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Supplementary Material

Structural diversity in nudibranch chemistry: elucidation of norditerpenes with a dendrillane scaffold from the Australian nudibranch *Goniobranchus coi*

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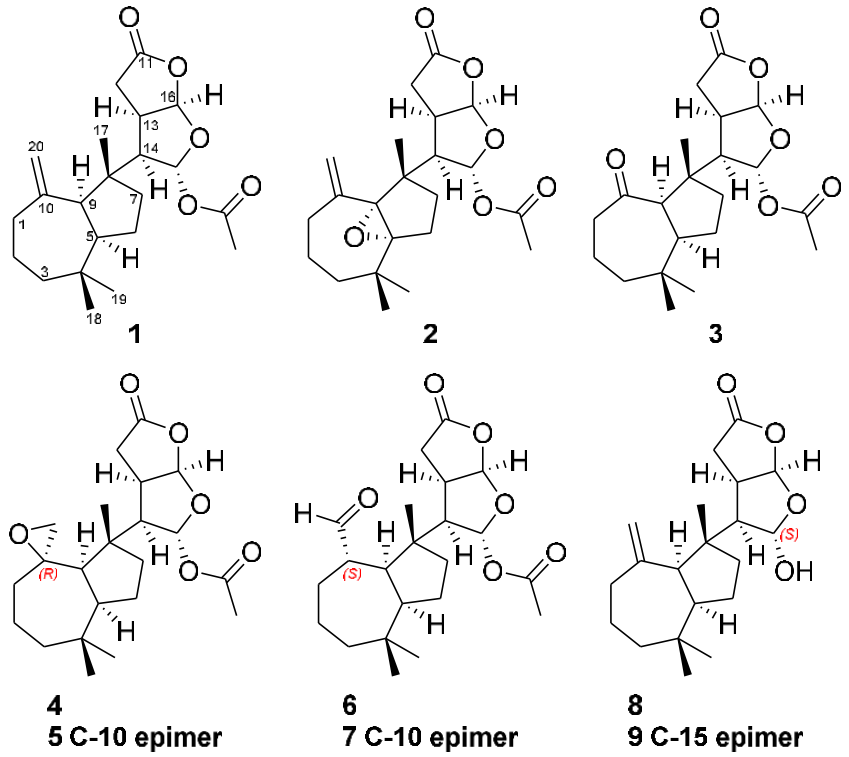


Figure S1. Structures of terpenes **1–9**.

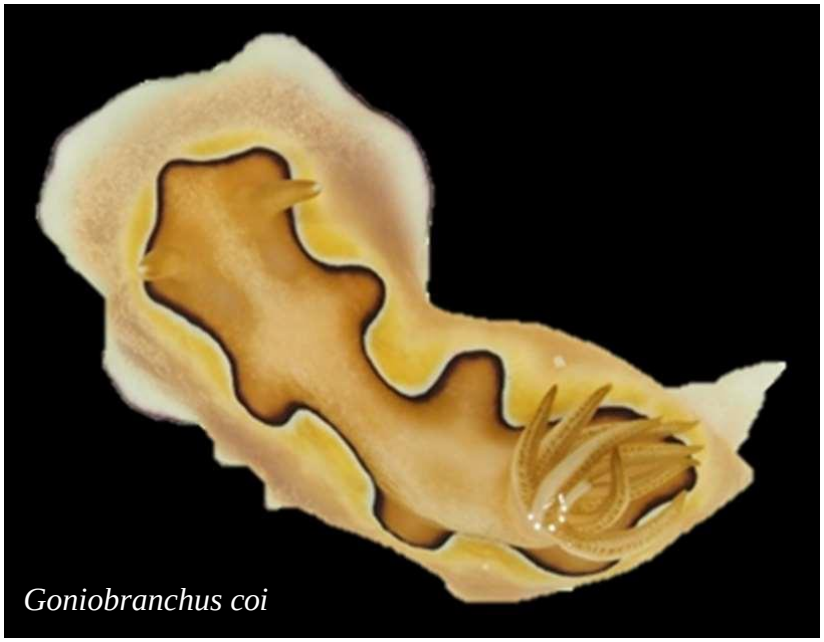


Figure S2. Image of the specimen of *Goniobranchus coi.*

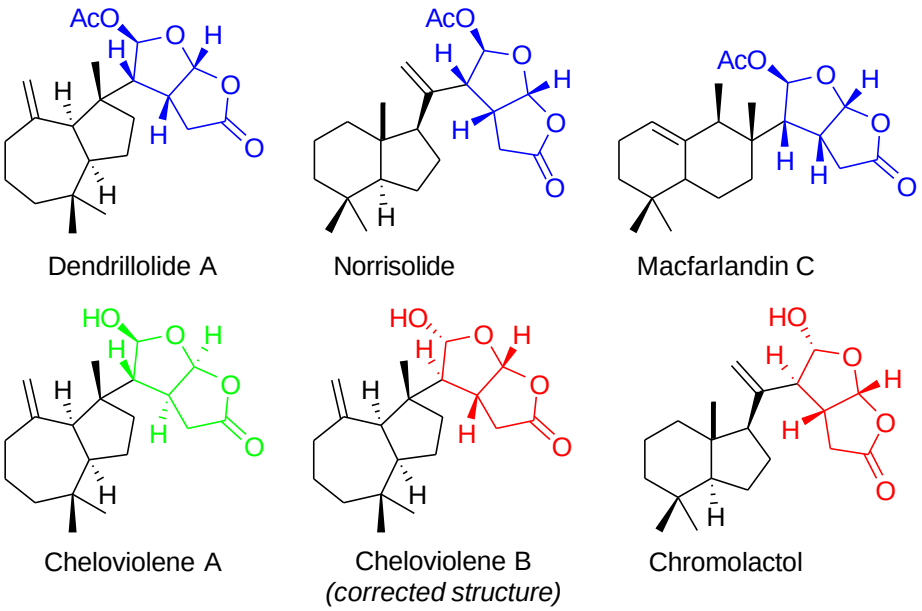
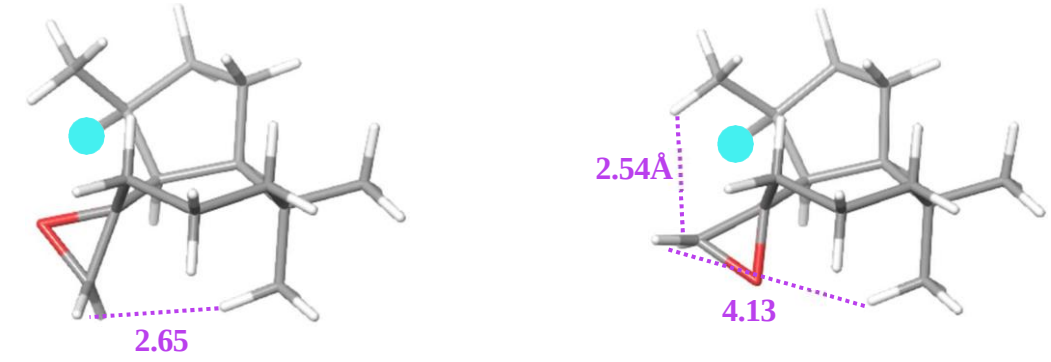


Figure S3. Comparison of selected structures for rearranged metabolites possessing a 2,8-dioxabicyclo[3.3.0]octane moiety, with the three established configurations indicated in blue, green and red.



4
Epoxide protons "inside"

5
Epoxide proton "outside"

Figure S4. Truncated structures of candidate diastereomers **4** and **5** for spiroepoxide, showing distances between key atoms for each stereoisomer; with the blue dot indicating the location of the 2,8-dioxabicyclo[3.3.0]octane moiety.

Assorted spectra

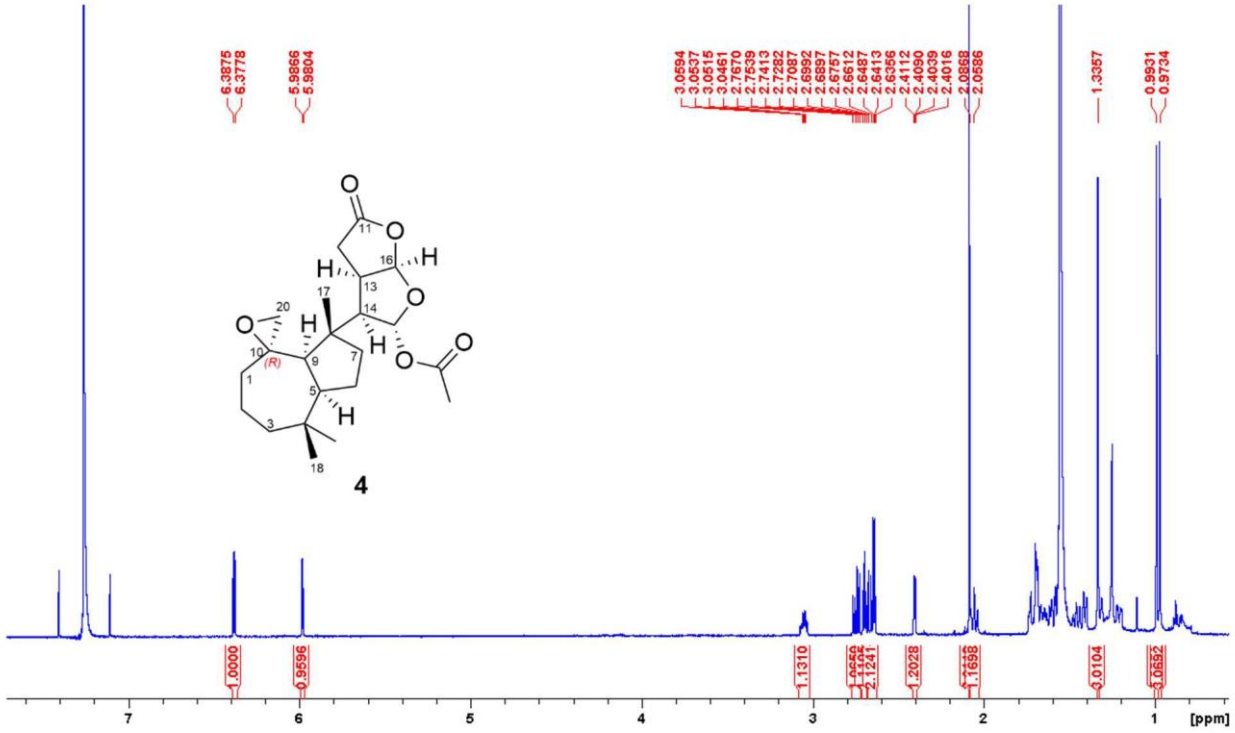


Figure S5. ^{1}H NMR spectrum of **4** (700 MHz, $CDCl_3$).

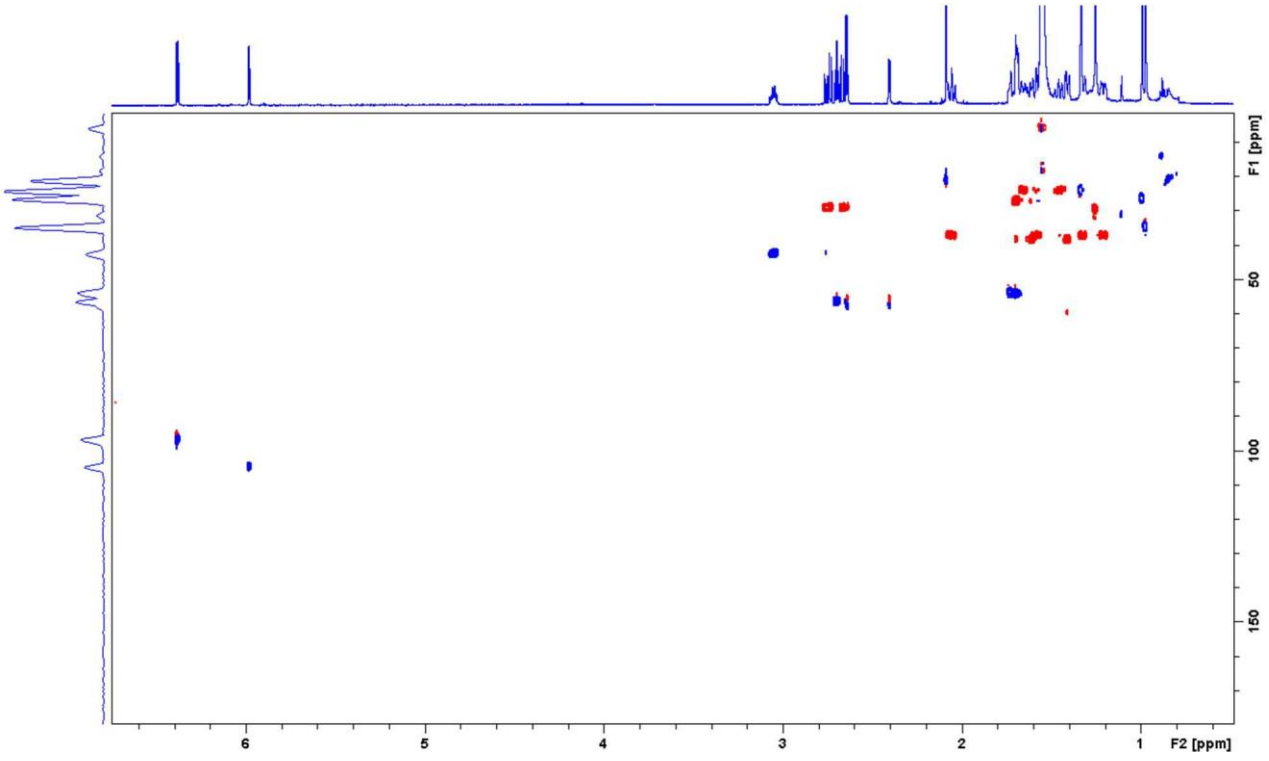


Figure S6. HSQC spectrum of **4** (700 MHz, $CDCl_3$).

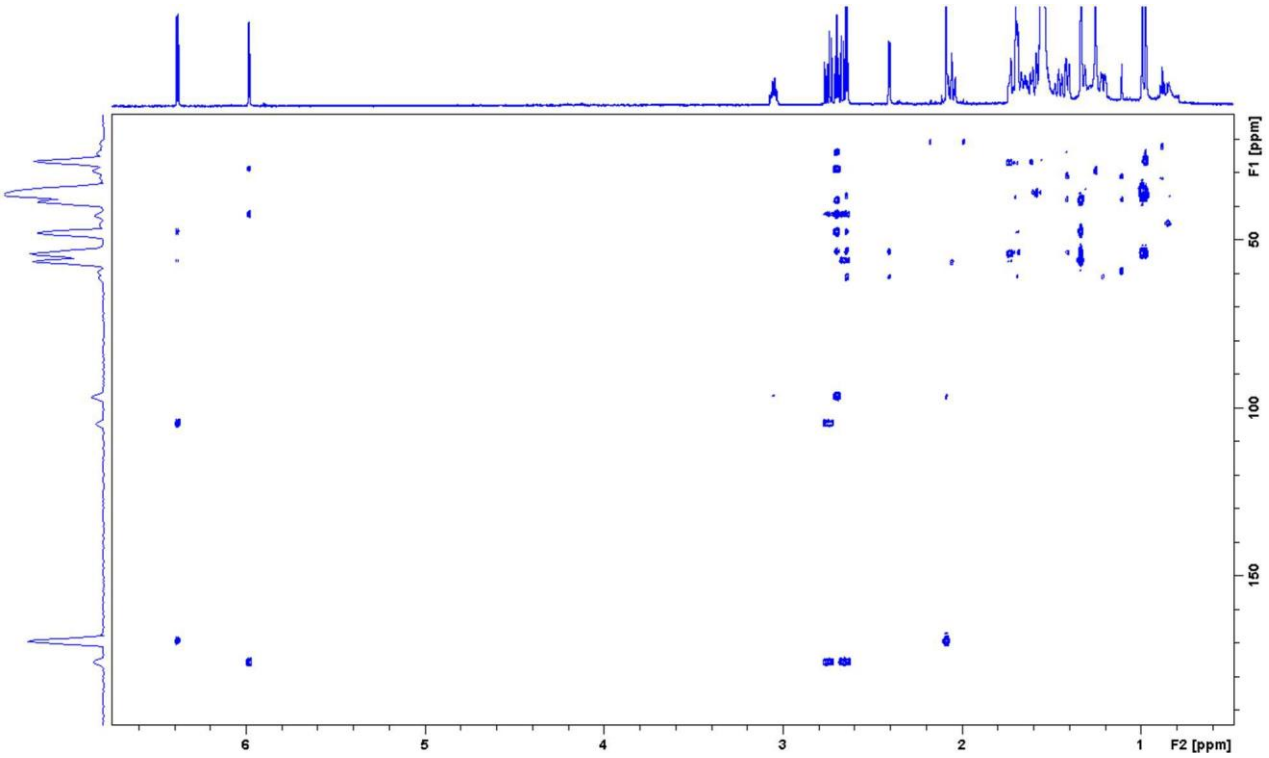


Figure S7. HMBC spectrum of **4** (700 MHz, $CDCl_3$).

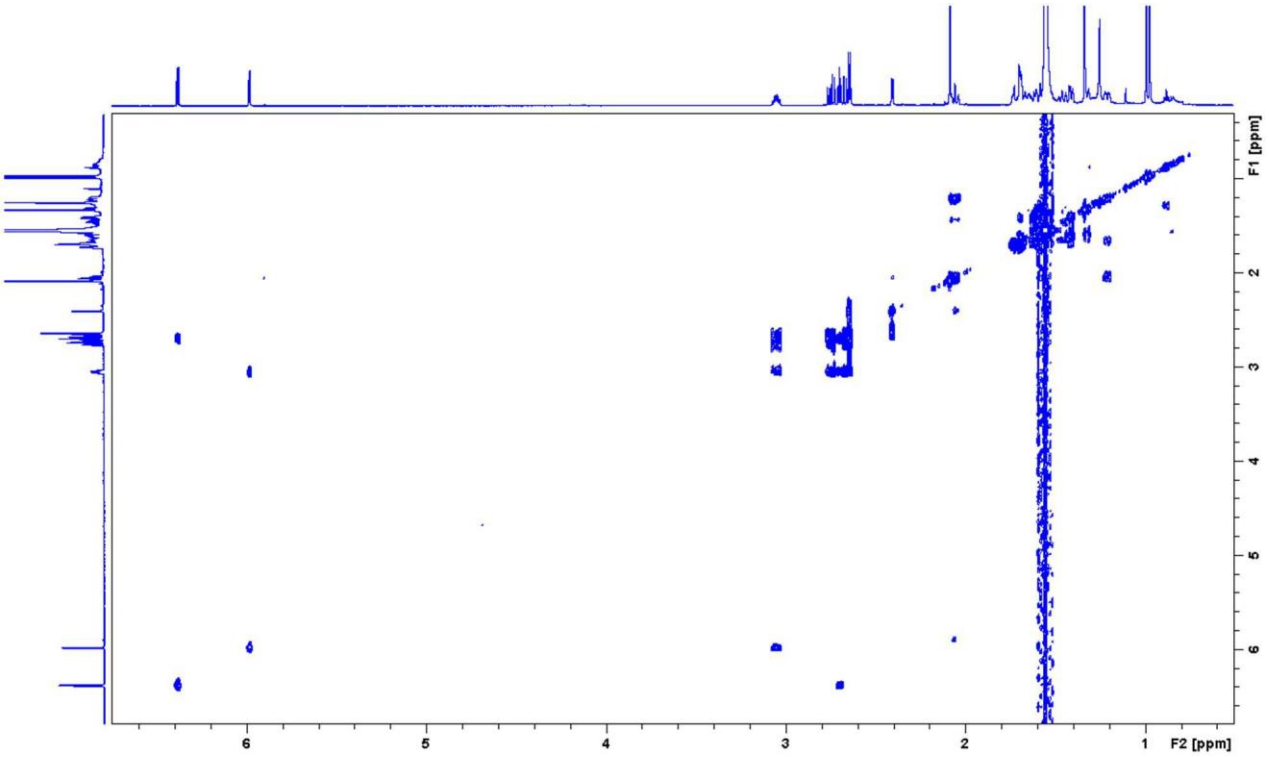


Figure S8. COSY spectrum of **4** (700 MHz, $CDCl_3$).

