4859	1.25359205359
5	H	30.1090	1.60184800185
7	H	26.5002	4.93638253638
10	H	25.1157	6.21566181566
11	H	28.2087	3.35772695773
12	H	27.9239	3.62088242088
17	H	25.5593	5.80577500578
19	H	23.9414	7.30071610072
21	H	29.6683	2.00905520906
22	H	29.2586	2.38761838762
24	H	28.1391	3.42203742204
26	H	28.9025	2.71665511666
27	H	27.9308	3.61450681451
28	H	28.0190	3.53300993301
30	H	29.8145	1.87396627397
31	H	30.6352	1.11563871564
33	H	28.9408	2.68126588127
35	H	30.9854	0.792053592054
36	H	30.7896	0.972972972973
37	H	30.7190	1.03820743821
39	H	27.0784	4.40212520213
43	H	27.8678	3.67271887272
46	H	29.1036	2.53083853084
48	H	30.5298	1.21302841303
49	H	31.2238	0.571771771772
50	H	30.7468	1.01252021252
52	H	25.7768	5.6048048048
54	H	24.9081	6.40748440748
56	H	25.2525	6.08925848926
58	H	25.2957	6.04934164934
60	H	29.2439	2.4012012012
61	H	29.0025	2.62425502426
62	H	29.9718	1.72862092862
63	H	30.5629	1.18244398244
65	H	30.1678	1.54751674752
66	H	30.5996	1.14853314853
70	H	25.5312	5.83173943174
71	H	27.5105	4.00286440286
73	H	29.8547	1.83682143682
74	H	31.0314	0.74954954955
78	H	30.0656	1.64194964195
79	H	30.5428	1.20101640102
80	H	30.6940	1.06130746131
81	H	27.7679	3.76502656503

83	H	27.4961	4.01617001617
85	H	30.0510	1.65544005544
88	H	29.4827	2.18054978055
89	H	27.1887	4.30020790021
93	H	28.5296	3.06121506122
94	H	28.2475	3.32187572188
95	H	28.0095	3.54178794179
96	H	28.1921	3.37306537307

Supporting Information: Original-MandelalideA184.log

Using Gaussian 09: AM64L-G09RevC.01 23-Sep-2011

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#Atoms= 96

Charge = 0 Multiplicity = 1

SCF Energy= -2116.22863251

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Optimization incomplete.

Atomic Type	Coordinates (Angstroms) X	Y	Z
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C	5.198329	1.201305	-1.073405
C	5.522675	2.321230	-0.066010
H	6.489674	2.801442	-0.226452
H	5.680236	1.916393	0.936359
C	4.288493	3.293885	-0.001628
H	3.773888	3.453452	-0.952212
C	4.773192	4.688135	0.376098
O	3.769343	5.682974	0.027295
H	2.854794	5.398036	0.203927
H	5.757307	4.931437	-0.031353
H	4.877802	4.776753	1.460307
O	3.325220	2.728727	0.960856
C	2.048353	3.101142	1.023047
O	1.602145	4.013729	0.401121
C	1.250687	2.191602	1.924269
H	1.767932	1.395744	2.457936
C	-0.022223	2.316197	2.084928
H	-0.554801	3.055886	1.492098
C	-0.905957	1.359349	2.943597
H	-1.609251	1.976284	3.505918
H	-0.327974	0.883228	3.738379
C	-1.790162	0.357646	2.199124
H	-2.446201	-0.166921	2.897980
O	5.023293	1.776511	-2.386068
H	5.220994	0.975577	-2.903914
H	4.320902	0.616390	-0.786028
H	7.210413	0.926368	-1.350057
C	6.560166	-0.546541	0.123429
H	7.027980	0.094870	0.873825
H	5.642469	-0.973599	0.534864
C	7.549672	-1.681501	-0.322332
H	8.513387	-1.179135	-0.430616
C	7.764362	-2.865983	0.528014
H	8.140111	-2.565994	1.508288
H	8.418578	-3.554563	-0.010631
H	6.840568	-3.436142	0.645593
C	7.066374	-1.900511	-1.763918
H	7.872700	-2.103488	-2.472906
O	6.380468	-0.735381	-2.236599
O	-0.972279	-0.500339	1.416075
C	-1.578484	-1.684117	0.825698
H	-2.302950	-2.243289	1.422115
C	-0.452169	-2.668347	0.481170
C	0.549750	-2.996328	1.628046
H	0.811232	-2.070002	2.144611
C	-0.097289	-4.027644	2.668793
H	0.471110	-4.035104	3.600687
H	-0.006711	-5.061505	2.328794
H	-1.059267	-3.768660	3.116252
C	1.925619	-3.562214	1.124600
H	2.342849	-4.345806	1.751670
C	2.689205	-3.045685	0.098724
H	2.241826	-2.209863	-0.437526
C	4.010716	-3.362718	-0.370887
H	4.529418	-4.075596	0.267931
C	4.606961	-2.832519	-1.485502
H	4.069264	-2.027779	-1.981259
C	6.056639	-3.131193	-1.946058
H	6.445603	-3.997730	-1.406614
H	5.887587	-3.292006	-3.013038
H	0.101068	-2.231708	-0.353539
H	-0.917454	-3.616229	0.202807
C	-2.188950	-1.064994	-0.417482
H	-2.476824	-1.961811	-0.969526
H	-1.489997	-0.512341	-1.047612
C	-3.255353	-0.158735	0.277977
O	-4.230680	0.412995	-0.641193
C	-5.488906	0.891624	-0.189354
H	-5.338264	1.872151	0.286477
H	-3.870981	-0.775878	0.937753
C	-2.670800	0.976738	1.105575
H	-3.414410	1.582417	1.628149
H	-2.049139	1.618156	0.477743
O	-6.081963	0.112674	0.916131
C	-6.519155	-1.243335	0.447184
C	-7.089796	-1.869267	1.709362
H	-7.442554	-2.840627	1.354648
H	-7.811866	-1.202099	2.184019
H	-6.241127	-2.035254	2.377334
H	-5.650216	-1.813267	0.108790
C	-7.564366	-1.165805	-0.749905
H	-8.519328	-0.710100	-0.478388
O	-7.733279	-2.480780	-1.374152
H	-7.930347	-2.309155	-2.312971
C	-6.916473	-0.328961	-1.864009
O	-7.864375	-0.250501	-2.949380
H	-8.576086	0.391992	-2.777446
H	-6.032930	-0.865045	-2.220708
C	-6.461281	1.040905	-1.395402
O	-7.724104	1.772374	-1.024186
C	-7.843816	3.027715	-1.496753
H	-8.293076	3.182381	-2.481846
H	-6.888945	3.558306	-1.476548
H	-8.452983	3.504745	-0.724910
H	-5.998272	1.616687	-2.200980

NMR-Shifts

Original-MandelalideA184ps-NMR.txt

Atom	Type	Isotropic	Scaled Shift
1	C	96.3988	85.8182583893
2	C	110.5900	72.235303126
3	C	146.0871	38.2596336071
6	C	101.6266	80.814525546
8	C	112.6382	70.2748904075
14	C	18.1516	160.711728785
16	C	60.0918	120.569115029

18	C	39.8049	139.986504336
20	C	148.3661	36.0783131377
23	C	109.9608	72.8375351749
29	C	150.3517	34.1778173395
32	C	147.5054	36.902122935
34	C	175.4204	10.1835793181
38	C	101.1563	81.2646681598
42	C	107.3595	75.3273416413
44	C	142.2006	41.9795555045
45	C	147.2718	37.1257106759
47	C	169.1827	16.1539271426
51	C	36.3757	143.26872643
53	C	46.7786	133.311701985
55	C	47.1637	132.94310764
57	C	38.4029	141.328413637
59	C	145.1900	39.1182832749
64	C	143.8142	40.4351155267
67	C	106.3919	76.25346963
69	C	83.9747	97.709852792
72	C	149.6598	34.8400620226
76	C	102.5402	79.9400830797
77	C	168.7045	16.6116311568
82	C	105.8131	76.807461858
86	C	107.7341	74.9687972588
90	C	91.1430	90.8487911331
92	C	132.4151	51.3456421448
4	H	30.1675	1.54779394779
5	H	30.0404	1.66523446523
7	H	26.2090	5.20545160545
10	H	27.7172	3.81187341187
11	H	28.0807	3.475999076
12	H	27.6417	3.88163548164
17	H	25.6848	5.68981288981
19	H	24.6269	6.66731346731
21	H	29.6350	2.03982443982
22	H	29.4360	2.2237006237
24	H	28.1618	3.40106260106
26	H	29.4321	2.2273042273
27	H	28.1169	3.44255024255
28	H	27.8237	3.71346731347
30	H	30.2726	1.45068145068
31	H	30.3320	1.3957957958
33	H	29.4156	2.24255024255
35	H	30.4326	1.30284130284
36	H	30.5860	1.1610995611
37	H	30.8269	0.938507738508
39	H	27.4013	4.10376530377
43	H	28.2659	3.30487410487
46	H	28.7073	2.89702009702
48	H	30.6736	1.08015708016
49	H	30.9827	0.794548394548
50	H	30.6738	1.07997227997
52	H	25.7908	5.59186879187
54	H	25.1295	6.20291060291
56	H	25.1433	6.19015939016
58	H	25.2856	6.05867405867
60	H	29.2605	2.38586278586
61	H	28.9991	2.6273966274
62	H	29.8732	1.81972741973
63	H	30.3280	1.39949179949
65	H	29.8096	1.87849387849
66	H	30.0776	1.63086163086
70	H	26.1432	5.26625086625
71	H	27.2899	4.2066990067
73	H	29.5576	2.11134211134
74	H	30.1616	1.55324555325
78	H	30.2713	1.45188265188
79	H	30.5183	1.22365442365
80	H	30.4537	1.28334488334
81	H	28.0586	3.49641949642
83	H	28.1520	3.41011781012
85	H	28.8371	2.77708477708
88	H	29.8933	1.80115500116
89	H	27.9526	3.59436359436
93	H	28.3291	3.24647724648
94	H	28.4641	3.12173712174
95	H	27.8670	3.67345807346
96	H	28.1110	3.448001848

Supporting Information: Original-MandelalideA186.log

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 Using  Gaussian 09:  AM64L-G09RevC.01 23-Sep-2011
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#Atoms= 96
 Charge = 0                Multiplicity = 1
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 SCF Energy= -2116.24319866
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 Optimization incomplete.


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      Type      X              Y              Z
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      C      -5.601248      1.485002      1.059779
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      H      -6.576438      2.981900     -0.243427
      H      -5.706359      1.733988     -1.162589
      C      -4.409277      3.238679     -0.294241
      H      -4.064523      3.443249      0.722910
      C      -4.618880      4.525797     -1.046475
      O      -3.637504      5.474106     -0.663329
      H      -2.843884      4.921698     -0.544419
      H      -5.576210      5.009855     -0.833643
      H      -4.481992      4.252500     -2.095535
      O      -3.404269      2.387285     -0.885727
      C      -2.153957      2.732711     -0.917755
      O      -1.791940      3.644714     -0.230596
      C      -1.392823      1.822163     -1.785493
      H      -1.990142      1.049964     -2.267954
      C      -0.089847      1.895043     -1.998505
      H       0.518401      2.637573     -1.488236
      C       0.636087      0.992760     -2.942340
      H       1.180519      1.617577     -3.654087
      H      -0.145517      0.450646     -3.478334
      C       1.593668      0.010734     -2.172591
      H       2.157138     -0.510544     -2.949760
      O      -5.730221      2.454613      2.198091
      H      -5.763951      1.823542      2.938661
      H      -4.625436      1.013576      1.199141
      H      -7.715607      0.951771      0.956097
      C      -6.504625     -0.518118     -0.135543
      H      -6.802179     -0.041639     -1.072693
      H      -5.472654     -0.830162     -0.309864
      C      -7.416741     -1.724046      0.289515
      H      -8.428256     -1.325393      0.186727
      C      -7.289883     -3.031616     -0.462434
      H      -7.469380     -2.875017     -1.528280
      H      -7.982384     -3.771869     -0.057103
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C	-7.043488	-1.778504	1.786606
H	-7.965497	-2.051238	2.306550
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O	0.818717	-0.949790	-1.331571
C	1.568813	-2.070731	-0.837827
H	1.936170	-2.693320	-1.658643
C	0.611405	-3.029178	-0.209280
C	-0.575753	-3.395625	-1.175082
H	-0.808681	-2.562074	-1.840623
C	-0.167274	-4.547721	-2.205895
H	-0.945734	-4.808320	-2.926650
H	0.313762	-5.304086	-1.582868
H	0.678870	-4.300550	-2.851140
C	-1.858215	-3.821171	-0.449078
H	-2.125286	-4.874494	-0.428694
C	-2.748244	-2.862275	0.001554
H	-2.473255	-1.809254	-0.036470
C	-3.927976	-3.250124	0.672137
H	-4.206504	-4.297144	0.569576
C	-4.548676	-2.416949	1.479376
H	-4.241279	-1.376607	1.544332
C	-5.807808	-2.650498	2.207807
H	-6.001298	-3.724011	2.147744
H	-5.625732	-2.491867	3.273099
H	0.124315	-2.504185	0.615448
H	1.028391	-3.949968	0.204690
C	2.795615	-1.523295	-0.082553
H	3.447379	-2.368058	0.149999
H	2.470107	-1.281805	0.931216
C	3.609427	-0.332209	-0.748049
O	4.442460	0.166365	0.389178
C	5.556587	0.989953	-0.047007
H	5.296239	1.975465	-0.461246
H	4.237320	-0.751115	-1.538403
C	2.569683	0.704579	-1.166907
H	3.080887	1.453385	-1.775346
H	2.046163	1.129756	-0.307848
O	6.387279	0.242062	-0.994801
C	7.140961	-0.920264	-0.482070
C	8.009240	-1.617713	-1.496501
H	8.615505	-2.413038	-1.058581
H	8.731663	-0.991771	-2.024877
H	7.390064	-2.131506	-2.234872
H	6.376533	-1.685490	-0.324432
C	7.790297	-0.744726	0.859775
H	8.664639	-0.099530	0.740455
O	8.196590	-1.980050	1.519741
H	8.443723	-1.767933	2.437196
C	6.859758	0.007928	1.824950
O	7.437842	0.243002	3.132419
H	8.208065	0.838188	3.103254
H	6.022690	-0.653843	2.063221
C	6.305596	1.282263	1.280681
O	7.366033	2.218866	1.017604
C	7.084138	3.572449	1.551177
H	6.977735	3.534332	2.638478
H	6.137307	4.006467	1.220990
H	7.937936	4.206755	1.302920
H	5.592520	1.718344	1.984925

NMR-Shifts
Original-MandelalideA186ps-NMR.txt

Atom	Type	Isotropic	Scaled Shift
1	C	99.4217	82.9249219931
2	C	99.6257	82.7296655755
3	C	143.1080	41.1110473018
6	C	106.3954	76.2501196424
8	C	114.7343	68.2686307165
14	C	17.0870	161.730699286
16	C	60.2844	120.384769999
18	C	29.8959	149.47079768
20	C	143.5323	40.704933096
23	C	100.7151	81.6869580199
29	C	142.7486	41.455043167
32	C	144.2896	39.9800915025
34	C	177.8999	7.81035241869
38	C	93.2174	88.8633013649
42	C	115.3705	67.6596986925
44	C	142.8453	41.3624877965
45	C	148.0239	36.4058462069
47	C	167.5118	17.7532112024
51	C	30.2019	149.177913053
53	C	38.5098	141.226095446
55	C	52.7850	127.562740481
57	C	53.4218	126.953234174
59	C	150.2631	34.2626198817
64	C	148.8943	35.5727521583
67	C	107.6560	75.0435498382
69	C	80.1157	101.403453359
72	C	149.7769	34.7279810104
76	C	117.1366	65.9692949712
77	C	173.0061	12.4944007351
82	C	113.6497	69.3067440035
86	C	108.6366	74.1049790386
90	C	100.2642	82.1185321312
92	C	120.5290	62.7222956029
4	H	30.2689	1.4541002541
5	H	29.8769	1.81630861631
7	H	25.9947	5.40346500347
10	H	26.5890	4.85433125433
11	H	27.8642	3.67604527605
12	H	27.8711	3.66966966967
17	H	25.3093	6.03677523678
19	H	24.2097	7.05280665281
21	H	29.2794	2.3683991684
22	H	29.0638	2.56761376761
24	H	28.1270	3.43321783322
26	H	29.7281	1.9537999538
27	H	27.4568	4.05248325248
28	H	27.9731	3.57542157542
30	H	30.3280	1.39949179949
31	H	29.8279	1.86158466158
33	H	29.5883	2.08297528298
35	H	30.9544	0.820697620698
36	H	30.9910	0.786879186879
37	H	30.4772	1.26163086163
39	H	27.0709	4.40905520906
43	H	28.1216	3.43820743821
46	H	28.4588	3.12663432663
48	H	30.4731	1.26541926542
49	H	30.8884	0.881681681682
50	H	30.7857	0.976576576577
52	H	25.3611	5.98891198891
54	H	24.5440	6.74391314391
56	H	25.2813	6.06264726265
58	H	25.9510	5.44384384384
60	H	29.7807	1.9051975052
61	H	29.5467	2.12141372141
62	H	30.5686	1.17717717718
63	H	30.3960	1.33665973666
65	H	30.4313	1.30404250404
66	H	30.7350	1.02342342342
70	H	26.0728	5.3313005313
71	H	27.0348	4.44241164241
73	H	29.6468	2.02892122892
74	H	29.9806	1.72048972049
78	H	30.2821	1.4419034419
79	H	30.8736	0.895356895357

80	H	30.5199	1.22217602218
81	H	27.8254	3.7118965119
83	H	28.2862	3.28611688612
85	H	29.0291	2.59967659968
88	H	30.1868	1.52996072996
89	H	27.7623	3.7702009702
93	H	28.4683	3.11785631786
94	H	28.3484	3.22864402864
95	H	28.1285	3.43183183183
96	H	28.1828	3.38165858166

Supporting Information: Original-MandelalideA188.log

Using Gaussian 09: AM64L-G09RevC.01 23-Sep-2011

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#Atoms= 96

Charge = 0 Multiplicity = 1

SCF Energy= -2116.26204867

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Optimization incomplete.

Atomic Type	Coordinates (Angstroms) X	Y	Z
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C	-5.674760	1.190888	1.249383
C	-5.919320	2.298421	0.205890
H	-6.846867	2.815606	0.460115
H	-6.062427	1.881017	-0.793124
C	-4.683322	3.245228	0.050301
H	-4.185530	3.421925	1.007493
C	-5.017099	4.486892	-0.839268
O	-3.890578	5.468487	-0.802512
H	-3.058432	5.031138	-0.548135
H	-5.993313	4.890050	-0.557039
H	-5.004227	4.135475	-1.873588
O	-3.653087	2.351227	-0.643747
C	-2.349804	2.726872	-0.698372
O	-1.970496	3.681040	-0.062280
C	-1.470023	1.872955	-1.633288
H	-1.960995	1.098340	-2.220044
C	-0.196427	2.262655	-1.729688
H	0.143639	3.090809	-1.113377
C	0.792527	1.748961	-2.722353
H	1.387644	2.606987	-3.040678
H	0.300163	1.445176	-3.648559
C	1.717428	0.626877	-2.248917
H	2.313898	0.350175	-3.121486
O	-5.652962	1.810265	2.576646
H	-5.561686	1.061315	3.193013
H	-4.706876	0.704293	1.103755
H	-7.688353	0.608425	1.803445
C	-7.233422	-0.573817	0.071991
H	-7.973754	0.052199	-0.430708
H	-6.382460	-0.695014	-0.600815
C	-7.654983	-1.951679	0.461567
H	-8.714531	-1.975459	0.726187
C	-7.426844	-2.988286	-0.709784
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H	-6.453011	-2.939959	-1.202878
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H	-7.430531	-2.606158	2.611231
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C	-0.341968	-3.190634	-1.635186
H	-0.726703	-2.402423	-2.286414
C	0.278320	-4.157417	-2.651467
H	-0.389246	-4.754618	-3.276660
H	0.877426	-4.892147	-2.109500
H	0.978757	-3.702950	-3.355472
C	-1.540991	-3.703566	-0.928988
H	-1.538171	-4.786962	-0.832447
C	-2.461519	-2.906636	-0.306690
H	-2.380997	-1.823854	-0.394347
C	-3.636920	-3.337419	0.433489
H	-3.735991	-4.422009	0.411632
C	-4.518284	-2.501012	0.941605
H	-4.443428	-1.417108	0.907379
C	-5.625333	-3.017962	1.785809
H	-5.900349	-4.028089	1.475116
H	-5.286455	-3.241206	2.800061
H	0.036283	-1.955185	0.162753
H	1.103818	-3.339537	-0.007724
C	2.794764	-1.321879	-0.372654
H	3.389833	-2.231682	-0.262557
H	2.350678	-1.029184	0.581281
C	3.603684	-0.149488	-0.793054
O	4.396049	0.186103	0.388741
C	5.636931	0.772647	0.044155
H	5.350047	1.615714	-0.601706
H	4.297116	-0.497978	-1.562535
C	2.785600	1.141291	-1.156368
H	3.407307	1.922404	-1.597605
H	2.304626	1.507117	-0.246886
O	6.490740	-0.008940	-0.801190
C	7.053283	-1.200640	-0.208430
C	8.026965	-1.787588	-1.197993
H	8.428143	-2.694130	-0.740892
H	8.900847	-1.139985	-1.287653
H	7.598970	-1.937920	-2.190597
H	6.292466	-1.923896	0.095524
C	7.756110	-0.945692	1.152769
H	8.692623	-0.401432	1.006373
O	8.006319	-2.168271	1.872451
H	8.060566	-1.989542	2.828012
C	6.827274	-0.046406	2.040764
O	7.336024	0.282760	3.285644
H	8.005194	0.979910	3.162943
H	5.895338	-0.591454	2.212365
C	6.370577	1.232678	1.318215
O	7.634029	1.894315	1.027337
C	7.335057	3.307221	0.928106
H	7.391349	3.840143	1.880562
H	6.339348	3.603820	0.585379
H	8.065854	3.838540	0.313224
H	5.718350	1.947219	1.827208

NMR-Shifts

Original-MandelalideA188ps-NMR.txt

Atom	Type	Isotropic	Scaled Shift
1	C	95.2926	86.8770458853
2	C	108.5377	74.1996401156
3	C	150.6415	33.9004383698
6	C	93.5945	88.5023641341
8	C	107.6174	75.0804954153

14	C	6.7187	171.654606711
16	C	53.7281	126.660062405
18	C	30.5876	148.808744425
20	C	150.1074	34.411646471
23	C	105.8641	76.7586477536
29	C	151.1201	33.4423514998
32	C	145.2781	39.0339593024
34	C	167.5202	17.7451712322
38	C	102.2811	80.1880778729
42	C	116.7140	66.3737820402
44	C	133.7458	50.0719768755
45	C	154.9885	29.7397538238
47	C	172.8628	12.6315587971
51	C	38.1398	141.580236988
53	C	44.7343	135.26838186
55	C	52.9369	127.417351021
57	C	57.0182	123.510978388
59	C	148.3178	36.124542966
64	C	146.2207	38.1317597963
67	C	112.1103	70.7801642451
69	C	89.5000	92.4213710063
72	C	145.8482	38.4882941863
76	C	114.0966	68.8789984494
77	C	168.8826	16.4411646471
82	C	105.3731	77.2286031509
86	C	114.0926	68.8828270066
90	C	95.2553	86.9127471812
92	C	127.9772	55.5933306533
4	H	30.1667	1.54853314853
5	H	30.0948	1.61496881497
7	H	25.3389	6.00942480942
10	H	27.8688	3.67179487179
11	H	27.8258	3.71152691153
12	H	27.3159	4.18267498267
17	H	25.0475	6.27867867868
19	H	23.8602	7.37574497574
21	H	29.5873	2.0838992839
22	H	29.0053	2.62166782167
24	H	28.1513	3.41076461076
26	H	29.3836	2.27211827212
27	H	27.3631	4.13906213906
28	H	27.5777	3.94077154077
30	H	29.9672	1.73287133287
31	H	30.5797	1.16692076692
33	H	29.2371	2.40748440748
35	H	30.6326	1.11804111804
36	H	30.5399	1.2036960037
37	H	30.9539	0.82115962116
39	H	27.3072	4.19071379071
43	H	28.3104	3.26375606376
46	H	28.8964	2.72229152229
48	H	30.7486	1.01085701086
49	H	31.3696	0.437052437052
50	H	30.8301	0.935550935551
52	H	25.6342	5.73656733657
54	H	25.2621	6.08038808039
56	H	25.2695	6.07355047355
58	H	25.2209	6.11845691846
60	H	29.6552	2.02115962116
61	H	29.1478	2.48999769
62	H	30.4872	1.25239085239
63	H	30.3652	1.36511896512
65	H	29.8780	1.81529221529
66	H	30.7146	1.04227304227
70	H	26.4831	4.95218295218
71	H	27.0547	4.42402402402
73	H	29.4458	2.21464541465
74	H	30.4807	1.2583968584
78	H	30.4007	1.33231693232
79	H	30.8380	0.928251328251
80	H	30.5543	1.19039039039
81	H	28.2671	3.30376530377
83	H	28.3118	3.26246246246
85	H	29.3714	2.28339108339
88	H	29.9255	1.7714021714
89	H	28.2157	3.35125895126
93	H	28.5910	3.00448140448
94	H	28.8247	2.78854238854
95	H	28.5680	3.02573342573
96	H	28.1235	3.43645183645

Supporting Information: Original-MandelalideA190.log

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 density=current SCRF=(PCM,SOLVENT=Chloroform)
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#Atoms= 96
 Charge = 0                Multiplicity = 1
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 SCF Energy= -2116.23453148
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 Optimization incomplete.


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      Type      X              Y              Z
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      C      -6.865353      0.097995      1.024724
      C      -5.718513      1.124138      1.053288
      C      -5.927266      2.470196      0.277613
      H      -6.737544      3.016193      0.765581
      H      -6.334581      2.255691     -0.712080
      C      -4.591815      3.355871      0.129722
      H      -4.391331      3.631727      1.168092
      C      -4.878180      4.655042     -0.675810
      O      -3.934513      5.708921     -0.327121
      H      -3.018959      5.382919     -0.386475
      H      -5.937291      4.904812     -0.570833
      H      -4.676061      4.410246     -1.721483
      O      -3.413349      2.628828     -0.443290
      C      -2.164662      3.137327     -0.520535
      O      -1.875889      4.241388     -0.091399
      C      -1.268667      2.286425     -1.313146
      H      -1.659981      1.399122     -1.808622
      C      -0.003377      2.659150     -1.519309
      H       0.389379      3.578972     -1.095896
      C       0.903811      1.950094     -2.535092
      H       1.495595      2.713701     -3.043799
      H       0.371986      1.537410     -3.394575
      C       1.760985      0.787903     -2.085116
      H       2.365359      0.417873     -2.918000
      O      -5.356479      1.389984      2.395277
      H      -5.155202      0.539227      2.825063
      H      -4.863306      0.670524      0.544630
      H      -7.804120      0.602919      1.266375
      C      -6.945990     -0.704512     -0.290144
      H      -7.450851     -0.251225     -1.145263
      H      -5.911990     -0.907735     -0.576965
      C      -7.615500     -2.003035      0.071934
      H      -8.696125     -1.911567     -0.054367
      C      -7.259677     -3.160632     -0.949508
      H      -7.609002     -2.848469     -1.936106
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H	-7.722919	-4.122809	-0.722202
H	-6.173706	-3.161627	-1.070040
C	-7.159407	-2.302551	1.518510
H	-8.006191	-2.571533	2.154959
O	-6.721922	-0.961289	2.020518
O	0.917505	-0.290473	-1.660907
C	1.494007	-1.568707	-1.227438
H	1.911228	-2.062779	-2.108652
C	0.440218	-2.438525	-0.547487
C	-0.574343	-2.953151	-1.549000
H	-1.069045	-2.096245	-2.012229
C	0.078084	-3.879653	-2.586969
H	-0.683651	-4.422798	-3.150873
H	0.795889	-4.551634	-2.113655
H	0.594988	-3.275000	-3.335171
C	-1.734391	-3.586832	-0.787706
H	-2.039893	-4.579131	-1.110737
C	-2.508705	-2.956152	0.136588
H	-2.302245	-1.924483	0.419704
C	-3.744230	-3.455340	0.731196
H	-3.843578	-4.537111	0.658670
C	-4.655309	-2.747752	1.277329
H	-4.544781	-1.681917	1.458619
C	-6.014550	-3.280112	1.760968
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H	-5.908955	-3.251348	2.847913
H	-0.029693	-1.844176	0.238870
H	0.915079	-3.332475	-0.138655
C	2.641431	-1.335113	-0.216069
H	3.042814	-2.339687	-0.067233
H	2.125057	-1.044766	0.701722
C	3.610751	-0.210177	-0.580669
O	4.404676	0.204302	0.516272
C	5.685590	0.884089	0.223188
H	5.552694	1.916674	-0.132112
H	4.154884	-0.584137	-1.451335
C	2.771162	1.062773	-0.970362
H	3.560390	1.723579	-1.335465
H	2.217104	1.573411	-0.179715
O	6.328524	0.111462	-0.855875
C	6.798421	-1.235314	-0.577207
C	7.623235	-1.563601	-1.803093
H	7.432830	-2.552818	-2.224744
H	8.661032	-1.537286	-1.463743
H	7.416011	-0.934045	-2.671001
H	5.994757	-1.956189	-0.409304
C	7.614231	-1.245265	0.739880
H	8.529576	-0.676669	0.555103
O	8.056145	-2.562831	1.075060
H	8.540556	-2.456277	1.913137
C	7.027410	-0.542367	1.922745
O	8.103998	-0.353021	2.932559
H	8.631525	0.367875	2.543251
H	6.245215	-1.213287	2.286051
C	6.494302	0.897885	1.551879
O	7.655353	1.819132	1.463135
C	7.435971	3.266433	1.384180
H	6.884229	3.624515	2.257089
H	6.869370	3.383420	0.457298
H	8.416963	3.745104	1.426146
H	5.866237	1.283311	2.359005

NMR-Shifts
Original-MandelalideA190ps-NMR.txt

Atom	Type	Isotropic	Scaled Shift
1	C	103.3259	79.1880587301
2	C	111.8511	71.0282547522
3	C	146.3621	37.996420299
6	C	95.3708	86.8021975918
8	C	112.1696	70.7234058845
14	C	10.7541	167.792166772
16	C	52.5685	127.76996114
18	C	27.5267	151.738452114
20	C	150.2801	34.2463485136
23	C	111.1994	71.6520224353
29	C	144.2375	40.0299584602
32	C	146.2460	38.107544172
34	C	168.5017	16.8057390073
38	C	97.3370	84.9202702961
42	C	109.1116	73.6503378702
44	C	137.3528	46.619575413
45	C	154.6251	30.0875782461
47	C	167.9746	17.3102471334
51	C	36.4501	143.197515266
53	C	47.0553	133.04686154
55	C	60.2964	120.373284328
57	C	61.0199	119.680794043
59	C	150.6957	33.8485614196
64	C	145.5741	38.750646069
67	C	117.0853	66.0183962174
69	C	81.2272	100.339593024
72	C	149.3404	35.1457723157
76	C	116.6779	66.408334769
77	C	167.3303	17.9269319857
82	C	104.7138	77.8596450927
86	C	108.8472	73.9034055016
90	C	100.4118	81.9772583702
92	C	125.2212	58.2312065698
4	H	30.0050	1.69794409794
5	H	30.0455	1.66052206052
7	H	26.0271	5.37352737353
10	H	25.6480	5.72381612382
11	H	28.1361	3.42480942481
12	H	27.5787	3.93984753985
17	H	25.0021	6.32062832063
19	H	23.8281	7.40540540541
21	H	29.5054	2.15957495957
22	H	29.1405	2.49674289674
24	H	28.2085	3.35791175791
26	H	29.5394	2.12815892816
27	H	27.7423	3.78868098868
28	H	28.1443	3.41723261723
30	H	29.9339	1.76364056364
31	H	30.5787	1.16784476784
33	H	29.2143	2.42855162855
35	H	30.9859	0.791591591592
36	H	30.6303	1.12016632017
37	H	30.8350	0.931023331023
39	H	26.9635	4.50829290829
43	H	27.9454	3.60101640102
46	H	29.0072	2.61991221991
48	H	30.4420	1.29415569416
49	H	31.1509	0.639131439131
50	H	30.3648	1.36548856549
52	H	25.9456	5.44883344883
54	H	25.3076	6.03834603835
56	H	25.6675	5.7057981058
58	H	25.3073	6.03862323862
60	H	29.5979	2.0741048741
61	H	29.2852	2.36303996304
62	H	29.7465	1.9367983368
63	H	30.4066	1.32686532687
65	H	30.2980	1.42721182721
66	H	30.6412	1.11009471009
70	H	25.6771	5.69692769693
71	H	27.6017	3.9185955186
73	H	29.8480	1.84301224301
74	H	30.6820	1.0723954724

78	H	30.2683	1.45465465465
79	H	30.2329	1.48736428736
80	H	30.3506	1.37860937861
81	H	28.1069	3.45179025179
83	H	28.5061	3.08292908293
85	H	29.4508	2.21002541003
88	H	29.2285	2.41543081543
89	H	27.8019	3.73361053361
93	H	28.3761	3.20304920305
94	H	27.5398	3.97579117579
95	H	27.7909	3.74377454377
96	H	27.7419	3.78905058905

Supporting Information: Original-MandelalideA192.log

Using Gaussian 09: AM64L-G09RevC.01 23-Sep-2011

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Pointgroup= C1 Stoichiometry= C33H52O11 C1[X(C33H52O11)]

#Atoms= 96

Charge = 0 Multiplicity = 1

SCF Energy= -2116.26536224

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Optimization incomplete.

Atomic Type	Coordinates (Angstroms) X	Y	Z
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C	-5.733417	2.369272	0.152282
H	-6.573468	2.899890	0.605737
H	-6.121650	1.967335	-0.786062
C	-4.420063	3.237754	-0.019844
H	-4.090669	3.578028	0.964766
C	-4.740820	4.454585	-0.879543
O	-3.756536	5.450998	-0.549965
H	-2.915446	4.981666	-0.409582
H	-5.773275	4.735429	-0.659892
H	-4.592572	4.122258	-1.910352
O	-3.436730	2.484748	-0.769810
C	-2.105021	2.659941	-0.636270
O	-1.740038	3.431327	0.204795
C	-1.245853	2.027408	-1.622267
H	-1.671865	1.246421	-2.249758
C	0.023369	2.348481	-1.788760
H	0.399702	3.116559	-1.117288
C	0.988630	1.693213	-2.763569
H	1.572415	2.508876	-3.194100
H	0.389490	1.267730	-3.571553
C	1.867854	0.595559	-2.222248
H	2.354999	0.181685	-3.108465
O	-5.151034	1.601153	2.426872
H	-5.347276	0.802557	2.948758
H	-4.559972	0.583927	0.711877
H	-7.594354	0.839177	1.184559
C	-6.774014	-0.642346	-0.078306
H	-7.179168	-0.005168	-0.867495
H	-5.784389	-1.006829	-0.362361
C	-7.695184	-1.722856	0.429257
H	-8.718846	-1.347314	0.490169
C	-7.640749	-2.970490	-0.511965
H	-8.143524	-2.804536	-1.466589
H	-8.132662	-3.781059	0.029812
H	-6.631561	-3.229178	-0.841525
C	-7.079383	-1.961887	1.885038
H	-7.914315	-2.200438	2.549341
O	-6.625809	-0.645319	2.244472
O	1.003323	-0.441230	-1.794599
C	1.537010	-1.625611	-1.282569
H	2.104373	-2.118577	-2.077772
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C	-0.695031	-2.825938	-1.796961
H	-1.078685	-1.901858	-2.234457
C	-0.222861	-3.591242	-3.023095
H	-1.031428	-3.516034	-3.754325
H	-0.146229	-4.675108	-2.919535
H	0.749750	-3.194961	-3.322629
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H	-2.223934	-4.405568	-1.339049
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H	-2.464610	-1.659315	-0.000009
C	-3.948338	-3.246678	0.416663
H	-4.437138	-4.101007	-0.049694
C	-4.538356	-2.567009	1.380730
H	-4.109630	-1.701281	1.880479
C	-5.885678	-3.024410	1.978048
H	-6.113717	-4.027052	1.609472
H	-5.804900	-3.111003	3.063483
H	0.074355	-1.947600	0.105390
H	0.888249	-3.465399	-0.321136
C	2.486480	-1.248741	-0.166514
H	2.961602	-2.126578	0.276003
H	1.933275	-0.637576	0.549524
C	3.578101	-0.244988	-0.613034
O	4.388110	0.055687	0.588191
C	5.564103	0.873224	0.441334
H	5.131202	1.864491	0.240844
H	4.166135	-0.723939	-1.400033
C	2.916178	1.056014	-1.153601
H	3.697404	1.689690	-1.579144
H	2.359425	1.589937	-0.381612
O	6.451898	0.523456	-0.604672
C	7.001224	-0.825924	-0.635036
C	8.047321	-1.025753	-1.736957
H	8.568500	-1.953636	-1.494426
H	8.849629	-0.285471	-1.763027
H	7.551061	-1.043242	-2.708939
H	6.151124	-1.488870	-0.816709
C	7.669355	-1.177830	0.753521
H	8.655714	-0.708532	0.784388
O	7.835701	-2.593104	0.895969
H	8.287876	-2.698985	1.752567
C	6.817811	-0.643947	1.943244
O	7.603392	-0.885319	3.109815
H	8.065884	-0.106705	3.468778
H	5.886515	-1.211137	2.024035
C	6.363385	0.839403	1.787052
O	7.518224	1.696940	1.784357
C	7.208892	3.131881	1.731117
H	6.708332	3.473522	2.640827
H	6.626115	3.430464	0.855796
H	8.171202	3.650404	1.740787
H	5.738526	1.045211	2.659481

NMR-Shifts

Original-MandelalideA192ps-NMR.txt

Atom	Type	Isotropic	Scaled Shift
1	C	99.9830	82.3876797029
2	C	111.5578	71.3089837095
3	C	138.9718	45.069966883

6	C	105.8443	76.7775991118
8	C	109.5197	73.259729321
14	C	14.2042	164.489940466
16	C	62.1439	118.604969467
18	C	28.3238	150.975516377
20	C	148.0703	36.3614349432
23	C	113.1398	69.7947893336
29	C	143.1164	41.1030073317
32	C	141.9546	42.2150117728
34	C	170.7282	14.6746683512
38	C	93.2898	88.7940044794
42	C	117.9647	65.1766879152
44	C	137.3560	46.6165125672
45	C	152.1356	32.4703765386
47	C	173.3042	12.2090775091
51	C	36.2458	143.393058826
53	C	45.0774	134.939987366
55	C	49.5153	130.692298857
57	C	49.6933	130.521928061
59	C	147.2929	37.1055150367
64	C	143.7477	40.4987652903
67	C	104.5377	78.0281973238
69	C	90.5321	91.4335075327
72	C	151.0642	33.4958555868
76	C	109.4638	73.313233408
77	C	169.4129	15.9335936752
82	C	103.4130	79.1046918969
86	C	108.0046	74.7098910775
90	C	103.1472	79.3590995233
92	C	128.3472	55.2391891116
4	H	30.1808	1.5355047355
5	H	30.1984	1.51924231924
7	H	25.8658	5.52256872257
10	H	29.5081	2.15708015708
11	H	28.0954	3.46241626242
12	H	27.9038	3.63945483945
17	H	25.6348	5.73601293601
19	H	24.0837	7.16923076923
21	H	29.2068	2.43548163548
22	H	29.0737	2.55846615847
24	H	27.9687	3.57948717949
26	H	28.6528	2.94737814738
27	H	28.1344	3.42638022638
28	H	27.8504	3.6887964888
30	H	30.0297	1.67512127512
31	H	30.4493	1.28741048741
33	H	29.2662	2.3805959806
35	H	30.7358	1.02268422268
36	H	30.5080	1.23317163317
37	H	30.8431	0.923538923539
39	H	27.0476	4.43058443058
43	H	28.3201	3.25479325479
46	H	28.7982	2.81302841303
48	H	30.5750	1.17126357126
49	H	31.2173	0.577777777778
50	H	30.3360	1.3920997921
52	H	25.7611	5.61931161931
54	H	25.0485	6.27775467775
56	H	25.1424	6.19099099099
58	H	25.2310	6.10912450912
60	H	29.5099	2.15541695542
61	H	29.3041	2.34557634558
62	H	30.3211	1.40586740587
63	H	30.1217	1.59011319011
65	H	30.0760	1.63234003234
66	H	30.7440	1.01510741511
70	H	25.4843	5.87507507508
71	H	27.5707	3.94723954724
73	H	29.2117	2.43095403095
74	H	30.5263	1.21626241626
78	H	30.1600	1.55472395472
79	H	30.7145	1.04236544237
80	H	30.4536	1.28343728344
81	H	27.7991	3.7361977362
83	H	28.2297	3.33832293832
85	H	29.2890	2.35952875953
88	H	29.8067	1.88117348117
89	H	27.5827	3.93615153615
93	H	28.7004	2.9033957034
94	H	28.1491	3.4127974128
95	H	28.3031	3.2705012705
96	H	27.9650	3.58290598291

Supporting Information: Original-MandelalideA194.log

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 Using  Gaussian 09:  AM64L-G09RevC.01 23-Sep-2011
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 #mPW1pw91/6-311+G(2d,p) scf=(maxcycle=300,direct,tight) NMR
 density=current SCRF=(PCM,SOLVENT=Chloroform)
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 Pointgroup= C1   Stoichiometry= C33H52O11   C1[X(C33H52O11)]
#Atoms= 96
 Charge = 0                 Multiplicity = 1
-----------------------------------------------------------------------
 SCF Energy= -2116.23659246
=======================================================================
 Optimization incomplete.


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     Atomic      Coordinates (Angstroms)
      Type      X              Y              Z
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      C       6.810253       0.265696      -1.102504
      C       5.392883       0.967177      -0.922512
      C       5.400887       2.186116       0.099458
      H       6.340762       2.672852      -0.170892
      H       5.519180       1.786192       1.108451
      C       4.169033       3.120262      -0.031477
      H       3.877588       3.373261      -1.054139
      C       4.349243       4.514952       0.675398
      O       3.516130       5.578678       0.128175
      H       2.634268       5.217069      -0.072671
      H       5.396700       4.810871       0.577426
      H       4.092478       4.366406       1.726897
      O       3.006218       2.463767       0.630515
      C       1.788743       2.995011       0.534921
      O       1.404447       3.806293      -0.329170
      C       0.849722       2.352793       1.512642
      H       1.354905       1.568977       2.073839
      C      -0.478894       2.577623       1.616358
      H      -0.890449       3.421048       1.068654
      C      -1.299845       2.053881       2.750300
      H      -2.166147       2.675948       2.983882
      H      -0.805272       2.167652       3.716899
      C      -1.967731       0.656079       2.415287
      H      -2.559445       0.215008       3.221563
      O       5.142560       1.430142      -2.230956
      H       5.505281       0.708622      -2.775106
      H       4.647462       0.251381      -0.564382
      H       7.636754       0.914346      -1.404151
      C       7.264850      -0.639131       0.036035
      H       8.034513      -0.266371       0.715623
      H       6.376770      -0.986242       0.568385
      C       7.816358      -1.917825      -0.693564
      H       8.851170      -1.850547      -1.035710
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C	7.852185	-3.177863	0.227448
H	8.717444	-3.002370	0.870216
H	8.089953	-4.073922	-0.349055
H	6.921133	-3.310096	0.781597
C	7.062270	-1.962933	-1.996612
H	7.750473	-2.293491	-2.778919
O	6.649866	-0.578833	-2.266881
O	-0.973864	-0.279529	1.946878
C	-1.466208	-1.558814	1.469716
H	-2.015389	-1.947881	2.330915
C	-0.350190	-2.544769	1.074643
C	0.905833	-2.466776	1.968581
H	1.182072	-1.429964	2.169981
C	0.635731	-3.182601	3.238038
H	1.530929	-3.315250	3.848145
H	0.161940	-4.145636	3.034519
H	-0.155083	-2.597544	3.712081
C	2.129569	-3.117700	1.354015
H	2.257654	-4.182711	1.532135
C	2.955961	-2.441496	0.572585
H	2.829973	-1.364222	0.477237
C	4.148495	-3.004054	-0.124993
H	4.538714	-3.954505	0.235802
C	4.686719	-2.429406	-1.193082
H	4.126585	-1.549740	-1.498891
C	5.884070	-2.856212	-2.064893
H	6.180491	-3.801652	-1.607418
H	5.526722	-3.059465	-3.077181
H	-0.039684	-2.443126	0.032801
H	-0.896512	-3.486853	0.984763
C	-2.277779	-1.298601	0.190934
H	-2.600176	-2.229684	-0.279116
H	-1.690836	-0.728727	-0.532250
C	-3.501490	-0.397621	0.587636
O	-4.232729	-0.104092	-0.631027
C	-5.500870	0.631239	-0.545961
H	-5.317533	1.681999	-0.280397
H	-4.173061	-0.905606	1.283948
C	-2.905102	0.825260	1.240225
H	-3.735543	1.469132	1.537532
H	-2.440836	1.448672	0.474030
O	-6.309147	0.229644	0.577924
C	-6.911332	-1.050259	0.466448
C	-7.860220	-1.221494	1.652967
H	-8.074576	-2.225517	2.024708
H	-8.845772	-0.788231	1.467921
H	-7.364483	-0.709593	2.481088
H	-6.085532	-1.764590	0.502947
C	-7.754864	-1.245270	-0.828848
H	-8.642007	-0.609388	-0.868118
O	-8.167064	-2.655983	-0.945694
H	-8.390559	-2.783519	-1.885070
C	-6.838674	-0.869786	-1.999526
O	-7.399764	-0.965218	-3.264551
H	-7.650516	-0.024519	-3.288965
H	-5.949679	-1.505599	-2.017941
C	-6.233243	0.559248	-1.858106
O	-7.353094	1.477162	-1.885634
C	-7.223069	2.865894	-1.700043
H	-6.147367	3.059541	-1.673820
H	-7.612198	3.063304	-0.698637
H	-7.742090	3.415628	-2.489198
H	-5.559409	0.700695	-2.707685

NMR-Shifts

Original-MandelalideA194ps-NMR.txt

Atom	Type	Isotropic	Scaled Shift
1	C	97.7168	84.5567487892
2	C	108.4907	74.2446256628
3	C	149.7546	34.7493252168
6	C	98.4678	83.8379371734
8	C	105.4059	77.1972089818
14	C	3.2380	174.98612148
16	C	43.3161	136.625796818
18	C	34.5695	144.997511438
20	C	150.8999	33.6531135741
23	C	107.8479	74.8598748062
29	C	147.3656	37.0359310094
32	C	141.5845	42.5692490285
34	C	170.6396	14.7594708934
38	C	104.1786	78.3719060472
42	C	110.8007	72.0336338751
44	C	136.8206	47.1289649496
45	C	152.7110	31.9196385842
47	C	166.6251	18.6019066215
51	C	37.7857	141.919160015
53	C	50.6645	129.592354371
55	C	49.2347	130.960872145
57	C	45.9006	134.152070292
59	C	152.3896	32.2272631559
64	C	142.5762	41.6200539827
67	C	112.0275	70.8594153793
69	C	87.2535	94.5715844484
72	C	150.8407	33.7097762208
76	C	117.3287	65.7854285113
77	C	167.0057	18.2376194031
82	C	103.0489	79.4531863167
86	C	113.4379	69.5094661077
90	C	101.6282	80.8129941232
92	C	132.5241	51.2413139608
4	H	30.0950	1.61478401478
5	H	29.9349	1.76271656272
7	H	25.5572	5.80771540772
10	H	28.0259	3.52663432663
11	H	28.1477	3.41409101409
12	H	27.6676	3.8577038577
17	H	25.1994	6.13832293832
19	H	24.0999	7.15426195426
21	H	29.5352	2.13203973204
22	H	28.8459	2.76895356895
24	H	27.7362	3.79431739432
26	H	27.3214	4.17759297759
27	H	27.6363	3.88662508663
28	H	27.4687	4.04148764149
30	H	29.5310	2.13592053592
31	H	30.2455	1.47572187572
33	H	28.9122	2.70769230769
35	H	30.5880	1.15925155925
36	H	30.7352	1.02323862324
37	H	30.7096	1.04689304689
39	H	27.5040	4.00887040887
43	H	27.9698	3.57847077847
46	H	28.9308	2.69050589051
48	H	30.5271	1.21552321552
49	H	31.0185	0.761469161469
50	H	30.2476	1.47378147378
52	H	25.9072	5.48431508432
54	H	25.5513	5.81316701317
56	H	25.5087	5.85252945253
58	H	25.8227	5.56239316239
60	H	29.6544	2.0218988219
61	H	29.3083	2.3416955417
62	H	30.2219	1.49752829753
63	H	30.3712	1.35957495957
65	H	30.1571	1.5574035574
66	H	30.6628	1.09013629014
70	H	26.0458	5.35624855625
71	H	27.8104	3.72575652576

73	H	29.9286	1.76853776854
74	H	30.6878	1.06703626704
78	H	30.0954	1.61441441441
79	H	30.6557	1.0966966967
80	H	30.7353	1.02314622315
81	H	28.0576	3.49734349734
83	H	28.0247	3.52774312774
85	H	29.7839	1.90224070224
88	H	29.1711	2.46846846847
89	H	28.0255	3.527003927
93	H	28.1458	3.41584661585
94	H	27.9376	3.60822360822
95	H	27.8845	3.65728805729
96	H	27.8670	3.67345807346

Supporting Information: Original-MandelalideA196.log

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 Using  Gaussian 09:  AM64L-G09RevC.01 23-Sep-2011
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 #mPW1pw91/6-311+G(2d,p) scf=(maxcycle=300,direct,tight) NMR
 density=current SCRF=(PCM,SOLVENT=Chloroform)
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 Pointgroup= C1   Stoichiometry= C33H52O11   C1[X(C33H52O11)]
#Atoms= 96
 Charge = 0                Multiplicity = 1
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 SCF Energy= -2116.26053401
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 Optimization incomplete.


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     Atomic      Coordinates (Angstroms)
      Type      X              Y              Z
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C	-6.727012	0.061790	1.148451
C	-5.530014	1.048413	1.118430
C	-5.694966	2.227863	0.171466
H	-6.514043	2.909423	0.411110
H	-5.883204	1.757266	-0.794973
C	-4.480159	3.114795	0.048585
H	-4.049486	3.323839	1.031426
C	-4.771564	4.432875	-0.677915
O	-4.059571	5.486865	-0.065486
H	-3.152841	5.160597	0.073581
H	-5.827866	4.696147	-0.578018
H	-4.450609	4.342663	-1.719015
O	-3.416638	2.422500	-0.720773
C	-2.140049	2.862132	-0.646120
O	-1.803089	3.710967	0.119636
C	-1.195206	2.183007	-1.510679
H	-1.593916	1.314182	-2.034317
C	0.074677	2.624309	-1.664297
H	0.413912	3.506441	-1.127967
C	0.985886	2.070509	-2.693666
H	1.635110	2.895846	-2.993565
H	0.494549	1.712723	-3.600134
C	1.793422	0.878228	-2.082889
H	2.280577	0.269178	-2.847364
O	-5.513779	1.575168	2.439159
H	-5.692969	0.794775	2.993150
H	-4.638723	0.424727	1.016644
H	-7.664004	0.597506	1.319940
C	-7.002453	-0.689509	-0.180530
H	-7.585830	-0.035385	-0.832077
H	-6.139181	-1.072215	-0.729768
C	-7.674222	-1.949144	0.406641
H	-8.734392	-1.692352	0.452425
C	-7.715051	-3.080650	-0.554788
H	-8.211749	-2.715759	-1.455928
H	-8.302050	-3.904033	-0.143900
H	-6.691071	-3.414010	-0.741574
C	-7.031344	-2.232517	1.792751
H	-7.855927	-2.474774	2.467387
O	-6.459979	-0.944641	2.171444
O	0.894432	-0.110294	-1.562271
C	1.533270	-1.415788	-1.232176
H	2.082991	-1.882067	-2.053923
C	0.421163	-2.312428	-0.729915
C	-0.698746	-2.559079	-1.773004
H	-1.087551	-1.618563	-2.169028
C	-0.133234	-3.244633	-3.095034
H	-0.827349	-3.250768	-3.937317
H	0.227912	-4.257968	-2.906398
H	0.681740	-2.664934	-3.533392
C	-1.931072	-3.227044	-1.198355
H	-1.960343	-4.309231	-1.288941
C	-2.847934	-2.572704	-0.424028
H	-2.915051	-1.491527	-0.313185
C	-3.985197	-3.319153	0.189300
H	-4.267504	-4.268392	-0.262358
C	-4.577410	-2.759042	1.271569
H	-4.248231	-1.806658	1.678603
C	-5.891671	-3.257091	1.904480
H	-6.116832	-4.220584	1.444570
H	-5.657040	-3.519692	2.938022
H	0.093206	-2.016439	0.269227
H	0.827412	-3.302208	-0.512838
C	2.552628	-1.105341	-0.152434
H	3.035516	-1.998518	0.247793
H	1.996590	-0.626083	0.655256
C	3.588932	-0.128585	-0.601363
O	4.505049	0.021769	0.539932
C	5.695820	0.808438	0.432162
H	5.407136	1.856381	0.264325
H	3.993792	-0.495518	-1.548549
C	2.927115	1.230510	-0.965398
H	3.648645	1.924677	-1.400548
H	2.464414	1.695478	-0.092699
O	6.487643	0.420481	-0.758412
C	6.947823	-0.904922	-0.617449
C	7.778528	-1.234340	-1.888037
H	7.966220	-2.301440	-1.751975
H	8.750773	-0.738330	-1.862793
H	7.211911	-1.048228	-2.803391
H	6.062463	-1.545848	-0.588691
C	7.829535	-1.212737	0.619985
H	8.798963	-0.712729	0.698914
O	8.027703	-2.596618	0.648572
H	8.317940	-2.756905	1.563654
C	7.077868	-0.851822	1.915509
O	7.841615	-1.054937	3.020431
H	8.452085	-0.295480	3.047591
H	6.253818	-1.568477	1.935428
C	6.538414	0.613203	1.770492
O	7.612724	1.533662	1.775845
C	7.351088	2.956710	1.979255
H	6.702573	3.119817	2.844685
H	6.850004	3.351590	1.091911
H	8.243818	3.532089	2.237576
H	5.831627	0.762871	2.590801

NMR-Shifts

Original-MandelalideA196ps-NMR.txt

Atom	Type	Isotropic	Scaled Shift
1	C	93.2169	88.8637799345

2	C	112.4864	70.4201841536
3	C	151.4572	33.1196998411
6	C	102.3783	80.0950439327
8	C	110.0788	72.7245927372
14	C	15.4665	163.281743525
16	C	53.6284	126.755489194
18	C	28.3688	150.932445108
20	C	149.4163	35.0731254427
23	C	105.0098	77.5763318593
29	C	144.8450	39.4484963342
32	C	146.7315	37.6428530408
34	C	170.8040	14.6021171921
38	C	102.9059	79.5900572369
42	C	105.3687	77.2328145638
44	C	142.9665	41.2464825131
45	C	151.8157	32.7765654013
47	C	169.2568	16.0830031203
51	C	36.1525	143.482359923
53	C	41.0962	138.750550355
55	C	43.9831	135.987384904
57	C	41.7537	138.121231264
59	C	152.2797	32.3324527652
64	C	145.6522	38.6758934895
67	C	109.3137	73.4569000172
69	C	82.7060	98.9241754245
72	C	144.7389	39.5500488141
76	C	114.2768	68.7065219472
77	C	167.3189	17.9378433737
82	C	109.4760	73.3015563085
86	C	111.9104	70.9714963916
90	C	102.2593	80.2089435096
92	C	126.6413	56.871973047
4	H	30.0514	1.65507045507
5	H	30.0440	1.66190806191
7	H	26.1514	5.25867405867
10	H	28.5372	3.05419265419
11	H	28.1059	3.45271425271
12	H	27.6512	3.87285747286
17	H	25.3149	6.0316008316
19	H	23.8209	7.41205821206
21	H	29.2461	2.39916839917
22	H	28.8150	2.79750519751
24	H	27.8351	3.70293370293
26	H	29.1907	2.45035805036
27	H	27.5605	3.95666435666
28	H	27.8776	3.66366366366
30	H	30.1742	1.5416031416
31	H	30.6078	1.14095634096
33	H	28.8831	2.73458073458
35	H	30.6698	1.08366828367
36	H	30.8139	0.95051975052
37	H	30.5931	1.15453915454
39	H	27.2155	4.27544467544
43	H	28.0457	3.50833910834
46	H	28.6402	2.95902055902
48	H	30.8259	0.939431739432
49	H	31.2417	0.555232155232
50	H	30.6298	1.12062832063
52	H	25.4855	5.87396627397
54	H	24.7787	6.52705012705
56	H	24.8717	6.44111804112
58	H	24.7921	6.51466851467
60	H	29.6709	2.00665280665
61	H	29.3590	2.29484869485
62	H	30.3661	1.36428736429
63	H	30.4997	1.24084084084
65	H	30.2394	1.48135828136
66	H	30.7341	1.02425502426
70	H	25.8026	5.58096558097
71	H	27.8715	3.6693000693
73	H	29.6305	2.04398244398
74	H	30.5343	1.20887040887
78	H	30.1284	1.58392238392
79	H	30.7669	0.993947793948
80	H	30.6590	1.09364749365
81	H	28.0583	3.4966966967
83	H	28.6129	2.98424578425
85	H	29.5945	2.07724647725
88	H	30.1256	1.58650958651
89	H	28.4219	3.16072996073
93	H	28.7198	2.88547008547
94	H	27.9989	3.55158235158
95	H	27.9748	3.57385077385
96	H	28.1275	3.43275583276

Supporting Information: Original-MandelalideA198.log

```
-----------------------------------------------------------------------
 Using  Gaussian 09:  AM64L-G09RevC.01 23-Sep-2011
=======================================================================
 #mPW1pw91/6-311+G(2d,p) scf=(maxcycle=300,direct,tight) NMR
 density=current SCRF=(PCM,SOLVENT=Chloroform)
-----------------------------------------------------------------------
 Pointgroup= C1   Stoichiometry= C33H52O11   C1[X(C33H52O11)]
#Atoms= 96
 Charge = 0                Multiplicity = 1
-----------------------------------------------------------------------
 SCF Energy= -2116.24216216
=======================================================================
 Optimization incomplete.


-----------------------------------------------------------------------
     Atomic     Coordinates (Angstroms)
      Type      X              Y              Z
-----------------------------------------------------------------------
      C      -6.666732      0.687368      0.960026
      C      -5.237415      1.190035      0.853545
      C      -5.174233      2.528354      0.038986
      H      -5.860421      3.224977      0.526147
      H      -5.525642      2.309339     -0.971753
      C      -3.828790      3.215045      0.043567
      H      -3.406099      3.364855      1.040315
      C      -4.122749      4.665196     -0.547722
      O      -3.183768      5.664337     -0.003483
      H      -2.309670      5.576788     -0.423863
      H      -5.155526      4.929541     -0.304581
      H      -4.037270      4.746193     -1.634127
      O      -2.944897      2.524516     -0.849319
      C      -1.688237      2.920717     -0.915111
      O      -1.088290      3.901753     -0.474283
      C      -1.000436      2.026364     -1.869276
      H      -1.607573      1.410081     -2.529777
      C       0.304801      2.015843     -1.958352
      H       0.862891      2.687941     -1.311195
      C       1.189467      1.198807     -2.848679
      H       1.991988      1.813261     -3.263143
      H       0.585322      0.826312     -3.679182
      C       1.904887      0.088176     -2.038513
      H       2.303424     -0.597007     -2.790478
      O      -4.736481      1.317763      2.196239
      H      -5.373106      0.769072      2.688261
      H      -4.698069      0.363457      0.383754
      H      -7.399257      1.466389      1.183395
      C      -7.205211     -0.014143     -0.222112
      H      -7.807266      0.643460     -0.852375
      H      -6.332265     -0.424856     -0.733461
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C	-7.955918	-1.181795	0.300175
H	-8.993753	-0.893877	0.479155
C	-8.146372	-2.270611	-0.822017
H	-9.000030	-1.942651	-1.418299
H	-8.466437	-3.224041	-0.396365
H	-7.244482	-2.426580	-1.418784
C	-7.403394	-1.551582	1.688048
H	-8.276437	-1.693889	2.329768
O	-6.696640	-0.312203	2.065779
O	0.790815	-0.750890	-1.430878
C	1.359243	-1.834303	-0.545279
H	1.893444	-2.559368	-1.163197
C	0.149292	-2.675549	-0.024727
C	-0.758205	-3.242526	-1.144436
H	-1.077018	-2.424651	-1.793537
C	-0.037940	-4.322031	-2.086797
H	-0.745280	-4.666552	-2.843886
H	0.234545	-5.217997	-1.525325
H	0.761983	-3.890240	-2.691662
C	-2.078731	-3.817995	-0.642649
H	-2.077337	-4.903706	-0.590818
C	-3.113267	-3.064232	-0.204527
H	-2.958263	-1.986560	-0.188648
C	-4.411607	-3.431821	0.301140
H	-4.905478	-4.376501	0.079746
C	-5.064721	-2.522832	1.091695
H	-4.625869	-1.553053	1.317685
C	-6.424324	-2.767495	1.777336
H	-6.815527	-3.707737	1.384288
H	-6.194377	-2.919481	2.833852
H	-0.459660	-2.141453	0.707784
H	0.546698	-3.594092	0.411749
C	2.354047	-1.314440	0.417763
H	2.700961	-2.175861	0.991575
H	1.854490	-0.674235	1.148620
C	3.485560	-0.565040	-0.262107
O	4.363061	-0.026433	0.733337
C	5.531152	0.661503	0.252138
H	5.216134	1.595672	-0.235120
H	4.017215	-1.184099	-0.988553
C	2.924513	0.617641	-0.976367
H	3.765959	1.061218	-1.511678
H	2.509430	1.302882	-0.234157
O	6.210793	-0.025598	-0.784448
C	6.653144	-1.287503	-0.387169
C	7.274508	-1.954002	-1.643364
H	7.180678	-3.035946	-1.528093
H	8.325580	-1.668143	-1.720569
H	6.710167	-1.732586	-2.551727
H	5.864132	-1.951675	-0.025123
C	7.736716	-0.952194	0.720969
H	8.476739	-0.301500	0.248204
O	8.218154	-2.208697	1.101488
H	8.522913	-2.070706	2.016519
C	7.022856	-0.264512	1.881098
O	7.896804	-0.063916	2.961459
H	8.250041	0.838667	2.867012
H	6.339231	-1.036159	2.242421
C	6.418715	1.049392	1.439355
O	7.461613	2.025939	0.978467
C	6.965982	3.372820	0.708654
H	6.792615	3.745126	1.721084
H	5.981509	3.278351	0.243508
H	7.763168	3.962921	0.248663
H	5.831945	1.470229	2.259347

NMR-Shifts
Original-MandelalideA198ps-NMR.txt

Atom	Type	Isotropic	Scaled Shift
1	C	97.0822	85.1641493903
2	C	109.0369	73.721836176
3	C	146.5112	37.8537108291
6	C	107.0115	75.6604261184
8	C	102.2215	80.2451233753
14	C	9.7856	168.719156186
16	C	57.3862	123.158751125
18	C	35.8259	143.794961619
20	C	146.3395	38.0180516472
23	C	101.6997	80.7445586631
29	C	148.6990	35.759681464
32	C	145.7611	38.5716610195
34	C	168.2508	17.0458852581
38	C	99.9252	82.4430023546
42	C	106.4299	76.2170983365
44	C	141.0840	43.0482972492
45	C	148.2780	36.1626371102
47	C	166.2568	18.9544210264
51	C	43.0218	136.907482915
53	C	48.5259	131.639292483
55	C	50.1260	130.107773885
57	C	33.4812	146.03916614
59	C	147.3152	37.0841708302
64	C	152.3100	32.3034514443
67	C	115.3937	67.6374930607
69	C	93.7276	88.374968893
72	C	149.0706	35.4040084994
76	C	113.6583	69.2985126055
77	C	166.3463	18.8687570589
82	C	107.1406	75.5368594345
86	C	112.4050	70.4980952928
90	C	103.5024	79.0191236433
92	C	127.7324	55.8276383545
4	H	30.1056	1.60498960499
5	H	29.8567	1.83497343497
7	H	26.5655	4.87604527605
10	H	28.6376	2.96142296142
11	H	28.0533	3.50131670132
12	H	27.2461	4.24717024717
17	H	25.6046	5.76391776392
19	H	24.3652	6.90912450912
21	H	29.4721	2.19034419034
22	H	29.1183	2.51725571726
24	H	27.5235	3.99085239085
26	H	27.8024	3.73314853315
27	H	27.9360	3.6097020097
28	H	27.7319	3.79829059829
30	H	29.5227	2.14358974359
31	H	30.6629	1.09004389004
33	H	28.9560	2.66722106722
35	H	30.4239	1.31088011088
36	H	30.5961	1.15176715177
37	H	31.0296	0.751212751213
39	H	27.2243	4.26731346731
43	H	28.2206	3.34673134673
46	H	29.1194	2.51623931624
48	H	30.7853	0.976946176946
49	H	31.1813	0.611041811042
50	H	30.5636	1.1817971818
52	H	26.0708	5.33314853315
54	H	24.9308	6.38650958651
56	H	24.9450	6.37338877339
58	H	24.9723	6.34816354816
60	H	29.4169	2.24134904135
61	H	29.4871	2.17648417648
62	H	30.1499	1.56405636406
63	H	30.4262	1.30875490875
65	H	30.2965	1.4285978286
66	H	30.5730	1.17311157311

70	H	25.9831	5.41418341418
71	H	28.1147	3.44458304458
73	H	29.0032	2.62360822361
74	H	30.1124	1.59870639871
78	H	30.2986	1.42665742666
79	H	30.3944	1.33813813814
80	H	30.6530	1.09919149919
81	H	28.1363	3.42462462462
83	H	28.3766	3.20258720259
85	H	29.7398	1.94298914299
88	H	30.3116	1.41464541465
89	H	27.8011	3.73434973435
93	H	28.1492	3.41270501271
94	H	27.6784	3.84772464772
95	H	27.6967	3.83081543082
96	H	28.0413	3.5124047124

Mandelalide B Revised Configuration

Supporting Information: Revised-MandelalideB-0001.log

