Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics.

Supporting information: A combined Raman optical activity and vibrational circular dichroism study on artemisinin-type products

Jonathan Bogaerts,[†] Filip Desmet,[†] Roy Aerts,[†] Patrick Bultinck,[‡] Wouter Herrebout,[†] and Christian Johannessen[*,†]

[†]*Department of Chemistry, University of Antwerp, Groenenborgerlaan 171, B-2020 Antwerp, Belgium*

[‡]*Department of Chemistry, Ghent University, Krijgslaan 281 (S3), B-9000 Ghent, Belgium.*

E-mail: christian.johannessen@uantwerpen.be

Contents

S1 Description of the Scaldis spectroscopy SCP-ROA spectrometer

The optical layout and operating principles of the home-built SCP-ROA spectrometer used in this study are based on the instrument designed by Hug and Hangartner[1].

A 532 nm diode-pumped solid-state laser (Laser Quantum Gem 532) is used as the excitation light source. The degree of linear polarization of the laser light is increased using a Glan-Taylor polarizer (Leysop). The laser light is focused into the sample solution using a plano-convex lens with a focal length of 50 mm (f/2.0) (Thorlabs). Back-scattered light is collected and collimated using the same lens. The collimated collected light beam passes through a long-pass edge filter (Semrock 532 nm Razoredge) to reject Rayleigh scattered laser light. The collected light then passes through a circular polarization analyzer consisting of a Liquid-Crystal Retarder (LVR-300-VIS-1L-TSC, Meadowlark Optics) combined with two polarizing beam-splitter cubes (Thorlabs). The left- and right-circularly polarized components are spatially separated by the analyzer into two beams. Using two 60 mm

achromatic doublets (f/2.4), each beam is focused onto a different entrance of a Y-shaped round-to-linear fiber bundle consisting of a total of 2×18 fibers with a core diameter of 75 μm (Ceramoptec). The linear end of the fiber bundle is coupled to the entrance of an Andor Holospec spectrograph (model f/1.8-VIS) equipped with an Andor HS-HSG-532-LF holographic transmission grating and the dispersed light is imaged onto a CCD camera (Andor Newton DU920P-BVF).

The four-phase virtual enantiomer deterministic offset correction scheme[2] is implemented using half-wave plates (Thorlabs, Edmund Optics) mounted on motorized computer-controlled translation stages (Thorlabs) in both the incident laser beam and the collimated collected light beam. Rotating half-wave plates are positioned in both the incident laser beam (181 Hz rotation, Koford Engineering, series 4851) and the collimated collected light beam (11 Hz rotation, Faulhaber, series 1628-B) to average out linearly polarized components over time[2].

Raman and ROA-spectra of standard reference samples obtained on the home-built instrument are presented below. All compounds were obtained from Sigma-Aldrich.

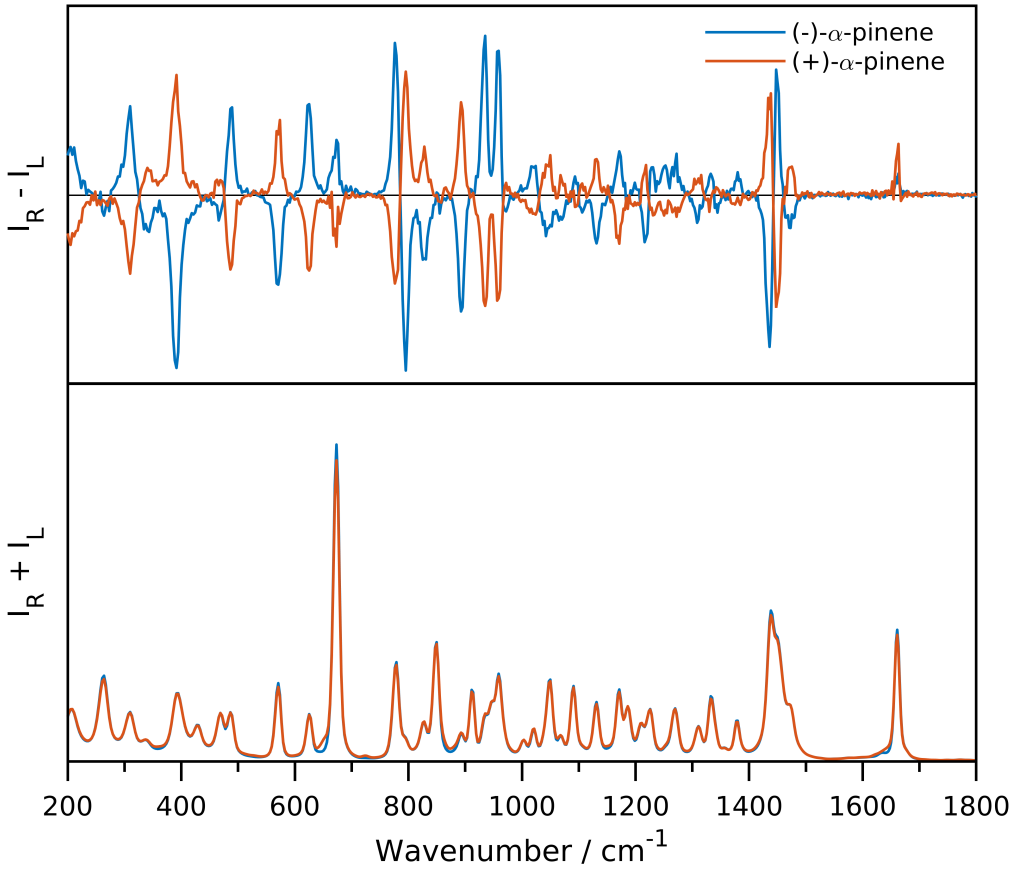

Figure S1: Raman (bottom) and ROA (top) spectra of α-pinene. Blue: (−)-α-pinene, orange: (+)-α-pinene ($\geq$ 80% e.e.). Both spectra were recorded with a laser power of 224 mW and an illumination time of 41 minutes. The difference in intensity between the two spectra is due to the lower e.e. of (+)-α-pinene.

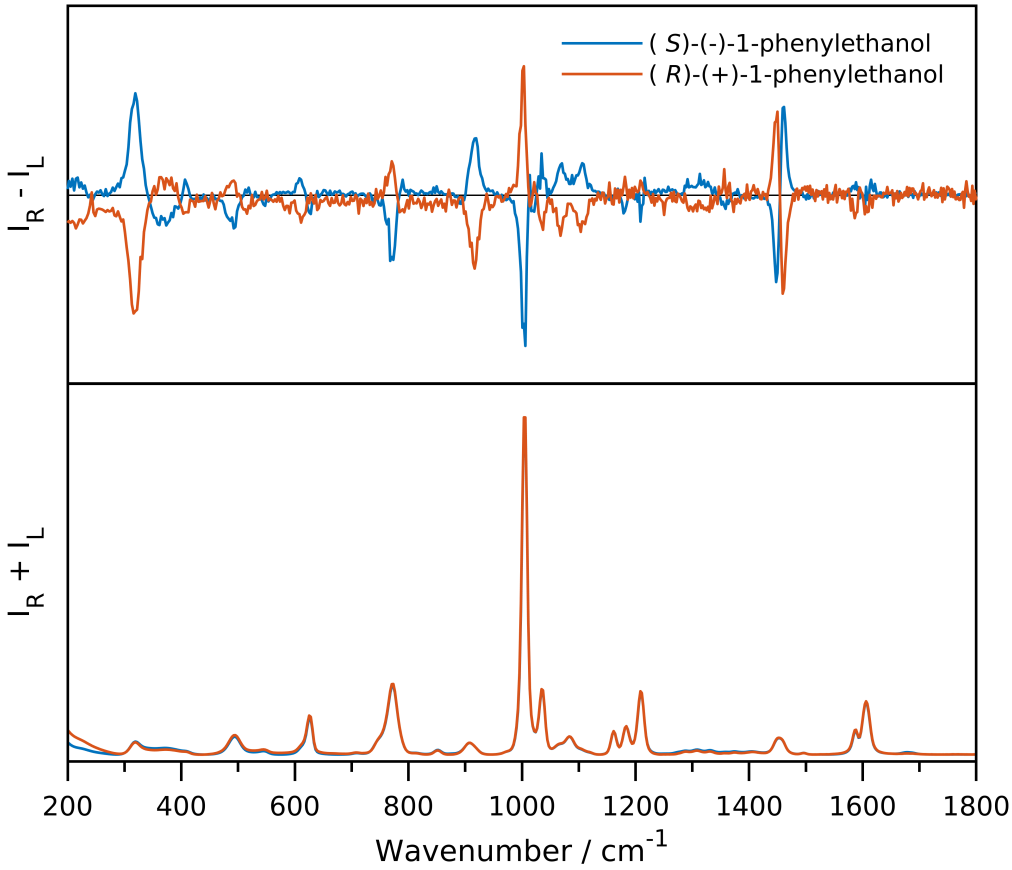

Figure S2: Raman (bottom) and ROA (top) spectra of 1-phenylethanol. Blue: (*S*)-(−)-1-phenylethanol (97%) (131 min., 74 mW), orange: (*R*)-(+)1-phenylethanol (97%) (821 min., 55 mW). A scaling factor in the y-range was calculated to adjust for the difference in exposure time and used Laser power.