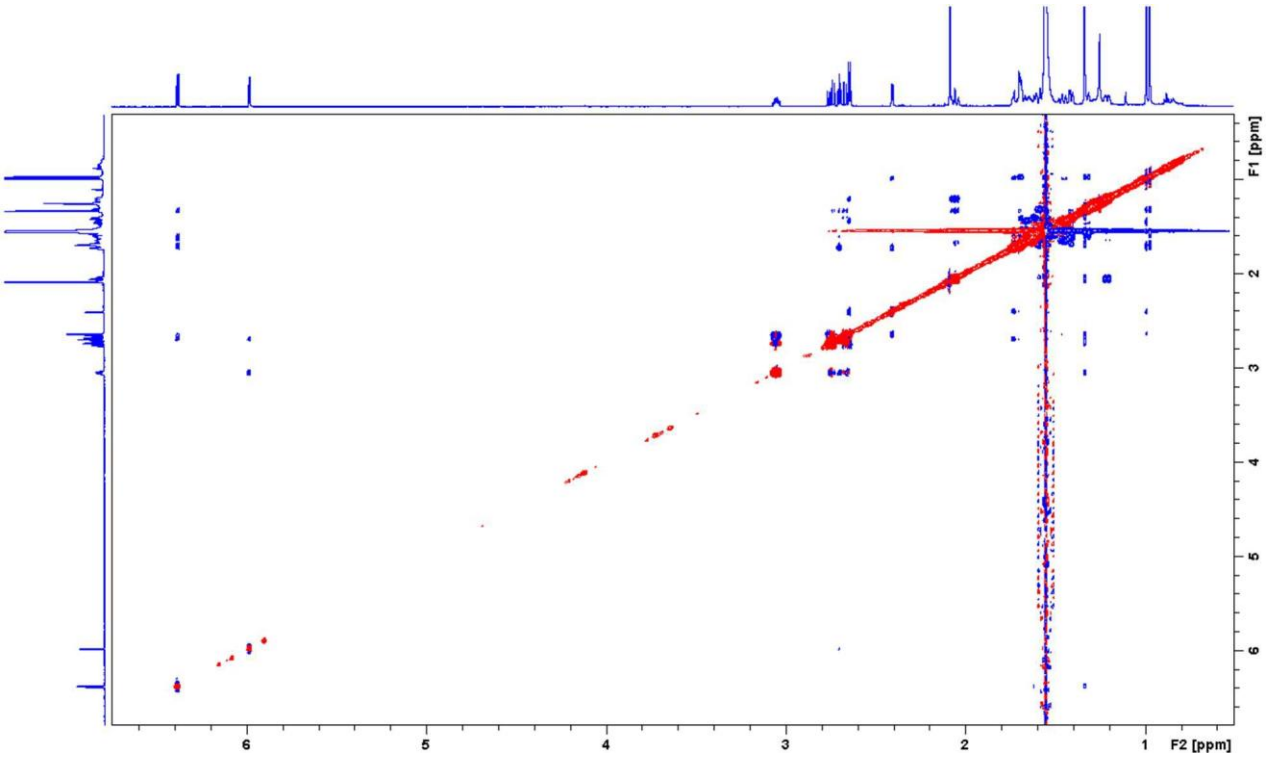
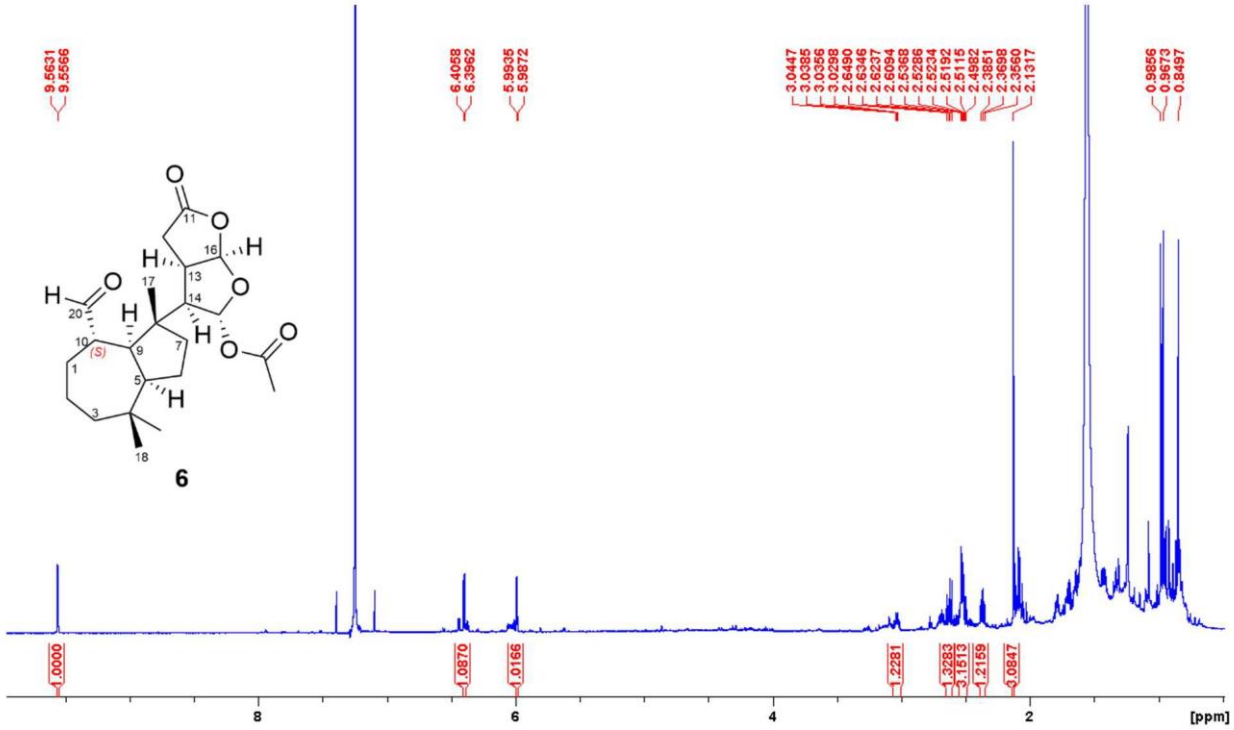


Figure S9. NOESY spectrum of **4** (700 MHz, $CDCl_3$).



6

Figure S10. ^1H NMR spectrum of **6** (700 MHz, $CDCl_3$).

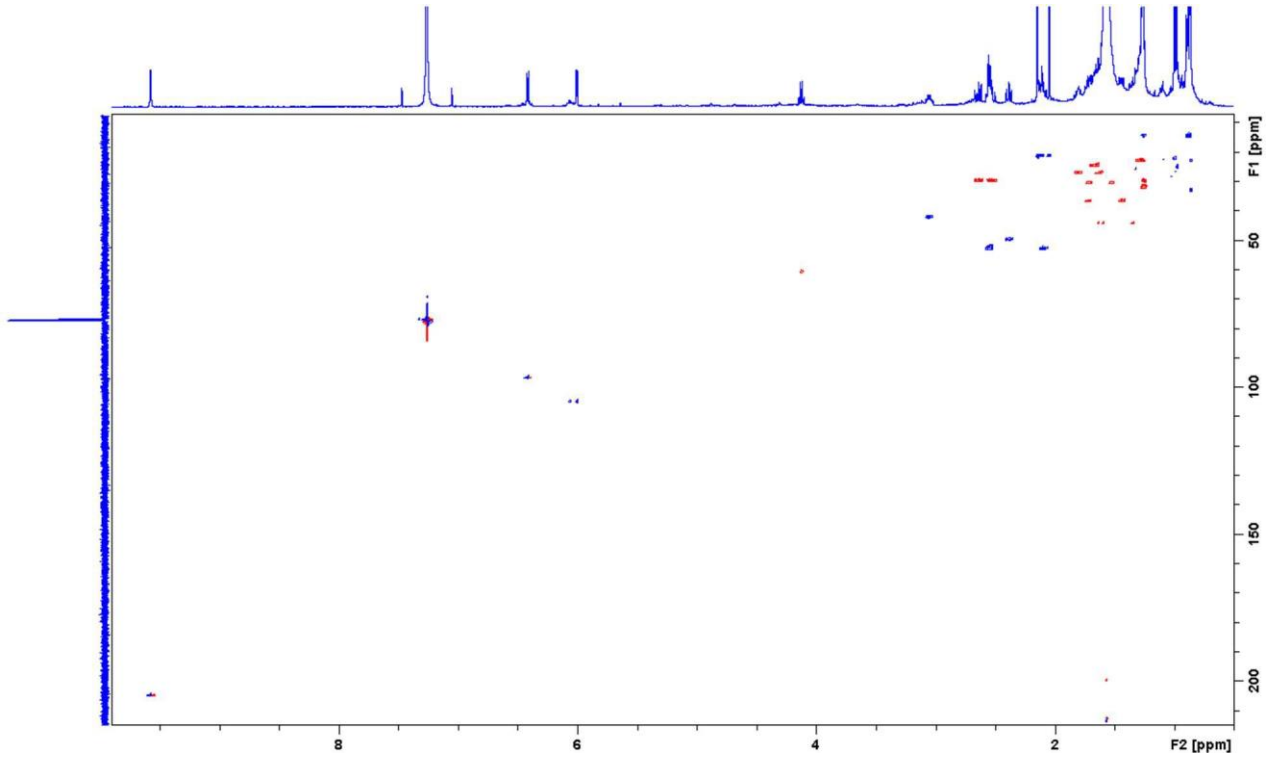


Figure S11. HSQC spectrum of **6** (500 MHz, $CDCl_3$).

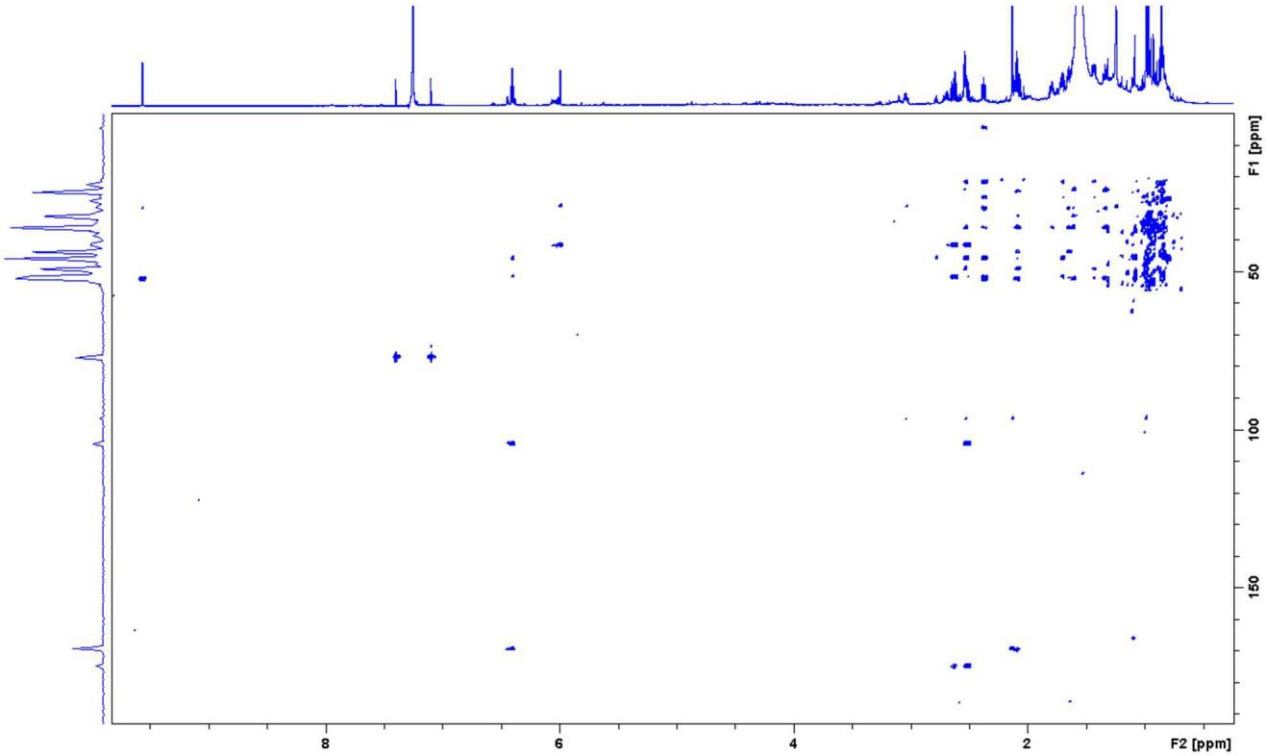


Figure S12. HMBC spectrum of **6** (700 MHz, $CDCl_3$).

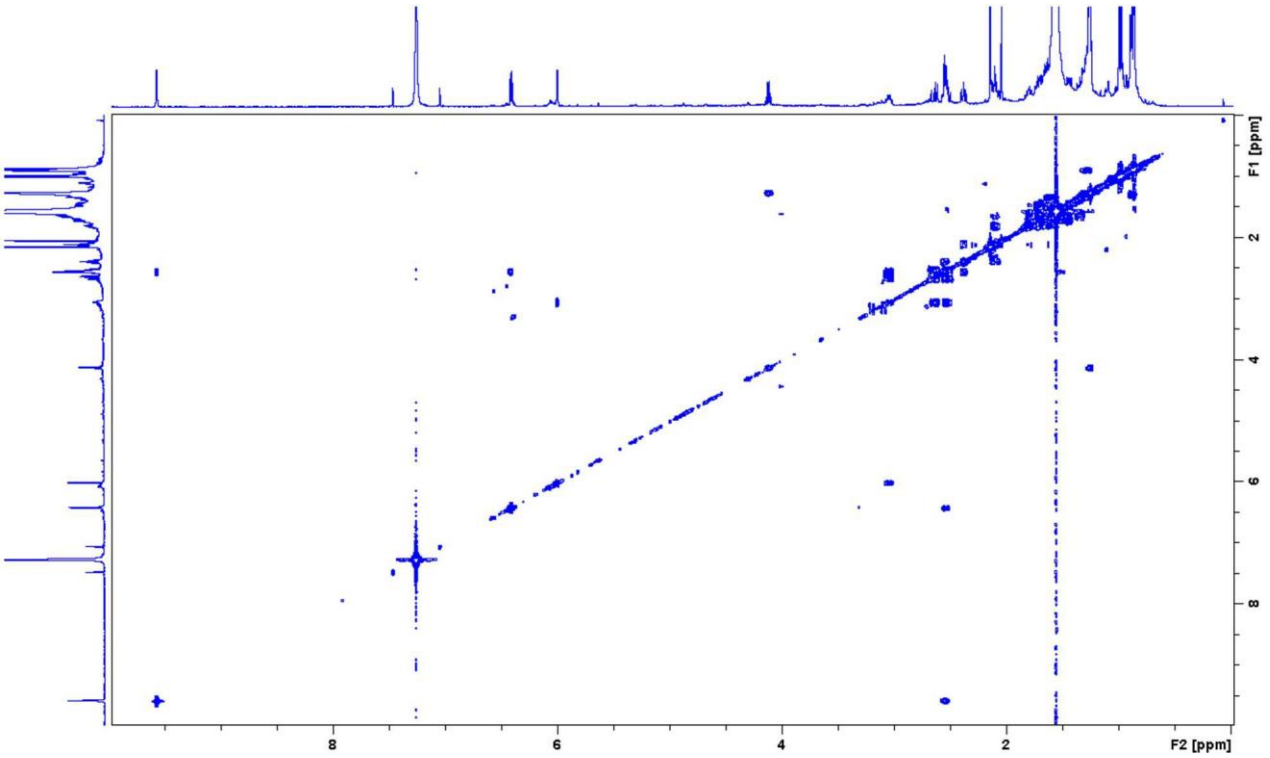


Figure S13. COSY spectrum of **6** (500 MHz, $CDCl_3$).

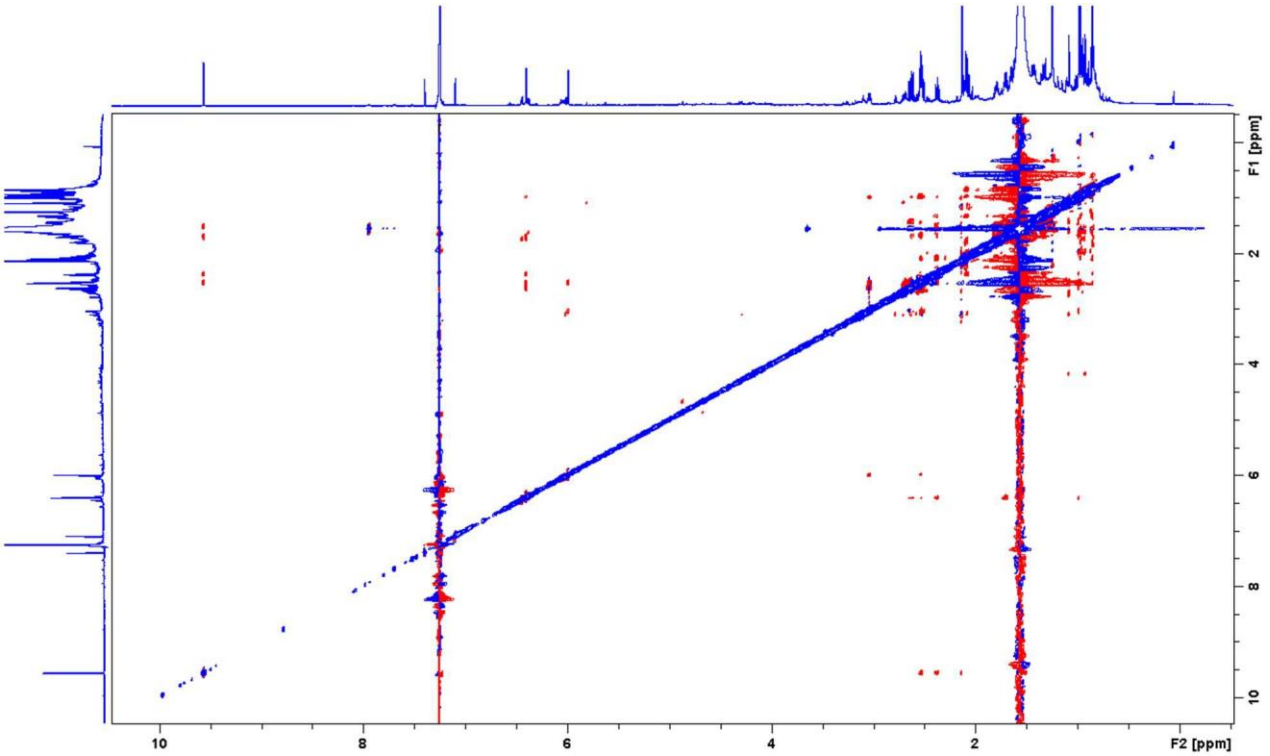


Figure S14. NOESY spectrum of **6** (700 MHz, $CDCl_3$).

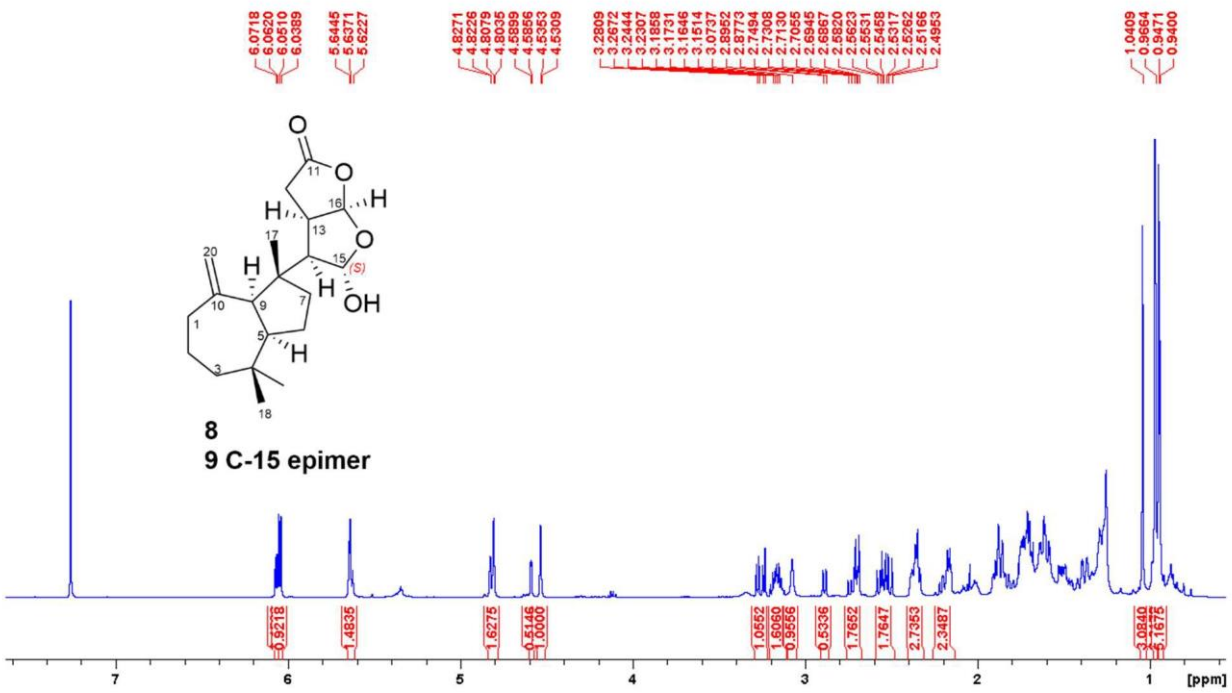


Figure S15. ^{1}H NMR spectrum of diastereomeric mixture of **8** and **9** (500 MHz, $CDCl_3$).