```
---------------------------------------------------------------------------
 Using  Gaussian 09:  AM64L-G09RevC.01 23-Sep-2011
=============================================================================
 #b3lyp/6-31G(d,p) scf=(maxcycle=300,direct,tight) density=current
 SCRF=(PCM,SOLVENT=Chloroform) opt=(maxcycle=250)
freq=noraman
 #N Geom=AllCheck Guess=TCheck SCRF=Check GenChk RB3LYP/6-
31G(d,p) Freq
---------------------------------------------------------------------------
 Pointgroup= C1   Stoichiometry= C37H58O13   C1[X(C37H58O13)]
#Atoms= 108
 Charge = 0                Multiplicity = 1
---------------------------------------------------------------------------
 SCF Energy= -2422.84519468      Predicted Change= -8.518173D-09
=============================================================================
 Optimization completed.          {Found       2       times}
 Item      Max Val.    Criteria    Pass?      RMS Val.    Criteria    Pass?
 Force      0.00001 ||  0.00045   [ YES ]      0.00000 ||  0.00030   [ YES ]
 Displ      0.00164 ||  0.00180   [ YES ]      0.00164 ||  0.00180   [ YES ]
---------------------------------------------------------------------------
     Atomic      Coordinates (Angstroms)
      Type      X                Y               Z
---------------------------------------------------------------------------
      C      -5.781727     -1.442681     -0.993299
      H      -6.333751     -1.060003     -1.866347
      C      -4.859485     -0.334599     -0.469284
      C      -3.924126      0.196252     -1.567294
      H      -3.283364     -0.633425     -1.888253
      H      -4.492644      0.516701     -2.448132
      C      -3.040324      1.343955     -1.100224
      H      -2.851159      1.263139     -0.028805
      O      -4.092825     -0.802610      0.642502
      H      -3.643910     -1.603407      0.326116
      H      -5.482399      0.481149     -0.083457
      O      -4.942994     -2.540227     -1.403348
      C      -5.551091     -3.810196     -1.082802
      C      -4.607844     -4.596256     -0.151913
      H      -4.519261     -4.072595      0.804642
      C      -3.265043     -4.820653     -0.790242
      H      -3.290301     -5.393401     -1.717243
      C      -2.067942     -4.362662     -0.378618
      H      -1.200540     -4.589218     -0.998535
      C      -1.790939     -3.573983      0.816229
      H      -2.600732     -3.442866      1.530421
      C      -0.592832     -3.017912      1.075552
      C      -0.231134     -2.167113      2.272492
      H       0.777248     -2.470523      2.589293
      C      -1.169484     -2.360658      3.473573
      H      -0.798732     -1.802936      4.339061
      H      -1.243319     -3.415701      3.753319
      H      -2.178780     -1.994178      3.256717
      C      -0.180626     -0.660725      1.906165
      H       0.072189     -0.085518      2.805929
      H      -1.186808     -0.351022      1.599817
      C       0.788383     -0.239692      0.798609
      H       0.548954     -0.781142     -0.132750
      H       0.204031     -3.171279      0.346283
      H      -5.074953     -5.568473      0.056375
      H      -5.653739     -4.374833     -2.019727
      C      -6.953193     -3.466702     -0.509280
      C      -7.544749     -4.456051      0.495319
      H      -6.935939     -4.527773      1.402007
      H      -7.635271     -5.460008      0.066986
      H      -8.547419     -4.135397      0.795363
      H      -7.636148     -3.404744     -1.366837
      C      -6.749967     -2.040064      0.025986
      H      -6.280871     -2.054145      1.015856
      H      -7.684646     -1.476633      0.095586
      C      -1.722924      1.508360     -1.864703
      H      -0.945495      0.895943     -1.416169
      H      -1.848606      1.217240     -2.912793
      C      -1.456065      3.016386     -1.837525
      O      -0.883768      3.453950     -3.059955
      H      -1.156386      4.379205     -3.176734
      C      -2.892524      3.571375     -1.709068
      O      -3.217790      4.709823     -1.967300
      O      -3.746828      2.622210     -1.299618
      C       2.269117     -0.460219      1.133689
      H       2.485446     -1.528929      1.235042
      H       2.495761      0.018860      2.094336
      C       3.164671      0.145926      0.054622
      O       4.528653      0.026397      0.502119
      C       5.493014     -0.068248     -0.521068
      H       5.310454      0.677057     -1.304963
      H       3.049528     -0.426206     -0.875881
      C       2.792417      1.612895     -0.184008
      H       3.364499      2.030973     -1.020210
      H       3.041538      2.189092      0.715153
      C       1.287899      1.744926     -0.468147
      C       0.872522      3.213770     -0.602470
      H       1.289209      3.778374      0.237541
      H       1.337145      3.611379     -1.510936
      C      -0.616079      3.591885     -0.669945
      O      -1.337866      3.275934      0.546030
      C      -1.220376      4.136619      1.587279
      O      -0.514225      5.124863      1.559559
      C      -2.094012      3.711881      2.746040
      H      -1.819842      4.337166      3.599648
      H      -1.857861      2.670265      2.988913
      C      -3.601928      3.843155      2.441424
      H      -4.149700      3.489321      3.322124
      H      -3.862709      3.169115      1.618822
      C      -4.037507      5.270955      2.098401
      H      -5.120112      5.319711      1.946452
      H      -3.561233      5.627074      1.178757
      H      -3.778541      5.970213      2.901143
      H      -0.647115      4.680980     -0.784531
      H       1.070639      1.210020     -1.407730
      O       0.530836      1.156191      0.589267
      O       5.453428     -1.306133     -1.205411
      C       5.726158     -2.463563     -0.383833
      H       4.987477     -2.501429      0.428502
      C       5.574508     -3.681679     -1.279773
      H       4.581681     -3.695065     -1.737133
      H       5.700527     -4.597987     -0.695078
      H       6.330317     -3.668843     -2.068026
```

C	7.118966	-2.345248	0.257295
O	8.180267	-2.447524	-0.692695
H	8.114545	-1.659773	-1.260406
H	7.258920	-3.182256	0.950446
C	7.231983	-1.024984	1.043695
O	8.522224	-0.873004	1.605449
H	9.134988	-1.063944	0.877984
H	6.518636	-1.043286	1.873564
C	6.863240	0.167043	0.140916
O	7.877578	0.272644	-0.861059
C	8.042556	1.571012	-1.419266
H	8.876987	1.510105	-2.120283
H	8.279329	2.305020	-0.638154
H	7.149876	1.906548	-1.962175
H	6.827773	1.087134	0.737636

Statistical Thermodynamic Analysis

Temperature= 298.150 Kelvin Pressure= 1.00000 Atm

==========

SCF Energy= -2422.84519468 Predicted Change= -8.518173D-09

Zero-point correction (ZPE)= -2421.9097 0.93542

Internal Energy (U)= -2421.8580 0.98711

Enthalpy (H)= -2421.8571 0.98806

Gibbs Free Energy (G)= -2421.9997 0.84548

Frequencies -- 10.6889 14.3146 15.8395

NMR-Shifts

Revised-MandelalideB-0001-NMR.txt

Atom	Type	Isotropic	Scaled Shift
1	C	100.4921	81.9004000842
3	C	115.2765	67.7496697869
4	C	142.5695	41.626466816
7	C	105.9753	76.6522138632
13	C	102.4228	80.0524512338
14	C	152.3084	32.3049828672
16	C	49.3448	130.855491108
18	C	50.3027	129.938647371
20	C	58.1596	122.418499588
22	C	38.7135	141.03112617
23	C	151.0518	33.5077241142
25	C	167.4016	17.8586879534
29	C	137.7130	46.2748138364
32	C	111.0244	71.8195218132
37	C	145.4912	38.8299929172
38	C	172.8099	12.6821914661
43	C	150.3236	34.2047129539
46	C	145.5094	38.8125729819
49	C	105.5036	77.103696472
52	C	-2.4812	180.460192576
55	C	148.1190	36.3148222592
58	C	113.2409	69.6980225502
60	C	90.9634	91.0206933517
63	C	147.1209	37.2701429966
66	C	112.2450	70.6512375811
67	C	151.3947	33.1795210475
70	C	106.7414	75.9189494439
72	C	5.4929	172.827868068
74	C	146.6014	37.767376864
77	C	163.3492	21.7373992611
80	C	173.3220	12.1920404296
88	C	115.2760	67.7501483566
90	C	169.9992	15.3724229024
94	C	110.0523	72.7499569287
98	C	117.8307	65.3049445816
102	C	101.9351	80.5192480714
104	C	128.2251	55.3560558204
2	H	27.6713	3.85428505429
5	H	30.0020	1.70071610072
6	H	30.0191	1.68491568492
8	H	26.4783	4.95661815662
10	H	30.8253	0.939986139986
11	H	28.1815	3.38285978286
15	H	29.2221	2.42134442134
17	H	26.1563	5.25414645415
19	H	25.1228	6.2091014091
21	H	25.0269	6.29771309771
24	H	29.3185	2.33227073227
26	H	30.7596	1.00069300069
27	H	30.6357	1.11517671518
28	H	30.5671	1.17856317856
30	H	30.1553	1.55906675907
31	H	30.1045	1.60600600601
33	H	28.2869	3.28547008547
34	H	25.2945	6.05045045045
35	H	29.7588	1.92543312543
36	H	27.5770	3.94141834142
39	H	30.9215	0.851097251097
40	H	30.7053	1.05086625087
41	H	30.5201	1.22199122199
42	H	29.1164	2.51901131901
44	H	29.7474	1.93596673597
45	H	29.9316	1.76576576577
47	H	29.0774	2.55504735505
48	H	29.7700	1.91508431508
51	H	29.6770	2.00101640102
56	H	29.6580	2.01857241857
57	H	30.7131	1.04365904366
61	H	26.4233	5.00743820744
62	H	27.6456	3.87803187803
64	H	29.7578	1.92635712636
65	H	30.8949	0.875675675676
68	H	29.4773	2.18553938554
69	H	29.7192	1.96202356202
75	H	29.7617	1.92275352275
76	H	29.1513	2.48676368676
78	H	30.2016	1.51628551629
79	H	29.9985	1.70395010395
81	H	30.7758	0.985724185724
82	H	31.0428	0.739015939016
83	H	31.0445	0.737445137445
84	H	26.8143	4.64615384615
85	H	27.9427	3.60351120351
89	H	27.6448	3.87877107877
91	H	30.5810	1.16571956572
92	H	30.8462	0.920674520675
93	H	30.0860	1.6231000231
96	H	29.7098	1.97070917071
97	H	28.2475	3.32187572188
100	H	29.1195	2.51614691615
101	H	28.0622	3.49309309309
105	H	28.1862	3.37851697852
106	H	28.6577	2.94285054285
107	H	28.1787	3.38544698545
108	H	28.3717	3.20711480711

Supporting Information: Revised-MandelalideB-0002.log

Using Gaussian 09: AM64L-G09RevC.01 23-Sep-2011

==========

#b3lyp/6-31G(d,p) scf=(maxcycle=300,direct,tight) density=current SCRF=(PCM,SOLVENT=Chloroform) opt=(maxcycle=250) freq=noraman

#N Geom=AllCheck Guess=TCheck SCRF=Check GenChk RB3LYP/6-31G(d,p) Freq

---

Pointgroup= C1 Stoichiometry= C37H58O13 C1[X(C37H58O13)]
#Atoms= 108
Charge = 0 Multiplicity = 1

SCF Energy= -2422.84595680 Predicted Change= -1.149442D-08

==========

Optimization completed. {Found 2 times}

Item	Max Val.	Criteria	Pass?	RMS Val.	Criteria	Pass?
Force	0.00001	0.00045	[YES]	0.00000	0.00030	[YES]
Displ	0.00159	0.00180	[YES]	0.00159	0.00180	[YES]

Atomic Type	Coordinates (Angstroms) X	Y	Z
C	-5.902990	-1.454464	-0.805916
H	-6.564251	-1.072555	-1.599830
C	-4.948962	-0.332936	-0.375858
C	-4.162845	0.240721	-1.565042
H	-3.543329	-0.565530	-1.974887
H	-4.838149	0.558849	-2.367708
C	-3.263836	1.408576	-1.179024
H	-3.000673	1.349479	-0.122072
O	-4.045176	-0.800489	0.627910
H	-3.615795	-1.582131	0.243873
H	-5.539119	0.460704	0.097855
O	-5.096960	-2.526585	-1.333539
C	-5.617608	-3.814568	-0.939155
C	-4.545888	-4.559552	-0.120164
H	-4.364815	-4.024850	0.817254
C	-3.279321	-4.743449	-0.909725
H	-3.397815	-5.303951	-1.837024
C	-2.051879	-4.267605	-0.627941
H	-1.256506	-4.469320	-1.345445
C	-1.653519	-3.492716	0.541362
H	-2.380639	-3.381506	1.342834
C	-0.439272	-2.927747	0.677155
C	0.042643	-2.093642	1.843425
H	1.089382	-2.375618	2.028049
C	-0.736894	-2.342608	3.143734
H	-1.775311	-2.004042	3.060900
H	-0.279772	-1.792657	3.972182
H	-0.745784	-3.405352	3.403296
C	0.010126	-0.578636	1.512926
H	0.348161	-0.016986	2.393204
H	-1.032177	-0.291584	1.330526
C	0.836327	-0.106555	0.313958
H	0.513598	-0.643364	-0.594980
H	0.275122	-3.060530	-0.136669
H	-4.949918	-5.546250	0.145543
H	-5.806231	-4.389450	-1.856209
C	-6.954522	-3.514436	-0.210224
C	-7.404427	-4.527203	0.842721
H	-7.516531	-5.529484	0.415492
H	-8.375042	-4.236014	1.256542
H	-6.696145	-4.590528	1.674687
H	-7.729953	-3.464491	-0.986241
C	-6.728625	-2.087131	0.313130
H	-6.145596	-2.096985	1.240581
H	-7.663139	-1.550299	0.498548
C	-2.001668	1.576122	-2.031923
H	-1.187357	0.986218	-1.619628
H	-2.190422	1.259772	-3.063068
C	-1.757360	3.088204	-2.052903
O	-1.278996	3.512925	-3.319485
H	-1.580724	4.429503	-3.433984
C	-3.190283	3.624410	-1.839206
O	-3.550711	4.750800	-2.103568
O	-3.999570	2.673534	-1.352295
C	2.351143	-0.280567	0.482483
H	2.613963	-1.340313	0.545555
H	2.663234	0.201350	1.417492
C	3.100719	0.372148	-0.684270
O	4.525601	0.385074	-0.490845
C	5.226494	-0.775285	-0.867581
H	4.789661	-1.205393	-1.778269
H	2.882695	-0.186397	-1.608594
C	2.656648	1.823680	-0.856448
H	3.127017	2.257202	-1.745505
H	2.990270	2.400511	0.014642
C	1.127201	1.911424	-0.964996
C	0.656248	3.367816	-1.025591
H	1.126635	3.927342	-0.210664
H	1.028037	3.800306	-1.960208
C	-0.844961	3.690954	-0.955956
O	-1.439298	3.325486	0.313446
C	-1.245286	4.158856	1.364539
O	-0.616730	5.195264	1.290725
C	-1.905400	3.608811	2.608759
H	-1.460663	2.623605	2.800295
H	-2.958749	3.413706	2.371628
C	-1.771029	4.523830	3.826892
H	-2.214218	5.498539	3.594377
H	-0.708865	4.711972	4.018461
C	-2.432207	3.931222	5.074022
H	-3.503077	3.761746	4.915041
H	-2.324916	4.602062	5.931949
H	-1.981672	2.969476	5.344134
H	-0.929586	4.779134	-1.050751
H	0.820396	1.385652	-1.884727
O	0.509613	1.282458	0.158688
O	5.151486	-1.823182	0.082794
C	5.725009	-1.513855	1.373301
H	5.206148	-0.638413	1.786853
C	5.486727	-2.723986	2.261090
H	4.419163	-2.953399	2.314303
H	5.849713	-2.525349	3.274053
H	6.018837	-3.593360	1.868729
C	7.211312	-1.149693	1.223974
O	8.023210	-2.261473	0.844206
H	7.746158	-2.505165	-0.056302
H	7.591758	-0.823313	2.198275
C	7.376998	0.002638	0.215048
O	8.742144	0.325070	0.025462
H	9.181064	-0.527130	-0.123841
H	6.886391	0.896594	0.612831
C	6.688095	-0.351695	-1.115167
O	7.418612	-1.434301	-1.696890
C	7.304690	-1.550522	-3.110223
H	6.279529	-1.780441	-3.427456
H	7.957647	-2.370868	-3.413697
H	7.630594	-0.626927	-3.606004
H	6.706350	0.516180	-1.786307

Statistical Thermodynamic Analysis
Temperature= 298.150 Kelvin Pressure= 1.00000 Atm

==========

SCF Energy= -2422.84595680 Predicted Change= -1.149442D-08
Zero-point correction (ZPE)= -2421.9110 0.93494
Internal Energy (U)= -2421.8591 0.98679
Enthalpy (H)= -2421.8582 0.98773
Gibbs Free Energy (G)= -2422.0007 0.84521

Frequencies -- 11.5395 14.7024 17.0163

NMR-Shifts
Revised-MandelalideB-0002-NMR.txt

Atom	Type	Isotropic	Scaled Shift
1	C	100.5560	81.8392388828
3	C	114.2981	68.6861348801
4	C	142.5578	41.6376653458
7	C	106.0078	76.6211068359
13	C	102.0838	80.3769214571
14	C	152.4457	32.173567641
16	C	48.9702	131.214035491
18	C	50.1653	130.070158311
20	C	58.6015	121.995539731
22	C	38.1405	141.57956699
23	C	151.7074	32.8802235877
25	C	166.9565	18.2847106568
29	C	137.4428	46.5334328758
32	C	111.1752	71.6751852065
37	C	145.1812	39.1267061008
38	C	173.1488	12.3578169567
43	C	150.3777	34.1529317177
46	C	144.9416	39.3560366776
49	C	105.3719	77.2297517181
52	C	-2.8784	180.840368307
55	C	146.4409	37.920997722
58	C	103.6114	78.9147954593
60	C	83.9491	97.7343555581
63	C	145.4665	38.8536342579
66	C	112.1289	70.7623614541
67	C	151.3467	33.225463734
70	C	107.2124	75.4681368326
72	C	5.0840	173.219242329
74	C	148.1908	36.2460996573
77	C	166.3893	18.8276000689
80	C	172.6745	12.8117881276
88	C	114.9319	68.0794999904
90	C	169.9732	15.3973085243
94	C	109.6872	73.0994084879
98	C	118.0537	65.0915025173
102	C	101.1558	81.2651467295
104	C	128.2227	55.3583529547
2	H	27.6931	3.83414183414
5	H	29.9126	1.78332178332
6	H	29.8854	1.80845460845
8	H	26.4756	4.95911295911
10	H	30.7738	0.987572187572
11	H	28.2165	3.35051975052
15	H	29.3150	2.3355047355
17	H	26.1930	5.22023562024
19	H	25.1027	6.22767382767
21	H	25.0212	6.30297990298
24	H	29.2788	2.36895356895
26	H	30.4883	1.25137445137
27	H	30.7936	0.969276969277
28	H	30.6164	1.13300993301
30	H	30.1065	1.60415800416
31	H	30.0312	1.67373527374
33	H	28.2886	3.2838992839
34	H	25.2141	6.12474012474
35	H	29.7361	1.94640794641
36	H	27.5845	3.93448833449
39	H	30.7555	1.00448140448
40	H	30.5354	1.20785400785
41	H	30.8719	0.896927696928
42	H	29.1495	2.48842688843
44	H	29.8356	1.85446985447
45	H	29.8892	1.80494340494
47	H	28.9815	2.64365904366
48	H	29.7298	1.95222915223
51	H	29.6683	2.00905520906
56	H	29.0362	2.59311619312
57	H	30.6331	1.11757911758
61	H	26.4174	5.01288981289
62	H	28.0196	3.53245553246
64	H	29.9690	1.73120813121
65	H	30.6634	1.08958188958
68	H	29.5485	2.11975051975
69	H	29.7906	1.89604989605
75	H	29.3937	2.26278586279
76	H	29.3984	2.25844305844
78	H	30.2672	1.45567105567
79	H	30.1933	1.52395472395
81	H	30.9701	0.806190806191
82	H	30.6095	1.13938553939
83	H	30.9729	0.803603603604
84	H	26.7531	4.7027027027
85	H	27.8710	3.66976206976
89	H	27.6254	3.8966966967
91	H	30.5223	1.21995841996
92	H	30.8671	0.901362901363
93	H	30.1302	1.58225918226
96	H	29.7285	1.95343035343
97	H	28.2626	3.30792330792
100	H	29.1080	2.52677292677
101	H	28.1060	3.45262185262
105	H	28.1344	3.42638022638
106	H	28.1340	3.42674982675
107	H	28.6051	2.99145299145
108	H	28.2850	3.28722568723

Supporting Information: Revised-MandelalideB-0003.log

Using Gaussian 09: AM64L-G09RevC.01 23-Sep-2011

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#b3lyp/6-31G(d,p) scf=(maxcycle=300,direct,tight) density=current SCRF=(PCM,SOLVENT=Chloroform) opt=(maxcycle=250) freq=noraman

#N Geom=AllCheck Guess=TCheck SCRF=Check GenChk RB3LYP/6-31G(d,p) Freq

---

Pointgroup= C1 Stoichiometry= C37H58O13 C1[X(C37H58O13)] #Atoms= 108

Charge = 0 Multiplicity = 1

SCF Energy= -2422.84635293 Predicted Change= -1.531123D-08

==========

Optimization completed. {Found 1 times}

Item	Max Val.	Criteria	Pass?	RMS Val.	Criteria	Pass?
Force	0.00001	0.00045	[YES]	0.00000	0.00030	[YES]
Displ	0.00626	0.00180	[NO]	0.00626	0.00180	[YES]

Atomic Type	Coordinates (Angstroms) X	Y	Z
C	-5.897609	-1.325004	-1.071959
H	-6.425900	-1.006088	-1.984372
C	-4.948910	-0.202778	-0.631583
C	-3.981454	0.206188	-1.753048
H	-3.361393	-0.665575	-1.992262
H	-4.525757	0.467892	-2.667779
C	-3.072688	1.365568	-1.364126
H	-2.959204	1.408108	-0.280049
O	-4.213031	-0.596272	0.528963
H	-3.789423	-1.436926	0.290610

H	-5.551717	0.661041	-0.326473
O	-5.087261	-2.478706	-1.368789
C	-5.733632	-3.696306	-0.939072
C	-4.822661	-4.414067	0.074862
H	-4.727097	-3.802215	0.976986
C	-3.482227	-4.736119	-0.525616
H	-3.520042	-5.378622	-1.405305
C	-2.272177	-4.292812	-0.136501
H	-1.409525	-4.600558	-0.727463
C	-1.971893	-3.427708	0.998109
H	-2.780561	-3.209021	1.692095
C	-0.752192	-2.906736	1.228443
C	-0.361325	-1.989087	2.365582
H	0.637294	-2.303192	2.702051
C	-1.302542	-2.073504	3.576985
H	-1.407664	-3.104838	3.926443
H	-2.300823	-1.692075	3.336838
H	-0.913116	-1.470863	4.403301
C	-0.262985	-0.512509	1.900581
H	0.004309	0.113098	2.761779
H	-1.257470	-0.192128	1.568263
C	0.722511	-0.198288	0.772407
H	0.471528	-0.799102	-0.118736
H	0.042168	-3.148415	0.520571
H	-5.319720	-5.347996	0.370994
H	-5.839235	-4.344350	-1.820030
C	-7.133057	-3.263739	-0.422834
C	-7.765682	-4.140379	0.658525
H	-8.763093	-3.767397	0.911961
H	-7.171296	-4.144939	1.577555
H	-7.877920	-5.176630	0.322020
H	-7.802072	-3.263390	-1.293592
C	-6.896796	-1.799587	-0.017945
H	-6.440980	-1.735775	0.976221
H	-7.815630	-1.206653	-0.015180
C	-1.698325	1.379233	-2.042778
H	-0.985661	0.799164	-1.462380
H	-1.764792	0.962683	-3.053214
C	-1.359118	2.866558	-2.180268
O	-0.693764	3.130342	-3.405712
H	-0.919064	4.043706	-3.649215
C	-2.770755	3.492498	-2.221204
O	-3.019853	4.601802	-2.640903
O	-3.697171	2.638739	-1.764714
C	2.194699	-0.437521	1.132328
H	2.377909	-1.502408	1.310632
H	2.431453	0.101255	2.058375
C	3.112795	0.063545	0.019051
O	4.470898	-0.070647	0.480111
C	5.438003	-0.223972	-0.533711
H	5.280676	0.500795	-1.341818
H	2.981301	-0.566467	-0.871071
C	2.786056	1.520909	-0.321570
H	3.375165	1.865443	-1.178999
H	3.043909	2.150664	0.538429
C	1.288486	1.673802	-0.629938
C	0.916410	3.138429	-0.877862
H	1.313509	3.749713	-0.061285
H	1.426894	3.461412	-1.790960
C	-0.560290	3.536762	-1.035036
O	-1.330836	3.330590	0.173826
C	-1.213914	4.251428	1.161416
O	-0.511384	5.238440	1.077025
C	-2.061642	3.866239	2.352825
H	-1.704134	2.888082	2.700280
H	-3.084787	3.694441	1.995935
C	-2.033007	4.897989	3.481535
H	-2.383161	5.862137	3.096022
H	-0.995566	5.056280	3.796140
C	-2.885610	4.472749	4.679720
H	-2.850074	5.225258	5.473447
H	-2.533733	3.524982	5.102644
H	-3.935082	4.338239	4.394553
H	-0.568307	4.612251	-1.243930
H	1.062961	1.078099	-1.529991
O	0.505686	1.185693	0.460637
O	5.367819	-1.481083	-1.179458
C	5.609153	-2.619170	-0.321937
H	4.870293	-2.611425	0.491164
C	5.423241	-3.860620	-1.178390
H	6.177441	-3.893969	-1.967679
H	4.429587	-3.861969	-1.634144
H	5.525572	-4.760792	-0.564733
C	7.005158	-2.517520	0.314461
O	8.061970	-2.672239	-0.633219
H	8.013579	-1.900487	-1.223973
H	7.125821	-3.337732	1.030932
C	7.150686	-1.178763	1.063307
O	8.444332	-1.042102	1.621108
H	9.052249	-1.262816	0.898048
H	6.437606	-1.156209	1.893393
C	6.811045	-0.003736	0.127541
O	7.829600	0.051835	-0.874462
C	8.030933	1.333050	-1.459702
H	7.146231	1.684143	-2.005888
H	8.859981	1.232920	-2.162601
H	8.293117	2.075437	-0.694807
H	6.795286	0.932509	0.699386

Statistical Thermodynamic Analysis
Temperature= 298.150 Kelvin Pressure= 1.00000 Atm
==========
==========
SCF Energy= -2422.84635293 Predicted Change= -1.531123D-08
Zero-point correction (ZPE)= -2421.9113 0.93502
Internal Energy (U)= -2421.8594 0.98688
Enthalpy (H)= -2421.8585
0.98783
Gibbs Free Energy (G)= -2422.0016
0.84469

Frequencies -- 10.0871 11.3845 15.9724

NMR-Shifts
Revised-MandelalideB-0003-NMR.txt

Atom	Type	Isotropic	Scaled Shift
1	C	100.9721	81.4409732192
3	C	114.6277	68.3706617661
4	C	142.6917	41.5095043933
7	C	106.1321	76.5021344206
13	C	102.3322	80.1391680545
14	C	152.1799	32.4279752675
16	C	49.3189	130.880281016
18	C	50.1981	130.038764142
20	C	56.4731	124.032715021
22	C	38.4904	141.244663948
23	C	150.7602	33.7868259346
25	C	167.2261	18.026665901
29	C	137.5789	46.4031662168
32	C	110.8610	71.9759183752
37	C	145.5940	38.7315989969
38	C	172.5459	12.9348762419
43	C	150.3281	34.2004058271
46	C	145.0750	39.2283542947
49	C	105.6117	77.0002297134
52	C	-2.8475	180.810792703
55	C	147.9598	36.4671988361
58	C	113.4216	69.5250674783

60	C	91.1551	90.8372097475
63	C	147.4528	36.9524684623
66	C	112.0191	70.8674553495
67	C	151.2021	33.3638660771
70	C	107.4888	75.2035835295
72	C	5.1899	173.117881276
74	C	148.1337	36.3007523115
77	C	166.3419	18.8729684718
80	C	172.8839	12.6113631578
88	C	115.3005	67.7266984437
90	C	170.0003	15.3713700492
94	C	109.8490	72.9445433488
98	C	117.7796	65.3538544
102	C	102.0223	80.4357855242
104	C	128.1812	55.3980742357
2	H	27.7358	3.79468699469
5	H	30.0320	1.672996073
6	H	30.0196	1.68445368445
8	H	26.5166	4.92122892123
10	H	30.8253	0.939986139986
11	H	28.1737	3.39006699007
15	H	29.2170	2.42605682606
17	H	26.1169	5.29055209055
19	H	25.0628	6.26454146454
21	H	24.8705	6.44222684223
24	H	29.3542	2.29928389928
26	H	30.6100	1.13892353892
27	H	30.5549	1.18983598984
28	H	30.7483	1.01113421113
30	H	30.1226	1.58928158928
31	H	30.1303	1.58216678217
33	H	28.2779	3.29378609379
34	H	25.2588	6.08343728344
35	H	29.7549	1.92903672904
36	H	27.6072	3.91351351351
39	H	30.5355	1.20776160776
40	H	30.9034	0.867821667822
41	H	30.7028	1.05317625318
42	H	29.1027	2.53167013167
44	H	29.8117	1.87655347655
45	H	29.9912	1.7106953107
47	H	28.9766	2.64818664819
48	H	29.7892	1.89734349734
51	H	29.6471	2.02864402864
56	H	29.7009	1.97893277893
57	H	30.7248	1.03284823285
61	H	26.4171	5.01316701317
62	H	27.6447	3.87886347886
64	H	29.7478	1.9355971356
65	H	30.8941	0.876414876415
68	H	29.5477	2.12048972049
69	H	29.7314	1.95075075075
75	H	29.4035	2.25373065373
76	H	29.3824	2.27322707323
78	H	30.2451	1.47609147609
79	H	30.1967	1.52081312081
81	H	30.5678	1.17791637792
82	H	31.0027	0.776068376068
83	H	30.9752	0.801478401478
84	H	26.7547	4.70122430122
85	H	27.9969	3.55343035343
89	H	27.6544	3.8699006699
91	H	30.0939	1.6158004158
92	H	30.6026	1.14576114576
93	H	30.8330	0.932871332871
96	H	29.7511	1.93254793255
97	H	28.2331	3.33518133518
100	H	29.1232	2.51272811273
101	H	28.0689	3.4869022869
105	H	28.1694	3.39404019404
106	H	28.1769	3.38711018711
107	H	28.6423	2.95708015708
108	H	28.3893	3.19085239085

Supporting Information: Revised-MandelalideB-0004.log

```
-----------------------------------------------------------------------
 Using  Gaussian 09:  AM64L-G09RevC.01 23-Sep-2011
=======================================================================
 #b3lyp/6-31G(d,p) scf=(maxcycle=300,direct,tight) density=current
 SCRF=(PCM,SOLVENT=Chloroform) opt=(maxcycle=250)
freq=noraman
 #N Geom=AllCheck Guess=TCheck SCRF=Check GenChk RB3LYP/6-
31G(d,p) Freq
-----------------------------------------------------------------------
 Pointgroup= C1   Stoichiometry= C37H58O13   C1[X(C37H58O13)]
#Atoms= 108
 Charge = 0                Multiplicity = 1
-----------------------------------------------------------------------
 SCF Energy= -2422.85096883      Predicted Change= -1.300864D-08
=======================================================================
 Optimization completed.          {Found       1       times}
 Item      Max Val.    Criteria    Pass?      RMS Val.    Criteria    Pass?
 Force      0.00000 ||  0.00045   [ YES ]      0.00000 ||  0.00030   [ YES ]
 Displ      0.00185 ||  0.00180   [ NO ]       0.00185 ||  0.00180   [ YES ]
-----------------------------------------------------------------------
     Atomic      Coordinates (Angstroms)
      Type      X                  Y                Z
-----------------------------------------------------------------------
      C      -6.912387     -0.195412     -0.259042
      H      -7.504147      0.592363     -0.743844
      C      -5.430480      0.193732     -0.282855
      C      -5.099331      1.535878      0.371657
      H      -5.483337      2.350135     -0.254261
      H      -5.572363      1.614801      1.356551
      C      -3.594704      1.703189      0.524938
      H      -3.110911      1.482761     -0.429992
      O      -4.963792      0.253791     -1.627745
      H      -5.201713     -0.600518     -2.020727
      H      -4.890298     -0.590468      0.266886
      O      -7.051768     -1.388128     -1.071352
      C      -7.489373     -2.500269     -0.269294
      C      -6.301724     -3.400265      0.143730
      H      -5.580201     -2.819166      0.725526
      C      -5.652208     -4.075490     -1.034423
      H      -6.267265     -4.835991     -1.515623
      C      -4.436302     -3.842765     -1.566009
      H      -4.148913     -4.434386     -2.435491
      C      -3.459328     -2.849349     -1.140842
      H      -3.683235     -2.266534     -0.249902
      C      -2.321688     -2.580317     -1.806132
      C      -1.363070     -1.465778     -1.472653
      H      -1.740517     -0.946350     -0.585107
      C      -1.330351     -0.457513     -2.640518
      H      -0.717941      0.417259     -2.404542
      H      -2.344126     -0.106528     -2.854916
      H      -0.931487     -0.920316     -3.551724
      C       0.036080     -2.025841     -1.121417
      H       0.406131     -2.643786     -1.950788
      H      -0.059995     -2.689167     -0.253162
      C       1.102551     -0.971025     -0.819163
      H       1.304666     -0.384001     -1.730174
      H      -2.084423     -3.163794     -2.699425
      H      -6.692112     -4.177887      0.813617
      H      -8.162745     -3.091320     -0.902233
      C      -8.271503     -1.836339      0.887169
      C      -8.526791     -2.686158      2.131423
```

H	-9.060801	-3.609378	1.881880
H	-9.141172	-2.134594	2.850211
H	-7.594814	-2.959825	2.635882
H	-9.241016	-1.541088	0.465332
C	-7.456831	-0.552765	1.133315
H	-6.634455	-0.753769	1.831757
H	-8.062041	0.250200	1.561768
C	-3.080768	3.019248	1.123594
H	-2.937503	3.794576	0.369599
H	-3.769768	3.393985	1.887467
C	-1.778182	2.585344	1.815130
O	-1.446066	3.386311	2.928850
H	-1.133357	2.779164	3.619829
C	-2.172360	1.172712	2.273818
O	-1.722436	0.594170	3.238417
O	-3.127667	0.673058	1.477615
C	2.421526	-1.589194	-0.331886
H	2.849713	-2.228537	-1.111687
H	2.221958	-2.218308	0.544147
C	3.420982	-0.501053	0.058294
O	4.566752	-1.145983	0.648583
C	5.790997	-0.471998	0.472639
H	5.684661	0.599571	0.682604
H	3.746724	0.030888	-0.845541
C	2.782011	0.488671	1.040029
H	3.457870	1.327834	1.242321
H	2.590769	-0.026990	1.988736
C	1.457958	1.011558	0.470949
C	0.696929	1.917768	1.439872
H	0.462524	1.329139	2.332164
H	1.328991	2.752517	1.756443
C	-0.594944	2.474127	0.819091
O	-0.360843	3.816789	0.316040
C	-0.143416	3.979401	-1.011357
O	-0.101263	3.064920	-1.810918
C	0.005377	5.448808	-1.352167
H	0.561070	5.936658	-0.544076
H	-1.005347	5.877295	-1.321595
C	0.654412	5.701408	-2.717103
H	0.534876	6.763677	-2.958364
H	0.104260	5.140502	-3.479956
C	2.138746	5.326238	-2.767678
H	2.715624	5.891586	-2.026805
H	2.563059	5.539761	-3.753642
H	2.282355	4.260144	-2.567570
H	-0.886797	1.843764	-0.022896
H	1.657019	1.558857	-0.464570
O	0.583665	-0.085079	0.180198
O	6.260115	-0.516980	-0.862126
C	6.532582	-1.845410	-1.362508
H	5.613308	-2.442611	-1.294312
C	6.943590	-1.691135	-2.817353
H	6.165242	-1.166106	-3.377319
H	7.095865	-2.674633	-3.272299
H	7.877024	-1.128734	-2.891195
C	7.600039	-2.529114	-0.492535
O	8.887936	-1.924284	-0.615243
H	8.804944	-1.030473	-0.239661
H	7.723234	-3.563333	-0.832863
C	7.153645	-2.541304	0.982396
O	8.141913	-3.124248	1.811303
H	8.968725	-2.683546	1.559798
H	6.251764	-3.154198	1.075474
C	6.796677	-1.116186	1.444953
O	8.009548	-0.359057	1.463293
C	8.014578	0.751826	2.351886
H	7.815845	0.429462	3.382222
H	7.276155	1.513294	2.070016
H	9.011166	1.194063	2.299619
H	6.360865	-1.151514	2.451407

Statistical Thermodynamic Analysis
Temperature= 298.150 Kelvin Pressure= 1.00000 Atm
==========
SCF Energy= -2422.85096883 Predicted Change= -1.300864D-08
Zero-point correction (ZPE)= -2421.9157 0.93519
Internal Energy (U)= -2421.8641 0.98680
Enthalpy (H)= -2421.8632
0.98774
Gibbs Free Energy (G)= -2422.0040
0.84689

Frequencies -- 12.6858 16.2504 20.6561

NMR-Shifts
Revised-MandelalideB-0004-NMR.txt

Atom	Type	Isotropic	Scaled Shift
1	C	100.5851	81.8113861291
3	C	109.9822	72.8170523938
4	C	148.0882	36.3443021497
7	C	107.5282	75.165872241
13	C	100.4573	81.9337085319
14	C	152.6444	31.9833840617
16	C	52.0480	128.268152147
18	C	49.2466	130.949482188
20	C	58.1393	122.437929516
22	C	36.1625	143.47278853
23	C	147.8489	36.5733455847
25	C	168.5484	16.7610406018
29	C	142.9583	41.2543310553
32	C	111.0338	71.8105247038
37	C	143.9542	40.3011160244
38	C	172.5606	12.9208062941
43	C	150.2004	34.3226325159
46	C	144.6329	39.6515055801
49	C	103.5491	78.9744252378
52	C	0.4611	177.644001608
55	C	145.9806	38.3615689427
58	C	112.1146	70.7760485461
60	C	91.0283	90.958575011
63	C	148.5651	35.8878424166
66	C	111.0219	71.8219146615
67	C	147.8010	36.6191925573
70	C	114.0826	68.8923983997
72	C	4.1336	174.128907521
74	C	149.7052	34.7966078983
77	C	166.1668	19.0405635636
80	C	173.1649	12.3424070139
88	C	115.3050	67.7223913168
90	C	170.0235	15.3491644174
94	C	109.7553	73.0342273014
98	C	118.2973	64.8583433833
102	C	101.8462	80.6043377553
104	C	127.9667	55.603380616
2	H	27.7850	3.74922614923
5	H	30.1928	1.52441672442
6	H	30.1907	1.52635712636
8	H	26.6518	4.7963039963
10	H	29.3336	2.31831831832
11	H	27.8573	3.68242088242
15	H	29.3227	2.32838992839
17	H	26.1263	5.28186648187
19	H	25.3299	6.01774081774
21	H	24.9296	6.38761838762
24	H	28.9893	2.63645183645
26	H	29.9114	1.78443058443
27	H	30.6606	1.09216909217

28	H	31.1895	0.603465003465
30	H	30.5235	1.21884961885
31	H	30.2031	1.5148995149
33	H	28.0339	3.51924231924
34	H	25.8433	5.54335874336
35	H	29.8370	1.85317625318
36	H	27.8415	3.69702009702
39	H	30.6623	1.0905982906
40	H	30.4964	1.24389004389
41	H	30.9927	0.785308385308
42	H	29.1502	2.48778008778
44	H	30.3212	1.40577500578
45	H	29.7242	1.9574035574
47	H	29.2407	2.40415800416
48	H	29.8007	1.88671748672
51	H	29.1835	2.45701085701
56	H	29.9861	1.71540771541
57	H	30.5515	1.19297759298
61	H	26.4409	4.99117579118
62	H	27.6224	3.89946869947
64	H	29.9291	1.76807576808
65	H	30.8204	0.944513744514
68	H	29.6517	2.02439362439
69	H	30.1967	1.52081312081
75	H	29.4443	2.21603141603
76	H	29.1024	2.53194733195
78	H	30.2961	1.42896742897
79	H	29.7841	1.90205590206
81	H	31.1597	0.631000231
82	H	30.6829	1.07156387156
83	H	30.6736	1.08015708016
84	H	25.8113	5.57292677293
85	H	28.1276	3.43266343266
89	H	27.6786	3.84753984754
91	H	30.6701	1.08339108339
92	H	30.8615	0.906537306537
93	H	30.1202	1.5914991915
96	H	29.7841	1.90205590206
97	H	28.2809	3.29101409101
100	H	29.0772	2.55523215523
101	H	28.1690	3.39440979441
105	H	28.6789	2.92326172326
106	H	28.2019	3.36401016401
107	H	28.1763	3.38766458766
108	H	28.3629	3.21524601525

Supporting Information: Revised-MandelalideB-0005.log

Using Gaussian 09: AM64L-G09RevC.01 23-Sep-2011

==========

#b3lyp/6-31G(d,p) scf=(maxcycle=300,direct,tight) density=current SCRF=(PCM,SOLVENT=Chloroform) opt=(maxcycle=250) freq=noraman

#N Geom=AllCheck Guess=TCheck SCRF=Check GenChk RB3LYP/6-31G(d,p) Freq

---

Pointgroup= C1 Stoichiometry= C37H58O13 C1[X(C37H58O13)] #Atoms= 108

Charge = 0 Multiplicity = 1

SCF Energy= -2422.85102635 Predicted Change= -4.276799D-08

==========

Optimization completed. {Found 1 times}

Item	Max Val.	Criteria	Pass?	RMS Val.	Criteria	Pass?
Force	0.00001	0.00045	[YES]	0.00000	0.00030	[YES]
Displ	0.00605	0.00180	[NO]	0.00605	0.00180	[YES]

Atomic Type	Coordinates (Angstroms) X	Y	Z
C	-6.794151	-0.407770	-0.168889
H	-7.412008	0.374349	-0.629844
C	-5.324714	0.025629	-0.192189
C	-5.029062	1.360784	0.492994
H	-5.449522	2.177559	-0.105657
H	-5.490091	1.397509	1.486036
C	-3.528709	1.575581	0.628416
H	-3.053079	1.393522	-0.338680
O	-4.870806	0.133176	-1.538463
H	-5.082402	-0.718937	-1.950778
H	-4.757070	-0.755429	0.334083
O	-6.903377	-1.583153	-1.010308
C	-7.312513	-2.725792	-0.237174
C	-6.103169	-3.608402	0.149597
H	-5.394073	-3.025184	0.744506
C	-5.441061	-4.237833	-1.046808
H	-6.035829	-5.005653	-1.541655
C	-4.236331	-3.955882	-1.579916
H	-3.936276	-4.518306	-2.464353
C	-3.288209	-2.942204	-1.137661
H	-3.523992	-2.388558	-0.231412
C	-2.165105	-2.620698	-1.804253
C	-1.239733	-1.483856	-1.452485
H	-1.626657	-0.995165	-0.551596
C	-1.247456	-0.450276	-2.598450
H	-2.273443	-0.128277	-2.799049
H	-0.839358	-0.879533	-3.521875
H	-0.662684	0.438701	-2.346381
C	0.179038	-2.007187	-1.123814
H	0.556263	-2.604910	-1.964698
H	0.113031	-2.682635	-0.262157
C	1.219067	-0.925908	-0.823724
H	1.390234	-0.322429	-1.730311
H	-1.916432	-3.174868	-2.712991
H	-6.474141	-4.411158	0.800438
H	-7.973985	-3.315644	-0.883656
C	-8.105693	-2.111530	0.938956
C	-8.336202	-3.000257	2.160774
H	-7.396073	-3.265474	2.654568
H	-8.849319	-3.928739	1.887955
H	-8.960770	-2.483161	2.896240
H	-9.083453	-1.827709	0.528421
C	-7.320019	-0.816242	1.216533
H	-6.488358	-1.016986	1.904023
H	-7.941135	-0.040173	1.670967
C	-3.049888	2.894583	1.249019
H	-2.946146	3.690895	0.510558
H	-3.738529	3.228400	2.031933
C	-1.722060	2.490226	1.909992
O	-1.399434	3.275779	3.037463
H	-1.058530	2.663155	3.710020
C	-2.060349	1.054677	2.341523
O	-1.575142	0.470632	3.285513
O	-3.011760	0.540788	1.549787
C	2.562265	-1.512225	-0.364370
H	2.995129	-2.131365	-1.157741
H	2.394600	-2.155398	0.508092
C	3.537170	-0.400722	0.020848
O	4.710520	-1.019344	0.584626
C	5.913787	-0.313914	0.388966
H	5.785970	0.752913	0.611003
H	3.832286	0.149555	-0.882405
C	2.887488	0.559520	1.024566
H	3.542557	1.415485	1.224835
H	2.728030	0.027937	1.970366
C	1.538548	1.050534	0.485715

C	0.769031	1.920019	1.481493
H	0.570643	1.312557	2.369933
H	1.381229	2.769533	1.797729
C	-0.551766	2.444015	0.893888
O	-0.375957	3.805457	0.418215
C	-0.176826	4.003218	-0.907031
O	-0.134839	3.109373	-1.729782
C	0.019435	5.475999	-1.207132
H	1.057954	5.709654	-0.936366
H	-0.608035	6.058490	-0.524488
C	-0.247411	5.840222	-2.672060
H	0.362712	5.195142	-3.313020
H	0.097142	6.867434	-2.835949
C	-1.721783	5.719463	-3.069163
H	-2.352007	6.375080	-2.457377
H	-2.078630	4.692487	-2.944512
H	-1.870023	5.997991	-4.117091
H	-0.834688	1.823472	0.041655
H	1.704515	1.616811	-0.445060
O	0.691242	-0.067072	0.194691
O	6.355240	-0.335860	-0.955779
C	6.648735	-1.652861	-1.474413
H	5.745372	-2.272340	-1.393507
C	7.026260	-1.475240	-2.935646
H	7.944614	-0.890327	-3.022556
H	6.224693	-0.963459	-3.474713
H	7.192229	-2.450503	-3.403346
C	7.749518	-2.319523	-0.633307
O	9.020768	-1.685057	-0.778165
H	8.926614	-0.796389	-0.393126
H	7.888502	-3.347732	-0.985571
C	7.334886	-2.354590	0.850403
O	8.353590	-2.921631	1.653101
H	9.164602	-2.459996	1.388073
H	6.449438	-2.988926	0.956649
C	6.955423	-0.942277	1.333369
O	8.150625	-0.157512	1.332177
C	8.149467	0.946210	2.229667
H	7.389206	1.693566	1.968879
H	9.134993	1.410484	2.161162
H	7.978617	0.611570	3.261093
H	6.542749	-0.996429	2.348705

Statistical Thermodynamic Analysis
Temperature= 298.150 Kelvin Pressure= 1.00000 Atm
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SCF Energy= -2422.85102635 Predicted Change= -4.276799D-08
Zero-point correction (ZPE)= -2421.9156 0.93540
Internal Energy (U)= -2421.8640 0.98694
Enthalpy (H)= -2421.8631
0.98789
Gibbs Free Energy (G)= -2422.0040
0.84694

Frequencies -- 12.7802 14.3833 17.2766

NMR-Shifts
Revised-MandelalideB-0005-NMR.txt

Atom	Type	Isotropic	Scaled Shift
1	C	100.3812	82.0065468328
3	C	110.0431	72.7587626103
4	C	148.0282	36.4017305079
7	C	107.6163	75.0815482685
13	C	100.2113	82.1691648002
14	C	152.7133	31.9174371638
16	C	52.0208	128.294186336
18	C	49.2185	130.976377802
20	C	57.9259	122.642183043
22	C	35.9177	143.707096231
23	C	147.8956	36.5286471793
25	C	168.6617	16.6525967189
29	C	142.8788	41.3304236299
32	C	110.9493	71.8914029748
37	C	143.6112	40.629414805
38	C	172.3320	13.1396083386
43	C	150.2068	34.3165068244
46	C	144.5210	39.758609468
49	C	103.5817	78.9432224966
52	C	0.5008	177.606003178
55	C	145.9330	38.4071287735
58	C	112.0856	70.8038055859
60	C	91.0917	90.8978923793
63	C	148.5394	35.9124408966
66	C	110.8980	71.940504221
67	C	147.9026	36.5219472042
70	C	114.2947	68.6893891537
72	C	4.2318	174.034916442
74	C	148.9659	35.5042209843
77	C	166.2550	18.9561438772
80	C	173.2338	12.276460116
88	C	115.4404	67.5927946553
90	C	170.0688	15.305806007
94	C	109.8462	72.9472233389
98	C	118.3468	64.8109649878
102	C	101.9940	80.4628725665
104	C	127.9686	55.6015620513
2	H	27.7627	3.76983136983
5	H	30.2038	1.51425271425
6	H	30.2111	1.50750750751
8	H	26.5991	4.844998845
10	H	29.3068	2.34308154308
11	H	27.8438	3.69489489489
15	H	29.3371	2.31508431508
17	H	26.1179	5.28962808963
19	H	25.3131	6.03326403326
21	H	24.8707	6.44204204204
24	H	29.0058	2.62120582121
26	H	30.6268	1.1234003234
27	H	31.1613	0.629521829522
28	H	29.9132	1.78276738277
30	H	30.5480	1.19621159621
31	H	30.1823	1.53411873412
33	H	28.0807	3.475999076
34	H	25.8040	5.57967197967
35	H	29.8400	1.8504042504
36	H	27.7975	3.73767613768
39	H	30.9648	0.811088011088
40	H	30.6381	1.11295911296
41	H	30.4715	1.2668976669
42	H	29.1066	2.52806652807
44	H	30.3505	1.3787017787
45	H	29.7239	1.95768075768
47	H	29.1821	2.4583044583
48	H	29.7511	1.93254793255
51	H	29.1637	2.47530607531
56	H	29.9983	1.70413490413
57	H	30.5562	1.18863478863
61	H	26.4866	4.94894894895
62	H	27.6152	3.90612150612
64	H	29.9496	1.74913374913
65	H	30.8261	0.939246939247
68	H	29.6791	1.99907599908
69	H	30.2162	1.5027951028
75	H	29.1354	2.50145530146
76	H	29.3570	2.2966966967
78	H	29.8080	1.87997227997
79	H	30.2947	1.43026103026

81	H	31.1236	0.664356664357
82	H	30.7511	1.00854700855
83	H	30.6963	1.05918225918
84	H	25.7790	5.60277200277
85	H	28.1624	3.40050820051
89	H	27.6887	3.83820743821
91	H	30.1306	1.58188958189
92	H	30.6809	1.07341187341
93	H	30.8656	0.902748902749
96	H	29.7825	1.90353430353
97	H	28.2779	3.29378609379
100	H	29.0871	2.54608454608
101	H	28.1596	3.4030954031
105	H	28.2042	3.36188496188
106	H	28.1835	3.38101178101
107	H	28.6834	2.9191037191
108	H	28.3695	3.20914760915

Supporting Information: Revised-MandelalideB-0006.log

Using Gaussian 09: AM64L-G09RevC.01 23-Sep-2011

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#b3lyp/6-31G(d,p) scf=(maxcycle=300,direct,tight) density=current SCRF=(PCM,SOLVENT=Chloroform) opt=(maxcycle=250) freq=noraman

#N Geom=AllCheck Guess=TCheck SCRF=Check GenChk RB3LYP/6-31G(d,p) Freq

---

Pointgroup= C1 Stoichiometry= C37H58O13 C1[X(C37H58O13)] #Atoms= 108

Charge = 0 Multiplicity = 1

SCF Energy= -2422.85009592 Predicted Change= -3.990542D-08

==========

Optimization completed. {Found 1 times}

Item	Max Val.	Criteria	Pass?	RMS Val.	Criteria	Pass?
Force	0.00002 ||	0.00045	[YES]	0.00000 ||	0.00030	[YES]
Displ	0.00260 ||	0.00180	[NO]	0.00260 ||	0.00180	[YES]

Atomic Type	Coordinates (Angstroms) X	Y	Z
C	-6.791408	-0.497909	-0.255355
H	-7.405045	0.238245	-0.791567
C	-5.321093	-0.069450	-0.308580
C	-5.030812	1.326132	0.245704
H	-5.440353	2.080203	-0.436812
H	-5.505118	1.462394	1.223717
C	-3.532220	1.550360	0.381582
H	-3.042723	1.274830	-0.555870
O	-4.854826	-0.093758	-1.654613
H	-5.062744	-0.982557	-1.982606
H	-4.758510	-0.795355	0.296168
O	-6.897137	-1.746743	-0.983947
C	-7.313394	-2.811792	-0.109948
C	-6.106679	-3.656876	0.360270
H	-5.399299	-3.023221	0.903298
C	-5.440188	-4.390766	-0.772697
H	-6.033638	-5.199305	-1.199596
C	-4.233614	-4.157473	-1.325020
H	-3.931746	-4.796269	-2.155366
C	-3.285147	-3.109828	-0.971365
H	-3.519914	-2.480635	-0.115487
C	-2.161281	-2.847490	-1.662452
C	-1.235230	-1.685960	-1.406400
H	-1.623593	-1.122778	-0.550701
C	-1.237112	-0.750602	-2.633595
H	-2.261627	-0.444578	-2.864581
H	-0.824615	-1.254165	-3.516675
H	-0.651590	0.154526	-2.450196
C	0.182636	-2.180395	-1.031267
H	0.563328	-2.843945	-1.819597
H	0.113547	-2.783823	-0.117946
C	1.220111	-1.076357	-0.815694
H	1.395284	-0.548778	-1.767688
H	-1.912322	-3.477376	-2.520344
H	-6.479213	-4.399171	1.078704
H	-7.973984	-3.457452	-0.701685
C	-8.110196	-2.089650	1.000882
C	-8.344720	-2.859024	2.300013
H	-7.405807	-3.075136	2.819502
H	-8.856609	-3.809530	2.114961
H	-8.971516	-2.274673	2.981204
H	-9.086378	-1.845435	0.562152
C	-7.325760	-0.773725	1.158879
H	-6.498268	-0.907438	1.867143
H	-7.949644	0.041455	1.534107
C	-3.057942	2.922511	0.878595
H	-2.942758	3.642401	0.067121
H	-3.756330	3.332032	1.615724
C	-1.740535	2.580633	1.593997
O	-1.428850	3.471286	2.643767
H	-1.097169	2.925890	3.376274
C	-2.092042	1.195488	2.159570
O	-1.624003	0.705244	3.163732
O	-3.033048	0.608991	1.407175
C	2.561832	-1.620617	-0.302996
H	3.000979	-2.298971	-1.042726
H	2.390385	-2.193951	0.616263
C	3.531334	-0.479042	-0.000767
O	4.704851	-1.049141	0.611259
C	5.902045	-0.340550	0.390009
H	5.762058	0.733975	0.561851
H	3.827095	0.001953	-0.942531
C	2.873040	0.553132	0.922825
H	3.524726	1.423572	1.061841
H	2.706549	0.095478	1.905345
C	1.528613	0.998945	0.336077
C	0.748847	1.943022	1.252602
H	0.531142	1.403282	2.179245
H	1.361208	2.810258	1.516079
C	-0.556963	2.429989	0.603544
O	-0.347838	3.740490	0.014229
C	-0.148278	3.824650	-1.323965
O	-0.131088	2.865493	-2.070372
C	0.058786	5.261694	-1.750964
H	0.230933	5.253567	-2.830209
H	0.974826	5.624807	-1.267918
C	-1.110542	6.195762	-1.387394
H	-1.263086	6.171386	-0.303713
H	-2.031869	5.814657	-1.845431
C	-0.863565	7.633731	-1.850403
H	-1.705574	8.280271	-1.584757
H	-0.732241	7.685283	-2.936751
H	0.037189	8.049909	-1.385616
H	-0.837837	1.740858	-0.194852
H	1.703745	1.489827	-0.635005
O	0.684310	-0.138940	0.126211
O	6.352734	-0.418933	-0.949352
C	6.664295	-1.754142	-1.406446
H	5.767378	-2.379948	-1.304270
C	7.050379	-1.637100	-2.871605
H	6.247123	-1.158569	-3.438051
H	7.230308	-2.630010	-3.294896
H	7.962776	-1.046149	-2.978145
C	7.766229	-2.369617	-0.528486

O	9.031484	-1.727838	-0.692588
H	8.924587	-0.823998	-0.348358
H	7.919344	-3.410980	-0.832863
C	7.341692	-2.342274	0.952794
O	8.361414	-2.860986	1.786324
H	9.169718	-2.405653	1.502666
H	6.462474	-2.980889	1.082376
C	6.943369	-0.913828	1.369059
O	8.129740	-0.116331	1.340690
C	8.111240	1.024421	2.190412
H	7.343270	1.750612	1.895045
H	9.091406	1.497372	2.106164
H	7.939799	0.731764	3.234420
H	6.523622	-0.926765	2.382840

Statistical Thermodynamic Analysis
Temperature= 298.150 Kelvin Pressure= 1.00000 Atm
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SCF Energy= -2422.85009592 Predicted Change= -3.990542D-08
Zero-point correction (ZPE)= -2421.9147 0.93532
Internal Energy (U)= -2421.8630 0.98702
Enthalpy (H)= -2421.8621
0.98796
Gibbs Free Energy (G)= -2422.0035
0.84659

Frequencies -- 12.9967 16.2341 19.2732

NMR Shifts
Revised-MandelalideB-0006-NMR.txt

Atom	Type	Isotropic	Scaled Shift
1	C	100.5175	81.876088746
3	C	109.8955	72.9000363713
4	C	148.0454	36.3852677119
7	C	107.7056	74.9960757289
13	C	101.2000	81.2228411723
14	C	152.5916	32.0339210169
16	C	52.7193	127.625624533
18	C	49.3209	130.878366737
20	C	57.7278	122.831792339
22	C	35.8885	143.735044698
23	C	148.1682	36.2677310056
25	C	168.8692	16.4539903138
29	C	142.7648	41.4395375103
32	C	111.0586	71.7867876491
37	C	144.4715	39.8059878635
38	C	172.6313	12.8531365455
43	C	149.9764	34.5370317196
46	C	144.5475	39.7332452765
49	C	103.4808	79.0397978522
52	C	0.4898	177.61653171
55	C	145.8178	38.5173912211
58	C	112.5561	70.3534715442
60	C	91.3935	90.6090277379
63	C	148.6344	35.821512663
66	C	110.9240	71.9156185991
67	C	147.6414	36.7719519899
70	C	114.2778	68.7055648079
72	C	4.5644	173.71657191
74	C	144.9592	39.3391910259
77	C	162.6242	22.4313252551
80	C	171.5738	13.8653113574
88	C	115.3509	67.6784586229
90	C	170.0296	15.3433258676
94	C	109.8625	72.9316219683
98	C	118.3415	64.8160378261
102	C	101.8929	80.5596393499
104	C	127.9390	55.6298933747
2	H	27.8436	3.69507969508
5	H	30.1785	1.53762993763
6	H	30.1737	1.54206514207
8	H	26.6284	4.81792561793
10	H	29.2705	2.37662277662
11	H	27.8391	3.69923769924
15	H	29.2609	2.38549318549
17	H	26.1094	5.29748209748
19	H	25.3089	6.03714483714
21	H	24.8884	6.42568722569
24	H	29.0258	2.60272580273
26	H	30.6612	1.09161469161
27	H	31.2344	0.561977361977
28	H	29.9726	1.72788172788
30	H	30.5745	1.17172557173
31	H	30.2101	1.50843150843
33	H	28.0939	3.4638022638
34	H	25.8076	5.57634557635
35	H	29.8135	1.87489027489
36	H	27.9042	3.63908523909
39	H	31.0113	0.768121968122
40	H	30.6528	1.09937629938
41	H	30.5228	1.2194964195
42	H	29.1578	2.48075768076
44	H	30.2735	1.44984984985
45	H	29.7787	1.90704550705
47	H	29.1500	2.48796488796
48	H	29.8191	1.86971586972
51	H	29.2119	2.43076923077
56	H	30.0201	1.68399168399
57	H	30.5765	1.16987756988
61	H	26.5473	4.89286209286
62	H	27.6086	3.91221991222
64	H	29.9168	1.77944097944
65	H	30.8457	0.921136521137
68	H	29.6771	2.00092400092
69	H	30.2249	1.49475629476
75	H	29.4484	2.21224301224
76	H	29.2809	2.36701316701
78	H	29.7951	1.89189189189
79	H	30.1471	1.56664356664
81	H	30.5160	1.22577962578
82	H	30.8863	0.883622083622
83	H	30.8720	0.896835296835
84	H	25.8530	5.5343959344
85	H	28.2180	3.34913374913
89	H	27.7152	3.81372141372
91	H	30.6747	1.07914067914
92	H	30.8717	0.897112497112
93	H	30.1304	1.58207438207
96	H	29.7930	1.89383229383
97	H	28.2688	3.30219450219
100	H	29.0715	2.5604989605
101	H	28.1560	3.40642180642
105	H	28.1881	3.37676137676
106	H	28.1814	3.38295218295
107	H	28.6812	2.92113652114
108	H	28.3691	3.20951720952

Supporting Information: Revised-MandelalideB-0007.log

Using Gaussian 09: AM64L-G09RevC.01 23-Sep-2011
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#b3lyp/6-31G(d,p) scf=(maxcycle=300,direct,tight) density=current
SCRF=(PCM,SOLVENT=Chloroform) opt=(maxcycle=250)
freq=noraman
#N Geom=AllCheck Guess=TCheck SCRF=Check GenChk RB3LYP/6-
31G(d,p) Freq

Pointgroup= C1 Stoichiometry= C37H58O13 C1[X(C37H58O13)]
#Atoms= 108
Charge = 0 Multiplicity = 1

SCF Energy= -2422.85065320 Predicted Change= -7.865775D-10
==========
==========
Optimization completed. {Found 2 times}

Item	Max Val.	Criteria	Pass?	RMS Val.	Criteria	Pass?
Force	0.00000 ||	0.00045	[YES]	0.00000 ||	0.00030	[YES]
Displ	0.00053 ||	0.00180	[YES]	0.00053 ||	0.00180	[YES]

Atomic Type	Coordinates (Angstroms) X	Y	Z
C	-6.734613	-0.609790	-0.256417
H	-7.409383	0.140905	-0.689153
C	-5.304409	-0.060566	-0.243818
C	-5.123014	1.264552	0.498083
H	-5.606977	2.068218	-0.069478
H	-5.589461	1.221294	1.488325
C	-3.645538	1.594657	0.652402
H	-3.154065	1.492155	-0.318500
O	-4.849647	0.137316	-1.579433
H	-4.993752	-0.710903	-2.027646
H	-4.680385	-0.814652	0.257508
O	-6.742670	-1.750903	-1.150748
C	-7.079312	-2.954813	-0.437332
C	-5.813815	-3.766429	-0.074944
H	-5.153750	-3.160891	0.553270
C	-5.096138	-4.294392	-1.288580
H	-5.624131	-5.087278	-1.818378
C	-3.914150	-3.897097	-1.798686
H	-3.563961	-4.399733	-2.700585
C	-3.051998	-2.829003	-1.310558
H	-3.335019	-2.327844	-0.387735
C	-1.953156	-2.396180	-1.954366
C	-1.123901	-1.203427	-1.551382
H	-1.550849	-0.784151	-0.633522
C	-1.212346	-0.126538	-2.653110
H	-2.260386	0.122175	-2.843819
H	-0.770208	-0.481809	-3.592126
H	-0.698706	0.793215	-2.359476
C	0.331927	-1.622586	-1.236264
H	0.757842	-2.155792	-2.096950
H	0.319246	-2.333201	-0.400851
C	1.282118	-0.473269	-0.892211
H	1.404950	0.173643	-1.776739
H	-1.655195	-2.894534	-2.880304
H	-6.131269	-4.622017	0.535652
H	-7.690538	-3.558621	-1.119372
C	-7.926259	-2.453671	0.755176
C	-8.106374	-3.411983	1.931706
H	-7.154743	-3.635710	2.424109
H	-8.552923	-4.359268	1.610698
H	-8.771024	-2.973007	2.682689
H	-8.917209	-2.220032	0.344604
C	-7.238047	-1.120736	1.102438
H	-6.398509	-1.293571	1.787891
H	-7.916863	-0.414337	1.587067
C	-3.273181	2.921127	1.327855
H	-3.232334	3.751978	0.622028
H	-3.985498	3.168775	2.121408
C	-1.916740	2.595603	1.974704
O	-1.655019	3.359058	3.132392
H	-1.260961	2.750651	3.779268
C	-2.141476	1.122280	2.348438
O	-1.611469	0.540162	3.269159
O	-3.050069	0.567668	1.533968
C	2.666364	-0.969058	-0.448822
H	3.145479	-1.530430	-1.256013
H	2.545210	-1.644127	0.407233
C	3.551620	0.208940	-0.026018
O	4.792053	-0.209009	0.570955
C	5.833902	-0.555125	-0.308595
H	5.827147	0.103948	-1.186534
H	3.785247	0.819111	-0.913201
C	2.829819	1.079268	1.003607
H	3.424617	1.973179	1.221013
H	2.722854	0.511484	1.935894
C	1.441280	1.473816	0.488997
C	0.609664	2.234719	1.522746
H	0.460890	1.572452	2.381090
H	1.155494	3.112939	1.879132
C	-0.748610	2.681918	0.958354
O	-0.677273	4.072556	0.545715
C	-0.516758	4.351786	-0.770028
O	-0.386385	3.507447	-1.634554
C	-0.557485	5.849066	-1.002512
H	-0.001223	6.337715	-0.194879
H	-1.603961	6.153850	-0.868755
C	-0.044385	6.276611	-2.381082
H	-0.311078	7.328992	-2.530479
H	-0.574986	5.704429	-3.149426
C	1.467332	6.100581	-2.554760
H	1.756329	5.050370	-2.451166
H	2.021294	6.680678	-1.807798
H	1.789585	6.438438	-3.544675
H	-0.986675	2.078438	0.080367
H	1.553545	2.089813	-0.417991
O	0.685799	0.303887	0.154156
O	5.717015	-1.858819	-0.850619
C	5.749650	-2.924988	0.124747
H	4.930424	-2.771704	0.840094
C	5.535302	-4.223256	-0.635496
H	4.596610	-4.185749	-1.194323
H	5.490333	-5.065008	0.062232
H	6.358400	-4.397046	-1.332303
C	7.069983	-2.887774	0.911455
O	8.204573	-3.233010	0.115494
H	8.295552	-2.526384	-0.547466
H	7.025755	-3.639318	1.707517
C	7.268696	-1.499429	1.548825
O	8.502897	-1.425809	2.238492
H	9.155588	-1.787642	1.618502
H	6.476364	-1.329156	2.284580
C	7.151131	-0.399623	0.478023
O	8.266258	-0.543447	-0.405385
C	8.648825	0.641908	-1.092562
H	8.904043	1.440027	-0.383354
H	7.862088	1.004866	-1.766203
H	9.530644	0.393102	-1.685821
H	7.176539	0.587699	0.956038

Statistical Thermodynamic Analysis
Temperature= 298.150 Kelvin Pressure= 1.00000 Atm
==========
==========
SCF Energy= -2422.85065320 Predicted Change= -7.865775D-10
Zero-point correction (ZPE)= -2421.9151 0.93552
Internal Energy (U)= -2421.8636 0.98703
Enthalpy (H)= -2421.8626
0.98798
Gibbs Free Energy (G)= -2422.0036
0.84697

Frequencies -- 11.9078 13.7541 15.4760

NMR-Shifts
Revised-MandelalideB-0007-NMR.txt

Atom	Type	Isotropic	Scaled Shift
1	C	100.3229	82.0623480541
3	C	109.7437	73.0453301173
4	C	148.1081	36.3252550776
7	C	108.4905	74.2448170907
13	C	100.0857	82.2893814966
14	C	153.1194	31.5287428932
16	C	51.6340	128.664407818
18	C	49.0884	131.100901625
20	C	56.9962	123.532035452
22	C	35.5628	144.046784969
23	C	147.7047	36.7113650721
25	C	168.7851	16.5344857291
29	C	142.9267	41.2845766573
32	C	111.5009	71.3634449358
37	C	143.4497	40.7839928023
38	C	171.8748	13.5772124275
43	C	149.9556	34.5569402171
46	C	144.7591	39.5307146002
49	C	103.5384	78.9846666284
52	C	0.8516	177.270238711
55	C	144.1354	40.1276823829
58	C	102.6804	79.8058921495
60	C	84.3380	97.3621240835
63	C	146.2049	38.1468825973
66	C	110.7887	72.0451195467
67	C	147.8299	36.5915312315
70	C	114.5706	68.4253144203
72	C	4.2729	173.995578016
74	C	149.5084	34.984972913
77	C	166.5535	18.6704377955
80	C	173.1430	12.3633683646
88	C	115.3669	67.663144394
90	C	170.1324	15.2449319474
94	C	109.1289	73.6337793602
98	C	118.6449	64.5256417619
102	C	101.6003	80.8396983097
104	C	128.5975	54.9996171443
2	H	27.8111	3.72510972511
5	H	30.3100	1.41612381612
6	H	30.2790	1.44476784477
8	H	26.6070	4.8376992377
10	H	29.1991	2.4425964426
11	H	27.8468	3.69212289212
15	H	29.3542	2.29928389928
17	H	26.1386	5.2705012705
19	H	25.2867	6.05765765766
21	H	24.8008	6.50662970663
24	H	29.0667	2.56493416493
26	H	30.6362	1.11471471471
27	H	31.1165	0.670917070917
28	H	29.9688	1.73139293139
30	H	30.5604	1.18475398475
31	H	30.1815	1.53485793486
33	H	28.1620	3.40087780088
34	H	25.7380	5.64065604066
35	H	29.8663	1.8261030261
36	H	27.7667	3.76613536614
39	H	30.9391	0.834834834835
40	H	30.5600	1.18512358512
41	H	30.4571	1.2802032802
42	H	29.0570	2.5738969739
44	H	30.3966	1.33610533611
45	H	29.7309	1.95121275121
47	H	29.3342	2.31776391776
48	H	29.7910	1.89568029568
51	H	29.1654	2.47373527374
56	H	29.4742	2.1884037884
57	H	30.5210	1.22115962116
61	H	26.5079	4.92926772927
62	H	28.0199	3.53217833218
64	H	30.0937	1.61598521599
65	H	30.6083	1.14049434049
68	H	29.7832	1.90288750289
69	H	30.2436	1.47747747748
75	H	29.3761	2.27904827905
76	H	29.0186	2.60937860938
78	H	30.3309	1.39681219681
79	H	29.8586	1.83321783322
81	H	30.6950	1.06038346038
82	H	31.1559	0.634511434511
83	H	30.6817	1.07267267267
84	H	25.9244	5.46842226842
85	H	28.0820	3.4747978748
89	H	27.6906	3.83645183645
91	H	30.6916	1.06352506353
92	H	30.8924	0.877985677986
93	H	30.1878	1.52903672904
96	H	29.8259	1.86343266343
97	H	28.2477	3.32169092169
100	H	29.0542	2.57648417648
101	H	28.1614	3.40143220143
105	H	28.6597	2.941002541
106	H	28.2416	3.32732732733
107	H	28.1871	3.37768537769
108	H	28.4084	3.1732039732

Mandelalide B Original Configuration

Supporting Information: Original-MandelalideB-0001.log

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-----------------------------------------------------------------------
 Using  Gaussian 09:  AM64L-G09RevC.01 23-Sep-2011
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 #b3lyp/6-31G(d,p) scf=(maxcycle=300,direct,tight) density=current
 SCRF=(PCM,SOLVENT=Chloroform) opt=(maxcycle=250)
freq=noraman
 #N Geom=AllCheck Guess=TCheck SCRF=Check GenChk RB3LYP/6-
31G(d,p) Freq
-----------------------------------------------------------------------
 Pointgroup= C1   Stoichiometry= C37H58O13   C1[X(C37H58O13)]
#Atoms= 108
 Charge = 0                  Multiplicity = 1
-----------------------------------------------------------------------
 SCF Energy= -2422.84621068      Predicted Change= -8.777232D-08
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 Optimization completed.          {Found       1       times}
 Item     Max Val.    Criteria    Pass?     RMS Val.    Criteria    Pass?
 Force     0.00002 ||  0.00045   [ YES ]     0.00000 ||  0.00030   [ YES ]
 Displ     0.01298 ||  0.00180   [ NO ]      0.01298 ||  0.00180   [ NO ]
-----------------------------------------------------------------------
     Atomic      Coordinates (Angstroms)
      Type      X                  Y                Z
-----------------------------------------------------------------------
      C       -6.595862      0.123447      0.516801
      H       -7.089905      0.824634      1.205164
      C       -5.197612      0.658925      0.158737
      C       -4.460692      1.248445      1.370186
      H       -5.061853      2.070946      1.775702
      H       -4.367916      0.493250      2.159847
      C       -3.088625      1.798144      1.000328
      H       -3.167487      2.427651      0.107840
      O       -4.440875     -0.371591     -0.472388
      H       -4.522346     -1.133744      0.124653
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H	-5.319064	1.447819	-0.594733
O	-6.430151	-1.145078	1.187714
C	-7.348530	-2.132809	0.658942
C	-6.568623	-3.228900	-0.092301
H	-7.303345	-3.890497	-0.571764
C	-5.722284	-4.071542	0.821691
H	-6.282373	-4.593717	1.597740
C	-4.391682	-4.274615	0.786768
H	-3.973607	-4.954556	1.529212
C	-3.413042	-3.679553	-0.114609
H	-3.755632	-2.944332	-0.841723
C	-2.102544	-3.979514	-0.075125
C	-1.027654	-3.365215	-0.935210
H	-1.422454	-2.442173	-1.377201
C	-0.630443	-4.323420	-2.077757
H	0.171817	-3.903606	-2.694203
H	-1.484864	-4.525975	-2.730297
H	-0.278958	-5.281477	-1.677280
C	0.191562	-2.995372	-0.056325
H	0.751582	-3.908839	0.182440
H	-0.151126	-2.574606	0.896093
C	1.147705	-1.972809	-0.668937
H	1.364556	-2.231594	-1.720328
H	-1.764854	-4.734248	0.639185
H	-5.979918	-2.775870	-0.895782
H	-7.853026	-2.594753	1.517430
C	-8.360157	-1.322952	-0.189535
C	-9.120194	-2.082324	-1.276622
H	-9.667663	-2.936171	-0.862950
H	-8.451885	-2.454825	-2.059169
H	-9.851966	-1.423423	-1.754697
H	-9.095639	-0.911607	0.515030
C	-7.493219	-0.159209	-0.688050
H	-8.079206	0.716247	-0.981522
H	-6.883620	-0.468207	-1.544983
C	-1.942050	0.787177	0.853126
H	-2.066828	-0.026225	1.574099
H	-1.894143	0.349029	-0.139840
C	-0.701660	1.583915	1.266011
O	0.226403	0.789352	1.987403
H	0.646210	1.387799	2.628652
C	-1.315702	2.609924	2.240513
O	-0.695578	3.225622	3.080549
O	-2.643981	2.691729	2.083124
C	2.478562	-1.895308	0.093241
H	3.007625	-2.850660	0.006915
H	2.278262	-1.715054	1.156132
C	3.346531	-0.763787	-0.446847
O	4.527618	-0.687320	0.375490
C	5.658594	-0.124625	-0.248014
H	5.405599	0.817215	-0.750064
H	3.653221	-0.996820	-1.475522
C	2.557333	0.547045	-0.417879
H	3.128701	1.364122	-0.873463
H	2.354049	0.803130	0.625086
C	1.229278	0.375153	-1.171948
C	0.338709	1.621505	-1.184086
H	0.825929	2.361894	-1.827748
H	-0.607134	1.359081	-1.668554
C	0.041130	2.351711	0.134944
O	-0.806753	3.490042	-0.204175
C	-0.193385	4.664340	-0.513112
O	1.012253	4.801452	-0.531373
C	-1.206648	5.729462	-0.861251
H	-0.694438	6.693851	-0.815283
H	-2.002189	5.721606	-0.108460
C	-1.815646	5.512278	-2.262518
H	-2.305767	4.532765	-2.291436
H	-1.007060	5.482167	-3.002869
C	-2.815816	6.609566	-2.633660
H	-3.232947	6.437081	-3.630608
H	-2.339061	7.595705	-2.636358
H	-3.648821	6.644088	-1.922900
H	0.962727	2.747958	0.567469
H	1.464295	0.152330	-2.228401
O	0.468327	-0.711398	-0.645639
O	6.182940	-0.936156	-1.282840
C	6.646104	-2.236870	-0.856680
H	5.809313	-2.773833	-0.389215
C	7.097547	-2.973060	-2.107255
H	7.400008	-3.994040	-1.855262
H	7.949767	-2.463534	-2.562495
H	6.281972	-3.021778	-2.833558
C	7.752577	-2.086505	0.199911
O	8.959531	-1.538386	-0.331802
H	8.751392	-0.622900	-0.588317
H	8.017597	-3.081000	0.575938
C	7.251326	-1.227014	1.376730
O	8.270291	-1.036178	2.340406
H	9.048207	-0.762333	1.829562
H	6.429289	-1.749721	1.875444
C	6.700095	0.115823	0.860572
O	7.805170	0.857753	0.338470
C	7.635390	2.270598	0.331239
H	7.437766	2.645668	1.343734
H	6.819107	2.587982	-0.329893
H	8.570072	2.699362	-0.034834
H	6.234246	0.667678	1.686707

Statistical Thermodynamic Analysis
Temperature= 298.150 Kelvin Pressure= 1.00000 Atm
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SCF Energy= -2422.84621068 Predicted Change= -8.777232D-08
Zero-point correction (ZPE)= -2421.9105 0.93563
Internal Energy (U)= -2421.8589 0.98724
Enthalpy (H)= -2421.8580
0.98818
Gibbs Free Energy (G)= -2422.0002
0.84595

Frequencies -- 12.6411 13.0617 15.4272

NMR-Shifts
Original-MandelalideB-0001-NMR.txt

Atom	Type	Isotropic	Scaled Shift
1	C	101.0675	81.3496621298
3	C	113.9607	69.0090736806
4	C	143.0749	41.1427286127
7	C	103.3406	79.1739887823
13	C	99.7474	82.6131817225
14	C	153.0402	31.604548326
16	C	51.2435	129.038170715
18	C	50.0220	130.207316373
20	C	57.9318	122.636535921
22	C	34.2862	145.268669002
23	C	149.7708	34.7338195601
25	C	165.9937	19.2062443768
29	C	141.6430	42.5132563793
32	C	110.7902	72.0436838377
37	C	145.5721	38.7525603476
38	C	171.8971	13.5558682211
43	C	148.5825	35.8711881927
46	C	142.2962	41.8880529872
49	C	103.6767	78.8522942629
52	C	-2.3544	180.338827313
55	C	146.7673	37.6085874538
58	C	113.3796	69.565267329

60	C	91.8115	90.2089435096
63	C	152.7308	31.900687226
66	C	110.1244	72.6809471851
67	C	149.1964	35.2836003752
70	C	109.3695	73.4034916442
72	C	5.4784	172.841746588
74	C	145.6072	38.7189647581
77	C	161.8044	23.2159880549
80	C	171.4911	13.9444667777
88	C	115.4066	67.6251459637
90	C	169.7652	15.5963934991
94	C	109.8107	72.9812017841
98	C	117.9298	65.2100920768
102	C	101.5946	80.8451540037
104	C	128.0823	55.4927353127
2	H	27.6800	3.84624624625
5	H	29.6664	2.01081081081
6	H	30.0006	1.70200970201
8	H	26.9864	4.48713328713
10	H	30.0770	1.63141603142
11	H	28.1860	3.3787017787
15	H	29.7117	1.96895356895
17	H	26.2203	5.19501039501
19	H	25.2925	6.0522984523
21	H	24.8834	6.43030723031
24	H	29.2752	2.37227997228
26	H	30.3883	1.34377454377
27	H	30.8909	0.879371679372
28	H	31.1297	0.65872025872
30	H	30.5581	1.18687918688
31	H	30.1496	1.56433356433
33	H	28.2344	3.33398013398
34	H	25.8760	5.51314391314
35	H	29.1989	2.44278124278
36	H	27.5191	3.99491799492
39	H	30.5464	1.19768999769
40	H	30.9242	0.848602448602
41	H	30.4554	1.28177408177
42	H	29.0802	2.55246015246
44	H	29.8733	1.81963501964
45	H	29.9370	1.76077616078
47	H	29.8159	1.87267267267
48	H	28.2002	3.36558096558
51	H	29.4459	2.21455301455
56	H	30.2114	1.50723030723
57	H	30.5330	1.21007161007
61	H	26.4004	5.0285978286
62	H	27.6212	3.90057750058
64	H	29.7110	1.9696003696
65	H	29.9221	1.77454377454
68	H	29.7679	1.91702471702
69	H	29.6576	2.01894201894
75	H	29.6641	2.01293601294
76	H	29.4884	2.17528297528
78	H	30.0712	1.63677523678
79	H	30.1714	1.54419034419
81	H	30.5745	1.17172557173
82	H	30.8975	0.873273273273
83	H	30.8692	0.899422499423
84	H	26.2861	5.13421113421
85	H	28.1053	3.45326865327
89	H	27.6738	3.85197505198
91	H	30.8385	0.927789327789
92	H	30.1437	1.56978516979
93	H	30.7240	1.03358743359
96	H	29.7601	1.92423192423
97	H	28.1971	3.36844536845
100	H	29.1167	2.51873411873
101	H	28.0919	3.46565026565
105	H	28.6074	2.98932778933
106	H	28.1559	3.40651420651
107	H	28.1388	3.42231462231
108	H	28.4032	3.17800877801

Supporting Information: Original-MandelalideB-0002.log

```
-----------------------------------------------------------------------
 Using  Gaussian 09:  AM64L-G09RevC.01 23-Sep-2011
=======================================================================
 #b3lyp/6-31G(d,p) scf=(maxcycle=300,direct,tight) density=current
 SCRF=(PCM,SOLVENT=Chloroform) opt=(maxcycle=250)
freq=noraman
 #N Geom=AllCheck Guess=TCheck SCRF=Check GenChk RB3LYP/6-
31G(d,p) Freq
-----------------------------------------------------------------------
 Pointgroup= C1   Stoichiometry= C37H58O13   C1[X(C37H58O13)]
#Atoms= 108
 Charge = 0                Multiplicity = 1
-----------------------------------------------------------------------
 SCF Energy= -2422.84482764      Predicted Change= -1.173022D-08
=======================================================================
 Optimization completed.          {Found       1       times}
 Item     Max Val.    Criteria    Pass?     RMS Val.    Criteria    Pass?
 Force     0.00001 ||  0.00045   [ YES ]     0.00000 ||  0.00030   [ YES ]
 Displ     0.00331 ||  0.00180   [ NO ]      0.00331 ||  0.00180   [ YES ]
-----------------------------------------------------------------------
     Atomic     Coordinates (Angstroms)
      Type      X                Y                Z
-----------------------------------------------------------------------
      C       5.331298     -1.414716      1.572837
      H       6.263732     -0.843878      1.700852
      C       4.210220     -0.452143      1.143840
      C       4.686505      0.557931      0.087929
      H       5.574947      1.069729      0.476786
      H       4.988678      0.032414     -0.825686
      C       3.639921      1.619397     -0.227340
      H       3.235928      2.029283      0.703330
      O       3.070569     -1.189059      0.708851
      H       3.420234     -1.851252      0.089193
      H       3.888217      0.102949      2.034803
      O       5.509128     -2.384166      0.520613
      C       5.772231     -3.697721      1.072299
      C       4.652862     -4.669294      0.658668
      H       4.893500     -5.650617      1.091143
      C       4.535070     -4.820353     -0.831888
      H       5.435506     -5.181270     -1.328768
      C       3.461675     -4.562651     -1.602739
      H       3.558016     -4.734574     -2.674642
      C       2.167549     -4.051166     -1.170213
      H       2.015698     -3.873400     -0.106290
      C       1.162578     -3.758840     -2.014042
      C      -0.156952     -3.146996     -1.619313
      H      -0.185961     -3.100316     -0.521956
      C      -1.329569     -4.023739     -2.099394
      H      -2.295642     -3.582125     -1.836906
      H      -1.280670     -5.022322     -1.654148
      H      -1.303710     -4.139748     -3.188999
      C      -0.238533     -1.692098     -2.170522
      H      -0.796667     -1.670578     -3.114810
      H       0.770296     -1.335514     -2.399109
      C      -0.835958     -0.663991     -1.205358
      H      -0.330821     -0.766331     -0.227867
      H       1.306087     -3.929549     -3.083431
      H       3.707479     -4.350245      1.107085
      H       6.716623     -4.050727      0.637246
      C       5.926433     -3.475041      2.599872
      C       5.621726     -4.668020      3.505812
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H	4.574378	-4.977155	3.435792
H	5.820076	-4.408200	4.550497
H	6.247600	-5.531887	3.257530
H	6.969412	-3.176688	2.770934
C	5.049054	-2.235948	2.828230
H	5.300784	-1.696413	3.745627
H	3.987201	-2.506196	2.864951
C	2.499920	1.233262	-1.181722
H	2.851223	0.498332	-1.911842
H	1.655188	0.803380	-0.653615
C	2.188020	2.525659	-1.947928
O	1.937002	2.275950	-3.321993
H	2.221324	3.072738	-3.800171
C	3.528868	3.280875	-1.833924
O	3.853336	4.220808	-2.527478
O	4.317807	2.741937	-0.895661
C	-2.352748	-0.773627	-0.998583
H	-2.607202	-1.720585	-0.514713
H	-2.847895	-0.747193	-1.977166
C	-2.873085	0.393980	-0.153702
O	-4.309842	0.429984	-0.091653
C	-4.920209	-0.316421	0.932443
H	-4.323486	-0.260604	1.852218
H	-2.484945	0.295860	0.872696
C	-2.409182	1.727317	-0.736499
H	-2.704239	2.547378	-0.073032
H	-2.900270	1.886184	-1.704463
C	-0.886955	1.724092	-0.935856
C	-0.392500	2.998100	-1.625239
H	-0.546756	2.885271	-2.702388
H	-1.011738	3.839463	-1.298021
C	1.059795	3.435310	-1.396923
O	1.332898	3.618717	0.020462
C	1.006489	4.817132	0.573760
O	0.484202	5.718196	-0.048538
C	1.352447	4.843053	2.048368
H	2.333733	4.373333	2.180842
H	0.633286	4.180999	2.548719
C	1.315701	6.246015	2.663761
H	1.369499	6.139767	3.753183
H	0.347356	6.705634	2.438959
C	2.447241	7.157203	2.178089
H	2.394403	7.307598	1.095961
H	3.428511	6.729539	2.413515
H	2.389258	8.140350	2.655484
H	1.178765	4.409599	-1.881649
H	-0.407228	1.625399	0.053329
O	-0.504044	0.617770	-1.755793
O	-5.006690	-1.703191	0.658875
C	-5.808275	-2.048152	-0.493186
H	-5.379034	-1.559264	-1.378315
C	-5.729704	-3.558185	-0.646618
H	-4.688531	-3.878950	-0.737153
H	-6.269207	-3.874274	-1.544637
H	-6.179782	-4.051809	0.217558
C	-7.245681	-1.528847	-0.324240
O	-7.973511	-2.217223	0.693985
H	-7.539552	-1.994353	1.536109
H	-7.794561	-1.710028	-1.255058
C	-7.236185	-0.014758	-0.039621
O	-8.548189	0.473551	0.169609
H	-8.949584	-0.152357	0.792893
H	-6.830767	0.509187	-0.910967
C	-6.317561	0.295500	1.155927
O	-6.920466	-0.279066	2.318096
C	-6.563080	0.335275	3.550334
H	-6.822692	1.401874	3.545148
H	-5.493090	0.231833	3.771704
H	-7.133029	-0.169316	4.332637
H	-6.224022	1.381600	1.280195