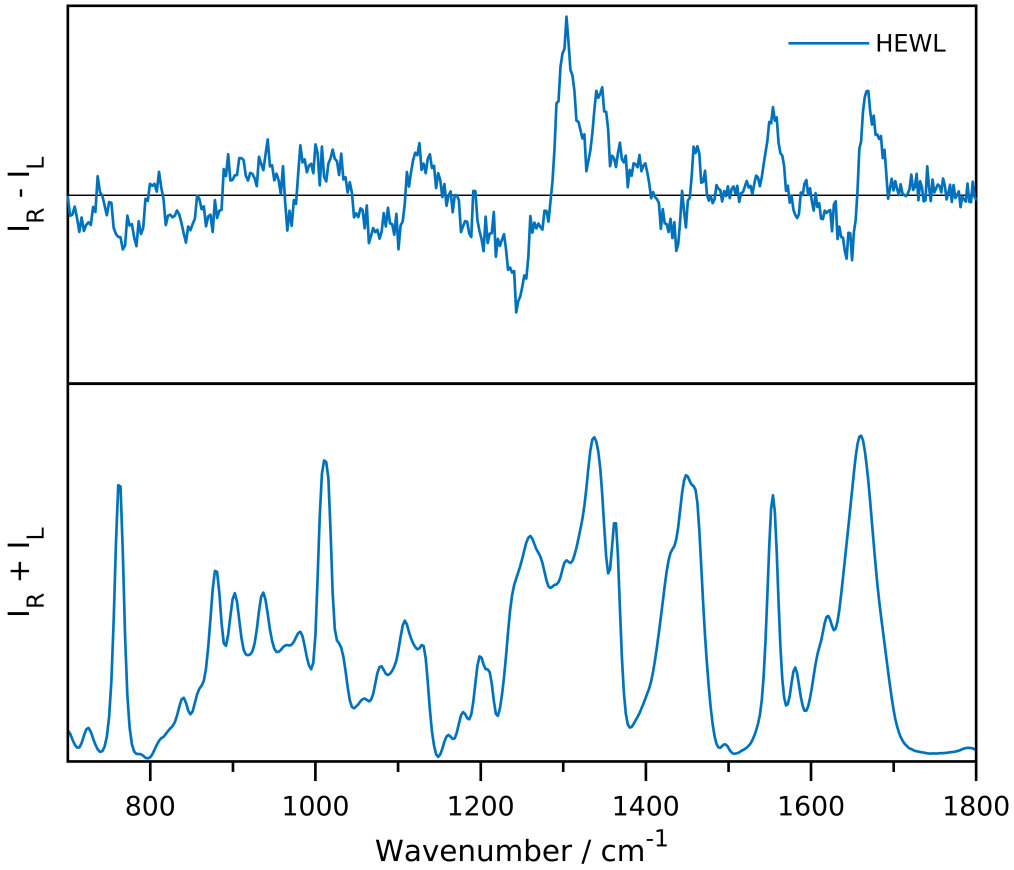

Figure S3: Raman (bottom) and ROA (top) spectra of hen egg-white lysozyme (HEWL, 100 mg/ml) (579 min., 705 mW).

S2 Optimising the scaling factor

To find the best scaling factor (σ), S_{fg}(Raman), S_{fg}(IR), S_{fg}(ROA), S_{fg}(VCD) for artemisinin were calculated over the range σ = 0.95 - 1.06 (with increments of 0.001) and are shown in figure S4. The scaling factor that gives the highest value for the function $|S_{fg}(IR) * S_{fg}(Raman) * S_{fg}(VCD) * S_{fg}(ROA)|^{1/4}$ was determined as scaling factor (σ) being 0.982.

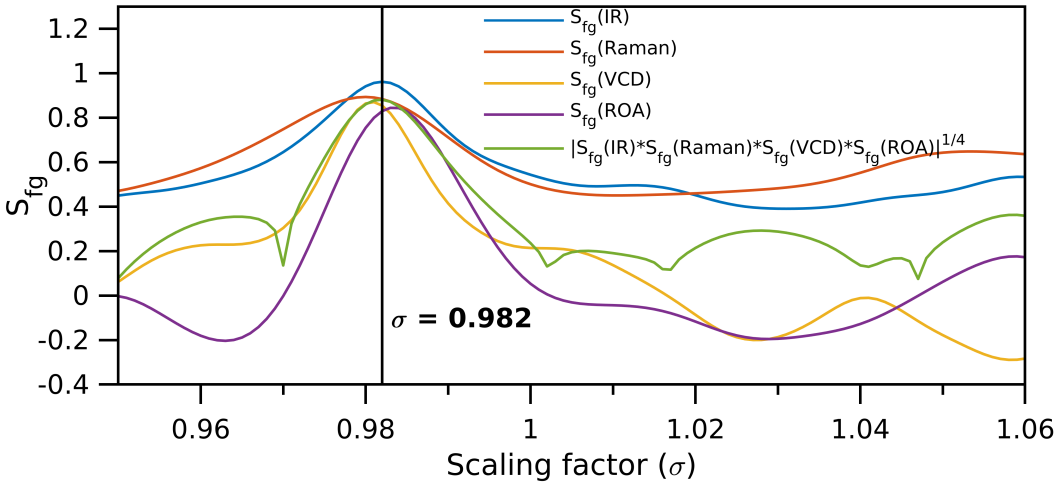

Figure S4: Similarity values S_{fg} for the wavenumber range 950 - 1550 cm^{-1} as a function of the scaling factor (σ) for Raman, IR, ROA and VCD spectra of artemisinin. The chosen scaling factor ($\sigma = 0.982$) is the one that gives the overall highest value for the function $|S_{fg}(IR) * S_{fg}(Raman) * S_{fg}(VCD) * S_{fg}(ROA)|^{1/4}$ (green curve).

S3 S_{fg} values for Raman, IR, ROA and VCD with different ratios for α and β epimers of dihydroartemisinin

Table S1: S_{fg} values for Raman, IR, ROA and VCD with different ratios for α and β epimers of dihydroartemisinin

$\boldsymbol{\alpha}$ (%)	$\boldsymbol{\beta}$ (%)	$\boldsymbol{S_{fg}}$**(Raman)** (%)	$\boldsymbol{S_{fg}}$**(IR)** (%)	$\boldsymbol{S_{fg}}$**(ROA)** (%)	$\boldsymbol{S_{fg}}$**(VCD)** (%)
0	100	88.6	90.9	70.5	76.0
5	95	88.8	91.9	71.8	79.4
10	90	88.9	92.8	73.1	82.5
15	85	89.1	93.5	74.2	85.3
20	80	89.2	94.0	75.2	87.8
25	75	89.3	94.4	76.1	89.9
30	70	89.4	94.5	76.9	91.5
35	65	89.4	94.6	77.6	92.7
40	60	89.5	94.4	78.1	93.5
45	55	89.5	94.2	78.4	93.8
50	50	89.5	93.8	78.6	93.7
55	45	89.4	93.2	78.7	93.3
60	40	89.4	92.6	78.6	92.5
65	35	89.3	91.9	78.3	91.5
70	30	89.2	91.1	77.9	90.4
75	25	89.1	90.3	77.3	89.1
80	20	89.0	89.3	76.7	87.6
85	15	88.8	88.4	75.9	86.1
90	10	88.7	87.4	75.0	84.6
95	5	88.5	86.4	74.1	83.1
100	0	88.3	85.3	73.0	81.5

S4 Calculated Raman and IR spectra of different dihydroartemisinin ratios

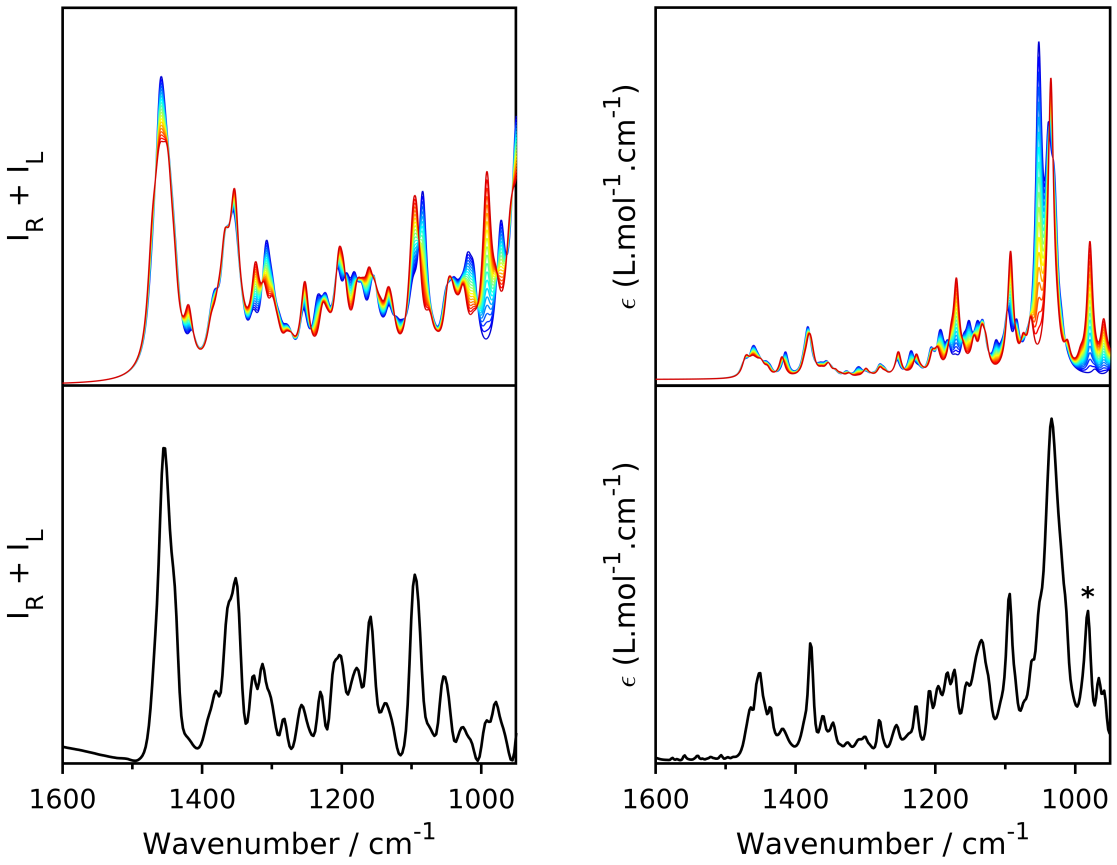

Figure S5: Comparison of experimental (bottom) and calculated (top) Raman (left) and IR spectra (right) of dihydroartemisinin with different ratios of α- and β-dihydroartemisinin. The 100% α-dihydroartemisinin spectra is shown in blue which gradually changes to red representing 100% β-dihydroartemisinin in the same way as presented in table 6. A global scaling factor (σ) of 0.982 was used on the calculated wavenumbers. The bands highlighted by an asterisk are those discussed in the main text. Note that the presented wavenumber range differs from previous figures as dihydroartemisinin does not exhibit a carbonyl stretching mode.