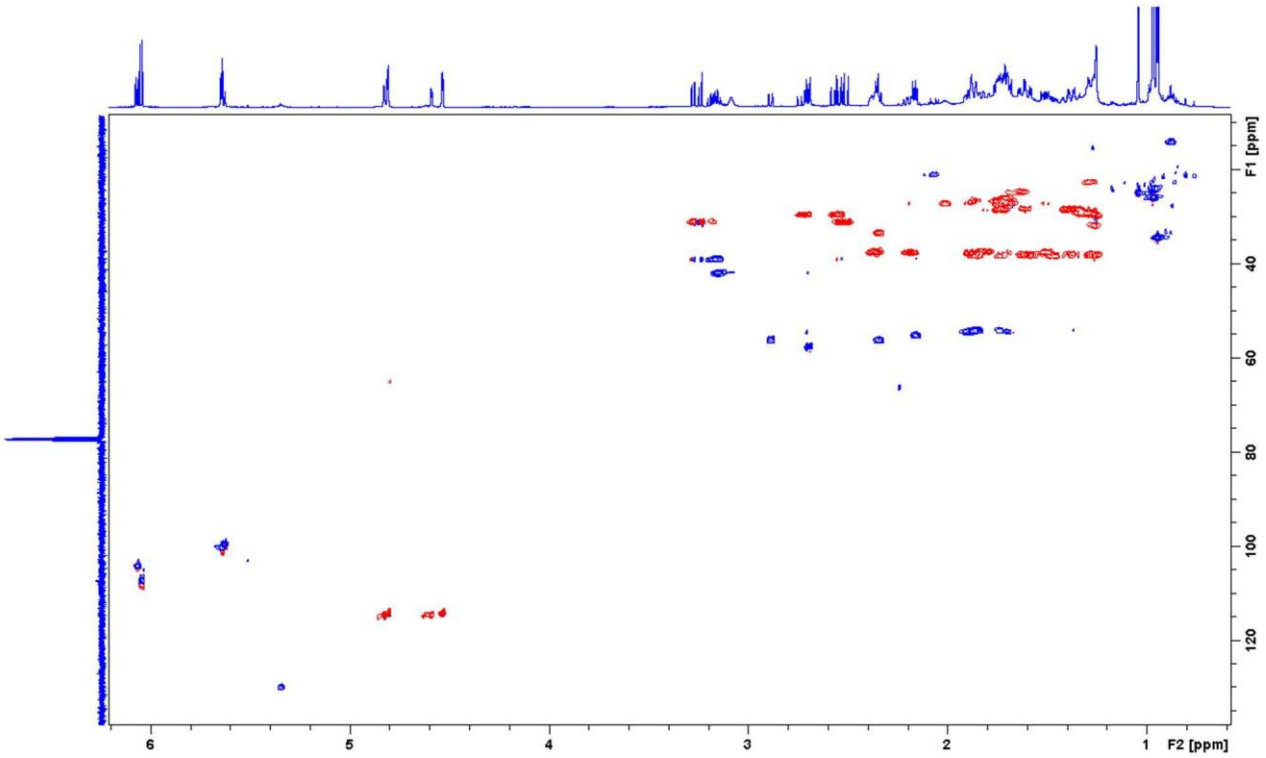


Figure S16. HSQC spectrum of diastereomeric mixture of **8** and **9** (500 MHz, $CDCl_3$).

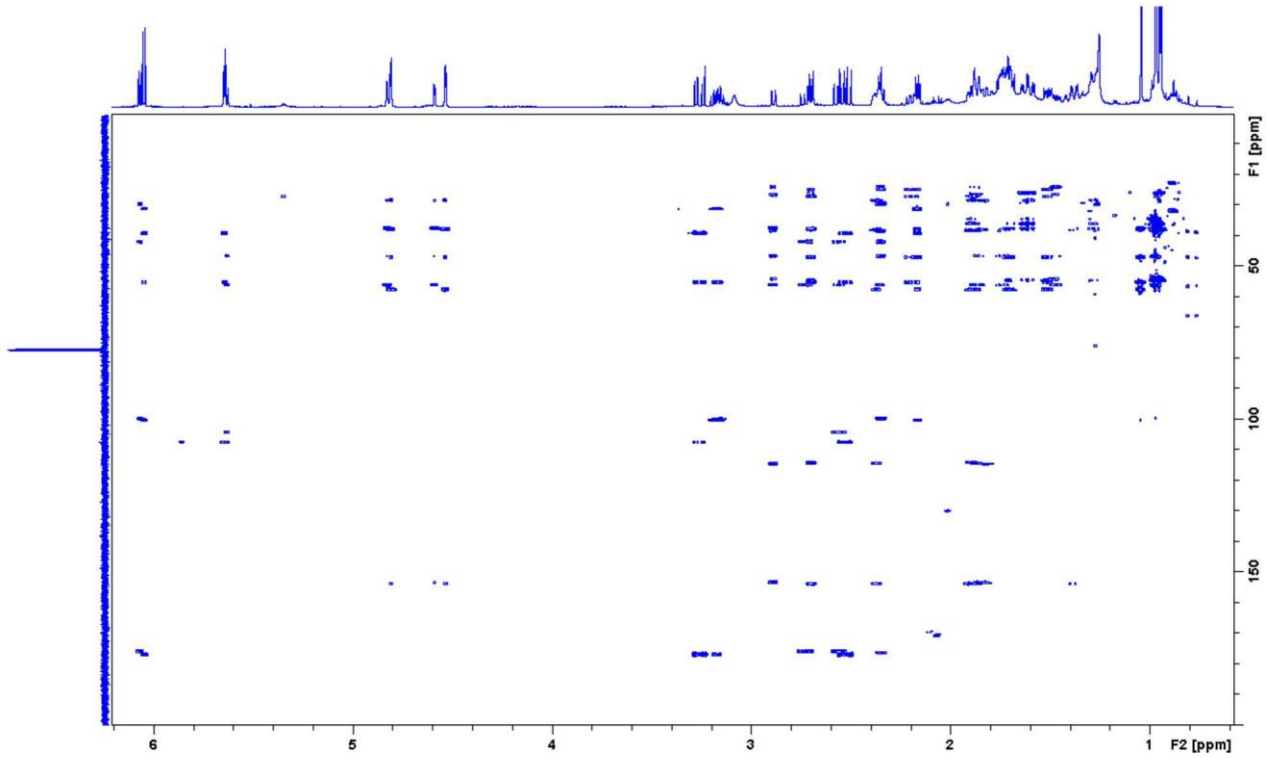


Figure S17. HMBC spectrum of diastereomeric mixture of **8** and **9** (500 MHz, $CDCl_3$).

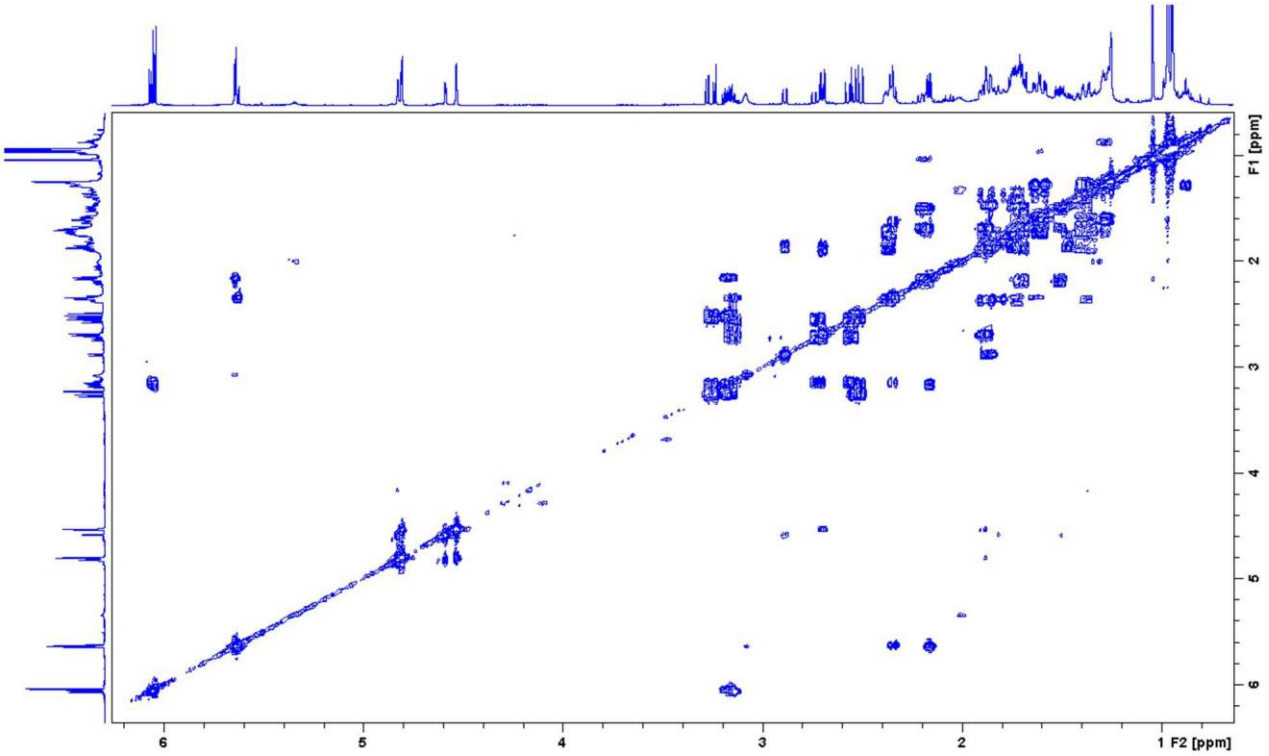


Figure S18. COSY spectrum of diastereomeric mixture of **8** and **9** (500 MHz, $CDCl_3$).

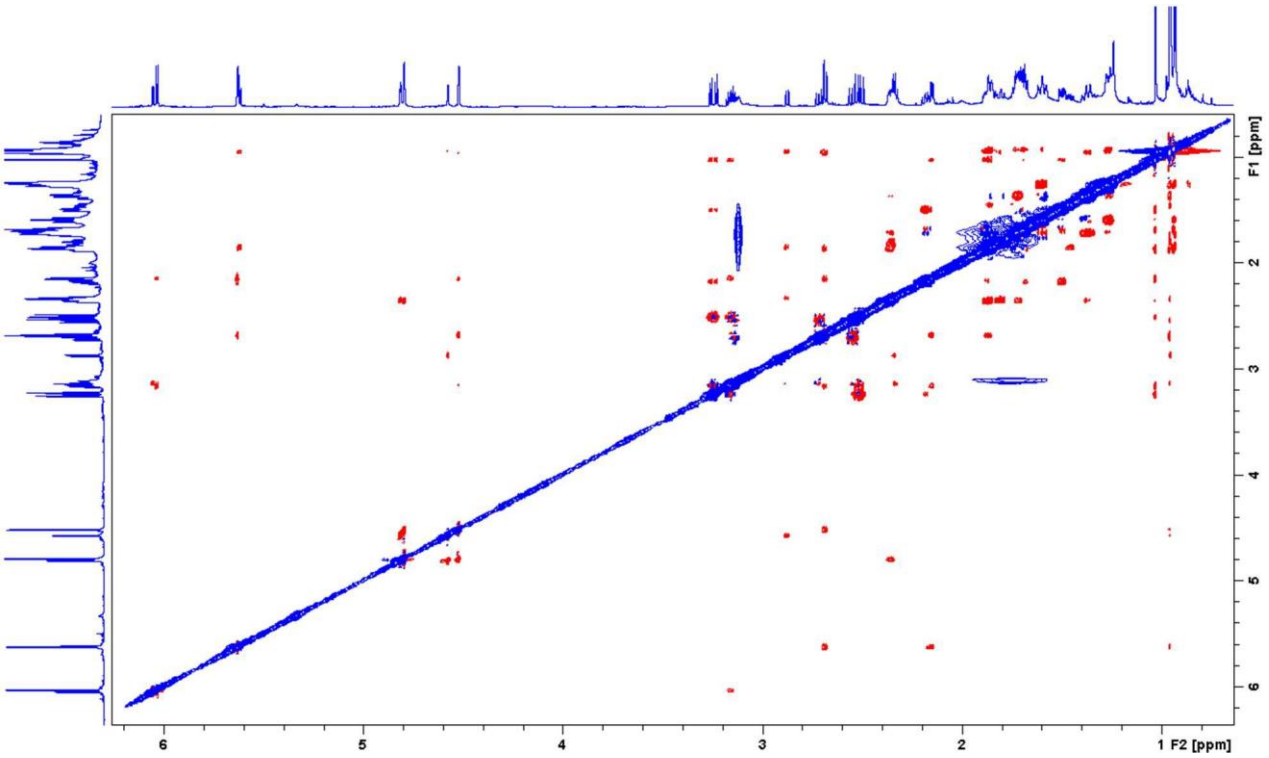


Figure S19. NOESY spectrum of diastereomeric mixture of **8** and **9** (700 MHz, $CDCl_3$).

Computational methods for 10,20-epoxydendrillolide A (4)

A conformational search was with the Monte Carlo Multiple Minimum (MCMM) using *MacroModel* (ver. 2018-1, Schrödinger Inc., New York, NY, USA). All conformers less then 3 kcal mol^{-1} from the lowest energy conformer were then further optimised by DFT calculations using B3LYP/6-31G(d,p) method with IEFPCM chloroform solvent (*Gaussian*, ver. 16W, rev. B.01, Gaussian, Inc., Wallingford, CT, USA). A single point energy was calculated using M062X/6-31+g(d,p) with IEFPCM chloroform solvent. Duplicates and high energy conformers (>3 kcal mol^{-1}) were removed and the free energies were calculated using a single point calculations at M062X/6-31+g(d,p) with IEFPCM chloroform solvent and the vibrational frequencies where checked for a true minimum, i.e. no negative frequencies. The free energies were used to calculate the Boltzmann populations.

The magnetic field tensors were calculated using mpw1pw91/6-311+g(2d,p) and wB97XD/6-311+g(2d,p) for ^{1}H and ^{13}C respectively. The unscaled chemical shifts (δ_u) were computed using TMS as reference standard according to:

$$\delta_u = \sigma_0 - \sigma_x$$

where σ_x is the Boltzmann averaged magnetic field tensors (over all significantly populated conformations) and σ_0 is the magnetic field tensors of TMS computed at the same level of theory employed for σ_x. The scaled chemical shifts (δ_s) were computed as:

$$\delta_s = \delta_u m - b$$

where m and b are the slope and intercept respectively, resulting from a linear regression calculation on a plot of δ_u against δ_{exp}.[1,2] The DP4 probabilities were calculated using the procedure of Sarotti[3]

using their supplied spreadsheet using scaled shifts.

Table S1. DFT modelling for 10,20-epoxydendrillolide A (4).

Spiro epoxide	Unique structures after MM	After DFT opt (<3 kcal mol^{-1} + removal of duplicates)
R	8	6
S	12	5

Table S2. Computed DP4 probabilities for the *R* and *S* isomers of 10,20-epoxydendrillolide A 4 and 5 respectively.

Spiro Epoxide	^{1}H	^{13}C	$^{1}H + ^{13}C$
R-isomer (4)	99.97	80.23	99.99
S-isomer (5)	0.03	19.77	0.01

The mean absolute error (MAE) of Spiro-R compared to the experimental chemical shifts was 0.08 and 1.0 for proton and carbon respectively. The maximum deviations were 0.27 and 2.6 ppm.

Table S3. Proton experimental and calculated chemical shifts for the *R* and *S* isomer of 10,20-epoxydendrillolide A 4 and 5 respectively.

^{1}H NMR chemical shift: experimental vs scaled

^{1}H	Expt	R-isomer (**4**)	S-isomer (**5**)
1a	2.06	2.07	1.76
1b	1.21	1.11	1.19
2a	1.66	1.56	1.79
2b	1.45	1.48	1.38
3a	1.58	1.61	1.63
3b	1.32	1.27	1.25
5	1.69	1.75	1.73
6a	1.69	1.70	1.75
6b	1.69	1.62	1.72
7a	1.62	1.65	1.67
7b	1.41	1.37	1.46
9	1.73	1.92	1.87
12a	2.75	2.75	2.64
12b	2.67	2.63	2.41
13	3.05	3.04	3.08
14	2.7	2.73	2.77
15	6.38	6.11	6.04
16	5.98	6.14	6.19
17	1.34	1.25	1.09
18	0.97	0.95	1.07
19	0.99	0.90	0.88
20a	2.64	2.64	2.87
20b	2.4	2.52	2.51
15-$OCOCH_3$	2.09	2.32	2.29

Table S4. Carbon experimental and calculated chemical shifts for the *R* and *S* isomer of 10,20-epoxydendrillolide A 4 and 5 respectively.

^{13}C NMR chemical shift: experimental vs scaled

^{13}C	Expt	R-isomer (**4**)	S-isomer (**5**)
1	37.2	37.3	35.5
2	24.1	24.6	23.4
3	37.2	36.2	37.1
4	36.3	38.1	38.7
5	54.1	53.5	55.6
6	27.2	27.5	27.7
7	38.4	37.9	37.5
8	47.7	49.9	49.2
9	53.4	53.4	55.0
10	61.2	61.3	60.0
11	175.7	175.2	175.0
12	29.1	30.3	29.9
13	42.4	44.3	44.0
14	56.2	57.4	57.1
15	96.9	98.9	99.0
16	104.8	103.0	103.2
17	24.1	23.3	23.8
18	34.8	32.2	32.7
19	26.5	25.2	24.7
20	56.7	55.1	55.2
15-$OCOCH_3$	169.5	169.5	169.3
15-$OCOCH_3$	21.1	20.5	20.8

XYZ Coordinates and energies for (*R*)-10,20-epoxydendrillolide A (4) at 228 K

Compound: Conf1R, Conformer: 01, Energy:-1308.015347 Hartree, Solvent: chloroform, Boltzmann percentage: 2.86

Zero-point correction=	0.522704 (Hartree/Particle)
Thermal correction to Energy=	0.548253
Thermal correction to Enthalpy=	0.549198
Thermal correction to Gibbs Free Energy=	0.470180
Sum of electronic and zero-point Energies=	-1307.962823
Sum of electronic and thermal Energies=	-1307.937274
Sum of electronic and thermal Enthalpies=	-1307.936330
Sum of electronic and thermal Free Energies=	-1308.015347

C	1.942552	-2.500393	-0.440303
C	1.014166	-1.343404	-0.789527
C	3.659393	0.243962	-0.138518
C	4.165235	-1.221240	-0.087294
C	3.397260	-2.284209	-0.879438
H	1.915022	-2.712788	0.631820
H	1.539677	-3.386344	-0.942828
H	5.201551	-1.218509	-0.449952
H	4.222491	-1.536666	0.962795
H	3.424844	-2.052660	-1.951124
H	3.928987	-3.236703	-0.765545
C	0.937854	-0.083044	0.087306
C	2.313183	0.497022	0.614823
C	2.298263	0.206045	2.128787
C	0.843600	0.481300	2.510342
C	0.001286	-0.187637	1.383964
H	0.502400	0.669658	-0.574088
H	2.193791	1.586874	0.540580
H	2.564614	-0.835880	2.340602
H	2.997079	0.836036	2.684961
H	0.568830	0.091169	3.495766
H	0.680200	1.564199	2.540692
O	-0.290072	-1.771184	-1.285635
C	0.649158	-1.217487	-2.217748
H	0.380188	-0.244287	-2.627259
H	1.048628	-1.926774	-2.942166
C	3.550243	0.743566	-1.594798
H	3.292047	1.808349	-1.618343
H	4.508099	0.623239	-2.113291
H	2.793767	0.210522	-2.172755
C	4.744796	1.107592	0.551443
H	4.431634	2.154843	0.629526
H	4.976777	0.748354	1.558543
H	5.673311	1.081144	-0.028657
C	-0.249164	-1.651649	1.828994
H	-0.955825	-1.667783	2.663744
H	-0.660479	-2.276888	1.037302
H	0.675592	-2.113198	2.182878
C	-1.393614	0.512076	1.270103
C	-2.371519	-0.064638	0.228935

H	-1.884624	0.309401	2.228521
H	-1.889096	-0.327949	-0.712617
O	-3.363900	0.950774	0.021738
C	-2.770057	2.194977	0.146489
C	-1.539940	2.068453	1.086804
C	-0.484143	2.918634	0.367852
C	-0.944333	2.982455	-1.075084
H	-3.534697	2.916105	0.438588
H	-1.771629	2.506710	2.057597
H	-0.502731	3.943565	0.757370
H	0.546678	2.582070	0.429673
O	-2.253219	2.622238	-1.146229
O	-0.314184	3.309943	-2.051699
O	-3.040916	-1.187205	0.769869
C	-3.768017	-2.039490	-0.023400
O	-4.355701	-2.940362	0.527938
C	-3.768366	-1.810192	-1.514728
H	-4.474254	-2.506884	-1.964385
H	-4.048618	-0.782876	-1.759131
H	-2.767327	-1.995858	-1.916674

Compound: Conf1R, Conformer: 02, Energy:-1308.017182 Hartree, Solvent: chloroform, Boltzmann percentage: 19.97

Zero-point correction=	0.522047 (Hartree/Particle)
Thermal correction to Energy=	0.547923
Thermal correction to Enthalpy=	0.548867
Thermal correction to Gibbs Free Energy=	0.468694
Sum of electronic and zero-point Energies=	-1307.963829
Sum of electronic and thermal Energies=	-1307.937953
Sum of electronic and thermal Enthalpies=	-1307.937009
Sum of electronic and thermal Free Energies=	-1308.017182

C	2.562997	-2.322866	-0.197686
C	1.412341	-1.445477	-0.674622
C	3.650630	0.742231	-0.280291
C	4.465525	-0.562879	-0.080758
C	3.937300	-1.859835	-0.704134
H	2.579306	-2.388697	0.894028
H	2.362113	-3.334195	-0.567220
H	5.469298	-0.383333	-0.487882
H	4.610235	-0.723232	0.995456
H	3.909878	-1.771109	-1.797028
H	4.662200	-2.653787	-0.487302
C	1.069531	-0.125822	0.034719
C	2.286960	0.774346	0.481022
C	2.343402	0.598772	2.011065
C	0.866678	0.636023	2.399408
C	0.145734	-0.248606	1.338668
H	0.507786	0.434395	-0.714561
H	1.925034	1.801295	0.326798
H	2.793520	-0.361145	2.288955