Statistical Thermodynamic Analysis
Temperature= 298.150 Kelvin Pressure= 1.00000 Atm
==========
SCF Energy= -2422.84482764 Predicted Change= -1.173022D-08
Zero-point correction (ZPE)= -2421.9099 0.93486
Internal Energy (U)= -2421.8581 0.98665
Enthalpy (H)= -2421.8572 0.98760
Gibbs Free Energy (G)= -2421.9999 0.84491

Frequencies -- 7.9953 12.5929 16.5894

NMR-Shifts
Original-MandelalideB-0002-NMR.txt

Atom	Type	Isotropic	Scaled Shift
1	C	100.3950	81.9933383105
3	C	113.8075	69.1557074217
4	C	142.1048	42.0712494496
7	C	102.0555	80.4040084994
13	C	100.3878	82.0002297134
14	C	152.3910	32.2259231609
16	C	50.6268	129.628438523
18	C	49.7584	130.459618293
20	C	59.7920	120.856065392
22	C	34.9654	144.618579988
23	C	147.0304	37.3567641034
25	C	163.9573	21.1553628515
29	C	141.3168	42.8254752197
32	C	107.9095	74.8009150252
37	C	145.6670	38.6617278279
38	C	172.6890	12.7979096078
43	C	149.1078	35.3684029174
46	C	142.1589	42.0194682134
49	C	105.7202	76.8963800992
52	C	-3.2514	181.197381267
55	C	144.5525	39.72845958
58	C	102.5152	79.9640115622
60	C	84.0244	97.6622829687
63	C	145.4270	38.8914412604
66	C	114.0800	68.8948869618
67	C	149.4680	35.0236413408
70	C	107.5313	75.1629051092
72	C	6.0004	172.342119872
74	C	149.7926	34.7129539233
77	C	166.5478	18.6758934895
80	C	173.2669	12.2447788051
88	C	115.3091	67.7184670457
90	C	169.7021	15.6567889891
94	C	109.6390	73.1455426023
98	C	117.6626	65.4658396983
102	C	101.7424	80.7036888149
104	C	128.3092	55.2755604051
2	H	27.7696	3.76345576346
5	H	29.6916	1.98752598753
6	H	29.8818	1.81178101178
8	H	26.9181	4.55024255024
10	H	30.1465	1.5671979672
11	H	28.1144	3.44486024486
15	H	29.7592	1.92506352506
17	H	26.1534	5.25682605683
19	H	25.1678	6.16752136752
21	H	25.0160	6.30778470778
24	H	29.6694	2.00803880804
26	H	30.4106	1.32316932317
27	H	30.8071	0.956802956803

28	H	30.8376	0.928620928621
30	H	30.4456	1.29082929083
31	H	30.0531	1.6534996535
33	H	28.3630	3.21515361515
34	H	25.6660	5.70718410718
35	H	29.2609	2.38549318549
36	H	27.4556	4.05359205359
39	H	30.9180	0.854331254331
40	H	30.5109	1.23049203049
41	H	30.6827	1.07174867175
42	H	29.1164	2.51901131901
44	H	29.9756	1.72510972511
45	H	29.8606	1.83136983137
47	H	29.7837	1.90242550243
48	H	28.5696	3.02425502426
51	H	29.7980	1.88921228921
56	H	29.2427	2.40231000231
57	H	30.5712	1.17477477477
61	H	26.4874	4.94820974821
62	H	27.9982	3.55222915223
64	H	30.1969	1.52062832063
65	H	30.4832	1.25608685609
68	H	29.5079	2.15726495726
69	H	29.8278	1.86167706168
75	H	29.4790	2.18396858397
76	H	29.1900	2.451004851
78	H	30.3739	1.35708015708
79	H	29.9450	1.75338415338
81	H	30.6781	1.075999076
82	H	31.2052	0.588958188958
83	H	30.7560	1.00401940402
84	H	26.5771	4.86532686533
85	H	28.0240	3.52838992839
89	H	27.5662	3.9513975514
91	H	30.5972	1.15075075075
92	H	30.8442	0.922522522523
93	H	30.0813	1.62744282744
96	H	29.7027	1.97726957727
97	H	28.2696	3.30145530146
100	H	29.0825	2.55033495033
101	H	28.0770	3.47941787942
105	H	28.6575	2.94303534304
106	H	28.1976	3.36798336798
107	H	28.1749	3.38895818896
108	H	28.3545	3.22300762301

Mandelalide C Revised Configuration

Supporting Information: Revised-MandelalideC-0001.log

Using Gaussian 09: AM64L-G09RevD.01 24-Apr-2013

==========

#b3lyp/6-31G(d,p) scf=(maxcycle=300,direct,tight) density=current SCRF=(PCM,SOLVENT=Chloroform) opt=(maxcycle=250) freq=noraman

#N Geom=AllCheck Guess=TCheck SCRF=Check GenChk RB3LYP/6-31G(d,p) Freq

---

Pointgroup= C1 Stoichiometry= C30H46O10 C1[X(C30H46O10)] #Atoms= 86

Charge = 0 Multiplicity = 1

SCF Energy= -1923.20161079 Predicted Change= -8.839230D-09

==========

Optimization completed. {Found 1 times}

Item	Max Val.	Criteria	Pass?	RMS Val.	Criteria	Pass?
Force	0.00001 ||	0.00045	[YES]	0.00000 ||	0.00030	[YES]
Displ	0.00389 ||	0.00180	[NO]	0.00389 ||	0.00180	[YES]

Atomic Type	Coordinates (Angstroms) X	Y	Z
C	-4.489394	-1.421567	0.777986
H	-4.620574	-2.288663	1.438941
C	-2.994796	-1.116251	0.630394
C	-2.146362	-2.286184	0.132139
H	-2.091803	-3.053194	0.913431
H	-2.583483	-2.743610	-0.759053
C	-0.736954	-1.816701	-0.191893
H	-0.340839	-1.245708	0.651168
O	-2.455396	-0.706620	1.883864
H	-3.033128	0.010188	2.189729
H	-2.909051	-0.298261	-0.100260
O	-5.092972	-0.285931	1.447535
C	-6.058268	0.354437	0.593274
C	-5.456232	1.598196	-0.101121
H	-4.590144	1.302208	-0.700314
C	-5.111758	2.697559	0.868278
H	-5.972920	3.191451	1.318353
C	-3.891379	3.122211	1.249965
H	-3.848275	3.935020	1.975325
C	-2.599576	2.590174	0.837273
H	-2.591076	1.802565	0.087207
C	-1.422675	2.982099	1.357462
C	-0.086380	2.353844	1.053431
H	-0.244418	1.552589	0.322933
C	0.483059	1.721665	2.340706
H	1.403460	1.164905	2.144011
H	-0.244373	1.023298	2.764578
H	0.699272	2.487109	3.096281
C	0.876424	3.382475	0.413665
H	0.971090	4.257641	1.070710
H	0.435058	3.740155	-0.524687
C	2.288684	2.867092	0.129145
H	2.786768	2.622465	1.081808
H	-1.417234	3.776169	2.108451
H	-6.207278	1.983809	-0.803156
H	-6.876092	0.686517	1.244600
C	-6.533259	-0.779489	-0.344115
C	-7.245664	-0.364450	-1.630835
H	-8.126603	0.251423	-1.419598
H	-7.586113	-1.248247	-2.179820
H	-6.587286	0.203462	-2.295729
H	-7.222179	-1.394287	0.249644
C	-5.240889	-1.591153	-0.551537
H	-4.658767	-1.172719	-1.382415
H	-5.439440	-2.639958	-0.786041
C	0.282219	-2.874675	-0.643475
O	-0.357132	-3.857457	-1.432341
C	1.224741	-2.031020	-1.538515
O	1.836184	-2.825507	-2.536175
H	1.703785	-2.362059	-3.380905
C	0.200774	-1.077799	-2.171569
O	0.284164	-0.597582	-3.280350
O	-0.826535	-0.884896	-1.337415
C	3.148660	3.889846	-0.625917
H	3.273895	4.798118	-0.026158
H	2.640821	4.170875	-1.556759
C	4.515840	3.302981	-0.972371
O	5.205198	4.263191	-1.773004
H	5.071165	3.129444	-0.035000
C	4.347760	1.959586	-1.694553
H	5.325137	1.485376	-1.852509
H	3.898741	2.140843	-2.678816

C	3.440558	1.028770	-0.883050
C	3.125843	-0.286622	-1.596567
H	2.600767	-0.044846	-2.525707
H	4.050151	-0.803570	-1.869871
C	2.265143	-1.224023	-0.732593
O	3.109359	-2.200340	-0.067290
C	3.443121	-1.988058	1.230190
O	3.106571	-1.008933	1.865664
C	4.254819	-3.149483	1.766924
H	4.947881	-3.476647	0.984144
H	3.549804	-3.979648	1.907499
C	4.987138	-2.837121	3.076001
H	5.363895	-3.780471	3.487058
H	4.265732	-2.443198	3.799595
C	6.146458	-1.849972	2.908741
H	6.893564	-2.232920	2.204086
H	6.650054	-1.672292	3.864046
H	5.791451	-0.884710	2.535290
H	1.755373	-0.634251	0.031452
H	3.916802	0.815368	0.087655
O	2.178613	1.661901	-0.641129
H	6.086476	3.910800	-1.959438
H	0.798204	-3.319831	0.215418
H	0.301379	-4.123511	-2.096826

Statistical Thermodynamic Analysis
Temperature= 298.150 Kelvin Pressure= 1.00000 Atm
==========
==========
SCF Energy= -1923.20161079 Predicted Change= -8.839230D-09
Zero-point correction (ZPE)= -1922.4585 0.74310
Internal Energy (U)= -1922.4177 0.78389
Enthalpy (H)= -1922.4167
0.78483
Gibbs Free Energy (G)= -1922.5324
0.66913

Frequencies -- 15.7323 24.0622 25.9977

NMR-Shifts
Revised-MandelalideC-0001-NMR.txt

Atom	Type	Isotropic	Scaled Shift
1	C	100.7130	81.6889680124
3	C	109.7240	73.0641857616
4	C	153.3939	31.2660081548
7	C	103.5161	79.0060108348
13	C	100.4835	81.9086314822
14	C	153.5559	31.1109515879
16	C	51.8123	128.49374988
18	C	48.9394	131.243515381
20	C	56.9534	123.573001015
22	C	35.1123	144.477976225
23	C	147.6380	36.7752062635
25	C	168.7705	16.5484599629
29	C	143.3647	40.865349643
32	C	110.8939	71.9444284921
37	C	143.7793	40.4685196884
38	C	172.3712	13.102088478
43	C	149.8795	34.629778518
46	C	111.0459	71.7989433182
48	C	100.9435	81.4683474033
51	C	1.6601	176.496391585
54	C	145.7239	38.6072666016
57	C	114.8641	68.1443940351
60	C	143.3447	40.884492429
63	C	111.7759	71.1002316277
64	C	147.3465	37.0542123701
67	C	114.7493	68.254273627
69	C	4.6587	173.626313674
71	C	149.5206	34.9732958135
74	C	166.5561	18.6679492333
77	C	173.2131	12.2962728996
2	H	27.8259	3.71143451143
5	H	30.2875	1.43691383691
6	H	29.8634	1.82878262878
8	H	26.4797	4.95532455532
10	H	29.2396	2.40517440517
11	H	27.8744	3.66662046662
15	H	29.3725	2.28237468237
17	H	26.1750	5.23686763687
19	H	25.1336	6.19912219912
21	H	24.7943	6.51263571264
24	H	29.0680	2.56373296373
26	H	29.9654	1.73453453453
27	H	30.7364	1.02212982213
28	H	31.2298	0.566227766228
30	H	30.5195	1.22254562255
31	H	30.2374	1.48320628321
33	H	28.1283	3.43201663202
34	H	25.8188	5.565996766
35	H	29.7432	1.93984753985
36	H	27.7403	3.79052899053
39	H	30.6575	1.09503349503
40	H	30.5399	1.2036960037
41	H	30.9940	0.784107184107
42	H	29.1729	2.46680526681
44	H	30.4363	1.29942249942
45	H	29.7172	1.96387156387
50	H	28.9834	2.6419034419
55	H	29.9741	1.7264957265
56	H	30.7169	1.04014784015
59	H	27.8707	3.67003927004
61	H	30.2072	1.51111111111
62	H	30.7064	1.04984984985
65	H	29.7076	1.97274197274
66	H	30.1861	1.53060753061
72	H	29.4137	2.24430584431
73	H	29.0906	2.54285054285
75	H	30.2976	1.42758142758
76	H	29.8518	1.8395010395
78	H	31.1745	0.617325017325
79	H	30.7037	1.05234465234
80	H	30.6780	1.07609147609
81	H	25.8189	5.5659043659
82	H	28.2166	3.35042735043
84	H	30.9733	0.803234003234
85	H	27.5400	3.97560637561
86	H	29.2148	2.42808962809

Supporting Information: Revised-MandelalideC-0002.log

Using Gaussian 09: AM64L-G09RevD.01 24-Apr-2013
==========
==========
#b3lyp/6-31G(d,p) scf=(maxcycle=300,direct,tight) density=current
SCRF=(PCM,SOLVENT=Chloroform) opt=(maxcycle=250)
freq=noraman
#N Geom=AllCheck Guess=TCheck SCRF=Check GenChk RB3LYP/6-
31G(d,p) Freq

Pointgroup= C1 Stoichiometry= C30H46O10 C1[X(C30H46O10)]
#Atoms= 86
Charge = 0 Multiplicity = 1

SCF Energy= -1923.20167834 Predicted Change= -1.023128D-08
==========
==========
Optimization completed. {Found 2 times}

Item	Max Val.	Criteria	Pass?	RMS Val.	Criteria	Pass?
Force	0.00001 ||	0.00045	[YES]	0.00000 ||	0.00030	[YES]
Displ	0.00147 ||	0.00180	[YES]	0.00147 ||	0.00180	[YES]

Atomic Type	Coordinates (Angstroms) X	Y	Z
C	-4.383934	-1.417524	0.560149
H	-4.516119	-2.331695	1.154120
C	-2.890017	-1.096913	0.447007
C	-2.031701	-2.217809	-0.139554
H	-1.982965	-3.049200	0.573305
H	-2.456766	-2.597774	-1.072000
C	-0.620084	-1.718790	-0.404228
H	-0.231461	-1.232809	0.493924
O	-2.361534	-0.789566	1.734341
H	-2.933638	-0.089939	2.086850
H	-2.803463	-0.221390	-0.213061
O	-4.994139	-0.335693	1.308117
C	-5.965933	0.355537	0.502485
C	-5.377173	1.654761	-0.095508
H	-4.505765	1.414963	-0.712106
C	-5.048939	2.678874	0.958314
H	-5.917776	3.136727	1.431197
C	-3.835941	3.068928	1.396004
H	-3.806934	3.818966	2.186781
C	-2.535924	2.571232	0.966042
H	-2.510864	1.863877	0.140086
C	-1.372515	2.902676	1.554507
C	-0.028377	2.303370	1.227134
H	-0.161824	1.592326	0.404257
C	0.492153	1.523445	2.452893
H	1.425630	0.998460	2.231343
H	-0.246510	0.776002	2.756059
H	0.668579	2.193493	3.303483
C	0.958601	3.392452	0.744341
H	1.034037	4.184593	1.501683
H	0.549919	3.860276	-0.159730
C	2.377671	2.903171	0.447322
H	2.847144	2.554550	1.381973
H	-1.387195	3.617009	2.381713
H	-6.130846	2.083646	-0.768999
H	-6.787878	0.629669	1.175259
C	-6.429054	-0.710868	-0.516735
C	-7.147522	-0.209140	-1.768552
H	-8.029387	0.387252	-1.510587
H	-7.487778	-1.052940	-2.377379
H	-6.493887	0.406329	-2.394711
H	-7.111094	-1.374881	0.030126
C	-5.128325	-1.491321	-0.781958
H	-4.548153	-1.004177	-1.576077
H	-5.315548	-2.520765	-1.097531
C	0.404857	-2.727191	-0.947557
O	-0.224417	-3.626398	-1.838103
C	1.355938	-1.798374	-1.742947
O	1.981066	-2.487819	-2.807703
H	1.864968	-1.937376	-3.601120
C	0.338406	-0.787275	-2.289958
O	0.435568	-0.197544	-3.343437
O	-0.699858	-0.679908	-1.454376
C	3.261371	3.997207	-0.166729
H	3.374166	4.831712	0.534223
H	2.779574	4.384998	-1.072709
C	4.635340	3.444003	-0.541448
O	5.348662	4.482802	-1.212081
H	5.164749	3.163246	0.384964
C	4.481663	2.189564	-1.411907
H	5.461355	1.730315	-1.597530
H	4.057268	2.480196	-2.380749
C	3.552410	1.180108	-0.729516
C	3.251259	-0.048510	-1.589004
H	2.736779	0.294429	-2.491817
H	4.180019	-0.531441	-1.906049
C	2.382856	-1.075853	-0.843966
O	3.224537	-2.112450	-0.273788
C	3.530821	-2.042402	1.045815
O	3.136866	-1.165256	1.788265
C	4.451421	-3.179392	1.440225
H	5.445750	-2.917007	1.054659
H	4.146950	-4.078685	0.894097
C	4.508007	-3.427134	2.951415
H	4.745134	-2.484348	3.455534
H	5.339815	-4.111636	3.152398
C	3.211661	-4.009619	3.522924
H	2.370683	-3.326727	3.368440
H	3.302746	-4.186335	4.599127
H	2.964700	-4.965896	3.047761
H	1.858140	-0.574211	-0.028848
H	4.005271	0.861732	0.223747
O	2.286358	1.788670	-0.450995
H	6.231284	4.145514	-1.418945
H	0.911144	-3.256273	-0.131617
H	0.441172	-3.822766	-2.519534

Statistical Thermodynamic Analysis
Temperature= 298.150 Kelvin Pressure= 1.00000 Atm
==========
SCF Energy= -1923.20167834 Predicted Change= -1.023128D-08
Zero-point correction (ZPE)= -1922.4583 0.74334
Internal Energy (U)= -1922.4176 0.78403
Enthalpy (H)= -1922.4167 0.78497
Gibbs Free Energy (G)= -1922.5319 0.66968

Frequencies -- 18.9754 20.7303 27.9514

NMR-Shifts
Revised-MandelalideC-0002-NMR.txt

Atom	Type	Isotropic	Scaled Shift
1	C	100.6281	81.7702291391
3	C	109.8125	72.9794789334
4	C	153.5497	31.1168858516
7	C	103.6539	78.874117039
13	C	100.6364	81.7622848829
14	C	153.7926	30.8843967151
16	C	51.8723	128.436321522
18	C	48.9293	131.253182488
20	C	57.2116	123.325867647
22	C	35.1228	144.467926262
23	C	148.0848	36.3475564234
25	C	168.8260	16.4953387316
29	C	143.4661	40.7682957178
32	C	110.7967	72.0374624323
37	C	143.6821	40.5615536285
38	C	172.2022	13.26384502
43	C	149.8460	34.6618426846
46	C	111.1104	71.7372078332
48	C	101.0453	81.3709106223
51	C	1.8622	176.302953732
54	C	145.7996	38.5348111564
57	C	114.9240	68.0870613909
60	C	143.1153	41.1040601849
63	C	111.5683	71.2989337468
64	C	147.8499	36.5723884454
67	C	115.3431	67.6859243094
69	C	4.3558	173.916231168

71	C	149.0900	35.3854399969
74	C	166.4858	18.7352361263
77	C	173.1369	12.3692069144
2	H	27.8510	3.68824208824
5	H	30.2980	1.42721182721
6	H	29.8387	1.85160545161
8	H	26.4729	4.96160776161
10	H	29.2560	2.39002079002
11	H	27.8402	3.69822129822
15	H	29.3405	2.31194271194
17	H	26.1882	5.22467082467
19	H	25.1050	6.22554862555
21	H	24.8418	6.46874566875
24	H	29.1496	2.48833448833
26	H	29.9782	1.72270732271
27	H	30.6409	1.11037191037
28	H	31.2409	0.555971355971
30	H	30.5494	1.19491799492
31	H	30.2335	1.48680988681
33	H	28.1460	3.41566181566
34	H	25.8147	5.56978516979
35	H	29.7309	1.95121275121
36	H	27.8022	3.73333333333
39	H	30.6912	1.06389466389
40	H	30.5386	1.2048972049
41	H	30.9514	0.82346962347
42	H	29.1510	2.48704088704
44	H	30.3869	1.34506814507
45	H	29.7581	1.92607992608
50	H	28.9309	2.69041349041
55	H	29.9658	1.73416493416
56	H	30.7801	0.981750981751
59	H	27.9250	3.61986601987
61	H	30.2380	1.48265188265
62	H	30.7356	1.02286902287
65	H	29.7689	1.9161007161
66	H	30.2636	1.458997459
72	H	29.1699	2.46957726958
73	H	29.3675	2.28699468699
75	H	29.8604	1.83155463155
76	H	30.3315	1.39625779626
78	H	30.7597	1.0006006006
79	H	30.7022	1.05373065373
80	H	31.1853	0.607345807346
81	H	25.8439	5.5428043428
82	H	28.3085	3.26551166551
84	H	31.0051	0.773850773851
85	H	27.6150	3.90630630631
86	H	29.2050	2.43714483714

Supporting Information: Revised-MandelalideC-0003.log

Using Gaussian 09: AM64L-G09RevD.01 24-Apr-2013

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#b3lyp/6-31G(d,p) scf=(maxcycle=300,direct,tight) density=current SCRF=(PCM,SOLVENT=Chloroform) opt=(maxcycle=250) freq=noraman

#N Geom=AllCheck Guess=TCheck SCRF=Check GenChk RB3LYP/6-31G(d,p) Freq

---

Pointgroup= C1 Stoichiometry= C30H46O10 C1[X(C30H46O10)] #Atoms= 86

Charge = 0 Multiplicity = 1

SCF Energy= -1923.20215489 Predicted Change= -9.211523D-09

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Optimization completed. {Found 1 times}

Item	Max Val.	Criteria	Pass?	RMS Val.	Criteria	Pass?
Force	0.00001 ||	0.00045	[YES]	0.00000 ||	0.00030	[YES]
Displ	0.00299 ||	0.00180	[NO]	0.00299 ||	0.00180	[YES]

Atomic Type	Coordinates (Angstroms) X	Y	Z
C	-4.487392	-1.428072	0.768551
H	-4.618206	-2.299134	1.424324
C	-2.992941	-1.121348	0.622580
C	-2.143953	-2.287810	0.117282
H	-2.090583	-3.060345	0.893189
H	-2.579781	-2.738883	-0.777773
C	-0.733921	-1.816393	-0.201104
H	-0.338740	-1.252013	0.646834
O	-2.453634	-0.719079	1.878445
H	-3.031937	-0.004753	2.189002
H	-2.907660	-0.298913	-0.103164
O	-5.090899	-0.296492	1.445074
C	-6.057879	0.347729	0.595719
C	-5.457808	1.596131	-0.092112
H	-4.592228	1.304273	-0.694083
C	-5.112930	2.689781	0.883550
H	-5.973890	3.181260	1.336625
C	-3.892425	3.111473	1.268097
H	-3.849088	3.919613	1.998637
C	-2.600769	2.581551	0.852195
H	-2.592424	1.799403	0.096429
C	-1.423898	2.969168	1.375668
C	-0.087361	2.343725	1.066823
H	-0.245373	1.545791	0.332693
C	0.485550	1.706669	2.349980
H	1.407142	1.153331	2.149289
H	-0.239526	1.004350	2.771325
H	0.700835	2.468898	3.109025
C	0.872465	3.377158	0.430250
H	0.966565	4.249329	1.091344
H	0.427963	3.738529	-0.505337
C	2.285478	2.866893	0.140115
H	2.787056	2.620053	1.090312
H	-1.418470	3.757669	2.132501
H	-6.210050	1.985285	-0.790897
H	-6.875338	0.675168	1.249823
C	-6.532608	-0.781107	-0.347927
C	-7.246985	-0.359043	-1.631262
H	-8.127978	0.255076	-1.415216
H	-7.587711	-1.239782	-2.184965
H	-6.589864	0.213130	-2.293757
H	-7.220142	-1.400271	0.242874
C	-5.239454	-1.589871	-0.561583
H	-4.658441	-1.165218	-1.390100
H	-5.436881	-2.637344	-0.802854
C	0.285314	-2.871310	-0.659351
O	-0.353699	-3.847362	-1.456883
C	1.229586	-2.021386	-1.546431
O	1.842032	-2.808934	-2.548904
H	1.712192	-2.339185	-3.390475
C	0.207429	-1.062334	-2.173435
O	0.293163	-0.572220	-3.277809
O	-0.821264	-0.875649	-1.339647
C	3.143246	3.895207	-0.612065
H	3.269270	4.801419	-0.009429
H	2.619109	4.178920	-1.535489
C	4.515544	3.313646	-0.972162
O	5.310374	4.229472	-1.725157
H	5.084062	3.153089	-0.047020
C	4.352467	1.965735	-1.686358
H	5.334061	1.504398	-1.841862
H	3.899934	2.130678	-2.674206

C	3.443156	1.035131	-0.876433
C	3.133204	-0.280617	-1.591317
H	2.612735	-0.039355	-2.523249
H	4.059857	-0.795588	-1.860202
C	2.269345	-1.220611	-0.733242
O	3.109763	-2.201674	-0.070757
C	3.445845	-1.992231	1.226750
O	3.112957	-1.012765	1.863587
C	4.254282	-3.157067	1.760742
H	4.950656	-3.479964	0.979076
H	3.548266	-3.987726	1.893092
C	4.981174	-2.852680	3.074705
H	5.353732	-3.798958	3.482893
H	4.257280	-2.460649	3.796869
C	6.143612	-1.867535	2.917609
H	6.893304	-2.249159	2.215039
H	6.642821	-1.695278	3.876208
H	5.792941	-0.899839	2.546502
H	1.758550	-0.633810	0.032437
H	3.917915	0.823053	0.095052
O	2.178911	1.666164	-0.636972
H	4.836226	4.411770	-2.549340
H	0.799883	-3.323528	0.196656
H	0.306078	-4.109968	-2.121458

Statistical Thermodynamic Analysis
Temperature= 298.150 Kelvin Pressure= 1.00000 Atm
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==========
SCF Energy= -1923.20215489 Predicted Change= -9.211523D-09
Zero-point correction (ZPE)= -1922.4588 0.74327
Internal Energy (U)= -1922.4181 0.78401
Enthalpy (H)= -1922.4171
0.78496
Gibbs Free Energy (G)= -1922.5326
0.66952

Frequencies -- 16.3997 24.3259 26.5261

NMR-Shifts
Revised-MandelalideC-0003-NMR.txt

Atom	Type	Isotropic	Scaled Shift
1	C	100.7290	81.6736537836
3	C	109.7302	73.0582514979
4	C	153.4049	31.2554796225
7	C	103.5218	79.0005551408
13	C	100.5139	81.8795344474
14	C	153.5870	31.0811845556
16	C	51.7594	128.544382549
18	C	48.9794	131.205229809
20	C	56.9467	123.579413848
22	C	35.2079	144.386473707
23	C	147.6178	36.7945404774
25	C	168.8045	16.5159172266
29	C	143.2644	40.961350715
32	C	110.6395	72.1879247306
37	C	143.7870	40.4611497157
38	C	172.3495	13.1228584008
43	C	149.8652	34.64346561
46	C	111.0975	71.7495549302
48	C	100.9667	81.4461417715
51	C	1.6155	176.539079998
54	C	141.9501	42.2193188997
57	C	114.3219	68.6633549647
60	C	142.7734	41.4313061123
63	C	110.9377	71.9025057907
64	C	147.2758	37.1218821187
67	C	114.7836	68.2214437489
69	C	4.6599	173.625165107
71	C	149.5602	34.9353930971
74	C	166.5359	18.6872834472
77	C	173.2028	12.3061314344
2	H	27.8293	3.70829290829
5	H	30.2883	1.43617463617
6	H	29.8641	1.82813582814
8	H	26.4823	4.95292215292
10	H	29.2413	2.4036036036
11	H	27.8799	3.66153846154
15	H	29.3774	2.27784707785
17	H	26.1740	5.23779163779
19	H	25.1296	6.20281820282
21	H	24.8005	6.50690690691
24	H	29.0762	2.55615615616
26	H	29.9618	1.73786093786
27	H	30.7391	1.01963501964
28	H	31.2274	0.568445368445
30	H	30.5334	1.2097020097
31	H	30.2864	1.43793023793
33	H	28.1338	3.42693462693
34	H	25.8263	5.55906675907
35	H	29.7445	1.93864633865
36	H	27.7455	3.78572418572
39	H	30.6602	1.09253869254
40	H	30.5399	1.2036960037
41	H	30.9966	0.781704781705
42	H	29.1727	2.46699006699
44	H	30.4362	1.29951489951
45	H	29.7211	1.96026796027
50	H	28.9841	2.64125664126
55	H	29.8907	1.80355740356
56	H	30.9246	0.848232848233
59	H	28.1535	3.40873180873
61	H	29.9660	1.73398013398
62	H	30.9537	0.821344421344
65	H	29.7401	1.94271194271
66	H	30.1736	1.54215754216
72	H	29.4110	2.2468006468
73	H	29.0953	2.53850773851
75	H	30.2992	1.4261030261
76	H	29.8531	1.8382998383
78	H	31.1659	0.625271425271
79	H	30.7024	1.05354585355
80	H	30.6620	1.09087549088
81	H	25.8407	5.54576114576
82	H	28.2056	3.36059136059
84	H	31.5989	0.225179025179
85	H	27.5445	3.97144837145
86	H	29.2148	2.42808962809

Supporting Information: Revised-MandelalideC-0004.log

Using Gaussian 09: AM64L-G09RevD.01 24-Apr-2013
==========
==========
#b3lyp/6-31G(d,p) scf=(maxcycle=300,direct,tight) density=current
SCRF=(PCM,SOLVENT=Chloroform) opt=(maxcycle=250)
freq=noraman
#N Geom=AllCheck Guess=TCheck SCRF=Check GenChk RB3LYP/6-
31G(d,p) Freq

Pointgroup= C1 Stoichiometry= C30H46O10 C1[X(C30H46O10)]
#Atoms= 86
Charge = 0 Multiplicity = 1

SCF Energy= -1923.20219806 Predicted Change= -1.314850D-08
==========
==========
Optimization completed. {Found 1 times}

Item	Max Val.	Criteria	Pass?	RMS Val.	Criteria	Pass?
Force	0.00001 ||	0.00045	[YES]	0.00000 ||	0.00030	[YES]
Displ	0.00194 ||	0.00180	[NO]	0.00194 ||	0.00180	[YES]

Atomic Type	Coordinates (Angstroms) X	Y	Z
C	-4.384581	-1.418473	0.556270
H	-4.517018	-2.333911	1.148147
C	-2.890588	-1.097865	0.444033
C	-2.032382	-2.217618	-0.144813
H	-1.984408	-3.050834	0.565960
H	-2.457053	-2.595080	-1.078455
C	-0.620359	-1.718650	-0.407273
H	-0.231783	-1.235690	0.492515
O	-2.362172	-0.793250	1.732019
H	-2.935208	-0.095459	2.086653
H	-2.803863	-0.220964	-0.214198
O	-4.994701	-0.338261	1.306723
C	-5.965321	0.355793	0.502112
C	-5.375011	1.655983	-0.092337
H	-4.503550	1.416980	-0.709186
C	-5.046379	2.676857	0.964478
H	-5.915107	3.133962	1.438283
C	-3.833342	3.064576	1.404148
H	-3.804244	3.812070	2.197319
C	-2.533439	2.567060	0.973569
H	-2.508398	1.862441	0.145275
C	-1.370257	2.895201	1.564347
C	-0.026204	2.296346	1.235702
H	-0.159535	1.587555	0.410865
C	0.494602	1.513554	2.459418
H	1.428163	0.989257	2.236695
H	-0.243905	0.765224	2.760717
H	0.670838	2.181579	3.311609
C	0.960568	3.386987	0.755759
H	1.037014	4.176293	1.515949
H	0.550283	3.858193	-0.145973
C	2.379314	2.899218	0.454549
H	2.850737	2.546884	1.386760
H	-1.385049	3.606452	2.394193
H	-6.127991	2.087377	-0.765014
H	-6.787368	0.629131	1.175065
C	-6.428848	-0.707806	-0.519817
C	-7.146303	-0.202504	-1.770772
H	-8.027551	0.394340	-1.511761
H	-7.487353	-1.044530	-2.381597
H	-6.491743	0.413581	-2.395377
H	-7.111772	-1.372406	0.025200
C	-5.128743	-1.488949	-0.786172
H	-4.547889	-1.000881	-1.579237
H	-5.316912	-2.517590	-1.103777
C	0.404071	-2.725948	-0.953438
O	-0.225802	-3.621697	-1.847050
C	1.356064	-1.795369	-1.745595
O	1.981140	-2.482346	-2.811959
H	1.866891	-1.929516	-3.603911
C	0.339683	-0.781532	-2.289574
O	0.437985	-0.187167	-3.340466
O	-0.698931	-0.676292	-1.454238
C	3.265091	3.995677	-0.154966
H	3.382394	4.826263	0.549837
H	2.768655	4.389136	-1.053163
C	4.642315	3.443928	-0.543135
O	5.464148	4.430376	-1.166255
H	5.183602	3.173055	0.372617
C	4.488062	2.186546	-1.408561
H	5.470061	1.736470	-1.591936
H	4.060208	2.464885	-2.381902
C	3.554322	1.179980	-0.727482
C	3.253035	-0.048297	-1.587282
H	2.739951	0.294993	-2.490829
H	4.182072	-0.531318	-1.903203
C	2.383045	-1.075730	-0.844240
O	3.223033	-2.113751	-0.274935
C	3.530263	-2.043874	1.044669
O	3.136361	-1.166824	1.787216
C	4.451283	-3.180607	1.438358
H	5.445660	-2.916689	1.053979
H	4.148031	-4.079462	0.890839
C	4.506918	-3.430036	2.949306
H	4.743333	-2.487705	3.454582
H	5.338927	-4.114342	3.150056
C	3.210471	-4.013798	3.519273
H	2.369221	-3.331168	3.364993
H	3.300873	-4.191655	4.595349
H	2.964276	-4.969679	3.042897
H	1.857979	-0.574833	-0.028851
H	4.006063	0.861601	0.226103
O	2.288173	1.790365	-0.450199
H	5.014339	4.708727	-1.977055
H	0.909796	-3.257992	-0.139093
H	0.440358	-3.817871	-2.527970

Statistical Thermodynamic Analysis
Temperature= 298.150 Kelvin Pressure= 1.00000 Atm
==========
SCF Energy= -1923.20219806 Predicted Change= -1.314850D-08
Zero-point correction (ZPE)= -1922.4588 0.74336
Internal Energy (U)= -1922.4181 0.78407
Enthalpy (H)= -1922.4171 0.78501
Gibbs Free Energy (G)= -1922.5325 0.66962

Frequencies -- 18.9230 20.8506 27.0995

NMR-Shifts
Revised-MandelalideC-0004-NMR.txt

Atom	Type	Isotropic	Scaled Shift
1	C	100.6243	81.7738662685
3	C	109.8135	72.9785217941
4	C	153.5600	31.1070273168
7	C	103.6214	78.9052240663
13	C	100.6546	81.7448649476
14	C	153.7833	30.8932981106
16	C	51.7857	128.519209786
18	C	48.9758	131.208675511
20	C	57.2061	123.331131913
22	C	35.2318	144.363598078
23	C	148.0551	36.3759834606
25	C	168.8570	16.4656674132
29	C	143.3385	40.8904266927
32	C	110.5509	72.2727272727
37	C	143.6791	40.5644250464
38	C	172.2023	13.2637493061
43	C	149.8478	34.6601198338
46	C	111.1334	71.7151936293
48	C	101.0425	81.3735906124
51	C	1.7841	176.377706311
54	C	142.0196	42.1527977182
57	C	114.4047	68.5841038305
60	C	142.7162	41.4860544804
63	C	110.7073	72.1230306859
64	C	147.8078	36.61268401
67	C	115.4021	67.6294530906
69	C	4.3358	173.935373954

71	C	149.0841	35.3910871188
74	C	166.4880	18.7331304198
77	C	173.1337	12.3722697601
2	H	27.8519	3.68741048741
5	H	30.2973	1.42785862786
6	H	29.8386	1.8516978517
8	H	26.4762	4.95855855856
10	H	29.2578	2.38835758836
11	H	27.8487	3.69036729037
15	H	29.3449	2.30787710788
17	H	26.1868	5.22596442596
19	H	25.1035	6.22693462693
21	H	24.8473	6.46366366366
24	H	29.1613	2.47752367752
26	H	29.9772	1.72363132363
27	H	30.6424	1.10898590899
28	H	31.2403	0.556525756526
30	H	30.5588	1.18623238623
31	H	30.2792	1.44458304458
33	H	28.1546	3.40771540772
34	H	25.8237	5.56146916147
35	H	29.7334	1.9489027489
36	H	27.8029	3.73268653269
39	H	30.6940	1.06130746131
40	H	30.5392	1.20434280434
41	H	30.9553	0.819866019866
42	H	29.1499	2.48805728806
44	H	30.3925	1.33989373989
45	H	29.7582	1.92598752599
50	H	28.9392	2.68274428274
55	H	29.8716	1.82120582121
56	H	30.9824	0.794825594826
59	H	28.2116	3.35504735505
61	H	30.0015	1.70117810118
62	H	30.9784	0.798521598522
65	H	29.8013	1.88616308616
66	H	30.2404	1.48043428043
72	H	29.1553	2.48306768307
73	H	29.3662	2.2881958882
75	H	29.8505	1.8407022407
76	H	30.3258	1.40152460152
78	H	30.7623	0.998198198198
79	H	30.7001	1.05567105567
80	H	31.1841	0.608454608455
81	H	25.8646	5.52367752368
82	H	28.2933	3.27955647956
84	H	31.6354	0.191452991453
85	H	27.6113	3.90972510973
86	H	29.2042	2.43788403788

Supporting Information: Revised-MandelalideC-0005.log

Using Gaussian 09: AM64L-G09RevD.01 24-Apr-2013

==========

#b3lyp/6-31G(d,p) scf=(maxcycle=300,direct,tight) density=current SCRF=(PCM,SOLVENT=Chloroform) opt=(maxcycle=250) freq=noraman

#N Geom=AllCheck Guess=TCheck SCRF=Check GenChk RB3LYP/6-31G(d,p) Freq

---

Pointgroup= C1 Stoichiometry= C30H46O10 C1[X(C30H46O10)] #Atoms= 86

Charge = 0 Multiplicity = 1

SCF Energy= -1923.20208967 Predicted Change= -3.659753D-08

==========

Optimization completed. {Found 2 times}

Item	Max Val.	Criteria	Pass?	RMS Val.	Criteria	Pass?
Force	0.00003 ||	0.00045	[YES]	0.00000 ||	0.00030	[YES]
Displ	0.00173 ||	0.00180	[YES]	0.00173 ||	0.00180	[YES]

Atomic Type	Coordinates (Angstroms) X	Y	Z
C	4.335906	-1.364779	-0.504114
H	4.476478	-2.279807	-1.094703
C	2.839634	-1.050528	-0.401988
C	1.981402	-2.177113	0.174841
H	1.939838	-3.004822	-0.542631
H	2.402410	-2.559788	1.108157
C	0.567285	-1.682202	0.431956
H	0.180788	-1.193846	-0.465287
O	2.319946	-0.741664	-1.692026
H	2.897567	-0.045413	-2.042179
H	2.744506	-0.177072	0.260135
O	4.947083	-0.282396	-1.250921
C	5.907919	0.417133	-0.439659
C	5.306798	1.716255	0.146634
H	4.426275	1.475695	0.749926
C	4.993424	2.736999	-0.915111
H	5.869092	3.198395	-1.371679
C	3.787656	3.120136	-1.378211
H	3.771262	3.868369	-2.171056
C	2.481488	2.616905	-0.974173
H	2.443162	1.909479	-0.148744
C	1.328959	2.942576	-1.586878
C	-0.018862	2.337746	-1.285606
H	0.099509	1.636606	-0.452010
C	-0.504566	1.542112	-2.515185
H	-1.438141	1.010917	-2.310140
H	0.243946	0.794869	-2.792126
H	-0.665951	2.202531	-3.376164
C	-1.024057	3.426187	-0.838901
H	-1.098011	4.201161	-1.613887
H	-0.632068	3.917270	0.060316
C	-2.441759	2.928927	-0.546469
H	-2.897115	2.549080	-1.476261
H	1.357558	3.655091	-2.415256
H	6.048713	2.148909	0.830608
H	6.734484	0.692842	-1.106114
C	6.368290	-0.642954	0.587501
C	7.072553	-0.132883	1.843940
H	7.952947	0.468257	1.591993
H	7.412710	-0.972684	2.458324
H	6.409537	0.480266	2.462488
H	7.059414	-1.304207	0.048794
C	5.070478	-1.431157	0.843789
H	4.480775	-0.946290	1.632276
H	5.261832	-2.458756	1.162889
C	-0.463465	-2.691294	0.960226
O	0.152104	-3.590708	1.860732
C	-1.423219	-1.761809	1.745178
O	-2.078231	-2.456111	2.787829
H	-1.974209	-1.915186	3.589449
C	-0.403514	-0.768079	2.319895
O	-0.508352	-0.191603	3.380337
O	0.640260	-0.651493	1.493022
C	-3.348685	4.027875	0.026081
H	-3.472223	4.837002	-0.702184
H	-2.866008	4.453548	0.917135
C	-4.721064	3.466802	0.418295
O	-5.563120	4.458286	1.004545
H	-5.249845	3.160846	-0.493821
C	-4.556165	2.237770	1.321850
H	-5.532798	1.779172	1.511926
H	-4.138829	2.550228	2.289261

C	-3.603540	1.224539	0.678945
C	-3.284341	0.027133	1.574215
H	-2.759167	0.399169	2.458818
H	-4.205449	-0.453619	1.915308
C	-2.419330	-1.004666	0.837621
O	-3.307535	-1.973149	0.222711
C	-3.212705	-2.178151	-1.115839
O	-2.381788	-1.645243	-1.824426
C	-4.295523	-3.126822	-1.587015
H	-5.233172	-2.555392	-1.571424
H	-4.414560	-3.914381	-0.834815
C	-4.042139	-3.709883	-2.981197
H	-3.860549	-2.887661	-3.681376
H	-4.960424	-4.208580	-3.311251
C	-2.873867	-4.699441	-3.028460
H	-1.935361	-4.215740	-2.741300
H	-2.744002	-5.103397	-4.037274
H	-3.042638	-5.543846	-2.350389
H	-1.860807	-0.504343	0.045576
H	-4.052494	0.867228	-0.264946
O	-2.346242	1.842894	0.384734
H	-5.123565	4.770766	1.808497
H	-0.951201	-3.221267	0.134272
H	-0.527148	-3.796114	2.525627

Statistical Thermodynamic Analysis
Temperature= 298.150 Kelvin Pressure= 1.00000 Atm
==========
SCF Energy= -1923.20208967 Predicted Change= -3.659753D-08
Zero-point correction (ZPE)= -1922.4587 0.74338
Internal Energy (U)= -1922.4180 0.78406
Enthalpy (H)= -1922.4170 0.78500
Gibbs Free Energy (G)= -1922.5323 0.66978

Frequencies -- 19.9357 22.4472 25.8179

NMR-Shifts
Revised-MandelalideC-0005-NMR.txt

Atom	Type	Isotropic	Scaled Shift
1	C	100.5744	81.8216275197
3	C	109.6649	73.1207526943
4	C	153.5291	31.1366029212
7	C	103.5572	78.9666724095
13	C	100.6384	81.7603706043
14	C	153.8237	30.8546296828
16	C	51.5840	128.712264783
18	C	48.9836	131.201209824
20	C	57.2448	123.294090622
22	C	35.5225	144.085357683
23	C	148.1878	36.2489710753
25	C	168.5645	16.7456306591
29	C	143.0975	41.1210972645
32	C	110.6409	72.1865847355
37	C	143.5675	40.6712417925
38	C	172.1720	13.2927506269
43	C	149.8080	34.6982139781
46	C	111.1950	71.6562338483
48	C	100.5815	81.8148318306
51	C	1.7713	176.389957694
54	C	142.1226	42.0542123701
57	C	114.4641	68.5272497559
60	C	142.9158	41.2950094757
63	C	111.1934	71.6577652712
64	C	149.0418	35.4315741113
67	C	115.7407	67.3053657229
69	C	4.2301	174.036543579
71	C	149.4413	35.0491969601
74	C	166.3269	18.8873255614
77	C	173.2184	12.2912000613
2	H	27.8399	3.6984984985
5	H	30.2982	1.42702702703
6	H	29.8797	1.81372141372
8	H	26.2110	5.2036036036
10	H	29.2261	2.41764841765
11	H	27.8337	3.70422730423
15	H	29.3381	2.31416031416
17	H	26.1846	5.227997228
19	H	25.0851	6.24393624394
21	H	24.8501	6.46107646108
24	H	29.1331	2.50358050358
26	H	30.2403	1.48052668053
27	H	30.5485	1.19574959575
28	H	31.2665	0.532316932317
30	H	30.5773	1.16913836914
31	H	30.2607	1.46167706168
33	H	28.2375	3.33111573112
34	H	25.8262	5.55915915916
35	H	29.7243	1.95731115731
36	H	27.7949	3.74007854008
39	H	30.6960	1.05945945946
40	H	30.5372	1.20619080619
41	H	30.9471	0.827442827443
42	H	29.1453	2.49230769231
44	H	30.3929	1.33952413952
45	H	29.7542	1.92968352968
50	H	29.0079	2.61926541927
55	H	29.8419	1.84864864865
56	H	30.9729	0.803603603604
59	H	28.2100	3.35652575653
61	H	29.9529	1.74608454608
62	H	30.9255	0.847401247401
65	H	29.9174	1.77888657889
66	H	30.1463	1.56738276738
72	H	29.0662	2.5653961654
73	H	29.3398	2.31258951259
75	H	29.8031	1.8844998845
76	H	30.2873	1.4370986371
78	H	30.7201	1.03719103719
79	H	30.6931	1.06213906214
80	H	31.1321	0.656502656503
81	H	25.7303	5.64777084777
82	H	28.5499	3.04245784246
84	H	31.6300	0.196442596443
85	H	27.8249	3.71235851236
86	H	29.3181	2.33264033264

Supporting Information: Revised-MandelalideC-0006.log

Using Gaussian 09: AM64L-G09RevD.01 24-Apr-2013
==========
#b3lyp/6-31G(d,p) scf=(maxcycle=300,direct,tight) density=current SCRF=(PCM,SOLVENT=Chloroform) opt=(maxcycle=250) freq=noraman
#N Geom=AllCheck Guess=TCheck SCRF=Check GenChk RB3LYP/6-31G(d,p) Freq

---

Pointgroup= C1 Stoichiometry= C30H46O10 C1[X(C30H46O10)] #Atoms= 86
Charge = 0 Multiplicity = 1

SCF Energy= -1923.20132065 Predicted Change= -8.943363D-09
==========
Optimization completed. {Found 1 times}

Item	Max Val.	Criteria	Pass?	RMS Val.	Criteria	Pass?
Force	0.00001 ||	0.00045	[YES]	0.00000 ||	0.00030	[YES]
Displ	0.00308 ||	0.00180	[NO]	0.00308 ||	0.00180	[YES]

Atomic Type	Coordinates (Angstroms) X	Y	Z
C	4.463672	-1.621250	-0.754635
H	4.567857	-2.476218	-1.435851
C	2.986696	-1.223764	-0.659929
C	2.047456	-2.346218	-0.218380
H	1.970113	-3.091625	-1.018438
H	2.424422	-2.849338	0.675601
C	0.661083	-1.793629	0.072377
H	0.325935	-1.185023	-0.771014
O	2.524204	-0.755985	-1.923847
H	3.153007	-0.066667	-2.189120
H	2.923712	-0.416334	0.084216
O	5.168387	-0.509831	-1.362199
C	6.127702	0.046872	-0.445882
C	5.570473	1.307676	0.255174
H	4.662077	1.051635	0.808474
C	5.336220	2.447294	-0.700317
H	6.244698	2.895072	-1.103210
C	4.162036	2.955294	-1.122689
H	4.200568	3.782614	-1.831683
C	2.822881	2.498052	-0.775818
H	2.732800	1.702987	-0.038901
C	1.697704	2.969622	-1.342275
C	0.310965	2.426877	-1.107491
H	0.383467	1.602251	-0.389855
C	-0.245459	1.862175	-2.430900
H	-1.214372	1.376038	-2.287763
H	0.445028	1.115850	-2.834485
H	-0.365288	2.654357	-3.180211
C	-0.605361	3.505622	-0.481953
H	-0.623216	4.394651	-1.126849
H	-0.172134	3.820236	0.475516
C	-2.055212	3.076180	-0.247758
H	-2.539322	2.876613	-1.217808
H	1.777217	3.772593	-2.079528
H	6.311442	1.630309	0.998458
H	6.994568	0.344978	-1.048515
C	6.488885	-1.138973	0.478755
C	7.160460	-0.802496	1.809747
H	8.083226	-0.231957	1.658880
H	7.424184	-1.719675	2.345949
H	6.502946	-0.217456	2.460556
H	7.169161	-1.777227	-0.099985
C	5.142456	-1.876818	0.600429
H	4.548737	-1.449945	1.418670
H	5.267531	-2.942479	0.808345
C	-0.434825	-2.792607	0.476580
O	0.118992	-3.826842	1.264623
C	-1.347422	-1.907082	1.361848
O	-2.033712	-2.678691	2.328440
H	-1.897522	-2.237867	3.184542
C	-0.284680	-1.029553	2.038947
O	-0.369264	-0.561548	3.152989
O	0.775440	-0.887637	1.236614
C	-2.873988	4.140649	0.497537
H	-2.931663	5.060910	-0.094182
H	-2.360000	4.381678	1.438740
C	-4.286784	3.634087	0.812665
O	-5.047383	4.583104	1.559722
H	-4.838630	3.520254	-0.129401
C	-4.220305	2.268652	1.508429
H	-5.230567	1.863382	1.633463
H	-3.782541	2.391912	2.509054
C	-3.347256	1.298948	0.704347
C	-3.133888	-0.044828	1.402329
H	-2.617972	0.148388	2.347757
H	-4.095867	-0.505362	1.644886
C	-2.313719	-1.022929	0.544437
O	-3.202711	-1.929729	-0.158494
C	-3.481861	-1.673596	-1.462681
O	-3.027352	-0.731115	-2.079947
C	-4.446123	-2.697387	-2.016570
H	-4.063259	-3.699158	-1.791612
H	-4.466453	-2.570904	-3.101880
C	-5.864497	-2.547213	-1.428245
H	-6.227770	-1.530960	-1.623906
H	-5.812488	-2.660958	-0.340209
C	-6.842103	-3.567574	-2.015995
H	-6.928751	-3.454689	-3.102123
H	-7.840884	-3.443877	-1.586257
H	-6.514208	-4.592757	-1.811965
H	-1.749215	-0.458238	-0.199619
H	-3.810042	1.132461	-0.281894
O	-2.042636	1.857515	0.507960
H	-4.587952	4.722191	2.400467
H	-0.952745	-3.189830	-0.404306
H	-0.572803	-4.059236	1.907613

Statistical Thermodynamic Analysis
Temperature= 298.150 Kelvin Pressure= 1.00000 Atm
==========
SCF Energy= -1923.20132065 Predicted Change= -8.943363D-09
Zero-point correction (ZPE)= -1922.4579 0.74336
Internal Energy (U)= -1922.4171 0.78420
Enthalpy (H)= -1922.4161 0.78515
Gibbs Free Energy (G)= -1922.5322 0.66905

Frequencies -- 15.5803 21.4896 24.4415

NMR-Shifts
Revised-MandelalideC-0006-NMR.txt

Atom	Type	Isotropic	Scaled Shift
1	C	100.1576	82.2205631808
3	C	109.6156	73.1679396619
4	C	153.8326	30.846111143
7	C	103.1447	79.3614923716
13	C	100.7355	81.6674323781
14	C	153.3182	31.3384636
16	C	52.1779	128.143819752
18	C	48.9404	131.242558242
20	C	56.9206	123.604395184
22	C	35.2829	144.31468826
23	C	147.6255	36.7871705048
25	C	168.7760	16.5431956967
29	C	143.1186	41.1009016252
32	C	110.7162	72.1145121461
37	C	143.8839	40.3684029174
38	C	172.9055	12.5906889489
43	C	150.1087	34.4104021899
46	C	111.2141	71.6379524876
48	C	100.9730	81.4401117939
51	C	1.4066	176.739026398
54	C	141.9278	42.2406631061
57	C	114.5978	68.3992802312
60	C	142.5830	41.6135454354
63	C	110.9844	71.8578073853
64	C	147.5522	36.8573288156
67	C	115.0332	67.9825417791
69	C	3.7776	174.469649113

71	C	145.6427	38.6849863129
74	C	162.2827	22.7581883267
77	C	171.3325	14.096269071
2	H	27.8359	3.70219450219
5	H	30.2531	1.4686994687
6	H	29.8748	1.81824901825
8	H	26.5028	4.93398013398
10	H	29.2959	2.35315315315
11	H	27.8833	3.6583968584
15	H	29.4129	2.24504504505
17	H	26.2006	5.21321321321
19	H	25.1408	6.19246939247
21	H	24.7846	6.5215985216
24	H	29.1002	2.53398013398
26	H	29.9918	1.71014091014
27	H	30.6873	1.0674982675
28	H	31.2344	0.561977361977
30	H	30.5585	1.18650958651
31	H	30.2911	1.43358743359
33	H	28.1577	3.40485100485
34	H	25.8220	5.56303996304
35	H	29.6951	1.98429198429
36	H	27.7632	3.76936936937
39	H	30.6449	1.10667590668
40	H	30.5286	1.21413721414
41	H	31.0650	0.718503118503
42	H	29.1711	2.46846846847
44	H	30.4636	1.2741972742
45	H	29.7281	1.9537999538
50	H	29.0029	2.62388542389
55	H	29.9148	1.78128898129
56	H	30.9461	0.828366828367
59	H	28.2081	3.35828135828
61	H	29.9565	1.74275814276
62	H	30.9498	0.824948024948
65	H	29.6922	1.98697158697
66	H	30.1501	1.56387156387
72	H	29.3664	2.28801108801
73	H	29.5537	2.11494571495
75	H	30.1467	1.56701316701
76	H	29.9213	1.77528297528
78	H	30.8470	0.919935319935
79	H	30.5106	1.23076923077
80	H	30.8584	0.909401709402
81	H	25.8292	5.55638715639
82	H	28.2749	3.29655809656
84	H	31.6224	0.203465003465
85	H	27.5376	3.97782397782
86	H	29.2046	2.43751443751

Supporting Information: Revised-MandelalideC-0007.log

Using Gaussian 09: AM64L-G09RevD.01 24-Apr-2013

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#b3lyp/6-31G(d,p) scf=(maxcycle=300,direct,tight) density=current SCRF=(PCM,SOLVENT=Chloroform) opt=(maxcycle=250) freq=noraman

#N Geom=AllCheck Guess=TCheck SCRF=Check GenChk RB3LYP/6-31G(d,p) Freq

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Pointgroup= C1 Stoichiometry= C30H46O10 C1[X(C30H46O10)] #Atoms= 86

Charge = 0 Multiplicity = 1

SCF Energy= -1923.19506701 Predicted Change= -4.964652D-07

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Optimization completed. {Found 1 times}

Item	Max Val.	Criteria	Pass?	RMS Val.	Criteria	Pass?
Force	0.00000 ||	0.00045	[YES]	0.00000 ||	0.00030	[YES]
Displ	0.14461 ||	0.00180	[NO]	0.14461 ||	0.00180	[NO]

Atomic Type	Coordinates (Angstroms) X	Y	Z
C	4.303685	-1.354287	-0.508341
H	4.446158	-2.265530	-1.104749
C	2.806797	-1.040651	-0.409927
C	1.948278	-2.174561	0.153131
H	1.908599	-2.987476	-0.582927
H	2.380029	-2.568064	1.078252
C	0.534653	-1.686480	0.429346
H	0.140246	-1.187647	-0.457992
O	2.291219	-0.722109	-1.698648
H	2.866421	-0.019422	-2.039857
H	2.706854	-0.174468	0.260723
O	4.918233	-0.267229	-1.244186
C	5.885843	0.418631	-0.428313
C	5.295214	1.719423	0.164178
H	4.410260	1.482870	0.762556
C	4.994884	2.749414	-0.892554
H	5.875911	3.211836	-1.337549
C	3.794182	3.138756	-1.363405
H	3.785907	3.893147	-2.150506
C	2.484114	2.634985	-0.973255
H	2.438587	1.922006	-0.152981
C	1.336128	2.967778	-1.590675
C	-0.014699	2.365437	-1.298858
H	0.099381	1.653391	-0.474029
C	-0.503977	1.587666	-2.538282
H	-1.441810	1.061352	-2.339584
H	0.238629	0.837437	-2.822890
H	-0.660172	2.258844	-3.391874
C	-1.016058	3.451614	-0.838535
H	-1.094240	4.232668	-1.607098
H	-0.619171	3.935019	0.062506
C	-2.431032	2.949461	-0.540878
H	-2.892280	2.577289	-1.471258
H	1.371123	3.686579	-2.413372
H	6.038263	2.141139	0.853591
H	6.715227	0.690401	-1.092837
C	6.336432	-0.651168	0.593071
C	7.041341	-0.153982	1.854322
H	7.927088	0.441687	1.608273
H	7.373280	-1.000075	2.464547
H	6.381469	0.460631	2.474698
H	7.023935	-1.314230	0.051893
C	5.032574	-1.431455	0.841933
H	4.443400	-0.945738	1.630258
H	5.216217	-2.461572	1.157663
C	-0.487352	-2.716764	0.962144
O	0.088565	-3.623995	1.885203
C	-1.442326	-1.794509	1.765438
O	-2.171403	-2.437292	2.777016
H	-1.936433	-1.997485	3.610204
C	-0.411773	-0.819457	2.351379
O	-0.493377	-0.267998	3.426405
O	0.619873	-0.680069	1.507918
C	-3.335189	4.039592	0.051424
H	-3.456147	4.855496	-0.673066
H	-2.860722	4.456429	0.948280
C	-4.703899	3.467662	0.441660
O	-5.500740	4.412701	1.155151
H	-5.228250	3.152813	-0.476909
C	-4.527759	2.244427	1.340471
H	-5.500437	1.780680	1.538456
H	-4.108128	2.567576	2.301131

C	-3.579273	1.235705	0.686135
C	-3.250244	0.039923	1.579058
H	-2.715419	0.410635	2.458129
H	-4.167189	-0.439496	1.931954
C	-2.395912	-0.994380	0.836137
O	-3.308249	-1.923581	0.192328
C	-3.149751	-2.180570	-1.128491
O	-2.231170	-1.748379	-1.798052
C	-4.282059	-3.046532	-1.641977
H	-5.168555	-2.399956	-1.685376
H	-4.505074	-3.805089	-0.883500
C	-4.007902	-3.677695	-3.010781
H	-3.721307	-2.888466	-3.713844
H	-4.946979	-4.104504	-3.380756
C	-2.926964	-4.762577	-2.981660
H	-1.966404	-4.352085	-2.656120
H	-2.782454	-5.197566	-3.975529
H	-3.199520	-5.575125	-2.298434
H	-1.817867	-0.494519	0.059217
H	-4.035847	0.876922	-0.253726
O	-2.325509	1.856230	0.378921
H	-5.625211	5.181641	0.581800
H	-0.982384	-3.238547	0.138143
H	0.577756	-4.290066	1.384677

Statistical Thermodynamic Analysis
Temperature= 298.150 Kelvin Pressure= 1.00000 Atm
==========
==========
SCF Energy= -1923.19506701 Predicted Change= -4.964652D-07
Zero-point correction (ZPE)= -1922.4525 0.74252
Internal Energy (U)= -1922.4113 0.78368
Enthalpy (H)= -1922.4104
0.78463
Gibbs Free Energy (G)= -1922.5287
0.66635

Frequencies -- 4.5985 12.0690 21.7705

NMR-Shifts
Revised-MandelalideC-0007-NMR.txt

Atom	Type	Isotropic	Scaled Shift
1	C	100.6194	81.7785562511
3	C	109.8644	72.9298034036
4	C	153.8231	30.8552039664
7	C	103.4005	79.1166561381
13	C	100.5203	81.8734087559
14	C	153.9014	30.780259959
16	C	51.6454	128.65349643
18	C	48.9561	131.227531155
20	C	57.2393	123.299354888
22	C	35.5911	144.019697927
23	C	148.2240	36.2143226325
25	C	168.5673	16.742950669
29	C	143.2246	40.9994448592
32	C	111.6444	71.2260954459
37	C	143.5804	40.6588946955
38	C	172.1865	13.278872107
43	C	149.7546	34.7493252168
46	C	108.8988	73.8540171137
48	C	101.2174	81.2061869484
51	C	1.0597	177.071058022
54	C	142.4806	41.7115564999
57	C	114.8571	68.1510940102
60	C	146.5540	37.8127452669
63	C	111.4548	71.4075690576
64	C	148.7929	35.6698060836
67	C	113.0579	69.8731790425
69	C	3.7149	174.529661747
71	C	149.3588	35.1281609525
74	C	166.3640	18.8518156933
77	C	173.2589	12.2524359195
2	H	27.8539	3.68556248556
5	H	30.4753	1.26338646339
6	H	30.0642	1.64324324324
8	H	26.1029	5.30348810349
10	H	29.2233	2.42023562024
11	H	27.7799	3.75393855394
15	H	29.3270	2.32441672442
17	H	26.1773	5.23474243474
19	H	25.0796	6.24901824902
21	H	24.8498	6.46135366135
24	H	29.0914	2.54211134211
26	H	30.3539	1.37556017556
27	H	30.5728	1.1732963733
28	H	31.2917	0.509032109032
30	H	30.6066	1.14206514207
31	H	30.2330	1.48727188727
33	H	28.2753	3.29618849619
34	H	25.8284	5.55712635713
35	H	29.7134	1.96738276738
36	H	27.7953	3.73970893971
39	H	30.6842	1.07036267036
40	H	30.5321	1.2109032109
41	H	30.9337	0.839824439824
42	H	29.1407	2.49655809656
44	H	30.3676	1.3629013629
45	H	29.7713	1.91388311388
50	H	29.3615	2.29253869254
55	H	30.0937	1.61598521599
56	H	30.7027	1.05326865327
59	H	27.9197	3.62476322476
61	H	30.0260	1.67854007854
62	H	30.7096	1.04689304689
65	H	29.9258	1.77112497112
66	H	30.0312	1.67373527374
72	H	29.0576	2.57334257334
73	H	29.2897	2.35888195888
75	H	29.8277	1.86176946177
76	H	30.2949	1.43007623008
78	H	30.7148	1.04208824209
79	H	30.7002	1.05557865558
80	H	31.1347	0.6541002541
81	H	25.8101	5.57403557404
82	H	28.5255	3.065003465
84	H	31.0002	0.778378378378
85	H	27.6629	3.86204666205
86	H	30.8522	0.915130515131

Supporting Information: Revised-MandelalideC-0008.log

Using Gaussian 09: AM64L-G09RevD.01 24-Apr-2013
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==========
#b3lyp/6-31G(d,p) scf=(maxcycle=300,direct,tight) density=current
SCRF=(PCM,SOLVENT=Chloroform) opt=(maxcycle=250)
freq=noraman
#N Geom=AllCheck Guess=TCheck SCRF=Check GenChk RB3LYP/6-
31G(d,p) Freq

Pointgroup= C1 Stoichiometry= C30H46O10 C1[X(C30H46O10)]
#Atoms= 86
Charge = 0 Multiplicity = 1

SCF Energy= -1923.19474017 Predicted Change= -1.679405D-08
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Optimization completed. {Found 1 times}

Item	Max Val.	Criteria	Pass?	RMS Val.	Criteria	Pass?
Force	0.00002 ||	0.00045	[YES]	0.00000 ||	0.00030	[YES]
Displ	0.00358 ||	0.00180	[NO]	0.00358 ||	0.00180	[YES]

Atomic Type	Coordinates (Angstroms) X	Y	Z
C	-4.461981	-1.388148	0.789031
H	-4.600754	-2.247781	1.458607
C	-2.964823	-1.091940	0.646860
C	-2.122166	-2.274287	0.167903
H	-2.072893	-3.021895	0.969440
H	-2.572011	-2.743787	-0.711694
C	-0.711390	-1.823368	-0.178739
H	-0.304396	-1.234458	0.646610
O	-2.428957	-0.672309	1.897790
H	-2.999178	0.055927	2.190495
H	-2.868730	-0.284628	-0.094001
O	-5.063875	-0.242767	1.441259
C	-6.033656	0.383456	0.580774
C	-5.438241	1.623804	-0.124698
H	-4.571152	1.326504	-0.721891
C	-5.097917	2.733056	0.834988
H	-5.960548	3.232382	1.276064
C	-3.878450	3.159068	1.217830
H	-3.836145	3.978914	1.935243
C	-2.586945	2.618944	0.815212
H	-2.578874	1.824706	0.072156
C	-1.410132	3.010563	1.335783
C	-0.076183	2.373191	1.041384
H	-0.236570	1.562533	0.321709
C	0.490352	1.757294	2.337650
H	1.407433	1.192932	2.148683
H	-0.240061	1.068243	2.771548
H	0.709837	2.532858	3.081929
C	0.891681	3.388163	0.387748
H	0.997440	4.268327	1.036374
H	0.448754	3.741002	-0.551698
C	2.297280	2.856366	0.100028
H	2.798463	2.614829	1.051960
H	-1.403555	3.811567	2.079348
H	-6.191400	1.999844	-0.829523
H	-6.853439	0.716784	1.228950
C	-6.502365	-0.761742	-0.346088
C	-7.213318	-0.362651	-1.638669
H	-8.097818	0.250860	-1.435771
H	-7.547880	-1.253507	-2.179770
H	-6.555898	0.201919	-2.307279
H	-7.190189	-1.373532	0.252089
C	-5.206488	-1.570315	-0.542583
H	-4.622084	-1.155836	-1.373832
H	-5.400813	-2.621443	-0.770503
C	0.291237	-2.914922	-0.621707
O	-0.319682	-3.919192	-1.410520
C	1.228313	-2.099911	-1.551563
O	1.905329	-2.857900	-2.518954
H	1.636752	-2.509566	-3.384411
C	0.198915	-1.163769	-2.198849
O	0.258046	-0.720021	-3.323693
O	-0.810004	-0.928737	-1.348038
C	3.163103	3.864454	-0.668173
H	3.301883	4.775853	-0.076090
H	2.652344	4.143894	-1.597890
C	4.521414	3.260060	-1.018907
O	5.216576	4.206866	-1.830591
H	5.080681	3.087156	-0.083674
C	4.334041	1.913614	-1.730060
H	5.305248	1.428000	-1.891171
H	3.880260	2.092320	-2.712603
C	3.422644	0.997587	-0.906125
C	3.091100	-0.318665	-1.609673
H	2.557576	-0.081073	-2.534900
H	4.008617	-0.842402	-1.891733
C	2.235178	-1.247970	-0.735113
O	3.093764	-2.193006	-0.040509
C	3.393768	-1.963970	1.260902
O	3.007719	-0.997614	1.888475
C	4.240128	-3.091401	1.817838
H	4.948621	-3.405895	1.043928
H	3.562197	-3.942656	1.965781
C	4.953137	-2.737529	3.127054
H	5.360737	-3.661706	3.552092
H	4.214262	-2.360002	3.841722
C	6.077804	-1.712172	2.952958
H	6.841731	-2.077493	2.257128
H	6.569461	-1.504264	3.908396
H	5.690805	-0.765071	2.564972
H	1.709686	-0.652142	0.012250
H	3.904567	0.787254	0.062783
O	2.169671	1.646491	-0.659243
H	6.089306	3.838973	-2.027152
H	0.820057	-3.340302	0.237049
H	-0.777275	-4.529785	-0.817499

Statistical Thermodynamic Analysis
Temperature= 298.150 Kelvin Pressure= 1.00000 Atm
==========
SCF Energy= -1923.19474017 Predicted Change= -1.679405D-08
Zero-point correction (ZPE)= -1922.4526 0.74208
Internal Energy (U)= -1922.4113 0.78343
Enthalpy (H)= -1922.4103 0.78438
Gibbs Free Energy (G)= -1922.5278 0.66688

Frequencies -- 15.7303 18.4079 24.2173

NMR-Shifts
Revised-MandelalideC-0008-NMR.txt

Atom	Type	Isotropic	Scaled Shift
1	C	100.7091	81.6927008557
3	C	109.9980	72.8019295928
4	C	153.4861	31.1777599112
7	C	103.2107	79.2983211777
13	C	100.4115	81.977545512
14	C	153.5577	31.1092287372
16	C	51.9878	128.325771933
18	C	48.8842	131.296349471
20	C	57.1552	123.379850303
22	C	35.0056	144.580102988
23	C	147.5851	36.8258389326
25	C	168.7495	16.5685598882
29	C	143.2122	41.0113133866
32	C	111.0785	71.767740577
37	C	143.7958	40.4527268899
38	C	172.4656	13.0117345278
43	C	149.8501	34.6579184134
46	C	108.8011	73.9475296235
48	C	101.5980	80.8418997301
51	C	0.8501	177.271674419
54	C	145.7243	38.6068837459
57	C	114.7932	68.2122552116
60	C	143.2935	40.9334979613
63	C	111.9430	70.9402936503
64	C	147.1229	37.268228718
67	C	113.0095	69.9195045847
69	C	4.4932	173.784720228

71	C	149.3081	35.1766879152
74	C	166.5187	18.7037462432
77	C	173.1865	12.321732805
2	H	27.8370	3.70117810118
5	H	30.4800	1.25904365904
6	H	30.0264	1.67817047817
8	H	26.4763	4.95846615847
10	H	29.2390	2.40572880573
11	H	27.8237	3.71346731347
15	H	29.3632	2.29096789097
17	H	26.1673	5.24398244398
19	H	25.1292	6.20318780319
21	H	24.7979	6.50930930931
24	H	29.0465	2.5835989836
26	H	29.9258	1.77112497112
27	H	30.7586	1.00161700162
28	H	31.2413	0.555601755602
30	H	30.5213	1.22088242088
31	H	30.2293	1.49069069069
33	H	28.1423	3.41908061908
34	H	25.8056	5.57819357819
35	H	29.7377	1.94492954493
36	H	27.7313	3.79884499884
39	H	30.6482	1.10362670363
40	H	30.5371	1.20628320628
41	H	30.9872	0.79039039039
42	H	29.1671	2.47216447216
44	H	30.4124	1.32150612151
45	H	29.7362	1.94631554632
50	H	29.3637	2.29050589051
55	H	29.9691	1.73111573112
56	H	30.7123	1.0443982444
59	H	27.8679	3.67262647263
61	H	30.1973	1.52025872026
62	H	30.6887	1.0662046662
65	H	29.7446	1.93855393855
66	H	30.1353	1.57754677755
72	H	29.3730	2.28191268191
73	H	29.0852	2.54784014784
75	H	30.2919	1.43284823285
76	H	29.8348	1.85520905521
78	H	31.1638	0.627211827212
79	H	30.7022	1.05373065373
80	H	30.6663	1.0869022869
81	H	25.7902	5.59242319242
82	H	28.2604	3.30995610996
84	H	30.9708	0.805544005544
85	H	27.3926	4.1118041118
86	H	30.7130	1.04375144375

Supporting Information: Revised-MandelalideC-0009.log

Using Gaussian 09: AM64L-G09RevD.01 24-Apr-2013

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#b3lyp/6-31G(d,p) scf=(maxcycle=300,direct,tight) density=current SCRF=(PCM,SOLVENT=Chloroform) opt=(maxcycle=250) freq=noraman

#N Geom=AllCheck Guess=TCheck SCRF=Check GenChk RB3LYP/6-31G(d,p) Freq

---

Pointgroup= C1 Stoichiometry= C30H46O10 C1[X(C30H46O10)] #Atoms= 86

Charge = 0 Multiplicity = 1

SCF Energy= -1923.19813765 Predicted Change= -4.928879D-09

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Optimization completed. {Found 2 times}

Item	Max Val.	Criteria	Pass?	RMS Val.	Criteria	Pass?
Force	0.00000 ||	0.00045	[YES]	0.00000 ||	0.00030	[YES]
Displ	0.00116 ||	0.00180	[YES]	0.00116 ||	0.00180	[YES]

