

Brief Overview of Recently Reported Misassigned Natural Products and Their *in Silico* Revisions Enabled by DU8ML, a Machine Learning-Augmented DFT Computational NMR Method.

Srinivas Beduru and Andrei G. Kutateladze*

Department of Chemistry and Biochemistry, University of Denver, Denver, CO 80208

SUPPORTING INFORMATION

Table of contents

NMR computations (DU8ML).....	4
How to read the NMR tables below:.....	4
REVISED AND VALIDATED STRUCTURES.....	5
Originally assigned (incorrect) structure of 1{2} (CDCl ₃).....	5
Revised structure of 1{2}, i.e. 2{2-rev} (CDCl ₃).....	7
Originally assigned (incorrect) structure of 3{1} (CDCl ₃).....	12
Revised structure of 3{1}, i.e. 4{1-rev} (CDCl ₃).....	17
Originally assigned (incorrect) structure of 5{7} (DMSO- <i>d</i> ₆).....	23
Revised structure of 5{7}, i.e. 6{7-rev} (DMSO- <i>d</i> ₆).....	25
Originally assigned (incorrect) structure of 7 {unknown} (CD ₃ OD).....	27
Revised structure of 7{unknown}, i.e. 8{unknown-rev} (CD ₃ OD)	28
Originally assigned (incorrect) structure of 9{2} (CD ₃ OD).....	32
Revised structure of 9{2}, i.e. 10{2-rev} (CD ₃ OD).....	34
Originally assigned (incorrect) structure of 11{1} (DMSO- <i>d</i> ₆).....	37
Revised structure of 11{1}, i.e. 15{1-rev} (DMSO- <i>d</i> ₆).....	39
Originally assigned (incorrect) structure of 12{3} (CDCl ₃).....	42
Revised structure of 12{3}, i.e. 16{3-rev} (CDCl ₃).....	44
Originally assigned (incorrect) structure of 13{4} (CDCl ₃).....	48
Revised structure of 13{4}, i.e. 17{4-rev} (CDCl ₃).....	51
Originally assigned (incorrect) structure of 14{5} (CDCl ₃).....	54

Revised structure of 14{5}, i.e. 18{5-rev} (CDCl ₃).....	57
Originally assigned (incorrect) structure of 19{9} (CDCl ₃).....	60
Revised structure of 19{9}, i.e. 22{9-rev} (CDCl ₃).....	62
Originally assigned correct structure of 21{10} (CDCl ₃).....	64
Originally assigned (incorrect) structure of 23{1} (CDCl ₃).....	66
Revised structure of 23{1}, i.e. 24{1-rev} (CDCl ₃).....	68
Originally assigned correct structure of 26{2} (CDCl ₃).....	70
Originally assigned (incorrect) structure of 27{4} (CDCl ₃).....	72
Revised structure of 27{4}, i.e. 28{4-rev} (CDCl ₃).....	75
Originally assigned correct structure of 29{1} (CDCl ₃).....	77
Originally assigned correct structure of 30{15} (CDCl ₃).....	81
Originally assigned (incorrect) structure of 31{13} (CDCl ₃).....	84
Revised structure of 31{13}, i.e. 32{13-rev} (CDCl ₃).....	86
Originally assigned correct structure of 33{5} (CDCl ₃).....	88
Originally assigned correct structure of 34{10} (CDCl ₃).....	91
Originally assigned (incorrect) structure of 35{9} (CDCl ₃).....	94
Revised structure of 35{9}, i.e. 36{9-rev} (CDCl ₃).....	97
Originally assigned correct structure of 38{1} (CDCl ₃).....	99
Originally assigned (incorrect) structure of 39{3} (CDCl ₃).....	102
Revised structure of 39{3}, i.e. 40{3-rev} (CDCl ₃).....	105
Originally assigned correct structure of 41{1} (CDCl ₃).....	108
Originally assigned (incorrect) structure of 42{2} (CDCl ₃).....	113
Originally assigned (incorrect) structure of 45{3} (Acetone- <i>d</i> ₆).....	119
Revised structure of 45{3}, i.e. 47{3-rev} (Acetone- <i>d</i> ₆).....	121
Originally assigned (incorrect) structure of 46{2} (Acetone- <i>d</i> ₆).....	124
Revised structure of 46{2}, i.e. 48{2-rev} (Acetone- <i>d</i> ₆).....	129
Originally assigned (incorrect) structure of 49{1} (CD ₃ OD).....	132
Revised structure of 49{1}, i.e. 50{1-rev} (CD ₃ OD).....	137
Originally assigned (incorrect) structure of 51{1} (CD ₃ OD).....	142
Revised structure of 51{1}, i.e. 54{1-rev} (CD ₃ OD).....	146
Originally assigned (incorrect) structure of 52{2} (CD ₃ OD).....	150
Revised structure of 52{2}, i.e. 55{2-rev} (CD ₃ OD).....	155
Originally assigned (incorrect) structure of 53{3} (CD ₃ OD).....	157

Revised structure of 53{3}, i.e. 56{3-rev} (CD ₃ OD).....	163
Originally assigned (incorrect) structure of 57{3} (CDCl ₃).....	166
Revised structure of 57{3}, i.e. 59{3-rev} (CDCl ₃).....	169
Originally assigned (incorrect) structure of 58{4} (CDCl ₃).....	174
Revised structure of 58{4}, i.e. 60{4-rev} (CDCl ₃).....	176
Originally assigned correct structure of 61{1} (CDCl ₃).....	180
Originally assigned correct structure of 62{2} (CDCl ₃).....	183
Originally assigned correct structure of 63{3} (CDCl ₃).....	185
Originally assigned (incorrect) structure of 64{18} (CDCl ₃).....	187
Revised structure of 64{18}, i.e. 66{18-rev} (CDCl ₃).....	190
Originally assigned (incorrect) structure of 68{1} (CDCl ₃).....	193
Revised structure of 68{1}, i.e. 70{1-rev} (CDCl ₃).....	197
Originally assigned (incorrect) structure of 69{2} (CDCl ₃).....	200
Revised structure of 69{2}, i.e. 71{2-rev} (CDCl ₃).....	203

NMR computations (DU8ML)

How to read the NMR tables below:

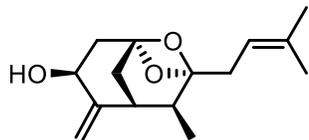
C-nom	iGau	Exp	Calc	diff	1	2	3
C-C	18	141.80	142.33	0.53	[140.66	142.98	145.37]
C-C-Br	6	137.90	139.50	1.60	[139.59	139.40	139.65]
C-C	3	79.60	80.83	1.23	[80.81	80.86	80.81]
.....							
C-CH3	19	16.80	18.48	1.68	[20.11	16.58	20.97]
					13C chem shifts: RMSD=1.52ppm (MAE=1.38) N=15 {-0.57 2.85}		
					Fractions: 0.397 0.490 0.113		

Annotations:

- Gaussian atom numbers
- Experimental chem shifts
- Calculated chem shifts, averaged over conformers
- Columns represent individual conformers
- Calculated chem shifts for individual conformers
- Curly brackets show max negative and positive deviations
- RMSD and MAE values over N atoms (CRMSD for PCM runs means corrected RMSD)
- Conformer populations for averaging

REVISED AND VALIDATED STRUCTURES

Originally assigned (incorrect) structure of 1{2} (CDCl₃)



					Conf1	Conf2
Rel energy (kcal/mol):					0.00	0.17
C-nom	iGau	Exp	Calc	diff	1	2
C1-C	6	102.90	119.00	16.10	[119.51	118.33]
C2-CH	5	39.60	49.59	9.99	[47.84	51.90]
C3-CH	4	43.70	51.35	7.65	[51.26	51.46]
C4-C	8	144.90	163.02	18.12	[162.97	163.09]
C5-CH	9	75.40	81.17	5.77	[81.13	81.22]
C6-CH2	7	42.20	51.22	9.02	[51.20	51.24]
C7-C	2	94.30	125.30	31.00	[124.96	125.74]
C8-CH2	3	42.90	38.56	-4.34	[38.87	38.14]
C9-CH2	13	36.30	34.39	-1.91	[34.80	33.84]
C10-CH	14	117.40	116.41	-0.99	[114.89	118.41]
C11-C	15	133.90	135.91	2.01	[138.91	131.94]
C12-CH2	11	108.70	105.38	-3.32	[105.38	105.38]
C13-CH3	18	14.90	12.08	-2.82	[12.02	12.16]
C14-CH3	17	18.20	17.22	-0.98	[17.40	16.98]
C15-CH3	16	26.00	25.19	-0.81	[25.13	25.27]

13C chem shifts: RMSD=11.16ppm (MAE=7.66) N=15 {-4.34 31.00}
Fractions: 0.569 0.431

Conformer 1

Energy: -810.35194 Hartree (Rel: 0.0 kcal/mol)

XYZ coordinates for conf 1:

O	-0.09960	-0.31420	-0.68154
C	-1.29348	0.39994	-1.17565
C	-2.16564	1.17576	-0.13773
C	-1.44708	0.75022	1.11953
C	0.01435	1.33164	0.90737
C	0.46128	0.97864	-0.55714
C	-2.12506	-0.77218	-1.62515
C	-1.66379	-0.79015	1.08408
C	-2.33710	-1.45519	-0.18202
O	-3.75790	-1.50701	0.00301
C	-1.45218	-1.56986	2.15000
O	-0.39891	1.45472	-1.67175
C	1.93188	1.12243	-0.91862
C	2.89429	0.49404	0.06123
C	3.41155	-0.74426	0.00527
C	4.38758	-1.21984	1.05532
C	3.09560	-1.75739	-1.06765
C	0.11400	2.81135	1.29006
H	-3.20876	0.85441	-0.15200
H	-2.11625	2.24340	-0.35115
H	-1.85631	1.16032	2.04999
H	0.71256	0.75848	1.53025
H	-3.10500	-0.51250	-2.02892
H	-1.59865	-1.44725	-2.30331
H	-1.93741	-2.47531	-0.24146
H	-3.90933	-1.78723	0.92108
H	-1.61667	-2.64555	2.12394
H	-1.08514	-1.16188	3.08931
H	2.04011	0.70587	-1.92409
H	2.13898	2.19757	-1.00121
H	3.19397	1.12834	0.89549
H	4.58988	-0.44986	1.80663
H	4.00604	-2.11146	1.57191
H	5.34375	-1.51176	0.59864

H	2.34894	-1.40786	-1.78313
H	4.00501	-2.03645	-1.61805
H	2.71133	-2.68109	-0.61428
H	1.13816	3.18008	1.16089
H	-0.15955	2.96131	2.34062
H	-0.54164	3.43951	0.67767

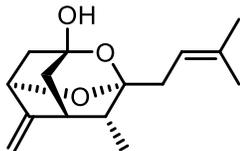
Conformer 2

Energy: -810.35168 Hartree (Rel: 0.2 kcal/mol)

XYZ coordinates for conf 2:

O	-0.29642	-0.50106	0.51317
C	-0.78665	-0.61086	-0.87584
C	-1.80745	0.45917	-1.37781
C	-2.01505	1.19683	-0.07744
C	-0.56594	1.75805	0.24630
C	0.46267	0.58656	0.01934
C	-1.55247	-1.90328	-0.77546
C	-2.61101	0.07139	0.81653
C	-2.67693	-1.40940	0.26675
O	-3.92662	-1.61519	-0.40466
C	-3.22288	0.32506	1.97851
O	0.49427	-0.04551	-1.32050
C	1.84828	0.77985	0.60972
C	2.69848	-0.46273	0.55588
C	4.00115	-0.55448	0.24882
C	4.70284	-1.89287	0.27286
C	4.88739	0.60695	-0.13217
C	-0.26706	3.05845	-0.50636
H	-2.72782	0.00816	-1.75325
H	-1.34927	1.05132	-2.16982
H	-2.71431	2.03934	-0.12782
H	-0.49949	1.95399	1.32475
H	-2.05040	-2.21498	-1.69507
H	-0.96827	-2.72670	-0.35909
H	-2.61940	-2.06515	1.14458
H	-4.61149	-1.20331	0.14817
H	-3.64831	-0.46498	2.59468
H	-3.30529	1.33698	2.36935
H	2.31990	1.62184	0.09247
H	1.70495	1.10056	1.65309
H	2.16937	-1.37721	0.81932
H	4.02523	-2.70443	0.55638
H	5.12887	-2.13162	-0.71188
H	5.54378	-1.88657	0.98087
H	4.35809	1.56154	-0.18395
H	5.70775	0.71964	0.59056
H	5.35815	0.42848	-1.10877
H	0.72265	3.44625	-0.24017
H	-1.00153	3.83168	-0.25409
H	-0.28521	2.91710	-1.59215

Revised structure of 1{2}, i.e. 2{2-rev} (CDCl₃)



Rel energy (kcal/mol):					Conf1	Conf2	Conf3	Conf4	Conf5	Conf6
					0.00	0.78	0.79	0.86	1.91	3.02
C-nom	iGau	Exp	Calc	diff	1	2	3	4	5	6
C-C	8	144.90	146.19	1.29	[146.25	146.06	146.40	145.92	145.81	145.77]
C-C	13	133.90	133.30	-0.60	[133.16	131.37	137.36	131.99	130.14	137.05]
C-C	6	102.90	102.97	0.07	[102.94	102.54	103.78	102.85	101.85	103.06]
C-C	2	94.30	94.06	-0.24	[94.10	93.93	94.08	94.06	93.85	93.88]
C-CH	12	117.40	118.66	1.26	[118.70	119.81	116.41	119.29	121.03	118.14]
C-CH	9	75.40	75.68	0.28	[75.71	75.65	75.71	75.48	75.89	75.70]
C-CH	4	43.70	43.98	0.28	[43.86	44.21	43.80	44.28	44.85	45.30]
C-CH	5	39.60	41.01	1.41	[40.10	43.36	39.77	43.04	43.61	43.31]
C-CH2	10	108.70	108.27	-0.43	[108.26	108.34	108.15	108.29	108.59	108.21]
C-CH2	7	42.90	43.99	1.09	[44.12	43.72	43.99	43.70	44.12	44.06]
C-CH2	3	42.20	41.80	-0.40	[41.79	41.82	41.72	41.93	41.82	41.79]
C-CH2	11	36.30	37.24	0.94	[37.37	36.94	37.07	36.63	40.21	40.18]
C-CH3	14	26.00	25.37	-0.63	[25.35	25.41	25.34	25.48	25.25	25.27]
C-CH3	15	18.20	17.07	-1.13	[17.07	16.80	17.60	16.82	16.93	17.92]
C-CH3	16	14.90	15.22	0.32	[15.00	15.49	15.48	15.33	16.08	17.10]
¹³C chem shifts: RMSD=0.82ppm (MAE=0.69) N=15 {-1.13 1.41}										
Fractions:					0.551	0.148	0.145	0.130	0.022	0.003

Conformer 1

Energy: -810.47838 Hartree (Rel: 0.0 kcal/mol)

XYZ coordinates for conf 1:

H	-1.72098	3.36256	-0.46591
C	-1.66457	1.54141	0.15840
C	-1.87276	0.79690	1.47881
C	-1.51639	-0.69360	1.26350
C	-0.03372	-0.78546	0.80522
C	0.07628	0.01158	-0.51872
C	-2.55873	0.97226	-0.95176
C	-2.39396	-1.25528	0.16332
C	-2.17519	-0.50759	-1.13503
C	-3.26137	-2.25915	0.30048
C	1.47371	0.05878	-1.14938
C	2.52581	0.64190	-0.24377
C	3.75296	0.16283	0.01831
C	4.68715	0.90983	0.94238
C	4.33373	-1.10512	-0.56061
C	0.45485	-2.23326	0.68938
H	-2.91178	0.90937	1.80770
H	-1.22241	1.24562	2.23779
H	-1.65587	-1.25447	2.19474
H	0.58600	-0.26308	1.54425
H	-3.61558	1.07287	-0.68276
H	-2.37543	1.52007	-1.88390
H	-2.71877	-0.96662	-1.96448
O	-0.77860	-0.56323	-1.50749
H	-3.86336	-2.61270	-0.53391
H	-3.40564	-2.76197	1.25428
H	1.72758	-0.94811	-1.48860
H	1.36579	0.67918	-2.05024
H	2.23714	1.58030	0.22859
H	4.22863	1.82191	1.33743
H	4.98693	0.28116	1.79282
H	5.61482	1.19077	0.42382
H	3.63871	-1.64790	-1.20568
H	5.23213	-0.88056	-1.15255
H	4.65486	-1.78509	0.24060

H	1.53288	-2.27484	0.50490
H	-0.05464	-2.76422	-0.12020
H	0.25798	-2.77290	1.62345
O	-1.86025	2.90505	0.38130
O	-0.29687	1.37473	-0.27448

Conformer 2

Energy: -810.47962 Hartree (Rel: 0.8 kcal/mol)

XYZ coordinates for conf 2:

H	-0.15571	3.22568	-0.46603
C	0.92328	1.63168	-0.47963
C	2.05507	1.04419	-1.32546
C	2.33264	-0.39764	-0.83674
C	1.02971	-1.23293	-0.99398
C	-0.05096	-0.54510	-0.11727
C	1.30342	1.67847	1.00665
C	2.70326	-0.35551	0.63197
C	1.57664	0.23186	1.45541
C	3.86457	-0.75868	1.14955
C	-1.42389	-1.22822	-0.15812
C	-2.48054	-0.49531	0.62632
C	-3.72170	-0.16598	0.23655
C	-4.65946	0.54733	1.18381
C	-4.31339	-0.45445	-1.12232
C	1.24592	-2.71462	-0.66604
H	2.95042	1.66915	-1.23468
H	1.74140	1.04481	-2.37516
H	3.13861	-0.84877	-1.42668
H	0.69573	-1.14526	-2.03607
H	2.18645	2.30862	1.15659
H	0.46826	2.09367	1.58320
H	1.78248	0.17161	2.52693
O	0.36840	-0.53544	1.24811
H	4.06687	-0.69736	2.21673
H	4.65909	-1.16023	0.52434
H	-1.70453	-1.34943	-1.20843
H	-1.29242	-2.23562	0.25796
H	-2.17901	-0.23047	1.63869
H	-4.19280	0.73585	2.15606
H	-4.98330	1.51190	0.76730
H	-5.57429	-0.03862	1.35270
H	-3.61564	-0.94212	-1.80712
H	-5.19836	-1.09990	-1.03004
H	-4.65725	0.47466	-1.59784
H	0.36795	-3.31612	-0.92249
H	1.46298	-2.86073	0.39630
H	2.09327	-3.10712	-1.24079
O	0.57988	2.88011	-1.00096
O	-0.24425	0.79100	-0.59411

Conformer 3

Energy: -810.47480 Hartree (Rel: 0.8 kcal/mol)

XYZ coordinates for conf 3:

H	-0.09792	3.35640	-0.02648
C	-0.87313	1.63759	0.36482
C	-1.43557	0.90778	1.58674
C	-1.74574	-0.55418	1.18496
C	-0.42839	-1.22218	0.69889
C	0.06769	-0.40077	-0.51774
C	-1.88068	1.64519	-0.79326
C	-2.73450	-0.54889	0.03684
C	-2.16323	0.17769	-1.16244
C	-3.95422	-1.08801	0.06214
C	1.37189	-0.88972	-1.16696
C	2.53323	-1.05381	-0.22023
C	3.54408	-0.19657	-0.00516
C	4.64776	-0.53530	0.96959
C	3.69120	1.14636	-0.67722
C	-0.60775	-2.71474	0.39921
H	-2.33841	1.41809	1.94015
H	-0.68751	0.94016	2.38651

H	-2.15022	-1.10473	2.04201
H	0.32316	-1.10527	1.48931
H	-2.80120	2.15959	-0.49755
H	-1.44389	2.16547	-1.65403
H	-2.81711	0.09817	-2.03450
O	-0.91261	-0.43149	-1.55737
H	-4.61589	-1.04582	-0.80043
H	-4.33891	-1.58761	0.94862
H	1.15173	-1.84798	-1.65109
H	1.59581	-0.17857	-1.96734
H	2.54518	-1.98811	0.34240
H	4.50131	-1.51762	1.43020
H	5.62791	-0.53410	0.47188
H	4.70772	0.21327	1.77212
H	2.86772	1.37992	-1.35404
H	3.73494	1.94396	0.07709
H	4.63393	1.19863	-1.23991
H	0.34959	-3.20033	0.18267
H	-1.27129	-2.87367	-0.45589
H	-1.04616	-3.22298	1.26627
O	-0.47202	2.91614	0.75626
O	0.30635	0.94916	-0.10252

Conformer 4

Energy: -810.47836 Hartree (Rel: 0.9 kcal/mol)

XYZ coordinates for conf 4:

H	0.77960	3.45064	-0.19120
C	1.41550	1.63297	-0.23198
C	2.58029	0.86145	-0.85593
C	2.37085	-0.64694	-0.58100
C	1.01601	-1.08336	-1.20830
C	-0.08876	-0.23448	-0.52269
C	1.34700	1.41149	1.28510
C	2.29943	-0.86730	0.91640
C	1.14451	-0.09624	1.51961
C	3.13978	-1.61841	1.62960
C	-1.50669	-0.51518	-1.03821
C	-2.55742	0.38637	-0.44518
C	-3.71209	0.03397	0.14155
C	-4.66347	1.08997	0.65662
C	-4.18964	-1.38332	0.34917
C	0.79006	-2.59612	-1.10489
H	3.52781	1.21022	-0.43051
H	2.59343	1.06209	-1.93294
H	3.18977	-1.22845	-1.01962
H	1.02555	-0.79724	-2.26802
H	2.26637	1.76349	1.76493
H	0.49565	1.96623	1.69720
H	1.01201	-0.32668	2.57956
O	-0.09366	-0.48243	0.88044
H	3.03233	-1.73120	2.70630
H	3.97035	-2.14447	1.16397
H	-1.47398	-0.38135	-2.12936
H	-1.73137	-1.56715	-0.85204
H	-2.33561	1.44878	-0.52933
H	-4.28249	2.10195	0.48554
H	-5.64647	1.00902	0.17091
H	-4.84091	0.96930	1.73485
H	-3.48113	-2.13855	0.00123
H	-4.38409	-1.57105	1.41428
H	-5.14231	-1.55107	-0.17288
H	-0.08330	-2.91386	-1.68343
H	0.64521	-2.90748	-0.06607
H	1.65969	-3.13426	-1.50041
O	1.53016	2.97707	-0.58979
O	0.17495	1.15060	-0.79093

Conformer 5

Energy: -810.47657 Hartree (Rel: 1.9 kcal/mol)

XYZ coordinates for conf 5:

H	2.70951	-2.99408	-0.62768
---	---------	----------	----------

C	2.23283	-1.24205	0.01550
C	2.56929	-0.35242	1.21290
C	1.66295	0.89933	1.15664
C	0.17429	0.44590	1.20167
C	-0.05713	-0.45554	-0.04079
C	2.48284	-0.51232	-1.31168
C	1.90172	1.62131	-0.15404
C	1.57130	0.72802	-1.33068
C	2.35926	2.86785	-0.28021
C	-1.44894	-1.09536	-0.18151
C	-2.56035	-0.18638	-0.63631
C	-3.83098	-0.15921	-0.20219
C	-4.83376	0.78660	-0.82228
C	-4.39283	-1.03089	0.89534
C	-0.77629	1.64235	1.31794
H	3.62844	-0.07330	1.18452
H	2.38881	-0.92165	2.13148
H	1.87557	1.55878	2.00576
H	0.04222	-0.19677	2.08188
H	3.53617	-0.22575	-1.39973
H	2.22380	-1.17408	-2.14683
H	1.63739	1.26523	-2.27989
O	0.20097	0.27272	-1.23737
H	2.51020	3.32553	-1.25557
H	2.60513	3.47580	0.58770
H	-1.31019	-1.89295	-0.92554
H	-1.67978	-1.59271	0.76518
H	-2.28654	0.48685	-1.44681
H	-4.38553	1.39584	-1.61363
H	-5.68233	0.23700	-1.25416
H	-5.25694	1.46442	-0.06721
H	-3.64572	-1.67487	1.36542
H	-4.85203	-0.41532	1.68137
H	-5.19129	-1.67727	0.50433
H	-1.81228	1.32287	1.45265
H	-0.73188	2.27640	0.42753
H	-0.49280	2.25546	2.18240
O	2.94785	-2.43554	0.13241
O	0.83178	-1.58325	0.05560

Conformer 6

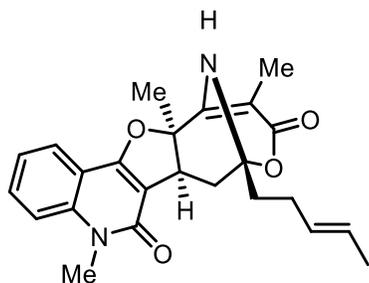
Energy: -810.47826 Hartree (Rel: 3.0 kcal/mol)

XYZ coordinates for conf 6:

H	-2.44710	-3.09576	0.09967
C	-2.12604	-1.20651	-0.09021
C	-2.80018	-0.01151	-0.76497
C	-1.86206	1.21083	-0.63513
C	-0.50323	0.87971	-1.31984
C	0.08776	-0.34548	-0.57119
C	-1.87248	-0.93695	1.39942
C	-1.60315	1.47949	0.83318
C	-0.94281	0.28644	1.49034
C	-1.92068	2.59947	1.48419
C	1.40880	-0.92903	-1.11596
C	2.68135	-0.15094	-0.88570
C	3.53686	-0.27782	0.14167
C	4.80379	0.54371	0.19463
C	3.34447	-1.21173	1.31077
C	0.41307	2.10769	-1.37228
H	-3.76978	0.18539	-0.29423
H	-2.97370	-0.25802	-1.81828
H	-2.31417	2.08623	-1.11505
H	-0.71400	0.55024	-2.34552
H	-2.81692	-0.75171	1.92206
H	-1.38238	-1.80826	1.85014
H	-0.65341	0.49984	2.52216
O	0.28786	-0.03708	0.80227
H	-1.70636	2.72537	2.54333
H	-2.41168	3.43089	0.98316
H	1.48058	-1.92511	-0.66827
H	1.26267	-1.08407	-2.19193

H	2.94638	0.56305	-1.66395
H	4.90370	1.20060	-0.67551
H	4.83162	1.16822	1.09876
H	5.69192	-0.10278	0.23834
H	2.41313	-1.77763	1.25760
H	4.18403	-1.91730	1.38664
H	3.32988	-0.64390	2.25129
H	1.27008	1.94537	-2.03105
H	0.79061	2.37029	-0.38001
H	-0.14331	2.96875	-1.76244
O	-2.90087	-2.34496	-0.32093
O	-0.84258	-1.43719	-0.70639

Originally assigned (incorrect) structure of 3{1} (CDCl₃)



Rel energy (kcal/mol):					Conf1	Conf2	Conf3	Conf4
					0.00	1.32	1.78	1.84
C-nom	iGau	Exp	Calc	diff	1	2	3	4
C2-C	8	162.30	161.02	-1.28	[161.05	160.86	160.92	160.95]
C3-C	9	105.30	107.32	2.02	[107.38	107.06	107.03	106.94]
C4-C	10	155.90	163.28	7.38	[163.43	162.56	162.51	162.65]
C4a-C	1	114.90	114.11	-0.79	[114.22	113.57	113.53	113.50]
C5-CH	2	122.70	124.64	1.94	[124.63	124.66	124.65	124.71]
C6-CH	3	121.80	121.11	-0.69	[121.02	121.56	121.54	121.58]
C7-CH	4	131.30	131.71	0.41	[131.58	132.31	132.33	132.35]
C8-CH	5	114.50	114.43	-0.07	[114.39	114.64	114.63	114.62]
C8a-C	6	139.60	141.37	1.77	[141.33	141.57	141.57	141.58]
C9-CH3	11	29.90	27.79	-2.11	[27.75	28.00	27.97	28.02]
C1'-CH3	28	18.10	17.92	-0.18	[17.94	17.79	17.88	17.92]
C2'-CH	27	127.00	126.85	-0.15	[126.89	126.30	126.84	127.28]
C3'-CH	26	129.90	129.70	-0.20	[129.68	130.03	129.70	129.40]
C4'-CH2	25	26.90	27.57	0.67	[27.51	28.35	27.34	27.38]
C5'-CH2	24	39.40	41.91	2.51	[42.11	40.88	40.99	41.00]
C6'-C	17	89.20	97.92	8.72	[98.06	97.47	96.88	97.06]
C7'-CH2	16	31.10	32.07	0.97	[31.49	36.65	32.96	32.87]
C8'-CH	13	34.70	60.73	26.03	[60.33	62.68	62.69	62.67]
C9'-C	14	82.00	96.30	14.30	[96.09	97.28	97.35	97.37]
C10'-C	18	165.60	151.84	-13.76	[151.81	152.33	151.61	151.53]
C11'-C	20	101.20	128.59	27.39	[129.95	121.69	122.00	122.13]
C12'-C	21	173.50	163.69	-9.81	[163.68	163.76	163.76	163.78]
C13'-CH3	30	26.00	23.44	-2.56	[23.36	23.81	23.79	23.82]
C14'-CH3	29	6.50	14.59	8.09	[14.66	14.24	14.23	14.21]
13C chem shifts: RMSD=9.46ppm (MAE=5.57) N=24 {-13.76 27.39}								
Fractions:					0.831	0.090	0.041	0.037

Conformer 1

Energy: -1340.58072 Hartree (Rel: 0.0 kcal/mol)

XYZ coordinates for conf 1:

C	-3.03383	-0.67590	-0.49740
C	-3.72668	-1.44594	-1.44827
C	-4.93588	-1.00654	-1.96296
C	-5.46288	0.21739	-1.52260
C	-4.79624	0.99426	-0.58291
C	-3.56354	0.56627	-0.04648
N	-2.87660	1.32699	0.89740
C	-1.63940	0.93707	1.46734
C	-1.11954	-0.31342	0.98667
C	-1.78238	-1.06967	0.07422
C	-3.43951	2.60110	1.34729
O	-1.07252	1.64680	2.31039
C	0.14811	-1.00451	1.41183
C	0.06434	-2.34687	0.53485
O	-1.18136	-2.23296	-0.24987
C	1.46655	-0.18485	1.24175
C	1.96428	-0.03828	-0.23138
C	1.24101	-2.19773	-0.38600
N	1.15585	-0.90876	-1.03405

C	2.46510	-2.76037	-0.31896
C	3.61806	-1.82424	-0.57293
O	3.38617	-0.50082	-0.35169
O	4.75162	-2.19796	-0.80485
C	1.96845	1.39050	-0.77596
C	2.94073	2.35921	-0.07478
C	2.93159	3.72204	-0.71605
C	2.56602	4.85588	-0.11031
C	2.55585	6.21625	-0.74885
C	2.86154	-4.13307	0.15253
C	-0.06256	-3.60235	1.38202
H	0.09496	-1.27729	2.47361
H	-3.29208	-2.38777	-1.76744
H	-5.46949	-1.60140	-2.69759
H	-6.41037	0.57145	-1.91908
H	-5.23483	1.93224	-0.26715
H	-4.41535	2.44829	1.81923
H	-2.74594	3.01895	2.07364
H	-3.55053	3.29301	0.50630
H	2.25686	-0.65534	1.83293
H	1.28585	0.79905	1.68102
H	1.50232	-0.94554	-1.99103
H	2.21395	1.34215	-1.84546
H	0.94246	1.76802	-0.69772
H	2.68222	2.45273	0.98706
H	3.95038	1.93142	-0.12225
H	3.24683	3.75981	-1.76159
H	2.24865	4.81353	0.93366
H	2.88449	6.17376	-1.79307
H	1.55065	6.65907	-0.72577
H	3.21520	6.91277	-0.21301
H	2.02367	-4.83022	0.14115
H	3.64568	-4.51584	-0.50882
H	3.28805	-4.11109	1.16393
H	0.82016	-3.74135	2.01222
H	-0.93569	-3.50493	2.03484
H	-0.19908	-4.49095	0.75909

Conformer 2

Energy: -1340.57988 Hartree (Rel: 1.3 kcal/mol)

XYZ coordinates for conf 2:

C	-2.74835	-0.77001	-0.82208
C	-3.19134	-1.01458	-2.13425
C	-4.43729	-0.57193	-2.54781
C	-5.25306	0.12237	-1.64092
C	-4.83632	0.37349	-0.33937
C	-3.57148	-0.06732	0.10307
N	-3.13095	0.17107	1.40394
C	-1.87373	-0.25367	1.89649
C	-1.05268	-0.95112	0.93966
C	-1.47627	-1.19811	-0.32681
C	-3.99772	0.89105	2.33947
O	-1.53056	-0.02466	3.06304
C	0.31079	-1.54883	1.16862
C	0.55509	-2.27511	-0.24932
O	-0.59297	-1.87446	-1.10028
C	1.42830	-0.54712	1.61562
C	2.02896	0.33587	0.45761
C	1.79426	-1.58227	-0.74867
N	1.58992	-0.17306	-0.83420
C	3.07758	-1.96765	-0.56678
C	4.03089	-0.86598	-0.21810
O	3.48707	0.21064	0.42973
O	5.23784	-0.92629	-0.33792
C	1.72695	1.82385	0.63185
C	2.26314	2.73440	-0.48847
C	1.98295	4.18803	-0.21404
C	1.24163	4.98875	-0.98598
C	0.96160	6.44026	-0.71503
C	3.65630	-3.35496	-0.48996
C	0.50697	-3.79068	-0.15371

H	0.25834	-2.32076	1.94580
H	-2.53698	-1.55551	-2.81022
H	-4.77916	-0.76018	-3.56059
H	-6.23197	0.47352	-1.95482
H	-5.49466	0.91129	0.33076
H	-4.93691	0.34963	2.48990
H	-3.46255	0.96073	3.28371
H	-4.21612	1.89674	1.96693
H	2.23786	-1.10925	2.08878
H	0.99614	0.09058	2.39194
H	0.61885	0.05755	-1.01921
H	0.63846	1.93673	0.72047
H	2.14753	2.13032	1.59790
H	3.34541	2.57051	-0.57392
H	1.82393	2.44234	-1.44917
H	2.42679	4.59738	0.69677
H	0.79855	4.57646	-1.89513
H	1.43822	6.77590	0.21250
H	1.32607	7.07597	-1.53363
H	-0.11748	6.62928	-0.63095
H	3.05039	-4.08681	-1.02465
H	4.65338	-3.33413	-0.94136
H	3.78597	-3.69872	0.54564
H	1.27978	-4.16785	0.52020
H	-0.46722	-4.08784	0.24777
H	0.63060	-4.25429	-1.13664

Conformer 3

Energy: -1340.57998 Hartree (Rel: 1.8 kcal/mol)

XYZ coordinates for conf 3:

C	-2.95817	-0.80762	-0.55916
C	-3.58846	-1.53425	-1.58509
C	-4.83181	-1.14634	-2.05723
C	-5.45568	-0.02006	-1.49842
C	-4.85210	0.71137	-0.48278
C	-3.58625	0.33487	0.01301
N	-2.96038	1.05105	1.03218
C	-1.69364	0.71214	1.56500
C	-1.07091	-0.43862	0.96189
C	-1.67670	-1.15040	-0.02339
C	-3.62859	2.21944	1.60951
O	-1.18213	1.37523	2.47603
C	0.25156	-1.05987	1.32759
C	0.24204	-2.35604	0.37130
O	-0.96705	-2.21151	-0.47714
C	1.50306	-0.12780	1.19236
C	2.02339	0.07392	-0.28058
C	1.46170	-2.12693	-0.47945
N	1.37632	-0.88152	-1.17077
C	2.71840	-2.56749	-0.24521
C	3.80246	-1.56717	-0.50711
O	3.44736	-0.25208	-0.37061
O	4.97219	-1.83956	-0.68682
C	1.87298	1.49825	-0.81642
C	2.71966	2.56042	-0.08784
C	2.58022	3.91825	-0.72447
C	2.08896	5.00448	-0.12030
C	1.94937	6.36047	-0.75299
C	3.17733	-3.84667	0.40179
C	0.07219	-3.65624	1.13876
H	0.23265	-1.40115	2.36963
H	-3.07964	-2.40089	-1.99468
H	-5.31820	-1.70661	-2.84941
H	-6.43071	0.29243	-1.86143
H	-5.36553	1.57352	-0.07688
H	-4.58505	1.93417	2.05873
H	-2.97029	2.61854	2.37786
H	-3.80234	2.98174	0.84364
H	2.31282	-0.53421	1.80393
H	1.23045	0.83224	1.63803
H	0.41475	-0.62179	-1.36707

H	2.14307	1.47593	-1.87880
H	0.81113	1.76996	-0.75427
H	2.43156	2.61993	0.96871
H	3.76964	2.24134	-0.11616
H	2.90786	3.99400	-1.76397
H	1.76057	4.92339	0.91802
H	2.29694	6.35808	-1.79190
H	0.90391	6.69813	-0.74418
H	2.52556	7.11747	-0.20348
H	2.44525	-4.64816	0.29984
H	4.10581	-4.16148	-0.08517
H	3.40798	-3.71834	1.46844
H	0.89010	-3.80484	1.84767
H	-0.86344	-3.61185	1.70544
H	0.02446	-4.51364	0.46135

Conformer 4

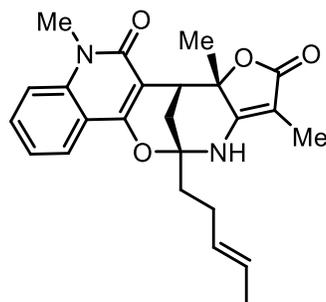
Energy: -1340.58282 Hartree (Rel: 1.8 kcal/mol)

XYZ coordinates for conf 4:

C	-3.11079	-0.25397	-0.64449
C	-3.80192	-0.79008	-1.74575
C	-4.94683	-0.17314	-2.22309
C	-5.40947	0.99307	-1.59383
C	-4.74349	1.53902	-0.50332
C	-3.57596	0.92751	-0.00049
N	-2.89052	1.45444	1.09299
C	-1.71625	0.87870	1.63440
C	-1.25672	-0.30841	0.95945
C	-1.92373	-0.83719	-0.09904
C	-3.39262	2.66614	1.74457
O	-1.14626	1.38228	2.61062
C	-0.06738	-1.16178	1.31553
C	-0.23511	-2.35968	0.25143
O	-1.37123	-1.96076	-0.61600
C	1.32079	-0.43728	1.30380
C	1.92883	-0.19715	-0.12901
C	1.03993	-2.25603	-0.54089
N	1.17940	-0.95909	-1.11984
C	2.20180	-2.90878	-0.31242
C	3.43854	-2.07460	-0.45206
O	3.28741	-0.73632	-0.20692
O	4.55798	-2.51337	-0.62272
C	2.02427	1.27348	-0.53682
C	3.01272	2.11418	0.29493
C	3.00936	3.56065	-0.12494
C	4.05735	4.21330	-0.63666
C	4.05964	5.65551	-1.05885
C	2.42819	-4.29509	0.22825
C	-0.63291	-3.67516	0.89935
H	-0.18990	-1.57665	2.32331
H	-3.41827	-1.69327	-2.20918
H	-5.48008	-0.58640	-3.07332
H	-6.30607	1.48481	-1.96043
H	-5.13163	2.43952	-0.04486
H	-4.40301	2.50473	2.13303
H	-2.71777	2.89074	2.56738
H	-3.40576	3.50500	1.04165
H	2.02825	-1.02047	1.89902
H	1.18483	0.51243	1.82747
H	0.27989	-0.53349	-1.32055
H	2.31544	1.30679	-1.59252
H	1.01596	1.70299	-0.46115
H	2.74505	2.04427	1.35914
H	4.01869	1.69429	0.19180
H	2.06441	4.09439	0.00200
H	4.99857	3.67451	-0.76349
H	3.08162	6.12334	-0.90116
H	4.80735	6.23317	-0.49829
H	4.31934	5.75840	-2.12136
H	1.58730	-4.95962	0.02802
H	3.31936	-4.70830	-0.25477

H	2.62488	-4.29749	1.30931
H	0.12416	-4.00693	1.61391
H	-1.57207	-3.53099	1.44317
H	-0.78529	-4.45709	0.14991

Revised structure of 3{1}, i.e. 4{1-rev} (CDCl₃)



Rel energy (kcal/mol): **Conf1** **Conf2** **Conf3** **Conf4** **Conf5** **Conf6**
 0.00 0.02 0.07 0.09 0.39 0.49

C-nom	iGau	Exp	Calc	diff	1	2	3	4	5	6
C2-C	8	162.30	162.57	0.27	[162.56	162.58	162.57	162.55	162.57	162.59]
C3-C	9	105.30	105.77	0.47	[105.76	105.86	105.64	105.63	105.94	105.96]
C4-C	10	155.90	155.96	0.06	[155.92	155.85	156.10	156.15	155.78	155.86]
C4a-C	1	114.90	116.26	1.36	[116.18	116.23	116.28	116.26	116.32	116.38]
C5-CH	2	122.70	123.86	1.16	[123.92	123.91	123.79	123.83	123.85	123.87]
C6-CH	3	121.80	120.75	-1.05	[120.71	120.75	120.79	120.75	120.77	120.76]
C7-CH	4	131.30	131.31	0.01	[131.29	131.28	131.33	131.34	131.32	131.31]
C8-CH	5	114.50	114.02	-0.48	[113.99	114.00	114.03	114.04	114.03	114.01]
C8a-C	6	139.60	139.99	0.39	[139.97	139.98	139.98	140.01	140.01	140.02]
C9-CH3	11	29.90	28.59	-1.31	[28.56	28.59	28.63	28.58	28.62	28.61]
C1'-CH3	30	18.10	17.97	-0.13	[17.97	18.00	17.93	17.93	18.00	17.99]
C2'-CH	29	127.00	127.95	0.95	[127.93	127.91	127.80	127.89	128.06	128.36]
C3'-CH	28	129.90	128.86	-1.04	[128.93	128.87	128.98	128.85	128.80	128.54]
C4'-CH2	27	26.90	28.44	1.54	[29.57	29.57	28.55	28.45	25.95	26.09]
C5'-CH2	26	39.40	40.58	1.18	[40.50	40.62	40.39	40.75	40.61	40.70]
C6'-C	23	89.20	89.26	0.06	[89.83	89.86	89.18	89.20	88.18	88.17]
C7'-CH2	24	31.10	30.58	-0.52	[30.35	30.07	29.48	29.28	33.50	33.54]
C8'-CH	25	34.70	36.02	1.32	[36.12	36.01	35.89	35.95	36.13	36.12]
C9'-C	20	82.00	83.68	1.68	[83.43	83.48	83.92	83.87	83.77	83.75]
C10'-C	21	165.60	166.15	0.55	[166.42	166.35	165.94	166.02	165.98	166.03]
C11'-C	19	101.20	101.61	0.41	[101.88	101.76	101.44	101.32	101.63	101.55]
C12'-C	18	173.50	173.19	-0.31	[173.13	173.15	173.22	173.21	173.23	173.24]
C13'-CH3	14	26.00	26.67	0.67	[26.65	26.64	26.72	26.67	26.70	26.65]
C14'-CH3	16	6.50	6.45	-0.05	[6.34	6.46	6.60	6.46	6.48	6.30]

13C chem shifts: RMSD=0.87ppm (MAE=0.71) N=24 {-1.31 1.68}
 Fractions: 0.214 0.206 0.191 0.185 0.111 0.094

Conformer 1

Energy: -1340.63716 Hartree (Rel: 0.0 kcal/mol)

XYZ coordinates for conf 1:

C	1.64358	-1.92625	0.27753
C	1.29471	-2.95365	1.17349
C	2.23751	-3.87665	1.59883
C	3.55454	-3.77804	1.12790
C	3.92391	-2.77342	0.24260
C	2.97571	-1.82876	-0.20225
N	3.32093	-0.82317	-1.09844
C	2.40117	0.13073	-1.57119
C	1.05127	0.06015	-1.03058
C	0.68785	-0.94049	-0.17442
C	4.69069	-0.74098	-1.60814
O	2.73623	0.96723	-2.41660
O	-0.57262	-1.10570	0.30771
C	-0.97005	3.40878	-1.10797
O	2.38548	3.60058	1.51570
C	0.27841	2.23295	3.26314
O	1.22294	2.91059	-0.29904
C	1.40712	3.04084	1.06377
C	0.31433	2.36208	1.77231
C	-0.05858	2.30214	-0.54905

C	-0.49298	1.83708	0.82416
N	-1.56758	0.97573	0.91208
C	-1.61497	-0.13018	-0.04551
C	-1.34642	0.37901	-1.46355
C	0.03147	1.07154	-1.49158
C	-2.91843	-0.91637	0.12214
C	-4.20678	-0.11328	-0.14197
C	-5.44058	-0.91246	0.18773
C	-6.38826	-1.25961	-0.68819
C	-7.61997	-2.05649	-0.36340
H	0.27079	-3.00580	1.52562
H	1.95879	-4.66570	2.29041
H	4.30346	-4.49388	1.45492
H	4.94818	-2.72388	-0.10391
H	5.39753	-0.58999	-0.78634
H	4.95712	-1.65415	-2.15014
H	4.73102	0.10910	-2.28499
H	-0.61654	3.71158	-2.09879
H	-2.01091	3.08617	-1.18705
H	-0.93364	4.27719	-0.44433
H	-0.29638	3.04307	3.73031
H	-0.17130	1.28412	3.57977
H	1.29477	2.28065	3.66581
H	-1.77208	0.66804	1.85945
H	-2.14921	1.05001	-1.77321
H	-1.34927	-0.47664	-2.14574
H	0.28636	1.40714	-2.49996
H	-2.87379	-1.78288	-0.54586
H	-2.93426	-1.31576	1.14567
H	-4.18158	0.80183	0.46574
H	-4.24671	0.20308	-1.19115
H	-5.54228	-1.22630	1.22925
H	-6.28080	-0.94583	-1.72863
H	-7.65331	-2.33363	0.69584
H	-8.53229	-1.49068	-0.59631
H	-7.66470	-2.97858	-0.95875

Conformer 2

Energy: -1340.63719 Hartree (Rel: 0.0 kcal/mol)

XYZ coordinates for conf 2:

C	1.70179	-1.91027	0.19929
C	1.30850	-3.01278	0.98015
C	2.24287	-3.92759	1.44037
C	3.59607	-3.74433	1.12212
C	4.00968	-2.66434	0.35265
C	3.07107	-1.72691	-0.12644
N	3.46218	-0.64587	-0.90902
C	2.55441	0.30504	-1.40988
C	1.15981	0.14086	-1.02688
C	0.75441	-0.93154	-0.28436
C	4.87263	-0.47398	-1.26095
O	2.93675	1.21708	-2.15075
O	-0.54084	-1.17749	0.04807
C	-0.98047	3.41254	-1.09183
O	2.07613	3.53874	1.87355
C	-0.14349	1.98697	3.29713
O	1.13857	2.93179	-0.09476
C	1.17417	2.97705	1.28556
C	0.04323	2.21433	1.82960
C	-0.08551	2.30064	-0.51688
C	-0.63784	1.72521	0.76968
N	-1.67721	0.82125	0.68734
C	-1.58231	-0.21437	-0.34240
C	-1.19267	0.40360	-1.68735
C	0.15022	1.14423	-1.52464
C	-2.86191	-1.05584	-0.36146
C	-4.15511	-0.27882	-0.67506
C	-5.36171	-1.18106	-0.67722
C	-6.40996	-1.06191	0.14312
C	-7.61582	-1.95832	0.14508
H	0.25682	-3.12946	1.21570

H	1.92968	-4.77505	2.04228
H	4.33876	-4.45265	1.47844
H	5.06138	-2.55022	0.12345
H	5.48143	-0.35244	-0.35962
H	5.23717	-1.33584	-1.82918
H	4.94385	0.42203	-1.87288
H	-0.54229	3.79568	-2.01894
H	-1.99411	3.06101	-1.29861
H	-1.04635	4.23306	-0.37194
H	-0.75742	2.77228	3.75683
H	-0.62976	1.02584	3.50204
H	0.82630	1.99440	3.80422
H	-1.96407	0.44021	1.58537
H	-1.98645	1.06677	-2.03451
H	-1.08903	-0.40096	-2.42183
H	0.49259	1.55848	-2.47620
H	-2.71650	-1.85851	-1.09325
H	-2.95705	-1.54383	0.61750
H	-4.29076	0.52692	0.05529
H	-4.05921	0.19925	-1.66035
H	-5.35344	-1.99017	-1.41105
H	-6.41316	-0.25187	0.87552
H	-7.53588	-2.74313	-0.61489
H	-7.74977	-2.44210	1.12219
H	-8.53472	-1.38856	-0.04902

Conformer 3

Energy: -1340.63706 Hartree (Rel: 0.1 kcal/mol)

XYZ coordinates for conf 3:

C	-0.82618	2.07420	0.39290
C	-0.19821	2.86517	1.37272
C	-0.77690	4.04597	1.81160
C	-2.00543	4.45016	1.26995
C	-2.64565	3.68690	0.30196
C	-2.06828	2.48495	-0.15761
N	-2.68584	1.71267	-1.13531
C	-2.13699	0.51326	-1.62372
C	-0.89396	0.06677	-1.01150
C	-0.25698	0.83093	-0.07546
C	-3.95532	2.15200	-1.71672
O	-2.68612	-0.10776	-2.53993
O	0.94339	0.50822	0.47733
C	-0.22639	-3.78094	-1.19812
O	-3.58691	-2.85005	1.24529
C	-1.24818	-2.42578	3.17190
O	-2.13807	-2.54526	-0.46622
C	-2.44528	-2.66323	0.87571
C	-1.23040	-2.46072	1.67575
C	-0.70900	-2.44053	-0.61665
C	-0.22747	-2.22233	0.80151
N	1.07826	-1.81763	0.98973
C	1.58497	-0.75948	0.11027
C	1.24835	-1.08303	-1.34753
C	-0.28054	-1.22800	-1.48426
C	3.07516	-0.55885	0.40322
C	3.76522	0.55395	-0.40810
C	5.18219	0.78453	0.04833
C	6.26955	0.62338	-0.71174
C	7.68459	0.85627	-0.26337
H	0.74822	2.52819	1.77994
H	-0.28468	4.64933	2.56806
H	-2.47058	5.37237	1.60673
H	-3.59311	4.02538	-0.09739
H	-4.72614	2.22673	-0.94343
H	-3.84036	3.12397	-2.20719
H	-4.24646	1.40542	-2.45169
H	-0.60058	-3.89460	-2.22057
H	0.86357	-3.85671	-1.20996
H	-0.61703	-4.60173	-0.59019
H	-1.13686	-3.42870	3.60394
H	-0.44088	-1.80227	3.57330

H	-2.20120	-2.02306	3.52936
H	1.32223	-1.64980	1.96252
H	1.78436	-1.98561	-1.64959
H	1.59426	-0.26437	-1.98379
H	-0.57070	-1.40572	-2.52266
H	3.17411	-0.33669	1.47486
H	3.57803	-1.51664	0.23088
H	3.76427	0.30192	-1.47512
H	3.18310	1.47846	-0.29542
H	5.30448	1.10471	1.08569
H	6.14188	0.30184	-1.74756
H	7.72871	1.17376	0.78408
H	8.29016	-0.05406	-0.36977
H	8.17272	1.62812	-0.87390

Conformer 4

Energy: -1340.63709 Hartree (Rel: 0.1 kcal/mol)

XYZ coordinates for conf 4:

C	-0.40826	2.10268	0.32826
C	0.44067	2.78313	1.22072
C	0.11866	4.05006	1.68221
C	-1.07109	4.65462	1.25200
C	-1.92638	4.00343	0.37235
C	-1.61180	2.71529	-0.10833
N	-2.44820	2.05051	-0.99823
C	-2.16277	0.77071	-1.50766
C	-0.95461	0.12530	-1.01344
C	-0.10739	0.77686	-0.16248
C	-3.67948	2.69414	-1.45951
O	-2.90281	0.24456	-2.34561
O	1.07100	0.25948	0.27837
C	-0.96045	-3.78192	-1.18068
O	-3.86734	-2.27886	1.54800
C	-1.31572	-2.24045	3.23578
O	-2.55966	-2.23931	-0.29887
C	-2.75165	-2.29222	1.06849
C	-1.44876	-2.29232	1.74585
C	-1.15481	-2.37632	-0.58546
C	-0.50953	-2.23292	0.77568
N	0.85680	-2.05181	0.83212
C	1.44902	-1.10241	-0.11571
C	0.92207	-1.37294	-1.52736
C	-0.61583	-1.25713	-1.51488
C	2.97233	-1.15992	0.03643
C	3.76824	-0.17570	-0.84112
C	5.25076	-0.28323	-0.59496
C	6.02434	0.70279	-0.13085
C	7.50277	0.60189	0.11776
H	1.35205	2.29223	1.54246
H	0.78001	4.56687	2.37074
H	-1.33565	5.64662	1.60726
H	-2.83740	4.49618	0.05786
H	-4.33852	2.91154	-0.61331
H	-3.45426	3.62491	-1.99010
H	-4.17111	1.99935	-2.13629
H	-1.44369	-3.83647	-2.16142
H	0.09527	-4.04068	-1.29173
H	-1.42367	-4.52167	-0.52185
H	-1.28162	-3.24454	3.67805
H	-0.40602	-1.71242	3.54541
H	-2.17629	-1.72300	3.67101
H	1.21661	-1.92100	1.77407
H	1.26550	-2.35507	-1.85977
H	1.33671	-0.62869	-2.21202
H	-1.03053	-1.38867	-2.51738
H	3.21077	-0.96498	1.09048
H	3.28168	-2.19058	-0.17275
H	3.56213	-0.38545	-1.90023
H	3.42866	0.84713	-0.64506
H	5.70415	-1.25274	-0.81422
H	5.56604	1.66959	0.08762

H	7.88518	-0.39587	-0.12343
H	8.05785	1.33403	-0.48440
H	7.74457	0.81511	1.16793

Conformer 5

Energy: -1340.63642 Hartree (Rel: 0.4 kcal/mol)

XYZ coordinates for conf 5:

C	-1.10182	2.05591	0.11784
C	-0.35171	3.04517	0.78038
C	-0.96252	4.18243	1.28563
C	-2.34711	4.34222	1.13325
C	-3.10996	3.38077	0.48297
C	-2.50293	2.21992	-0.03977
N	-3.24679	1.25236	-0.70609
C	-2.67643	0.08606	-1.24732
C	-1.24827	-0.10203	-1.03497
C	-0.49741	0.85368	-0.41079
C	-4.68693	1.43955	-0.88987
O	-3.36508	-0.71763	-1.88511
O	0.85066	0.77344	-0.24813
C	-0.01018	-3.81057	-1.16234
O	-2.58874	-3.08633	2.15056
C	0.10982	-2.10245	3.20412
O	-1.79657	-2.78726	0.05197
C	-1.66144	-2.78464	1.42677
C	-0.31695	-2.31512	1.78531
C	-0.52123	-2.49442	-0.55019
C	0.31877	-2.04171	0.62437
N	1.53043	-1.43263	0.36667
C	1.55935	-0.43096	-0.70093
C	0.85769	-0.97022	-1.95066
C	-0.59320	-1.34335	-1.58842
C	2.99570	0.02187	-0.98148
C	3.76695	0.60330	0.22207
C	5.09182	1.18573	-0.19666
C	6.28704	0.75342	0.21605
C	7.60968	1.33130	-0.20122
H	0.71680	2.89814	0.88883
H	-0.37458	4.93960	1.79514
H	-2.83846	5.22788	1.52621
H	-4.17674	3.53265	0.38014
H	-5.19242	1.50709	0.07848
H	-4.88778	2.34844	-1.46616
H	-5.05596	0.57399	-1.43479
H	-0.64701	-4.09612	-2.00570
H	1.02247	-3.73055	-1.51012
H	-0.05406	-4.60151	-0.40844
H	0.56829	-3.00354	3.63166
H	0.83825	-1.28778	3.29340
H	-0.75762	-1.85438	3.82361
H	2.01095	-1.11669	1.20375
H	1.42101	-1.81889	-2.34410
H	0.86145	-0.18786	-2.71564
H	-1.14814	-1.68217	-2.46685
H	3.54327	-0.83680	-1.38566
H	2.94523	0.77599	-1.77533
H	3.15240	1.38238	0.69264
H	3.94325	-0.17320	0.97764
H	5.04339	2.02093	-0.89892
H	6.32900	-0.08369	0.91605
H	7.48304	2.16330	-0.90234
H	8.17362	1.69979	0.66645
H	8.24036	0.57195	-0.68317

Conformer 6

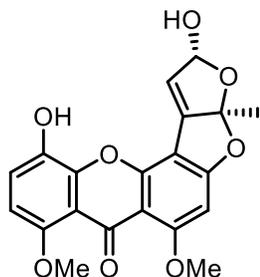
Energy: -1340.63658 Hartree (Rel: 0.5 kcal/mol)

XYZ coordinates for conf 6:

C	-0.63483	2.12052	0.12736
C	0.28475	2.93616	0.81241
C	-0.09453	4.17262	1.31143
C	-1.41434	4.60972	1.12994

C	-2.34114	3.82369	0.45737
C	-1.96992	2.56487	-0.05933
N	-2.87911	1.76863	-0.74682
C	-2.54388	0.51287	-1.28481
C	-1.18810	0.03961	-1.04358
C	-0.27432	0.82166	-0.39519
C	-4.24901	2.24083	-0.95491
O	-3.36674	-0.13360	-1.94193
O	1.02495	0.46890	-0.20029
C	-0.72976	-3.84377	-1.16392
O	-3.20523	-2.60548	2.07736
C	-0.39368	-2.18421	3.21367
O	-2.30600	-2.47891	0.00457
C	-2.21454	-2.50069	1.38282
C	-0.81387	-2.31380	1.78286
C	-0.98056	-2.45153	-0.55838
C	-0.10145	-2.17835	0.64234
N	1.21609	-1.82870	0.42436
C	1.48219	-0.85632	-0.63793
C	0.71991	-1.24040	-1.90957
C	-0.78599	-1.30843	-1.58948
C	2.98817	-0.71087	-0.87929
C	3.82957	-0.26906	0.33608
C	5.28549	-0.11738	-0.02108
C	5.97679	1.02388	0.05269
C	7.42735	1.18368	-0.30465
H	1.29849	2.57527	0.94335
H	0.62274	4.79423	1.83840
H	-1.72497	5.57583	1.51773
H	-3.35253	4.18849	0.33232
H	-4.74790	2.40655	0.00495
H	-4.25369	3.17245	-1.52982
H	-4.77406	1.46749	-1.51039
H	-1.38314	-3.99243	-2.02957
H	0.30837	-3.97678	-1.47739
H	-0.95950	-4.60956	-0.41784
H	-0.08622	-3.14819	3.63925
H	0.44656	-1.48904	3.32975
H	-1.22898	-1.81388	3.81573
H	1.72418	-1.61583	1.27767
H	1.10816	-2.18617	-2.29328
H	0.90566	-0.47491	-2.66900
H	-1.37401	-1.52431	-2.48502
H	3.35421	-1.67517	-1.25119
H	3.12054	0.01841	-1.68583
H	3.44183	0.67613	0.73102
H	3.74129	-1.01715	1.13849
H	5.78949	-1.02126	-0.37055
H	5.46645	1.92412	0.40127
H	7.86547	0.23897	-0.64433
H	7.56006	1.92755	-1.10194
H	8.01108	1.54051	0.55478

Originally assigned (incorrect) structure of 5{7} (DMSO-*d*₆)



					Conf1	Conf2
Rel energy (kcal/mol):					0.00	1.46
C-nom	iGau	Exp	Calc	diff	1	2
C1-C	11	162.50	164.62	2.12	[164.64 164.42]	
C2-CH	12	91.00	91.61	0.61	[91.64 91.29]	
C3-C	13	163.50	170.62	7.12	[170.61 170.74]	
C4-C	14	108.70	100.47	-8.23	[100.45 100.70]	
C4a-C	5	152.70	152.56	-0.14	[152.49 153.32]	
C5-C	7	138.00	140.38	2.38	[140.35 140.73]	
C6-CH	8	120.20	122.08	1.88	[122.11 121.75]	
C7-CH	9	107.00	106.57	-0.43	[106.63 105.82]	
C8-C	10	151.20	151.42	0.22	[151.40 151.69]	
C8a-C	2	114.10	113.48	-0.62	[113.38 114.63]	
C9-C	3	173.50	172.62	-0.88	[172.60 172.86]	
C9a-C	4	108.20	108.21	0.01	[108.19 108.41]	
C10a-C	1	144.80	146.77	1.97	[146.70 147.62]	
C1'-CH	18	117.30	117.07	-0.23	[117.08 116.94]	
C2'-C	19	89.00	139.03	50.03	[138.97 139.71]	
C3'-CH	22	148.20	120.11	-28.09	[120.15 119.58]	
C4'-CH	21	107.10	111.09	3.99	[111.09 111.15]	
C1-OMe-CH3	28	56.50	56.65	0.15	[56.65 56.63]	
C8-OMe-CH3	26	56.40	55.67	-0.73	[55.67 55.70]	

13C chem shifts: RMSD=13.47ppm (MAE=5.78) N=19 {-28.09 50.03}
 Fractions: 0.921 0.079

Conformer 1
 Energy: -1334.15471 Hartree (Rel: 0.0 kcal/mol)
 XYZ coordinates for conf 1:

C	1.50925	-1.37822	-0.07859
C	2.46407	-0.35346	-0.01354
C	2.00586	1.06465	-0.00275
C	0.53421	1.25968	-0.04249
C	-0.31713	0.13802	-0.10418
O	0.16103	-1.13383	-0.12077
C	1.83380	-2.74308	-0.10934
C	3.17476	-3.09156	-0.06447
C	4.16494	-2.10676	0.00864
C	3.83697	-0.74792	0.03354
C	-0.08990	2.55599	-0.01079
C	-1.48490	2.70117	-0.04578
C	-2.25826	1.55120	-0.11713
C	-1.70309	0.25938	-0.16639
O	2.79908	2.00415	0.03594
O	0.86991	-3.70776	-0.18082
O	-3.62408	1.56188	-0.11894
C	-4.02338	0.20277	-0.48034
C	-2.83457	-0.64307	-0.09300
O	-5.10792	-0.30050	0.22945
C	-4.78292	-1.67057	0.61375
C	-3.27453	-1.75027	0.51223
O	-5.38748	-2.59424	-0.24840
H	-4.23880	0.24344	-1.55649

O	4.77378	0.23160	0.10331
C	6.14802	-0.14367	0.15284
O	0.72738	3.62203	0.05332
C	0.16364	4.93556	0.08658
H	3.44674	-4.14207	-0.08699
H	5.19997	-2.42044	0.04353
H	-1.96257	3.67019	-0.01043
H	0.00279	-3.27095	-0.23930
H	-5.15293	-1.79607	1.63780
H	-2.70304	-2.54604	0.97240
H	-6.33764	-2.62167	-0.04495
H	6.70434	0.79325	0.20483
H	6.36799	-0.74784	1.04121
H	6.44672	-0.69527	-0.74666
H	1.01633	5.61328	0.13352
H	-0.41899	5.13959	-0.81834
H	-0.46558	5.07478	0.97243

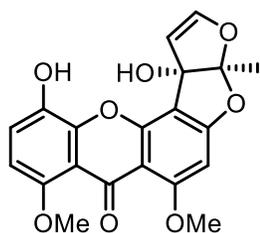
Conformer 2

Energy: -1334.15239 Hartree (Rel: 1.5 kcal/mol)

XYZ coordinates for conf 2:

C	1.48908	-1.37768	-0.11494
C	2.44806	-0.35381	-0.05895
C	1.99941	1.06687	-0.12500
C	0.53126	1.26928	-0.09426
C	-0.31892	0.14783	-0.15813
O	0.14886	-1.12336	-0.20264
C	1.82014	-2.74423	-0.09042
C	3.16114	-3.08383	0.00253
C	4.15141	-2.09753	0.07254
C	3.82038	-0.74207	0.04423
C	-0.08962	2.56446	-0.01069
C	-1.48486	2.71068	-0.00145
C	-2.26024	1.56208	-0.08936
C	-1.70622	0.27422	-0.19507
O	2.79807	1.99967	-0.20406
O	0.79298	-3.64337	-0.15788
O	-3.62637	1.56967	-0.04711
C	-4.03447	0.22089	-0.43510
C	-2.83117	-0.63349	-0.12025
O	-5.09059	-0.31248	0.29707
C	-4.74983	-1.69836	0.60715
C	-3.24610	-1.77012	0.44648
O	-5.38639	-2.58384	-0.27249
H	-4.28962	0.29427	-1.50087
O	4.75150	0.24242	0.12226
C	6.12190	-0.12764	0.24979
O	0.73241	3.62668	0.06978
C	0.17193	4.93736	0.17727
H	3.44946	-4.13155	0.02462
H	5.18416	-2.41078	0.15001
H	-1.96073	3.67770	0.08166
H	1.16124	-4.54196	-0.13783
H	-5.08236	-1.87023	1.63738
H	-2.65264	-2.58458	0.84145
H	-6.32899	-2.61839	-0.03737
H	6.67420	0.81169	0.30147
H	6.29884	-0.70570	1.16482
H	6.46495	-0.70423	-0.61772
H	1.02628	5.61274	0.22807
H	-0.43740	5.18080	-0.69994
H	-0.43072	5.03769	1.08661

Revised structure of 5{7}, i.e. 6{7-rev} (DMSO-*d*₆)



					Conf1	Conf2
Rel energy (kcal/mol):					0.00	1.99
C-nom	iGau	Exp	Calc	diff	1	2
C1-C	11	162.50	163.18	0.68	[163.20	162.55]
C2-CH	12	91.00	90.55	-0.45	[90.55	90.43]
C3-C	13	163.50	165.04	1.54	[165.04	164.94]
C4-C	14	108.70	106.70	-2.00	[106.65	108.26]
C4a-C	5	152.70	152.86	0.16	[152.86	152.80]
C5-C	7	138.00	140.51	2.51	[140.51	140.40]
C6-CH	8	120.20	121.76	1.56	[121.76	121.64]
C7-CH	9	107.00	106.21	-0.79	[106.23	105.65]
C8-C	10	151.20	151.19	-0.01	[151.17	151.84]
C8a-C	2	114.10	113.26	-0.84	[113.22	114.34]
C9-C	3	173.50	172.71	-0.79	[172.71	172.76]
C9a-C	4	108.20	108.17	-0.03	[108.17	108.03]
C10a-C	1	144.80	146.72	1.92	[146.69	147.44]
C1'-CH	18	117.30	116.14	-1.16	[116.14	116.22]
C2'-C	19	89.00	90.75	1.75	[90.78	89.77]
C3'-CH***	22	107.10	105.01	-2.09	[104.97	106.22]
C4'-CH***	21	148.20	147.95	-0.25	[147.97	147.44]
C1-OMe-CH3	28	56.50	56.58	0.08	[56.58	56.55]
C8-OMe-CH3	26	56.40	55.63	-0.77	[55.63	55.62]
13C chem shifts: RMSD=1.27ppm (MAE=1.02) N=19 {-2.09 2.51}					Fractions: 0.966 0.034	

Conformer 1

Energy: -1334.16075 Hartree (Rel: 0.0 kcal/mol)

XYZ coordinates for conf 1:

C	1.53344	-1.25429	-0.04977
C	2.33948	-0.11298	0.05339
C	1.69102	1.22944	0.10013
C	0.21169	1.22702	-0.02951
C	-0.47911	-0.00018	-0.10791
O	0.16754	-1.19573	-0.08753
C	2.03301	-2.56284	-0.12959
C	3.40758	-2.73295	-0.08274
C	4.25708	-1.62649	0.03364
C	3.75226	-0.32421	0.09861
C	-0.58547	2.42321	-0.06883
C	-1.98169	2.36687	-0.18520
C	-2.57820	1.11202	-0.24724
C	-1.86150	-0.07354	-0.21363
O	2.34491	2.26321	0.23339
O	1.19465	-3.63460	-0.24997
O	-3.92556	0.92537	-0.36126
C	-4.18687	-0.48705	-0.45276
C	-2.81315	-1.24325	-0.26477
O	-5.04215	-0.88279	0.60400
C	-4.29797	-1.67305	1.45900
C	-3.05456	-1.93265	1.05614
O	-2.52466	-2.21120	-1.26319
H	-4.69062	-0.67812	-1.40133
O	4.55000	0.76948	0.20025
C	5.96240	0.58067	0.23025
O	0.07199	3.59674	0.00360
C	-0.67278	4.81546	-0.03965

H	3.81894	-3.73566	-0.14117
H	5.32460	-1.80076	0.06692
H	-2.59211	3.25811	-0.22373
H	0.28301	-3.30186	-0.33633
H	-2.31301	-2.51777	1.58141
H	-4.83316	-1.98871	2.34530
H	-2.21221	-1.74186	-2.05600
H	6.38900	1.58178	0.30694
H	6.27025	-0.01374	1.09891
H	6.32320	0.09982	-0.68696
H	0.06988	5.61031	0.03479
H	-1.22137	4.91275	-0.98308
H	-1.37019	4.88473	0.80259

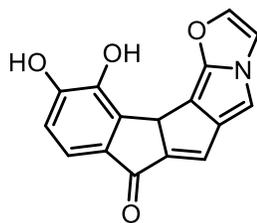
Conformer 2

Energy: -1334.15759 Hartree (Rel: 2.0 kcal/mol)

XYZ coordinates for conf 2:

C	1.51901	-1.25500	-0.04818
C	2.32548	-0.10969	0.04377
C	1.68172	1.23760	0.08716
C	0.20404	1.23968	-0.02049
C	-0.48243	0.01117	-0.09599
O	0.15505	-1.18990	-0.08998
C	2.03364	-2.56141	-0.10636
C	3.41018	-2.71774	-0.06482
C	4.25602	-1.60664	0.03109
C	3.74126	-0.31002	0.08557
C	-0.59675	2.43377	-0.05329
C	-1.99322	2.37427	-0.16963
C	-2.58510	1.11631	-0.23533
C	-1.86273	-0.06264	-0.19265
O	2.34151	2.27018	0.20173
O	1.13168	-3.58497	-0.20325
O	-3.93006	0.91452	-0.36400
C	-4.17251	-0.50189	-0.47020
C	-2.80369	-1.23713	-0.26932
O	-5.04119	-0.91624	0.56715
C	-4.30410	-1.70963	1.42822
C	-3.04927	-1.94420	1.04585
O	-2.56089	-2.11173	-1.36784
H	-4.65155	-0.69314	-1.43097
O	4.53282	0.78893	0.17499
C	5.94616	0.60824	0.20722
O	0.05868	3.60949	0.02469
C	-0.69001	4.82552	-0.01173
H	3.83989	-3.71530	-0.10722
H	5.32427	-1.77579	0.06100
H	-2.60505	3.26450	-0.20986
H	1.61487	-4.42631	-0.24884
H	-2.30857	-2.52409	1.57919
H	-4.85588	-2.04557	2.29685
H	-1.68155	-2.50431	-1.22769
H	6.36697	1.61243	0.27525
H	6.25698	0.02324	1.08122
H	6.31026	0.12151	-0.70559
H	0.04951	5.62282	0.06849
H	-1.23816	4.92719	-0.95506
H	-1.38894	4.88733	0.82998

Originally assigned (incorrect) structure of 7 (CD₃OD)



Rel energy (kcal/mol): **Conf1** 0.00

C-nom	iGau	Exp	Calc	diff	1
C2-CH	17	147.13	138.51	-8.62	[138.51]
C3-CH	16	113.93	113.74	-0.19	[113.74]
C5-CH	13	117.59	99.71	-17.88	[99.71]
C5a-C	11	135.08	138.82	3.74	[138.82]
C6-CH	10	120.38	130.08	9.70	[130.08]
C6a-C	8	135.09	153.36	18.27	[153.36]
C7-C	7	195.24	187.04	-8.20	[187.04]
C7a-C	4	132.04	135.49	3.45	[135.49]
C8-CH	3	118.19	119.86	1.67	[119.86]
C9-CH	2	117.23	115.44	-1.79	[115.44]
C10-C	1	154.19	152.50	-1.69	[152.50]
C11-C	6	143.00	140.27	-2.73	[140.27]
C11a-C	5	138.70	131.35	-7.35	[131.35]
C11b-CH	9	30.19	44.64	14.45	[44.64]
C11c-C	12	117.59	95.83	-21.76	[95.83]
C11d-C	15	153.78	139.65	-14.13	[139.65]