H	2.921694	1.382335	2.507506
H	0.670128	0.282286	3.416568
H	0.518170	1.673373	2.348271
O	0.230154	-2.192641	-1.094077
C	1.047569	-1.583791	-2.102056
H	0.589713	-0.748021	-2.630731
H	1.592969	-2.282891	-2.735470
C	3.430768	1.036354	-1.779192
H	2.944383	2.009504	-1.912933
H	4.390616	1.072738	-2.306567
H	2.811834	0.286447	-2.274614
C	4.522282	1.894132	0.278979
H	3.989969	2.851153	0.240148
H	4.821757	1.716327	1.316134
H	5.437426	1.998622	-0.313534
C	0.078759	-1.688492	1.905683
H	-0.590983	-1.709761	2.770807
H	-0.289526	-2.414756	1.181139
H	1.059650	-2.021587	2.252588
C	-1.325292	0.240869	1.146682
C	-2.157461	-0.467058	0.052645
H	-1.831223	-0.017878	2.084781
H	-1.564058	-0.875238	-0.763051
O	-3.064215	0.485452	-0.478747
C	-3.090608	1.642509	0.348749
C	-1.673476	1.736230	0.940267
C	-0.972364	2.616651	-0.109686
C	-2.105677	3.376327	-0.781906
H	-3.916130	1.599438	1.063517
H	-1.693744	2.263910	1.896292
H	-0.244692	3.317917	0.300602
H	-0.473740	2.048777	-0.899102
O	-3.301580	2.781294	-0.469818
O	-2.048925	4.342476	-1.496751
O	-2.882744	-1.529542	0.691359
C	-3.516200	-2.499238	-0.036346
O	-4.175523	-3.312329	0.570811
C	-3.337577	-2.507660	-1.535841
H	-3.960102	-3.300613	-1.947763
H	-3.622039	-1.546832	-1.972065
H	-2.289700	-2.699442	-1.788199

Compound: Conf1R, Conformer: 03, Energy:-1308.017720 Hartree, Solvent: chloroform, Boltzmann percentage: 35.305

Zero-point correction=	0.522042 (Hartree/Particle)
Thermal correction to Energy=	0.547916
Thermal correction to Enthalpy=	0.548860
Thermal correction to Gibbs Free Energy=	0.468527
Sum of electronic and zero-point Energies=	-1307.964206
Sum of electronic and thermal Energies=	-1307.938331
Sum of electronic and thermal Enthalpies=	-1307.937387
Sum of electronic and thermal Free Energies=	-1308.017720

C	-3.157105	-1.212011	1.723385
C	-2.064836	-0.170795	1.520916
C	-3.504686	-0.032789	-1.309336
C	-4.423701	-1.007482	-0.526870
C	-4.472673	-0.893579	1.000953
H	-2.807962	-2.202332	1.415154
H	-3.339650	-1.269908	2.802137
H	-5.444511	-0.860373	-0.903728
H	-4.156980	-2.038262	-0.796157
H	-4.819894	0.103953	1.296555
H	-5.234084	-1.594856	1.363910
C	-1.242407	-0.110009	0.226746
C	-1.976889	-0.310916	-1.154724
C	-1.451194	-1.661869	-1.673514
C	0.026311	-1.623177	-1.271119
C	0.021837	-1.091034	0.190994
H	-0.846160	0.904915	0.218779
H	-1.511582	0.439652	-1.811438
H	-1.958618	-2.504473	-1.188961
H	-1.581061	-1.783702	-2.752133
H	0.512407	-2.599716	-1.352717
H	0.554199	-0.941143	-1.949403
O	-1.241030	0.049751	2.701895
C	-2.176263	1.068308	2.322954
H	-1.729708	1.992966	1.958733
H	-3.018541	1.196696	3.003128
C	-3.805119	1.432307	-0.926817
H	-3.252148	2.119454	-1.577400
H	-4.872340	1.650731	-1.046728
H	-3.533151	1.665449	0.104621
C	-3.861550	-0.193653	-2.807168
H	-3.195375	0.401681	-3.441852
H	-3.795847	-1.236007	-3.133937
H	-4.886800	0.144851	-2.991534
C	-0.107329	-2.311743	1.131527
H	0.788699	-2.935684	1.060277
H	-0.234306	-2.018864	2.175227
H	-0.949982	-2.946896	0.849436
C	1.288698	-0.295634	0.636991
C	1.690234	0.950169	-0.192528
H	1.041381	0.096468	1.629574
H	1.367028	0.931698	-1.235685
O	3.101260	1.039412	-0.179363
C	3.651597	0.103831	0.745618
C	2.631704	-1.041960	0.797792
C	3.156550	-1.954791	-0.325476
C	4.625841	-1.587061	-0.455088
H	3.897627	0.589633	1.692357
H	2.683694	-1.562407	1.756135
H	3.055571	-3.022890	-0.128195
H	2.690957	-1.754736	-1.294391
O	4.858994	-0.404970	0.204183
O	5.506955	-2.171610	-1.029015

O	1.115535	2.099751	0.452568
C	1.151568	3.346238	-0.114405
O	0.645276	4.252624	0.506311
C	1.802046	3.508210	-1.467508
H	1.818239	4.569274	-1.711866
H	2.816721	3.104725	-1.466339
H	1.230444	2.977083	-2.236121

Compound: Conf1R, Conformer: 04, Energy:-1308.014514 Hartree, Solvent: chloroform, Boltzmann percentage: 1.184

Zero-point correction=	0.522370 (Hartree/Particle)
Thermal correction to Energy=	0.548192
Thermal correction to Enthalpy=	0.549136
Thermal correction to Gibbs Free Energy=	0.469097
Sum of electronic and zero-point Energies=	-1307.961240
Sum of electronic and thermal Energies=	-1307.935418
Sum of electronic and thermal Enthalpies=	-1307.934474
Sum of electronic and thermal Free Energies=	-1308.014514

C	2.015439	-2.652424	-0.317822
C	1.028149	-1.563725	-0.720162
C	3.586247	0.174361	-0.073763
C	4.175418	-1.257634	0.005530
C	3.461714	-2.380200	-0.755042
H	1.986087	-2.821058	0.763462
H	1.664628	-3.578787	-0.785504
H	5.207168	-1.205690	-0.366584
H	4.258792	-1.545375	1.061857
H	3.482237	-2.180630	-1.833328
H	4.038233	-3.302174	-0.610844
C	0.888822	-0.273576	0.105717
C	2.222002	0.357883	0.665841
C	2.192658	0.032217	2.172745
C	0.724613	0.251005	2.547591
C	-0.089609	-0.363778	1.365206
H	0.451551	0.441062	-0.593323
H	2.051919	1.439948	0.600604
H	2.484916	-1.007265	2.361658
H	2.866289	0.665195	2.756412
H	0.449903	-0.219060	3.497299
H	0.528592	1.319275	2.670209
O	-0.248138	-2.086124	-1.189086
C	0.648271	-1.515941	-2.150143
H	0.315964	-0.577127	-2.590909
H	1.085926	-2.227680	-2.850151
C	3.454278	0.641608	-1.538998
H	3.099761	1.677057	-1.582786
H	4.426433	0.597563	-2.043083
H	2.756615	0.032362	-2.116650
C	4.612663	1.112611	0.608218
H	4.244776	2.143989	0.646406
H	4.841904	0.796966	1.630676

H	5.553318	1.116342	0.047229
C	-0.413573	-1.818667	1.801599
H	-1.156980	-1.801430	2.605686
H	-0.795448	-2.448430	0.998803
H	0.476747	-2.307271	2.205186
C	-1.463546	0.371512	1.179887
C	-2.380692	-0.286894	0.127013
H	-1.963622	0.261150	2.145387
H	-2.090788	-1.287445	-0.175555
O	-2.339411	0.510272	-1.036914
C	-2.123643	1.853183	-0.687220
C	-1.607407	1.888693	0.774013
C	-0.429061	2.869314	0.679189
C	-0.095804	2.962076	-0.798676
H	-3.022476	2.445137	-0.879168
H	-2.387265	2.306527	1.411471
H	-0.733405	3.869064	1.008328
H	0.464871	2.617370	1.242346
O	-1.089144	2.380874	-1.531773
O	0.865527	3.471232	-1.319625
O	-3.713499	-0.283597	0.680336
C	-4.738490	-0.961449	0.081688
O	-5.843279	-0.845728	0.562605
C	-4.430713	-1.820405	-1.122338
H	-5.368606	-2.226698	-1.498129
H	-3.933560	-1.239267	-1.902318
H	-3.767349	-2.647668	-0.849461

Compound: Conf1R, Conformer: 05, Energy:-1308.017845 Hartree, Solvent: chloroform, Boltzmann percentage: 40.303

Zero-point correction=	0.522155 (Hartree/Particle)
Thermal correction to Energy=	0.547840
Thermal correction to Enthalpy=	0.548784
Thermal correction to Gibbs Free Energy=	0.469358
Sum of electronic and zero-point Energies=	-1307.965048
Sum of electronic and thermal Energies=	-1307.939363
Sum of electronic and thermal Enthalpies=	-1307.938419
Sum of electronic and thermal Free Energies=	-1308.017845

C	3.069359	-1.506114	1.316098
C	2.077769	-1.471566	0.160066
C	3.918894	0.972000	-0.615020
C	4.705442	0.366215	0.577369
C	4.498996	-1.114939	0.914187
H	2.732340	-0.865285	2.136755
H	3.068797	-2.531601	1.701350
H	5.773497	0.513866	0.369521
H	4.496233	0.963633	1.474299
H	4.823977	-1.742958	0.075653
H	5.165383	-1.363658	1.749158
C	1.440593	-0.153297	-0.294238
C	2.382519	1.112215	-0.372442

C	1.942984	1.981111	0.820290
C	0.422912	1.844766	0.774633
C	0.159511	0.323594	0.546927
H	1.089454	-0.352153	-1.311434
H	2.024059	1.651104	-1.261294
H	2.343117	1.598445	1.766645
H	2.265101	3.021830	0.730096
H	-0.076765	2.209711	1.678302
H	0.037318	2.433089	-0.063142
O	1.136539	-2.583411	0.152697
C	2.185256	-2.572917	-0.822292
H	1.863745	-2.417285	-1.851924
H	2.945903	-3.342454	-0.690840
C	4.180529	0.178286	-1.912473
H	3.708689	0.675273	-2.767883
H	5.255782	0.120406	-2.116176
H	3.797519	-0.842806	-1.871357
C	4.486382	2.395823	-0.838282
H	3.932866	2.926584	-1.620950
H	4.446283	3.001059	0.072313
H	5.534870	2.341440	-1.150490
C	0.036821	-0.337112	1.937443
H	-0.909415	-0.056136	2.412264
H	0.093870	-1.424124	1.907909
H	0.827374	0.019860	2.602742
C	-1.118718	0.132839	-0.325891
C	-2.415538	0.836164	0.137042
H	-0.892805	0.614339	-1.286794
H	-2.552432	0.869112	1.220846
O	-3.501998	0.120874	-0.431173
C	-3.031586	-0.958542	-1.237738
C	-1.632473	-1.275134	-0.691070
C	-1.979230	-2.300301	0.403887
C	-3.305163	-2.890517	-0.040048
H	-3.108304	-0.710269	-2.298630
H	-1.001489	-1.746338	-1.446374
H	-1.226401	-3.076923	0.527730
H	-2.149472	-1.844156	1.383625
O	-3.858072	-2.088957	-1.010508
O	-3.863958	-3.884697	0.344935
O	-2.403710	2.172239	-0.375003
C	-3.345729	3.094632	-0.003288
O	-3.291783	4.184947	-0.523401
C	-4.374256	2.701788	1.030690
H	-5.086023	3.520128	1.128093
H	-4.892594	1.784663	0.742641
H	-3.898272	2.529690	2.001886

Compound: Conf1R, Conformer: 07, Energy:-1308.013439 Hartree, Solvent: chloroform, Boltzmann percentage: 0.379

Zero-point correction=	0.522348 (Hartree/Particle)
Thermal correction to Energy=	0.548159
Thermal correction to Enthalpy=	0.549103
Thermal correction to Gibbs Free Energy=	0.468838
Sum of electronic and zero-point Energies=	-1307.959928
Sum of electronic and thermal Energies=	-1307.934118
Sum of electronic and thermal Enthalpies=	-1307.933174
Sum of electronic and thermal Free Energies=	-1308.013439

C	3.177085	0.443662	-1.876230
C	2.286376	1.155389	-0.869158
C	3.514871	-1.032962	1.021563
C	4.358296	-1.230100	-0.267979
C	4.489497	-0.065958	-1.259205
H	2.641107	-0.385365	-2.351755
H	3.406603	1.163945	-2.669027
H	5.372368	-1.506513	0.049645
H	3.975959	-2.105123	-0.808819
H	5.008881	0.775674	-0.784829
H	5.142891	-0.398057	-2.075128
C	1.367763	0.358555	0.062816
C	1.973514	-0.916236	0.772496
C	1.338593	-2.158176	0.072048
C	0.384214	-1.621526	-1.000347
C	0.021430	-0.164498	-0.604650
H	1.108921	1.069166	0.849784
H	1.553612	-0.881318	1.785553
H	2.088448	-2.814832	-0.375792
H	0.802965	-2.769543	0.804957
H	0.889111	-1.592187	-1.972377
H	-0.501273	-2.247674	-1.127727
O	1.654555	2.371377	-1.367244
C	2.730454	2.497539	-0.432436
H	2.450905	2.870901	0.552575
H	3.648547	2.922391	-0.838517
C	4.025942	0.172054	1.838236
H	3.480235	0.253045	2.785421
H	5.087604	0.046947	2.079670
H	3.918599	1.121141	1.312038
C	3.740131	-2.289991	1.898468
H	3.153203	-2.236433	2.822336
H	3.463048	-3.211617	1.378255
H	4.795598	-2.374289	2.178946
C	-0.461987	0.562881	-1.878069
H	-1.236318	-0.036873	-2.368565
H	-0.870707	1.559018	-1.707875
H	0.350675	0.670600	-2.597834
C	-1.083857	-0.186614	0.507335
C	-2.499682	-0.605775	0.067042
H	-0.800813	-0.957978	1.231286
H	-2.813289	-0.162839	-0.881920

O	-3.368140	-0.156079	1.112152
C	-2.888966	1.057948	1.593208
C	-1.352475	1.099386	1.369684
C	-1.121080	2.505231	0.793560
C	-2.481819	2.962992	0.307777
H	-3.238126	1.177665	2.619426
H	-0.838941	0.993361	2.325494
H	-0.820050	3.194998	1.591147
H	-0.375110	2.593536	0.003883
O	-3.448452	2.146374	0.817675
O	-2.752953	3.904175	-0.396272
O	-2.598153	-2.014047	0.006786
C	-3.699879	-2.637956	-0.533292
O	-3.716947	-3.844784	-0.505072
C	-4.790222	-1.782550	-1.131314
H	-5.620646	-2.433295	-1.400681
H	-5.123386	-1.015734	-0.428890
H	-4.429066	-1.278610	-2.034207

XYZ Coordinates and energies for (*S*)-10,20-epoxydendrillolide A (5) at 228 K

Compound: Conf1S, Conformer: 01, Energy:-1308.016556 Hartree, Solvent: chloroform, Boltzmann percentage: 84.575

Zero-point correction=	0.521887 (Hartree/Particle)
Thermal correction to Energy=	0.547774
Thermal correction to Enthalpy=	0.548718
Thermal correction to Gibbs Free Energy=	0.468408
Sum of electronic and zero-point Energies=	-1307.963078
Sum of electronic and thermal Energies=	-1307.937190
Sum of electronic and thermal Enthalpies=	-1307.936246
Sum of electronic and thermal Free Energies=	-1308.016556

C	-3.291850	-1.563952	1.363735
C	-2.189811	-0.519844	1.505007
C	-3.338578	0.220634	-1.370429
C	-4.377268	-0.819777	-0.875546
C	-4.536094	-1.037007	0.633322
H	-2.911045	-2.454011	0.852064
H	-3.588010	-1.887274	2.367844
H	-5.354469	-0.512553	-1.271512
H	-4.159771	-1.785619	-1.351009
H	-4.857709	-0.111586	1.122662
H	-5.347655	-1.759755	0.783303
C	-1.248423	-0.198726	0.335619
C	-1.854075	-0.187362	-1.116222
C	-1.380083	-1.516937	-1.728528
C	0.073195	-1.598738	-1.258949
C	0.052491	-1.139271	0.231523
H	-0.913308	0.814831	0.564876
H	-1.273997	0.589613	-1.638819
H	-1.956548	-2.364670	-1.340531

H	-1.461495	-1.543174	-2.818407
H	0.499352	-2.599830	-1.371393
H	0.674759	-0.923161	-1.878766
O	-2.673061	0.661603	2.207125
C	-1.720373	-0.175161	2.865207
H	-0.738953	0.275105	3.013053
H	-2.097146	-0.736372	3.720644
C	-3.614205	1.613748	-0.765137
H	-2.953177	2.362460	-1.218032
H	-4.645895	1.920534	-0.972880
H	-3.461429	1.648068	0.314291
C	-3.535089	0.344058	-2.901736
H	-2.791091	1.015501	-3.345381
H	-3.459762	-0.623802	-3.407110
H	-4.526024	0.754097	-3.124438
C	-0.029365	-2.400765	1.120177
H	0.865086	-3.016004	0.986232
H	-0.110262	-2.161133	2.183319
H	-0.883919	-3.025480	0.851405
C	1.310726	-0.334266	0.683484
C	1.645742	0.964322	-0.096472
H	1.102338	0.004200	1.704573
H	1.228609	1.015112	-1.103733
O	3.051026	1.047071	-0.211092
C	3.667325	0.126134	0.687938
C	2.681261	-1.048765	0.770157
C	3.188281	-1.936741	-0.380832
C	4.641348	-1.527762	-0.560231
H	3.932465	0.614116	1.628632
H	2.788334	-1.577911	1.719354
H	3.123655	-3.008744	-0.190059
H	2.685092	-1.740593	-1.330530
O	4.865262	-0.342131	0.097785
O	5.516828	-2.083907	-1.168954
O	1.145212	2.065734	0.679386
C	1.174285	3.353220	0.205241
O	0.832357	4.231529	0.961565
C	1.608190	3.587887	-1.222144
H	1.626083	4.662376	-1.397964
H	2.596207	3.161214	-1.408350
H	0.902930	3.125656	-1.920943

Compound: Conf1S, Conformer: 02, Energy:-1308.014251 Hartree, Solvent: chloroform, Boltzmann percentage: 7.362

Zero-point correction=	0.522025 (Hartree/Particle)
Thermal correction to Energy=	0.547972
Thermal correction to Enthalpy=	0.548916
Thermal correction to Gibbs Free Energy=	0.468253
Sum of electronic and zero-point Energies=	-1307.960479
Sum of electronic and thermal Energies=	-1307.934532
Sum of electronic and thermal Enthalpies=	-1307.933588
Sum of electronic and thermal Free Energies=	-1308.014251

C	3.454704	-0.496926	-1.793718
C	2.404068	0.548378	-1.437591
C	3.379367	-0.335096	1.459086
C	4.463685	-0.985996	0.558887
C	4.676655	-0.448048	-0.861191
H	3.010475	-1.498332	-1.791053
H	3.794292	-0.311601	-2.818663
H	5.418677	-0.897035	1.093759
H	4.268916	-2.064147	0.496611
H	5.036049	0.585830	-0.830438
H	5.479612	-1.036847	-1.321465
C	1.399929	0.291359	-0.304008
C	1.914965	-0.513820	0.942512
C	1.467954	-1.991618	0.713542
C	0.513790	-1.981917	-0.496093
C	0.090521	-0.503191	-0.713996
H	1.128362	1.300924	0.015336
H	1.304046	-0.132345	1.771472
H	2.315999	-2.654264	0.524684
H	0.974129	-2.382494	1.608323
H	1.033330	-2.331336	-1.395054
H	-0.350713	-2.635344	-0.360312
O	2.984600	1.887334	-1.398159
C	2.064419	1.576973	-2.444669
H	1.114945	2.107914	-2.395587
H	2.492510	1.507824	-3.445101
C	3.683494	1.159409	1.693792
H	2.962844	1.589488	2.400014
H	4.681122	1.279250	2.132011
H	3.643648	1.749492	0.777109
C	3.465896	-1.043910	2.833154
H	2.727686	-0.638137	3.534241
H	3.293091	-2.121653	2.749892
H	4.457743	-0.901459	3.275736
C	-0.370150	-0.321605	-2.171751
H	-1.175216	-1.025319	-2.405842
H	-0.730507	0.683450	-2.403948
H	0.446382	-0.542435	-2.862534
C	-1.051209	-0.167766	0.316675
C	-2.488849	-0.578145	-0.048816
H	-0.841678	-0.746503	1.223816
H	-2.781075	-0.314447	-1.068539
O	-3.338336	0.110161	0.869787
C	-2.651630	1.177277	1.495989
C	-1.271709	1.278737	0.811973
C	-1.493007	2.409671	-0.207022
C	-2.727853	3.144952	0.288776
H	-2.649119	1.024336	2.576497
H	-0.512717	1.573364	1.538835
H	-0.657729	3.106789	-0.291427
H	-1.719665	2.051800	-1.215440
O	-3.341454	2.406023	1.262721

O	-3.167878	4.204920	-0.074597
O	-2.642943	-1.975614	0.143302
C	-3.772614	-2.642704	-0.266614
O	-3.833480	-3.824379	-0.025192
C	-4.841670	-1.867061	-0.998035
H	-5.700774	-2.522178	-1.134202
H	-5.134352	-0.972703	-0.444015
H	-4.478921	-1.553163	-1.982909

Compound: Conf1S, Conformer: 07, Energy:-1308.012267 Hartree, Solvent: chloroform, Boltzmann percentage: 0.9

Zero-point correction=	0.521703 (Hartree/Particle)
Thermal correction to Energy=	0.547666
Thermal correction to Enthalpy=	0.548610
Thermal correction to Gibbs Free Energy=	0.468219
Sum of electronic and zero-point Energies=	-1307.958783
Sum of electronic and thermal Energies=	-1307.932820
Sum of electronic and thermal Enthalpies=	-1307.931876
Sum of electronic and thermal Free Energies=	-1308.012267