S5 Calculated enthalpies and free energies for the most stable conformers of α- and β-dihydroartemisinin

Table S2: Enthalpies and free energies of the most stable conformers of α- and β-dihydroartemisinin

Compound	**H° (kcal/mol)**	**G°(kcal/mol)**	**ΔH° (kcal/mol)**[a]	**ΔG°(kcal/mol)**[a]
α-Dihydroartemisinin	-603284.78	-603323.43	0.28	0.17
β-Dihydroartemisinin	-603285.06	-603323.60	0.00	0.00

[a] Referenced to H° and G° of β-Dihydroartemisinin

S6 NMR spectra of dihydroartemisinin and artesunate

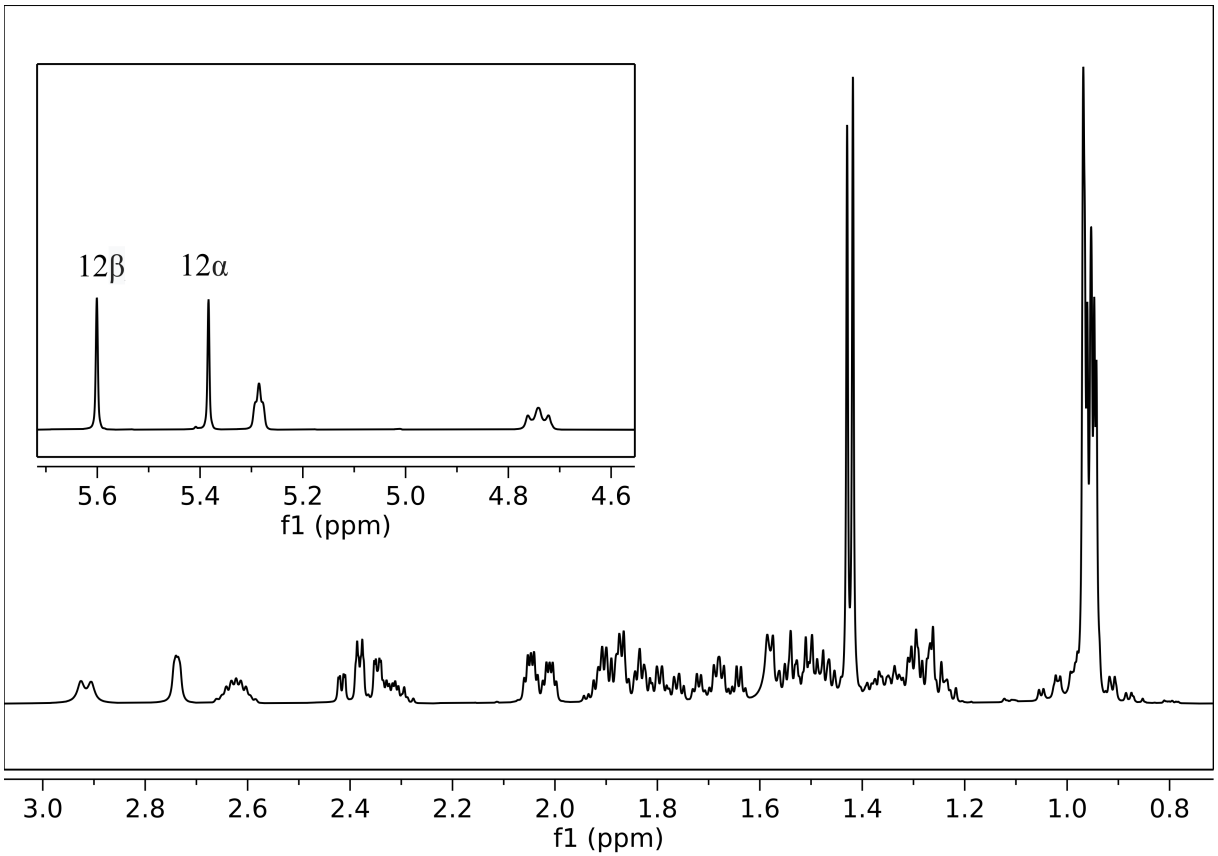

Figure S6: ^{1}H-NMR of dihydroartemisinin in $CDCl_3$ ($\sim$ 20 mg.mL^{-1}). NMR spectra were recorded on a Bruker Avance III 400 Fourier Transform NMR spectrometer at 300 K, using the non or partly deuterated solvent as internal standard (1H: δ 7.26 ppm for for $CDCl_3$).

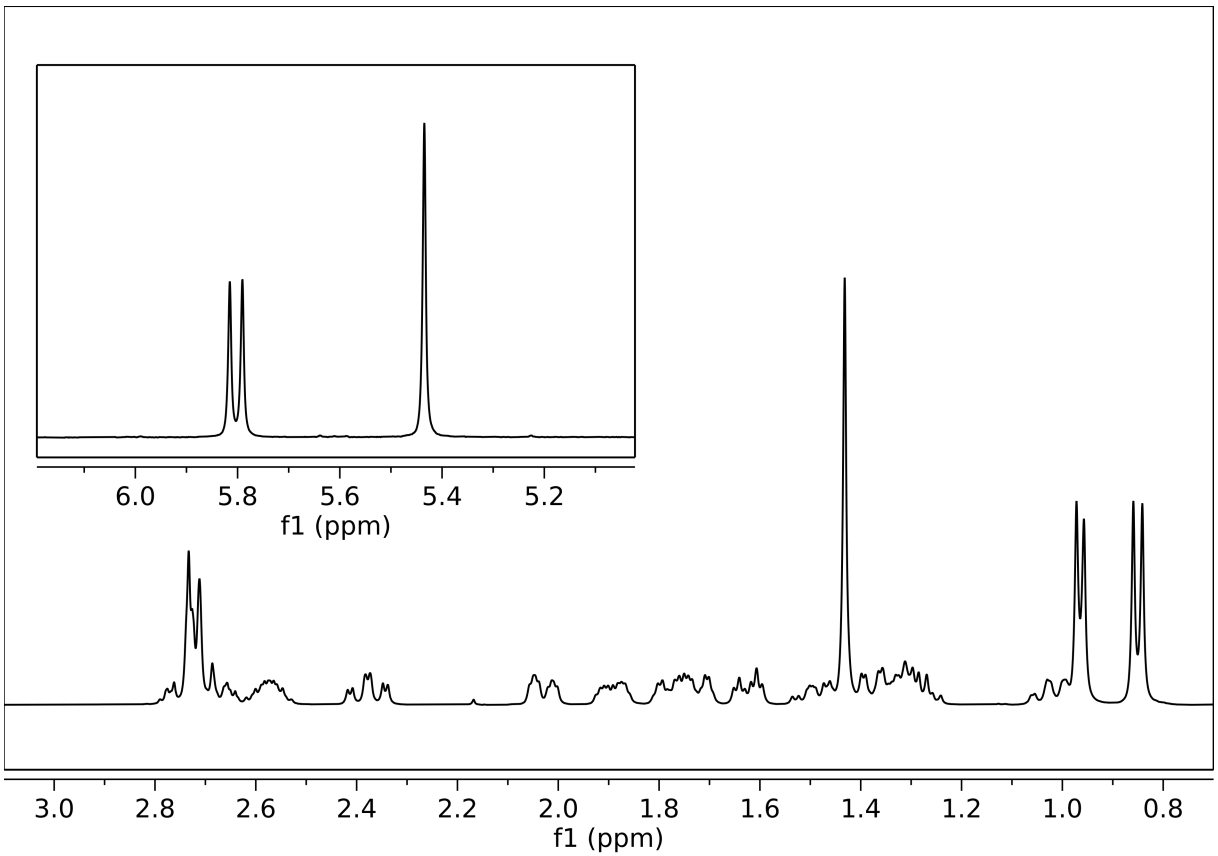

Figure S7: ^{1}H-NMR of artesunate in $CDCl_3$ ($\sim$ 20 mg.mL^{-1}). NMR spectra were recorded on a Bruker Avance III 400 Fourier Transform NMR spectrometer at 300 K, using the non or partly deuterated solvent as internal standard (1H: δ 7.26 ppm for for $CDCl_3$).

S7 Overlay of experimental and calculated Raman/ROA and IR/VCD spectra of the three artemisinin type compounds