13C chem shifts: RMSD=10.80ppm (MAE=8.48) N=16 {-21.76 18.27}

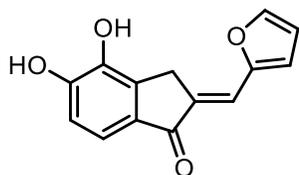
Conformer 1

Energy: -970.67283 Hartree (Rel: 0.0 kcal/mol)

XYZ coordinates for conf 1:

C	-2.94869	-1.74418	-0.23422
C	-3.92234	-0.76384	-0.46282
C	-3.60446	0.58615	-0.32158
C	-2.30702	0.93579	0.05498
C	-1.32222	-0.04849	0.30095
C	-1.63900	-1.38918	0.16013
C	-1.72808	2.30299	0.17664
C	-0.28888	2.06859	0.41740
C	-0.04946	0.60944	0.81195
C	0.82407	2.64296	-0.11688
C	1.88048	1.64832	-0.17626
C	1.34041	0.38759	0.28335
C	3.20936	1.49595	-0.55553
N	3.49831	0.16357	-0.31961
C	2.38856	-0.48459	0.19908
C	4.51310	-0.78964	-0.45306
C	3.99934	-1.95742	-0.01361
O	2.68001	-1.80001	0.40007
O	-2.31827	3.37003	0.00969
O	-0.79729	-2.45166	0.38687
O	-3.27043	-3.05484	-0.38811
H	-4.91498	-1.08464	-0.76305
H	-4.34556	1.35635	-0.51246
H	-0.04169	0.51370	1.91076
H	0.87370	3.63946	-0.54314
H	3.94475	2.17596	-0.95535
H	5.49395	-0.55993	-0.83708
H	4.41112	-2.94876	0.07701
H	0.13163	-2.16975	0.39271
H	-2.46425	-3.57828	-0.22330

Revised structure of 7{unknown}, i.e. {8-rev} (CD₃OD)



Rel energy (kcal/mol): **Conf1** **Conf2** **Conf3** **Conf4** **Conf5** **Conf6**
 0.00 0.28 0.82 1.23 2.53 3.47

C-nom	iGau	Exp	Calc	diff	1	2	3	4	5	6
C2-CH	16	147.13	147.48	0.35	[147.61	147.66	146.77	146.90	147.69	146.89]
C3-CH	17	113.93	113.01	-0.92	[112.89	112.96	113.41	113.40	112.94	113.39]
C5-CH	18	117.59	115.60	-1.99	[116.15	116.30	112.94	112.97	116.30	112.98]
C11d-C	14	153.78	156.24	2.46	[156.29	156.11	156.40	156.22	156.10	156.21]
C6-CH	13	120.38	120.30	-0.08	[120.11	120.15	121.05	121.09	120.15	121.09]
C6a-C	10	135.05	135.01	-0.04	[135.29	134.45	135.51	134.64	134.55	134.71]
C7-C	9	195.24	195.45	0.21	[195.76	195.05	195.53	194.83	195.20	194.99]
C7a-C	4	132.04	132.79	0.75	[133.36	131.83	133.43	131.90	132.45	132.58]
C8-CH	3	118.19	118.16	-0.03	[117.46	119.27	117.54	119.37	118.24	118.28]
C9-CH	2	117.23	115.54	-1.69	[115.18	116.04	115.32	116.19	116.92	117.04]
C10-C	1	154.19	151.77	-2.42	[150.86	153.18	151.02	153.42	152.38	152.58]
C11-C	6	143.00	143.26	0.26	[143.96	142.05	144.06	142.12	143.61	143.66]
C11a-C	5	138.70	136.70	-2.00	[137.62	135.69	136.62	134.68	136.85	135.78]
C11b-CH	11	30.19	29.23	-0.96	[29.96	28.16	29.72	27.94	28.10	27.85]

13C chem shifts: RMSD=1.34ppm (MAE=1.01) N=14 {-2.42 2.46}
 Fractions: 0.495 0.311 0.124 0.063 0.007 0.001

Conformer 1

Energy: -840.37047 Hartree (Rel: 0.0 kcal/mol)

XYZ coordinates for conf 1:

C	-3.70156	-0.55315	0.00018
C	-3.90180	0.83400	0.00041
C	-2.80772	1.69699	0.00025
C	-1.52553	1.14336	-0.00016
C	-1.31734	-0.24635	-0.00030
C	-2.40463	-1.10790	-0.00016
O	-2.22291	-2.46072	-0.00030
O	-4.71178	-1.47296	0.00031
C	-0.22073	1.83427	-0.00064
C	0.82203	0.76899	-0.00032
C	0.15581	-0.59253	-0.00047
O	-0.02634	3.05177	0.00019
C	2.13609	1.09046	-0.00013
C	3.27193	0.22082	0.00004
O	3.08866	-1.14473	0.00013
C	4.32122	-1.71680	0.00027
C	5.29876	-0.76207	0.00028
C	4.62372	0.49197	0.00013
H	-4.91746	1.22176	0.00067
H	-2.94502	2.77379	0.00036
H	-3.10245	-2.87906	-0.00018
H	-5.57610	-1.02998	0.00048
H	0.43519	-1.19220	-0.87652
H	0.43526	-1.19234	0.87547
H	2.37558	2.15279	-0.00012
H	4.33823	-2.79630	0.00036
H	6.36559	-0.93532	0.00039
H	5.06870	1.47749	0.00009

Conformer 2

Energy: -840.37178 Hartree (Rel: 0.3 kcal/mol)

XYZ coordinates for conf 2:

C	-3.71633	-0.55061	-0.00004
C	-3.91163	0.83785	-0.00007
C	-2.81669	1.69757	-0.00003

C	-1.53291	1.14604	0.00003
C	-1.32486	-0.24500	0.00005
C	-2.41637	-1.09949	0.00002
O	-2.36570	-2.47085	0.00002
O	-4.79692	-1.37470	-0.00008
C	-0.23073	1.83835	0.00009
C	0.81444	0.77602	0.00007
C	0.15266	-0.58804	0.00010
O	-0.03665	3.05598	0.00001
C	2.12853	1.09621	0.00002
C	3.26396	0.22607	-0.00001
O	3.07939	-1.13915	0.00005
C	4.31161	-1.71242	-0.00000
C	5.28981	-0.75842	-0.00010
C	4.61591	0.49626	-0.00010
H	-4.93002	1.21367	-0.00012
H	-2.95130	2.77488	-0.00005
H	-1.44571	-2.77920	0.00012
H	-4.47306	-2.29403	-0.00005
H	0.44070	-1.18162	-0.87813
H	0.44065	-1.18155	0.87839
H	2.36774	2.15857	0.00000
H	4.32782	-2.79191	0.00004
H	6.35645	-0.93288	-0.00016
H	5.06148	1.48146	-0.00015

Conformer 3

Energy: -840.37134 Hartree (Rel: 0.8 kcal/mol)

XYZ coordinates for conf 3:

C	-3.76860	-0.50485	-0.00013
C	-3.92781	0.88747	-0.00017
C	-2.80871	1.71816	-0.00007
C	-1.54326	1.12770	0.00009
C	-1.37716	-0.26746	0.00012
C	-2.48811	-1.09747	0.00002
O	-2.34523	-2.45455	0.00005
O	-4.80400	-1.39571	-0.00023
C	-0.21788	1.77952	0.00024
C	0.79142	0.68250	0.00020
C	0.08595	-0.65589	0.00027
O	0.01410	2.98983	0.00009
C	2.11644	0.95379	0.00007
C	3.20458	0.02201	0.00001
O	4.46661	0.58067	-0.00036
C	5.36294	-0.43647	-0.00035
C	4.72248	-1.64404	0.00000
C	3.32866	-1.35312	0.00030
H	-4.93148	1.30538	-0.00029
H	-2.91479	2.79847	-0.00009
H	-3.23613	-2.84825	-0.00007
H	-5.65604	-0.92963	-0.00040
H	0.34477	-1.26384	-0.87840
H	0.34460	-1.26364	0.87913
H	2.39988	2.00527	0.00000
H	6.40358	-0.14891	-0.00064
H	5.18819	-2.61939	0.00008
H	2.51992	-2.06856	0.00066

Conformer 4

Energy: -840.36983 Hartree (Rel: 1.2 kcal/mol)

XYZ coordinates for conf 4:

C	3.78530	-0.49806	-0.00009
C	3.93669	0.89562	-0.00006
C	2.81525	1.72065	0.00002
C	1.54963	1.12935	0.00004
C	1.38591	-0.26774	0.00002
C	2.50289	-1.08823	-0.00005
O	2.49797	-2.46024	-0.00008
O	4.89085	-1.28759	-0.00017
C	0.22632	1.78107	0.00003
C	-0.78439	0.68599	0.00012

C	-0.08167	-0.65419	0.00015
O	-0.00644	2.99139	0.00021
C	-2.10945	0.95590	0.00003
C	-3.19838	0.02515	0.00002
O	-4.45941	0.58580	-0.00045
C	-5.35735	-0.42975	-0.00035
C	-4.71901	-1.63845	0.00014
C	-3.32479	-1.34984	0.00048
H	4.94274	1.30322	-0.00009
H	2.91605	2.80161	0.00003
H	1.58994	-2.80209	0.00004
H	4.59648	-2.21683	-0.00017
H	-0.34851	-1.25604	0.88135
H	-0.34871	-1.25622	-0.88085
H	-2.39179	2.00763	-0.00006
H	-6.39751	-0.14046	-0.00071
H	-5.18630	-2.61303	0.00030
H	-2.51789	-2.06737	0.00097

Conformer 5

Energy: -840.36626 Hartree (Rel: 2.5 kcal/mol)

XYZ coordinates for conf 5:

C	3.70991	-0.58050	-0.00005
C	3.90532	0.80986	-0.00006
C	2.82014	1.68229	-0.00003
C	1.53563	1.13796	0.00002
C	1.32548	-0.25192	0.00004
C	2.40564	-1.12527	0.00001
O	2.29893	-2.48853	0.00004
O	4.73943	-1.47037	-0.00008
C	0.23543	1.83499	0.00005
C	-0.81246	0.77539	0.00006
C	-0.15378	-0.59001	0.00008
O	0.04542	3.05307	0.00006
C	-2.12560	1.09969	0.00002
C	-3.26327	0.23253	-0.00000
O	-3.08238	-1.13319	0.00010
C	-4.31612	-1.70315	0.00002
C	-5.29169	-0.74648	-0.00011
C	-4.61441	0.50626	-0.00014
H	4.92285	1.19389	-0.00010
H	2.96610	2.75795	-0.00004
H	1.35992	-2.73497	0.00004
H	5.58130	-0.98508	-0.00012
H	-0.44481	-1.18210	0.87867
H	-0.44485	-1.18216	-0.87845
H	-2.36170	2.16262	-0.00000
H	-4.33512	-2.78260	0.00009
H	-6.35879	-0.91788	-0.00019
H	-5.05736	1.49265	-0.00024

Conformer 6

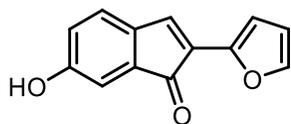
Energy: -840.36776 Hartree (Rel: 3.5 kcal/mol)

XYZ coordinates for conf 6:

C	-3.77859	-0.53016	-0.00007
C	-3.93183	0.86528	-0.00010
C	-2.82075	1.70466	-0.00005
C	-1.55356	1.12205	0.00005
C	-1.38598	-0.27376	0.00007
C	-2.49103	-1.11463	0.00002
O	-2.42736	-2.48006	0.00002
O	-4.83342	-1.38889	-0.00012
C	-0.23176	1.77967	0.00010
C	0.78222	0.68744	0.00010
C	0.08314	-0.65409	0.00015
O	-0.00372	2.99054	0.00009
C	2.10645	0.96097	0.00002
C	3.19754	0.03213	0.00000
O	4.45735	0.59440	-0.00019
C	5.35742	-0.41920	-0.00018
C	4.72087	-1.62880	-0.00000

C	3.32653	-1.34268	0.00014
H	-4.93738	1.27979	-0.00017
H	-2.93397	2.78426	-0.00006
H	-1.49724	-2.75814	0.00022
H	-5.66085	-0.87943	-0.00024
H	0.35359	-1.25474	-0.88132
H	0.35352	-1.25463	0.88171
H	2.38758	2.01298	-0.00002
H	6.39713	-0.12820	-0.00032
H	5.19041	-2.60230	0.00003
H	2.52031	-2.06095	0.00032

Originally assigned (incorrect) structure of 9{2} (CD₃OD)



					Conf1	Conf2	Conf3	Conf4
Rel energy (kcal/mol):					0.00	0.15	2.83	2.98
C-nom	iGau	Exp	Calc	diff	1	2	3	4
C1-C	7	172.10	199.28	27.18	[199.22	199.38	197.84	198.01]
C2-C	8	124.10	131.47	7.37	[131.58	131.32	131.63	131.35]
C3-CH	9	124.30	136.91	12.61	[136.93	136.86	138.24	138.23]
C3a-C	5	149.10	135.85	-13.25	[135.65	136.11	135.11	135.54]
C4-CH	6	111.90	125.99	14.09	[125.85	126.18	125.61	125.94]
C5-CH	1	118.40	118.66	0.26	[118.12	119.36	117.89	119.13]
C6-C	2	155.40	160.27	4.87	[160.34	160.17	160.52	160.34]
C7-CH	3	112.70	113.34	0.64	[113.80	112.76	113.52	112.46]
C7a-C	4	118.80	133.29	14.49	[133.51	133.01	132.93	132.46]
C1'-C	12	152.60	146.84	-5.76	[146.85	146.80	147.82	147.78]
C3'-CH	14	148.90	143.66	-5.24	[143.65	143.68	143.43	143.43]
C4'-CH	15	114.90	112.16	-2.74	[112.16	112.16	111.89	111.89]
C5'-CH	16	123.00	111.42	-11.58	[111.45	111.39	110.62	110.67]
13C chem shifts: RMSD=11.64ppm (MAE=9.24) N=13 {-13.25 27.18}								
Fractions:					0.559	0.433	0.005	0.004

Conformer 1

Energy: -725.82773 Hartree (Rel: 0.0 kcal/mol)

XYZ coordinates for conf 1:

C	-3.55077	-1.18663	-0.00002
C	-3.67801	0.20540	0.00000
C	-2.52797	1.02847	0.00001
C	-1.29797	0.40871	-0.00000
C	-1.15210	-0.99366	-0.00002
C	-2.28316	-1.79759	-0.00002
C	0.08023	1.00524	0.00001
C	1.02997	-0.16881	-0.00001
C	0.28409	-1.30973	-0.00002
O	0.36595	2.19204	0.00001
O	-4.88385	0.83986	0.00002
C	2.45875	-0.02063	0.00000
O	3.21610	-1.16945	0.00006
C	4.52591	-0.78893	0.00003
C	4.62909	0.57074	-0.00004
C	3.29133	1.07361	-0.00002
H	-4.44550	-1.80441	-0.00003
H	-2.63109	2.10931	0.00002
H	-2.20800	-2.88127	-0.00004
H	0.67931	-2.31934	-0.00003
H	-5.59828	0.18117	0.00008
H	5.24705	-1.59212	0.00006
H	5.54448	1.14586	-0.00008
H	2.97002	2.10399	-0.00005

Conformer 2

Energy: -725.82322 Hartree (Rel: 0.2 kcal/mol)

XYZ coordinates for conf 2:

C	-3.54825	-1.20514	-0.00001
C	-3.68160	0.18753	0.00000
C	-2.53570	1.01399	0.00000
C	-1.30133	0.39765	0.00000
C	-1.15093	-1.00182	-0.00001
C	-2.28106	-1.81052	-0.00001
C	0.07408	0.99972	0.00001
C	1.02910	-0.17103	-0.00000
C	0.28713	-1.31401	-0.00001
O	0.35439	2.18765	0.00001
O	-4.94529	0.69885	-0.00000

C	2.45718	-0.01727	0.00000
O	3.21881	-1.16320	0.00003
C	4.52719	-0.77781	0.00001
C	4.62528	0.58225	-0.00003
C	3.28567	1.08011	-0.00001
H	-4.44889	-1.81106	-0.00001
H	-2.62529	2.09797	0.00001
H	-2.20080	-2.89386	-0.00001
H	0.68502	-2.32254	-0.00001
H	-4.90435	1.66942	0.00003
H	5.25131	-1.57832	0.00003
H	5.53853	1.16075	-0.00005
H	2.96058	2.10932	-0.00003

Conformer 3

Energy: -725.82346 Hartree (Rel: 2.8 kcal/mol)

XYZ coordinates for conf 3:

C	-3.59339	1.13210	0.00006
C	-3.66742	-0.26428	0.00009
C	-2.48705	-1.04311	0.00002
C	-1.28162	-0.37715	-0.00010
C	-1.18969	1.02812	-0.00011
C	-2.35006	1.79008	-0.00003
C	0.11793	-0.92532	-0.00029
C	1.02802	0.28737	-0.00011
C	0.23221	1.39534	-0.00014
O	0.43183	-2.10295	-0.00011
O	-4.84788	-0.94485	0.00018
C	2.47013	0.24865	-0.00001
O	3.08773	-0.97928	0.00004
C	4.43131	-0.76015	0.00013
C	4.69761	0.57800	0.00016
C	3.43071	1.23494	0.00006
H	-4.51083	1.71574	0.00013
H	-2.54860	-2.12716	0.00002
H	-2.31532	2.87588	-0.00002
H	0.58088	2.42275	-0.00009
H	-5.58798	-0.31520	0.00028
H	5.05085	-1.64407	0.00018
H	5.67487	1.04018	0.00024
H	3.25050	2.30097	0.00003

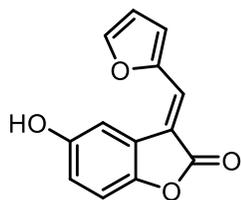
Conformer 4

Energy: -725.82798 Hartree (Rel: 3.0 kcal/mol)

XYZ coordinates for conf 4:

C	3.59119	1.14943	0.00009
C	3.67110	-0.24763	0.00013
C	2.49455	-1.03001	0.00002
C	1.28493	-0.36678	-0.00013
C	1.18864	1.03594	-0.00014
C	2.34828	1.80244	-0.00004
C	-0.11245	-0.91996	-0.00039
C	-1.02728	0.28943	-0.00015
C	-0.23502	1.39966	-0.00019
O	-0.42170	-2.09876	-0.00014
O	4.91478	-0.80585	0.00026
C	-2.46880	0.24542	-0.00001
O	-3.08218	-0.98475	0.00004
C	-4.42645	-0.76980	0.00017
C	-4.69730	0.56751	0.00021
C	-3.43281	1.22852	0.00010
H	4.51433	1.72046	0.00017
H	2.54147	-2.11672	0.00002
H	2.30895	2.88809	-0.00003
H	-0.58633	2.42615	-0.00013
H	4.83825	-1.77425	0.00027
H	-5.04261	-1.65605	0.00022
H	-5.67592	1.02686	0.00031
H	-3.25673	2.29524	0.00008

Revised structure of 9{2}, i.e. 10{2-rev} (CD₃OD)



Rel energy (kcal/mol):					Conf1	Conf2	Conf3	Conf4
					0.00	0.06	3.00	3.12
C-nom	iGau	Exp	Calc	diff	1	2	3	4
C-C	9	172.10	173.52	1.42	[173.50	173.54	173.19	173.13]
C-C	1	155.40	154.48	-0.92	[154.45	154.52	154.55	154.49]
C-C	13	152.60	152.27	-0.33	[152.27	152.26	152.49	152.48]
C-C	4	149.10	147.69	-1.41	[147.76	147.62	147.67	147.84]
C-C	5	124.10	123.96	-0.14	[123.71	124.24	124.07	123.55]
C-C	10	118.80	117.38	-1.42	[117.36	117.39	118.00	118.09]
C-CH	16	148.90	150.51	1.61	[150.44	150.59	149.83	149.77]
C-CH	11	124.30	126.59	2.29	[126.49	126.68	128.78	128.62]
C-CH	14	123.00	124.72	1.72	[124.71	124.80	119.73	119.33]
C-CH	2	118.40	116.18	-2.22	[116.69	115.60	115.88	117.19]
C-CH	15	114.90	113.97	-0.93	[113.98	113.96	114.26	114.17]
C-CH	3	112.70	112.32	-0.38	[112.66	111.93	112.63	113.35]
C-CH	6	111.90	112.29	0.39	[111.85	112.80	110.76	109.77]

13C chem shifts: RMSD=1.36ppm (MAE=1.17) N=13 {-2.22 2.29}
 Fractions: 0.523 0.471 0.003 0.003

Conformer 1

Energy: -801.06730 Hartree (Rel: 0.0 kcal/mol)

XYZ coordinates for conf 1:

C	2.12190	-1.96047	-0.00006
C	3.34271	-1.26835	0.00012
C	3.36745	0.12971	0.00016
C	2.15166	0.78846	0.00005
C	0.91427	0.12400	-0.00007
C	0.90038	-1.27564	-0.00016
O	2.18807	-3.32845	-0.00024
O	2.00986	2.17027	0.00012
C	0.65589	2.45583	-0.00004
C	-0.09918	1.17306	-0.00006
C	-1.46205	1.24656	-0.00013
O	0.25854	3.60125	-0.00006
C	-2.47688	0.25211	-0.00005
C	-3.85245	0.39665	-0.00012
C	-4.40805	-0.90970	0.00010
C	-3.34523	-1.77136	0.00011
O	-2.17187	-1.09043	0.00022
H	4.26706	-1.83676	0.00021
H	4.30377	0.67729	0.00031
H	-0.03514	-1.82167	-0.00032
H	1.28800	-3.69316	0.00032
H	-1.86045	2.25950	-0.00011
H	-4.38499	1.33769	-0.00020
H	-5.45385	-1.18138	0.00012
H	-3.26370	-2.84781	0.00024

Conformer 2

Energy: -801.06261 Hartree (Rel: 0.1 kcal/mol)

XYZ coordinates for conf 2:

C	2.13240	-1.94344	-0.00000
C	3.34667	-1.24213	0.00001
C	3.36061	0.15877	0.00001
C	2.14127	0.80631	-0.00000
C	0.90789	0.13004	-0.00001
C	0.90468	-1.26721	-0.00002
O	2.08034	-3.31224	-0.00001

O	1.98663	2.18657	0.00001
C	0.63009	2.46040	-0.00001
C	-0.11406	1.17159	-0.00001
C	-1.47746	1.23421	-0.00001
O	0.22355	3.60256	0.00001
C	-2.48436	0.23187	-0.00000
C	-3.86110	0.36579	0.00000
C	-4.40645	-0.94472	0.00000
C	-3.33661	-1.79794	0.00004
O	-2.16890	-1.10818	-0.00002
H	4.28623	-1.78849	0.00002
H	4.29332	0.71237	0.00003
H	-0.01612	-1.83427	-0.00004
H	2.98358	-3.66886	-0.00001
H	-1.88382	2.24396	-0.00001
H	-4.40091	1.30268	-0.00000
H	-5.45011	-1.22453	-0.00000
H	-3.24664	-2.87372	0.00005

Conformer 3

Energy: -801.06243 Hartree (Rel: 3.0 kcal/mol)

XYZ coordinates for conf 3:

C	-2.32305	-1.88214	-0.08594
C	-3.48956	-1.11068	0.01353
C	-3.41598	0.28631	0.08487
C	-2.16000	0.85949	0.06886
C	-0.97057	0.11200	-0.00372
C	-1.05731	-1.27953	-0.09630
O	-2.35416	-3.24706	-0.17807
O	-1.92233	2.22684	0.09472
C	-0.55386	2.42071	0.01655
C	0.11151	1.08917	-0.02151
C	1.47457	1.06875	-0.06680
O	-0.08097	3.53617	0.00119
C	2.41482	-0.00065	0.00326
C	2.41719	-1.33279	0.37585
C	3.75732	-1.79179	0.28272
C	4.49656	-0.71975	-0.13953
O	3.71305	0.36787	-0.30467
H	-4.46019	-1.59929	0.02871
H	-4.31201	0.89451	0.14408
H	-0.18574	-1.91108	-0.20229
H	-3.27691	-3.54974	-0.17780
H	1.93832	2.04965	-0.15953
H	1.56984	-1.90119	0.72482
H	4.12682	-2.78279	0.50406
H	5.54530	-0.58533	-0.35853

Conformer 4

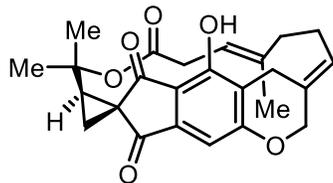
Energy: -801.06740 Hartree (Rel: 3.1 kcal/mol)

XYZ coordinates for conf 4:

C	-2.31595	-1.89624	-0.08884
C	-3.48767	-1.13040	0.01116
C	-3.42266	0.26389	0.08478
C	-2.16828	0.84565	0.07033
C	-0.97579	0.10721	-0.00338
C	-1.05414	-1.28755	-0.09841
O	-2.47322	-3.25240	-0.17749
O	-1.94094	2.21476	0.09753
C	-0.57409	2.41819	0.01784
C	0.10009	1.09078	-0.02141
C	1.46312	1.07932	-0.06867
O	-0.10852	3.53664	0.00260
C	2.40966	0.01533	0.00440
C	2.42149	-1.31148	0.39498
C	3.76298	-1.76575	0.29573
C	4.49329	-0.69614	-0.14743
O	3.70308	0.38574	-0.31971
H	-4.44551	-1.64001	0.02217
H	-4.32148	0.86795	0.14476
H	-0.16619	-1.89870	-0.20897

H	-1.60190	-3.67713	-0.23358
H	1.92056	2.06279	-0.16541
H	1.58019	-1.87816	0.76139
H	4.13933	-2.75178	0.52747
H	5.53935	-0.55968	-0.37767

Originally assigned (incorrect) structure of 11{1} (DMSO-*d*₆)



Rel energy (kcal/mol): **Conf1** 0.00

C-nom	iGau	Exp	Calc	diff	1
C2-C	18	82.20	80.36	-1.84	[80.32]
C3-CH	17	46.10	44.69	-1.41	[43.92]
C4-CH2	16	19.00	20.21	1.21	[18.93]
C4a-C	12	42.80	42.31	-0.49	[41.49]
C5-C	11	192.40	197.84	5.44	[200.23]
C5a-C	8	121.00	121.22	0.22	[122.03]
C6-C	7	161.60	156.36	-5.24	[157.89]
C7-C	1	119.50	120.09	0.59	[120.87]
C8-C	2	153.20	162.14	8.94	[163.79]
C9-CH	10	99.60	104.88	5.28	[105.35]
C9a-C	9	143.30	138.91	-4.39	[140.08]
C10-C	13	196.90	195.77	-1.13	[198.11]
C10a-C	22	170.90	168.00	-2.90	[169.77]
C11-CH2	24	31.10	33.96	2.86	[32.97]
C12-CH	25	118.60	115.39	-3.21	[116.07]
C13-C	26	134.00	135.75	1.75	[136.85]
C14-CH2	27	38.90	37.34	-1.56	[36.41]
C15-CH2	29	25.40	26.61	1.21	[25.46]
C16-CH	30	129.60	130.11	0.51	[131.10]
C17-C	5	129.40	123.21	-6.19	[124.06]
C18-CH2	6	24.80	24.38	-0.42	[23.19]
C19-CH2	4	72.90	72.77	-0.13	[72.58]
C20-CH3	20	29.20	27.16	-2.04	[26.02]
C21-CH3	21	24.40	28.14	3.74	[27.03]
C22-CH3	28	16.20	16.76	0.56	[15.41]

13C chem shifts: CRMSD=3.37ppm (CMAE=2.53) N=25 {-6.19 8.94}

Conformer 1

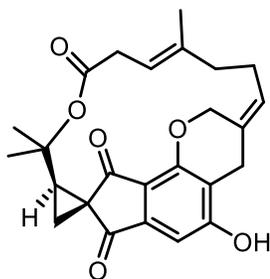
Energy: -1419.61846 Hartree (Rel: 0.0 kcal/mol)

XYZ coordinates for conf 1:

C	1.87456	-1.39645	0.83312
C	1.77802	-2.26210	-0.28241
O	2.86159	-2.71699	-0.94865
C	4.18094	-2.26291	-0.52910
C	4.11850	-0.87416	0.03222
C	3.21593	-0.81253	1.23931
C	0.68925	-0.98662	1.46512
C	-0.54141	-1.37315	0.92397
C	-0.60579	-2.19101	-0.21633
C	0.53583	-2.67831	-0.81544
C	-1.85567	-0.88740	1.31645
C	-2.80196	-1.32174	0.23409
C	-2.02959	-2.27936	-0.64303
O	-2.09254	-0.22816	2.33583
O	-2.49026	-2.94175	-1.55868
C	-4.30523	-1.36828	0.34259
C	-3.70066	-0.33230	-0.54680
C	-3.75358	1.18585	-0.30129
O	-2.42654	1.74929	0.01174
C	-4.57510	1.57598	0.93007
C	-4.30747	1.87553	-1.55490
C	-1.34531	1.60399	-0.77787
O	-1.31502	0.97665	-1.81946
C	-0.18301	2.35588	-0.14311

C	1.16805	2.12527	-0.77859
C	2.31319	2.67830	-0.34551
C	3.63873	2.44560	-1.04552
C	2.37233	3.63319	0.82633
C	4.67732	1.61406	-0.21827
C	4.69885	0.15710	-0.59599
O	0.74490	-0.16772	2.54010
H	4.79904	-2.33032	-1.42579
H	4.54865	-2.98387	0.21283
H	3.06566	0.20904	1.59573
H	3.64855	-1.38238	2.07602
H	0.51353	-3.30808	-1.69772
H	-4.79302	-2.21855	-0.12668
H	-4.71504	-1.06470	1.30085
H	-3.70780	-0.59253	-1.60179
H	-5.60933	1.23877	0.81465
H	-4.57617	2.66488	1.03845
H	-4.15228	1.13749	1.83696
H	-3.69430	1.65264	-2.43080
H	-4.33512	2.95934	-1.40460
H	-5.32852	1.52814	-1.74552
H	-0.17888	2.09461	0.92250
H	-0.46152	3.41955	-0.16962
H	1.18082	1.47314	-1.64947
H	3.47447	1.95926	-2.01396
H	4.08633	3.42618	-1.25958
H	1.43341	3.68966	1.38202
H	2.61729	4.64669	0.47784
H	3.16093	3.35308	1.53576
H	4.48799	1.74064	0.85234
H	5.67708	2.02543	-0.40284
H	5.24579	-0.06674	-1.51341
H	-0.18489	0.01139	2.81421

Revised structure of 11{1}, i.e. 15{1-rev} (DMSO-*d*₆)



Rel energy (kcal/mol): **Conf1** **Conf2**
 0.00 1.20

iGau	jGau	Jexp	Jcalc	diff	1	2
55	56	11.20	8.82	-2.38	[8.82	8.85]
54	56	4.60	7.83	3.23	[7.82	7.87]

For Js: RMSD=2.83Hz N=2 {-2.38 3.23}

C-nom	iGau	Exp	Calc	diff	1	2
C2-C	18	82.20	81.15	-1.05	[81.37	81.33]
C3-CH	17	46.10	43.71	-2.39	[43.41	43.49]
C4-CH2	16	19.00	20.76	1.76	[20.13	20.39]
C4a-C	12	42.80	41.22	-1.58	[40.89	40.95]
C5-C	11	192.40	191.75	-0.65	[193.46	193.39]
C5a-C	8	121.00	123.28	2.28	[124.13	123.51]
C6-C***	7	153.20	154.01	0.81	[155.20	155.25]
C7-C	1	119.50	120.81	1.31	[121.86	119.25]
C8-C***	2	161.60	161.35	-0.25	[162.57	163.23]
C9-CH	10	99.60	102.21	2.61	[102.56	103.78]
C9a-C	9	143.30	142.58	-0.72	[143.60	143.81]
C10-C	13	196.90	197.35	0.45	[199.11	199.27]
C10a-C	22	170.90	170.54	-0.36	[171.97	171.90]
C11-CH2	24	31.10	34.54	3.44	[34.12	34.10]
C12-CH	25	118.60	118.33	-0.27	[119.03	119.18]
C13-C	26	134.00	134.82	0.82	[135.78	135.60]
C14-CH2	27	38.90	40.04	1.14	[39.71	39.59]
C15-CH2	29	25.40	24.78	-0.62	[24.24	24.15]
C16-CH	30	129.60	129.44	-0.16	[130.21	131.03]
C17-C	5	129.40	125.73	-3.67	[126.71	125.33]
C18-CH2	6	24.80	25.27	0.47	[24.92	23.26]
C19-CH2	4	72.90	72.83	-0.07	[72.99	72.44]
C20-CH3	21	29.20	27.56	-1.64	[27.05	27.07]
C21-CH3	20	24.40	25.80	1.40	[25.25	25.34]
C22-CH3	28	16.20	15.21	-0.99	[14.53	14.54]

13C chem shifts: CRMSD=1.57ppm (CMAE=1.23) N=25 {-3.67 3.44}
 Fractions: 0.883 0.117

Conformer 1

Energy: -1419.61065 Hartree (Rel: 0.0 kcal/mol)

XYZ coordinates for conf 1:

C	2.07786	-1.85668	0.14787
C	1.73642	-2.52636	-1.04583
O	2.77873	-2.95514	-1.80265
C	2.68042	-0.57326	2.57844
C	3.50641	-0.29934	1.35942
C	3.52461	-1.49448	0.44005
C	1.05444	-1.41277	1.01001
C	-0.28835	-1.55576	0.60650
C	-0.57679	-2.18265	-0.61825
C	0.40312	-2.70538	-1.44453
C	-1.53199	-1.05800	1.23452
C	-2.62840	-1.27745	0.21914
C	-2.03740	-2.10717	-0.88015
O	-1.66829	-0.58624	2.35615
O	-2.63678	-2.58955	-1.83010
C	-4.09816	-1.35126	0.56661

C	-3.62430	-0.19261	-0.24465
C	-3.62982	1.27165	0.22034
O	-2.27084	1.85401	0.27210
C	-4.13403	1.46746	1.65176
C	-4.47385	2.09877	-0.75938
C	-1.42972	1.82213	-0.77624
O	-1.63558	1.23375	-1.82218
C	-0.18109	2.64207	-0.48409
C	1.09116	1.96427	-0.94983
C	2.32368	2.49599	-0.93222
C	3.51813	1.65944	-1.34732
C	2.61685	3.91114	-0.49539
C	4.56677	1.40385	-0.21929
C	3.94032	0.93463	1.07126
O	1.29081	-0.80295	2.19048
H	3.01730	-1.46614	3.12024
H	2.44622	-3.35967	-2.62144
H	4.04824	-2.33892	0.91377
H	4.04498	-1.29331	-0.49911
H	0.15106	-3.19432	-2.38117
H	-4.67519	-2.12370	0.06507
H	-4.32994	-1.19785	1.61608
H	-3.80438	-0.29522	-1.31084
H	-5.17325	1.13474	1.73081
H	-4.09241	2.53009	1.91009
H	-3.52215	0.90735	2.36172
H	-4.08069	2.02848	-1.77631
H	-4.48397	3.14922	-0.45190
H	-5.50496	1.72971	-0.75942
H	-0.15110	2.86972	0.58666
H	-0.32762	3.60481	-0.99604
H	0.97574	0.93785	-1.29174
H	3.16364	0.69244	-1.72101
H	4.04575	2.14906	-2.17923
H	1.70978	4.50438	-0.35104
H	3.24369	4.42330	-1.23758
H	3.17577	3.93053	0.45031
H	5.12846	2.32528	-0.02952
H	5.29089	0.67275	-0.59825
H	3.76186	1.70776	1.81904
H	2.64018	0.27120	3.26802

Conformer 2

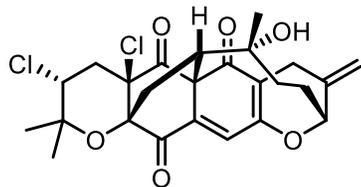
Energy: -1419.60874 Hartree (Rel: 1.2 kcal/mol)

XYZ coordinates for conf 2:

C	2.08712	-1.86434	0.13866
C	1.73887	-2.55999	-1.03927
O	2.68286	-3.06178	-1.87564
C	2.69146	-0.57030	2.56333
C	3.51125	-0.28524	1.34350
C	3.53349	-1.47752	0.41926
C	1.06389	-1.41009	1.00033
C	-0.27869	-1.55430	0.60212
C	-0.57166	-2.19272	-0.61709
C	0.40327	-2.73271	-1.43451
C	-1.51933	-1.05075	1.23105
C	-2.62015	-1.28078	0.22282
C	-2.03359	-2.11662	-0.87427
O	-1.65093	-0.56764	2.34849
O	-2.63765	-2.60414	-1.81843
C	-4.08784	-1.36186	0.57927
C	-3.62557	-0.20460	-0.24012
C	-3.63922	1.26169	0.21893
O	-2.28423	1.85266	0.26927
C	-4.14507	1.46004	1.64945
C	-4.48782	2.07970	-0.76448
C	-1.44175	1.82135	-0.77779
O	-1.64276	1.22766	-1.82163
C	-0.19862	2.65011	-0.48699
C	1.07759	1.98224	-0.95585
C	2.30760	2.51930	-0.92942

C	3.50593	1.69351	-1.35461
C	2.59365	3.93063	-0.47592
C	4.55858	1.43197	-0.23166
C	3.93853	0.95124	1.05755
O	1.30210	-0.79141	2.17555
H	3.02908	-1.46899	3.09493
H	3.56829	-2.97955	-1.48570
H	4.08502	-2.30981	0.88355
H	4.04646	-1.23639	-0.51818
H	0.16589	-3.23829	-2.36377
H	-4.66206	-2.14088	0.08472
H	-4.31485	-1.20474	1.62919
H	-3.81082	-0.31325	-1.30486
H	-5.18184	1.12014	1.73002
H	-4.11104	2.52404	1.90325
H	-3.52891	0.90754	2.36171
H	-4.09360	2.00762	-1.78089
H	-4.50450	3.13131	-0.46131
H	-5.51665	1.70434	-0.76366
H	-0.16856	2.87745	0.58377
H	-0.35314	3.61210	-0.99816
H	0.96660	0.95990	-1.31130
H	3.15510	0.72927	-1.73885
H	4.02996	2.19421	-2.18205
H	1.68342	4.51656	-0.32223
H	3.21543	4.45550	-1.21349
H	3.15494	3.94210	0.46849
H	5.11732	2.35371	-0.03557
H	5.28524	0.70735	-0.61828
H	3.76035	1.71828	1.81139
H	2.65617	0.26780	3.26058

Originally assigned (incorrect) structure of 12{3} (CDCl₃)



Rel energy (kcal/mol): **Conf1** 0.00

C-nom	iGau	Exp	Calc	diff	1
C2-C	2	80.10	79.53	-0.57	[79.53]
C3-CH	1	58.70	57.42	-1.28	[57.42]
C4-CH2	6	36.70	37.07	0.37	[37.07]
C4a-C	5	70.50	69.20	-1.30	[69.20]
C5-C	10	192.30	194.57	2.27	[194.57]
C5a-C	9	60.40	62.99	2.59	[62.99]
C6-C	14	184.10	191.16	7.06	[191.16]
C7-C	13	121.70	129.80	8.10	[129.80]
C8-C	12	162.70	161.77	-0.93	[161.77]
C9-CH	11	131.10	133.41	2.31	[133.41]
C9a-C	8	138.80	132.76	-6.04	[132.76]
C10-C	7	194.30	192.75	-1.55	[192.75]
C10a-C	4	83.10	82.41	-0.69	[82.41]
C11-CH2	27	35.30	34.66	-0.64	[34.66]
C12-CH	21	43.80	47.54	3.74	[47.54]
C13-C	29	86.30	73.35	-12.95	[73.35]
C14-CH2***	30	27.40	28.51	1.11	[28.51]
C15-CH2***	31	30.27	36.54	6.27	[36.54]
C16-CH	16	80.50	81.27	0.77	[81.27]
C17-C	17	139.00	153.78	14.78	[153.78]
C18-CH2	19	113.80	105.47	-8.33	[105.47]
C19-CH2	18	23.10	27.58	4.48	[27.58]
C20-CH3	26	29.60	29.08	-0.52	[29.08]
C21-CH3	25	23.40	24.48	1.08	[24.48]
C22-CH3	32	15.20	33.35	18.15	[33.35]

13C chem shifts: RMSD=6.45ppm (MAE=4.32) N=25 {-12.95 18.15}

Conformer 1

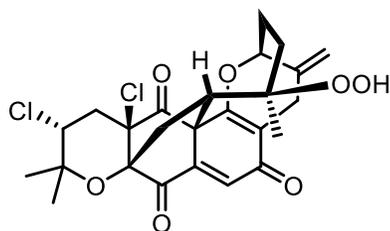
Energy: -2339.92779 Hartree (Rel: 0.0 kcal/mol)

XYZ coordinates for conf 1:

C	-4.32306	0.35394	-0.02391
C	-4.04686	-1.16269	0.16564
O	-2.70977	-1.31243	0.75224
C	-1.59545	-0.56410	0.33896
C	-1.90776	0.93241	0.13757
C	-3.17543	1.10548	-0.69656
C	-0.91097	-1.08770	-0.97228
C	0.37536	-0.39167	-1.20664
C	0.62739	0.79525	-0.29757
C	-0.66687	1.62683	-0.46189
C	1.38197	-0.94466	-1.91419
C	2.71556	-0.40967	-1.71995
C	2.95432	0.85087	-1.27094
C	1.86814	1.62333	-0.66522
O	3.74371	-1.29648	-1.83970
C	4.64998	-1.23395	-0.68884
C	5.17657	0.17767	-0.45984
C	4.38426	1.28354	-1.13417
C	6.26459	0.40361	0.28193
O	1.96825	2.79913	-0.34689
C	0.71099	0.22224	1.19636
O	-0.75896	2.65072	-1.09554
Cl	-2.17094	1.79756	1.76441
Cl	-5.86280	0.64960	-0.96809

C	-4.19333	-1.98484	-1.12084
C	-4.95884	-1.73452	1.25572
C	-0.48580	-0.75156	1.41162
O	-1.30380	-2.04252	-1.61689
C	2.07614	-0.38697	1.69717
C	2.54027	-1.72143	0.99532
C	4.02107	-1.92670	0.56368
C	1.93264	-0.65647	3.21064
O	3.01543	0.68034	1.54394
H	-4.52342	0.79914	0.95016
H	-3.41003	2.16601	-0.80506
H	-2.99153	0.70616	-1.70159
H	1.24642	-1.87241	-2.46241
H	5.48189	-1.86892	-1.00237
H	4.80914	1.46278	-2.13350
H	4.44662	2.22138	-0.57855
H	6.62521	1.41259	0.46321
H	6.84097	-0.40620	0.72403
H	0.57267	1.10108	1.83241
H	-3.76885	-2.97697	-0.95472
H	-5.25196	-2.09015	-1.37205
H	-3.67950	-1.54096	-1.97474
H	-4.80388	-1.20603	2.20146
H	-6.00897	-1.64058	0.96469
H	-4.73433	-2.79445	1.40962
H	-0.16347	-1.79706	1.37109
H	-0.94228	-0.59401	2.39035
H	1.90376	-1.96406	0.14731
H	2.35711	-2.53190	1.71033
H	4.10291	-3.00389	0.37729
H	4.70104	-1.72559	1.40152
H	2.89365	-1.00627	3.60780
H	1.18762	-1.42778	3.43038
H	1.65959	0.26232	3.73943
H	3.89501	0.37461	1.81856

Revised structure of 12{3}, i.e. 16{3-rev} (CDCl₃)



Rel energy (kcal/mol): **Conf1** **Conf2** **Conf3**
 0.00 1.39 3.51

iGau	jGau	Jexp	Jcalc	diff	1	2	3		
34	36	12.10	12.18	0.08	[12.18	12.19	12.19]	H3	H4b
34	35	3.70	3.82	0.12	[3.82	3.81	3.82]	H3	H4a
35	36	14.30	15.08	0.78	[-15.07	-15.13	-15.10]	H4a	H4b

For Js: RMSD=0.46Hz N=3 {0.08 0.78}

H-nom	iGau	Exp	Calc	diff	1	2	3		
H3	34	4.48	4.47	-0.01	[4.47	4.42	4.45]		
H4a	35	2.75	2.69	-0.06	[2.69	2.67	2.68]		
H4b	36	1.89	1.91	0.02	[1.91	1.88	1.89]		

1H chem shifts: RMSD=0.04ppm (MAE=0.03) N=3 {-0.06 0.02}
 m=1.000 b=0.00

C-nom	iGau	Exp	Calc	diff	1	2	3		
C2-C	2	80.10	79.75	-0.35	[79.74	79.90	79.79]		
C3-CH	1	58.70	56.94	-1.76	[56.96	56.76	56.99]		
C4-CH2	6	36.70	37.59	0.89	[37.61	37.40	37.48]		
C4a-C	5	70.50	69.11	-1.39	[69.15	68.73	68.98]		
C5-C	10	192.30	195.60	3.30	[195.66	195.02	195.37]		
C5a-C	9	60.40	58.40	-2.00	[58.42	58.16	58.63]		
C6-C**	14	162.70	162.70	0.00	[162.70	162.72	162.84]		
C7-C	13	121.70	121.80	0.10	[121.78	122.04	121.67]		
C8-C**	12	184.10	186.51	2.41	[186.52	186.37	186.48]		
C9-CH	11	131.10	132.09	0.99	[132.06	132.39	131.94]		
C9a-C	8	138.80	138.53	-0.27	[138.58	138.05	138.29]		
C10-C	7	194.30	195.97	1.67	[196.01	195.61	195.71]		
C10a-C	4	83.10	82.04	-1.06	[82.08	81.68	81.93]		
C11-CH2	27	35.30	35.30	0.00	[35.33	35.04	34.93]		
C12-CH	21	43.80	45.60	1.80	[45.49	46.68	49.24]		
C13-C	29	86.30	87.75	1.45	[87.51	90.15	89.50]		
C14-CH2	30	36.60	37.12	0.52	[37.32	34.94	38.87]		
C15-CH2	31	27.40	27.74	0.34	[27.72	27.90	27.92]		
C16-CH	16	80.50	81.21	0.71	[81.18	81.49	80.85]		
C17-C	17	139.00	139.97	0.97	[139.97	139.99	139.82]		
C18-CH2	19	113.80	114.68	0.88	[114.69	114.60	114.72]		
C19-CH2	18	23.10	24.64	1.54	[24.64	24.60	24.61]		
C20-CH3	26	29.60	28.92	-0.68	[28.93	28.87	28.91]		
C21-CH3	25	23.40	23.83	0.43	[23.84	23.74	23.84]		
C22-CH3	32	15.20	15.52	0.32	[15.71	13.58	14.86]		

13C chem shifts: RMSD=1.31ppm (MAE=1.03) N=25 {-2.00 3.30}
 Fractions: 0.910 0.088 0.002

Conformer 1

Energy: -2415.08626 Hartree (Rel: 0.0 kcal/mol)

XYZ coordinates for conf 1:

C	-4.09836	-0.41299	-0.86661
C	-4.20735	0.20693	0.55417
O	-2.97888	0.96827	0.81240
C	-1.70018	0.47758	0.50388
C	-1.62465	-0.13536	-0.91268
C	-2.77012	-1.12457	-1.12651
C	-1.13850	-0.55248	1.53051
C	0.23970	-0.99177	1.17226
C	0.79961	-0.30799	-0.05182
C	-0.22581	-0.74254	-1.14236

C	0.89606	-1.96418	1.83002
C	2.26276	-2.38993	1.43897
C	2.87736	-1.70013	0.30025
C	2.17551	-0.76938	-0.39379
O	2.84815	-3.27554	2.06746
C	4.11541	0.20533	-1.27674
C	4.86046	-1.09889	-1.12600
C	4.31096	-2.01933	-0.04983
C	5.90554	-1.40437	-1.89722
O	2.69268	-0.07802	-1.42993
C	0.70606	1.27525	0.06017
O	0.01524	-1.51564	-2.03692
Cl	-1.75661	1.18363	-2.21382
Cl	-5.46866	-1.57599	-1.20843
C	-4.48144	-0.82293	1.65747
C	-5.28678	1.29337	0.57610
C	-0.68845	1.64620	0.64850
O	-1.69720	-0.86874	2.56208
C	1.86757	2.03459	0.80565
C	3.18581	2.26699	-0.00262
C	4.27952	1.17696	-0.09126
C	2.15470	1.52434	2.22265
O	1.34673	3.36294	1.10201
H	-4.23346	0.37643	-1.60507
H	-2.73325	-1.52719	-2.14077
H	-2.64286	-1.96575	-0.43364
H	0.44490	-2.45988	2.68472
H	4.91035	-1.94885	0.86944
H	4.39671	-3.06543	-0.36761
H	6.43891	-2.34587	-1.79116
H	6.27190	-0.71879	-2.65725
H	0.74266	1.64176	-0.96645
H	-4.32189	-0.35126	2.62874
H	-5.51866	-1.16184	1.59397
H	-3.83305	-1.69903	1.59937
H	-5.05706	2.07642	-0.15303
H	-6.26571	0.86553	0.34172
H	-5.33487	1.74842	1.57006
H	-0.62229	1.90907	1.70707
H	-1.09507	2.51758	0.13380
H	2.92224	2.60188	-1.01116
H	3.64385	3.12581	0.50233
H	5.24946	1.67018	-0.22139
H	4.35383	0.62623	0.85139
H	2.88193	2.18173	2.70915
H	2.56690	0.51440	2.20228
H	1.24948	1.51200	2.83548
O	0.99938	4.04795	-0.13651
H	4.38173	0.70378	-2.21083
H	1.73170	4.68886	-0.19659

Conformer 2

Energy: -2415.08847 Hartree (Rel: 1.4 kcal/mol)

XYZ coordinates for conf 2:

C	-4.14699	-0.53298	-0.76817
C	-4.22873	0.39515	0.47531
O	-2.98342	1.17063	0.54409
C	-1.71800	0.59634	0.34670
C	-1.66876	-0.32658	-0.89124
C	-2.83571	-1.31332	-0.86734
C	-1.16008	-0.17763	1.57934
C	0.20878	-0.70670	1.32291
C	0.76454	-0.33815	-0.03276
C	-0.28400	-0.99858	-0.98079
C	0.85906	-1.50876	2.18463
C	2.21539	-2.03662	1.89443
C	2.82256	-1.65191	0.61691
C	2.12621	-0.89895	-0.27146
O	2.79604	-2.75516	2.71196
C	4.06689	-0.21243	-1.39114
C	4.78960	-1.45826	-0.93983

C	4.24285	-2.07911	0.33417
C	5.81502	-1.96440	-1.62737
O	2.63562	-0.49250	-1.45087
C	0.69764	1.22918	-0.29367
O	-0.06869	-1.96989	-1.66309
Cl	-1.78655	0.66091	-2.46031
Cl	-5.54282	-1.71334	-0.82829
C	-4.50718	-0.35095	1.78626
C	-5.28830	1.47952	0.25787
C	-0.68631	1.74899	0.21066
O	-1.71350	-0.23972	2.65919
C	1.89517	2.10773	0.23949
C	3.18705	2.10728	-0.63712
C	4.26956	1.01470	-0.47982
C	2.19349	1.93152	1.72960
O	1.28962	3.42499	0.01251
H	-4.27450	0.07147	-1.66550
H	-2.81764	-1.93684	-1.76343
H	-2.71772	-1.97742	-0.00228
H	0.41001	-1.78377	3.13463
H	4.86084	-1.80367	1.20104
H	4.30195	-3.17272	0.27696
H	6.33304	-2.86371	-1.30312
H	6.18029	-1.49128	-2.53545
H	0.72429	1.34724	-1.37874
H	-4.33167	0.32757	2.62304
H	-5.54983	-0.67817	1.80808
H	-3.87231	-1.22768	1.92647
H	-5.05417	2.07127	-0.63242
H	-6.27735	1.02912	0.13499
H	-5.31632	2.14964	1.12246
H	-0.60212	2.24171	1.18238
H	-1.09286	2.48657	-0.48195
H	2.88184	2.18301	-1.68725
H	3.66452	3.05845	-0.38703
H	5.24254	1.44447	-0.74385
H	4.35846	0.70682	0.56678
H	2.93878	2.66642	2.04516
H	2.59242	0.93883	1.94485
H	1.29498	2.07325	2.33814
O	2.15916	4.47944	0.49796
H	4.32332	0.03847	-2.42212
H	1.70134	4.71948	1.32499

Conformer 3

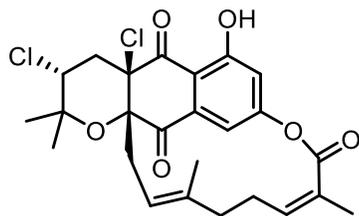
Energy: -2415.08288 Hartree (Rel: 3.5 kcal/mol)

XYZ coordinates for conf 3:

C	-4.09115	-0.67578	-0.75289
C	-4.20016	0.32190	0.43347
O	-2.97558	1.13092	0.45897
C	-1.69477	0.57878	0.29764
C	-1.61895	-0.41337	-0.88246
C	-2.76023	-1.42688	-0.80367
C	-1.12138	-0.10573	1.57663
C	0.26358	-0.61014	1.35614
C	0.80974	-0.31199	-0.01879
C	-0.21724	-1.05218	-0.92899
C	0.93853	-1.33111	2.26938
C	2.30908	-1.83781	2.01115
C	2.90265	-1.52467	0.70741
C	2.18297	-0.85258	-0.22580
O	2.91271	-2.48214	2.87292
C	4.09860	-0.19572	-1.40252
C	4.85556	-1.38923	-0.87191
C	4.33335	-1.93125	0.44742
C	5.88733	-1.91744	-1.53278
O	2.67616	-0.51287	-1.43396
C	0.70785	1.24071	-0.36781
O	0.02629	-2.05381	-1.55650
Cl	-1.75675	0.47739	-2.50749
Cl	-5.45662	-1.89326	-0.74595

C	-4.46546	-0.35286	1.78525
C	-5.28610	1.36436	0.15044
C	-0.69176	1.74672	0.10097
O	-1.67758	-0.11981	2.65669
C	1.87934	2.18797	0.09855
C	3.17225	2.15406	-0.79304
C	4.27504	1.09165	-0.57393
C	2.21830	2.11787	1.58548
O	1.44064	3.54367	-0.26910
H	-4.23120	-0.12900	-1.68468
H	-2.72316	-2.10100	-1.66176
H	-2.62877	-2.03604	0.09914
H	0.49868	-1.55476	3.23697
H	4.94729	-1.57509	1.28750
H	4.42425	-3.02388	0.46988
H	6.42933	-2.77990	-1.15258
H	6.23351	-1.49985	-2.47495
H	0.73207	1.29344	-1.45833
H	-4.31256	0.37811	2.58131
H	-5.49916	-0.70610	1.82249
H	-3.80818	-1.20234	1.97911
H	-5.06318	1.90924	-0.77203
H	-6.26302	0.88259	0.05148
H	-5.33429	2.08271	0.97444
H	-0.62710	2.29365	1.04213
H	-1.11082	2.43637	-0.63303
H	2.86690	2.16099	-1.84586
H	3.63553	3.12735	-0.60518
H	5.23449	1.52928	-0.87169
H	4.37691	0.85528	0.48941
H	2.96439	2.88061	1.83439
H	2.63939	1.14392	1.84116
H	1.34044	2.28228	2.21251
O	0.61795	4.17074	0.75109
H	4.34553	-0.00739	-2.44905
H	1.27338	4.76397	1.16281

Originally assigned (incorrect) structure of 13{4} (CDCl₃)



Rel energy (kcal/mol):					Conf1	Conf2
					0.00	0.91
C-nom	iGau	Exp	Calc	diff	1	2
C2-C	2	78.80	79.01	0.21	[78.99	79.08]
C3-CH	1	58.80	56.31	-2.49	[56.25	56.57]
C4-CH2	6	42.60	42.77	0.17	[43.05	41.45]
C4a-C	5	83.60	77.57	-6.03	[77.17	79.39]
C5-C	10	193.70	192.83	-0.87	[192.72	193.35]
C5a-C	9	109.20	110.59	1.39	[110.54	110.80]
C6-C	14	164.90	164.71	-0.19	[164.83	164.17]
C7-CH	13	109.50	110.30	0.80	[110.19	110.82]
C8-C	12	165.00	164.74	-0.26	[164.78	164.55]
C9-CH	11	108.20	106.47	-1.73	[105.73	109.89]
C9a-C	8	135.00	139.05	4.05	[139.13	138.67]
C10-C	7	195.10	193.95	-1.15	[193.93	194.02]
C10a-C	4	79.30	84.80	5.50	[84.51	86.15]
C11-CH2	23	40.60	43.39	2.79	[43.45	43.09]
C12-CH	17	116.50	116.82	0.32	[116.37	118.90]
C13-C	25	140.10	141.18	1.08	[141.66	138.96]
C14-CH2	27	37.70	38.83	1.13	[38.94	38.32]
C15-CH2	28	26.70	31.59	4.89	[32.29	28.38]
C16-CH	29	144.50	150.58	6.08	[151.38	146.86]
C17-C	30	127.10	126.03	-1.07	[125.72	127.47]
C18-C	32	172.80	165.58	-7.22	[165.34	166.68]
C19-CH3	31	12.00	23.35	11.35	[23.61	22.17]
C20-CH3	22	28.90	28.46	-0.44	[28.31	29.14]
C21-CH3	21	22.20	21.43	-0.77	[21.18	22.58]
C22-CH3	26	16.50	15.78	-0.72	[16.19	13.91]

13C chem shifts: RMSD=3.75ppm (MAE=2.51) N=25 {-7.22 11.35}
 Fractions: 0.822 0.178

Conformer 1

Energy: -2339.99676 Hartree (Rel: 0.0 kcal/mol)

XYZ coordinates for conf 1:

C	-4.24125	-0.28795	-0.38788
C	-3.55933	-1.67254	-0.43228
O	-2.48229	-1.62106	0.55040
C	-1.49374	-0.60388	0.59232
C	-2.15114	0.80875	0.53721
C	-3.24335	0.84966	-0.55962
C	-0.41740	-0.76905	-0.50863
C	0.46694	0.40252	-0.77460
C	0.06301	1.71469	-0.43114
C	-1.20015	1.98389	0.22998
C	1.73658	0.13920	-1.26059
C	2.66654	1.19033	-1.31175
C	2.28022	2.50969	-1.08549
C	0.97765	2.78801	-0.66084
O	4.00306	0.97667	-1.46086
O	0.65729	4.06285	-0.41870
C	0.59553	-0.30645	2.23397
O	-1.56671	3.13430	0.50553
Cl	-2.97824	1.19059	2.13989
Cl	-5.55163	-0.11753	-1.65473
C	-3.06639	-2.07915	-1.82703
C	-4.48317	-2.75578	0.13106
C	-0.72267	-0.97132	1.92119

O	-0.19809	-1.85877	-1.00570
C	1.81196	-0.88649	2.23988
C	2.07583	-2.33031	1.88184
C	3.03464	-0.09633	2.68268
C	4.00954	0.39111	1.56498
C	4.78143	-0.69883	0.87831
C	5.02601	-1.01259	-0.41764
C	5.85734	-2.23209	-0.76529
C	4.49909	-0.33271	-1.62252
O	4.54254	-0.80099	-2.73445
H	-4.76542	-0.18028	0.56152
H	-2.75924	0.78174	-1.54144
H	-3.74661	1.81782	-0.51123
H	2.01286	-0.88227	-1.48943
H	3.00393	3.31339	-1.15759
H	-0.26436	4.06228	-0.04557
H	0.53500	0.73849	2.53930
H	-2.43596	-2.96552	-1.73763
H	-3.92226	-2.31324	-2.46527
H	-2.48251	-1.30139	-2.32528
H	-4.78863	-2.50517	1.15169
H	-5.37652	-2.85977	-0.49103
H	-3.95850	-3.71576	0.15184
H	-0.60254	-2.05293	1.84176
H	-1.42989	-0.78947	2.73567
H	1.18678	-2.86836	1.54847
H	2.49375	-2.86508	2.74585
H	2.82155	-2.40376	1.08140
H	2.70947	0.80038	3.22154
H	3.60880	-0.70115	3.39969
H	3.47708	1.04539	0.88109
H	4.75763	1.01954	2.07333
H	5.25166	-1.37738	1.59284
H	6.25022	-2.70466	0.13859
H	5.26227	-2.96996	-1.31466
H	6.70051	-1.96318	-1.41165

Conformer 2

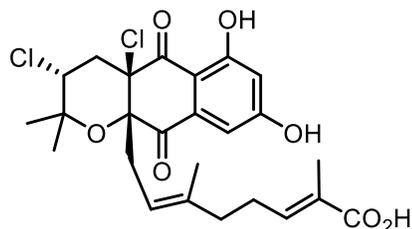
Energy: -2339.99821 Hartree (Rel: 0.9 kcal/mol)

XYZ coordinates for conf 2:

C	-4.26497	-0.43943	-0.42364
C	-3.55399	-1.78991	-0.16592
O	-2.45014	-1.52243	0.75801
C	-1.52666	-0.46013	0.60802
C	-2.24801	0.88677	0.29879
C	-3.29979	0.67751	-0.80932
C	-0.47695	-0.74326	-0.49504
C	0.44470	0.38334	-0.80174
C	0.02820	1.71995	-0.61079
C	-1.30615	2.04085	-0.12931
C	1.74325	0.06467	-1.15402
C	2.69260	1.09700	-1.20606
C	2.31439	2.43289	-1.10602
C	0.97655	2.76011	-0.84310
O	4.03687	0.83081	-1.16709
O	0.64987	4.05389	-0.75473
C	0.63254	-1.07774	1.97135
O	-1.71735	3.20568	-0.06717
Cl	-3.14324	1.47441	1.80354
Cl	-5.55436	-0.57505	-1.71606
C	-3.09594	-2.50245	-1.44552
C	-4.45433	-2.72237	0.65074
C	-0.72660	-0.41387	1.97723
O	-0.30819	-1.85437	-0.96037
C	1.76048	-0.61009	2.53647
C	1.83892	0.61995	3.40990
C	3.08395	-1.31199	2.27944
C	4.11853	-0.34363	1.60794
C	5.14918	-1.07178	0.79366
C	5.36388	-1.11113	-0.54173
C	6.40358	-2.02903	-1.14841

C	4.52425	-0.42382	-1.55401
O	4.29218	-0.85446	-2.65864
H	-4.81473	-0.15122	0.47143
H	-2.78345	0.42941	-1.74515
H	-3.83870	1.61402	-0.97072
H	2.02080	-0.97505	-1.26603
H	3.05483	3.22182	-1.17217
H	-0.31386	4.09370	-0.51958
H	0.69656	-2.01440	1.42017
H	-2.42212	-3.31728	-1.17650
H	-3.96536	-2.91503	-1.96389
H	-2.56887	-1.84739	-2.14235
H	-4.72886	-2.25369	1.60077
H	-5.36600	-2.95883	0.09467
H	-3.92477	-3.65580	0.86450
H	-1.40520	-0.89412	2.69120
H	-0.62955	0.62812	2.28406
H	0.86380	1.06736	3.61392
H	2.29080	0.36190	4.37753
H	2.47769	1.39397	2.96572
H	3.51490	-1.69785	3.21382
H	2.91379	-2.17437	1.62583
H	3.58535	0.38821	1.00746
H	4.63952	0.21673	2.39542
H	5.79607	-1.72326	1.38384
H	6.97553	-2.53683	-0.36746
H	5.93171	-2.78537	-1.78506
H	7.10354	-1.47136	-1.78218

Revised structure of 13{4}, i.e. 17{4-rev} (CDCl₃)



Rel energy (kcal/mol): **Conf1** **Conf2**
 0.00 0.29

C-nom	iGau	Exp	Calc	diff	1	2
C2-C	2	78.80	78.95	0.15	[78.93	78.99]
C3-CH	1	58.80	56.86	-1.94	[56.76	57.03]
C4-CH2	6	42.60	42.17	-0.43	[42.16	42.19]
C4a-C**	5	79.30	79.59	0.29	[79.70	79.41]
C5-C	10	193.70	192.17	-1.53	[192.32	191.92]
C5a-C	9	109.20	107.99	-1.21	[108.32	107.45]
C6-C	14	164.90	164.84	-0.06	[164.78	164.95]
C7-CH	13	109.50	109.01	-0.49	[109.38	108.39]
C8-C	12	165.00	165.17	0.17	[164.38	166.48]
C9-CH	11	108.20	107.18	-1.02	[107.29	107.01]
C9a-C	8	135.00	135.05	0.05	[135.01	135.11]
C10-C	7	195.10	192.21	-2.89	[192.58	191.59]
C10a-C	4	83.60	84.86	1.26	[83.93	86.39]
C11-CH2	23	40.60	39.84	-0.76	[38.86	41.46]
C12-CH	17	116.50	117.17	0.67	[119.59	113.18]
C13-C	25	140.10	137.27	-2.83	[134.16	142.38]
C14-CH2	27	37.70	37.81	0.11	[39.24	35.45]
C15-CH2	28	26.70	26.36	-0.34	[25.99	26.97]
C16-CH	29	144.50	146.52	2.02	[144.88	149.22]
C17-C	30	127.10	126.61	-0.49	[127.81	124.64]
C18-C	32	172.80	172.01	-0.79	[171.87	172.25]
C19-CH3	31	12.00	12.58	0.58	[12.23	13.15]
C20-CH3	22	28.90	28.86	-0.04	[28.73	29.07]
C21-CH3	21	22.20	21.99	-0.21	[22.00	21.97]
C22-CH3	26	16.50	16.14	-0.36	[14.89	18.19]

13C chem shifts: RMSD=1.16ppm (MAE=0.83) N=25 {-2.89 2.02}

Fractions: 0.622 0.378

Conformer 1

Energy: -2416.46212 Hartree (Rel: 0.0 kcal/mol)

XYZ coordinates for conf 1:

C	-4.12999	-0.55548	-0.56138
C	-3.17472	-1.63643	-1.12180
O	-2.05705	-1.73407	-0.18448
C	-1.33933	-0.61557	0.30298
C	-2.30068	0.49487	0.82524
C	-3.41423	0.74703	-0.21558
C	-0.36937	-0.02899	-0.75778
C	0.21343	1.31464	-0.48844
C	-0.40062	2.19863	0.43329
C	-1.62340	1.85069	1.13343
C	1.37927	1.65492	-1.15173
C	1.99971	2.88935	-0.87314
C	1.40941	3.79479	0.00854
C	0.21283	3.46976	0.65605
O	3.18822	3.22919	-1.42456
O	-0.31226	4.37431	1.49094
C	0.67075	-2.10581	0.94123
O	-2.17711	2.63223	1.91883
Cl	-3.12300	-0.05445	2.38171
Cl	-5.50314	-0.18322	-1.71412
C	-2.72038	-1.37190	-2.56371
C	-3.81587	-3.02413	-1.02695

C	-0.42894	-1.19073	1.43458
O	-0.00485	-0.69639	-1.70954
C	1.72908	-2.52645	1.65201
C	1.96458	-2.17218	3.10133
C	2.75176	-3.44173	1.00553
C	4.22253	-2.92482	1.03639
C	4.36603	-1.50538	0.56538
C	4.58918	-1.07323	-0.69237
C	4.74390	-1.94004	-1.91603
C	4.56759	0.38420	-0.95229
O	4.39959	0.86482	-2.07574
H	-4.62510	-0.94608	0.32680
H	-2.96408	1.18510	-1.11499
H	-4.11958	1.47746	0.18754
H	1.81701	0.95428	-1.85257
H	1.88239	4.74914	0.21136
H	-1.14027	3.97263	1.86628
H	0.56789	-2.45752	-0.08196
H	-1.89751	-2.04575	-2.80737
H	-3.55092	-1.56188	-3.24838
H	-2.37782	-0.34809	-2.73037
H	-4.07776	-3.25407	0.01044
H	-4.71983	-3.07189	-1.64074
H	-3.11216	-3.78265	-1.38309
H	-1.10826	-1.72858	2.10407
H	-0.01667	-0.35404	2.00955
H	1.14472	-1.59261	3.53283
H	2.08039	-3.08389	3.70344
H	2.88794	-1.59297	3.23675
H	2.74808	-4.41988	1.50921
H	2.46557	-3.61888	-0.03699
H	4.83042	-3.60760	0.43341
H	4.60354	-2.98688	2.06270
H	4.22932	-0.74443	1.32905
H	4.81430	-2.99750	-1.65320
H	3.89077	-1.81127	-2.59196
H	5.64053	-1.66409	-2.48234
H	3.55182	2.47179	-1.94856
O	4.71267	1.16591	0.13401
H	4.59091	2.09641	-0.14427

Conformer 2

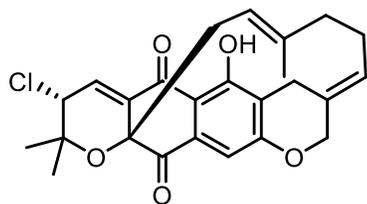
Energy: -2416.46259 Hartree (Rel: 0.3 kcal/mol)

XYZ coordinates for conf 2:

C	3.91254	-0.42631	0.77735
C	2.91029	-1.56153	1.09708
O	1.91883	-1.55944	0.02313
C	1.24702	-0.39459	-0.41776
C	2.24610	0.76816	-0.69313
C	3.22740	0.90599	0.49027
C	0.13980	0.06229	0.56016
C	-0.44655	1.41103	0.32558
C	0.26726	2.39793	-0.39989
C	1.59108	2.14943	-0.93326
C	-1.71537	1.65185	0.81532
C	-2.34681	2.88649	0.55337
C	-1.65766	3.89328	-0.12795
C	-0.35835	3.66911	-0.59333
O	-3.61349	3.12546	0.93376
O	0.25824	4.66727	-1.23893
C	-0.79439	-1.61245	-1.53516
O	2.24106	3.02373	-1.52510
Cl	3.25156	0.39104	-2.19584
Cl	5.13215	-0.18318	2.12222
C	2.27669	-1.45211	2.49069
C	3.57958	-2.92996	0.93911
C	0.48394	-0.83207	-1.72450
O	-0.32912	-0.70124	1.38488
C	-0.95121	-2.94380	-1.59998
C	0.18219	-3.92216	-1.79895
C	-2.30887	-3.61859	-1.50218

C	-3.57194	-2.73731	-1.45150
C	-3.83406	-2.08193	-0.12488
C	-4.40068	-0.87814	0.10399
C	-4.85521	0.10469	-0.94728
C	-4.58664	-0.43213	1.50578
O	-4.73390	0.74069	1.85190
H	4.51624	-0.71820	-0.08116
H	2.66911	1.24500	1.37153
H	3.96559	1.67575	0.25323
H	-2.21721	0.87961	1.38178
H	-2.13365	4.84898	-0.31694
H	1.15319	4.32678	-1.50556
H	-1.67787	-1.00092	-1.36795
H	1.44264	-2.15225	2.55792
H	3.01974	-1.70735	3.25066
H	1.89606	-0.45357	2.71697
H	3.97700	-3.04675	-0.07391
H	4.39790	-3.04192	1.65602
H	2.84771	-3.72329	1.11866
H	1.21453	-1.39457	-2.30681
H	0.25407	0.07574	-2.29384
H	1.16404	-3.44878	-1.76296
H	0.07816	-4.45110	-2.75667
H	0.15893	-4.69108	-1.01507
H	-2.40373	-4.28991	-2.36826
H	-2.30556	-4.28930	-0.62879
H	-4.42958	-3.39935	-1.64955
H	-3.56193	-2.01088	-2.27042
H	-3.56153	-2.67903	0.74301
H	-4.53853	-0.19514	-1.94780
H	-5.94968	0.18605	-0.95292
H	-4.46715	1.10778	-0.74880
H	-4.02524	2.30227	1.29221
O	-4.58776	-1.41664	2.42109
H	-4.65409	-0.98993	3.29726

Originally assigned (incorrect) structure of 14{5} (CDCl₃)