Atomic Type	Coordinates (Angstroms) X	Y	Z
C	-4.472048	-0.496581	0.574961
H	-4.424982	-0.788764	1.636955
C	-4.412187	-1.767010	-0.285699
C	-3.263971	-2.731398	0.081695
H	-3.376218	-3.021421	1.134328
H	-3.373610	-3.643026	-0.510134
C	-1.835561	-2.225115	-0.088459
H	-1.671030	-1.289516	0.448286
O	-4.432937	-1.454555	-1.673250
H	-3.602351	-0.994654	-1.864788
H	-5.343804	-2.315992	-0.098477
O	-3.335113	0.326912	0.259951
C	-3.690739	1.726731	0.224221
C	-3.421966	2.257069	-1.205821
H	-2.568972	1.680367	-1.579773
C	-3.108815	3.733419	-1.267144
H	-3.895543	4.397756	-1.616672
C	-1.929502	4.275317	-0.900925
H	-1.802236	5.354862	-0.976590
C	-0.790005	3.519890	-0.400410
H	-0.911634	2.441529	-0.314958
C	0.393772	4.039513	-0.032868
C	1.549838	3.211230	0.465573
H	1.189676	2.184049	0.598805
C	2.055727	3.731809	1.823807
H	2.904636	3.143724	2.188567
H	1.266514	3.683844	2.580290
H	2.383387	4.775402	1.744898
C	2.687863	3.163069	-0.586220
H	3.295379	4.074738	-0.520619
H	2.259277	3.137069	-1.594432
C	3.600390	1.943928	-0.455763
H	3.922947	1.821759	0.592791
H	0.555021	5.117496	-0.105451
H	-4.265579	2.013884	-1.860411
H	-3.021415	2.252040	0.914744
C	-5.152507	1.784684	0.734790
C	-5.996220	2.971172	0.269370
H	-5.540100	3.923289	0.558182
H	-6.992302	2.928813	0.721717
H	-6.128560	2.974883	-0.817286
H	-5.101493	1.814622	1.831607
C	-5.685905	0.400075	0.333338
H	-5.952611	0.375354	-0.729093
H	-6.558338	0.093572	0.917565
C	-0.743638	-3.250200	0.276356
O	-1.181920	-4.561454	-0.015219
C	0.408031	-2.870729	-0.691676
O	1.149831	-4.028780	-1.040137
H	1.249289	-4.019689	-2.007261
C	-0.396416	-2.379984	-1.906072
O	-0.016389	-2.419715	-3.055615
O	-1.596400	-1.931204	-1.521462
C	4.847974	2.047718	-1.342337
H	5.463851	2.896390	-1.025124
H	4.541981	2.226612	-2.380658
C	5.664571	0.760230	-1.284637
O	6.741976	0.888783	-2.211788
H	6.062194	0.641868	-0.262054
C	4.766418	-0.439101	-1.603433
H	5.318471	-1.378094	-1.468826
H	4.461310	-0.377533	-2.655343

C	3.516981	-0.442176	-0.710840
C	2.555591	-1.560532	-1.107965
H	2.194100	-1.367009	-2.123393
H	3.108367	-2.504089	-1.131170
C	1.347532	-1.738399	-0.186547
O	1.857692	-2.101096	1.121876
C	1.372276	-1.444744	2.207179
O	0.491491	-0.609673	2.152664
C	2.048608	-1.933948	3.471145
H	3.117032	-2.061355	3.264380
H	1.659560	-2.943917	3.656937
C	1.811380	-1.031294	4.686039
H	2.146606	-1.569943	5.579476
H	0.734467	-0.868599	4.800456
C	2.532486	0.316990	4.596685
H	3.616360	0.180730	4.506469
H	2.346450	0.919910	5.490899
H	2.188663	0.890672	3.730862
H	0.788666	-0.805495	-0.088159
H	3.829187	-0.583714	0.337585
O	2.816326	0.797898	-0.824524
H	7.275202	0.083789	-2.154496
H	-0.467442	-3.156510	1.331810
H	-0.396552	-5.026420	-0.352465

Statistical Thermodynamic Analysis
Temperature= 298.150 Kelvin Pressure= 1.00000 Atm
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==========
SCF Energy= -1923.19813765 Predicted Change= -4.928879D-09
Zero-point correction (ZPE)= -1922.4553 0.74278
Internal Energy (U)= -1922.4143 0.78377
Enthalpy (H)= -1922.4134
0.78472
Gibbs Free Energy (G)= -1922.5304
0.66766

Frequencies -- 14.5459 19.5227 22.2883

NMR-Shifts
Revised-MandelalideC-0009-NMR.txt

Atom	Type	Isotropic	Scaled Shift
1	C	100.2516	82.1305920864
3	C	114.6185	68.3794674477
4	C	149.3706	35.1168667088
7	C	99.6278	82.727655583
13	C	97.8772	84.4032236452
14	C	151.9192	32.6775014836
16	C	51.3627	128.924079711
18	C	49.2602	130.936465093
20	C	55.9153	124.566607324
22	C	38.8169	140.932157966
23	C	147.8292	36.592201229
25	C	166.9282	18.311797699
29	C	139.9036	44.1781044813
32	C	110.5107	72.3112042727
37	C	145.3073	39.0060108348
38	C	172.9717	12.5273263271
43	C	149.0594	35.4147284596
46	C	111.4286	71.4326461073
48	C	101.9115	80.5418365589
51	C	1.4941	176.655276709
54	C	146.1114	38.236375122
57	C	115.1357	67.8844350007
60	C	142.7859	41.419341871
63	C	113.8046	69.1584831256
64	C	149.5819	34.9146231743
67	C	114.9832	68.0303987442
69	C	4.1557	174.107754743
71	C	149.5780	34.9183560175
74	C	166.6960	18.534045445
77	C	172.8410	12.6524244339
2	H	27.6122	3.90889350889
5	H	30.1038	1.60665280665
6	H	29.1134	2.52178332178
8	H	25.8652	5.52312312312
10	H	30.0156	1.68814968815
11	H	28.0105	3.54086394086
15	H	29.0170	2.61085701086
17	H	25.9386	5.4553014553
19	H	25.3352	6.01284361284
21	H	24.7874	6.51901131901
24	H	29.0859	2.54719334719
26	H	30.6054	1.14317394317
27	H	30.8071	0.956802956803
28	H	31.0905	0.694941094941
30	H	30.5673	1.17837837838
31	H	30.3975	1.33527373527
33	H	28.3699	3.20877800878
34	H	25.8306	5.55509355509
35	H	29.6138	2.05941325941
36	H	27.5636	3.9537999538
39	H	30.6289	1.12145992146
40	H	30.5559	1.18891198891
41	H	30.7852	0.977038577039
42	H	29.2089	2.43354123354
44	H	29.6874	1.99140679141
45	H	30.1356	1.57726957727
50	H	29.1634	2.47558327558
55	H	30.0334	1.6717024717
56	H	30.7406	1.01824901825
59	H	27.8845	3.65728805729
61	H	30.0812	1.62753522754
62	H	30.6060	1.14261954262
65	H	29.8184	1.87036267036
66	H	29.6662	2.010995611
72	H	29.3826	2.27304227304
73	H	29.1010	2.53324093324
75	H	30.3333	1.39459459459
76	H	29.8547	1.83682143682
78	H	31.1853	0.607345807346
79	H	30.7173	1.03977823978
80	H	30.6609	1.09189189189
81	H	25.8517	5.5355971356
82	H	28.3214	3.25359205359
84	H	30.9726	0.803880803881
85	H	27.6742	3.85160545161
86	H	28.9685	2.65567105567

Supporting Information: Revised-MandelalideC-0010.log

Using Gaussian 09: AM64L-G09RevD.01 24-Apr-2013
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==========
#b3lyp/6-31G(d,p) scf=(maxcycle=300,direct,tight) density=current
SCRF=(PCM,SOLVENT=Chloroform) opt=(maxcycle=250)
freq=noraman
#N Geom=AllCheck Guess=TCheck SCRF=Check GenChk RB3LYP/6-
31G(d,p) Freq

Pointgroup= C1 Stoichiometry= C30H46O10 C1[X(C30H46O10)]
#Atoms= 86
Charge = 0 Multiplicity = 1

SCF Energy= -1923.19813767 Predicted Change= -1.655685D-09
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==========
Optimization completed. {Found 2 times}

Item	Max Val.	Criteria	Pass?	RMS Val.	Criteria	Pass?
Force	0.00000 ||	0.00045	[YES]	0.00000 ||	0.00030	[YES]
Displ	0.00071 ||	0.00180	[YES]	0.00071 ||	0.00180	[YES]

Atomic Type	Coordinates (Angstroms) X	Y	Z
C	-4.472094	-0.496560	0.574794
H	-4.424971	-0.788623	1.636821
C	-4.412229	-1.767076	-0.285736
C	-3.263988	-2.731406	0.081739
H	-3.376231	-3.021345	1.134393
H	-3.373609	-3.643084	-0.510016
C	-1.835589	-2.225105	-0.088453
H	-1.671072	-1.289478	0.448249
O	-4.432988	-1.454744	-1.673314
H	-3.602475	-0.994710	-1.864852
H	-5.343834	-2.316054	-0.098454
O	-3.335223	0.326931	0.259594
C	-3.690818	1.726770	0.224149
C	-3.421898	2.257370	-1.205769
H	-2.568871	1.680723	-1.579723
C	-3.108749	3.733724	-1.266809
H	-3.895475	4.398134	-1.616205
C	-1.929435	4.275553	-0.900490
H	-1.802165	5.355111	-0.975972
C	-0.789948	3.520043	-0.400078
H	-0.911640	2.441690	-0.314612
C	0.393895	4.039591	-0.032640
C	1.549953	3.211234	0.465702
H	1.189752	2.184066	0.598917
C	2.055951	3.731745	1.823920
H	2.904838	3.143598	2.188627
H	1.266773	3.683817	2.580443
H	2.383676	4.775320	1.745023
C	2.687900	3.163068	-0.586178
H	3.295428	4.074731	-0.520604
H	2.259230	3.137092	-1.594355
C	3.600426	1.943919	-0.455823
H	3.923074	1.821725	0.592700
H	0.555207	5.117564	-0.105234
H	-4.265443	2.014293	-1.860491
H	-3.021546	2.251941	0.914833
C	-5.152630	1.784667	0.734635
C	-5.996351	2.971137	0.269170
H	-5.540294	3.923268	0.558038
H	-6.992466	2.928731	0.721441
H	-6.128610	2.974864	-0.817496
H	-5.101693	1.814609	1.831454
C	-5.685978	0.400048	0.333145
H	-5.952642	0.375324	-0.729297
H	-6.558417	0.093508	0.917343
C	-0.743654	-3.250155	0.276456
O	-1.181903	-4.561445	-0.014985
C	0.408016	-2.870746	-0.691609
O	1.149819	-4.028815	-1.039992
H	1.249293	-4.019798	-2.007113
C	-0.396430	-2.380074	-1.906033
O	-0.016407	-2.419856	-3.055575
O	-1.596419	-1.931277	-1.521451
C	4.847943	2.047711	-1.342497
H	5.463848	2.896385	-1.025345
H	4.541863	2.226597	-2.380793
C	5.664546	0.760224	-1.284843
O	6.741870	0.888753	-2.212090
H	6.062249	0.641885	-0.262290
C	4.766370	-0.439115	-1.603556
H	5.318431	-1.378104	-1.468960
H	4.461221	-0.377567	-2.655455
C	3.516971	-0.442180	-0.710909
C	2.555552	-1.560524	-1.108020
H	2.194036	-1.366983	-2.123433
H	3.108316	-2.504086	-1.131242
C	1.347529	-1.738381	-0.186550
O	1.857770	-2.101032	1.121850
C	1.372285	-1.444787	2.207185
O	0.491452	-0.609762	2.152706
C	2.048592	-1.934054	3.471137
H	3.117001	-2.061570	3.264374
H	1.659421	-2.943974	3.656937
C	1.811470	-1.031387	4.686045
H	2.146775	-1.570038	5.579451
H	0.734569	-0.868683	4.800563
C	2.532573	0.316896	4.596619
H	3.616426	0.180624	4.506151
H	2.346752	0.919755	5.490918
H	2.188564	0.890635	3.730910
H	0.788664	-0.805478	-0.088163
H	3.829215	-0.583741	0.337500
O	2.816325	0.797900	-0.824543
H	7.275371	0.083966	-2.154485
H	-0.467478	-3.156344	1.331903
H	-0.396537	-5.026419	-0.352225

Statistical Thermodynamic Analysis
Temperature= 298.150 Kelvin Pressure= 1.00000 Atm
==========
SCF Energy= -1923.19813767 Predicted Change= -1.655685D-09
Zero-point correction (ZPE)= -1922.4553 0.74278
Internal Energy (U)= -1922.4143 0.78377
Enthalpy (H)= -1922.4134 0.78472
Gibbs Free Energy (G)= -1922.5304 0.66767

Frequencies -- 14.5623 19.5272 22.2946

NMR-Shifts
Revised-MandelalideC-0010-NMR.txt

Atom	Type	Isotropic	Scaled Shift
1	C	100.2533	82.1289649496
3	C	114.6195	68.3785103084
4	C	149.3705	35.1169624227
7	C	99.6310	82.7245927372
13	C	97.8775	84.4029365034
14	C	151.9213	32.675491491
16	C	51.3645	128.92235686
18	C	49.2593	130.937326519
20	C	55.9156	124.566320182
22	C	38.8163	140.93273225
23	C	147.8293	36.592105515
25	C	166.9285	18.3115105572
29	C	139.9041	44.1776259117
32	C	110.5108	72.3111085587
37	C	145.3087	39.0046708398
38	C	172.9713	12.5277091828
43	C	149.0577	35.4163555964
46	C	111.4282	71.433028963
48	C	101.9117	80.541645131
51	C	1.4941	176.655276709
54	C	146.1116	38.2361836942
57	C	115.1360	67.8841478589
60	C	142.7854	41.4198204407
63	C	113.8047	69.1583874117
64	C	149.5820	34.9145274603
67	C	114.9830	68.0305901721
69	C	4.1554	174.108041884

71	C	149.5772	34.919121729
74	C	166.6950	18.5350025843
77	C	172.8414	12.6520415781
2	H	27.6124	3.90870870871
5	H	30.1039	1.60656040656
6	H	29.1135	2.52169092169
8	H	25.8655	5.52284592285
10	H	30.0156	1.68814968815
11	H	28.0105	3.54086394086
15	H	29.0171	2.61076461076
17	H	25.9384	5.45548625549
19	H	25.3353	6.01275121275
21	H	24.7874	6.51901131901
24	H	29.0860	2.5471009471
26	H	30.6054	1.14317394317
27	H	30.8072	0.956710556711
28	H	31.0905	0.694941094941
30	H	30.5674	1.17828597829
31	H	30.3976	1.33518133518
33	H	28.3700	3.20868560869
34	H	25.8305	5.55518595519
35	H	29.6137	2.05950565951
36	H	27.5635	3.95389235389
39	H	30.6288	1.12155232155
40	H	30.5559	1.18891198891
41	H	30.7850	0.977223377223
42	H	29.2089	2.43354123354
44	H	29.6875	1.99131439131
45	H	30.1357	1.57717717718
50	H	29.1635	2.47549087549
55	H	30.0334	1.6717024717
56	H	30.7406	1.01824901825
59	H	27.8845	3.65728805729
61	H	30.0810	1.62772002772
62	H	30.6061	1.14252714253
65	H	29.8184	1.87036267036
66	H	29.6662	2.010995611
72	H	29.3826	2.27304227304
73	H	29.1010	2.53324093324
75	H	30.3333	1.39459459459
76	H	29.8547	1.83682143682
78	H	31.1853	0.607345807346
79	H	30.7173	1.03977823978
80	H	30.6609	1.09189189189
81	H	25.8519	5.53541233541
82	H	28.3213	3.25368445368
84	H	30.9723	0.804158004158
85	H	27.6743	3.85151305151
86	H	28.9684	2.65576345576

Supporting Information: Revised-MandelalideC-0011.log

Using Gaussian 09: AM64L-G09RevD.01 24-Apr-2013

==========

#b3lyp/6-31G(d,p) scf=(maxcycle=300,direct,tight) density=current SCRF=(PCM,SOLVENT=Chloroform) opt=(maxcycle=250) freq=noraman

#N Geom=AllCheck Guess=TCheck SCRF=Check GenChk RB3LYP/6-31G(d,p) Freq

---

Pointgroup= C1 Stoichiometry= C30H46O10 C1[X(C30H46O10)] #Atoms= 86

Charge = 0 Multiplicity = 1

SCF Energy= -1923.19827983 Predicted Change= -4.964966D-08

==========

Optimization completed. {Found 1 times}

Item	Max Val.	Criteria	Pass?	RMS Val.	Criteria	Pass?
Force	0.00001 ||	0.00045	[YES]	0.00000 ||	0.00030	[YES]
Displ	0.00904 ||	0.00180	[NO]	0.00904 ||	0.00180	[NO]

Atomic Type	Coordinates (Angstroms) X	Y	Z
C	-4.420568	-0.467021	0.309088
H	-4.434114	-0.878731	1.331708
C	-4.315097	-1.633178	-0.684908
C	-3.183301	-2.635372	-0.371275
H	-3.342762	-3.035830	0.638160
H	-3.264147	-3.478611	-1.061221
C	-1.749241	-2.118708	-0.421847
H	-1.609657	-1.246597	0.218641
O	-4.270702	-1.170122	-2.029213
H	-3.420809	-0.719420	-2.140239
H	-5.253197	-2.196959	-0.604154
O	-3.266861	0.378176	0.155468
C	-3.619365	1.775736	0.246996
C	-3.275251	2.450883	-1.103488
H	-2.404415	1.911179	-1.490954
C	-2.958557	3.923527	-0.994857
H	-3.726217	4.625644	-1.311295
C	-1.797741	4.416684	-0.517413
H	-1.664859	5.497379	-0.474897
C	-0.685054	3.605700	-0.044040
H	-0.814585	2.525245	-0.070672
C	0.483734	4.076090	0.424073
C	1.612978	3.192374	0.886905
H	1.246613	2.158783	0.891698
C	2.051743	3.561740	2.316296
H	2.882498	2.934315	2.656347
H	1.226659	3.435843	3.023934
H	2.382028	4.606303	2.365562
C	2.802035	3.252086	-0.106610
H	3.405553	4.147653	0.088298
H	2.424606	3.338021	-1.131869
C	3.706067	2.020754	-0.063376
H	3.969646	1.780950	0.981458
H	0.653045	5.154501	0.465927
H	-4.083505	2.281045	-1.822310
H	-2.987831	2.222547	1.023110
C	-5.106932	1.788513	0.680484
C	-5.922853	3.024042	0.300750
H	-5.482139	3.936728	0.714094
H	-6.941962	2.940318	0.691961
H	-5.996743	3.145033	-0.784785
H	-5.116557	1.699495	1.775286
C	-5.618807	0.459291	0.102613
H	-5.828982	0.551763	-0.968696
H	-6.521309	0.096929	0.603193
C	-0.673656	-3.181030	-0.121269
O	-1.098320	-4.452341	-0.568862
C	0.518634	-2.705908	-0.992085
O	1.275713	-3.823718	-1.427564
H	1.427040	-3.708149	-2.381037
C	-0.230955	-2.084509	-2.181251
O	0.200497	-2.000174	-3.309924
O	-1.447205	-1.673991	-1.803504
C	5.001640	2.212698	-0.861733
H	5.599064	3.017313	-0.419185
H	4.754987	2.505341	-1.889888
C	5.811682	0.920919	-0.898058
O	6.944995	1.143739	-1.736455
H	6.144204	0.685722	0.127617
C	4.934008	-0.227451	-1.403474
H	5.477061	-1.179377	-1.344656
H	4.690275	-0.045073	-2.457410

C	3.634950	-0.322274	-0.588829
C	2.694832	-1.382796	-1.157808
H	2.395966	-1.084422	-2.168277
H	3.243137	-2.325378	-1.242085
C	1.432078	-1.633003	-0.331244
O	1.856351	-2.114850	0.969553
C	1.338823	-1.518147	2.075001
O	0.474281	-0.665321	2.039287
C	2.005935	-2.046847	3.327667
H	3.005572	-1.593175	3.359034
H	2.170580	-3.122746	3.202747
C	1.234116	-1.738071	4.614736
H	1.035357	-0.662143	4.658384
H	1.884143	-1.974387	5.464636
C	-0.080750	-2.513695	4.741366
H	-0.763995	-2.266811	3.923033
H	-0.587768	-2.273436	5.681042
H	0.093658	-3.595599	4.724153
H	0.873395	-0.706491	-0.184507
H	3.888223	-0.582554	0.452835
O	2.942990	0.927710	-0.600282
H	7.467726	0.329878	-1.744956
H	-0.441018	-3.201524	0.948475
H	-0.299149	-4.881547	-0.920738

Statistical Thermodynamic Analysis
Temperature= 298.150 Kelvin Pressure= 1.00000 Atm
==========
SCF Energy= -1923.19827983 Predicted Change= -4.964966D-08
Zero-point correction (ZPE)= -1922.4553 0.74291
Internal Energy (U)= -1922.4144 0.78385
Enthalpy (H)= -1922.4134 0.78479
Gibbs Free Energy (G)= -1922.5303 0.66795

Frequencies -- 14.2389 17.4579 23.7101

NMR-Shifts
Revised-MandelalideC-0011-NMR.txt

Atom	Type	Isotropic	Scaled Shift
1	C	99.7629	82.5983460633
3	C	113.8248	69.1391489117
4	C	149.7801	34.7249181646
7	C	99.7412	82.6191159861
13	C	97.8201	84.4578762993
14	C	152.3339	32.280575815
16	C	51.6743	128.625835104
18	C	49.0643	131.123968682
20	C	55.9734	124.510997531
22	C	38.1783	141.543387125
23	C	148.0554	36.3756963188
25	C	167.3583	17.9001320852
29	C	140.4127	43.6908248627
32	C	110.3105	72.5028235609
37	C	145.7402	38.591665231
38	C	172.8811	12.6140431478
43	C	149.3623	35.124810965
46	C	111.2451	71.6082811692
48	C	102.2737	80.1951607037
51	C	1.5842	176.569038458
54	C	145.7458	38.5863052509
57	C	114.8911	68.118551274
60	C	142.5058	41.6874365895
63	C	113.7313	69.2286414365
64	C	149.4222	35.0674783208
67	C	115.0309	67.9847431995
69	C	4.5041	173.77428741
71	C	149.6040	34.8934703957
74	C	166.7200	18.5110741017
77	C	173.2026	12.3063228622
2	H	27.5626	3.95472395472
5	H	30.0544	1.6522984523
6	H	29.1174	2.51808731809
8	H	25.8098	5.57431277431
10	H	29.9723	1.72815892816
11	H	27.9409	3.60517440517
15	H	29.0993	2.53481173481
17	H	25.9529	5.44208824209
19	H	25.3738	5.97717717718
21	H	24.8112	6.49702009702
24	H	29.0433	2.58655578656
26	H	30.5934	1.15426195426
27	H	30.8514	0.91586971587
28	H	31.1845	0.608085008085
30	H	30.6681	1.08523908524
31	H	30.4306	1.30468930469
33	H	28.4254	3.1574959575
34	H	25.7812	5.60073920074
35	H	29.5551	2.11365211365
36	H	27.6090	3.91185031185
39	H	30.6117	1.13735273735
40	H	30.5598	1.18530838531
41	H	30.7622	0.998290598291
42	H	29.2272	2.41663201663
44	H	29.6258	2.04832524833
45	H	30.1193	1.59233079233
50	H	29.2921	2.35666435666
55	H	30.0538	1.65285285285
56	H	30.7858	0.976484176484
59	H	27.8916	3.65072765073
61	H	30.1344	1.57837837838
62	H	30.6059	1.14271194271
65	H	29.9430	1.75523215523
66	H	29.7337	1.94862554863
72	H	29.0750	2.55726495726
73	H	29.4163	2.2419034419
75	H	29.8634	1.82878262878
76	H	30.3096	1.41649341649
78	H	30.7166	1.04042504043
79	H	30.6772	1.07683067683
80	H	31.1532	0.637006237006
81	H	25.8556	5.53199353199
82	H	28.3678	3.21071841072
84	H	31.0201	0.759990759991
85	H	27.6526	3.87156387156
86	H	28.9652	2.65872025872

Supporting Information: Revised-MandelalideC-0012.log

Using Gaussian 09: AM64L-G09RevD.01 24-Apr-2013
==========
#b3lyp/6-31G(d,p) scf=(maxcycle=300,direct,tight) density=current SCRF=(PCM,SOLVENT=Chloroform) opt=(maxcycle=250) freq=noraman
#N Geom=AllCheck Guess=TCheck SCRF=Check GenChk RB3LYP/6-31G(d,p) Freq

---

Pointgroup= C1 Stoichiometry= C30H46O10 C1[X(C30H46O10)] #Atoms= 86
Charge = 0 Multiplicity = 1

SCF Energy= -1923.19547635 Predicted Change= -1.714035D-08
==========
Optimization completed. {Found 1 times}

Item	Max Val.	Criteria	Pass?	RMS Val.	Criteria	Pass?
Force	0.00000 ||	0.00045	[YES]	0.00000 ||	0.00030	[YES]
Displ	0.00321 ||	0.00180	[NO]	0.00321 ||	0.00180	[YES]

Atomic Type	Coordinates (Angstroms) X	Y	Z
C	-4.502048	-0.493121	0.579773
H	-4.506160	-0.820465	1.632832
C	-4.424659	-1.740812	-0.313288
C	-3.275388	-2.708464	0.044726
H	-3.393412	-3.009908	1.094165
H	-3.385280	-3.609845	-0.564305
C	-1.847982	-2.194248	-0.120365
H	-1.681865	-1.283628	0.458338
O	-4.432296	-1.402668	-1.694219
H	-3.557525	-1.041780	-1.901623
H	-5.356522	-2.296540	-0.145150
O	-3.343472	0.327511	0.350480
C	-3.693446	1.725401	0.265555
C	-3.392954	2.220820	-1.171697
H	-2.536890	1.630161	-1.514684
C	-3.071354	3.693736	-1.259058
H	-3.853485	4.355754	-1.623269
C	-1.891807	4.237189	-0.895780
H	-1.759986	5.314844	-0.989039
C	-0.756971	3.485889	-0.378968
H	-0.881201	2.408797	-0.281909
C	0.426125	4.007617	-0.012140
C	1.579638	3.182665	0.497233
H	1.222387	2.153146	0.619780
C	2.066497	3.697130	1.864766
H	2.915492	3.111967	2.234259
H	1.269304	3.638505	2.612165
H	2.387876	4.743459	1.797046
C	2.731567	3.145764	-0.540003
H	3.342198	4.053489	-0.452408
H	2.316708	3.136583	-1.554184
C	3.635750	1.919605	-0.415934
H	3.945755	1.781397	0.634684
H	0.589452	5.084562	-0.095499
H	-4.224754	1.967204	-1.837434
H	-3.037674	2.266212	0.957047
C	-5.165433	1.796535	0.738044
C	-5.984251	2.993728	0.256414
H	-5.526398	3.939657	0.562432
H	-6.993040	2.959712	0.680484
H	-6.085685	3.003812	-0.833492
H	-5.142310	1.819045	1.836103
C	-5.699519	0.419802	0.311549
H	-5.936373	0.407207	-0.757888
H	-6.591218	0.116985	0.867939
C	-0.751186	-3.225697	0.201207
O	-1.123576	-4.553945	-0.171385
C	0.402291	-2.839800	-0.764670
O	1.173056	-3.949522	-1.140523
H	0.574203	-4.713618	-1.069622
C	-0.397218	-2.245746	-1.955893
O	-0.035632	-2.123208	-3.099693
O	-1.620540	-1.848682	-1.531030
C	4.894060	2.028881	-1.286796
H	5.512631	2.867621	-0.948792
H	4.600683	2.227195	-2.325223
C	5.700265	0.734214	-1.242547
O	6.789893	0.871592	-2.154402
H	6.085202	0.594710	-0.217559
C	4.796974	-0.452125	-1.592259
H	5.340634	-1.397660	-1.469866
H	4.501653	-0.369715	-2.645462
C	3.539600	-0.462696	-0.711116
C	2.573907	-1.566916	-1.134493
H	2.221886	-1.361367	-2.149946
H	3.112656	-2.517250	-1.165691
C	1.354360	-1.737733	-0.225955
O	1.849582	-2.127927	1.083142
C	1.360542	-1.488225	2.174048
O	0.465736	-0.666321	2.132264
C	2.053672	-1.974181	3.431160
H	3.129441	-2.030112	3.229432
H	1.728261	-3.011571	3.584148
C	1.757408	-1.123772	4.670501
H	2.113713	-1.671457	5.550275
H	0.672386	-1.022174	4.779894
C	2.405781	0.263368	4.630631
H	3.496066	0.187646	4.546869
H	2.180743	0.826862	5.541499
H	2.038514	0.844047	3.779604
H	0.813224	-0.796105	-0.116248
H	3.842656	-0.621825	0.337823
O	2.848871	0.785122	-0.809692
H	7.304934	0.053538	-2.119814
H	-0.462813	-3.187883	1.252893
H	-1.464366	-5.019681	0.601968

Statistical Thermodynamic Analysis
Temperature= 298.150 Kelvin Pressure= 1.00000 Atm
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SCF Energy= -1923.19547635 Predicted Change= -1.714035D-08
Zero-point correction (ZPE)= -1922.4529 0.74254
Internal Energy (U)= -1922.4117 0.78371
Enthalpy (H)= -1922.4108 0.78465
Gibbs Free Energy (G)= -1922.5280 0.66737

Frequencies -- 14.3078 18.4435 23.2950

NMR-Shifts
Revised-MandelalideC-0012-NMR.txt

Atom	Type	Isotropic	Scaled Shift
1	C	99.6643	82.6927199985
3	C	114.0932	68.8822527231
4	C	149.6302	34.868393346
7	C	102.9441	79.5534945156
13	C	97.3822	84.8770075997
14	C	151.4592	33.1177855625
16	C	51.1165	129.159727407
18	C	49.3906	130.811654128
20	C	55.9944	124.490897605
22	C	38.8137	140.935220812
23	C	147.8129	36.6078025996
25	C	166.8077	18.4271329849
29	C	140.0002	44.0856448247
32	C	110.5607	72.2633473076
37	C	145.2782	39.0338635885
38	C	172.9099	12.5864775359
43	C	149.3625	35.1246195371
46	C	108.8434	73.907042631
48	C	103.7384	78.793238768
51	C	4.0837	174.176668772
54	C	146.0294	38.3148605448
57	C	114.9439	68.0680143188
60	C	142.8719	41.337027891
63	C	113.3825	69.562491625
64	C	149.9149	34.5958957867
67	C	114.4599	68.531269741
69	C	3.8791	174.372499474

71	C	149.6787	34.8219720898
74	C	166.6592	18.5692681713
77	C	172.8460	12.6476387373
2	H	27.6063	3.91434511435
5	H	30.2561	1.46592746593
6	H	29.1825	2.45793485793
8	H	25.8863	5.50362670363
10	H	29.6380	2.03705243705
11	H	28.0080	3.54317394317
15	H	29.0208	2.60734580735
17	H	25.9771	5.41972741973
19	H	25.3319	6.01589281589
21	H	24.7978	6.5094017094
24	H	29.1030	2.53139293139
26	H	30.6028	1.14557634558
27	H	30.8339	0.93203973204
28	H	31.1065	0.680157080157
30	H	30.5717	1.17431277431
31	H	30.3837	1.34802494802
33	H	28.3773	3.20194040194
34	H	25.8406	5.54585354585
35	H	29.6234	2.05054285054
36	H	27.6124	3.90870870871
39	H	30.6504	1.10159390159
40	H	30.5654	1.18013398013
41	H	30.7966	0.966504966505
42	H	29.2280	2.41589281589
44	H	29.6323	2.04231924232
45	H	30.1303	1.58216678217
50	H	27.9140	3.63003003003
55	H	30.0480	1.65821205821
56	H	30.7384	1.02028182028
59	H	27.8937	3.64878724879
61	H	30.0966	1.61330561331
62	H	30.5790	1.16756756757
65	H	29.5259	2.14063294063
66	H	29.5445	2.12344652345
72	H	29.3591	2.29475629476
73	H	29.1265	2.50967890968
75	H	30.3389	1.38942018942
76	H	29.9006	1.79440979441
78	H	31.1716	0.620004620005
79	H	30.7177	1.03940863941
80	H	30.6091	1.13975513976
81	H	25.9051	5.48625548626
82	H	28.3445	3.23224763225
84	H	30.9957	0.782536382536
85	H	27.6918	3.83534303534
86	H	30.0299	1.67493647494

Mandelalide C Original Configuration

Supporting Information: Original_MandelalideC-0001.log

Using Gaussian 09: AM64L-G09RevD.01 24-Apr-2013

==========

#b3lyp/6-31G(d,p) scf=(maxcycle=300,direct,tight) density=current SCRF=(PCM,SOLVENT=Chloroform) opt=(maxcycle=250) freq=noraman

#N Geom=AllCheck Guess=TCheck SCRF=Check GenChk RB3LYP/6-31G(d,p) Freq

---

Pointgroup= C1 Stoichiometry= C30H46O10 C1[X(C30H46O10)] #Atoms= 86

Charge = 0 Multiplicity = 1

SCF Energy= -1923.19787677 Predicted Change= -5.934326D-09

==========

Optimization completed. {Found 2 times}

Item	Max Val.	Criteria	Pass?	RMS Val.	Criteria	Pass?
Force	0.00000	0.00045	[YES]	0.00000	0.00030	[YES]
Displ	0.00142	0.00180	[YES]	0.00142	0.00180	[YES]

Atomic Type	Coordinates (Angstroms) X	Y	Z
C	3.717006	-2.608012	0.175264
H	3.691046	-3.522809	0.787181
C	2.273399	-2.174095	-0.133108
C	1.363728	-2.260765	1.099810
H	1.338660	-3.300435	1.445690
H	1.765622	-1.649719	1.912820
C	-0.064618	-1.832463	0.795553
H	-0.430829	-2.320838	-0.112759
O	2.260631	-0.869429	-0.708654
H	2.627554	-0.282485	-0.028382
H	1.881292	-2.842186	-0.911071
O	4.360033	-1.562731	0.933727
C	5.678163	-1.282329	0.408032
C	5.704957	0.113109	-0.243809
H	6.681797	0.232630	-0.732796
C	5.551264	1.232006	0.748419
H	6.317039	1.257938	1.523985
C	4.616691	2.200748	0.773749
H	4.694504	2.951571	1.560084
C	3.478749	2.362265	-0.121638
H	3.311414	1.601063	-0.882651
C	2.612164	3.387015	-0.042414
C	1.383221	3.568310	-0.896569
H	1.155507	2.610723	-1.380757
C	1.628746	4.625833	-1.992627
H	0.734072	4.787687	-2.603473
H	2.438673	4.314209	-2.658849
H	1.910202	5.588214	-1.549240
C	0.185200	3.949788	0.004863
H	0.285706	5.000125	0.307774
H	0.215393	3.350052	0.921625
C	-1.197421	3.742257	-0.612896
H	-1.215190	4.121841	-1.649525
H	2.790744	4.164749	0.704050
H	4.947343	0.159904	-1.030939
H	6.371059	-1.280961	1.259891
C	5.989908	-2.466602	-0.540961
C	7.043473	-2.232236	-1.623215
H	8.001762	-1.921585	-1.192884
H	6.728442	-1.466141	-2.338462
H	7.219400	-3.155412	-2.184690
H	6.332522	-3.293448	0.095931
C	4.591523	-2.826765	-1.059309
H	4.525536	-3.850988	-1.437297
H	4.286323	-2.144105	-1.860616
C	-0.342403	-0.317284	0.709668
O	0.474988	0.373034	1.636265
H	-0.176733	0.051972	-0.302300
C	-1.820836	-0.234300	1.160428
O	-2.069172	0.956311	1.892159
H	-2.605257	0.693542	2.660971
C	-1.901087	-1.425576	2.132677
O	-2.707722	-1.525783	3.032397
O	-0.925842	-2.305987	1.893578
C	-2.299426	4.453177	0.183470
H	-2.142872	5.536820	0.146652
H	-2.247480	4.141346	1.233582
C	-3.680497	4.107269	-0.363462
O	-4.647264	4.730267	0.482233

H	-3.766022	4.507874	-1.388454
C	-3.847089	2.585903	-0.409655
H	-4.799699	2.316589	-0.884302
H	-3.855363	2.212478	0.617854
C	-2.689081	1.943251	-1.187384
C	-2.734487	0.412941	-1.252542
H	-3.592876	0.137594	-1.874737
H	-1.840008	0.065607	-1.779035
C	-2.896299	-0.388521	0.050398
O	-2.904127	-1.798829	-0.314119
C	-4.108340	-2.371172	-0.591981
O	-5.153551	-1.756701	-0.584724
C	-3.941303	-3.841658	-0.900418
H	-3.431774	-4.302378	-0.044593
H	-3.239437	-3.926628	-1.740151
C	-5.259502	-4.554230	-1.208413
H	-5.748045	-4.057298	-2.053935
H	-5.937030	-4.438884	-0.355319
C	-5.055927	-6.039312	-1.518808
H	-6.010309	-6.528528	-1.735828
H	-4.597221	-6.563887	-0.673187
H	-4.404239	-6.179143	-2.388720
H	-3.858387	-0.164768	0.516137
H	-2.741005	2.298973	-2.232137
O	-1.422953	2.325732	-0.648256
H	-0.087989	1.074887	2.004699
H	-5.523282	4.515859	0.132594

Statistical Thermodynamic Analysis
Temperature= 298.150 Kelvin Pressure= 1.00000 Atm
==========
SCF Energy= -1923.19787677 Predicted Change= -5.934326D-09
Zero-point correction (ZPE)= -1922.4552 0.74262
Internal Energy (U)= -1922.4142 0.78366
Enthalpy (H)= -1922.4132 0.78460
Gibbs Free Energy (G)= -1922.5298 0.66807

Frequencies -- 18.4072 23.6299 27.5775

NMR-Shifts
Original_MandelalideC-0001-NMR.txt

Atom	Type	Isotropic	Scaled Shift
1	C	101.5982	80.8417083022
3	C	113.3822	69.5627787668
4	C	151.8062	32.7856582247
7	C	98.8960	83.4280901242
13	C	99.8848	82.4816707824
14	C	153.7308	30.943547924
16	C	50.5508	129.70118111
18	C	49.5227	130.685216026
20	C	57.1121	123.421103007
22	C	36.7693	142.891996401
23	C	148.9834	35.4874710465
25	C	166.1098	19.0951205038
29	C	141.3652	42.7791496774
32	C	111.1151	71.7327092785
37	C	145.4275	38.8909626907
38	C	172.2526	13.2156051992
43	C	148.5951	35.8591282375
46	C	112.5462	70.3629472233
49	C	102.7792	79.7113267865
52	C	-1.5626	179.580964414
55	C	146.0413	38.3034705871
58	C	114.4587	68.5324183082
61	C	146.7596	37.6159574264
64	C	111.1453	71.7038036716
65	C	148.4211	36.0256704761
68	C	110.1661	72.6410344762
70	C	5.2123	173.096441356
72	C	148.0675	36.3641149333
75	C	166.5770	18.6479450219
78	C	172.9049	12.5912632325
2	H	27.6473	3.87646107646
5	H	30.0079	1.69526449526
6	H	29.1322	2.50441210441
8	H	26.8196	4.64125664126
10	H	30.2516	1.47008547009
11	H	28.1822	3.38221298221
15	H	29.7633	1.92127512128
17	H	26.2136	5.2012012012
19	H	25.1054	6.22517902518
21	H	25.1181	6.21344421344
24	H	29.1655	2.47364287364
26	H	30.4352	1.30043890044
27	H	30.8613	0.906722106722
28	H	31.1425	0.646893046893
30	H	30.5135	1.22808962809
31	H	30.2242	1.4954030954
33	H	28.2320	3.3361977362
34	H	25.9326	5.46084546085
35	H	29.1507	2.48731808732
36	H	27.5717	3.94631554632
39	H	30.7378	1.02083622084
40	H	30.9619	0.813767613768
41	H	30.5539	1.19075999076
42	H	29.2527	2.39306999307
44	H	29.9745	1.72612612613
45	H	29.8723	1.82055902056
48	H	26.5913	4.85220605221
51	H	29.2020	2.43991683992
56	H	30.1000	1.61016401016
57	H	30.6077	1.14104874105
60	H	27.8235	3.71365211365
62	H	30.0535	1.65313005313
63	H	29.9157	1.78045738046
66	H	29.8026	1.88496188496
67	H	29.5363	2.13102333102
73	H	29.3593	2.29457149457
74	H	29.4294	2.2297990298
76	H	30.2382	1.48246708247
77	H	30.2330	1.48727188727
79	H	30.6165	1.13291753292
80	H	30.9846	0.792792792793
81	H	31.0127	0.766828366828
82	H	26.2305	5.18558558559
83	H	28.1090	3.44984984985
85	H	29.1875	2.45331485331
86	H	30.9176	0.854700854701

Supporting Information: Original_MandelalideC-0002.log

Using Gaussian 09: AM64L-G09RevD.01 24-Apr-2013
==========
#b3lyp/6-31G(d,p) scf=(maxcycle=300,direct,tight) density=current SCRF=(PCM,SOLVENT=Chloroform) opt=(maxcycle=250) freq=noraman
#N Geom=AllCheck Guess=TCheck SCRF=Check GenChk RB3LYP/6-31G(d,p) Freq

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Pointgroup= C1 Stoichiometry= C30H46O10 C1[X(C30H46O10)] #Atoms= 86
Charge = 0 Multiplicity = 1

SCF Energy= -1923.19660121 Predicted Change= -1.440458D-08

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Optimization completed. {Found 1 times}

Item	Max Val.	Criteria	Pass?	RMS Val.	Criteria	Pass?
Force	0.00000	0.00045	[YES]	0.00000	0.00030	[YES]
Displ	0.00286	0.00180	[NO]	0.00286	0.00180	[YES]

Atomic Type	Coordinates (Angstroms) X	Y	Z
C	-3.952926	2.075981	0.360683
H	-4.061112	2.941637	1.032011
C	-2.460970	1.870633	0.045614
C	-1.577806	2.011840	1.292871
H	-1.702963	3.021548	1.700498
H	-1.891352	1.300899	2.062469
C	-0.101572	1.811767	0.980459
H	0.189057	2.391680	0.099056
O	-2.262105	0.616025	-0.601767
H	-2.565985	-0.051714	0.033771
H	-2.163617	2.631261	-0.688034
O	-4.443165	0.900709	1.038925
C	-5.708031	0.475261	0.480267
C	-5.538285	-0.862397	-0.265240
H	-6.487900	-1.081773	-0.772900
C	-5.234632	-2.015355	0.650563
H	-5.997740	-2.206027	1.405562
C	-4.170113	-2.839228	0.631499
H	-4.149396	-3.646332	1.363915
C	-3.007193	-2.775197	-0.243989
H	-2.938714	-1.951151	-0.952614
C	-2.003500	-3.668752	-0.204268
C	-0.748135	-3.620453	-1.037449
H	-0.649937	-2.611104	-1.455960
C	-0.825700	-4.628764	-2.202541
H	0.093119	-4.627293	-2.798836
H	-1.659309	-4.388321	-2.868980
H	-0.979198	-5.647202	-1.826822
C	0.478832	-3.888811	-0.133722
H	0.522769	-4.960155	0.101881
H	0.351948	-3.359314	0.817481
C	1.825687	-3.452158	-0.709112
H	1.910272	-3.763941	-1.764960
H	-2.081433	-4.508511	0.490305
H	-4.779964	-0.749531	-1.045294
H	-6.395603	0.318797	1.321830
C	-6.180729	1.666614	-0.389584
C	-7.193973	1.361988	-1.492588
H	-8.093924	0.884012	-1.090535
H	-6.775799	0.704415	-2.261085
H	-7.506298	2.288198	-1.985580
H	-6.634264	2.392833	0.298597
C	-4.845200	2.250984	-0.868250
H	-4.921373	3.296963	-1.178714
H	-4.445900	1.670883	-1.708093
C	0.396493	0.360254	0.824344
O	-0.307761	-0.486381	1.713466
H	0.285030	0.019040	-0.204747
C	1.871852	0.476160	1.279619
O	2.295095	-0.698555	1.954650
H	2.785226	-0.396439	2.739556
C	1.774386	1.616620	2.309737
O	2.556466	1.789113	3.220031
O	0.679827	2.354076	2.106007
C	3.010381	-4.044035	0.065553
H	3.009987	-5.135187	-0.033138
H	2.907612	-3.802966	1.130254
C	4.332423	-3.475838	-0.441166
O	5.371858	-4.001779	0.384041
H	4.480722	-3.802963	-1.484812
C	4.281748	-1.945576	-0.403265
H	5.189921	-1.518339	-0.848197
H	4.228658	-1.632041	0.642772
C	3.049608	-1.432672	-1.163096
C	2.874733	0.089298	-1.152839
H	3.685806	0.515220	-1.752992
H	1.940615	0.327417	-1.671190
C	2.913835	0.841599	0.187358
O	2.712449	2.253203	-0.111391
C	3.816381	3.003442	-0.383084
O	4.941147	2.549474	-0.395570
C	3.434928	4.430627	-0.696770
H	4.339027	5.037883	-0.605610
H	2.707636	4.774366	0.046444
C	2.836029	4.571028	-2.112475
H	1.950515	3.930556	-2.191640
H	3.561339	4.198334	-2.845699
C	2.464979	6.019162	-2.440115
H	2.044422	6.095958	-3.447479
H	3.341848	6.673786	-2.392604
H	1.721007	6.406506	-1.735432
H	3.897856	0.742064	0.650801
H	3.157850	-1.722931	-2.223705
O	1.847765	-2.018344	-0.661291
H	0.353962	-1.112887	2.052502
H	6.211777	-3.652579	0.055043

Statistical Thermodynamic Analysis
Temperature= 298.150 Kelvin Pressure= 1.00000 Atm
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==========
SCF Energy= -1923.19660121 Predicted Change= -1.440458D-08
Zero-point correction (ZPE)= -1922.4532 0.74335
Internal Energy (U)= -1922.4124 0.78419
Enthalpy (H)= -1922.4114
0.78513
Gibbs Free Energy (G)= -1922.5271
0.66944

Frequencies -- 21.1940 21.8250 27.9450

NMR-Shifts
Original_MandelalideC-0002-NMR.txt

Atom	Type	Isotropic	Scaled Shift
1	C	101.1434	81.2770152568
3	C	113.4896	69.4599820058
4	C	151.6558	32.9296119757
7	C	98.8455	83.476425659
13	C	99.7421	82.6182545608
14	C	153.3664	31.2923294856
16	C	50.4787	129.770190854
18	C	49.5902	130.620609123
20	C	57.4578	123.090219951
22	C	35.7029	143.912689753
23	C	148.7642	35.6972759815
25	C	165.4719	19.7056796646
29	C	141.5380	42.613756006
32	C	110.7788	72.0545952258
37	C	145.3269	38.9872509045
38	C	172.1221	13.3405118781
43	C	148.7419	35.718620188
46	C	112.7517	70.1662550968
49	C	103.0602	79.4423706426
52	C	-1.5179	179.538180287
55	C	146.3110	38.0453301173
58	C	114.9258	68.0853385402
61	C	146.3967	37.9633032792
64	C	110.6655	72.1630391087

65	C	148.9245	35.5438465514
68	C	110.8283	72.0072168303
70	C	5.4814	172.83887517
72	C	145.5778	38.7471046536
75	C	161.8205	23.2005781121
78	C	171.3345	14.0943547924
2	H	27.5681	3.94964194964
5	H	30.0226	1.68168168168
6	H	29.0838	2.54913374913
8	H	26.8506	4.61261261261
10	H	30.1245	1.58752598753
11	H	28.1546	3.40771540772
15	H	29.7365	1.94603834604
17	H	26.2367	5.17985677986
19	H	25.0937	6.23598983599
21	H	24.8932	6.42125202125
24	H	29.2486	2.39685839686
26	H	30.5336	1.20951720952
27	H	30.8145	0.949965349965
28	H	31.0990	0.687087087087
30	H	30.5456	1.19842919843
31	H	30.1913	1.5258027258
33	H	28.2895	3.28306768307
34	H	25.8691	5.51951951952
35	H	29.1720	2.46763686764
36	H	27.5351	3.98013398013
39	H	30.7444	1.01473781474
40	H	30.9606	0.814968814969
41	H	30.5892	1.15814275814
42	H	29.1782	2.46190806191
44	H	29.9129	1.78304458304
45	H	29.8464	1.84449064449
48	H	26.6468	4.80092400092
51	H	29.2159	2.42707322707
56	H	30.1327	1.57994917995
57	H	30.6535	1.09872949873
60	H	27.9181	3.62624162624
62	H	30.0857	1.62337722338
63	H	29.8564	1.83525063525
66	H	29.8232	1.86592746593
67	H	29.6126	2.06052206052
73	H	29.6472	2.02855162855
74	H	29.4720	2.19043659044
76	H	30.0496	1.65673365673
77	H	30.1424	1.57098637099
79	H	30.5106	1.23076923077
80	H	30.8447	0.922060522061
81	H	30.9031	0.868098868099
82	H	26.2930	5.12783552784
83	H	28.0552	3.49956109956
85	H	29.1677	2.47161007161
86	H	30.9379	0.835943635944

Mandelalide D Revised Configuration

Supporting Information: Revised-MandelalideD-0001.log

Using Gaussian 09: AM64L-G09RevD.01 24-Apr-2013

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#b3lyp/6-31G(d,p) scf=(maxcycle=300,direct,tight) density=current SCRF=(PCM,SOLVENT=Chloroform) opt=(maxcycle=250) freq=noraman

#N Geom=AllCheck Guess=TCheck SCRF=Check GenChk RB3LYP/6-31G(d,p) Freq

---

Pointgroup= C1 Stoichiometry= C34H52O11 C1[X(C34H52O11)] #Atoms= 97

Charge = 0 Multiplicity = 1

SCF Energy= -2154.49924888 Predicted Change= -1.251231D-08

==========

Optimization completed. {Found 1 times}

Item	Max Val.	Criteria	Pass?	RMS Val.	Criteria	Pass?
Force	0.00001 ||	0.00045	[YES]	0.00000 ||	0.00030	[YES]
Displ	0.00464 ||	0.00180	[NO]	0.00464 ||	0.00180	[YES]

Atomic Type	Coordinates (Angstroms) X	Y	Z
C	4.416699	0.276429	1.051677
H	4.587164	0.990300	1.868702
C	2.909637	0.074417	0.859518
C	2.116386	1.357830	0.606713
H	2.067414	1.939560	1.534217
H	2.597187	1.975736	-0.156287
C	0.701915	1.018236	0.163090
H	0.276026	0.277283	0.843351
O	2.348415	-0.545176	2.012253
H	2.887155	-1.336592	2.168550
H	2.787491	-0.580828	-0.015996
O	4.965398	-0.994808	1.479516
C	5.910484	-1.493990	0.516262
C	5.266582	-2.560731	-0.399616
H	4.413857	-2.126884	-0.930333
C	4.880176	-3.807238	0.351249
H	5.722404	-4.407727	0.695049
C	3.645596	-4.247366	0.662557
H	3.573340	-5.175725	1.229527
C	2.373835	-3.601564	0.366379
H	2.393213	-2.695605	-0.235534
C	1.186456	-4.034615	0.826800
C	-0.127699	-3.317114	0.652785
H	0.051791	-2.415743	0.056378
C	-0.654917	-2.880129	2.035126
H	-1.561779	-2.275225	1.948178
H	0.097960	-2.273021	2.545292
H	-0.880005	-3.748796	2.665848
C	-1.138752	-4.191778	-0.126474
H	-1.280379	-5.148421	0.394276
H	-0.712706	-4.428064	-1.109183
C	-2.519961	-3.563789	-0.329613
H	-3.017248	-3.448123	0.647994
H	1.157593	-4.946274	1.428890
H	6.006397	-2.834711	-1.163086
H	6.712897	-1.974856	1.089300
C	6.433854	-0.219770	-0.186389
C	7.131764	-0.406624	-1.533014
H	7.981736	-1.092519	-1.450433
H	7.515860	0.550628	-1.899770
H	6.449863	-0.801326	-2.292860
H	7.146125	0.239172	0.511550
C	5.176840	0.669227	-0.224856
H	4.579595	0.443688	-1.117455
H	5.419761	1.734505	-0.253270
C	-0.302572	2.162183	-0.018992
O	0.371917	3.309896	-0.548171
C	-1.245987	1.587745	-1.112406
O	-1.876018	2.569301	-1.893852
H	-1.703314	2.335240	-2.821063
C	-0.225961	0.796822	-1.944819
O	-0.301443	0.591863	-3.135837
O	0.789228	0.390191	-1.172119
C	-3.422388	-4.402800	-1.243876
H	-3.614707	-5.382547	-0.792856
H	-2.912049	-4.569850	-2.200498

C	-4.744341	-3.686248	-1.514884
O	-5.470280	-4.470391	-2.461019
H	-5.309719	-3.621369	-0.569493
C	-4.481425	-2.262007	-2.022671
H	-5.425291	-1.710755	-2.122292
H	-4.019049	-2.319698	-3.015714
C	-3.542273	-1.520291	-1.066012
C	-3.123190	-0.136595	-1.562270
H	-2.548248	-0.269458	-2.483094
H	-4.001086	0.467985	-1.806038
C	-2.282267	0.598501	-0.511624
O	-3.199680	1.346667	0.325645
C	-3.059394	1.272185	1.672001
O	-2.192768	0.623237	2.226160
C	-4.088063	2.139894	2.365247
H	-5.035607	2.058761	1.821743
H	-3.749485	3.175083	2.224531
C	-4.258310	1.822039	3.854232
H	-4.848761	2.625892	4.307979
H	-3.274526	1.842458	4.334543
C	-4.935492	0.473475	4.117600
H	-5.933918	0.437107	3.666931
H	-5.048151	0.294792	5.191479
H	-4.346319	-0.350516	3.703643
H	-1.766549	-0.131539	0.113079
H	-4.040087	-1.421520	-0.084796
O	-2.329204	-2.260173	-0.894900
H	-6.320378	-4.034438	-2.612243
H	-0.801346	2.426252	0.910486
C	-0.151181	4.529957	-0.232003
C	0.571847	5.623989	-0.981995
C	0.150275	7.033038	-0.561008
C	0.884828	8.119082	-1.351038
O	-1.062121	4.682344	0.551605
H	0.381203	5.459291	-2.050720
H	1.649868	5.471559	-0.848780
H	0.567724	9.116974	-1.033198
H	0.686780	8.032926	-2.425346
H	0.337249	7.158832	0.511491
H	-0.931757	7.137421	-0.695164
H	1.969236	8.052671	-1.207799

Statistical Thermodynamic Analysis
Temperature= 298.150 Kelvin Pressure= 1.00000 Atm
==========
==========
SCF Energy= -2154.49924888 Predicted Change= -1.251231D-08
Zero-point correction (ZPE)= -2153.6619 0.83730
Internal Energy (U)= -2153.6147 0.88447
Enthalpy (H)= -2153.6138
0.88542
Gibbs Free Energy (G)= -2153.7455
0.75368

Frequencies -- 15.6648 19.3883 21.3232

NMR Shifts
Revised-MandelalideD-0001-NMR.txt

Atom	Type	Isotropic	Scaled Shift
1	C	99.9176	82.4502766133
3	C	109.5692	73.2123509256
4	C	152.7592	31.8735044698
7	C	104.8254	77.7528283466
13	C	100.7103	81.6915522885
14	C	152.6135	32.0129596661
16	C	52.0803	128.237236547
18	C	49.0682	131.120235839
20	C	57.3894	123.155688279
22	C	35.7377	143.879381305
23	C	147.7328	36.6844694577
25	C	168.2182	17.0770879994
29	C	142.8314	41.3757920328
32	C	111.5647	71.3023794483
37	C	143.3602	40.8696567698
38	C	172.4550	13.0218802044
43	C	150.3396	34.1893987251
46	C	109.4714	73.3059591493
48	C	100.4703	81.921265721
51	C	1.1579	176.977066942
54	C	145.6749	38.6541664274
57	C	114.7981	68.207565229
60	C	142.7400	41.463274565
63	C	112.2527	70.6438676085
64	C	149.4656	35.0259384751
67	C	115.1999	67.8229866575
69	C	3.3367	174.891651831
71	C	149.4677	35.0239284826
74	C	166.4408	18.7783073949
77	C	173.0726	12.4307509715
86	C	5.2562	173.054422941
87	C	148.9617	35.5082409694
88	C	165.8590	19.3351710408
89	C	172.9159	12.5807347001
2	H	27.8405	3.69794409794
5	H	30.3584	1.3714021714
6	H	29.9450	1.75338415338
8	H	26.0240	5.37639177639
10	H	29.2144	2.42845922846
11	H	27.8415	3.69702009702
15	H	29.3304	2.32127512128
17	H	26.1069	5.29979209979
19	H	25.2584	6.08380688381
21	H	24.8507	6.46052206052
24	H	29.0574	2.57352737353
26	H	30.3717	1.35911295911
27	H	30.5007	1.23991683992
28	H	31.2145	0.580364980365
30	H	30.5446	1.19935319935
31	H	30.1840	1.53254793255
33	H	28.2326	3.33564333564
34	H	25.7969	5.58623238623
35	H	29.7386	1.9440979441
36	H	27.7438	3.78729498729
39	H	30.6624	1.09050589051
40	H	30.5267	1.21589281589
41	H	30.9751	0.801570801571
42	H	29.0491	2.5811965812
44	H	30.4399	1.2960960961
45	H	29.6867	1.99205359205
50	H	29.4974	2.16696696697
55	H	29.9734	1.72714252714
56	H	30.7352	1.02323862324
59	H	27.8845	3.65728805729
61	H	30.1520	1.56211596212
62	H	30.6417	1.10963270963
65	H	29.7617	1.92275352275
66	H	30.0302	1.67465927466
72	H	29.3626	2.29152229152
73	H	28.8940	2.72450912451
75	H	30.3178	1.40891660892
76	H	29.8088	1.87923307923
78	H	31.1455	0.644121044121
79	H	30.7025	1.05345345345
80	H	30.7643	0.99635019635
81	H	25.8432	5.54345114345
82	H	28.5214	3.06879186879
84	H	30.9301	0.843150843151
85	H	26.1297	5.27872487872

91	H	29.3759	2.27923307923
92	H	29.3705	2.28422268422
93	H	30.5729	1.1732039732
94	H	30.9953	0.782905982906
95	H	30.2351	1.48533148533
96	H	30.0546	1.65211365211
97	H	31.0052	0.773758373758