Artemisinin

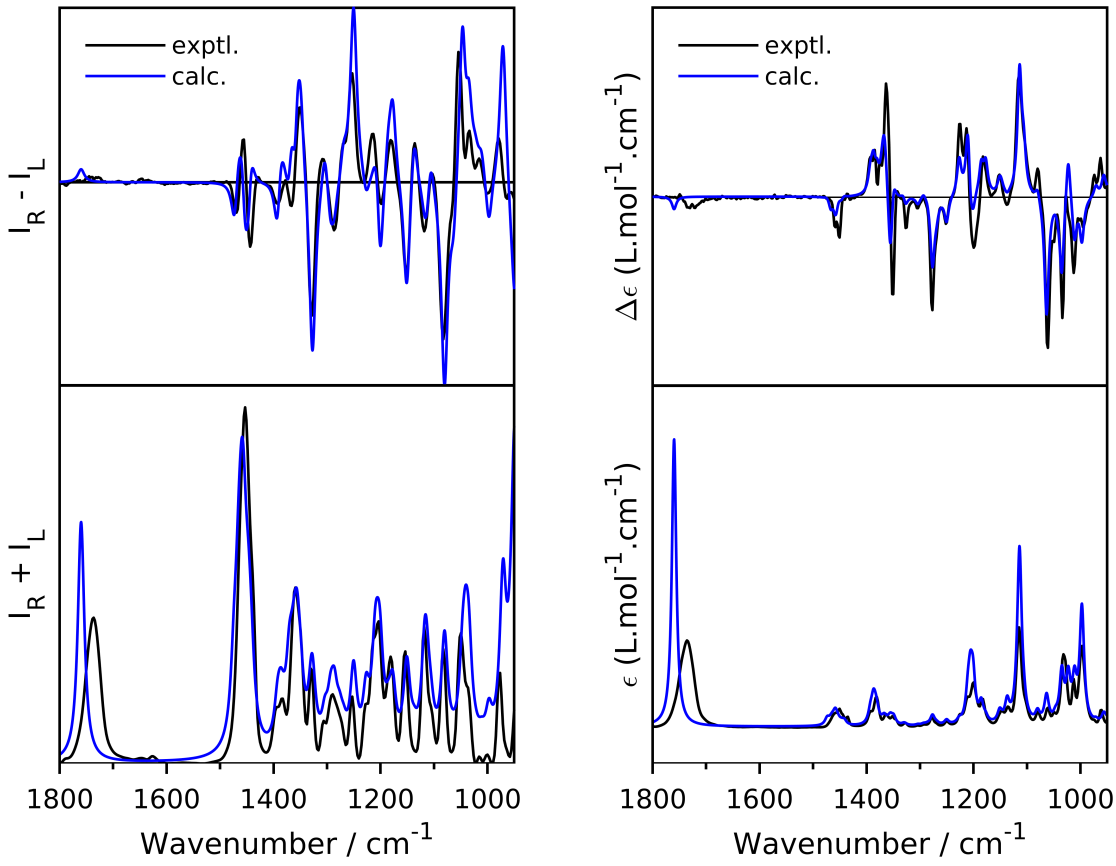

Figure S8: Left: Comparison of the experimental (black) and calculated (blue) Raman (bottom) and ROA (top) spectra of artemisinin in $CDCl_3$. Right: Comparison of the experimental (black) and calculated (blue) IR (bottom) and VCD (top) spectra of artemisinin in $CDCl_3$. A global scaling factor (σ) of 0.982 was used on the calculated wavenumbers.

Dihydroartemisinin

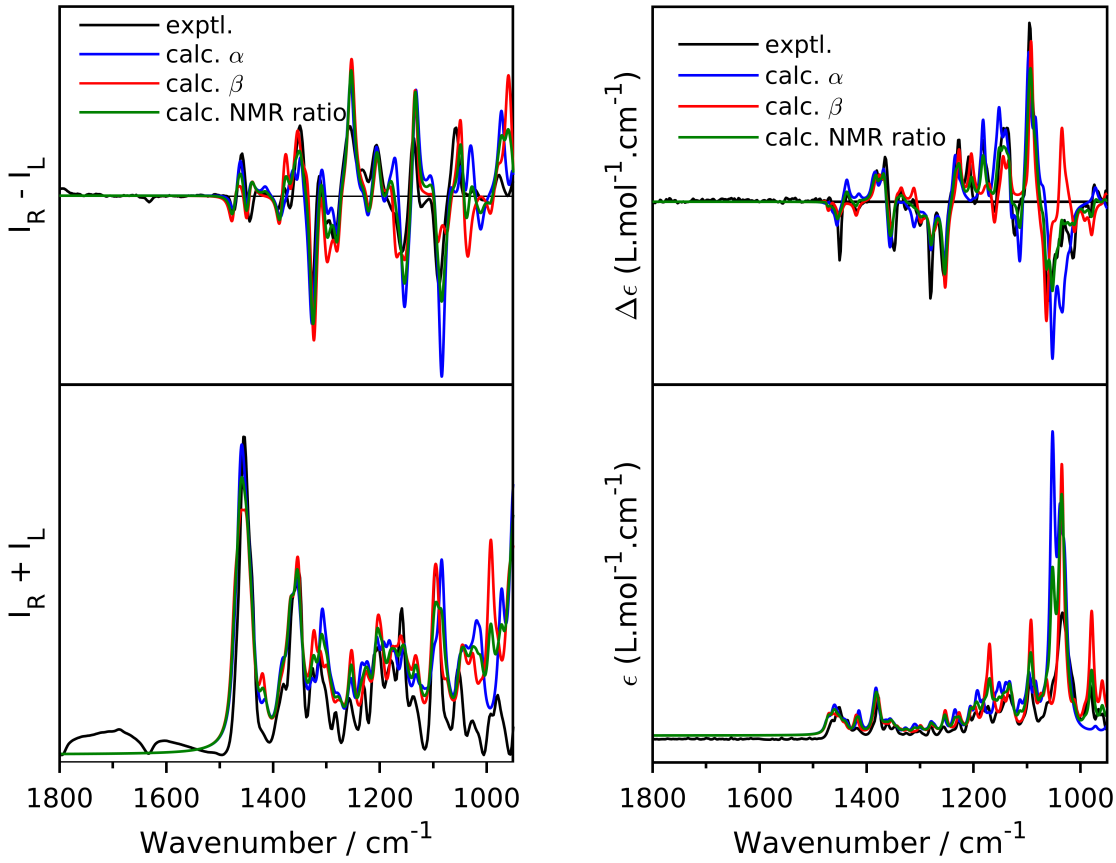

Figure S9: Left: Comparison of the experimental (black) and calculated Raman (bottom) and ROA (top) spectra of dihydroartemisinin in $CDCl_3$. Right: Comparison of the experimental (black) and calculated IR (bottom) and VCD (top) spectra of dihydroartemisinin in $CDCl_3$. The calculated α- and β-epimeric forms are shown in blue and red respectively. The green spectra correspond to a α and β combined spectrum with ^{1}H-NMR determined weights. A global scaling factor (σ) of 0.982 was used on the calculated wavenumbers.

Artesunate

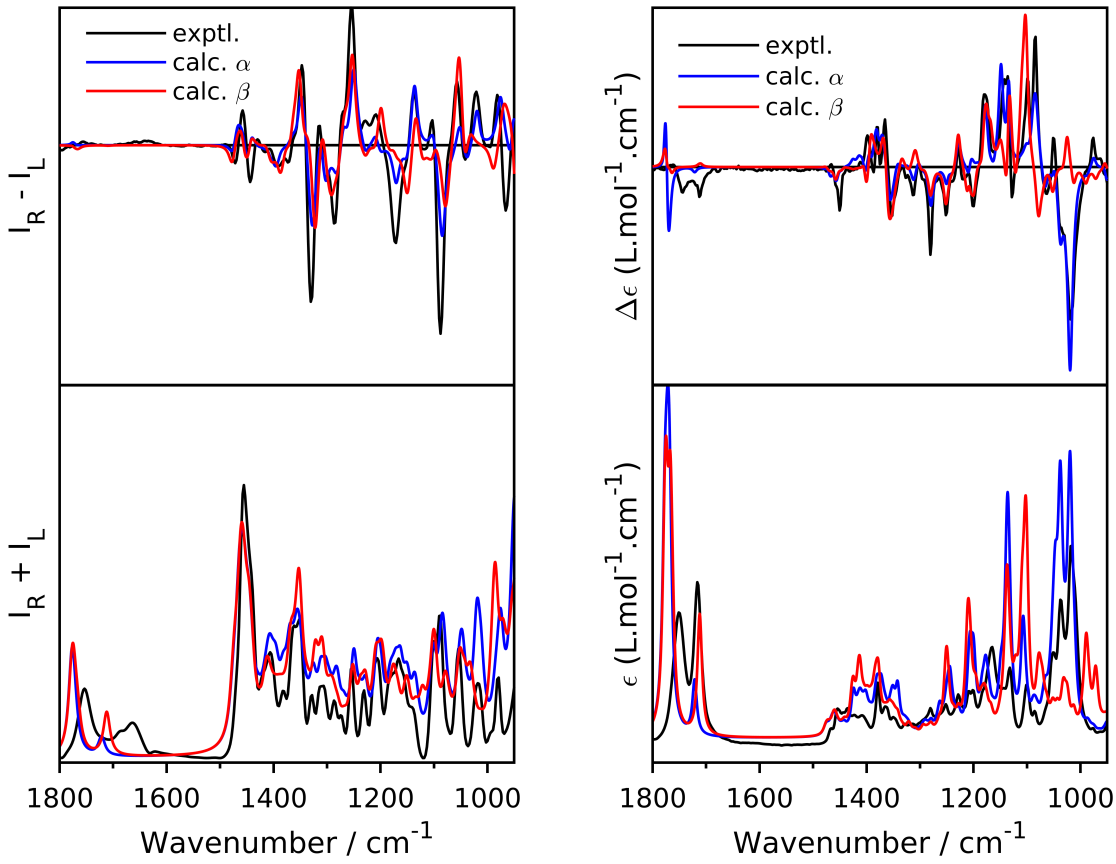

Figure S10: Left: Comparison of the experimental (black) and calculated Raman (bottom) and ROA (top) spectra of artesunate in $CDCl_3$. Right: Comparison of the experimental (black) and calculated IR (bottom) and VCD (top) spectra of artesunate in $CDCl_3$. The calculated α- and β-epimeric forms are shown in blue and red respectively. A global scaling factor (σ) of 0.982 was used on the calculated wavenumbers.