C	2.881837	-2.233373	0.028062
C	1.577316	-1.621602	-0.475477
C	3.483907	0.927103	-0.409114
C	4.505774	-0.213496	-0.169441
C	4.135437	-1.629260	-0.622783
H	2.945012	-2.151414	1.118020
H	2.860216	-3.305193	-0.196732
H	5.434977	0.069186	-0.681951
H	4.756784	-0.238446	0.899225
H	4.006907	-1.663216	-1.709924
H	4.983778	-2.286592	-0.395796
C	1.073770	-0.266944	0.061545
C	2.174560	0.792912	0.429535
C	2.328895	0.647904	1.954855
C	0.877502	0.551309	2.424390
C	0.142584	-0.340188	1.366076
H	0.488117	0.121644	-0.775646
H	1.670388	1.758951	0.286672
H	2.884671	-0.257533	2.219831
H	2.852395	1.491055	2.413767
H	0.773497	0.138753	3.432583
H	0.456702	1.560432	2.452773
O	1.464169	-1.745902	-1.925447
C	0.601897	-2.534958	-1.105526
H	-0.452914	-2.272890	-1.152120
H	0.796287	-3.607489	-1.106883
C	3.143496	1.065320	-1.908374
H	2.498784	1.936867	-2.074329
H	4.058285	1.220398	-2.491956
H	2.630272	0.191253	-2.311772
C	4.180896	2.241458	0.021394
H	3.507530	3.100191	-0.079514

H	4.526724	2.204122	1.059051
H	5.055985	2.430960	-0.609422
C	0.049992	-1.767987	1.957574
H	-0.545234	-1.745756	2.875718
H	-0.420199	-2.485955	1.286430
H	1.040881	-2.145340	2.222550
C	-1.321529	0.187654	1.168155
C	-2.205421	-0.433105	0.066643
H	-1.842336	-0.078691	2.097874
H	-1.692930	-0.577792	-0.889427
O	-3.292144	0.463634	-0.136328
C	-3.101609	1.674856	0.577924
C	-1.618835	1.695779	0.989056
C	-0.986465	2.499163	-0.161233
C	-2.144633	3.273192	-0.771383
H	-3.832868	1.754976	1.384719
H	-1.500084	2.238492	1.928109
H	-0.207932	3.195020	0.153513
H	-0.564953	1.876272	-0.955328
O	-3.328833	2.776021	-0.294053
O	-2.111619	4.183908	-1.557002
O	-2.705307	-1.683817	0.530093
C	-3.484985	-2.495860	-0.259262
O	-3.916645	-3.504434	0.246390
C	-3.737048	-2.088096	-1.690746
H	-4.403117	-2.823167	-2.139833
H	-4.184346	-1.093284	-1.739914
H	-2.802275	-2.061786	-2.260718

Compound: Conf1S, Conformer: 08, Energy:-1308.013839 Hartree, Solvent: chloroform, Boltzmann percentage: 4.759

Zero-point correction=	0.521919 (Hartree/Particle)
Thermal correction to Energy=	0.547903
Thermal correction to Enthalpy=	0.548847
Thermal correction to Gibbs Free Energy=	0.467852
Sum of electronic and zero-point Energies=	-1307.959772
Sum of electronic and thermal Energies=	-1307.933788
Sum of electronic and thermal Enthalpies=	-1307.932844
Sum of electronic and thermal Free Energies=	-1308.013839

C	3.528303	0.276732	-1.737016
C	2.484675	1.132831	-1.029516
C	3.336045	-0.813001	1.332558
C	4.421325	-1.124466	0.267733
C	4.710972	-0.089661	-0.825948
H	3.064382	-0.629683	-2.141227
H	3.912997	0.837618	-2.595897
H	5.359237	-1.304556	0.809861
H	4.179042	-2.080568	-0.213920
H	5.098818	0.835113	-0.386209
H	5.514822	-0.488983	-1.456589
C	1.426399	0.484526	-0.125512

C	1.879269	-0.729694	0.770168
C	1.383512	-2.017839	0.038145
C	0.543423	-1.549810	-1.161917
C	0.145310	-0.077046	-0.877135
H	1.123770	1.306556	0.530282
H	1.268260	-0.632008	1.676269
H	2.210964	-2.647935	-0.297027
H	0.787433	-2.634807	0.716962
H	1.142802	-1.572872	-2.078314
H	-0.322424	-2.190965	-1.343003
O	3.086939	2.329816	-0.451611
C	2.203653	2.483641	-1.562500
H	1.263504	2.984030	-1.334656
H	2.669006	2.798419	-2.496877
C	3.681579	0.471269	2.115514
H	2.964366	0.623756	2.931080
H	4.676332	0.383344	2.567752
H	3.670967	1.365860	1.491967
C	3.363829	-1.984507	2.345516
H	2.613176	-1.844614	3.131627
H	3.171020	-2.949024	1.865407
H	4.344472	-2.046810	2.829671
C	-0.196906	0.623220	-2.204056
H	-1.060057	0.150025	-2.683529
H	-0.418295	1.685429	-2.099681
H	0.635848	0.534344	-2.906180
C	-1.049425	-0.069822	0.140643
C	-2.387231	-0.698095	-0.323094
H	-0.745952	-0.711744	0.974199
H	-2.591262	-0.614918	-1.391942
O	-3.428864	-0.033121	0.369839
C	-2.891195	0.842862	1.358050
C	-1.510978	1.241998	0.814780
C	-1.877986	2.484919	-0.015607
C	-3.161154	2.994670	0.621670
H	-2.917331	0.380368	2.347191
H	-0.844789	1.526742	1.631999
H	-1.122015	3.271188	-0.020969
H	-2.122362	2.248632	-1.054757
O	-3.694577	2.008724	1.415426
O	-3.699597	4.062497	0.494999
O	-2.359984	-2.083843	0.045680
C	-3.345454	-2.954315	-0.344629
O	-3.281911	-4.087515	0.071295
C	-4.426276	-2.453117	-1.272462
H	-5.152789	-3.252619	-1.409362
H	-4.916057	-1.566438	-0.864155
H	-4.004085	-2.187118	-2.247311

Compound: Conf1S, Conformer: 12, Energy:-1308.013194 Hartree, Solvent: chloroform, Boltzmann percentage: 2.403

Zero-point correction=	0.521969 (Hartree/Particle)
Thermal correction to Energy=	0.547728
Thermal correction to Enthalpy=	0.548672
Thermal correction to Gibbs Free Energy=	0.468931
Sum of electronic and zero-point Energies=	-1307.960157
Sum of electronic and thermal Energies=	-1307.934398
Sum of electronic and thermal Enthalpies=	-1307.933453
Sum of electronic and thermal Free Energies=	-1308.013194

C	3.235082	-1.420542	1.380373
C	2.171768	-1.518477	0.290698
C	3.809611	1.009721	-0.711962
C	4.727516	0.483904	0.422622
C	4.608253	-0.984773	0.845037
H	2.906144	-0.741266	2.173393
H	3.342361	-2.406980	1.844720
H	5.765004	0.654444	0.105296
H	4.584670	1.118274	1.307345
H	4.875606	-1.645336	0.013527
H	5.350995	-1.167744	1.631370
C	1.440725	-0.262857	-0.208979
C	2.296203	1.054207	-0.332663
C	1.922076	1.855459	0.927085
C	0.407095	1.683411	0.975385
C	0.141106	0.179551	0.631506
H	1.111835	-0.545261	-1.214031
H	1.824744	1.596095	-1.166242
H	2.395545	1.440955	1.824243
H	2.211322	2.908020	0.867128
H	-0.033589	1.958234	1.939764
H	-0.041486	2.334879	0.221719
O	2.603449	-2.407431	-0.782078
C	1.535242	-2.834138	0.061905
H	0.567419	-2.900708	-0.430796
H	1.762408	-3.664471	0.731046
C	4.013361	0.208904	-2.015679
H	3.439220	0.662133	-2.832814
H	5.069379	0.226305	-2.309491
H	3.702973	-0.832819	-1.930047
C	4.260113	2.463296	-1.002480
H	3.621448	2.933158	-1.758832
H	4.237926	3.090442	-0.106004
H	5.287144	2.472027	-1.383253
C	-0.020025	-0.581909	1.963134
H	-0.951736	-0.295263	2.462826
H	-0.018003	-1.666341	1.851725
H	0.790522	-0.324423	2.650090
C	-1.125554	0.080536	-0.280925
C	-2.392844	0.845409	0.183700
H	-0.849956	0.577556	-1.220103
H	-2.521267	0.892614	1.267739

O	-3.515068	0.176034	-0.365922
C	-3.095082	-0.866732	-1.242426
C	-1.716595	-1.283407	-0.706345
C	-2.138576	-2.332408	0.342650
C	-3.488123	-2.833290	-0.147460
H	-3.146266	-0.549957	-2.286259
H	-1.119943	-1.752410	-1.492275
H	-1.455558	-3.173862	0.458143
H	-2.299690	-1.903427	1.335375
O	-3.978861	-1.963462	-1.089135
O	-4.098798	-3.814055	0.186668
O	-2.324948	2.173858	-0.344759
C	-3.223893	3.143103	0.019210
O	-3.124973	4.221139	-0.518621
C	-4.260098	2.811939	1.066587
H	-4.931375	3.664261	1.159663
H	-4.824453	1.917451	0.794249
H	-3.783906	2.629315	2.035726

Computational methods for 15-dendrillactol (8) and 15-epidendrillactol (9)

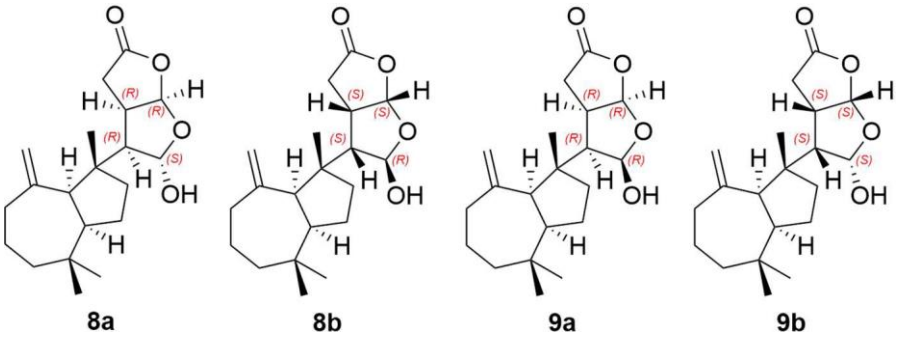


Figure S20. Candidate structures (**8a**, **8b**, **9a** and **9b**) proposed for lactols **8** and **9**.

A Monte Carlo conformational search for four diastereomers (**8a**,**b**, **9a,b**) was undertaken in gas phase with Merck Molecular Force Field (MMFF) using *MacroModel* (ver. 2018-1, Schrödinger Inc.). The selected conformers (<5 kcal mol^{-1} of the global minimum, **8a**: 5 conformers, and **8b**: 10 conformers**,** **9a**: 5 conformers, **9b**: 6 conformers) were optimised by density functional theory (DFT) calculations at the B3LYP/6-31+G(d,p) level with chloroform solvent (IEF-PCM) using *Gaussian* software (ver. 16W, revision B.01). A single point energy of the optimised conformers was calculated using M062X/6-31+G(d,p) with chloroform solvent (IEF-PCM) and duplicate conformers and conformers with <1% of the Boltzmann population removed. The free energies of the resulting diastereomers for **8a**, **8b**, **9a** and **9b** were calculated with M062X/6-31+G(d,p) with PCM implicit solvent model for chloroform were used to scale the calculated NMR parameters relative to their Boltzmann population and the vibrational frequencies where checked for a true minimum, i.e. no negative frequencies. The Boltzmann population were calculated by:

$$\rho_i = \frac{e^{-\varepsilon_i \div kT}}{\sum_{i=1}^{M} e^{-\varepsilon_i \div kT}}$$

where ρ_i is the probability of state i, ε_i the energy of state i, k the Boltzmann constant, T the temperature of the system and M is the number of all states accessible to the system of interest.

The magnetic field tensors were calculated using B3LYP/6-311+G(d,p) and their DP4+ probabilities calculated relative to the experimental chemical shifts using the *Excel* spreadsheet available for free at sarotti-nmr.weebly.com. It was found that **8a** had a 99.9% probability for the minor component and **9a** had a 100% probability for the major component.

The unscaled chemical shifts (δ_u) were computed using TMS as reference standard according to:

$$\delta_u = \sigma_0 - \sigma_x$$

where σ_x is the Boltzmann averaged magnetic field tensors (over all significantly populated conformations) and σ_0 is the magnetic field tensors of TMS computed at the same level of theory employed for σ_x. The scaled chemical shifts (δ_s) were computed as:

$$\delta_s = \delta_u m - b$$

where m and b are the slope and intercept respectively, resulting from a linear regression calculation on a plot of δ_u against δ_{exp}.[1,2] The DP4 probabilities were calculated and supported the DP4+ result that **8a** had a 98.5% probability for the minor component and **9a** had a 99.7% probability of representing the major component (see tables).

Table S5. Computed DP4 probabilities for 15-dendrillactol (8) and 15-epidendrillactol (9).

Major (**9**)	DP4+	DP4
9a	100	99.7
9b	0	0.3

Minor (**8**)	DP4+	DP4
8a	99.9	98.5
8b	0.1	1.5

The final NMR chemical shifts were calculated with mpw1pw91/6-311+G(2d,p) for proton NMR and wB97XD/6-311+g(2d,p) for carbon NMR with chloroform solvent (IEF-PCM). The DP4 probabilities were calculated using the procedure of Sarotti[3] using their supplied spreadsheet using scaled shifts. The magnetic field tensors were converted to scaled chemical shifts and weighted by their Boltzmann populations for diastereomers **8a** and **9a** only. The mean absolute error (MAE) of **8a** compared to the experimental chemical shifts was 0.09 and 1.5 for proton and carbon respectively. The maximum deviations were 0.24 and 2.8 ppm. The mean absolute error (MAE) of **9a** compared to the experimental chemical shifts was 0.07 and 1.5 for proton and carbon respectively. The maximum deviations were 0.30 and 3.6 ppm.

The coupling constants for the 2,8-dioxabicyclo[3.3.0]octane moiety in **8** and **9** were calculated using the method of Kutateladze and Mukhina.[3] For both metabolites **8** and **9**, the calculated and experimental coupling constants were in agreement, which further supported the proposed configuration of 15*S* for **8** and 15*R* for **9**.

Table S6. Proton and carbon experimental and calculated chemical shifts for 15-dendrillactol (8).

^{1}H NMR experimental	δ scaled
2.20	2.29
1.82	1.87
1.72	1.68
1.38	1.34
1.72	1.62
1.46	1.22
1.72	1.84
1.74	1.71
1.74	1.69
1.72	1.92
1.38	1.39
2.88	2.95
2.72	2.60
2.55	2.39
3.15	3.01
2.35	2.36
5.63	5.61
6.06	5.92
0.96	0.88
0.94	0.87
0.97	0.91
4.82	4.95
4.59	4.73
MAE	**0.09**
MAX	**0.24**

^{13}C NMR experimental	δ scaled
37.6	37.5
28.5	30.0
38.4	37.0
36.2	38.5
54.4	53.4
26.8	27.1
37.8	37.8
46.6	49.1
56.2	56.3
153.5	156.1
176.2	174.7
29.7	30.7
41.9	44.0
56.2	55.4
99.7	97.6
104.1	102.3
24.1	22.3
34.5	32.0
26.0	24.5
114.7	111.9
MAE	**1.5**
MAX	**2.8**

Table S7. Proton and carbon experimental and calculated chemical shifts for 15-epidendrillactol (9).

^{1}H NMR experimental	δ scaled
2.37	2.34
1.88	1.95
1.73	1.69
1.38	1.38
1.61	1.63
1.27	1.25
1.87	1.88
1.70	1.71
1.70	1.63
1.82	2.12
1.51	1.53
2.70	2.77
3.26	3.10
2.53	2.43
3.17	3.10
2.16	2.16
5.64	5.54
6.05	5.90
1.04	1.02
0.95	0.89
0.97	0.94
4.81	4.97
4.53	4.72
MAE	**0.07**
MAX	**0.30**

^{13}C NMR experimental	δ scaled
37.6	38.0
28.5	29.9
38.3	37.3
36.2	38.4
54.5	53.9
27.1	27.8
37.6	37.4
47.0	49.4
57.7	57.8
153.8	157.4
177.0	175.9
31.2	32.8
39.1	41.2
55.2	54.8
100.3	98.8
107.4	105.8
24.9	22.5
34.5	32.2
26.0	24.5
114.2	112.2
MAE	**1.5**
MAX	**3.6**

Table S8. Key coupling constants (Hz) computed for 15-dendrillactol (8) and 15-epidendrillactol (9).

Major (9)	**12b**	**13**	**14**	**15**	**16**
12a	18.5	7.5	-	-	-
12b	-	10.8	-	-	-
13	-	-	6.9	-	6.0
14	-	-	-	3.7	-

Minor (8)	**12b**	**13**	**14**	**15**	**16**
12a	17.1	10.5	-	-	-
12b	-	9.2	-	-	-
13	-	-	6.9	-	4.2
14	-	-	-	5.9	-

XYZ Coordinates and Energies for 15-dendrillactol 8a

Compound: 8a, Conformer: 1, Energy:-1080.272591 Hartree, Solvent: chloroform, Boltzmann percentage: 46.612

Zero-point correction=	0.478355 (Hartree/Particle)
Thermal correction to Energy=	0.500393
Thermal correction to Enthalpy=	0.501337
Thermal correction to Gibbs Free Energy=	0.429846
Sum of electronic and zero-point Energies=	-1080.224082
Sum of electronic and thermal Energies=	-1080.202043
Sum of electronic and thermal Enthalpies=	-1080.201099
Sum of electronic and thermal Free Energies=	-1080.272591

C	-1.367902	0.725366	0.169621
C	-1.584609	0.073771	1.560357
O	-3.002345	-0.054667	1.748593
H	-1.150066	1.779114	0.389628
H	-1.178470	-0.937830	1.663634
C	-3.691157	0.727520	0.786655
C	-2.785097	0.721198	-0.453697
C	-3.314915	-0.517458	-1.202322
C	-4.730779	-0.694596	-0.684268
O	-4.905527	0.060423	0.442418
H	-3.971811	1.704185	1.190336
H	-2.952909	1.616254	-1.059043
H	-3.325444	-0.421155	-2.289824
H	-2.772745	-1.435138	-0.958439
O	-5.620803	-1.377866	-1.131869
C	-0.150079	-1.307727	-0.994835
C	1.327638	-1.713821	-0.982338
C	-0.161838	0.220904	-0.683570
H	1.821947	-1.390340	-1.906126
H	1.454137	-2.798354	-0.909935
H	-0.640767	-1.534011	-1.947036
O	-1.028379	0.916996	2.544644
H	-1.096071	0.477829	3.409960
C	1.867479	-0.956184	0.243826
C	1.197322	0.461266	0.151088
C	2.045240	1.623142	-0.349584
C	3.062613	1.428885	-1.457728
C	4.393881	0.823587	-0.967679
C	4.332767	-0.660167	-0.584679
C	3.388167	-1.088654	0.569398
H	1.372989	-1.427453	1.108245
H	0.901168	0.746632	1.161313
H	2.665360	0.789086	-2.254051
H	3.270755	2.403524	-1.914412
H	5.131549	0.929180	-1.774245
H	4.770464	1.421580	-0.128786
H	4.078959	-1.244143	-1.479910
H	5.348007	-0.974992	-0.306088
C	3.683768	-2.582560	0.852029
H	4.712784	-2.706896	1.208275

H	3.014148	-2.981168	1.623408
H	3.569787	-3.199736	-0.045349
C	3.709621	-0.304498	1.860659
H	4.767474	-0.419566	2.126050
H	3.501840	0.763879	1.765873
H	3.114888	-0.686825	2.699319
C	1.912121	2.831675	0.222170
H	2.477757	3.691690	-0.129474
H	1.239934	2.998376	1.060306
C	-0.195527	0.990799	-2.022276
H	-0.096757	2.070056	-1.875261
H	0.606236	0.668898	-2.691055
H	-1.137786	0.802774	-2.546186
H	-0.673209	-1.879226	-0.218387

Compound: 8a, Conformer: 2, Energy:-1080.271853 Hartree, Solvent: chloroform, Boltzmann pecentage: 21.333

Zero-point correction=	0.478197 (Hartree/Particle)
Thermal correction to Energy=	0.500168
Thermal correction to Enthalpy=	0.501112
Thermal correction to Gibbs Free Energy=	0.430034
Sum of electronic and zero-point Energies=	-1080.223690
Sum of electronic and thermal Energies=	-1080.201719
Sum of electronic and thermal Enthalpies=	-1080.200775
Sum of electronic and thermal Free Energies=	-1080.271853

C	1.333488	0.886009	0.178415
C	2.395845	1.842737	-0.410338
O	3.653918	1.476093	0.201630
H	0.990396	1.401153	1.087331
H	2.542422	1.752751	-1.492963
C	3.480544	0.410279	1.115729
C	2.187769	-0.297327	0.680752
C	2.741742	-1.344355	-0.304060
C	4.180698	-1.546091	0.132940
O	4.555385	-0.523972	0.958595
H	3.529882	0.763510	2.149203
H	1.716948	-0.800559	1.529409
H	2.203074	-2.293274	-0.304531
H	2.778013	-0.985186	-1.337036
O	4.945223	-2.433951	-0.163676
C	-0.657281	1.986586	-0.989873
C	-2.156855	1.695585	-0.917629
C	0.044406	0.629702	-0.664194
H	-2.494250	1.148187	-1.805986
H	-2.749809	2.613502	-0.859502
H	-0.335030	2.383941	-1.958720
O	2.072184	3.166692	-0.079632
H	2.680190	3.766994	-0.543538
C	-2.257589	0.832039	0.353314
C	-1.028467	-0.147669	0.254758
C	-1.316193	-1.583734	-0.162822