Supporting Information: Revised-MandelalideD-0002.log

```
-----------------------------------------------------------------------
 Using  Gaussian 09:  AM64L-G09RevD.01 24-Apr-2013
=========================================================
=====================
 #b3lyp/6-31G(d,p) scf=(maxcycle=300,direct,tight) density=current
 SCRF=(PCM,SOLVENT=Chloroform) opt=(maxcycle=250)
freq=noraman
 #N Geom=AllCheck Guess=TCheck SCRF=Check GenChk RB3LYP/6-
31G(d,p) Freq
-----------------------------------------------------------------------
 Pointgroup= C1   Stoichiometry= C34H52O11   C1[X(C34H52O11)]
#Atoms= 97
 Charge = 0                Multiplicity = 1
-----------------------------------------------------------------------
 SCF Energy= -2154.49784005      Predicted Change= -7.234901D-09
=========================================================
=====================
 Optimization completed.          {Found       1       times}
 Item     Max Val.    Criteria    Pass?     RMS Val.    Criteria    Pass?
 Force     0.00000 ||  0.00045   [ YES ]     0.00000 ||  0.00030   [ YES ]
 Displ     0.00394 ||  0.00180   [ NO ]      0.00394 ||  0.00180   [ YES ]
-----------------------------------------------------------------------
     Atomic     Coordinates (Angstroms)
      Type      X                Y                Z
-----------------------------------------------------------------------
      C       4.300359     -0.442229      1.079036
      H       4.584743      0.241417      1.889987
      C       2.784423     -0.370081      0.862136
      C       2.243719      1.035701      0.594082
      H       2.295812      1.622971      1.517928
      H       2.838258      1.547243     -0.167445
      C       0.794963      0.960711      0.137637
      H       0.234525      0.315253      0.817575
      O       2.101588     -0.871770      2.006001
      H       2.488930     -1.744791      2.176042
      H       2.558384     -0.995102     -0.015086
      O       4.605473     -1.784047      1.532911
      C       5.445269     -2.465521      0.583347
      C       4.616428     -3.406766     -0.320970
      H       3.858038     -2.830073     -0.858577
      C       4.006258     -4.551346      0.443524
      H       4.723265     -5.291123      0.799557
      C       2.710682     -4.755140      0.751778
      H       2.468309     -5.648223      1.328245
      C       1.579311     -3.891914      0.440530
      H       1.766255     -3.008977     -0.166915
      C       0.328943     -4.097025      0.892301
      C      -0.828928     -3.151356      0.698122
      H      -0.479250     -2.303372      0.098820
      C      -1.283299     -2.612573      2.070313
      H      -2.053750     -1.843401      1.966830
      H      -0.435868     -2.159136      2.591836
      H      -1.682362     -3.417528      2.699727
      C      -1.974939     -3.832059     -0.087941
      H      -2.299035     -4.738644      0.440831
      H      -1.587652     -4.156380     -1.061524
      C      -3.212131     -2.960659     -0.317971
      H      -3.690561     -2.738729      0.650750
      H       0.127588     -4.982307      1.500768
      H       5.292519     -3.822642     -1.079687
      H       6.140488     -3.078996      1.169632
      C       6.201221     -1.322555     -0.132226
      C       6.856221     -1.655203     -1.472170
      H       7.561979     -2.487405     -1.376748
      H       7.414505     -0.792000     -1.848397
      H       6.115004     -1.924785     -2.231112
      H       6.984957     -0.997005      0.564031
      C       5.135971     -0.211714     -0.190312
      H       4.516802     -0.325636     -1.089272
      H       5.577705      0.787493     -0.221646
      C       0.017720      2.267723     -0.059579
      O       0.890760      3.269877     -0.593867
      C      -1.009420      1.863982     -1.154111
      O      -1.452799      2.937008     -1.942986
      H      -1.323214      2.671363     -2.868659
      C      -0.143775      0.898303     -1.976504
      O      -0.247226      0.703067     -3.166921
      O       0.776413      0.319291     -1.194015
      C      -4.247241     -3.627546     -1.234771
      H      -4.618251     -4.549112     -0.767884
      H      -3.768168     -3.901989     -2.182569
      C      -5.413105     -2.676226     -1.532692
      O      -6.299079     -3.201060     -2.520996
      H      -5.965179     -2.491437     -0.595346
      C      -4.884786     -1.340113     -2.053410
      H      -5.711233     -0.631261     -2.174653
      H      -4.429386     -1.498230     -3.038799
      C      -3.833557     -0.776431     -1.093364
      C      -3.163707      0.501053     -1.598855
      H      -2.619371      0.257798     -2.515846
      H      -3.915321      1.253599     -1.852558
      C      -2.205820      1.079248     -0.550391
      O      -2.973093      1.985282      0.281932
      C      -2.857078      1.885743      1.628947
      O      -2.131770      1.084507      2.186965
      C      -3.708295      2.931668      2.316577
      H      -4.651357      3.028059      1.767904
      H      -3.181633      3.885229      2.177158
      C      -3.943431      2.653940      3.804743
      H      -4.381949      3.552804      4.252499
      H      -2.975604      2.497880      4.292724
      C      -4.855393      1.450963      4.064970
      H      -5.840755      1.594697      3.606875
      H      -5.006214      1.298474      5.138216
      H      -4.422111      0.532992      3.656155
      H      -1.829314      0.272141      0.078809
      H      -4.313066     -0.576091     -0.118691
      O      -2.777846     -1.725055     -0.899145
      H      -6.651681     -4.036178     -2.183582
      H      -0.430338      2.627399      0.863569
      C       0.607862      4.566100     -0.273867
      C       1.540244      5.513386     -0.991106
      C       3.019297      5.333862     -0.596152
      C       3.930647      6.331856     -1.314677
      O      -0.266237      4.884002      0.502656
      H       1.201608      6.527837     -0.766601
      H       1.427065      5.347763     -2.069151
      H       4.975261      6.188604     -1.021622
      H       3.654977      7.364704     -1.075742
      H       3.330594      4.309885     -0.827649
      H       3.119396      5.456352      0.489164
      H       3.868384      6.213095     -2.402012
-----------------------------------------------------------------------
 Statistical Thermodynamic Analysis
 Temperature= 298.150 Kelvin       Pressure= 1.00000 Atm
=========================================================
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 SCF Energy=     -2154.49784005   Predicted Change= -7.234901D-09
 Zero-point correction (ZPE)=           -2153.6603              0.83744
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Internal Energy (U)= -2153.6131 0.88469
Enthalpy (H)= -2153.6122
0.88563
Gibbs Free Energy (G)= -2153.7452
0.75263

Frequencies -- 10.9615 15.3383 20.4928

NMR Shifts
Revised-MandelalideD-0002-NMR.txt

Atom	Type	Isotropic	Scaled Shift
1	C	100.6989	81.7024636766
3	C	109.7854	73.0054174084
4	C	152.8633	31.7738662685
7	C	104.9115	77.6704186527
13	C	101.1157	81.3035280155
14	C	153.2696	31.3849805701
16	C	51.3905	128.897471238
18	C	49.2263	130.968912115
20	C	58.0931	122.482149352
22	C	36.4218	143.224602309
23	C	147.6414	36.7719519899
25	C	168.1012	17.1890732977
29	C	143.5094	40.726851586
32	C	111.5837	71.2841938016
37	C	143.8458	40.4048699248
38	C	172.6069	12.8764907445
43	C	149.4191	35.0704454526
46	C	109.7853	73.0055131224
48	C	101.7616	80.6853117403
51	C	1.5907	176.562817052
54	C	142.4230	41.7666877237
57	C	115.1250	67.8946763912
60	C	146.9133	37.4688451157
63	C	111.5592	71.3076437145
64	C	150.1705	34.3512509811
67	C	114.7731	68.2314937116
69	C	3.0008	175.213154923
71	C	148.9501	35.5193437853
74	C	166.5702	18.6544535692
77	C	173.1404	12.3658569268
86	C	5.6713	172.657114416
87	C	145.7437	38.5883152434
88	C	162.5502	22.5021535634
89	C	171.5165	13.9201554394
2	H	27.8710	3.66976206976
5	H	30.4500	1.28676368676
6	H	30.0071	1.696003696
8	H	25.9895	5.40826980827
10	H	29.2172	2.42587202587
11	H	27.8665	3.67392007392
15	H	29.2983	2.35093555094
17	H	26.1299	5.27854007854
19	H	25.2339	6.10644490644
21	H	24.9505	6.36830676831
24	H	29.0924	2.54118734119
26	H	30.1974	1.52016632017
27	H	30.5880	1.15925155925
28	H	31.2599	0.538415338415
30	H	30.5216	1.22060522061
31	H	30.2344	1.48597828598
33	H	28.2520	3.31771771772
34	H	25.8617	5.52635712636
35	H	29.7164	1.96461076461
36	H	27.7796	3.75421575422
39	H	30.7076	1.04874104874
40	H	30.5811	1.16562716563
41	H	30.9411	0.832986832987
42	H	29.1165	2.51891891892
44	H	30.3559	1.37371217371
45	H	29.7523	1.93143913144
50	H	29.4406	2.21945021945
55	H	30.1484	1.56544236544
56	H	30.6937	1.06158466158
59	H	27.8975	3.64527604528
61	H	29.9490	1.74968814969
62	H	30.7191	1.03811503812
65	H	29.8548	1.83672903673
66	H	30.0359	1.66939246939
72	H	29.3328	2.31905751906
73	H	28.8623	2.7537999538
75	H	30.2946	1.43035343035
76	H	29.7695	1.91554631555
78	H	31.1813	0.611041811042
79	H	30.7012	1.05465465465
80	H	30.7146	1.04227304227
81	H	25.7546	5.62531762532
82	H	28.4932	3.09484869485
84	H	31.0116	0.767844767845
85	H	26.2984	5.12284592285
91	H	29.6041	2.06837606838
92	H	29.3565	2.29715869716
93	H	30.5740	1.17218757219
94	H	30.8931	0.877338877339
95	H	29.9676	1.7325017325
96	H	30.1664	1.54881034881
97	H	30.8991	0.871794871795

Supporting Information: Revised-MandelalideD-0003.log

Using Gaussian 09: AM64L-G09RevD.01 24-Apr-2013
==========
#b3lyp/6-31G(d,p) scf=(maxcycle=300,direct,tight) density=current
SCRF=(PCM,SOLVENT=Chloroform) opt=(maxcycle=250)
freq=noraman
#N Geom=AllCheck Guess=TCheck SCRF=Check GenChk RB3LYP/6-
31G(d,p) Freq

Pointgroup= C1 Stoichiometry= C34H52O11 C1[X(C34H52O11)]
#Atoms= 97
Charge = 0 Multiplicity = 1

SCF Energy= -2154.49778271 Predicted Change= -2.169505D-08
==========
Optimization completed. {Found 1 times}

Item	Max Val.	Criteria	Pass?	RMS Val.	Criteria	Pass?
Force	0.00001 ||	0.00045	[YES]	0.00000 ||	0.00030	[YES]
Displ	0.00267 ||	0.00180	[NO]	0.00267 ||	0.00180	[YES]

Atomic Type	Coordinates (Angstroms) X	Y	Z
C	4.300582	-0.442580	1.077334
H	4.585961	0.241286	1.887760
C	2.784546	-0.369457	0.861408
C	2.244580	1.036665	0.593517
H	2.297524	1.623919	1.517319
H	2.838881	1.547883	-0.168414
C	0.795489	0.962219	0.138160
H	0.235668	0.316069	0.817925
O	2.101998	-0.870343	2.005735
H	2.488460	-1.743787	2.175604
H	2.557508	-0.994486	-0.015572
O	4.605080	-1.784325	1.531652
C	5.443090	-2.467104	0.581423
C	4.612323	-3.407760	-0.321677

H	3.853668	-2.830574	-0.858396
C	4.002303	-4.551872	0.443667
H	4.719325	-5.291884	0.799183
C	2.706880	-4.755274	0.752804
H	2.464665	-5.648387	1.329278
C	1.575368	-3.891978	0.442253
H	1.762163	-3.008333	-0.164232
C	0.324929	-4.098170	0.893339
C	-0.833416	-3.153015	0.699458
H	-0.483532	-2.303839	0.101929
C	-1.289462	-2.616719	2.072092
H	-2.060517	-1.848096	1.968997
H	-0.442956	-2.163447	2.595319
H	-1.688636	-3.422945	2.699760
C	-1.978017	-3.833363	-0.088790
H	-2.302658	-4.740586	0.438374
H	-1.589279	-4.156744	-1.062112
C	-3.215433	-2.962620	-0.320013
H	-3.695330	-2.741414	0.648012
H	0.123665	-4.984342	1.500498
H	5.287131	-3.824183	-1.081239
H	6.138236	-3.081117	1.167228
C	6.199571	-1.325177	-0.135282
C	6.852953	-1.659013	-1.475728
H	7.557965	-2.491880	-1.380621
H	7.411752	-0.796526	-1.852854
H	6.110757	-1.928202	-2.233851
H	6.984317	-1.000179	0.560094
C	5.135437	-0.213231	-0.192757
H	4.515413	-0.326725	-1.091182
H	5.578181	0.785513	-0.224686
C	0.017833	2.269172	-0.057292
O	0.889952	3.271208	-0.593458
C	-1.010945	1.865512	-1.150353
O	-1.456760	2.938493	-1.938064
H	-1.323473	2.675274	-2.863911
C	-0.145454	0.901459	-1.974922
O	-0.250115	0.708202	-3.165611
O	0.775880	0.322195	-1.194303
C	-4.246760	-3.633476	-1.236987
H	-4.623717	-4.553003	-0.775664
H	-3.764732	-3.908149	-2.183286
C	-5.409105	-2.688401	-1.537614
O	-6.254364	-3.337104	-2.487244
H	-5.965975	-2.507348	-0.602417
C	-4.880051	-1.344857	-2.056695
H	-5.704172	-0.630211	-2.178472
H	-4.421225	-1.501615	-3.040579
C	-3.833764	-0.776651	-1.092948
C	-3.164156	0.502223	-1.595426
H	-2.619631	0.260862	-2.512773
H	-3.915747	1.255349	-1.847723
C	-2.206100	1.079037	-0.546293
O	-2.974042	1.982691	0.288054
C	-2.852335	1.884913	1.634835
O	-2.121186	1.087549	2.190601
C	-3.705809	2.927468	2.324808
H	-4.653798	3.014674	1.783023
H	-3.187399	3.884312	2.177369
C	-3.927687	2.654161	3.815836
H	-4.368343	3.552079	4.263399
H	-2.955146	2.506203	4.296893
C	-4.829972	1.446577	4.088061
H	-5.819991	1.582515	3.637649
H	-4.971053	1.297331	5.163070
H	-4.394409	0.529709	3.679263
H	-1.828530	0.271008	0.081072
H	-4.317216	-0.577874	-0.119740
O	-2.779290	-1.725021	-0.897896
H	-7.006538	-2.753140	-2.656832
H	-0.428436	2.628782	0.866714
C	0.606180	4.567661	-0.275356
C	1.536484	5.514749	-0.995591
C	3.017004	5.335000	-0.606487
C	3.925597	6.332809	-1.328757
O	-0.267518	4.886039	0.501428
H	1.198783	6.529254	-0.769874
H	1.419185	5.349283	-2.073255
H	4.971375	6.189333	-1.040019
H	3.651155	7.365732	-1.088722
H	3.327250	4.310984	-0.839186
H	3.121452	5.457515	0.478408
H	3.858821	6.214030	-2.415829

Statistical Thermodynamic Analysis
Temperature= 298.150 Kelvin Pressure= 1.00000 Atm
==========
==========
SCF Energy= -2154.49778271 Predicted Change= -2.169505D-08
Zero-point correction (ZPE)= -2153.6603 0.83738
Internal Energy (U)= -2153.6131 0.88466
Enthalpy (H)= -2153.6121
0.88560
Gibbs Free Energy (G)= -2153.7452
0.75257

Frequencies -- 12.4787 15.0617 19.8402

NMR-Shifts
Revised-MandelalideD-0003-NMR.txt

Atom	Type	Isotropic	Scaled Shift
1	C	100.7110	81.690882291
3	C	109.7885	73.0024502766
4	C	152.8580	31.7789391068
7	C	104.8869	77.6939642796
13	C	101.1075	81.3113765577
14	C	153.2669	31.3875648462
16	C	51.4649	128.826260074
18	C	49.1778	131.015333372
20	C	58.1441	122.433335248
22	C	36.2935	143.347403281
23	C	147.6534	36.7604663183
25	C	168.0834	17.2061103773
29	C	143.5061	40.7300101457
32	C	110.9849	71.8573288156
37	C	143.8424	40.4081241984
38	C	172.6037	12.8795535902
43	C	149.4108	35.0783897088
46	C	109.7608	73.0289630353
48	C	101.7150	80.7299144317
51	C	1.5617	176.590574092
54	C	145.7624	38.5704167385
57	C	115.0808	67.9369819484
60	C	143.5236	40.7132602079
63	C	112.1718	70.721300178
64	C	150.1442	34.3764237447
67	C	114.7872	68.2179980474
69	C	3.0440	175.171806505
71	C	148.9699	35.5003924271
74	C	166.5799	18.6451693179
77	C	173.1289	12.3768640288
86	C	5.6705	172.657880128
87	C	145.7387	38.5931009399
88	C	162.5681	22.4850207699
89	C	171.5226	13.9143168897
2	H	27.8690	3.67161007161
5	H	30.4476	1.28898128898
6	H	30.0072	1.69591129591

8	H	25.9789	5.41806421806
10	H	29.2098	2.43270963271
11	H	27.8639	3.67632247632
15	H	29.2969	2.35222915223
17	H	26.1304	5.27807807808
19	H	25.2260	6.11374451374
21	H	24.9508	6.36802956803
24	H	29.0938	2.53989373989
26	H	30.1976	1.51998151998
27	H	30.5921	1.15546315546
28	H	31.2429	0.554123354123
30	H	30.4741	1.2644952645
31	H	30.2213	1.49808269808
33	H	28.2118	3.35486255486
34	H	25.8462	5.54067914068
35	H	29.7144	1.96645876646
36	H	27.7772	3.75643335643
39	H	30.7055	1.05068145068
40	H	30.5808	1.1659043659
41	H	30.9389	0.83501963502
42	H	29.1157	2.51965811966
44	H	30.3550	1.37454377454
45	H	29.7519	1.93180873181
50	H	29.4422	2.21797181797
55	H	29.9529	1.74608454608
56	H	30.7043	1.05179025179
59	H	27.8558	3.68380688381
61	H	30.1056	1.60498960499
62	H	30.6450	1.10658350658
65	H	29.8580	1.83377223377
66	H	30.0656	1.64194964195
72	H	29.3467	2.30621390621
73	H	28.8631	2.75306075306
75	H	30.2983	1.42693462693
76	H	29.7674	1.91748671749
78	H	31.1904	0.602633402633
79	H	30.6971	1.05844305844
80	H	30.7026	1.05336105336
81	H	25.7529	5.62688842689
82	H	28.5096	3.0796950797
84	H	31.0443	0.73762993763
85	H	26.2977	5.12349272349
91	H	29.6055	2.06708246708
92	H	29.3592	2.29466389466
93	H	30.5737	1.17246477246
94	H	30.8945	0.876045276045
95	H	29.9662	1.7337953338
96	H	30.1661	1.54908754909
97	H	30.9003	0.870686070686

Mandelalide D Original Configuration

Supporting Information: Original-MandelalideD-0001.log

Using Gaussian 09: AM64L-G09RevD.01 24-Apr-2013

==========

#b3lyp/6-31G(d,p) scf=(maxcycle=300,direct,tight) density=current SCRF=(PCM,SOLVENT=Chloroform) opt=(maxcycle=250) freq=noraman

#N Geom=AllCheck Guess=TCheck SCRF=Check GenChk RB3LYP/6-31G(d,p) Freq

---

Pointgroup= C1 Stoichiometry= C34H52O11 C1[X(C34H52O11)] #Atoms= 97

Charge = 0 Multiplicity = 1

SCF Energy= -2154.49744005 Predicted Change= -2.446362D-09

==========

Optimization completed on the basis of negligible forces.

{Found 2 times}

Item	Max Val.	Criteria	Pass?	RMS Val.	Criteria	Pass?
Force	0.00000 ||	0.00045	[YES]	0.00000 ||	0.00030	[YES]
Displ	0.00195 ||	0.00180	[NO]	0.00195 ||	0.00180	[YES]

Atomic Type	Coordinates (Angstroms) X	Y	Z
C	-3.853752	1.654108	1.527744
H	-3.564426	2.286837	2.377272
C	-2.623684	0.880646	1.037421
C	-1.440576	1.778975	0.678921
H	-1.744215	2.540647	-0.043979
H	-1.086304	2.291683	1.581103
C	-0.287289	0.970819	0.107111
H	-0.015091	0.176929	0.806164
O	-2.189286	-0.030094	2.040255
H	-2.985423	-0.520382	2.299802
H	-2.923428	0.328532	0.134006
O	-4.802501	0.684595	2.032972
C	-5.995660	0.680895	1.229367
C	-5.962678	-0.451365	0.180776
H	-6.876963	-0.370147	-0.423821
C	-5.936130	-1.815127	0.813878
H	-6.802985	-2.039891	1.435834
C	-4.997989	-2.775132	0.703344
H	-5.182531	-3.710328	1.232628
C	-3.743100	-2.732154	-0.037805
H	-3.475158	-1.810069	-0.550460
C	-2.899797	-3.777518	-0.106905
C	-1.573873	-3.810597	-0.823554
H	-1.347932	-2.803592	-1.192638
C	-1.639030	-4.768087	-2.030341
H	-0.703314	-4.761120	-2.597625
H	-2.443680	-4.474141	-2.710771
H	-1.832497	-5.798324	-1.707676
C	-0.472514	-4.212320	0.187835
H	-0.711168	-5.202191	0.600375
H	-0.494787	-3.507783	1.028107
C	0.959903	-4.267748	-0.343498
H	1.026854	-4.987254	-1.176781
H	-3.181421	-4.703615	0.401043
H	-5.121727	-0.308477	-0.504217
H	-6.828680	0.486666	1.916366
C	-6.070568	2.120136	0.671936
C	-6.981420	2.349290	-0.533721
H	-8.011891	2.046072	-0.319288
H	-6.640552	1.792460	-1.412318
H	-6.999802	3.410392	-0.802246
H	-6.426482	2.747757	1.499139
C	-4.584971	2.452475	0.435449
H	-4.383022	3.524698	0.498511
H	-4.275374	2.118039	-0.562931
C	0.974395	1.736889	-0.315831
O	0.599077	3.002364	-0.872869
H	1.658995	1.889259	0.514785
C	1.534144	0.834753	-1.450473
O	2.270569	1.530882	-2.424298
H	1.894050	1.280029	-3.284254
C	0.217824	0.317340	-2.050926
O	0.056011	-0.000365	-3.208927
O	-0.752452	0.315755	-1.130643
C	1.953681	-4.692719	0.748366
H	1.728909	-5.719399	1.064880
H	1.836080	-4.040328	1.622330
C	3.399997	-4.589408	0.255776

O	4.345421	-4.825051	1.298681
H	3.552052	-5.316733	-0.560167
C	3.653873	-3.186278	-0.286356
H	4.664599	-3.118538	-0.703511
H	3.584914	-2.480186	0.548909
C	2.616837	-2.838491	-1.361556
C	2.722321	-1.413769	-1.916007
H	3.733137	-1.230047	-2.290297
H	2.045275	-1.338541	-2.769942
C	2.366342	-0.343624	-0.872339
O	3.603378	0.210165	-0.356764
C	3.737898	0.364615	0.983469
O	2.873700	0.070476	1.787132
C	5.084834	0.963603	1.317241
H	5.102328	1.966047	0.868978
H	5.852966	0.389139	0.785910
C	5.370238	1.027932	2.818603
H	5.330927	0.015469	3.236388
H	4.570056	1.591192	3.310569
C	6.727277	1.667371	3.123496
H	6.910225	1.703804	4.201798
H	6.778405	2.693122	2.741341
H	7.546635	1.101917	2.665470
H	1.821946	-0.801473	-0.045835
H	2.739865	-3.540501	-2.203491
O	1.285917	-2.965256	-0.844962
C	1.518937	4.005277	-0.787258
H	4.186966	-5.715167	1.642458
C	1.064154	5.209423	-1.581640
C	1.819504	6.496380	-1.235883
C	1.486897	7.046272	0.154648
O	2.553283	3.910030	-0.163152
H	-0.017078	5.326740	-1.448496
H	1.209973	4.945187	-2.637381
H	1.577691	7.247183	-1.996559
H	2.895048	6.305213	-1.311780
H	2.039003	7.970282	0.352807
H	0.417964	7.270770	0.246325
H	1.749986	6.326998	0.936049

Statistical Thermodynamic Analysis
Temperature= 298.150 Kelvin Pressure= 1.00000 Atm
==========
==========
SCF Energy= -2154.49744005 Predicted Change= -2.446362D-09
Zero-point correction (ZPE)= -2153.6602 0.83720
Internal Energy (U)= -2153.6128 0.88456
Enthalpy (H)= -2153.6119
0.88550
Gibbs Free Energy (G)= -2153.7462
0.75122

Frequencies -- 8.7356 9.3302 18.5901

NMR Shifts
Original-MandelalideD-0001-NMR.txt

Atom	Type	Isotropic	Scaled Shift
1	C	100.1609	82.2174046211
3	C	109.9220	72.8746721798
4	C	153.5317	31.134114359
7	C	105.9273	76.6981565497
13	C	100.3663	82.0208082084
14	C	153.0499	31.5952640747
16	C	51.1946	129.084974827
18	C	49.4063	130.796627041
20	C	57.8172	122.746224085
22	C	35.3817	144.220122897
23	C	148.9896	35.4815367829
25	C	167.4763	17.7871896476
29	C	141.6713	42.4861693371
32	C	112.6515	70.2621604548
37	C	144.0848	40.1761136316
38	C	172.5083	12.9708646796
43	C	149.5818	34.9147188882
46	C	109.2214	73.5452439748
49	C	101.0359	81.3799077318
52	C	0.8012	177.318478531
55	C	142.1459	42.0319110243
58	C	115.0177	67.9973774383
61	C	148.2275	36.210972645
64	C	111.3515	71.5064415475
65	C	151.6746	32.9116177568
68	C	117.2146	65.8946381056
70	C	2.7726	175.431574111
72	C	148.1438	36.2910852045
75	C	166.0979	19.1065104615
78	C	172.6407	12.8441394361
85	C	6.0010	172.341545589
87	C	150.2244	34.2996611727
88	C	166.5351	18.6880491587
89	C	173.2012	12.3076628573
2	H	27.8402	3.69822129822
5	H	29.9449	1.75347655348
6	H	30.4597	1.2778008778
8	H	26.1628	5.24814044814
10	H	29.1705	2.46902286902
11	H	27.8998	3.64315084315
15	H	29.7184	1.96276276276
17	H	26.1961	5.21737121737
19	H	25.1738	6.16197736198
21	H	24.9706	6.34973434973
24	H	29.1010	2.53324093324
26	H	30.5799	1.16673596674
27	H	30.8788	0.890552090552
28	H	31.2595	0.538784938785
30	H	30.6375	1.11351351351
31	H	30.0847	1.6243012243
33	H	28.1998	3.36595056595
34	H	25.9320	5.4613998614
35	H	29.3213	2.32968352968
36	H	27.6822	3.84421344421
39	H	30.7044	1.0516978517
40	H	30.9809	0.796211596212
41	H	30.5722	1.17385077385
42	H	29.1194	2.51623931624
44	H	29.6729	2.0048048048
45	H	30.3691	1.36151536152
48	H	26.1440	5.26551166551
51	H	29.3829	2.27276507277
56	H	30.2439	1.4772002772
57	H	30.6370	1.11397551398
60	H	27.9125	3.63141603142
62	H	30.1850	1.53162393162
63	H	30.8100	0.954123354123
66	H	30.1779	1.53818433818
67	H	29.3208	2.33014553015
73	H	29.1414	2.49591129591
74	H	29.3406	2.31185031185
76	H	30.1635	1.55148995149
77	H	29.9951	1.70709170709
79	H	30.4944	1.24573804574
80	H	30.9536	0.821436821437
81	H	30.9513	0.823562023562
82	H	25.8507	5.53652113652
83	H	28.2074	3.35892815893
86	H	30.9821	0.795102795103
91	H	29.4395	2.22046662047
92	H	29.0843	2.54867174867

93	H	30.3419	1.38664818665
94	H	29.8297	1.85992145992
95	H	30.7191	1.03811503812
96	H	31.1985	0.595148995149
97	H	30.7612	0.999214599215

Supporting Information: Original-MandelalideD-0002.log

Using Gaussian 09: AM64L-G09RevD.01 24-Apr-2013

==========

#b3lyp/6-31G(d,p) scf=(maxcycle=300,direct,tight) density=current SCRF=(PCM,SOLVENT=Chloroform) opt=(maxcycle=250) freq=noraman

#N Geom=AllCheck Guess=TCheck SCRF=Check GenChk RB3LYP/6-31G(d,p) Freq

---

Pointgroup= C1 Stoichiometry= C34H52O11 C1[X(C34H52O11)] #Atoms= 97

Charge = 0 Multiplicity = 1

SCF Energy= -2154.49744018 Predicted Change= -4.874605D-09

==========

Optimization completed. {Found 2 times}

Item	Max Val.	Criteria	Pass?	RMS Val.	Criteria	Pass?
Force	0.00000	0.00045	[YES]	0.00000	0.00030	[YES]
Displ	0.00145	0.00180	[YES]	0.00145	0.00180	[YES]

Atomic Type	Coordinates (Angstroms) X	Y	Z
C	-3.853873	1.653497	1.528173
H	-3.564556	2.286030	2.377848
C	-2.623772	0.880206	1.037655
C	-1.440746	1.778696	0.679287
H	-1.744475	2.540428	-0.043511
H	-1.086526	2.291325	1.581535
C	-0.287353	0.970759	0.107374
H	-0.014966	0.176892	0.806378
O	-2.189291	-0.030707	2.040297
H	-2.985384	-0.521105	2.299768
H	-2.923503	0.328257	0.134137
O	-4.802589	0.683844	2.033207
C	-5.995671	0.680155	1.229487
C	-5.962467	-0.451878	0.180653
H	-6.876691	-0.370621	-0.424030
C	-5.935871	-1.815762	0.813491
H	-6.802767	-2.040699	1.435329
C	-4.997654	-2.775682	0.702876
H	-5.182190	-3.710981	1.231980
C	-3.742703	-2.732507	-0.038154
H	-3.474757	-1.810325	-0.550631
C	-2.899349	-3.777822	-0.107367
C	-1.573365	-3.810700	-0.823912
H	-1.347492	-2.803634	-1.192870
C	-1.638324	-4.768072	-2.030801
H	-0.702573	-4.760925	-2.598023
H	-2.442966	-4.474155	-2.711254
H	-1.831684	-5.798367	-1.708256
C	-0.472041	-4.212410	0.187522
H	-0.710607	-5.202356	0.599935
H	-0.494458	-3.507965	1.027868
C	0.960415	-4.267609	-0.343729
H	1.027504	-4.987047	-1.177060
H	-3.180969	-4.704023	0.400391
H	-5.121449	-0.308770	-0.504210
H	-6.828725	0.485666	1.916370
C	-6.070714	2.119507	0.672369
C	-6.981505	2.348830	-0.533301
H	-8.011960	2.045455	-0.319008
H	-6.640519	1.792231	-1.411999
H	-6.999981	3.409990	-0.801595
H	-6.426763	2.746895	1.499690
C	-4.585140	2.452087	0.436066
H	-4.383328	3.524317	0.499451
H	-4.275440	2.117988	-0.562395
C	0.974163	1.737073	-0.315628
O	0.598528	3.002440	-0.872717
H	1.658766	1.889623	0.514952
C	1.534034	0.835030	-1.450282
O	2.270340	1.531291	-2.424102
H	1.893841	1.280383	-3.284052
C	0.217766	0.317454	-2.050710
O	0.055954	-0.000207	-3.208724
O	-0.752468	0.315660	-1.130384
C	1.954197	-4.692520	0.748153
H	1.729544	-5.719249	1.064597
H	1.836476	-4.040197	1.622152
C	3.400522	-4.588994	0.255632
O	4.345933	-4.824572	1.298565
H	3.552707	-5.316255	-0.560343
C	3.654241	-3.185800	-0.286408
H	4.664975	-3.117908	-0.703519
H	3.585168	-2.479773	0.548903
C	2.617200	-2.838068	-1.361622
C	2.722514	-1.413293	-1.915972
H	3.733311	-1.229417	-2.290236
H	2.045468	-1.338098	-2.769909
C	2.366392	-0.343271	-0.872224
O	3.603383	0.210592	-0.356602
C	3.737843	0.365037	0.983636
O	2.873577	0.070970	1.787253
C	5.084806	0.963926	1.317490
H	5.102365	1.966423	0.869344
H	5.852917	0.389486	0.786109
C	5.370185	1.028084	2.818867
H	5.330783	0.015582	3.236547
H	4.570038	1.591360	3.310871
C	6.727271	1.667377	3.123856
H	6.910195	1.703693	4.202166
H	6.778502	2.693159	2.741798
H	7.546591	1.101893	2.665798
H	1.822048	-0.801248	-0.045759
H	2.740348	-3.540006	-2.203599
O	1.286280	-2.965039	-0.845086
C	1.518255	4.005498	-0.787412
H	4.187601	-5.714738	1.642269
C	1.063205	5.209435	-1.581960
C	1.818427	6.496560	-1.236545
C	1.485985	7.046648	0.153946
O	2.552694	3.910509	-0.163422
H	-0.018026	5.326632	-1.448703
H	1.208929	4.945020	-2.637669
H	1.576371	7.247196	-1.997309
H	2.893984	6.305533	-1.312599
H	2.038019	7.970757	0.351851
H	0.417042	7.271039	0.245764
H	1.749290	6.327539	0.935425

Statistical Thermodynamic Analysis

Temperature= 298.150 Kelvin Pressure= 1.00000 Atm

==========

SCF Energy= -2154.49744018 Predicted Change= -4.874605D-09

Zero-point correction (ZPE)=	-2153.6602	0.83720
Internal Energy (U)=	-2153.6128	0.88456

Enthalpy (H)= -2153.6119
0.88550
Gibbs Free Energy (G)= -2153.7461
0.75124

Frequencies -- 8.7817 9.3800 18.6076

NMR Shifts
Original-MandelalideD-0002-NMR.txt

Atom	Type	Isotropic	Scaled Shift
1	C	100.1594	82.21884033
3	C	109.9223	72.874385038
4	C	153.5328	31.1330615058
7	C	105.9273	76.6981565497
13	C	100.3635	82.0234881985
14	C	153.0520	31.5932540822
16	C	51.1941	129.085453397
18	C	49.4064	130.796531327
20	C	57.8172	122.746224085
22	C	35.3840	144.217921476
23	C	148.9891	35.4820153525
25	C	167.4764	17.7870939337
29	C	141.6701	42.4873179042
32	C	112.6510	70.2626390245
37	C	144.0852	40.1757307759
38	C	172.5086	12.9705775379
43	C	149.5834	34.9131874653
46	C	109.2185	73.5480196788
49	C	101.0365	81.3793334482
52	C	0.7999	177.319722812
55	C	142.1464	42.0314324547
58	C	115.0183	67.9968031547
61	C	148.2279	36.2105897892
64	C	111.3512	71.5067286893
65	C	151.6738	32.9123834683
68	C	117.2128	65.8963609564
70	C	2.7735	175.430712686
72	C	148.1432	36.2916594881
75	C	166.0983	19.1061276058
78	C	172.6406	12.84423515
85	C	6.0008	172.341737016
87	C	150.2241	34.2999483145
88	C	166.5345	18.6886234423
89	C	173.2015	12.3073757155
2	H	27.8402	3.69822129822
5	H	29.9450	1.75338415338
6	H	30.4599	1.27761607762
8	H	26.1625	5.24841764842
10	H	29.1705	2.46902286902
11	H	27.8998	3.64315084315
15	H	29.7184	1.96276276276
17	H	26.1959	5.21755601756
19	H	25.1741	6.1617001617
21	H	24.9706	6.34973434973
24	H	29.1009	2.53333333333
26	H	30.5800	1.16664356664
27	H	30.8787	0.890644490644
28	H	31.2592	0.539062139062
30	H	30.6373	1.1136983137
31	H	30.0845	1.62448602449
33	H	28.1997	3.36604296604
34	H	25.9320	5.4613998614
35	H	29.3214	2.32959112959
36	H	27.6821	3.84430584431
39	H	30.7045	1.05160545161
40	H	30.9810	0.796119196119
41	H	30.5723	1.17375837376
42	H	29.1196	2.51605451605
44	H	29.6730	2.00471240471
45	H	30.3692	1.36142296142
48	H	26.1439	5.2656040656
51	H	29.3827	2.27294987295
56	H	30.2437	1.47738507739
57	H	30.6370	1.11397551398
60	H	27.9126	3.63132363132
62	H	30.1848	1.53180873181
63	H	30.8102	0.953938553939
66	H	30.1778	1.53827673828
67	H	29.3207	2.33023793024
73	H	29.1417	2.49563409563
74	H	29.3407	2.31175791176
76	H	30.1637	1.55130515131
77	H	29.9951	1.70709170709
79	H	30.4944	1.24573804574
80	H	30.9536	0.821436821437
81	H	30.9512	0.823654423654
82	H	25.8509	5.53633633634
83	H	28.2072	3.35911295911
86	H	30.9820	0.795195195195
91	H	29.4396	2.22037422037
92	H	29.0843	2.54867174867
93	H	30.3419	1.38664818665
94	H	29.8300	1.85964425964
95	H	30.7189	1.0382998383
96	H	31.1988	0.594871794872
97	H	30.7612	0.999214599215

Coibamide A - [D-N,O-diMe-Ser] Revised Configuration

Supporting Information: CoibamideA-D-N.OdiMeSer0001.log

Using Gaussian 09: AM64L-G09RevD.01 24-Apr-2013
==========
#mPW1PW91/6-311+G(2d,p) scf=(maxcycle=300,direct,tight,xqc,vshift=200) NMR density=current SCRF=(PCM,SOLVENT=Chloroform)

Pointgroup= C1 Stoichiometry= C65H110N10O16 C1[X(C65H110N10O16)] #Atoms= 201
Charge = 0 Multiplicity = 1

SCF Energy= -4294.54519875
==========
Optimization incomplete.

Atomic Type	Coordinates (Angstroms) X	Y	Z
N	8.056972	-2.706907	1.991699
C	6.783625	-3.186074	2.531473
H	5.918560	-2.740383	2.029928
H	6.716611	-4.274279	2.426929
H	6.710015	-2.975859	3.604184
C	8.165347	-3.036585	0.570624
H	8.131523	-4.123949	0.436004
H	7.356747	-2.604276	-0.025603
H	9.121740	-2.709077	0.152149
C	8.283768	-1.267422	2.304088
H	8.073782	-1.126915	3.374890
C	9.767799	-0.825462	2.119859

H	10.028461	-0.812406	1.054401
C	10.742572	-1.776269	2.828767
H	10.510465	-1.858085	3.896114
H	10.710764	-2.780194	2.394047
H	11.773058	-1.416762	2.734162
C	9.991114	0.593904	2.665331
H	9.768665	0.645441	3.736641
H	11.032289	0.903045	2.522783
H	9.361416	1.328215	2.154924
C	7.285304	-0.345060	1.570334
O	6.191374	-0.023016	2.024644
C	6.901789	0.966176	-0.348691
H	6.586337	1.740375	0.355272
O	7.760732	0.061753	0.359512
C	7.714485	1.650302	-1.477192
H	7.035452	2.253551	-2.091937
C	8.410185	0.646668	-2.404699
H	9.120444	0.015215	-1.860808
H	7.684494	-0.004493	-2.901133
H	8.965345	1.171304	-3.190066
C	8.765083	2.596190	-0.885180
H	9.511868	2.051626	-0.298227
H	9.291572	3.135307	-1.680009
H	8.295543	3.340826	-0.233998
C	5.667340	0.254419	-0.959002
O	5.736353	-0.928678	-1.305766
C	3.497262	0.453541	-2.103550
H	2.645300	1.140732	-2.075206
N	4.498958	0.986423	-1.146909
C	4.342375	2.381170	-0.751644
H	3.285020	2.655866	-0.722632
H	4.748340	2.546054	0.247884
H	4.866132	3.019247	-1.467344
C	4.037852	0.484003	-3.552984
H	3.272405	0.129802	-4.253668
H	4.919849	-0.158366	-3.657351
O	4.382733	1.830854	-3.919856
C	4.937061	1.883802	-5.229250
H	5.170186	2.926322	-5.461303
H	5.861566	1.300267	-5.276153
H	4.217484	1.513319	-5.965569
C	2.120164	-2.715154	-0.273697
H	1.873215	-3.201057	-1.222382
C	2.874508	-0.945343	-1.807638
O	2.606525	-1.702433	-2.753217
N	2.459960	-1.291077	-0.521334
C	2.588613	-0.415016	0.634616
H	1.804312	-0.620904	1.364670
H	3.564598	-0.579697	1.097429
H	2.483627	0.629892	0.347430
C	3.365397	-3.463450	0.268273
H	4.267548	-2.984610	-0.135225
H	3.439154	-3.364774	1.358256
C	3.426916	-4.955814	-0.131106
H	3.394701	-5.022485	-1.226283
C	2.271251	-5.784530	0.427989
H	2.205117	-5.691573	1.517100
H	1.315314	-5.478445	-0.005247
H	2.403452	-6.845582	0.189252
C	4.755731	-5.562828	0.326373
H	4.839493	-5.552878	1.418050
H	4.845857	-6.601285	-0.009669
H	5.602714	-5.006264	-0.087742
C	0.887827	-2.880955	0.661821
O	1.053022	-3.073415	1.872264
C	-0.721317	-2.270210	-1.246789
H	0.228598	-2.166899	-1.756858
N	-0.397693	-2.802458	0.119375
C	-1.502029	-3.212099	0.981435
H	-1.214647	-3.253968	2.035398
H	-2.348724	-2.531341	0.897453
H	-1.810722	-4.218842	0.686589
C	-1.611740	-3.189046	-2.126582
H	-1.778897	-2.692728	-3.090122
C	-0.922624	-4.533988	-2.370968
H	-0.832246	-5.109405	-1.444129
H	-1.503222	-5.154081	-3.061129
H	0.074674	-4.395593	-2.799645
O	-2.891982	-3.409837	-1.498703
C	-1.631093	1.454317	-2.054434
H	-2.584648	1.363509	-1.524827
C	-1.316929	-0.833171	-1.176165
O	-1.969325	-0.482778	-0.186216
N	-1.115794	0.052479	-2.236191
C	-1.849669	2.232609	-3.371240
H	-0.928653	2.271414	-3.965365
H	-2.134538	3.270636	-3.173878
C	-3.138058	2.320272	-5.351927
H	-2.240422	2.325542	-5.977592
H	-3.937177	1.804501	-5.890860
H	-3.460247	3.345249	-5.145030
O	-2.893136	1.621192	-4.138181
C	-0.635235	2.258448	-1.168865
O	0.530173	1.860487	-1.029702
C	-5.208025	-4.053876	-1.493659
H	-5.167790	-5.130454	-1.275510
C	-3.923523	-3.792979	-2.308128
O	-3.806188	-4.029118	-3.505590
C	-6.467999	-3.830541	-2.329665
H	-6.539476	-2.810171	-2.717003
H	-7.367733	-4.035943	-1.741065
H	-6.475473	-4.499021	-3.197871
C	-5.198571	-4.228970	0.996543
H	-6.109754	-4.833845	1.020097
H	-4.328330	-4.886976	0.914603
H	-5.118060	-3.673977	1.929750
N	-5.248553	-3.369546	-0.177830
C	-5.432366	-1.226351	1.182472
H	-4.695528	-1.641746	1.870804
N	-5.080705	0.177222	0.939872
H	-5.481232	0.569691	0.091446
C	-4.119156	0.981772	1.473270
O	-3.974664	2.086314	0.944673
C	-3.314468	0.529805	2.722433
H	-3.082792	-0.526687	2.559806
C	-4.184610	0.614130	3.993829
H	-5.072236	-0.013902	3.858505
H	-4.581470	1.629269	4.109400
C	-3.482346	0.188684	5.299416
H	-2.586858	0.803330	5.448890
C	-3.059418	-1.281241	5.278324
H	-2.301399	-1.468930	4.512752
H	-2.626331	-1.574357	6.240768
H	-3.913819	-1.937059	5.079013
C	-4.412787	0.437444	6.490712
H	-5.330194	-0.155462	6.409711
H	-3.919540	0.172555	7.432024
H	-4.695146	1.494050	6.549323
N	-2.005549	1.224687	2.827870
C	-1.952620	2.589626	3.115334
O	-2.935375	3.231422	3.497712
C	-0.577535	3.298047	3.002509
H	0.077543	2.761784	2.321342
C	-0.822232	0.457568	2.458837
H	-0.526462	0.726901	1.443676
H	0.001974	0.691785	3.137141
H	-1.005859	-0.616728	2.524749
C	0.069998	3.350956	4.383265

H	-0.549097	3.914227	5.091158
H	0.210883	2.347841	4.797843
H	1.047491	3.842637	4.333854
N	-0.767783	4.660769	2.497030
H	-1.291924	5.286060	3.099895
C	-0.585714	5.167725	1.241749
O	-0.981212	6.316155	1.027051
C	0.004342	4.267757	0.120422
H	0.678123	3.556017	0.608154
N	-1.029899	3.464136	-0.587923
C	-2.394242	4.000931	-0.623644
H	-2.387051	4.967549	-1.132685
H	-3.094133	3.349077	-1.142810
H	-2.757317	4.143522	0.395958
C	0.929417	5.043697	-0.877712
H	1.399860	4.289927	-1.524364
C	2.072714	5.754394	-0.116532
H	2.520326	5.050985	0.596605
H	1.680344	6.593712	0.468899
C	3.184587	6.270593	-1.020891
H	2.839545	7.092395	-1.654616
H	4.013808	6.649319	-0.414547
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H	-0.282090	6.825582	-1.290471
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H	-8.517141	-2.682199	0.053271
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NMR-Shifts

CoibamideA-D-N.OdiMeSer0001-NMR.txt

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22	C	3.0819	175.135530925
24	C	107.2325	75.4488983327
27	C	151.8799	32.7151170581
29	C	170.1926	15.1873121614
33	C	163.9586	21.1541185704
37	C	5.3719	172.943681923
39	C	115.3910	67.6400773369
42	C	147.8881	36.5358257241
46	C	110.8294	72.0061639771
50	C	126.7668	56.7518520645
54	C	125.7171	57.7565611899
56	C	6.3499	172.007599686
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63	C	143.0895	41.1287543789
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76	C	6.6351	171.734623557
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85	C	111.3361	71.5211814928
87	C	167.7667	17.5092363943
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94	C	7.3983	171.004134842
97	C	114.2599	68.7226976014
100	C	127.3658	56.1785256226
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21	H	30.9750	0.801663201663
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Supporting Information: CoibamideA-D-N.OdiMeSer0002.log

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 Using  Gaussian 09:  AM64L-G09RevD.01 24-Apr-2013
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H	-9.728621	1.621792	-1.032884
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NMR-Shifts
CoibamideA-D-N.OdiMeSer0002-NMR.txt

Atom	Type	Isotropic	Scaled Shift
2	C	141.5008	42.6493615881
6	C	148.1927	36.2442810927
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12	C	153.6851	30.9872891901
14	C	166.0593	19.1434560386
18	C	165.5177	19.6618426846
22	C	1.8617	176.303432302
24	C	105.6685	76.9458642011
27	C	154.1206	30.570455024
29	C	169.2946	16.0468232547
33	C	165.1791	19.9859300523
37	C	5.8495	172.486552193
39	C	117.8693	65.2679990046
42	C	146.6817	37.6905185781
46	C	111.7992	71.077930282
50	C	127.5685	55.9845134861
54	C	132.1151	51.6327839354
56	C	5.5777	172.746702655
59	C	156.5156	28.2781063956
63	C	142.2850	41.8987729474
66	C	159.5155	25.4067842034
68	C	165.4921	19.6863454507
72	C	160.6711	24.3007140259
76	C	3.5654	174.672754073
78	C	121.2117	62.0688566014
81	C	154.4896	30.2172706216
85	C	111.2631	71.5910526618
87	C	167.9399	17.3434598671
92	C	121.6911	61.61000402
94	C	7.0418	171.345355003
97	C	114.6183	68.3796588756
100	C	127.5268	56.024426195
105	C	7.1837	171.209536936
107	C	120.1160	63.1175941347
109	C	3.7014	174.542583128
111	C	171.1624	14.2590784663
115	C	148.3047	36.1370814908
120	C	131.3470	52.3679626333
124	C	7.1343	171.256819618
126	C	116.5156	66.5636784778
128	C	144.8714	39.4232278566
131	C	157.1993	27.6237102548
133	C	165.3897	19.7843565152
137	C	162.1708	22.8652922146
142	C	2.8609	175.347058711
144	C	134.1630	49.6726583587
146	C	144.2422	40.0254599054
150	C	167.5292	17.7365569785
156	C	8.5333	169.917781734
158	C	125.8655	57.6145217175
161	C	147.9874	36.4407817914
165	C	145.7526	38.5797967036
167	C	159.0953	25.8089741381
170	C	174.5112	11.0538103716
174	C	174.7245	10.8496525584
178	C	152.7889	31.8450774326
182	C	7.8204	170.600126342
184	C	147.9888	36.4394417964
187	C	22.6183	156.436474665
188	C	64.6842	116.173548498
189	C	49.7814	130.437604089
190	C	54.7549	125.67727177
191	C	47.5884	132.536610578
192	C	73.1542	108.06657861
198	C	131.6104	52.1158521411
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4	H	29.3678	2.28671748672
5	H	29.2974	2.35176715177
7	H	29.5176	2.1483021483
8	H	29.2220	2.42143682144
9	H	29.0687	2.56308616309
11	H	28.7537	2.85414645415
13	H	29.5210	2.14516054516
15	H	31.2735	0.525848925849
16	H	30.3226	1.40448140448
17	H	30.8755	0.893601293601
19	H	31.1059	0.680711480711
20	H	30.6040	1.14446754447
21	H	30.9486	0.826056826057
25	H	26.4847	4.9507045507
28	H	29.4849	2.17851697852
30	H	30.6894	1.06555786556
31	H	30.7424	1.01658581659
32	H	30.8636	0.904596904597
34	H	30.5399	1.2036960037
35	H	30.8292	0.936382536383
36	H	30.6336	1.11711711712
40	H	27.0434	4.43446523447
43	H	28.7046	2.89951489951
44	H	28.6798	2.92243012243
45	H	28.4268	3.1562023562
47	H	28.0474	3.50676830677

48	H	27.1640	4.32303072303
51	H	28.2689	3.3021021021
52	H	28.7252	2.88048048048
53	H	28.8119	2.80036960037
55	H	26.4755	4.95920535921
60	H	28.3683	3.21025641026
61	H	28.8097	2.8024024024
62	H	29.1661	2.47308847309
64	H	29.5308	2.13610533611
65	H	30.8587	0.909124509125
67	H	30.1799	1.53633633634
69	H	31.6322	0.19440979441
70	H	30.5386	1.2048972049
71	H	31.0918	0.69373989374
73	H	31.2361	0.560406560407
74	H	30.6008	1.14742434742
75	H	30.8239	0.94127974128
79	H	26.4775	4.95735735736
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88	H	30.6575	1.09503349503
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98	H	28.3605	3.21746361746
99	H	28.0746	3.48163548164
101	H	28.6872	2.91559251559
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108	H	27.8834	3.6583044583
112	H	29.4638	2.19801339801
113	H	30.6019	1.14640794641
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132	H	30.0605	1.64666204666
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151	H	30.5503	1.19408639409
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153	H	30.5045	1.23640563641
155	H	25.8508	5.53642873643
159	H	26.8726	4.59228459228
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166	H	29.5460	2.12206052206
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169	H	30.3963	1.33638253638
171	H	30.6564	1.09604989605
172	H	30.8310	0.934719334719
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176	H	30.8737	0.895264495264
177	H	31.0245	0.755925155925
179	H	29.0569	2.57398937399
180	H	28.7633	2.84527604528
181	H	29.0292	2.59958419958
185	H	28.6752	2.92668052668
186	H	28.7487	2.85876645877
193	H	24.6232	6.67073227073
194	H	24.3455	6.92732732733
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Supporting Information: CoibamideA-D-N.OdiMeSer0003.log

Using Gaussian 09: AM64L-G09RevD.01 24-Apr-2013

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Pointgroup= C1 Stoichiometry= C65H110N10O16 C1[X(C65H110N10O16)] #Atoms= 201

Charge = 0 Multiplicity = 1

SCF Energy= -4294.54703171

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Optimization incomplete.

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H	9.751393	-1.756291	1.324297
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H	11.501878	-2.064691	1.254511
C	9.071566	-3.838913	-0.245753
H	8.977446	-4.595414	0.542101
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H	8.957791	-4.376654	-1.191512
C	10.680371	-2.245524	-1.272999
H	11.676972	-1.825079	-1.071047
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C	11.771571	-4.131790	-2.619095
H	12.766585	-3.818226	-2.285553
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H	11.875638	-4.583034	-3.611897
C	11.280375	-1.958813	-3.739051
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H	10.572894	-1.135188	-3.875312
C	9.729671	-1.031208	-1.310081
O	10.004824	0.062250	-0.826198
C	7.608215	-0.241629	-1.983481
H	8.136406	0.650192	-2.338660
O	8.557469	-1.320369	-1.940257
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H	5.696789	0.133483	-2.951523
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H	5.413917	-1.998166	-1.694664
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N	3.911875	0.121736	1.968414
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C	-5.190125	1.427028	1.362973
H	-5.467616	0.801639	2.215801
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H	-5.519121	2.442562	1.585924
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H	-8.020170	3.782027	-0.878125
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H	-6.964205	5.026390	-0.197240
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H	-0.601560	5.491332	2.599043
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C	-4.237282	-4.709138	-0.490964
H	-3.383734	-4.786319	-1.177819
H	-4.053012	-5.461741	0.286913
C	-7.885278	-5.727997	-2.587833
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C	-5.502259	-5.075772	-1.232034
C	-5.742676	-4.587434	-2.521267
C	-6.925964	-4.911043	-3.189493
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H	-5.016159	-3.947709	-3.018050
H	-7.101002	-4.521825	-4.189852
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H	-10.796778	-6.911838	-3.526210
H	-9.593714	-7.816952	-2.599167
H	-10.417199	-6.375292	-1.884893

NMR-Shifts
CoibamideA-D-N.OdiMeSer0003-NMR.txt

Atom	Type	Isotropic	Scaled Shift
2	C	142.1459	42.0319110243
6	C	149.7106	34.7914393461
10	C	106.3840	76.2610310305
12	C	154.4951	30.2120063554
14	C	165.9437	19.2541013419
18	C	165.7188	19.4693619709
22	C	3.0823	175.135148069
24	C	106.6795	75.9781963667
27	C	152.9601	31.6812151841
29	C	169.5488	15.8035184441
33	C	164.6783	20.4652654147
37	C	6.3305	172.026168189
39	C	126.7176	56.7989433182
42	C	154.2337	30.462202569
46	C	114.8048	68.2011523957
50	C	127.1448	56.3900534084
54	C	129.8383	53.8119986983
56	C	5.2374	173.07241716
59	C	154.7216	29.9952143035
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193	H	24.5201	6.765996766
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Supporting Information: CoibamideA-D-N.OdiMeSer0004.log

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 Using  Gaussian 09:  AM64L-G09RevD.01 24-Apr-2013
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NMR-Shifts

CoibamideA-D-N.OdiMeSer0004-NMR.txt

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24	C	106.0631	76.5681770325
27	C	151.7113	32.8764907445
29	C	169.4187	15.9280422673
33	C	163.9832	21.1305729436
37	C	6.0195	172.323838511
39	C	127.0954	56.4373360899
42	C	154.9439	29.7824422366
46	C	114.2220	68.758973181
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54	C	130.1031	53.5585482111
56	C	4.7028	173.58410383
59	C	156.0130	28.7591646088
63	C	147.9849	36.4431746396
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124	C	7.5995	170.811558414
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128	C	145.4609	38.858994238
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Supporting Information: CoibamideA-D-N.OdiMeSer0005.log

Using Gaussian 09: AM64L-G09RevD.01 24-Apr-2013

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Pointgroup= C1 Stoichiometry= C65H110N10O16

C1[X(C65H110N10O16)] #Atoms= 201

Charge = 0 Multiplicity = 1

SCF Energy= -4294.54687065

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Optimization incomplete.

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H	11.582067	-1.893564	-0.915599
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NMR-Shifts

CoibamideA-D-N.OdiMeSer0005-NMR.txt

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12	C	153.9850	30.7002431134
14	C	166.7043	18.5261011888
18	C	165.8819	19.3132525508
22	C	3.4153	174.816420682
24	C	106.2797	76.3608606597
27	C	152.2662	32.3453741458
29	C	169.4812	15.8682210609
33	C	164.0987	21.0200233542
37	C	6.2043	172.146959168
39	C	126.3095	57.1895518674
42	C	154.6573	30.0567583606
46	C	113.8448	69.1200061257
50	C	127.5144	56.0362947223
54	C	129.5546	54.0835391183
56	C	4.6591	173.625930818
59	C	155.6640	29.0932062252
63	C	148.0010	36.4277646969
66	C	157.5526	27.2855529394
68	C	165.1543	20.009667107
72	C	162.0821	22.9501904707
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78	C	114.6800	68.3206033806
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85	C	108.5570	74.1811673271
87	C	168.6426	16.6708780796
92	C	120.5336	62.7178927621
94	C	8.7245	169.734776699
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100	C	127.2379	56.3009437394
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107	C	118.8102	64.3674266353
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158	C	128.7120	54.8900246942
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165	C	146.1213	38.2268994429
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178	C	150.9547	33.6006623404
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191	C	49.0616	131.126552959
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11	H	29.0133	2.61427581428
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25	H	26.4777	4.95717255717
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55	H	26.4154	5.01473781474
60	H	28.2612	3.30921690922
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64	H	29.6623	2.0145992146
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98	H	28.0680	3.48773388773

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175	H	29.8329	1.85696465696
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177	H	30.7238	1.03377223377
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193	H	24.5450	6.74298914299
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200	H	28.0000	3.55056595057
201	H	28.0151	3.53661353661

Supporting Information: CoibamideA -D-N.OdiMeSer0006.log

Using Gaussian 09: AM64L-G09RevD.01 24-Apr-2013

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Pointgroup= C1 Stoichiometry= C65H110N10O16 C1[X(C65H110N10O16)] #Atoms= 201

Charge = 0 Multiplicity = 1

SCF Energy= -4294.54582318

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Optimization incomplete.

Atomic Type	Coordinates (Angstroms) X	Y	Z
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H	-10.510372	2.452174	-4.015750
C	-12.521553	0.851087	-1.843823
H	-13.393541	0.802075	-2.506350
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H	-12.915456	1.053132	-0.843502
C	-10.474580	2.173264	-1.362412
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H	-11.483765	2.048845	0.576197
C	-11.820697	4.019717	-0.203692
H	-11.316162	4.785830	-0.802295
H	-12.756656	3.755544	-0.705574
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H	-10.035063	3.665248	1.784729
H	-9.093335	2.339606	1.107171
C	-9.620703	0.911349	-1.125362
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C	-7.613012	-0.170245	-1.743917
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H	-5.841725	-0.947466	-2.736600
C	-5.969203	1.124491	-3.233257
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H	3.207669	0.347083	5.315905
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H	1.169083	-2.269466	0.569544
C	0.652991	-2.161226	3.187299
O	0.485278	-2.343104	4.399995
N	0.415421	-3.208090	2.296275
C	-0.440198	-3.610237	-0.013008
H	-1.363317	-3.462705	0.560711
H	-0.398991	-4.656533	-0.337832
C	-1.637751	-3.081228	-1.979150
H	-2.568879	-3.006458	-1.410703
H	-1.673687	-2.369303	-2.807869
H	-1.529449	-4.090009	-2.388980
O	-0.517104	-2.760935	-1.162726
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C	3.020306	1.672714	2.567438
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H	1.375386	3.791412	1.712920
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H	5.616901	4.549267	2.165172
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C	8.561767	0.264285	-0.977284
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C	7.198488	-4.435521	-0.102729
H	8.018211	-4.471797	-0.829735
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N	5.542169	-4.620477	-1.892131
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NMR-Shifts

CoibamideA-D-N.OdiMeSer0006-NMR.txt

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18	C	165.7279	19.4606520033
22	C	4.8532	173.440150079
24	C	108.4604	74.2736269837
27	C	152.6055	32.0206167806
29	C	170.3561	15.0308198855
33	C	163.6685	21.4317846819
37	C	5.7485	172.583223262
39	C	126.6790	56.8358888953
42	C	153.8026	30.8748253221
46	C	114.0313	68.9414996459
50	C	127.3988	56.1469400257
54	C	126.2360	57.2599016061
56	C	5.0920	173.211585214
59	C	153.1155	31.5324757365
63	C	150.3409	34.188154444
66	C	151.1263	33.4364172362
68	C	161.4380	23.5666838952
72	C	165.7557	19.4340435307
76	C	1.1551	176.979746932
78	C	115.7652	67.28191581
81	C	145.4176	38.9004383698
85	C	109.0851	73.6757020617
87	C	168.3666	16.935048527
92	C	120.6855	62.5725033021
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97	C	107.0687	75.6056777503
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105	C	4.3472	173.924462566
107	C	119.6559	63.5579739275
109	C	0.8624	177.259901606
111	C	169.4662	15.8825781504
115	C	149.0813	35.3937671089
120	C	128.9829	54.6307356573
124	C	8.0781	170.353471544
126	C	117.6512	65.4767510864
128	C	144.5620	39.7193667566
131	C	157.3835	27.4474051954
133	C	165.3593	19.81345355
137	C	162.9123	22.1555734222
142	C	0.7868	177.332261337
144	C	133.4762	50.3300216313
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189	C	49.1808	131.012461954
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44	H	28.7133	2.89147609148
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67	H	30.0423	1.66347886348
69	H	31.0241	0.756294756295
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73	H	30.4964	1.24389004389
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75	H	30.8997	0.87124047124
79	H	27.1394	4.34576114576
82	H	29.1782	2.46190806191
83	H	27.9131	3.63086163086
84	H	28.1970	3.36853776854
86	H	25.9924	5.40559020559
88	H	30.0539	1.65276045276
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93	H	27.0040	4.47087087087
98	H	27.7700	3.76308616309
99	H	27.9383	3.60757680758
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108	H	28.1937	3.37158697159
112	H	28.9907	2.63515823516
113	H	30.5113	1.23012243012
114	H	30.1897	1.52728112728
116	H	29.7973	1.88985908986

117	H	29.1391	2.49803649804
118	H	29.6519	2.02420882421
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127	H	27.7391	3.79163779164
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135	H	30.6569	1.09558789559
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138	H	31.0337	0.747424347424
139	H	30.7165	1.04051744052
140	H	30.6492	1.1027027027
145	H	27.3379	4.16234696235
147	H	28.7079	2.89646569647
148	H	28.6170	2.98045738046
149	H	28.4858	3.10168630169
151	H	30.5901	1.15731115731
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153	H	30.3592	1.37066297066
155	H	25.6785	5.69563409563
159	H	26.6226	4.82328482328
162	H	28.7844	2.82577962578
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166	H	29.7696	1.91545391545
168	H	30.4347	1.3009009009
169	H	30.1561	1.55832755833
171	H	30.5959	1.15195195195
172	H	30.6848	1.06980826981
173	H	31.0910	0.694479094479
175	H	30.0379	1.66754446754
176	H	30.6912	1.06389466389
177	H	30.8219	0.943127743128
179	H	28.7453	2.86190806191
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181	H	28.2368	3.33176253176
185	H	28.6966	2.90690690691
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193	H	24.5074	6.77773157773
194	H	24.1250	7.13106953107
195	H	23.9994	7.24712404712
196	H	24.4724	6.81007161007
199	H	27.7276	3.80226380226
200	H	28.1297	3.43072303072
201	H	28.2398	3.32899052899

Supporting Information: CoibamideA-D-N.OdiMeSer0007.log

Using Gaussian 09: AM64L-G09RevD.01 24-Apr-2013

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#mPW1PW91/6-311+G(2d,p) scf=(maxcycle=300,direct,tight,xqc,vshift=200) NMR density=current SCRF=(PCM,SOLVENT=Chloroform)

Pointgroup= C1 Stoichiometry= C65H110N10O16 C1[X(C65H110N10O16)] #Atoms= 201

Charge = 0 Multiplicity = 1

SCF Energy= -4294.54570814

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Optimization incomplete.

Atomic Type	Coordinates (Angstroms) X	Y	Z
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H	9.705299	-4.344481	0.886428
H	10.934448	-3.231704	0.311983
C	8.048601	-4.109106	-1.173735
H	7.870897	-5.001496	-0.562191
H	7.391595	-3.319300	-0.800553
H	7.733117	-4.373877	-2.187117
C	9.854697	-2.642106	-2.051009
H	10.931999	-2.472703	-1.905228
C	9.693812	-2.998953	-3.559916
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C	10.388148	-4.322310	-3.909873
H	11.453792	-4.288674	-3.658740
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H	11.333749	-1.730006	-4.252139
H	10.167776	-2.159604	-5.514687
H	9.746937	-0.942595	-4.311647
C	9.182424	-1.300442	-1.691954
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H	7.885709	0.844706	-2.083593
O	7.924439	-1.208127	-2.205515
C	5.973982	0.091730	-2.799602
H	5.366919	0.957580	-2.511284
C	5.073891	-1.146343	-2.701484
H	5.599455	-2.056984	-3.007384
H	4.708577	-1.290012	-1.679798
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H	2.598055	-2.283180	3.742286
H	1.263932	-2.467159	2.651421
C	3.102416	-3.308790	1.897927

H	4.167306	-3.051632	1.866753
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H	2.805398	-2.547527	-0.126236
H	3.118632	-4.278230	-0.048358
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H	3.363184	-4.587783	3.639486
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H	0.882342	4.119224	-1.121520
C	1.981970	2.126123	-2.359674
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H	1.945402	1.238593	-2.996931
H	1.913840	3.014985	-2.994151
O	0.879176	2.077534	-1.461768
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H	-1.070771	-3.171188	4.911237
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O	-3.588192	-0.134220	-1.525196
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H	-5.509839	-0.732650	0.915065
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H	-5.291855	2.706469	1.377136
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NMR-Shifts

CoibamideA-D-N.OdiMeSer0007-NMR.txt

Atom	Type	Isotropic	Scaled Shift
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10	C	107.5892	75.1074867436
12	C	153.3530	31.3051551523
14	C	166.2665	18.9451367752
18	C	165.4350	19.7409981049
22	C	4.0140	174.243381382
24	C	106.1259	76.5080686843
27	C	153.4473	31.2148969161
29	C	169.8177	15.5461436858
33	C	164.6882	20.4557897356
37	C	6.3632	171.994869733
39	C	125.2662	58.1881353012
42	C	153.4873	31.176611344
46	C	115.0864	67.9316219683
50	C	126.9702	56.5571699305
54	C	129.5405	54.0970347824
56	C	5.1445	173.161335401
59	C	154.0627	30.6258733896
63	C	147.5855	36.8254560769
66	C	156.9655	27.8474894236
68	C	165.7690	19.421313578
72	C	161.8293	23.1921552863
76	C	1.3803	176.764199162
78	C	116.0948	66.9664426961
81	C	144.8662	39.428204981
85	C	108.9684	73.7874002182
87	C	168.6380	16.6752809204
92	C	120.4212	62.8254752197
94	C	7.8559	170.566147897
97	C	108.0953	74.6230785429
100	C	128.1595	55.4188441586
105	C	4.4713	173.805681579
107	C	119.8615	63.361186087
109	C	1.9011	176.265721013
111	C	168.8677	16.4554260227
115	C	149.1450	35.3327973353
120	C	126.6603	56.8537874002
124	C	7.7551	170.662627539
126	C	118.2674	64.8869618484
128	C	145.9739	38.3679817761
131	C	156.8367	27.9707689657
133	C	166.2427	18.9679166906
137	C	162.8357	22.2288902927
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144	C	134.2119	49.6258542468
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150	C	166.6324	18.5949195046
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161	C	146.3619	37.9966117269
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167	C	155.6194	29.1358946381
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174	C	168.5623	16.7477363656
178	C	151.1349	33.4281858382
182	C	2.1375	176.039453282
184	C	147.3248	37.0749822929
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188	C	73.0312	108.184306744
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190	C	50.0189	130.210283505
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198	C	131.3886	52.3281456383
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7	H	29.8026	1.88496188496
8	H	29.0762	2.55615615616
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36	H	30.7295	1.02850542851
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73	H	30.7022	1.05373065373
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75	H	30.5907	1.15675675676
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82	H	29.2508	2.39482559483
83	H	27.8502	3.68898128898
84	H	28.2786	3.29313929314
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88	H	29.8821	1.8115038115
89	H	30.5995	1.14862554863
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93	H	26.9388	4.53111573112
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127	H	27.7086	3.81981981982
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135	H	30.8595	0.908385308385
136	H	31.5064	0.310649110649
138	H	31.6541	0.174174174174
139	H	30.8801	0.889350889351
140	H	31.0980	0.688011088011
145	H	27.4852	4.02624162624
147	H	28.9370	2.68477708478
148	H	28.8371	2.77708477708
149	H	28.5525	3.04005544006
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153	H	30.3513	1.37796257796
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159	H	26.3503	5.07489027489
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166	H	29.3459	2.30695310695
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172	H	30.7009	1.05493185493
173	H	30.8723	0.896558096558
175	H	29.7393	1.94345114345
176	H	31.1073	0.679417879418
177	H	30.4542	1.28288288288
179	H	28.8427	2.77191037191
180	H	29.6134	2.05978285978
181	H	28.1736	3.39015939016
185	H	29.0277	2.60097020097
186	H	29.0507	2.57971817972
193	H	24.5451	6.7428967429
194	H	23.9935	7.25257565258
195	H	23.9546	7.28851928852
196	H	24.4473	6.83326403326
199	H	27.7838	3.75033495033
200	H	28.2225	3.34497574498
201	H	28.2135	3.35329175329

Coibamide A - [D-Hiv], [D-MeAla] Revision

Supporting Information: NMR-CoibamideA.D-MeAla.D-HIV-0001.log

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Using Gaussian 09: AM64L-G09RevD.01 24-Apr-2013

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#mPW1PW91/6-311+G(2d,p) scf=(maxcycle=300,direct,tight,xqc,vshift=200) NMR density=current SCRF=(PCM,SOLVENT=Chloroform)

Pointgroup= C1 Stoichiometry= C65H110N10O16 C1[X(C65H110N10O16)] #Atoms= 201

Charge = 0 Multiplicity = 1

SCF Energy= -4294.55868915

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Optimization incomplete.

Atomic Type	Coordinates (Angstroms) X	Y	Z
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C	6.098975	-0.176660	4.283826
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H	7.156469	-0.021412	4.524259
C	4.256592	-1.715599	4.358198
H	3.681239	-1.028547	4.989541
H	3.982036	-1.514946	3.317109
H	3.918567	-2.722330	4.621318
C	6.551951	-2.556980	3.937896
H	7.599803	-2.259013	4.088409
C	6.421929	-3.976757	4.566774
H	5.430319	-4.391758	4.346733
C	6.597938	-3.947358	6.090871
H	7.562884	-3.510032	6.369456
H	5.806879	-3.366063	6.574682
H	6.553810	-4.959975	6.506524
C	7.458615	-4.942520	3.971834
H	8.478994	-4.582681	4.142645
H	7.370226	-5.934466	4.428215
H	7.318907	-5.068271	2.893713
C	6.301856	-2.623887	2.416664
O	5.387275	-3.237847	1.878000
C	7.098765	-1.886011	0.317210
H	6.931095	-2.915270	-0.016987
O	7.261711	-1.920780	1.747293
C	8.408235	-1.350525	-0.310883
H	8.267863	-1.220692	-1.390473
C	9.548389	-2.355116	-0.111088
H	9.772149	-2.506098	0.950319
H	9.289566	-3.326300	-0.545712
H	10.463188	-2.005038	-0.601205
C	8.824956	0.008491	0.264383
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H	8.049155	0.762679	0.098848
C	5.894394	-1.004358	-0.103199
O	5.426205	-0.193890	0.704525
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H	3.879394	1.382083	-3.223773
H	4.965007	0.131640	-3.850217
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C	1.111667	-2.463609	-1.593455
H	1.255606	-2.711024	-2.646222
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H	1.552362	-1.526695	0.802572
C	0.991905	-3.773280	-0.786210
H	0.810446	-3.541049	0.270607
H	0.098799	-4.323428	-1.108202
C	2.215792	-4.707815	-0.894957
H	3.117032	-4.168230	-0.581611
C	2.438216	-5.213098	-2.321520
H	1.542345	-5.707478	-2.711861
H	2.699519	-4.394454	-2.998541
H	3.262796	-5.933407	-2.353953

C	2.042708	-5.898407	0.052625
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H	2.917235	-6.556480	0.014890
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H	-1.724183	-2.805914	-4.157328
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H	-2.704126	-0.744257	-4.265544
C	-3.973721	0.622055	-3.215210
H	-4.033945	1.131544	-2.248567
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H	-4.880629	0.029871	-3.357181
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O	-4.415348	-2.469575	-3.046858
N	-4.242011	-2.541971	-0.759630
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H	-6.175030	-5.369161	-0.336126
H	-4.662462	-4.980701	0.508090
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H	-5.193128	-7.316778	-1.285201
H	-3.675038	-7.136753	-2.190730
H	-3.662353	-6.944991	-0.424534
O	-4.481694	-5.380196	-1.514305
C	-6.465089	-2.785729	0.445203
O	-6.865577	-3.550244	1.326509
C	0.346290	1.875338	-4.009371
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H	-1.723843	6.765772	1.140902
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H	-1.966383	5.174361	4.591699
N	-4.213353	3.260706	1.051748
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H	-4.938396	2.809305	-0.845755
C	-7.093860	2.722111	2.741744
H	-6.849444	2.913485	3.792977
H	-7.173542	3.692958	2.243580
H	-8.077111	2.241777	2.714282
N	-5.903988	0.576098	2.809439
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N	-6.892919	-1.453618	0.375012
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C	-8.852179	-1.549565	2.048372
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C	-9.841231	-1.936013	0.924460
H	-10.654569	-2.528504	1.362961
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C	-10.461498	-0.770473	0.165466
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H	-10.486907	-1.198578	3.450348
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C	2.230197	4.138834	0.562292
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C	4.726500	8.533250	0.290341
H	5.588611	9.149480	0.017533
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NMR-Shifts

NMR-CoibamideA.D-MeAla.D-HIV-0001-NMR.txt

Atom	Type	Isotropic	Scaled Shift
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6	C	149.2419	35.240050537
10	C	109.5808	73.2012481096
12	C	155.2251	29.5132946649

14	C	166.6099	18.6164551389
18	C	165.8412	19.3522081204
22	C	3.6297	174.611210016
24	C	106.9005	75.7666685809
27	C	154.0398	30.6477918796
29	C	165.0244	20.1339995023
33	C	170.3701	15.0174199353
37	C	8.5548	169.897203239
39	C	126.8932	56.6308696568
42	C	158.1517	26.7121307835
46	C	113.4890	69.4605562894
50	C	126.8048	56.7154807711
54	C	129.5283	54.1087118819
56	C	4.7982	173.492792741
59	C	153.0847	31.561955627
63	C	147.3976	37.0053025517
66	C	156.7791	28.0259001895
68	C	166.4057	18.8119029844
72	C	162.6115	22.4434809242
76	C	3.6760	174.566894466
78	C	125.7445	57.730335573
81	C	154.2596	30.437412661
85	C	115.6514	67.3908382626
87	C	166.8333	18.4026302188
92	C	124.9369	58.5033212734
94	C	8.1436	170.29077892
97	C	111.9552	70.9286165509
100	C	126.7824	56.7369206914
105	C	5.6125	172.713394207
107	C	127.3629	56.1813013266
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111	C	170.0867	15.2886732135
115	C	157.4831	27.3520741209
120	C	126.5304	56.9781197956
124	C	8.6034	169.850686269
126	C	114.6150	68.3828174352
128	C	143.6437	40.5983077777
131	C	156.5468	28.2482436494
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142	C	0.4090	177.693868566
144	C	133.7138	50.1026053332
146	C	148.5762	35.8772181703
150	C	165.7354	19.4534734585
156	C	11.7336	166.854648826
158	C	117.4086	65.708953081
161	C	145.8983	38.4403415073
165	C	151.7813	32.8094909933
167	C	160.9399	24.0434349815
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174	C	170.5153	14.8784433086
178	C	155.9727	28.7977373227
182	C	8.4226	170.023737055
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188	C	74.4346	106.841057448
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190	C	51.1231	129.153410287
191	C	46.4354	133.640192194
192	C	63.1471	117.644767319
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73	H	31.1039	0.682559482559
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79	H	25.6561	5.71633171633
82	H	28.6830	2.91947331947
83	H	29.1763	2.46366366366
84	H	28.7348	2.87161007161
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89	H	30.8265	0.938877338877
90	H	30.6185	1.13106953107
93	H	26.1167	5.29073689074
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99	H	28.2473	3.32206052206
101	H	28.4802	3.10686070686
102	H	28.1924	3.37278817279
103	H	28.6747	2.92714252714
108	H	26.2612	5.15721875722
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113	H	29.8890	1.80512820513
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118	H	28.9717	2.65271425271
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153	H	30.4044	1.3288981289