S8 Distinguish between the diastereomers of artemisinin

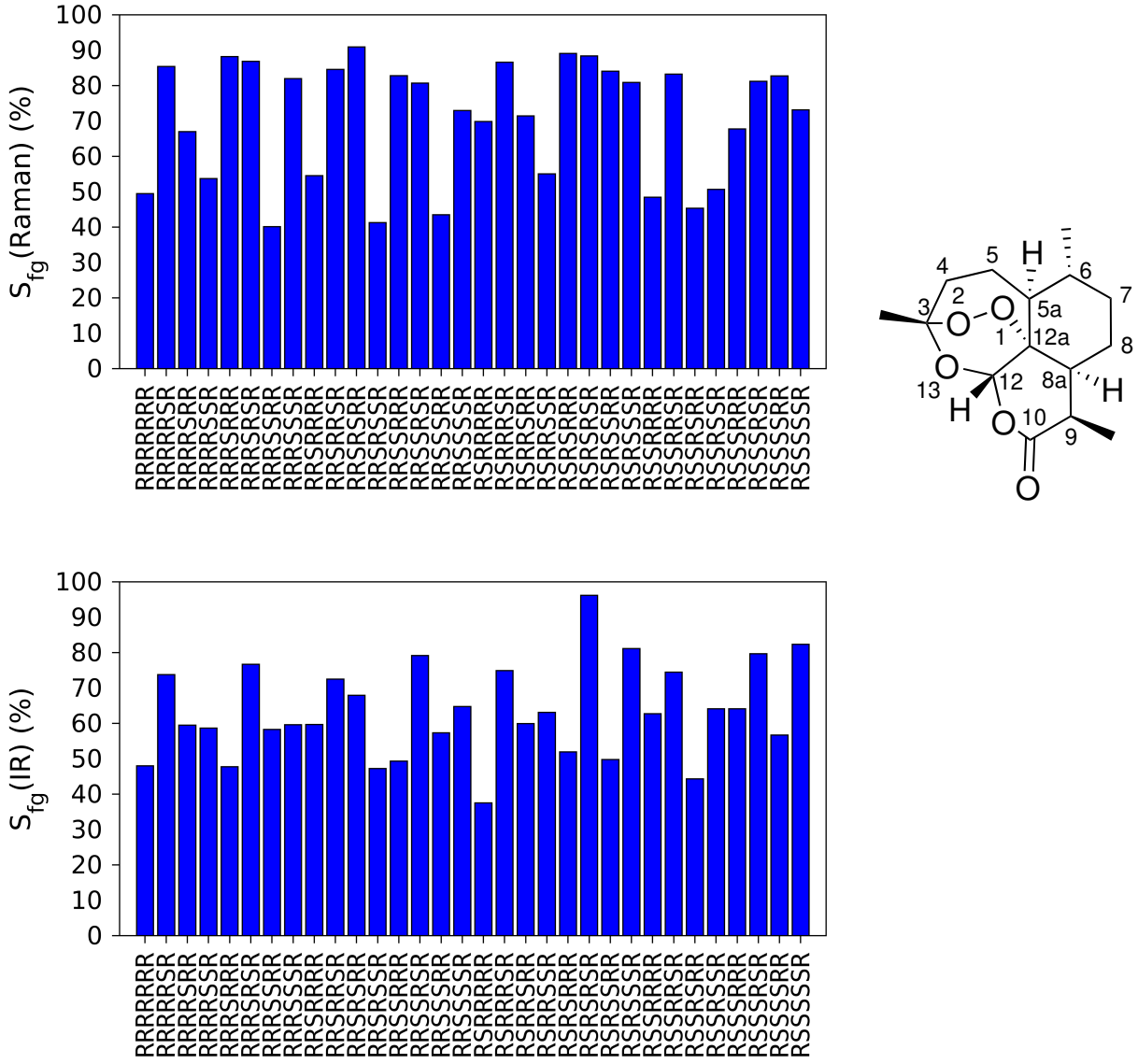

Figure S11: S_{fg}(Raman) (top) and S_{fg}(IR) (bottom) for all possible diastereomers of artemisinin. The blue bars show the S_{fg} value of the diastereomer as indicated in the labels in which the order is the same as indicated in shown structure (e.g. atom numbers 3, 5a, 6, 8a, 9, 12 and 12a).

Table S3: Scaling factors (σ) for the different diastereomers of artemisinin

Diastereomer	**Scaling factor (σ)**
RRRRRRR	1.019
RRRRRSR	0.978
RRRRSRR	0.992
RRRRSSR	1.039
RRRSRRR	0.976
RRRSRSR	0.980
RRRSSRR	1.009
RRRSSSR	0.986
RRSRRRR	1.002
RRSRRSR	0.980
RRSRSRR	0.978
RRSRSSR	1.016
RRSSRRR	0.979
RRSSRSR	0.984
RRSSSRR	0.950
RRSSSSR	0.990
RSRRRRR	0.966
RSRRRSR	0.977
RSRRSRR	0.989
RSRRSSR	1.043
RSRSRRR	0.979
RSRSRSR	0.982
RSRSSRR	0.972
RSRSSSR	0.985
RSSRRRR	1.008
RSSRRSR	0.975
RSSRSRR	1.013
RSSRSSR	1.041
RSSSRRR	0.992
RSSSRSR	0.983
RSSSSRR	0.981
RSSSSSR	0.989

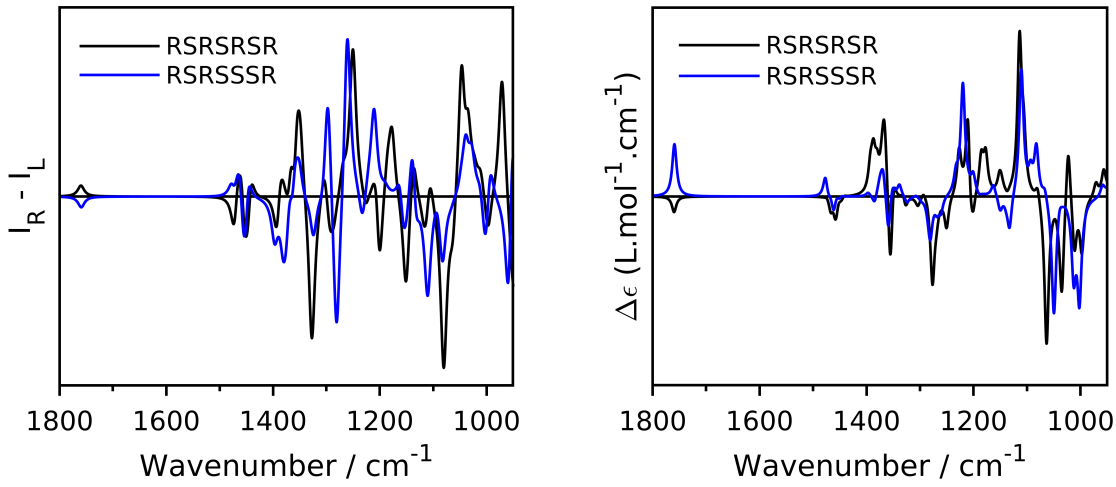

Figure S12: Left: Calculated ROA spectra of artemisinin (black, RSRSRSR) and its RSRSSSR diastereomer (blue). Right: Calculated VCD spectra of artemisinin (black, RSRSRSR) and its RSRSSSR diastereomer (blue). The scale factor (σ) is 0.982 and 0.985 respectively (see table S3).

S9 Distinguish between the diastereomers of artesunate

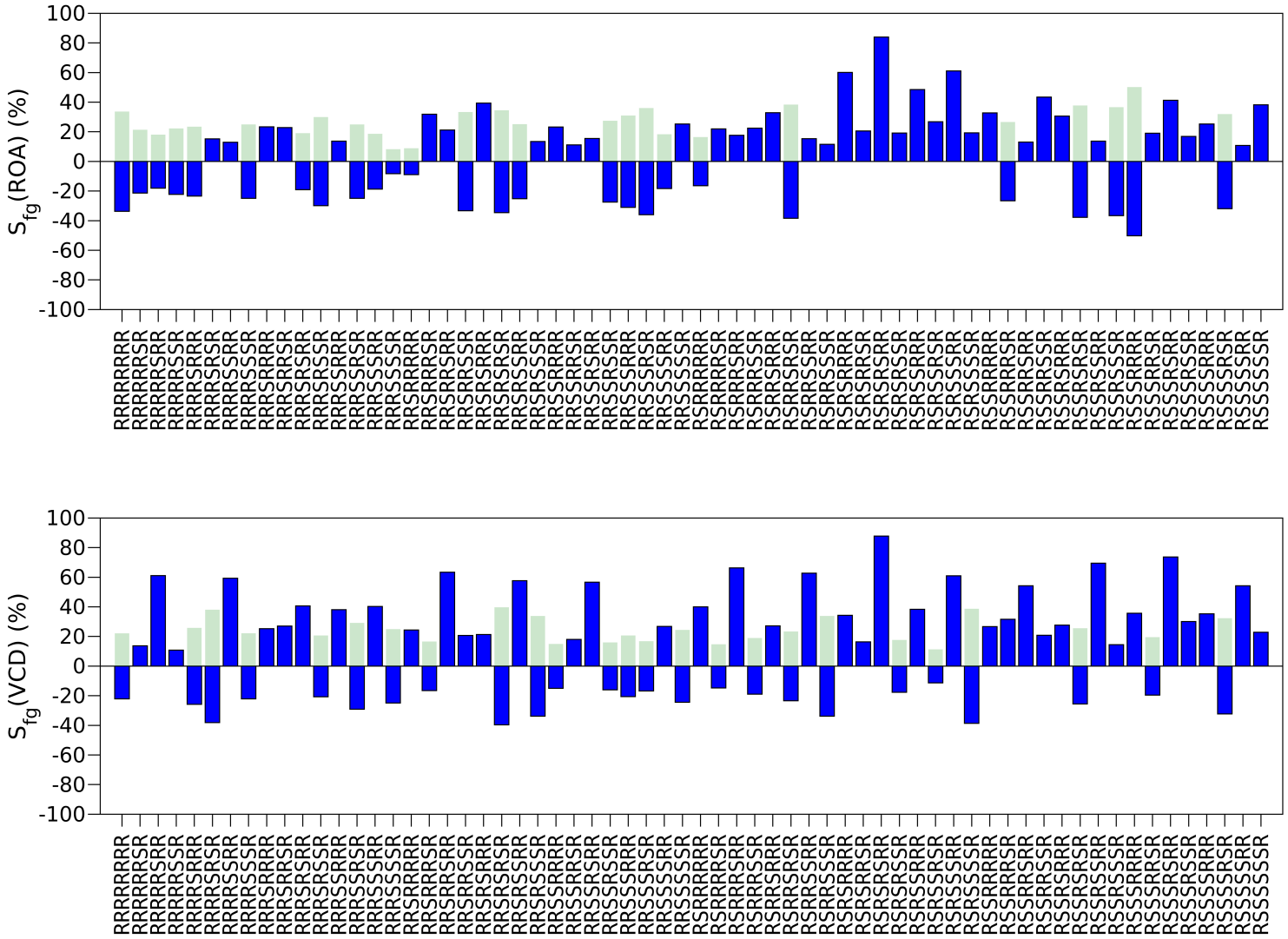

Figure S13: S_{fg}(ROA) (top) and S_{fg}(VCD) (bottom) for all possible diastereomers of artesunate. The blue bars show the S_{fg} value of the diastereomer as indicated in the labels in which the order is the same as indicated in shown artemisinin structure (e.g. atom numbers 3, 5a, 6, 8a, 9, 10, 12 and 12a). For the calculated diastereomers that give a negative S_{fg} value, the green bars indicate the S_{fg} value of the corresponding enantiomer (e.g. absolute value of the S_{fg} value). This to make the comparison with the positive value of the correct AC (RSRSRSRR) more clear. Note that those enantiomers are not explicitly calculated.