C	-2.331437	-1.882509	-1.250165
C	-3.782703	-1.908872	-0.727023
C	-4.369149	-0.541092	-0.355085
C	-3.668077	0.292499	0.750549
H	-1.990433	1.509608	1.178879
H	-0.594196	-0.221414	1.256709
H	-2.267200	-1.155115	-2.066358
H	-2.101008	-2.862285	-1.684298
H	-4.418159	-2.341929	-1.510856
H	-3.839397	-2.595204	0.126694
H	-4.434956	0.071937	-1.264065
H	-5.407250	-0.700898	-0.032333
C	-4.578952	1.514854	1.026488
H	-5.546120	1.186926	1.424380
H	-4.126639	2.188448	1.763932
H	-4.776028	2.092919	0.117706
C	-3.569727	-0.509192	2.067039
H	-4.563087	-0.849985	2.382968
H	-2.927219	-1.388002	1.977787
H	-3.166263	0.120596	2.869541
C	-0.714251	-2.604503	0.469554
H	-0.892632	-3.637230	0.178790
H	-0.040373	-2.446909	1.308069
C	0.334721	-0.086498	-2.000940
H	0.565646	-1.145987	-1.878553
H	-0.529264	-0.017309	-2.667330
H	1.168990	0.390971	-2.525909
H	-0.401106	2.740252	-0.239214

Compound: 8a, Conformer: 3, Energy:-1080.271998 Hartree, Solvent: chloroform, Boltzmann percentage: 24.874

Zero-point correction=	0.477894 (Hartree/Particle)
Thermal correction to Energy=	0.500165
Thermal correction to Enthalpy=	0.501109
Thermal correction to Gibbs Free Energy=	0.428940
Sum of electronic and zero-point Energies=	-1080.223044
Sum of electronic and thermal Energies=	-1080.200773
Sum of electronic and thermal Enthalpies=	-1080.199829
Sum of electronic and thermal Free Energies=	-1080.271998

C	1.264430	0.855029	-0.011946
C	2.493149	1.598492	-0.563494
O	3.521382	1.408875	0.446863
H	0.904928	1.511907	0.790771
H	2.880343	1.185073	-1.502836
C	3.225089	0.305867	1.263840
C	1.930673	-0.335547	0.714922
C	2.466352	-1.521818	-0.107745
C	3.881189	-1.741901	0.395932
O	4.267320	-0.689824	1.166936
H	3.212929	0.615015	2.311273
H	1.314491	-0.701623	1.539804

H	1.887521	-2.441443	0.000985
H	2.541632	-1.312847	-1.179068
O	4.616639	-2.677208	0.177773
C	-0.787796	1.930064	-1.031735
C	-1.697397	1.918127	0.216572
C	0.050336	0.621706	-0.986219
H	-2.708380	2.242797	-0.044418
H	-1.340900	2.621557	0.976270
H	-1.394340	1.924613	-1.944195
O	2.238442	2.961503	-0.705030
H	2.985468	3.383363	-1.162996
C	-1.672084	0.460089	0.773402
C	-0.961569	-0.407090	-0.320764
C	-1.854038	-1.143872	-1.312605
C	-3.163361	-0.538673	-1.778592
C	-4.313225	-0.777324	-0.775833
C	-4.253251	0.059035	0.509103
C	-3.000954	-0.049452	1.421042
H	-0.963829	0.462014	1.613279
H	-0.383529	-1.191762	0.174325
H	-3.065230	0.537727	-1.962179
H	-3.439035	-0.996192	-2.735683
H	-5.260846	-0.542916	-1.278617
H	-4.350209	-1.847281	-0.536917
H	-4.403774	1.113148	0.242511
H	-5.122737	-0.211137	1.124071
C	-3.278894	0.837245	2.659782
H	-4.171151	0.488089	3.192087
H	-2.438298	0.807995	3.363247
H	-3.447667	1.883101	2.381104
C	-2.816302	-1.499937	1.916526
H	-3.714762	-1.842188	2.443912
H	-2.621469	-2.199058	1.099475
H	-1.976845	-1.563537	2.619931
C	-1.507821	-2.370296	-1.735067
H	-2.112875	-2.915319	-2.455914
H	-0.612057	-2.871821	-1.376508
C	0.496186	0.233370	-2.406299
H	1.033096	-0.718211	-2.449136
H	-0.373249	0.129241	-3.059503
H	1.135345	1.009402	-2.839516
H	-0.149098	2.814844	-1.082835

Compound: 8a, Conformer: 5, Energy:-1080.270825 Hartree, Solvent: chloroform, Boltzmann percentage: 7.181

Zero-point correction=	0.477908 (Hartree/Particle)
Thermal correction to Energy=	0.500142
Thermal correction to Enthalpy=	0.501087
Thermal correction to Gibbs Free Energy=	0.428871
Sum of electronic and zero-point Energies=	-1080.221788
Sum of electronic and thermal Energies=	-1080.199554
Sum of electronic and thermal Enthalpies=	-1080.198610

Sum of electronic and thermal Free Energies= -1080.270825

C	1.260010	0.828080	-0.083574
C	2.479937	1.554282	-0.695622
O	3.489373	1.485556	0.349229
H	0.879976	1.529971	0.672842
H	2.871945	1.068811	-1.594246
C	3.226843	0.427905	1.234594
C	1.952203	-0.288526	0.731145
C	2.524181	-1.515445	-0.002741
C	3.940595	-1.661176	0.522724
O	4.298092	-0.539594	1.205323
H	3.203203	0.806349	2.258773
H	1.343814	-0.611773	1.579491
H	1.967033	-2.439298	0.165848
H	2.604569	-1.379718	-1.085262
O	4.698917	-2.592967	0.384617
C	-0.785132	1.790423	-1.229074
C	-1.698649	1.923478	0.009004
C	0.050955	0.494884	-1.032989
H	-2.705555	2.226195	-0.290877
H	-1.340879	2.703148	0.690096
H	-1.390203	1.678963	-2.135338
O	2.301420	2.887227	-1.050112
H	2.002929	3.387686	-0.269279
C	-1.687757	0.534536	0.721807
C	-0.968089	-0.450773	-0.261814
C	-1.852337	-1.297574	-1.169358
C	-3.153703	-0.748853	-1.720031
C	-4.316471	-0.865540	-0.710913
C	-4.267508	0.114163	0.468851
C	-3.027828	0.105836	1.404505
H	-0.990474	0.624719	1.566109
H	-0.393994	-1.173039	0.324762
H	-3.050145	0.298206	-2.028398
H	-3.418973	-1.315401	-2.619974
H	-5.256906	-0.687869	-1.249093
H	-4.361317	-1.900264	-0.349619
H	-4.407699	1.130964	0.079748
H	-5.146509	-0.078326	1.099245
C	-3.318100	1.127774	2.531139
H	-4.217946	0.842569	3.088068
H	-2.486570	1.176605	3.244283
H	-3.480524	2.135712	2.134019
C	-2.855992	-1.279623	2.063512
H	-3.763781	-1.558421	2.611778
H	-2.650800	-2.067022	1.334072
H	-2.027906	-1.264731	2.782950
C	-1.506297	-2.566613	-1.437911
H	-2.104806	-3.192129	-2.096099
H	-0.617047	-3.024174	-1.010830
C	0.499881	-0.051232	-2.399456
H	1.014821	-1.013200	-2.334895

H	-0.367469	-0.207339	-3.045183
H	1.157939	0.660156	-2.908390
H	-0.149600	2.664815	-1.389839

XYZ Coordinates and Energies for 15-epidendrillactol 9a.

Compound: 9a, Conformer: 1, Energy:-1080.273984 Hartree, Solvent: chloroform, Boltzmann percentage: 49.36

Zero-point correction=	0.478783 (Hartree/Particle)
Thermal correction to Energy=	0.500674
Thermal correction to Enthalpy=	0.501618
Thermal correction to Gibbs Free Energy=	0.430534
Sum of electronic and zero-point Energies=	-1080.225736
Sum of electronic and thermal Energies=	-1080.203844
Sum of electronic and thermal Enthalpies=	-1080.202900
Sum of electronic and thermal Free Energies=	-1080.273984

C	-1.342408	0.760889	0.237763
C	-1.698582	-0.059977	1.491798
O	-2.936833	0.523542	1.929265
H	-1.104847	1.752415	0.649892
H	-1.010868	0.070105	2.332595
C	-3.676299	0.971037	0.816362
C	-2.739542	0.936924	-0.419465
C	-3.311297	-0.203614	-1.281329
C	-4.610284	-0.606558	-0.613101
O	-4.783715	0.086155	0.544503
H	-4.118198	1.936371	1.068397
H	-2.799699	1.885622	-0.956258
H	-3.519386	0.094473	-2.312803
H	-2.676964	-1.089726	-1.315497
O	-5.426326	-1.415444	-0.994382
C	-0.078914	-1.006417	-1.309083
C	1.403521	-1.396344	-1.350079
C	-0.106321	0.403837	-0.643170
H	1.931020	-0.851300	-2.142564
H	1.538581	-2.464299	-1.547216
H	-0.536895	-0.991316	-2.304080
O	-1.861087	-1.425117	1.186725
H	-2.138758	-1.893044	1.993403
C	1.890559	-0.976530	0.048589
C	1.205316	0.416132	0.295166
C	2.056496	1.672514	0.170196
C	3.125888	1.787338	-0.899406
C	4.442098	1.074047	-0.529760
C	4.383180	-0.458034	-0.565920
C	3.399413	-1.183405	0.389902
H	1.368045	-1.652779	0.741927
H	0.858630	0.421244	1.331317
H	2.774383	1.385879	-1.856235
H	3.339617	2.849683	-1.065068

H	5.212349	1.394976	-1.243564
H	4.774289	1.423045	0.455625
H	4.170145	-0.777260	-1.595265
H	5.390518	-0.835963	-0.342527
C	3.705720	-2.697234	0.275771
H	4.720131	-2.909136	0.632748
H	3.008968	-3.290189	0.880004
H	3.640153	-3.050827	-0.758490
C	3.657296	-0.772176	1.856392
H	4.705696	-0.947814	2.126213
H	3.436163	0.281627	2.042329
H	3.036867	-1.369148	2.536129
C	1.879418	2.682513	1.038477
H	2.446493	3.607150	0.958864
H	1.169456	2.617104	1.859751
C	-0.052053	1.458896	-1.773072
H	0.053865	2.476447	-1.385139
H	0.778879	1.271338	-2.456628
H	-0.967031	1.414976	-2.372194
H	-0.617141	-1.735774	-0.700743

Compound: 9a, Conformer: 2, Energy:-1080.273744 Hartree, Solvent: chloroform, Boltzmann percentage: 38.281

Zero-point correction=	0.478609 (Hartree/Particle)
Thermal correction to Energy=	0.500467
Thermal correction to Enthalpy=	0.501411
Thermal correction to Gibbs Free Energy=	0.430558
Sum of electronic and zero-point Energies=	-1080.225692
Sum of electronic and thermal Energies=	-1080.203835
Sum of electronic and thermal Enthalpies=	-1080.202891
Sum of electronic and thermal Free Energies=	-1080.273744

C	1.275931	-0.834811	-0.255114
C	2.346224	-1.842805	0.204369
O	3.346329	-1.757806	-0.826697
H	0.866476	-1.316363	-1.155146
H	2.012461	-2.884673	0.196956
C	3.352133	-0.466611	-1.399699
C	2.157012	0.317589	-0.800447
C	2.833863	1.297628	0.175883
C	4.307976	1.252937	-0.169723
O	4.554945	0.246019	-1.053034
H	3.370492	-0.573755	-2.485880
H	1.637791	0.868913	-1.587577
H	2.464928	2.322869	0.096138
H	2.750732	0.991159	1.219280
O	5.197448	1.962283	0.243385
C	-0.618415	-1.931232	1.031151
C	-2.129895	-1.703187	0.970969
C	0.028205	-0.564084	0.638582
H	-2.473123	-1.142392	1.848188
H	-2.687938	-2.644288	0.950209

H	-0.264693	-2.276836	2.008253
O	2.877062	-1.502410	1.463090
H	3.558197	-2.154944	1.700950
C	-2.282361	-0.882699	-0.323792
C	-1.097411	0.151172	-0.270082
C	-1.436200	1.581679	0.128767
C	-2.457972	1.862614	1.214375
C	-3.912363	1.815531	0.701700
C	-4.444653	0.415519	0.370510
C	-3.718787	-0.416453	-0.720147
H	-1.995470	-1.573291	-1.132286
H	-0.689441	0.228272	-1.282859
H	-2.357270	1.158365	2.047289
H	-2.266326	2.861068	1.624011
H	-4.560197	2.242695	1.478620
H	-4.003211	2.476056	-0.169294
H	-4.476958	-0.175832	1.295545
H	-5.491223	0.523433	0.053611
C	-4.578585	-1.683539	-0.954622
H	-5.563417	-1.408284	-1.349065
H	-4.105492	-2.355766	-1.680249
H	-4.740710	-2.245942	-0.029235
C	-3.666682	0.354177	-2.057530
H	-4.676541	0.643510	-2.372390
H	-3.062147	1.261926	-1.996426
H	-3.243126	-0.277929	-2.847813
C	-0.866392	2.611942	-0.517466
H	-1.075320	3.642551	-0.240064
H	-0.183051	2.463278	-1.350059
C	0.338534	0.210538	1.936335
H	0.566441	1.262686	1.754101
H	-0.522363	0.179267	2.610284
H	1.179812	-0.249602	2.457554
H	-0.356565	-2.706273	0.299295

Compound: 9a, Conformer: 3, Energy:-1080.272495 Hartree, Solvent: chloroform, Boltzmann percentage: 10.197

Zero-point correction=	0.478429 (Hartree/Particle)
Thermal correction to Energy=	0.500431
Thermal correction to Enthalpy=	0.501375
Thermal correction to Gibbs Free Energy=	0.430002
Sum of electronic and zero-point Energies=	-1080.224068
Sum of electronic and thermal Energies=	-1080.202066
Sum of electronic and thermal Enthalpies=	-1080.201121
Sum of electronic and thermal Free Energies=	-1080.272495

C	1.170949	-0.612960	0.217268
C	2.176343	-1.395985	1.081578
O	3.097499	-1.937453	0.117145
H	0.658444	-1.416826	-0.325255
H	1.749756	-2.268090	1.586234
C	3.156583	-1.113646	-1.029377

C	2.108662	0.012900	-0.849313
C	2.976153	1.237452	-0.498857
C	4.391658	0.841253	-0.865202
O	4.448599	-0.489995	-1.148003
H	3.047117	-1.744657	-1.913575
H	1.579010	0.185303	-1.789486
H	2.697348	2.147511	-1.035085
H	2.985821	1.462933	0.568412
O	5.379002	1.539530	-0.909339
C	-0.708581	-0.673206	1.921814
C	-1.685958	-1.557576	1.122482
C	0.036116	0.224796	0.897125
H	-2.631786	-1.665978	1.660632
H	-1.292273	-2.572166	0.997145
H	-1.264910	-0.023689	2.605913
O	2.828893	-0.559757	2.006289
H	3.461235	-1.093107	2.518220
C	-1.871224	-0.877160	-0.271621
C	-1.084065	0.483125	-0.208132
C	-1.894030	1.752673	0.011743
C	-3.071857	1.764414	0.965834
C	-4.368489	1.237354	0.316820
C	-4.406964	-0.274721	0.061578
C	-3.324001	-0.909718	-0.852324
H	-1.306363	-1.483415	-0.991397
H	-0.577717	0.630932	-1.167842
H	-2.860616	1.176194	1.866899
H	-3.244033	2.794817	1.297607
H	-5.208513	1.483409	0.979815
H	-4.542413	1.788533	-0.615495
H	-4.396183	-0.789720	1.031293
H	-5.383006	-0.513064	-0.383046
C	-3.712993	-2.398385	-1.031135
H	-4.695778	-2.483913	-1.508750
H	-2.987888	-2.922848	-1.664749
H	-3.764651	-2.925424	-0.072325
C	-3.340854	-0.256906	-2.251440
H	-4.339855	-0.332634	-2.697465
H	-3.065220	0.799802	-2.224174
H	-2.640283	-0.769034	-2.922529
C	-1.588586	2.864889	-0.675251
H	-2.130477	3.795294	-0.521617
H	-0.790015	2.883449	-1.413203
C	0.537571	1.511954	1.570872
H	0.888422	2.251935	0.847688
H	-0.276154	1.984237	2.128460
H	1.345913	1.290578	2.271313
H	-0.025461	-1.252245	2.550865

Compound: 9a, Conformer: 5, Energy:-1080.271030 Hartree, Solvent: chloroform, Boltzmann percentage: 2.161

Zero-point correction=	0.478317 (Hartree/Particle)
Thermal correction to Energy=	0.500352
Thermal correction to Enthalpy=	0.501297
Thermal correction to Gibbs Free Energy=	0.429837
Sum of electronic and zero-point Energies=	-1080.222550
Sum of electronic and thermal Energies=	-1080.200515
Sum of electronic and thermal Enthalpies=	-1080.199571
Sum of electronic and thermal Free Energies=	-1080.271030

C	-1.557169	-1.067041	0.823536
C	-2.349275	-1.657613	-0.353278
O	-3.710062	-1.307292	-0.045217
H	-1.912083	-1.663198	1.677357
H	-2.338040	-2.749928	-0.408838
C	-3.743102	-0.086204	0.660545
C	-2.281275	0.296340	1.020007
C	-1.988892	1.494625	0.097277
C	-3.323568	1.872914	-0.512869
O	-4.277569	0.968462	-0.163326
H	-4.436094	-0.193322	1.497015
H	-2.232717	0.613359	2.063858
H	-1.580331	2.359745	0.625654
H	-1.320216	1.263642	-0.732169
O	-3.579865	2.822377	-1.218384
C	0.481286	-0.709947	2.292779
C	1.794011	0.037988	2.046022
C	-0.003773	-1.237837	0.897416
H	2.635896	-0.660702	2.014499
H	2.008436	0.760941	2.839427
H	0.584723	-1.529524	3.012508
O	-1.941413	-1.086137	-1.572696
H	-2.483970	-1.458437	-2.289187
C	1.559960	0.702291	0.674998
C	0.853800	-0.407783	-0.176083
C	1.759305	-1.251320	-1.075556
C	3.173940	-1.608765	-0.657519
C	4.189553	-0.476452	-0.920342
C	4.085370	0.739106	0.010260
C	2.744697	1.518881	0.067277
H	0.774772	1.454051	0.848568
H	0.155390	0.064528	-0.864196
H	3.221852	-1.893410	0.400026
H	3.488908	-2.489673	-1.228941
H	5.200415	-0.891921	-0.812211
H	4.098635	-0.163187	-1.967730
H	4.348885	0.425813	1.029263
H	4.864941	1.454111	-0.287284
C	2.987187	2.749871	0.975649
H	3.757306	3.398932	0.543297
H	2.074088	3.346638	1.086547
H	3.324884	2.460492	1.976438

C	2.357046	2.048827	-1.330278
H	3.160098	2.674613	-1.737892
H	2.162731	1.245426	-2.044599
H	1.454568	2.669514	-1.270767
C	1.322178	-1.636951	-2.284950
H	1.942451	-2.245097	-2.940056
H	0.335365	-1.365698	-2.646234
C	0.271216	-2.757217	0.821302
H	0.052779	-3.169901	-0.166476
H	1.318820	-2.979418	1.042575
H	-0.337681	-3.287970	1.562521
H	-0.248497	-0.011963	2.716855

XYZ Coordinates and Energies for 15-dendrillactol 8b

Compound: 8b, Conformer: 01, Energy:-1080.270882 Hartree, Solvent: chloroform, Boltzmann percentage: 41.039

Zero-point correction=	0.477892 (Hartree/Particle)
Thermal correction to Energy=	0.500191
Thermal correction to Enthalpy=	0.501135
Thermal correction to Gibbs Free Energy=	0.428847
Sum of electronic and zero-point Energies=	-1080.221837
Sum of electronic and thermal Energies=	-1080.199538
Sum of electronic and thermal Enthalpies=	-1080.198594
Sum of electronic and thermal Free Energies=	-1080.270882

C	-1.229858	-0.042078	0.360428
C	-1.939529	0.902285	1.343864
O	-3.093536	0.151362	1.811156
H	-0.744880	-0.779133	1.012166
H	-2.316979	1.824621	0.886022
C	-3.378598	-0.924286	0.951103
C	-2.425127	-0.802816	-0.257381
C	-3.314528	-0.116148	-1.310841
C	-4.736450	-0.358686	-0.837701
O	-4.724981	-0.817036	0.443672
H	-3.348466	-1.864081	1.507089
H	-2.130242	-1.794711	-0.609320
H	-3.180981	0.968983	-1.356077
H	-3.188924	-0.499157	-2.325744
O	-5.768764	-0.183585	-1.443167
C	0.208533	-0.412216	-1.730868
C	1.140167	-1.501333	-1.162322
C	-0.112894	0.561021	-0.566934
H	1.916644	-1.758942	-1.888204
H	0.591243	-2.428707	-0.964831
H	0.726041	0.151684	-2.514566
O	-1.116574	1.204658	2.428627
H	-1.535941	1.895158	2.969916
C	1.730129	-0.932008	0.166859
C	1.249094	0.560103	0.262232
C	2.236798	1.641900	-0.152819