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172	H	30.7413	1.0176022176
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175	H	31.0825	0.702333102333
176	H	31.1009	0.685331485331
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181	H	29.0594	2.57167937168
185	H	28.6472	2.95255255255
186	H	27.8764	3.66477246477
193	H	24.7527	6.55107415107
194	H	23.7927	7.43811503812
195	H	23.7229	7.50261030261
196	H	24.4155	6.86264726265
199	H	27.8627	3.67743127743
200	H	28.1379	3.42314622315
201	H	28.1755	3.3884037884

Supporting Information: NMR-CoibamideA.D-MeAla.D-HIV-0002.log

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Using Gaussian 09: AM64L-G09RevD.01 24-Apr-2013

==========

#mPW1PW91/6-311+G(2d,p) scf=(maxcycle=300,direct,tight,xqc,vshift=200) NMR density=current SCRF=(PCM,SOLVENT=Chloroform)

Pointgroup= C1 Stoichiometry= C65H110N10O16 C1[X(C65H110N10O16)] #Atoms= 201

Charge = 0 Multiplicity = 1

SCF Energy= -4294.55857835

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Optimization incomplete.

Atomic Type	Coordinates (Angstroms) X	Y	Z
N	5.861000	-2.120307	4.557255
C	6.120795	-0.685980	4.411832
H	5.879794	-0.312770	3.412593
H	5.528702	-0.117295	5.137788
H	7.171329	-0.458309	4.623567
C	4.441058	-2.400706	4.341054
H	3.838260	-1.869249	5.086678
H	4.091879	-2.088031	3.351257
H	4.214769	-3.463008	4.472134
C	6.780706	-2.935747	3.711565
H	7.802842	-2.567813	3.883020
C	6.803107	-4.442578	4.107149
H	5.844194	-4.909157	3.848998
C	7.038986	-4.638092	5.610674
H	7.973310	-4.163664	5.929550
H	6.221515	-4.215576	6.203080
H	7.099800	-5.703429	5.858617
C	7.896042	-5.200582	3.337091
H	8.886655	-4.777087	3.534990
H	7.915790	-6.255804	3.630913
H	7.722481	-5.168480	2.257085
C	6.479919	-2.787848	2.205193
O	5.578411	-3.361329	1.604103
C	7.200247	-1.734540	0.214329
H	7.071519	-2.717609	-0.250471
O	7.387410	-1.949326	1.624913
C	8.478545	-1.066210	-0.348480
H	8.319899	-0.802797	-1.400623
C	9.662041	-2.038502	-0.290067
H	9.905355	-2.317210	0.740733
H	9.438161	-2.954833	-0.846397
H	10.555186	-1.588536	-0.736620
C	8.845393	0.223166	0.396507
H	9.059588	0.035367	1.453786
H	9.736288	0.681536	-0.046619
H	8.036125	0.957693	0.337382
C	5.954402	-0.858891	-0.079971
O	5.454772	-0.189139	0.831205
C	4.305030	0.100319	-1.655456
H	4.063788	0.667281	-0.754631
N	5.428407	-0.842768	-1.369720
C	5.911786	-1.656890	-2.482977
H	5.070832	-2.161964	-2.964390
H	6.411651	-1.006878	-3.205940
H	6.621027	-2.423058	-2.175790
C	4.681745	1.153891	-2.719301
H	3.826168	1.812314	-2.909130
H	4.955862	0.683423	-3.670690
O	5.784997	1.949723	-2.258884
C	6.107681	2.978290	-3.185571
H	6.955063	3.544276	-2.789521
H	6.393572	2.548909	-4.150520
H	5.260737	3.659816	-3.310722
C	1.213605	-2.263165	-1.658671
H	1.384941	-2.434998	-2.722355
C	3.053219	-0.683880	-2.120368
O	2.776456	-0.746724	-3.325532
N	2.325035	-1.409841	-1.176784
C	2.504783	-1.249270	0.264070
H	3.283862	-1.938072	0.597220
H	2.780425	-0.225815	0.518678
H	1.579576	-1.472512	0.800927
C	1.126356	-3.627516	-0.942697
H	0.923388	-3.473140	0.124389
H	0.256258	-4.183158	-1.313753
C	2.380151	-4.515110	-1.094481
H	3.256855	-3.975886	-0.717468
C	2.650493	-4.900963	-2.549741
H	1.777893	-5.385006	-3.000955
H	2.906785	-4.025480	-3.153609
H	3.494555	-5.596036	-2.616488
C	2.220580	-5.781108	-0.247612
H	1.363606	-6.376888	-0.579925
H	3.115908	-6.408513	-0.312725
H	2.069631	-5.526734	0.806923
C	-0.134867	-1.491691	-1.546845
O	-0.258736	-0.560066	-0.740408
C	-2.502615	-1.155284	-2.170639
H	-2.471222	-0.589492	-1.240463
N	-1.220219	-1.899789	-2.323386

C	-1.189260	-2.962077	-3.329748
H	-0.187151	-3.333365	-3.533592
H	-1.792510	-3.800976	-2.971063
H	-1.604269	-2.589274	-4.269400
C	-2.688698	-0.106336	-3.302100
H	-2.672352	-0.579984	-4.289811
C	-3.995802	0.677814	-3.175155
H	-4.072230	1.142756	-2.187685
H	-4.021633	1.493235	-3.906967
H	-4.876487	0.052429	-3.338075
O	-1.651417	0.899223	-3.183232
C	-5.322088	-3.471024	-0.798381
H	-5.869048	-3.396430	-1.745123
C	-3.714030	-2.114849	-2.105950
O	-4.294902	-2.439424	-3.147460
N	-4.106489	-2.615021	-0.866904
C	-4.956909	-4.964009	-0.628382
H	-5.873717	-5.563923	-0.569795
H	-4.384618	-5.126590	0.292185
C	-3.864672	-6.806213	-1.623149
H	-4.776663	-7.410117	-1.596207
H	-3.275876	-7.101298	-2.495808
H	-3.267780	-6.982369	-0.723165
O	-4.184177	-5.426238	-1.745736
C	-6.308125	-3.036888	0.324479
O	-6.654197	-3.857493	1.177908
C	0.326135	2.082178	-3.871385
H	1.280283	1.579915	-3.680257
C	-0.671565	0.930364	-4.126656
O	-0.601543	0.160942	-5.078480
C	0.507976	2.912666	-5.141159
H	-0.446493	3.271407	-5.539074
H	0.968517	2.307557	-5.930270
H	1.154477	3.776939	-4.957065
C	-1.147898	3.813810	-2.743873
H	-1.404596	4.069099	-3.772560
H	-2.009904	3.342100	-2.265261
H	-0.909430	4.740092	-2.214230
N	-0.004991	2.912578	-2.679812
C	-0.014573	3.052241	-0.146722
H	-0.540692	3.999491	-0.264837
N	-0.981831	1.993439	0.179700
H	-0.680330	1.036353	-0.045210
C	-2.283460	2.042096	0.568575
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C	-2.976370	3.382999	0.959845
H	-2.883851	4.033422	0.081310
C	-2.314775	4.104008	2.148632
H	-1.321344	4.440584	1.844816
H	-2.127252	3.396454	2.964391
C	-3.076449	5.333930	2.685538
H	-4.090863	5.040488	2.978992
C	-3.181287	6.447458	1.641921
H	-3.761815	6.127841	0.772402
H	-3.681751	7.326575	2.062045
H	-2.190561	6.758474	1.292902
C	-2.376312	5.869040	3.938397
H	-1.353236	6.191230	3.715966
H	-2.919171	6.725771	4.351739
H	-2.328688	5.098989	4.715591
N	-4.426088	3.096804	1.137317
C	-4.820368	2.311227	2.222641
O	-4.120863	2.178581	3.232839
C	-6.162579	1.546918	2.132417
H	-6.417904	1.342357	1.093233
C	-5.292352	3.400379	0.009360
H	-6.343494	3.406118	0.301215
H	-5.046808	4.389222	-0.387310
H	-5.139484	2.644950	-0.764335
C	-7.265076	2.338463	2.821498
H	-7.026943	2.510984	3.877452
H	-7.406371	3.317840	2.354693
H	-8.217263	1.799954	2.782092
N	-5.946175	0.267198	2.813184
H	-5.229282	0.282431	3.535991
C	-6.499659	-0.964059	2.629543
O	-6.089048	-1.880115	3.345757
C	-7.533618	-1.183639	1.493183
H	-7.928237	-0.204309	1.204893
N	-6.816920	-1.731653	0.307353
C	-6.574721	-0.807077	-0.789882
H	-6.453874	-1.331244	-1.737639
H	-7.423948	-0.127866	-0.903274
H	-5.675917	-0.226375	-0.568659
C	-8.755157	-2.014257	1.984633
H	-8.402486	-2.941492	2.450913
C	-9.723387	-2.425869	0.851722
H	-10.496262	-3.081612	1.273138
H	-9.191804	-3.033114	0.110567
C	-10.418386	-1.277712	0.131920
H	-9.702054	-0.595802	-0.331994
H	-11.060897	-1.672984	-0.661944
H	-11.054057	-0.703013	0.811592
C	-9.511835	-1.259778	3.091307
H	-9.830559	-0.266419	2.760441
H	-10.401547	-1.817308	3.403207
H	-8.883178	-1.128150	3.977886
C	-3.404259	-2.346396	0.387492
H	-3.854526	-1.469272	0.856948
H	-3.494325	-3.200778	1.062776
H	-2.342536	-2.164883	0.223398
C	0.638681	2.595696	-1.481186
O	1.631168	1.861030	-1.470736
C	1.055508	3.166518	0.957278
H	0.580613	3.240219	1.943679
H	1.662905	2.253141	1.013963
C	3.627324	6.604936	0.372664
C	2.384359	6.754459	0.987248
C	1.556182	5.642507	1.185051
C	1.958362	4.366297	0.770563
C	3.209484	4.223110	0.159630
C	4.033133	5.334186	-0.037887
H	2.028321	7.721205	1.328227
H	0.597390	5.788498	1.676142
H	3.559098	3.245036	-0.168764
H	5.002176	5.202199	-0.513422
O	4.526237	7.604066	0.118792
C	4.172780	8.912428	0.552394
H	4.995041	9.584876	0.289521
H	3.273949	9.268425	0.038318
H	4.047903	8.947976	1.639682

NMR-Shifts

NMR-CoibamideA.D-MeAla.D-HIV-0002-NMR.txt

Atom	Type	Isotropic	Scaled Shift
2	C	141.9024	42.2649744444
6	C	149.1895	35.2902046364
10	C	108.9935	73.7633760217
12	C	154.6057	30.1061467486
14	C	166.6087	18.617603706
18	C	165.8469	19.3467524263
22	C	1.9931	176.177664197
24	C	107.0384	75.6346790712
27	C	153.1227	31.5255843335
29	C	164.8180	20.3315530542
33	C	170.0728	15.3019774498
37	C	8.7162	169.742720956
39	C	127.0742	56.4576274431

42	C	158.5332	26.3469821398
46	C	113.4757	69.4732862421
50	C	126.8286	56.6927008557
54	C	129.3270	54.3013840234
56	C	5.5063	172.815042401
59	C	152.8424	31.7938704799
63	C	148.0650	36.3665077815
66	C	157.3014	27.5259863321
68	C	166.4063	18.8113287008
72	C	162.4547	22.5935603668
76	C	3.3040	174.922950286
78	C	126.0891	57.4005053696
81	C	154.1176	30.5733264419
85	C	115.8459	67.2046746684
87	C	167.0319	18.2125423534
92	C	125.4506	58.0116388139
94	C	8.1933	170.243209097
97	C	112.3000	70.5985949195
100	C	127.0110	56.518118647
105	C	6.7421	171.632209652
107	C	127.4787	56.0704645954
109	C	2.6693	175.530446601
111	C	169.8763	15.4900553227
115	C	157.3212	27.5070349739
120	C	127.0417	56.4887344704
124	C	8.4636	169.984494343
126	C	114.4606	68.5305997435
128	C	143.6444	40.5976377802
131	C	156.6850	28.1159669978
133	C	165.0988	20.0627883382
137	C	162.6862	22.3719826184
142	C	0.5549	177.554221941
144	C	133.5227	50.2855146538
146	C	147.8943	36.5298914604
150	C	165.5918	19.5909186623
156	C	11.9277	166.668868087
158	C	116.8283	66.264381018
161	C	145.6483	38.6796263328
165	C	151.7723	32.818105247
167	C	160.0717	24.8744233236
170	C	178.1728	7.54914910316
174	C	170.1335	15.2438790942
178	C	155.6085	29.1463274565
182	C	8.6597	169.796799326
184	C	146.5683	37.7990581749
187	C	24.0493	155.066808323
188	C	74.4249	106.850341699
189	C	51.4429	128.847317139
190	C	51.2990	128.985049484
191	C	46.4840	133.593675223
192	C	63.2030	117.591263232
198	C	131.7324	51.9990811463
3	H	28.7328	2.87345807346
4	H	29.4233	2.23543543544
5	H	29.3529	2.30048510049
7	H	29.6935	1.98577038577
8	H	30.0087	1.69452529453
9	H	29.3886	2.2674982675
11	H	28.6404	2.95883575884
13	H	29.5829	2.08796488796
15	H	31.2921	0.508662508663
16	H	30.3670	1.36345576346
17	H	30.9159	0.856271656272
19	H	31.1736	0.618156618157
20	H	30.7619	0.998567798568
21	H	30.9751	0.801570801571
25	H	26.3936	5.03488103488
28	H	29.4857	2.17777777778
30	H	30.6229	1.127003927
31	H	30.7772	0.984430584431
32	H	30.5445	1.19944559945
34	H	30.6595	1.09318549319
35	H	30.9305	0.842781242781
36	H	30.5294	1.2133980134
40	H	24.8928	6.42162162162
43	H	29.0482	2.58202818203
44	H	29.1659	2.47327327327
45	H	28.4768	3.11000231
47	H	27.8720	3.66883806884
48	H	27.6210	3.90076230076
51	H	28.0941	3.46361746362
52	H	28.4671	3.11896511897
53	H	28.4773	3.10954030954
55	H	26.2900	5.13060753061
60	H	29.1596	2.47909447909
61	H	27.8613	3.67872487872
62	H	28.4622	3.12349272349
64	H	29.8132	1.87516747517
65	H	30.4391	1.29683529684
67	H	30.0895	1.61986601987
69	H	31.3264	0.476969276969
70	H	30.6956	1.05982905983
71	H	30.7519	1.00780780781
73	H	31.1313	0.657241857242
74	H	30.6606	1.09216909217
75	H	30.7705	0.990621390621
79	H	25.7559	5.62411642412
82	H	28.7315	2.87465927466
83	H	29.2271	2.41672441672
84	H	28.7450	2.86218526219
86	H	25.9901	5.40771540772
88	H	30.8415	0.925017325017
89	H	30.8401	0.926310926311
90	H	30.5943	1.15343035343
93	H	26.1960	5.21746361746
98	H	28.0961	3.46176946177
99	H	28.3011	3.27234927235
101	H	28.5501	3.04227304227
102	H	28.2443	3.32483252483
103	H	28.6855	2.91716331716
108	H	26.3315	5.09226149226
112	H	30.5812	1.16553476553
113	H	29.8455	1.84532224532
114	H	30.9323	0.841118041118
116	H	28.9916	2.63432663433
117	H	28.7924	2.81838761839
118	H	29.0112	2.61621621622
121	H	27.3210	4.17796257796
123	H	22.2538	8.86006006006
127	H	27.3509	4.15033495033
129	H	29.7763	1.90926310926
130	H	28.4603	3.12524832525
132	H	29.7658	1.91896511897
134	H	30.4325	1.30293370293
135	H	30.3240	1.40318780319
136	H	30.8889	0.88121968122
138	H	30.6560	1.09641949642
139	H	30.5394	1.20415800416
140	H	30.3833	1.34839454839
145	H	26.9509	4.51993531994
147	H	28.3838	3.19593439593
148	H	28.9686	2.65557865558
149	H	28.7767	2.83289443289
151	H	30.1848	1.53180873181
152	H	30.5211	1.22106722107
153	H	30.2517	1.46999306999
155	H	25.0440	6.28191268191
159	H	28.2138	3.35301455301

162	H	28.6310	2.96752136752
163	H	28.9547	2.66842226842
164	H	28.3890	3.19112959113
166	H	27.7953	3.73970893971
168	H	30.4022	1.33093093093
169	H	29.8598	1.83210903211
171	H	31.1685	0.622869022869
172	H	30.7851	0.977130977131
173	H	30.6193	1.13033033033
175	H	31.1108	0.676183876184
176	H	31.0364	0.74492954493
177	H	30.8001	0.963270963271
179	H	28.7365	2.87003927004
180	H	29.2116	2.43104643105
181	H	29.1068	2.52788172788
185	H	28.6439	2.9556017556
186	H	27.9439	3.6024024024
193	H	24.7049	6.59524139524
194	H	23.8237	7.40947100947
195	H	23.7648	7.46389466389
196	H	24.4239	6.85488565489
199	H	27.9659	3.58207438207
200	H	28.1017	3.4565950566
201	H	28.1157	3.44365904366

Supporting Information: NMR-CoibamideA.D-MeAla.D-HIV-0003.log

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Using Gaussian 09: AM64L-G09RevD.01 24-Apr-2013

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#mPW1PW91/6-311+G(2d,p) scf=(maxcycle=300,direct,tight,xqc,vshift=200) NMR density=current SCRF=(PCM,SOLVENT=Chloroform)

Pointgroup= C1 Stoichiometry= C65H110N10O16 C1[X(C65H110N10O16)] #Atoms= 201

Charge = 0 Multiplicity = 1

SCF Energy= -4294.55858722

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Optimization incomplete.

Atomic Type	Coordinates (Angstroms) X	Y	Z
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H	5.061435	-0.451475	3.313737
H	4.681881	-0.227983	5.029266
H	6.353514	-0.157839	4.499067
C	4.236005	-2.769036	4.404671
H	3.515093	-2.368989	5.127324
H	3.813012	-2.622241	3.405740
H	4.296304	-3.842645	4.605091
C	6.646770	-2.705505	3.789523
H	7.537325	-2.091364	3.987561
C	7.016579	-4.153676	4.225680
H	6.203588	-4.840543	3.959084
C	7.252074	-4.252795	5.738717
H	8.041689	-3.565747	6.061860
H	6.344097	-4.018477	6.302847
H	7.553086	-5.268128	6.018937
C	8.277552	-4.648023	3.499573
H	9.131240	-3.989997	3.694903
H	8.546042	-5.656687	3.831996
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C	6.384194	-2.668985	2.269385
O	5.510181	-3.296307	1.682043
C	7.152748	-1.744406	0.231469
H	7.003992	-2.750028	-0.175368
O	7.308750	-1.872021	1.656794
C	8.454994	-1.144618	-0.351356
H	8.318816	-0.949365	-1.421551
C	9.612782	-2.138672	-0.206336
H	9.832588	-2.352149	0.845106
H	9.375046	-3.085234	-0.703060
H	10.523879	-1.741564	-0.666683
C	8.842203	0.182856	0.311409
H	9.031607	0.062548	1.383156
H	9.753171	0.587170	-0.143523
H	8.054447	0.932212	0.185776
C	5.934071	-0.856416	-0.124109
O	5.453499	-0.114967	0.740925
C	4.289964	0.019973	-1.750301
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H	3.822893	1.667017	-3.091267
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C	6.115940	2.791429	-3.440600
H	6.971228	3.368610	-3.079279
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H	5.275787	3.474390	-3.598947
C	1.192588	-2.332056	-1.619437
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H	2.801052	-0.219019	0.455334
H	1.594579	-1.443945	0.802484
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C	-2.519412	-1.207534	-2.137121
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H	-1.625464	-2.710346	-4.199348
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H	-4.073452	1.101494	-2.222281
H	-3.997613	1.416017	-3.947710

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H	-4.508696	-5.064222	0.443161
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H	-4.897920	-7.401913	-1.373720
H	-3.374182	-7.147994	-2.251899
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NMR-Shifts

NMR-CoibamideA.D-MeAla.D-HIV-0003-NMR.txt

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12	C	153.7542	30.9211508643
14	C	166.2244	18.9854323398
18	C	165.4787	19.6991711174
22	C	0.3173	177.78163824
24	C	107.7670	74.9373073757
27	C	153.5453	31.1210972645
29	C	164.9561	20.1993721166
33	C	170.2415	15.1405080495
37	C	8.6428	169.81297498
39	C	127.0765	56.4554260227
42	C	159.1235	25.7819828098
46	C	113.4749	69.4740519535
50	C	126.7939	56.7259135895
54	C	129.3961	54.2352456977
56	C	5.3100	173.002928846
59	C	152.4889	32.1322192232
63	C	147.7264	36.6905951492
66	C	157.3285	27.500047857
68	C	166.4169	18.8011830242

72	C	162.5866	22.4673136928
76	C	3.4682	174.765788013
78	C	125.9981	57.487605046
81	C	154.1850	30.508815253
85	C	115.7453	67.3009628821
87	C	166.9863	18.2561879056
92	C	125.1986	58.252837918
94	C	8.1523	170.282451808
97	C	112.2602	70.6366890637
100	C	126.9196	56.6056011792
105	C	6.1752	172.174811922
107	C	127.5744	55.9788663642
109	C	2.4934	175.698807404
111	C	170.0106	15.3615115144
115	C	157.5197	27.3170428224
120	C	126.9140	56.6109611593
124	C	8.5202	169.930320259
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128	C	143.5821	40.6572675587
131	C	156.7536	28.0503072417
133	C	165.1662	19.9982771493
137	C	162.7571	22.3041214418
142	C	0.5311	177.577001857
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146	C	148.5895	35.8644882176
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158	C	116.9617	66.1366986351
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167	C	160.6343	24.3359367522
170	C	178.1290	7.59107180459
174	C	170.2957	15.0886310994
178	C	155.7138	29.045540688
182	C	8.5451	169.90648749
184	C	146.5643	37.8028867321
187	C	23.9662	155.146346599
188	C	74.3138	106.956679875
189	C	51.2686	129.014146519
190	C	51.4634	128.827695783
191	C	46.3404	133.731120427
192	C	63.0806	117.708417083
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7	H	29.7584	1.9258027258
8	H	29.7972	1.88995148995
9	H	29.1108	2.52418572419
11	H	28.5902	3.00522060522
13	H	29.8348	1.85520905521
15	H	31.2352	0.561238161238
16	H	30.4499	1.28685608686
17	H	30.9295	0.843705243705
19	H	31.1021	0.684222684223
20	H	30.7757	0.985816585817
21	H	30.9613	0.814322014322
25	H	26.3976	5.03118503119
28	H	29.5281	2.1386001386
30	H	30.6461	1.10556710557
31	H	30.7544	1.0054978055
32	H	30.6344	1.11637791638
34	H	30.7057	1.0504966505
35	H	30.9503	0.824486024486
36	H	30.6030	1.14539154539
40	H	24.7982	6.50903210903
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44	H	29.1330	2.50367290367
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62	H	28.4439	3.1404019404
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65	H	30.4262	1.30875490875
67	H	30.1069	1.60378840379
69	H	31.3348	0.469207669208
70	H	30.5780	1.16849156849
71	H	30.7247	1.03294063294
73	H	31.1338	0.654931854932
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79	H	25.6715	5.7021021021
82	H	28.6940	2.90930930931
83	H	29.2095	2.43298683299
84	H	28.7516	2.85608685609
86	H	25.9423	5.45188265188
88	H	30.7993	0.96401016401
89	H	30.8347	0.931300531301
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93	H	26.1412	5.2680988681
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99	H	28.2699	3.30117810118
101	H	28.5197	3.07036267036
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112	H	30.5261	1.21644721645
113	H	29.8543	1.83719103719
114	H	30.9226	0.850080850081
116	H	28.9717	2.65271425271
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118	H	28.9613	2.66232386232
121	H	27.3314	4.16835296835
123	H	22.0502	9.04818664819
127	H	27.3655	4.13684453684
129	H	29.8084	1.8796026796
130	H	28.4701	3.11619311619
132	H	29.7690	1.91600831601
134	H	30.4527	1.28426888427
135	H	30.3213	1.40568260568
136	H	30.8918	0.87854007854
138	H	30.6837	1.07082467082
139	H	30.5523	1.19223839224
140	H	30.4057	1.3276969277
145	H	27.0221	4.45414645415
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148	H	29.0441	2.58581658582
149	H	28.7417	2.86523446523
151	H	30.1830	1.53347193347
152	H	30.4791	1.25987525988
153	H	30.3048	1.42092862093
155	H	24.9209	6.39565719566
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163	H	29.0667	2.56493416493
164	H	28.1789	3.38526218526
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169	H	30.0640	1.64342804343
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172	H	30.7816	0.980364980365
173	H	30.6059	1.14271194271

175	H	31.1101	0.676830676831
176	H	31.1096	0.677292677293
177	H	30.7097	1.0468006468
179	H	28.6704	2.93111573112
180	H	29.1984	2.44324324324
181	H	29.0391	2.59043659044
185	H	28.6618	2.93906213906
186	H	27.9309	3.61441441441
193	H	24.7205	6.58082698083
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195	H	23.7165	7.50852390852
196	H	24.4103	6.86745206745
199	H	27.8940	3.64851004851
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Supporting Information: NMR-CoibamideA.D-MeAla.D-HIV-0004.log

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Using Gaussian 09: AM64L-G09RevD.01 24-Apr-2013

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Pointgroup= C1 Stoichiometry= C65H110N10O16 C1[X(C65H110N10O16)] #Atoms= 201

Charge = 0 Multiplicity = 1

SCF Energy= -4294.55301863

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Optimization incomplete.

Atomic Type	Coordinates (Angstroms) X	Y	Z
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H	6.759098	-0.702375	3.505692
C	3.699236	-1.905466	2.794102
H	3.180990	-1.405142	3.620485
H	3.488130	-1.342327	1.879252
H	3.246399	-2.897659	2.707581
C	5.901802	-2.807341	2.096955
H	6.973383	-2.684374	2.311597
C	5.617323	-4.334010	2.232088
H	4.592187	-4.551544	1.906740
C	5.769291	-4.820909	3.679553
H	6.768324	-4.597693	4.069404
H	5.032230	-4.352944	4.339491
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H	7.609035	-4.977941	1.601944
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H	6.430254	-4.907744	0.280712
C	5.667181	-2.344183	0.644278
O	4.753462	-2.723855	-0.079789
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H	8.596645	-1.859974	-2.486094
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NMR-Shifts

NMR-CoibamideA.D-MeAla.D-HIV-0004-NMR.txt

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14	C	166.6566	18.5717567335
18	C	165.7741	19.4164321675
22	C	1.5066	176.643312468
24	C	108.2769	74.4492620456
27	C	152.2430	32.3675797776
29	C	164.5655	20.573230728
33	C	170.2035	15.176879343
37	C	6.2689	172.08512797
39	C	131.3252	52.3888282701
42	C	156.0689	28.7056605218
46	C	114.1404	68.837075748
50	C	128.1358	55.44152836
54	C	131.6874	52.0421524149
56	C	5.1251	173.179903903
59	C	151.0800	33.4807327858
63	C	146.7682	37.6077260284
66	C	155.7392	29.0212293497
68	C	165.7706	19.4197821551
72	C	162.6370	22.419073872
76	C	1.6984	176.45973315
78	C	128.6292	54.9692758284
81	C	156.7118	28.0903156645
85	C	112.5253	70.3829514348
87	C	169.4806	15.8687953445
92	C	123.7663	59.6237485404
94	C	7.4822	170.923830854
97	C	107.0257	75.6468347403

100	C	126.8558	56.6666666667
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107	C	126.7841	56.7352935546
109	C	3.2451	174.979325791
111	C	169.9163	15.4517697506
115	C	153.8644	30.8156741132
120	C	128.5114	55.0820268382
124	C	10.1305	168.389038841
126	C	117.2766	65.8352954689
128	C	146.8871	37.4939221654
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133	C	160.9796	24.0054365512
137	C	166.7798	18.4538371715
142	C	2.5010	175.691533146
144	C	135.6070	48.2905492065
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150	C	167.3417	17.9160205976
156	C	13.8785	164.801680737
158	C	128.1264	55.4505254695
161	C	151.2097	33.3565918184
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167	C	155.8732	28.8929726832
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174	C	169.1012	16.2319339957
178	C	157.9354	26.9191600145
182	C	6.5106	171.8537874
184	C	140.6121	43.4999712858
187	C	23.0016	156.06960317
188	C	73.9971	107.259805892
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5	H	29.5320	2.134996535
7	H	29.6902	1.98881958882
8	H	29.9774	1.72344652345
9	H	29.2787	2.36904596905
11	H	28.8657	2.75065835066
13	H	29.5231	2.14322014322
15	H	31.2004	0.593393393393
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17	H	30.8456	0.921228921229
19	H	31.3092	0.492862092862
20	H	30.7170	1.04005544006
21	H	30.8165	0.948117348117
25	H	26.3018	5.1197043197
28	H	29.7856	1.90066990067
30	H	30.5866	1.16054516055
31	H	30.7642	0.996442596443
32	H	30.6080	1.14077154077
34	H	30.6335	1.11720951721
35	H	30.9626	0.813120813121
36	H	30.5166	1.22522522523
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65	H	30.6753	1.07858627859
67	H	30.3102	1.41593901594
69	H	31.4594	0.354077154077
70	H	30.6332	1.11748671749
71	H	30.6036	1.14483714484
73	H	31.1284	0.659921459921
74	H	30.6595	1.09318549319
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79	H	25.8005	5.58290598291
82	H	28.1315	3.42905982906
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84	H	28.9031	2.7161007161
86	H	26.0221	5.37814737815
88	H	30.6249	1.12515592516
89	H	30.7714	0.98978978979
90	H	30.5231	1.21921921922
93	H	26.2799	5.13993993994
98	H	28.0794	3.4772002772
99	H	27.8878	3.65423885424
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113	H	29.9110	1.7848001848
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118	H	30.3740	1.35698775699
121	H	26.8625	4.60161700162
123	H	25.3539	5.99556479556
127	H	27.8340	3.70395010395
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132	H	29.9275	1.76955416955
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139	H	30.7936	0.969276969277
140	H	30.3437	1.38498498498
145	H	27.5974	3.92256872257
147	H	28.4919	3.09604989605
148	H	28.8425	2.7720951721
149	H	28.1767	3.38729498729
151	H	30.4070	1.3264957265
152	H	30.6993	1.05641025641
153	H	30.4787	1.26024486024
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159	H	27.0088	4.46643566644
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166	H	29.6114	2.06163086163
168	H	30.1328	1.57985677986
169	H	30.5516	1.19288519289
171	H	31.1224	0.665465465465
172	H	30.7302	1.02785862786
173	H	30.9724	0.804065604066
175	H	30.0171	1.68676368676
176	H	31.1774	0.614645414645
177	H	30.9597	0.8158004158
179	H	29.9651	1.73481173481
180	H	29.4328	2.22665742666
181	H	27.4318	4.07558327558
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186	H	29.0233	2.60503580504
193	H	24.5500	6.73836913837

194	H	23.7976	7.43358743359
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196	H	24.4780	6.8048972049
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Supporting Information: NMR-CoibamideA.D-MeAla.D-HIV-0005.log

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Using Gaussian 09: AM64L-G09RevD.01 24-Apr-2013

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Pointgroup= C1 Stoichiometry= C65H110N10O16 C1[X(C65H110N10O16)] #Atoms= 201

Charge = 0 Multiplicity = 1

SCF Energy= -4294.55334971

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Optimization incomplete.

Atomic Type	Coordinates (Angstroms) X	Y	Z
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H	-3.095759	0.616549	-3.817315
H	-4.759456	0.999146	-3.408570
C	-3.282038	-2.013406	-3.578180
H	-2.415431	-1.683422	-4.163499
H	-2.952303	-2.118927	-2.540449
H	-3.541414	-3.003582	-3.963580
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H	-6.396216	-0.678490	-3.359587
C	-6.273219	-2.777570	-3.779940
H	-5.644098	-3.638540	-3.521515
C	-6.349083	-2.677617	-5.309312
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H	-8.779131	-2.202572	1.148934
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C	-2.323117	-0.455501	2.849840
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H	0.051452	-4.036785	1.350631
C	-2.094254	-4.152078	1.129842
H	-2.936112	-3.473941	0.953707
C	-2.327549	-4.855327	2.468242
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H	-1.978659	-4.694939	-0.973749
C	0.717691	-1.561344	2.119394
O	1.112774	-0.760765	1.264021
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C	1.139841	-2.942020	4.166207
H	1.972531	-3.325289	4.754719
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H	0.624899	-3.796154	3.719281
C	2.934175	-0.463077	4.541303
H	2.506555	-0.996412	5.397440
C	4.315515	0.061486	4.927587
H	4.756197	0.646043	4.116073
H	4.234900	0.741546	5.783221
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H	3.617000	-1.516162	0.759830
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N	4.682646	-2.769405	2.087472
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C	1.832425	0.269303	-2.983751
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NMR-Shifts

NMR-CoibamideA.D-MeAla.D-HIV-0005-NMR.txt

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14	C	166.1761	19.0316621681
18	C	165.1735	19.9912900324
22	C	-0.7556	178.808552997
24	C	110.3797	72.4365895212
27	C	153.2214	31.4311146844
29	C	164.7258	20.4198012979
33	C	170.3988	14.9899500373
37	C	7.3759	171.025574762
39	C	131.8266	51.908918624
42	C	158.0745	26.7860219376
46	C	113.2235	69.7146767741
50	C	128.7666	54.8377648883
54	C	131.4090	52.3086199966
56	C	4.7484	173.540458278
59	C	149.8393	34.6682555179
63	C	146.0489	38.2961963284
66	C	155.7172	29.0422864144
68	C	166.2885	18.9240797106
72	C	162.3371	22.7061199487
76	C	1.9645	176.205038381
78	C	128.2675	55.315473114
81	C	156.3755	28.4122016118
85	C	112.6795	70.2353605544
87	C	169.6912	15.6672218075
92	C	124.5011	58.9204425812
94	C	7.2159	171.17871705
97	C	108.3316	74.3969065258
100	C	126.7006	56.8152146863
105	C	8.5738	169.879017592
107	C	126.7325	56.7846819426
109	C	3.8302	174.419303585
111	C	169.2950	16.0464403989
115	C	153.1450	31.5042401271
120	C	125.5969	57.871609334
124	C	12.1277	166.477440227
126	C	118.2815	64.8734661843

128	C	148.6230	35.832424051
131	C	152.9617	31.6796837612
133	C	161.1287	23.8627270813
137	C	164.8352	20.3150902582
142	C	6.3150	172.041003848
144	C	135.1453	48.7324604223
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150	C	167.0819	18.1646853883
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182	C	6.0604	172.284691514
184	C	144.2566	40.0116770995
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188	C	73.1699	108.051551523
189	C	47.7984	132.335611325
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7	H	29.4948	2.16936936937
8	H	29.2561	2.38992838993
9	H	29.3299	2.32173712174
11	H	28.6200	2.97768537769
13	H	29.9294	1.7677985678
15	H	31.2594	0.538877338877
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17	H	30.9345	0.839085239085
19	H	31.0714	0.71258951259
20	H	30.6865	1.06823746824
21	H	30.9678	0.808316008316
25	H	26.4162	5.013998614
28	H	29.7402	1.94261954262
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31	H	30.8045	0.959205359205
32	H	30.6903	1.06472626473
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36	H	30.4732	1.26532686533
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44	H	28.9346	2.68699468699
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65	H	30.9539	0.82115962116
67	H	29.8185	1.87027027027
69	H	31.5037	0.313143913144
70	H	30.5063	1.23474243474
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73	H	31.1855	0.607161007161
74	H	30.5317	1.21127281127
75	H	30.8377	0.928528528529
79	H	25.6173	5.75218295218
82	H	28.2898	3.28279048279
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84	H	29.1404	2.49683529684
86	H	25.8496	5.53753753754
88	H	30.5365	1.20683760684
89	H	30.5680	1.17773157773
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99	H	28.0021	3.54862554863
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117	H	28.3300	3.24564564565
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121	H	26.8837	4.58202818203
123	H	25.2322	6.10801570802
127	H	28.9964	2.62989142989
129	H	30.8771	0.892122892123
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132	H	31.4802	0.334857934858
134	H	31.3233	0.479833679834
135	H	30.9950	0.783183183183
136	H	31.2630	0.535550935551
138	H	31.3800	0.427442827443
139	H	30.9414	0.83270963271
140	H	30.8728	0.896096096096
145	H	27.8945	3.64804804805
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148	H	29.2878	2.36063756064
149	H	28.1720	3.39163779164
151	H	30.6547	1.09762069762
152	H	30.7599	1.00041580042
153	H	30.3149	1.4115962116
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159	H	26.8433	4.61935781936
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163	H	29.1132	2.52196812197
164	H	29.2298	2.41422961423
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168	H	29.9403	1.75772695773
169	H	30.4472	1.28935088935
171	H	31.0583	0.724693924694
172	H	30.7493	1.01021021021
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199	H	27.7844	3.74978054978
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Supporting Information: NMR-CoibamideA.D-MeAla.D-HIV-0006.log

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 Using  Gaussian 09:  AM64L-G09RevD.01 24-Apr-2013
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 SCF Energy= -4294.55402610
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 Optimization incomplete.


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     Type      X                Y              Z
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     H       4.985582    -0.999571    -3.310092
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NMR-Shifts

NMR-CoibamideA.D-MeAla.D-HIV-0006-NMR.txt

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22	C	-1.0252	179.066597753
24	C	109.4830	73.2948563334
27	C	152.2331	32.3770554567
29	C	164.4142	20.7180459044
33	C	170.3584	15.0286184651
37	C	6.8758	171.504240127
39	C	132.4835	51.2801738165
42	C	158.7109	26.1768984858
46	C	113.2591	69.6806026149
50	C	129.3989	54.2325657076
54	C	131.4101	52.3075671433
56	C	4.4730	173.804054442
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63	C	147.9820	36.4459503436
66	C	158.7608	26.1291372346
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76	C	2.3105	175.873868183
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81	C	156.9952	27.8190623863
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97	C	107.6691	75.0310113134
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189	C	51.0411	129.23189571
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Supporting Information: NMR-CoibamideA.D-MeAla.D-HIV-0007.log

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 Using  Gaussian 09:  AM64L-G09RevD.01 24-Apr-2013
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SCF Energy= -4294.55584001
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Optimization incomplete.

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H	0.985516	1.519001	-6.132129
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NMR-Shifts

NMR-CoibamideA.D-MeAla.D-HIV-0007-NMR.txt

Atom	Type	Isotropic	Scaled Shift
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14	C	166.4166	18.801470166
18	C	165.7385	19.4505063267
22	C	1.5389	176.612396868
24	C	107.3551	75.3315530542
27	C	152.3494	32.2657401558
29	C	164.8953	20.2575661862
33	C	169.8340	15.5305423151
37	C	8.0943	170.337965888
39	C	131.5747	52.1500220142
42	C	156.5518	28.2434579529
46	C	114.7110	68.2909320623
50	C	127.1776	56.3586592393
54	C	129.1172	54.502191849
56	C	3.1658	175.055226938
59	C	153.7777	30.8986580907
63	C	146.4610	37.901759222
66	C	156.7360	28.0671528934
68	C	166.4859	18.7351404123
72	C	162.6623	22.3948582477
76	C	3.0092	175.205114952
78	C	125.8077	57.6698443691
81	C	153.9328	30.7502057849
85	C	115.0997	67.9188920155
87	C	166.5215	18.7010662532
92	C	124.8849	58.5530925171
94	C	8.0746	170.356821532
97	C	112.2957	70.6027106185
100	C	126.8995	56.6248396792
105	C	4.2723	173.9961523
107	C	127.1166	56.4170447367
109	C	2.5090	175.683876031
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115	C	157.3022	27.5252206206
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124	C	8.7096	169.749038075
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128	C	143.8986	40.3543329696
131	C	156.5651	28.2307280002
133	C	165.1795	19.9855471965
137	C	162.8163	22.2474587952
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150	C	166.0522	19.1502517276
156	C	12.4988	166.122245832
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161	C	146.2802	38.0748100078
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167	C	151.5938	32.9889546125
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174	C	164.5294	20.6077834568
178	C	156.6057	28.1918681445
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184	C	145.7994	38.5350025843
187	C	23.4468	155.643484753
188	C	74.4209	106.854170256
189	C	53.1539	127.209651793
190	C	50.4572	129.790769349
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7	H	29.5947	2.07706167706
8	H	29.8851	1.80873180873
9	H	28.9708	2.65354585355
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13	H	29.7733	1.91203511204
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17	H	30.8923	0.878078078078
19	H	31.2016	0.592284592285
20	H	30.7144	1.04245784246
21	H	31.0111	0.768306768307
25	H	26.5125	4.92501732502
28	H	29.4469	2.21362901363
30	H	30.5544	1.1902979903
31	H	30.7983	0.964934164934
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34	H	30.5938	1.15389235389
35	H	30.8950	0.875583275583
36	H	30.5070	1.2340956341
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44	H	29.3132	2.33716793717
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69	H	31.2980	0.503210903211
70	H	30.5279	1.21478401478
71	H	30.7031	1.0528990529
73	H	31.0759	0.708431508432
74	H	30.6156	1.13374913375
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88	H	30.6816	1.07276507277
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98	H	28.0141	3.53753753754
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117	H	28.6628	2.93813813814
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129	H	29.7827	1.90334950335
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135	H	30.3575	1.37223377223
136	H	30.8580	0.909771309771
138	H	30.8264	0.93896973897
139	H	30.5280	1.21469161469
140	H	30.5495	1.19482559483
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148	H	29.0497	2.58064218064
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151	H	30.3594	1.37047817048
152	H	30.5730	1.17311157311
153	H	30.5459	1.19815199815
155	H	25.0986	6.23146223146
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164	H	27.9869	3.56267036267
166	H	28.1540	3.40826980827
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175	H	31.4404	0.371633171633
176	H	30.6912	1.06389466389
177	H	30.8131	0.951258951259
179	H	28.6298	2.96863016863
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193	H	24.6660	6.63118503119
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Supporting Information: NMR-CoibamideA.D-MeAla.D-HIV-0008.log

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 Using  Gaussian 09:  AM64L-G09RevD.01 24-Apr-2013
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 density=current SCRF=(PCM,SOLVENT=Chloroform)
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H	-9.081171	-2.313321	-0.705114
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NMR-Shifts

NMR-CoibamideA.D-MeAla.D-HIV-0008-NMR.txt

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14	C	166.4047	18.8128601237
18	C	165.6880	19.4988418614
22	C	2.6859	175.514558089
24	C	107.0120	75.6599475488
27	C	153.0522	31.5930626543
29	C	164.9672	20.1887478704
33	C	169.9746	15.3959685293
37	C	8.0758	170.355672965
39	C	131.4758	52.2446830912
42	C	156.2432	28.5388311415
46	C	114.6149	68.3829131492
50	C	127.0584	56.4727502441
54	C	129.1381	54.4821876376
56	C	3.4210	174.810964988
59	C	153.0646	31.581194127
63	C	146.6048	37.7641225904
66	C	156.5452	28.2497750723
68	C	166.3801	18.8364057505
72	C	162.7078	22.3513084094
76	C	3.0871	175.130553801
78	C	125.6317	57.8383008863
81	C	153.8792	30.8015084515
85	C	115.3360	67.6927199985
87	C	166.7197	18.5113612435
92	C	124.9745	58.4673328356
94	C	8.1315	170.302360306
97	C	112.1408	70.7509714964
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105	C	3.8941	174.358142384
107	C	127.0063	56.5226172017
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111	C	170.0283	15.3445701487
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124	C	8.7157	169.743199525
126	C	114.5460	68.4488600471
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131	C	156.5723	28.2238365972
133	C	165.0242	20.1341909301
137	C	162.8375	22.2271674419
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178	C	156.4467	28.3440532935
182	C	9.0203	169.451654894
184	C	145.6356	38.691782002
187	C	23.5984	155.498382435
188	C	74.5457	106.734719271
189	C	53.5164	126.862688796
190	C	50.2791	129.961235858
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8	H	29.9281	1.768999769
9	H	29.2204	2.42291522292
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19	H	31.1981	0.595518595519
20	H	30.7976	0.965580965581
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25	H	26.4755	4.95920535921
28	H	29.4812	2.18193578194
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32	H	30.5895	1.15786555787
34	H	30.6010	1.14723954724
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36	H	30.5414	1.20231000231
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67	H	29.9762	1.72455532456
69	H	31.3097	0.4924000924
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71	H	30.6693	1.08413028413
73	H	31.0826	0.702240702241
74	H	30.6197	1.12996072996
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82	H	28.6099	2.98701778702
83	H	29.1124	2.52270732271
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88	H	30.6752	1.07867867868
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152	H	30.5428	1.20101640102
153	H	30.5681	1.17763917764
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175	H	31.4289	0.382259182259
176	H	30.7253	1.03238623239
177	H	30.7458	1.01344421344
179	H	28.6107	2.98627858628
180	H	29.2105	2.43206283206
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Supporting Information: NMR-CoibamideA.D-MeAla.D-HIV-0009.log

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 Using  Gaussian 09:  AM64L-G09RevD.01 24-Apr-2013
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 density=current SCRF=(PCM,SOLVENT=Chloroform)
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C1[X(C65H110N10O16)]  #Atoms= 201
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 SCF Energy= -4294.55528195
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 Optimization incomplete.


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     Atomic     Coordinates (Angstroms)
      Type     X                Y              Z
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H	-5.012014	2.802892	-1.147818
C	-7.220332	3.075461	2.384567
H	-6.994750	3.368949	3.416314
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C	-6.705867	-0.264754	2.675655
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C	-6.711255	-0.619457	-0.751076
H	-6.571440	-1.299184	-1.590952
H	-7.552062	0.034030	-1.002576
H	-5.811049	-0.017112	-0.607221
C	-9.037070	-1.211715	2.066191
H	-8.842524	-2.178747	2.540629
C	-10.110567	-1.401397	0.965723
H	-10.209259	-0.484066	0.372544
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H	-9.675092	-3.497637	0.596647
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H	-9.071844	-2.402977	-0.669582
C	-9.651491	-0.311448	3.158314
H	-9.881350	0.685109	2.766347
H	-10.581858	-0.745284	3.541471
H	-8.979863	-0.196354	4.014205
C	-3.619660	-2.109200	0.753682
H	-4.033137	-1.150728	1.074943
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C	1.129472	2.911214	0.679429
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C	1.925878	5.316400	0.486555
C	2.218075	3.946567	0.508083
C	3.554598	3.545403	0.397934
C	4.570647	4.494384	0.258612
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H	3.820480	2.488902	0.419906
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H	6.074377	8.587112	-0.030549
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NMR-Shifts

NMR-CoibamideA.D-MeAla.D-HIV-0009-NMR.txt

Atom	Type	Isotropic	Scaled Shift
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14	C	166.3318	18.8826355788
18	C	165.7670	19.4232278566
22	C	0.0757	178.012883095
24	C	107.7489	74.9546315971
27	C	153.2329	31.4201075825
29	C	165.0501	20.1094010222
33	C	169.9883	15.3828557208
37	C	7.9312	170.494075308
39	C	131.5849	52.1402591933
42	C	155.7714	28.9904094642
46	C	114.6739	68.3264419304
50	C	126.9440	56.5822469802
54	C	129.2379	54.3866651352
56	C	3.4996	174.735733839
59	C	153.0715	31.5745898658
63	C	146.2723	38.0823714083
66	C	156.2549	28.5276326117
68	C	166.4816	18.7392561113
72	C	162.7286	22.3313999119
76	C	3.0304	175.184823599
78	C	125.8007	57.6765443443
81	C	153.7872	30.8895652673
85	C	115.2398	67.7847967993
87	C	166.8179	18.4173701641
92	C	124.9843	58.4579528705
94	C	8.1265	170.307146002
97	C	112.1856	70.7080916557
100	C	126.9177	56.6074197439
105	C	3.8621	174.388770842
107	C	126.9795	56.548268535
109	C	2.4920	175.700147399
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120	C	126.9657	56.5614770574
124	C	8.7889	169.673136928
126	C	114.3040	68.6804877582
128	C	143.7102	40.5346580141
131	C	156.6352	28.1636325351
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137	C	162.8446	22.2203717529
142	C	0.1064	177.983498918
144	C	133.7046	50.1114110148
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167	C	151.6196	32.9642604185
170	C	172.8975	12.5983460633
174	C	164.4936	20.6420490438
178	C	156.6456	28.1536782863
182	C	8.6764	169.7808151
184	C	145.3869	38.9298225464
187	C	23.6450	155.453779743
188	C	74.7191	106.568751316
189	C	53.7727	126.617373993
190	C	50.4068	129.839009169
191	C	46.1865	133.878424166
192	C	62.6437	118.126591244
198	C	131.5945	52.131070656
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4	H	29.4541	2.20697620698
5	H	29.1361	2.50080850081
7	H	29.6290	2.04536844537
8	H	29.6036	2.06883806884
9	H	29.1504	2.4875952876
11	H	28.5477	3.04449064449
13	H	29.7475	1.93587433587
15	H	31.2616	0.536844536845
16	H	30.3269	1.40050820051

17	H	30.8592	0.908662508663
19	H	31.0576	0.725340725341
20	H	30.7571	1.003003003
21	H	30.9394	0.834557634558
25	H	26.4468	4.98572418572
28	H	29.4985	2.16595056595
30	H	30.5818	1.16498036498
31	H	30.8072	0.956710556711
32	H	30.6732	1.08052668053
34	H	30.5493	1.19501039501
35	H	30.9199	0.852575652576
36	H	30.5182	1.22374682375
40	H	24.7956	6.51143451143
43	H	28.6260	2.97214137214
44	H	29.1754	2.4644952645
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47	H	28.0491	3.5051975052
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52	H	29.2369	2.40766920767
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61	H	28.7540	2.85386925387
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64	H	29.7549	1.92903672904
65	H	30.5042	1.23668283668
67	H	29.9935	1.70857010857
69	H	31.3308	0.472903672904
70	H	30.5408	1.20286440286
71	H	30.6516	1.10048510049
73	H	31.0753	0.708985908986
74	H	30.5973	1.15065835066
75	H	30.7079	1.04846384846
79	H	25.3562	5.99343959344
82	H	28.6196	2.97805497805
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84	H	28.7946	2.81635481635
86	H	25.8529	5.53448833449
88	H	30.6187	1.13088473088
89	H	30.8138	0.950612150612
90	H	30.5618	1.18346038346
93	H	26.1422	5.26717486717
98	H	27.9840	3.56534996535
99	H	28.2074	3.35892815893
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151	H	30.3715	1.3592977593
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155	H	24.9454	6.37301917302
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162	H	29.0616	2.56964656965
163	H	29.3163	2.3343035343
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169	H	29.8421	1.84846384846
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175	H	31.4274	0.383645183645
176	H	30.7110	1.0455994456
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179	H	28.6291	2.96927696928
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181	H	28.9121	2.70778470778
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194	H	23.9556	7.2875952876
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199	H	27.9151	3.62901362901
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Supporting Information: NMR-CoibamideA.D-MeAla.D-HIV-0010.log

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 Using  Gaussian 09:  AM64L-G09RevD.01 24-Apr-2013
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scf=(maxcycle=300,direct,tight,xqc,vshift=200) NMR
 density=current SCRF=(PCM,SOLVENT=Chloroform)
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C1[X(C65H110N10O16)]  #Atoms= 201
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 SCF Energy= -4294.55540159
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 Optimization incomplete.


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H	-9.565512	-3.613651	0.594710
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H	-8.980854	-2.494371	-0.658430
C	-9.518916	-0.481619	3.217822
H	-9.758000	0.522408	2.851143
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C	0.768507	2.332843	-1.838109
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C	1.261796	3.067933	0.558008
H	0.795413	3.081457	1.551962
H	1.931876	2.198841	0.580997
C	3.611987	6.681766	0.086375
C	2.604928	6.617010	1.047765
C	1.851986	5.446243	1.202599
C	2.090711	4.324912	0.397618
C	3.111414	4.394878	-0.556570
C	3.860031	5.564350	-0.712270
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H	1.083487	5.420542	1.971682
H	3.344320	3.537146	-1.182625
H	4.649123	5.602010	-1.459455
O	4.416249	7.758241	-0.167899
C	4.227501	8.908437	0.648404
H	4.949935	9.666077	0.329958
H	3.224549	9.326731	0.513803
H	4.424456	8.681853	1.701518

NMR-Shifts

NMR-CoibamideA.D-MeAla.D-HIV-0010-NMR.txt

Atom	Type	Isotropic	Scaled Shift
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14	C	166.5045	18.7173376213
18	C	165.8743	19.3205268095
22	C	2.7163	175.485461054
24	C	107.2543	75.4280326959
27	C	153.4499	31.2124083539
29	C	165.0832	20.0777197113
33	C	170.0473	15.326384502
37	C	8.4464	170.000957139
39	C	132.2621	51.492084458
42	C	156.6975	28.1040027566
46	C	115.0316	67.984073202
50	C	127.7661	55.79538276
54	C	129.0333	54.5824958364
56	C	3.7668	174.479986217
59	C	153.1502	31.4992630027
63	C	146.4057	37.9546890254
66	C	156.0855	28.6897720094
68	C	166.4719	18.7485403626
72	C	162.7388	22.3216370911
76	C	3.4463	174.786749364
78	C	125.5801	57.8876892743
81	C	153.7322	30.9422079289
85	C	115.3711	67.659124409
87	C	166.7924	18.4417772163
92	C	124.9174	58.5219854898
94	C	8.2162	170.221290607
97	C	112.0682	70.8204598097
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105	C	3.7411	174.504584697
107	C	126.8502	56.6720266468
109	C	2.0818	176.092765941
111	C	169.7263	15.633626218
115	C	157.2315	27.5928903693
120	C	126.5670	56.9430884971
124	C	8.7331	169.726545301
126	C	114.6756	68.3248147935
128	C	144.2679	40.0008614254
131	C	156.5133	28.280307816
133	C	165.4762	19.7015639656
137	C	162.6219	22.4335266755
142	C	0.5015	177.60533318
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178	C	156.4220	28.3676946343
182	C	8.4439	170.003349988
184	C	145.8233	38.512126955
187	C	24.3699	154.759949463
188	C	74.5649	106.716342196
189	C	51.2494	129.032523593
190	C	50.4215	129.824939222
191	C	49.9076	130.316813109
192	C	64.0118	116.817128965
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5	H	29.4177	2.24060984061
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9	H	29.2706	2.37653037653
11	H	28.7283	2.87761607762
13	H	29.8076	1.88034188034
15	H	31.3420	0.462554862555
16	H	30.4575	1.27983367983
17	H	30.9332	0.840286440286
19	H	31.2269	0.568907368907
20	H	30.8301	0.935550935551
21	H	30.9732	0.803326403326
25	H	26.5235	4.91485331485
28	H	29.5738	2.09637329637
30	H	30.5372	1.20619080619
31	H	30.7854	0.976853776854
32	H	30.6644	1.08865788866

34	H	30.7745	0.986925386925
35	H	31.0154	0.764333564334
36	H	30.7859	0.976391776392
40	H	24.8783	6.43501963502
43	H	28.6220	2.97583737584
44	H	29.2271	2.41672441672
45	H	29.2091	2.43335643336
47	H	27.8092	3.72686532687
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51	H	28.3585	3.21931161931
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55	H	26.3963	5.03238623239
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62	H	28.5237	3.06666666667
64	H	29.8403	1.85012705013
65	H	30.5171	1.22476322476
67	H	30.0122	1.69129129129
69	H	31.3507	0.454516054516
70	H	30.5356	1.20766920767
71	H	30.6224	1.12746592747
73	H	31.0996	0.686532686533
74	H	30.6228	1.1270963271
75	H	30.7461	1.01316701317
79	H	25.4631	5.89466389466
82	H	28.6520	2.94811734812
83	H	29.1408	2.49646569647
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86	H	25.8766	5.51258951259
88	H	30.7064	1.04984984985
89	H	30.8182	0.946546546547
90	H	30.5466	1.19750519751
93	H	26.1492	5.26070686071
98	H	27.9644	3.58346038346
99	H	28.1980	3.36761376761
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113	H	29.7744	1.91101871102
114	H	30.7610	0.999399399399
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121	H	27.4026	4.10256410256
123	H	21.6451	9.4224994225
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139	H	30.5149	1.2267960268
140	H	30.4124	1.32150612151
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151	H	30.3503	1.37888657889
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Supporting Information: NMR-CoibamideA.D-MeAla.D-HIV-0011.log

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 Using  Gaussian 09:  AM64L-G09RevD.01 24-Apr-2013
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 Optimization incomplete.


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C	2.747501	4.861348	-0.262045
C	3.386756	6.101683	-0.339606
H	1.800587	7.668328	2.231148
H	0.694769	5.510092	2.369093
H	3.042755	4.078262	-0.955967
H	4.152619	6.265372	-1.094068
O	3.758807	8.290204	0.360639
C	3.483884	9.356952	1.261508
H	4.127355	10.198883	0.988417
H	2.444409	9.689517	1.172929
H	3.723508	9.074897	2.292047

NMR-Shifts
NMR-CoibamideA.D-MeAla.D-HIV-0011-NMR.txt

Atom	Type	Isotropic	Scaled Shift
2	C	141.8898	42.2770343996
6	C	149.4996	34.9933957388
10	C	109.3422	73.4296215471
12	C	153.7815	30.8950209614
14	C	166.3457	18.8693313425
18	C	165.3344	19.8372863187
22	C	-0.0332	178.117115565
24	C	108.6371	74.104500469
27	C	152.8708	31.7666877237
29	C	164.5344	20.6029977603
33	C	170.2106	15.170083654
37	C	6.6990	171.673462356
39	C	132.9440	50.8394111679
42	C	157.7756	27.072110875
46	C	114.5356	68.4588142958
50	C	127.7012	55.8575011007
54	C	129.4180	54.2142843469
56	C	4.3740	173.898811233
59	C	151.8826	32.712532782
63	C	146.5495	37.8170523938
66	C	156.0292	28.7436589521
68	C	166.2193	18.9903137503
72	C	162.2857	22.7553169088
76	C	3.3182	174.909358908
78	C	125.6407	57.8296866326
81	C	153.6963	30.9765692299
85	C	115.5159	67.520530638
87	C	167.2061	18.045808687
92	C	125.0751	58.3710446218
94	C	8.3140	170.127682383
97	C	112.3744	70.5273837554
100	C	126.9013	56.6231168284
105	C	4.0545	174.20461724
107	C	126.6330	56.8799173032
109	C	2.7860	175.418748445
111	C	169.8190	15.5448994047
115	C	157.0694	27.7480426501
120	C	126.8707	56.6524052911
124	C	8.6297	169.825513505
126	C	114.4495	68.5412239897
128	C	144.1793	40.0856639675
131	C	156.4040	28.3849231417
133	C	165.5060	19.6730412144
137	C	162.6927	22.3657612129
142	C	0.8226	177.29799575
144	C	133.9933	49.8350848983
146	C	147.9871	36.4410689332
150	C	165.8112	19.3809222994
156	C	12.2756	166.335879324
158	C	112.9952	69.9331916767
161	C	146.5926	37.7757996899
165	C	149.6218	34.8764333161
167	C	151.4548	33.1219969754
170	C	173.3099	12.2036218151
174	C	164.4547	20.6792817627
178	C	155.9798	28.7909416336
182	C	7.8147	170.605582036
184	C	145.7115	38.6191351289
187	C	23.6087	155.4885239
188	C	74.2177	107.048660962
189	C	50.7475	129.512911809
190	C	48.8579	131.321522234
191	C	49.9593	130.267329007
192	C	63.2203	117.574704723
198	C	131.7474	51.9847240567
3	H	29.3831	2.27258027258
4	H	29.5475	2.12067452067
5	H	29.3919	2.26444906445
7	H	29.7511	1.93254793255
8	H	29.5178	2.14811734812
9	H	29.2420	2.40295680296
11	H	28.5995	2.99662739663
13	H	29.9581	1.74127974128
15	H	31.2790	0.520766920767
16	H	30.5620	1.18327558328
17	H	30.9811	0.796026796027
19	H	31.1432	0.646246246246
20	H	30.7684	0.992561792562
21	H	31.0516	0.730884730885
25	H	26.4498	4.98295218295
28	H	29.6380	2.03705243705
30	H	30.7182	1.03894663895
31	H	30.7947	0.968260568261
32	H	30.5451	1.19889119889
34	H	30.7404	1.01843381843
35	H	31.0058	0.773203973204
36	H	30.5728	1.1732963733
40	H	25.0919	6.23765303765
43	H	28.8094	2.80267960268
44	H	29.1145	2.52076692077
45	H	28.8147	2.79778239778
47	H	27.9486	3.59805959806
48	H	27.2056	4.28459228459

51	H	28.2762	3.29535689536
52	H	28.6358	2.96308616309
53	H	28.0463	3.50778470778
55	H	26.3851	5.04273504274
60	H	28.7102	2.89434049434
61	H	27.9878	3.56183876184
62	H	28.5037	3.08514668515
64	H	29.8129	1.87544467544
65	H	30.5003	1.24028644029
67	H	29.7729	1.9124047124
69	H	31.3455	0.459320859321
70	H	30.4361	1.29960729961
71	H	30.5773	1.16913836914
73	H	31.0686	0.715176715177
74	H	30.5545	1.19020559021
75	H	30.7986	0.964656964657
79	H	25.5444	5.81954261954
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84	H	28.7797	2.83012243012
86	H	25.8600	5.52792792793
88	H	30.7318	1.02638022638
89	H	30.7930	0.969831369831
90	H	30.5088	1.23243243243
93	H	26.2029	5.21108801109
98	H	27.9544	3.5927003927
99	H	28.2181	3.34904134904
101	H	28.4938	3.09429429429
102	H	28.2040	3.36206976207
103	H	28.6651	2.93601293601
108	H	26.1659	5.24527604528
112	H	30.4374	1.29840609841
113	H	29.7501	1.93347193347
114	H	30.7402	1.01861861862
116	H	28.9213	2.69928389928
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121	H	27.4081	4.09748209748
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127	H	27.4477	4.06089166089
129	H	29.8652	1.82711942712
130	H	28.4386	3.1452991453
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134	H	30.5284	1.21432201432
135	H	30.4186	1.31577731578
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139	H	30.5544	1.1902979903
140	H	30.3560	1.37361977362
145	H	27.1347	4.3501039501
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148	H	29.0070	2.6200970201
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151	H	30.3150	1.4115038115
152	H	30.5454	1.19861399861
153	H	30.3741	1.3568953569
155	H	25.0539	6.27276507277
159	H	28.7158	2.88916608917
162	H	28.9021	2.71702471702
163	H	29.1685	2.47087087087
164	H	28.1126	3.44652344652
166	H	28.2273	3.34054054054
168	H	30.2820	1.441995842
169	H	29.8275	1.86195426195
171	H	30.8285	0.937029337029
172	H	30.9044	0.866897666898
173	H	30.5057	1.2352968353
175	H	31.3905	0.417740817741
176	H	30.7992	0.964102564103
177	H	30.7086	1.04781704782
179	H	28.7196	2.88565488565
180	H	29.2827	2.36534996535
181	H	28.9995	2.62702702703
185	H	28.8800	2.73744513745
186	H	27.3662	4.1361977362
193	H	24.5926	6.69900669901
194	H	23.8657	7.37066297066
195	H	24.0403	7.20933240933
196	H	24.6298	6.66463386463
199	H	27.8885	3.65359205359
200	H	28.0836	3.47331947332
201	H	28.0698	3.48607068607

Supporting Information: NMR-CoibamideA.D-MeAla.D-HIV-0012.log

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Using Gaussian 09: AM64L-G09RevD.01 24-Apr-2013

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Pointgroup= C1 Stoichiometry= C65H110N10O16 C1[X(C65H110N10O16)] #Atoms= 201

Charge = 0 Multiplicity = 1

SCF Energy= -4294.55531297

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Optimization incomplete.

Atomic Type	Coordinates (Angstroms) X	Y	Z
N	6.238448	-0.754489	4.446476
C	6.544951	0.542168	3.838277
H	6.228050	0.602590	2.793279
H	6.047538	1.347915	4.390029
H	7.619259	0.750847	3.888032
C	4.793653	-0.986671	4.440799
H	4.289444	-0.211694	5.029931
H	4.363479	-0.966734	3.433841
H	4.535838	-1.939390	4.912693
C	7.038547	-1.853915	3.832454
H	8.086240	-1.521418	3.799209
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C	7.411581	-2.894745	6.144082
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H	6.674378	-2.252899	6.636448
H	7.453415	-3.831469	6.710693
C	8.015360	-4.195569	4.103020
H	9.036937	-3.801344	4.073865
H	8.022388	-5.105075	4.713470
H	7.735760	-4.489701	3.086691
C	6.601727	-2.162471	2.385131
O	5.606372	-2.804016	2.067370
C	7.192713	-1.872543	0.114296
H	6.947155	-2.933907	0.001592
O	7.505745	-1.647989	1.501040
C	8.450034	-1.544931	-0.727648
H	8.202914	-1.610285	-1.793605
C	9.561211	-2.563092	-0.448487
H	9.888952	-2.527067	0.595922
H	9.216768	-3.580548	-0.661896

H	10.433334	-2.368044	-1.081692
C	8.982002	-0.130476	-0.467385
H	9.290664	0.002958	0.574679
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C	5.988532	-1.014025	-0.349704
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H	4.066125	0.341833	-1.273269
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H	6.074094	-2.153963	-3.300688
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H	1.245326	-3.091878	-2.210564
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N	2.274055	-1.733171	-1.028558
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H	1.676561	-1.246077	0.935524
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H	0.927511	-3.350151	0.827531
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H	-6.031919	-3.521289	-1.081247
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C	0.277344	1.345309	-4.232495
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H	-2.033957	2.746262	-2.831079
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C	-2.119579	4.374507	1.398121
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C	-7.168962	3.037900	2.296291
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H	-7.251464	3.926863	1.664017
H	-8.150058	2.554434	2.335946
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H	-6.529662	-1.487657	-1.500383
H	-7.518254	-0.144516	-0.948703
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C	-8.924989	-1.279265	2.205025
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C	-9.803503	-2.738089	0.247758
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H	2.400624	7.205506	1.976928
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H	4.962690	9.505288	0.749375
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H	4.499189	8.353942	2.008390

NMR-Shifts

NMR-CoibamideA.D-MeAla.D-HIV-0012-NMR.txt

Atom	Type	Isotropic	Scaled Shift
2	C	142.1221	42.0546909397
6	C	149.1837	35.2957560443
10	C	108.3560	74.3735523268
12	C	153.6860	30.9864277647
14	C	166.4299	18.7887402133
18	C	165.8058	19.3860908517
22	C	2.3591	175.827351213
24	C	106.9795	75.6910545761
27	C	152.7543	31.8781944524
29	C	165.0048	20.1527594326
33	C	169.8784	15.4880453301
37	C	8.4668	169.981431498
39	C	132.3131	51.4432703536
42	C	156.5121	28.2814563832
46	C	115.1005	67.9181263041
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Supporting Information: NMR-CoibamideA.D-MeAla.D-HIV-0013.log

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 Using  Gaussian 09:  AM64L-G09RevD.01 24-Apr-2013
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 Optimization incomplete.


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NMR-Shifts

NMR-CoibamideA.D-MeAla.D-HIV-0013-NMR.txt

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22	C	1.6745	176.482608779
24	C	106.9472	75.7219701755
27	C	152.2443	32.3663354965
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33	C	169.7236	15.6362104941
37	C	7.4967	170.909952334
39	C	131.4696	52.2506173548
42	C	156.4444	28.3462547139
46	C	114.4651	68.5262926166
50	C	127.2722	56.2681138613
54	C	129.0032	54.6113057294
56	C	3.1054	175.113038152
59	C	154.2538	30.442964069
63	C	147.2054	37.1892647256
66	C	157.1458	27.6749172075
68	C	166.5453	18.6782863378
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87	C	166.7436	18.4884856142
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190	C	50.0764	130.155247995
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5	H	29.2250	2.41866481866
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9	H	29.0420	2.58775698776
11	H	28.6154	2.98193578194
13	H	29.7551	1.92885192885
15	H	31.2965	0.504596904597
16	H	30.3219	1.40512820513
17	H	30.9709	0.805451605452
19	H	31.2252	0.570478170478
20	H	30.7307	1.0273966274
21	H	31.0240	0.756387156387
25	H	26.4489	4.98378378378
28	H	29.4715	2.1908985909
30	H	30.5383	1.20517440517
31	H	30.7930	0.969831369831
32	H	30.4572	1.28011088011
34	H	30.5611	1.18410718411
35	H	30.8296	0.936012936013
36	H	30.3951	1.33749133749
40	H	24.8927	6.42171402171
43	H	28.6688	2.93259413259
44	H	29.3795	2.27590667591
45	H	28.8620	2.75407715408
47	H	28.1010	3.45724185724
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52	H	29.1929	2.44832524833
53	H	28.0724	3.48366828367
55	H	26.3795	5.04790944791
60	H	28.6848	2.91781011781
61	H	28.1994	3.36632016632
62	H	28.2535	3.31633171633
64	H	29.7104	1.97015477015
65	H	30.4175	1.31679371679
67	H	30.0582	1.64878724879
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70	H	30.5520	1.19251559252
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73	H	31.0602	0.722938322938
74	H	30.6599	1.09281589282
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79	H	25.2046	6.13351813352
82	H	28.7411	2.86578886579

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99	H	27.6707	3.85483945484
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103	H	28.7569	2.85118965119
108	H	26.3908	5.03746823747
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114	H	30.9398	0.834188034188
116	H	28.9414	2.68071148071
117	H	28.6475	2.95227535228
118	H	28.7322	2.87401247401
121	H	27.0813	4.39944559945
123	H	21.4838	9.57154077154
127	H	27.1774	4.31064911065
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132	H	29.8818	1.81178101178
134	H	30.2321	1.4881034881
135	H	30.3870	1.34497574498
136	H	30.8630	0.905151305151
138	H	30.8974	0.873365673366
139	H	30.5101	1.23123123123
140	H	30.6200	1.12968352968
145	H	27.0900	4.39140679141
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149	H	28.7701	2.83899283899
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152	H	30.5729	1.1732039732
153	H	30.5455	1.19852159852
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163	H	29.3436	2.30907830908
164	H	27.8929	3.64952644953
166	H	28.0403	3.51332871333
168	H	30.3911	1.34118734119
169	H	29.8927	1.80170940171
171	H	30.7874	0.975005775006
172	H	30.8132	0.951166551167
173	H	30.5086	1.23261723262
175	H	31.4054	0.403973203973
176	H	30.6744	1.07941787942
177	H	30.7697	0.991360591361
179	H	28.8027	2.80887040887
180	H	28.7074	2.89692769693
181	H	29.2869	2.36146916147
185	H	28.4437	3.14058674059
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193	H	24.6366	6.65835065835
194	H	23.9248	7.31605451605
195	H	23.3732	7.82573342573
196	H	24.7304	6.57167937168
199	H	27.9170	3.62725802726
200	H	28.1310	3.42952182952
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Supporting Information: NMR-CoibamideA.D-MeAla.D-HIV-0014.log

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Using Gaussian 09: AM64L-G09RevD.01 24-Apr-2013

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#mPW1PW91/6-311+G(2d,p) scf=(maxcycle=300,direct,tight,xqc,vshift=200) NMR density=current SCRF=(PCM,SOLVENT=Chloroform)

Pointgroup= C1 Stoichiometry= C65H110N10O16 C1[X(C65H110N10O16)] #Atoms= 201

Charge = 0 Multiplicity = 1

SCF Energy= -4294.55625667

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Optimization incomplete.

Atomic Type	Coordinates (Angstroms) X	Y	Z
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H	7.100479	1.404838	3.429456
C	4.768871	-0.655852	4.705258
H	4.208310	0.114655	5.247656
H	4.210036	-0.884618	3.792167
H	4.763297	-1.539389	5.349914
C	7.049775	-1.217306	3.882346
H	8.012684	-0.717218	3.702978
C	7.348657	-2.386801	4.866066
H	6.444252	-2.991232	5.009405
C	7.807888	-1.876929	6.238334
H	8.698366	-1.245427	6.147898
H	7.025070	-1.293830	6.733039
H	8.054161	-2.713870	6.900857
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C	6.560019	-1.782760	2.532924
O	5.549749	-2.456446	2.366281
C	7.093527	-1.936228	0.232909
H	6.802328	-2.988005	0.324604
O	7.450494	-1.468265	1.546342
C	8.339044	-1.827029	-0.679376
H	8.060963	-2.081578	-1.708599
C	9.416530	-2.821280	-0.232348
H	9.772542	-2.602999	0.780047