Rel energy (kcal/mol):					Conf1	Conf2
					0.00	0.72
C-nom	iGau	Exp	Calc	diff	1	2
C2-C	2	77.20	77.42	0.22	[77.43	77.40]
C3-CH	1	59.40	58.32	-1.08	[58.40	58.07]
C4-CH	6	135.60	136.86	1.26	[137.31	135.36]
C4a-C	5	137.50	136.68	-0.82	[136.13	138.51]
C5-C	10	187.90	188.36	0.46	[188.39	188.26]
C5a-C	9	113.40	114.34	0.94	[114.38	114.21]
C6-C	14	161.90	158.49	-3.41	[158.36	158.92]
C7-C	13	119.20	126.57	7.37	[126.89	125.50]
C8-C	12	162.80	165.20	2.40	[165.31	164.85]
C9-CH	11	109.50	112.49	2.99	[112.48	112.54]
C9a-C	8	136.40	136.25	-0.15	[136.01	137.06]
C10-C	7	195.50	194.51	-0.99	[194.81	193.50]
C10a-C	4	84.00	83.17	-0.83	[83.13	83.29]
C11-CH2	22	43.10	46.04	2.94	[45.82	46.79]
C12-CH	16	118.00	118.43	0.43	[118.84	117.05]
C13-C	24	138.30	140.33	2.03	[140.39	140.14]
C14-CH2	26	38.70	38.59	-0.11	[38.05	40.40]
C15-CH2	27	25.50	28.30	2.80	[29.35	24.77]
C16-CH	32	133.30	134.62	1.32	[134.19	136.06]
C17-C	30	133.20	130.20	-3.00	[130.90	127.87]
C18-CH2	31	20.80	26.80	6.00	[26.91	26.44]
C19-CH2	29	70.10	76.16	6.06	[76.15	76.18]
C20-CH3	21	27.40	27.03	-0.37	[27.05	26.97]
C21-CH3	20	20.20	20.12	-0.08	[20.12	20.12]
C22-CH3	25	13.90	18.32	4.42	[19.10	15.71]
13C chem shifts: RMSD=2.90ppm (MAE=2.10) N=25 {-3.41 7.37}						
Fractions:					0.770	0.230

Conformer 1

Energy: -1803.95254 Hartree (Rel: 0.0 kcal/mol)

XYZ coordinates for conf 1:

C	-4.24033	0.37091	0.66729
C	-4.06539	-0.83883	-0.29657
O	-2.83099	-1.46340	0.11930
C	-1.61373	-0.73101	0.13067
C	-1.82024	0.74758	0.35131
C	-3.03049	1.25066	0.63852
C	-0.81624	-0.95330	-1.17434
C	0.38963	-0.09166	-1.30287
C	0.46455	1.14205	-0.60353
C	-0.65360	1.64855	0.18289
C	1.49463	-0.62186	-1.95051
C	2.74877	-0.01813	-1.75538
C	2.86728	1.18736	-1.04555
C	1.71438	1.80909	-0.54455
O	1.85856	2.98057	0.09744
C	0.44947	-0.83415	1.89982
O	-0.63843	2.77949	0.71290
H	-3.14282	2.31688	0.80823
Cl	-5.73395	1.36455	0.27491
C	-4.04126	-0.44492	-1.77849
C	-5.12567	-1.90959	-0.03783
O	-0.82019	-1.42064	1.32325
C	-1.08671	-1.84716	-1.95706
C	1.68718	-1.36933	1.89821

C	2.05997	-2.62122	1.13804
C	2.78574	-0.79883	2.79696
C	3.87792	0.14931	2.20315
O	3.83933	-0.69968	-2.19193
C	5.09195	-0.58399	-1.41039
C	4.79990	0.19515	-0.16687
C	4.24275	1.55682	-0.53893
C	4.61826	-0.41137	1.01825
H	-4.43242	-0.00843	1.67472
H	1.42540	-1.57669	-2.45820
H	0.95522	3.22201	0.44516
H	0.29749	0.06457	2.49935
H	-3.75373	-1.31748	-2.36973
H	-5.03070	-0.10901	-2.09997
H	-3.32955	0.35955	-1.98415
H	-5.09900	-2.23115	1.00826
H	-6.12415	-1.52620	-0.26505
H	-4.93202	-2.77996	-0.67179
H	-0.67950	-2.45924	1.01017
H	-1.56541	-1.43965	2.12771
H	1.23426	-3.03502	0.55515
H	2.88291	-2.42220	0.44181
H	2.41336	-3.40042	1.82728
H	2.31769	-0.24303	3.61764
H	3.30286	-1.65085	3.26113
H	3.41307	1.10533	1.94508
H	4.57715	0.35503	3.02727
H	5.40654	-1.61093	-1.21071
H	5.81897	-0.10194	-2.07193
H	4.16765	2.25155	0.29756
H	4.86705	2.03177	-1.30667
H	4.96140	-1.44233	1.11784

Conformer 2

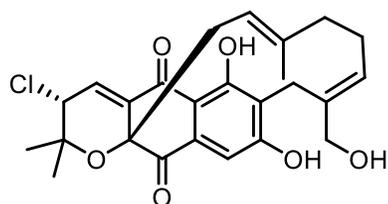
Energy: -1803.95139 Hartree (Rel: 0.7 kcal/mol)

XYZ coordinates for conf 2:

C	-4.23324	-0.68886	0.06389
C	-4.05918	0.68538	-0.64286
O	-2.83826	0.54938	-1.40434
C	-1.60716	0.25083	-0.76001
C	-1.80396	-0.56917	0.49488
C	-3.00961	-1.03973	0.84830
C	-0.81442	1.53021	-0.41134
C	0.38956	1.28440	0.43295
C	0.49347	0.10013	1.21122
C	-0.61817	-0.82862	1.34309
C	1.47658	2.12677	0.26798
C	2.74178	1.70448	0.71355
C	2.89717	0.49502	1.41115
C	1.75874	-0.25186	1.74424
O	1.92978	-1.36884	2.47188
C	0.67942	-0.61348	-2.00035
O	-0.58242	-1.81333	2.11186
H	-3.10585	-1.65672	1.73621
Cl	-5.70380	-0.72718	1.16415
C	-4.00861	1.87245	0.32674
C	-5.13468	0.90129	-1.70790
C	-0.83161	-0.58331	-1.87852
O	-1.08974	2.61813	-0.88527
C	1.52460	-1.62940	-1.73259
C	1.12038	-2.89795	-1.01974
C	2.95180	-1.61437	-2.27121
C	4.15546	-1.72023	-1.26532
O	3.80198	2.46459	0.34495
C	5.09764	1.78777	0.14167
C	4.86632	0.30828	0.14197
C	4.27940	-0.12089	1.46971
C	4.77271	-0.37017	-1.01190
H	-4.44959	-1.44841	-0.69254
H	1.39063	3.01975	-0.34005
H	1.02688	-1.78478	2.56186

H	1.10073	0.26026	-2.49771
H	-3.71313	2.76715	-0.22603
H	-4.99191	2.03979	0.77423
H	-3.29204	1.71748	1.13827
H	-5.12323	0.08410	-2.43629
H	-6.12592	0.95275	-1.24921
H	-4.94508	1.83931	-2.23815
H	-1.21120	-0.13797	-2.80507
H	-1.24517	-1.59488	-1.82503
H	0.04651	-2.95538	-0.82568
H	1.62588	-2.97715	-0.04800
H	1.41108	-3.78456	-1.59862
H	3.02623	-2.47399	-2.95280
H	3.09212	-0.72449	-2.89581
H	3.84345	-2.20333	-0.33477
H	4.90983	-2.37720	-1.71813
H	5.47125	2.16312	-0.81359
H	5.75647	2.12647	0.94844
H	4.19862	-1.20234	1.58822
H	4.88364	0.25658	2.30509
H	5.10734	0.14302	-1.91571

Revised structure of 14{5}, i.e. 18{5-rev} (CDCl₃)



Rel energy (kcal/mol): **Conf1** **Conf2**
 0.00 3.72

C-nom	iGau	Exp	Calc	diff	1	2
C2-C	2	77.20	77.27	0.07	[77.27	77.02]
C3-CH	1	59.40	58.34	-1.06	[58.34	58.32]
C4-CH	6	135.60	135.81	0.21	[135.81	136.18]
C4a-C	5	137.50	138.28	0.78	[138.28	138.19]
C5-C	10	187.90	187.63	-0.27	[187.63	187.92]
C5a-C	9	113.40	112.56	-0.84	[112.56	111.58]
C6-C	14	161.90	161.69	-0.21	[161.69	162.76]
C7-C	13	119.20	119.90	0.70	[119.90	118.93]
C8-C	12	162.80	164.46	1.66	[164.46	164.41]
C9-CH	11	109.50	110.09	0.59	[110.09	109.21]
C9a-C	8	136.40	137.22	0.82	[137.22	137.53]
C10-C	7	195.50	194.38	-1.12	[194.38	194.44]
C10a-C	4	84.00	83.63	-0.37	[83.63	83.24]
C11-CH2	22	43.10	44.97	1.87	[44.97	44.70]
C12-CH	16	118.00	117.76	-0.24	[117.77	112.97]
C13-C	24	138.30	138.30	0.00	[138.30	138.86]
C14-CH2	26	38.70	39.40	0.70	[39.41	36.22]
C15-CH2	27	25.50	26.23	0.73	[26.24	22.14]
C16-CH	32	133.30	133.70	0.40	[133.70	134.19]
C17-C	30	133.20	129.48	-3.72	[129.48	127.71]
C18-CH2	31	20.80	23.33	2.53	[23.33	24.49]
C19-CH2	29	70.10	71.15	1.05	[71.15	71.87]
C20-CH3	21	27.40	26.94	-0.46	[26.94	26.94]
C21-CH3	20	20.20	19.98	-0.22	[19.98	20.07]
C22-CH3	25	13.90	13.43	-0.47	[13.42	17.47]

13C chem shifts: RMSD=1.18ppm (MAE=0.84) N=25 {-3.72 2.53}

Fractions: 0.998 0.002

Conformer 1

Energy: -1880.39392 Hartree (Rel: 0.0 kcal/mol)

XYZ coordinates for conf 1:

C	4.50982	0.58867	0.32470
C	4.38689	-0.69700	-0.54227
O	3.24907	-0.44972	-1.39676
C	1.96704	-0.18312	-0.84405
C	2.04798	0.48127	0.51064
C	3.22166	0.87711	1.02743
C	1.10844	-1.46719	-0.73408
C	-0.15580	-1.30797	0.04492
C	-0.29847	-0.25381	0.98564
C	0.79989	0.64641	1.29487
C	-1.23455	-2.10950	-0.27735
C	-2.52251	-1.79453	0.20986
C	-2.71787	-0.71068	1.08792
C	-1.58245	-0.01429	1.54114
O	-1.76106	0.95967	2.45210
C	-0.17348	0.91897	-1.98408
O	0.72069	1.52517	2.18213
H	3.24201	1.37679	1.99074
Cl	5.87098	0.47484	1.55326
C	4.22347	-1.98081	0.28042
C	5.55883	-0.82313	-1.51609
C	1.32506	0.78571	-1.92996
O	1.39718	-2.49088	-1.32826
C	-0.95378	1.97877	-1.70534

C	-0.45409	3.32343	-1.23899
C	-2.46011	1.83898	-1.85536
C	-3.26900	2.10179	-0.54150
O	-3.52065	-2.56956	-0.24470
C	-6.28067	-0.30615	0.16674
C	-4.92760	0.33771	0.32304
C	-4.09972	-0.23259	1.48346
C	-4.55704	1.32161	-0.51476
H	4.80586	1.42000	-0.32118
H	-1.12415	-2.91763	-0.99135
H	-0.86279	1.37503	2.59998
H	-0.68367	0.01853	-2.32286
H	3.97609	-2.80319	-0.39506
H	5.15364	-2.21944	0.80298
H	3.42963	-1.89841	1.02808
H	5.63173	0.06914	-2.14616
H	6.49919	-0.95082	-0.97293
H	5.40771	-1.69177	-2.16388
H	1.67241	0.35910	-2.87916
H	1.82793	1.74903	-1.80620
H	0.63646	3.38650	-1.20671
H	-0.82817	3.55518	-0.23307
H	-0.82037	4.12084	-1.90009
H	-2.82394	2.53085	-2.62923
H	-2.68372	0.82804	-2.21231
H	-2.66009	1.87094	0.33267
H	-3.50414	3.17296	-0.47545
H	-6.85115	0.15860	-0.64549
H	-6.86080	-0.21019	1.09470
H	-3.99123	0.52138	2.26751
H	-4.66218	-1.06158	1.93035
H	-5.26793	1.59059	-1.29856
H	-4.42779	-2.21919	-0.05383
O	-6.08888	-1.71080	-0.12591
H	-6.77984	-2.23246	0.31056

Conformer 2

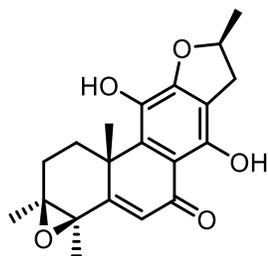
Energy: -1880.38799 Hartree (Rel: 3.7 kcal/mol)

XYZ coordinates for conf 2:

C	-4.56644	-0.49322	-0.59887
C	-4.37346	0.61494	0.47568
O	-3.21400	1.35329	0.03243
C	-1.96142	0.70507	-0.14425
C	-2.11102	-0.75382	-0.50925
C	-3.31343	-1.29279	-0.76386
C	-1.06816	0.83081	1.11477
C	0.16063	-0.01572	1.09704
C	0.24111	-1.15509	0.25157
C	-0.89641	-1.60551	-0.53384
C	1.26816	0.41535	1.80235
C	2.53159	-0.16583	1.55681
C	2.67063	-1.22523	0.64129
C	1.50480	-1.77920	0.08050
O	1.63616	-2.85763	-0.71072
C	0.15491	1.38144	-1.62226
O	-0.87240	-2.65805	-1.20941
H	-3.38328	-2.33731	-1.05071
Cl	-5.96537	-1.61531	-0.19973
C	-4.19968	0.06929	1.89845
C	-5.50605	1.64057	0.42318
C	-1.31473	1.55049	-1.32554
O	-1.30548	1.63781	1.99601
C	1.13596	2.25763	-1.34358
C	0.90980	3.61617	-0.71595
C	2.61944	1.98024	-1.54535
C	3.09941	0.56984	-1.98660
O	3.56926	0.39565	2.20202
C	6.27551	-0.52609	0.04034
C	4.87098	-0.58838	-0.50216
C	4.02638	-1.68611	0.15744
C	4.47392	0.31385	-1.41631

H	-4.86564	-0.02215	-1.53926
H	1.19970	1.27656	2.45705
H	0.72120	-3.06870	-1.05352
H	0.42775	0.44040	-2.09411
H	-3.89967	0.88906	2.55552
H	-5.14063	-0.35112	2.26328
H	-3.43756	-0.71310	1.95474
H	-5.58448	2.07460	-0.57876
H	-6.46051	1.17459	0.68293
H	-5.30511	2.44750	1.13404
H	-1.55072	2.58379	-1.06181
H	-1.91451	1.29947	-2.20904
H	-0.14043	3.90939	-0.66711
H	1.31107	3.64010	0.30634
H	1.44734	4.38980	-1.28010
H	3.02912	2.73100	-2.23775
H	3.09482	2.21067	-0.58020
H	2.39997	-0.19847	-1.66215
H	3.13687	0.51880	-3.08301
H	6.88799	0.19870	-0.50758
H	6.76689	-1.50654	-0.01124
H	3.88021	-2.51119	-0.54532
H	4.60186	-2.10054	0.99484
H	5.23237	1.02429	-1.75187
H	4.45562	0.06688	1.91047
O	6.17288	-0.11516	1.42690
H	6.81524	-0.60587	1.96210

Originally assigned (incorrect) structure of 19{9} (CDCl₃)



Conf1

Rel energy (kcal/mol): 0.00

C-nom	iGau	Exp	Calc	diff	1
C	8	189.40	189.50	0.10	[189.50]
C	4	165.40	163.18	-2.22	[163.18]
C	18	154.50	156.14	1.64	[156.14]
C	16	154.50	155.53	1.03	[155.53]
C	10	134.70	139.49	4.79	[139.49]
C	19	131.20	130.62	-0.58	[130.62]
C	7	125.50	126.76	1.26	[126.76]
C	17	111.70	112.29	0.59	[112.29]
C	9	109.30	108.92	-0.38	[108.92]
C	23	83.50	83.42	-0.08	[83.42]
C	2	61.60	67.64	6.04	[67.64]
C	3	60.20	63.01	2.81	[63.01]
C	5	39.70	42.95	3.25	[42.95]
C	22	34.50	35.43	0.93	[35.43]
C	6	27.90	31.16	3.26	[31.16]
C	1	24.90	28.06	3.16	[28.06]
C	11	22.10	21.06	-1.04	[21.06]
C	25	19.80	20.76	0.96	[20.76]
C	14	19.60	19.68	0.08	[19.68]
C	12	17.60	17.75	0.15	[17.75]

13C chem shifts: RMSD=2.37ppm (MAE=1.72) N=20 {-2.22 6.04}

Conformer 1

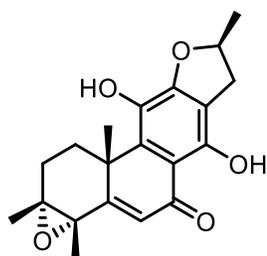
Energy: -1151.46039 Hartree (Rel: 0.0 kcal/mol)

XYZ coordinates for conf 1:

C	3.01398	-2.01241	-0.69100
C	4.05164	-0.94968	-0.33892
C	3.59381	0.39043	0.15958
C	2.10836	0.65996	0.22806
C	1.14048	-0.51808	0.31782
C	1.57547	-1.50012	-0.81546
C	1.66763	1.93018	0.12645
C	0.25906	2.29820	0.04429
C	-0.73808	1.24144	-0.00089
C	-0.33206	-0.12492	0.10302
C	5.39517	-1.15404	-1.01286
C	4.49967	1.60465	0.05687
O	4.10252	-0.62875	1.06363
C	1.22952	-1.15602	1.74080
O	-0.04528	3.51705	-0.01611
C	-2.11048	1.61334	-0.15160
C	-3.06658	0.60737	-0.21211
C	-2.65663	-0.70772	-0.09610
C	-1.32576	-1.11118	0.06583
O	-2.50509	2.89807	-0.23740
O	-1.05737	-2.45651	0.19143
C	-4.56973	0.63004	-0.32127
C	-4.90886	-0.87922	-0.48007
O	-3.67051	-1.61097	-0.14416
C	-6.02891	-1.39487	0.40318
H	3.29378	-2.48229	-1.64125
H	3.08239	-2.79903	0.07118

H	0.89154	-2.34882	-0.84761
H	1.46759	-0.96330	-1.76715
H	2.34375	2.77436	0.06435
H	5.30928	-0.99709	-2.09427
H	6.16940	-0.49257	-0.62197
H	5.72493	-2.18789	-0.85254
H	5.54588	1.30383	0.10236
H	4.33724	2.15161	-0.87764
H	4.31962	2.28999	0.89181
H	0.89136	-0.42843	2.48656
H	0.58310	-2.03418	1.79592
H	2.25246	-1.44033	1.98214
H	-1.66489	3.43986	-0.16746
H	-1.90546	-2.92827	0.11720
H	-5.03336	1.05113	0.58096
H	-4.93239	1.21247	-1.17413
H	-5.10975	-1.11520	-1.53105
H	-6.15941	-2.47469	0.27992
H	-6.96957	-0.90258	0.13279
H	-5.81789	-1.18383	1.45704

Revised structure of 19{9}, i.e. 22{9-rev} (CDCl₃)



Conf1

Rel energy (kcal/mol): 0.00

C-nom	iGau	Exp	Calc	diff	1
C	8	189.40	190.28	0.88	[190.28]
C	4	165.40	162.99	-2.41	[162.99]
C	16	154.50	155.63	1.13	[155.63]
C	18	154.50	155.99	1.49	[155.99]
C	10	134.70	136.84	2.14	[136.84]
C	19	131.20	131.19	-0.01	[131.19]
C	7	125.50	125.70	0.20	[125.70]
C	17	111.70	112.71	1.01	[112.71]
C	9	109.30	109.22	-0.08	[109.22]
C	23	83.50	83.46	-0.04	[83.46]
C	2	61.60	61.23	-0.37	[61.23]
C	3	60.20	60.36	0.16	[60.36]
C	5	39.70	40.42	0.72	[40.42]
C	22	34.50	35.43	0.93	[35.43]
C	1	27.90	28.22	0.32	[28.22]
C	6	24.90	24.98	0.08	[24.98]
C	25	22.10	20.75	-1.35	[20.75]
C	11	19.80	19.94	0.14	[19.94]
C	14	19.60	19.36	-0.24	[19.36]
C	12	17.60	17.16	-0.44	[17.16]

13C chem shifts: RMSD=0.99ppm (MAE=0.71) N=20 {-2.41 2.14}

Conformer 1

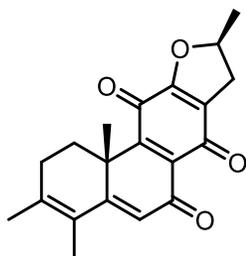
Energy: -1151.46273 Hartree (Rel: 0.0 kcal/mol)

XYZ coordinates for conf 1:

C	3.01600	-1.98320	-0.73270
C	4.04096	-0.92302	-0.36263
C	3.57738	0.40198	0.13097
C	2.08955	0.69039	0.16627
C	1.14890	-0.49541	0.23808
C	1.59143	-1.45235	-0.91651
C	1.65684	1.96025	0.07783
C	0.24313	2.31403	-0.00739
C	-0.74478	1.24304	-0.02606
C	-0.32891	-0.12102	0.07888
C	5.40100	-1.49287	-0.00578
C	4.43138	1.27133	1.03423
O	4.06153	0.23193	-1.23137
C	1.33317	-1.15340	1.64130
O	-0.07805	3.52684	-0.08031
C	-2.12417	1.59794	-0.14796
C	-3.07151	0.58116	-0.17372
C	-2.64918	-0.72998	-0.05568
C	-1.31029	-1.11796	0.07414
O	-2.53649	2.87689	-0.23728
O	-1.01362	-2.45706	0.19998
C	-4.57716	0.59070	-0.24615
C	-4.90748	-0.92226	-0.38586
O	-3.65629	-1.64149	-0.07049
C	-6.00445	-1.43973	0.52482
H	3.34615	-2.47604	-1.65700
H	3.03197	-2.75636	0.04583

H	0.89941	-2.29320	-0.97933
H	1.52105	-0.89584	-1.85785
H	2.34106	2.80148	0.02543
H	5.72020	-2.19326	-0.78679
H	6.16519	-0.71852	0.07915
H	5.35456	-2.04698	0.93910
H	5.49027	1.02574	0.94343
H	4.31397	2.33010	0.78293
H	4.13161	1.14151	2.08028
H	0.97445	-0.47219	2.41950
H	0.76435	-2.08340	1.70273
H	2.38458	-1.37378	1.84663
H	-1.70186	3.42949	-0.19838
H	-1.85239	-2.94681	0.13838
H	-5.02204	1.01463	0.66420
H	-4.96516	1.16405	-1.09395
H	-5.12849	-1.16800	-1.43053
H	-6.12915	-2.52143	0.41241
H	-6.95444	-0.95674	0.27079
H	-5.77286	-1.21903	1.57239

Originally assigned correct structure of 21{10} (CDCl₃)



Conf1					
Rel energy (kcal/mol): 0.00					
C-nom	iGau	Exp	Calc	diff	1
C	8	184.00	183.11	-0.89	[183.11]
C	15	182.60	182.56	-0.04	[182.56]
C	18	180.90	182.16	1.26	[182.16]
C	4	162.80	163.28	0.48	[163.28]
C	17	157.70	158.39	0.69	[158.39]
C	10	153.40	153.24	-0.16	[153.24]
C	2	141.20	140.14	-1.06	[140.14]
C	9	130.60	130.64	0.04	[130.64]
C	3	124.80	125.94	1.14	[125.94]
C	7	122.60	123.32	0.72	[123.32]
C	16	121.20	120.32	-0.88	[120.32]
C	22	83.20	82.77	-0.43	[82.77]
C	5	39.90	39.88	-0.02	[39.88]
C	21	34.30	34.18	-0.12	[34.18]
C	6	30.80	30.41	-0.39	[30.41]
C	1	30.00	29.76	-0.24	[29.76]
C	13	24.30	25.16	0.86	[25.16]
C	24	22.00	21.61	-0.39	[21.61]
C	11	20.90	20.34	-0.56	[20.34]
C	12	14.90	14.98	0.08	[14.98]

13C chem shifts: RMSD=0.65ppm (MAE=0.52) N=20 {-1.06 1.26}

Conformer 1

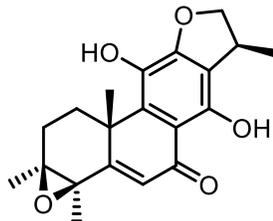
Energy: -1075.01844 Hartree (Rel: 0.0 kcal/mol)

XYZ coordinates for conf 1:

C	3.15629	-2.04432	-0.59765
C	4.14516	-0.93688	-0.32654
C	3.73961	0.32020	-0.00415
C	2.30168	0.63797	0.11824
C	1.31658	-0.51422	0.27688
C	1.71335	-1.57891	-0.78695
C	1.86812	1.92272	0.15309
C	0.46310	2.30046	0.23762
C	-0.53082	1.20728	-0.01328
C	-0.13791	-0.09413	0.07972
C	5.57990	-1.37517	-0.47685
C	4.70413	1.47080	0.19934
C	1.46635	-1.06668	1.73135
O	0.11933	3.45046	0.51047
C	-1.95389	1.60163	-0.36837
C	-2.94427	0.54079	-0.32187
C	-2.58232	-0.74267	-0.13196
C	-1.18705	-1.18246	0.09901
O	-2.24155	2.73647	-0.73784
O	-0.94268	-2.36134	0.32585
C	-4.42454	0.59787	-0.58660
C	-4.83843	-0.89111	-0.38337
O	-3.57344	-1.64376	-0.18078
C	-5.73221	-1.14107	0.81906
H	3.21440	-2.77252	0.22623
H	3.47955	-2.59979	-1.48903
H	1.03990	-2.43400	-0.73600

H	1.60154	-1.12475	-1.77999
H	2.55479	2.76139	0.13339
H	5.71693	-2.36526	-0.02346
H	5.83562	-1.48509	-1.54045
H	6.30688	-0.69720	-0.02767
H	5.74363	1.14404	0.21816
H	4.61409	2.21113	-0.60588
H	4.50161	1.99543	1.14037
H	2.51224	-1.29865	1.94676
H	1.13489	-0.31380	2.45358
H	0.86690	-1.96967	1.86023
H	-4.94812	1.26155	0.11142
H	-4.64362	0.95600	-1.59892
H	-5.27786	-1.31795	-1.28795
H	-5.27943	-0.73315	1.72950
H	-5.90331	-2.21245	0.96132
H	-6.70101	-0.65251	0.66652

Originally assigned (incorrect) structure of 23{1} (CDCl₃)



Rel energy (kcal/mol):					Conf1	Conf2
					0.00	0.16
C-nom	iGau	Exp	Calc	diff	1	2
C1-CH2	6	33.20	33.14	-0.06	[34.58	31.27]
C2-CH2	1	29.80	29.36	-0.44	[30.40	28.00]
C3-C	2	67.80	68.06	0.26	[68.37	67.66]
C4-C	3	62.60	62.63	0.03	[62.36	62.99]
C5-C	4	168.00	166.68	-1.32	[169.31	163.27]
C6-CH	7	124.50	125.11	0.61	[123.86	126.74]
C7-C	8	189.10	189.46	0.36	[189.31	189.65]
C8-C	9	108.90	109.03	0.13	[108.92	109.18]
C9-C	10	139.10	140.07	0.97	[140.43	139.60]
C10-C	5	41.80	43.19	1.39	[43.37	42.96]
C11-C	14	130.40	130.80	0.40	[130.72	130.90]
C12-C	13	154.70	155.86	1.16	[155.61	156.19]
C13-C	12	115.70	115.78	0.08	[116.13	115.32]
C14-C	11	154.70	156.14	1.44	[155.85	156.52]
C15-CH	15	35.80	37.54	1.74	[37.39	37.73]
C16-CH2	16	81.10	79.81	-1.29	[79.88	79.73]
C17-CH3	25	18.60	18.58	-0.02	[19.37	17.55]
C18-CH3	19	19.40	19.38	-0.02	[18.06	21.09]
C19-CH3	20	16.90	17.33	0.43	[17.04	17.70]
C20-CH3	22	26.30	24.28	-2.02	[27.89	19.58]
13C chem shifts: RMSD=0.95ppm (MAE=0.71) N=20 {-2.02 1.74}						
Fractions:					0.565	0.435

Conformer 1

Energy: -1151.45494 Hartree (Rel: 0.0 kcal/mol)

XYZ coordinates for conf 1:

C	2.88009	-1.35174	-1.34518
C	3.98469	-0.60077	-0.61631
C	3.52018	0.45937	0.32778
C	2.03100	0.65420	0.33126
C	1.14966	-0.57646	0.47946
C	1.72684	-1.74876	-0.41491
C	1.52407	1.88969	0.14358
C	0.10491	2.14933	-0.05805
C	-0.81503	1.02014	-0.07279
C	-0.32700	-0.30222	0.15826
C	-2.20023	1.27673	-0.31518
C	-3.08464	0.20342	-0.32179
C	-2.59261	-1.06491	-0.07498
C	-1.24720	-1.35582	0.17606
C	-4.58887	0.12183	-0.47567
C	-4.78543	-1.42013	-0.54802
O	-3.54239	-2.03920	-0.08657
O	4.00356	-0.82209	0.80753
C	5.32457	-0.55179	-1.31467
C	4.38978	1.64361	0.70493
O	-0.28048	3.33344	-0.23630
C	1.20906	-0.97710	1.99259
O	-2.67452	2.51937	-0.53236
O	-0.87471	-2.65522	0.43435
C	-5.35008	0.78210	0.68681
H	2.52176	-0.72080	-2.17073
H	3.29027	-2.26017	-1.80522

H	2.07241	-2.54615	0.24756
H	0.92732	-2.17411	-1.02167
H	2.15734	2.76810	0.08098
H	-4.91693	0.57921	-1.41622
H	-4.95918	-1.76787	-1.57115
H	-5.58591	-1.78656	0.09864
H	5.21331	-0.12030	-2.31629
H	6.06308	0.03395	-0.76427
H	5.71503	-1.56980	-1.43280
H	5.42048	1.31780	0.85233
H	4.38092	2.41839	-0.06876
H	4.03966	2.09296	1.64034
H	0.80940	-0.16866	2.61368
H	0.60947	-1.87533	2.15688
H	2.24002	-1.17946	2.28782
H	-1.87708	3.12360	-0.46778
H	-1.67397	-3.20638	0.36974
H	-6.43279	0.67564	0.55167
H	-5.11293	1.84879	0.73950
H	-5.07597	0.32260	1.64349

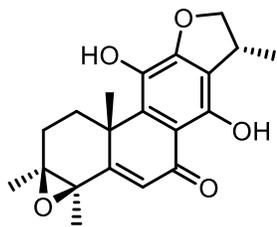
Conformer 2

Energy: -1151.45518 Hartree (Rel: 0.2 kcal/mol)

XYZ coordinates for conf 2:

C	3.20081	-1.83907	-0.63793
C	4.11684	-0.66656	-0.29706
C	3.51443	0.62854	0.16527
C	2.00819	0.74176	0.21053
C	1.16803	-0.52897	0.31667
C	1.71830	-1.48354	-0.78983
C	1.43796	1.95577	0.07304
C	-0.00009	2.17200	-0.03243
C	-0.88197	1.01636	-0.05515
C	-0.33458	-0.29702	0.07815
C	-2.28496	1.23887	-0.22112
C	-3.13614	0.13884	-0.23998
C	-2.58363	-1.12219	-0.11837
C	-1.21905	-1.38209	0.05451
C	-4.63352	0.00222	-0.42670
C	-4.81884	-1.52827	-0.20629
O	-3.48949	-2.13534	-0.17670
O	4.11401	-0.31185	1.09840
C	5.48413	-0.74337	-0.94948
C	4.28911	1.92874	0.04452
O	-0.42799	3.35077	-0.13056
C	1.30500	-1.12440	1.75422
O	-2.80240	2.47461	-0.36308
O	-0.81213	-2.68976	0.20126
C	-5.49420	0.84577	0.52449
H	3.54119	-2.29572	-1.57475
H	3.34092	-2.59893	0.14142
H	1.12792	-2.40009	-0.81090
H	1.56725	-0.98135	-1.75444
H	2.02252	2.86469	-0.00286
H	-4.90058	0.26365	-1.45987
H	-5.38204	-2.02249	-1.00014
H	-5.29329	-1.74131	0.75787
H	5.39881	-0.61615	-2.03484
H	6.17990	0.00172	-0.56145
H	5.91641	-1.73441	-0.76432
H	5.36042	1.74062	0.10737
H	4.08193	2.43518	-0.90389
H	4.02752	2.60920	0.86170
H	0.88671	-0.41922	2.48061
H	0.75021	-2.06226	1.82262
H	2.34872	-1.29834	2.01081
H	-2.02136	3.10056	-0.30104
H	-1.61079	-3.24575	0.17840
H	-6.55953	0.64356	0.36293
H	-5.31708	1.91144	0.35810
H	-5.25660	0.61760	1.56993

Revised structure of 23{1}, i.e. 24{1-rev} (CDCl₃)



Rel energy (kcal/mol):					Conf1	Conf2
					0.00	0.10
C-nom	iGau	Exp	Calc	diff	1	2
C1-CH2	6	33.20	33.03	-0.17	[34.65	31.12]
C2-CH2	1	29.80	29.31	-0.49	[30.40	28.03]
C3-C	2	67.80	68.05	0.25	[68.39	67.65]
C4-C	3	62.60	62.61	0.01	[62.33	62.95]
C5-C	4	168.00	166.50	-1.50	[169.25	163.25]
C6-CH	7	124.50	125.21	0.71	[123.90	126.75]
C7-C	8	189.10	189.45	0.35	[189.30	189.63]
C8-C	9	108.90	109.01	0.11	[108.86	109.19]
C9-C	10	139.10	140.01	0.91	[140.38	139.57]
C10-C	5	41.80	43.16	1.36	[43.35	42.93]
C11-C	14	130.40	130.73	0.33	[130.66	130.82]
C12-C	13	154.70	156.07	1.37	[155.97	156.19]
C13-C	12	115.70	115.26	-0.44	[115.19	115.34]
C14-C	11	154.70	156.39	1.69	[156.29	156.51]
C15-CH	15	35.80	37.69	1.89	[37.67	37.71]
C16-CH2	16	81.10	79.73	-1.37	[79.72	79.74]
C17-CH3	25	18.60	17.72	-0.88	[17.79	17.64]
C18-CH3	19	19.40	19.45	0.05	[18.06	21.10]
C19-CH3	20	16.90	17.34	0.44	[17.05	17.69]
C20-CH3	22	26.30	24.07	-2.23	[27.81	19.66]
13C chem shifts: RMSD=1.06ppm (MAE=0.83) N=20 {-2.23 1.89}					Fractions: 0.541 0.459	

Conformer 1

Energy: -1151.45495 Hartree (Rel: 0.0 kcal/mol)

XYZ coordinates for conf 1:

C	-2.77089	-1.27700	1.49226
C	-3.92634	-0.56373	0.80563
C	-3.53302	0.44293	-0.22529
C	-2.04843	0.63415	-0.34715
C	-1.17727	-0.60433	-0.49011
C	-1.68770	-1.72627	0.50360
C	-1.53146	1.87709	-0.26702
C	-0.10184	2.14473	-0.18399
C	0.81864	1.01619	-0.16537
C	0.31742	-0.31564	-0.28706
C	2.21699	1.28250	-0.03093
C	3.10187	0.20885	-0.01147
C	2.59535	-1.06825	-0.16715
C	1.23651	-1.36956	-0.31096
C	4.61182	0.12977	0.08210
C	4.82564	-1.41303	0.11184
O	3.54167	-2.04514	-0.18540
O	-4.04781	-0.86154	-0.59913
C	-5.21210	-0.47397	1.59562
C	-4.42973	1.60713	-0.60121
O	0.29273	3.33680	-0.10591
C	-1.34224	-1.08523	-1.97166
O	2.70108	2.53631	0.06900
O	0.85156	-2.68018	-0.47848
C	5.22925	0.83780	1.29671
H	-2.35453	-0.60327	2.25430
H	-3.14534	-2.15824	2.02925
H	-2.07995	-2.55601	-0.08951
H	-0.84634	-2.12194	1.07269

H	-2.16013	2.75915	-0.20960
H	5.06033	0.54974	-0.82856
H	5.13400	-1.75848	1.10464
H	5.54164	-1.77163	-0.63023
H	-5.02849	0.00864	2.56269
H	-5.98896	0.08485	1.07061
H	-5.59255	-1.48313	1.79467
H	-5.46780	1.27608	-0.65591
H	-4.36609	2.42200	0.12745
H	-4.14916	2.00527	-1.58214
H	-0.98652	-0.31302	-2.66174
H	-0.75643	-1.99378	-2.12865
H	-2.39158	-1.29829	-2.18275
H	1.89863	3.13623	0.02516
H	1.65650	-3.22615	-0.44971
H	6.31508	0.68835	1.32088
H	5.03060	1.91199	1.25528
H	4.80846	0.44685	2.23034

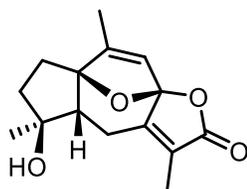
Conformer 2

Energy: -1151.45510 Hartree (Rel: 0.1 kcal/mol)

XYZ coordinates for conf 2:

C	3.13462	-1.83086	-0.77485
C	4.07762	-0.67062	-0.46734
C	3.51489	0.61428	0.06760
C	2.01586	0.73211	0.21875
C	1.17746	-0.53782	0.34649
C	1.64736	-1.46579	-0.81791
C	1.44472	1.95197	0.15835
C	0.00399	2.17649	0.15929
C	-0.88338	1.02481	0.14966
C	-0.33620	-0.29382	0.21348
C	-2.29245	1.25678	0.07472
C	-3.14706	0.15985	0.04258
C	-2.59725	-1.10516	0.12876
C	-1.22637	-1.37454	0.21702
C	-4.65622	0.03753	-0.00330
C	-4.82368	-1.50805	-0.09920
O	-3.51292	-2.11101	0.13595
O	4.17143	-0.35208	0.93367
C	5.39685	-0.73531	-1.21336
C	4.28672	1.91424	-0.07235
O	-0.42349	3.35919	0.13634
C	1.40637	-1.17036	1.75617
O	-2.81374	2.49851	0.03689
O	-0.81868	-2.68648	0.31565
C	-5.33845	0.78148	-1.16025
H	3.40887	-2.26510	-1.74350
H	3.32262	-2.61048	-0.02571
H	1.05152	-2.37906	-0.82190
H	1.43504	-0.93851	-1.75727
H	2.02819	2.86067	0.07175
H	-5.08363	0.39975	0.94170
H	-5.14703	-1.81713	-1.09921
H	-5.50793	-1.92338	0.64308
H	5.23845	-0.57868	-2.28661
H	6.12175	-0.00364	-0.85426
H	5.83496	-1.73267	-1.08442
H	5.35871	1.72040	-0.09025
H	4.01623	2.44725	-0.98975
H	4.08729	2.57307	0.77935
H	1.03958	-0.48322	2.52635
H	0.85379	-2.10849	1.83740
H	2.46416	-1.35284	1.93851
H	-2.02744	3.11986	0.07153
H	-1.61764	-3.24140	0.28289
H	-6.41939	0.59879	-1.15353
H	-5.17088	1.85827	-1.07437
H	-4.94040	0.44832	-2.12568

Originally assigned correct structure of 26{2} (CDCl₃)



Rel energy (kcal/mol): **Conf1** 0.00

C-nom	iGau	Exp	Calc	diff	1
C1-C	5	93.60	94.74	1.14	[94.74]
C2-CH2	1	28.90	29.31	0.41	[29.31]
C3-CH2	2	41.30	39.42	-1.88	[39.42]
C4-C	3	75.10	73.28	-1.82	[73.28]
C5-CH	4	55.60	57.12	1.52	[57.12]
C6-CH2	6	20.80	21.14	0.34	[21.14]
C7-C	7	154.80	155.81	1.01	[155.81]
C8-C	8	108.80	110.87	2.07	[110.87]
C9-CH	9	128.40	127.84	-0.56	[127.84]
C10-C	10	146.00	146.97	0.97	[146.97]
C11-C	12	121.20	121.57	0.37	[121.57]
C12-C	13	172.30	172.85	0.55	[172.85]
C13-CH3	15	8.40	8.38	-0.02	[8.38]
C14-CH3	18	26.60	26.12	-0.48	[26.12]
C15-CH3	11	14.50	14.14	-0.36	[14.14]

13C chem shifts: RMSD=1.10ppm (MAE=0.90) N=15 {-1.88 2.07}

Conformer 1

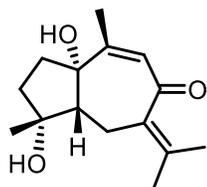
Energy: -883.28971 Hartree (Rel: 0.0 kcal/mol)

XYZ coordinates for conf 1:

C	-2.12570	-1.02556	-1.46103
C	-3.22975	-0.17394	-0.78614
C	-2.53738	1.05113	-0.10207
C	-1.02346	0.74332	-0.27623
C	-0.90863	-0.78562	-0.57192
C	0.04386	1.22883	0.73127
C	1.34427	0.56746	0.35744
C	1.26070	-0.88073	-0.10347
C	0.57207	-1.75793	0.91755
C	-0.73955	-1.69146	0.66758
C	-1.83992	-2.38337	1.41274
C	2.61531	0.98047	0.25396
C	3.41143	-0.16369	-0.26353
O	2.57202	-1.24712	-0.47003
C	3.25859	2.30131	0.53296
O	4.59508	-0.23037	-0.49540
O	0.37764	-0.94690	-1.22592
C	-2.99981	1.27180	1.34094
O	-2.90404	2.20329	-0.88263
H	-0.76974	1.19213	-1.24389
H	-2.39686	-2.08121	-1.55733
H	-1.89912	-0.64654	-2.46365
H	-3.97485	0.18326	-1.50152
H	-3.76083	-0.76732	-0.03475
H	0.13994	2.32019	0.72747
H	-0.22717	0.93303	1.75320
H	1.08279	-2.26138	1.72997
H	-1.42517	-3.04262	2.18106
H	-2.52033	-1.68110	1.90755
H	-2.45203	-2.99337	0.73666
H	2.52337	3.04433	0.85369
H	4.01755	2.20583	1.31881
H	3.77104	2.68012	-0.35893
H	-2.54271	2.17596	1.76276

H	-4.08712	1.40027	1.36549
H	-2.73830	0.43576	1.99724
H	-2.47804	2.97935	-0.48230

Originally assigned (incorrect) structure of 27{4} (CDCl₃)



					Conf1	Conf2	Conf3
Rel energy (kcal/mol):					0.00	0.11	3.19
C-nom	iGau	Exp	Calc	diff	1	2	3
C1-C	5	88.20	85.35	-2.85	[84.25	86.65	87.10]
C2-CH2	1	30.40	35.01	4.61	[34.67	35.44	32.49]
C3-CH2	2	38.00	37.45	-0.55	[35.82	39.39	39.62]
C4-C	3	83.70	80.96	-2.74	[82.60	79.00	77.77]
C5-CH	4	61.90	51.63	-10.27	[51.27	52.07	51.42]
C6-CH2	6	28.50	24.17	-4.33	[23.74	24.69	23.93]
C7-C	7	132.30	133.63	1.33	[133.54	133.72	138.07]
C8-C	8	205.10	204.18	-0.92	[204.46	203.82	209.24]
C9-CH2	9	46.70	45.57	-1.13	[45.65	45.46	47.58]
C10-CH	10	37.60	39.57	1.97	[38.38	41.02	36.69]
C11-C	12	144.40	148.19	3.79	[147.57	148.98	139.53]
C12-CH3	15	21.80	23.91	2.11	[23.73	24.15	20.10]
C13-CH3	13	22.50	25.21	2.71	[25.04	25.43	21.57]
C14-CH3	17	25.10	25.72	0.62	[25.77	25.66	25.30]
C15-CH3	11	18.00	15.42	-2.58	[15.25	15.63	15.35]
13C chem shifts: RMSD=3.67ppm (MAE=2.83) N=15 {-10.27 4.61}							
Fractions:					0.544	0.453	0.003

Conformer 1

Energy: -811.69498 Hartree (Rel: 0.0 kcal/mol)

XYZ coordinates for conf 1:

C	2.71123	-1.03178	0.63567
C	3.17368	0.44191	0.78350
C	2.02562	1.33110	0.24228
C	0.79591	0.37581	0.19907
C	1.42542	-0.98308	-0.22537
C	-0.37533	0.86071	-0.68314
C	-1.73999	0.32228	-0.27726
C	-1.86952	-1.16799	-0.23506
C	-0.80862	-2.02405	-0.92232
C	0.49996	-2.21337	-0.10070
C	0.19707	-2.66873	1.33567
C	-2.80590	1.12264	0.00839
C	-4.19545	0.61628	0.33335
O	-2.79179	-1.73751	0.34890
C	-2.75188	2.63367	0.01637
O	1.78595	-0.94128	-1.61723
C	1.81172	2.60904	1.04983
O	2.42545	1.68795	-1.11282
H	0.44523	0.27867	1.23586
H	3.45967	-1.67085	0.15802
H	2.50097	-1.45120	1.62346
H	3.38113	0.68667	1.82976
H	4.08301	0.65997	0.21588
H	-0.40124	1.95218	-0.67532
H	-0.15961	0.57561	-1.72037
H	-0.54545	-1.62070	-1.90468
H	-1.27034	-3.00561	-1.06484
H	1.04337	-3.02577	-0.60170
H	1.08991	-3.05841	1.83343
H	-0.55208	-3.46759	1.32443
H	-0.20885	-1.85973	1.95405
H	-4.93460	1.39458	0.11123
H	-4.45385	-0.29618	-0.20417
H	-4.27985	0.37886	1.40172
H	-3.30941	3.03479	-0.84188

H	-3.26036	3.01038	0.91315
H	-1.74989	3.06275	-0.00304
H	2.19009	-0.06301	-1.77092
H	1.00853	3.22481	0.62557
H	2.72799	3.20920	1.05421
H	1.54352	2.37684	2.08606
H	1.73181	2.25375	-1.49244

Conformer 2

Energy: -811.69481 Hartree (Rel: 0.1 kcal/mol)

XYZ coordinates for conf 2:

C	2.68124	-1.01091	0.70767
C	3.19824	0.44844	0.71778
C	2.02986	1.34908	0.19718
C	0.79607	0.38837	0.18660
C	1.41597	-0.98185	-0.17132
C	-0.36835	0.85198	-0.71585
C	-1.73446	0.32475	-0.30198
C	-1.88215	-1.16175	-0.26851
C	-0.80189	-2.02866	-0.91714
C	0.48168	-2.20792	-0.05699
C	0.14020	-2.63326	1.38124
C	-2.78798	1.13491	0.00578
C	-4.17800	0.64090	0.34844
O	-2.82900	-1.73048	0.27634
C	-2.71204	2.64423	0.02756
O	1.82429	-0.85671	-1.56342
C	1.82128	2.59645	1.05139
O	2.30777	1.82418	-1.12646
H	0.43635	0.31467	1.22199
H	3.41834	-1.73030	0.33007
H	2.42126	-1.32604	1.72248
H	3.51497	0.74403	1.72354
H	4.05887	0.58795	0.05717
H	-0.36996	1.94093	-0.73557
H	-0.15218	0.55320	-1.74762
H	-0.51474	-1.63749	-1.89833
H	-1.26048	-3.01139	-1.06051
H	1.03212	-3.04268	-0.51792
H	1.02234	-3.00141	1.91331
H	-0.60133	-3.43897	1.36642
H	-0.28996	-1.81200	1.96529
H	-4.90590	1.44691	0.20221
H	-4.47546	-0.22872	-0.23890
H	-4.23249	0.33149	1.39990
H	-3.30127	3.06131	-0.80142
H	-3.17695	3.01799	0.94924
H	-1.70578	3.05808	-0.03259
H	2.38697	-1.61895	-1.77799
H	0.98019	3.19285	0.68074
H	2.71760	3.22587	1.01743
H	1.62562	2.32933	2.09530
H	2.34937	1.01878	-1.67703

Conformer 3

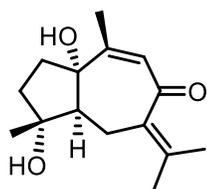
Energy: -811.68991 Hartree (Rel: 3.2 kcal/mol)

XYZ coordinates for conf 3:

C	2.55440	1.16411	-0.27257
C	3.22677	-0.20604	-0.56072
C	2.12867	-1.30930	-0.37249
C	0.81792	-0.47124	-0.32704
C	1.22913	0.80932	0.42733
C	-0.43580	-1.15677	0.21728
C	-1.74495	-0.42900	-0.11228
C	-1.69388	0.74399	-1.05344
C	-0.73901	1.92310	-0.79467
C	0.11911	1.88510	0.47718
C	0.65652	3.28430	0.82158
C	-2.93739	-0.84030	0.38283
C	-4.26704	-0.17690	0.10775
O	-2.44536	0.82283	-2.01890

C	-3.05609	-2.01981	1.32028
O	1.51861	0.39454	1.79302
C	2.14685	-2.35644	-1.48271
O	2.32360	-2.03240	0.84824
H	0.63298	-0.16925	-1.36732
H	3.17905	1.82617	0.33763
H	2.34516	1.69849	-1.20723
H	3.64696	-0.23026	-1.57163
H	4.04671	-0.41412	0.13281
H	-0.49141	-2.16709	-0.20974
H	-0.32427	-1.29083	1.29735
H	-1.39585	2.80284	-0.75872
H	-0.12479	2.06325	-1.69472
H	-0.53784	1.57259	1.29969
H	1.27164	3.27117	1.72970
H	-0.17035	3.98034	1.00091
H	1.26761	3.69452	0.00927
H	-4.81647	-0.04172	1.04904
H	-4.18377	0.78565	-0.39585
H	-4.88839	-0.82655	-0.52397
H	-3.34840	-1.68250	2.32483
H	-3.85443	-2.69104	0.97688
H	-2.13982	-2.60441	1.41319
H	1.98890	1.11959	2.23505
H	1.35116	-3.09531	-1.33721
H	3.10398	-2.88972	-1.47575
H	2.01704	-1.89210	-2.46610
H	2.21849	-1.36436	1.55310

Revised structure of 27{4}, i.e. 28{4-rev} (CDCl₃)



					Conf1	Conf2
Rel energy (kcal/mol):					0.00	0.55
C-nom	iGau	Exp	Calc	diff	1	2
C1-C	5	88.20	87.36	-0.84	[86.33	89.95]
C2-CH2	1	30.40	32.41	2.01	[32.60	31.93]
C3-CH2	2	38.00	38.38	0.38	[38.47	38.17]
C4-C	3	83.70	83.40	-0.30	[84.25	81.26]
C5-CH	4	61.90	61.03	-0.87	[60.87	61.45]
C6-CH2	6	28.50	29.53	1.03	[29.56	29.46]
C7-C	7	132.30	133.59	1.29	[133.62	133.51]
C8-C	8	205.10	204.60	-0.50	[204.86	203.93]
C9-CH2	9	46.70	46.58	-0.12	[46.43	46.97]
C10-CH	10	37.60	37.86	0.26	[37.81	37.99]
C11-C	12	144.40	146.98	2.58	[146.64	147.83]
C12-CH3	15	21.80	21.51	-0.29	[21.44	21.67]
C13-CH3	13	22.50	22.46	-0.04	[22.39	22.62]
C14-CH3	17	25.10	24.61	-0.49	[24.79	24.17]
C15-CH3	11	18.00	17.91	-0.09	[18.18	17.23]
13C chem shifts: RMSD=1.03ppm (MAE=0.74) N=15 {-0.87 2.58}						
Fractions:					0.717	0.283

Conformer 1

Energy: -811.69050 Hartree (Rel: 0.0 kcal/mol)

XYZ coordinates for conf 1:

C	2.21301	1.16188	-0.70697
C	2.73689	-0.22007	-1.16917
C	2.11778	-1.25918	-0.20980
C	0.76116	-0.61318	0.20304
C	1.14732	0.89506	0.40482
C	-0.35859	-0.89758	-0.82504
C	-1.74847	-0.45247	-0.39288
C	-2.09180	0.95408	-0.74366
C	-0.93685	1.94818	-0.80645
C	-0.00689	1.93222	0.43296
C	0.54626	3.35102	0.66877
C	-2.61045	-1.24832	0.29372
C	-3.98712	-0.82254	0.75125
O	-3.23734	1.33930	-0.96422
C	-2.28121	-2.66171	0.71312
O	1.75266	1.02628	1.70169
C	2.07107	-2.67532	-0.78311
O	2.88659	-1.31136	1.02701
H	0.44518	-1.02454	1.16843
H	3.00263	1.78970	-0.28647
H	1.78967	1.71082	-1.55471
H	2.41511	-0.43544	-2.19445
H	3.83143	-0.28938	-1.16710
H	-0.11108	-0.43558	-1.78887
H	-0.38205	-1.97023	-1.02282
H	-1.40097	2.93384	-0.90689
H	-0.35992	1.78747	-1.72728
H	-0.61377	1.67188	1.31091
H	1.21738	3.36779	1.53006
H	1.09848	3.71497	-0.20635
H	-0.27675	4.05081	0.85335
H	-4.21659	-1.28126	1.72070
H	-4.10479	0.25794	0.82040
H	-4.74569	-1.18200	0.04212
H	-2.23490	-2.72246	1.80905

H	-3.08745	-3.34005	0.40300
H	-1.34102	-3.04757	0.31761
H	2.39174	0.28837	1.76385
H	1.58392	-3.36361	-0.08387
H	3.09363	-3.03608	-0.95240
H	1.54916	-2.71860	-1.74341
H	3.80870	-1.51300	0.79590

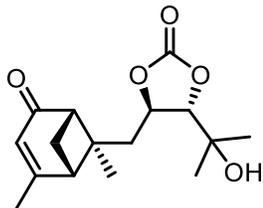
Conformer 2

Energy: -811.69138 Hartree (Rel: 0.6 kcal/mol)

XYZ coordinates for conf 2:

C	2.19539	1.11567	-0.78252
C	2.80805	-0.27006	-1.11002
C	2.11959	-1.30177	-0.17133
C	0.75829	-0.61199	0.19700
C	1.16275	0.88448	0.35169
C	-0.36713	-0.87247	-0.83132
C	-1.75539	-0.43069	-0.38888
C	-2.09874	0.98144	-0.70938
C	-0.94229	1.97498	-0.78477
C	0.02416	1.94027	0.42831
C	0.58568	3.35906	0.65204
C	-2.61830	-1.23799	0.28472
C	-3.99211	-0.81763	0.75564
O	-3.24533	1.37836	-0.90174
C	-2.29323	-2.66100	0.67285
O	1.85327	0.91330	1.63804
C	2.02406	-2.69320	-0.79506
O	2.89112	-1.49445	1.02318
H	0.42358	-0.99549	1.16764
H	2.94865	1.84866	-0.47216
H	1.70816	1.54060	-1.66603
H	2.62769	-0.52552	-2.16029
H	3.88955	-0.30569	-0.95074
H	-0.11933	-0.40061	-1.79050
H	-0.39270	-1.94175	-1.04234
H	-1.40844	2.96200	-0.85514
H	-0.39354	1.83013	-1.72468
H	-0.56093	1.67938	1.32046
H	1.23079	3.41520	1.53526
H	1.15698	3.70995	-0.21551
H	-0.23583	4.06476	0.81346
H	-4.22782	-1.31095	1.70627
H	-4.10080	0.26054	0.86545
H	-4.75221	-1.14221	0.03154
H	-2.24516	-2.74524	1.76716
H	-3.10330	-3.32884	0.35026
H	-1.35572	-3.04241	0.26745
H	2.40622	1.71037	1.66767
H	1.47120	-3.37717	-0.14106
H	3.03659	-3.09421	-0.91508
H	1.54746	-2.67939	-1.77921
H	2.79167	-0.66452	1.53052

Originally assigned correct structure of 29{1} (CDCl₃)



Rel energy (kcal/mol):					Conf1	Conf2	Conf3	Conf4	Conf5
					0.00	0.27	0.28	1.11	1.18
C-nom	iGau	Exp	Calc	diff	1	2	3	4	5
C1-CH2	8	40.20	41.38	1.18	[41.19	41.49	41.53	41.35	41.61]
C2-CH	3	48.50	47.49	-1.01	[49.54	45.53	45.91	49.71	46.23]
C3-C	2	168.90	169.27	0.37	[168.63	169.88	169.68	168.92	169.61]
C4-CH	1	122.00	123.44	1.44	[123.23	123.63	123.61	123.24	123.53]
C5-C	6	202.90	201.17	-1.73	[201.48	200.89	200.88	201.56	201.16]
C6-CH	5	56.00	55.46	-0.54	[53.68	57.14	56.73	54.03	56.59]
C7-C	4	55.20	57.17	1.97	[56.65	57.66	57.55	56.77	57.48]
C8-CH2	9	44.70	44.02	-0.68	[44.62	43.41	43.47	45.18	43.60]
C9-CH	11	76.00	76.66	0.66	[76.91	76.15	76.32	77.58	77.66]
C10-CH	16	87.20	87.56	0.36	[87.86	87.86	87.68	85.84	85.41]
C11-C	15	70.40	68.94	-1.46	[68.71	68.71	68.76	70.50	70.82]
C12-CH3	13	25.60	22.36	-3.24	[21.54	21.50	21.53	28.73	29.01]
C13-CH3	14	25.30	26.04	0.74	[26.57	26.65	26.60	21.55	21.91]
C14-CH3	10	19.80	18.46	-1.34	[17.77	19.36	18.91	17.50	18.46]
C15-CH3	7	23.70	22.93	-0.77	[22.88	23.01	22.94	22.90	22.93]
C16-C	19	154.20	154.47	0.27	[154.47	154.39	154.45	154.63	154.67]
13C chem shifts: RMSD=1.33ppm (MAE=1.11) N=16 {-3.24 1.97}									
Fractions:					0.393	0.249	0.244	0.060	0.054

Conformer 1

Energy: -999.03740 Hartree (Rel: 0.0 kcal/mol)

XYZ coordinates for conf 1:

C	4.24019	0.02747	0.55534
C	3.90297	-0.82436	-0.43852
C	2.55831	-0.60216	-1.10502
C	1.41724	-0.41314	-0.01799
C	1.98920	1.05907	0.09397
C	3.25712	1.05760	0.94917
C	4.77037	-1.94976	-0.91286
C	2.43575	0.92672	-1.39331
C	0.03050	-0.50003	-0.70337
C	1.41269	-1.29995	1.23220
C	-1.15490	0.09601	0.05360
O	-3.59393	-0.58866	1.57281
C	-2.78053	-2.52276	0.47516
C	-4.80959	-1.31296	-0.41064
C	-3.44127	-1.15723	0.26924
C	-2.53016	-0.23658	-0.57501
O	3.43543	1.84538	1.87254
O	-3.16695	1.05800	-0.69076
C	-2.29495	2.05083	-0.39074
O	-1.10683	1.54649	-0.00436
O	-2.55353	3.22234	-0.46427
H	5.18006	-0.03079	1.09770
H	2.37205	-1.31344	-1.91636
H	1.32355	1.86856	0.39555
H	5.71953	-1.99122	-0.37096
H	4.25455	-2.91178	-0.78822
H	4.98283	-1.84983	-1.98587
H	1.64010	1.18230	-2.09547
H	3.35369	1.44113	-1.68964
H	-0.18585	-1.56573	-0.86194
H	0.04031	-0.04418	-1.69862
H	2.38954	-1.34690	1.71657

H	0.70160	-0.92514	1.97715
H	1.11690	-2.32512	0.97586
H	-1.15564	-0.16825	1.11298
H	-4.10818	0.23060	1.47498
H	-2.57123	-3.00773	-0.48390
H	-3.45468	-3.16746	1.04701
H	-1.84619	-2.43600	1.03832
H	-5.45696	-1.93628	0.21375
H	-5.29176	-0.33985	-0.55062
H	-4.71392	-1.78733	-1.39368
H	-2.42142	-0.63649	-1.58954

Conformer 2

Energy: -999.03695 Hartree (Rel: 0.3 kcal/mol)

XYZ coordinates for conf 2:

C	4.21482	0.00000	0.47884
C	3.19738	-0.25278	1.33233
C	1.87132	-0.66964	0.72002
C	1.47323	0.32013	-0.45671
C	2.51655	-0.52416	-1.29801
C	3.94149	-0.07965	-0.97018
C	3.30565	-0.15301	2.82275
C	2.18865	-1.73558	-0.37231
C	0.04122	0.07427	-0.99897
C	1.71197	1.82611	-0.29966
C	-1.12409	0.31214	-0.03943
O	-3.25338	-1.09480	1.45930
C	-2.29871	-2.57873	-0.11969
C	-4.56453	-1.55551	-0.54277
C	-3.16595	-1.32884	0.05054
C	-2.49930	-0.10471	-0.61931
O	4.77153	0.18265	-1.83464
O	-3.33083	1.05480	-0.37580
C	-2.58803	2.09042	0.08254
O	-1.30105	1.72538	0.24106
O	-3.02473	3.18620	0.31396
H	5.20796	0.29507	0.80644
H	1.12456	-0.89960	1.48583
H	2.37852	-0.60527	-2.38005
H	4.31221	0.13195	3.14182
H	2.59328	0.58836	3.20987
H	3.04423	-1.10921	3.29583
H	1.31614	-2.30290	-0.70184
H	3.00223	-2.43173	-0.15228
H	-0.06255	-0.95807	-1.34879
H	-0.10853	0.70779	-1.88315
H	2.72927	2.05833	0.01985
H	1.53859	2.33086	-1.25787
H	1.01953	2.26018	0.42657
H	-0.96387	-0.17311	0.92688
H	-3.89090	-0.37347	1.59503
H	-2.12340	-2.79744	-1.17819
H	-2.81004	-3.43612	0.32812
H	-1.33326	-2.46909	0.38396
H	-5.04192	-2.39990	-0.03626
H	-5.19444	-0.66922	-0.41359
H	-4.51057	-1.77845	-1.61420
H	-2.44950	-0.24556	-1.70486

Conformer 3

Energy: -999.03697 Hartree (Rel: 0.3 kcal/mol)

XYZ coordinates for conf 3:

C	4.19339	-0.08241	0.51395
C	3.16895	-0.57616	1.24499
C	1.86653	-0.84401	0.51096
C	1.46315	0.41425	-0.37044
C	2.54228	-0.15385	-1.38032
C	3.94819	0.21998	-0.91090
C	3.24780	-0.87430	2.71057
C	2.23454	-1.57479	-0.81655
C	0.04551	0.28465	-0.98042

C	1.65792	1.82857	0.18670
C	-1.13190	0.37102	-0.00877
O	-3.18967	-1.27041	1.33847
C	-2.15649	-2.54427	-0.36903
C	-4.47421	-1.60665	-0.70495
C	-3.08972	-1.36450	-0.08563
C	-2.48640	-0.04943	-0.63122
O	4.78572	0.72149	-1.65374
O	-3.37159	1.03878	-0.27606
C	-2.67600	2.05931	0.28071
O	-1.37273	1.74186	0.40438
O	-3.16294	3.10591	0.61605
H	5.17188	0.13765	0.93215
H	1.11059	-1.28479	1.16855
H	2.42572	0.05164	-2.44828
H	4.24031	-0.66292	3.11849
H	2.50873	-0.27816	3.26326
H	3.00409	-1.92732	2.90607
H	1.38739	-2.05721	-1.30749
H	3.06546	-2.28324	-0.76690
H	-0.05773	-0.66902	-1.50776
H	-0.08444	1.06575	-1.74130
H	2.66984	1.99695	0.55873
H	1.46045	2.56873	-0.59786
H	0.95953	2.03024	1.00407
H	-0.94948	-0.19711	0.90746
H	-3.85902	-0.59418	1.53849
H	-1.96951	-2.65131	-1.44251
H	-2.62000	-3.46687	-0.00700
H	-1.19815	-2.43014	0.14716
H	-4.90633	-2.51947	-0.28364
H	-5.15022	-0.77131	-0.49468
H	-4.40908	-1.72311	-1.79247
H	-2.43165	-0.08017	-1.72529

Conformer 4

Energy: -999.03563 Hartree (Rel: 1.1 kcal/mol)

XYZ coordinates for conf 4:

C	4.25180	0.03662	0.52226
C	3.88214	-0.91660	-0.36215
C	2.53855	-0.73609	-1.04251
C	1.41255	-0.38717	0.02222
C	2.02673	1.07057	-0.04517
C	3.30113	1.13381	0.79744
C	4.71225	-2.11611	-0.70274
C	2.45763	0.75092	-1.50853
C	0.01967	-0.51253	-0.64125
C	1.39464	-1.11425	1.37195
C	-1.16229	0.09854	0.10612
O	-2.61958	-2.29953	0.45255
C	-4.67771	-1.52634	-0.60704
C	-3.89764	-0.54926	1.58634
C	-3.45841	-1.15175	0.24567
C	-2.52805	-0.21445	-0.55324
O	3.50918	2.01869	1.62159
O	-3.13983	1.07801	-0.71982
C	-2.27224	2.06298	-0.38245
O	-1.10897	1.54955	0.06797
O	-2.51317	3.23677	-0.47685
H	5.19428	0.01541	1.06278
H	2.32515	-1.53182	-1.76362
H	1.38508	1.92765	0.16346
H	5.66422	-2.12170	-0.16410
H	4.16874	-3.04006	-0.46168
H	4.91870	-2.15153	-1.78097
H	1.66530	0.94459	-2.23373
H	3.38779	1.19979	-1.86701
H	-0.20429	-1.58338	-0.73801
H	0.01563	-0.10275	-1.65652
H	2.39086	-1.21045	1.80744
H	0.77805	-0.57279	2.09844

H	0.97294	-2.12115	1.26459
H	-1.15803	-0.19012	1.15760
H	-3.14124	-2.96843	0.92502
H	-5.26741	-0.64015	-0.86338
H	-5.32822	-2.21679	-0.05717
H	-4.35967	-2.01655	-1.53324
H	-4.51425	-1.27520	2.12905
H	-3.04145	-0.30061	2.22115
H	-4.49689	0.35382	1.43716
H	-2.38087	-0.63890	-1.55245

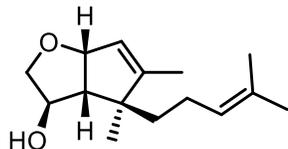
Conformer 5

Energy: -999.03552 Hartree (Rel: 1.2 kcal/mol)

XYZ coordinates for conf 5:

C	4.14476	-0.14201	0.54048
C	3.10397	-0.72280	1.17898
C	1.81591	-0.87899	0.39149
C	1.43836	0.48961	-0.32316
C	2.53236	0.05187	-1.37892
C	3.92984	0.34919	-0.83613
C	3.15515	-1.21778	2.59175
C	2.20468	-1.42844	-1.01507
C	0.02973	0.44401	-0.95792
C	1.62602	1.81869	0.41563
C	-1.14290	0.47145	0.02210
O	-1.77779	-2.22183	-0.46615
C	-4.12368	-1.86188	-1.03857
C	-3.28831	-1.50813	1.31763
C	-2.93618	-1.42203	-0.17290
C	-2.47419	-0.01127	-0.59596
O	4.78555	0.93897	-1.48826
O	-3.43129	0.97870	-0.17477
C	-2.79301	2.04576	0.36525
O	-1.46364	1.82659	0.43989
O	-3.34367	3.05154	0.72590
H	5.11612	0.01259	1.00242
H	1.03899	-1.39921	0.95993
H	2.43871	0.39914	-2.41192
H	4.14046	-1.06922	3.04272
H	2.40773	-0.69907	3.20765
H	2.90553	-2.28652	2.63730
H	1.36054	-1.83345	-1.57536
H	3.03045	-2.14422	-1.04581
H	-0.09446	-0.46403	-1.55283
H	-0.08269	1.29028	-1.64858
H	2.62342	1.92490	0.84579
H	1.46673	2.65414	-0.27660
H	0.89722	1.92794	1.22509
H	-0.90463	-0.08757	0.93031
H	-2.00424	-3.14946	-0.28927
H	-4.98032	-1.19411	-0.90019
H	-4.43899	-2.87594	-0.76576
H	-3.84533	-1.86043	-2.09762
H	-3.56859	-2.53811	1.56692
H	-2.44022	-1.23157	1.95175
H	-4.13491	-0.86054	1.56325
H	-2.41983	0.02904	-1.68998

Originally assigned correct structure of 30{15} (CDCl₃)



Rel energy (kcal/mol):					Conf1	Conf2	Conf3
					0.00	0.50	2.49
C-nom	iGau	Exp	Calc	diff	1	2	3
C1-CH2	7	72.30	70.91	-1.39	[70.96	70.81	70.65]
C2-CH	8	75.10	74.76	-0.34	[74.76	74.79	74.24]
C3-C	4	150.80	151.83	1.03	[150.91	153.94	152.54]
C4-CH	5	123.50	123.30	-0.20	[123.83	122.02	124.44]
C5-CH	1	86.30	86.02	-0.28	[86.01	86.08	85.28]
C6-CH	2	59.00	59.71	0.71	[59.81	59.26	65.90]
C7-C	3	50.30	51.91	1.61	[51.95	51.81	52.03]
C8-CH2	14	41.70	42.16	0.46	[41.79	42.76	49.56]
C9-CH2	15	23.30	24.62	1.32	[24.40	25.09	25.97]
C10-CH	16	124.20	123.75	-0.45	[123.78	123.68	123.88]
C11-C	17	131.70	130.74	-0.96	[130.71	130.83	130.46]
C12-CH3	19	17.70	16.45	-1.25	[16.39	16.57	16.56]
C13-CH3	18	25.80	25.30	-0.50	[25.26	25.38	25.30]
C14-CH3	13	22.20	22.89	0.69	[24.20	19.95	20.20]
C15-CH3	12	12.40	13.11	0.71	[13.10	13.01	16.57]

13C chem shifts: RMSD=0.90ppm (MAE=0.79) N=15 {-1.39 1.61}
 Fractions: 0.691 0.298 0.010

Conformer 1

Energy: -736.44201 Hartree (Rel: 0.0 kcal/mol)

XYZ coordinates for conf 1:

C	1.80115	0.00606	-1.35917
C	1.48620	-0.68431	0.00834
C	0.62287	0.33761	0.83844
C	0.66078	1.60418	-0.02245
C	1.27262	1.40206	-1.19573
O	3.24087	-0.03423	-1.52973
C	3.79479	-0.05567	-0.21123
C	2.90392	-1.06070	0.51928
O	3.24356	-2.39410	0.13401
H	1.39131	-0.50697	-2.23610
H	0.93882	-1.62128	-0.11917
C	0.03700	2.89436	0.42790
C	1.16374	0.61171	2.25851
C	-0.83660	-0.18801	0.99796
C	-1.63527	-0.41669	-0.30174
C	-2.98197	-1.03490	-0.02735
C	-4.20329	-0.51886	-0.24195
C	-5.44584	-1.30290	0.11359
C	-4.47665	0.84087	-0.83946
H	1.39980	2.15556	-1.96929
H	3.75386	0.93981	0.25617
H	4.83614	-0.37951	-0.28437
H	3.00952	-1.03107	1.60403
H	3.31269	-2.38433	-0.83641
H	0.51887	3.27882	1.33584
H	0.11641	3.66319	-0.34693
H	-1.02629	2.76436	0.66935
H	0.51922	1.32509	2.78374
H	1.18566	-0.30741	2.85537
H	2.17531	1.03217	2.24167
H	-0.79235	-1.12927	1.56411
H	-1.39857	0.51453	1.62760
H	-1.73249	0.52827	-0.84462
H	-1.06869	-1.08973	-0.96214
H	-2.93478	-2.03114	0.41810

H	-5.20410	-2.28124	0.54137
H	-6.06440	-0.75621	0.83964
H	-6.07846	-1.46436	-0.77092
H	-3.56924	1.40049	-1.07817
H	-5.06665	0.74703	-1.76204
H	-5.07763	1.45088	-0.15054

Conformer 2

Energy: -736.44122 Hartree (Rel: 0.5 kcal/mol)

XYZ coordinates for conf 2:

C	2.02723	-0.34932	-1.34318
C	1.11028	-0.60170	-0.10150
C	0.65671	0.81437	0.41774
C	1.51100	1.77600	-0.42037
C	2.20625	1.14001	-1.37071
O	3.26837	-1.05941	-1.09881
C	3.41848	-1.11359	0.32232
C	2.01448	-1.48152	0.80335
O	1.76151	-2.87007	0.58050
H	1.64331	-0.75497	-2.28549
H	0.23676	-1.20407	-0.36031
C	1.51668	3.26008	-0.18480
C	0.88289	1.05185	1.92545
C	-0.84353	1.04557	0.05998
C	-1.87293	0.20503	0.84720
C	-3.28232	0.49174	0.39673
C	-4.16902	-0.33920	-0.17519
C	-5.54442	0.15137	-0.56617
C	-3.91962	-1.79688	-0.48081
H	2.85806	1.62440	-2.09365
H	3.74567	-0.14411	0.72752
H	4.16572	-1.87585	0.55733
H	1.86428	-1.32156	1.87158
H	2.05070	-3.05327	-0.33019
H	1.89593	3.50489	0.81564
H	2.14803	3.77143	-0.91806
H	0.50810	3.68776	-0.25094
H	0.48773	2.02999	2.22340
H	0.37980	0.29674	2.53741
H	1.94820	1.03504	2.18187
H	-1.08362	2.10692	0.21023
H	-0.97513	0.85129	-1.01268
H	-1.63789	-0.86053	0.75611
H	-1.79147	0.44775	1.91595
H	-3.59985	1.52495	0.55453
H	-5.68455	1.21060	-0.32741
H	-5.72053	0.01797	-1.64310
H	-6.32970	-0.42092	-0.05193
H	-2.91841	-2.13464	-0.20333
H	-4.64626	-2.43214	0.04495
H	-4.05694	-1.99467	-1.55314

Conformer 3

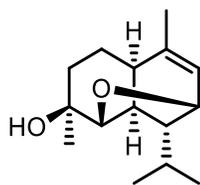
Energy: -736.43804 Hartree (Rel: 2.5 kcal/mol)

XYZ coordinates for conf 3:

C	2.42536	0.15289	-1.26871
C	1.60339	-0.71887	-0.26563
C	0.50361	0.23057	0.34793
C	0.98871	1.62516	-0.07633
C	1.97117	1.55524	-0.98390
O	3.82430	-0.04170	-0.94000
C	3.86151	-0.31401	0.46389
C	2.71091	-1.30199	0.65573
O	3.09752	-2.60640	0.21758
H	2.33075	-0.13787	-2.32039
H	1.12454	-1.57113	-0.75417
C	0.45664	2.90655	0.50585
C	0.35235	0.11437	1.87673
C	-0.83929	-0.17184	-0.34811
C	-2.10300	0.67653	-0.09092
C	-3.30930	0.07126	-0.76359

C	-4.43470	-0.40348	-0.20515
C	-5.53481	-0.98564	-1.06309
C	-4.73189	-0.41232	1.27545
H	2.45467	2.41411	-1.44318
H	3.71109	0.60277	1.05346
H	4.83800	-0.74331	0.70175
H	2.40736	-1.41999	1.69639
H	3.50967	-2.48643	-0.65546
H	0.65057	2.95266	1.58558
H	0.94079	3.77249	0.04314
H	-0.62562	3.01586	0.38089
H	-0.44031	0.77223	2.24737
H	0.09288	-0.91008	2.16844
H	1.27321	0.39404	2.40037
H	-0.66295	-0.20206	-1.43203
H	-1.05786	-1.20560	-0.04580
H	-2.27309	0.79658	0.98325
H	-1.95102	1.68430	-0.49956
H	-3.22932	0.00883	-1.85114
H	-5.28071	-0.95983	-2.12766
H	-5.74132	-2.02940	-0.78660
H	-6.47736	-0.43713	-0.92395
H	-3.92360	-0.00026	1.88405
H	-5.64267	0.16404	1.49063
H	-4.92626	-1.43657	1.62313

Originally assigned (incorrect) structure of 31{13} (CDCl₃)



Rel energy (kcal/mol): **Conf1** **Conf2**
 0.00 3.18

C-nom	iGau	Exp	Calc	diff	1	2
C1-CH2	6	21.60	25.39	3.79	[25.41	21.94]
C2-CH2	1	29.30	31.80	2.50	[31.80	31.01]
C3-C	2	70.30	68.26	-2.04	[68.28	64.74]
C4-CH	3	86.10	85.65	-0.45	[85.66	84.34]
C5-CH	4	37.80	41.15	3.35	[41.16	40.04]
C6-CH	5	37.50	38.76	1.26	[38.78	35.29]
C7-C	10	140.70	141.73	1.03	[141.71	145.34]
C8-CH	9	126.70	124.03	-2.67	[124.07	116.09]
C9-CH	8	73.60	74.54	0.94	[74.53	76.09]
C10-CH	7	54.30	54.82	0.52	[54.83	52.97]
C11-CH	14	25.40	26.57	1.17	[26.57	26.30]
C12-CH3	15	21.80	20.67	-1.13	[20.67	21.20]
C13-CH3	16	21.50	21.00	-0.50	[21.00	21.06]
C14-CH3	11	19.50	19.90	0.40	[19.90	20.67]
C15-CH3	17	28.00	24.05	-3.95	[24.02	30.24]

13C chem shifts: RMSD=2.09ppm (MAE=1.71) N=15 {-3.95 3.79}

Fractions: 0.995 0.005

Conformer 1

Energy: -736.47274 Hartree (Rel: 0.0 kcal/mol)

XYZ coordinates for conf 1:

C	2.45022	0.87085	0.25059
C	2.41183	-0.64465	-0.02671
C	0.96055	-1.14686	-0.20327
C	-0.13005	-0.57797	0.72510
C	0.01355	0.95543	0.96515
C	1.47291	1.29065	1.35541
C	-1.37493	-0.91689	-0.13001
C	-0.85604	-0.30985	-1.45270
C	-0.84932	1.19752	-1.35831
C	-0.45383	1.79364	-0.22445
C	-0.47041	3.29185	-0.05602
H	-0.62411	1.22591	1.82139
H	-0.12102	-1.09499	1.69043
C	-2.75792	-0.47244	0.38163
C	-3.84662	-0.72978	-0.67384
C	-3.10948	-1.18636	1.69761
C	3.11583	-1.43670	1.07938
O	3.13251	-0.93703	-1.23167
O	0.50165	-0.82761	-1.54168
H	3.47774	1.15912	0.50279
H	2.19117	1.39427	-0.67828
H	0.97408	-2.24363	-0.11646
H	1.57336	2.36194	1.56303
H	1.71348	0.77651	2.29522
H	-1.40970	-2.00929	-0.25967
H	-1.38142	-0.66123	-2.34354
H	-1.18463	1.78446	-2.21159
H	-0.93481	3.78178	-0.91761
H	-1.02949	3.58003	0.84492
H	0.53999	3.70508	0.05841
H	-2.73377	0.60617	0.57733
H	-4.83429	-0.44919	-0.28936
H	-3.67068	-0.15244	-1.58857
H	-3.88620	-1.79203	-0.94904
H	-4.09352	-0.86657	2.06018

H	-2.37992	-0.97356	2.48707
H	-3.14445	-2.27495	1.55863
H	3.09509	-2.50749	0.85124
H	4.16308	-1.12310	1.14800
H	2.64753	-1.28295	2.05685
H	2.52142	-0.69740	-1.95198

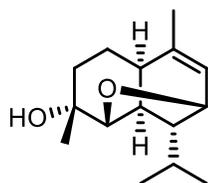
Conformer 2

Energy: -736.46767 Hartree (Rel: 3.2 kcal/mol)

XYZ coordinates for conf 2:

C	2.44932	0.04710	1.39618
C	2.32583	-0.65132	0.03671
C	0.88736	-1.25295	-0.06731
C	-0.20070	-0.56182	0.78364
C	0.05432	0.96030	0.91199
C	1.46138	1.22239	1.54545
C	-1.45575	-0.88472	-0.05986
C	-0.86826	-0.47890	-1.42373
C	-0.66221	1.01692	-1.48063
C	-0.19783	1.68513	-0.41236
C	0.01055	3.17747	-0.44316
H	-0.68681	1.37155	1.61498
H	-0.24038	-1.00901	1.78231
C	-2.79779	-0.25887	0.36319
C	-3.89944	-0.56912	-0.66439
C	-3.21646	-0.74874	1.75948
C	3.38099	-1.75226	-0.13809
O	2.51673	0.33649	-0.97738
O	0.41627	-1.17634	-1.43615
H	2.27893	-0.69905	2.18380
H	3.47621	0.40918	1.52912
H	0.93510	-2.31563	0.20449
H	1.90422	2.11667	1.10154
H	1.33773	1.43867	2.61298
H	-1.58829	-1.97738	-0.06937
H	-1.42075	-0.85251	-2.28811
H	-0.87697	1.54035	-2.41071
H	-0.38405	3.61323	-1.36649
H	-0.48620	3.66434	0.40724
H	1.07388	3.44021	-0.37987
H	-2.68111	0.83085	0.40500
H	-4.86058	-0.15265	-0.34061
H	-3.66947	-0.14532	-1.64845
H	-4.03062	-1.65236	-0.78712
H	-4.17433	-0.30438	2.05454
H	-2.47843	-0.48486	2.52525
H	-3.33828	-1.83987	1.77381
H	3.24031	-2.26368	-1.09780
H	4.38442	-1.31327	-0.12879
H	3.32182	-2.50159	0.66078
H	1.87185	0.10168	-1.67288

Revised structure of 31{13}, i.e. 32{13-rev} (CDCl₃)



					Conf1	Conf2
Rel energy (kcal/mol):					0.00	0.08
C-nom	iGau	Exp	Calc	diff	1	2
C1-CH2	6	21.60	23.07	1.47	[23.03	23.12]
C2-CH2	1	29.30	29.74	0.44	[28.51	31.15]
C3-C	2	70.30	69.29	-1.01	[69.10	69.50]
C4-CH	3	86.10	85.92	-0.18	[87.39	84.24]
C5-CH	4	37.80	40.13	2.33	[40.23	40.02]
C6-CH	5	37.50	38.77	1.27	[38.75	38.79]
C7-C	10	140.70	141.22	0.52	[141.36	141.06]
C8-CH	9	126.70	124.61	-2.09	[124.46	124.79]
C9-CH	8	73.60	74.84	1.24	[74.98	74.69]
C10-CH	7	54.30	53.74	-0.56	[53.75	53.72]
C11-CH	14	25.40	26.45	1.05	[26.44	26.47]
C12-CH3	15	21.80	20.78	-1.02	[20.77	20.80]
C13-CH3	16	21.50	21.14	-0.36	[21.14	21.15]
C14-CH3	11	19.50	20.02	0.52	[20.02	20.02]
C15-CH3	17	28.00	27.78	-0.22	[27.75	27.82]
13C chem shifts: RMSD=1.14ppm (MAE=0.95) N=15 {-2.09 2.33}						
Fractions:					0.532	0.468

Conformer 1

Energy: -736.47105 Hartree (Rel: 0.0 kcal/mol)

XYZ coordinates for conf 1:

C	2.45756	0.87164	0.26008
C	2.40550	-0.64219	0.02494
C	0.95992	-1.13065	-0.21644
C	-0.13197	-0.56329	0.71186
C	0.00653	0.97254	0.93525
C	1.46102	1.31210	1.33797
C	-1.37529	-0.91725	-0.13670
C	-0.85731	-0.32632	-1.46685
C	-0.85614	1.18323	-1.39118
C	-0.45734	1.79478	-0.26674
C	-0.47082	3.29542	-0.11994
H	-0.63864	1.25158	1.78356
H	-0.10833	-1.06997	1.68128
C	-2.75927	-0.47087	0.37010
C	-3.84874	-0.74564	-0.68007
C	-3.10687	-1.16760	1.69630
C	3.32913	-1.06924	-1.11901
O	2.85287	-1.23531	1.26147
O	0.50372	-0.83218	-1.55242
H	3.48067	1.14237	0.54719
H	2.23671	1.37872	-0.68652
H	0.97885	-2.22963	-0.10521
H	1.56145	2.38625	1.53058
H	1.69567	0.79927	2.27760
H	-1.40707	-2.01174	-0.25230
H	-1.38243	-0.68949	-2.35359
H	-1.19176	1.75891	-2.25223
H	-0.93378	3.77429	-0.98864
H	-1.02937	3.59822	0.77666
H	0.54051	3.70795	-0.01067
H	-2.73815	0.61040	0.55108
H	-4.83692	-0.46224	-0.29870
H	-3.67496	-0.18100	-1.60310
H	-3.88600	-1.81183	-0.94030
H	-4.09050	-0.84470	2.05752

H	-2.37502	-0.94362	2.48047
H	-3.14064	-2.25807	1.57172
H	4.35685	-0.75371	-0.90833
H	3.32258	-2.16146	-1.23439
H	3.00639	-0.63207	-2.06793
H	2.86591	-2.19844	1.13448

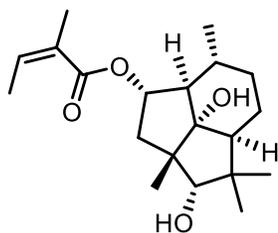
Conformer 2

Energy: -736.47118 Hartree (Rel: 0.1 kcal/mol)

XYZ coordinates for conf 2:

C	2.45307	0.86745	0.24451
C	2.39811	-0.65280	0.02201
C	0.95470	-1.14045	-0.20872
C	-0.13382	-0.56216	0.71644
C	0.00896	0.97456	0.93261
C	1.46607	1.31244	1.32829
C	-1.37751	-0.91673	-0.13142
C	-0.85663	-0.33263	-1.46351
C	-0.85438	1.17743	-1.39390
C	-0.45562	1.79308	-0.27168
C	-0.46967	3.29422	-0.12970
H	-0.63202	1.25955	1.78208
H	-0.11251	-1.06484	1.68787
C	-2.76115	-0.46591	0.37214
C	-3.85046	-0.74642	-0.67673
C	-3.10997	-1.15421	1.70246
C	3.31698	-1.08928	-1.12263
O	2.77625	-1.33803	1.23534
O	0.50322	-0.84030	-1.54571
H	3.48020	1.14896	0.51738
H	2.22796	1.37406	-0.70198
H	0.97897	-2.23435	-0.08735
H	1.57006	2.38579	1.52299
H	1.70434	0.79509	2.26515
H	-1.41082	-2.01155	-0.24201
H	-1.38147	-0.69861	-2.34929
H	-1.19044	1.75014	-2.25682
H	-0.93014	3.77027	-1.00130
H	-1.03114	3.59979	0.76415
H	0.54122	3.70750	-0.01868
H	-2.73938	0.61650	0.54655
H	-4.83862	-0.45969	-0.29775
H	-3.67570	-0.18811	-1.60345
H	-3.88842	-1.81427	-0.92992
H	-4.09381	-0.82873	2.06090
H	-2.37852	-0.92566	2.48566
H	-3.14369	-2.24539	1.58481
H	4.34940	-0.77526	-0.92059
H	3.30454	-2.17998	-1.22608
H	3.00048	-0.64606	-2.07082
H	3.68159	-1.05994	1.45030

Originally assigned correct structure of 33{5} (CDCl₃)



					Conf1	Conf2
Rel energy (kcal/mol):					0.00	0.06
C-nom	iGau	Exp	Calc	diff	1	2
C1-CH	11	57.90	56.03	-1.87	[57.67	54.21]
C2-CH	1	84.60	84.90	0.30	[83.51	86.44]
C3-CH2	2	39.80	39.26	-0.54	[38.75	39.83]
C4-C	3	58.80	57.92	-0.88	[57.80	58.06]
C5-CH	5	87.20	85.99	-1.21	[85.97	86.02]
C6-C	6	52.20	52.93	0.73	[52.87	52.99]
C7-CH	7	54.00	52.81	-1.19	[52.86	52.76]
C8-C	4	95.30	92.06	-3.24	[92.23	91.88]
C9-CH	10	36.20	35.26	-0.94	[35.03	35.51]
C10-CH2	9	34.80	33.63	-1.17	[33.71	33.55]
C11-CH2	8	27.00	26.83	-0.17	[26.82	26.84]
C12-CH3	24	27.80	26.63	-1.17	[26.66	26.60]
C13-CH3	22	27.90	27.27	-0.63	[27.29	27.24]
C14-CH3	21	30.50	28.96	-1.54	[28.96	28.96]
C15-CH3	20	21.90	21.16	-0.74	[21.37	20.92]
C1'-C	13	168.30	166.50	-1.80	[166.43	166.58]
C2'-C	14	129.40	127.32	-2.08	[127.11	127.55]
C3'-CH	17	136.80	138.38	1.58	[138.68	138.05]
C4'-CH3	18	15.90	16.46	0.56	[16.49	16.43]
C5'-CH3	16	20.80	22.73	1.93	[22.88	22.57]
13C chem shifts: RMSD=1.41ppm (MAE=1.21) N=20 {-3.24 1.93}						
Fractions:					0.526	0.474

Conformer 1

Energy: -1082.25694 Hartree (Rel: 0.0 kcal/mol)

XYZ coordinates for conf 1:

C	-0.96880	0.18326	0.82425
C	-0.08420	-0.93952	1.46639
C	1.34220	-0.46681	1.10375
C	1.10020	-0.03981	-0.37127
C	2.60690	-1.35302	0.92664
C	3.46751	-0.59578	-0.19029
C	2.45874	0.42128	-0.89987
C	2.65769	1.94634	-0.75387
C	1.37075	2.69801	-1.14944
C	0.15409	2.35696	-0.25786
C	-0.14679	0.84092	-0.34923
O	-2.17900	-0.44174	0.33276
C	-3.35905	0.18750	0.51082
O	-4.53293	-0.52467	-0.07394
C	-3.47381	1.24217	1.11930
C	-5.85825	0.04475	0.38490
C	-4.48734	-1.54711	-0.95362
C	-3.34095	-2.26737	-1.60032
H	-0.69505	0.66965	-1.28227
C	-1.07203	3.19591	-0.64537
C	4.01218	-1.58502	-1.24299
C	4.69426	0.08270	0.45273
O	2.30259	-2.68643	0.47039
C	1.70167	0.62396	2.14446
O	0.67833	-1.20195	-1.12818
H	-1.26725	0.93019	1.56083
H	-0.26029	-1.01763	2.54431
H	-0.34485	-1.89276	1.00368

H	3.18541	-1.43460	1.85559
H	2.93615	2.23880	0.26300
H	1.11999	2.46727	-2.19632
H	1.55226	3.78003	-1.10698
H	0.42135	2.62069	0.77343
H	-5.94991	1.10098	0.10777
H	-6.69275	-0.50565	-0.05891
H	-5.95481	0.00043	1.47632
H	-5.46255	-1.92128	-1.27025
H	-2.36956	-1.81630	-1.41027
H	-3.31407	-3.30845	-1.24655
H	-3.51188	-2.32120	-2.68369
H	-1.93835	2.94909	-0.02245
H	-0.86511	4.26724	-0.53420
H	-1.34959	3.01601	-1.69252
H	4.64168	-1.04000	-1.95669
H	4.62294	-2.36726	-0.77984
H	3.21159	-2.06898	-1.80723
H	5.37391	-0.67763	0.85647
H	5.25077	0.65799	-0.29590
H	4.44387	0.76243	1.27123
H	1.79318	-3.12351	1.17265
H	0.89128	1.33746	2.30623
H	1.87683	0.12076	3.10351
H	2.59972	1.19372	1.91270
H	1.17760	-1.97650	-0.79927
H	2.47300	0.21597	-1.97617
H	3.48457	2.27185	-1.39757

Conformer 2

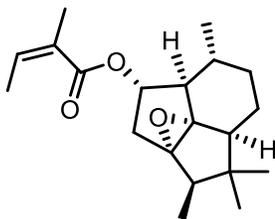
Energy: -1082.25703 Hartree (Rel: 0.1 kcal/mol)

XYZ coordinates for conf 2:

C	0.99801	0.40870	-0.66125
C	0.32903	-0.90887	-1.19602
C	-1.17348	-0.59959	-0.99561
C	-1.11398	0.04939	0.41466
C	-2.32400	-1.62177	-0.77495
C	-3.36577	-0.84845	0.16340
C	-2.55860	0.38455	0.78416
C	-2.93763	1.83554	0.41066
C	-1.79430	2.80502	0.77594
C	-0.47770	2.51673	0.01877
C	0.00545	1.08431	0.34724
O	2.23386	0.13139	0.04119
C	3.32551	-0.13573	-0.70520
C	4.54951	-0.45711	0.08512
O	3.32194	-0.09279	-1.92675
C	5.82245	-0.36910	-0.72822
C	4.57393	-0.84323	1.37743
C	3.47304	-1.06196	2.37385
H	0.49170	1.11850	1.32806
C	0.60316	3.55442	0.35212
C	-3.86441	-1.75462	1.30973
C	-4.61201	-0.43882	-0.64765
O	-1.88975	-2.82612	-0.11172
C	-1.58558	0.28021	-2.20341
O	-0.60908	-0.93094	1.35566
H	1.24551	1.07297	-1.49289
H	0.60691	-1.09993	-2.23605
H	0.67243	-1.74519	-0.58402
H	-2.80734	-1.90753	-1.71783
H	-3.16712	1.94957	-0.65307
H	-1.60185	2.75255	1.85860
H	-2.10963	3.83591	0.56773
H	-0.69416	2.59966	-1.05392
H	5.95774	0.63440	-1.14965
H	6.69514	-0.60619	-0.11298
H	5.79469	-1.06153	-1.57708
H	5.56813	-1.05045	1.77713
H	3.50636	-0.27671	3.14321
H	2.47592	-1.06208	1.93735

H	3.64196	-2.01056	2.89963
H	1.53855	3.34501	-0.18078
H	0.27989	4.56509	0.07577
H	0.82664	3.55393	1.42672
H	-4.61484	-1.21158	1.89681
H	-4.33017	-2.66816	0.92495
H	-3.05768	-2.04438	1.98698
H	-5.15065	-1.33316	-0.98379
H	-5.29946	0.14522	-0.02515
H	-4.38488	0.15694	-1.53540
H	-1.26887	-3.27721	-0.70742
H	-0.86543	1.07267	-2.41584
H	-1.61332	-0.36674	-3.08889
H	-2.56675	0.74294	-2.11339
H	-0.97636	-1.80406	1.11016
H	-2.63563	0.32336	1.87553
H	-3.84904	2.12660	0.94785

Originally assigned correct structure of 34{10} (CDCl₃)



Rel energy (kcal/mol): **Conf1** **Conf2**
 0.00 0.17

C-nom	iGau	Exp	Calc	diff	1	2
C1-CH	11	53.00	52.52	-0.48	[53.66	51.00]
C2-CH	1	82.90	84.28	1.38	[83.83	84.88]
C3-CH2	2	33.00	34.15	1.15	[33.42	35.12]
C4-C	3	79.70	78.54	-1.16	[78.75	78.25]
C5-CH	5	43.80	43.33	-0.47	[43.30	43.37]
C6-C	6	49.30	51.39	2.09	[51.35	51.44]
C7-CH	7	46.30	45.26	-1.04	[45.29	45.23]
C8-C	4	79.90	78.56	-1.34	[78.48	78.66]
C9-CH	10	36.30	35.35	-0.95	[35.32	35.39]
C10-CH2	9	33.30	31.99	-1.31	[32.06	31.89]
C11-CH2	8	29.60	29.20	-0.40	[29.18	29.22]
C12-CH3	24	14.42	15.42	1.00	[15.44	15.40]
C13-CH3	21	35.60	34.13	-1.47	[34.11	34.15]
C14-CH3	22	22.20	21.74	-0.46	[21.74	21.73]
C15-CH3	20	22.20	20.23	-1.97	[20.30	20.13]
C1'-CO	13	168.20	166.66	-1.54	[166.56	166.79]
C2'-C	14	129.20	127.26	-1.94	[127.14	127.42]
C3'-CH	17	137.00	138.81	1.81	[139.06	138.47]
C4'-CH3***	16	20.80	22.61	1.81	[22.72	22.47]
C5'-CH3***	18	16.00	16.26	0.26	[16.29	16.23]
13C chem shifts: RMSD=1.32ppm (MAE=1.20) N=20 {-1.97 2.09}						
					Fractions: 0.573	0.427

NOTICE:
 there is xray

Conformer 1
 Energy: -1005.83760 Hartree (Rel: 0.0 kcal/mol)
 XYZ coordinates for conf 1:

C	-0.92717	0.43606	0.93266
C	0.01570	-0.50595	1.73093
C	1.09689	-0.88987	0.74014
C	1.01189	-0.01597	-0.43151
C	2.53276	-1.34294	0.96743
C	3.28060	-0.91693	-0.37854
C	2.38656	0.22836	-1.01441
C	2.79383	1.68302	-0.68638
C	1.65261	2.67082	-0.97352
C	0.42646	2.42275	-0.07288
C	-0.11642	0.98765	-0.28803
O	-2.05793	-0.35505	0.49086
C	-3.24653	0.26811	0.34429
C	-4.34791	-0.60763	-0.15116
O	-3.42212	1.44657	0.61937
C	-5.71802	0.01453	0.01256
C	-4.20024	-1.81572	-0.73387
C	-2.98232	-2.62901	-1.05880
H	-0.75765	0.98413	-1.17878
C	-0.66385	3.47864	-0.29799
C	3.32290	-2.12536	-1.34142
C	4.73758	-0.47613	-0.15037
O	0.53762	-1.38046	-0.50628
C	3.10464	-0.76568	2.27288
H	-1.31787	1.24582	1.54984
H	0.45260	0.03608	2.57685

H	-0.54159	-1.35789	2.13324
H	2.56989	-2.43726	1.05033
H	3.06463	1.77125	0.37402
H	1.34973	2.59721	-2.02928
H	2.00705	3.69871	-0.82305
H	0.77168	2.50075	0.97066
H	-5.78712	0.96331	-0.53127
H	-6.49707	-0.65759	-0.35848
H	-5.92948	0.24271	1.06425
H	-5.13267	-2.29254	-1.04145
H	-2.04196	-2.10488	-0.90036
H	-2.97513	-3.54182	-0.44504
H	-3.04126	-2.96764	-2.10179
H	-1.55945	3.27011	0.29559
H	-0.29881	4.47875	-0.03611
H	-0.96643	3.49823	-1.35314
H	3.80447	-1.84628	-2.28739
H	3.90618	-2.94520	-0.90279
H	2.31987	-2.49608	-1.56134
H	5.32747	-1.30311	0.26302
H	5.20029	-0.19279	-1.10351
H	4.83522	0.37321	0.53081
H	3.06684	0.32956	2.29870
H	4.14647	-1.06717	2.41467
H	2.53726	-1.13676	3.13398
H	2.37866	0.11957	-2.10776
H	3.68785	1.95665	-1.25806

Conformer 2

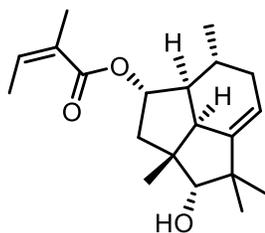
Energy: -1005.83787 Hartree (Rel: 0.2 kcal/mol)

XYZ coordinates for conf 2:

C	0.95484	0.71579	-0.61669
C	0.25054	-0.35918	-1.49885
C	-0.89090	-0.86122	-0.63714
C	-1.06354	0.03128	0.51033
C	-2.21994	-1.49783	-1.02237
C	-3.17513	-1.15576	0.21180
C	-2.51780	0.10280	0.91979
C	-3.06566	1.48977	0.51138
C	-2.09794	2.62103	0.89350
C	-0.75968	2.51526	0.13643
C	-0.06460	1.17169	0.46954
O	2.10550	0.16241	0.06845
C	3.25511	0.07783	-0.63488
C	4.39526	-0.52417	0.11471
O	3.36207	0.48727	-1.78168
C	5.74001	-0.23703	-0.51698
C	4.29204	-1.29714	1.21530
C	3.09622	-1.77271	1.98707
H	0.45694	1.27331	1.42954
C	0.15550	3.71158	0.42625
C	-3.18210	-2.34842	1.19500
C	-4.63708	-0.90916	-0.20176
O	-0.43230	-1.25846	0.68219
C	-2.69606	-1.01367	-2.40192
H	1.31144	1.54836	-1.22560
H	-0.13585	0.10759	-2.41160
H	0.95256	-1.14116	-1.80365
H	-2.10855	-2.58873	-1.07950
H	-3.22538	1.53042	-0.57404
H	-1.90721	2.60356	1.97747
H	-2.56100	3.59173	0.67441
H	-0.99673	2.51787	-0.93961
H	5.92633	0.84167	-0.58654
H	6.54794	-0.69030	0.06450
H	5.78461	-0.62681	-1.54010
H	5.24104	-1.65980	1.61414
H	3.06244	-1.27181	2.96587
H	2.14682	-1.59567	1.48453
H	3.20373	-2.84459	2.19807
H	1.10757	3.63631	-0.11194

H	-0.32266	4.65137	0.12670
H	0.38321	3.77625	1.49785
H	-3.80687	-2.12290	2.06877
H	-3.59937	-3.24130	0.71189
H	-2.17472	-2.58472	1.54306
H	-5.06229	-1.81013	-0.66021
H	-5.24542	-0.67669	0.68073
H	-4.75721	-0.08773	-0.91288
H	-2.79752	0.07671	-2.45126
H	-3.66474	-1.45091	-2.66064
H	-1.98369	-1.31529	-3.17815
H	-2.62694	0.00569	2.00880
H	-4.04515	1.65351	0.97470

Originally assigned (incorrect) structure of 35{9} (CDCl₃)



					Conf1	Conf2
Rel energy (kcal/mol):					0.00	0.25
iGau	jGau	Jexp	Jcalc	diff	1	2
26	28	11.30	8.50	-2.80	[8.76	8.09]
26	27	9.30	6.46	-2.84	[6.68	6.12]
19	26	6.30	3.34	-2.96	[3.21	3.54]
19	25	12.00	10.28	-1.72	[10.28	10.28]
For Js: RMSD=2.63Hz N=4					{-2.96	-1.72}
C-nom	iGau	Exp	Calc	diff	1	2
C1-CH***	11	56.90	45.41	-11.49	[46.32	44.01]
C2-CH	1	76.30	84.73	8.43	[83.41	86.75]
C3-CH2	2	42.90	40.19	-2.71	[40.21	40.15]
C4-C	3	44.90	51.23	6.33	[51.13	51.39]
C5-CH	5	88.80	84.38	-4.42	[84.36	84.42]
C6-C	6	50.10	50.91	0.81	[50.86	50.98]
C7-C	7	154.80	146.14	-8.66	[146.02	146.33]
C8-CH***	4	57.50	53.53	-3.97	[53.66	53.32]
C9-CH	10	32.50	32.31	-0.19	[32.11	32.62]
C10-CH2	9	36.80	35.06	-1.74	[35.11	34.99]
C11-CH	8	114.30	112.57	-1.73	[112.74	112.31]
C12-CH3	24	30.70	22.89	-7.81	[22.86	22.93]
C13-CH3	21	22.20	24.12	1.92	[24.10	24.15]
C14-CH3???	22	28.00	26.42	-1.58	[26.44	26.40]
C15-CH3	20	20.10	19.67	-0.43	[19.79	19.48]
C1'-CH3	13	168.50	166.51	-1.99	[166.41	166.67]
C2'-CO	14	128.60	127.59	-1.01	[127.40	127.89]
C3'-C	17	137.80	137.81	0.01	[138.13	137.33]
C4'-CH	18	15.70	16.51	0.81	[16.53	16.47]
C5'-CH3	16	20.60	23.06	2.46	[23.13	22.94]
13C chem shifts: RMSD=4.73ppm (MAE=3.42) N=20 {-11.49 8.43}						
Fractions:					0.605	0.395

NOTICE:

typo in Table 4 for C14 (two entries both wrong); SI shows a peak labeled "14" at approx 28ppm

Conformer 1

Energy: -1005.81627 Hartree (Rel: 0.0 kcal/mol)

XYZ coordinates for conf 1:

C	-0.88645	0.02321	0.65664
C	-0.04870	-1.22310	1.10852
C	1.39313	-0.70237	0.95686
C	1.24924	-0.01820	-0.41962
C	2.66095	-1.54839	0.66476
C	3.57537	-0.55979	-0.24862
C	2.59451	0.56987	-0.62186
C	2.73206	1.87288	-0.88069
C	1.49444	2.75064	-1.02950
C	0.28356	2.30396	-0.15672
C	-0.02783	0.80766	-0.40764
O	-2.13273	-0.44262	0.07862
C	-3.28625	0.14323	0.47014
C	-4.51642	-0.39876	-0.17904
O	-3.33138	1.06456	1.27254
C	-5.73696	0.46391	0.06141
C	-4.60938	-1.54178	-0.88965
C	-3.59250	-2.58857	-1.23567
H	-0.54460	0.73110	-1.37266

C	-0.93642	3.19928	-0.40668
C	4.05473	-1.27919	-1.52821
C	4.81291	-0.07067	0.52298
O	2.25935	-2.74358	0.00354
C	1.70495	0.22675	2.15325
H	1.11466	-0.85060	-1.12621
H	-1.14372	0.65854	1.50410
H	-0.32130	-1.54154	2.12053
H	-0.23566	-2.05461	0.42210
H	3.21047	-1.80557	1.58218
H	3.70841	2.35033	-0.95809
H	1.17817	2.79165	-2.08495
H	1.74869	3.78445	-0.76161
H	0.58860	2.42845	0.89019
H	-5.58052	1.48579	-0.30388
H	-6.61370	0.04593	-0.44142
H	-5.95550	0.54688	1.13200
H	-5.60433	-1.75895	-1.28163
H	-3.35127	-2.53621	-2.30731
H	-2.66566	-2.49412	-0.67442
H	-4.02142	-3.58434	-1.06637
H	-1.78166	2.90377	0.22450
H	-0.70637	4.25077	-0.19559
H	-1.26037	3.13281	-1.45396
H	4.65219	-0.59118	-2.13607
H	4.69523	-2.13914	-1.28792
H	3.22045	-1.63585	-2.13833
H	5.48227	-0.90973	0.75006
H	5.38117	0.65177	-0.07465
H	4.55125	0.41324	1.46855
H	3.05634	-3.24114	-0.23588
H	0.85530	0.85922	2.42348
H	1.93695	-0.39063	3.02996
H	2.55441	0.88867	1.97160

Conformer 2

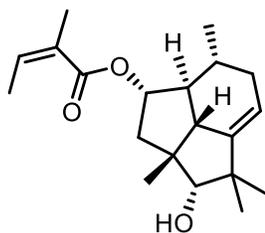
Energy: -1005.81667 Hartree (Rel: 0.3 kcal/mol)

XYZ coordinates for conf 2:

C	0.90346	-0.03157	-0.58741
C	0.17991	-1.42667	-0.57942
C	-1.30262	-1.00686	-0.62696
C	-1.25907	0.12678	0.41896
C	-2.51663	-1.79357	-0.06348
C	-3.53176	-0.62135	0.43256
C	-2.64802	0.64152	0.38852
C	-2.88587	1.93772	0.17079
C	-1.71927	2.90721	0.01164
C	-0.45104	2.27690	-0.63651
C	-0.04488	0.99423	0.12890
O	2.16439	-0.08147	0.12944
C	3.23558	-0.55400	-0.54609
C	4.50784	-0.58583	0.23412
O	3.16723	-0.95294	-1.69890
C	5.57953	-1.43149	-0.41923
C	4.75182	0.07428	1.38449
C	3.89652	1.00309	2.19497
H	0.43624	1.30367	1.06490
C	0.69812	3.28965	-0.70888
C	-4.00188	-0.87711	1.88117
C	-4.77432	-0.53716	-0.47029
O	-2.05589	-2.64171	0.98254
C	-1.64197	-0.58785	-2.07682
H	-1.09178	-0.39000	1.37559
H	1.13052	0.27298	-1.61126
H	0.51340	-2.05031	-1.41381
H	0.41261	-1.94293	0.35753
H	-3.01344	-2.40065	-0.83438
H	-3.89541	2.33418	0.06690
H	-1.44479	3.34078	0.98751
H	-2.03605	3.75757	-0.60617
H	-0.72716	2.00173	-1.66244

H	5.82384	-1.05254	-1.41795
H	6.49169	-1.43824	0.18427
H	5.24379	-2.46684	-0.55301
H	5.74796	-0.07882	1.80245
H	3.02919	1.37302	1.65152
H	3.53687	0.49281	3.10027
H	4.50051	1.85219	2.53778
H	1.58231	2.85623	-1.19178
H	0.40995	4.18033	-1.28007
H	0.99531	3.61754	0.29585
H	-4.66744	-0.06801	2.20104
H	-4.57073	-1.81406	1.95763
H	-3.16554	-0.92804	2.58360
H	-5.37330	-1.45267	-0.38771
H	-5.41313	0.30261	-0.17236
H	-4.51656	-0.40085	-1.52466
H	-2.82332	-3.08717	1.37325
H	-0.83533	-0.02051	-2.54827
H	-1.79184	-1.49187	-2.67990
H	-2.54698	0.01936	-2.14716

Revised structure of 35{9}, i.e. 36{9-rev} (CDCl₃)



					Conf1
Rel energy (kcal/mol):					0.00
iGau	jGau	Jexp	Jcalc	diff	1
19	26	11.30	11.41	0.11	[11.41]
26	28	9.30	9.46	0.16	[9.46]
26	27	6.30	6.28	-0.02	[6.28]
19	25	12.00	11.12	-0.88	[11.12]
For Js: RMSD=0.45Hz N=4					{-0.88 0.16}

C-nom	iGau	Exp	Calc	diff	1
C1-CH***	11	56.90	54.87	-2.03	[54.87]
C2-CH	1	76.30	78.13	1.83	[78.13]
C3-CH2	2	42.90	42.27	-0.63	[42.27]
C4-C	3	44.90	46.08	1.18	[46.08]
C5-CH	5	88.80	88.96	0.16	[88.96]
C6-C	6	50.10	51.96	1.86	[51.96]
C7-C	7	154.80	153.75	-1.05	[153.75]
C8-CH***	4	57.50	57.81	0.31	[57.81]
C9-CH	10	32.50	33.96	1.46	[33.96]
C10-CH2	9	36.80	36.97	0.17	[36.97]
C11-CH	8	114.30	114.95	0.65	[114.95]
C12-CH3	24	30.70	30.38	-0.32	[30.38]
C13-CH3	21	22.20	21.96	-0.24	[21.96]
C14-CH3???	22	28.00	27.43	-0.57	[27.43]
C15-CH3	20	20.10	20.20	0.10	[20.20]
C1'-CH3	13	168.50	167.05	-1.45	[167.05]
C2'-CO	14	128.60	127.96	-0.64	[127.96]
C3'-C	17	137.80	137.30	-0.50	[137.30]
C4'-CH	18	15.70	16.63	0.93	[16.63]
C5'-CH3	16	20.60	22.78	2.18	[22.78]
13C chem shifts: RMSD=1.13ppm (MAE=0.91) N=20 {-2.03 2.18}					

NOTICE:

typo in Table 4 for C14 (two entries both wrong); SI shows a peak labeled "14" at approx 28ppm

Conformer 1

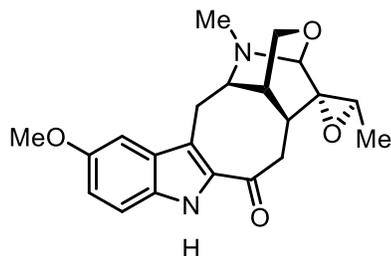
Energy: -1005.83009 Hartree (Rel: 0.0 kcal/mol)

XYZ coordinates for conf 1:

C	0.81881	-0.34491	-0.67889
C	0.11177	-1.56236	-0.02576
C	-1.39951	-1.41043	-0.40805
C	-1.49300	0.05694	-0.90429
C	-2.44546	-1.45411	0.76318
C	-3.50455	-0.30451	0.47469
C	-2.64606	0.73916	-0.22635
C	-2.62968	2.07438	-0.14358
C	-1.49024	2.91750	-0.70083
C	-0.18387	2.14700	-1.13025
C	-0.20421	0.76653	-0.46565
O	2.07311	-0.02325	-0.02855
C	3.16475	-0.71940	-0.41544
C	4.43162	-0.33257	0.27336
O	3.13000	-1.57528	-1.28649
C	5.66832	-0.84182	-0.43480
C	4.52802	0.35675	1.42839
C	3.47569	0.91434	2.34083
H	-0.26195	0.91484	0.62248

C	1.06011	2.98811	-0.81836
C	-4.15721	0.20976	1.76753
C	-4.62766	-0.80966	-0.46360
O	-1.75548	-1.23980	1.99392
C	-1.74387	-2.44683	-1.49326
H	-1.56672	0.09704	-2.00125
H	1.02626	-0.52518	-1.73811
H	0.53541	-2.51076	-0.36815
H	0.25077	-1.49766	1.05577
H	-2.95476	-2.42926	0.79922
H	-3.39610	2.61465	0.41162
H	-1.22257	3.64548	0.07996
H	-1.83699	3.52847	-1.54750
H	-0.22221	1.98988	-2.21832
H	5.72287	-0.46387	-1.46289
H	6.57458	-0.53514	0.09521
H	5.65752	-1.93516	-0.50596
H	5.54670	0.53388	1.77709
H	3.44348	2.01007	2.25344
H	2.47844	0.53147	2.13312
H	3.74084	0.69560	3.38277
H	1.97261	2.50295	-1.17992
H	0.99094	3.97629	-1.28997
H	1.16899	3.14044	0.26294
H	-4.87991	1.00164	1.54170
H	-4.70811	-0.59115	2.27899
H	-3.41477	0.62396	2.45520
H	-5.12625	-1.69089	-0.04034
H	-5.38130	-0.02483	-0.59380
H	-4.26183	-1.07310	-1.45906
H	-2.39899	-1.32980	2.71352
H	-1.04104	-2.36755	-2.33127
H	-1.66737	-3.46483	-1.09226
H	-2.75223	-2.32415	-1.89852

Originally assigned correct structure of 38{1} (CDCl₃)



					Conf1	Conf2
Rel energy (kcal/mol):					0.00	1.09
C-nom	iGau	Exp	Calc	diff	1	2
C2-C	8	135.80	136.92	1.12	[136.81	137.64]
C3-C	10	191.70	192.99	1.29	[192.92	193.42]
C5-CH	14	59.40	59.84	0.44	[59.86	59.74]
C6-CH2	15	31.20	32.22	1.02	[32.22	32.22]
C7-C	9	119.70	119.75	0.05	[119.80	119.44]
C8-C	5	128.30	129.00	0.70	[128.88	129.73]
C9-CH	6	100.80	100.67	-0.13	[99.73	106.61]
C10-C	1	154.90	153.78	-1.12	[153.88	153.12]
C11-CH	2	119.00	118.41	-0.59	[119.46	111.76]
C12-CH	3	113.30	113.17	-0.13	[113.30	112.33]
C13-C	4	131.90	132.26	0.36	[132.22	132.48]
C14-CH2	11	42.10	44.10	2.00	[44.09	44.16]
C15-CH	12	31.10	33.46	2.36	[33.46	33.43]
C16-CH	13	33.10	32.60	-0.50	[32.60	32.57]
C17-CH2	21	70.90	70.42	-0.48	[70.42	70.39]
C18-CH3	23	13.70	13.40	-0.30	[13.40	13.40]
C19-CH	22	59.00	58.00	-1.00	[57.99	58.03]
C20-C	17	63.80	64.43	0.63	[64.43	64.44]
C21-CH	18	89.20	88.58	-0.62	[88.58	88.55]
COMe-CH3	27	56.00	55.42	-0.58	[55.42	55.40]
CNMe-CH3	19	41.90	40.31	-1.59	[40.31	40.30]
13C chem shifts: RMSD=1.01ppm (MAE=0.81) N=21 {-1.59 2.36}						
Fractions:					0.864	0.136

Conformer 1

Energy: -1225.01510 Hartree (Rel: 0.0 kcal/mol)

XYZ coordinates for conf 1:

C	-4.84214	0.39003	0.03501
C	-5.22804	-0.92642	0.41332
C	-4.31257	-1.95882	0.47996
C	-2.97505	-1.66755	0.16189
C	-2.56820	-0.35741	-0.22013
C	-3.52415	0.68470	-0.28194
N	-1.86559	-2.46780	0.14072
C	-0.76440	-1.72393	-0.24338
C	-1.16026	-0.40423	-0.47943
C	0.53373	-2.39866	-0.29744
C	1.76208	-1.62166	-0.74305
C	2.35802	-0.70311	0.35623
C	1.36234	0.22754	1.09384
C	0.71572	1.27295	0.15799
C	-0.29027	0.74266	-0.90901
N	1.81564	2.01557	-0.50436
C	3.44985	0.23761	-0.19654
C	3.09476	1.69499	0.09083
C	1.55487	3.44639	-0.63332
O	3.11334	1.88111	1.51963
C	2.15598	1.01133	2.15221
C	4.86612	-0.13556	-0.34973
C	5.42599	-1.49801	-0.03048
O	3.99464	-0.01993	-1.49944
O	0.61459	-3.58936	0.01743

O	-5.87119	1.29364	0.02031
C	-5.57437	2.63234	-0.34957
H	-6.27376	-1.09651	0.64971
H	-4.61985	-2.95923	0.76978
H	-3.22123	1.68450	-0.57059
H	-1.80001	-3.44993	0.36835
H	2.51394	-2.36182	-1.02683
H	1.53753	-1.03779	-1.63898
H	2.79833	-1.36096	1.11699
H	0.58680	-0.35241	1.59960
H	0.15606	1.95681	0.81798
H	0.28275	0.47847	-1.80280
H	-0.93067	1.57917	-1.21092
H	3.85830	2.36403	-0.31080
H	2.36084	3.91696	-1.20609
H	0.62150	3.59971	-1.18445
H	1.47006	3.96087	0.33918
H	1.48087	1.62765	2.75985
H	2.68805	0.32353	2.82451
H	5.59403	0.67725	-0.28668
H	6.21736	-1.75919	-0.74231
H	5.86649	-1.49598	0.97361
H	4.66114	-2.27812	-0.07165
H	-6.51902	3.17640	-0.29778
H	-5.17790	2.68812	-1.37180
H	-4.85316	3.08933	0.34071

Conformer 2

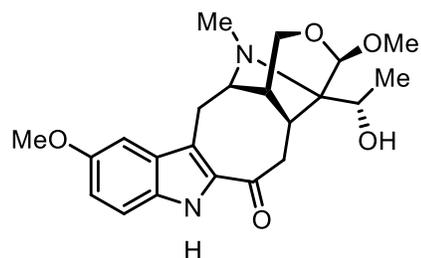
Energy: -1225.01684 Hartree (Rel: 1.1 kcal/mol)

XYZ coordinates for conf 2:

C	4.76286	-0.59253	-0.08401
C	5.19661	0.69529	0.32467
C	4.30216	1.75263	0.43604
C	2.95617	1.51391	0.13582
C	2.50227	0.22522	-0.27753
C	3.42606	-0.83077	-0.38430
N	1.86827	2.34608	0.15695
C	0.74032	1.64368	-0.22934
C	1.08960	0.32176	-0.51029
C	-0.53941	2.35775	-0.24410
C	-1.79607	1.63154	-0.69505
C	-2.40574	0.69872	0.38471
C	-1.42922	-0.28097	1.08303
C	-0.82525	-1.31797	0.11006
C	0.18045	-0.78730	-0.95710
N	-1.95481	-2.01105	-0.55635
C	-3.53063	-0.19372	-0.18179
C	-3.21661	-1.66831	0.06228
C	-1.73849	-3.44539	-0.72428
O	-3.22513	-1.89183	1.48595
C	-2.23275	-1.07076	2.12947
C	-4.93633	0.22572	-0.31000
C	-5.45175	1.59499	0.05202
O	-4.07991	0.11542	-1.47154
O	-0.57910	3.53998	0.10657
O	5.60480	-1.66845	-0.20913
C	6.98452	-1.49100	0.07852
H	6.24072	0.86946	0.55590
H	4.64544	2.73426	0.74909
H	3.12480	-1.82663	-0.69471
H	1.83434	3.32256	0.41286
H	-2.52833	2.40233	-0.94664
H	-1.60041	1.06838	-1.61077
H	-2.81819	1.34662	1.16932
H	-0.63087	0.26152	1.59491
H	-0.27619	-2.03497	0.74296
H	-0.39731	-0.48291	-1.83497
H	0.79296	-1.63271	-1.28993
H	-4.00469	-2.30310	-0.34758
H	-2.56427	-3.87684	-1.29966
H	-0.81596	-3.61247	-1.28934

H	-1.65922	-3.98655	0.23400
H	-1.56882	-1.72468	2.70953
H	-2.73441	-0.38697	2.82866
H	-5.68768	-0.56640	-0.26121
H	-6.24058	1.89993	-0.64507
H	-5.88390	1.57797	1.05960
H	-4.66384	2.35248	0.02591
H	7.45156	-2.46330	-0.08876
H	7.14651	-1.18852	1.12132
H	7.44631	-0.75047	-0.58738

Originally assigned (incorrect) structure of 39{3} (CDCl₃)



					Conf1	Conf2
Rel energy (kcal/mol):					0.00	1.89
C-nom	iGau	Exp	Calc	diff	1	2
C2-C	9	136.80	137.66	0.86	[137.68	137.24]
C3-C	11	192.70	193.20	0.50	[193.20	193.28]
C5-CH	15	63.60	65.05	1.45	[65.09	63.96]
C6-CH2	16	34.50	36.01	1.51	[36.02	35.85]
C7-C	10	120.40	120.27	-0.13	[120.21	121.61]
C8-C	6	128.40	128.85	0.45	[128.84	129.02]
C9-CH	7	100.80	99.59	-1.21	[99.58	99.84]
C10-C	2	154.70	153.75	-0.95	[153.76	153.63]
C11-CH	3	118.60	119.15	0.55	[119.15	119.20]
C12-CH	4	113.20	113.24	0.04	[113.25	113.10]
C13-C	5	131.80	132.06	0.26	[132.05	132.23]
C14-CH2	12	40.60	41.02	0.42	[41.02	40.94]
C15-CH	13	37.50	41.55	4.05	[41.61	40.13]
C16-CH	14	40.40	41.13	0.73	[41.16	40.45]
C17-CH2	20	66.80	67.09	0.29	[67.12	66.39]
C18-CH3	27	18.70	20.68	1.98	[20.67	20.95]
C19-CH	21	67.50	64.67	-2.83	[64.27	74.47]
C20-C	1	71.10	72.42	1.32	[72.47	71.26]
C21-CH	18	100.90	99.41	-1.49	[99.46	98.22]
COMe-CH3	25	55.90	55.33	-0.57	[55.33	55.33]
COMe-CH3	29	55.00	54.72	-0.28	[54.72	54.67]
CNMe-CH3	26	33.50	35.49	1.99	[35.52	34.83]
13C chem shifts: RMSD=1.44ppm (MAE=1.09) N=22 {-2.83 4.05}						
Fractions:					0.961	0.039

Conformer 1

Energy: -1340.76293 Hartree (Rel: 0.0 kcal/mol)

XYZ coordinates for conf 1:

C	-2.75855	-0.20548	-0.33959
C	5.26278	-0.72772	0.15002
C	5.74451	0.56215	0.50871
C	4.91134	1.66375	0.53581
C	3.56108	1.47016	0.19795
C	3.05825	0.18853	-0.16505
C	3.93175	-0.92533	-0.18735
N	2.51873	2.35344	0.13853
C	1.36875	1.69222	-0.25219
C	1.66164	0.33855	-0.45253
C	0.13017	2.47553	-0.32610
C	-1.13950	1.79775	-0.80933
C	-1.83423	0.90053	0.25566
C	-0.88569	-0.01381	1.05353
C	-0.51812	-1.07997	0.00517
C	0.73481	-0.76364	-0.89401
N	-1.75389	-1.18997	-0.82764
C	-3.59341	-0.78931	0.83449
O	-2.77044	-1.41153	1.80166
C	-1.65419	-0.62162	2.23027
C	-3.66576	0.29626	-1.52164
O	-2.92238	0.24742	-2.73750
O	0.14849	3.66929	-0.01480
O	6.21762	-1.70969	0.17333

C	5.82280	-3.02890	-0.17374
C	-2.17558	-2.56928	-1.08059
C	-5.00992	-0.41834	-1.71869
O	-4.37311	0.25456	1.36831
C	-5.33960	-0.17850	2.32220
H	6.79594	0.65530	0.76196
H	5.29080	2.64353	0.81034
H	3.55929	-1.90482	-0.46366
H	2.52168	3.33974	0.35730
H	-0.90858	1.21762	-1.70450
H	-1.82582	2.59315	-1.11153
H	-2.40748	1.54800	0.92383
H	-0.01304	0.49996	1.46079
H	-0.33942	-2.03830	0.50766
H	1.32503	-1.68030	-0.99778
H	0.35523	-0.54520	-1.89883
H	-4.24704	-1.59992	0.49083
H	-1.02016	-1.30707	2.80104
H	-1.99219	0.17768	2.90456
H	-3.89365	1.35034	-1.31593
H	-2.17458	-0.35548	-2.53106
H	6.72075	-3.64394	-0.09292
H	5.44051	-3.07672	-1.20180
H	5.05632	-3.41261	0.51241
H	-1.35388	-3.10228	-1.57051
H	-2.44347	-3.11788	-0.16523
H	-3.02639	-2.58523	-1.76634
H	-5.49800	0.01266	-2.59895
H	-4.89423	-1.49223	-1.89870
H	-5.67125	-0.27256	-0.85919
H	-6.04172	-0.89624	1.87388
H	-5.88809	0.71117	2.63890
H	-4.86197	-0.64417	3.19127

Conformer 2

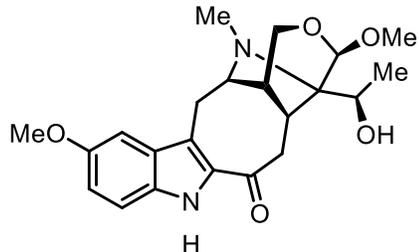
Energy: -1340.76595 Hartree (Rel: 1.9 kcal/mol)

XYZ coordinates for conf 2:

C	-2.72145	-0.22507	-0.41589
C	5.33017	-0.68197	0.10804
C	5.78675	0.59573	0.53619
C	4.93415	1.68005	0.61322
C	3.58982	1.48098	0.25541
C	3.11192	0.21134	-0.17677
C	4.00526	-0.88447	-0.24979
N	2.53286	2.34787	0.23356
C	1.39657	1.68646	-0.19819
C	1.71415	0.35040	-0.46656
C	0.14785	2.45140	-0.24158
C	-1.11564	1.78288	-0.75395
C	-1.81888	0.84284	0.26954
C	-0.85354	-0.12050	0.99190
C	-0.47521	-1.09929	-0.13756
C	0.81519	-0.74731	-0.97170
N	-1.67800	-1.10135	-1.00591
C	-3.51449	-0.99394	0.68670
O	-2.65655	-1.67254	1.57991
C	-1.60473	-0.85377	2.10504
C	-3.67081	0.32752	-1.52541
O	-4.55093	-0.69277	-2.02896
O	0.14562	3.63139	0.12198
O	6.30187	-1.64772	0.08847
C	5.93127	-2.95427	-0.32650
C	-2.03739	-2.41489	-1.52598
C	-4.49805	1.56659	-1.16780
O	-4.36916	-0.09184	1.35479
C	-5.26835	-0.71978	2.26513
H	6.83457	0.69380	0.80229
H	5.29423	2.65089	0.94069
H	3.65196	-1.85446	-0.57945
H	2.51627	3.32082	0.50471
H	-0.87531	1.21184	-1.65612

H	-1.79008	2.59365	-1.03829
H	-2.38548	1.44666	0.98325
H	0.00847	0.37752	1.43953
H	-0.32579	-2.09947	0.29220
H	1.42113	-1.65415	-1.07224
H	0.47117	-0.50693	-1.98487
H	-4.10813	-1.79565	0.22973
H	-0.94112	-1.54322	2.63579
H	-2.00777	-0.13383	2.83125
H	-3.02246	0.56206	-2.37492
H	-5.32141	-0.73010	-1.43926
H	6.83852	-3.55820	-0.26872
H	5.55748	-2.95736	-1.35880
H	5.16593	-3.38361	0.33337
H	-1.21538	-2.79003	-2.14796
H	-2.22427	-3.16130	-0.73348
H	-2.92916	-2.33478	-2.14837
H	-5.06021	1.87962	-2.05406
H	-5.20063	1.34557	-0.36007
H	-3.87922	2.40753	-0.84417
H	-5.89766	-1.46080	1.75054
H	-5.90294	0.06922	2.67473
H	-4.73081	-1.21859	3.07877

Revised structure of 39{3}, i.e. 40{3-rev} (CDCl₃)



Rel energy (kcal/mol):					Conf1	Conf2
					0.00	0.78
C-nom	iGau	Exp	Calc	diff	1	2
C2-C	9	136.80	137.69	0.89	[137.72	137.57]
C3-C	11	192.70	193.53	0.83	[193.37	194.11]
C5-CH	15	63.60	64.38	0.78	[63.98	65.88]
C6-CH2	16	34.50	36.07	1.57	[36.13	35.87]
C7-C	10	120.40	120.50	0.10	[120.46	120.63]
C8-C	6	128.40	128.86	0.46	[128.82	129.02]
C9-CH	7	100.80	99.62	-1.18	[99.60	99.70]
C10-C	2	154.70	153.72	-0.98	[153.75	153.63]
C11-CH	3	118.60	119.11	0.51	[119.14	118.98]
C12-CH	4	113.20	113.24	0.04	[113.26	113.16]
C13-C	5	131.80	132.07	0.27	[132.08	132.05]
C14-CH2	12	40.60	41.84	1.24	[42.16	40.67]
C15-CH	13	37.50	39.12	1.62	[38.43	41.69]
C16-CH	14	40.40	41.07	0.67	[41.56	39.26]
C17-CH2	20	66.80	66.85	0.05	[66.67	67.50]
C18-CH3	27	18.70	18.37	-0.33	[17.89	20.15]
C19-CH	21	67.50	67.47	-0.03	[66.74	70.18]
C20-C	1	71.10	73.11	2.01	[73.62	71.20]
C21-CH	18	100.90	101.37	0.47	[101.79	99.82]
COMe-CH3	25	55.90	55.33	-0.57	[55.33	55.31]
COMe-CH3	29	55.00	54.97	-0.03	[55.04	54.72]
CNMe-CH3	26	33.50	33.00	-0.50	[32.41	35.19]

13C chem shifts: RMSD=0.88ppm (MAE=0.69) N=22 {-1.18 2.01}
 Fractions: 0.788 0.212

Conformer 1

Energy: -1340.76634 Hartree (Rel: 0.0 kcal/mol)

XYZ coordinates for conf 1:

C	2.77379	-0.30980	0.41451
C	-5.26783	-0.64382	-0.11544
C	-5.70521	0.61375	-0.61709
C	-4.83800	1.68091	-0.74973
C	-3.49824	1.48467	-0.37387
C	-3.03952	0.23506	0.13143
C	-3.94746	-0.84343	0.26047
N	-2.42969	2.33789	-0.39518
C	-1.30517	1.68823	0.08016
C	-1.64202	0.37354	0.42023
C	-0.04251	2.43462	0.08601
C	1.20143	1.77908	0.66084
C	1.89714	0.76455	-0.29431
C	0.91987	-0.19912	-1.00430
C	0.50359	-1.13894	0.14397
C	-0.75206	-0.70101	0.98658
N	1.72336	-1.19282	0.99914
C	3.57616	-1.07299	-0.68651
O	2.71766	-1.77777	-1.56120
C	1.66164	-0.97118	-2.09846
C	3.72853	0.14095	1.56780
O	2.97729	0.40553	2.74842
O	-0.01813	3.58724	-0.35430
O	-6.25237	-1.59396	-0.04732

C	-5.90261	-2.87886	0.44593
C	2.10137	-2.53897	1.42883
C	4.61098	1.35437	1.28502
O	4.39636	-0.15878	-1.37224
C	5.33151	-0.77497	-2.25421
H	-6.75031	0.71031	-0.89412
H	-5.18329	2.63652	-1.13309
H	-3.60868	-1.79804	0.64573
H	-2.39997	3.29429	-0.71931
H	0.94078	1.29373	1.60276
H	1.89438	2.58825	0.89994
H	2.49011	1.32429	-1.02166
H	0.07221	0.30406	-1.47252
H	0.30301	-2.13818	-0.26187
H	-1.36831	-1.58686	1.17354
H	-0.37920	-0.39067	1.96969
H	4.19703	-1.85677	-0.23073
H	0.99172	-1.67323	-2.60406
H	2.06021	-0.27300	-2.84744
H	4.40199	-0.71426	1.76043
H	2.18856	-0.16954	2.65692
H	-6.81778	-3.47282	0.41709
H	-5.53554	-2.82632	1.47928
H	-5.13924	-3.35653	-0.18228
H	1.27899	-2.96900	2.01057
H	2.32182	-3.21792	0.59123
H	2.97593	-2.49464	2.08556
H	5.19994	1.57642	2.18147
H	5.29002	1.15741	0.45398
H	4.01636	2.24091	1.04671
H	5.99985	-1.45468	-1.70623
H	5.92119	0.03016	-2.69761
H	4.82383	-1.33730	-3.04554

Conformer 2

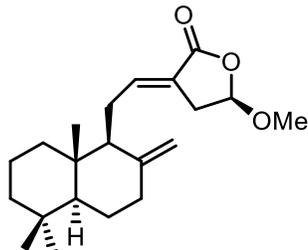
Energy: -1340.76758 Hartree (Rel: 0.8 kcal/mol)

XYZ coordinates for conf 2:

C	-2.70246	-0.26564	-0.42634
C	5.33274	-0.66989	0.11991
C	5.78294	0.61594	0.52967
C	4.92531	1.69755	0.58824
C	3.58277	1.48729	0.23049
C	3.11108	0.20917	-0.18294
C	4.00934	-0.88363	-0.23735
N	2.52201	2.34923	0.19256
C	1.38954	1.67710	-0.23098
C	1.71324	0.33838	-0.47774
C	0.13617	2.43742	-0.28847
C	-1.11960	1.75001	-0.78839
C	-1.79927	0.81182	0.24805
C	-0.84112	-0.13621	0.98968
C	-0.45880	-1.13059	-0.12113
C	0.81992	-0.77067	-0.96910
N	-1.66972	-1.17047	-0.99037
C	-3.51778	-0.98406	0.68866
O	-2.69421	-1.62397	1.63327
C	-1.60451	-0.82783	2.12136
C	-3.64631	0.36295	-1.50159
O	-4.23585	1.56334	-0.98969
O	0.13125	3.62228	0.05761
O	6.30872	-1.63173	0.11670
C	5.94509	-2.94556	-0.28061
C	-2.02053	-2.52441	-1.40259
C	-4.76004	-0.52184	-2.07877
O	-4.38622	-0.02807	1.28178
C	-5.34949	-0.59110	2.17385
H	6.82975	0.72261	0.79648
H	5.28028	2.67491	0.90162
H	3.66101	-1.86018	-0.55274
H	2.50018	3.32633	0.44835
H	-0.87074	1.17796	-1.68801

H	-1.83003	2.53084	-1.06656
H	-2.37129	1.42528	0.94678
H	0.02257	0.36503	1.43102
H	-0.29352	-2.12120	0.32319
H	1.43306	-1.67261	-1.07060
H	0.46375	-0.53957	-1.97984
H	-4.11986	-1.79948	0.26963
H	-0.96024	-1.52895	2.66045
H	-1.97460	-0.07957	2.83617
H	-3.00224	0.67956	-2.32708
H	-4.62982	1.31257	-0.13280
H	6.85499	-3.54444	-0.21259
H	5.57345	-2.96495	-1.31353
H	5.18042	-3.36932	0.38368
H	-1.16249	-2.96406	-1.92367
H	-2.27913	-3.19130	-0.56217
H	-2.85234	-2.51824	-2.10881
H	-5.34065	0.08440	-2.78141
H	-4.38088	-1.39183	-2.62191
H	-5.44797	-0.87078	-1.30063
H	-5.99716	-1.30777	1.65010
H	-5.95357	0.23786	2.54762
H	-4.85787	-1.09668	3.01094

Originally assigned correct structure of 41{1} (CDCl₃)



Rel energy (kcal/mol):					Conf1	Conf2	Conf3	Conf4	Conf5
					0.00	0.10	1.13	2.16	2.47
C-nom	iGau	Exp	Calc	diff	1	2	3	4	5
C1-CH2	6	39.30	40.08	0.78	[40.07	39.86	41.07	41.72	41.05]
C2-CH2	1	19.30	21.01	1.71	[21.03	21.03	20.85	21.00	20.79]
C3-CH2	2	42.00	42.10	0.10	[42.11	42.08	42.20	42.15	41.99]
C4-C	3	33.50	33.13	-0.37	[33.11	33.17	33.02	32.98	32.96]
C5-CH	4	55.40	54.83	-0.57	[54.77	54.85	54.99	55.21	55.00]
C6-CH2	7	24.10	26.18	2.08	[26.08	26.31	26.17	26.18	25.18]
C7-CH2	8	37.80	38.65	0.85	[38.50	38.81	38.81	38.75	38.33]
C8-C	9	147.90	148.32	0.42	[148.33	147.67	151.35	151.51	149.32]
C9-CH	10	56.20	56.65	0.45	[57.54	55.52	56.80	59.08	55.08]
C10-C	5	39.40	40.29	0.89	[40.02	40.46	41.10	40.68	39.83]
C11-CH2	15	25.50	27.42	1.92	[27.62	26.48	30.84	29.36	29.90]
C12-CH	17	143.10	141.86	-1.24	[142.88	140.36	143.69	142.39	140.31]
C13-C	18	123.90	124.07	0.17	[123.86	124.64	122.05	125.78	123.21]
C14-CH2	19	32.80	33.41	0.61	[33.44	33.33	33.82	32.87	32.97]
C15-CH	20	102.20	101.33	-0.87	[101.24	101.42	101.38	101.44	101.45]
C16-C	22	169.70	169.10	-0.60	[168.98	169.22	169.22	169.29	169.04]
C17-CH2	16	107.60	107.72	0.12	[108.01	107.61	106.58	106.49	107.92]
C18-CH3	12	33.50	33.22	-0.28	[33.20	33.23	33.33	33.13	33.45]
C19-CH3	11	21.70	22.06	0.36	[22.07	22.01	22.21	22.09	22.19]
C20-CH3	14	14.30	15.49	1.19	[15.65	15.33	15.26	14.83	17.56]
C21-CH3	25	56.60	55.84	-0.76	[55.86	55.84	55.76	55.87	55.91]
13C chem shifts: RMSD=0.96ppm (MAE=0.78) N=21 {-1.24 2.08}									
Fractions:					0.491	0.416	0.073	0.013	0.008

Conformer 1

Energy: -1045.14723 Hartree (Rel: 0.0 kcal/mol)

XYZ coordinates for conf 1:

C	3.38824	-2.55501	-0.44244
C	4.51780	-1.68493	-0.99678
C	4.65934	-0.31261	-0.29229
C	3.25139	0.38781	-0.26385
C	2.02521	-0.47186	0.23538
C	2.03964	-1.82746	-0.51583
C	3.26306	1.78123	0.39410
C	1.95483	2.54352	0.11421
C	0.74442	1.71983	0.48652
C	0.72402	0.34343	-0.16356
C	5.31990	-0.48864	1.09307
C	5.62746	0.53614	-1.15075
H	3.03224	0.56126	-1.33107
C	2.00707	-0.73112	1.75818
C	-0.60382	-0.42228	0.03488
C	-0.17813	2.18309	1.33795
C	-1.76867	0.22466	-0.65813
C	-3.04155	0.23072	-0.23981
C	-3.66510	-0.32604	1.01290
C	-5.17231	-0.23626	0.71688
O	-5.31143	0.68969	-0.39145
C	-4.11567	0.87264	-1.03481
O	-4.04229	1.49416	-2.07243
O	-5.63690	-1.49712	0.36286
C	-7.04336	-1.55790	0.12809

H	3.32653	-3.48949	-1.01514
H	3.60436	-2.85015	0.59227
H	5.47616	-2.21936	-0.94033
H	4.32583	-1.50853	-2.06604
H	1.79529	-1.65061	-1.57464
H	1.25779	-2.48684	-0.12013
H	4.10205	2.37419	0.01555
H	3.40735	1.69687	1.47782
H	1.94667	3.50153	0.64688
H	1.91417	2.77535	-0.96179
H	0.81545	0.51000	-1.24994
H	4.80956	-1.21806	1.72642
H	6.35194	-0.83864	0.96517
H	5.36272	0.45781	1.64314
H	5.91297	1.47204	-0.65880
H	6.55090	-0.02592	-1.33767
H	5.18679	0.78521	-2.12417
H	2.02457	0.19535	2.33816
H	1.09455	-1.27042	2.03775
H	2.84784	-1.34537	2.08490
H	-0.82753	-0.57635	1.09594
H	-0.49361	-1.42460	-0.40024
H	-1.05472	1.61483	1.63081
H	-0.08547	3.17533	1.77390
H	-1.56844	0.70476	-1.61651
H	-3.39299	-1.36354	1.22256
H	-3.41413	0.27622	1.89479
H	-5.77267	0.19120	1.52827
H	-7.28334	-2.60788	-0.04985
H	-7.60314	-1.20006	1.00388
H	-7.32720	-0.96361	-0.74725

Conformer 2

Energy: -1045.14379 Hartree (Rel: 0.1 kcal/mol)

XYZ coordinates for conf 2:

C	-2.59919	-2.47015	-1.00279
C	-3.51839	-2.43616	0.21920
C	-4.08852	-1.03188	0.53820
C	-2.89832	-0.00530	0.59032
C	-1.87545	-0.02324	-0.61230
C	-1.42941	-1.48926	-0.84843
C	-3.33233	1.43094	0.94056
C	-2.11923	2.31394	1.28651
C	-1.07757	2.26197	0.19394
C	-0.63033	0.84489	-0.14385
C	-5.20824	-0.66878	-0.46225
C	-4.74245	-1.11989	1.93792
H	-2.29873	-0.35454	1.44795
C	-2.42349	0.56390	-1.93113
C	0.59164	0.78340	-1.09608
C	-0.65897	3.37713	-0.41702
C	1.85960	1.23500	-0.43142
C	3.02675	0.57644	-0.43702
C	3.42134	-0.72673	-1.08121
C	4.77057	-1.04451	-0.41552
O	5.24340	0.20664	0.14895
C	4.22241	1.11323	0.25962
O	4.37098	2.16878	0.83541
O	4.56952	-1.98815	0.58422
C	5.76587	-2.41491	1.23513
H	-2.20349	-3.48494	-1.13967
H	-3.16645	-2.24338	-1.91454
H	-4.35032	-3.14264	0.09256
H	-2.94712	-2.78568	1.09254
H	-0.80981	-1.81377	0.00167
H	-0.79541	-1.55325	-1.74051
H	-4.01592	1.42373	1.79572
H	-3.88270	1.88437	0.10745
H	-2.43589	3.34753	1.46781
H	-1.67780	1.94402	2.22514
H	-0.30544	0.38461	0.80317

H	-4.89812	-0.74855	-1.50681
H	-6.05771	-1.34959	-0.32469
H	-5.57811	0.34991	-0.30191
H	-5.31204	-0.21968	2.19200
H	-5.44155	-1.96476	1.97024
H	-3.99171	-1.27913	2.72202
H	-2.80689	1.58014	-1.80767
H	-1.62597	0.60855	-2.68227
H	-3.22268	-0.04571	-2.35651
H	0.40827	1.41100	-1.97933
H	0.72751	-0.23357	-1.47036
H	0.07581	3.38285	-1.21608
H	-1.04887	4.34960	-0.12515
H	1.83121	2.17735	0.11300
H	2.71763	-1.54384	-0.90243
H	3.55022	-0.62004	-2.16472
H	5.55759	-1.36492	-1.10786
H	5.47763	-3.21137	1.92378
H	6.48979	-2.80748	0.50698
H	6.22829	-1.59523	1.79561

Conformer 3

Energy: -1045.14330 Hartree (Rel: 1.1 kcal/mol)

XYZ coordinates for conf 3:

C	-1.00265	-2.43355	-0.01978
C	-2.34981	-2.64883	0.67284
C	-3.45225	-1.65341	0.23237
C	-2.88887	-0.18857	0.34254
C	-1.46821	0.08800	-0.28939
C	-0.49079	-1.00501	0.20606
C	-3.90498	0.89701	-0.06145
C	-3.41640	2.30152	0.33857
C	-2.01988	2.56616	-0.17338
C	-1.01044	1.50780	0.25719
C	-3.98634	-2.03456	-1.16632
C	-4.62803	-1.81627	1.22523
H	-2.72351	-0.05927	1.42549
C	-1.46118	0.11628	-1.83386
C	0.45382	1.92014	-0.04117
C	-1.75390	3.61600	-0.95971
C	1.50048	1.29289	0.83020
C	2.72957	0.91626	0.45154
C	3.39143	0.93532	-0.90063
C	4.60875	0.01985	-0.69329
O	4.82751	-0.03240	0.74110
C	3.70417	0.36052	1.42078
O	3.61907	0.24990	2.62453
O	4.31093	-1.24313	-1.19016
C	5.39023	-2.17355	-1.11006
H	-0.26697	-3.14679	0.37373
H	-1.08398	-2.64662	-1.09328
H	-2.70661	-3.67517	0.50951
H	-2.20029	-2.54373	1.75811
H	-0.32013	-0.86941	1.28433
H	0.48370	-0.88375	-0.27946
H	-4.87132	0.71190	0.41907
H	-4.08716	0.87380	-1.14239
H	-4.11139	3.06714	-0.02534
H	-3.41431	2.36642	1.43807
H	-1.08997	1.43611	1.35430
H	-3.20133	-2.11728	-1.92161
H	-4.48752	-3.00926	-1.11352
H	-4.72277	-1.30932	-1.52955
H	-5.51986	-1.26219	0.91345
H	-4.91243	-2.87344	1.29682
H	-4.35247	-1.47720	2.23163
H	-2.17542	0.83548	-2.24249
H	-0.46928	0.39995	-2.20416
H	-1.68664	-0.86040	-2.26499
H	0.51746	3.00177	0.15124
H	0.70629	1.79292	-1.09913

H	-0.76787	3.82386	-1.36396
H	-2.53807	4.31817	-1.23385
H	1.26130	1.18175	1.88816
H	2.76643	0.54943	-1.71037
H	3.72013	1.94464	-1.17609
H	5.54601	0.40009	-1.11540
H	5.05361	-3.08340	-1.61057
H	6.28174	-1.78482	-1.62237
H	5.64413	-2.40035	-0.06892

Conformer 4

Energy: -1045.14708 Hartree (Rel: 2.2 kcal/mol)

XYZ coordinates for conf 4:

C	-2.55848	-2.40369	-0.81607
C	-3.36163	-2.28184	0.48042
C	-3.91801	-0.86068	0.74624
C	-2.74138	0.17471	0.61731
C	-1.82133	0.06461	-0.66195
C	-1.38864	-1.41128	-0.83644
C	-3.16809	1.63273	0.87723
C	-1.94973	2.56604	1.01214
C	-1.00077	2.40925	-0.15376
C	-0.55103	0.96774	-0.36077
C	-5.12620	-0.57878	-0.17418
C	-4.44418	-0.84804	2.20132
H	-2.06963	-0.09696	1.44895
C	-2.49416	0.55118	-1.96482
C	0.64439	0.84031	-1.35659
C	-0.65994	3.44980	-0.92287
C	1.54477	-0.34255	-1.12980
C	2.59211	-0.36495	-0.29250
C	3.14525	0.69921	0.61725
C	4.52488	0.13910	1.00153
O	4.47585	-1.28221	0.70709
C	3.43875	-1.57354	-0.13861
O	3.30331	-2.67656	-0.62146
O	5.49690	0.76536	0.23194
C	6.83354	0.37549	0.54597
H	-2.16671	-3.42431	-0.91366
H	-3.20894	-2.24676	-1.68584
H	-4.19294	-3.00020	0.48540
H	-2.70749	-2.56153	1.32016
H	-0.69229	-1.67963	-0.02875
H	-0.83710	-1.52461	-1.77734
H	-3.76107	1.69676	1.79548
H	-3.81153	1.99704	0.06789
H	-2.27553	3.60842	1.10653
H	-1.41974	2.30977	1.94302
H	-0.17263	0.62090	0.61333
H	-4.90332	-0.71393	-1.23507
H	-5.94439	-1.26620	0.07478
H	-5.50580	0.44027	-0.04133
H	-4.99081	0.07022	2.44114
H	-5.13527	-1.68594	2.35588
H	-3.62576	-0.95452	2.92428
H	-2.91938	1.55304	-1.87044
H	-1.76267	0.58783	-2.78025
H	-3.29022	-0.12086	-2.29021
H	1.25089	1.74485	-1.24175
H	0.28569	0.83326	-2.39148
H	-0.00128	3.36524	-1.78198
H	-1.04566	4.44527	-0.71466
H	1.35700	-1.25686	-1.68816
H	3.25803	1.67666	0.14008
H	2.52684	0.83035	1.51302
H	4.76354	0.20448	2.06929
H	7.49018	1.00043	-0.06221
H	7.05192	0.54536	1.60983
H	7.00696	-0.67940	0.30722

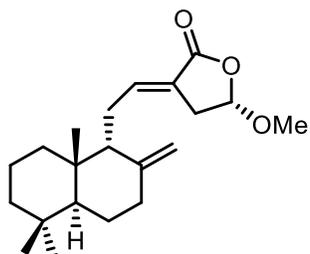
Conformer 5

Energy: -1045.14543 Hartree (Rel: 2.5 kcal/mol)

XYZ coordinates for conf 5:

C	1.97541	-2.61609	-0.15000
C	3.46554	-2.43032	-0.44711
C	4.06586	-1.12471	0.13241
C	3.15672	0.08779	-0.29253
C	1.59944	-0.06873	-0.10286
C	1.16078	-1.43330	-0.68734
C	3.63068	1.44890	0.25035
C	2.91647	2.60881	-0.46529
C	1.40881	2.46135	-0.47775
C	0.93404	1.09266	-0.94981
C	4.28604	-1.27508	1.65480
C	5.46295	-0.94446	-0.50824
H	3.29114	0.13295	-1.38638
C	1.15387	0.03244	1.37352
C	-0.59615	0.97674	-1.19809
C	0.61812	3.49073	-0.15053
C	-1.52953	0.95607	-0.02123
C	-2.62481	0.18977	0.08934
C	-3.19858	-0.85005	-0.83746
C	-4.59771	-1.10189	-0.24910
O	-4.56691	-0.57790	1.10402
C	-3.50517	0.26894	1.28049
O	-3.37410	0.92071	2.29356
O	-5.53715	-0.42369	-1.01563
C	-6.88829	-0.63494	-0.60699
H	1.61978	-3.54529	-0.61399
H	1.80909	-2.73351	0.92850
H	4.04205	-3.28750	-0.07283
H	3.60032	-2.42177	-1.53943
H	1.27304	-1.40486	-1.78239
H	0.09520	-1.59844	-0.48565
H	4.71053	1.56488	0.10934
H	3.45078	1.51722	1.32949
H	3.19964	3.56950	-0.01978
H	3.26873	2.62931	-1.50933
H	1.36329	0.97367	-1.95841
H	3.39671	-1.61770	2.18954
H	5.07410	-2.01631	1.83778
H	4.61026	-0.33472	2.11359
H	6.02606	-0.12020	-0.05735
H	6.05787	-1.85606	-0.37171
H	5.38814	-0.75408	-1.58614
H	1.31660	1.03285	1.78469
H	0.08614	-0.18681	1.46664
H	1.68015	-0.67651	2.01409
H	-0.78441	0.09890	-1.82360
H	-0.87064	1.84296	-1.82007
H	-0.46549	3.44924	-0.18288
H	1.04533	4.44306	0.15567
H	-1.33703	1.64186	0.80050
H	-3.29134	-0.51937	-1.87490
H	-2.60934	-1.77492	-0.82630
H	-4.86499	-2.15965	-0.14354
H	-7.51748	-0.12710	-1.34038
H	-7.13235	-1.70675	-0.59786
H	-7.07342	-0.21570	0.38791

Originally assigned (incorrect) structure of 42{2} (CDCl₃)



Rel energy (kcal/mol):					Conf1	Conf2	Conf3	Conf4	Conf5	Conf6
					0.00	0.14	1.36	1.97	2.29	3.84
C-nom	iGau	Exp	Calc	diff	1	2	3	4	5	6
C1-CH2	6	39.30	28.36	-10.94	[28.58	27.59	27.93	39.08	30.01	31.03]
C2-CH2	1	19.30	20.66	1.36	[20.67	20.61	20.57	21.87	20.73	21.06]
C3-CH2	2	42.00	35.61	-6.39	[35.44	35.60	35.42	41.20	35.02	34.84]
C4-C	3	33.80	33.89	0.09	[33.95	33.84	33.97	33.22	34.06	34.27]
C5-CH	4	55.30	52.48	-2.82	[51.90	53.44	52.16	48.68	52.23	53.02]
C6-CH2	7	24.10	29.65	5.55	[29.72	29.64	30.90	24.94	29.17	29.78]
C7-CH2	8	37.80	37.48	-0.32	[37.47	37.64	38.87	29.45	38.61	38.94]
C8-C	9	148.10	148.22	0.12	[147.99	147.95	152.03	148.59	150.04	151.40]
C9-CH	10	56.20	53.57	-2.63	[54.76	51.79	55.27	55.07	52.91	54.87]
C10-C	5	39.40	41.68	2.28	[41.55	41.91	42.53	37.86	42.07	42.59]
C11-CH2	15	25.40	28.61	3.21	[28.45	28.24	31.12	32.43	31.31	32.66]
C12-CH	17	143.20	142.10	-1.10	[143.20	140.48	144.81	140.50	140.34	140.51]
C13-C	18	123.80	123.97	0.17	[124.01	124.30	120.98	124.16	123.30	125.02]
C14-CH2	19	32.80	33.52	0.72	[33.88	33.10	33.41	33.20	33.35	33.15]
C15-CH	20	102.10	101.34	-0.76	[101.29	101.41	101.30	101.41	101.40	101.41]
C16-C	22	169.70	169.17	-0.53	[169.08	169.29	169.16	169.11	169.03	169.18]
C17-CH2	16	107.30	107.53	0.23	[107.95	107.05	105.81	111.73	106.45	105.77]
C18-CH3	12	33.50	32.87	-0.63	[33.22	32.79	33.11	24.01	33.30	33.13]
C19-CH3	11	21.70	31.48	9.78	[31.80	30.92	31.70	33.95	31.84	31.88]
C20-CH3	14	14.30	27.10	12.80	[26.82	26.91	27.86	37.01	27.13	26.75]
C21-CH3	25	56.60	55.84	-0.76	[55.79	55.87	55.99	55.87	55.86	55.94]
13C chem shifts: RMSD=4.82ppm (MAE=3.01) N=21 {-10.94 12.80}										
Fractions:					0.512	0.406	0.052	0.019	0.011	0.001

Conformer 1

Energy: -1045.13736 Hartree (Rel: 0.0 kcal/mol)

XYZ coordinates for conf 1:

C	3.42954	-1.46596	-1.76302
C	4.53278	-0.43045	-1.51839
C	4.66530	0.00840	-0.03833
C	3.24723	0.45077	0.53038
C	2.06650	-0.57379	0.24091
C	2.06690	-0.97341	-1.25542
C	2.91710	1.89217	0.06739
C	1.55103	2.40319	0.54002
C	0.47701	1.46365	0.07307
C	0.65918	0.06433	0.63008
C	5.32652	-1.12267	0.79277
C	5.67311	1.18394	0.01977
H	3.35021	0.49913	1.62607
C	2.22998	-1.82631	1.13537
C	-0.55579	-0.84820	0.33657
C	-0.48224	1.85483	-0.77445
C	-1.80604	-0.41317	1.04651
C	-3.06243	-0.57995	0.61150
C	-3.58630	-1.17988	-0.66594
C	-5.05491	-0.72498	-0.67883
O	-5.37127	-0.35904	0.68985
C	-4.22945	-0.15018	1.41862
O	-4.26819	0.29897	2.54334
O	-5.17891	0.37277	-1.52141
C	-6.51515	0.85356	-1.66344

H	3.35985	-1.67940	-2.83760
H	3.68890	-2.41929	-1.28498
H	5.50084	-0.81967	-1.86332
H	4.32366	0.45391	-2.13684
H	1.75469	-0.10903	-1.85722
H	1.31510	-1.75419	-1.42720
H	2.95033	1.96072	-1.02780
H	3.68239	2.57435	0.44610
H	1.54688	2.45826	1.63974
H	1.37993	3.41879	0.16455
H	0.70026	0.18189	1.72635
H	4.92659	-2.11632	0.58575
H	6.39811	-1.16772	0.56453
H	5.22694	-0.93808	1.86908
H	5.77841	1.57533	1.04000
H	6.66080	0.83248	-0.30098
H	5.39934	2.01392	-0.63704
H	2.27477	-1.54411	2.19446
H	1.39548	-2.52264	1.01327
H	3.12889	-2.39426	0.90911
H	-0.34057	-1.86912	0.67506
H	-0.73978	-0.92714	-0.74055
H	-1.25605	1.19385	-1.14961
H	-0.52911	2.88540	-1.11938
H	-1.68559	0.04875	2.02680
H	-3.07820	-0.82721	-1.56786
H	-3.52858	-2.27491	-0.65210
H	-5.77453	-1.50863	-0.94245
H	-6.48072	1.65075	-2.40839
H	-7.18404	0.05523	-2.01516
H	-6.89733	1.25204	-0.71742

Conformer 2

Energy: -1045.13930 Hartree (Rel: 0.1 kcal/mol)

XYZ coordinates for conf 2:

C	-3.35832	-1.74637	1.61282
C	-4.61026	-1.11178	0.99763
C	-4.44198	-0.70225	-0.48694
C	-3.14069	0.19093	-0.66249
C	-1.83203	-0.41079	0.01120
C	-2.13150	-0.83419	1.47066
C	-3.42629	1.64900	-0.22911
C	-2.21312	2.57648	-0.36511
C	-1.08184	2.03355	0.46040
C	-0.64435	0.65365	-0.00041
C	-4.43012	-1.96029	-1.39139
C	-5.71033	0.07946	-0.91059
H	-2.93525	0.23480	-1.74362
C	-1.32992	-1.62016	-0.82008
C	0.63648	0.16478	0.73431
C	-0.59298	2.71585	1.50381
C	1.86825	0.87627	0.25665
C	2.99977	0.29478	-0.16448
C	3.37868	-1.15923	-0.27883
C	4.89738	-1.10155	-0.51541
O	5.18599	0.25388	-0.94682
C	4.15377	1.09945	-0.63747
O	4.25073	2.29843	-0.78202
O	5.55035	-1.38536	0.67761
C	6.97294	-1.42727	0.57042
H	-3.53524	-1.94964	2.67697
H	-3.16151	-2.72236	1.15112
H	-5.46425	-1.79777	1.08480
H	-4.87477	-0.22152	1.58569
H	-2.28851	0.06769	2.07815
H	-1.25494	-1.34002	1.89491
H	-3.77482	1.68419	0.81136
H	-4.23432	2.05438	-0.84341
H	-1.91568	2.62933	-1.42379
H	-2.47841	3.59270	-0.05163
H	-0.38024	0.76352	-1.06524

H	-3.73478	-2.73478	-1.06798
H	-5.42779	-2.41582	-1.39875
H	-4.18034	-1.69845	-2.42684
H	-5.62917	0.45347	-1.93943
H	-6.57985	-0.58727	-0.87097
H	-5.92608	0.92817	-0.25566
H	-1.37592	-1.40177	-1.89330
H	-0.29314	-1.87437	-0.58597
H	-1.90852	-2.52547	-0.64110
H	0.77512	-0.91099	0.61679
H	0.51873	0.33335	1.81286
H	0.19910	2.34868	2.14829
H	-0.98265	3.70127	1.74876
H	1.83933	1.96456	0.23683
H	3.16814	-1.74723	0.61783
H	2.88040	-1.64192	-1.12814
H	5.25868	-1.74582	-1.32524
H	7.34839	-1.74873	1.54375
H	7.28723	-2.14848	-0.19737
H	7.38319	-0.44125	0.32673

Conformer 3

Energy: -1045.13952 Hartree (Rel: 1.4 kcal/mol)

XYZ coordinates for conf 3:

C	2.59377	-1.25474	-2.08412
C	4.01342	-1.20095	-1.50659
C	4.06632	-1.19032	0.04269
C	3.09578	-0.06775	0.61234
C	1.62960	-0.08672	0.00182
C	1.71305	-0.11719	-1.54442
C	3.77348	1.32220	0.48733
C	2.90399	2.50301	0.94053
C	1.59038	2.47224	0.21307
C	0.82286	1.19397	0.49900
C	3.74905	-2.60459	0.59631
C	5.53144	-0.91768	0.46724
H	2.98386	-0.26377	1.69056
C	0.83888	-1.31197	0.51014
C	-0.65837	1.28483	0.03907
C	1.21653	3.44915	-0.62191
C	-1.65480	0.49663	0.83748
C	-2.78899	-0.04764	0.37425
C	-3.34637	-0.10948	-1.02340
C	-4.78341	-0.61189	-0.79937
O	-4.81114	-1.17345	0.53851
C	-3.73143	-0.75656	1.27154
O	-3.63717	-0.99750	2.45555
O	-5.65666	0.46440	-0.89681
C	-7.03458	0.11325	-0.77396
H	2.64323	-1.18461	-3.17856
H	2.13147	-2.22625	-1.86799
H	4.60447	-2.04966	-1.87798
H	4.50955	-0.29733	-1.88769
H	2.10762	0.84093	-1.90642
H	0.70538	-0.21336	-1.96856
H	4.07809	1.50293	-0.55142
H	4.68851	1.32950	1.08516
H	2.72838	2.42774	2.02477
H	3.43521	3.44541	0.76307
H	0.79990	1.10271	1.59773
H	2.90183	-3.09055	0.11070
H	4.61284	-3.26206	0.44135
H	3.54671	-2.57575	1.67363
H	5.62832	-0.85030	1.55869
H	6.16810	-1.74450	0.13111
H	5.93928	-0.00154	0.03192
H	0.80855	-1.33504	1.60644
H	-0.19328	-1.28402	0.15124
H	1.25478	-2.25885	0.17438
H	-0.76634	1.07306	-1.02983
H	-0.95409	2.33687	0.16352

H	0.29269	3.42556	-1.19222
H	1.84377	4.32589	-0.76682
H	-1.47256	0.40636	1.90868
H	-3.37128	0.85559	-1.53588
H	-2.78877	-0.81425	-1.65232
H	-5.09004	-1.42901	-1.46256
H	-7.60518	1.02479	-0.96153
H	-7.31269	-0.64933	-1.51526
H	-7.26220	-0.26156	0.22986

Conformer 4

Energy: -1045.13340 Hartree (Rel: 2.0 kcal/mol)

XYZ coordinates for conf 4:

C	1.85529	-2.38008	0.90455
C	3.21486	-2.48643	0.21450
C	3.53701	-1.28181	-0.70200
C	3.39078	0.05448	0.12675
C	2.18426	0.21369	1.14446
C	1.81611	-1.14236	1.80926
C	3.59592	1.34523	-0.71168
C	2.30653	1.96348	-1.28758
C	1.29913	2.20564	-0.19229
C	0.90264	0.96639	0.59273
C	5.01806	-1.42663	-1.12888
C	2.69287	-1.36956	-1.99042
H	4.26422	-0.00052	0.79109
C	2.69293	1.12525	2.29797
C	-0.14403	0.12656	-0.20603
C	0.82045	3.42286	0.08973
C	-1.44597	0.85317	-0.36922
C	-2.64977	0.40991	0.01826
C	-3.05877	-0.87083	0.69904
C	-4.58984	-0.86588	0.55199
O	-4.95966	0.50341	0.24361
C	-3.87583	1.22128	-0.18756
O	-3.99315	2.34278	-0.63042
O	-4.94600	-1.71539	-0.48804
C	-6.35418	-1.84739	-0.67968
H	1.05626	-2.36207	0.15516
H	1.67733	-3.27427	1.51641
H	3.99416	-2.56118	0.98812
H	3.27611	-3.41095	-0.37559
H	0.83781	-1.04702	2.30109
H	2.53638	-1.32114	2.62024
H	4.30079	1.15634	-1.52834
H	4.07145	2.10437	-0.07847
H	2.54524	2.90351	-1.79866
H	1.88025	1.29442	-2.04655
H	0.36634	1.29696	1.49199
H	5.17587	-2.39671	-1.61619
H	5.68952	-1.37601	-0.26299
H	5.32713	-0.65292	-1.84015
H	2.92141	-0.55119	-2.68118
H	1.61681	-1.36251	-1.80306
H	2.92052	-2.30638	-2.51444
H	2.88748	2.14889	1.96463
H	1.94530	1.17795	3.09925
H	3.61615	0.72492	2.73174
H	-0.32067	-0.82460	0.29985
H	0.24197	-0.10534	-1.20583
H	0.11561	3.58907	0.90153
H	1.11425	4.29822	-0.48586
H	-1.41174	1.83413	-0.84011
H	-2.64701	-1.77221	0.23858
H	-2.78048	-0.87236	1.75961
H	-5.13752	-1.11399	1.46852
H	-6.49250	-2.60285	-1.45545
H	-6.84633	-2.18071	0.24503
H	-6.80229	-0.90210	-1.00446

Conformer 5

Energy: -1045.13587 Hartree (Rel: 2.3 kcal/mol)

XYZ coordinates for conf 5:

C	-1.48656	-1.68738	1.53822
C	-3.01691	-1.77461	1.49575
C	-3.62385	-1.51031	0.09430
C	-3.02585	-0.16883	-0.51094
C	-1.44352	-0.05864	-0.45943
C	-0.96596	-0.35071	0.98511
C	-3.70684	1.05522	0.15628
C	-3.19313	2.41730	-0.32499
C	-1.69690	2.50922	-0.20134
C	-1.00609	1.38842	-0.95510
C	-3.40092	-2.74234	-0.82267
C	-5.16176	-1.40333	0.25130
H	-3.30957	-0.14713	-1.57557
C	-0.77315	-1.04601	-1.44250
C	0.51637	1.62300	-1.18061
C	-1.10518	3.50350	0.47134
C	1.46603	1.42725	-0.03368
C	2.69556	0.89848	-0.12324
C	3.44623	0.33830	-1.30240
C	4.62767	-0.39052	-0.64091
O	4.73703	0.15854	0.69868
C	3.58218	0.79903	1.06211
O	3.40805	1.20335	2.19100
O	4.34806	-1.75037	-0.59156
C	5.40322	-2.54581	-0.05197
H	-1.14337	-1.80537	2.57410
H	-1.04261	-2.52178	0.98041
H	-3.34901	-2.76094	1.84882
H	-3.42765	-1.04531	2.20771
H	-1.28834	0.46192	1.64946
H	0.12847	-0.35753	1.01777
H	-3.58659	1.00585	1.24577
H	-4.78158	1.01976	-0.03788
H	-3.47160	2.54772	-1.38300
H	-3.68490	3.22103	0.23550
H	-1.42439	1.44751	-1.97414
H	-2.40242	-3.17508	-0.74499
H	-4.10344	-3.53785	-0.54720
H	-3.57978	-2.49610	-1.87622
H	-5.64792	-1.15920	-0.70242
H	-5.56213	-2.36696	0.58748
H	-5.46511	-0.65598	0.98924
H	-1.09320	-0.85227	-2.47430
H	0.31603	-0.94834	-1.40354
H	-0.99246	-2.08703	-1.22177
H	0.60941	2.67110	-1.50452
H	0.85467	1.02953	-2.03462
H	-0.02952	3.60901	0.56562
H	-1.70039	4.27462	0.95540
H	1.16425	1.77705	0.95086
H	2.86885	-0.36462	-1.90896
H	3.81342	1.13330	-1.96235
H	5.60044	-0.20395	-1.11027
H	5.09011	-3.58665	-0.15303
H	6.33679	-2.39047	-0.61114
H	5.57475	-2.31546	1.00506

Conformer 6

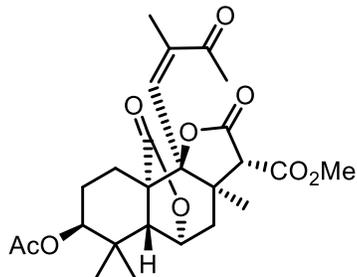
Energy: -1045.13638 Hartree (Rel: 3.8 kcal/mol)

XYZ coordinates for conf 6:

C	2.77283	-2.01303	-1.04212
C	4.14366	-1.32983	-1.11865
C	4.49089	-0.47244	0.12535
C	3.28363	0.50175	0.46427
C	1.85842	-0.19786	0.54227
C	1.63846	-1.01453	-0.75650
C	3.28785	1.69638	-0.53004
C	2.12865	2.69304	-0.37534
C	0.81035	1.97024	-0.36023

C	0.76931	0.94240	0.75089
C	4.87942	-1.39235	1.31325
C	5.77555	0.33413	-0.19155
H	3.48292	0.91843	1.46454
C	1.74008	-1.12074	1.77608
C	-0.67246	0.53774	1.19587
C	-0.15957	2.22250	-1.24584
C	-1.52051	-0.36853	0.35188
C	-2.78891	-0.14095	-0.02087
C	-3.68776	1.04797	0.19729
C	-5.07313	0.50945	-0.19850
O	-4.83066	-0.68818	-0.98252
C	-3.55598	-1.15017	-0.79290
O	-3.19337	-2.21660	-1.23949
O	-5.78399	0.20340	0.95511
C	-7.11896	-0.24300	0.71886
H	2.56844	-2.52552	-1.99097
H	2.78225	-2.79856	-0.27574
H	4.93187	-2.08126	-1.26602
H	4.16548	-0.69104	-2.01238
H	1.53935	-0.32900	-1.60724
H	0.69487	-1.56628	-0.70353
H	3.27735	1.32174	-1.56094
H	4.22095	2.25346	-0.41428
H	2.25069	3.24165	0.57176
H	2.16837	3.43371	-1.18285
H	1.14162	1.47787	1.64001
H	4.23374	-2.26474	1.42460
H	5.89477	-1.77799	1.16312
H	4.87265	-0.84527	2.26360
H	6.04476	1.00337	0.63619
H	6.61297	-0.35744	-0.34117
H	5.69007	0.93479	-1.10090
H	1.90096	-0.55878	2.70495
H	0.74509	-1.57402	1.82819
H	2.44819	-1.94484	1.76541
H	-1.21217	1.47500	1.36999
H	-0.58681	0.05799	2.18016
H	-1.09964	1.68161	-1.25645
H	-0.03187	2.98672	-2.00949
H	-1.11371	-1.33658	0.07042
H	-3.71204	1.40478	1.22987
H	-3.40972	1.89134	-0.44602
H	-5.65062	1.17167	-0.85367
H	-7.58564	-0.35855	1.69890
H	-7.68183	0.49705	0.13250
H	-7.13023	-1.20327	0.19192

Originally assigned (incorrect) structure of 45{3} (Acetone-*d*₆)



Conf1					
Rel energy (kcal/mol): 0.00					
C-nom	iGau	Exp	Calc	diff	1
C1-CH2	8	19.70	20.55	0.85	[22.05]
C2-CH2	3	22.50	21.79	-0.71	[23.28]
C3-CH	4	76.00	76.11	0.11	[77.46]
C4-C	5	35.20	33.42	-1.78	[34.88]
C5-CH	6	47.20	47.29	0.09	[48.72]
C6-CH	9	76.10	76.05	-0.05	[77.40]
C7-CH2	10	36.60	43.65	7.05	[45.08]
C8-C	11	46.50	48.15	1.65	[49.57]
C9-C	12	88.60	92.32	3.72	[93.62]
C10-C	7	50.60	51.11	0.51	[52.52]
C11-CH	22	119.80	117.64	-2.16	[118.88]
C12-C	23	143.70	144.21	0.51	[145.37]
C13-C	25	207.90	207.28	-0.62	[208.27]
C14-CH	18	57.50	62.61	5.11	[63.99]
C15-C	19	168.40	169.58	1.18	[170.68]
C19-C	32	166.80	165.13	-1.67	[166.24]
C20-CH3	26	29.00	30.57	1.57	[32.04]
C21-CH3	24	20.90	22.13	1.23	[23.62]
C22-CH3	17	25.80	21.88	-3.92	[23.37]
C23-C	2	176.80	176.52	-0.28	[177.60]
C24-CH3	13	22.40	20.76	-1.64	[22.26]
C25-CH3	14	26.50	24.41	-2.09	[25.90]
C26-C	30	170.30	168.41	-1.89	[169.51]
C27-CH3	31	20.80	19.20	-1.60	[20.70]
C28-CH3	35	52.70	52.45	-0.25	[53.86]

13C chem shifts: CRMSD=2.36ppm (CMAE=1.69) N=25 {-3.92 7.05}

NOTICE:

HMBC C9-H14 is not observed, but J(6-14)=4.5Hz for the orig. str., while it is = 0.8Hz for the revised epiE (i.e. epi-14)

Conformer 1

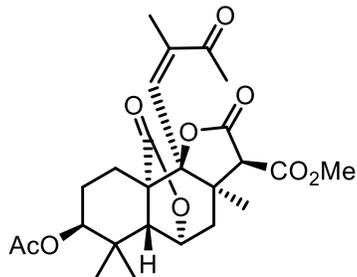
Energy: -1648.96144 Hartree (Rel: 0.0 kcal/mol)

XYZ coordinates for conf 1:

O	0.59460	-2.95936	1.03628
C	0.66253	-1.81217	1.75313
C	3.09857	0.32829	1.46506
C	3.66610	-0.13808	0.12387
C	3.04795	-1.47025	-0.35858
C	1.48957	-1.32110	-0.41935
C	0.80856	-0.62564	0.78780
C	1.58205	0.55158	1.40272
C	0.70544	-2.63908	-0.38995
C	-0.68321	-2.44693	-0.98095
C	-1.55860	-1.37151	-0.25056
C	-0.67400	-0.19156	0.38358
C	3.54838	-2.58959	0.58742
C	3.55671	-1.80326	-1.77710
H	1.26247	-0.76749	-1.33319
O	0.59821	-1.80042	2.96145
C	-2.47760	-2.07484	0.76703

C	-2.36480	-0.60706	-1.35309
C	-1.54366	0.64787	-1.62099
O	-0.55361	0.77126	-0.69623
O	-1.67067	1.43753	-2.52186
C	-1.33265	0.47200	1.57279
C	-1.73045	1.73914	1.75823
C	-2.38541	2.15350	3.06097
C	-1.67030	2.91085	0.79222
C	-0.35184	3.63307	0.60024
O	-2.70142	3.33173	0.29358
O	3.37466	0.87414	-0.88471
O	5.29295	1.98132	-0.40730
C	4.26787	1.87425	-1.05221
C	3.81956	2.81856	-2.14112
C	-3.81652	-0.27282	-1.01649
O	-4.19535	0.67741	-0.36707
O	-4.63011	-1.20679	-1.53632
C	-6.03755	-1.03944	-1.26027
H	3.35279	-0.40722	2.23550
H	3.59078	1.26195	1.75635
H	4.75267	-0.23880	0.18490
H	1.38754	1.43950	0.79889
H	1.19718	0.75159	2.40622
H	1.21323	-3.48565	-0.85317
H	-0.53276	-2.18071	-2.03292
H	-1.23002	-3.39548	-0.97741
H	3.20744	-3.57207	0.24770
H	4.64413	-2.60584	0.57988
H	3.22987	-2.47188	1.62565
H	3.28227	-1.02603	-2.49538
H	4.64871	-1.90068	-1.77914
H	3.14084	-2.75507	-2.12695
H	-3.09875	-2.80784	0.24295
H	-1.90356	-2.61440	1.52419
H	-3.14070	-1.37077	1.27547
H	-2.39298	-1.18978	-2.27603
H	-1.46132	-0.20262	2.41549
H	-2.42103	1.32356	3.77204
H	-1.84853	2.98801	3.53069
H	-3.40807	2.49921	2.86848
H	0.22324	3.67379	1.53125
H	0.24938	3.09633	-0.14061
H	-0.54423	4.64378	0.23145
H	4.54128	3.62951	-2.24445
H	3.73005	2.28016	-3.09042
H	2.83260	3.22770	-1.90247
H	-6.53022	-1.87604	-1.75380
H	-6.39089	-0.08926	-1.66677
H	-6.21772	-1.06679	-0.18322

Revised structure of 45{3}, i.e. 47{3-rev} (Acetone-*d*₆)



					Conf1	Conf2
Rel energy (kcal/mol):					0.00	2.09
C-nom	iGau	Exp	Calc	diff	1	2
C1-CH2	8	19.70	20.77	1.07	[21.08	21.11]
C2-CH2	3	22.50	22.81	0.31	[23.14	22.85]
C3-CH	4	76.00	76.83	0.83	[77.56	77.53]
C4-C	5	35.20	34.29	-0.91	[34.70	34.68]
C5-CH	6	47.20	47.91	0.71	[48.42	48.46]
C6-CH	9	76.10	76.97	0.87	[77.71	77.50]
C7-CH2	10	36.60	35.25	-1.35	[35.66	35.74]
C8-C	11	46.50	49.27	2.77	[49.77	50.48]
C9-C	12	88.60	90.91	2.31	[91.73	92.28]
C10-C	7	50.60	51.87	1.27	[52.43	51.79]
C11-CH	22	119.80	117.87	-1.93	[118.90	119.14]
C12-C	23	143.70	143.77	0.07	[144.96	146.21]
C13-C	25	207.90	209.84	1.94	[211.65	208.56]
C14-CH	18	57.50	57.95	0.45	[58.53	58.81]
C15-C	19	168.40	168.89	0.49	[170.36	168.65]
C19-C	32	166.80	165.45	-1.35	[166.87	166.06]
C20-CH3	26	29.00	29.25	0.25	[29.63	29.41]
C21-CH3	24	20.90	21.28	0.38	[21.57	22.50]
C22-CH3	17	25.80	25.04	-0.76	[25.37	25.81]
C23-C	2	176.80	176.25	-0.55	[177.73	177.35]
C24-CH3	13	22.40	21.74	-0.66	[22.06	21.96]
C25-CH3	14	26.50	25.46	-1.04	[25.80	25.84]
C26-C	30	170.30	168.16	-2.14	[169.57	169.58]
C27-CH3	31	20.80	20.44	-0.36	[20.74	20.81]
C28-CH3	35	52.70	53.40	0.70	[53.95	54.07]
13C chem shifts: CRMSD=1.23ppm (CMAE=1.02) N=25 {-2.14 2.77}						
Fractions:					0.972	0.028

NOTICE:

HMBC C9-H14 is not observed, but J(6-14)=4.5Hz for the orig. str., while it is = 0.8Hz for the revised epiE (i.e. epi-14)

Conformer 1

Energy: -1648.96747 Hartree (Rel: 0.0 kcal/mol)

XYZ coordinates for conf 1:

O	0.35147	-2.41667	1.90609
C	0.67377	-1.15862	2.28931
C	3.28578	0.46364	1.17479
C	3.59300	-0.41638	-0.03816
C	2.75884	-1.71870	-0.06656
C	1.23910	-1.34779	-0.00855
C	0.82954	-0.28101	1.03907
C	1.81167	0.88703	1.22588
C	0.29898	-2.47369	0.44005
C	-1.12661	-2.21403	-0.03206
C	-1.73616	-0.87579	0.49974
C	-0.62390	0.25871	0.68553
C	3.24581	-2.61737	1.09632
C	3.02151	-2.48191	-1.38200
H	0.96448	-1.00227	-1.00708
O	0.78536	-0.84489	3.45325
C	-2.58167	-1.14622	1.75726

C	-2.60459	-0.18948	-0.60030
C	-1.58346	0.56315	-1.43321
O	-0.51591	0.85984	-0.63597
O	-1.63268	0.91926	-2.58157
C	-1.02985	1.29829	1.70616
C	-1.43881	2.56185	1.53246
C	-1.78432	3.44581	2.71291
C	-1.67073	3.24297	0.20064
C	-0.58922	4.16335	-0.31552
O	-2.73532	3.09431	-0.38311
O	3.27991	0.33168	-1.25014
O	5.35891	1.23093	-1.30029
C	4.24785	1.11162	-1.77957
C	3.76182	1.79280	-3.03581
C	-3.50725	-1.10204	-1.40906
O	-3.15718	-1.77105	-2.36068
O	-4.75330	-1.09357	-0.91128
C	-5.70474	-1.95520	-1.57340
H	3.56561	-0.07603	2.08567
H	3.91962	1.35559	1.13859
H	4.65764	-0.66207	-0.06814
H	1.62647	1.61579	0.43199
H	1.60534	1.38554	2.17724
H	0.62331	-3.47790	0.16495
H	-1.11108	-2.23305	-1.12620
H	-1.77544	-3.03995	0.27752
H	2.74046	-3.58761	1.07958
H	4.31907	-2.80755	0.98193
H	3.09426	-2.18483	2.08804
H	2.74607	-1.88474	-2.25537
H	4.08274	-2.74358	-1.46729
H	2.44882	-3.41585	-1.41179
H	-3.38763	-1.84190	1.50241
H	-1.99408	-1.60420	2.55684
H	-3.03990	-0.23047	2.14000
H	-3.22371	0.58051	-0.12499
H	-0.93866	0.94581	2.73108
H	-1.63285	2.91654	3.65772
H	-1.17105	4.35537	2.72576
H	-2.83203	3.76723	2.65799
H	-0.23532	4.83983	0.47020
H	0.26934	3.55931	-0.63196
H	-0.96111	4.73907	-1.16615
H	4.53191	2.46879	-3.40896
H	3.52967	1.04290	-3.79957
H	2.84154	2.34950	-2.83348
H	-5.81855	-1.65711	-2.61797
H	-5.37297	-2.99460	-1.52297
H	-6.64014	-1.82276	-1.03163

Conformer 2

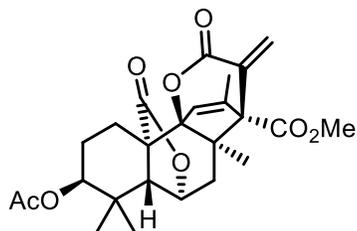
Energy: -1648.97080 Hartree (Rel: 2.1 kcal/mol)

XYZ coordinates for conf 2:

O	0.16438	-2.50441	1.83920
C	0.55279	-1.27311	2.24910
C	3.26289	0.21198	1.14660
C	3.49579	-0.64372	-0.09910
C	2.59309	-1.89862	-0.14430
C	1.09899	-1.44261	-0.05760
C	0.76309	-0.37761	1.01910
C	1.81719	0.71889	1.24430
C	0.09698	-2.52091	0.37370
C	-1.31512	-2.16140	-0.07520
C	-1.83831	-0.80870	0.50950
C	-0.65701	0.25579	0.67990
C	3.04108	-2.85072	0.99070
C	2.79618	-2.64382	-1.48040
H	0.83569	-1.05761	-1.04420
O	0.67639	-0.99111	3.41750
C	-2.66941	-1.06920	1.77940
C	-2.70021	-0.05190	-0.54700

C	-1.66601	0.67790	-1.38620
O	-0.53770	0.84259	-0.64850
O	-1.76220	1.11250	-2.49670
C	-0.99340	1.33130	1.68780
C	-1.03870	2.66370	1.54440
C	-1.37810	3.55590	2.72230
C	-0.68410	3.45569	0.29810
C	-1.81669	4.08780	-0.48430
O	0.48540	3.65899	0.01310
O	3.18899	0.15608	-1.27910
O	5.29619	0.98608	-1.33900
C	4.16850	0.93268	-1.79060
C	3.66610	1.71498	-2.97980
C	-3.65941	-0.89770	-1.36610
O	-3.35941	-1.53590	-2.35180
O	-4.88831	-0.86669	-0.83110
C	-5.88821	-1.67019	-1.49590
H	3.53179	-0.37312	2.03260
H	3.94590	1.06738	1.12510
H	4.54519	-0.94302	-0.16540
H	1.65960	1.51069	0.50870
H	1.65510	1.16809	2.22840
H	0.35628	-3.53561	0.06930
H	-1.30991	-2.14250	-1.16940
H	-2.01002	-2.95710	0.21260
H	2.48578	-3.79271	0.95190
H	4.10248	-3.09312	0.86380
H	2.91738	-2.43742	1.99440
H	2.54719	-2.01042	-2.33610
H	3.83928	-2.96492	-1.58460
H	2.16928	-3.54171	-1.52540
H	-3.49901	-1.73780	1.52850
H	-2.08561	-1.55330	2.56570
H	-3.09951	-0.14740	2.17990
H	-3.28511	0.71500	-0.02540
H	-1.17691	0.94010	2.68520
H	-1.55810	2.96390	3.62390
H	-0.55699	4.25509	2.92490
H	-2.27190	4.16030	2.52530
H	-2.41000	3.31860	-0.99150
H	-2.49809	4.62860	0.18170
H	-1.40869	4.77230	-1.23140
H	4.48410	2.29118	-3.41360
H	3.24669	1.03778	-3.73050
H	2.86480	2.39198	-2.66480
H	-6.02261	-1.32759	-2.52410
H	-5.59012	-2.72089	-1.49500
H	-6.80181	-1.52829	-0.92040

Originally assigned (incorrect) structure of 46{2} (Acetone-*d*₆)



Rel energy (kcal/mol):					Conf1	Conf2	Conf3	Conf4
					0.00	0.89	0.91	1.19
C-nom	iGau	Exp	Calc	diff	1	2	3	4
C1-CH2	10	18.40	18.23	-0.17	[19.58	19.58	19.54	0.00]
C2-CH2	5	22.60	20.91	-1.69	[22.37	22.21	22.19	0.00]
C3-CH	6	75.90	75.65	-0.25	[78.22	78.38	78.41	0.00]
C4-C	7	35.10	33.12	-1.98	[34.80	34.78	34.81	0.00]
C5-CH	8	47.80	50.63	2.83	[52.65	52.81	52.85	0.00]
C6-CH	11	76.90	76.32	-0.58	[78.98	78.95	78.89	0.00]
C7-CH2	12	36.90	35.09	-1.81	[36.91	36.60	36.56	0.00]
C8-C	13	49.50	49.81	0.31	[51.68	52.21	52.32	0.00]
C9-C	14	85.50	96.78	11.28	[100.04	99.42	99.59	0.00]
C10-C	9	48.10	49.73	1.63	[51.78	51.78	51.76	0.00]
C11-CH	16	124.60	125.29	0.69	[128.75	129.29	130.02	0.00]
C12-C	1	139.20	148.53	9.33	[153.06	152.44	151.82	0.00]
C13-C	23	139.60	131.21	-8.39	[134.86	135.43	135.67	0.00]
C14-C	15	69.40	70.58	1.18	[72.70	74.16	73.82	0.00]
C17-C	24	169.10	156.62	-12.48	[161.02	161.06	161.19	0.00]
C19-C	31	166.90	166.15	-0.75	[170.78	170.64	171.01	0.00]
C20-CH2	25	119.00	125.19	6.19	[128.83	128.72	129.56	0.00]
C21-CH3	2	18.50	14.30	-4.20	[15.32	16.33	15.88	0.00]
C22-CH3	21	22.70	31.70	9.00	[32.98	35.52	32.81	0.00]
C23-C	4	176.50	173.69	-2.81	[178.46	178.63	178.57	0.00]
C24-CH3	17	22.70	20.46	-2.24	[21.90	21.77	21.73	0.00]
C25-CH3	18	26.60	24.81	-1.79	[26.31	26.29	26.28	0.00]
C26-C	29	170.40	164.78	-5.62	[169.40	169.38	169.38	0.00]
C27-CH3	30	20.90	19.49	-1.41	[20.87	20.87	20.87	0.00]
C28-CH3	34	52.60	51.53	-1.07	[53.58	53.78	53.67	0.00]

13C chem shifts: CRMSD=5.11ppm (CMAE=3.59) N=25 {-12.48 11.28}
 Fractions: 0.636 0.141 0.138 0.086

Conformer 1

Energy: -1572.49338 Hartree (Rel: 0.0 kcal/mol)

XYZ coordinates for conf 1:

C	-2.46624	0.79890	1.71135
C	-3.46805	1.46638	2.60176
O	0.24195	-2.78269	-0.24625
C	0.61897	-2.26083	0.94988
C	3.34303	-0.58944	1.50382
C	3.72100	-0.36855	0.03593
C	2.85053	-1.18410	-0.95353
C	1.35881	-0.77893	-0.71598
C	0.88768	-0.75895	0.77890
C	1.88687	-0.19723	1.79849
C	0.28645	-1.72706	-1.27064
C	-1.09928	-1.04233	-1.40540
C	-1.62332	-0.64047	-0.00617
C	-0.46896	0.03514	0.79000
C	-2.69947	0.49931	0.19764
C	-1.19590	0.49655	2.03020
C	3.17681	-2.68472	-0.76556
C	3.22683	-0.81350	-2.40451
H	1.25016	0.21129	-1.14862
O	0.73601	-2.94147	1.94393
C	-2.21326	-1.90255	0.72745
O	-0.03747	1.30418	0.11811
C	-2.32451	1.77888	-0.54087

C	-0.88456	2.17195	-0.46772
C	-3.17071	2.59907	-1.17621
O	-0.43198	3.20585	-0.92349
O	3.52373	1.03873	-0.29019
O	5.59011	1.59052	0.45567
C	4.52318	1.90701	-0.03535
C	4.14693	3.30343	-0.47220
C	-4.11508	0.06884	-0.18890
O	-5.11754	0.23395	0.47668
O	-4.11910	-0.50609	-1.40215
C	-5.40405	-0.94248	-1.89597
H	-3.85436	2.38224	2.13797
H	-4.33199	0.82132	2.78521
H	-3.00841	1.73008	3.55910
H	3.51824	-1.63994	1.75834
H	4.01642	-0.00209	2.13621
H	4.77770	-0.60221	-0.12110
H	1.80239	0.89302	1.79150
H	1.60816	-0.54147	2.80048
H	0.56000	-2.22593	-2.20136
H	-1.80699	-1.71405	-1.89606
H	-0.97554	-0.17767	-2.06698
H	-0.72099	0.69532	2.98431
H	2.62600	-3.29493	-1.48781
H	4.24564	-2.84780	-0.94651
H	2.95122	-3.07073	0.23071
H	3.06666	0.24931	-2.60441
H	4.28187	-1.04237	-2.59648
H	2.62989	-1.39037	-3.12008
H	-2.28021	-2.74932	0.04347
H	-1.63038	-2.21907	1.59141
H	-3.21675	-1.70401	1.11173
H	-2.80011	3.51208	-1.62968
H	-4.23313	2.39527	-1.26040
H	4.67226	4.03511	0.14472
H	4.45967	3.44570	-1.51358
H	3.06698	3.45868	-0.41798
H	-5.20396	-1.37957	-2.87319
H	-5.83505	-1.68581	-1.22177
H	-6.08340	-0.09193	-1.98601

Conformer 2

Energy: -1572.49149 Hartree (Rel: 0.9 kcal/mol)

XYZ coordinates for conf 2:

C	-2.52344	0.57600	1.56002
C	-3.58187	1.15719	2.44632
O	0.40613	-2.80631	-0.44375
C	0.71425	-2.33493	0.79199
C	3.34448	-0.58567	1.54878
C	3.76772	-0.26793	0.11141
C	2.97777	-1.07008	-0.95364
C	1.46165	-0.73963	-0.76120
C	0.92880	-0.81680	0.71167
C	1.86124	-0.27488	1.80308
C	0.45315	-1.69772	-1.41070
C	-0.95020	-1.05769	-1.57230
C	-1.54578	-0.74133	-0.18040
C	-0.45511	-0.07087	0.70242
C	-2.67042	0.34664	0.01901
C	-1.25948	0.29834	1.92568
C	3.36049	-2.56336	-0.82548
C	3.39743	-0.61111	-2.36702
H	1.32962	0.26682	-1.14687
O	0.82143	-3.06298	1.75321
C	-2.11836	-2.05508	0.47217
O	-0.03637	1.24817	0.12641
C	-2.30007	1.67456	-0.63688
C	-0.88401	2.11772	-0.45333
C	-3.12682	2.48576	-1.30853
O	-0.45043	3.19501	-0.81859
O	3.50909	1.14273	-0.15118

O	5.49679	1.76607	0.73802
C	4.44077	2.04943	0.20488
C	4.00568	3.44457	-0.17855
C	-4.00751	-0.13667	-0.54917
O	-4.09206	-0.83489	-1.54019
O	-5.06984	0.33068	0.11929
C	-6.36538	-0.05861	-0.39162
H	-3.98918	2.08140	2.02015
H	-4.42539	0.47056	2.57030
H	-3.16513	1.38263	3.43261
H	3.55861	-1.63968	1.75391
H	3.96449	-0.00430	2.23850
H	4.84047	-0.44016	-0.01401
H	1.72809	0.80915	1.85557
H	1.55842	-0.69005	2.77066
H	0.78663	-2.13737	-2.35170
H	-1.61562	-1.72654	-2.12185
H	-0.83086	-0.15751	-2.18604
H	-0.84084	0.46016	2.91265
H	2.86854	-3.15694	-1.60209
H	4.44226	-2.67336	-0.96520
H	3.10809	-3.00949	0.13873
H	3.20223	0.45353	-2.52068
H	4.46791	-0.78882	-2.52465
H	2.85437	-1.17321	-3.13533
H	-2.16752	-2.85916	-0.26284
H	-1.53596	-2.41210	1.32026
H	-3.12751	-1.89734	0.85929
H	-2.75529	3.42511	-1.70366
H	-4.17133	2.25080	-1.48010
H	4.44956	4.16913	0.50699
H	4.36808	3.66362	-1.19012
H	2.91684	3.53334	-0.18120
H	-7.08899	0.40911	0.27428
H	-6.49242	0.30131	-1.41478
H	-6.46610	-1.14566	-0.37010

Conformer 3

Energy: -1572.49194 Hartree (Rel: 0.9 kcal/mol)

XYZ coordinates for conf 3:

C	-2.52018	0.66869	1.53306
C	-3.55816	1.31235	2.40189
O	0.33704	-2.79105	-0.45194
C	0.64765	-2.32855	0.78675
C	3.31712	-0.64277	1.56104
C	3.75614	-0.33443	0.12629
C	2.95365	-1.11765	-0.94359
C	1.44484	-0.75058	-0.76016
C	0.90135	-0.81633	0.70946
C	1.83995	-0.29809	1.80703
C	0.41741	-1.68315	-1.41722
C	-0.96852	-1.00698	-1.58677
C	-1.56295	-0.68153	-0.19729
C	-0.46405	-0.03709	0.69257
C	-2.66509	0.43513	-0.00526
C	-1.26708	0.35680	1.90935
C	3.29933	-2.61973	-0.81278
C	3.39330	-0.66918	-2.35429
H	1.33967	0.25923	-1.14531
O	0.72752	-3.05975	1.74814
C	-2.17505	-1.98327	0.44350
O	-0.01129	1.27165	0.11892
C	-2.25867	1.74975	-0.66140
C	-0.83751	2.16496	-0.45813
C	-3.06170	2.57503	-1.34441
O	-0.37792	3.23590	-0.81004
O	3.53240	1.08179	-0.13799
O	5.52387	1.66029	0.77256
C	4.47997	1.96744	0.22884
C	4.07922	3.37211	-0.15740
C	-3.99902	-0.03921	-0.58661

O	-4.10173	-0.43759	-1.73071
O	-5.02604	0.02878	0.26846
C	-6.30722	-0.40564	-0.24216
H	-3.95823	2.21702	1.92822
H	-4.40761	0.64582	2.57723
H	-3.12432	1.59095	3.36697
H	3.50599	-1.70148	1.76685
H	3.94630	-0.07606	2.25460
H	4.82526	-0.53189	0.00712
H	1.73172	0.78867	1.86020
H	1.52171	-0.70723	2.77224
H	0.74550	-2.12973	-2.35676
H	-1.64564	-1.65760	-2.14492
H	-0.82299	-0.10787	-2.19586
H	-0.84725	0.52200	2.89528
H	2.79894	-3.20147	-1.59296
H	4.37912	-2.75588	-0.94453
H	3.02926	-3.05950	0.14959
H	3.22356	0.39956	-2.50972
H	4.46054	-0.87132	-2.50427
H	2.84315	-1.21918	-3.12629
H	-2.22451	-2.78689	-0.29248
H	-1.61695	-2.35394	1.30212
H	-3.18740	-1.80450	0.81298
H	-2.67188	3.51158	-1.72859
H	-4.10285	2.34714	-1.54567
H	4.53832	4.08683	0.52840
H	4.44887	3.58113	-1.16847
H	2.99272	3.48670	-0.16306
H	-7.00445	-0.27631	0.58423
H	-6.60041	0.20910	-1.09575
H	-6.25551	-1.45355	-0.54463

Conformer 4

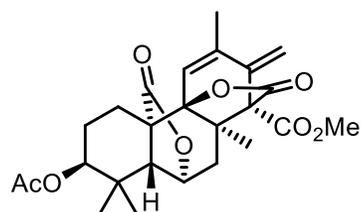
Energy: -1572.49196 Hartree (Rel: 1.2 kcal/mol)

XYZ coordinates for conf 4:

C	-2.60535	0.55018	1.55630
C	-3.67671	1.10397	2.44567
O	0.35695	-2.72597	-0.56461
C	0.63110	-2.33313	0.70848
C	3.24121	-0.72836	1.65740
C	3.75164	-0.34864	0.26455
C	2.95917	-1.01578	-0.89072
C	1.44425	-0.65869	-0.72277
C	0.86102	-0.81446	0.72382
C	1.76808	-0.34871	1.86827
C	0.44234	-1.56135	-1.46025
C	-0.95264	-0.90380	-1.62226
C	-1.58676	-0.67401	-0.23053
C	-0.51791	-0.05861	0.71604
C	-2.71675	0.40275	0.00356
C	-1.35075	0.24929	1.93670
C	3.29669	-2.52672	-0.88280
C	3.43715	-0.45022	-2.24534
H	1.34237	0.37234	-1.05039
O	0.70373	-3.12848	1.63944
C	-2.18545	-2.02156	0.32201
O	-0.08306	1.28692	0.21737
C	-2.33180	1.76208	-0.56817
C	-0.91976	2.19134	-0.33080
C	-3.14743	2.60969	-1.20719
O	-0.47708	3.28899	-0.63024
O	3.63050	1.09865	0.13630
O	5.88616	1.39135	0.18199
C	4.75686	1.84702	0.11223
C	4.41741	3.31428	0.00320
C	-4.03236	-0.05649	-0.63126
O	-4.08537	-0.54389	-1.75220
O	-5.10914	0.15761	0.13690
C	-6.38164	-0.23244	-0.42838
H	-4.08593	2.03459	2.03501

H	-4.51589	0.40914	2.54722
H	-3.27088	1.31259	3.44018
H	3.38365	-1.80403	1.80542
H	3.85969	-0.22781	2.41078
H	4.81022	-0.59891	0.16778
H	1.68602	0.73895	1.94725
H	1.40787	-0.77679	2.81031
H	0.79923	-1.94623	-2.41650
H	-1.60213	-1.53392	-2.23357
H	-0.81334	0.03286	-2.17359
H	-0.95361	0.36398	2.93907
H	2.79952	-3.04306	-1.70940
H	4.37677	-2.65443	-1.01950
H	3.02102	-3.04112	0.04025
H	3.25446	0.62542	-2.32184
H	4.51117	-0.62563	-2.37822
H	2.91782	-0.94170	-3.07597
H	-2.21222	-2.77993	-0.46140
H	-1.63486	-2.43361	1.16620
H	-3.20652	-1.88092	0.68489
H	-2.77388	3.57293	-1.53767
H	-4.18569	2.37795	-1.41957
H	5.32934	3.89260	-0.14951
H	3.71888	3.48621	-0.82102
H	3.92562	3.64673	0.92402
H	-7.12062	0.00919	0.33404
H	-6.57478	0.32809	-1.34551
H	-6.38439	-1.30270	-0.64481

Revised structure of 46{2}, i.e. 48{2-rev} (Acetone-*d*₆)



					Conf1	Conf2
Rel energy (kcal/mol):					0.00	0.30
C-nom	iGau	Exp	Calc	diff	1	2
C1-CH2	8	18.40	19.76	1.36	[20.02	20.03]
C2-CH2	3	22.60	22.69	0.09	[22.97	22.98]
C3-CH	4	75.90	77.00	1.10	[77.51	77.52]
C4-C	5	35.10	34.24	-0.86	[34.58	34.56]
C5-CH	6	47.80	48.86	1.06	[49.30	49.18]
C6-CH	9	76.90	77.71	0.81	[78.22	78.23]
C7-CH2	10	36.90	34.46	-2.44	[34.79	34.80]
C8-C	11	49.50	52.51	3.01	[53.06	52.68]
C9-C	12	85.50	88.79	3.29	[89.45	89.20]
C10-C	7	48.10	49.15	1.05	[49.54	49.55]
C11-CH	22	124.60	123.16	-1.44	[123.81	123.96]
C12-C**	23	139.60	140.16	0.56	[140.97	140.91]
C13-C**	25	139.20	136.78	-2.42	[137.61	137.44]
C14-C	18	69.40	70.92	1.52	[71.28	71.61]
C17-C	19	169.10	169.44	0.34	[170.38	170.31]
C19-C	32	166.90	165.71	-1.19	[166.66	166.51]
C20-CH2	26	119.00	121.54	2.54	[122.16	122.38]
C21-CH3	24	18.50	18.55	0.05	[18.86	18.74]
C22-CH3	17	22.70	20.57	-2.13	[20.50	21.39]
C23-C	2	176.50	176.23	-0.27	[177.12	177.24]
C24-CH3	13	22.70	21.87	-0.83	[22.13	22.18]
C25-CH3	14	26.60	25.60	-1.00	[25.87	25.92]
C26-C	30	170.40	168.69	-1.71	[169.59	169.60]
C27-CH3	31	20.90	20.50	-0.40	[20.77	20.76]
C28-CH3	35	52.60	53.55	0.95	[53.95	53.97]
13C chem shifts: CRMSD=1.57ppm (CMAE=1.30) N=25 {-2.44 3.29}						
Fractions:					0.623	0.377

Conformer 1

Energy: -1572.51863 Hartree (Rel: 0.0 kcal/mol)

XYZ coordinates for conf 1:

O	-0.41879	1.52972	-2.39378
C	-0.72342	2.13826	-1.21827
C	-3.35354	1.37413	0.58074
C	-3.69582	0.04751	-0.09886
C	-2.87010	-0.20687	-1.38250
C	-1.35108	-0.13986	-1.01722
C	-0.90428	1.06412	-0.13831
C	-1.87481	1.46568	0.98450
C	-0.38793	0.07531	-2.19185
C	1.03393	-0.38312	-1.83423
C	1.63874	0.45175	-0.66442
C	0.53095	0.74555	0.41532
C	-3.32721	0.81364	-2.45269
C	-3.17533	-1.61766	-1.92950
H	-1.11619	-1.07087	-0.50182
O	-0.80702	3.33973	-1.11226
C	2.38583	1.66376	-1.26183
C	2.58878	-0.38676	0.28156
C	1.57541	-1.23219	1.07473
O	0.39762	-0.56595	1.09863
O	1.73713	-2.27400	1.66059
C	1.06892	1.70974	1.44412
C	2.33121	1.58631	1.90081
C	2.86165	2.51432	2.96429

C	3.22312	0.53612	1.34770
C	4.47381	0.35704	1.80246
H	4.88204	0.98688	2.58493
O	-3.41102	-1.04061	0.82914
O	-5.48582	-0.89310	1.72732
C	-4.38856	-1.41513	1.68321
C	-3.93282	-2.56274	2.55140
C	3.59910	-1.18980	-0.53702
O	4.63906	-0.73310	-0.97016
O	3.16667	-2.42834	-0.80361
C	4.01973	-3.22810	-1.65233
H	-3.61854	2.19519	-0.09374
H	-3.98103	1.49204	1.47003
H	-4.76247	0.00916	-0.33475
H	-1.69487	0.80946	1.84156
H	-1.66036	2.48937	1.30571
H	-0.71169	-0.36620	-3.13502
H	0.97450	-1.44896	-1.59281
H	1.68634	-0.29747	-2.70924
H	-2.81944	0.63457	-3.40511
H	-4.40262	0.69680	-2.62915
H	-3.15224	1.85641	-2.17789
H	-2.91766	-2.39481	-1.20496
H	-4.24110	-1.71283	-2.16848
H	-2.61344	-1.80887	-2.85080
H	3.28639	1.29628	-1.76352
H	1.78170	2.17758	-2.00940
H	2.69313	2.38746	-0.50746
H	5.13320	-0.40448	1.40594
H	0.42130	2.48415	1.83766
H	2.09936	3.24229	3.25406
H	3.16328	1.96181	3.86235
H	3.74288	3.06361	2.61163
H	-4.70721	-2.80198	3.28099
H	-3.73016	-3.44141	1.92962
H	-3.00199	-2.30331	3.06512
H	4.13565	-2.75134	-2.62805
H	4.99934	-3.35497	-1.18692
H	3.51161	-4.18639	-1.74831

Conformer 2

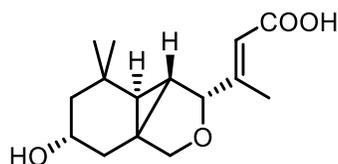
Energy: -1572.51911 Hartree (Rel: 0.3 kcal/mol)

XYZ coordinates for conf 2:

O	0.38707	-2.76299	0.53397
C	0.69744	-1.88635	1.52377
C	3.37878	-0.01127	1.49885
C	3.74753	-0.18912	0.02520
C	2.90338	-1.27393	-0.68529
C	1.39041	-0.91244	-0.52367
C	0.92681	-0.50236	0.90424
C	1.90683	0.37958	1.69485
C	0.39910	-2.05990	-0.75592
C	-1.00429	-1.52872	-1.08307
C	-1.60913	-0.70699	0.09637
C	-0.48766	0.16915	0.77244
C	3.31018	-2.64942	-0.10351
C	3.23800	-1.29365	-2.19214
H	1.19264	-0.09560	-1.21727
O	0.75097	-2.21329	2.68666
C	-2.39815	-1.66589	1.01386
C	-2.50929	0.49984	-0.38453
C	-1.44721	1.49414	-0.88965
O	-0.29902	1.26329	-0.21231
O	-1.55508	2.38965	-1.68960
C	-1.03635	0.80653	2.02528
C	-2.28128	1.32354	2.03635
C	-2.82404	2.00549	3.26681
C	-3.14003	1.22149	0.82873
C	-4.34632	1.80861	0.76755
H	-4.74834	2.35807	1.61139
O	3.51741	1.07208	-0.66951

O	5.60585	1.79310	-0.16791
C	4.52506	1.97162	-0.69568
C	4.12591	3.20343	-1.47137
C	-3.45294	0.07218	-1.50818
O	-3.17545	0.15271	-2.68767
O	-4.57690	-0.49571	-1.04783
C	-5.47635	-1.01769	-2.05181
H	3.60347	-0.93990	2.03415
H	4.02114	0.75940	1.93695
H	4.80953	-0.42937	-0.07101
H	1.76483	1.41699	1.37677
H	1.66747	0.32876	2.76127
H	0.71685	-2.79499	-1.49610
H	-0.92032	-0.93307	-1.99788
H	-1.67263	-2.36320	-1.31792
H	2.79019	-3.46131	-0.62072
H	4.38502	-2.80245	-0.25363
H	3.11041	-2.75910	0.96490
H	3.01771	-0.33341	-2.66613
H	4.30091	-1.51467	-2.34532
H	2.66280	-2.07029	-2.70896
H	-3.26263	-2.04119	0.45863
H	-1.79913	-2.52934	1.30285
H	-2.76531	-1.18165	1.91817
H	-4.97545	1.75737	-0.11247
H	-0.41162	0.87081	2.90840
H	-2.09376	1.96992	4.07942
H	-3.06067	3.05804	3.06916
H	-3.74724	1.52636	3.61419
H	4.92367	3.94514	-1.41934
H	3.93806	2.93909	-2.51756
H	3.19876	3.62207	-1.06791
H	-5.80962	-0.21477	-2.71261
H	-4.97803	-1.79258	-2.63819
H	-6.31573	-1.43334	-1.49638

Originally assigned (incorrect) structure of 49{1} (CD₃OD)



					Conf1	Conf2	Conf3	Conf4	Conf5	Conf6	Conf7
Rel energy (kcal/mol):					0.00	0.23	0.44	1.59	1.89	1.97	2.35
C-nom	iGau	Exp	Calc	diff	1	2	3	4	5	6	7
C1-C	6	33.90	29.28	-4.62	[29.77	30.14	27.09	29.96	30.14	27.41	27.51]
C2-CH2	1	27.40	44.23	16.83	[45.17	45.54	40.56	45.22	45.55	40.42	40.76]
C3-CH	2	74.20	66.12	-8.08	[66.02	65.93	66.60	66.02	65.92	66.59	66.56]
C4-CH2	3	21.80	33.10	11.30	[34.07	34.16	29.75	33.96	34.18	29.63	29.83]
C5-C	4	30.70	31.03	0.33	[32.07	32.25	27.50	30.88	32.31	26.41	27.58]
C6-CH	5	30.80	28.13	-2.67	[27.13	28.90	28.89	27.98	28.92	29.86	30.54]
C7-CH	10	37.50	28.49	-9.01	[28.57	26.45	30.57	31.51	26.58	33.57	28.57]
C8-CH	9	87.60	85.16	-2.44	[84.48	86.27	84.37	87.27	86.78	87.18	86.85]
C9-C	16	159.10	153.66	-5.44	[152.01	156.92	152.32	155.04	152.63	155.35	152.65]
C10-CH	17	115.70	118.17	2.47	[117.74	118.51	117.57	121.42	120.90	121.26	120.76]
C11-C	19	170.50	169.54	-0.96	[169.33	169.98	169.42	169.14	169.66	169.14	169.69]
C12-CH3	18	15.70	17.70	2.00	[18.53	16.17	18.56	15.49	18.16	15.60	18.30]
C13-CH2	7	75.40	74.78	-0.62	[74.89	74.23	75.20	75.38	74.28	75.67	74.65]
C14-CH3	12	23.70	29.15	5.45	[28.29	28.56	31.66	28.37	28.53	31.63	32.30]
C15-CH3	11	27.30	33.87	6.57	[34.37	34.54	31.90	34.59	34.53	31.99	32.15]
13C chem shifts: RMSD=6.86ppm (MAE=5.25) N=15 {-9.01 16.83}											
Fractions:					0.432	0.291	0.205	0.030	0.018	0.016	0.008

Conformer 1

Energy: -885.68908 Hartree (Rel: 0.0 kcal/mol)

XYZ coordinates for conf 1:

C	-3.18671	1.10775	-0.33593
C	-3.50131	-0.12600	0.50555
C	-2.82874	-1.36369	-0.10062
C	-1.34687	-1.15322	-0.33487
C	-0.78088	0.24793	-0.47882
C	-1.68420	1.49882	-0.36307
C	-0.55648	-2.24979	-1.03293
O	0.81874	-2.03080	-0.69572
C	0.88901	-1.40790	0.58691
C	-0.41247	-0.60716	0.71654
C	-1.44151	2.37573	-1.60940
C	-1.32425	2.32872	0.88779
O	-4.92459	-0.26844	0.52700
H	0.01867	0.35570	-1.21179
H	-0.75652	-0.35261	1.71374
C	2.14805	-0.57649	0.73769
C	2.97223	-0.41847	-0.31817
C	2.31500	0.00850	2.11674
C	4.22484	0.34522	-0.42617
O	4.93575	0.31316	-1.42061
O	4.55016	1.11375	0.64327
H	-3.77912	1.95513	0.03113
H	-3.52939	0.89998	-1.35925
H	-3.13746	0.02115	1.53486
H	-2.99030	-2.23977	0.54455
H	-3.32831	-1.57319	-1.05732
H	-0.62783	-2.23265	-2.12606
H	-0.88950	-3.23742	-0.67571
H	0.89845	-2.17830	1.37831
H	-1.62634	1.81042	-2.53071
H	-2.10719	3.24728	-1.60794
H	-0.40756	2.74065	-1.63767
H	-1.55598	1.80063	1.81918
H	-0.25495	2.57102	0.89921
H	-1.88466	3.27160	0.89484

H	-5.12995	-1.06024	1.05059
H	2.71827	-0.92428	-1.24216
H	1.75827	0.95186	2.19658
H	1.90204	-0.67034	2.87148
H	3.35632	0.21859	2.35517
H	5.39831	1.54367	0.41996

Conformer 2

Energy: -885.68981 Hartree (Rel: 0.2 kcal/mol)

XYZ coordinates for conf 2:

C	3.08936	1.16134	0.27531
C	3.30749	0.15963	-0.85483
C	2.83675	-1.23321	-0.42009
C	1.42064	-1.21939	0.11727
C	0.80887	0.06181	0.65064
C	1.59964	1.39287	0.64696
C	0.85242	-2.50397	0.70291
O	-0.56987	-2.35051	0.68913
C	-0.91710	-1.52562	-0.43971
C	0.26332	-0.57850	-0.61353
C	1.55047	1.97521	2.07533
C	0.96470	2.42135	-0.31308
O	4.70610	0.16342	-1.15575
H	0.16294	-0.05795	1.51997
H	0.40161	-0.10669	-1.58140
C	-2.30613	-0.95898	-0.19900
C	-2.54223	0.34429	-0.45082
C	-3.32465	-1.96647	0.25659
C	-3.83450	1.04453	-0.33573
O	-4.91828	0.59778	0.00887
O	-3.68886	2.35204	-0.67767
H	3.55184	2.11836	0.00356
H	3.63177	0.78460	1.15377
H	2.74493	0.47523	-1.74778
H	2.91787	-1.94224	-1.25720
H	3.52550	-1.58164	0.36283
H	1.14693	-2.69752	1.74032
H	1.15780	-3.36390	0.08432
H	-0.98409	-2.16052	-1.34352
H	1.94183	1.25799	2.80672
H	2.15148	2.89000	2.14377
H	0.52180	2.22474	2.36260
H	1.01921	2.10425	-1.36031
H	-0.09100	2.58509	-0.06747
H	1.48059	3.38604	-0.23336
H	4.85389	-0.48698	-1.86172
H	-1.72416	0.97682	-0.77559
H	-3.32812	-2.82687	-0.42565
H	-3.03745	-2.35562	1.24028
H	-4.32417	-1.54006	0.31053
H	-4.56802	2.76556	-0.58074

Conformer 3

Energy: -885.69212 Hartree (Rel: 0.4 kcal/mol)

XYZ coordinates for conf 3:

C	-3.02180	1.09143	0.73263
C	-3.73974	-0.20448	0.32639
C	-2.82571	-1.43218	0.43297
C	-1.38547	-1.18602	-0.00024
C	-0.85069	0.21121	-0.25232
C	-1.74496	1.44507	-0.07594
C	-0.64734	-2.30159	-0.72622
O	0.75085	-2.05368	-0.53784
C	0.93877	-1.37959	0.70704
C	-0.35305	-0.58525	0.92831
C	-2.10743	1.98310	-1.47904
C	-0.97167	2.54847	0.67547
O	-4.23866	-0.17429	-1.01891
H	-0.13887	0.30672	-1.07346
H	-0.61416	-0.29858	1.94330
C	2.19710	-0.53348	0.70088

C	2.91085	-0.40900	-0.43684
C	2.49279	0.10534	2.03369
C	4.13775	0.35918	-0.69747
O	4.74604	0.29542	-1.75646
O	4.56072	1.16911	0.30537
H	-2.76586	0.99680	1.79774
H	-3.72668	1.93266	0.67163
H	-4.58841	-0.35015	1.01272
H	-2.84454	-1.79909	1.46710
H	-3.26991	-2.22255	-0.18424
H	-0.82667	-2.33390	-1.80683
H	-0.92762	-3.27692	-0.29684
H	1.03495	-2.11794	1.52301
H	-2.60602	1.22003	-2.08027
H	-2.77562	2.85023	-1.40051
H	-1.20292	2.30774	-2.00838
H	-0.67880	2.22192	1.67999
H	-0.06026	2.82488	0.13108
H	-1.58575	3.45196	0.78079
H	-4.75097	0.64400	-1.12354
H	2.57231	-0.95132	-1.31167
H	1.93398	1.04556	2.13354
H	2.16621	-0.54818	2.85057
H	3.54972	0.33475	2.15884
H	5.37785	1.59563	-0.01781

Conformer 4

Energy: -885.69283 Hartree (Rel: 1.6 kcal/mol)

XYZ coordinates for conf 4:

C	3.34429	0.96554	-0.20776
C	3.28106	-0.25995	-1.11543
C	2.72786	-1.46247	-0.34101
C	1.41489	-1.14502	0.34400
C	1.04024	0.28610	0.67501
C	1.96082	1.46914	0.28633
C	0.78589	-2.19818	1.24718
O	-0.60550	-1.86515	1.34404
C	-0.99854	-1.24856	0.11118
C	0.24661	-0.49135	-0.35811
C	2.18817	2.32643	1.54910
C	1.30101	2.36020	-0.78769
O	4.61142	-0.50948	-1.57841
H	0.54163	0.42268	1.63273
H	0.29138	-0.21547	-1.40703
C	-2.25504	-0.41422	0.31251
C	-3.19459	-0.50183	-0.65420
C	-2.31199	0.44803	1.54364
C	-4.47074	0.21536	-0.81615
O	-5.26678	-0.05277	-1.70435
O	-4.71474	1.21091	0.06999
H	3.86259	1.77710	-0.73359
H	3.96721	0.69862	0.65744
H	2.63109	-0.05102	-1.97989
H	2.60775	-2.32574	-1.01201
H	3.47974	-1.74283	0.41066
H	1.18530	-2.21576	2.26709
H	0.91405	-3.19819	0.80245
H	-1.21375	-2.02535	-0.63955
H	2.60270	1.72307	2.36561
H	2.88907	3.14442	1.34346
H	1.24709	2.76845	1.89855
H	1.19006	1.84444	-1.74761
H	0.30381	2.68356	-0.46673
H	1.90739	3.25710	-0.96339
H	4.57876	-1.29595	-2.14733
H	-3.03646	-1.20259	-1.46968
H	-1.89056	-0.10002	2.39042
H	-1.69751	1.34729	1.40462
H	-3.32573	0.76798	1.77607
H	-5.59058	1.57474	-0.16407

Conformer 5

Energy: -885.68970 Hartree (Rel: 1.9 kcal/mol)

XYZ coordinates for conf 5:

C	3.10853	1.14621	0.27085
C	3.32091	0.13102	-0.84827
C	2.83223	-1.25199	-0.40215
C	1.41418	-1.21700	0.12906
C	0.81415	0.07623	0.64638
C	1.61956	1.39848	0.63195
C	0.82980	-2.48915	0.72576
O	-0.59055	-2.32031	0.70417
C	-0.92403	-1.50479	-0.43601
C	0.26677	-0.57149	-0.61330
C	1.56945	1.99729	2.05348
C	1.00156	2.42332	-0.34297
O	4.72093	0.11575	-1.14234
H	0.16341	-0.02736	1.51415
H	0.41483	-0.11125	-1.58533
C	-2.31292	-0.92605	-0.20941
C	-2.52077	0.38194	-0.46449
C	-3.32883	-1.94245	0.23469
C	-3.74797	1.19568	-0.39434
O	-3.75868	2.38250	-0.68749
O	-4.87360	0.56640	0.01993
H	3.58335	2.09518	-0.00773
H	3.64184	0.77194	1.15593
H	2.76631	0.44415	-1.74705
H	2.90884	-1.96998	-1.23200
H	3.51362	-1.60063	0.38709
H	1.11790	-2.67496	1.76637
H	1.12844	-3.35879	0.11748
H	-0.99047	-2.14931	-1.33299
H	1.94873	1.28388	2.79492
H	2.18048	2.90590	2.11498
H	0.54219	2.26170	2.33236
H	1.05751	2.09365	-1.38625
H	-0.05329	2.60276	-0.10487
H	1.52871	3.38255	-0.27158
H	4.86435	-0.54225	-1.84215
H	-1.67843	0.98696	-0.78026
H	-3.29427	-2.81423	-0.43163
H	-3.06156	-2.30937	1.23249
H	-4.34179	-1.54831	0.25681
H	-5.58133	1.23954	0.00776

Conformer 6

Energy: -885.69030 Hartree (Rel: 2.0 kcal/mol)

XYZ coordinates for conf 6:

C	2.88838	1.06937	-1.11654
C	3.60954	-0.28378	-1.02068
C	2.62912	-1.45768	-0.89438
C	1.40884	-1.16875	-0.02964
C	1.07169	0.22796	0.45076
C	1.94920	1.42735	0.06661
C	0.84423	-2.29228	0.83137
O	-0.52991	-1.96545	1.07617
C	-1.02157	-1.24619	-0.06278
C	0.18525	-0.45211	-0.56595
C	2.76256	1.84776	1.31214
C	1.06042	2.61747	-0.35001
O	4.50279	-0.36727	0.09965
H	0.67125	0.29391	1.46160
H	0.15661	-0.09389	-1.59186
C	-2.25063	-0.43310	0.31572
C	-3.27319	-0.44385	-0.56704
C	-2.19199	0.32726	1.61208
C	-4.55401	0.28289	-0.55672
O	-5.42946	0.08323	-1.38639
O	-4.70962	1.20830	0.42084
H	2.31167	1.06113	-2.05257
H	3.63206	1.87014	-1.23485

H	4.19154	-0.42258	-1.94502
H	2.30840	-1.76124	-1.89911
H	3.18865	-2.30461	-0.47881
H	1.32888	-2.40011	1.80817
H	0.92327	-3.25112	0.29394
H	-1.30566	-1.95665	-0.85537
H	3.36865	1.02110	1.68854
H	3.43211	2.68383	1.07304
H	2.08990	2.17967	2.11288
H	0.44307	2.37363	-1.22202
H	0.38951	2.90864	0.46789
H	1.67408	3.49101	-0.60454
H	5.07628	0.41608	0.07654
H	-3.19256	-1.07746	-1.44632
H	-1.70103	-0.28716	2.37141
H	-1.58517	1.23416	1.49083
H	-3.17862	0.62794	1.95888
H	-5.60037	1.58915	0.29510

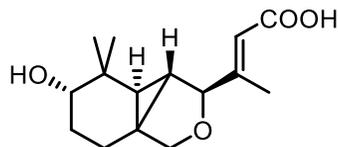
Conformer 7

Energy: -885.69245 Hartree (Rel: 2.4 kcal/mol)

XYZ coordinates for conf 7:

C	2.77662	1.31638	-0.77899
C	3.62851	0.04011	-0.71756
C	2.77961	-1.22741	-0.87402
C	1.43383	-1.17738	-0.16078
C	0.86843	0.11291	0.39820
C	1.64376	1.43192	0.27599
C	0.91896	-2.44810	0.50079
O	-0.49783	-2.29311	0.61758
C	-0.95001	-1.49334	-0.49349
C	0.20600	-0.54790	-0.78907
C	2.21765	1.77836	1.66922
C	0.69458	2.57210	-0.14642
O	4.35446	-0.09440	0.51309
H	0.31756	0.02141	1.33482
H	0.26712	-0.10047	-1.77782
C	-2.32093	-0.93613	-0.13890
C	-2.57040	0.37085	-0.35962
C	-3.27767	-1.97238	0.38427
C	-3.80003	1.16221	-0.17172
O	-3.85955	2.34985	-0.45567
O	-4.87148	0.51089	0.34108
H	2.34293	1.36437	-1.78825
H	3.43104	2.19575	-0.69588
H	4.34939	0.07380	-1.54929
H	2.62684	-1.42030	-1.94352
H	3.37272	-2.06624	-0.48975
H	1.30938	-2.62331	1.50972
H	1.16472	-3.32102	-0.12636
H	-1.09236	-2.14815	-1.37417
H	2.85492	0.97577	2.04626
H	2.81347	2.69894	1.62475
H	1.40399	1.94368	2.38642
H	0.25753	2.38769	-1.13471
H	-0.12671	2.68512	0.57159
H	1.23240	3.52764	-0.19259
H	4.83116	0.73796	0.66447
H	-1.76868	0.99337	-0.74046
H	-3.28677	-2.83963	-0.28876
H	-2.91832	-2.34030	1.35239
H	-4.29124	-1.59608	0.49794
H	-5.58936	1.17092	0.39714

Revised structure of 49{1}, i.e. 50{1-rev} (CD₃OD)



					Conf1	Conf2	Conf3	Conf4	Conf5	Conf6	Conf7
Rel energy (kcal/mol):					0.00	0.63	0.63	0.96	1.57	1.58	2.22
C-nom	iGau	Exp	Calc	diff	1	2	3	4	5	6	7
C1-C	6	33.90	32.97	-0.93	[33.33	32.36	32.36	33.38	33.31	32.43	32.26]
C2-CH*	1	74.20	73.67	-0.53	[74.14	72.93	72.92	74.05	74.23	72.83	73.19]
C3-CH2*	2	27.40	26.88	-0.52	[27.75	25.46	25.46	27.73	27.83	25.47	25.52]
C4-CH2	3	21.80	21.41	-0.39	[23.72	17.59	17.59	24.09	23.41	17.81	17.48]
C5-C	4	30.70	29.65	-1.05	[29.01	30.03	30.03	30.95	28.95	32.03	30.02]
C6-CH**	5	37.50	34.71	-2.79	[37.07	30.56	30.56	38.62	35.35	32.09	28.85]
C7-CH**	10	30.80	29.40	-1.40	[30.07	27.77	27.78	32.75	26.89	30.48	24.56]
C8-CH	9	87.60	87.17	-0.43	[86.66	86.98	86.98	90.34	84.90	90.51	84.84]
C9-C	16	159.10	158.33	-0.77	[158.02	158.18	158.18	160.70	155.70	160.98	155.92]
C10-CH	17	115.70	115.21	-0.49	[114.47	114.43	114.43	118.72	118.96	118.50	118.70]
C11-C	19	170.50	169.86	-0.64	[169.88	169.90	169.90	169.70	169.86	169.75	169.87]
C12-CH3	18	15.70	16.25	0.55	[16.66	16.62	16.62	13.20	17.87	13.14	17.85]
C13-CH2	7	75.40	74.21	-1.19	[73.87	73.90	73.91	77.19	71.59	77.01	71.78]
C14-CH3***	12	27.30	27.13	-0.17	[27.34	26.78	26.78	27.36	27.34	26.85	26.85]
C15-CH3***	11	23.70	24.27	0.57	[21.73	28.39	28.39	21.71	21.85	28.32	28.46]
¹³C chem shifts: RMSD=1.03ppm (MAE=0.83) N=15 {-2.79 0.57}											
Fractions:					0.487	0.168	0.168	0.097	0.035	0.034	0.011

NOTICE:

omitting the C=C-COOH moiety (need parameterization in methanol)

Conformer 1

Energy: -885.69168 Hartree (Rel: 0.0 kcal/mol)

XYZ coordinates for conf 1:

C	-3.07436	0.18253	1.09485
C	-2.71292	-1.25853	1.47259
C	-1.23418	-1.59432	1.20830
C	-0.70531	-1.00069	-0.09416
C	-1.51727	-0.00331	-0.89856
C	-2.90034	0.46813	-0.42872
C	0.31292	-1.79402	-0.89555
O	1.01597	-0.84459	-1.71456
C	1.00840	0.43785	-1.07845
C	-0.24961	0.44000	-0.20930
C	-3.96985	-0.28132	-1.25463
C	-3.05014	1.98069	-0.68587
O	-4.38432	0.52517	1.55933
H	-1.44021	-0.09058	-1.98371
H	-0.29714	1.10944	0.64406
C	2.27458	0.74900	-0.29059
C	3.27081	-0.15747	-0.25008
C	2.29762	2.10911	0.35523
C	4.55529	0.00611	0.44638
O	4.91847	0.93437	1.15461
O	5.36516	-1.06102	0.21323
H	-2.41655	0.86622	1.64720
H	-4.99865	-0.15093	1.23034
H	-2.94687	-1.41034	2.53234
H	-0.61726	-1.24241	2.04583
H	-3.35469	-1.94748	0.90734
H	-0.12719	-2.53313	-1.57441
H	1.00556	-2.31332	-0.21611
H	0.94063	1.17869	-1.88966
H	-3.89071	-1.36900	-1.15121
H	-4.98218	0.02177	-0.96410
H	-3.85463	-0.04480	-2.31844
H	-2.29153	2.55262	-0.13876
H	-2.93687	2.20741	-1.75283

H	-4.03634	2.33062	-0.36375
H	-1.11816	-2.68499	1.18377
H	3.14582	-1.09047	-0.78786
H	3.31574	2.46895	0.49956
H	1.73024	2.82951	-0.24555
H	1.82160	2.07188	1.34430
H	6.19334	-0.89365	0.70227

Conformer 2

Energy: -885.69267 Hartree (Rel: 0.6 kcal/mol)

XYZ coordinates for conf 2:

C	-3.47397	-0.26276	0.90232
C	-2.38022	-0.73769	1.86267
C	-1.31400	-1.56855	1.13306
C	-0.77960	-0.86155	-0.09518
C	-1.57742	0.24738	-0.75614
C	-2.93520	0.72021	-0.18756
C	0.15616	-1.61675	-1.02215
O	0.88103	-0.62070	-1.76522
C	0.96116	0.58622	-0.99985
C	-0.25767	0.55503	-0.07702
C	-3.93947	0.78860	-1.35737
C	-2.83135	2.13414	0.42446
O	-4.04273	-1.45540	0.34702
H	-1.52973	0.26640	-1.84533
H	-0.23750	1.14134	0.83529
C	2.27221	0.75559	-0.24254
C	3.22135	-0.19630	-0.33742
C	2.39109	2.03963	0.53516
C	4.53878	-0.16535	0.31418
O	4.97491	0.66522	1.09852
O	5.28555	-1.23676	-0.06466
H	-4.24789	0.27183	1.47537
H	-4.84321	-1.20451	-0.13859
H	-1.92317	0.13064	2.35211
H	-0.48975	-1.81095	1.81726
H	-2.83940	-1.34027	2.65435
H	-0.35426	-2.25084	-1.75560
H	0.84480	-2.24450	-0.43646
H	0.89686	1.41124	-1.72573
H	-3.99993	-0.16559	-1.89111
H	-4.94423	1.05621	-1.00455
H	-3.63057	1.55278	-2.07967
H	-2.20429	2.16044	1.32178
H	-2.40224	2.83532	-0.30008
H	-3.82435	2.50533	0.70582
H	-1.76254	-2.52121	0.82648
H	3.02766	-1.06239	-0.96007
H	3.43122	2.33574	0.66748
H	1.83612	2.84347	0.03754
H	1.95579	1.92253	1.53670
H	6.13949	-1.15912	0.40204

Conformer 3

Energy: -885.69066 Hartree (Rel: 0.6 kcal/mol)

XYZ coordinates for conf 3:

C	3.47388	-0.26265	-0.90249
C	2.38004	-0.73771	-1.86269
C	1.31395	-1.56863	-1.13296
C	0.77960	-0.86164	0.09529
C	1.57745	0.24736	0.75613
C	2.93514	0.72026	0.18746
C	-0.15597	-1.61688	1.02242
O	-0.88104	-0.62089	1.76535
C	-0.96117	0.58604	1.00007
C	0.25758	0.55488	0.07714
C	3.93952	0.78866	1.35718
C	2.83118	2.13420	-0.42451
O	4.04286	-1.45520	-0.34726
H	1.52984	0.26638	1.84532
H	0.23729	1.14113	-0.83520

C	-2.27222	0.75550	0.24277
C	-3.22133	-0.19646	0.33733
C	-2.39115	2.03970	-0.53464
C	-4.53866	-0.16531	-0.31443
O	-4.97444	0.66520	-1.09901
O	-5.28579	-1.23643	0.06455
H	4.24765	0.27202	-1.47568
H	4.84310	-1.20413	0.13867
H	1.92288	0.13057	-2.35211
H	0.48969	-1.81113	-1.81711
H	2.83917	-1.34028	-2.65442
H	0.35469	-2.25074	1.75591
H	-0.84450	-2.24492	0.43692
H	-0.89678	1.41107	1.72592
H	4.00019	-0.16557	1.89082
H	4.94419	1.05649	1.00430
H	3.63056	1.55269	2.07961
H	2.20409	2.16050	-1.32180
H	2.40205	2.83533	0.30007
H	3.82414	2.50549	-0.70591
H	1.76260	-2.52124	-0.82639
H	-3.02774	-1.06266	0.95986
H	-3.43129	2.33583	-0.66690
H	-1.83625	2.84346	-0.03681
H	-1.95584	1.92288	-1.53621
H	-6.13962	-1.15865	-0.40232

Conformer 4

Energy: -885.69170 Hartree (Rel: 1.0 kcal/mol)

XYZ coordinates for conf 4:

C	2.97999	0.57563	-1.07018
C	3.08415	-0.92899	-1.34391
C	1.76225	-1.67637	-1.09218
C	1.01622	-1.18504	0.14563
C	1.45550	0.06122	0.88912
C	2.65634	0.89509	0.42168
C	0.24931	-2.19644	0.98146
O	-0.78958	-1.47726	1.66408
C	-1.08677	-0.24089	0.98519
C	0.14630	0.05718	0.13759
C	3.85913	0.55776	1.33106
C	2.33597	2.39606	0.56565
O	4.14760	1.26643	-1.52666
H	1.35602	0.02680	1.97583
H	0.02527	0.65525	-0.76170
C	-2.36827	-0.32831	0.16701
C	-3.28755	0.64420	0.34248
C	-2.49189	-1.49053	-0.77674
C	-4.57118	0.78950	-0.36735
O	-5.06072	0.05576	-1.21327
O	-5.21328	1.91309	0.04680
H	2.17449	0.99077	-1.68994
H	4.92002	0.83294	-1.12881
H	3.40280	-1.07362	-2.38237
H	1.11041	-1.58403	-1.97145
H	3.87443	-1.35367	-0.71061
H	0.85780	-2.68614	1.75143
H	-0.17666	-2.97664	0.33319
H	-1.22488	0.50880	1.77380
H	4.11215	-0.50777	1.31068
H	4.74836	1.13067	1.04437
H	3.62764	0.81919	2.36980
H	1.46979	2.67676	-0.04492
H	2.10773	2.64732	1.60841
H	3.18835	3.00389	0.24510
H	1.97615	-2.74693	-0.98531
H	-3.09345	1.42618	1.07161
H	-3.41976	-1.45453	-1.34383
H	-1.64268	-1.50854	-1.47155
H	-2.45215	-2.42728	-0.20749
H	-6.05101	1.95607	-0.45285

Conformer 5

Energy: -885.69319 Hartree (Rel: 1.6 kcal/mol)

XYZ coordinates for conf 5:

C	-2.82312	1.17586	-0.35714
C	-2.50144	1.59139	1.08291
C	-1.07585	1.20211	1.51341
C	-0.65174	-0.17420	1.01150
C	-1.48849	-0.95064	0.01405
C	-2.78854	-0.37047	-0.56042
C	0.23980	-1.03440	1.89405
O	0.84188	-2.00665	1.02722
C	1.01183	-1.40508	-0.28054
C	-0.13602	-0.41874	-0.39638
C	-3.97541	-1.04622	0.16220
C	-2.88333	-0.69069	-2.06533
O	-4.06000	1.74789	-0.79593
H	-1.53106	-2.03043	0.16441
H	-0.07003	0.38417	-1.12437
C	2.42724	-0.83572	-0.37465
C	2.64826	0.49264	-0.30286
C	3.48612	-1.89616	-0.49355
C	3.95980	1.16833	-0.33072
O	5.07008	0.67346	-0.45227
O	3.79731	2.51107	-0.20070
H	-2.07814	1.62471	-1.02702
H	-4.73933	1.51525	-0.14226
H	-2.63630	2.67525	1.17181
H	-0.36181	1.95810	1.15966
H	-3.23083	1.12725	1.76004
H	-0.29729	-1.59334	2.66851
H	1.00514	-0.40948	2.38086
H	0.92769	-2.23617	-0.99270
H	-3.94350	-0.89711	1.24695
H	-4.93491	-0.67076	-0.21122
H	-3.95815	-2.12668	-0.01999
H	-2.04520	-0.25060	-2.61826
H	-2.86540	-1.77403	-2.23466
H	-3.81296	-0.29331	-2.48565
H	-1.01857	1.22261	2.60891
H	1.80806	1.17183	-0.21175
H	4.49238	-1.49220	-0.40446
H	3.32037	-2.65958	0.27617
H	3.39057	-2.40438	-1.46342
H	4.69049	2.90460	-0.22722

Conformer 6

Energy: -885.69420 Hartree (Rel: 1.6 kcal/mol)

XYZ coordinates for conf 6:

C	3.47077	0.27647	-0.90797
C	2.58823	-0.60497	-1.79561
C	1.82139	-1.64561	-0.96643
C	1.07557	-1.01739	0.19301
C	1.48614	0.34294	0.72436
C	2.64205	1.15010	0.08934
C	0.40849	-1.92899	1.20792
O	-0.64644	-1.17027	1.82219
C	-1.03338	-0.06310	0.98467
C	0.14474	0.16295	0.04185
C	3.56025	1.63860	1.22962
C	2.11762	2.39589	-0.65736
O	4.37179	-0.62226	-0.24887
H	1.41870	0.45623	1.80720
H	-0.04731	0.62311	-0.92263
C	-2.34071	-0.32926	0.24994
C	-3.29897	0.61888	0.31809
C	-2.44348	-1.62687	-0.49975
C	-4.61453	0.59969	-0.34610
O	-5.09863	-0.27229	-1.05248
O	-5.29652	1.74274	-0.07225
H	4.04969	0.96319	-1.54547

H	5.04712	-0.09013	0.19870
H	1.89185	0.02704	-2.35953
H	1.12387	-2.20077	-1.60822
H	3.22021	-1.11330	-2.53238
H	1.07694	-2.25828	2.01249
H	0.00540	-2.82277	0.70844
H	-1.17803	0.78903	1.65998
H	3.90319	0.80697	1.85396
H	4.43918	2.16546	0.83533
H	3.02124	2.33864	1.87808
H	1.52371	2.13893	-1.54071
H	1.48529	3.00074	0.00220
H	2.95263	3.02302	-0.99265
H	2.53817	-2.37567	-0.57174
H	-3.11538	1.51054	0.91147
H	-3.39539	-1.72114	-1.01817
H	-1.62520	-1.71152	-1.22608
H	-2.32874	-2.46209	0.20185
H	-6.15384	1.67353	-0.53423

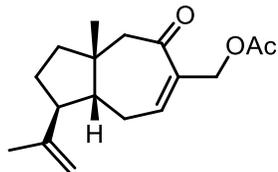
Conformer 7

Energy: -885.69319 Hartree (Rel: 2.2 kcal/mol)

XYZ coordinates for conf 7:

C	3.25693	1.08021	0.14891
C	2.08237	2.01874	-0.14018
C	1.14311	1.43102	-1.20435
C	0.72501	0.01343	-0.87665
C	1.54571	-0.83682	0.07404
C	2.80384	-0.27762	0.77814
C	-0.06523	-0.77697	-1.90705
O	-0.67797	-1.86153	-1.19207
C	-0.94754	-1.41734	0.16080
C	0.14345	-0.40458	0.45649
C	3.93405	-1.31704	0.62160
C	2.56556	-0.07073	2.28981
O	3.93599	0.91695	-1.10270
H	1.62914	-1.88883	-0.19899
H	-0.00025	0.29853	1.26977
C	-2.39127	-0.91940	0.22987
C	-2.66979	0.39818	0.30065
C	-3.40393	-2.02795	0.15529
C	-4.01084	1.01307	0.32314
O	-5.10210	0.46393	0.31326
O	-3.90431	2.36721	0.36299
H	3.93688	1.56594	0.86652
H	4.77321	0.46064	-0.92875
H	1.53546	2.21446	0.78985
H	0.25722	2.06994	-1.32112
H	2.47351	2.98261	-0.48481
H	0.54732	-1.22654	-2.69641
H	-0.82587	-0.13379	-2.37726
H	-0.86551	-2.31886	0.78186
H	4.10140	-1.57399	-0.42961
H	4.87699	-0.94719	1.04566
H	3.67617	-2.24153	1.15069
H	1.83793	0.72046	2.49865
H	2.19277	-0.99307	2.74923
H	3.50145	0.20212	2.79248
H	1.66352	1.43274	-2.16977
H	-1.85822	1.11577	0.34374
H	-4.42121	-1.65729	0.04805
H	-3.15538	-2.68685	-0.68538
H	-3.34292	-2.64373	1.06371
H	-4.81511	2.71878	0.37714

Originally assigned (incorrect) structure of 51{1} (CD₃OD)



Rel energy (kcal/mol):					Conf1	Conf2	Conf3	Conf4
					0.00	0.55	0.97	1.34
C-nom	iGau	Exp	Calc	diff	1	2	3	4
C1-C	1	41.60	44.22	2.62	[44.53	44.90	44.47	45.11]
C2-CH2	8	42.90	40.61	-2.29	[42.20	38.38	42.21	37.85]
C3-CH2	9	29.80	30.46	0.66	[30.83	29.51	33.30	32.93]
C4-CH	10	50.70	56.40	5.70	[58.69	54.39	55.08	50.54]
C5-CH	2	49.60	52.25	2.65	[52.55	54.25	50.18	51.93]
C6-CH2	3	31.20	31.36	0.16	[32.95	29.25	32.92	28.89]
C7-CH	4	146.00	145.51	-0.49	[144.98	146.80	144.88	146.76]
C8-C	5	137.10	137.01	-0.09	[137.34	136.38	137.24	136.24]
C9-C	6	202.90	203.56	0.66	[203.20	203.59	203.19	203.58]
C10-CH2	7	59.70	56.19	-3.51	[56.28	57.20	56.32	57.31]
C11-C	13	147.30	147.55	0.25	[147.56	147.32	147.70	147.87]
C12-CH2	14	113.90	112.26	-1.64	[113.39	113.58	107.47	107.55]
C13-CH3	15	24.10	18.80	-5.30	[18.26	17.76	24.88	25.13]
C14-CH3	11	19.50	29.68	10.18	[29.25	32.18	29.67	32.26]
C15-CH2	17	67.50	60.79	-6.71	[60.61	62.43	60.64	62.35]
C16-C	20	172.50	172.42	-0.08	[172.35	172.17	172.37	172.16]
C17-CH3	21	20.80	20.84	0.04	[21.45	21.16	21.45	21.14]
13C chem shifts: CRMSD=3.79ppm (CMAE=2.53) N=17 {-6.71 10.18}					Fractions: 0.590 0.233 0.116 0.061			

Conformer 1

Energy: -887.91176 Hartree (Rel: 0.0 kcal/mol)

XYZ coordinates for conf 1:

C	1.55710	-1.42115	-0.01291
C	1.53800	0.15425	0.02813
C	0.37601	0.83432	-0.72465
C	-0.99785	0.58273	-0.15817
C	-1.59961	-0.59842	0.08259
C	-0.98758	-1.92868	-0.16792
C	0.38259	-2.04358	-0.81216
C	2.90181	-1.76667	-0.71572
C	3.83541	-0.60006	-0.37592
C	2.91668	0.62749	-0.54602
C	1.55988	-1.99018	1.42073
H	1.46360	0.46514	1.07689
C	3.41931	1.93628	0.03302
C	3.44314	3.05005	-0.71195
C	3.88938	1.95042	1.47028
O	-1.61245	-2.94226	0.14913
C	-2.99360	-0.69356	0.67512
O	-3.61194	0.59411	0.85308
O	-4.72593	0.37861	-1.11153
C	-4.46418	1.01784	-0.11315
C	-5.02580	2.37501	0.23087
H	0.40282	0.53731	-1.78305
H	0.55855	1.91419	-0.71730
H	-1.56895	1.47372	0.09417
H	0.56810	-3.11494	-0.94324
H	0.34412	-1.59716	-1.81453
H	3.28794	-2.74308	-0.40140
H	2.75515	-1.81001	-1.80329
H	4.71964	-0.55138	-1.02110
H	4.19023	-0.68365	0.65829
H	2.77968	0.77697	-1.62638
H	2.44170	-1.65133	1.97620
H	0.67636	-1.66694	1.98378

H	1.57103	-3.08681	1.40832
H	3.78521	4.00111	-0.30961
H	3.12699	3.04873	-1.75279
H	4.80228	1.35429	1.59743
H	4.10694	2.96956	1.80401
H	3.14165	1.52336	2.15054
H	-3.63064	-1.31902	0.04761
H	-2.95589	-1.13826	1.67324
H	-5.77367	2.66107	-0.50936
H	-5.47338	2.35878	1.22927
H	-4.22108	3.11816	0.24359

Conformer 2

Energy: -887.91264 Hartree (Rel: 0.6 kcal/mol)

XYZ coordinates for conf 2:

C	2.11019	-1.40464	0.22038
C	1.91028	0.07490	0.72055
C	0.72723	0.32372	1.68038
C	-0.66206	0.18414	1.10993
C	-1.16773	-0.80726	0.35027
C	-0.41944	-2.02246	-0.05729
C	0.92662	-2.34914	0.56291
C	2.32522	-1.27505	-1.31866
C	2.78063	0.17400	-1.54002
C	1.89402	0.96755	-0.55771
C	3.36939	-2.00023	0.88335
H	2.80560	0.33866	1.29684
C	2.27408	2.41724	-0.32217
C	1.35962	3.38988	-0.43881
C	3.70585	2.73705	0.04566
O	-0.92622	-2.79068	-0.87732
C	-2.57633	-0.77636	-0.20083
O	-3.25286	0.40591	0.26118
O	-5.09523	-0.21770	-0.88769
C	-4.52570	0.57090	-0.15947
C	-5.11813	1.84299	0.39465
H	0.82169	1.34224	2.07169
H	0.83302	-0.33555	2.55516
H	-1.33585	1.00838	1.32916
H	0.80822	-2.39087	1.65447
H	1.17318	-3.36074	0.22416
H	3.04225	-2.01406	-1.69366
H	1.38336	-1.44571	-1.85454
H	2.66364	0.50843	-2.57683
H	3.84031	0.28371	-1.27753
H	0.87262	0.95479	-0.95999
H	4.26155	-1.42184	0.61607
H	3.28241	-1.99201	1.97711
H	3.53184	-3.03668	0.56453
H	1.60817	4.43421	-0.26264
H	0.33035	3.17651	-0.71897
H	4.39297	2.49604	-0.77566
H	3.82386	3.79943	0.27985
H	4.04576	2.16015	0.91513
H	-2.56400	-0.78384	-1.29520
H	-3.13875	-1.66165	0.11339
H	-6.14077	1.95870	0.03434
H	-5.11266	1.81401	1.48917
H	-4.51666	2.70405	0.08578

Conformer 3

Energy: -887.91049 Hartree (Rel: 1.0 kcal/mol)

XYZ coordinates for conf 3:

C	1.49794	-1.44638	0.09528
C	1.51510	0.13048	0.13466
C	0.38447	0.83432	-0.64645
C	-1.01189	0.59104	-0.13373
C	-1.64101	-0.58511	0.05566
C	-1.04080	-1.91894	-0.20342
C	0.36072	-2.04245	-0.77468
C	2.87458	-1.82897	-0.52096

C	3.80816	-0.66988	-0.16085
C	2.91031	0.56915	-0.39321
C	1.39965	-2.01184	1.52709
H	1.42107	0.43006	1.18388
C	3.49196	1.87141	0.13058
C	2.96108	2.59893	1.12156
C	4.75732	2.32518	-0.56425
O	-1.69947	-2.92907	0.04987
C	-3.05867	-0.67091	0.59050
O	-3.66126	0.62232	0.78166
O	-4.69894	0.48371	-1.23102
C	-4.46708	1.08888	-0.20442
C	-5.02029	2.44485	0.15755
H	0.44510	0.55040	-1.70685
H	0.57635	1.91182	-0.61871
H	-1.57828	1.48509	0.11825
H	0.53929	-3.11442	-0.91021
H	0.38188	-1.58323	-1.77195
H	3.22646	-2.80287	-0.16195
H	2.79022	-1.89685	-1.61390
H	4.72092	-0.65646	-0.76498
H	4.11045	-0.71999	0.89337
H	2.82470	0.68138	-1.48731
H	2.25955	-1.69912	2.13046
H	0.49656	-1.65924	2.03911
H	1.37694	-3.10833	1.51621
H	3.43332	3.52143	1.45150
H	2.04972	2.31953	1.64105
H	4.59664	2.42420	-1.64659
H	5.10353	3.28964	-0.18017
H	5.56953	1.59809	-0.43571
H	-3.68112	-1.26636	-0.07938
H	-3.06827	-1.14444	1.57595
H	-5.73015	2.76696	-0.60496
H	-5.51165	2.40581	1.13454
H	-4.20472	3.17266	0.22884

Conformer 4

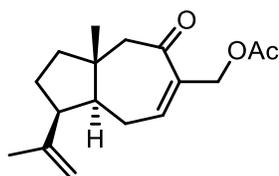
Energy: -887.91110 Hartree (Rel: 1.3 kcal/mol)

XYZ coordinates for conf 4:

C	2.16244	-1.41011	0.19582
C	1.92820	0.03128	0.78641
C	0.73782	0.17895	1.76010
C	-0.64575	0.07218	1.16851
C	-1.12948	-0.85370	0.31734
C	-0.35696	-2.01535	-0.18975
C	0.97759	-2.38614	0.43004
C	2.42841	-1.17756	-1.32309
C	2.83097	0.29785	-1.44415
C	1.89966	0.99770	-0.42403
C	3.40243	-2.03926	0.86332
H	2.82023	0.26957	1.37758
C	2.24048	2.45737	-0.17633
C	2.82191	2.92337	0.93645
C	1.88309	3.39265	-1.31044
O	-0.83523	-2.70529	-1.09230
C	-2.53177	-0.79234	-0.24696
O	-3.23444	0.32760	0.31935
O	-5.03958	-0.18779	-0.93731
C	-4.49827	0.52424	-0.11477
C	-5.11962	1.72491	0.55505
H	0.81483	1.15777	2.24403
H	0.84858	-0.55640	2.57136
H	-1.33281	0.86482	1.45351
H	0.83494	-2.52040	1.51112
H	1.24000	-3.36393	0.01298
H	3.18874	-1.86344	-1.71322
H	1.51466	-1.35226	-1.90423
H	2.72256	0.68467	-2.46261
H	3.87703	0.44476	-1.14400
H	0.88785	0.97155	-0.85662

H	4.29891	-1.44151	0.66083
H	3.27945	-2.09794	1.95211
H	3.58214	-3.05382	0.48819
H	3.05941	3.97933	1.04343
H	3.08603	2.28924	1.77745
H	0.80434	3.36270	-1.51659
H	2.15923	4.42712	-1.08384
H	2.38531	3.10322	-2.24277
H	-2.50665	-0.69313	-1.33655
H	-3.08189	-1.71334	-0.02752
H	-6.13776	1.86289	0.18988
H	-5.13151	1.58525	1.64088
H	-4.52655	2.62106	0.34554

Revised structure of 51{1}, i.e. 54{1-rev} (CD₃OD)



Rel energy (kcal/mol):					Conf1	Conf2	Conf3	Conf4
					0.00	0.22	0.39	1.72
C-nom	iGau	Exp	Calc	diff	1	2	3	4
C1-C	1	41.60	43.02	1.42	[42.85	42.56	43.00	42.51]
C2-CH2	8	42.90	42.02	-0.88	[41.77	41.87	41.57	42.95]
C3-CH2	9	29.80	29.95	0.15	[28.66	28.88	32.38	32.98]
C4-CH	10	50.70	51.25	0.55	[51.75	51.75	48.59	52.11]
C5-CH	2	49.60	51.27	1.67	[51.30	51.21	50.17	53.26]
C6-CH2	3	31.20	31.13	-0.07	[30.45	30.81	31.55	32.80]
C7-CH	4	146.00	146.98	0.98	[150.50	144.04	144.49	144.51]
C8-C	5	137.10	133.81	-3.29	[135.55	132.66	132.14	132.01]
C9-C	6	202.90	203.05	0.15	[203.32	203.19	203.01	203.29]
C10-CH2	7	59.70	59.92	0.22	[59.79	59.76	59.31	62.20]
C11-C	13	147.30	148.05	0.75	[147.79	147.78	148.74	150.70]
C12-CH2	14	113.90	115.04	1.14	[115.99	115.73	112.26	112.89]
C13-CH3	15	24.10	23.91	-0.19	[21.94	22.17	28.46	27.39]
C14-CH3	11	19.50	19.96	0.46	[19.64	19.61	19.41	23.61]
C15-CH2	17	67.50	65.83	-1.67	[68.82	63.18	63.13	63.10]
C16-C	20	172.50	172.23	-0.27	[172.68	172.04	172.03	172.03]
C17-CH3	21	20.80	21.48	0.68	[21.15	21.23	21.23	21.24]
13C chem shifts: CRMSD=1.17ppm (CMAE=0.85) N=17 {-3.29 1.67}								
Fractions:					0.441	0.306	0.229	0.024

Conformer 1

Energy: -887.90205 Hartree (Rel: 0.0 kcal/mol)

XYZ coordinates for conf 1:

C	-1.36831	-1.31306	0.02766
C	-1.62570	0.12755	0.55211
C	-1.04677	1.26352	-0.28907
C	0.44602	1.29462	-0.46898
C	1.39674	0.33386	-0.47354
C	1.23253	-1.14919	-0.30621
C	0.04676	-1.78911	0.40268
C	-2.44105	-2.11699	0.80252
C	-3.69657	-1.23313	0.74840
C	-3.17240	0.22291	0.90677
C	-1.57694	-1.47925	-1.49158
H	-1.11138	0.18535	1.52040
C	-3.99091	1.29662	0.20180
C	-4.33328	2.41287	0.86084
C	-4.43364	1.09565	-1.23108
O	2.13599	-1.87786	-0.71188
C	2.81549	0.73906	-0.79285
O	3.61716	0.52960	0.40267
O	5.49449	0.80963	-0.82393
C	4.95371	0.57937	0.24133
C	5.66846	0.31426	1.54487
H	-1.33800	2.22083	0.16030
H	-1.49161	1.28596	-1.29527
H	0.81134	2.29822	-0.69045
H	0.14542	-2.86541	0.22336
H	0.20329	-1.63000	1.48043
H	-2.59993	-3.11725	0.38306
H	-2.11786	-2.24629	1.84458
H	-4.42606	-1.48638	1.52494
H	-4.20203	-1.36739	-0.21316
H	-3.21349	0.47512	1.97167
H	-2.58523	-1.19513	-1.80609

H	-0.86866	-0.87878	-2.07343
H	-1.42689	-2.52794	-1.77483
H	-4.90963	3.20428	0.38677
H	-4.05185	2.57425	1.89922
H	-5.14093	0.26144	-1.32147
H	-4.93032	1.99221	-1.61450
H	-3.59482	0.86511	-1.89833
H	3.23365	0.13162	-1.59626
H	2.87896	1.79347	-1.07281
H	6.74600	0.39145	1.39580
H	5.34657	1.03333	2.30493
H	5.41740	-0.68626	1.91232

Conformer 2

Energy: -887.90178 Hartree (Rel: 0.2 kcal/mol)

XYZ coordinates for conf 2:

C	1.66291	-1.37295	0.06001
C	1.63599	0.03024	-0.60928
C	0.63849	1.02706	-0.02560
C	-0.81747	0.65331	-0.04324
C	-1.46987	-0.52718	-0.10228
C	-0.91384	-1.91305	-0.15391
C	0.53212	-2.25780	-0.48793
C	3.04372	-1.90734	-0.39458
C	3.98590	-0.70225	-0.25734
C	3.14492	0.51935	-0.72385
C	1.59074	-1.33934	1.60047
H	1.31397	-0.14023	-1.64514
C	3.50233	1.84916	-0.07333
C	3.64491	2.94586	-0.83114
C	3.71691	1.92607	1.42257
O	-1.70127	-2.84447	0.02517
C	-2.98950	-0.56887	-0.03002
O	-3.52274	0.76768	-0.05333
O	-5.61216	-0.07619	0.11197
C	-4.86595	0.87922	0.02641
C	-5.29144	2.32656	-0.00742
H	0.73308	1.97959	-0.56261
H	0.88652	1.27766	1.01690
H	-1.46598	1.52132	0.05351
H	0.66431	-3.29498	-0.15933
H	0.59256	-2.27219	-1.58716
H	3.36939	-2.77755	0.18721
H	2.98622	-2.21984	-1.44635
H	4.90252	-0.81147	-0.84675
H	4.29494	-0.59161	0.78691
H	3.32810	0.65671	-1.79488
H	2.39983	-0.74952	2.04130
H	0.64385	-0.92132	1.95916
H	1.67196	-2.35803	1.99830
H	3.88944	3.91362	-0.39875
H	3.52482	2.91468	-1.91194
H	4.60898	1.36550	1.73001
H	3.85198	2.96325	1.74439
H	2.87650	1.50507	1.98699
H	-3.40256	-1.13367	-0.87111
H	-3.32310	-1.07199	0.88188
H	-6.37774	2.39135	0.06169
H	-4.83426	2.87276	0.82403
H	-4.95115	2.79646	-0.93592

Conformer 3

Energy: -887.89965 Hartree (Rel: 0.4 kcal/mol)

XYZ coordinates for conf 3:

C	1.65499	-1.39333	0.07445
C	1.66176	0.01379	-0.59020
C	0.65511	1.00739	-0.01661
C	-0.80071	0.63389	-0.03124
C	-1.46248	-0.53970	-0.11931
C	-0.91680	-1.92624	-0.21226
C	0.53707	-2.26979	-0.50989

C	3.04473	-1.93841	-0.33467
C	3.99106	-0.74553	-0.14483
C	3.18064	0.49012	-0.62309
C	1.53658	-1.35539	1.61267
H	1.37743	-0.14406	-1.63877
C	3.50423	1.80811	0.07454
C	3.78537	1.92352	1.37881
C	3.50247	3.02606	-0.82209
O	-1.71541	-2.85809	-0.09392
C	-2.98241	-0.57165	-0.04988
O	-3.50508	0.76890	-0.01856
O	-5.60287	-0.06417	0.08351
C	-4.84826	0.88786	0.04987
C	-5.26211	2.33874	0.07605
H	0.73367	1.95702	-0.56234
H	0.91499	1.27014	1.01982
H	-1.44412	1.50308	0.08735
H	0.65889	-3.31007	-0.18664
H	0.62693	-2.27741	-1.60723
H	3.33837	-2.81996	0.24721
H	3.02289	-2.23655	-1.39209
H	4.92617	-0.85296	-0.70492
H	4.26709	-0.64977	0.90935
H	3.41811	0.64536	-1.68233
H	2.31548	-0.74046	2.07285
H	0.57004	-0.95881	1.94074
H	1.63163	-2.36990	2.01818
H	4.00213	2.89201	1.82348
H	3.81637	1.07333	2.05438
H	2.54529	3.13846	-1.34849
H	3.69376	3.94719	-0.26268
H	4.27108	2.93117	-1.60192
H	-3.39904	-1.09820	-0.91366
H	-3.32126	-1.10916	0.84034
H	-6.34863	2.40938	0.13535
H	-4.81066	2.84343	0.93635
H	-4.90716	2.84690	-0.82650

Conformer 4

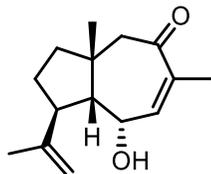
Energy: -887.90240 Hartree (Rel: 1.7 kcal/mol)

XYZ coordinates for conf 4:

C	1.68452	-1.18213	0.17009
C	1.58635	0.12456	-0.67541
C	0.55738	1.14132	-0.19567
C	-0.87968	0.70586	-0.13198
C	-1.48048	-0.50231	-0.09236
C	-0.86882	-1.86516	-0.06275
C	0.60626	-2.17927	-0.29052
C	3.11071	-1.73595	-0.17291
C	3.78389	-0.71064	-1.11479
C	3.05070	0.63431	-0.89813
C	1.55647	-0.96100	1.69204
H	1.26296	-0.18884	-1.67882
C	3.65148	1.55212	0.16502
C	4.46413	1.13446	1.14515
C	3.36177	3.02946	0.00115
O	-1.63006	-2.81873	0.11574
C	-2.99627	-0.60132	0.00146
O	-3.58313	0.71111	-0.06634
O	-5.63500	-0.20789	0.15825
C	-4.92876	0.77228	0.02660
C	-5.41225	2.19933	-0.05548
H	0.58455	2.01958	-0.85517
H	0.82313	1.52969	0.79963
H	-1.56274	1.55118	-0.08703
H	0.76332	-3.15520	0.18300
H	0.71261	-2.34807	-1.37338
H	3.68917	-1.86293	0.74866
H	3.05624	-2.72571	-0.64015
H	3.63517	-1.01665	-2.15710
H	4.86369	-0.63294	-0.95611

H	3.05975	1.21245	-1.83237
H	2.30065	-0.24776	2.05612
H	0.56506	-0.59180	1.97708
H	1.71526	-1.91105	2.21702
H	4.89492	1.83648	1.85546
H	4.73906	0.09270	1.27852
H	2.28925	3.25158	0.03546
H	3.85301	3.62221	0.77921
H	3.71960	3.38450	-0.97534
H	-3.39559	-1.21444	-0.81181
H	-3.29908	-1.08125	0.93627
H	-6.49995	2.22295	0.01787
H	-4.97387	2.79186	0.75415
H	-5.09508	2.65003	-1.00149

Originally assigned (incorrect) structure of 52{2} (CD₃OD)



Rel energy (kcal/mol):					Conf1	Conf2	Conf3	Conf4	Conf5	Conf6
					0.00	1.53	2.56	2.60	3.52	3.61
C-nom	iGau	Exp	Calc	diff	1	2	3	4	5	6
C1-C	1	42.30	43.64	1.34	[43.11	43.53	43.24	43.65	43.23	43.26]
C2-CH2	8	43.80	38.69	-5.11	[38.06	37.53	43.11	37.63	42.99	42.99]
C3-CH2	9	32.30	30.81	-1.49	[29.71	34.41	30.55	31.77	30.89	33.44]
C4-CH***	10	49.80	52.43	2.63	[52.32	49.19	52.42	52.65	53.87	49.25]
C5-CH***	2	57.90	59.73	1.83	[59.82	57.19	55.59	57.94	55.48	52.95]
C6-CH	3	70.70	70.95	0.25	[71.01	71.33	66.78	71.96	67.16	67.24]
C7-CH	4	145.70	151.47	5.77	[153.09	154.03	145.02	153.38	143.36	145.19]
C8-C	5	134.50	134.87	0.37	[136.04	135.90	141.21	135.73	140.30	141.03]
C9-C	6	203.60	201.39	-2.21	[203.89	203.73	204.77	203.52	204.88	204.81]
C10-CH2	7	59.60	56.76	-2.84	[56.51	56.79	55.62	57.17	54.45	55.77]
C11-C	13	149.50	147.78	-1.72	[149.23	150.16	147.74	148.99	147.13	148.06]
C12-CH2	14	113.00	110.40	-2.60	[111.41	107.62	113.61	111.02	113.72	107.02]
C13-CH3	15	26.00	19.40	-6.60	[17.89	25.63	18.13	18.41	18.04	25.12]
C14-CH3	11	20.20	32.77	12.57	[32.12	32.13	29.25	32.21	29.25	29.64]
C15-CH3	18	22.10	21.79	-0.31	[20.88	20.68	21.66	20.73	21.60	21.66]

¹³C chem shifts: CRMSD=4.46ppm (CMAE=3.18) N=15 {-6.60 12.57}
 Fractions: 0.903 0.069 0.012 0.011 0.002 0.002

Conformer 1

Energy: -735.24456 Hartree (Rel: 0.0 kcal/mol)

XYZ coordinates for conf 1:

C	0.37702	1.61140	0.34645
C	-0.62129	0.43225	0.64081
C	-0.05082	-0.74641	1.46530
C	0.95747	-1.62203	0.74848
C	2.03177	-1.28585	0.00587
C	2.45429	0.12167	-0.23275
C	1.86846	1.25311	0.59596
C	0.11823	1.98119	-1.14800
C	-1.25807	1.38927	-1.48304
C	-1.24393	0.04061	-0.73245
C	0.03765	2.80499	1.26213
H	-1.42285	0.83522	1.27048
C	-2.56863	-0.70039	-0.66233
C	-2.66085	-1.97106	-1.08744
C	-3.77655	0.02616	-0.11573
O	-1.11253	-1.55749	1.97857
O	3.31573	0.36215	-1.07844
C	2.88023	-2.33698	-0.67015
H	0.42158	-0.32911	2.36547
H	0.74223	-2.68381	0.86533
H	2.00856	1.01949	1.66036
H	2.47796	2.13550	0.37594
H	0.17053	3.06315	-1.31199
H	0.87858	1.52448	-1.79266
H	-1.42500	1.26799	-2.55886
H	-2.05572	2.03558	-1.09632
H	-0.53025	-0.61124	-1.25234
H	-0.97876	3.16745	1.06907
H	0.09603	2.52220	2.32063
H	0.73059	3.63824	1.09618
H	-3.59852	-2.52049	-1.04723
H	-1.80568	-2.49774	-1.50545
H	-4.03843	0.88719	-0.74310
H	-4.64663	-0.63553	-0.07165

H	-3.59568	0.41509	0.89368
H	-1.64240	-1.85267	1.21548
H	2.52065	-3.34313	-0.43725
H	2.86955	-2.20395	-1.75785
H	3.92829	-2.25877	-0.35761

Conformer 2

Energy: -735.24871 Hartree (Rel: 1.5 kcal/mol)

XYZ coordinates for conf 2:

C	0.49628	1.62951	0.25077
C	-0.56768	0.55365	0.68781
C	-0.01785	-0.57825	1.59007
C	0.86131	-1.59326	0.88625
C	1.90768	-1.40730	0.05608
C	2.41829	-0.06143	-0.32350
C	1.97132	1.17564	0.43893
C	0.17911	1.91463	-1.25117
C	-1.23939	1.37846	-1.48203
C	-1.27312	0.09563	-0.61601
C	0.30334	2.90566	1.09450
H	-1.30430	1.07166	1.31227
C	-2.65715	-0.53071	-0.51493
C	-3.53603	-0.27463	0.46611
C	-3.01755	-1.45013	-1.65945
O	-1.07464	-1.25539	2.27635
O	3.23837	0.04274	-1.23555
C	2.62335	-2.57414	-0.58260
H	0.56298	-0.10847	2.39595
H	0.56373	-2.61932	1.09998
H	2.16727	1.01920	1.50862
H	2.62632	1.98754	0.10691
H	0.27661	2.97952	-1.48934
H	0.88226	1.37832	-1.89930
H	-1.45754	1.18710	-2.53794
H	-1.99210	2.08583	-1.11088
H	-0.62113	-0.63664	-1.11225
H	-0.69221	3.33413	0.92976
H	0.40238	2.69210	2.16618
H	1.04669	3.66759	0.83201
H	-4.52835	-0.71903	0.45788
H	-3.31694	0.38932	1.29722
H	-2.33645	-2.31068	-1.69853
H	-4.04185	-1.82515	-1.57384
H	-2.92128	-0.93324	-2.62333
H	-1.78267	-1.42723	1.63024
H	2.20357	-3.52587	-0.24502
H	2.54848	-2.52614	-1.67485
H	3.69324	-2.55933	-0.34318

Conformer 3

Energy: -735.24628 Hartree (Rel: 2.6 kcal/mol)

XYZ coordinates for conf 3:

C	0.17775	1.25938	-0.06436
C	-0.58802	-0.10123	0.14935
C	0.05145	-1.37382	-0.42908
C	1.39788	-1.73274	0.17702
C	2.51604	-0.99014	0.31459
C	2.64400	0.43700	-0.11522
C	1.51328	1.13798	-0.84181
C	-0.82054	2.12253	-0.88679
C	-2.20960	1.63625	-0.46004
C	-2.03597	0.10418	-0.41802
C	0.44004	1.93126	1.30025
H	-0.65270	-0.28691	1.22819
C	-3.10460	-0.68114	0.31795
C	-3.68696	-1.74372	-0.25508
C	-3.48970	-0.24003	1.71218
O	0.11296	-1.26509	-1.86369
O	3.69629	1.03280	0.11282
C	3.75744	-1.57232	0.94890
H	-0.63336	-2.19671	-0.17975

H	1.45373	-2.75632	0.54816
H	1.87842	2.14336	-1.07784
H	1.32553	0.60578	-1.77938
H	-0.66342	3.19520	-0.72404
H	-0.68031	1.92999	-1.95851
H	-3.00518	1.94522	-1.14741
H	-2.46421	2.03181	0.53053
H	-2.01808	-0.24840	-1.45525
H	-0.49716	2.13073	1.83214
H	1.05419	1.29542	1.94914
H	0.96297	2.88659	1.17072
H	-4.44214	-2.33209	0.26173
H	-3.43177	-2.05911	-1.26439
H	-3.99483	0.73442	1.69702
H	-4.16717	-0.95996	2.18147
H	-2.61327	-0.12561	2.36287
H	0.48400	-2.09540	-2.20376
H	3.59774	-2.61261	1.24570
H	4.60701	-1.53214	0.25727
H	4.05107	-0.99562	1.83329

Conformer 4

Energy: -735.24295 Hartree (Rel: 2.6 kcal/mol)

XYZ coordinates for conf 4:

C	0.38343	1.60600	0.29846
C	-0.62566	0.44112	0.62562
C	-0.03038	-0.68350	1.49572
C	0.92888	-1.60557	0.77265
C	2.01111	-1.30506	0.02646
C	2.46490	0.09006	-0.22928
C	1.87694	1.25395	0.55277
C	0.12737	1.93598	-1.20470
C	-1.24882	1.33868	-1.52499
C	-1.24949	0.01059	-0.73155
C	0.05169	2.82654	1.18083
H	-1.42386	0.86950	1.24182
C	-2.59736	-0.68610	-0.68628
C	-2.81377	-1.78922	-1.41468
C	-3.69244	-0.08567	0.16471
O	-1.12981	-1.43212	2.02335
O	3.34800	0.29596	-1.06179
C	2.82194	-2.38258	-0.65361
H	0.49785	-0.20228	2.33488
H	0.66407	-2.65889	0.86618
H	2.02657	1.06554	1.62500
H	2.48483	2.12681	0.29365
H	0.18542	3.01296	-1.39786
H	0.88686	1.45829	-1.83544
H	-1.41130	1.17934	-2.59629
H	-2.04889	1.99904	-1.16609
H	-0.54491	-0.66167	-1.23727
H	-0.96202	3.19050	0.97660
H	0.10684	2.57256	2.24690
H	0.75039	3.65053	0.99350
H	-3.78308	-2.28278	-1.43230
H	-2.02892	-2.23952	-2.01889
H	-3.82153	0.98701	-0.02834
H	-4.65117	-0.58003	-0.02116
H	-3.45701	-0.19338	1.23032
H	-0.78214	-2.03061	2.70426
H	2.43350	-3.37695	-0.41624
H	2.80944	-2.25199	-1.74156
H	3.87357	-2.33599	-0.34690

Conformer 5

Energy: -735.24463 Hartree (Rel: 3.5 kcal/mol)

XYZ coordinates for conf 5:

C	0.19202	1.26028	-0.05125
C	-0.58816	-0.09190	0.15811
C	0.04664	-1.38071	-0.40931
C	1.38819	-1.73418	0.20278

C	2.50820	-0.99292	0.31823
C	2.64677	0.41822	-0.15928
C	1.50430	1.12478	-0.86367
C	-0.80981	2.15408	-0.83646
C	-2.19658	1.66916	-0.40243
C	-2.03282	0.13537	-0.40524
C	0.49797	1.90779	1.31597
H	-0.66480	-0.27270	1.23760
C	-3.11365	-0.66433	0.29719
C	-3.73038	-1.67843	-0.32522
C	-3.47775	-0.28531	1.71518
O	0.20934	-1.38095	-1.84143
O	3.71652	1.00012	0.01544
C	3.74964	-1.56605	0.96122
H	-0.64010	-2.19587	-0.14490
H	1.44127	-2.75061	0.59092
H	1.87353	2.12532	-1.11326
H	1.28865	0.59310	-1.79559
H	-0.64055	3.22055	-0.64840
H	-0.68773	1.98917	-1.91523
H	-3.00093	2.00244	-1.06752
H	-2.43209	2.03498	0.60406
H	-2.02814	-0.17094	-1.46025
H	-0.42389	2.12342	1.86809
H	1.10794	1.24869	1.94516
H	1.04199	2.85152	1.18790
H	-4.49743	-2.27133	0.16797
H	-3.49760	-1.94778	-1.35328
H	-3.95135	0.70412	1.75366
H	-4.17644	-1.00718	2.14866
H	-2.59609	-0.23410	2.36642
H	-0.66276	-1.53493	-2.23754
H	3.58113	-2.59329	1.29628
H	4.59235	-1.56087	0.26031
H	4.05872	-0.96214	1.82189

Conformer 6

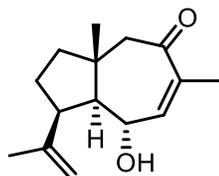
Energy: -735.24309 Hartree (Rel: 3.6 kcal/mol)

XYZ coordinates for conf 6:

C	0.20177	1.24767	0.12080
C	-0.54799	-0.13648	0.22439
C	0.07983	-1.33613	-0.50679
C	1.46164	-1.72700	-0.00940
C	2.57885	-0.98391	0.13222
C	2.66849	0.47787	-0.17155
C	1.48533	1.23039	-0.74774
C	-0.84620	2.19344	-0.52998
C	-2.20688	1.63740	-0.10151
C	-2.01100	0.10888	-0.24845
C	0.54793	1.75925	1.53543
H	-0.55620	-0.42021	1.28188
C	-3.11269	-0.72154	0.38815
C	-2.95680	-1.51907	1.45278
C	-4.46369	-0.59327	-0.28196
O	0.06415	-1.08776	-1.92530
O	3.73047	1.06295	0.03852
C	3.86036	-1.60337	0.63862
H	-0.57737	-2.19324	-0.30521
H	1.54847	-2.77896	0.26328
H	1.82411	2.26096	-0.89984
H	1.24374	0.79585	-1.72268
H	-0.68967	3.23876	-0.23925
H	-0.76326	2.14220	-1.62362
H	-3.03249	2.02119	-0.70961
H	-2.42358	1.88987	0.94468
H	-2.03616	-0.10265	-1.32697
H	-0.35598	1.89090	2.14111
H	1.19849	1.05585	2.06887
H	1.06381	2.72589	1.48600
H	-3.79670	-2.07850	1.85840
H	-2.00785	-1.65362	1.96268

H	-4.40038	-0.86317	-1.34503
H	-5.21159	-1.23719	0.19099
H	-4.83369	0.43956	-0.24521
H	0.42028	-1.87764	-2.36359
H	3.72708	-2.66798	0.85003
H	4.66705	-1.49064	-0.09502
H	4.20121	-1.10350	1.55237

Revised structure of 52{2}, i.e. 55{2-rev} (CD₃OD)



Rel energy (kcal/mol):					Conf1	Conf2
					0.00	3.96
C-nom	iGau	Exp	Calc	diff	1	2
C1-C	1	42.30	44.31	2.01	[44.03	42.75]
C2-CH2	8	43.80	43.16	-0.64	[42.76	41.92]
C3-CH2	9	32.30	30.32	-1.98	[28.60	32.33]
C4-CH***	10	49.80	50.80	1.00	[51.47	46.79]
C5-CH***	2	57.90	59.56	1.66	[58.54	60.72]
C6-CH	3	70.70	69.18	-1.52	[69.57	66.70]
C7-CH	4	145.70	145.14	-0.56	[145.92	144.54]
C8-C	5	134.50	134.42	-0.08	[133.51	138.21]
C9-C	6	203.60	204.17	0.57	[204.15	208.17]
C10-CH2	7	59.60	58.70	-0.90	[59.21	55.48]
C11-C	13	149.50	149.60	0.10	[148.61	154.21]
C12-CH2	14	113.00	112.52	-0.48	[114.66	106.78]
C13-CH3	15	26.00	23.93	-2.07	[22.16	25.81]
C14-CH3	11	20.20	21.98	1.78	[19.79	24.99]
C15-CH3	18	22.10	24.53	2.43	[24.30	22.07]
13C chem shifts: CRMSD=1.40ppm (CMAE=1.18) N=15 {-2.07 2.43}						
Fractions:					0.740	0.260
Fractions-derived rel energies:					0.00	0.62
Energy discrepancy:					0.00	3.34

Conformer 1

Energy: -735.23055 Hartree (Rel: 0.0 kcal/mol)

XYZ coordinates for conf 1:

C	0.21729	1.30474	-0.05138
C	-0.46510	0.02294	-0.60712
C	-0.06010	-1.30437	0.04148
C	1.40950	-1.65400	0.03946
C	2.56149	-0.95172	0.01074
C	2.72785	0.53402	-0.07835
C	1.64473	1.46492	-0.60341
C	-0.70492	2.40873	-0.62382
C	-2.12812	1.86633	-0.43031
C	-2.02382	0.33409	-0.69192
C	0.25289	1.39303	1.48926
H	-0.14007	-0.06825	-1.65145
C	-2.98974	-0.50994	0.13672
C	-3.81379	-1.37403	-0.48077
C	-3.06174	-0.34591	1.63981
O	-0.68183	-2.40716	-0.63660
O	3.82193	1.01380	0.21438
C	3.87784	-1.69196	0.14823
H	-0.37086	-1.31589	1.09962
H	1.51979	-2.73387	0.13996
H	2.00957	2.47937	-0.40792
H	1.62200	1.34010	-1.69652
H	-0.54522	3.37837	-0.13807
H	-0.49382	2.53948	-1.69377
H	-2.85502	2.33678	-1.10021
H	-2.46633	2.06843	0.59055
H	-2.30354	0.15452	-1.73448
H	-0.74641	1.36089	1.93149
H	0.83945	0.58293	1.93664
H	0.71591	2.33937	1.79353
H	-4.52522	-1.98149	0.07362
H	-3.81739	-1.48810	-1.56282

H	-3.40734	0.65807	1.91527
H	-3.76036	-1.06630	2.07533
H	-2.08934	-0.48503	2.12449
H	-1.64204	-2.30991	-0.50336
H	3.71914	-2.77346	0.17147
H	4.55239	-1.45489	-0.68269
H	4.39840	-1.39539	1.06537

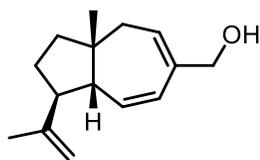
Conformer 2

Energy: -735.23686 Hartree (Rel: 4.0 kcal/mol)

XYZ coordinates for conf 2:

C	-0.09944	-1.23541	0.53712
C	0.24236	0.06634	-0.23822
C	-0.19494	1.39037	0.41358
C	-1.67300	1.66144	0.25047
C	-2.68203	0.82455	-0.05479
C	-2.54540	-0.66683	-0.20172
C	-1.62983	-1.41611	0.75331
C	0.49707	-2.27396	-0.44212
C	1.85524	-1.67616	-0.87446
C	1.70130	-0.11032	-0.77875
C	0.58686	-1.36853	1.91203
H	-0.35334	0.00636	-1.15981
C	2.90415	0.53103	-0.09876
C	2.94992	1.02977	1.14650
C	4.13838	0.56367	-0.97456
O	0.45086	2.52227	-0.18537
O	-3.25584	-1.26867	-1.00128
C	-4.07652	1.34641	-0.32199
H	0.02749	1.38004	1.49313
H	-1.90587	2.72258	0.33497
H	-1.88732	-1.06906	1.76250
H	-1.89045	-2.47808	0.69617
H	0.60145	-3.26495	0.01464
H	-0.16760	-2.38204	-1.30876
H	2.13913	-1.99454	-1.88192
H	2.64898	-2.01396	-0.19983
H	1.70501	0.29499	-1.79748
H	1.67698	-1.35750	1.83705
H	0.28759	-0.56799	2.59826
H	0.29309	-2.31898	2.37401
H	3.86824	1.46021	1.53872
H	2.10709	1.00881	1.82802
H	3.95553	1.14655	-1.88705
H	4.99513	0.99950	-0.45230
H	4.41533	-0.44743	-1.30064
H	1.39827	2.43589	0.02471
H	-4.11862	2.43376	-0.21488
H	-4.39265	1.07844	-1.33600
H	-4.80826	0.90098	0.36385

Originally assigned (incorrect) structure of 53{3} (CD₃OD)



Rel energy (kcal/mol):					Conf1	Conf2	Conf3	Conf4	Conf5	Conf6	Conf7	Conf8	Conf9
C-nom	iGau	Exp	Calc	diff	1	2	3	4	5	6	7	8	9
C1-C	1	46.80	49.93	3.13	[43.86	67.47	43.74	52.47	65.03	43.75	43.49	68.11	66.14
C2-CH2	8	40.50	38.21	-2.29	[43.32	37.33	43.33	43.11	37.79	42.26	42.15	37.20	37.22
C3-CH2	9	29.70	25.87	-3.83	[26.64	30.41	26.55	32.42	30.50	29.20	29.17	32.75	31.38
C4-CH	10	48.70	55.53	6.83	[59.05	59.24	59.00	54.82	61.93	54.80	54.83	56.23	57.97
C5-CH	2	45.70	52.90	7.20	[55.73	54.97	55.78	55.09	54.71	54.16	54.18	62.79	62.12
C6-CH	3	144.50	136.73	-7.77	[135.90	142.45	135.10	137.96	141.80	135.78	134.87	142.29	141.64
C7-CH	4	122.80	125.89	3.09	[125.89	131.70	124.71	126.25	129.29	125.98	124.82	131.98	129.73
C8-C	5	134.60	137.33	2.73	[136.99	141.98	136.58	138.79	140.72	137.04	136.51	141.89	140.74
C9-CH	6	129.80	130.44	0.64	[131.77	132.09	132.07	131.12	132.21	131.80	131.99	132.00	132.54
C10-CH2	7	29.50	36.07	6.57	[37.36	40.67	37.37	42.11	40.40	37.53	37.62	40.46	40.35
C11-C	13	146.70	146.92	0.22	[147.51	147.86	147.52	148.32	147.72	149.08	149.13	151.73	151.02
C12-CH2	14	112.90	109.52	-3.38	[113.05	112.76	113.10	108.28	112.45	106.14	106.14	108.54	108.52
C13-CH3	15	24.30	16.62	-7.68	[17.59	17.50	17.55	25.53	17.42	25.09	25.10	27.11	26.76
C14-CH3	11	19.00	25.17	6.17	[25.56	32.35	25.53	29.00	32.63	25.59	25.59	32.54	32.77
C15-CH2	18	70.70	66.35	-4.35	[70.24	67.59	69.16	68.74	66.95	70.24	69.20	67.45	66.90
					¹³C chem shifts: CRMSD=5.01ppm (CMAE=4.39) N=15 {-7.77 7.20}								
					Fractions: 0.225 0.209 0.193 0.115 0.080 0.067 0.059 0.035 0.017								

Conformer 1

Energy: -659.99591 Hartree (Rel: 0.0 kcal/mol)

XYZ coordinates for conf 1:

C	-0.10224	1.41249	0.24277
C	-0.68320	-0.00104	0.50697
C	0.22580	-1.19455	0.53506
C	1.50810	-1.34400	0.14740
C	2.44897	-0.38481	-0.44524
C	2.14269	0.83077	-0.94233
C	0.78146	1.46698	-1.03482
C	-1.40171	2.22492	-0.00126
C	-2.37141	1.29001	-0.75911
C	-1.84994	-0.16695	-0.52889
C	0.67439	1.95794	1.45060
H	-1.15081	0.05582	1.50275
C	-2.92343	-1.16575	-0.13686
C	-3.22742	-2.19337	-0.94104
C	-3.64562	-0.96713	1.17733
O	4.35493	-1.10096	0.82097
H	0.23029	1.01961	-1.87602
C	3.87992	-0.86947	-0.51088
H	1.93731	-2.33339	0.30488
H	-0.25533	-2.08977	0.93129
H	2.96522	1.42253	-1.34296

H	-1.83313	2.50020	0.96952
H	-1.20694	3.16033	-0.53857
H	-2.38858	1.50886	-1.83181
H	-3.39890	1.41405	-0.40239
H	-1.40455	-0.52682	-1.46281
H	0.04238	1.96023	2.34713
H	1.56515	1.35926	1.66335
H	1.00031	2.99018	1.26874
H	-4.00545	-2.90974	-0.68628
H	-2.70944	-2.35397	-1.88404
H	-4.04759	0.04954	1.27264
H	-4.47745	-1.67059	1.27990
H	-2.97506	-1.11828	2.03332
H	5.18786	-1.59374	0.74902
H	3.92388	-1.80527	-1.09142
H	4.50667	-0.12955	-1.02896
H	0.91653	2.52197	-1.30325

Conformer 2

Energy: -659.99500 Hartree (Rel: 0.0 kcal/mol)

XYZ coordinates for conf 2:

C	-0.52784	1.80456	0.01173
C	-0.78562	0.40760	0.71698
C	0.26080	-0.13475	1.66448
C	1.56945	-0.32272	1.40959
C	2.27523	0.11931	0.19905
C	1.97319	1.28321	-0.40930
C	0.95017	2.25719	0.11662
C	-0.95758	1.58158	-1.47223
C	-1.82691	0.31725	-1.47094
C	-1.10552	-0.58830	-0.45388
C	-1.41137	2.88099	0.66886
H	-1.70912	0.51922	1.29810
C	-1.83085	-1.85352	-0.04137
C	-1.21063	-3.03997	-0.09927
C	-3.26189	-1.74330	0.43437
O	2.82261	-2.04404	-0.66001
H	1.05429	3.21491	-0.40844
C	3.38009	-0.77107	-0.30768
H	2.16730	-0.86146	2.14641
H	-0.11688	-0.50618	2.61638
H	2.52023	1.55842	-1.31010
H	-1.47264	2.45775	-1.88283
H	-0.07339	1.40620	-2.09686
H	-1.91549	-0.14658	-2.46038
H	-2.84243	0.54925	-1.12493
H	-0.14500	-0.88256	-0.89256
H	-2.47567	2.64025	0.55707
H	-1.19874	2.96526	1.74228
H	-1.24097	3.86428	0.21307
H	-1.70664	-3.96108	0.19995
H	-0.18146	-3.12775	-0.44036
H	-3.92471	-1.38411	-0.36349
H	-3.64036	-2.71253	0.77361
H	-3.36230	-1.03265	1.26510
H	3.56336	-2.64383	-0.84318
H	3.87524	-0.30409	-1.17140
H	4.13922	-0.89980	0.48137
H	1.16095	2.45097	1.17924

Conformer 3

Energy: -659.99355 Hartree (Rel: 0.1 kcal/mol)

XYZ coordinates for conf 3:

C	-0.21251	1.50117	0.16868
C	-0.72829	0.09189	0.56141
C	0.24566	-1.01391	0.84496
C	1.56841	-1.11441	0.60780
C	2.50650	-0.16637	-0.00776
C	2.18136	0.94188	-0.70300
C	0.80209	1.46404	-1.00727
C	-1.52647	2.17084	-0.31448

C	-2.34033	1.07409	-1.03776
C	-1.75816	-0.29632	-0.55704
C	0.38662	2.25543	1.36517
H	-1.30766	0.23969	1.48652
C	-2.80395	-1.31595	-0.14410
C	-2.94702	-2.46174	-0.82370
C	-3.68367	-1.00326	1.04605
O	4.22366	-1.78700	-0.43845
H	0.37423	0.88097	-1.83717
C	3.96778	-0.51872	0.17786
H	2.04090	-2.04493	0.91992
H	-0.21805	-1.88312	1.31340
H	3.00425	1.52973	-1.10907
H	-2.08224	2.52962	0.56117
H	-1.33417	3.04439	-0.94818
H	-2.24552	1.15207	-2.12579
H	-3.40825	1.16230	-0.81405
H	-1.18860	-0.73896	-1.38145
H	-0.34177	2.32436	2.18241
H	1.28280	1.75922	1.74981
H	0.66639	3.27764	1.07957
H	-3.70155	-3.19754	-0.55405
H	-2.31504	-2.70402	-1.67531
H	-4.15993	-0.01885	0.95429
H	-4.47380	-1.75175	1.15919
H	-3.10752	-0.98439	1.98034
H	5.07023	-2.11143	-0.09319
H	4.60201	0.26498	-0.26102
H	4.20288	-0.57205	1.25247
H	0.90304	2.48610	-1.39310

Conformer 4

Energy: -659.99423 Hartree (Rel: 0.4 kcal/mol)

XYZ coordinates for conf 4:

C	-0.04546	1.41734	0.20717
C	-0.58700	-0.05668	0.32256
C	0.22976	-1.21181	-0.19877
C	1.53719	-1.32892	-0.50728
C	2.58501	-0.30384	-0.52973
C	2.33652	1.00686	-0.71777
C	0.97039	1.58197	-0.95869
C	-1.31780	2.27291	-0.10926
C	-2.52747	1.36596	0.14510
C	-2.01853	-0.02741	-0.28641
C	0.58753	1.86851	1.53549
H	-0.72173	-0.24499	1.40030
C	-2.97258	-1.15589	0.06504
C	-2.84711	-1.94349	1.14108
C	-4.13597	-1.32158	-0.88693
O	4.14548	-1.45175	0.88080
H	0.52776	1.11359	-1.85200
C	4.00158	-0.80460	-0.38940
H	1.88149	-2.33213	-0.76281
H	-0.35216	-2.13163	-0.26054
H	3.17729	1.69925	-0.70844
H	-1.34578	3.19501	0.48215
H	-1.30920	2.57200	-1.16522
H	-3.42140	1.68641	-0.40035
H	-2.78280	1.33776	1.21252
H	-1.91340	-0.01216	-1.38306
H	-0.15468	1.86044	2.34332
H	1.41349	1.21196	1.82932
H	0.98177	2.88947	1.45316
H	-3.58418	-2.71201	1.36234
H	-2.01976	-1.86097	1.83984
H	-3.78117	-1.57435	-1.89555
H	-4.82080	-2.10935	-0.55785
H	-4.70891	-0.38991	-0.98395
H	5.00324	-1.90569	0.87665
H	4.21862	-1.51895	-1.20064
H	4.70803	0.03231	-0.48860