C	3.181457	1.429590	-1.319329
C	4.443692	0.633764	-0.925986
C	4.222235	-0.860569	-0.659629
C	3.226823	-1.285192	0.453666
H	1.197452	-1.438711	0.981750
H	0.995485	0.779241	1.301873
H	2.682024	0.916182	-2.149989
H	3.494710	2.408777	-1.699844
H	5.172604	0.720575	-1.742717
H	4.902322	1.115212	-0.053553
H	3.922947	-1.339104	-1.601565
H	5.195926	-1.302210	-0.406301
C	3.321757	-2.826958	0.567432
H	4.338860	-3.130843	0.840481
H	2.641755	-3.208477	1.338327
H	3.071315	-3.322186	-0.377103
C	3.648495	-0.693011	1.815817
H	4.674880	-0.991085	2.061796
H	3.603431	0.398448	1.829419
H	2.995280	-1.064040	2.614946
C	2.304501	2.782618	0.552353
H	2.982677	3.585290	0.271054
H	1.687092	2.949410	1.431490
C	-0.491618	1.952115	-1.103396
H	-0.598592	2.691667	-0.304561
H	0.284704	2.324656	-1.776283
H	-1.424249	1.925592	-1.674280
H	-0.687776	-0.825880	-2.202989

Compound: 8b, Conformer: 02, Energy:-1080.270284 Hartree, Solvent: chloroform, Boltzmann percentage: 21.784

Zero-point correction=	0.477994 (Hartree/Particle)
Thermal correction to Energy=	0.500127
Thermal correction to Enthalpy=	0.501071
Thermal correction to Gibbs Free Energy=	0.429474
Sum of electronic and zero-point Energies=	-1080.221764
Sum of electronic and thermal Energies=	-1080.199631
Sum of electronic and thermal Enthalpies=	-1080.198687
Sum of electronic and thermal Free Energies=	-1080.270284

C	1.324958	0.024460	-0.481435
C	1.830346	1.485186	-0.506706
O	3.209262	1.430919	-0.938699
H	0.944191	-0.145905	-1.499023
H	1.834011	1.984423	0.468546
C	3.589563	0.100749	-1.238224
C	2.640763	-0.785160	-0.418100
C	3.434172	-0.919572	0.896503
C	4.879491	-0.708495	0.481537
O	4.917655	-0.127651	-0.754379
H	3.620923	-0.071086	-2.317525
H	2.528165	-1.769120	-0.881369

H	3.205537	-0.128666	1.617827
H	3.319345	-1.878365	1.405327
O	5.889094	-0.970434	1.091443
C	-0.142905	-1.885585	0.333376
C	-1.664680	-2.035567	0.272312
C	0.142517	-0.352196	0.470358
H	-2.101742	-1.972287	1.274907
H	-1.964045	-3.000229	-0.149431
H	0.316300	-2.457937	1.147016
O	1.073083	2.228916	-1.425952
H	1.352069	3.159749	-1.384789
C	-2.074784	-0.837588	-0.604425
C	-1.207791	0.351436	-0.062866
C	-1.875618	1.300999	0.928738
C	-2.889589	0.797329	1.939291
C	-4.303450	0.619931	1.346548
C	-4.473962	-0.571698	0.395583
C	-3.596910	-0.631871	-0.883209
H	-1.646618	-1.049167	-1.597308
H	-0.928137	0.978333	-0.910570
H	-2.574473	-0.153590	2.384681
H	-2.948508	1.520962	2.760647
H	-5.006934	0.484541	2.178858
H	-4.595757	1.552295	0.847990
H	-4.324145	-1.499356	0.964331
H	-5.523728	-0.592101	0.071367
C	-4.096268	-1.844997	-1.706547
H	-5.139343	-1.698322	-2.009632
H	-3.500678	-1.977899	-2.617456
H	-4.048470	-2.776839	-1.133221
C	-3.802955	0.628562	-1.751137
H	-4.863457	0.751043	-2.002386
H	-3.468989	1.541018	-1.251711
H	-3.247760	0.541395	-2.693130
C	-1.602038	2.614932	0.876845
H	-2.047818	3.313887	1.581202
H	-0.931330	3.027681	0.128852
C	0.432401	-0.025641	1.949165
H	0.615957	1.038138	2.120848
H	-0.415844	-0.308693	2.577475
H	1.290543	-0.591267	2.317060
H	0.278424	-2.267912	-0.604346

Compound: 8b, Conformer: 03, Energy:-1080.269335 Hartree, Solvent: chloroform, Boltzmann percentage: 7.973

Zero-point correction=	0.478135 (Hartree/Particle)
Thermal correction to Energy=	0.500245
Thermal correction to Enthalpy=	0.501189
Thermal correction to Gibbs Free Energy=	0.429338
Sum of electronic and zero-point Energies=	-1080.220538
Sum of electronic and thermal Energies=	-1080.198428
Sum of electronic and thermal Enthalpies=	-1080.197483

Sum of electronic and thermal Free Energies= -1080.269335

C	1.502892	-1.045498	0.139708
C	2.665726	-1.514826	-0.772485
O	3.828646	-0.755389	-0.393728
H	1.471519	-1.786983	0.949701
H	2.513779	-1.314172	-1.838438
C	3.580353	-0.051741	0.809436
C	2.069739	0.232308	0.806795
C	2.023493	1.605840	0.110733
C	3.407804	2.188811	0.334910
O	4.257640	1.205125	0.756173
H	3.979978	-0.585500	1.676222
H	1.703579	0.334280	1.832177
H	1.884194	1.544199	-0.972151
H	1.264228	2.286389	0.500555
O	3.782621	3.326925	0.181571
C	-0.026512	-0.399359	-1.914810
C	-1.460160	0.137763	-1.988664
C	0.079519	-1.069079	-0.510958
H	-2.169318	-0.679779	-2.165226
H	-1.587414	0.858136	-2.802158
H	0.204242	-1.109253	-2.716539
O	2.887600	-2.889099	-0.566881
H	3.562764	-3.195599	-1.196360
C	-1.653111	0.763961	-0.594864
C	-0.973830	-0.257525	0.392867
C	-1.871913	-1.135936	1.254914
C	-3.154518	-1.723757	0.698745
C	-4.334823	-0.732296	0.689873
C	-4.234825	0.385643	-0.354730
C	-3.047975	1.380611	-0.260551
H	-0.978521	1.633552	-0.583260
H	-0.399645	0.332519	1.109961
H	-3.008164	-2.093600	-0.321878
H	-3.432172	-2.591109	1.308841
H	-5.251526	-1.300431	0.483524
H	-4.457047	-0.309879	1.694704
H	-4.234716	-0.066950	-1.355813
H	-5.158526	0.978077	-0.299443
C	-3.327280	2.502638	-1.291106
H	-4.230809	3.057535	-1.013951
H	-2.497730	3.218292	-1.335229
H	-3.482739	2.103380	-2.298804
C	-2.997095	2.041448	1.134796
H	-3.959926	2.508872	1.373577
H	-2.765169	1.328296	1.929462
H	-2.233520	2.828707	1.158205
C	-1.534693	-1.373913	2.533165
H	-2.133388	-2.022670	3.168243
H	-0.653163	-0.927992	2.988059
C	-0.298483	-2.559551	-0.690587
H	-0.430087	-3.065394	0.269907

H	-1.221451	-2.672006	-1.264608
H	0.493015	-3.082188	-1.233460
H	0.669840	0.437524	-2.026020

Compound: 8b, Conformer: 04, Energy:-1080.269264 Hartree, Solvent: chloroform, Boltzmann percentage: 7.396

Zero-point correction=	0.478007 (Hartree/Particle)
Thermal correction to Energy=	0.500136
Thermal correction to Enthalpy=	0.501080
Thermal correction to Gibbs Free Energy=	0.429480
Sum of electronic and zero-point Energies=	-1080.220737
Sum of electronic and thermal Energies=	-1080.198608
Sum of electronic and thermal Enthalpies=	-1080.197664
Sum of electronic and thermal Free Energies=	-1080.269264

C	1.473496	-0.865924	0.886744
C	1.640176	-1.669803	-0.419994
O	3.041444	-1.570567	-0.770409
H	1.758603	-1.577878	1.675387
H	1.077123	-1.271147	-1.272245
C	3.733126	-0.716215	0.117140
C	2.655535	0.125230	0.820744
C	2.587653	1.360901	-0.092854
C	3.932307	1.387845	-0.797153
O	4.557738	0.186015	-0.635444
H	4.412485	-1.285874	0.756338
H	2.986719	0.419844	1.819908
H	1.827184	1.272289	-0.874783
H	2.413706	2.303563	0.428231
O	4.436075	2.286804	-1.428864
C	-0.790431	-1.622696	1.759678
C	-2.170168	-1.509928	1.106721
C	0.043917	-0.370764	1.305472
H	-2.848673	-0.917580	1.727289
H	-2.637085	-2.491101	0.974875
H	-0.845846	-1.676800	2.852767
O	1.302554	-3.013757	-0.211372
H	1.321720	-3.482393	-1.063257
C	-1.879672	-0.810636	-0.236078
C	-0.813038	0.285358	0.115486
C	-1.366442	1.680854	0.398173
C	-2.682990	1.861190	1.131953
C	-3.899213	1.751993	0.185022
C	-4.218306	0.345586	-0.342866
C	-3.118751	-0.436676	-1.111981
H	-1.325161	-1.546933	-0.837635
H	-0.158155	0.409212	-0.751653
H	-2.794324	1.144778	1.952651
H	-2.693368	2.858456	1.586572
H	-4.785667	2.112425	0.723719
H	-3.746793	2.445524	-0.651099
H	-4.561424	-0.274484	0.495370

H	-5.083849	0.433388	-1.014047
C	-3.771654	-1.756443	-1.593482
H	-4.606274	-1.545244	-2.271794
H	-3.050881	-2.378802	-2.136815
H	-4.166011	-2.347052	-0.760074
C	-2.669558	0.335889	-2.371065
H	-3.527873	0.532025	-3.024819
H	-2.204891	1.295152	-2.132690
H	-1.945742	-0.254179	-2.946966
C	-0.747254	2.773350	-0.076637
H	-1.132653	3.770785	0.122080
H	0.144287	2.719053	-0.692720
C	0.224157	0.574527	2.511458
H	0.703658	1.518465	2.239417
H	-0.739372	0.817253	2.968296
H	0.834435	0.086588	3.280523
H	-0.305701	-2.539106	1.417003

Compound: 8b, Conformer: 05, Energy:-1080.269022 Hartree, Solvent: chloroform, Boltzmann percentage: 5.723

Zero-point correction=	0.477947 (Hartree/Particle)
Thermal correction to Energy=	0.500048
Thermal correction to Enthalpy=	0.500992
Thermal correction to Gibbs Free Energy=	0.429661
Sum of electronic and zero-point Energies=	-1080.220736
Sum of electronic and thermal Energies=	-1080.198635
Sum of electronic and thermal Enthalpies=	-1080.197691
Sum of electronic and thermal Free Energies=	-1080.269022

C	1.378507	-1.050802	0.269934
C	2.617303	-1.714333	-0.380147
O	3.764010	-0.951186	0.048259
H	1.265210	-1.589105	1.221713
H	2.624019	-1.687636	-1.476781
C	3.380583	0.022429	1.002464
C	1.914625	0.345362	0.671018
C	2.104400	1.471657	-0.367042
C	3.469058	2.055319	-0.047680
O	4.148771	1.206414	0.778677
H	3.599374	-0.303986	2.022834
H	1.394373	0.736048	1.550410
H	2.148089	1.109044	-1.398497
H	1.353219	2.260789	-0.327965
O	3.951132	3.097349	-0.423830
C	-0.125446	-0.490155	-1.822092
C	-0.975804	0.783553	-1.607042
C	0.002389	-1.240271	-0.461732
H	-1.873954	0.736774	-2.228619
H	-0.443885	1.688104	-1.917916
H	-0.622391	-1.149971	-2.541298
O	2.728156	-3.038169	0.074865
H	3.455743	-3.474484	-0.400155

C	-1.337810	0.840114	-0.098757
C	-1.146675	-0.613494	0.452895
C	-2.396922	-1.473172	0.562135
C	-3.472000	-1.389721	-0.502287
C	-4.462236	-0.233259	-0.244325
C	-3.913550	1.177184	-0.499102
C	-2.636931	1.640157	0.255280
H	-0.545369	1.417752	0.391967
H	-0.753641	-0.547441	1.473325
H	-3.033044	-1.275697	-1.501751
H	-4.033881	-2.330869	-0.511890
H	-5.333813	-0.372240	-0.897597
H	-4.833521	-0.319621	0.784175
H	-3.745474	1.294173	-1.577331
H	-4.709110	1.893483	-0.251848
C	-2.398995	3.115289	-0.152816
H	-3.251788	3.737588	0.141488
H	-1.506471	3.523099	0.336661
H	-2.269368	3.223639	-1.234963
C	-2.867182	1.613367	1.781746
H	-3.727845	2.237979	2.049286
H	-3.054378	0.605430	2.159167
H	-1.992992	2.012991	2.310600
C	-2.569135	-2.275284	1.624080
H	-3.440562	-2.919906	1.714455
H	-1.847096	-2.315265	2.436276
C	-0.183801	-2.753592	-0.699978
H	-0.103758	-3.331818	0.224313
H	-1.163727	-2.955872	-1.139267
H	0.574742	-3.130061	-1.391947
H	0.852484	-0.270268	-2.261908

Compound: 8b, Conformer: 07, Energy:-1080.268416 Hartree, Solvent: chloroform, Boltzmann percentage: 3.012

Zero-point correction=	0.478358 (Hartree/Particle)
Thermal correction to Energy=	0.500419
Thermal correction to Enthalpy=	0.501364
Thermal correction to Gibbs Free Energy=	0.429907
Sum of electronic and zero-point Energies=	-1080.219964
Sum of electronic and thermal Energies=	-1080.197903
Sum of electronic and thermal Enthalpies=	-1080.196958
Sum of electronic and thermal Free Energies=	-1080.268416

C	1.344749	0.100123	-0.694353
C	1.945910	1.511587	-0.568600
O	3.160058	1.466509	-1.364812
H	0.837816	0.109931	-1.667591
H	2.230422	1.779303	0.456641
C	3.724018	0.208962	-1.260717
C	2.604958	-0.812825	-0.920218
C	3.220107	-1.645748	0.216678
C	4.394327	-0.833574	0.724741

O	4.666272	0.174675	-0.137907
H	4.313220	0.012522	-2.158151
H	2.419487	-1.451689	-1.785181
H	2.559368	-1.910095	1.039204
H	3.625205	-2.587900	-0.172828
O	5.050993	-1.016641	1.726924
C	-0.042797	-1.845951	0.225506
C	-1.562962	-1.999898	0.125747
C	0.258743	-0.310427	0.359259
H	-2.013702	-2.020442	1.122676
H	-1.844342	-2.934132	-0.370717
H	0.375358	-2.417055	1.061174
O	1.105335	2.477094	-1.114674
H	1.455148	3.361129	-0.909204
C	-1.988877	-0.747106	-0.660409
C	-1.133456	0.405968	-0.039577
C	-1.791718	1.226289	1.067120
C	-2.753354	0.590822	2.053351
C	-4.182509	0.441069	1.487497
C	-4.367766	-0.631973	0.405392
C	-3.519280	-0.540246	-0.891628
H	-1.572535	-0.878841	-1.672239
H	-0.905247	1.127022	-0.825632
H	-2.394505	-0.388263	2.391737
H	-2.804988	1.226451	2.944989
H	-4.854741	0.191869	2.319424
H	-4.510275	1.418686	1.112858
H	-4.204618	-1.619213	0.857491
H	-5.424430	-0.619227	0.103963
C	-4.015207	-1.671020	-1.826590
H	-5.071383	-1.523351	-2.079795
H	-3.447370	-1.686241	-2.764383
H	-3.923514	-2.657864	-1.360654
C	-3.767091	0.798774	-1.619195
H	-4.833340	0.918810	-1.846175
H	-3.450288	1.661741	-1.029077
H	-3.221449	0.826239	-2.570409
C	-1.565143	2.548161	1.137593
H	-2.010703	3.156754	1.921569
H	-0.930632	3.055646	0.417196
C	0.689552	0.030581	1.800514
H	0.722783	1.107523	1.978379
H	-0.018499	-0.389556	2.521490
H	1.673520	-0.379162	2.043396
H	0.409776	-2.245101	-0.689058

Compound:8b, Conformer: 08, Energy:-1080.267958 Hartree, Solvent: chloroform, Boltzmann percentage: 1.855

Zero-point correction=	0.478085 (Hartree/Particle)
Thermal correction to Energy=	0.500164
Thermal correction to Enthalpy=	0.501108
Thermal correction to Gibbs Free Energy=	0.429674
Sum of electronic and zero-point Energies=	-1080.219547
Sum of electronic and thermal Energies=	-1080.197468
Sum of electronic and thermal Enthalpies=	-1080.196524
Sum of electronic and thermal Free Energies=	-1080.267958

C	1.485343	-0.859157	0.883365
C	1.677703	-1.624101	-0.447394
O	3.117804	-1.661056	-0.635146
H	1.769767	-1.580894	1.666207
H	1.223259	-1.120927	-1.307095
C	3.765377	-0.700324	0.163732
C	2.662573	0.140543	0.840324
C	2.583550	1.371168	-0.078767
C	3.906923	1.388368	-0.821158
O	4.540863	0.194043	-0.658075
H	4.484232	-1.190987	0.823845
H	2.973222	0.443576	1.843140
H	1.800687	1.291368	-0.838744
H	2.431648	2.316479	0.444779
O	4.385212	2.278588	-1.484986
C	-0.775781	-1.639895	1.741453
C	-2.161521	-1.520387	1.104043
C	0.050200	-0.378365	1.299895
H	-2.831024	-0.929179	1.735474
H	-2.632068	-2.499689	0.972178
H	-0.816636	-1.716778	2.833831
O	1.195374	-2.930300	-0.500748
H	1.629839	-3.457614	0.193914
C	-1.878939	-0.815868	-0.237568
C	-0.812761	0.280770	0.114056
C	-1.366856	1.674900	0.403483
C	-2.680734	1.851607	1.143159
C	-3.900613	1.743522	0.200812
C	-4.219891	0.337770	-0.328435
C	-3.123152	-0.440569	-1.105280
H	-1.325197	-1.548181	-0.843422
H	-0.162988	0.407973	-0.756016
H	-2.788615	1.132892	1.962262
H	-2.690280	2.847572	1.600666
H	-4.785116	2.102080	0.743991
H	-3.752176	2.438896	-0.634469
H	-4.557171	-0.284746	0.510500
H	-5.089440	0.425285	-0.994468
C	-3.776151	-1.760137	-1.587406
H	-4.613178	-1.548086	-2.262528
H	-3.056327	-2.380705	-2.133650
H	-4.167815	-2.352528	-0.753886

C	-2.681095	0.335732	-2.364690
H	-3.543074	0.532532	-3.013429
H	-2.216524	1.295116	-2.126389
H	-1.959624	-0.252299	-2.945312
C	-0.753410	2.769927	-0.072967
H	-1.141200	3.765798	0.128919
H	0.134258	2.720008	-0.694972
C	0.216133	0.557597	2.515416
H	0.683210	1.510224	2.252465
H	-0.751061	0.783066	2.973261
H	0.831863	0.071217	3.281259
H	-0.297875	-2.550269	1.372909

Compound: 8b, Conformer: 09, Energy:-1080.269284 Hartree, Solvent: chloroform, Boltzmann percentage: 7.554

Zero-point correction=	0.478373 (Hartree/Particle)
Thermal correction to Energy=	0.500512
Thermal correction to Enthalpy=	0.501456
Thermal correction to Gibbs Free Energy=	0.429680
Sum of electronic and zero-point Energies=	-1080.220591
Sum of electronic and thermal Energies=	-1080.198452
Sum of electronic and thermal Enthalpies=	-1080.197508
Sum of electronic and thermal Free Energies=	-1080.269284

C	1.304245	0.374093	-0.853056
C	1.643471	1.808037	-0.394215
O	2.971077	1.785957	0.127695
H	0.780446	0.466947	-1.808635
H	1.024021	2.187589	0.419990
C	3.721582	0.791926	-0.518095
C	2.731218	-0.205042	-1.177071
C	3.213132	-1.568727	-0.651316
C	4.205599	-1.256879	0.452681
O	4.475385	0.074522	0.477512
H	4.455779	1.241068	-1.193015
H	2.860687	-0.163916	-2.260186
H	2.443778	-2.234359	-0.267446
H	3.751121	-2.126034	-1.426892
O	4.736967	-2.028690	1.218734
C	-0.011976	-1.798775	-0.461976
C	-1.535813	-1.944983	-0.491374
C	0.306639	-0.369501	0.099289
H	-1.906660	-2.266039	0.487135
H	-1.857466	-2.698704	-1.216977
H	0.454086	-2.586627	0.138923
O	1.556095	2.661088	-1.519553
H	1.778666	3.566725	-1.241701
C	-2.021841	-0.528363	-0.840818
C	-1.103748	0.416579	0.007686
C	-1.671492	0.904497	1.336089
C	-2.524377	-0.006408	2.198623
C	-4.002028	-0.028626	1.748793

C	-4.290505	-0.762454	0.431247
C	-3.566857	-0.297408	-0.861967
H	-1.702241	-0.353377	-1.880394
H	-0.934939	1.323100	-0.580670
H	-2.136299	-1.031035	2.211953
H	-2.485778	0.354678	3.232772
H	-4.591056	-0.517621	2.536009
H	-4.363080	1.005785	1.694820
H	-4.091136	-1.832552	0.574453
H	-5.370432	-0.689485	0.242107
C	-4.154025	-1.137405	-2.023407
H	-5.227254	-0.942984	-2.131320
H	-3.672984	-0.886021	-2.976010
H	-4.029962	-2.212410	-1.855854
C	-3.877244	1.184038	-1.166541
H	-4.959673	1.337124	-1.253429
H	-3.504840	1.859064	-0.392853
H	-3.423905	1.483787	-2.119437
C	-1.487945	2.177520	1.721830
H	-1.873147	2.543644	2.670662
H	-0.965772	2.902236	1.102097
C	0.842058	-0.464477	1.541176
H	1.006162	0.516585	1.993017
H	0.140700	-1.005523	2.182674
H	1.787804	-1.010675	1.580259
H	0.376619	-1.899855	-1.482621