H	9.027055	-3.844751	-0.242356
H	10.278749	-2.787373	-0.906849
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C	2.008652	-4.874280	0.249940
H	2.971316	-4.352388	0.296060
C	2.024501	-5.787636	-0.977211
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H	2.796925	-6.557927	-0.877408
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H	-5.793788	-5.270893	-1.977678
H	-4.607508	-6.588342	-1.941397
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H	-0.418793	2.109241	-6.004617
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H	-2.213250	7.422313	3.093180
H	-1.820902	5.820031	3.730603
N	-4.191986	3.517290	0.496977
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C	-6.098383	2.383637	1.721114
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C	5.346443	7.782425	-0.659217
H	6.315513	8.249441	-0.859937
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NMR-Shifts

NMR-CoibamideA.D-MeAla.D-HIV-0014-NMR.txt

Atom	Type	Isotropic	Scaled Shift
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6	C	149.6222	34.8760504604
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12	C	153.8932	30.7881085013
14	C	166.3194	18.8945041061
18	C	165.3114	19.8593005226
22	C	0.1168	177.97354467
24	C	107.7657	74.9385516568
27	C	152.9228	31.71691648
29	C	164.6525	20.4899596087
33	C	170.1925	15.1874078753
37	C	6.9915	171.39349911
39	C	130.4959	53.1825838933
42	C	157.4844	27.3508298398
46	C	114.2306	68.750741783
50	C	127.8475	55.7174716208
54	C	129.0443	54.5719673041
56	C	3.2051	175.017611363
59	C	154.9866	29.7415723884
63	C	147.8864	36.5374528609
66	C	157.2663	27.5595819216
68	C	166.4858	18.7352361263
72	C	162.7399	22.3205842378
76	C	2.7608	175.442868355
78	C	126.4380	57.0665594671
81	C	154.2552	30.441624074
85	C	114.8643	68.1442026072
87	C	166.7507	18.4816899252
92	C	128.3866	55.2014778231
94	C	7.8068	170.613143437
97	C	114.2959	68.6882405865
100	C	128.0589	55.5151323724
105	C	4.4715	173.805490151
107	C	127.6442	55.9120580409
109	C	2.1464	176.030934742
111	C	170.5634	14.8324049082
115	C	157.2811	27.5454162599
120	C	127.0363	56.4939030226
124	C	8.6410	169.814697831
126	C	114.7374	68.2656635847
128	C	143.5798	40.6594689791
131	C	156.7175	28.0848599705
133	C	165.3016	19.8686804878
137	C	162.8828	22.1838090316
142	C	0.1692	177.92339057
144	C	133.3234	50.4762725167
146	C	148.6239	35.8315626256
150	C	166.0106	19.1900687226
156	C	11.9101	166.685713739
158	C	112.3455	70.5550450813
161	C	146.3822	37.977181799
165	C	147.6325	36.7804705297
167	C	151.9312	32.6660158119
170	C	172.5153	12.9641647045
174	C	163.9478	21.1644556749
178	C	156.7080	28.0939527939
182	C	9.0924	169.38264515
184	C	145.8478	38.4886770421
187	C	24.2004	154.922184575
188	C	74.7698	106.520224353
189	C	53.7961	126.594976933
190	C	50.0609	130.170083654
191	C	45.8939	134.158483126
192	C	62.9633	117.820689523
198	C	131.8102	51.9246157086
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8	H	29.6879	1.99094479094
9	H	29.2482	2.39722799723
11	H	28.6669	2.93434973435
13	H	29.6665	2.01071841072
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16	H	30.3037	1.42194502195
17	H	30.9362	0.837514437514
19	H	31.0972	0.68875028875
20	H	30.5841	1.16285516286
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25	H	26.3051	5.11665511666
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44	H	29.4669	2.19514899515
45	H	28.9016	2.71748671749
47	H	28.1916	3.37352737353
48	H	27.2697	4.22536382536
51	H	28.3735	3.20545160545
52	H	29.1432	2.49424809425
53	H	28.0567	3.49817509818
55	H	26.3723	5.05456225456
60	H	28.8769	2.74030954031
61	H	28.4235	3.15925155925
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64	H	29.6919	1.98724878725
65	H	30.4321	1.3033033033
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69	H	31.2557	0.542296142296
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73	H	31.0463	0.735781935782
74	H	30.6667	1.08653268653
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88	H	30.6393	1.11185031185
89	H	30.8480	0.919011319011
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93	H	26.1574	5.25313005313
98	H	28.3141	3.26033726034
99	H	27.6763	3.84966504967

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103	H	28.8063	2.80554400554
108	H	26.3902	5.03802263802
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114	H	30.9943	0.78382998383
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117	H	28.7323	2.87392007392
118	H	28.7640	2.84462924463
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132	H	29.9022	1.79293139293
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135	H	30.4654	1.27253407253
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139	H	30.4906	1.24924924925
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145	H	27.0190	4.45701085701
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159	H	28.8492	2.7659043659
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166	H	28.0016	3.54908754909
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169	H	29.9552	1.74395934396
171	H	30.7476	1.01178101178
172	H	30.8053	0.958466158466
173	H	30.4718	1.26662046662
175	H	31.3798	0.427627627628
176	H	30.6519	1.10020790021
177	H	30.8089	0.95513975514
179	H	28.8135	2.79889119889
180	H	28.7434	2.86366366366
181	H	29.2891	2.35943635944
185	H	28.5493	3.04301224301
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193	H	24.6825	6.61593901594
194	H	23.9320	7.3094017094
195	H	23.4141	7.78794178794
196	H	24.7068	6.59348579349
199	H	27.9376	3.60822360822
200	H	28.1383	3.42277662278
201	H	28.1034	3.45502425502

Supporting Information: NMR-CoibamideA.D-MeAla.D-HIV-0015.log

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Using Gaussian 09: AM64L-G09RevD.01 24-Apr-2013

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Pointgroup= C1 Stoichiometry= C65H110N10O16 C1[X(C65H110N10O16)] #Atoms= 201

Charge = 0 Multiplicity = 1

SCF Energy= -4294.55330714

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Optimization incomplete.

Atomic Type	Coordinates (Angstroms) X	Y	Z
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H	5.535086	-1.135127	4.534412
C	3.707156	-3.834197	3.703747
H	2.856721	-3.611190	4.358855
H	3.416479	-3.553591	2.686780
H	3.837369	-4.919349	3.743068
C	6.168067	-3.499086	3.493314
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C	6.599448	-5.359990	5.198300
H	7.273301	-4.709616	5.766440
H	5.601082	-5.285623	5.640103
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C	7.981489	-5.259395	3.125193
H	8.737203	-4.603979	3.571329
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H	7.997216	-5.109174	2.041148
C	6.143122	-3.178163	1.984841
O	5.366561	-3.655103	1.165694
C	7.175825	-1.880155	0.304458
H	7.065441	-2.767019	-0.329330
O	7.149546	-2.308252	1.676772
C	8.546438	-1.224052	0.011588
H	8.525944	-0.779438	-0.990981
C	9.656192	-2.281290	0.029765
H	9.752275	-2.747644	1.016111
H	9.451402	-3.070931	-0.700871
H	10.622295	-1.833875	-0.227090
C	8.898201	-0.108123	1.002868
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H	0.331298	-4.050070	-1.412513
C	2.449583	-4.397992	-1.159925
H	3.324731	-3.861695	-0.776585
C	2.725691	-4.774922	-2.616278
H	1.856778	-5.261044	-3.072408
H	2.978804	-3.895137	-3.215153
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H	-4.165764	-4.894948	-1.584925
C	-5.937858	-6.813553	-1.496465
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O	-6.153309	-5.408518	-1.544569
C	-6.275602	-2.767835	0.199762
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C	-0.515184	1.134339	-4.101480
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C	-9.608824	-2.759065	-0.402368
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H	-2.334776	-2.016529	0.147096
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H	5.295813	5.019079	-0.193242

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NMR-Shifts
NMR-CoibamideA.D-MeAla.D-HIV-0015-NMR.txt

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12	C	152.9750	31.6669538085
14	C	166.0729	19.1304389441
18	C	165.1698	19.9948314478
22	C	-1.0140	179.055877792
24	C	109.1858	73.579318134
27	C	152.5083	32.1136507207
29	C	164.1598	20.9615421428
33	C	170.2766	15.10691246
37	C	6.3194	172.036792435
39	C	128.2685	55.3145159747
42	C	157.3346	27.4942093072
46	C	112.9237	70.0016271368
50	C	126.8217	56.6993051169
54	C	129.7352	53.9106797603
56	C	5.3143	172.998813147
59	C	151.8621	32.7321541377
63	C	147.7545	36.6636995348
66	C	157.9795	26.8769501713
68	C	166.5053	18.7165719099
72	C	162.3391	22.7042056701
76	C	3.1378	175.082026838
78	C	126.4577	57.0477038228
81	C	153.8978	30.7837056605
85	C	115.9599	67.0955607879
87	C	167.0775	18.1688968012
92	C	124.3063	59.1068933173
94	C	9.0756	169.39872509
97	C	111.6385	71.2317425678
100	C	127.1611	56.3744520377
105	C	6.9983	171.386990563
107	C	127.5987	55.9556078792
109	C	2.7362	175.466413982
111	C	169.9565	15.4132927506
115	C	157.3047	27.5228277724
120	C	127.1021	56.4309232566
124	C	8.3341	170.108443883
126	C	114.7229	68.2795421046
128	C	143.6514	40.5909378051
131	C	156.7143	28.0879228163
133	C	165.0529	20.1067210322
137	C	162.7698	22.2919657727
142	C	0.7303	177.386339708
144	C	133.6748	50.139933766
146	C	148.1672	36.2686881449
150	C	165.7391	19.4499320431
156	C	13.0853	165.560883631
158	C	113.4251	69.5217174908
161	C	145.9149	38.4244529949
165	C	149.5131	34.9804743582
167	C	150.8910	33.6616321139
170	C	172.9756	12.5235934838
174	C	164.0963	21.0223204885
178	C	153.1160	31.5319971669
182	C	8.3889	170.055992649
184	C	146.5448	37.8215509485
187	C	23.8841	155.224927736
188	C	74.3311	106.940121365
189	C	51.1781	129.100767626
190	C	51.9492	128.36271751
191	C	46.1596	133.904171213
192	C	62.5907	118.177319627
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9	H	29.3075	2.34243474243
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69	H	31.3583	0.447493647494
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73	H	31.1530	0.637191037191
74	H	30.6512	1.10085470085
75	H	30.8163	0.948302148302
79	H	25.7062	5.67003927004
82	H	28.6721	2.92954492954
83	H	29.3637	2.29050589051
84	H	28.6103	2.98664818665
86	H	25.9740	5.42259182259
88	H	30.7889	0.97361977362
89	H	30.7950	0.967983367983
90	H	30.6628	1.09013629014
93	H	26.7824	4.67562947563
98	H	27.6834	3.8431046431
99	H	28.7364	2.87013167013
101	H	28.6136	2.9835989836
102	H	28.1839	3.38064218064
103	H	28.6906	2.91245091245
108	H	26.3267	5.0966966967
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113	H	29.8875	1.80651420651
114	H	30.9689	0.8072996073
116	H	28.9906	2.63525063525
117	H	28.8408	2.77366597367

118	H	29.0094	2.61787941788
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123	H	22.2962	8.82088242088
127	H	27.4333	4.0741972742
129	H	29.8048	1.88292908293
130	H	28.5140	3.07562947563
132	H	29.8357	1.85437745438
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135	H	30.3586	1.37121737122
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138	H	30.7226	1.03488103488
139	H	30.5603	1.18484638485
140	H	30.4756	1.26310926311
145	H	26.9938	4.4802956803
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148	H	29.0193	2.60873180873
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151	H	30.2595	1.46278586279
152	H	30.5358	1.20748440748
153	H	30.3253	1.40198660199
155	H	25.3675	5.982998383
159	H	28.4516	3.13328713329
162	H	28.4420	3.14215754216
163	H	28.8317	2.78207438207
164	H	28.2528	3.31697851698
166	H	28.0495	3.50482790483
168	H	30.3217	1.40531300531
169	H	29.7707	1.91443751444
171	H	30.7289	1.02905982906
172	H	30.8132	0.951166551167
173	H	30.6955	1.05992145992
175	H	31.3094	0.492677292677
176	H	30.8236	0.941556941557
177	H	30.5518	1.1927003927
179	H	28.7752	2.83428043428
180	H	29.3635	2.29069069069
181	H	29.0710	2.56096096096
185	H	28.6619	2.93896973897
186	H	28.0598	3.49531069531
193	H	24.6864	6.61233541234
194	H	23.8708	7.36595056595
195	H	23.7917	7.43903903904
196	H	24.4422	6.83797643798
199	H	27.8967	3.64601524602
200	H	28.1191	3.44051744052
201	H	28.1433	3.41815661816

Supporting Information: NMR-CoibamideA.D-MeAla.D-HIV-0016.log

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Using Gaussian 09: AM64L-G09RevD.01 24-Apr-2013

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#mPW1PW91/6-311+G(2d,p) scf=(maxcycle=300,direct,tight,xqc,vshift=200) NMR density=current SCRF=(PCM,SOLVENT=Chloroform)

Pointgroup= C1 Stoichiometry= C65H110N10O16 C1[X(C65H110N10O16)] #Atoms= 201

Charge = 0 Multiplicity = 1

SCF Energy= -4294.55442567

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Optimization incomplete.

Atomic Coordinates (Angstroms)

Type	X	Y	Z
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H	4.313875	-0.844982	4.969758
H	6.022101	-0.793528	4.569695
C	3.833482	-3.298943	4.071415
H	3.068839	-2.932535	4.766549
H	3.499808	-3.051341	3.058862
H	3.840381	-4.387119	4.181134
C	6.287666	-3.275172	3.653004
H	7.179873	-2.728056	3.991208
C	6.562057	-4.777007	3.957273
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C	6.665099	-5.045314	5.464488
H	7.452679	-4.436519	5.921582
H	5.723591	-4.825759	5.977338
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C	7.859194	-5.253011	3.284749
H	8.718647	-4.660703	3.616952
H	8.058888	-6.302586	3.526778
H	7.795954	-5.179264	2.194554
C	6.162152	-3.063741	2.129942
O	5.311907	-3.569854	1.406847
C	7.135002	-1.953619	0.283254
H	6.972542	-2.890488	-0.261554
O	7.172886	-2.259751	1.687659
C	8.503778	-1.359639	-0.129518
H	8.445280	-0.999585	-1.163811
C	9.590665	-2.438989	-0.073140
H	9.725025	-2.822940	0.943746
H	9.333845	-3.281908	-0.723363
H	10.552206	-2.039026	-0.412277
C	8.925826	-0.173002	0.745472
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H	4.142004	0.600008	-0.747170
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C	2.520493	-1.263731	0.226289
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H	1.593397	-1.497714	0.754802
C	1.092571	-3.597103	-1.029182
H	0.874950	-3.454666	0.036591
H	0.215869	-4.124869	-1.424973
C	2.327579	-4.511245	-1.173536
H	3.210764	-3.996058	-0.779085

C	2.607992	-4.887491	-2.629321
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H	2.885460	-4.010799	-3.221998
H	3.440798	-5.596072	-2.693323
C	2.129167	-5.781797	-0.342114
H	1.262815	-6.354309	-0.690475
H	3.010659	-6.428798	-0.403550
H	1.972003	-5.534748	0.713280
C	-0.103641	-1.417804	-1.599899
O	-0.209747	-0.507740	-0.767126
C	-2.456308	-0.994099	-2.230216
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H	-1.557683	-2.376269	-4.373924
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H	-2.609324	-0.370856	-4.336420
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C	-3.695777	-1.917088	-2.193002
O	-4.225977	-2.285101	-3.246875
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C	-5.193625	-4.631026	-0.913071
H	-4.993779	-4.994920	0.101546
H	-4.317718	-4.864094	-1.531494
C	-6.136400	-6.737352	-1.414501
H	-6.047950	-7.070295	-0.375983
H	-7.013197	-7.214412	-1.860558
H	-5.249592	-7.033132	-1.983232
O	-6.316983	-5.327781	-1.470941
C	-6.357763	-2.673696	0.257590
O	-6.626035	-3.471894	1.157524
C	0.463884	2.193613	-3.864059
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C	-0.568384	1.077998	-4.140379
O	-0.520523	0.325048	-5.106650
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C	-1.992047	5.830697	4.108457
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H	-2.491836	6.689739	4.568542
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N	-4.201309	3.279445	1.216928
C	-4.624510	2.478691	2.280183
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H	-4.937656	2.918023	-0.695559
C	-7.056184	2.642220	2.907435
H	-6.797902	2.774014	3.964504
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H	-8.040252	2.164526	2.865509
N	-5.870887	0.494068	2.836580
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C	-6.505104	-0.694980	2.631909
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C	-9.690635	-2.583761	-0.332136
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C	1.909718	5.548614	1.174563
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C	4.747112	8.636696	0.574768
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H	3.894960	9.030970	0.011364
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NMR-Shifts

NMR-CoibamideA.D-MeAla.D-HIV-0016-NMR.txt

Atom	Type	Isotropic	Scaled Shift

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6	C	149.5350	34.9595130075
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12	C	154.9791	29.7487509332
14	C	166.3239	18.8901969793
18	C	165.7024	19.4850590555
22	C	0.1136	177.976607515
24	C	108.5366	74.2006929689
27	C	152.0971	32.5072264017
29	C	164.2341	20.8904266927
33	C	170.2074	15.1731464997
37	C	6.9446	171.438388943
39	C	127.9667	55.603380616
42	C	156.9905	27.8235609411
46	C	112.8707	70.0523555198
50	C	126.7982	56.7217978905
54	C	129.6731	53.970118111
56	C	5.5132	172.80843814
59	C	153.0391	31.6056011792
63	C	147.6124	36.7997090297
66	C	157.2783	27.5480962499
68	C	166.4808	18.7400218228
72	C	162.4535	22.5947089339
76	C	3.2270	174.996650012
78	C	126.5007	57.0065468328
81	C	154.0540	30.6342005015
85	C	115.9110	67.1423648998
87	C	167.0117	18.2318765673
92	C	124.1714	59.2360114091
94	C	9.0740	169.400256513
97	C	111.6676	71.2038898141
100	C	127.0837	56.4485346197
105	C	7.0219	171.364402075
107	C	127.6793	55.8784624514
109	C	2.7573	175.446218343
111	C	170.0148	15.3574915293
115	C	157.3092	27.5185206455
120	C	127.0166	56.5127586669
124	C	8.3003	170.140795191
126	C	115.0303	67.9853174831
128	C	143.3132	40.914642317
131	C	156.5699	28.2261337315
133	C	165.1234	20.0392427114
137	C	162.7427	22.3179042478
142	C	0.7118	177.404046785
144	C	133.7705	50.0483355348
146	C	148.3221	36.120427267
150	C	165.7732	19.4172935929
156	C	13.1253	165.522598059
158	C	113.4366	69.5107103888
161	C	146.0133	38.3302704876
165	C	149.8878	34.6218342618
167	C	150.9827	33.5738624399
170	C	173.0524	12.4500851854
174	C	164.2419	20.8829610061
178	C	153.1249	31.5234786271
182	C	8.1480	170.286567507
184	C	146.5395	37.8266237868
187	C	23.9636	155.148835161
188	C	74.2604	107.007791114
189	C	51.3099	128.974616666
190	C	51.7821	128.522655487
191	C	46.0715	133.988495186
192	C	62.7210	118.052604376
198	C	131.7409	51.9909454622
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5	H	29.3731	2.28182028182
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8	H	29.6989	1.98078078078
9	H	29.3122	2.33809193809
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44	H	28.6946	2.90875490875
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52	H	28.5961	2.99976899977
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62	H	28.5073	3.08182028182
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65	H	30.5026	1.23816123816
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70	H	30.5932	1.15444675445
71	H	30.6985	1.05714945715
73	H	31.1367	0.652252252252
74	H	30.6218	1.12802032802
75	H	30.8532	0.914206514207
79	H	25.7270	5.65082005082
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83	H	29.3683	2.28625548626
84	H	28.6111	2.98590898591
86	H	25.9836	5.41372141372
88	H	30.7934	0.969461769462
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90	H	30.6648	1.08828828829
93	H	26.6997	4.75204435204
98	H	27.6342	3.88856548857
99	H	28.7386	2.8680988681
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102	H	28.1976	3.36798336798
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117	H	28.8501	2.76507276507
118	H	29.0064	2.62065142065
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123	H	22.2651	8.84961884962
127	H	27.4474	4.06116886117
129	H	29.8418	1.84874104874
130	H	28.5662	3.0273966274
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135	H	30.3512	1.37805497805

136	H	30.9289	0.84425964426
138	H	30.7632	0.997366597367
139	H	30.5283	1.21441441441
140	H	30.5278	1.21487641488
145	H	27.0049	4.47003927004
147	H	28.4289	3.15426195426
148	H	29.0427	2.58711018711
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151	H	30.2628	1.45973665974
152	H	30.4940	1.24610764611
153	H	30.3686	1.36197736198
155	H	25.3503	5.99889119889
159	H	28.4505	3.1343035343
162	H	28.4062	3.17523677524
163	H	28.8465	2.7683991684
164	H	28.2819	3.29009009009
166	H	28.1145	3.44476784477
168	H	30.3114	1.41483021483
169	H	29.7693	1.91573111573
171	H	30.7702	0.990898590899
172	H	30.8551	0.912450912451
173	H	30.7848	0.977408177408
175	H	31.3020	0.499514899515
176	H	30.8183	0.946454146454
177	H	30.5532	1.19140679141
179	H	28.7270	2.87881727882
180	H	29.3478	2.3051975052
181	H	29.0854	2.54765534766
185	H	28.6633	2.93767613768
186	H	28.0668	3.48884268884
193	H	24.7267	6.5750981751
194	H	23.8683	7.36826056826
195	H	23.7712	7.45798105798
196	H	24.4024	6.87475167475
199	H	27.8616	3.67844767845
200	H	28.1372	3.42379302379
201	H	28.1490	3.41288981289

Supporting Information: NMR-CoibamideA.D-MeAla.D-HIV-0017.log

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Using Gaussian 09: AM64L-G09RevD.01 24-Apr-2013

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#mPW1PW91/6-311+G(2d,p) scf=(maxcycle=300,direct,tight,xqc,vshift=200) NMR density=current SCRF=(PCM,SOLVENT=Chloroform)

Pointgroup= C1 Stoichiometry= C65H110N10O16 C1[X(C65H110N10O16)] #Atoms= 201

Charge = 0 Multiplicity = 1

SCF Energy= -4294.55418341

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Optimization incomplete.

Atomic Type	Coordinates (Angstroms) X	Y	Z
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C	5.943740	-1.213210	4.449000
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H	6.996459	-1.162247	4.748127
C	4.050311	-2.648438	4.100289
H	3.469924	-2.092062	4.845440
H	3.833291	-2.212339	3.119841
H	3.664571	-3.671990	4.120503
C	6.333773	-3.471009	3.586239
H	7.380886	-3.278454	3.861976
C	6.104678	-4.991740	3.837659
H	5.112421	-5.284186	3.471821
C	6.186059	-5.345383	5.328657
H	7.150124	-5.046652	5.754320
H	5.392924	-4.854407	5.901196
H	6.071038	-6.424422	5.478579
C	7.134783	-5.840538	3.076009
H	8.156879	-5.590781	3.380573
H	6.976561	-6.907115	3.269249
H	7.056956	-5.692650	1.994444
C	6.184412	-3.151091	2.084151
O	5.289776	-3.568768	1.357591
C	7.158766	-1.975548	0.281628
H	7.008038	-2.889676	-0.303802
O	7.209619	-2.352437	1.667745
C	8.519738	-1.345774	-0.105842
H	8.452755	-0.932598	-1.119591
C	9.619906	-2.413003	-0.111127
H	9.764241	-2.847885	0.883606
H	9.370092	-3.223588	-0.803751
H	10.574728	-1.983753	-0.432958
C	8.931350	-0.201561	0.828922
H	9.057429	-0.544325	1.861187
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H	3.994841	1.794147	-2.845947
H	5.184895	0.692864	-3.554156
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H	1.427805	-2.344455	-2.774356
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C	1.120481	-3.572765	-1.027040
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H	0.248184	-4.103466	-1.428547
C	2.361466	-4.478468	-1.173869
H	3.241068	-3.958704	-0.777248
C	2.645162	-4.847608	-2.630785
H	1.773146	-5.317044	-3.098469
H	2.916617	-3.967076	-3.220366
H	3.483063	-5.550158	-2.696864
C	2.171225	-5.753352	-0.347097
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H	3.057112	-6.394367	-0.410528
H	2.012048	-5.511317	0.709080
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C	-3.900120	0.882913	-3.200432
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C	-5.134620	-4.658795	-0.910417
H	-4.932607	-5.017045	0.105737
H	-4.254465	-4.882561	-1.526175
C	-6.048824	-6.778656	-1.408069
H	-5.959182	-7.107636	-0.368364
H	-6.917870	-7.268201	-1.855444
H	-5.156472	-7.064297	-1.973286
O	-6.247645	-5.371613	-1.468779
C	-6.324609	-2.711976	0.252392
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H	-4.968694	2.897981	-0.723121
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H	-8.065658	2.112107	2.838886
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C	-9.401847	-1.009482	3.167827
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H	-10.303016	-1.545393	3.485757
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H	-2.373711	-2.014438	0.158947
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C	3.468259	4.082924	0.268834
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NMR-Shifts

NMR-CoibamideA.D-MeAla.D-HIV-0017-NMR.txt

Atom	Type	Isotropic	Scaled Shift
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6	C	149.0360	35.4371255192
10	C	108.6273	74.1138804342
12	C	154.7919	29.9279274106
14	C	166.7316	18.4999712858
18	C	165.8660	19.3284710657
22	C	1.4171	176.728976435
24	C	107.4025	75.2861846513
27	C	151.8153	32.776948257

29	C	164.2530	20.8723367599
33	C	170.1169	15.2597676066
37	C	6.8058	171.571239878
39	C	128.0993	55.4764639446
42	C	157.1437	27.6769272
46	C	112.9088	70.0158885124
50	C	126.7930	56.7267750148
54	C	129.6679	53.9750952354
56	C	5.4915	172.829208063
59	C	153.2126	31.4395375103
63	C	147.6431	36.7703248531
66	C	157.4358	27.3973468099
68	C	166.4553	18.764428875
72	C	162.3704	22.6742472099
76	C	3.1995	175.022971343
78	C	126.4702	57.0357395815
81	C	153.9522	30.7316372825
85	C	115.9148	67.1387277704
87	C	167.0635	18.1822967515
92	C	124.2039	59.2049043818
94	C	9.0631	169.410689332
97	C	111.6210	71.2484925056
100	C	127.1340	56.4003905128
105	C	6.9546	171.42881755
107	C	127.6439	55.9123451827
109	C	2.7360	175.46660541
111	C	169.9175	15.4506211834
115	C	157.2464	27.5786289937
120	C	127.0090	56.5200329256
124	C	8.2961	170.144815176
126	C	114.8568	68.151381152
128	C	143.4223	40.8102184192
131	C	156.6942	28.1071613163
133	C	165.0850	20.0759968606
137	C	162.7412	22.3193399567
142	C	0.6617	177.451999464
144	C	133.6970	50.1186852735
146	C	148.2456	36.1936484236
150	C	165.7412	19.4479220506
156	C	13.0484	165.596202071
158	C	113.5073	69.4430406401
161	C	146.0487	38.2963877563
165	C	149.9793	34.5342560156
167	C	150.9983	33.5589310668
170	C	173.0441	12.4580294416
174	C	164.1876	20.9349336702
178	C	153.1433	31.5058672639
182	C	8.2698	170.16998794
184	C	146.6079	37.7611554586
187	C	23.9882	155.125289535
188	C	74.2324	107.034591014
189	C	51.1425	129.134841785
190	C	51.7346	128.568119604
191	C	46.1686	133.895556959
192	C	62.7344	118.039778709
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7	H	29.7143	1.96655116655
8	H	30.1362	1.57671517672
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52	H	28.5817	3.01307461307
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70	H	30.6247	1.12534072534
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73	H	31.1447	0.64486024486
74	H	30.6388	1.11231231231
75	H	30.8257	0.939616539617
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82	H	28.6839	2.91864171864
83	H	29.3718	2.28302148302
84	H	28.6102	2.98674058674
86	H	25.9896	5.40817740818
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89	H	30.7889	0.97361977362
90	H	30.6644	1.08865788866
93	H	26.7357	4.71878031878
98	H	27.6586	3.86601986602
99	H	28.7400	2.86680526681
101	H	28.6028	2.99357819358
102	H	28.1876	3.37722337722
103	H	28.6854	2.91725571726
108	H	26.3234	5.09974589975
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114	H	30.9577	0.817648417648
116	H	28.9774	2.64744744745
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118	H	29.0106	2.61677061677
121	H	27.3121	4.18618618619
123	H	22.2958	8.82125202125
127	H	27.4164	4.08981288981
129	H	29.8213	1.86768306768
130	H	28.5353	3.05594825595
132	H	29.8405	1.84994224994
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139	H	30.5520	1.19251559252
140	H	30.4839	1.25544005544
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147	H	28.4207	3.16183876184
148	H	29.0273	2.60133980134
149	H	28.7150	2.88990528991
151	H	30.2464	1.47489027489

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166	H	28.0969	3.46103026103
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173	H	30.7387	1.02000462
175	H	31.3017	0.499792099792
176	H	30.8296	0.936012936013
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179	H	28.7540	2.85386925387
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181	H	29.0934	2.54026334026
185	H	28.6587	2.94192654193
186	H	28.0422	3.51157311157
193	H	24.7158	6.58516978517
194	H	23.8525	7.38285978286
195	H	23.7943	7.43663663664
196	H	24.4033	6.87392007392
199	H	27.8842	3.65756525757
200	H	28.1247	3.43534303534
201	H	28.1449	3.41667821668

Supporting Information: NMR-CoibamideA.D-MeAla.D-HIV-0018.log

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Using Gaussian 09: AM64L-G09RevD.01 24-Apr-2013

==========

#mPW1PW91/6-311+G(2d,p) scf=(maxcycle=300,direct,tight,xqc,vshift=200) NMR density=current SCRF=(PCM,SOLVENT=Chloroform)

Pointgroup= C1 Stoichiometry= C65H110N10O16 C1[X(C65H110N10O16)] #Atoms= 201

Charge = 0 Multiplicity = 1

SCF Energy= -4294.55472903

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Optimization incomplete.

Atomic Type	Coordinates (Angstroms) X	Y	Z
N	5.868578	-1.956108	4.561541
C	6.322253	-0.585877	4.312617
H	6.142571	-0.260876	3.284149
H	5.807765	0.112088	4.982843
H	7.392295	-0.486811	4.525636
C	4.424811	-2.057791	4.343133
H	3.894967	-1.392220	5.034481
H	4.128634	-1.780863	3.325712
H	4.055814	-3.066325	4.552233
C	6.671901	-2.952858	3.795118
H	7.734631	-2.706116	3.933835
C	6.504500	-4.407494	4.328304
H	5.492145	-4.769803	4.109341
C	6.722343	-4.492071	5.844894
H	7.710734	-4.111677	6.124528
H	5.967745	-3.917628	6.390991
H	6.650101	-5.529224	6.190192
C	7.487632	-5.366178	3.638217
H	8.525173	-5.056800	3.803976
H	7.373269	-6.384005	4.026871
H	7.314948	-5.410721	2.558445
C	6.378312	-2.902904	2.280888
O	5.436613	-3.457197	1.724676
C	7.143167	-2.033838	0.219230
H	6.953649	-3.035206	-0.181807
O	7.335110	-2.171027	1.638849
C	8.449033	-1.473500	-0.395533
H	8.290732	-1.261903	-1.459371
C	9.575810	-2.507652	-0.293925
H	9.816840	-2.741255	0.748545
H	9.292319	-3.439546	-0.794476
H	10.486936	-2.136174	-0.774851
C	8.899260	-0.167032	0.269344
H	9.119379	-0.306345	1.332949
H	9.807329	0.214054	-0.210559
H	8.131619	0.607859	0.178281
C	5.943822	-1.110052	-0.118267
O	5.492848	-0.358045	0.753387
C	4.321610	-0.168441	-1.729069
H	4.102527	0.443122	-0.852286
N	5.400353	-1.147735	-1.400203
C	5.824339	-2.052375	-2.466761
H	4.953514	-2.565401	-2.882113
H	6.316020	-1.470993	-3.251033
H	6.523454	-2.814869	-2.128441
C	4.749551	0.825783	-2.829788
H	3.925536	1.515430	-3.047284
H	5.003624	0.307624	-3.761671
O	5.888016	1.585845	-2.395637
C	6.251535	2.571747	-3.353176
H	7.125163	3.110463	-2.976984
H	6.512951	2.102125	-4.306256
H	5.435175	3.286579	-3.494948
C	1.125374	-2.384441	-1.650025
H	1.277740	-2.586060	-2.710915
C	3.033896	-0.908753	-2.165932
O	2.741351	-0.985326	-3.366418
N	2.282797	-1.578580	-1.198338
C	2.490427	-1.399109	0.236561
H	3.245916	-2.112919	0.571092
H	2.813118	-0.383798	0.467037
H	1.565359	-1.573596	0.791128
C	0.974677	-3.728334	-0.906666
H	0.784780	-3.543238	0.157873
H	0.075447	-4.245423	-1.264386
C	2.180180	-4.681992	-1.045088
H	3.083320	-4.184407	-0.672938
C	2.432629	-5.100443	-2.494373
H	1.536827	-5.544746	-2.941076
H	2.734718	-4.247558	-3.109293
H	3.239726	-5.839013	-2.550043
C	1.952770	-5.926973	-0.182487
H	1.066777	-6.481682	-0.509652
H	2.814227	-6.601006	-0.236850
H	1.812742	-5.651440	0.868180
C	-0.182966	-1.545963	-1.538827
O	-0.258341	-0.606541	-0.735808
C	-2.533125	-1.091465	-2.159068
H	-2.466917	-0.514887	-1.237300
N	-1.291377	-1.904931	-2.308518
C	-1.309446	-2.966046	-3.316788
H	-0.330761	-3.401716	-3.505146
H	-1.969153	-3.766254	-2.969439
H	-1.684178	-2.567266	-4.262456
C	-2.674929	-0.050750	-3.303865

H	-2.683300	-0.538635	-4.284558
C	-3.948132	0.788137	-3.185310
H	-4.004555	1.269483	-2.204209
H	-3.942971	1.593260	-3.928750
H	-4.852291	0.194171	-3.338541
O	-1.593545	0.908104	-3.200205
C	-5.566295	-3.099723	-0.771110
H	-6.129252	-2.929224	-1.695898
C	-3.792766	-1.984462	-2.081406
O	-4.336384	-2.378998	-3.118704
N	-4.269354	-2.372181	-0.834317
C	-5.329351	-4.621537	-0.678864
H	-5.143115	-4.940896	0.353187
H	-4.452447	-4.896077	-1.278434
C	-6.299580	-6.734834	-1.090273
H	-6.224802	-7.020555	-0.036691
H	-7.179479	-7.219275	-1.521762
H	-5.412484	-7.069371	-1.636562
O	-6.458695	-5.326758	-1.213364
C	-6.466432	-2.592720	0.393931
O	-6.760203	-3.346334	1.323804
C	0.422358	2.003542	-3.925088
H	1.359435	1.461488	-3.758433
C	-0.627746	0.894776	-4.158628
O	-0.606557	0.120608	-5.108958
C	0.607548	2.828677	-5.198025
H	-0.341008	3.225816	-5.573182
H	1.024971	2.207220	-5.998349
H	1.292138	3.666086	-5.028252
C	-0.946187	3.797125	-2.761874
H	-1.210778	4.069993	-3.783925
H	-1.819516	3.362523	-2.268955
H	-0.655788	4.708704	-2.232758
N	0.154989	2.843905	-2.724628
C	0.217677	2.986164	-0.191627
H	-0.248496	3.965605	-0.297874
N	-0.806785	1.990650	0.157417
H	-0.569545	1.015673	-0.066999
C	-2.098489	2.124952	0.559569
O	-2.801851	1.107246	0.533059
C	-2.690709	3.509534	0.962606
H	-2.551557	4.160012	0.090371
C	-1.973746	4.168603	2.155991
H	-0.959469	4.436892	1.850898
H	-1.833697	3.440054	2.962672
C	-2.643920	5.443226	2.710579
H	-3.675741	5.219872	3.004569
C	-2.672472	6.573736	1.680527
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H	-1.663232	6.818008	1.331598
C	-1.903815	5.911339	3.967260
H	-0.860706	6.161268	3.745041
H	-2.382235	6.800040	4.392574
H	-1.909946	5.130602	4.735191
N	-4.156901	3.330133	1.138209
C	-4.609723	2.577289	2.224212
O	-3.918296	2.384806	3.230367
C	-6.014181	1.934885	2.144157
H	-6.286457	1.739535	1.107961
C	-4.994138	3.693366	0.005542
H	-6.045434	3.764879	0.286819
H	-4.682369	4.666562	-0.383428
H	-4.881833	2.933800	-0.771441
C	-7.042223	2.833224	2.818210
H	-6.791286	2.998415	3.872463
H	-7.093728	3.814895	2.337861
H	-8.039132	2.382245	2.783557
N	-5.918268	0.652238	2.845740
H	-5.216571	0.617405	3.582410
C	-6.590725	-0.522790	2.686434
O	-6.298871	-1.445119	3.450655
C	-7.613858	-0.673156	1.525661
H	-7.924781	0.336698	1.235814
N	-6.917442	-1.264050	0.352608
C	-6.658352	-0.369456	-0.766534
H	-6.541162	-0.907428	-1.706366
H	-7.498210	0.320404	-0.891989
H	-5.747046	0.195962	-0.556935
C	-8.923565	-1.393936	1.968982
H	-8.715630	-2.420611	2.287110
C	-10.011054	-1.423947	0.865656
H	-10.120630	-0.429709	0.415623
H	-10.978197	-1.658548	1.329135
C	-9.795523	-2.454672	-0.232568
H	-9.564028	-3.438816	0.185760
H	-10.706924	-2.552137	-0.832279
H	-8.997572	-2.163952	-0.918148
C	-9.529594	-0.672960	3.191198
H	-9.764406	0.371207	2.957937
H	-10.455531	-1.163014	3.512041
H	-8.850671	-0.687370	4.048912
C	-3.560847	-2.152419	0.426734
H	-3.974976	-1.266464	0.912826
H	-3.692571	-3.021539	1.077582
H	-2.490893	-2.015574	0.271964
C	0.808927	2.492042	-1.541243
O	1.757408	1.701655	-1.554196
C	1.317922	3.029964	0.887012
H	0.873941	3.152535	1.882668
H	1.851556	2.071657	0.941207
C	4.140219	6.244847	0.198737
C	2.897822	6.512894	0.773317
C	1.987803	5.473704	1.005573
C	2.307031	4.153062	0.665338
C	3.558095	3.891035	0.095015
C	4.463263	4.929274	-0.136859
H	2.604624	7.518732	1.055934
H	1.030858	5.711432	1.463450
H	3.843240	2.875667	-0.177302
H	5.430133	4.704286	-0.581256
O	5.113169	7.164235	-0.082547
C	4.844174	8.514950	0.274584
H	5.717564	9.113723	-0.001141
H	3.984250	8.905323	-0.279604
H	4.698431	8.616180	1.355176

NMR-Shifts

NMR-CoibamideA.D-MeAla.D-HIV-0018-NMR.txt

Atom	Type	Isotropic	Scaled Shift
2	C	141.9084	42.2592316086
6	C	149.3052	35.1794636191
10	C	109.3230	73.4479986217
12	C	154.4985	30.2087520818
14	C	166.6570	18.5713738778
18	C	165.7755	19.4150921725
22	C	3.6854	174.557897356
24	C	106.4921	76.1575642719
27	C	153.4565	31.2060912345
29	C	164.8066	20.3424644423
33	C	170.2269	15.1544822834
37	C	8.4603	169.987652903
39	C	127.2503	56.289075212
42	C	157.9536	26.9017400793
46	C	113.8190	69.1447003197
50	C	126.9228	56.6025383334
54	C	129.5846	54.0548249392
56	C	5.0582	173.243936523

59	C	152.9910	31.6516395796
63	C	147.4785	36.9278699822
66	C	156.8033	28.0027374184
68	C	166.4861	18.7349489845
72	C	162.4802	22.5691533146
76	C	3.3788	174.851356266
78	C	126.2871	57.2109917877
81	C	154.0163	30.6702846532
85	C	115.8755	67.176343345
87	C	167.0302	18.2141694902
92	C	124.2012	59.2074886579
94	C	8.9793	169.490897605
97	C	111.7640	71.1116215854
100	C	127.0780	56.4539903138
105	C	6.2246	172.127529241
107	C	127.4749	56.0741017248
109	C	2.6127	175.584620686
111	C	170.0735	15.3013074523
115	C	157.3477	27.4816707824
120	C	126.8036	56.7166293382
124	C	8.4676	169.980665786
126	C	115.0454	67.9708646796
128	C	143.5763	40.6628189667
131	C	156.6355	28.1633453933
133	C	165.0943	20.0670954651
137	C	162.7645	22.297038611
142	C	0.7293	177.387296847
144	C	133.9105	49.9143360325
146	C	148.6568	35.8000727426
150	C	166.0104	19.1902601505
156	C	13.1344	165.513888091
158	C	113.3552	69.588621528
161	C	146.2052	38.1465954555
165	C	149.9687	34.5444016922
167	C	151.0510	33.5084898256
170	C	173.0473	12.4549665958
174	C	164.4090	20.7230230288
178	C	153.0399	31.6048354678
182	C	8.1256	170.308007427
184	C	146.5376	37.8284423515
187	C	24.1268	154.992630027
188	C	74.4046	106.869771627
189	C	51.7696	128.534619729
190	C	51.2312	129.049943529
191	C	46.4595	133.617125136
192	C	63.2582	117.538429143
198	C	131.7188	52.0120982408
3	H	28.7286	2.87733887734
4	H	29.4773	2.18553938554
5	H	29.4679	2.19422499422
7	H	29.7036	1.97643797644
8	H	30.0557	1.6510972511
9	H	29.3590	2.29484869485
11	H	28.7977	2.81349041349
13	H	29.7501	1.93347193347
15	H	31.2949	0.506075306075
16	H	30.2945	1.43044583045
17	H	30.9281	0.844998844999
19	H	31.2609	0.537491337491
20	H	30.6820	1.0723954724
21	H	30.9700	0.806283206283
25	H	26.4306	5.00069300069
28	H	29.5425	2.12529452529
30	H	30.6299	1.12053592054
31	H	30.7284	1.02952182952
32	H	30.5859	1.16119196119
34	H	30.8152	0.949318549319
35	H	30.9667	0.809332409332
36	H	30.6714	1.08218988219
40	H	24.8727	6.44019404019
43	H	29.2036	2.43843843844
44	H	29.1022	2.53213213213
45	H	28.5485	3.04375144375
47	H	27.9338	3.61173481173
48	H	27.6761	3.84984984985
51	H	28.0562	3.49863709864
52	H	28.4880	3.09965349965
53	H	28.5214	3.06879186879
55	H	26.2820	5.137999538
60	H	28.9929	2.63312543313
61	H	27.9892	3.56054516055
62	H	28.5619	3.03136983137
64	H	29.8210	1.86796026796
65	H	30.4707	1.26763686764
67	H	30.0206	1.68352968353
69	H	31.3517	0.453592053592
70	H	30.5723	1.17375837376
71	H	30.7275	1.03035343035
73	H	31.1253	0.662785862786
74	H	30.6205	1.12922152922
75	H	30.8696	0.899052899053
79	H	25.6918	5.68334488334
82	H	28.6447	2.95486255486
83	H	29.3333	2.3185955186
84	H	28.5889	3.00642180642
86	H	25.9574	5.43793023793
88	H	30.7738	0.987572187572
89	H	30.7979	0.965303765304
90	H	30.6728	1.0808962809
93	H	26.6203	4.82541002541
98	H	27.5596	3.9574959575
99	H	28.7168	2.88824208824
101	H	28.5545	3.03820743821
102	H	28.1768	3.3872025872
103	H	28.6608	2.93998613999
108	H	26.2920	5.12875952876
112	H	30.5532	1.19140679141
113	H	29.9065	1.78895818896
114	H	30.9876	0.790020790021
116	H	28.9864	2.63913143913
117	H	28.8518	2.7635019635
118	H	29.0058	2.62120582121
121	H	27.3287	4.17084777085
123	H	22.3193	8.79953799954
127	H	27.4016	4.10348810349
129	H	29.8731	1.81981981982
130	H	28.5320	3.058997459
132	H	29.8496	1.84153384153
134	H	30.5020	1.23871563872
135	H	30.3330	1.39487179487
136	H	30.9315	0.841857241857
138	H	30.7535	1.00632940633
139	H	30.5674	1.17828597829
140	H	30.4938	1.24629244629
145	H	27.0364	4.44093324093
147	H	28.4250	3.15786555787
148	H	29.0802	2.55246015246
149	H	28.6952	2.9082005082
151	H	30.2727	1.45058905059
152	H	30.4700	1.26828366828
153	H	30.4813	1.25784245784
155	H	25.2765	6.06708246708
159	H	28.5040	3.08486948487
162	H	28.5127	3.07683067683
163	H	28.9600	2.66352506353
164	H	28.1718	3.39182259182
166	H	28.1944	3.37094017094
168	H	30.3248	1.40244860245

169	H	29.7369	1.94566874567
171	H	30.8067	0.957172557173
172	H	30.8612	0.906814506815
173	H	30.7321	1.0261030261
175	H	31.3222	0.48085008085
176	H	30.7597	1.0006006006
177	H	30.5975	1.15047355047
179	H	28.6756	2.92631092631
180	H	29.3397	2.31268191268
181	H	29.0185	2.60947100947
185	H	28.6672	2.93407253407
186	H	27.9987	3.55176715177
193	H	24.7525	6.55125895126
194	H	23.8542	7.38128898129
195	H	23.7849	7.44532224532
196	H	24.3747	6.90034650035
199	H	27.8606	3.67937167937
200	H	28.1495	3.41242781243
201	H	28.1477	3.41409101409

Supporting Information: NMR-CoibamideA.D-MeAla.D-HIV-0019.log

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Using Gaussian 09: AM64L-G09RevD.01 24-Apr-2013

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#mPW1PW91/6-311+G(2d,p) scf=(maxcycle=300,direct,tight,xqc,vshift=200) NMR density=current SCRF=(PCM,SOLVENT=Chloroform)

Pointgroup= C1 Stoichiometry= C65H110N10O16 C1[X(C65H110N10O16)] #Atoms= 201

Charge = 0 Multiplicity = 1

SCF Energy= -4294.55458897

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Optimization incomplete.

Atomic Type	Coordinates (Angstroms) X	Y	Z
N	5.179908	-1.979348	4.688575
C	5.337274	-0.562168	4.352363
H	5.110362	-0.352887	3.303228
H	4.672191	0.050826	4.971188
H	6.357101	-0.221861	4.563161
C	3.797619	-2.401487	4.460765
H	3.123463	-1.828699	5.108369
H	3.469122	-2.246962	3.427907
H	3.645493	-3.452323	4.723613
C	6.206688	-2.823036	4.009309
H	7.184793	-2.360964	4.207482
C	6.294436	-4.269912	4.578018
H	5.384893	-4.826514	4.319508
C	6.442339	-4.276583	6.105280
H	7.324790	-3.708894	6.419729
H	5.565169	-3.842932	6.595449
H	6.548574	-5.300219	6.480585
C	7.478738	-5.034906	3.966899
H	8.426200	-4.521718	4.163816
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H	7.369694	-5.143830	2.883284
C	6.014604	-2.871274	2.479113
O	5.100078	-3.441494	1.895012
C	6.955240	-2.177941	0.422731
H	6.727694	-3.190220	0.069841
O	7.042473	-2.222800	1.858185
C	8.330286	-1.738252	-0.137141
H	8.248077	-1.576729	-1.218700
C	9.374208	-2.837204	0.090573
H	9.533460	-3.027352	1.157357
H	9.058202	-3.775063	-0.378372
H	10.336899	-2.554225	-0.348481
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H	8.979309	-0.520617	1.564605
H	9.791292	-0.138145	0.041287
H	8.128117	0.389552	0.302906
C	5.845449	-1.206394	-0.049593
O	5.442055	-0.325487	0.717819
C	4.288876	-0.378919	-1.780656
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H	5.164711	-0.005537	-3.759482
O	5.933751	1.330193	-2.381745
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C	0.996560	-2.454562	-1.842981
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O	2.778756	-1.172411	-3.495736
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H	2.724216	-0.599358	0.358010
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H	-0.158036	-4.268863	-1.543350
C	1.914898	-4.825705	-1.301938
H	2.834711	-4.391589	-0.893395
C	2.174031	-5.203838	-2.761146
H	1.265119	-5.582710	-3.240596
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H	-4.899973	0.453428	-3.304171
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C	-6.589841	-6.467240	-1.303435
H	-6.469256	-6.816726	-0.273554
H	-7.516057	-6.884480	-1.707511
H	-5.753267	-6.810500	-1.919545
O	-6.685478	-5.048650	-1.339059
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N	-3.912815	3.405709	1.243708
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H	-7.718209	2.507758	3.099314
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C	2.278461	5.344653	0.881507
C	2.541958	4.020406	0.508717
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NMR-Shifts

NMR-CoibamideA.D-MeAla.D-HIV-0019-NMR.txt

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12	C	152.8733	31.7642948755
14	C	166.2806	18.931641111
18	C	165.7276	19.4609391451
22	C	1.5897	176.563774192
24	C	107.2949	75.3891728402
27	C	152.6621	31.9664426961
29	C	164.6206	20.5204923525
33	C	170.4175	14.9720515324
37	C	7.4209	170.982503494
39	C	127.3080	56.2338482743
42	C	157.0395	27.7766611153
46	C	112.3271	70.5726564444
50	C	126.8715	56.6516395796
54	C	129.4088	54.2230900285
56	C	5.9891	172.352935546
59	C	154.0136	30.6728689293
63	C	147.1933	37.2008461111
66	C	155.9234	28.8449242903
68	C	166.6984	18.5317483106
72	C	162.5053	22.5451291181
76	C	3.2618	174.963341565
78	C	126.4268	57.0772794272
81	C	154.4073	30.2960431861
85	C	115.5939	67.4458737725

87	C	166.9481	18.2927506269
92	C	124.0247	59.3764237447
94	C	9.1224	169.353930971
97	C	111.7962	71.0808016999
100	C	126.8294	56.6919351442
105	C	6.2703	172.083787975
107	C	128.0082	55.563659335
109	C	2.4215	175.76762572
111	C	170.3033	15.0813568407
115	C	157.2825	27.5440762649
120	C	126.6536	56.8602002335
124	C	8.2356	170.202722104
126	C	114.9326	68.0788299929
128	C	143.3147	40.9132066081
131	C	156.0160	28.7562931909
133	C	165.1144	20.0478569651
137	C	162.6179	22.4373552327
142	C	0.6095	177.501962136
144	C	133.9587	49.8682019181
146	C	147.7640	36.6546067115
150	C	166.0841	19.1197189839
156	C	12.6836	165.945366489
158	C	113.1833	69.753153774
161	C	146.8476	37.5317291679
165	C	150.7136	33.8314286261
167	C	151.3288	33.2425965275
170	C	172.7044	12.7831696625
174	C	164.6766	20.4668925515
178	C	153.3610	31.2974980379
182	C	7.4079	170.994946304
184	C	146.4990	37.8653879286
187	C	24.0262	155.088918241
188	C	74.4586	106.818086104
189	C	52.2380	128.086295679
190	C	50.6992	129.559141637
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192	C	63.1746	117.618445989
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4	H	29.5626	2.10672210672
5	H	29.4002	2.25677985678
7	H	29.7666	1.91822591823
8	H	29.7845	1.90168630169
9	H	29.5298	2.13702933703
11	H	28.7893	2.82125202125
13	H	29.8462	1.84467544468
15	H	31.2440	0.553106953107
16	H	30.2501	1.47147147147
17	H	30.9434	0.830861630862
19	H	31.2620	0.536474936475
20	H	30.6263	1.12386232386
21	H	31.1577	0.632848232848
25	H	26.5276	4.91106491106
28	H	29.6165	2.05691845692
30	H	30.5409	1.20277200277
31	H	30.7288	1.02915222915
32	H	30.6356	1.11526911527
34	H	30.8401	0.926310926311
35	H	30.8916	0.878724878725
36	H	30.6899	1.0650958651
40	H	24.8592	6.45266805267
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44	H	28.6373	2.9617001617
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53	H	28.5084	3.0808038808
55	H	26.1034	5.30302610303
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61	H	28.2061	3.36012936013
62	H	28.5374	3.05400785401
64	H	29.7352	1.94723954724
65	H	30.4216	1.31300531301
67	H	29.8989	1.79598059598
69	H	31.3696	0.437052437052
70	H	30.4912	1.24869484869
71	H	30.6765	1.07747747748
73	H	31.1029	0.683483483483
74	H	30.5826	1.16424116424
75	H	30.8710	0.897759297759
79	H	25.7435	5.63557403557
82	H	28.6646	2.93647493647
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84	H	28.5913	3.0042042042
86	H	26.0017	5.396996997
88	H	30.7370	1.02157542158
89	H	30.7749	0.986555786556
90	H	30.6902	1.06481866482
93	H	26.5767	4.8656964657
98	H	27.3821	4.12150612151
99	H	28.6939	2.9094017094
101	H	28.4820	3.1051975052
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108	H	26.2590	5.15925155925
112	H	30.5375	1.20591360591
113	H	29.9269	1.77010857011
114	H	30.9789	0.79805959806
116	H	28.9924	2.63358743359
117	H	28.8630	2.75315315315
118	H	29.0709	2.56105336105
121	H	27.3027	4.19487179487
123	H	22.3277	8.79177639178
127	H	27.4440	4.06431046431
129	H	29.8800	1.81344421344
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132	H	29.7984	1.88884268884
134	H	30.4856	1.25386925387
135	H	30.3081	1.41787941788
136	H	30.9651	0.810810810811
138	H	30.7804	0.981473781474
139	H	30.5095	1.23178563179
140	H	30.5475	1.19667359667
145	H	26.9572	4.51411411411
147	H	28.4300	3.15324555325
148	H	28.9771	2.64772464772
149	H	28.6617	2.93915453915
151	H	30.3097	1.4164010164
152	H	30.5332	1.20988680989
153	H	30.4548	1.28232848233
155	H	25.4477	5.90889350889
159	H	28.4872	3.10039270039
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163	H	28.9579	2.66546546547
164	H	28.3429	3.23372603373
166	H	28.1279	3.43238623239
168	H	30.3489	1.38018018018
169	H	29.9416	1.75652575653
171	H	30.7474	1.01196581197
172	H	30.9027	0.868468468468
173	H	30.8589	0.90893970894
175	H	31.3004	0.500993300993
176	H	30.8160	0.948579348579
177	H	30.5961	1.15176715177
179	H	28.6667	2.93453453453
180	H	29.3786	2.27673827674

181	H	29.1168	2.51864171864
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186	H	28.0113	3.54012474012
193	H	24.7567	6.54737814738
194	H	23.8427	7.39191499191
195	H	23.8178	7.41492261492
196	H	24.3914	6.88491568492
199	H	27.8613	3.67872487872
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Supporting Information: NMR-CoibamideA.D-MeAla.D-HIV-0020.log

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Using Gaussian 09: AM64L-G09RevD.01 24-Apr-2013

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Pointgroup= C1 Stoichiometry= C65H110N10O16

C1[X(C65H110N10O16)] #Atoms= 201

Charge = 0 Multiplicity = 1

SCF Energy= -4294.55410367

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Optimization incomplete.

Atomic Type	Coordinates (Angstroms) X	Y	Z
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H	7.130559	-0.769817	4.684159
C	4.182233	-2.331570	4.265259
H	3.615983	-1.707773	4.966721
H	3.935737	-1.996320	3.252145
H	3.806819	-3.350754	4.397044
C	6.458736	-3.190006	3.779737
H	7.511253	-2.956373	3.996904
C	6.260448	-4.675810	4.205094
H	5.262582	-5.018854	3.904488
C	6.390448	-4.860837	5.722936
H	7.361454	-4.504444	6.083339
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H	6.297041	-5.917940	5.994440
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H	7.144860	-6.631612	3.824886
H	7.170821	-5.563863	2.422603
C	6.254822	-3.039811	2.257478
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H	8.393518	-1.177435	-1.249071
C	9.598354	-2.546995	-0.134294
H	9.781522	-2.873797	0.894820
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C	8.944053	-0.245849	0.591227
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H	8.198552	0.553134	0.530461
C	5.994093	-1.093076	-0.044438
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C	4.384698	-0.150839	-1.668898
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H	4.028457	1.552756	-2.975157
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N	2.332853	-1.582378	-1.271979
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H	1.574773	-1.688700	0.701590
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H	3.085989	-4.225397	-0.872240
C	2.459747	-5.024144	-2.757668
H	1.566640	-5.427187	-3.246925
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H	1.763464	-5.761233	0.553841
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C	-2.460224	-0.968259	-2.268432
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C	-3.865676	0.931938	-3.271624
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H	-7.663211	-6.699515	-1.699174
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NMR-Shifts

NMR-CoibamideA.D-MeAla.D-HIV-0020-NMR.txt

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12	C	154.0271	30.6599475488
14	C	166.4896	18.7315989969
18	C	165.8475	19.3461781428
22	C	2.4120	175.776718544
24	C	107.1023	75.5735178698
27	C	152.1180	32.4872221903
29	C	164.3262	20.802274163
33	C	170.1137	15.2628304523
37	C	7.1996	171.194318421
39	C	127.4467	56.1010930531
42	C	156.5191	28.274756408
46	C	112.7034	70.2124849251
50	C	126.8279	56.6933708532
54	C	129.4004	54.2311299987
56	C	5.6839	172.645054461
59	C	153.6709	31.0008805682
63	C	147.3884	37.0141082333
66	C	156.2649	28.5180612186
68	C	166.5595	18.6646949597
72	C	162.4113	22.6351002125
76	C	3.4470	174.786079366
78	C	125.7671	57.7087042248
81	C	154.2671	30.4302341163
85	C	115.7770	67.2706215663
87	C	167.1817	18.069162886
92	C	125.7947	57.6822871801
94	C	8.0757	170.355768679
97	C	112.9135	70.0113899577
100	C	126.7130	56.803346159
105	C	6.8112	171.566071326
107	C	127.5820	55.9715921055
109	C	2.8332	175.37357147
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115	C	157.0494	27.7671854362
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128	C	143.8857	40.3666800666
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174	C	163.9745	21.1389000555
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182	C	8.2182	170.219376328
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187	C	24.0383	155.077336856
188	C	74.2708	106.997836865
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190	C	51.6059	128.691303432
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192	C	62.9250	117.857347958
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8	H	30.1211	1.59066759067
9	H	29.2306	2.41349041349
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13	H	29.6202	2.0534996535
15	H	31.2598	0.538507738508
16	H	30.3157	1.41085701086
17	H	30.8506	0.916608916609
19	H	31.1906	0.602448602449
20	H	30.6634	1.08958188958
21	H	30.8577	0.910048510049
25	H	26.5124	4.92510972511
28	H	29.5656	2.10395010395
30	H	30.6382	1.11286671287
31	H	30.7664	0.99440979441
32	H	30.4394	1.29655809656
34	H	30.7052	1.05095865096
35	H	30.9409	0.833171633172
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65	H	30.4469	1.28962808963
67	H	29.9477	1.75088935089
69	H	31.3547	0.45082005082
70	H	30.6321	1.1185031185
71	H	30.7168	1.04024024024
73	H	31.0967	0.689212289212
74	H	30.6028	1.14557634558
75	H	30.8581	0.909678909679
79	H	25.6934	5.68186648187
82	H	28.6691	2.93231693232
83	H	29.3416	2.31092631093
84	H	28.6224	2.97546777547
86	H	25.9810	5.41612381612
88	H	30.7627	0.997828597829
89	H	30.7770	0.984615384615
90	H	30.4816	1.25756525757
93	H	26.7348	4.71961191961
98	H	27.3214	4.17759297759
99	H	28.6386	2.9604989605
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112	H	30.5646	1.18087318087
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116	H	28.9863	2.63922383922
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118	H	29.0348	2.59440979441
121	H	27.3088	4.18923538924
123	H	22.3430	8.77763917764
127	H	27.4488	4.05987525988
129	H	29.9048	1.79052899053
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132	H	29.8932	1.80124740125
134	H	30.5220	1.22023562024
135	H	30.3611	1.36890736891
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138	H	30.7615	0.998937398937
139	H	30.6006	1.14760914761
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145	H	27.2090	4.28145068145
147	H	28.4082	3.17338877339
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149	H	28.7432	2.86384846385
151	H	30.3367	1.39145299145
152	H	30.5152	1.22651882652
153	H	30.5993	1.14881034881
155	H	25.4703	5.88801108801
159	H	28.5707	3.02323862324
162	H	28.1305	3.42998382998
163	H	28.7617	2.84675444675
164	H	28.2021	3.36382536383
166	H	28.7239	2.88168168168
168	H	30.0906	1.61884961885
169	H	30.0879	1.62134442134
171	H	31.0105	0.768861168861
172	H	30.8535	0.913929313929
173	H	31.0141	0.765534765535
175	H	31.3121	0.490182490182
176	H	30.6093	1.13957033957
177	H	30.6201	1.12959112959
179	H	28.8661	2.75028875029
180	H	29.2035	2.43853083853
181	H	28.9500	2.67276507277
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186	H	28.0711	3.48486948487
193	H	24.7532	6.55061215061
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195	H	23.8440	7.39071379071
196	H	24.4068	6.87068607069
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201 H 28.1705 3.39302379302

Supporting Information: NMR-Coibamide.D-MeAla.D-HIV-0021.log

Using Gaussian 09: AM64L-G09RevD.01 24-Apr-2013

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Pointgroup= C1 Stoichiometry= C65H110N10O16 C1[X(C65H110N10O16)] #Atoms= 201

Charge = 0 Multiplicity = 1

SCF Energy= -4294.55436396

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Optimization incomplete.

Atomic Type	Coordinates (Angstroms) X	Y	Z
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H	5.811421	-0.702805	-5.290984
C	7.821690	-2.900499	-3.725994
H	8.335579	-3.259039	-4.625464
H	8.494913	-2.203215	-3.216720
H	7.679271	-3.778252	-3.088587
C	5.674036	-1.940797	-2.931384
H	4.797021	-1.409286	-3.330477
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C	4.457130	-4.181114	-3.183835
H	3.671469	-3.700476	-3.776898
H	5.198380	-4.598286	-3.872417
H	4.006032	-5.023054	-2.647122
C	4.035255	-2.782597	-1.169372
H	3.202169	-2.253305	-1.643780
H	3.629630	-3.666074	-0.665328
H	4.451659	-2.131478	-0.397506
C	6.354046	-0.939017	-1.974543
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O	7.102972	-1.556534	-1.017327
C	8.818478	-1.470971	0.695295
H	8.321049	-2.262685	1.271359
C	9.596933	-0.587792	1.673670
H	10.118954	0.219768	1.149480
H	8.935643	-0.138813	2.421258
H	10.346515	-1.176204	2.214118
C	9.797711	-2.162058	-0.259925
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H	10.575348	-2.694830	0.298038
H	9.286210	-2.899221	-0.886553
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H	7.408114	3.115706	1.160745
H	8.384944	1.885377	0.370552
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H	6.422368	1.350063	3.699759
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C	4.572638	2.831484	1.157384
O	4.835706	4.008815	1.423111
N	3.636479	2.509852	0.177761
C	3.427123	1.160423	-0.343578
H	2.657524	0.670020	0.255898
H	3.118795	1.200736	-1.391603
H	4.336063	0.567962	-0.288693
C	3.388802	4.114903	-1.688130
H	4.472972	4.241963	-1.562719
H	3.267128	3.347682	-2.464156
C	2.794904	5.445033	-2.200033
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C	3.341470	5.745542	-3.598890
H	4.430805	5.859556	-3.584407
H	3.093454	4.937485	-4.295348
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C	3.102581	6.619241	-1.268647
H	4.178882	6.712048	-1.088146
H	2.751396	7.561494	-1.703473
H	2.602366	6.506819	-0.302571
C	1.316306	3.107320	-0.522760
O	0.802615	3.018430	-1.642499
C	-0.642437	1.948728	0.432804
H	-0.720836	1.750379	-0.634452
N	0.621102	2.709928	0.623973
C	1.111644	2.916594	1.985013
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H	1.600062	2.000177	2.327446
H	1.823149	3.740095	2.041006
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C	-1.249078	0.393499	2.460933
H	-0.789479	1.055882	3.198345
H	-2.326003	0.581381	2.424648
H	-1.138618	-0.635268	2.818299
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C	-3.957695	4.018401	0.290348
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H	-3.064887	7.990870	0.340842
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H	-2.065032	7.354972	-1.007121
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C	-0.513327	-1.037593	-0.719036
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H	-0.894482	-0.778969	-3.415826

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C	0.250941	-3.247395	-3.009128
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NMR-Shifts

NMR-CoibamideA.D-MeAla.D-HIV-0021-NMR.txt

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12	C	154.8028	29.9174945922
14	C	166.0838	19.1200061257
18	C	163.9707	21.1425371849
22	C	4.9375	173.359463236
24	C	108.1502	74.5705315952
27	C	151.7766	32.813989548
29	C	168.8358	16.4859587664
33	C	165.6566	19.5288960355
37	C	6.4821	171.88106587
39	C	128.6497	54.9496544727
42	C	153.5474	31.119087272
46	C	111.9620	70.9221080036
50	C	127.4203	56.1263615307
54	C	128.1715	55.407358487
56	C	8.8085	169.654376998
59	C	154.0272	30.6598518348
63	C	144.5526	39.7283638661
66	C	157.6184	27.2225731733
68	C	161.6888	23.3266333582
72	C	166.0877	19.1162732824
76	C	5.5553	172.768142575
78	C	128.4138	55.1754436341
81	C	156.9804	27.833228048
85	C	111.9681	70.9162694539
87	C	165.5634	19.6181014185
92	C	125.1941	58.2571450449
94	C	6.1764	172.173663355
97	C	111.5807	71.2870652195
100	C	127.0243	56.5053886943
105	C	2.9095	175.300541741
107	C	127.9548	55.6147705737
109	C	0.9447	177.181129042
111	C	168.4190	16.8848944275
115	C	155.7359	29.0243879094
120	C	128.4524	55.138498057
124	C	3.7060	174.538180287
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128	C	147.7865	36.6330710772
131	C	157.5346	27.3027814468
133	C	164.5270	20.6100805911
137	C	161.8915	23.1326212217
142	C	0.8548	177.267175865

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146	C	154.2799	30.4179827332
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156	C	1.4746	176.673940925
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182	C	4.4782	173.799077318
184	C	143.2454	40.9795363617
187	C	23.4882	155.603859186
188	C	62.4297	118.331419055
189	C	50.8523	129.41260361
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7	H	29.6202	2.0534996535
8	H	30.2562	1.46583506584
9	H	29.2371	2.40748440748
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13	H	29.4019	2.25520905521
15	H	31.3156	0.486948486948
16	H	30.0517	1.65479325479
17	H	30.7789	0.98285978286
19	H	30.9659	0.810071610072
20	H	30.4509	1.28593208593
21	H	30.3652	1.36511896512
25	H	26.4116	5.01824901825
28	H	29.3508	2.30242550243
30	H	31.0450	0.736983136983
31	H	30.6667	1.08653268653
32	H	30.7161	1.04088704089
34	H	31.2013	0.592561792562
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36	H	30.3242	1.403003003
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64	H	30.7309	1.02721182721
65	H	29.3741	2.2808962809
67	H	30.0598	1.64730884731
69	H	31.1156	0.671748671749
70	H	30.7582	1.00198660199
71	H	30.7021	1.05382305382
73	H	31.2468	0.55051975052
74	H	30.9563	0.818942018942
75	H	30.3767	1.35449295449
79	H	26.3025	5.11905751906
82	H	28.2773	3.29434049434
83	H	29.3924	2.26398706399
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86	H	26.7467	4.70861630862
88	H	30.3522	1.37713097713
89	H	31.0296	0.751212751213
90	H	31.4696	0.344652344652
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98	H	27.9847	3.5647031647
99	H	28.1547	3.40762300762
101	H	28.5678	3.02591822592
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127	H	26.1345	5.27428967429
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132	H	30.4372	1.29859089859
134	H	30.9494	0.825317625318
135	H	30.9857	0.791776391776
136	H	31.2522	0.54553014553
138	H	30.9097	0.862000462
139	H	30.5424	1.20138600139
140	H	30.5406	1.20304920305
145	H	27.1636	4.3234003234
147	H	28.6029	2.99348579349
148	H	28.3541	3.22337722338
149	H	28.8099	2.80221760222
151	H	31.1452	0.644398244398
152	H	30.0407	1.66495726496
153	H	30.4075	1.32603372603
155	H	26.1325	5.27613767614
159	H	28.5518	3.0407022407
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169	H	29.7673	1.91757911758
171	H	31.1340	0.654747054747
172	H	30.8311	0.934626934627
173	H	30.7965	0.966597366597
175	H	30.8248	0.940448140448
176	H	30.7205	1.03682143682
177	H	30.4045	1.32880572881
179	H	28.6954	2.90801570802
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193	H	24.4910	6.79288519289
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199	H	27.8076	3.72834372834
200	H	27.9653	3.58262878263
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Supporting Information: NMR-Coibamide.D-MeAla.D-HIV-0022.log

Using Gaussian 09: AM64L-G09RevD.01 24-Apr-2013

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density=current SCRF=(PCM,SOLVENT=Chloroform)

Pointgroup= C1 Stoichiometry= C65H110N10O16
C1[X(C65H110N10O16)] #Atoms= 201
Charge = 0 Multiplicity = 1

SCF Energy= -4294.55636808
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Optimization incomplete.

Atomic Type	Coordinates (Angstroms) X	Y	Z
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H	7.415578	-0.956415	-4.579789
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H	6.138411	-1.706375	-2.796657
C	6.526296	-3.266614	-1.398591
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C	6.357965	-4.464085	-2.343984
H	5.652940	-4.236118	-3.150668
H	7.311185	-4.755916	-2.795459
H	5.978382	-5.336656	-1.801059
C	5.190763	-3.027995	-0.678324
H	4.398884	-2.760561	-1.386521
H	4.873532	-3.930108	-0.144017
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H	8.493443	-1.358645	2.523318
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C	3.093835	4.230543	-3.573025
H	2.027192	4.053420	-3.752982
C	3.823392	4.047568	-4.907379
H	4.899628	4.220756	-4.799515
H	3.679481	3.033029	-5.293836
H	3.441188	4.746027	-5.659372
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NMR-Shifts

NMR-Coibamide.D-MeAla.D-HIV-0021-NMR.txt

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14	C	166.0838	19.1200061257
18	C	163.9707	21.1425371849
22	C	4.9375	173.359463236
24	C	108.1502	74.5705315952
27	C	151.7766	32.813989548
29	C	168.8358	16.4859587664
33	C	165.6566	19.5288960355
37	C	6.4821	171.88106587
39	C	128.6497	54.9496544727
42	C	153.5474	31.119087272
46	C	111.9620	70.9221080036
50	C	127.4203	56.1263615307
54	C	128.1715	55.407358487
56	C	8.8085	169.654376998
59	C	154.0272	30.6598518348
63	C	144.5526	39.7283638661
66	C	157.6184	27.2225731733
68	C	161.6888	23.3266333582
72	C	166.0877	19.1162732824
76	C	5.5553	172.768142575
78	C	128.4138	55.1754436341
81	C	156.9804	27.833228048
85	C	111.9681	70.9162694539
87	C	165.5634	19.6181014185
92	C	125.1941	58.2571450449
94	C	6.1764	172.173663355
97	C	111.5807	71.2870652195
100	C	127.0243	56.5053886943
105	C	2.9095	175.300541741
107	C	127.9548	55.6147705737
109	C	0.9447	177.181129042
111	C	168.4190	16.8848944275
115	C	155.7359	29.0243879094
120	C	128.4524	55.138498057
124	C	3.7060	174.538180287
126	C	127.7408	55.8195983843
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131	C	157.5346	27.3027814468
133	C	164.5270	20.6100805911
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8	H	30.2562	1.46583506584
9	H	29.2371	2.40748440748
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28	H	29.3508	2.30242550243
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64	H	30.7309	1.02721182721
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69	H	31.1156	0.671748671749
70	H	30.7582	1.00198660199
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73	H	31.2468	0.55051975052
74	H	30.9563	0.818942018942
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82	H	28.2773	3.29434049434
83	H	29.3924	2.26398706399
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86	H	26.7467	4.70861630862
88	H	30.3522	1.37713097713
89	H	31.0296	0.751212751213
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112	H	30.0896	1.61977361977
113	H	29.8023	1.88523908524
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136	H	31.2522	0.54553014553
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140	H	30.5406	1.20304920305
145	H	27.1636	4.3234003234
147	H	28.6029	2.99348579349
148	H	28.3541	3.22337722338
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151	H	31.1452	0.644398244398
152	H	30.0407	1.66495726496
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172	H	30.8311	0.934626934627
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175	H	30.8248	0.940448140448
176	H	30.7205	1.03682143682
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179	H	28.6954	2.90801570802
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193	H	24.4910	6.79288519289
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Coibamide A - Original Configuration

Supporting Information: CoibamideA-OriginalConfiguration-0001.log

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 Using  Gaussian 09:  AM64L-G09RevD.01 24-Apr-2013
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density=current
 SCRF=(PCM,SOLVENT=Chloroform)
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Pointgroup= C1 Stoichiometry= C65H110N10O16
C1[X(C65H110N10O16)] #Atoms= 201
Charge = 0 Multiplicity = 1

SCF Energy= -4294.53850382

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Optimization incomplete.

Atomic Type	Coordinates (Angstroms) X	Y	Z
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C	6.789488	-2.068753	-0.971077
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C	0.218932	1.199894	4.955636
H	0.550208	1.657202	5.898128
C	1.150292	-0.002617	4.762512
O	1.088704	-1.015880	5.448913
C	-1.231731	0.774160	5.165411
H	-1.582582	0.094056	4.385954
H	-1.898623	1.642020	5.194229
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H	0.715038	3.824593	5.224616
H	2.192950	3.088673	4.541364
H	1.200510	4.191569	3.569516