H	1.06391	2.65194	-1.18024
---	---------	---------	----------

Conformer 5

Energy: -659.99471 Hartree (Rel: 0.6 kcal/mol)

XYZ coordinates for conf 5:

C	0.45682	1.72547	-0.12647
C	0.79165	0.28963	-0.71334
C	-0.27593	-0.47276	-1.46546
C	-1.54950	-0.70594	-1.09449
C	-2.23226	-0.12933	0.07232
C	-1.99057	1.12800	0.49036
C	-1.04823	2.07554	-0.20579
C	0.96514	1.67794	1.34521
C	2.00254	0.54983	1.38391
C	1.35362	-0.53550	0.50167
C	1.23880	2.78901	-0.92158
H	1.62372	0.42832	-1.41371
C	2.23623	-1.71046	0.12844
C	1.84450	-2.96613	0.38341
C	3.56933	-1.43179	-0.52940
O	-4.30861	-1.29384	-0.17193
H	-1.18695	3.08588	0.19864
C	-3.25992	-0.99808	0.75964
H	-2.14307	-1.39665	-1.69239
H	0.07187	-0.98035	-2.36483
H	-2.53695	1.50242	1.35526
H	1.36458	2.64542	1.67098
H	0.13744	1.42519	2.01943
H	2.21686	0.19218	2.39776
H	2.95157	0.88500	0.94658
H	0.48648	-0.92838	1.04719
H	2.32061	2.62503	-0.84638
H	0.97072	2.76158	-1.98545
H	1.02602	3.79750	-0.54589
H	2.46085	-3.82343	0.12109
H	0.89275	-3.18117	0.86418
H	4.23652	-0.86927	0.13626
H	4.07552	-2.36287	-0.80216
H	3.45871	-0.82946	-1.44024
H	-4.80510	-2.04902	0.18075
H	-2.79025	-1.93209	1.10446
H	-3.65566	-0.47840	1.64490
H	-1.32072	2.12074	-1.27147

Conformer 6

Energy: -659.99584 Hartree (Rel: 0.7 kcal/mol)

XYZ coordinates for conf 6:

C	-0.05191	1.39539	0.35354
C	-0.63723	-0.02036	0.60193
C	0.26346	-1.22064	0.53509
C	1.52069	-1.36387	0.07023
C	2.43707	-0.39271	-0.54091
C	2.11480	0.84088	-0.97966
C	0.75559	1.48737	-0.97174
C	-1.35178	2.22971	0.21447
C	-2.37049	1.33956	-0.53192
C	-1.85846	-0.13424	-0.36310
C	0.80046	1.88861	1.53217
H	-1.04248	0.01096	1.62560
C	-2.96803	-1.10000	0.01721
C	-3.12015	-1.65082	1.22798
C	-3.94446	-1.39819	-1.09862
O	4.40144	-1.15117	0.60395
H	0.15244	1.07115	-1.79311
C	3.85896	-0.88365	-0.69524
H	1.94896	-2.36128	0.16956
H	-0.20020	-2.12542	0.92824
H	2.91862	1.44108	-1.40489
H	-1.72930	2.46434	1.21765
H	-1.17521	3.18648	-0.29047
H	-2.43580	1.60433	-1.59221

H	-3.37544	1.45707	-0.11333
H	-1.47307	-0.47006	-1.33556
H	0.21966	1.87060	2.46253
H	1.69157	1.27006	1.67509
H	1.13293	2.92134	1.36565
H	-3.95293	-2.31793	1.43841
H	-2.43724	-1.46727	2.05216
H	-3.43200	-1.86637	-1.95036
H	-4.40515	-0.47765	-1.48124
H	-4.74502	-2.06818	-0.77002
H	5.22573	-1.64711	0.47619
H	3.86611	-1.80471	-1.30034
H	4.46270	-0.13418	-1.22676
H	0.88263	2.54993	-1.21295

Conformer 7

Energy: -659.99598 Hartree (Rel: 0.8 kcal/mol)

XYZ coordinates for conf 7:

C	-0.15392	1.51546	0.23763
C	-0.68478	0.12127	0.66684
C	0.28298	-1.00211	0.90767
C	1.58707	-1.13321	0.59369
C	2.50834	-0.21662	-0.09081
C	2.16934	0.89408	-0.77520
C	0.78833	1.45134	-0.99598
C	-1.47498	2.21700	-0.17253
C	-2.35374	1.14216	-0.85149
C	-1.77700	-0.24132	-0.38698
C	0.53328	2.25711	1.39367
H	-1.20850	0.29386	1.62035
C	-2.86309	-1.21763	0.03166
C	-3.12075	-1.57826	1.29500
C	-3.68453	-1.76524	-1.11409
O	4.15283	-1.88689	-0.60994
H	0.29725	0.88036	-1.79900
C	3.96882	-0.60589	0.00584
H	2.05724	-2.06948	0.89190
H	-0.16736	-1.85367	1.41777
H	2.97980	1.45546	-1.23958
H	-1.97383	2.58688	0.73202
H	-1.29712	3.08673	-0.81557
H	-2.32172	1.22548	-1.94262
H	-3.40267	1.24905	-0.55604
H	-1.26184	-0.69667	-1.24381
H	-0.14469	2.34909	2.25106
H	1.43606	1.73748	1.72870
H	0.82423	3.27011	1.08726
H	-3.93071	-2.26621	1.52635
H	-2.54985	-1.21239	2.14329
H	-3.04991	-2.32119	-1.81797
H	-4.47563	-2.43520	-0.76327
H	-4.15286	-0.95632	-1.69061
H	5.01084	-2.22991	-0.31427
H	4.59382	0.15616	-0.48170
H	4.27021	-0.65405	1.06402
H	0.89235	2.47069	-1.38828

Conformer 8

Energy: -659.99534 Hartree (Rel: 1.1 kcal/mol)

XYZ coordinates for conf 8:

C	-0.61033	1.79812	0.03955
C	-0.82125	0.38397	0.72590
C	0.25736	-0.15062	1.64200
C	1.57043	-0.28418	1.37245
C	2.25367	0.21143	0.17021
C	1.90428	1.37435	-0.41412
C	0.85129	2.30025	0.13803
C	-1.04926	1.58398	-1.44203
C	-1.91068	0.31520	-1.44049
C	-1.16881	-0.59946	-0.45022
C	-1.52314	2.83438	0.72189

H	-1.73555	0.45767	1.32675
C	-1.88629	-1.86933	-0.01574
C	-3.18142	-1.89388	0.32413
C	-1.03835	-3.11848	0.02523
O	2.90961	-1.92050	-0.69161
H	0.91603	3.27026	-0.37054
C	3.39941	-0.61843	-0.34877
H	2.19130	-0.82085	2.09142
H	-0.09666	-0.56020	2.58754
H	2.43770	1.68880	-1.31019
H	-1.57097	2.46044	-1.84374
H	-0.16780	1.41643	-2.07303
H	-2.01563	-0.13828	-2.43296
H	-2.92109	0.53476	-1.07312
H	-0.21856	-0.88897	-0.91687
H	-2.57996	2.56108	0.61523
H	-1.30389	2.90786	1.79476
H	-1.38844	3.82998	0.28115
H	-3.66434	-2.81286	0.64845
H	-3.80827	-1.00584	0.29795
H	-0.15352	-2.96843	0.65724
H	-1.59603	-3.98135	0.40370
H	-0.66107	-3.36568	-0.97702
H	3.68068	-2.47974	-0.87785
H	3.85871	-0.12593	-1.21824
H	4.17324	-0.70215	0.43225
H	1.06585	2.48339	1.20187

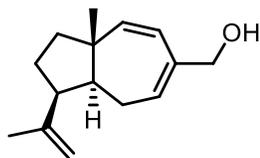
Conformer 9

Energy: -659.99483 Hartree (Rel: 1.5 kcal/mol)

XYZ coordinates for conf 9:

C	-0.51000	1.74623	0.17127
C	-0.82058	0.29459	0.73364
C	0.27029	-0.45902	1.46177
C	1.54155	-0.67034	1.06821
C	2.19403	-0.07586	-0.10686
C	1.92988	1.18355	-0.50445
C	0.99276	2.11086	0.22506
C	-1.04866	1.72526	-1.28991
C	-2.07946	0.59209	-1.32823
C	-1.40784	-0.50839	-0.48951
C	-1.28487	2.78363	1.00688
H	-1.65204	0.40048	1.44052
C	-2.26517	-1.70324	-0.10074
C	-3.56554	-1.60205	0.20397
O	-1.55651	-3.03715	-0.06230
O	4.28589	-1.22218	0.08290
H	1.11224	3.12849	-0.16705
C	3.21643	-0.92591	-0.82451
H	2.15635	-1.35400	1.65258
H	-0.05276	-0.97151	2.36773
H	2.45318	1.57482	-1.37611
H	-1.45994	2.69674	-1.58800
H	-0.23312	1.49139	-1.98559
H	-2.31909	0.25577	-2.34355
H	-3.01815	0.91385	-0.86064
H	-0.54935	-0.88066	-1.06503
H	-2.36653	2.61282	0.94788
H	-0.99662	2.73219	2.06454
H	-1.08650	3.80267	0.65227
H	-4.14531	-2.47402	0.49810
H	-4.10150	-0.65706	0.17810
H	-0.68884	-3.00266	0.60882
H	-2.21983	-3.84251	0.26936
H	-1.16759	-3.29982	-1.05608
H	4.78422	-1.96655	-0.28965
H	2.74927	-1.86036	-1.17150
H	3.58954	-0.39161	-1.71089
H	1.28732	2.14337	1.28526

Revised structure of 53{3}, i.e. 56{3-rev} (CD₃OD)



					Conf1	Conf2	Conf3	Conf4
Rel energy (kcal/mol):					0.00	0.04	2.61	2.63
C-nom	iGau	Exp	Calc	diff	1	2	3	4
C1-C	1	46.80	48.33	1.53	[48.94	49.38	43.28	42.26]
C2-CH2	8	40.50	39.82	-0.68	[40.46	40.62	42.01	41.87]
C3-CH2	9	29.70	30.30	0.60	[29.41	32.70	32.63	32.56]
C4-CH	10	48.70	48.57	-0.13	[50.83	47.65	50.99	50.98]
C5-CH	2	45.70	46.77	1.07	[48.15	46.62	56.03	56.03]
C6-CH2*	3	29.50	30.81	1.31	[29.81	30.74	133.30	133.32]
C7-CH*	4	129.90	130.99	1.09	[131.59	132.31	127.50	126.81]
C8-C*	5	134.60	133.50	-1.10	[134.42	134.36	134.41	134.48]
C9-CH*	6	122.80	123.97	1.17	[124.19	125.35	132.63	132.49]
C10-CH*	7	144.50	142.26	-2.24	[143.99	144.73	48.45	48.29]
C11-C	13	146.70	147.74	1.04	[148.91	148.35	149.80	149.75]
C12-CH2	14	112.90	112.72	-0.18	[115.01	112.06	112.38	112.35]
C13-CH3	15	24.30	24.49	0.19	[22.46	28.07	27.06	26.96]
C14-CH3	11	19.00	19.20	0.20	[20.30	19.33	25.04	25.03]
C15-CH2	18	70.70	70.48	-0.22	[71.01	71.54	71.48	71.22]
13C chem shifts: CRMSD=1.04ppm (CMAE=0.85) N=15 {-2.24 1.53}								
Fractions:					0.511	0.477	0.006	0.006

Conformer 1

Energy: -659.98900 Hartree (Rel: 0.0 kcal/mol)

XYZ coordinates for conf 1:

C	-0.13624	1.34840	0.11206
C	-0.49536	-0.04841	-0.48914
C	0.02067	-1.25853	0.28827
C	1.51683	-1.37193	0.41281
C	2.49302	-0.46255	0.19824
C	2.36691	0.95321	-0.19784
C	1.28025	1.74542	-0.23012
C	-1.17718	2.26277	-0.58021
C	-2.48117	1.45343	-0.54940
C	-2.04881	-0.01506	-0.82560
C	-0.30040	1.41887	1.64986
H	0.00709	-0.08267	-1.46322
C	-2.93160	-1.08445	-0.19582
C	-3.35505	-2.12070	-0.93381
C	-3.34964	-0.96581	1.25368
O	4.63611	-0.78850	-0.83585
H	1.42890	2.78794	-0.51413
C	3.93154	-0.89714	0.40745
H	1.84791	-2.36213	0.72876
H	-0.34114	-2.17120	-0.20540
H	3.31762	1.41010	-0.46830
H	-1.26603	3.24192	-0.09430
H	-0.86851	2.44018	-1.61963
H	-3.21647	1.80348	-1.28201
H	-2.94992	1.54701	0.43554
H	-2.11736	-0.17872	-1.90660
H	-1.30817	1.13462	1.97123
H	0.41424	0.76168	2.15462
H	-0.11549	2.44140	1.99953
H	-3.98011	-2.90599	-0.51416
H	-3.09276	-2.22044	-1.98495
H	-4.00059	-0.09714	1.41559
H	-3.90070	-1.85528	1.57468
H	-2.49177	-0.84057	1.92439
H	5.58486	-0.80939	-0.63399
H	4.40598	-0.25070	1.16244

H	3.96503	-1.92853	0.78626
H	-0.41422	-1.30256	1.29799

Conformer 2

Energy: -659.98906 Hartree (Rel: 0.0 kcal/mol)

XYZ coordinates for conf 2:

C	-0.04827	1.32815	0.03258
C	-0.59058	-0.01479	-0.56255
C	-0.04652	-1.27708	0.10526
C	1.44693	-1.46263	0.07711
C	2.44448	-0.61599	-0.26416
C	2.35360	0.80622	-0.63959
C	1.31831	1.65683	-0.51834
C	-1.12352	2.33797	-0.43400
C	-2.45297	1.60666	-0.21088
C	-2.17421	0.13581	-0.62385
C	0.03553	1.31240	1.57919
H	-0.24925	-0.03961	-1.60393
C	-2.99388	-0.92533	0.10296
C	-3.33055	-0.86553	1.39783
C	-3.43477	-2.09258	-0.75196
O	4.65195	-0.41628	0.66239
H	1.47511	2.68836	-0.83549
C	3.86163	-1.15289	-0.27850
H	1.75494	-2.46817	0.36712
H	-0.48588	-2.15699	-0.38671
H	3.28469	1.21717	-1.02791
H	-1.06187	3.29494	0.09819
H	-0.98302	2.54847	-1.50338
H	-3.27805	2.03664	-0.78924
H	-2.74199	1.67081	0.84245
H	-2.43760	0.04314	-1.68468
H	-0.91340	1.01663	2.03952
H	0.80705	0.61877	1.92582
H	0.29301	2.31129	1.95038
H	-3.91155	-1.65745	1.86497
H	-3.05036	-0.03785	2.04329
H	-2.57994	-2.58196	-1.23727
H	-3.97375	-2.84686	-0.16990
H	-4.09248	-1.74959	-1.56301
H	5.58247	-0.62762	0.48613
H	3.86451	-2.22563	-0.03869
H	4.28341	-1.03934	-1.29036
H	-0.39300	-1.34825	1.14689

Conformer 3

Energy: -659.98491 Hartree (Rel: 2.6 kcal/mol)

XYZ coordinates for conf 3:

C	0.37373	-1.20379	0.23194
C	0.44339	0.09862	-0.64320
C	-0.38937	1.25310	-0.16194
C	-1.69070	1.17839	0.17467
C	-2.57709	0.00522	0.18334
C	-2.24384	-1.29923	0.05314
C	-0.91148	-1.99125	-0.08511
C	1.63822	-2.00800	-0.22492
C	2.36884	-1.13881	-1.27482
C	1.95899	0.31997	-0.97279
C	0.43932	-0.91722	1.74479
H	0.01377	-0.19253	-1.61560
C	2.83771	1.03993	0.05248
C	3.78412	0.42964	0.77948
C	2.67918	2.54432	0.16359
O	-4.46598	1.19805	-0.70015
H	-0.93700	-2.88301	0.56067
C	-4.04010	0.35218	0.37483
H	-2.18462	2.11013	0.44654
H	0.07076	2.23557	-0.13147
H	-3.07965	-2.00047	0.04967
H	2.28654	-2.20453	0.63568
H	1.36486	-2.98567	-0.63884

H	2.00833	-1.39269	-2.27902
H	3.45215	-1.29076	-1.27983
H	2.01742	0.92463	-1.88956
H	1.32290	-0.32355	1.99686
H	-0.44618	-0.37996	2.09572
H	0.50060	-1.86354	2.29755
H	4.42520	0.99642	1.45114
H	3.96057	-0.64035	0.74608
H	1.80838	2.82206	0.76909
H	3.55720	2.99708	0.63539
H	2.54258	3.00774	-0.82178
H	-5.31908	1.58310	-0.44424
H	-4.64624	-0.56388	0.41720
H	-4.16703	0.87705	1.33541
H	-0.84924	-2.39556	-1.10841

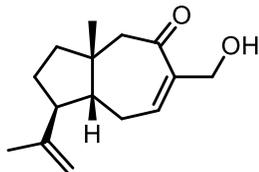
Conformer 4

Energy: -659.98487 Hartree (Rel: 2.6 kcal/mol)

XYZ coordinates for conf 4:

C	0.33401	-1.16285	0.29005
C	0.52377	-0.00302	-0.75088
C	-0.34942	1.20421	-0.55297
C	-1.68097	1.17158	-0.35883
C	-2.57658	0.00748	-0.27839
C	-2.24805	-1.29846	-0.15729
C	-0.91495	-1.99582	-0.05582
C	1.63337	-2.01927	0.10746
C	2.49648	-1.30621	-0.95952
C	2.07069	0.17846	-0.92118
C	0.22476	-0.65773	1.74209
H	0.21513	-0.43721	-1.71584
C	2.82638	1.04260	0.09058
C	3.67616	0.54871	1.00191
C	2.66412	2.54587	-0.02728
O	-4.39109	1.17991	0.76878
H	-1.01829	-2.79047	0.69930
C	-4.04720	0.36980	-0.36246
H	-2.19415	2.12776	-0.27140
H	0.11244	2.18370	-0.62770
H	-3.08743	-1.99507	-0.13342
H	2.17107	-2.08858	1.05915
H	1.39832	-3.04697	-0.19335
H	2.25717	-1.70343	-1.95339
H	3.57043	-1.45178	-0.81107
H	2.24703	0.64637	-1.90077
H	1.07955	-0.02909	2.00794
H	-0.68963	-0.08020	1.90382
H	0.20916	-1.51296	2.42998
H	4.23649	1.20972	1.65949
H	3.84816	-0.51376	1.13878
H	1.72598	2.89362	0.42107
H	3.47911	3.06928	0.48296
H	2.65405	2.86782	-1.07646
H	-5.23876	1.60861	0.57123
H	-4.23741	0.92824	-1.29251
H	-4.66158	-0.54136	-0.39162
H	-0.74356	-2.53563	-1.00123

Originally assigned (incorrect) structure of 57{3} (CDCl₃)



Rel energy (kcal/mol):					Conf1	Conf2	Conf3	Conf4
					0.00	0.21	0.30	0.79
C-nom	iGau	Exp	Calc	diff	1	2	3	4
C1-C	5	139.80	141.09	1.29	[141.62	140.34	140.65	142.04]
C2-CH	4	144.40	144.40	-0.00	[144.20	145.60	143.87	143.17]
C3-CH2	3	30.40	34.47	4.07	[32.71	36.58	35.88	32.36]
C4-CH	2	48.70	55.78	7.08	[57.09	55.58	53.46	56.66]
C5-C	1	40.70	47.40	6.70	[49.32	45.69	45.41	49.20]
C6-CH2	7	59.10	56.89	-2.21	[57.41	56.60	55.99	57.74]
C7-C	6	204.20	203.12	-1.08	[203.28	202.78	203.65	202.18]
C8-CH2	8	42.10	41.92	-0.18	[39.50	43.25	45.36	39.75]
C9-CH2	9	28.90	30.00	1.10	[31.23	29.22	28.43	30.94]
C10-CH	10	50.70	53.46	2.76	[51.94	55.65	54.30	51.53]
C11-C	13	146.00	149.02	3.02	[150.11	147.87	148.19	149.88]
C12-CH2	14	113.70	106.92	-6.78	[106.00	108.72	106.81	105.90]
C13-CH3	15	24.10	22.99	-1.11	[23.23	22.80	22.69	23.24]
C14-CH2	17	67.80	66.10	-1.70	[66.18	66.30	66.06	65.36]
C15-CH3	11	19.50	31.05	11.55	[31.71	30.90	29.94	31.44]
13C chem shifts: RMSD=4.62ppm (MAE=3.38) N=15 {-6.78 11.55}								
Fractions:					0.390	0.273	0.234	0.103

Conformer 1

Energy: -735.23894 Hartree (Rel: 0.0 kcal/mol)

XYZ coordinates for conf 1:

C	-0.45559	1.55229	0.23302
C	-1.00265	0.21822	0.85984
C	-0.10442	-0.42408	1.94477
C	1.17005	-1.07372	1.46272
C	2.09242	-0.59785	0.60175
C	2.02036	0.75007	-0.01788
C	1.05953	1.78712	0.52059
C	-0.71398	1.40494	-1.29177
C	-0.69073	-0.10366	-1.57372
C	-1.33702	-0.76017	-0.33429
C	-1.20531	2.76817	0.80996
H	-1.93917	0.46601	1.37180
C	-2.83571	-1.02393	-0.42088
C	-3.64112	-0.51806	-1.36244
C	-3.38349	-1.92322	0.66449
O	2.77384	1.03535	-0.95552
C	3.27904	-1.43778	0.16293
O	3.28205	-1.66743	-1.24332
H	3.32838	-0.77123	-1.62608
H	-0.69127	-1.19156	2.46157
H	0.12728	0.32774	2.71473
H	1.34457	-2.07939	1.84580
H	1.20330	1.87102	1.60563
H	1.35322	2.74198	0.07394
H	-1.70359	1.81360	-1.52876
H	0.01567	1.96224	-1.89019
H	0.34204	-0.45792	-1.66535
H	-1.19494	-0.37181	-2.50714
H	-0.85808	-1.73015	-0.14375
H	-2.28259	2.67587	0.63083
H	-1.04953	2.85906	1.89235
H	-0.86433	3.70064	0.34419
H	-4.70662	-0.73549	-1.36538
H	-3.28297	0.12266	-2.16239
H	-3.18030	-1.52002	1.66595

H	-4.46528	-2.05924	0.57110
H	-2.90853	-2.91337	0.62618
H	4.21392	-0.94524	0.47498
H	3.24344	-2.41869	0.64608

Conformer 2

Energy: -735.23802 Hartree (Rel: 0.2 kcal/mol)

XYZ coordinates for conf 2:

C	0.40067	-1.04097	0.07749
C	0.74955	0.45471	-0.27441
C	-0.11262	1.09096	-1.39532
C	-1.54905	1.37391	-1.03418
C	-2.45785	0.56631	-0.45147
C	-2.18309	-0.84289	-0.07742
C	-0.92768	-1.53558	-0.56612
C	1.58351	-1.88703	-0.50758
C	2.43098	-0.92587	-1.35646
C	2.26117	0.45385	-0.69364
C	0.31970	-1.22500	1.60597
H	0.60029	1.07376	0.61625
C	3.20253	0.76901	0.46446
C	4.05969	-0.10676	1.00357
C	3.15364	2.19898	0.95635
O	-2.99675	-1.46070	0.61818
C	-3.86263	1.05273	-0.13504
O	-4.17746	0.96309	1.25002
H	-4.06644	0.01554	1.45398
H	-0.06946	0.47251	-2.30419
H	0.34860	2.04495	-1.67210
H	-1.88219	2.38735	-1.26002
H	-1.05233	-2.59775	-0.33396
H	-0.86388	-1.44121	-1.65771
H	2.17775	-2.29837	0.31520
H	1.22363	-2.74170	-1.09090
H	2.03071	-0.87644	-2.37673
H	3.47715	-1.23522	-1.44544
H	2.42125	1.24969	-1.43535
H	1.25417	-0.90313	2.07727
H	-0.49789	-0.64118	2.04468
H	0.15399	-2.27802	1.86447
H	4.72344	0.18491	1.81403
H	4.14362	-1.13486	0.66592
H	2.15326	2.47730	1.31185
H	3.85879	2.36615	1.77612
H	3.40065	2.89783	0.14501
H	-3.96576	2.10477	-0.41770
H	-4.58676	0.47583	-0.73339

Conformer 3

Energy: -735.23880 Hartree (Rel: 0.3 kcal/mol)

XYZ coordinates for conf 3:

C	0.33858	-1.01828	0.27134
C	0.88937	0.43012	-0.02995
C	-0.03730	1.33054	-0.88296
C	-1.40019	1.60302	-0.30255
C	-2.36658	0.71832	0.01466
C	-2.23295	-0.74772	-0.17532
C	-0.91324	-1.38385	-0.57900
C	1.50549	-1.96188	-0.14277
C	2.27323	-1.20724	-1.23154
C	2.28281	0.25691	-0.75010
C	0.01233	-1.20018	1.76561
H	1.03611	0.94142	0.92743
C	3.44433	0.66456	0.14939
C	4.33690	-0.18564	0.67043
C	3.55045	2.15072	0.41071
O	-3.21829	-1.47205	0.00354
C	-3.68931	1.17187	0.61057
O	-4.81283	0.78084	-0.16989
H	-4.75093	-0.19220	-0.19730
H	-0.14143	0.89512	-1.88694

H	0.46977	2.28970	-1.03057
H	-1.62759	2.65419	-0.12364
H	-1.08451	-2.46311	-0.51958
H	-0.73032	-1.15420	-1.63819
H	2.15625	-2.12859	0.72335
H	1.14746	-2.94507	-0.46847
H	1.72996	-1.26789	-2.18333
H	3.27568	-1.60550	-1.41620
H	2.31521	0.93270	-1.61654
H	0.89900	-0.99726	2.37708
H	-0.78219	-0.52289	2.09883
H	-0.31241	-2.22723	1.97389
H	5.14737	0.17049	1.30194
H	4.30719	-1.25611	0.49246
H	2.63597	2.55108	0.86825
H	4.38797	2.38526	1.07467
H	3.69437	2.70150	-0.52930
H	-3.77546	0.77675	1.63614
H	-3.71194	2.26391	0.67576

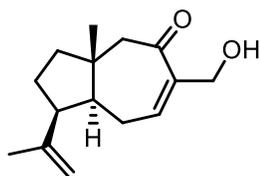
Conformer 4

Energy: -735.23928 Hartree (Rel: 0.8 kcal/mol)

XYZ coordinates for conf 4:

C	-0.48770	1.48792	0.42722
C	-1.02409	0.07490	0.85295
C	-0.07683	-0.74546	1.76070
C	1.14434	-1.33761	1.09981
C	2.01350	-0.76204	0.24394
C	1.95613	0.66851	-0.15107
C	1.05460	1.63436	0.59124
C	-0.90516	1.62628	-1.06106
C	-0.91636	0.19695	-1.61729
C	-1.45073	-0.68388	-0.46607
C	-1.12610	2.59330	1.28959
H	-1.92544	0.24494	1.45254
C	-2.94943	-0.96109	-0.47633
C	-3.83383	-0.31835	-1.24824
C	-3.39981	-2.04345	0.47893
O	2.70363	1.08486	-1.04280
C	3.10488	-1.57655	-0.43268
O	4.39643	-0.99176	-0.32834
H	4.30927	-0.13434	-0.78315
H	-0.64904	-1.57270	2.19509
H	0.22764	-0.12626	2.61848
H	1.31740	-2.39079	1.32315
H	1.29905	1.55913	1.65978
H	1.34500	2.63707	0.26270
H	-1.91406	2.05349	-1.11234
H	-0.24168	2.29809	-1.61755
H	0.10460	-0.11608	-1.86382
H	-1.50098	0.09754	-2.53672
H	-0.95024	-1.66133	-0.49169
H	-2.21832	2.56724	1.20290
H	-0.86859	2.47441	2.34960
H	-0.78617	3.58709	0.97401
H	-4.89426	-0.55476	-1.20229
H	-3.54896	0.45877	-1.95091
H	-3.12670	-1.80759	1.51644
H	-4.48360	-2.19013	0.44329
H	-2.91593	-3.00067	0.24021
H	3.16692	-2.56609	0.03027
H	2.83316	-1.72454	-1.49075

Revised structure of 57{3}, i.e. 59{3-rev} (CDCl₃)



Rel energy (kcal/mol): **Conf1** **Conf2** **Conf3** **Conf4** **Conf5** **Conf6**
 0.00 0.27 0.46 0.58 1.66 1.85

C-nom	iGau	Exp	Calc	diff	1	2	3	4	5	6
C1-C	5	139.80	138.54	-1.26	[138.93	138.35	138.50	138.01	138.36	137.80]
C2-CH	4	144.40	142.99	-1.41	[142.65	143.15	143.00	143.54	142.76	143.68]
C3-CH2	3	30.40	30.23	-0.17	[29.38	30.31	30.63	31.37	31.59	32.59]
C4-CH	2	48.70	50.20	1.50	[50.76	49.95	50.00	48.73	52.96	51.95]
C5-C	1	40.70	42.12	1.42	[42.13	42.50	41.62	42.14	42.11	41.59]
C6-CH2	7	59.10	59.04	-0.06	[59.03	58.60	59.27	58.85	61.69	61.30]
C7-C	6	204.20	203.01	-1.19	[204.00	203.46	201.40	201.52	203.71	202.57]
C8-CH2	8	42.10	41.18	-0.92	[41.18	40.86	41.40	41.15	41.89	42.68]
C9-CH2	9	28.90	29.57	0.67	[27.80	31.48	28.35	31.76	31.97	32.47]
C10-CH	10	50.70	49.83	-0.87	[51.14	47.84	50.94	47.94	51.63	51.19]
C11-C	13	146.00	146.78	0.78	[146.35	147.22	146.27	147.15	149.08	149.27]
C12-CH2	14	113.70	113.97	0.27	[115.53	112.02	115.36	111.84	112.79	112.39]
C13-CH3	15	24.10	24.14	0.04	[21.31	27.88	21.60	27.68	26.63	26.90]
C14-CH2	17	67.80	69.44	1.64	[69.77	69.77	68.71	68.85	69.71	69.17]
C15-CH3	11	19.50	18.97	-0.53	[18.85	18.64	18.94	18.79	22.88	22.82]

13C chem shifts: RMSD=1.00ppm (MAE=0.85) N=15 {-1.41 1.64}

Fractions: 0.388 0.248 0.178 0.146 0.024 0.017

Conformer 1

Energy: -735.23165 Hartree (Rel: 0.0 kcal/mol)

XYZ coordinates for conf 1:

C	-0.26515	1.25704	0.01157
C	-0.82017	-0.03786	-0.64668
C	-0.26352	-1.35661	-0.11274
C	1.21745	-1.58437	-0.25685
C	2.28046	-0.75290	-0.32046
C	2.29239	0.73886	-0.22445
C	1.10882	1.62695	-0.57717
C	-1.33701	2.29513	-0.40160
C	-2.67368	1.56141	-0.21386
C	-2.40334	0.10364	-0.68426
C	-0.15866	1.18784	1.54879
H	-0.50829	0.00943	-1.69864
C	-3.22236	-0.97475	0.01253
C	-3.83550	-1.91940	-0.71444
C	-3.35991	-0.96818	1.51926
O	3.35103	1.28752	0.09946
C	3.68107	-1.35397	-0.41281
O	4.46421	-1.13631	0.75520
H	4.50086	-0.16462	0.82956
H	-0.77182	-2.18532	-0.62111
H	-0.51027	-1.49449	0.95073
H	1.47184	-2.64569	-0.26354
H	1.39646	2.63806	-0.26900
H	1.03594	1.63576	-1.67530
H	-1.26920	3.22264	0.17875
H	-1.19994	2.56044	-1.45906
H	-3.49249	2.02241	-0.77621
H	-2.96440	1.58716	0.84114
H	-2.67821	0.04192	-1.74267
H	-1.12069	0.97114	2.02193
H	0.55152	0.42148	1.87865
H	0.19256	2.14951	1.94148
H	-4.42119	-2.70975	-0.25044
H	-3.77747	-1.93448	-1.80062
H	-3.91708	-0.08991	1.86941

H	-3.89566	-1.85738	1.86527
H	-2.38836	-0.94293	2.02666
H	3.60833	-2.43750	-0.54520
H	4.19032	-0.94455	-1.30011

Conformer 2

Energy: -735.23134 Hartree (Rel: 0.3 kcal/mol)

XYZ coordinates for conf 2:

C	-0.23743	1.27264	0.00139
C	-0.83983	-0.01972	-0.62238
C	-0.29697	-1.33258	-0.06087
C	1.18213	-1.58383	-0.17872
C	2.26312	-0.78006	-0.28742
C	2.30834	0.71291	-0.28300
C	1.12662	1.60627	-0.62795
C	-1.29614	2.32955	-0.39400
C	-2.63998	1.63158	-0.14343
C	-2.42088	0.16042	-0.59242
C	-0.09522	1.21530	1.53701
H	-0.56001	-0.00036	-1.68398
C	-3.22005	-0.89385	0.16845
C	-3.46217	-0.85455	1.48464
C	-3.75831	-2.02561	-0.67818
O	3.39082	1.25722	-0.03984
C	3.64939	-1.41740	-0.34819
O	4.45107	-1.13373	0.79265
H	4.51787	-0.16096	0.79036
H	-0.79463	-2.17160	-0.56402
H	-0.57366	-1.44781	0.99770
H	1.41697	-2.64844	-0.12542
H	1.43548	2.62096	-0.35361
H	1.02828	1.59042	-1.72422
H	-1.18457	3.26583	0.16518
H	-1.18992	2.57123	-1.46078
H	-3.46770	2.09813	-0.68805
H	-2.89737	1.68251	0.91843
H	-2.74600	0.08608	-1.63720
H	-1.04308	0.98713	2.03260
H	0.62998	0.45870	1.85514
H	0.25332	2.18366	1.91555
H	-4.03369	-1.63908	1.97477
H	-3.11350	-0.05047	2.12635
H	-2.95752	-2.53233	-1.23326
H	-4.28117	-2.77506	-0.07589
H	-4.45901	-1.64222	-1.43316
H	3.55211	-2.50578	-0.40061
H	4.15703	-1.08483	-1.26792

Conformer 3

Energy: -735.23337 Hartree (Rel: 0.5 kcal/mol)

XYZ coordinates for conf 3:

C	-0.27094	1.26165	0.08157
C	-0.77230	-0.05914	-0.56947
C	-0.29491	-1.34616	0.09670
C	1.18702	-1.57038	0.19890
C	2.26742	-0.75914	0.14467
C	2.32094	0.71901	-0.06052
C	1.13802	1.61134	-0.41867
C	-1.30631	2.28479	-0.44927
C	-2.65277	1.55338	-0.35408
C	-2.34225	0.09117	-0.77794
C	-0.28582	1.25018	1.62418
H	-0.34894	-0.07360	-1.58266
C	-3.23459	-0.97636	-0.15912
C	-3.73852	-1.95331	-0.92593
C	-3.56705	-0.91862	1.31586
O	3.42739	1.26598	0.01292
C	3.64467	-1.37068	0.39876
O	4.57656	-1.13252	-0.64861
H	4.68616	-0.16464	-0.64801
H	-0.71726	-2.20565	-0.44021

H	-0.69646	-1.44110	1.11714
H	1.41989	-2.61735	0.40271
H	1.42568	2.61628	-0.08827
H	1.12554	1.64967	-1.51919
H	-1.28767	3.22896	0.10752
H	-1.08245	2.52054	-1.49891
H	-3.42645	2.00311	-0.98549
H	-3.02382	1.59444	0.67502
H	-2.50285	0.02037	-1.85910
H	-1.27830	1.02896	2.02842
H	0.41171	0.51364	2.03688
H	0.01245	2.23407	2.00561
H	-4.36942	-2.73779	-0.51411
H	-3.54170	-2.00185	-1.99472
H	-4.20549	-0.05694	1.54958
H	-4.10177	-1.81981	1.63119
H	-2.67250	-0.82090	1.94248
H	4.03485	-0.98799	1.35489
H	3.55163	-2.45650	0.49088

Conformer 4

Energy: -735.23387 Hartree (Rel: 0.6 kcal/mol)

XYZ coordinates for conf 4:

C	-0.25304	1.28539	0.07153
C	-0.78985	-0.04031	-0.54385
C	-0.31460	-1.31231	0.15264
C	1.16471	-1.54218	0.27452
C	2.25687	-0.75115	0.17579
C	2.32979	0.71054	-0.11534
C	1.14823	1.60794	-0.46454
C	-1.28474	2.31496	-0.45118
C	-2.63781	1.61019	-0.29191
C	-2.36630	0.13396	-0.68772
C	-0.23975	1.29579	1.61496
H	-0.39763	-0.08252	-1.56854
C	-3.23835	-0.91140	0.00065
C	-3.63003	-0.84280	1.27915
C	-3.66206	-2.07068	-0.87308
O	3.44777	1.23902	-0.11847
C	3.62668	-1.36781	0.45492
O	4.54594	-1.22102	-0.62029
H	4.66556	-0.25694	-0.69353
H	-0.72200	-2.18861	-0.36984
H	-0.73923	-1.38289	1.16532
H	1.38395	-2.58025	0.53220
H	1.45358	2.61590	-0.15954
H	1.11322	1.62804	-1.56503
H	-1.23008	3.27226	0.08030
H	-1.09094	2.51967	-1.51342
H	-3.42411	2.05386	-0.91194
H	-2.97917	1.68305	0.74487
H	-2.57664	0.04217	-1.76029
H	-1.21992	1.05790	2.03893
H	0.47813	0.57819	2.02491
H	0.04597	2.29063	1.97725
H	-4.24672	-1.62177	1.72108
H	-3.36391	-0.01876	1.93510
H	-2.79617	-2.57858	-1.31866
H	-4.24221	-2.81310	-0.31622
H	-4.27496	-1.71604	-1.71357
H	4.03786	-0.92460	1.37548
H	3.51716	-2.44249	0.62608

Conformer 5

Energy: -735.23356 Hartree (Rel: 1.7 kcal/mol)

XYZ coordinates for conf 5:

C	0.37979	-1.09108	0.11090
C	0.78746	0.16175	-0.72313
C	0.14584	1.47985	-0.29941
C	-1.35504	1.56886	-0.37387
C	-2.34364	0.64928	-0.32857

C	-2.22718	-0.82710	-0.12566
C	-0.97006	-1.64344	-0.39087
C	1.52818	-2.11593	-0.18733
C	2.57389	-1.38848	-1.06538
C	2.34787	0.12773	-0.85625
C	0.28122	-0.83016	1.62885
H	0.43554	-0.03176	-1.74722
C	3.17393	0.77271	0.25511
C	3.75258	0.08915	1.25141
C	3.41027	2.26282	0.12484
O	-3.24093	-1.43844	0.22922
C	-3.79216	1.12562	-0.41229
O	-4.52472	0.92021	0.78985
H	-4.48837	-0.04555	0.91891
H	0.53743	2.28703	-0.93261
H	0.44443	1.75198	0.72458
H	-1.70014	2.60152	-0.44791
H	-1.16625	-2.62638	0.05084
H	-0.91582	-1.79349	-1.48021
H	1.97199	-2.45730	0.75422
H	1.14668	-3.01198	-0.68962
H	2.39061	-1.61885	-2.12158
H	3.60073	-1.69584	-0.84672
H	2.61081	0.66869	-1.77603
H	1.21772	-0.43302	2.02840
H	-0.51916	-0.12423	1.87856
H	0.06179	-1.76914	2.15166
H	4.36399	0.59190	1.99708
H	3.65123	-0.98575	1.36514
H	2.47772	2.83805	0.14220
H	4.04971	2.63740	0.93022
H	3.89845	2.49274	-0.83248
H	-3.81452	2.20071	-0.61335
H	-4.28711	0.61964	-1.25673

Conformer 6

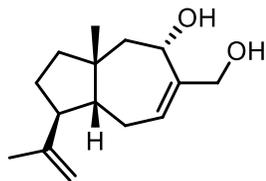
Energy: -735.23429 Hartree (Rel: 1.9 kcal/mol)

XYZ coordinates for conf 6:

C	0.39055	-1.09059	0.23812
C	0.72540	0.16147	-0.63188
C	0.17545	1.48244	-0.10821
C	-1.30964	1.58854	0.08835
C	-2.31455	0.68605	0.13995
C	-2.24857	-0.80039	0.01015
C	-0.98639	-1.64086	-0.16867
C	1.51100	-2.11871	-0.14453
C	2.44301	-1.41985	-1.16043
C	2.25752	0.10156	-0.95136
C	0.41455	-0.83212	1.75946
H	0.24398	-0.00922	-1.60613
C	3.21010	0.75447	0.04855
C	3.85614	0.09041	1.01621
C	3.48172	2.22827	-0.16874
O	-3.31805	-1.42119	0.02687
C	-3.73173	1.19251	0.40359
O	-4.64811	0.87777	-0.63770
H	-4.66678	-0.09653	-0.64118
H	0.45670	2.29308	-0.79549
H	0.64798	1.75035	0.84942
H	-1.62190	2.62422	0.23497
H	-1.19479	-2.57872	0.36051
H	-0.96713	-1.90672	-1.23679
H	2.06285	-2.41485	0.75409
H	1.08814	-3.03990	-0.56139
H	2.12566	-1.66618	-2.18086
H	3.48683	-1.73403	-1.06612
H	2.41795	0.62483	-1.90406
H	1.37439	-0.41696	2.07883
H	-0.37665	-0.14532	2.07834
H	0.26234	-1.77726	2.29509
H	4.55105	0.59999	1.67963

H	3.73293	-0.97500	1.18363
H	2.56941	2.83368	-0.11924
H	4.18576	2.61947	0.57232
H	3.90982	2.39587	-1.16691
H	-4.08500	0.78468	1.36365
H	-3.72169	2.28269	0.49090

Originally assigned (incorrect) structure of 58{4} (CDCl₃)



					Conf1	Conf2
Rel energy (kcal/mol):					0.00	1.88
iGau	jGau	Jexp	Jcalc	diff	1	2
20	22	10.00	4.49	-5.51	[4.29	9.38]
20	21	15.70	15.47	-0.23	[-15.45	-15.88]
12	21	10.00	3.16	-6.84	[3.17	2.82]
23	24	13.70	14.91	1.21	[-14.87	-15.96]
24	40	9.90	11.28	1.38	[11.60	3.67]
For Js: RMSD=4.01Hz N=5					{-6.84	1.38}

C-nom	iGau	Exp	Calc	diff	1	2
C1-C	5	142.30	133.35	-8.95	[133.27	135.15]
C2-CH	4	129.00	131.08	2.08	[131.14	129.71]
C3-CH2	3	26.60	33.42	6.82	[33.56	30.05]
C4-CH	2	49.90	55.44	5.54	[55.28	59.31]
C5-C	1	41.90	43.90	2.00	[43.79	46.51]
C6-CH2	7	51.00	44.07	-6.93	[44.03	44.91]
C7-CH	6	70.20	71.23	1.03	[71.00	76.78]
C8-CH2	8	42.30	45.19	2.89	[45.35	41.41]
C9-CH2	9	27.90	29.05	1.15	[28.93	31.93]
C10-CH	10	49.50	55.51	6.01	[55.65	52.19]
C11-C	13	147.00	148.65	1.65	[148.55	151.06]
C12-CH2	14	113.20	107.60	-5.60	[107.68	105.63]
C14-CH2	17	69.90	71.52	1.62	[71.62	69.21]
C15-CH3	11	18.40	31.14	12.74	[30.98	34.97]
13C chem shifts: RMSD=5.73ppm (MAE=4.65) N=14					{-8.95	12.74}
Fractions:					0.960	0.040

NOTICE:
Mel3 is off

Conformer 1
Energy: -736.42494 Hartree (Rel: 0.0 kcal/mol)
XYZ coordinates for conf 1:

C	0.47946	-1.00003	0.28144
C	0.87712	0.46671	-0.15893
C	-0.10060	1.15255	-1.14262
C	-1.45486	1.49384	-0.56363
C	-2.32473	0.69268	0.06996
C	-2.16363	-0.79975	0.31217
C	-0.90090	-1.46222	-0.24407
C	1.57705	-1.92082	-0.35516
C	2.32436	-1.06011	-1.38308
C	2.30803	0.36317	-0.79769
C	0.53330	-1.11711	1.81856
H	0.91017	1.10250	0.73256
C	3.42346	0.70403	0.18463
C	4.31222	-0.17619	0.66210
C	3.50786	2.16488	0.56990
O	-3.26015	-1.52749	-0.26978
C	-3.59203	1.29262	0.64287
O	-4.79673	0.74316	0.06077
H	-4.78947	0.98058	-0.88228
H	-0.21086	0.54624	-2.05198
H	0.36388	2.08912	-1.47198
H	-1.73377	2.54573	-0.64709
H	-1.00635	-2.52945	-0.01080
H	-0.93451	-1.39480	-1.33827
H	2.26577	-2.26581	0.42378

H	1.14156	-2.81835	-0.80858
H	1.77455	-1.05405	-2.33287
H	3.33282	-1.42444	-1.60538
H	2.38539	1.10288	-1.60800
H	1.53288	-0.85685	2.18454
H	-0.18278	-0.44689	2.30778
H	0.31178	-2.14186	2.14390
H	5.09765	0.13512	1.34694
H	4.30380	-1.22770	0.39319
H	2.57709	2.52182	1.02932
H	4.32343	2.34930	1.27585
H	3.67575	2.79120	-0.31745
H	-3.68130	1.05884	1.71014
H	-3.58826	2.38468	0.53516
H	-2.18992	-0.95186	1.40576
H	-4.06099	-0.98674	-0.12086

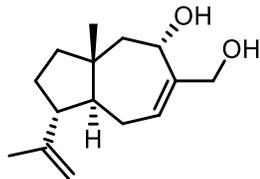
Conformer 2

Energy: -736.42794 Hartree (Rel: 1.9 kcal/mol)

XYZ coordinates for conf 2:

C	-0.43831	1.50960	0.25446
C	-1.01892	0.18280	0.88475
C	-0.12436	-0.49511	1.94544
C	1.13781	-1.14243	1.41890
C	2.09658	-0.60694	0.64952
C	2.17887	0.84566	0.22833
C	1.03880	1.79018	0.63699
C	-0.65438	1.34098	-1.27828
C	-0.68499	-0.17003	-1.53657
C	-1.39115	-0.78007	-0.30840
C	-1.24659	2.72046	0.76904
H	-1.94323	0.45288	1.40923
C	-2.90010	-0.96319	-0.42028
C	-3.66126	-0.43088	-1.38420
C	-3.51581	-1.81964	0.66375
O	2.41460	0.86351	-1.20364
C	3.25403	-1.46213	0.16717
O	3.17966	-1.75494	-1.22931
H	3.05514	-0.88505	-1.65333
H	-0.71901	-1.27344	2.43828
H	0.11395	0.22929	2.73796
H	1.26847	-2.18976	1.69227
H	1.10136	1.90882	1.72703
H	1.30248	2.77737	0.22945
H	-1.61967	1.78514	-1.55193
H	0.11548	1.85080	-1.86487
H	0.33798	-0.55474	-1.58196
H	-1.17254	-0.43487	-2.48081
H	-0.97108	-1.77434	-0.10278
H	-2.31313	2.59369	0.55049
H	-1.13799	2.84580	1.85422
H	-0.91462	3.65146	0.29202
H	-4.73648	-0.59353	-1.40543
H	-3.25446	0.17842	-2.18544
H	-3.30589	-1.41879	1.66465
H	-4.60201	-1.89678	0.55351
H	-3.09594	-2.83497	0.64234
H	4.20935	-0.96056	0.40300
H	3.25258	-2.42577	0.68585
H	3.09084	1.24618	0.70480
H	2.76297	1.73865	-1.43869

Revised structure of 58{4}, i.e. 60{4-rev} (CDCl₃)



Rel energy (kcal/mol):					Conf1	Conf2	Conf3	Conf4	Conf5	
					0.00	0.76	1.28	2.05	3.41	
iGau	jGau	Jexp	Jcalc	diff	1	2	3	4	5	
20	22	10.00	9.54	-0.46	[9.55	9.58	9.44	9.47	7.41]	
20	21	15.70	16.36	0.66	[-16.31	-16.08	-17.16	-16.99	-19.83]	
12	21	10.00	11.75	1.75	[11.77	11.64	11.88	11.78	11.28]	
23	24	13.70	12.98	-0.72	[-13.08	-13.09	-12.08	-12.09	-15.37]	
24	40	9.90	11.54	1.64	[11.54	11.56	11.64	11.65	4.70]	
For Js: RMSD=1.18Hz N=5					{ -0.72	1.75 }				
C-nom	iGau	Exp	Calc	diff	1	2	3	4	5	
C1-C	5	142.30	140.84	-1.46	[140.70	140.74	142.06	142.07	136.21]	
C2-CH	4	129.00	128.46	-0.54	[128.86	128.94	124.70	124.71	133.21]	
C3-CH2	3	26.60	26.19	-0.41	[26.00	26.49	26.79	27.24	27.44]	
C4-CH	2	49.90	48.88	-1.02	[49.14	47.94	49.14	47.99	47.59]	
C5-C	1	41.90	43.87	1.97	[43.90	43.90	43.60	43.62	44.76]	
C6-CH2	7	51.00	51.46	0.46	[51.75	51.81	49.01	49.08	40.92]	
C7-CH	6	70.20	68.27	-1.93	[67.99	68.04	70.51	70.52	72.67]	
C8-CH2	8	42.30	41.73	-0.57	[41.92	41.08	41.86	41.06	40.06]	
C9-CH2	9	27.90	26.74	-1.16	[26.12	28.89	26.32	29.11	27.47]	
C10-CH	10	49.50	51.65	2.15	[52.56	48.18	52.97	48.59	51.18]	
C11-C	13	147.00	147.26	0.26	[146.99	148.32	146.83	148.08	147.79]	
C12-CH2	14	113.20	111.52	-1.68	[113.13	105.65	113.13	105.72	112.56]	
C14-CH2	17	69.90	69.33	-0.57	[69.37	69.39	68.86	68.90	73.80]	
C15-CH3	11	18.40	17.84	-0.56	[17.78	18.05	17.73	17.98	22.27]	
13C chem shifts: RMSD=1.23ppm (MAE=1.05) N=14 {-1.93 2.15}										
					Fractions:	0.701	0.194	0.081	0.022	0.002

NOTICE:
Me13 is off

Conformer 1
Energy: -736.43156 Hartree (Rel: 0.0 kcal/mol)
XYZ coordinates for conf 1:

C	0.24350	1.36358	0.00325
C	0.85156	-0.06074	-0.12107
C	0.25830	-0.98119	-1.19779
C	-1.12677	-1.49715	-0.87579
C	-2.21046	-0.80412	-0.48726
C	-2.28950	0.72098	-0.33110
C	-1.19282	1.34367	0.56087
C	1.23437	2.00214	1.01005
C	2.63336	1.45433	0.62642
C	2.38020	0.18179	-0.25157
C	0.29560	2.16352	-1.31809
H	0.67416	-0.54636	0.84958
C	3.25250	-1.01135	0.09347
C	4.13351	-1.49487	-0.79265
C	3.10232	-1.64192	1.46008
O	-3.57522	1.12907	0.14681
C	-3.48727	-1.55619	-0.19107
O	-3.89726	-1.38031	1.18505
H	-3.16548	-1.69804	1.74046
H	0.92579	-1.84220	-1.32251
H	0.25988	-0.46842	-2.17111
H	-1.24898	-2.57687	-0.97020
H	-1.51294	2.37656	0.75150
H	-1.20074	0.82587	1.53116
H	1.19011	3.09744	0.99787
H	0.97155	1.68243	2.02682

H	3.22318	1.22119	1.51862
H	3.21328	2.18923	0.05850
H	2.59080	0.43578	-1.29769
H	1.32386	2.31085	-1.66481
H	-0.25536	1.68464	-2.13342
H	-0.14303	3.15729	-1.16635
H	4.77591	-2.34129	-0.55978
H	4.24676	-1.05827	-1.78254
H	2.12048	-2.11873	1.57751
H	3.86558	-2.40800	1.62719
H	3.18638	-0.89963	2.26397
H	-4.32544	-1.16707	-0.77531
H	-3.37155	-2.62318	-0.41842
H	-2.22163	1.16789	-1.33101
H	-3.81304	0.51401	0.86867

Conformer 2

Energy: -736.42734 Hartree (Rel: 0.8 kcal/mol)

XYZ coordinates for conf 2:

C	0.23587	1.32684	0.02237
C	0.81113	-0.11394	-0.08472
C	0.20006	-1.01767	-1.16818
C	-1.20151	-1.49552	-0.85783
C	-2.27121	-0.77402	-0.48267
C	-2.31206	0.75277	-0.33134
C	-1.20552	1.34834	0.56637
C	1.23002	1.94936	1.03442
C	2.62087	1.37177	0.66755
C	2.33980	0.08903	-0.19496
C	0.32100	2.11676	-1.30344
H	0.60690	-0.58605	0.88705
C	3.23392	-1.07902	0.18538
C	2.81976	-2.17187	0.83851
C	4.68240	-0.91918	-0.21861
O	-3.58966	1.19571	0.13742
C	-3.57007	-1.49202	-0.19808
O	-3.98946	-1.30339	1.17352
H	-3.27251	-1.64035	1.73688
H	0.84149	-1.89741	-1.28818
H	0.22192	-0.50220	-2.13958
H	-1.35072	-2.57204	-0.95008
H	-1.49829	2.39054	0.74985
H	-1.23581	0.83532	1.53869
H	1.20894	3.04530	1.01684
H	0.95215	1.63985	2.05006
H	3.19017	1.12017	1.56844
H	3.22142	2.09460	0.10571
H	2.57269	0.33017	-1.24286
H	1.35556	2.23163	-1.64390
H	-0.23848	1.65012	-2.11999
H	-0.08896	3.12399	-1.16040
H	3.51565	-2.96532	1.10116
H	1.78707	-2.32427	1.13752
H	5.11771	-0.00763	0.21236
H	5.29077	-1.77054	0.10222
H	4.77567	-0.82253	-1.30924
H	-4.39179	-1.08206	-0.79139
H	-3.47994	-2.56205	-0.42280
H	-2.22611	1.19508	-1.33196
H	-3.84932	0.58740	0.85747

Conformer 3

Energy: -736.43277 Hartree (Rel: 1.3 kcal/mol)

XYZ coordinates for conf 3:

C	-0.29437	1.32283	0.11385
C	-0.90590	-0.10212	0.03855
C	-0.22830	-1.19732	0.86954
C	1.14936	-1.61477	0.40208
C	2.19036	-0.86545	0.00399
C	2.24943	0.66698	0.02473
C	1.06289	1.41331	-0.60804

C	-1.37790	2.13812	-0.63750
C	-2.73530	1.52195	-0.21407
C	-2.40994	0.10580	0.37005
C	-0.17322	1.85740	1.55791
H	-0.83297	-0.40435	-1.01637
C	-3.33276	-1.00255	-0.10307
C	-4.12431	-1.65037	0.76219
C	-3.33688	-1.35687	-1.57346
O	3.47037	1.14888	-0.58587
C	3.47125	-1.55864	-0.43396
O	4.61320	-1.16641	0.32412
H	4.69914	-0.21232	0.13998
H	-0.87374	-2.08420	0.85284
H	-0.19008	-0.89317	1.92690
H	1.31129	-2.69331	0.40061
H	1.36275	2.46834	-0.66490
H	0.94191	1.05882	-1.64294
H	-1.31277	3.21112	-0.42256
H	-1.23319	2.01877	-1.71916
H	-3.42285	1.46328	-1.06372
H	-3.23614	2.13186	0.54488
H	-2.50585	0.15306	1.46182
H	-1.14996	1.92639	2.04816
H	0.46451	1.23444	2.19289
H	0.25820	2.86582	1.54672
H	-4.80159	-2.43859	0.44081
H	-4.12559	-1.41311	1.82378
H	-2.38033	-1.79672	-1.88419
H	-4.12500	-2.08053	-1.80261
H	-3.49425	-0.47388	-2.20594
H	3.36544	-2.64016	-0.30799
H	3.64823	-1.37747	-1.50852
H	2.35930	0.98859	1.06599
H	3.37851	1.05774	-1.54915

Conformer 4

Energy: -736.43073 Hartree (Rel: 2.1 kcal/mol)

XYZ coordinates for conf 4:

C	-0.28229	1.29212	0.05079
C	-0.86819	-0.14556	-0.01238
C	-0.18210	-1.20573	0.85899
C	1.21444	-1.60286	0.43084
C	2.24861	-0.84264	0.03576
C	2.27733	0.69037	0.01811
C	1.08552	1.39670	-0.64879
C	-1.36428	2.07587	-0.73345
C	-2.71956	1.45133	-0.31838
C	-2.37626	0.03970	0.27864
C	-0.19688	1.85406	1.48708
H	-0.76317	-0.46249	-1.05997
C	-3.32423	-1.04562	-0.20372
C	-2.99704	-2.00959	-1.07312
C	-4.72165	-0.95786	0.36757
O	3.49644	1.18114	-0.58907
C	3.55231	-1.52041	-0.35691
O	4.67061	-1.08150	0.41091
H	4.74135	-0.13209	0.19834
H	-0.80410	-2.10792	0.84970
H	-0.17184	-0.87372	1.90840
H	1.39913	-2.67737	0.46055
H	1.36342	2.45669	-0.72293
H	0.99013	1.01826	-1.67784
H	-1.31739	3.15410	-0.54085
H	-1.20216	1.93503	-1.80981
H	-3.38916	1.36109	-1.17996
H	-3.23730	2.07095	0.42109
H	-2.50098	0.09775	1.37027
H	-1.18254	1.90682	1.96149
H	0.44659	1.25882	2.14243
H	0.20933	2.87276	1.46456
H	-3.72985	-2.74590	-1.39505

H	-2.00240	-2.10935	-1.49710
H	-5.18129	0.01540	0.14921
H	-5.37473	-1.73942	-0.03302
H	-4.70299	-1.05428	1.46207
H	3.46689	-2.59985	-0.20106
H	3.74662	-1.36683	-1.43268
H	2.36719	1.04007	1.05227
H	3.41836	1.06509	-1.55092

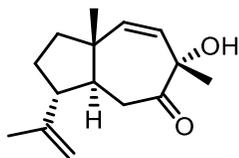
Conformer 5

Energy: -736.42950 Hartree (Rel: 3.4 kcal/mol)

XYZ coordinates for conf 5:

C	-0.40608	1.60021	0.10844
C	-0.69105	0.09534	0.34831
C	-0.09194	-0.52369	1.61279
C	1.38134	-0.82775	1.48853
C	2.28202	-0.31581	0.63221
C	2.08410	0.79674	-0.40366
C	1.10329	1.91823	-0.04807
C	-1.23705	1.82111	-1.18104
C	-2.53245	0.98844	-0.98013
C	-2.22529	-0.03179	0.17217
C	-0.96116	2.51198	1.22589
H	-0.23077	-0.42215	-0.50117
C	-2.72817	-1.44139	-0.07749
C	-3.67156	-1.98157	0.70592
C	-2.13511	-2.22341	-1.22831
O	1.76930	0.25368	-1.69770
C	3.65800	-0.93647	0.54917
O	3.85819	-1.55027	-0.74671
H	3.27278	-2.32591	-0.77807
H	-0.60347	-1.47307	1.82784
H	-0.28281	0.10400	2.49686
H	1.73736	-1.61390	2.15798
H	1.47832	2.34529	0.89123
H	1.22466	2.70699	-0.80291
H	-1.44283	2.88263	-1.36519
H	-0.66961	1.44422	-2.03875
H	-2.81838	0.47664	-1.90470
H	-3.38290	1.62005	-0.70251
H	-2.71250	0.32081	1.08934
H	-2.04886	2.44065	1.32974
H	-0.51482	2.28289	2.20087
H	-0.72426	3.55879	0.99809
H	-4.05319	-2.98605	0.53599
H	-4.09982	-1.43566	1.54381
H	-1.07645	-2.45437	-1.05302
H	-2.66350	-3.17024	-1.37649
H	-2.17733	-1.66049	-2.16921
H	4.44787	-0.18031	0.61568
H	3.81894	-1.67111	1.34862
H	3.06518	1.29620	-0.48101
H	2.46316	-0.41418	-1.85603

Originally assigned correct structure of 61{1} (CDCl₃)



					Conf1	Conf2	Conf3	Conf4
Rel energy (kcal/mol):					0.00	0.73	1.27	1.81
C-nom	iGau	Exp	Calc	diff	1	2	3	4
C1-C	1	46.30	47.61	1.31	[47.26	47.37	50.18	50.17]
C2-CH2	8	39.20	39.18	-0.02	[39.43	38.53	39.05	38.21]
C3-CH2	9	26.10	26.54	0.44	[25.80	28.18	27.47	29.85]
C4-CH	10	50.90	51.52	0.62	[52.45	47.99	53.25	49.13]
C5-CH	2	44.80	46.67	1.87	[47.40	46.46	42.93	41.79]
C6-CH2	3	39.30	38.37	-0.93	[37.58	37.86	43.99	44.28]
C7-C	6	210.30	209.36	-0.94	[209.12	209.33	210.79	210.96]
C8-C	5	78.40	78.45	0.05	[78.49	78.46	78.22	78.10]
C9-CH	4	130.30	131.44	1.14	[132.08	131.92	126.76	126.74]
C10-CH	7	139.40	136.42	-2.98	[135.09	135.18	146.60	146.84]
C11-C	13	145.70	145.99	0.29	[145.73	146.45	146.39	147.51]
C12-CH2	14	111.70	112.64	0.94	[114.39	107.50	112.88	106.56]
C13-CH3	15	18.70	18.32	-0.38	[16.61	23.89	16.83	24.07]
C14-CH3***	11	19.40	19.83	0.43	[19.93	20.22	18.47	18.61]
C15-CH3***	18	27.90	27.60	-0.30	[27.79	27.62	26.45	26.43]
13C chem shifts: RMSD=1.13ppm (MAE=0.84) N=15 {-2.98 1.87}								
Fractions:					0.687	0.199	0.081	0.033

Conformer 1

Energy: -735.23353 Hartree (Rel: 0.0 kcal/mol)

XYZ coordinates for conf 1:

C	-0.12188	1.54442	-0.09788
C	-0.61226	0.07468	-0.00414
C	0.21068	-0.88586	0.87566
C	2.29645	0.93244	-0.79876
C	2.64691	-0.35366	-0.05074
C	1.45432	-1.31696	0.13692
C	1.20095	1.70242	-0.81961
C	-1.29923	2.16523	-0.89857
C	-2.57996	1.48233	-0.35207
C	-2.10672	0.18957	0.39620
C	-0.01846	2.25666	1.27473
H	-0.58006	-0.31376	-1.03139
C	-2.93912	-1.04910	0.12236
C	-3.64245	-1.62698	1.10512
C	-2.94989	-1.61323	-1.28063
H	0.45920	-0.41425	1.83251
O	1.53846	-2.43274	-0.36092
C	3.27588	-0.02546	1.32377
H	1.27622	2.61504	-1.41332
H	-0.37219	-1.78890	1.08230
H	3.15278	1.26335	-1.38471
H	-1.32794	3.25687	-0.80756
H	-1.17138	1.93384	-1.96312
H	-3.27420	1.24590	-1.16413
H	-3.12306	2.13404	0.33959
H	-2.15400	0.37446	1.47585
H	-0.97752	2.27243	1.80378
H	0.72223	1.78903	1.93051
H	0.29228	3.29677	1.12542
H	-4.25711	-2.50673	0.92886
H	-3.63198	-1.23813	2.12093
H	-1.97240	-2.03301	-1.55188
H	-3.69125	-2.41193	-1.37781
H	-3.17987	-0.84467	-2.02941
H	4.17528	0.57575	1.15932
H	2.59828	0.53995	1.96892

H	3.56967	-0.95077	1.83184
O	3.62982	-1.03551	-0.82085
H	3.22956	-1.90823	-1.01649

Conformer 2

Energy: -735.23439 Hartree (Rel: 0.7 kcal/mol)

XYZ coordinates for conf 2:

C	-0.11966	1.51632	-0.13825
C	-0.57436	0.03381	-0.04508
C	0.26025	-0.88279	0.87392
C	2.33434	0.96732	-0.77067
C	2.70025	-0.30828	-0.01191
C	1.52319	-1.29265	0.15696
C	1.21874	1.70631	-0.82302
C	-1.28743	2.09957	-0.97786
C	-2.56673	1.39431	-0.45919
C	-2.07741	0.10911	0.30093
C	-0.07472	2.24347	1.22981
H	-0.49778	-0.36115	-1.06749
C	-2.92280	-1.11630	0.00032
C	-2.49991	-2.17618	-0.69984
C	-4.32755	-1.06087	0.55738
H	0.48330	-0.37847	1.81971
O	1.63197	-2.40515	-0.34402
C	3.29798	0.03933	1.37135
H	1.28554	2.61962	-1.41671
H	-0.29694	-1.79699	1.09462
H	3.19646	1.32111	-1.33444
H	-1.34439	3.19126	-0.90164
H	-1.12569	1.85806	-2.03529
H	-3.22684	1.12686	-1.29030
H	-3.14241	2.04353	0.20796
H	-2.16994	0.29704	1.38076
H	-1.04663	2.23058	1.73522
H	0.66541	1.80803	1.90803
H	0.20353	3.29242	1.07813
H	-3.16168	-3.01724	-0.89280
H	-1.49401	-2.26141	-1.09966
H	-4.87432	-0.18718	0.17840
H	-4.90022	-1.95718	0.30033
H	-4.31093	-0.96722	1.65213
H	4.18818	0.65745	1.21985
H	2.59768	0.59479	2.00085
H	3.60088	-0.87713	1.89003
O	3.71048	-0.97273	-0.76137
H	3.32610	-1.84865	-0.97360

Conformer 3

Energy: -735.23524 Hartree (Rel: 1.3 kcal/mol)

XYZ coordinates for conf 3:

C	-0.08785	1.52998	-0.03535
C	-0.55063	0.05246	0.07390
C	0.22332	-0.84008	1.05451
C	2.24721	0.84312	-0.92091
C	2.37405	-0.59987	-0.43567
C	1.73441	-0.71118	0.96618
C	1.23387	1.70621	-0.75167
C	-1.25105	2.13650	-0.87046
C	-2.53745	1.42362	-0.38391
C	-2.06938	0.13737	0.37655
C	0.00549	2.24436	1.33624
H	-0.42195	-0.37245	-0.92564
C	-2.85398	-1.11857	0.04314
C	-3.61225	-1.71803	0.97025
C	-2.75458	-1.67215	-1.36078
H	-0.05233	-0.63899	2.09527
O	2.42897	-0.66451	1.96721
C	3.85083	-1.00441	-0.38378
H	1.37674	2.70413	-1.17140
H	-0.03181	-1.88935	0.85225
H	3.12360	1.20294	-1.46058

H	-1.30343	3.22669	-0.77062
H	-1.08039	1.91885	-1.93203
H	-3.19231	1.18102	-1.22673
H	-3.12232	2.05968	0.28832
H	-2.19034	0.31312	1.45238
H	-0.95531	2.23369	1.86276
H	0.75502	1.77896	1.98424
H	0.29300	3.29292	1.19659
H	-4.19248	-2.61048	0.74671
H	-3.68106	-1.33676	1.98668
H	-1.74780	-2.05639	-1.57044
H	-3.46212	-2.49305	-1.51181
H	-2.96051	-0.90434	-2.11770
H	4.41060	-0.36529	0.30423
H	4.29153	-0.91653	-1.38349
H	3.94588	-2.04147	-0.05003
O	1.65425	-1.52137	-1.28187
H	1.82000	-1.25584	-2.20121

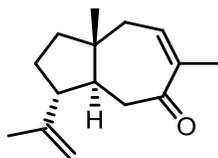
Conformer 4

Energy: -735.23641 Hartree (Rel: 1.8 kcal/mol)

XYZ coordinates for conf 4:

C	-0.08129	1.50562	-0.07741
C	-0.51124	0.01765	0.03577
C	0.26678	-0.83428	1.04984
C	2.28575	0.86488	-0.91139
C	2.43706	-0.56893	-0.40692
C	1.77609	-0.67620	0.98545
C	1.25009	1.70611	-0.76894
C	-1.23927	2.07689	-0.94137
C	-2.52079	1.35287	-0.46180
C	-2.03384	0.06473	0.29302
C	-0.03364	2.23556	1.28845
H	-0.34365	-0.41147	-0.95576
C	-2.83227	-1.17512	-0.07345
C	-2.35278	-2.19846	-0.79143
C	-4.25684	-1.17885	0.43333
H	-0.03146	-0.61479	2.08071
O	2.45309	-0.60788	1.99729
C	3.92154	-0.93863	-0.32525
H	1.37813	2.70311	-1.19554
H	0.03952	-1.89297	0.86869
H	3.16369	1.23971	-1.43812
H	-1.31193	3.16781	-0.86405
H	-1.04888	1.84073	-1.99543
H	-3.16178	1.09426	-1.31080
H	-3.11530	1.98866	0.20219
H	-2.19158	0.23047	1.36910
H	-1.00307	2.20127	1.79812
H	0.71732	1.79923	1.95464
H	0.22524	3.29084	1.14329
H	-2.98087	-3.05267	-1.03380
H	-1.33216	-2.23583	-1.16062
H	-4.81332	-0.30538	0.06784
H	-4.79584	-2.07914	0.12251
H	-4.28139	-1.12634	1.53068
H	4.45528	-0.27751	0.36273
H	4.37647	-0.85440	-1.31883
H	4.03455	-1.96852	0.02469
O	1.75403	-1.51841	-1.25313
H	1.91193	-1.24984	-2.17292

Originally assigned correct structure of 62{2} (CDCl₃)



					Conf1	Conf2
Rel energy (kcal/mol):					0.00	0.77
iGau	jGau	Jexp	Jcalc	diff	1	2
12	16	12.50	12.80	0.30	[12.82	12.72]
12	20	6.00	2.40	-3.60	[2.41	2.36]
16	20	17.00	16.51	-0.49	[-16.51	-16.52]
21	22	4.00	2.95	-1.05	[2.95	2.95]
19	21	17.50	18.21	0.71	[-18.19	-18.28]
For Js: RMSD=1.73Hz N=5					{-3.60	0.71}
C-nom	iGau	Exp	Calc	diff	1	2
C1-C	1	42.40	44.66	2.26	[44.68	44.60]
C2-CH2**	8	41.40	41.70	0.30	[41.90	40.95]
C3-CH2	9	28.30	27.88	-0.42	[27.37	29.74]
C4-CH	10	52.80	53.31	0.51	[54.23	49.91]
C5-CH**	2	45.50	45.70	0.20	[46.00	44.59]
C6-CH2	3	45.90	44.47	-1.43	[44.37	44.86]
C7-C	6	203.60	202.21	-1.39	[202.20	202.24]
C8-C	5	136.90	138.20	1.30	[138.22	138.13]
C9-CH	4	137.50	138.27	0.77	[138.24	138.36]
C10-CH2	7	43.50	43.90	0.40	[43.85	44.09]
C11-C	13	145.80	146.31	0.51	[146.13	146.98]
C12-CH2	14	111.40	111.92	0.52	[113.46	106.25]
C13-CH3	15	18.60	18.28	-0.32	[16.65	24.26]
C14-CH3***	11	20.00	18.98	-1.02	[18.91	19.23]
C15-CH3***	18	22.10	23.71	1.61	[23.71	23.72]
13C chem shifts: RMSD=1.04ppm (MAE=0.86) N=15 {-1.43 2.26}						
Fractions:					0.786	0.214

NOTICE:

this requires swap of C2(CH₂) and C5(CH) -- HMBC is uncertain

another inconsistency - J(H5-H6a) = 6Hz -- possible messy overlap misinterpretation?