Compound: 8b, Conformer: 10, Energy:-1080.268601 Hartree, Solvent: chloroform, Boltzmann percentage: 3.664

Zero-point correction=	0.478123 (Hartree/Particle)
Thermal correction to Energy=	0.500250
Thermal correction to Enthalpy=	0.501194
Thermal correction to Gibbs Free Energy=	0.429126
Sum of electronic and zero-point Energies=	-1080.219603
Sum of electronic and thermal Energies=	-1080.197477
Sum of electronic and thermal Enthalpies=	-1080.196533
Sum of electronic and thermal Free Energies=	-1080.268601

C	1.516783	-1.029453	0.144543
C	2.698015	-1.386426	-0.790603
O	3.882103	-0.976019	-0.056104
H	1.523747	-1.803653	0.927971
H	2.666970	-0.846578	-1.742761
C	3.562614	-0.060105	0.957956
C	2.050292	0.241097	0.850436
C	2.026784	1.599635	0.125286
C	3.430504	2.154556	0.283579
O	4.261946	1.185248	0.752167
H	3.916955	-0.437909	1.919702
H	1.624421	0.351845	1.850490
H	1.837633	1.526359	-0.949335
H	1.301348	2.308306	0.530348

O	3.825458	3.271344	0.040045
C	-0.032753	-0.432460	-1.908511
C	-1.472795	0.085590	-1.990513
C	0.083897	-1.069157	-0.489798
H	-2.175001	-0.742965	-2.140928
H	-1.611013	0.782367	-2.822460
H	0.212101	-1.156720	-2.692798
O	2.843362	-2.726445	-1.139225
H	2.921852	-3.260099	-0.327863
C	-1.662069	0.748511	-0.613185
C	-0.971544	-0.241273	0.398546
C	-1.859640	-1.103641	1.287926
C	-3.145909	-1.708061	0.758557
C	-4.328636	-0.719772	0.733117
C	-4.240511	0.368287	-0.343549
C	-3.056622	1.369243	-0.286039
H	-0.990831	1.620814	-0.629655
H	-0.401729	0.373034	1.097610
H	-3.008184	-2.104591	-0.253116
H	-3.416304	-2.559380	1.393982
H	-5.245522	-1.295786	0.551123
H	-4.442968	-0.269609	1.726766
H	-4.245977	-0.112580	-1.331344
H	-5.165900	0.958883	-0.298184
C	-3.347350	2.461207	-1.345241
H	-4.250937	3.020355	-1.077038
H	-2.520829	3.178264	-1.415331
H	-3.508545	2.033415	-2.340225
C	-2.997656	2.068628	1.090130
H	-3.960119	2.539757	1.322896
H	-2.758112	1.378411	1.902672
H	-2.236293	2.858357	1.086242
C	-1.510186	-1.311060	2.568316
H	-2.101569	-1.945752	3.224096
H	-0.627028	-0.850729	3.005588
C	-0.297341	-2.563048	-0.634030
H	-0.411227	-3.049522	0.339289
H	-1.233591	-2.686016	-1.183247
H	0.479947	-3.089395	-1.192318
H	0.648499	0.414296	-2.038793

XYZ Coordinates and Energies for 15-epidendrillactol 9b

Compound: 9b, Conformer: 1, Energy:-1080.272367 Hartree, Solvent: chloroform, Boltzmann percentage: 26.085

Zero-point correction=	0.478439 (Hartree/Particle)
Thermal correction to Energy=	0.500440
Thermal correction to Enthalpy=	0.501384
Thermal correction to Gibbs Free Energy=	0.430190
Sum of electronic and zero-point Energies=	-1080.224117
Sum of electronic and thermal Energies=	-1080.202117
Sum of electronic and thermal Enthalpies=	-1080.201173
Sum of electronic and thermal Free Energies=	-1080.272367

C	-1.178293	-0.424066	-0.116483
C	-1.620971	-0.515719	1.354677
O	-2.698222	-1.470330	1.326739
H	-0.741654	-1.414121	-0.298707
H	-0.874812	-0.953946	2.024324
C	-3.321259	-1.480968	0.057989
C	-2.546297	-0.493325	-0.848623
C	-3.478231	0.734003	-0.887839
C	-4.815466	0.233869	-0.381287
O	-4.678627	-1.013128	0.150298
H	-3.384154	-2.514275	-0.289181
H	-2.436260	-0.912184	-1.851986
H	-3.167314	1.527021	-0.205758
H	-3.600290	1.168541	-1.882606
O	-5.884537	0.800417	-0.396648
C	0.449838	0.166075	-1.949049
C	1.495978	-0.944584	-1.709266
C	-0.081697	0.604873	-0.556479
H	2.370719	-0.787414	-2.346234
H	1.101567	-1.930522	-1.977130
H	0.916908	1.030712	-2.433197
O	-2.046106	0.734505	1.839867
H	-2.319622	0.634445	2.767989
C	1.857955	-0.899563	-0.191227
C	1.194135	0.403221	0.376928
C	2.081278	1.635203	0.502613
C	3.153896	1.925730	-0.528349
C	4.458856	1.145858	-0.260980
C	4.401984	-0.357012	-0.563766
C	3.344968	-1.231848	0.163486
H	1.299890	-1.715686	0.286449
H	0.847099	0.203625	1.393941
H	2.803802	1.701772	-1.543328
H	3.380915	2.997845	-0.505160
H	5.252499	1.579227	-0.883985
H	4.759221	1.316679	0.780103
H	4.281312	-0.486992	-1.647118
H	5.387433	-0.782536	-0.329199
C	3.605981	-2.694286	-0.274612
H	4.617286	-3.007138	0.009564

H	2.897888	-3.382082	0.202704
H	3.514628	-2.816653	-1.359394
C	3.542816	-1.161865	1.693167
H	4.561236	-1.467046	1.962018
H	3.378173	-0.157404	2.090558
H	2.849196	-1.842042	2.202754
C	1.947117	2.445499	1.564266
H	2.551448	3.343206	1.673748
H	1.226592	2.242901	2.352888
C	-0.583679	2.055603	-0.614295
H	-0.993994	2.391801	0.340330
H	0.236261	2.726755	-0.880311
H	-1.350771	2.167392	-1.385689
H	-0.358706	-0.153771	-2.615670

Compound: 9b, Conformer: 2, Energy:-1080.271645 Hartree, Solvent: chloroform, Boltzmann percentage: 12.142

Zero-point correction=	0.478492 (Hartree/Particle)
Thermal correction to Energy=	0.500447
Thermal correction to Enthalpy=	0.501391
Thermal correction to Gibbs Free Energy=	0.430202
Sum of electronic and zero-point Energies=	-1080.223355
Sum of electronic and thermal Energies=	-1080.201399
Sum of electronic and thermal Enthalpies=	-1080.200455
Sum of electronic and thermal Free Energies=	-1080.271645

C	-1.366838	-0.961529	-0.102809
C	-2.558710	-1.635741	0.598382
O	-3.633387	-1.517323	-0.351928
H	-1.125723	-1.660829	-0.917789
H	-2.439733	-2.710981	0.759036
C	-3.415585	-0.421123	-1.217177
C	-2.068767	0.225469	-0.814915
C	-2.517945	1.465978	-0.017862
C	-3.970879	1.671664	-0.395552
O	-4.441039	0.574846	-1.053158
H	-3.500044	-0.768559	-2.248978
H	-1.522241	0.535308	-1.709059
H	-2.510471	1.299560	1.061380
H	-1.944353	2.370369	-0.231493
O	-4.680104	2.624774	-0.166696
C	0.039676	0.240844	1.820577
C	1.494596	0.725126	1.831214
C	-0.021653	-0.801483	0.667177
H	2.159761	-0.035391	2.257939
H	1.618791	1.634515	2.427006
H	-0.290816	-0.189566	2.769992
O	-2.858084	-0.984066	1.809959
H	-3.609463	-1.434861	2.232133
C	1.770489	0.946692	0.332184
C	1.096256	-0.287383	-0.373549
C	1.990314	-1.388182	-0.927687

C	3.235894	-1.833145	-0.184654
C	4.444932	-0.899254	-0.391191
C	4.344034	0.457374	0.316219
C	3.196430	1.418578	-0.091117
H	1.124755	1.793987	0.053206
H	0.562176	0.100110	-1.245081
H	3.047054	-1.914698	0.891126
H	3.506988	-2.837021	-0.531697
H	5.336098	-1.411467	-0.004952
H	4.613885	-0.761198	-1.466120
H	4.289896	0.286146	1.400103
H	5.289199	0.992187	0.148815
C	3.476568	2.767989	0.615330
H	4.408103	3.207632	0.240922
H	2.670724	3.488413	0.431202
H	3.581097	2.648454	1.698735
C	3.218858	1.683542	-1.612834
H	4.205244	2.046884	-1.925427
H	2.990757	0.789622	-2.198399
H	2.484049	2.453636	-1.878128
C	1.685841	-1.958197	-2.105923
H	2.280724	-2.771420	-2.515228
H	0.839634	-1.627151	-2.703479
C	0.306440	-2.185385	1.277347
H	0.399331	-2.963494	0.513608
H	1.237557	-2.161634	1.847036
H	-0.481643	-2.477694	1.977270
H	-0.600141	1.102291	1.621948

Compound: 9b, Conformer: 3, Energy:-1080.271694 Hartree, Solvent: chloroform, Boltzmann percentage: 12.789

Zero-point correction=	0.478367 (Hartree/Particle)
Thermal correction to Energy=	0.500359
Thermal correction to Enthalpy=	0.501303
Thermal correction to Gibbs Free Energy=	0.430042
Sum of electronic and zero-point Energies=	-1080.223369
Sum of electronic and thermal Energies=	-1080.201377
Sum of electronic and thermal Enthalpies=	-1080.200433
Sum of electronic and thermal Free Energies=	-1080.271694

C	-1.273531	-0.363115	0.414046
C	-1.818264	0.809848	1.247530
O	-2.922849	0.221569	1.962404
H	-0.874484	-1.044627	1.179732
H	-1.135256	1.168206	2.023412
C	-3.485376	-0.832862	1.209919
C	-2.592169	-1.045695	-0.038482
C	-3.433758	-0.437270	-1.176723
C	-4.825054	-0.273024	-0.599609
O	-4.804994	-0.489606	0.744497
H	-3.615900	-1.693910	1.868213
H	-2.439764	-2.113064	-0.215045
H	-3.104425	0.562256	-1.464971

H	-3.477118	-1.055800	-2.076345
O	-5.847089	0.020071	-1.177784
C	0.278378	-1.566817	-1.190363
C	1.806916	-1.640198	-1.194026
C	-0.086530	-0.172266	-0.579803
H	2.220716	-1.063170	-2.028590
H	2.168667	-2.667562	-1.301053
H	-0.164137	-1.700214	-2.183469
O	-2.245524	1.870232	0.429433
H	-2.588109	2.583597	0.994861
C	2.166397	-1.011920	0.165292
C	1.220392	0.236916	0.274155
C	1.820964	1.596019	-0.069746
C	2.842146	1.739821	-1.182983
C	4.273960	1.367116	-0.745540
C	4.526361	-0.131117	-0.533717
C	3.679811	-0.884055	0.526898
H	1.770211	-1.712611	0.917360
H	0.911333	0.320452	1.320408
H	2.572554	1.132291	-2.054292
H	2.843334	2.782968	-1.519500
H	4.968238	1.714741	-1.522048
H	4.524010	1.929943	0.162199
H	4.414153	-0.645790	-1.497501
H	5.581940	-0.255516	-0.254994
C	4.265085	-2.314706	0.626242
H	5.301473	-2.279412	0.981090
H	3.692854	-2.929401	1.331159
H	4.266614	-2.825206	-0.342522
C	3.830921	-0.229689	1.917505
H	4.887765	-0.185358	2.206905
H	3.432442	0.787011	1.948940
H	3.304906	-0.819415	2.678442
C	1.486524	2.676733	0.652658
H	1.882868	3.661895	0.417889
H	0.808112	2.617255	1.499926
C	-0.375075	0.808365	-1.733469
H	-0.593471	1.815320	-1.378352
H	0.481833	0.859285	-2.410479
H	-1.220403	0.461222	-2.331934
H	-0.105880	-2.376018	-0.556524

Compound: 9b, Conformer: 4, Energy:-1080.270852 Hartree, Solvent: chloroform, Boltzmann percentage: 5.242

Zero-point correction=	0.478420 (Hartree/Particle)
Thermal correction to Energy=	0.500383
Thermal correction to Enthalpy=	0.501327
Thermal correction to Gibbs Free Energy=	0.430290
Sum of electronic and zero-point Energies=	-1080.222722
Sum of electronic and thermal Energies=	-1080.200759
Sum of electronic and thermal Enthalpies=	-1080.199815
Sum of electronic and thermal Free Energies=	-1080.270852

C	1.487517	-0.867238	0.986608
C	1.812121	-1.738940	-0.239745
O	3.244280	-1.859324	-0.186498
H	1.764960	-1.524018	1.824606
H	1.435593	-2.764645	-0.182898
C	3.807057	-0.698924	0.388051
C	2.643911	0.166446	0.939345
C	2.580555	1.347290	-0.043811
C	3.839330	1.244703	-0.881121
O	4.496488	0.085081	-0.605674
H	4.567899	-1.008585	1.106675
H	2.886357	0.523427	1.942511
H	1.740248	1.286365	-0.735906
H	2.544917	2.324309	0.443871
O	4.260720	2.031723	-1.698368
C	-0.763013	-1.772954	1.679327
C	-2.144576	-1.654520	1.033922
C	0.019250	-0.453704	1.338799
H	-2.831739	-1.112878	1.690851
H	-2.591936	-2.635847	0.846147
H	-0.809251	-1.934617	2.762143
O	1.398771	-1.122227	-1.435961
H	1.660291	-1.686027	-2.184362
C	-1.860449	-0.869608	-0.261519
C	-0.834334	0.236896	0.164926
C	-1.431177	1.600187	0.511229
C	-2.770573	1.710819	1.218006
C	-3.964334	1.610559	0.242588
C	-4.231910	0.219435	-0.349632
C	-3.096914	-0.489270	-1.137356
H	-1.267252	-1.544916	-0.895547
H	-0.168417	0.406065	-0.680067
H	-2.880640	0.953944	2.002219
H	-2.819967	2.685045	1.718092
H	-4.870684	1.923033	0.778340
H	-3.816356	2.343007	-0.560493
H	-4.562978	-0.447918	0.456932
H	-5.092584	0.308085	-1.027133
C	-3.700640	-1.801326	-1.697454
H	-4.528273	-1.580928	-2.381537
H	-2.950949	-2.374108	-2.255955
H	-4.093359	-2.444396	-0.902741
C	-2.650448	0.360802	-2.346403

H	-3.503403	0.565951	-3.004679
H	-2.218428	1.318812	-2.049094
H	-1.897794	-0.176080	-2.936356
C	-0.821884	2.731351	0.121027
H	-1.234579	3.707780	0.365070
H	0.090929	2.729708	-0.465671
C	0.102403	0.420340	2.609121
H	0.544203	1.400407	2.411263
H	-0.888817	0.589290	3.038763
H	0.706644	-0.082785	3.373342
H	-0.248053	-2.643564	1.258177

Compound: 9b, Conformer: 5, Energy:-1080.272723 Hartree, Solvent: chloroform, Boltzmann percentage: 38.03

Zero-point correction=	0.478591 (Hartree/Particle)
Thermal correction to Energy=	0.500514
Thermal correction to Enthalpy=	0.501458
Thermal correction to Gibbs Free Energy=	0.430610
Sum of electronic and zero-point Energies=	-1080.224742
Sum of electronic and thermal Energies=	-1080.202820
Sum of electronic and thermal Enthalpies=	-1080.201875
Sum of electronic and thermal Free Energies=	-1080.272723

C	1.307037	-1.074555	0.413937
C	2.576127	-1.783788	-0.091656
O	3.589205	-1.362672	0.836619
H	1.116161	-1.575747	1.373481
H	2.548865	-2.873579	-0.007199
C	3.291447	-0.076346	1.332662
C	1.878388	0.311949	0.820184
C	2.174928	1.375743	-0.254366
C	3.641990	1.718202	-0.094935
O	4.222903	0.895720	0.819703
H	3.431850	-0.083669	2.415075
H	1.296587	0.749877	1.634531
H	2.041531	1.016462	-1.275213
H	1.584370	2.287810	-0.140396
O	4.273381	2.581810	-0.661017
C	-0.138174	-0.530429	-1.749001
C	-0.916923	0.788708	-1.543612
C	-0.032189	-1.262013	-0.378674
H	-1.780477	0.820010	-2.213658
H	-0.311290	1.664562	-1.795982
H	-0.693813	-1.178809	-2.435993
O	2.884851	-1.392080	-1.408319
H	3.697564	-1.847110	-1.688938
C	-1.351345	0.831928	-0.052607
C	-1.214135	-0.631998	0.489224
C	-2.480108	-1.474157	0.522745
C	-3.501661	-1.356150	-0.589919
C	-4.482086	-0.185165	-0.360634
C	-3.898060	1.218677	-0.569651

C	-2.651250	1.650085	0.250635
H	-0.571111	1.388495	0.481241
H	-0.872187	-0.585326	1.529176
H	-3.013903	-1.235519	-1.565549
H	-4.079433	-2.286361	-0.639963
H	-5.324708	-0.299430	-1.055373
H	-4.902180	-0.279130	0.648294
H	-3.676484	1.345817	-1.636951
H	-4.692639	1.945376	-0.351096
C	-2.367574	3.125066	-0.127109
H	-3.223671	3.759516	0.129519
H	-1.494502	3.510950	0.412585
H	-2.179183	3.242035	-1.199672
C	-2.955332	1.608604	1.763696
H	-3.816866	2.245185	1.998406
H	-3.178062	0.599418	2.117997
H	-2.100617	1.985381	2.339139
C	-2.714819	-2.292149	1.560698
H	-3.598548	-2.925213	1.597495
H	-2.034507	-2.355664	2.406776
C	-0.183918	-2.782148	-0.601825
H	-0.113070	-3.348067	0.333473
H	-1.150200	-3.019074	-1.052824
H	0.592239	-3.141659	-1.285121
H	0.841509	-0.389134	-2.207901

Compound: 9b, Conformer: 6, Energy:-1080.270933 Hartree, Solvent: chloroform, Boltzmann percentage: 5.712

Zero-point correction=	0.478398 (Hartree/Particle)
Thermal correction to Energy=	0.500399
Thermal correction to Enthalpy=	0.501343
Thermal correction to Gibbs Free Energy=	0.429977
Sum of electronic and zero-point Energies=	-1080.222512
Sum of electronic and thermal Energies=	-1080.200511
Sum of electronic and thermal Enthalpies=	-1080.199567
Sum of electronic and thermal Free Energies=	-1080.270933

C	1.429714	-0.181720	1.273133
C	1.689208	-1.540956	0.602164
O	3.097752	-1.735160	0.811522
H	1.657113	-0.389996	2.327126
H	1.199032	-2.393982	1.081990
C	3.751762	-0.490415	0.698012
C	2.672262	0.622832	0.790285
C	2.675238	1.261120	-0.609332
C	3.794549	0.576811	-1.368145
O	4.394184	-0.362546	-0.588056
H	4.550185	-0.460701	1.440747
H	2.962795	1.358781	1.541746
H	1.753370	1.111622	-1.171566
H	2.876024	2.336521	-0.587419
O	4.169194	0.792049	-2.498994

C	-0.889079	-0.292345	2.332822
C	-1.709219	-1.315810	1.526157
C	0.013118	0.498964	1.338382
H	-2.745186	-1.332869	1.876900
H	-1.327182	-2.332850	1.668065
H	-1.564500	0.416117	2.825320
O	1.405587	-1.491600	-0.777140
H	1.673221	-2.336206	-1.179292
C	-1.596029	-0.903123	0.027687
C	-0.831169	0.470268	-0.011330
C	-1.670905	1.723275	-0.222507
C	-3.012929	1.870593	0.467213
C	-4.157667	1.189739	-0.311809
C	-4.146850	-0.343871	-0.283641
C	-2.898072	-1.094431	-0.820284
H	-0.888564	-1.598170	-0.431464
H	-0.137914	0.430424	-0.852940
H	-2.983603	1.462641	1.485257
H	-3.245156	2.937724	0.563158
H	-5.111873	1.524235	0.116648
H	-4.141400	1.554505	-1.346122
H	-4.339637	-0.671677	0.746565
H	-5.010302	-0.694247	-0.866073
C	-3.244158	-2.604267	-0.789741
H	-4.105893	-2.814436	-1.433865
H	-2.403369	-3.208803	-1.149964
H	-3.495790	-2.945980	0.220137
C	-2.625559	-0.716165	-2.292547
H	-3.510816	-0.914814	-2.909011
H	-2.362506	0.336991	-2.413389
H	-1.799632	-1.314558	-2.695483
C	-1.245686	2.688067	-1.053316
H	-1.816211	3.602227	-1.201938
H	-0.321096	2.596851	-1.617949
C	0.249532	1.919643	1.892964
H	0.792157	2.558538	1.190781
H	-0.696518	2.418231	2.116252
H	0.823924	1.869809	2.826181
H	-0.302795	-0.757130	3.133943

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