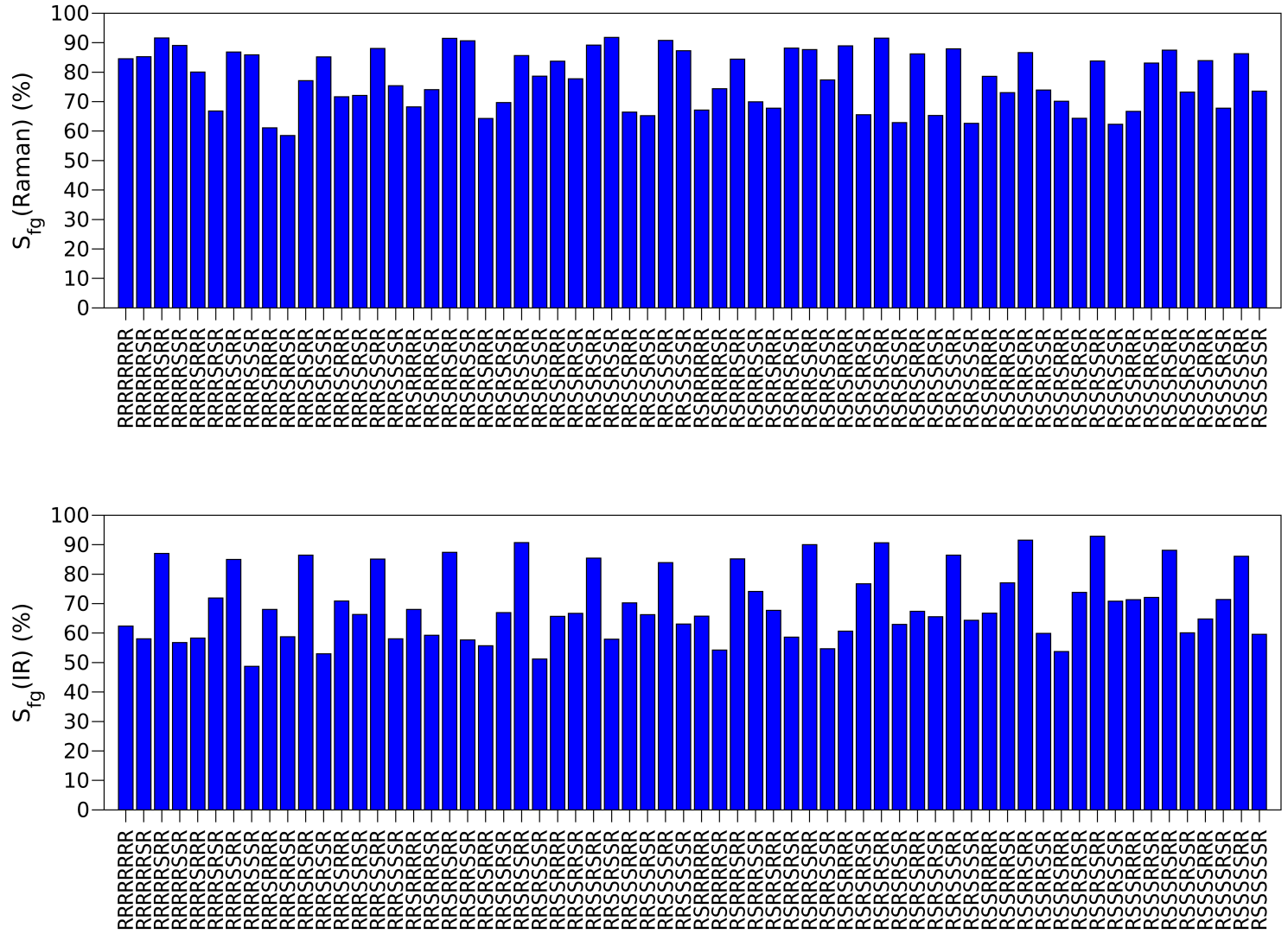

Figure S14: S_{fg}(Raman) (top) and S_{fg}(IR) (bottom) for all possible diastereomers of artesunate. The blue bars show the S_{fg} value of the diastereomer as indicated in the labels in which the order is the same as indicated in shown artemisinin structure (e.g. atom numbers 3, 5a, 6, 8a, 9, 10, 12 and 12a).

Table S4: Scaling factors (σ) for the different diastereomers of artesunate

Diastereomer	**Scaling factor (σ)**	**Diastereomer**	**Scaling factor (σ)**
RRRRRRRR	0.9830	RSRRRRRR	1.0020
RRRRRRSR	0.9700	RSRRRRSR	0.9500
RRRRRSRR	0.9780	RSRRRSRR	0.9830
RRRRRSSR	0.9830	RSRRRSSR	1.0380
RRRRSRRR	0.9840	RSRRSRRR	1.0270
RRRRSRSR	1.0080	RSRRSRSR	0.9750
RRRRSSRR	0.9720	RSRRSSRR	0.9810
RRRRSSSR	0.9700	RSRRSSSR	0.9580
RRRSRRRR	1.0290	RSRSRRRR	0.9830
RRRSRRSR	1.0380	RSRSRRSR	1.0100
RRRSRSRR	0.9610	RSRSRSRR	0.9820
RRRSRSSR	0.9690	RSRSRSSR	1.0230
RRRSSRRR	0.9500	RSRSSRRR	0.9850
RRRSSRSR	0.9520	RSRSSRSR	1.0260
RRRSSSRR	0.9800	RSRSSSRR	0.9830
RRRSSSSR	0.9930	RSRSSSSR	1.0370
RRSRRRRR	0.9990	RSSRRRRR	0.9650
RRSRRRSR	0.9520	RSSRRRSR	1.0020
RRSRRSRR	0.9780	RSSRRSRR	0.9760
RRSRRSSR	0.9830	RSSRRSSR	0.9560
RRSRSRRR	1.0310	RSSRSRRR	0.9500
RRSRSRSR	0.9980	RSSRSRSR	1.0170
RRSRSSRR	0.9840	RSSRSSRR	0.9840
RRSRSSSR	0.9660	RSSRSSSR	1.0150
RRSSRRRR	0.9870	RSSSRRRR	1.0220
RRSSRRSR	0.9920	RSSSRRSR	0.9860
RRSSRSRR	0.9780	RSSSRSRR	0.9830
RRSSRSSR	0.9760	RSSSRSSR	0.9530
RRSSSRRR	1.0060	RSSSSRRR	0.9870
RRSSSRSR	1.0030	RSSSSRSR	1.0110
RRSSSSRR	0.9790	RSSSSSRR	0.9810
RRSSSSSR	0.9720	RSSSSSSR	0.9500

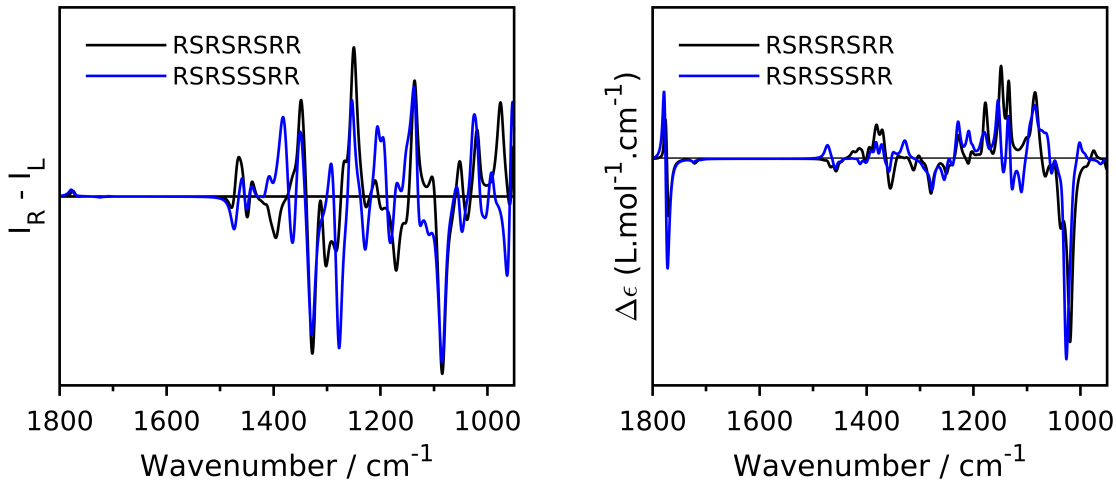

Figure S15: Left: Calculated ROA spectra of α-artesunate (black, RSRSRSRR) and its RSRSSSRR diastereomer (blue). Right: Calculated VCD spectra of α-artesunate (black, RSRSRSRR) and its RSRSSSRR diastereomer (blue). The scale factor (σ) is 0.982 and 0.983 respectively (see table S4).