Conformer 1

Energy: -660.02989 Hartree (Rel: 0.0 kcal/mol)

XYZ coordinates for conf 1:

C	-0.04329	1.48728	-0.06850
C	0.45145	0.02268	0.04916
C	-0.37271	-1.04298	-0.67574
C	-2.54287	0.97064	0.55418
C	-2.78356	-0.30182	0.16853
C	-1.77096	-1.35619	-0.15934
C	-1.27390	1.74672	0.81580
C	1.19195	2.25957	0.46006
C	2.42759	1.49832	-0.07505
C	1.92795	0.06200	-0.44624
C	-0.34812	1.91111	-1.52016
H	0.45849	-0.21744	1.12228
C	2.80405	-1.06851	0.06224
C	3.42779	-1.88820	-0.79428
C	2.95584	-1.24409	1.55674
H	-0.48360	-0.76014	-1.73347
O	-2.11598	-2.53406	-0.08730
C	-4.21012	-0.81539	0.13878
H	-1.52631	2.81423	0.75948
H	0.16586	-1.99640	-0.66867
H	-0.99598	1.57530	1.86880
H	-3.43643	1.54348	0.80645
H	1.18067	3.31488	0.16402
H	1.18733	2.23520	1.55768

H	3.23019	1.47335	0.66879
H	2.84551	1.98459	-0.96260
H	1.90782	-0.02083	-1.53981
H	0.49511	1.72056	-2.19292
H	-1.22396	1.39248	-1.92350
H	-0.55988	2.98649	-1.55537
H	4.06944	-2.69624	-0.45016
H	3.32085	-1.77906	-1.87122
H	2.01248	-1.55442	2.02442
H	3.70652	-2.00524	1.78971
H	3.25659	-0.31043	2.04900
H	-4.45686	-1.24710	-0.83854
H	-4.92134	-0.01257	0.35324
H	-4.35125	-1.61500	0.87375

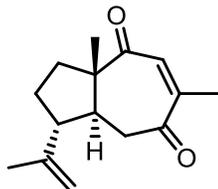
Conformer 2

Energy: -660.03112 Hartree (Rel: 0.8 kcal/mol)

XYZ coordinates for conf 2:

C	-0.05839	1.47212	0.00633
C	0.41251	-0.00201	0.11894
C	-0.40109	-1.03736	-0.66289
C	-2.58955	0.98642	0.52008
C	-2.83529	-0.27303	0.09707
C	-1.82759	-1.33537	-0.21869
C	-1.31967	1.73577	0.84479
C	1.16258	2.21921	0.59866
C	2.41243	1.45008	0.10954
C	1.90113	0.02698	-0.31043
C	-0.29763	1.92662	-1.44847
H	0.36985	-0.25671	1.18762
C	2.79819	-1.09442	0.18631
C	2.46555	-1.96751	1.14479
C	4.14924	-1.16154	-0.48988
H	-0.45973	-0.73061	-1.71799
O	-2.19715	-2.50800	-0.19959
C	-4.26762	-0.76245	0.00374
H	-1.55231	2.80828	0.79794
H	0.11631	-2.00140	-0.65086
H	-1.08718	1.54153	1.90482
H	-3.48276	1.56797	0.75297
H	1.17831	3.27836	0.31689
H	1.10997	2.18070	1.69430
H	3.16485	1.38185	0.90199
H	2.88895	1.95495	-0.73710
H	1.92593	-0.02307	-1.40940
H	0.57080	1.73831	-2.08916
H	-1.16199	1.42721	-1.89810
H	-0.49472	3.00513	-1.47154
H	3.16231	-2.73853	1.46511
H	1.50176	-1.95978	1.64459
H	4.69932	-0.21758	-0.37869
H	4.76843	-1.96557	-0.08032
H	4.03744	-1.33131	-1.56980
H	-4.48417	-1.17105	-0.99044
H	-4.97354	0.04780	0.20765
H	-4.44935	-1.57360	0.71690

Originally assigned correct structure of 63{3} (CDCl₃)



					Conf1	Conf2
Rel energy (kcal/mol):					0.00	0.06
C-nom	iGau	Exp	Calc	diff	1	2
C1-C	1	56.10	58.47	2.37	[57.75	59.26]
C2-CH2	8	34.70	35.03	0.33	[34.28	35.86]
C3-CH2	9	27.90	30.31	2.41	[34.62	25.55]
C4-CH	10	51.50	51.24	-0.26	[49.45	53.21]
C5-CH	2	41.80	41.56	-0.24	[41.39	41.75]
C6-CH2	3	42.80	43.28	0.48	[42.81	43.79]
C7-C	6	202.30	200.90	-1.40	[203.32	198.22]
C8-C	5	146.90	147.91	1.01	[150.02	145.58]
C9-CH	4	132.80	134.07	1.27	[132.15	136.20]
C10-C	7	204.80	203.15	-1.65	[203.34	202.93]
C11-C	12	144.70	145.91	1.21	[146.58	145.18]
C12-CH2	13	112.20	110.86	-1.34	[107.58	114.48]
C13-CH3	14	18.60	20.62	2.02	[24.51	16.32]
C14-CH3***	11	20.10	20.78	0.68	[22.70	18.66]
C15-CH3***	16	21.70	23.30	1.60	[23.05	23.58]
13C chem shifts: RMSD=1.40ppm (MAE=1.22) N=15 {-1.65 2.41}						
Fractions:					0.525	0.475

Conformer 1

Energy: -734.04490 Hartree (Rel: 0.0 kcal/mol)

XYZ coordinates for conf 1:

C	0.10938	1.28763	0.40446
C	-0.46672	-0.10445	-0.01925
C	0.17542	-1.30817	0.66191
C	2.32699	0.59224	-0.83736
C	2.51253	-0.68628	-0.43522
C	1.68960	-1.42894	0.59084
C	1.31683	1.62710	-0.47337
C	-1.07380	2.28713	0.18835
C	-2.26424	1.45394	-0.32382
C	-1.98813	0.02353	0.20193
C	0.58076	1.35402	1.87989
C	-2.88637	-1.03692	-0.41036
C	-2.53204	-1.81024	-1.44431
C	-4.25877	-1.14620	0.21331
O	2.26928	-2.20088	1.34388
C	3.70697	-1.46772	-0.92588
O	1.50350	2.76113	-0.90299
H	-0.30608	-0.19762	-1.10206
H	-0.09432	-1.36413	1.72277
H	-0.21740	-2.23021	0.21031
H	3.06658	1.00902	-1.51910
H	-1.32716	2.76305	1.14199
H	-0.78907	3.08632	-0.49950
H	-2.27953	1.42663	-1.42057
H	-3.22898	1.85212	0.00646
H	-2.17195	0.02771	1.28821
H	-0.23144	1.06738	2.55668
H	1.44100	0.71068	2.09079
H	0.87056	2.38220	2.12169
H	-3.22495	-2.53233	-1.86933
H	-1.55392	-1.75566	-1.91373
H	-4.78475	-0.18249	0.19029
H	-4.88050	-1.88495	-0.30159
H	-4.18613	-1.43625	1.27052

H	4.33270	-1.76613	-0.07852
H	4.30454	-0.88310	-1.62928
H	3.38818	-2.39422	-1.41981

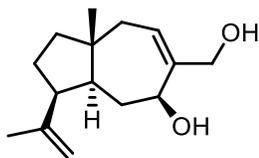
Conformer 2

Energy: -734.04499 Hartree (Rel: 0.1 kcal/mol)

XYZ coordinates for conf 2:

C	0.04974	1.35942	0.30387
C	-0.50495	-0.06613	0.03579
C	0.19284	-1.22701	0.74464
C	2.51232	0.66528	-0.38632
C	2.63981	-0.66098	-0.14139
C	1.56014	-1.64346	0.23598
C	1.36689	1.62246	-0.41184
C	-1.08843	2.25252	-0.24572
C	-2.40245	1.51366	0.10096
C	-2.00994	0.03465	0.42170
C	0.29528	1.65665	1.80567
C	-2.89964	-1.01809	-0.21477
C	-3.62848	-1.84419	0.54727
C	-2.94316	-1.10727	-1.72376
O	1.83170	-2.83696	0.16775
C	3.99267	-1.30899	-0.32362
O	1.56103	2.68482	-0.99599
H	-0.44196	-0.23134	-1.04899
H	0.30147	-0.99775	1.81479
H	-0.43047	-2.12531	0.68787
H	3.41303	1.18024	-0.71695
H	-1.04858	3.26700	0.16142
H	-0.97547	2.34563	-1.33094
H	-3.11471	1.57462	-0.72753
H	-2.90002	1.95918	0.96834
H	-2.07614	-0.10874	1.50704
H	-0.60869	1.47602	2.39639
H	1.10322	1.04995	2.22695
H	0.57144	2.70903	1.93014
H	-4.28339	-2.59588	0.11270
H	-3.60003	-1.79534	1.63349
H	-1.98245	-1.44102	-2.13706
H	-3.70839	-1.81618	-2.05357
H	-3.16116	-0.13556	-2.18467
H	4.29401	-1.83956	0.58660
H	4.75592	-0.56775	-0.57202
H	3.95472	-2.06133	-1.11874

Originally assigned (incorrect) structure of 64{18} (CDCl₃)



Rel energy (kcal/mol):					Conf1	Conf2	Conf3	Conf4
					0.00	0.78	2.03	2.06
C-nom	iGau	Exp	Calc	diff	1	2	3	4
C1-C	5	143.70	140.34	-3.36	[140.41	140.07	139.95	140.73]
C2-CH	4	68.80	73.68	4.88	[73.78	73.35	73.54	73.28]
C3-CH2	3	32.10	35.24	3.14	[35.33	35.45	34.88	30.79]
C4-CH	2	46.20	52.85	6.65	[52.78	53.00	53.29	53.55]
C5-C	1	43.80	43.25	-0.55	[43.12	43.66	43.86	43.40]
C6-CH2	7	42.90	41.77	-1.13	[41.90	41.38	41.54	41.33]
C7-CH	6	128.00	127.04	-0.96	[127.03	127.10	127.39	126.52]
C8-CH2	8	43.60	41.34	-2.26	[41.36	41.29	41.27	41.20]
C9-CH2	9	29.50	28.76	-0.74	[27.93	31.25	31.31	31.15]
C10-CH	10	51.70	50.90	-0.80	[52.02	47.53	47.62	47.52]
C11-C	13	148.90	147.48	-1.42	[147.03	148.83	148.71	148.84]
C12-CH2	14	113.70	114.42	0.72	[115.49	111.17	111.27	111.22]
C13-CH3	15	23.30	22.98	-0.32	[21.11	28.61	28.63	28.64]
C14-CH2	17	69.10	69.38	0.28	[69.41	69.28	69.95	68.85]
C15-CH3	11	19.40	19.20	-0.20	[19.35	18.79	18.76	18.55]
13C chem shifts: RMSD=2.59ppm (MAE=1.83) N=15 {-3.36 6.65}								
Fractions:					0.751	0.201	0.025	0.023

Conformer 1

Energy: -736.42360 Hartree (Rel: 0.0 kcal/mol)

XYZ coordinates for conf 1:

C	-0.50916	1.52139	0.02934
C	-0.74406	0.15894	-0.68653
C	0.20633	-0.99196	-0.34460
C	1.62195	-0.81284	-0.93684
C	2.46007	0.29592	-0.28611
C	2.07425	1.57412	-0.13143
C	0.76007	2.21536	-0.52406
C	-1.80000	2.27692	-0.36657
C	-2.92446	1.23666	-0.20041
C	-2.30193	-0.12593	-0.63790
C	-0.41264	1.43661	1.56583
H	-0.55797	0.37770	-1.74925
C	-2.78341	-1.34337	0.13865
C	-3.32181	-2.37951	-0.52020
C	-2.66882	-1.38705	1.64624
O	2.31469	-2.06210	-0.93495
C	3.83268	-0.11617	0.19247
O	3.75693	-1.14714	1.20401
H	3.23138	-0.78678	1.93803
H	-0.18662	-1.92074	-0.77456
H	0.28619	-1.15720	0.73704
H	1.49939	-0.56505	-2.00224
H	0.77036	3.25757	-0.18116
H	0.68038	2.25909	-1.62158
H	-1.96322	3.17989	0.23405
H	-1.73118	2.59227	-1.41712
H	-3.81258	1.48006	-0.79303
H	-3.24884	1.20245	0.84478
H	-2.60381	-0.31158	-1.67437
H	-1.30928	1.00477	2.01695
H	0.44492	0.84018	1.89044
H	-0.28809	2.44418	1.98285
H	-3.67886	-3.26610	-0.00093
H	-3.42576	-2.37904	-1.60297
H	-3.20998	-0.55970	2.12233
H	-3.08084	-2.32124	2.04031

H	-1.62705	-1.31382	1.97864
H	4.41530	-0.57081	-0.61356
H	4.38710	0.75010	0.57419
H	2.79515	2.24538	0.33635
H	2.70658	-2.16219	-0.04484

Conformer 2

Energy: -736.42365 Hartree (Rel: 0.8 kcal/mol)

XYZ coordinates for conf 2:

C	-0.48243	1.54204	-0.00926
C	-0.75571	0.16003	-0.67436
C	0.18623	-0.98392	-0.28624
C	1.60592	-0.84284	-0.88235
C	2.46522	0.27687	-0.28201
C	2.10003	1.56638	-0.18691
C	0.78941	2.20075	-0.59930
C	-1.76316	2.31015	-0.40836
C	-2.90227	1.30298	-0.17011
C	-2.32034	-0.08827	-0.55989
C	-0.36501	1.49269	1.52775
H	-0.58796	0.33075	-1.74875
C	-2.77947	-1.27082	0.29111
C	-3.00437	-1.22520	1.61015
C	-3.01869	-2.55357	-0.47550
O	2.27926	-2.10231	-0.83268
C	3.83305	-0.13634	0.20850
O	3.74577	-1.12557	1.25987
H	3.22493	-0.73100	1.97952
H	-0.19643	-1.92815	-0.68819
H	0.24785	-1.11078	0.80123
H	1.48511	-0.63614	-1.95674
H	0.80922	3.25612	-0.29964
H	0.70259	2.20039	-1.69723
H	-1.89224	3.24140	0.15638
H	-1.71060	2.57879	-1.47290
H	-3.79973	1.53891	-0.75216
H	-3.20254	1.31849	0.88145
H	-2.65837	-0.31565	-1.57845
H	-1.23547	1.02890	1.99735
H	0.51880	0.93628	1.85127
H	-0.27661	2.51212	1.92499
H	-3.33202	-2.10803	2.15408
H	-2.88407	-0.32315	2.20232
H	-2.13296	-2.85850	-1.04705
H	-3.29738	-3.37970	0.18627
H	-3.82533	-2.41578	-1.20957
H	4.40627	-0.63099	-0.58055
H	4.40139	0.73610	0.55413
H	2.83153	2.24953	0.24578
H	2.67333	-2.17243	0.05944

Conformer 3

Energy: -736.42563 Hartree (Rel: 2.0 kcal/mol)

XYZ coordinates for conf 3:

C	-0.49764	1.54177	-0.00330
C	-0.76378	0.15992	-0.67135
C	0.18526	-0.97856	-0.28491
C	1.60488	-0.82517	-0.87798
C	2.45593	0.29499	-0.26658
C	2.08330	1.58140	-0.17219
C	0.77113	2.20638	-0.59358
C	-1.78241	2.30402	-0.40019
C	-2.91606	1.29018	-0.16386
C	-2.32689	-0.09712	-0.55718
C	-0.37722	1.48901	1.53351
H	-0.59751	0.33384	-1.74560
C	-2.77972	-1.28406	0.29099
C	-3.00366	-1.24321	1.61028
C	-3.01243	-2.56605	-0.47889
O	2.28607	-2.08096	-0.83297
C	3.83145	-0.10515	0.20595

O	3.68365	-1.07359	1.27077
H	4.55458	-1.47386	1.42872
H	-0.18982	-1.92394	-0.69160
H	0.24700	-1.10787	0.80175
H	1.48541	-0.61353	-1.95182
H	0.78367	3.26301	-0.29793
H	0.68685	2.20102	-1.69177
H	-1.91632	3.23314	0.16701
H	-1.73201	2.57568	-1.46417
H	-3.81529	1.52262	-0.74470
H	-3.21554	1.30140	0.88798
H	-2.66419	-0.32376	-1.57623
H	-1.24854	1.02684	2.00335
H	0.50584	0.93032	1.85444
H	-0.28681	2.50788	1.93202
H	-3.32593	-2.12928	2.15217
H	-2.88574	-0.34257	2.20499
H	-2.12436	-2.86533	-1.04987
H	-3.28779	-3.39507	0.18068
H	-3.81884	-2.43059	-1.21370
H	4.40131	-0.55485	-0.61863
H	4.38130	0.77205	0.56876
H	2.80405	2.26744	0.27254
H	2.66806	-2.14819	0.06493

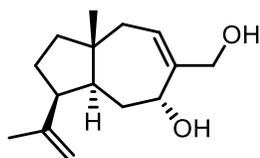
Conformer 4

Energy: -736.42688 Hartree (Rel: 2.1 kcal/mol)

XYZ coordinates for conf 4:

C	-0.54558	1.51908	-0.05623
C	-0.76406	0.08866	-0.63476
C	0.14155	-1.01651	-0.08367
C	1.60185	-0.88596	-0.55574
C	2.39855	0.26110	0.07808
C	2.04273	1.55410	0.01768
C	0.77807	2.13544	-0.57701
C	-1.78218	2.24844	-0.62921
C	-2.94249	1.25864	-0.41912
C	-2.33205	-0.15848	-0.63490
C	-0.56912	1.58939	1.48425
H	-0.50684	0.17944	-1.70081
C	-2.86594	-1.26635	0.27150
C	-3.21299	-1.10849	1.55486
C	-3.03142	-2.61351	-0.39816
O	2.21438	-2.15231	-0.31463
C	3.66975	-0.12272	0.79293
O	4.55495	-0.77701	-0.14571
H	5.27351	-1.18617	0.36392
H	-0.19523	-1.99014	-0.45646
H	0.10527	-1.07095	1.00982
H	1.57154	-0.70013	-1.64552
H	0.76601	3.21362	-0.37356
H	0.79942	2.03537	-1.67383
H	-1.95955	3.21994	-0.15210
H	-1.63146	2.43466	-1.70198
H	-3.77899	1.44221	-1.10213
H	-3.34268	1.35976	0.59365
H	-2.58064	-0.47544	-1.65537
H	-1.48849	1.17642	1.90553
H	0.26954	1.04850	1.93032
H	-0.49670	2.63599	1.80746
H	-3.58814	-1.94410	2.14105
H	-3.14904	-0.15772	2.07509
H	-2.09585	-2.95963	-0.85518
H	-3.37020	-3.38079	0.30512
H	-3.76585	-2.54797	-1.21356
H	4.15490	0.76780	1.21113
H	3.44304	-0.81192	1.61841
H	2.72231	2.27480	0.47228
H	3.16954	-2.02609	-0.48372

Revised structure of 64{18}, i.e. 66{18-rev} (CDCl₃)



					Conf1	Conf2	Conf3	Conf4
Rel energy (kcal/mol):					0.00	0.32	0.44	0.94
C-nom	iGau	Exp	Calc	diff	1	2	3	4
C1-C	5	143.70	141.34	-2.36	[141.43	141.90	140.50	141.27]
C2-CH	4	68.80	67.77	-1.03	[67.13	68.77	67.47	68.76]
C3-CH2	3	32.10	30.73	-1.37	[31.06	30.83	29.33	32.05]
C4-CH	2	46.20	46.88	0.68	[46.98	47.24	46.31	46.66]
C5-C	1	43.80	44.26	0.46	[44.13	44.36	44.14	44.83]
C6-CH2	7	42.90	42.27	-0.63	[42.67	42.24	41.55	42.11]
C7-CH	6	128.00	126.12	-1.88	[128.22	119.79	132.26	119.77]
C8-CH2	8	43.60	42.05	-1.55	[42.19	42.11	41.71	41.95]
C9-CH2	9	29.50	28.67	-0.83	[28.41	28.48	27.99	32.00]
C10-CH	10	51.70	51.75	0.05	[52.21	52.23	51.85	47.98]
C11-C	13	148.90	147.33	-1.57	[147.07	147.21	147.63	148.21]
C12-CH2	14	113.70	115.00	1.30	[115.52	115.42	115.00	111.30]
C13-CH3	15	23.30	21.70	-1.60	[21.00	21.01	21.20	28.17]
C14-CH2	17	69.10	68.58	-0.52	[70.39	65.33	70.17	65.33]
C15-CH3	11	19.40	19.09	-0.31	[19.21	19.12	18.72	19.26]
13C chem shifts: RMSD=1.25ppm (MAE=1.08) N=15 {-2.36 1.30}								
Fractions:					0.442	0.257	0.209	0.091

Conformer 1

Energy: -736.42131 Hartree (Rel: 0.0 kcal/mol)

XYZ coordinates for conf 1:

C	-0.38590	1.48747	0.02276
C	-0.68568	0.07626	-0.56505
C	0.11492	-1.08387	0.02947
C	1.58335	-1.16176	-0.41787
C	2.50014	0.02188	-0.13052
C	2.21586	1.33491	-0.20774
C	0.92914	2.06120	-0.54263
C	-1.61015	2.29052	-0.47901
C	-2.80442	1.34681	-0.26506
C	-2.26768	-0.07281	-0.61407
C	-0.33202	1.53014	1.56389
H	-0.39501	0.13251	-1.62440
C	-2.90053	-1.21552	0.16694
C	-3.44137	-2.25147	-0.48991
C	-2.93640	-1.17738	1.67884
O	1.69059	-1.50743	-1.81615
C	3.92577	-0.40092	0.16317
O	4.03565	-1.16075	1.37193
H	3.70131	-0.59822	2.08957
H	-0.34621	-2.03158	-0.27333
H	0.09092	-1.06439	1.12520
H	2.01702	-2.02580	0.09585
H	1.03376	3.09828	-0.19678
H	0.83952	2.13165	-1.63906
H	-1.72593	3.25207	0.03544
H	-1.49059	2.50603	-1.55023
H	-3.67024	1.61238	-0.88098
H	-3.13503	1.39809	0.77743
H	-2.51505	-0.26835	-1.66313
H	-1.22829	1.10717	2.02635
H	0.53353	0.98802	1.95637
H	-0.24718	2.57085	1.90083
H	-3.90363	-3.08471	0.03470
H	-3.44173	-2.30417	-1.57638
H	-3.49131	-0.30755	2.05229
H	-3.41975	-2.07393	2.07922

H	-1.93107	-1.11787	2.11134
H	4.28295	-1.07395	-0.62462
H	4.59108	0.47443	0.18815
H	3.06060	2.00635	-0.04213
H	1.55021	-0.69462	-2.32718

Conformer 2

Energy: -736.42202 Hartree (Rel: 0.3 kcal/mol)

XYZ coordinates for conf 2:

C	-0.30449	1.41664	-0.08615
C	-0.71630	-0.01868	-0.52916
C	-0.06595	-1.17412	0.23390
C	1.40780	-1.43697	-0.11837
C	2.41736	-0.32274	0.12586
C	2.27532	0.99161	-0.10713
C	1.09284	1.78580	-0.62534
C	-1.41102	2.26608	-0.75640
C	-2.70632	1.47361	-0.51494
C	-2.30040	-0.02372	-0.65621
C	-0.33087	1.63861	1.43998
H	-0.37103	-0.11282	-1.56926
C	-3.08359	-0.99337	0.21726
C	-3.70011	-2.04407	-0.34251
C	-3.18305	-0.76643	1.70965
O	1.54941	-1.92210	-1.47117
C	3.75860	-0.87697	0.58945
O	4.83833	0.04314	0.60343
H	5.00019	0.31316	-0.31527
H	-0.60469	-2.10227	0.00846
H	-0.13829	-1.02841	1.31787
H	1.71657	-2.29801	0.48875
H	1.28129	2.84484	-0.40427
H	1.07027	1.72127	-1.72548
H	-1.45560	3.28921	-0.36413
H	-1.21216	2.33879	-1.83509
H	-3.50421	1.74168	-1.21572
H	-3.08852	1.68509	0.48901
H	-2.51500	-0.32666	-1.68684
H	-1.29350	1.37260	1.88560
H	0.44544	1.05992	1.94913
H	-0.14719	2.69751	1.66095
H	-4.27075	-2.75624	0.24946
H	-3.65728	-2.23008	-1.41339
H	-3.65441	0.19582	1.94586
H	-3.78025	-1.55164	2.18356
H	-2.19785	-0.75943	2.18984
H	3.66904	-1.23831	1.62268
H	3.99894	-1.75743	-0.02894
H	3.16567	1.58927	0.08546
H	1.54238	-1.14781	-2.05572

Conformer 3

Energy: -736.42053 Hartree (Rel: 0.4 kcal/mol)

XYZ coordinates for conf 3:

C	-0.35083	1.46042	0.09020
C	-0.67868	0.10945	-0.61124
C	0.15468	-1.10898	-0.20388
C	1.60600	-1.07330	-0.70772
C	2.51083	0.01175	-0.12826
C	2.23510	1.32547	-0.05511
C	0.97055	2.05614	-0.45248
C	-1.57212	2.30987	-0.33611
C	-2.77692	1.36382	-0.18057
C	-2.25621	-0.04525	-0.60120
C	-0.28376	1.38883	1.62901
H	-0.43492	0.27643	-1.66670
C	-2.85864	-1.21413	0.16567
C	-3.46083	-2.20814	-0.50290
C	-2.79282	-1.25453	1.67649
O	1.54379	-0.97941	-2.14459
C	3.85311	-0.49243	0.35707

O	3.72375	-1.41425	1.44586
H	3.25021	-0.94711	2.15363
H	-0.30660	-2.00983	-0.62747
H	0.17677	-1.25333	0.88216
H	2.05633	-2.03872	-0.43437
H	1.05481	3.09501	-0.10824
H	0.90652	2.10414	-1.54974
H	-1.67401	3.23041	0.25154
H	-1.46024	2.60529	-1.38872
H	-3.63523	1.67222	-0.78694
H	-3.11683	1.36238	0.86028
H	-2.54693	-0.20823	-1.64478
H	-1.21466	1.02303	2.06982
H	0.52641	0.73961	1.97429
H	-0.09821	2.39023	2.03829
H	-3.90410	-3.05862	0.01051
H	-3.53266	-2.20753	-1.58829
H	-3.28621	-0.38615	2.13098
H	-3.28344	-2.15306	2.06357
H	-1.75905	-1.25387	2.04049
H	4.36331	-1.06528	-0.42775
H	4.50539	0.35040	0.62903
H	3.02665	1.96211	0.34395
H	2.44953	-0.85426	-2.46944

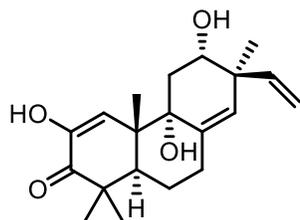
Conformer 4

Energy: -736.42151 Hartree (Rel: 0.9 kcal/mol)

XYZ coordinates for conf 4:

C	-0.27723	1.44801	-0.09773
C	-0.72653	0.00928	-0.49881
C	-0.09917	-1.12111	0.32046
C	1.37269	-1.42524	-0.00581
C	2.41031	-0.32058	0.14382
C	2.29371	0.98211	-0.15793
C	1.11452	1.78375	-0.66887
C	-1.38034	2.30755	-0.75833
C	-2.68193	1.55260	-0.45256
C	-2.31565	0.04876	-0.58859
C	-0.27049	1.69301	1.42628
H	-0.39163	-0.13200	-1.53680
C	-3.08212	-0.90907	0.31909
C	-3.41757	-0.64625	1.58815
C	-3.47790	-2.22004	-0.32322
O	1.50256	-2.01593	-1.31889
C	3.75410	-0.88237	0.59288
O	4.85709	0.00611	0.50813
H	4.99253	0.20988	-0.43164
H	-0.63475	-2.05769	0.13028
H	-0.19608	-0.92785	1.39440
H	1.66788	-2.24359	0.66395
H	1.32363	2.84356	-0.46946
H	1.07232	1.70195	-1.76746
H	-1.38714	3.34178	-0.39363
H	-1.21307	2.34517	-1.84436
H	-3.50213	1.82889	-1.12421
H	-3.01872	1.78319	0.56245
H	-2.56149	-0.25394	-1.61399
H	-1.20717	1.39045	1.90303
H	0.54206	1.15239	1.91991
H	-0.12413	2.76152	1.62797
H	-3.95990	-1.37292	2.18852
H	-3.17516	0.29037	2.08196
H	-2.60723	-2.74701	-0.73554
H	-3.97802	-2.88919	0.38411
H	-4.15821	-2.04409	-1.16857
H	3.69435	-1.17362	1.65008
H	3.94829	-1.80643	0.02450
H	3.20636	1.56377	-0.03127
H	1.49172	-1.28862	-1.96102

Originally assigned (incorrect) structure of 68{1} (CDCl₃)



Rel energy (kcal/mol):					Conf1	Conf2	Conf3	Conf4
					0.00	0.20	1.11	2.50
C-nom	iGau	Exp	Calc	diff	1	2	3	4
C1-CH	6	123.20	120.55	-2.65	[123.49	115.80	123.17	123.02]
C2-C	1	145.00	144.39	-0.61	[143.17	146.36	143.31	143.55]
C3-C	2	200.60	202.75	2.15	[202.66	202.89	202.67	202.53]
C4-C	3	42.90	44.21	1.31	[44.12	44.36	44.13	44.11]
C5-CH	4	42.10	43.47	1.37	[43.54	43.38	43.45	43.29]
C6-CH2	7	21.50	22.93	1.43	[23.62	21.84	23.44	23.72]
C7-CH2	8	31.80	33.42	1.62	[33.96	32.60	33.71	33.83]
C8-C	9	138.40	136.74	-1.66	[139.33	133.03	136.70	141.22]
C9-C	10	73.80	76.60	2.80	[75.91	77.80	75.61	75.30]
C10-C	5	43.60	43.57	-0.03	[43.12	44.35	42.87	43.64]
C11-CH2	14	31.00	32.46	1.46	[32.71	31.97	33.05	33.20]
C12-CH	13	71.70	73.42	1.72	[74.03	72.32	74.54	73.80]
C13-C	12	43.50	43.61	0.11	[43.73	43.81	42.03	42.36]
C14-CH	11	126.30	128.97	2.67	[125.79	133.78	127.83	124.03]
C15-CH	24	143.60	143.80	0.20	[144.68	142.88	142.54	142.15]
C16-CH2	25	117.10	114.06	-3.04	[114.72	113.30	113.23	114.46]
C17-CH3	23	25.30	22.58	-2.72	[24.64	20.24	20.17	20.53]
C18-CH3	20	19.20	20.42	1.22	[20.26	20.67	20.34	20.05]
C19-CH3	17	26.30	26.11	-0.19	[26.46	25.55	26.40	26.55]
C20-CH3	18	22.80	23.01	0.21	[23.11	22.86	23.08	23.08]
13C chem shifts: RMSD=1.75ppm (MAE=1.46) N=20 {-3.04 2.80}								
Fractions:					0.532	0.379	0.082	0.008

Conformer 1

Energy: -1079.80600 Hartree (Rel: 0.0 kcal/mol)

XYZ coordinates for conf 1:

C	-2.74628	1.63933	0.37043
C	-3.64481	0.52227	0.01622
C	-3.08248	-0.89174	-0.12066
C	-1.54483	-0.82656	-0.41165
C	-0.69522	0.17260	0.44635
C	-1.42473	1.48760	0.56699
C	-0.85101	-2.19737	-0.46838
C	0.52365	-2.05423	-1.14244
C	1.37783	-0.94995	-0.55661
C	0.67936	0.39345	-0.31739
C	2.69703	-1.11435	-0.38357
C	3.68777	-0.04070	0.01618
C	3.03929	1.35606	-0.16868
C	1.62278	1.37793	0.41376
O	-4.84659	0.77543	-0.10144
O	-3.37939	2.83661	0.51819
C	-3.80231	-1.56742	-1.31266
C	-3.49478	-1.65272	1.16875
H	-1.48972	-0.41133	-1.42495
C	-0.39219	-0.33880	1.88298
O	0.33576	0.95560	-1.59892
O	3.01571	1.67883	-1.57910
C	4.95628	-0.16337	-0.86594
C	4.13894	-0.17150	1.46730
C	3.71457	-1.06069	2.36648
H	-0.86082	2.36082	0.88497
H	-1.45038	-2.91059	-1.04391
H	-0.73834	-2.62376	0.53556

H	0.35086	-1.81991	-2.20314
H	1.07181	-3.00339	-1.11543
H	3.13087	-2.09214	-0.59759
H	3.66248	2.10068	0.34506
H	1.21367	2.39051	0.32952
H	1.70074	1.14051	1.47802
H	-4.32355	2.63430	0.34011
H	-3.57382	-2.63648	-1.35398
H	-3.50396	-1.11640	-2.26599
H	-4.88404	-1.45424	-1.20628
H	-3.20375	-1.13102	2.08411
H	-3.04697	-2.65143	1.18476
H	-4.58338	-1.76671	1.19039
H	0.36215	-1.13156	1.88126
H	-0.01798	0.47181	2.51526
H	-1.29096	-0.72607	2.36330
H	1.20067	1.16805	-2.00446
H	2.90248	2.64044	-1.65306
H	5.68084	0.62068	-0.61476
H	5.43613	-1.13408	-0.69985
H	4.70606	-0.06862	-1.92472
H	4.91784	0.53769	1.75565
H	4.12754	-1.08510	3.37160
H	2.94648	-1.79341	2.13404

Conformer 2

Energy: -1079.80777 Hartree (Rel: 0.2 kcal/mol)

XYZ coordinates for conf 2:

C	2.77167	-1.65845	0.27894
C	3.68428	-0.52712	-0.02120
C	3.14630	0.90086	0.01810
C	1.61230	0.87971	-0.29141
C	0.74308	-0.16784	0.48389
C	1.45938	-1.49719	0.53438
C	0.92732	2.25522	-0.26145
C	-0.43427	2.16611	-0.97222
C	-1.30429	1.01927	-0.49959
C	-0.61996	-0.33542	-0.32952
C	-2.62561	1.17412	-0.33457
C	-3.63453	0.08385	-0.01712
C	-2.98345	-1.31368	-0.29552
C	-1.57098	-1.38079	0.29878
O	4.86965	-0.79744	-0.21540
O	3.38710	-2.86623	0.32930
C	3.88568	1.72044	-1.06455
C	3.54820	1.47465	1.40462
H	1.56808	0.54433	-1.33545
C	0.39971	0.25688	1.93963
O	-0.31752	-0.76282	-1.69011
O	-2.96297	-1.64169	-1.68135
C	-4.87009	0.26679	-0.91594
C	-3.99263	0.19064	1.46155
C	-5.21010	0.33727	1.99040
H	0.89658	-2.37522	0.84427
H	1.53976	3.00279	-0.77535
H	0.79863	2.61004	0.76777
H	-0.24010	2.02583	-2.04582
H	-0.98412	3.10925	-0.87490
H	-3.04678	2.17195	-0.46583
H	-3.61342	-2.07346	0.18298
H	-1.17094	-2.38559	0.12265
H	-1.63200	-1.24782	1.38132
H	4.32954	-2.67227	0.13071
H	3.69267	2.79040	-0.94590
H	3.57313	1.42508	-2.07276
H	4.96307	1.55792	-0.98106
H	3.25733	0.82570	2.23478
H	3.09172	2.45779	1.55765
H	4.63569	1.59312	1.44760
H	-0.37151	1.03300	1.96260
H	0.03261	-0.59531	2.51906

H	1.27848	0.63919	2.45914
H	0.25810	-1.54776	-1.62861
H	-2.12070	-1.29825	-2.03885
H	-5.61290	-0.51620	-0.72464
H	-5.34268	1.23874	-0.73606
H	-4.58201	0.20356	-1.96667
H	-3.14291	0.15487	2.14324
H	-5.34548	0.40375	3.06706
H	-6.11202	0.39811	1.38836

Conformer 3

Energy: -1079.80378 Hartree (Rel: 1.1 kcal/mol)

XYZ coordinates for conf 3:

C	2.79156	-1.66375	0.26800
C	3.70167	-0.52680	0.02182
C	3.15061	0.89800	0.00610
C	1.61642	0.87127	-0.30814
C	0.74932	-0.19371	0.44683
C	1.46892	-1.51951	0.46285
C	0.93241	2.24686	-0.24833
C	-0.43680	2.17535	-0.94426
C	-1.30438	1.02722	-0.47209
C	-0.61580	-0.33684	-0.35209
C	-2.62453	1.18624	-0.30232
C	-3.63254	0.08933	0.00541
C	-2.98750	-1.29152	-0.29574
C	-1.56695	-1.38780	0.27091
O	4.90257	-0.77831	-0.10658
O	3.41481	-2.87392	0.31780
C	3.89005	1.67319	-1.11084
C	3.55100	1.53559	1.36426
H	1.57141	0.54943	-1.35528
C	0.42725	0.19569	1.91782
O	-0.26069	-0.77776	-1.67688
O	-2.95725	-1.48276	-1.73038
C	-4.88656	0.29364	-0.86510
C	-3.96669	0.16034	1.49408
C	-5.17221	0.32413	2.04384
H	0.89574	-2.41269	0.69826
H	1.54195	3.00385	-0.75292
H	0.81378	2.58302	0.78856
H	-0.25549	2.03958	-2.02056
H	-0.97955	3.12148	-0.83398
H	-3.05166	2.18255	-0.42336
H	-3.62067	-2.07111	0.14716
H	-1.16929	-2.38656	0.06085
H	-1.61989	-1.28851	1.35801
H	4.36219	-2.66455	0.16704
H	3.66945	2.74336	-1.05771
H	3.60086	1.31273	-2.10467
H	4.96950	1.54208	-1.00195
H	3.24566	0.93422	2.22442
H	3.10855	2.53165	1.46574
H	4.63984	1.63983	1.40932
H	-0.32726	0.98701	1.97211
H	0.04789	-0.66510	2.47680
H	1.31893	0.54252	2.44031
H	-1.12205	-0.95050	-2.10780
H	-2.86685	-2.43595	-1.89193
H	-5.62040	-0.50211	-0.69260
H	-5.36158	1.25279	-0.63294
H	-4.62105	0.28516	-1.92345
H	-3.10637	0.09532	2.15925
H	-5.28825	0.37656	3.12342
H	-6.08233	0.41440	1.45818

Conformer 4

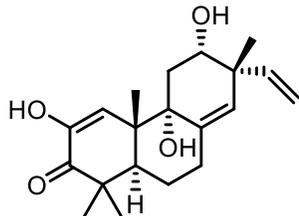
Energy: -1079.80745 Hartree (Rel: 2.5 kcal/mol)

XYZ coordinates for conf 4:

C	2.77063	-1.68474	0.18672
C	3.68356	-0.53165	0.04526

C	3.12815	0.89145	0.08789
C	1.60497	0.87887	-0.27653
C	0.72066	-0.23215	0.38699
C	1.44089	-1.55659	0.33977
C	0.91378	2.24775	-0.16067
C	-0.44548	2.21307	-0.88233
C	-1.31444	1.04352	-0.47334
C	-0.61835	-0.32626	-0.46232
C	-2.62350	1.20440	-0.21812
C	-3.61625	0.08350	0.07072
C	-3.00016	-1.23032	-0.49144
C	-1.57340	-1.44265	0.02338
O	4.88968	-0.77159	-0.05051
O	3.39790	-2.89330	0.18372
C	3.90031	1.72494	-0.96332
C	3.48346	1.45986	1.48856
H	1.59632	0.61787	-1.34122
C	0.35880	0.06174	1.86987
O	-0.21481	-0.64433	-1.81027
O	-2.97941	-1.23066	-1.93998
C	-4.96157	0.38655	-0.61954
C	-3.79436	-0.03566	1.58186
C	-4.94210	-0.01922	2.26378
H	0.86061	-2.46288	0.49416
H	1.52985	3.03007	-0.61618
H	0.77506	2.53195	0.88911
H	-0.24912	2.12672	-1.96053
H	-0.98853	3.15334	-0.73217
H	-3.04291	2.21077	-0.24127
H	-3.63179	-2.07718	-0.20240
H	-1.20314	-2.40095	-0.35413
H	-1.59852	-1.51730	1.11267
H	4.34923	-2.67277	0.08168
H	3.67349	2.79040	-0.86230
H	3.64541	1.41535	-1.98334
H	4.97612	1.59108	-0.82578
H	3.14758	0.81956	2.30819
H	3.04063	2.45176	1.62334
H	4.57038	1.55721	1.57510
H	-0.36219	0.87997	1.96092
H	-0.07619	-0.82068	2.34893
H	1.24500	0.32630	2.44699
H	-1.01849	-0.99955	-2.23638
H	-3.03491	-0.30665	-2.23532
H	-5.67175	-0.43430	-0.47280
H	-5.40244	1.30130	-0.21055
H	-4.84488	0.53280	-1.69709
H	-2.86755	-0.11857	2.14657
H	-4.94347	-0.10187	3.34757
H	-5.91419	0.07676	1.78949

Revised structure of 68{1}, i.e. 70{1-rev} (CDCl₃)



Rel energy (kcal/mol):					Conf1	Conf2	Conf3
					0.00	1.87	2.19
C-nom	iGau	Exp	Calc	diff	1	2	3
C1-CH	6	123.20	123.29	0.09	[123.48	123.37	115.70]
C2-C	1	145.00	143.36	-1.64	[143.29	143.33	146.41]
C3-C	2	200.60	202.63	2.03	[202.62	202.63	202.86]
C4-C	3	42.90	44.09	1.19	[44.08	44.11	44.35]
C5-CH	4	42.10	43.38	1.28	[43.38	43.36	43.42]
C6-CH2	7	21.50	23.55	2.05	[23.59	23.57	21.82]
C7-CH2	8	31.80	33.97	2.17	[34.01	33.82	32.70]
C8-C	9	138.40	140.39	1.99	[140.65	138.41	133.26]
C9-C	10	73.80	75.29	1.49	[75.23	75.44	77.65]
C10-C	5	43.60	43.03	-0.57	[43.00	42.96	44.33]
C11-CH2	14	31.00	30.46	-0.54	[30.41	30.81	32.09]
C12-CH	13	71.70	69.54	-2.16	[69.42	70.38	72.82]
C13-C	12	43.50	43.74	0.24	[43.77	43.81	42.52]
C14-CH	11	126.30	125.09	-1.21	[124.76	127.74	133.76]
C15-CH	24	143.60	141.34	-2.26	[141.16	144.10	143.87]
C16-CH2	25	117.10	116.43	-0.67	[116.78	111.23	111.25]
C17-CH3	23	25.30	25.54	0.24	[25.52	28.39	21.39]
C18-CH3	20	19.20	20.29	1.09	[20.28	20.23	20.64]
C19-CH3	17	26.30	26.44	0.14	[26.46	26.41	25.53]
C20-CH3	18	22.80	23.12	0.32	[23.13	23.13	22.87]
13C chem shifts: RMSD=1.39ppm (MAE=1.17) N=20 {-2.26 2.17}							
Fractions:					0.937	0.040	0.023

Conformer 1

Energy: -1079.80695 Hartree (Rel: 0.0 kcal/mol)

XYZ coordinates for conf 1:

C	2.83741	-1.64714	-0.03718
C	3.70027	-0.46437	-0.22995
C	3.12298	0.93769	-0.04238
C	1.56726	0.90218	-0.22004
C	0.79203	-0.26518	0.48108
C	1.53401	-1.56357	0.28281
C	0.86729	2.24210	0.05930
C	-0.56093	2.21021	-0.50939
C	-1.35849	0.99084	-0.09702
C	-0.63658	-0.35740	-0.20843
C	-2.65366	1.09627	0.23276
C	-3.59415	-0.05358	0.52633
C	-2.97210	-1.37681	-0.02324
C	-1.50119	-1.50399	0.36933
O	4.89047	-0.66486	-0.48561
O	3.48595	-2.83684	-0.17689
C	3.74267	1.84722	-1.13070
C	3.63439	1.43932	1.33536
H	1.43204	0.69961	-1.28902
C	0.59775	-0.05266	2.00969
O	-0.39392	-0.62698	-1.60089
O	-3.02057	-1.44366	-1.45697
C	-3.83298	-0.17047	2.05400
C	-4.95125	0.13535	-0.13655
C	-5.23437	0.93615	-1.16969
H	0.99937	-2.49320	0.46032
H	1.41224	3.06800	-0.40995
H	0.84209	2.45655	1.13432

H	-0.48159	2.20201	-1.60634
H	-1.10756	3.12169	-0.24010
H	-3.09794	2.09066	0.28451
H	-3.53838	-2.22451	0.39112
H	-1.12191	-2.45519	-0.01652
H	-1.44025	-1.54715	1.45890
H	4.41200	-2.58482	-0.38397
H	3.50448	2.89881	-0.94534
H	3.37317	1.58318	-2.12820
H	4.83012	1.73878	-1.13088
H	3.41318	0.74622	2.15111
H	3.19154	2.41025	1.57890
H	4.72165	1.56067	1.29623
H	-0.16523	0.70335	2.22108
H	0.28972	-0.98181	2.49860
H	1.52615	0.26142	2.48710
H	-1.27841	-0.84547	-1.95931
H	-3.84872	-1.01770	-1.74513
H	-4.28764	0.75044	2.43483
H	-4.51110	-1.00163	2.28430
H	-2.89711	-0.32800	2.59743
H	-5.74494	-0.49307	0.27113
H	-6.23636	0.98100	-1.58821
H	-4.48820	1.58564	-1.62053

Conformer 2

Energy: -1079.81044 Hartree (Rel: 1.9 kcal/mol)

XYZ coordinates for conf 2:

C	2.78483	-1.71236	0.12812
C	3.70657	-0.59220	-0.14941
C	3.19469	0.84628	-0.09183
C	1.64286	0.86706	-0.30229
C	0.79992	-0.19686	0.48083
C	1.48200	-1.54052	0.41344
C	1.00155	2.25733	-0.16032
C	-0.41612	2.23949	-0.75665
C	-1.27629	1.10139	-0.24975
C	-0.61810	-0.28262	-0.22979
C	-2.56861	1.29201	0.04819
C	-3.56593	0.21186	0.42784
C	-3.00615	-1.16802	-0.00890
C	-1.54864	-1.33584	0.41956
O	4.88924	-0.86973	-0.36456
O	3.37765	-2.93843	0.10523
C	3.87857	1.63234	-1.23623
C	3.70301	1.43635	1.25165
H	1.51959	0.57584	-1.35204
C	0.58712	0.15851	1.98013
O	-0.36283	-0.67961	-1.58934
O	-3.02891	-1.33947	-1.43711
C	-3.81248	0.23996	1.96305
C	-4.90716	0.51361	-0.23852
C	-5.84286	-0.37029	-0.60102
H	0.90017	-2.42484	0.66051
H	1.59366	3.01176	-0.68895
H	0.96620	2.56920	0.89034
H	-0.31740	2.12638	-1.84606
H	-0.92280	3.19630	-0.58370
H	-2.97099	2.30511	-0.00628
H	-3.61028	-1.96207	0.45464
H	-1.21191	-2.33133	0.11478
H	-1.50573	-1.29726	1.51010
H	4.31780	-2.74888	-0.10488
H	3.69084	2.70592	-1.14139
H	3.51408	1.30615	-2.21705
H	4.95894	1.47116	-1.20376
H	3.43705	0.82197	2.11572
H	3.29906	2.44185	1.40657
H	4.79512	1.50787	1.22621
H	-0.14139	0.96568	2.10682
H	0.22397	-0.70828	2.54060

H	1.52038	0.46883	2.45041
H	-1.25090	-0.87481	-1.95182
H	-3.85492	-0.94721	-1.76969
H	-4.24304	1.20317	2.25791
H	-4.51659	-0.54707	2.25624
H	-2.88070	0.10982	2.52209
H	-5.11440	1.57404	-0.38697
H	-6.78425	-0.04222	-1.03313
H	-5.72557	-1.44395	-0.46952

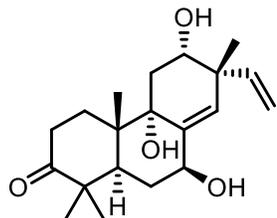
Conformer 3

Energy: -1079.80745 Hartree (Rel: 2.2 kcal/mol)

XYZ coordinates for conf 3:

C	2.83715	-1.64426	0.14316
C	3.71759	-0.49207	-0.17319
C	3.16802	0.92676	-0.05214
C	1.61785	0.89733	-0.26586
C	0.80920	-0.18714	0.52398
C	1.54135	-1.50834	0.48346
C	0.92245	2.26232	-0.14299
C	-0.47842	2.18180	-0.77322
C	-1.30598	1.00573	-0.29613
C	-0.59937	-0.34510	-0.21041
C	-2.61619	1.13911	-0.04484
C	-3.59753	0.02585	0.28902
C	-2.94645	-1.35247	-0.06585
C	-1.50204	-1.41399	0.44758
O	4.89140	-0.74078	-0.44890
O	3.46705	-2.84515	0.11393
C	3.82972	1.79127	-1.15005
C	3.64946	1.45857	1.32566
H	1.51137	0.59843	-1.31652
C	0.55109	0.18299	2.01216
O	-0.37454	-0.73237	-1.59787
O	-2.99457	-1.65079	-1.45903
C	-3.94605	0.08036	1.79228
C	-4.83238	0.22899	-0.57721
C	-6.06820	0.52192	-0.16623
H	1.00802	-2.40393	0.79506
H	1.49493	3.03590	-0.66439
H	0.85297	2.57725	0.90476
H	-0.34799	2.08586	-1.86132
H	-1.03243	3.11275	-0.60676
H	-3.05318	2.13624	-0.11186
H	-3.53741	-2.13412	0.42772
H	-1.10346	-2.41104	0.22934
H	-1.50228	-1.30161	1.53379
H	4.39332	-2.63291	-0.13554
H	3.63346	2.85421	-0.98320
H	3.45745	1.52598	-2.14626
H	4.91189	1.63953	-1.13966
H	3.41514	0.77951	2.14955
H	3.19503	2.43130	1.53918
H	4.73648	1.58693	1.30628
H	-0.23403	0.93915	2.10976
H	0.24053	-0.69564	2.58509
H	1.45277	0.56964	2.48737
H	0.21784	-1.50730	-1.59231
H	-2.17034	-1.29989	-1.85021
H	-4.37113	1.05438	2.05737
H	-4.67962	-0.69141	2.05337
H	-3.05808	-0.06600	2.41380
H	-4.64340	0.11836	-1.64196
H	-6.87500	0.65455	-0.88297
H	-6.33530	0.63884	0.88043

Originally assigned (incorrect) structure of 69{2} (CDCl₃)



Rel energy (kcal/mol):					Conf1	Conf2
					0.00	1.82
C-nom	iGau	Exp	Calc	diff	1	2
C1-CH2*	6	31.10	32.41	1.31	[32.41	32.37]
C2-CH2*	1	34.60	35.18	0.58	[35.18	35.19]
C3-C	2	216.50	215.65	-0.85	[215.65	215.62]
C4-C	3	47.40	47.81	0.41	[47.81	47.83]
C5-CH	4	39.40	43.22	3.82	[43.22	43.26]
C6-CH2	7	31.00	35.03	4.03	[35.03	35.05]
C7-CH	8	73.70	69.74	-3.96	[69.75	69.54]
C8-C	9	138.70	142.76	4.06	[142.85	140.79]
C9-C	10	75.50	74.79	-0.71	[74.78	75.01]
C10-C	5	37.00	37.21	0.21	[37.21	37.22]
C11-CH2	14	30.60	30.76	0.16	[30.74	31.19]
C12-CH	13	71.70	69.28	-2.42	[69.24	70.18]
C13-C	12	43.70	43.38	-0.32	[43.37	43.49]
C14-CH**	11	131.20	122.27	-8.93	[122.13	125.16]
C15-CH**	24	143.40	141.24	-2.16	[141.10	144.34]
C16-CH2	25	116.70	116.80	0.10	[117.06	111.26]
C17-CH3	23	25.00	25.70	0.70	[25.57	28.43]
C18-CH3	20	17.40	18.14	0.74	[18.15	18.03]
C19-CH3	17	26.10	25.44	-0.66	[25.44	25.46]
C20-CH3	18	19.70	20.03	0.33	[20.03	19.98]
13C chem shifts: RMSD=2.82ppm (MAE=1.82) N=20 {-8.93 4.06}						
Fractions:					0.955	0.045

Conformer 1

Energy: -1081.01802 Hartree (Rel: 0.0 kcal/mol)

XYZ coordinates for conf 1:

C	3.12550	-2.00637	0.38140
C	3.91083	-0.86609	-0.23550
C	3.34692	0.55687	-0.05058
C	1.77763	0.56524	-0.22394
C	0.95838	-0.63751	0.36375
C	1.64875	-1.95869	-0.04396
C	1.13103	1.89639	0.19705
C	-0.30137	2.00725	-0.34278
C	-1.14732	0.77980	-0.02543
C	-0.48090	-0.57432	-0.29348
C	-2.43251	0.90762	0.32911
C	-3.40804	-0.23162	0.53648
C	-2.85613	-1.51489	-0.16284
C	-1.38353	-1.74183	0.17310
O	4.95699	-1.06956	-0.83205
O	-0.90950	3.23495	0.05467
C	3.97228	1.47127	-1.12509
C	3.85667	1.04553	1.33376
H	1.63578	0.47913	-1.30793
C	0.81243	-0.57590	1.90466
O	-0.29326	-0.68304	-1.71996
O	-2.94052	-1.42891	-1.59440
C	-3.61000	-0.49405	2.05129
C	-4.77377	0.07363	-0.06226
C	-5.05411	0.98920	-0.99611
H	1.12798	-2.81392	0.40164
H	1.69577	2.75368	-0.18264
H	1.10981	1.99276	1.29076

H	-0.97877	3.22025	1.02430
H	-0.23902	2.07779	-1.43620
H	-2.83350	1.91072	0.45563
H	-3.44951	-2.37742	0.17638
H	-1.04798	-2.65776	-0.32313
H	-1.29869	-1.90767	1.24927
H	3.20404	-1.93912	1.47535
H	3.67772	2.51457	-0.97585
H	3.66270	1.16845	-2.13145
H	5.06255	1.41484	-1.08285
H	3.57492	0.38950	2.16123
H	3.47366	2.04736	1.55253
H	4.95064	1.10301	1.31930
H	0.07404	0.16861	2.21775
H	0.49345	-1.54280	2.30769
H	1.75186	-0.32384	2.39854
H	-1.19577	-0.83439	-2.06857
H	-3.75474	-0.93961	-1.81383
H	-4.01595	0.39999	2.53680
H	-4.31566	-1.31751	2.21735
H	-2.66728	-0.74294	2.54671
H	-5.57883	-0.56838	0.29943
H	-6.06457	1.11119	-1.37728
H	-4.29781	1.65884	-1.39773
H	3.59796	-2.94583	0.07919
H	1.57913	-2.07637	-1.13029

Conformer 2

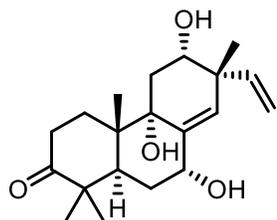
Energy: -1081.02092 Hartree (Rel: 1.8 kcal/mol)

XYZ coordinates for conf 2:

C	3.04441	-2.06629	0.54607
C	3.89559	-1.01250	-0.13437
C	3.40285	0.44667	-0.05895
C	1.83915	0.51994	-0.26386
C	0.95071	-0.59569	0.39231
C	1.57840	-1.97521	0.09091
C	1.25371	1.90922	0.04520
C	-0.16296	2.05054	-0.52894
C	-1.07249	0.89472	-0.13163
C	-0.47352	-0.50609	-0.29304
C	-2.35231	1.10930	0.19666
C	-3.38542	0.03280	0.47724
C	-2.89990	-1.30678	-0.13767
C	-1.44434	-1.59217	0.23073
O	4.93740	-1.30999	-0.69806
O	-0.71341	3.33359	-0.23551
C	4.09147	1.25105	-1.18183
C	3.91396	1.00623	1.29760
H	1.71151	0.36180	-1.34144
C	0.78613	-0.41819	1.92197
O	-0.27035	-0.72044	-1.70573
O	-2.95701	-1.29833	-1.57551
C	-3.59221	-0.11317	2.01156
C	-4.72780	0.46907	-0.10719
C	-5.70809	-0.32310	-0.55390
H	1.00764	-2.76973	0.58507
H	1.86712	2.70660	-0.38589
H	1.21998	2.08847	1.12829
H	-0.79458	3.39664	0.73120
H	-0.08136	2.03446	-1.62311
H	-2.70814	2.13779	0.23075
H	-3.53308	-2.12390	0.23891
H	-1.15468	-2.55236	-0.20710
H	-1.37935	-1.69938	1.31564
H	3.11006	-1.92667	1.63398
H	3.84870	2.31572	-1.11071
H	3.78258	0.89455	-2.17062
H	5.17665	1.14314	-1.11480
H	3.58582	0.42536	2.16315
H	3.57849	2.03872	1.43808
H	5.00955	1.00867	1.30107

H	0.09307	0.39165	2.16910
H	0.39941	-1.33266	2.38380
H	1.73257	-0.19301	2.41546
H	-1.17467	-0.83605	-2.06255
H	-3.76735	-0.82785	-1.83796
H	-3.97789	0.82261	2.43071
H	-4.31897	-0.90388	2.23009
H	-2.65276	-0.34263	2.52378
H	-4.89246	1.54712	-0.11263
H	-6.64397	0.09538	-0.91384
H	-5.63407	-1.40851	-0.56553
H	3.47305	-3.04681	0.31810
H	1.52003	-2.16583	-0.98566

Revised structure of 69{2}, i.e. 71{2-rev} (CDCl₃)



Rel energy (kcal/mol):					Conf1	Conf2	Conf3	Conf4	Conf5
					0.00	1.25	1.53	1.94	2.54
C-nom	iGau	Exp	Calc	diff	1	2	3	4	5
C1-CH2*	6	31.10	32.65	1.55	[32.66	32.85	32.27	32.53	32.49]
C2-CH2*	1	34.60	35.10	0.50	[35.20	34.16	35.17	35.21	35.10]
C3-C	2	216.50	215.84	-0.66	[215.60	218.52	215.08	215.56	214.95]
C4-C	3	47.40	47.79	0.39	[47.90	46.78	47.87	47.91	47.61]
C5-CH	4	39.40	41.03	1.63	[41.08	40.33	41.35	41.12	41.67]
C6-CH2	7	31.00	32.81	1.81	[32.94	33.33	30.00	33.08	33.42]
C7-CH	8	73.70	72.59	-1.11	[72.47	72.15	74.55	72.33	75.21]
C8-C	9	138.70	136.43	-2.27	[137.06	136.26	130.68	134.77	128.18]
C9-C	10	75.50	76.82	1.32	[76.81	76.68	76.98	77.12	76.83]
C10-C	5	37.00	37.35	0.35	[37.27	37.33	38.28	37.28	38.34]
C11-CH2	14	30.60	29.75	-0.85	[29.75	29.35	30.06	30.27	30.25]
C12-CH	13	71.70	69.28	-2.42	[68.99	69.18	72.22	70.09	72.32]
C13-C	12	43.70	43.55	-0.15	[43.61	43.65	42.64	43.85	42.71]
C14-CH**	11	131.20	128.56	-2.64	[127.92	127.74	135.49	130.63	137.91]
C15-CH**	24	143.40	141.07	-2.33	[140.79	140.80	143.42	143.49	143.67]
C16-CH2	25	116.70	116.95	0.25	[117.54	117.46	112.00	111.69	111.71]
C17-CH3	23	25.00	24.73	-0.27	[24.93	25.11	20.77	27.79	20.84]
C18-CH3	20	17.40	17.87	0.47	[17.75	19.35	17.29	17.61	17.60]
C19-CH3	17	26.10	25.78	-0.32	[25.49	28.46	25.53	25.52	25.47]
C20-CH3	18	19.70	19.82	0.12	[20.05	17.97	19.61	20.04	19.77]
13C chem shifts: RMSD=1.36ppm (MAE=1.07) N=20 {-2.64 1.81}									
Fractions:					0.801	0.097	0.061	0.030	0.011

Conformer 1

Energy: -1081.02445 Hartree (Rel: 0.0 kcal/mol)

XYZ coordinates for conf 1:

C	3.06571	-2.04780	-0.16693
C	3.87009	-0.78564	-0.41030
C	3.33087	0.52087	0.20593
C	1.76314	0.60860	0.03636
C	0.92285	-0.70254	0.24087
C	1.58928	-1.85137	-0.54920
C	1.12780	1.77276	0.81724
C	-0.30748	2.04012	0.33818
C	-1.16091	0.78408	0.32729
C	-0.52382	-0.43175	-0.34483
C	-2.43617	0.81414	0.73337
C	-3.43449	-0.31555	0.58814
C	-2.90956	-1.33120	-0.47869
C	-1.43791	-1.67407	-0.25229
O	4.91031	-0.81482	-1.04954
O	-0.29707	2.62050	-0.97790
C	3.97953	1.71160	-0.53150
C	3.83972	0.55103	1.67415
H	1.64184	0.84918	-1.02598
C	0.78368	-1.10075	1.73155
O	-0.36073	-0.09100	-1.75310
O	-2.99961	-0.81111	-1.81530
C	-3.63710	-1.02900	1.94937
C	-4.79261	0.19062	0.12239
C	-5.04347	1.34799	-0.49969
H	1.05523	-2.79301	-0.37779
H	1.69638	2.69720	0.67546
H	1.11675	1.56456	1.89417

H	-0.23162	1.86222	-1.59137
H	-0.77175	2.79101	0.98812
H	-2.81846	1.72913	1.18620
H	-3.51660	-2.24611	-0.41305
H	-1.12542	-2.39774	-1.01167
H	-1.34187	-2.16405	0.71868
H	3.14531	-2.31918	0.89469
H	3.71315	2.66143	-0.05837
H	3.66151	1.75085	-1.57912
H	5.06788	1.61624	-0.51834
H	3.55898	-0.33071	2.25553
H	3.45688	1.43420	2.19521
H	4.93376	0.60961	1.67823
H	0.07324	-0.46019	2.26270
H	0.43463	-2.13372	1.83199
H	1.73324	-1.03708	2.26354
H	-1.26890	-0.17184	-2.11899
H	-3.79993	-0.25636	-1.86717
H	-4.01813	-0.32028	2.69238
H	-4.36292	-1.84658	1.85973
H	-2.69925	-1.44084	2.33270
H	-5.61687	-0.50445	0.28996
H	-6.04980	1.60784	-0.81721
H	-4.26559	2.08150	-0.69700
H	3.52211	-2.85747	-0.74415
H	1.51817	-1.63672	-1.62080

Conformer 2

Energy: -1081.02135 Hartree (Rel: 1.3 kcal/mol)

XYZ coordinates for conf 2:

C	3.04414	-1.59908	-1.17378
C	3.81296	-0.87806	-0.09063
C	3.31968	0.54656	0.20529
C	1.77566	0.65501	-0.10752
C	0.96003	-0.67214	0.10854
C	1.57345	-1.82937	-0.74839
C	1.12788	1.84866	0.61530
C	-0.32320	2.07180	0.17771
C	-1.14783	0.80179	0.28234
C	-0.52804	-0.43036	-0.37202
C	-2.39979	0.82972	0.75595
C	-3.38483	-0.31985	0.71391
C	-2.90419	-1.36714	-0.34381
C	-1.41799	-1.67979	-0.18247
O	4.76089	-1.38248	0.49199
O	-0.37718	2.57663	-1.16750
C	4.08730	1.46469	-0.78935
C	3.73765	0.96311	1.62983
H	1.70335	0.86901	-1.18012
C	0.98544	-1.09241	1.59621
O	-0.45378	-0.13729	-1.80142
O	-3.07672	-0.89861	-1.69134
C	-3.49647	-0.98275	2.11069
C	-4.77645	0.14580	0.30879
C	-5.08484	1.27271	-0.34265
H	1.51574	-2.76465	-0.18081
H	1.68660	2.76728	0.40171
H	1.15208	1.70742	1.70200
H	-0.32216	1.78422	-1.73816
H	-0.77297	2.85100	0.80426
H	-2.77406	1.75952	1.18451
H	-3.49181	-2.28733	-0.21078
H	-1.13084	-2.43541	-0.92064
H	-1.27031	-2.12335	0.80331
H	3.54013	-2.54532	-1.40607
H	3.74776	2.50067	-0.68101
H	3.92649	1.16891	-1.83180
H	5.16337	1.43677	-0.58682
H	3.58579	2.03558	1.78313
H	3.18555	0.43003	2.40816
H	4.79912	0.74400	1.77099

H	0.52720	-0.34826	2.25514
H	0.46508	-2.04117	1.75427
H	2.01368	-1.25210	1.93227
H	-1.38196	-0.23783	-2.10819
H	-3.89027	-0.36159	-1.71912
H	-3.85138	-0.25250	2.84577
H	-4.20824	-1.81723	2.09346
H	-2.53010	-1.35977	2.45698
H	-5.57640	-0.55561	0.55131
H	-6.11266	1.50275	-0.61043
H	-4.33391	2.01056	-0.61405
H	3.06011	-0.97835	-2.07863
H	0.98576	-1.96659	-1.65803

Conformer 3

Energy: -1081.02201 Hartree (Rel: 1.5 kcal/mol)

XYZ coordinates for conf 3:

C	3.04503	-2.09629	0.04684
C	3.89668	-0.87358	-0.23415
C	3.36426	0.48701	0.26315
C	1.81058	0.59528	0.00440
C	0.92413	-0.67276	0.26767
C	1.59096	-1.89014	-0.40910
C	1.17574	1.83917	0.65530
C	-0.23887	2.09022	0.13348
C	-1.12103	0.86052	0.15984
C	-0.49073	-0.40750	-0.41046
C	-2.40706	0.94237	0.52703
C	-3.43145	-0.17664	0.41688
C	-2.89816	-1.24531	-0.59819
C	-1.44092	-1.61622	-0.29476
O	4.96966	-0.97103	-0.80849
O	-0.08945	2.52174	-1.25272
C	4.08243	1.60646	-0.52031
C	3.79932	0.60877	1.74988
H	1.75693	0.74773	-1.07985
C	0.70960	-0.95690	1.77459
O	-0.32121	-0.20185	-1.84801
O	-3.02533	-0.81436	-1.95151
C	-3.65345	-0.81245	1.80605
C	-4.71578	0.42491	-0.13490
C	-5.88873	0.53814	0.49213
H	1.02417	-2.80341	-0.19586
H	1.76791	2.73662	0.45211
H	1.12405	1.72862	1.74387
H	-0.96768	2.80992	-1.55548
H	-0.70720	2.90208	0.70426
H	-2.77975	1.89050	0.91825
H	-3.52751	-2.13880	-0.49332
H	-1.11875	-2.37905	-1.01101
H	-1.38084	-2.06136	0.69965
H	3.07367	-2.30394	1.12539
H	3.83396	2.59335	-0.11842
H	3.80774	1.58946	-1.58078
H	5.16494	1.47473	-0.45590
H	3.46276	-0.22034	2.37674
H	3.42085	1.53775	2.18815
H	4.89301	0.63714	1.80536
H	0.03162	-0.23424	2.23842
H	0.28208	-1.95269	1.92873
H	1.64428	-0.92814	2.33568
H	-0.11828	0.75032	-1.97107
H	-2.14413	-0.48150	-2.21729
H	-4.00391	-0.06448	2.52533
H	-4.40437	-1.60945	1.75439
H	-2.72778	-1.23696	2.20422
H	-4.62453	0.78851	-1.15537
H	-6.74197	0.99373	-0.00445
H	-6.05782	0.18756	1.50652
H	3.50361	-2.95098	-0.45927
H	1.56830	-1.74914	-1.49545

Conformer 4

Energy: -1081.02040 Hartree (Rel: 1.9 kcal/mol)

XYZ coordinates for conf 4:

C	2.98776	-2.14096	-0.00325
C	3.85816	-0.94438	-0.33529
C	3.38479	0.43294	0.17156
C	1.82447	0.58714	-0.01695
C	0.91718	-0.65903	0.28572
C	1.52446	-1.89863	-0.40884
C	1.24741	1.84293	0.66091
C	-0.17001	2.14493	0.14872
C	-1.08575	0.93684	0.24081
C	-0.51219	-0.36060	-0.32719
C	-2.35626	1.06064	0.64206
C	-3.40674	-0.03534	0.59756
C	-2.94529	-1.13687	-0.39487
C	-1.49232	-1.54205	-0.14772
O	4.89959	-1.07729	-0.95921
O	-0.12302	2.61271	-1.20998
C	4.09776	1.52563	-0.65301
C	3.88890	0.55451	1.63660
H	1.71983	0.74613	-1.09626
C	0.75554	-0.93149	1.80184
O	-0.32865	-0.14037	-1.75739
O	-3.00685	-0.70030	-1.76551
C	-3.60756	-0.63118	2.01981
C	-4.74335	0.57607	0.18130
C	-5.73303	-0.02774	-0.48488
H	0.94134	-2.79520	-0.16909
H	1.86461	2.72166	0.44899
H	1.22052	1.72470	1.75114
H	-0.09513	1.80360	-1.75783
H	-0.59608	2.97063	0.73063
H	-2.69643	2.03171	1.00526
H	-3.59080	-2.01884	-0.27376
H	-1.22275	-2.33025	-0.85755
H	-1.41805	-1.97135	0.85325
H	3.05062	-2.33513	1.07629
H	3.88209	2.52262	-0.25749
H	3.78464	1.49904	-1.70250
H	5.17923	1.37306	-0.62531
H	3.56047	-0.26182	2.28459
H	3.55015	1.49519	2.08206
H	4.98448	0.55701	1.64481
H	0.09127	-0.20581	2.28053
H	0.33838	-1.92798	1.98068
H	1.70875	-0.89170	2.32965
H	-1.24030	-0.19067	-2.11942
H	-3.79714	-0.14175	-1.86843
H	-3.97418	0.14169	2.70395
H	-4.34721	-1.43942	1.99783
H	-2.66976	-1.01797	2.43020
H	-4.89497	1.60472	0.51013
H	-6.66342	0.49289	-0.69398
H	-5.67281	-1.05702	-0.83200
H	3.40352	-3.01418	-0.51478
H	1.46703	-1.76369	-1.49417

Conformer 5

Energy: -1081.02245 Hartree (Rel: 2.5 kcal/mol)

XYZ coordinates for conf 5:

C	3.04057	-2.09853	0.05553
C	3.89110	-0.87710	-0.23227
C	3.36070	0.48317	0.26823
C	1.80706	0.59208	0.01000
C	0.91908	-0.67446	0.27114
C	1.58734	-1.89219	-0.40370
C	1.16748	1.83283	0.66079
C	-0.23649	2.09481	0.10243
C	-1.12215	0.86894	0.13736

C	-0.49619	-0.41130	-0.40882
C	-2.40777	0.96287	0.49886
C	-3.43445	-0.15592	0.41678
C	-2.90633	-1.25121	-0.57233
C	-1.44872	-1.61564	-0.26393
O	4.95914	-0.97333	-0.81579
O	-0.16292	2.46803	-1.30262
C	4.07951	1.60347	-0.51307
C	3.79666	0.60178	1.75500
H	1.74970	0.74549	-1.07452
C	0.70351	-0.95590	1.77905
O	-0.33070	-0.23289	-1.84984
O	-3.03903	-0.85932	-1.93610
C	-3.65719	-0.75708	1.82125
C	-4.71698	0.43697	-0.14858
C	-5.89274	0.55614	0.47201
H	1.01987	-2.80505	-0.19102
H	1.77824	2.72891	0.49281
H	1.09239	1.71551	1.74769
H	0.56290	3.10576	-1.41250
H	-0.71256	2.91418	0.65685
H	-2.77930	1.92304	0.85871
H	-3.53605	-2.14096	-0.44085
H	-1.12925	-2.39482	-0.96356
H	-1.38752	-2.03812	0.74024
H	3.06703	-2.30064	1.13513
H	3.83832	2.58989	-0.10480
H	3.80181	1.59137	-1.57309
H	5.16172	1.46757	-0.45417
H	3.47105	-0.23506	2.37727
H	3.40814	1.52357	2.19975
H	4.89004	0.64201	1.80910
H	-0.00570	-0.25567	2.23086
H	0.31242	-1.96587	1.93723
H	1.63101	-0.88667	2.34836
H	-0.17187	0.72420	-1.99803
H	-2.16449	-0.51501	-2.20902
H	-4.00588	0.00902	2.52208
H	-4.40964	-1.55370	1.78957
H	-2.73226	-1.17396	2.22925
H	-4.62137	0.78802	-1.17294
H	-6.74450	1.00408	-0.03396
H	-6.06560	0.21859	1.49021
H	3.49892	-2.95584	-0.44627
H	1.56667	-1.75195	-1.49006