N	0.399321	2.232384	3.910512
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H	1.350208	3.336795	1.705233
N	0.410216	2.228992	0.253110
H	-0.142967	1.375546	0.217897
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C	2.040471	3.722250	-0.924143
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C	1.633146	4.623829	-2.108610
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H	1.622990	4.052383	-3.043705
C	2.497565	5.887398	-2.294294
H	3.543113	5.593281	-2.443897
C	2.432592	6.822557	-1.085832
H	2.874671	6.360221	-0.198658
H	2.989255	7.746001	-1.279183
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C	2.048387	6.638626	-3.550763
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H	2.674047	7.521094	-3.721462
H	2.128203	5.998724	-4.436004
N	3.459633	3.292927	-0.890479
C	4.081424	2.748587	-2.025769
O	3.527263	2.658473	-3.125701
C	5.547747	2.305817	-1.896087
H	5.743231	1.887411	-0.912510
C	4.081891	3.311338	0.433812
H	5.169946	3.342520	0.387979
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H	3.769351	2.411183	0.970795
C	6.453748	3.498271	-2.186623
H	6.266033	3.898825	-3.189848
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C	6.728995	0.254745	-2.893888
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C	7.719977	0.144778	-1.717315
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H	12.003216	-1.387731	-0.470008
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C	9.746206	0.760820	-3.105024
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C	-2.940219	3.804824	2.385275
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H	-4.372973	2.909257	-1.092425
H	-1.996682	3.481980	-0.868494
H	-2.550904	4.048743	3.371059
H	-4.909034	3.496011	3.150454
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H	-8.022831	2.604360	1.458307
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NMR-Shifts
CoibamideA-OriginalConfiguration-0001-NMR.txt

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12	C	152.7257	31.9055686365
14	C	166.2441	18.9665766956
18	C	164.5354	20.602040621
22	C	4.7737	173.516242654
24	C	108.7205	74.0246750512
27	C	151.0226	33.5356725818
29	C	170.4243	14.9655429851
33	C	163.4083	21.6808323283
37	C	5.2846	173.027240185
39	C	128.0148	55.5573422156
42	C	150.3260	34.2024158196
46	C	109.3031	73.4670456938
50	C	127.5489	56.0032734164
54	C	127.5640	55.988820613
56	C	5.8994	172.438790942
59	C	154.4359	30.2686690021
63	C	149.1887	35.2909703478
66	C	151.2796	33.2896877812
68	C	161.5123	23.495568445
72	C	166.3557	18.8597599495
76	C	2.2411	175.94029365
78	C	128.3629	55.2241620245
81	C	156.4202	28.369417485
85	C	115.2190	67.8047052968
87	C	166.9557	18.2854763682
92	C	124.4150	59.0028522751
94	C	7.1076	171.282375237
97	C	111.2717	71.5828212638
100	C	126.5776	56.9329428205
105	C	5.3546	172.960240433
107	C	120.7721	62.4896150386
109	C	3.8770	174.374509466
111	C	169.2446	16.0946802198
115	C	148.1609	36.2747181225
120	C	130.1151	53.5470625395
124	C	9.3921	169.095790501
126	C	123.6007	59.7822508088
128	C	145.1279	39.1777216256
131	C	157.2037	27.6194988419
133	C	165.4111	19.7638737342
137	C	162.3881	22.6573058443
142	C	4.9114	173.384444572
144	C	136.1104	47.8087252819
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156	C	12.6646	165.963552135
158	C	114.0150	68.9571010165
161	C	143.9585	40.2970003254
165	C	147.6206	36.7918604874
167	C	159.3226	25.5914163747
170	C	174.1142	11.4337946745
174	C	171.6907	13.753421773
178	C	149.5972	34.8999789429
182	C	8.8531	169.611688585

184	C	146.0275	38.3166791095
187	C	21.8843	157.139014912
188	C	60.4800	120.197553552
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190	C	54.1356	126.27002814
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7	H	29.7579	1.92626472626
8	H	30.0248	1.67964887965
9	H	29.3820	2.2735966736
11	H	28.6827	2.91975051975
13	H	29.5116	2.15384615385
15	H	31.0993	0.68680988681
16	H	30.4029	1.33028413028
17	H	30.8770	0.892215292215
19	H	31.0509	0.731531531532
20	H	30.6212	1.12857472857
21	H	29.8990	1.79588819589
25	H	26.4954	4.94081774082
28	H	29.5088	2.15643335643
30	H	30.5834	1.1635019635
31	H	30.5404	1.20323400323
32	H	30.9136	0.858396858397
34	H	30.5238	1.21857241857
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44	H	29.0817	2.55107415107
45	H	28.2456	3.32363132363
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62	H	28.3718	3.20702240702
64	H	29.9971	1.70524370524
65	H	30.3271	1.40032340032
67	H	30.1353	1.57754677755
69	H	31.0558	0.727003927004
70	H	30.7086	1.04781704782
71	H	30.7885	0.973989373989
73	H	31.3423	0.462277662278
74	H	30.8742	0.894802494802
75	H	30.6096	1.13929313929
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82	H	28.5724	3.02166782167
83	H	29.1482	2.48962808963
84	H	28.2739	3.29748209748
86	H	26.2041	5.20997920998
88	H	30.9942	0.783922383922
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93	H	27.0252	4.45128205128
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99	H	28.0161	3.53568953569
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108	H	27.8680	3.67253407253
112	H	29.1109	2.52409332409
113	H	30.7077	1.04864864865
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116	H	28.7711	2.83806883807
117	H	28.6444	2.95513975514
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129	H	30.6168	1.13264033264
130	H	28.1046	3.45391545392
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134	H	30.5232	1.21912681913
135	H	30.5649	1.1805959806
136	H	31.2794	0.520397320397
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139	H	30.5361	1.20720720721
140	H	30.6966	1.05890505891
145	H	27.2258	4.26592746593
147	H	28.2574	3.31272811273
148	H	28.8607	2.75527835528
149	H	28.3706	3.20813120813
151	H	30.4375	1.29831369831
152	H	30.6638	1.08921228921
153	H	30.5474	1.19676599677
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173	H	31.0888	0.696511896512
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176	H	30.3731	1.35781935782
177	H	31.0854	0.699653499654
179	H	29.1652	2.47392007392
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193	H	24.3056	6.96419496419
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Supporting Information: CoibamideA-OriginalConfiguration-0002.log

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 Using  Gaussian 09:  AM64L-G09RevD.01 24-Apr-2013
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 Charge = 0                Multiplicity = 1
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 SCF Energy= -4294.53649847
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 Optimization incomplete.
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H	3.034318	3.776563	-2.964729
C	4.037711	5.480056	-2.073785
H	5.040308	5.037607	-2.049557

C	3.911041	6.439688	-0.889641
H	4.128496	5.936806	0.057009
H	4.620404	7.268972	-0.984432
H	2.902921	6.863199	-0.827923
C	3.913022	6.261374	-3.384820
H	2.931886	6.740618	-3.470748
H	4.678459	7.042327	-3.447074
H	4.044226	5.598439	-4.246655
N	4.367701	2.784205	-0.542151
C	5.120298	2.197761	-1.573509
O	4.752040	2.180501	-2.752042
C	6.496669	1.610100	-1.213457
H	6.413266	0.988576	-0.325369
C	4.718134	2.704395	0.876869
H	5.667651	2.212859	1.075736
H	4.767350	3.719629	1.281780
H	3.932272	2.147046	1.394889
C	7.499534	2.744901	-1.021471
H	7.609780	3.328642	-1.943056
H	7.189074	3.439051	-0.235075
H	8.488696	2.362641	-0.756311
N	6.922731	0.745868	-2.320059
H	6.561533	0.999376	-3.235820
C	7.802579	-0.313575	-2.329290
O	8.118857	-0.830768	-3.404010
C	8.376660	-0.820082	-0.989177
H	8.656012	0.095793	-0.455965
N	7.326327	-1.446190	-0.143054
C	7.431909	-1.158907	1.289503
H	7.581067	-0.085958	1.440436
H	6.551716	-1.452996	1.855071
H	8.293887	-1.703581	1.685183
C	9.688909	-1.659944	-1.072985
H	10.031925	-1.805845	-0.038471
C	10.845311	-0.946205	-1.813566
H	10.617887	-0.840414	-2.879966
H	11.740002	-1.579710	-1.755907
C	11.210694	0.416160	-1.243553
H	11.371699	0.362522	-0.162536
H	12.134225	0.779628	-1.705953
H	10.432752	1.156176	-1.446995
C	9.525012	-3.068934	-1.654139
H	9.127128	-3.051726	-2.672187
H	10.491131	-3.585491	-1.689805
H	8.871562	-3.683975	-1.029216
C	3.798386	-1.254793	-0.407596
H	2.825777	-1.662238	-0.689276
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H	4.429333	-1.220771	-1.297130
C	0.052237	2.249537	2.261847
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C	-2.576128	3.849274	0.823428
C	-1.391488	4.018972	0.097979
C	-1.427836	3.870186	-1.294449
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H	-4.677553	3.404187	0.748340
H	-2.581280	3.954072	1.905352
H	-0.523337	3.996446	-1.884603
H	-2.592433	3.444329	-3.030389
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H	-6.093869	2.493176	-3.388251
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NMR-Shifts

CoibamideA-OriginalConfiguration-0002-NMR.txt

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12	C	153.2243	31.4283389805
14	C	166.4508	18.7687360018
18	C	164.6394	20.5024981336
22	C	5.8779	172.459369437
24	C	108.4071	74.3246425085
27	C	151.5367	33.0436072666
29	C	165.4728	19.7048182392
33	C	168.2603	17.0367924348
37	C	4.1246	174.137521775
39	C	127.6502	55.9063152051
42	C	156.8357	27.971726105
46	C	114.6223	68.3758303183
50	C	127.8269	55.7371886904
54	C	131.7434	51.9885526139
56	C	4.0376	174.220792894
59	C	154.9514	29.7752636919
63	C	147.8479	36.574302724
66	C	156.5117	28.2818392389
68	C	166.0605	19.1423074714
72	C	162.2180	22.8201152396
76	C	2.9328	175.278240395
78	C	128.2843	55.2993931737
81	C	155.6655	29.0917705163
85	C	115.2680	67.757805471
87	C	167.4803	17.7833610904
92	C	126.5767	56.9338042459
94	C	6.8594	171.519937212
97	C	110.6292	72.1977832654
100	C	126.9845	56.5434828385
105	C	7.4074	170.995424874
107	C	120.6905	62.5677176056
109	C	4.1612	174.102490476
111	C	168.3553	16.9458642011
115	C	148.0806	36.3515764084
120	C	130.3371	53.3345776144
124	C	10.1342	168.385497425
126	C	125.6367	57.8335151898
128	C	145.3509	38.9642795612
131	C	158.4975	26.3811520129
133	C	165.5432	19.6374356324
137	C	162.8590	22.206588947
142	C	5.7362	172.594996076
144	C	135.4826	48.4096173357
146	C	146.7524	37.6228488294
150	C	166.4635	18.7565803327
156	C	12.5349	166.087693103
158	C	122.3615	60.9683378319
161	C	147.6528	36.7610406018
165	C	144.4110	39.8638947912
167	C	156.7267	28.0760542889
170	C	172.7414	12.7477555083
174	C	165.7925	19.3988208044
178	C	148.7720	35.689810295
182	C	8.4565	169.991290032
184	C	147.3141	37.0852236835
187	C	21.2072	157.787093934
188	C	63.8055	117.014586803
189	C	49.3996	130.803039874
190	C	55.4824	124.980952928
191	C	49.1215	131.069220314
192	C	73.4779	107.756752618
198	C	132.1817	51.5690384579

3	H	29.7543	1.92959112959
4	H	29.3297	2.32192192192
5	H	29.3621	2.29198429198
7	H	29.7309	1.95121275121
8	H	29.9545	1.74460614461
9	H	29.2983	2.35093555094
11	H	28.7563	2.85174405174
13	H	29.5576	2.11134211134
15	H	31.1854	0.607253407253
16	H	30.4729	1.2656040656
17	H	30.9512	0.823654423654
19	H	31.1669	0.624347424347
20	H	30.7462	1.01307461307
21	H	30.3715	1.3592977593
25	H	26.5649	4.8765996766
28	H	29.3224	2.32866712867
30	H	31.2237	0.571864171864
31	H	30.1521	1.56202356202
32	H	30.7326	1.02564102564
34	H	31.0704	0.713513513514
35	H	30.5421	1.20166320166
36	H	30.6540	1.09826749827
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43	H	29.2167	2.42633402633
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47	H	28.8497	2.76544236544
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55	H	26.7512	4.70445830446
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61	H	28.4172	3.16507276507
62	H	29.0544	2.5762993763
64	H	29.8730	1.81991221991
65	H	30.7115	1.04513744514
67	H	30.3499	1.37925617926
69	H	31.4697	0.34455994456
70	H	30.9113	0.860522060522
71	H	30.8942	0.876322476322
73	H	31.1801	0.612150612151
74	H	30.7972	0.965950565951
75	H	30.8577	0.910048510049
79	H	26.4504	4.9823977824
82	H	28.3556	3.22199122199
83	H	28.5489	3.04338184338
84	H	29.0975	2.53647493647
86	H	26.1769	5.23511203511
88	H	30.9478	0.826796026796
89	H	30.6800	1.07424347424
90	H	30.4832	1.25608685609
93	H	26.9333	4.5361977362
98	H	28.4712	3.11517671518
99	H	28.2089	3.35754215754
101	H	28.9571	2.6662046662
102	H	28.2988	3.27447447447
103	H	28.7459	2.86135366135
108	H	27.9721	3.57634557635
112	H	29.3449	2.30787710788
113	H	30.6707	1.08283668284
114	H	30.1780	1.53809193809
116	H	28.8660	2.75038115038
117	H	28.5795	3.01510741511
118	H	28.2182	3.34894894895
121	H	27.0382	4.43927003927
123	H	25.2742	6.06920766921
127	H	27.7000	3.82776622777
129	H	30.4691	1.26911526912
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132	H	30.0723	1.63575883576
134	H	30.4670	1.27105567106
135	H	30.6707	1.08283668284
136	H	31.1452	0.644398244398
138	H	31.0058	0.773203973204
139	H	30.6968	1.05872025872
140	H	30.6340	1.11674751675
145	H	27.3507	4.15051975052
147	H	28.1952	3.3702009702
148	H	28.7121	2.89258489258
149	H	28.6963	2.90718410718
151	H	30.5185	1.22346962347
152	H	30.5664	1.17920997921
153	H	30.3344	1.39357819358
155	H	25.5213	5.84088704089
159	H	28.3053	3.26846846847
162	H	29.2803	2.36756756757
163	H	28.6528	2.94737814738
164	H	28.5125	3.07701547702
166	H	29.6936	1.98567798568
168	H	29.7658	1.91896511897
169	H	30.2193	1.49993069993
171	H	31.2130	0.581750981751
172	H	30.6343	1.11647031647
173	H	30.9869	0.790667590668
175	H	29.2412	2.4036960037
176	H	31.1949	0.598475398475
177	H	30.2697	1.45336105336
179	H	28.8796	2.73781473781
180	H	29.0927	2.54091014091
181	H	29.2417	2.40323400323
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186	H	28.8992	2.7197043197
193	H	24.6618	6.63506583507
194	H	24.6137	6.67951027951
195	H	24.1148	7.14049434049
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199	H	27.9453	3.60110880111
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Supporting Information: CoibamideA-OriginalConfiguration-0004.log

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 Using  Gaussian 09:  AM64L-G09RevD.01 24-Apr-2013
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 density=current SCRF=(PCM,SOLVENT=Chloroform)
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 Pointgroup= C1   Stoichiometry= C65H110N10O16
C1[X(C65H110N10O16)]  #Atoms= 201
 Charge = 0                 Multiplicity = 1
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 SCF Energy= -4294.53769798
=========================================================================
 Optimization incomplete.


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     Atomic     Coordinates (Angstroms)
      Type     X                Y              Z
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      N       9.517746      3.663948     -1.124185
      C      10.780613      3.004709     -0.794596
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H	6.686368	3.952058	-1.501437
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H	-7.994396	-2.594702	1.092602
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H	-8.789241	-3.752440	-2.450460
H	-10.078230	-2.629245	-1.982741
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C	-5.589251	4.356685	-1.235940
O	-5.375597	4.986586	-2.276147
C	-5.316927	4.977493	0.149856
H	-6.004871	4.514837	0.865480
N	-3.936565	4.611306	0.557468
C	-3.800134	3.978805	1.869503
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H	-3.890478	2.896715	1.754238
H	-2.843484	4.221056	2.333616
C	-5.598722	6.511772	0.170879
H	-5.047860	6.999256	-0.642468
C	-5.149281	7.155099	1.502924
H	-4.082304	6.963610	1.663270
H	-5.684990	6.693876	2.341346
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H	-6.406455	8.932866	1.581838
H	-4.888295	9.067520	2.468169
H	-4.879254	9.154642	0.699026
C	-7.095500	6.766873	-0.076551
H	-7.702484	6.384460	0.751071
H	-7.303667	7.835478	-0.186649
H	-7.440730	6.285385	-0.996697
C	-2.072978	2.155565	-0.752918
H	-2.926444	1.614852	-0.334698
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H	-1.347495	1.444666	-1.145937
C	-2.142805	-3.505886	1.641251
O	-1.133177	-3.586372	0.935492
C	-4.142692	-4.764742	0.683386
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H	-5.149339	-4.638450	0.265746
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C	-1.682325	-7.359334	-0.642548
C	-2.430733	-6.570028	0.233020
C	-3.346815	-5.634692	-0.262008
C	-3.500002	-5.511030	-1.648450
C	-2.749981	-6.301567	-2.525291
H	-0.973106	-8.076799	-0.236548
H	-2.285789	-6.687206	1.304041
H	-4.204105	-4.792796	-2.061764
H	-2.904607	-6.163867	-3.590806
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H	-0.456580	-8.659732	-4.636361
H	-2.161243	-8.205116	-4.528058
H	-0.866350	-6.943746	-4.527813

NMR-Shifts
CoibamideA-OriginalConfiguration-0004-NMR.txt

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12	C	153.5325	31.1333486476
14	C	164.8526	20.2984360344
18	C	165.4370	19.7390838263
22	C	4.7577	173.531556883
24	C	109.4197	73.3554432512
27	C	153.3334	31.3239150826
29	C	170.3587	15.0283313233
33	C	164.3012	20.8262026455
37	C	5.9461	172.394092536
39	C	115.4216	67.6107888742
42	C	147.9298	36.4959130152
46	C	106.8558	75.8094527077
50	C	127.0259	56.5038572714
54	C	128.9666	54.6463370279
56	C	7.8558	170.566243611
59	C	152.1553	32.4515208944
63	C	146.3975	37.9625375677
66	C	157.8159	27.0335381611
68	C	162.1652	22.8706521947
72	C	166.6597	18.5687896016
76	C	7.5352	170.873102471
78	C	126.2514	57.2451616608
81	C	155.3905	29.3549838243
85	C	114.5425	68.4522100346
87	C	166.2912	18.9214954344
92	C	124.1141	59.2908554911
94	C	8.4703	169.97808151
97	C	112.2674	70.6297976608
100	C	127.3793	56.165604242
105	C	5.9429	172.397155382
107	C	119.9953	63.2331208484
109	C	3.2042	175.018472789
111	C	168.9172	16.4080476273
115	C	147.9570	36.4698788262
120	C	130.5281	53.1517640077
124	C	8.4190	170.027182756
126	C	123.2422	60.1253852486
128	C	143.9241	40.3299259174
131	C	156.6439	28.1553054232
133	C	165.4312	19.7446352342
137	C	162.4229	22.6239973966
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150	C	166.1103	19.0946419342
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158	C	113.7117	69.2474013668
161	C	144.3916	39.8824632937
165	C	147.3542	37.0468423974
167	C	159.3044	25.60883631
170	C	174.0512	11.4940944505
174	C	170.2910	15.0931296541
178	C	153.0118	31.6317310821
182	C	8.4739	169.974635808
184	C	146.9097	37.4722908172
187	C	22.7056	156.352916403
188	C	63.9989	116.829476062
189	C	48.5686	131.598422634
190	C	54.4431	125.975707805
191	C	47.9942	132.14820345
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5	H	29.8360	1.8541002541
7	H	29.6891	1.98983598984
8	H	30.0619	1.64536844537
9	H	29.3268	2.3246015246
11	H	28.6880	2.91485331485
13	H	29.4934	2.17066297066
15	H	31.2194	0.575837375837
16	H	30.3282	1.39930699931

17	H	31.1063	0.680341880342
19	H	31.2375	0.559112959113
20	H	30.9432	0.831046431046
21	H	30.5674	1.17828597829
25	H	26.2768	5.1428043428
28	H	29.7226	1.95888195888
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31	H	30.7509	1.00873180873
32	H	31.0774	0.707045507046
34	H	30.6251	1.12497112497
35	H	30.5337	1.20942480942
36	H	30.8198	0.945068145068
40	H	27.9333	3.6121968122
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44	H	28.5743	3.01991221991
45	H	29.0241	2.6042966043
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52	H	28.3532	3.22420882421
53	H	28.2571	3.31300531301
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64	H	30.8180	0.946731346731
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67	H	30.2899	1.4346962347
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74	H	31.0283	0.752413952414
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88	H	30.9549	0.820235620236
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90	H	30.3925	1.33989373989
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121	H	26.8474	4.61556941557
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127	H	27.5675	3.9501963502
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145	H	27.0304	4.44647724648
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155	H	25.4224	5.93227073227
159	H	28.8886	2.7294987295
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175	H	31.7259	0.107830907831
176	H	30.3148	1.41168861169
177	H	30.8827	0.886948486948
179	H	28.9860	2.6395010395
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185	H	28.7353	2.87114807115
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193	H	24.5646	6.72487872488
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Supporting Information: CoibamideA-OriginalConfiguration-0005.log

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 Using  Gaussian 09:  AM64L-G09RevD.01 24-Apr-2013
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density=current
 SCRF=(PCM,SOLVENT=Chloroform)
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C1[X(C65H110N10O16)]  #Atoms= 201
 Charge = 0                 Multiplicity = 1
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 SCF Energy= -4294.53234619
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 Optimization incomplete.


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      Type      X                  Y                  Z
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H	9.666240	-0.612798	-3.277688
C	3.684994	-1.772908	-0.698652
H	3.975661	-0.722854	-0.608313
H	4.092914	-2.182756	-1.626174
H	2.600232	-1.850922	-0.749229
C	0.244973	2.599821	2.087814
O	-0.570583	1.741531	1.737856
C	0.141092	4.742683	0.706713
H	0.038199	5.355775	1.610575
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C	-3.797511	3.947156	-0.903019
C	-2.691094	4.041633	-1.751384
C	-1.421992	4.314620	-1.237320
C	-1.238063	4.496532	0.138029
C	-2.352029	4.414459	0.983022
C	-3.622768	4.142848	0.467249
H	-2.810089	3.894218	-2.822226
H	-0.578022	4.372338	-1.920022
H	-2.238679	4.546639	2.056627
H	-4.451825	4.083799	1.164949
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C	-6.117640	3.480872	-0.689305
H	-6.964194	3.220044	-1.330948
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H	-6.371682	4.407502	-0.164180

NMR-Shifts

CoibamideA-OriginalConfiguration-0005-NMR.txt

Atom	Type	Isotropic	Scaled Shift
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12	C	153.0296	31.6146940026
14	C	167.2082	18.0437986945
18	C	165.5691	19.6126457245
22	C	6.1428	172.205823236
24	C	111.2445	71.6088554528
27	C	150.4835	34.0516663795
29	C	167.3434	17.9143934608
33	C	168.4185	16.8853729972
37	C	8.4449	170.002392848
39	C	130.5246	53.1551139953
42	C	154.6159	30.0963839277
46	C	112.7490	70.1688393729
50	C	127.5851	55.9686249737
54	C	131.1949	52.5135435211
56	C	4.0894	174.171213078
59	C	153.8477	30.8316583396
63	C	142.4478	41.742950669
66	C	158.8325	26.0605103467
68	C	161.8119	23.2088095101
72	C	164.1076	21.0115048144
76	C	3.1201	175.098968204
78	C	127.6416	55.9145466031
81	C	154.9716	29.755929478
85	C	116.3951	66.6790137637
87	C	166.3680	18.847987136
92	C	122.5265	60.810409847
94	C	7.8072	170.612760581
97	C	112.0604	70.8279254963
100	C	126.9138	56.6111525871
105	C	7.3746	171.026819043
107	C	120.1535	63.0817014108
109	C	3.3703	174.85949195
111	C	167.7371	17.5375677176
115	C	148.1230	36.310993702
120	C	130.3202	53.3507532686
124	C	8.9272	169.540764563
126	C	123.9016	59.4942475928
128	C	144.2500	40.0179942189
131	C	158.0740	26.7865005073
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142	C	4.6289	173.654836425
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161	C	142.6454	41.553819943
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174	C	164.5197	20.617067708
178	C	154.0765	30.6126648672
182	C	9.3237	169.16125883
184	C	146.8005	37.576810429
187	C	23.8932	155.216217768
188	C	64.5113	116.339037884
189	C	49.1190	131.071613163
190	C	54.8981	125.540209422
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192	C	72.8975	108.312276269
198	C	130.9112	52.7850839411
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8	H	30.2703	1.45280665281
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11	H	28.6173	2.98018018018
13	H	29.4886	2.1750981751
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16	H	30.4917	1.24823284823
17	H	31.0449	0.737075537076
19	H	31.1139	0.673319473319
20	H	30.8045	0.959205359205
21	H	30.8069	0.956987756988
25	H	26.1582	5.25239085239
28	H	29.5684	2.10136290136
30	H	31.1582	0.632386232386
31	H	30.5365	1.20683760684

32	H	30.6399	1.1112959113
34	H	30.8619	0.906167706168
35	H	30.8893	0.88085008085
36	H	29.9765	1.72427812428
40	H	26.4682	4.96595056595
43	H	29.1859	2.45479325479
44	H	28.9451	2.67729267729
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52	H	28.6930	2.91023331023
53	H	28.7217	2.88371448371
55	H	27.0611	4.41811041811
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61	H	29.3852	2.27063987064
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67	H	30.2139	1.50492030492
69	H	31.0720	0.712035112035
70	H	30.7476	1.01178101178
71	H	30.7188	1.03839223839
73	H	31.4652	0.348717948718
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86	H	26.1751	5.23677523678
88	H	31.0110	0.768399168399
89	H	30.7701	0.990990990991
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99	H	28.4520	3.13291753292
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112	H	29.1311	2.50542850543
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138	H	31.0507	0.731716331716
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149	H	28.4657	3.12025872026
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152	H	30.5622	1.18309078309
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193	H	24.4262	6.85276045276
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Supporting Information: CoibamideA-OriginalConfiguration-0006.log

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 SCRF=(PCM,SOLVENT=Chloroform)
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 Charge = 0                 Multiplicity = 1
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 SCF Energy= -4294.53183591
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 Optimization incomplete.


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      Type      X                Y              Z
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C	-5.955944	3.511128	-0.991906
H	-6.769215	3.242541	-1.672293
H	-5.807839	2.673998	-0.301632
H	-6.256123	4.417396	-0.455866

NMR-Shifts

CoibamideA-OriginalConfiguration-0006-NMR.txt

Atom	Type	Isotropic	Scaled Shift
2	C	141.8405	42.3242213672
6	C	149.8817	34.6276728115
10	C	110.7016	72.1284863799
12	C	153.3498	31.308217998
14	C	166.6200	18.6067880319
18	C	165.8890	19.3064568617
22	C	5.3002	173.012308811
24	C	111.5763	71.2912766324
27	C	150.0022	34.5123375256
29	C	167.4621	17.8007810257
33	C	168.3153	16.9841497732
37	C	8.6610	169.795555045
39	C	131.4635	52.2564559046
42	C	153.8004	30.8769310285
46	C	113.3760	69.5687130305
50	C	127.5947	55.9594364364
54	C	131.0216	52.6794157622
56	C	4.0630	174.196481556
59	C	153.4523	31.2101112196
63	C	142.9567	41.2558624782
66	C	158.6811	26.205421237
68	C	161.7028	23.313233408
72	C	164.3905	20.7407301059
76	C	3.2818	174.944198779
78	C	127.6282	55.9273722698
81	C	155.0845	29.6478684508
85	C	116.3907	66.6832251766
87	C	166.3080	18.9054154942
92	C	122.7820	60.5658607554
94	C	7.8815	170.541645131
97	C	112.0548	70.8332854764
100	C	126.8722	56.6509695821
105	C	7.4086	170.994276307
107	C	120.0281	63.2017266793
109	C	3.3348	174.893470396
111	C	167.7890	17.4878921878
115	C	148.0146	36.4147476024
120	C	130.5884	53.0940485078
124	C	8.7583	169.702425391
126	C	123.6543	59.7309481422
128	C	144.0377	40.2211948927
131	C	157.9858	26.8709201937
133	C	165.4252	19.75037807
137	C	162.8442	22.2207546086
142	C	4.3894	173.884071288
144	C	134.9254	48.9429353548
146	C	147.0056	37.3805011581
150	C	165.9284	19.2687455732
156	C	12.4656	166.154022856
158	C	112.7122	70.2040620992
161	C	142.4484	41.7423763855
165	C	149.0197	35.4527268899
167	C	152.4677	32.1525105764
170	C	171.7010	13.7435632382
174	C	164.3342	20.7946170486
178	C	153.9951	30.6905760064
182	C	9.1585	169.319378242
184	C	146.9765	37.4083539118
187	C	23.3526	155.733647275
188	C	64.5086	116.34162216
189	C	48.6306	131.539079998
190	C	54.8912	125.546813683
191	C	49.2909	130.907080917
192	C	72.4245	108.765003159
198	C	130.8048	52.8869235629
3	H	29.2317	2.41247401247
4	H	29.1752	2.46468006468
5	H	29.8215	1.8674982675
7	H	29.6191	2.05451605452
8	H	30.1314	1.58115038115
9	H	29.2011	2.44074844075
11	H	28.6590	2.94164934165
13	H	29.6313	2.04324324324
15	H	31.2136	0.581196581197
16	H	30.3612	1.36881496881
17	H	30.9633	0.812474012474
19	H	31.0193	0.76072996073
20	H	31.0143	0.76534996535
21	H	30.7844	0.977777777778
25	H	26.2928	5.12802032802
28	H	29.5947	2.07706167706
30	H	31.2244	0.571217371217
31	H	30.5543	1.19039039039
32	H	30.7594	1.00087780088
34	H	30.9503	0.824486024486
35	H	30.9265	0.846477246477
36	H	30.0416	1.66412566413
40	H	26.1677	5.24361284361
43	H	29.1972	2.44435204435
44	H	28.8356	2.77847077847
45	H	28.3634	3.21478401478

47	H	27.5850	3.93402633403
48	H	28.8541	2.76137676138
51	H	28.0873	3.4699006699
52	H	28.6957	2.90773850774
53	H	28.7172	2.88787248787
55	H	27.1203	4.36340956341
60	H	29.3467	2.30621390621
61	H	29.4519	2.20900900901
62	H	28.3928	3.18761838762
64	H	30.5651	1.18041118041
65	H	29.6827	1.99574959575
67	H	30.2633	1.45927465927
69	H	31.0887	0.696604296604
70	H	30.7694	0.991637791638
71	H	30.7317	1.02647262647
73	H	31.4897	0.32607992608
74	H	30.5935	1.15416955417
75	H	30.7680	0.992931392931
79	H	26.7131	4.73966273966
82	H	27.9635	3.58429198429
83	H	28.9794	2.6455994456
84	H	28.3250	3.25026565027
86	H	26.1759	5.23603603604
88	H	31.0190	0.761007161007
89	H	30.7766	0.984984984985
90	H	30.5911	1.15638715639
93	H	26.5660	4.87558327558
98	H	27.9022	3.64093324093
99	H	28.4635	3.12229152229
101	H	28.5908	3.00466620467
102	H	28.2118	3.35486255486
103	H	28.6847	2.9179025179
108	H	27.9147	3.62938322938
112	H	29.1511	2.48694848695
113	H	30.6155	1.13384153384
114	H	30.1671	1.54816354816
116	H	28.9001	2.71887271887
117	H	28.5653	3.02822822823
118	H	28.2830	3.28907368907
121	H	26.9163	4.55190575191
123	H	25.0308	6.29410949411
127	H	27.7041	3.82397782398
129	H	30.3477	1.38128898129
130	H	27.9480	3.59861399861
132	H	29.8931	1.80133980134
134	H	30.4543	1.28279048279
135	H	30.5816	1.16516516517
136	H	31.1278	0.660475860476
138	H	31.0397	0.74188034188
139	H	30.6044	1.1440979441
140	H	30.6339	1.11683991684
145	H	27.1195	4.36414876415
147	H	28.2476	3.32178332178
148	H	28.8371	2.77708477708
149	H	28.4826	3.10464310464
151	H	30.4113	1.32252252252
152	H	30.5868	1.16036036036
153	H	30.4209	1.31365211365
155	H	25.4223	5.93236313236
159	H	28.6792	2.92298452298
162	H	28.8759	2.74123354123
163	H	28.2336	3.33471933472
164	H	28.7539	2.85396165396
166	H	28.3426	3.234003234
168	H	30.1822	1.53421113421
169	H	29.9150	1.7811041811
171	H	30.5805	1.16618156618
172	H	30.8092	0.954862554863
173	H	30.8076	0.956340956341
175	H	31.2991	0.502194502195
176	H	30.7456	1.01362901363
177	H	30.7481	1.01131901132
179	H	28.9466	2.67590667591
180	H	29.2671	2.37976437976
181	H	29.1972	2.44435204435
185	H	28.9277	2.69337029337
186	H	28.8257	2.78761838762
193	H	24.4810	6.80212520213
194	H	24.2009	7.06093786094
195	H	24.4448	6.83557403557
196	H	24.6432	6.65225225225
199	H	27.7990	3.73629013629
200	H	27.8572	3.68251328251
201	H	28.1573	3.40522060522

Comparison of Computational and Experimental NMR Data

Revised Mandelalide A (DFT Methodologies)

Atom Number	Boltzmann Avg (Comp δ)	Exp δ	Δδ (|Comp δ – Exp δ|)
C1	83.22	82.2	1.02
C2	72.21	73	0.79
C3	32.98	34.1	1.12
C6	70.85	72.3	1.45
C8	64.37	66.1	1.73
C14	167.76	167.4	0.36
C16	121.34	123.1	1.76
C18	154.16	147.1	7.06
C20	40.73	38.8	1.93
C23	73.61	73.9	0.29
C29	35.35	36.8	1.45
C32	39.10	37.3	1.80
C34	12.99	14.5	1.51
C38	81.18	81	0.18
C42	71.09	72.5	1.41
C44	42.76	43.1	0.34

C45	35.70	34.2	1.50
C47	16.04	18.3	2.26
C51	143.40	141.5	1.90
C53	123.54	123.9	0.36
C55	130.81	131.3	0.49
C57	129.14	126.9	2.24
C59	33.35	31.1	2.25
C64	39.55	39.7	0.15
C67	75.76	73.1	2.66
C69	95.68	94.2	1.48
C72	37.86	37.6	0.26
C76	68.88	68.1	0.78
C77	16.13	17.7	1.57
C82	72.19	74.3	2.11
C86	69.93	71.7	1.77
C90	79.25	80.8	1.55
C92	55.32	59.1	3.78
		CMAD	1.56
		Largest Δδ	7.06
		stdev	1.29

Atom Number	Boltzmann Avg (Comp δ)	Exp δ	Δδ (|Comp δ – Exp δ|)
H4	1.51	1.46	0.05
H5	1.57	1.76	0.19
H7	5.12	5.23	0.11
H11	3.55	3.61	0.06
H12	3.39	3.81	0.42
H17	5.91	6.01	0.10
H19	7.17	6.97	0.20
H21	2.37	2.39	0.02
H22	2.33	2.36	0.03
H24	3.49	3.36	0.13
H27	3.53	3.42	0.11
H28	3.58	3.63	0.05
H30	1.37	1.17	0.20
H31	1.79	2.01	0.22
H33	2.51	2.52	0.01
H35	1.05	1.03	0.02
H36	1.02	1.03	0.01
H37	0.97	1.03	0.06
H39	3.77	3.98	0.21
H43	3.24	3.32	0.08
H46	2.52	2.37	0.15
H48	0.74	0.85	0.11
H49	0.80	0.85	0.05
H50	1.05	0.85	0.20
H52	5.56	5.45	0.11
H54	6.20	6.28	0.08
H56	6.29	6.05	0.24
H8	5.27	5.28	0.01
H60	1.77	1.88	0.11
H61	2.35	2.28	0.07
H62	1.38	1.51	0.13
H63	1.13	1.21	0.08
H65	2.00	1.87	0.13
H66	1.15	1.22	0.07
H70	4.81	5.02	0.21
H71	3.68	3.82	0.14
H73	1.84	2.02	0.18
H74	1.18	1.2	0.02
H78	1.13	1.27	0.14
H79	1.31	1.27	0.04
H80	1.06	1.27	0.21
H81	3.53	3.62	0.09
H83	3.38	3.34	0.04

H89	3.66	3.68	0.02
H93	3.20	3.45	0.25
H94	3.26	3.45	0.19
H95	3.19	3.45	0.26
H96	3.25	3.4	0.15
		CMAD	0.12
		Largest Δδ	0.42
		stdev	0.09

Original Mandelalide A (DFT Methodologies)

Atom Number	Boltzmann Avg (Comp δ)	Exp δ	Δδ (|Comp δ – Exp δ|)
C1	82.84	82.2	0.64
C2	70.55	73	2.45
C3	33.36	34.1	0.74
C6	71.67	72.3	0.63
C8	65.39	66.1	0.71
C14	167.70	167.4	0.30
C16	122.39	123.1	0.71
C18	152.07	147.1	4.97
C20	38.71	38.8	0.09
C23	73.33	73.9	0.57
C29	36.40	36.8	0.40
C32	40.51	37.3	3.21
C34	13.10	14.5	1.40
C38	79.94	81	1.06
C42	73.44	72.5	0.94
C44	42.31	43.1	0.79
C45	36.27	34.2	2.07
C47	18.79	18.3	0.49
C51	139.18	141.5	2.32
C53	127.83	123.9	3.93
C55	133.86	131.3	2.56
C57	129.96	126.9	3.06
C59	36.26	31.1	5.16
C64	38.39	39.7	1.31
C67	71.04	73.1	2.06
C69	91.57	94.2	2.63
C72	34.08	37.6	3.52
C76	67.87	68.1	0.23
C77	16.35	17.7	1.35
C82	72.34	74.3	1.96
C86	70.45	71.7	1.25
C90	79.67	80.8	1.13
C92	55.61	59.1	3.49
		CMAD	1.76
		Largest Δδ	5.16
		stdev	1.37

Atom Number	Boltzmann Avg (Comp δ)	Exp δ	Δδ (|Comp δ – Exp δ|)
H4	1.41	1.46	0.05
H5	1.70	1.76	0.06
H7	5.20	5.23	0.03
H11	3.68	3.61	0.07
H12	3.43	3.81	0.38
H17	5.95	6.01	0.06
H19	7.34	6.97	0.37
H21	2.31	2.39	0.08
H22	2.67	2.36	0.31
H24	3.50	3.36	0.14
H27	3.32	3.42	0.10
H28	3.60	3.63	0.03
H30	1.79	2.01	0.22
H31	1.26	1.17	0.09
H33	2.57	2.52	0.05
H35	1.03	1.03	0.00

H36	1.07	1.03	0.04
H37	1.11	1.03	0.08
H39	4.04	3.98	0.06
H43	3.35	3.32	0.03
H46	2.44	2.37	0.07
H48	1.04	0.85	0.19
H49	0.86	0.85	0.01
H50	1.00	0.85	0.15
H52	5.66	5.45	0.21
H54	5.85	6.28	0.43
H56	6.11	6.05	0.06
H8	5.51	5.28	0.23
H60	2.19	1.88	0.31
H61	2.25	2.28	0.03
H62	1.43	1.51	0.08
H63	1.24	1.21	0.03
H65	1.72	1.87	0.15
H66	1.17	1.22	0.05
H70	4.99	5.02	0.03
H71	3.84	3.82	0.02
H73	1.90	2.02	0.12
H74	1.42	1.2	0.22
H78	1.14	1.27	0.13
H79	1.30	1.27	0.03
H80	1.15	1.27	0.12
H81	3.57	3.62	0.05
H83	3.21	3.34	0.13
H89	3.37	3.68	0.31
H93	3.36	3.45	0.09
H94	3.25	3.45	0.20
H95	3.18	3.45	0.27
H96	3.31	3.4	0.09
		CMAD	0.13
		Largest Δδ	0.43
		Stdev	0.11

Revised Mandelalide A (MM Methodologies)

Atom Number	Boltzmann Avg (Comp δ)	Exp δ	Δδ (|Comp δ – Exp δ|)
C1	84.33	82.2	2.13
C2	72.21	73	0.79
C3	34.16	34.1	0.06
C6	69.24	72.3	3.06
C8	63.53	66.1	2.57
C14	164.27	167.4	3.13
C16	124.02	123.1	0.92
C18	152.33	147.1	5.23
C20	41.35	38.8	2.55
C23	72.03	73.9	1.87
C29	35.52	36.8	1.28
C32	36.56	37.3	0.74
C34	13.86	14.5	0.64
C38	80.48	81	0.52
C42	69.52	72.5	2.98
C44	43.11	43.1	0.01
C45	36.60	34.2	2.40
C47	16.93	18.3	1.37
C51	142.02	141.5	0.52
C53	123.05	123.9	0.85
C55	129.55	131.3	1.75
C57	128.95	126.9	2.05
C59	31.26	31.1	0.16
C64	40.00	39.7	0.30
C67	73.74	73.1	0.64
C69	96.78	94.2	2.58
C72	38.35	37.6	0.75
C76	67.43	68.1	0.67

C77	17.08	17.7	0.62
C82	74.25	74.3	0.05
C86	71.64	71.7	0.06
C90	79.22	80.8	1.58
C92	54.57	59.1	4.53
		CMAD	1.49
		Largest Δδ	5.23
		stdev	1.31

Atom Number	Boltzmann Avg (Comp δ)	Exp δ	Δδ (|Comp δ – Exp δ|)
H4	1.92	1.76	0.16
H5	1.49	1.46	0.03
H7	4.88	5.23	0.35
H11	3.39	3.61	0.22
H12	3.73	3.81	0.08
H17	5.93	6.01	0.08
H19	7.11	6.97	0.14
H21	2.28	2.39	0.11
H22	2.26	2.36	0.10
H24	3.22	3.36	0.14
H27	3.64	3.42	0.22
H28	3.65	3.63	0.02
H30	1.22	1.17	0.05
H31	1.74	2.01	0.27
H33	2.39	2.52	0.13
H35	0.82	1.03	0.21
H36	1.08	1.03	0.05
H37	1.06	1.03	0.03
H39	3.82	3.98	0.16
H43	3.12	3.32	0.20
H46	2.44	2.37	0.07
H48	0.82	0.85	0.03
H49	0.51	0.85	0.34
H50	1.15	0.85	0.30
H52	5.45	5.45	0.00
H54	6.23	6.28	0.05
H56	5.90	6.05	0.15
H8	5.20	5.28	0.08
H60	1.82	1.88	0.06
H61	2.22	2.28	0.06
H62	1.48	1.51	0.03
H63	1.17	1.21	0.04
H65	2.11	1.87	0.24
H66	1.10	1.22	0.12
H70	4.97	5.02	0.05
H71	3.62	3.82	0.20
H73	1.81	2.02	0.21
H74	1.18	1.20	0.02
H78	0.99	1.27	0.28
H79	1.11	1.27	0.16
H80	1.39	1.27	0.12
H81	3.39	3.62	0.23
H83	3.31	3.34	0.03
H89	3.64	3.68	0.04
H93	3.15	3.45	0.30
H94	2.97	3.45	0.48
H95	3.20	3.45	0.25
H96	3.37	3.40	0.03
		CMAD	0.14
		Largest Δδ	0.48
		stdev	0.11
		DP4	99.9%

Original Mandelalide A (MM Methodologies)

Atom Number	Boltzmann Avg (Comp δ)	Exp δ	Δδ (|Comp δ – Exp δ|)
C1	83.79	82.2	1.59
C2	71.41	73	1.59
C3	34.71	34.1	0.61
C6	69.81	72.3	2.49
C8	65.10	66.1	1.00
C14	165.71	167.4	1.69
C16	125.30	123.1	2.20
C18	151.79	147.1	4.69
C20	39.21	38.8	0.41
C23	72.78	73.9	1.12
C29	37.18	36.8	0.38
C32	37.17	37.3	0.13
C34	13.24	14.5	1.26
C38	78.13	81	2.87
C42	71.43	72.5	1.07
C44	43.32	43.1	0.22
C45	36.20	34.2	2.00
C47	20.14	18.3	1.84
C51	139.05	141.5	2.45
C53	128.43	123.9	4.53
C55	134.18	131.3	2.88
C57	130.81	126.9	3.91
C59	36.51	31.1	5.41
C64	39.03	39.7	0.67
C67	68.93	73.1	4.17
C69	92.93	94.2	1.27
C72	34.70	37.6	2.90
C76	65.64	68.1	2.46
C77	17.38	17.7	0.32
C82	74.04	74.3	0.26
C86	71.75	71.7	0.05
C90	79.93	80.8	0.87
C92	54.90	59.1	4.20
		CMAD	1.94
		Largest Δδ	5.41
		stdev	1.50

Atom Number	Boltzmann Avg (Comp δ)	Exp δ	Δδ (|Comp δ – Exp δ|)
H4	1.93	1.76	0.26
H5	1.50	1.46	0.47
H7	4.95	5.23	0.28
H11	3.84	3.61	0.23
H12	3.35	3.81	0.46
H17	6.00	6.01	0.01
H19	7.21	6.97	0.24
H21	2.30	2.39	0.09
H22	2.58	2.36	0.22
H24	3.33	3.36	0.03
H27	3.49	3.42	0.07
H28	3.61	3.63	0.02
H30	1.75	1.17	0.58
H31	1.13	2.01	0.88
H33	2.44	2.52	0.08
H35	0.88	1.03	0.15
H36	1.12	1.03	0.09
H37	1.07	1.03	0.04
H39	4.09	3.98	0.11
H43	3.23	3.32	0.09
H46	2.50	2.37	0.13
H48	0.85	0.85	0.00
H49	0.81	0.85	0.04

H50	1.19	0.85	0.34
H52	5.51	5.45	0.06
H54	5.75	6.28	0.53
H56	6.12	6.05	0.07
H8	5.55	5.28	0.27
H60	2.25	1.88	0.37
H61	2.28	2.28	0.00
H62	1.63	1.51	0.12
H63	1.28	1.21	0.07
H65	1.78	1.87	0.09
H66	2.07	1.22	0.85
H70	3.39	5.02	1.63
H71	2.92	3.82	0.90
H73	2.31	2.02	0.29
H74	2.10	1.2	0.90
H78	2.04	1.27	0.77
H79	2.11	1.27	0.84
H80	1.96	1.27	0.69
H81	2.87	3.62	0.75
H83	2.72	3.34	0.62
H89	2.79	3.68	0.89
H93	2.66	3.45	0.79
H94	2.66	3.45	0.79
H95	2.61	3.45	0.84
H96	2.67	3.4	0.73
		CMAD	0.39
		Largest Δδ	1.63
		Stdev	0.37
		DP4	0.11 %

Revised Mandelalide A (MD Methodologies)

Atom Number	Boltzmann Avg (Comp δ)	Exp δ	Δδ (|Comp δ – Exp δ|)
C1	89.89	82.2	7.69
C2	66.59	73	6.41
C3	36.68	34.1	2.58
C6	77.47	72.3	5.17
C8	72.41	66.1	6.31
C14	173.62	167.4	6.22
C16	118.39	123.1	4.71
C18	146.58	147.1	0.52
C20	39.52	38.8	0.72
C23	73.50	73.9	1.20
C29	36.85	36.8	0.05
C32	34.70	37.3	2.60
C34	13.06	14.5	1.44
C38	79.88	81	1.12
C42	75.00	72.5	2.50
C44	46.41	43.1	3.31
C45	32.86	34.2	1.34
C47	19.15	18.3	0.85
C51	134.15	141.5	7.35
C53	129.52	123.9	5.62
C55	134.29	131.3	2.99
C57	131.01	126.9	4.11
C59	37.29	31.1	6.19
C64	41.34	39.7	1.64
C67	67.85	73.1	5.25
C69	97.39	94.2	3.19
C72	34.97	37.6	2.63
C76	63.43	68.1	4.67
C77	17.47	17.7	0.23
C82	74.54	74.3	0.24
C86	73.43	71.7	1.73
C90	83.38	80.8	2.58

C92	58.81	59.1	0.29
		CMAD	3.13
		Largest Δδ	7.69
		stdev	2.31

Atom Number	Boltzmann Avg (Comp δ)	Exp δ	Δδ (|Comp δ – Exp δ|)
H4	1.29	1.76	0.47
H5	1.48	1.46	0.02
H7	5.39	5.23	0.16
H11	3.66	3.61	0.05
H12	3.80	3.81	0.01
H17	5.88	6.01	0.13
H19	7.28	6.97	0.31
H21	2.23	2.39	0.16
H22	2.53	2.36	0.17
H24	2.79	3.36	0.57
H27	3.36	3.42	0.06
H28	3.51	3.63	0.12
H30	1.77	1.17	0.60
H31	1.32	2.01	0.69
H33	2.40	2.52	0.12
H35	0.86	1.03	0.17
H36	0.92	1.03	0.11
H37	1.14	1.03	0.11
H39	4.00	3.98	0.02
H43	3.30	3.32	0.02
H46	3.44	2.37	1.07
H48	1.18	0.85	0.33
H49	0.70	0.85	0.15
H50	0.98	0.85	0.13
H52	5.54	5.45	0.09
H54	6.30	6.28	0.02
H56	6.01	6.05	0.04
H8	5.74	5.28	0.46
H60	2.13	1.88	0.25
H61	2.04	2.28	0.24
H62	2.13	1.51	0.62
H63	1.33	1.21	0.12
H65	1.59	1.87	0.28
H66	1.21	1.22	0.01
H70	5.40	5.02	0.38
H71	3.94	3.82	0.12
H73	2.06	2.02	0.04
H74	1.10	1.2	0.10
H78	1.75	1.27	0.48
H79	1.42	1.27	0.15
H80	1.00	1.27	0.27
H81	3.46	3.62	0.16
H83	3.20	3.34	0.14
H89	3.60	3.68	0.08
H93	3.55	3.45	0.10
H94	3.71	3.45	0.26
H95	3.89	3.45	0.44
H96	3.47	3.4	0.07
		CMAD	0.22
		Largest Δδ	1.07
		Stdev	0.21

Original Mandelalide A (MD Methodologies)

Atom Number	Boltzmann Avg (Comp δ)	Exp δ	Δδ (|Comp δ – Exp δ|)
C1	86.47	82.2	4.27
C2	82.14	73	9.14

C3	42.59	34.1	8.49
C6	83.85	72.3	11.55
C8	78.20	66.1	12.10
C14	171.81	167.4	4.41
C16	128.62	123.1	5.52
C18	156.34	147.1	9.24
C20	46.18	38.8	7.38
C23	76.64	73.9	4.34
C29	43.06	36.8	6.26
C32	50.45	37.3	13.15
C34	17.23	14.5	2.73
C38	96.44	81	15.44
C42	78.75	72.5	6.25
C44	53.15	43.1	10.05
C45	44.45	34.2	10.25
C47	24.04	18.3	5.74
C51	151.07	141.5	9.57
C53	130.66	123.9	6.76
C55	138.31	131.3	7.01
C57	130.17	126.9	3.27
C59	42.03	31.1	10.93
C64	46.51	39.7	6.81
C67	76.75	73.1	3.65
C69	96.05	94.2	1.85
C72	43.72	37.6	6.12
C76	75.11	68.1	7.01
C77	19.71	17.7	2.01
C82	88.15	74.3	13.85
C86	82.73	71.7	11.03
C90	85.16	80.8	4.36
C92	56.71	59.1	2.39
		CMAD	7.36
		Largest Δδ	15.4
		stdev	3.62

Atom Number	Boltzmann Avg (Comp δ)	Exp δ	Δδ (|Comp δ – Exp δ|)
H4	4.27	1.76	0.02
H5	9.14	1.46	0.07
H7	8.49	5.23	0.17
H11	4.03	3.61	0.42
H12	3.86	3.81	0.05
H17	6.36	6.01	0.35
H19	7.34	6.97	0.37
H21	2.55	2.39	0.16
H22	2.58	2.36	0.22
H24	3.47	3.36	0.11
H27	3.81	3.42	0.39
H28	3.64	3.63	0.01
H30	1.82	1.17	0.65
H31	1.84	2.01	0.17
H33	2.49	2.52	0.03
H35	0.77	1.03	0.26
H36	1.01	1.03	0.02
H37	1.17	1.03	0.14
H39	4.32	3.98	0.34
H43	3.88	3.32	0.56
H46	2.57	2.37	0.20
H48	0.39	0.85	0.46
H49	1.27	0.85	0.42
H50	0.96	0.85	0.11
H52	5.67	5.45	0.22
H54	6.88	6.28	0.60
H56	6.15	6.05	0.10
H8	5.55	5.28	0.27
H60	2.07	1.88	0.19

H61	3.05	2.28	0.77
H62	1.72	1.51	0.21
H63	1.60	1.21	0.39
H65	2.10	1.87	0.23
H66	1.27	1.22	0.05
H70	6.04	5.02	1.02
H71	4.18	3.82	0.36
H73	2.32	2.02	0.30
H74	0.87	1.2	0.33
H78	0.99	1.27	0.28
H79	1.13	1.27	0.14
H80	1.67	1.27	0.40
H81	3.61	3.62	0.01
H83	3.58	3.34	0.24
H89	3.95	3.68	0.27
H93	3.45	3.45	0.00
H94	2.82	3.45	0.63
H95	3.47	3.45	0.02
H96	3.28	3.4	0.12
		CMAD	0.28
		Largest Δδ	1.02
		Stdev	0.22

Revised Mandelalide B

Atom Number	Boltzmann Avg (Comp δ)	Exp δ	Δδ (|Comp δ – Exp δ|)
C1	81.92	82.1	0.18
C3	72.71	74.5	1.79
C4	36.54	37.9	1.36
C7	74.98	74.9	0.08
C13	81.90	81.5	0.40
C14	31.89	30.7	1.19
C16	128.34	127.1	1.24
C18	130.94	131	0.06
C20	122.81	123.3	0.49
C22	143.63	142.1	1.53
C23	36.43	33.9	2.53
C25	16.68	18.5	1.82
C29	41.49	42.2	0.71
C32	71.75	72.4	0.65
C37	40.37	38.3	2.07
C38	13.10	14.2	1.10
C43	34.40	35.6	1.20
C46	39.66	39.7	0.04
C49	78.91	79.3	0.39
C52	177.66	175.6	2.06
C55	38.70	39.6	0.90
C58	72.54	73.3	0.76
C60	92.21	94.8	2.59
C63	36.39	37.4	1.01
C66	71.88	72.7	0.82
C67	36.50	36.3	0.20
C70	68.93	69.5	0.57
C72	173.97	173.6	0.37
C74	35.85	36.3	0.45
C77	19.50	18.8	0.70
C80	12.59	14	1.41
C88	67.67	67.4	0.27
C90	15.32	16.6	1.28
C94	73.11	73.3	0.19
C98	64.79	66.6	1.81
C102	80.60	80.9	0.30

C104	55.48	59.6	4.12
		CMAD	1.04
		Largest Δδ	4.12
		stdev	0.87

Atom Number	Boltzmann Avg (Comp δ)	Exp δ	Δδ (|Comp δ – Exp δ|)
H2	3.74	3.77	0.03
H5	1.51	1.64	0.13
H6	1.51	1.51	0.00
H8	4.83	4.84	0.01
H11	3.68	3.76	0.08
H15	2.33	2.31	0.02
H17	5.28	5.28	0.00
H19	6.04	6.1	0.06
H21	6.43	6.4	0.03
H24	2.60	2.5	0.10
H26	1.32	1.07	0.25
H27	0.78	1.07	0.29
H28	1.38	1.07	0.31
H30	1.21	1.18	0.03
H31	1.53	1.57	0.04
H33	3.47	3.39	0.08
H34	5.60	5.5	0.10
H35	1.85	1.9	0.05
H36	3.72	3.95	0.23
H39	0.90	1.03	0.13
H40	1.16	1.03	0.13
H41	1.11	1.03	0.08
H42	2.52	2.52	0.00
H44	1.41	1.33	0.08
H45	1.94	2.05	0.11
H47	2.43	2.39	0.04
H48	1.90	1.93	0.03
H56	1.81	1.81	0.00
H57	1.19	1.23	0.04
H61	4.95	5.04	0.09
H62	3.83	3.75	0.08
H64	1.74	1.89	0.15
H65	0.98	1.1	0.12
H68	1.99	2.14	0.15
H69	1.52	1.59	0.07
H75	2.31	2.35	0.04
H76	2.44	2.35	0.09
H78	1.64	1.67	0.03
H79	1.68	1.67	0.01
H81	0.84	0.95	0.11
H82	0.93	0.95	0.02
H83	1.03	0.95	0.08
H84	5.53	5.48	0.05
H85	3.42	3.3	0.12
H89	3.84	3.85	0.01
H91	1.24	1.23	0.01
H92	0.96	1.23	0.27
H93	1.35	1.23	0.12
H97	3.30	3.49	0.19
H101	3.40	3.74	0.34
H105	3.15	3.45	0.30
H106	3.36	3.45	0.09
H107	3.15	3.45	0.30
H108	3.20	3.33	0.13
		CMAD	0.10

Largest Δδ	0.34
stdev	0.09

Original Mandelalide B

Atom Number	Boltzmann Avg (Comp δ)	Exp δ	Δδ (|Comp δ – Exp δ|)
C1	81.99	82.1	0.11
C3	69.16	74.5	5.34
C4	42.07	37.9	4.17
C7	80.40	74.9	5.50
C13	82.00	81.5	0.50
C14	32.23	30.7	1.53
C16	129.63	127.1	2.53
C18	130.46	131	0.54
C20	120.86	123.3	2.44
C22	144.62	142.1	2.52
C23	37.36	33.9	3.46
C25	21.16	18.5	2.66
C29	42.83	42.2	0.63
C32	74.80	72.4	2.40
C37	38.66	38.3	0.36
C38	12.80	14.2	1.40
C43	35.37	35.6	0.23
C46	42.02	39.7	2.32
C49	76.90	79.3	2.40
C52	181.20	175.6	5.60
C55	39.73	39.6	0.13
C58	79.96	73.3	6.66
C60	97.66	94.8	2.86
C63	38.89	37.4	1.49
C66	68.89	72.7	3.81
C67	35.02	36.3	1.28
C70	75.16	69.5	5.66
C72	172.34	173.6	1.26
C74	34.71	36.3	1.59
C77	18.68	18.8	0.12
C80	12.24	14	1.76
C88	67.72	67.4	0.32
C90	15.66	16.6	0.94
C94	73.15	73.3	0.15
C98	65.47	66.6	1.13
C102	80.70	80.9	0.20
C104	55.28	59.6	4.32
		CMAD	2.17
		Stdev	1.86
		Largest Δδ	6.66

Atom Number	Boltzmann Avg (Comp δ)	Exp δ	Δδ (|Comp δ – Exp δ|)
H2	3.81	3.77	0.04
H5	2.00	1.64	0.36
H6	1.75	1.51	0.24
H8	4.51	4.84	0.33
H11	3.41	3.76	0.35
H15	1.95	2.31	0.36
H17	5.22	5.28	0.06
H19	6.10	6.1	0.00
H21	6.38	6.4	0.02
H24	2.22	2.5	0.28
H26	1.34	1.07	0.27
H27	0.91	1.07	0.16
H28	0.77	1.07	0.30
H30	1.23	1.18	0.05
H31	1.60	1.57	0.03

H33	3.29	3.39	0.10
H34	5.59	5.5	0.09
H35	2.42	1.9	0.52
H36	4.02	3.95	0.07
H39	1.06	1.03	0.03
H40	1.00	1.03	0.03
H41	1.20	1.03	0.17
H42	2.54	2.52	0.02
H44	1.78	1.33	0.45
H45	1.79	2.05	0.26
H47	1.88	2.39	0.51
H48	3.23	1.93	1.30
H56	1.87	1.81	0.06
H57	1.20	1.23	0.03
H61	5.00	5.04	0.04
H62	3.76	3.75	0.01
H64	1.79	1.89	0.10
H65	1.56	1.1	0.46
H68	2.02	2.14	0.12
H69	1.95	1.59	0.36
H75	2.08	2.35	0.27
H76	2.29	2.35	0.06
H78	1.52	1.67	0.15
H79	1.63	1.67	0.04
H81	1.13	0.95	0.18
H82	0.76	0.95	0.19
H83	0.94	0.95	0.01
H84	5.02	5.48	0.46
H85	3.48	3.3	0.18
H89	3.89	3.85	0.04
H91	1.02	1.23	0.21
H92	1.31	1.23	0.08
H93	1.28	1.23	0.05
H97	3.34	3.49	0.15
H101	3.47	3.74	0.27
H105	2.97	3.45	0.48
H106	3.39	3.45	0.06
H107	3.41	3.45	0.04
H108	3.20	3.33	0.13
		CMAD	0.20
		stdev	0.21
		Largest Δδ	1.30

Revised Mandelalide C

Atom Number	Boltzmann Avg (Comp δ)	Exp δ	Δδ (|Comp δ – Exp δ|)
C1	81.84	82.4	0.56
C3	72.80	74.4	1.60
C4	31.36	32.1	0.74
C7	79.23	78.9	0.33
C13	81.95	81.6	0.35
C14	31.12	30.7	0.42
C16	128.51	127.1	1.41
C18	131.21	131.1	0.11
C20	123.53	123.2	0.33
C22	144.16	142.2	1.96
C23	36.57	34	2.57
C25	16.64	18.4	1.76
C29	41.13	42.1	0.97
C32	72.14	72.3	0.16
C37	40.42	38.3	2.12
C38	13.08	14.2	1.12
C43	34.66	35.7	1.04
C46	71.72	72.2	0.48

C48	81.42	82	0.58
C51	176.49	174.7	1.79
C54	40.96	41.2	0.24
C57	68.40	68.3	0.10
C60	41.31	41.2	0.11
C63	71.54	72.3	0.76
C64	36.55	36.4	0.15
C67	67.90	68.3	0.40
C69	173.91	173.4	0.51
C71	35.60	36.3	0.70
C74	19.27	18.7	0.57
C77	12.58	13.9	1.32
		CMAD	0.84
		Largest Δδ	2.57
		stdev	0.68

Atom Number	Boltzmann Avg (Comp δ)	Exp δ	Δδ (|Comp δ – Exp δ|)
H2	3.71	3.82	0.11
H5	1.45	1.59	0.14
H6	1.87	1.82	0.05
H8	5.02	5.01	0.01
H11	3.67	3.73	0.06
H15	2.31	2.3	0.01
H17	5.24	5.28	0.04
H19	6.20	6.1	0.10
H21	6.49	6.39	0.10
H24	2.53	2.49	0.04
H26	1.66	1.06	0.60
H27	1.07	1.06	0.01
H28	0.56	1.06	0.50
H30	1.19	1.19	0.00
H31	1.45	1.57	0.12
H33	3.39	3.37	0.02
H34	5.56	5.5	0.06
H35	1.96	1.9	0.06
H36	3.77	3.95	0.18
H39	1.08	1.03	0.05
H40	1.20	1.03	0.17
H41	0.80	1.03	0.23
H42	2.47	2.53	0.06
H44	1.36	1.33	0.03
H45	1.92	2.1	0.18
H55	1.78	1.83	0.05
H56	0.89	1.13	0.24
H59	3.47	3.76	0.29
H61	1.66	1.86	0.20
H62	0.90	1.11	0.21
H65	1.91	2.14	0.23
H66	1.55	1.65	0.10
H72	2.37	2.34	0.03
H73	2.37	2.34	0.03
H75	1.64	1.65	0.01
H76	1.64	1.65	0.01
H78	0.84	0.94	0.10
H79	1.08	0.94	0.14
H80	0.85	0.94	0.09
H81	5.56	5.51	0.05
H82	3.27	3.25	0.02
H85	3.91	3.98	0.07
		CMAD	0.18
		Largest Δδ	0.60
		stdev	0.12

Original Mandelalide C

Atom Number	Boltzmann Avg (Comp δ)	Exp δ	Δδ (|Comp δ – Exp δ|)
C1	80.87	82.4	1.53
C3	69.56	74.4	4.84
C4	32.79	32.1	0.69
C7	83.43	78.9	4.53
C13	82.49	81.6	0.89
C14	30.96	30.7	0.26
C16	129.71	127.1	2.61
C18	130.68	131.1	0.42
C20	123.40	123.2	0.20
C22	142.95	142.2	0.75
C23	35.50	34	1.50
C25	19.13	18.4	0.73
C29	42.77	42.1	0.67
C32	71.75	72.3	0.55
C37	38.90	38.3	0.60
C38	13.22	14.2	0.98
C43	35.85	35.7	0.15
C46	70.35	72.2	1.85
C49	79.70	82	2.30
C52	179.58	174.7	4.88
C55	38.29	41.8	3.51
C58	68.51	68.3	0.21
C61	37.64	41.2	3.56
C64	71.73	71.3	0.43
C65	36.00	36.4	0.40
C68	72.61	68.3	4.31
C70	173.08	173.4	0.32
C72	36.50	36.3	0.20
C75	18.90	18.7	0.20
C78	12.68	13.9	1.22
		CMAD	1.51
		Largest Δδ	4.88
		stdev	1.55

Atom Number	Boltzmann Avg (Comp δ)	Exp δ	Δδ (|Comp δ – Exp δ|)
H2	3.88	3.82	0.06
H5	1.69	1.59	0.10
H6	2.51	1.82	0.69
H8	4.64	5.01	0.37
H11	3.38	3.73	0.35
H15	1.92	2.30	0.38
H17	5.20	5.28	0.08
H19	6.23	6.10	0.13
H21	6.23	6.39	0.16
H24	2.47	2.49	0.02
H26	1.30	1.06	0.24
H27	0.91	1.06	0.15
H28	0.65	1.06	0.41
H30	1.23	1.19	0.04
H31	1.50	1.57	0.07
H33	3.33	3.37	0.04
H34	5.46	5.50	0.04
H35	2.49	1.90	0.59
H36	3.95	3.95	0.00
H39	1.02	1.03	0.01
H40	0.81	1.03	0.22
H41	1.19	1.03	0.16
H42	2.40	2.53	0.13
H44	1.73	1.33	0.40
H45	1.82	2.10	0.28
H48	4.85	3.98	0.87

H56	1.61	1.83	0.22
H57	1.14	1.13	0.01
H60	3.71	3.76	0.05
H62	1.65	1.11	0.54
H63	1.78	1.86	0.08
H66	1.88	1.65	0.23
H77	2.13	2.14	0.01
H73	2.28	2.34	0.06
H74	2.23	2.34	0.11
H76	1.49	1.65	0.16
H77	1.49	1.65	0.16
H79	1.14	0.94	0.20
H80	0.80	0.94	0.14
H81	0.77	0.94	0.17
H82	5.18	5.51	0.33
H83	3.45	3.25	0.20
		CMAD	0.20
		Largest Δδ	0.87
		Stdev	0.19

Revised Mandelalide D

Atom Number	Boltzmann Avg (Comp δ)	Exp δ	Δδ (|Comp δ – Exp δ|)
C1	82.01	82.2	0.19
C3	73.09	74.3	1.21
C4	31.82	32.5	0.68
C7	77.71	76.7	1.01
C13	81.46	81.6	0.14
C14	31.65	30.6	1.05
C16	128.59	127.1	1.49
C18	131.04	131.1	0.06
C20	122.75	123.1	0.35
C22	143.53	142.3	1.23
C23	36.73	34.2	2.53
C25	17.15	18.3	1.15
C29	41.00	42.1	1.10
C32	71.45	72.2	0.75
C37	40.60	38.3	2.30
C38	12.94	14.3	1.36
C43	34.70	35.7	1.00
C46	73.14	74	0.86
C48	81.22	81.3	0.08
C51	176.74	172.9	3.84
C54	39.52	41.8	2.28
C57	68.04	68.4	0.36
C60	40.09	41.2	1.11
C63	70.85	72.2	1.35
C64	34.64	36.2	1.56
C67	68.05	68.6	0.55
C69	175.06	173.6	1.46
C71	35.30	36.3	1.00
C74	18.70	18.6	0.10
C77	12.40	13.9	1.50
C86	172.82	173.1	0.28
C87	37.28	36	1.28
C88	21.16	18.6	2.56
C89	13.35	13.8	0.45
		CMAD	1.12
		Largest Δδ	3.84
		stdev	0.84

Atom Number	Boltzmann Avg (Comp δ)	Exp δ	Δδ (|Comp δ – Exp δ|)
H2	3.68	3.79	0.11

H5	1.32	1.47	0.15
H6	1.72	1.65	0.07
H8	5.40	5.13	0.27
H11	3.68	3.73	0.05
H15	2.34	2.29	0.05
H17	5.29	5.28	0.01
H19	6.10	6.1	0.00
H21	6.41	6.38	0.03
H24	2.55	2.48	0.07
H26	1.45	1.07	0.38
H27	1.19	1.07	0.12
H28	0.56	1.07	0.51
H30	1.22	1.19	0.03
H31	1.51	1.57	0.06
H33	3.34	3.36	0.02
H34	5.56	5.5	0.06
H35	1.96	1.9	0.06
H36	3.77	3.94	0.17
H39	1.07	1.04	0.03
H40	1.19	1.04	0.15
H41	0.82	1.04	0.22
H42	2.55	2.56	0.01
H44	1.34	1.34	0.00
H45	1.96	2.08	0.12
H55	1.69	1.83	0.14
H56	1.04	1.12	0.08
H59	3.66	3.75	0.09
H61	1.63	1.85	0.22
H62	1.09	1.12	0.03
H65	1.87	2.18	0.31
H66	1.66	1.68	0.02
H72	2.30	2.4	0.10
H73	2.74	2.43	0.31
H75	1.42	1.7	0.28
H76	1.90	1.7	0.20
H78	0.62	0.96	0.34
H79	1.06	0.96	0.10
H80	1.03	0.96	0.07
H81	5.59	5.56	0.03
H82	3.08	3.21	0.13
H85	5.19	5.17	0.02
H91	2.16	2.31	0.15
H92	2.29	2.33	0.04
H93	1.17	0.93	0.24
H94	0.84	0.93	0.09
H95	1.63	1.63	0.00
H96	1.59	1.63	0.04
H97	0.83	0.93	0.10
		CMAD	0.12
		Largest Δδ	0.51
		stdev	0.11

Original Mandelalide D

Atom Number	Boltzmann Avg (Comp δ)	Exp δ	Δδ (|Comp δ – Exp δ|)
C1	82.2	82.2	0.02
C3	72.9	74.3	1.43
C4	31.1	32.5	1.37
C7	76.7	76.7	0.00
C13	82.0	81.6	0.42
C14	31.6	30.6	0.99
C16	129.1	127.1	1.99
C18	130.8	131.1	0.30
C20	122.7	123.1	0.35
C22	144.2	142.3	1.92

C23	35.5	34.2	1.28
C25	17.8	18.3	0.51
C29	42.5	42.1	0.39
C32	70.3	72.2	1.94
C37	40.2	38.3	1.88
C38	13.0	14.3	1.33
C43	34.9	35.7	0.79
C46	73.5	74	0.45
C49	81.4	81.3	0.08
C52	177.3	172.9	4.42
C55	42.0	41.8	0.23
C58	68.0	68.4	0.40
C61	36.2	41.2	4.99
C64	71.5	72.2	0.69
C65	32.9	36.2	3.29
C68	65.9	68.6	2.70
C70	175.4	173.6	1.83
C72	36.3	36.3	0.01
C75	19.1	18.6	0.51
C78	12.8	13.9	1.06
C85	172.3	173.1	0.76
C87	34.3	36	1.70
C88	18.7	18.6	0.09
C89	12.3	13.8	1.49
		CMAD	1.25
		Largest Δδ	4.99
		stdev	1.26

Atom Number	Boltzmann Avg (Comp δ)	Exp δ	Δδ (|Comp δ – Exp δ|)
H2	3.70	3.79	0.09
H5	1.75	1.47	0.28
H6	1.28	1.65	0.37
H8	5.25	5.13	0.12
H11	3.64	3.73	0.09
H15	1.96	2.29	0.33
H17	5.22	5.28	0.06
H19	6.16	6.1	0.06
H21	6.35	6.38	0.03
H24	2.53	2.48	0.05
H26	1.17	1.07	0.10
H27	0.89	1.07	0.18
H28	0.54	1.07	0.53
H30	1.11	1.19	0.08
H31	1.62	1.57	0.05
H33	3.37	3.36	0.01
H34	5.46	5.5	0.04
H35	2.33	1.9	0.43
H36	3.84	3.94	0.10
H39	1.05	1.04	0.01
H40	0.80	1.04	0.24
H41	1.17	1.04	0.13
H42	2.52	2.56	0.04
H44	2.00	1.34	0.66
H45	1.36	2.08	0.72
H48	5.27	5.17	0.10
H56	1.48	1.83	0.35
H57	1.11	1.12	0.01
H60	3.63	3.75	0.12
H62	1.53	1.85	0.32
H63	0.95	1.12	0.17
H66	1.54	2.18	0.64
H67	2.33	1.68	0.65
H73	2.50	2.4	0.10
H74	2.31	2.43	0.12

H76	1.55	1.7	0.15
H78	1.71	1.7	0.01
H79	1.25	0.96	0.29
H80	0.82	0.96	0.14
H81	0.82	0.96	0.14
H82	5.54	5.56	0.02
H83	3.36	3.21	0.15
H91	2.22	2.31	0.09
H92	2.55	2.33	0.22
H93	1.39	1.63	0.24
H94	1.86	1.63	0.23
H95	1.04	0.93	0.11
H96	0.60	0.93	0.33
H97	1.00	0.93	0.07
		CMAD	0.20
		Largest Δδ	0.72
		stdev	0.19

Proposed Revised [D-N,O-diMe-Ser] Coibamide A

Atom Number	Boltzmann Avg (Comp δ)	Exp δ	Δδ (|Comp δ – Exp δ|)
C2	42.2	41.3	2.81
C6	34.8	Same as Atom 2	
C10	75.6	73.8	1.76
C12	30.6	27.6	3.01
C14	18.7	19.5	0.76
C18	19.4	19.6	0.17
C22	174.7	172.4	2.30
C24	76.1	74.7	1.40
C27	32.2	29.9	2.28
C29	15.7	18	0.31
C33	20.9	Same as Atom 29	
C37	172.2	170	2.21
C39	57.4	52.6	4.79
C42	30.5	30.2	0.35
C46	68.8	69.3	0.52
C50	56.2	58.6	2.38
C54	54.3	51.1	3.18
C56	173.3	170.5	2.81
C59	29.6	31.2	1.62
C63	36.5	37.9	1.40
C66	28.1	25.3	2.76
C68	20.3	23.1	2.84
C72	22.8	21.2	1.56
C76	176.8	170.5	6.32
C78	67.7	NOT OBSERVED	
C81	39.2	29.7	9.52
C85	74.1	68	6.08
C87	16.9	18.4	1.45
C92	62.4	52.8	9.64
C94	170.0	169.7	0.34
C97	75.0	68.6	6.41
C100	56.0	58.8	2.83
C105	173.8	168.7	5.13
C107	64.0	51.1	12.89
C109	176.9	170.4	6.46
C111	16.2	12.9	3.33
C115	35.7	30.1	5.64
C120	56.5	50	6.51
C124	171.1	171.2	0.06
C126	65.2	63.6	1.64
C128	38.9	36.1	2.78
C131	27.1	24.9	2.17
C133	19.1	21.4	2.25

C137	22.0	23.2	1.22
C142	176.5	171.5	5.03
C144	49.5	47	2.53
C146	39.2	39.4	0.25
C150	18.5	18.6	0.05
C156	167.6	167.2	0.38
C158	55.3	64.8	9.53
C161	37.7	28.9	8.77
C165	38.8	32	6.75
C167	28.2	24.2	4.01
C170	12.5	11.6	0.86
C174	15.6	15.7	0.06
C178	33.4	30	3.36
C182	175.5	171.4	4.12
C184	37.3	38.9	1.61
C187	156.0	158.6	2.55
C188	108.4	113.7	0.61
C189	128.4	130.4	0.75
C190	129.8	128.4	1.44
C191	130.9	Same as Atom 189	
C192	117.7	Same as Atom 188	
C198	52.0	55.3	3.34
		CMAD	3.17
		STDEV	2.83
		Largest Δδ	12.89

Atom Number	Boltzmann Avg (Comp δ)	Exp δ	Δδ (|Comp δ – Exp δ|)
H3	1.95	2.34	0.20
H4	2.24	Same as above (Methyl Group)	
H5	2.23	Same as above (Methyl Group)	
H7	1.95	2.34	0.12
H8	2.37	Same as above (Methyl Group)	
H9	2.33	Same as above (Methyl Group)	
H11	2.66	2.84	0.18
H13	2.12	2.02	0.10
H15	0.52	0.99	0.07
H16	1.37	Same as above (Methyl Group)	
H17	0.87	Same as above (Methyl Group)	
H19	0.62	1.04	0.19
H20	1.11	Same as above (Methyl Group)	
H21	0.83	Same as above (Methyl Group)	
H25	5.05	5	0.05
H28	2.06	2.21	0.15
H30	0.95	1.06	0.12
H31	1.04	Same as above (Methyl Group)	
H32	0.83	Same as above (Methyl Group)	
H34	1.16	1.06	0.02
H35	1.07	Same as above (Methyl Group)	
H36	1.01	Same as above (Methyl Group)	
H40	5.21	6.02	0.81
H43	3.44	3.04	0.08
H44	2.90	Same as above (Methyl Group)	
H45	3.00	Same as above (Methyl Group)	
H47	3.43	3.9	0.47
H48	3.63	3.64	0.01
H51	3.47	3.35	0.16
H52	3.05	Same as above (Methyl Group)	
H53	3.04	Same as above (Methyl Group)	
H55	4.92	5.34	0.42
H60	3.31	3.13	0.07
H61	2.92	Same as above (Methyl Group)	
H62	2.95	Same as above (Methyl Group)	
H64	1.90	1.68	0.22
H65	1.45	1.31	0.14
H67	1.58	1.36	0.22

H69	0.57	0.89	0.02
H70	1.13	Same as above (Methyl Group)	
H71	0.90	Same as above (Methyl Group)	
H73	1.02	0.92	0.00
H74	0.70	Same as above (Methyl Group)	
H75	1.05	Same as above (Methyl Group)	
H79	4.22	6.35	2.13
H82	2.54	2.89	0.31
H83	3.69	Same as above (Methyl Group)	
H84	3.36	Same as above (Methyl Group)	
H86	5.24	5.5	0.26
H88	1.75	1.07	0.50
H89	1.15	Same as above (Methyl Group)	
H90	1.81	Same as above (Methyl Group)	
H93	4.53	5.69	1.16
H98	3.51	3.83	0.32
H99	3.61	3.53	0.08
H101	3.35	3.3	0.04
H102	3.46	Same as above (Methyl Group)	
H103	2.98	Same as above (Methyl Group)	
H108	3.57	5.32	1.75
H112	2.60	1.11	0.74
H113	1.31	Same as above (Methyl Group)	
H114	1.64	Same as above (Methyl Group)	
H116	2.98	2.35	0.58
H117	3.11	Same as above (Methyl Group)	
H118	2.71	Same as above (Methyl Group)	
H121	3.78	5.11	1.33
H123	5.27	NH	
H127	3.86	3.62	0.24
H129	0.39	1.5	1.11
H130	2.79	1.5	1.29
H132	1.40	1.6	0.20
H134	1.03	0.89	0.13
H135	0.94	Same as above (Methyl Group)	
H136	0.30	Same as above (Methyl Group)	
H138	0.21	0.94	0.33
H139	0.85	Same as above (Methyl Group)	
H140	0.78	Same as above (Methyl Group)	
H145	4.12	4.73	0.61
H147	2.82	3.15	0.28
H148	2.73	Same as above (Methyl Group)	
H149	3.05	Same as above (Methyl Group)	
H151	1.21	1.28	0.04
H152	1.13	Same as above (Methyl Group)	
H153	1.38	Same as above (Methyl Group)	
H155	5.79	NH	
H159	5.00	3.75	1.25
H162	3.24	2.75	0.24
H163	2.87	Same as above (Methyl Group)	
H164	2.87	Same as above (Methyl Group)	
H166	2.16	2.05	0.11
H168	1.65	1.11	0.54
H169	1.36	1.35	0.01
H171	0.86	0.93	0.00
H172	1.04	Same as above (Methyl Group)	
H173	0.89	Same as above (Methyl Group)	
H175	1.86	0.83	0.39
H176	0.75	Same as above (Methyl Group)	
H177	1.06	Same as above (Methyl Group)	
H179	2.79	2.85	0.14
H180	2.11	Same as above (Methyl Group)	
H181	3.24	Same as above (Methyl Group)	
H185	2.71	2.85	0.14
H186	2.71	2.99	0.28

H193	6.75	6.77	0.02
H194	7.20	7.09	0.11
H195	7.33	7.09	0.24
H196	6.86	6.77	0.09
H199	3.78	3.77	0.16
H200	3.51	Same as above (Methyl Group)	
H201	3.52	Same as above (Methyl Group)	
		CMAD	0.36
		Largest Δδ	2.13
		Stdev	0.45
		DP4	13.1%

Coibamide A [D-HIV], [D-MeAla] Revision

Atom Number	Boltzmann Avg comp δ	Exp δ	Δδ (compδ-expδ)
C2	42.5	41.3	2.4
C6	35.4	Same as C6	
C10	74.1	73.8	0.3
C12	30.4	27.6	2.8
C14	18.9	19.5	0.6
C18	19.6	19.6	0.0
C22	177.2	172.4	4.8
C24	75.9	74.7	1.2
C27	31.4	29.9	1.5
C29	20.3	18.0	0.2
C33	15.3	Same as C29	
C37	170.9	170.0	0.9
C39	56.4	52.6	3.8
C42	26.7	30.2	3.5
C46	69.8	69.3	0.5
C50	57.0	58.6	1.6
C54	54.5	51.1	3.4
C56	174.2	170.5	3.7
C59	31.9	31.2	0.7
C63	37.0	37.9	0.9
C66	27.9	25.3	2.6
C68	18.9	23.1	4.2
C72	22.6	21.2	1.4
C76	175.8	170.5	5.3
C78	57.8	NOT OBSERVED	
C81	30.7	29.7	1.0
C85	67.8	68.0	0.2
C87	18.4	18.4	0.0
C92	58.5	52.8	5.7
C94	171.2	169.7	1.5
C97	71.1	68.6	2.5
C100	56.9	58.8	1.9
C105	173.3	168.7	4.6
C107	56.4	51.1	5.3
C109	176.6	170.4	6.2
C111	15.5	12.9	2.6
C115	27.6	30.1	2.5
C120	57.0	50.0	7.0
C124	170.9	171.2	0.3
C126	68.7	63.6	5.1
C128	40.8	36.1	4.7
C131	28.3	24.9	3.4
C133	20.2	21.4	1.2
C137	22.5	23.2	0.7
C142	178.6	171.5	7.1
C144	50.5	47.0	3.5
C146	36.2	39.4	3.2
C150	19.6	18.6	1.0
C156	167.7	167.2	0.5

C158	66.8	64.8	2.0
C161	38.7	28.9	9.8
C165	33.4	32.0	1.4
C167	25.5	24.2	1.3
C170	8.2	11.6	3.4
C174	15.8	15.7	0.1
C178	29.1	30.0	0.9
C182	170.9	171.4	0.5
C184	38.1	38.9	0.8
C187	156.0	158.6	2.6
C188	107.5	113.7	0.8
C189	129.4	130.4	1.5
C190	129.8	128.4	1.4
C191	134.3	Same as 189	
C192	118.3	Same as 188	
C198	52.3	55.3	3.0
		CMAD	2.5
		STDEV	2.1
		Largest Δδ	9.8

Atom Number	Boltzmann Avg comp δ	Exp δ	Δδ (compδ-expδ)
H3	2.78	2.34	0.06
H4	2.17	Same as above (Methyl Group)	
H5	2.25	Same as above (Methyl Group)	
H7	1.97	2.34	0.31
H8	1.76	Same as above (Methyl Group)	
H9	2.37	Same as above (Methyl Group)	
H11	2.93	2.84	0.09
H13	1.96	2.02	0.06
H15	0.52	0.99	0.07
H16	1.37	Same as above (Methyl Group)	
H17	0.86	Same as above (Methyl Group)	
H19	0.62	1.04	0.22
H20	1.03	Same as above (Methyl Group)	
H21	0.81	Same as above (Methyl Group)	
H25	5.04	5	0.04
H28	2.14	2.21	0.07
H30	1.14	1.06	0.04
H31	1.02	Same as above (Methyl Group)	
H32	1.14	Same as above (Methyl Group)	
H34	1.03	1.06	0.07
H35	0.83	Same as above (Methyl Group)	
H36	1.13	Same as above (Methyl Group)	
H40	6.51	6.02	0.49
H43	2.54	3.04	0.34
H44	2.53	Same as above (Methyl Group)	
H45	3.03		
H47	3.67	3.9	0.23
H48	3.95	3.64	0.31
H51	3.45	3.35	0.13
H52	3.07	Same as above (Methyl Group)	
H53	3.14		
H55	5.18	5.34	0.16
H60	2.62	3.13	0.01
H61	3.61	Same as above (Methyl Group)	
H62	3.13	Same as above (Methyl Group)	
H64	1.88	1.68	0.20
H65	1.31	1.31	0.00
H67	1.65	1.36	0.29
H69	0.48	0.89	0.01
H70	1.18	Same as above (Methyl Group)	
H71	1.04	Same as above (Methyl Group)	
H73	0.67	0.92	0.00
H74	1.10	Same as above (Methyl Group)	
H75	1.00	Same as above (Methyl Group)	

H79	5.74	6.35	0.61
H82	2.92	2.89	0.13
H83	2.48	Same as above (Methyl Group)	
H84	2.87	Same as above (Methyl Group)	
H86	5.48	5.5	0.02
H88	0.98	1.07	0.05
H89	0.94	Same as above (Methyl Group)	
H90	1.15	Same as above (Methyl Group)	
H93	5.28	5.69	0.41
H98	3.52	3.83	0.31
H99	3.34	3.53	0.19
H101	3.11	3.3	0.17
H102	3.36	Same as above (Methyl Group)	
H103	2.94	Same as above (Methyl Group)	
H108	5.14	5.32	0.18
H112	1.21	1.11	0.19
H113	1.84	Same as above (Methyl Group)	
H114	0.84	Same as above (Methyl Group)	
H116	2.66	2.35	0.37
H117	2.83	Same as above (Methyl Group)	
H118	2.68	Same as above (Methyl Group)	
H121	4.21	5.11	0.90
H123	9.06	NH	
H127	4.18	3.62	0.56
H129	1.89	1.5	0.39
H130	3.14	1.5	1.64
H132	1.91	1.6	0.31
H134	1.29	0.89	0.30
H135	1.40	Same as above (Methyl Group)	
H136	0.87	Same as above (Methyl Group)	
H138	1.07	0.94	0.26
H139	1.21	Same as above (Methyl Group)	
H140	1.32	Same as above (Methyl Group)	
H145	4.49	4.73	0.24
H147	3.20	3.15	0.25
H148	2.62	Same as above (Methyl Group)	
H149	2.87	Same as above (Methyl Group)	
H151	1.52	1.28	0.11
H152	1.26	Same as above (Methyl Group)	
H153	1.39	Same as above (Methyl Group)	
H155	6.39	NH	
H159	3.31	3.75	0.44
H162	2.87	2.75	0.19
H163	2.56	Same as above (Methyl Group)	
H164	3.40	Same as above (Methyl Group)	
H166	3.68	2.05	1.63
H168	1.19	1.11	0.08
H169	1.65	1.35	0.30
H171	0.66	0.93	0.00
H172	0.99	Same as above (Methyl Group)	
H173	1.16	Same as above (Methyl Group)	
H175	0.67	0.83	0.02
H176	0.74	Same as above (Methyl Group)	
H177	1.03	Same as above (Methyl Group)	
H179	2.94	2.85	0.18
H180	2.47	Same as above (Methyl Group)	
H181	2.59	Same as above (Methyl Group)	
H185	2.97	2.85	0.12
H186	3.65	2.99	0.66
H193	6.62	6.77	0.15
H194	7.45	7.09	0.36
H195	7.54	7.09	0.45
H196	6.88	6.77	0.11
H199	3.66	3.77	0.25
H200	3.46	Same as above (Methyl Group)	

H201	3.43	Same as above (Methyl Group)	
		CMAD	0.27
		Largest Δδ	1.64
		Stdev	0.32
		DP4	82.6 %

Coibamide A- Original Configuration

Atom Number	Boltzmann Avg (Comp δ)	Exp δ	Δδ (|Comp δ – Exp δ|)
C2	42.7	41.3	2.5
C6	34.9	Same as above (C2)	
C10	72.7	73.8	1.1
C12	31.7	27.6	4.1
C14	19.3	19.5	0.2
C18	20.4	19.6	0.8
C22	173.4	172.4	1.0
C24	73.9	74.7	0.8
C27	32.9	29.9	3.0
C29	15.3	18	0.2
C33	21.1	Same as above (C29)	
C37	172.9	170	2.9
C39	58.9	52.6	6.3
C42	34.4	30.2	4.2
C46	73.7	69.3	4.4
C50	56.1	58.6	2.5
C54	55.3	51.1	4.2
C56	172.1	170.5	1.6
C59	30.8	31.2	0.4
C63	36.1	37.9	1.8
C66	31.2	25.3	5.9
C68	23.0	23.1	0.1
C72	19.1	21.2	2.1
C76	174.5	170.5	4.0
C78	55.8	NOT OBSERVED	
C81	28.7	29.7	1.0
C85	68.0	68	0.0
C87	18.4	18.4	0.0
C92	58.9	52.8	6.1
C94	170.9	169.7	1.2
C97	71.4	68.6	2.8
C100	56.7	58.8	2.1
C105	172.7	168.7	4.0
C107	62.7	51.1	11.6
C109	174.5	170.4	4.1
C111	16.2	12.9	3.3
C115	36.3	30.1	6.2
C120	53.4	50	3.4
C124	169.3	171.2	1.9
C126	59.7	63.6	3.9
C128	39.5	36.1	3.4
C131	27.7	24.9	2.8
C133	19.7	21.4	1.7
C137	22.6	23.2	0.6
C142	173.3	171.5	1.8
C144	47.8	47	0.8
C146	37.6	39.4	1.8
C150	19.0	18.6	0.4
C156	166.0	167.2	1.2
C158	68.4	64.8	3.6
C161	39.9	28.9	11.0
C165	37.1	32	5.1
C167	25.8	24.2	1.6
C170	11.6	11.6	0.0
C174	14.6	15.7	1.1

C178	34.1	30	4.1
C182	169.7	171.4	1.7
C184	38.0	38.9	0.9
C187	157.0	158.6	1.6
C188	119.0	113.7	0.1
C189	130.9	130.4	0.2
C190	126.1	128.4	2.3
C191	130.3	Same as 189	
C192	108.6	Same as 188	
C198	51.5	55.3	3.8
		CMAD	2.6
		STDEV	2.4
		Largest Δδ	11.6

Atom Number	Boltzmann Avg (Comp δ)	Exp δ	Δδ (|Comp δ – Exp δ|)
H3	2.27	2.34	0.17
H4	2.33	Same as above (Methyl Group)	
H5	1.91	Same as above (Methyl Group)	
H7	1.95	2.34	0.37
H8	1.67	Same as above (Methyl Group)	
H9	2.29	Same as above (Methyl Group)	
H11	2.91	2.84	0.07
H13	2.16	2.02	0.14
H15	0.65	0.99	0.05
H16	1.34	Same as above (Methyl Group)	
H17	0.83	Same as above (Methyl Group)	
H19	0.68	1.04	0.06
H20	1.04	Same as above (Methyl Group)	
H21	1.59	Same as above (Methyl Group)	
H25	4.99	5	0.01
H28	2.12	2.21	0.09
H30	1.09	1.06	0.03
H31	1.18	Same as above (Methyl Group)	
H32	0.83	Same as above (Methyl Group)	
H34	1.15	1.06	0.07
H35	1.26	Same as above (Methyl Group)	
H36	0.98	Same as above (Methyl Group)	
H40	4.11	6.02	1.91
H43	2.54	3.04	0.26
H44	2.71	Same as above (Methyl Group)	
H45	3.08	Same as above (Methyl Group)	
H47	3.00	3.9	0.90
H48	3.04	3.64	0.60
H51	3.22	3.35	0.30
H52	2.92	Same as above (Methyl Group)	
H53	3.01	Same as above (Methyl Group)	
H55	4.64	5.34	0.70
H60	2.26	3.13	0.48
H61	2.66	Same as above (Methyl Group)	
H62	3.02	Same as above (Methyl Group)	
H64	1.51	1.68	0.17
H65	1.53	1.31	0.22
H67	1.52	1.36	0.16
H69	0.66	0.89	0.02
H70	0.98	Same as above (Methyl Group)	
H71	0.96	Same as above (Methyl Group)	
H73	0.51	0.92	0.11
H74	0.86	Same as above (Methyl Group)	
H75	1.06	Same as above (Methyl Group)	
H79	4.80	6.35	1.55
H82	2.92	2.89	0.02
H83	2.64	Same as above (Methyl Group)	
H84	3.04	Same as above (Methyl Group)	

H86	5.24	5.5	0.26
H88	0.80	1.07	0.03
H89	1.08	Same as above (Methyl Group)	
H90	1.24	Same as above (Methyl Group)	
H93	4.61	5.69	1.08
H98	3.24	3.83	0.59
H99	3.38	3.53	0.15
H101	2.82	3.3	0.27
H102	3.32	Same as above (Methyl Group)	
H103	2.95	Same as above (Methyl Group)	
H108	3.65	5.32	1.67
H112	2.46	1.11	0.62
H113	1.10	Same as above (Methyl Group)	
H114	1.61	Same as above (Methyl Group)	
H116	2.81	2.35	0.69
H117	3.00	Same as above (Methyl Group)	
H118	3.30	Same as above (Methyl Group)	
H121	4.61	5.11	0.50
H123	6.14	NH	
H127	3.79	3.62	0.17
H129	1.20	1.5	0.30
H130	3.52	1.5	2.02
H132	1.85	1.6	0.25
H134	1.27	0.89	0.11
H135	1.19	Same as above	
H136	0.56	Same as above	
H138	0.73	0.94	0.07
H139	1.22	Same as above	
H140	1.09	Same as above	
H145	4.31	4.73	0.42
H147	3.35	3.15	0.07
H148	2.75	Same as above (Methyl Group)	
H149	3.15	Same as above (Methyl Group)	
H151	1.31	1.28	0.07
H152	1.11	Same as above (Methyl Group)	
H153	1.22	Same as above (Methyl Group)	
H155	5.81	NH	
H159	2.67	3.75	1.08
H162	2.90	2.75	0.02
H163	2.72	Same as above (Methyl Group)	
H164	2.57	Same as above (Methyl Group)	
H166	3.08	2.05	1.03
H168	1.82	1.11	0.71
H169	0.90	1.35	0.45
H171	1.11	0.93	0.04
H172	1.12	Same as above (Methyl Group)	
H173	0.70	Same as above (Methyl Group)	
H175	0.28	0.83	0.03
H176	1.31	Same as above (Methyl Group)	
H177	0.81	Same as above (Methyl Group)	
H179	2.54	2.85	0.38
H180	2.52	Same as above (Methyl Group)	
H181	2.34	Same as above (Methyl Group)	
H185	2.75	2.85	0.10
H186	2.77	2.99	0.22
H193	6.87	6.77	0.10
H194	7.09	7.09	0.00
H195	7.04	7.09	0.05
H196	6.67	6.77	0.10
H199	3.69	3.77	0.24
H200	3.52	Same as above (Methyl Group)	
H201	3.38	Same as above (Methyl Group)	
		CMAD	0.39
		Largest Δδ	2.02
		Stdev	0.48

DP4	4.3 %