S10 Cartesian Coordinates artesunate

α-artesunate

Conformer 1: ΔH° = 0 kcal/mol, weight = 21.2%

O	2.31717	-0.53618	1.55129
O	2.20604	-1.91570	1.12736
C	2.83010	-2.07090	-0.12830
C	4.23259	-1.44228	-0.15478
C	4.26105	-0.00877	-0.68550
C	3.36250	1.00635	0.04136
C	2.00359	0.39500	0.47884
C	3.22316	2.31593	-0.76599
C	2.32749	3.30877	-0.02406
C	0.95798	2.71844	0.28645
C	1.06746	1.43855	1.12942
C	1.28439	-0.35050	-0.66228
C	-0.29426	0.79968	1.48505
O	0.00862	-0.83624	-0.26685
O	2.00138	-1.45196	-1.12952
C	-1.27265	1.77822	2.13413
C	4.58254	2.94942	-1.07643
C	2.82124	-3.56370	-0.38907
H	4.86807	-2.05712	-0.80165
H	4.64878	-1.50621	0.85614
H	3.98704	-0.03024	-1.74746
H	5.29630	0.34410	-0.64191
H	3.84544	1.26816	0.99562
H	2.73851	2.07635	-1.72632
H	2.82134	3.60964	0.91211
H	2.21262	4.22027	-0.62334
H	0.35262	3.45037	0.83061
H	0.42865	2.52498	-0.65615
H	1.55045	1.71636	2.07781
H	1.15986	0.33134	-1.51565
H	-0.09407	-0.01736	2.18834
H	-1.64340	2.52729	1.42661
H	-2.13861	1.24515	2.53477
H	-0.79017	2.30770	2.96270
H	4.44552	3.91555	-1.57427
H	5.14940	3.12745	-0.15381
H	5.19514	2.32615	-1.73373
H	3.10380	-3.74185	-1.42955
H	3.53761	-4.06658	0.26543
H	1.82195	-3.97090	-0.21949
C	-0.86610	0.14953	0.23498
H	-1.10909	0.87989	-0.54818
O	-2.05526	-0.54936	0.58110
C	-2.99357	-0.71005	-0.38068
C	-4.12867	-1.56490	0.12512
H	-3.74906	-2.59154	0.19154
H	-4.37245	-1.25788	1.14587
C	-5.34912	-1.52225	-0.77845
H	-6.07589	-2.28132	-0.46583
H	-5.08803	-1.75343	-1.81532
C	-6.05580	-0.19139	-0.74995
O	-5.83381	0.71169	0.03179
O	-2.91223	-0.24084	-1.49545
O	-7.00973	-0.11235	-1.69600
H	-7.43916	0.75497	-1.61296

Conformer 2: ΔH° = 0.18 kcal/mol, weight = 15.8%

O	-2.28757	0.69980	1.51340
O	-1.88114	2.01970	1.08074

C	-2.45341	2.29724	-0.17857
C	-3.95869	1.98629	-0.20672
C	-4.29486	0.58937	-0.72827
C	-3.64073	-0.59021	0.01039
C	-2.18202	-0.28506	0.44875
C	-3.78919	-1.90658	-0.78350
C	-3.13250	-3.06316	-0.02916
C	-1.66778	-2.78296	0.28096
C	-1.49553	-1.50114	1.10968
C	-1.31550	0.27925	-0.69573
C	-0.02805	-1.17136	1.46448
O	0.03460	0.48020	-0.29872
O	-1.77530	1.50643	-1.17229
C	0.71375	-2.33643	2.11947
C	-5.25306	-2.23289	-1.09368
C	-2.11938	3.75032	-0.44846
H	-4.44458	2.71942	-0.85990
H	-4.35347	2.14565	0.80213
H	-4.01846	0.54286	-1.78884
H	-5.38212	0.46950	-0.68807
H	-4.17098	-0.73067	0.96528
H	-3.26357	-1.78878	-1.74480
H	-3.68157	-3.24067	0.90777
H	-3.21763	-3.98357	-0.61977
H	-1.23977	-3.62391	0.83574
H	-1.10751	-2.72271	-0.66170
H	-2.02792	-1.65836	2.05947
H	-1.33902	-0.41929	-1.54441
H	-0.04589	-0.32767	2.16445
H	0.91553	-3.15012	1.41464
H	1.67228	-2.00144	2.52424
H	0.12545	-2.74708	2.94695
H	-5.32707	-3.20926	-1.58496
H	-5.84697	-2.27780	-0.17217
H	-5.71474	-1.49687	-1.75757
H	-2.35540	3.97967	-1.49052
H	-2.70869	4.40170	0.20178
H	-1.05516	3.92932	-0.27953
C	0.67585	-0.66523	0.21517
H	0.76507	-1.43520	-0.56337
O	1.98213	-0.23104	0.57155
C	2.94168	-0.25819	-0.38376
C	4.22385	0.32435	0.15081
H	4.02171	1.36002	0.44603
H	4.47900	-0.19911	1.07822
C	5.35972	0.25259	-0.85565
H	5.10665	0.78451	-1.77906
H	5.55728	-0.78148	-1.15957
C	6.64282	0.82956	-0.32085
O	6.81006	1.29075	0.79068
O	2.77471	-0.69911	-1.50071
O	7.62817	0.77755	-1.23785
H	8.42671	1.15911	-0.83764

Conformer 3: ΔH° = 0.24 kcal/mol, weight = 14.3%

O	1.43800	1.99343	-0.35760
O	0.42752	2.49652	-1.26370
C	-0.63843	3.04441	-0.51907
C	-0.14058	4.00317	0.57459
C	0.04106	3.34413	1.94185
C	0.98067	2.12774	1.99432
C	0.86214	1.22571	0.73498
C	0.83262	1.35782	3.32561
C	1.77638	0.15612	3.35555
C	1.55332	-0.77224	2.16839

C	1.74096	-0.04138	0.83027
C	-0.59462	0.85532	0.39586
C	1.53970	-0.93883	-0.41256
O	-0.67876	-0.02749	-0.71451
O	-1.37819	1.96492	0.08152
C	2.37639	-2.21735	-0.37766
C	1.07215	2.25617	4.54276
C	-1.54011	3.69706	-1.54719
H	-0.87488	4.80933	0.68052
H	0.78913	4.46133	0.22135
H	-0.94707	3.04709	2.31406
H	0.41439	4.10600	2.63349
H	2.01762	2.49574	1.95052
H	-0.19999	0.97806	3.38917
H	2.81679	0.51411	3.35473
H	1.63757	-0.39780	4.29205
H	2.25577	-1.61046	2.21668
H	0.54912	-1.21143	2.24029
H	2.78019	0.31818	0.80210
H	-1.05773	0.37708	1.27048
H	1.83331	-0.34882	-1.28879
H	2.01739	-2.92723	0.37514
H	2.34997	-2.71939	-1.34826
H	3.42157	-1.98421	-0.14823
H	1.03431	1.66393	5.46365
H	2.06160	2.72771	4.49074
H	0.32461	3.04919	4.63300
H	-2.48431	3.96715	-1.06789
H	-1.07083	4.60102	-1.94347
H	-1.74480	3.00190	-2.36461
C	0.05486	-1.22336	-0.57628
H	-0.35342	-1.82953	0.24417
O	-0.14383	-1.92431	-1.79742
C	-1.25306	-2.69350	-1.90973
C	-1.34057	-3.28241	-3.29356
H	-1.29709	-2.45921	-4.01470
H	-0.43497	-3.87349	-3.46927
C	-2.59111	-4.12285	-3.48902
H	-3.49865	-3.52679	-3.34603
H	-2.64898	-4.92531	-2.74481
C	-2.65455	-4.75642	-4.85274
O	-1.79449	-4.69654	-5.70889
O	-2.04323	-2.87892	-1.00924
O	-3.80704	-5.43027	-5.03169
H	-3.78761	-5.82078	-5.92081

Conformer 4: ΔH° = 0.55 kcal/mol, weight = 8.4%

O	-2.37596	0.64279	1.51542
O	-1.96560	2.00680	1.25742
C	-2.40469	2.39274	-0.02629
C	-3.88604	2.05164	-0.25464
C	-4.11474	0.70559	-0.94234
C	-3.50763	-0.52634	-0.24930
C	-2.11947	-0.23163	0.38214
C	-3.51645	-1.75981	-1.17891
C	-2.90896	-2.97036	-0.46929
C	-1.50071	-2.68847	0.03810
C	-1.47110	-1.49103	1.00002
C	-1.15269	0.46021	-0.59796
C	-0.06539	-1.16321	1.55360
O	0.14008	0.65087	-0.02938
O	-1.59376	1.71600	-1.00617
C	0.63944	-2.36838	2.17619
C	-4.92371	-2.08911	-1.68612
C	-2.08968	3.87166	-0.12116

H	-4.32167	2.83462	-0.88485
H	-4.39466	2.10030	0.71378
H	-3.72130	0.76974	-1.96419
H	-5.19506	0.55769	-1.03732
H	-4.13773	-0.77454	0.61891
H	-2.88980	-1.53283	-2.05665
H	-3.55487	-3.25612	0.37437
H	-2.89250	-3.82748	-1.15345
H	-1.11133	-3.56967	0.55787
H	-0.83589	-2.52234	-0.82020
H	-2.10181	-1.75295	1.86212
H	-1.05502	-0.15323	-1.50458
H	-0.19149	-0.39125	2.32173
H	0.94650	-3.10455	1.42579
H	1.53407	-2.05247	2.71909
H	-0.02328	-2.87154	2.88796
H	-4.90867	-3.01626	-2.26929
H	-5.61592	-2.23440	-0.84726
H	-5.33196	-1.30448	-2.32899
H	-2.21970	4.19451	-1.15699
H	-2.76615	4.44470	0.51777
H	-1.05598	4.05671	0.17966
C	0.75018	-0.52220	0.44322
H	0.95987	-1.21317	-0.38420
O	2.00150	-0.09080	0.99156
C	3.04504	0.02656	0.16715
C	4.28419	0.47758	0.89481
H	3.97518	1.16557	1.68647
H	4.69799	-0.40107	1.40708
C	5.34359	1.15495	0.01250
H	6.04085	1.69105	0.65777
H	4.86294	1.89789	-0.63578
C	6.18783	0.23785	-0.86140
O	7.40212	0.21486	-0.80398
O	2.99192	-0.22757	-1.02869
O	5.53628	-0.53729	-1.73272
H	4.55741	-0.41782	-1.63289

Conformer 5: ΔH° = 0.6 kcal/mol, weight = 7.8%

O	1.61063	1.83060	-0.48102
O	0.63030	2.36533	-1.40228
C	-0.42282	2.95860	-0.67434
C	0.09829	3.90698	0.41763
C	0.23971	3.25223	1.79167
C	1.13269	2.00236	1.86426
C	0.99371	1.09490	0.61093
C	0.94156	1.24978	3.19968
C	1.83928	0.01379	3.24987
C	1.59483	-0.91576	2.06761
C	1.82304	-0.20370	0.72587
C	-0.47289	0.77725	0.25878
C	1.60036	-1.10263	-0.51244
O	-0.57904	-0.11218	-0.84413
O	-1.20929	1.91330	-0.07368
C	2.38846	-2.41114	-0.45966
C	1.20132	2.14874	4.41225
C	-1.28762	3.63580	-1.71816
H	-0.60671	4.74054	0.50910
H	1.04834	4.32764	0.07182
H	-0.76286	2.99422	2.15409
H	0.63276	4.00503	2.48241
H	2.18314	2.33089	1.82895
H	-0.10504	0.90905	3.25504
H	2.89237	0.33262	3.25792
H	1.66972	-0.52690	4.18910

H	2.26591	-1.77851	2.12975
H	0.57470	-1.31767	2.13168
H	2.87522	0.11676	0.70570
H	-0.96350	0.32549	1.13262
H	1.92443	-0.53051	-1.38983
H	1.99519	-3.10186	0.29387
H	2.35346	-2.91874	-1.42714
H	3.43925	-2.21585	-0.22058
H	1.13302	1.56575	5.33728
H	2.20755	2.58414	4.36684
H	0.48191	2.96878	4.48848
H	-2.22559	3.94653	-1.25144
H	-0.77944	4.51725	-2.11721
H	-1.51096	2.94097	-2.53090
C	0.10728	-1.33277	-0.68731
H	-0.32987	-1.91515	0.13538
O	-0.10958	-2.03853	-1.90327
C	-1.23022	-2.79084	-2.00552
C	-1.33481	-3.39473	-3.38382
H	-1.31120	-2.57758	-4.11223
H	-0.43179	-3.98988	-3.55845
C	-2.57705	-4.25214	-3.56036
H	-2.66871	-4.99856	-2.76713
H	-2.51122	-4.80633	-4.50491
C	-3.85003	-3.44624	-3.62281
O	-3.92511	-2.26327	-3.88607
O	-2.01812	-2.96457	-1.10099
O	-4.93571	-4.20822	-3.39249
H	-5.71945	-3.64102	-3.48031

Conformer 6: ΔH° = 0.67 kcal/mol, weight = 6.9%

O	2.33151	-0.72948	1.43923
O	2.04267	-2.02712	0.86707
C	2.53440	-2.07662	-0.45452
C	3.98710	-1.58147	-0.54596
C	4.11729	-0.10101	-0.90313
C	3.39836	0.89044	0.02703
C	2.02636	0.35664	0.52146
C	3.32878	2.30164	-0.59701
C	2.61165	3.26848	0.34603
C	1.21986	2.77439	0.71891
C	1.26569	1.38978	1.38248
C	1.13600	-0.16633	-0.62345
C	-0.11879	0.83976	1.79182
O	-0.14502	-0.57767	-0.16433
O	1.69030	-1.26015	-1.28669
C	-0.92967	1.81251	2.64782
C	4.71487	2.84114	-0.96252
C	2.34508	-3.51583	-0.88906
H	4.49582	-2.16490	-1.32120
H	4.48142	-1.81175	0.40368
H	3.74824	0.03941	-1.92656
H	5.18345	0.14595	-0.92363
H	3.98810	0.97887	0.95277
H	2.74087	2.23800	-1.52700
H	3.21489	3.39682	1.25740
H	2.54185	4.25726	-0.12373
H	0.74817	3.48206	1.40817
H	0.59123	2.76098	-0.18167
H	1.85641	1.49391	2.30471
H	1.00918	0.62806	-1.37264
H	0.05507	-0.07635	2.36846
H	-1.27891	2.67896	2.07603
H	-1.80818	1.31402	3.06578
H	-0.32564	2.18283	3.48305

H	4.63612	3.87264	-1.32301
H	5.37648	2.84433	-0.08706
H	5.19861	2.25588	-1.74935
H	2.51845	-3.58534	-1.96582
H	3.05614	-4.16443	-0.37128
H	1.32532	-3.84333	-0.67417
C	-0.86356	0.41127	0.53690
H	-1.09889	1.25574	-0.12509
O	-2.08300	-0.21449	0.91729
C	-3.13745	-0.11795	0.07455
C	-4.32039	-0.87602	0.62302
H	-4.02429	-1.92436	0.73581
H	-4.52163	-0.50179	1.63241
C	-5.55872	-0.74863	-0.24906
H	-5.79109	0.29604	-0.47125
H	-6.42727	-1.15540	0.28382
C	-5.45314	-1.51336	-1.54411
O	-4.69537	-2.43768	-1.75828
O	-3.12653	0.51213	-0.96096
O	-6.34640	-1.08203	-2.45411
H	-6.25119	-1.63476	-3.24727

Conformer 7: ΔH° = 0.67 kcal/mol, weight = 6.9%

O	2.25162	0.47787	-1.64706
O	1.64915	1.79414	-1.65309
C	2.01613	2.48241	-0.47765
C	3.52872	2.40645	-0.21449
C	3.93978	1.26768	0.71871
C	3.52282	-0.14948	0.29011
C	2.11233	-0.18414	-0.36036
C	3.69901	-1.16331	1.44204
C	3.27756	-2.56265	0.99274
C	1.84711	-2.58726	0.47009
C	1.65564	-1.61946	-0.70753
C	1.04788	0.54169	0.48478
C	0.22343	-1.60802	-1.28891
O	-0.25428	0.43222	-0.08416
O	1.30077	1.90286	0.63060
C	-0.29651	-2.99887	-1.65207
C	5.13331	-1.18383	1.97903
C	1.49274	3.89151	-0.66792
H	3.84167	3.35145	0.24266
H	4.03494	2.33643	-1.18294
H	3.52856	1.47316	1.71455
H	5.02891	1.29646	0.82331
H	4.19016	-0.47067	-0.52460
H	3.03749	-0.86053	2.26972
H	3.96424	-2.91143	0.20700
H	3.37922	-3.26409	1.82979
H	1.58990	-3.59955	0.14245
H	1.16022	-2.34921	1.29353
H	2.32539	-1.95426	-1.51311
H	1.03117	0.10990	1.49526
H	0.24766	-0.99130	-2.19507
H	-0.49970	-3.61156	-0.76735
H	-1.22342	-2.92525	-2.22693
H	0.43667	-3.53123	-2.26697
H	5.24294	-1.96893	2.73506
H	5.84840	-1.39457	1.17393
H	5.41949	-0.23754	2.44617
H	1.56295	4.42529	0.28300
H	2.08870	4.41864	-1.41707
H	0.44694	3.86655	-0.98256
C	-0.68754	-0.88350	-0.31229
H	-0.81151	-1.42403	0.63565

O	-1.97876	-0.74349	-0.91766
C	-3.03439	-0.57186	-0.11809
C	-4.29136	-0.30042	-0.90065
H	-4.28543	0.76817	-1.15336
H	-4.21839	-0.83144	-1.85350
C	-5.59481	-0.69565	-0.18972
H	-5.49063	-1.69860	0.24284
H	-6.39353	-0.74577	-0.93101
C	-6.08756	0.23925	0.90603
O	-7.20366	0.72169	0.89806
O	-2.97308	-0.62816	1.10282
O	-5.24751	0.49113	1.91307
H	-4.37903	0.03871	1.75961

Conformer 8: ΔH° = 1.11 kcal/mol, weight = 3.3%

O	2.37240	-0.58095	1.50987
O	2.13935	-1.96847	1.17149
C	2.67789	-2.23393	-0.10533
C	4.11670	-1.70949	-0.24096
C	4.21340	-0.31327	-0.85498
C	3.43083	0.80150	-0.14114
C	2.06111	0.31339	0.40588
C	3.33462	2.07161	-1.01477
C	2.55394	3.16431	-0.28368
C	1.16863	2.69171	0.14038
C	1.24083	1.45398	1.04767
C	1.22647	-0.43613	-0.65040
C	-0.13583	0.93162	1.51753
O	-0.05460	-0.80774	-0.15905
O	1.83716	-1.60934	-1.09333
C	-1.00293	2.01008	2.16680
C	4.71431	2.58913	-1.43325
C	2.54995	-3.73339	-0.28167
H	4.67183	-2.40303	-0.88201
H	4.58227	-1.74656	0.74948
H	3.87780	-0.37217	-1.89756
H	5.27137	-0.03412	-0.88720
H	3.98583	1.08021	0.76814
H	2.78138	1.81650	-1.93307
H	3.12319	3.48097	0.60306
H	2.46391	4.04699	-0.92857
H	0.65252	3.49466	0.67649
H	0.56738	2.48889	-0.75586
H	1.79865	1.74669	1.94947
H	1.09982	0.20806	-1.53209
H	0.05293	0.14065	2.25295
H	-1.36571	2.74474	1.44017
H	-1.87521	1.56244	2.65027
H	-0.43419	2.54796	2.93289
H	4.61563	3.53608	-1.97511
H	5.34499	2.77215	-0.55416
H	5.24238	1.89076	-2.08823
H	2.76096	-3.98612	-1.32373
H	3.26440	-4.25240	0.36221
H	1.53522	-4.05669	-0.03855
C	-0.82883	0.25839	0.34363
H	-1.08022	0.96267	-0.46069
O	-2.03179	-0.34464	0.80499
C	-3.03718	-0.51011	-0.08569
C	-4.18178	-1.26285	0.54402
H	-3.81688	-2.26911	0.78140
H	-4.42112	-0.79364	1.50282
C	-5.40232	-1.35872	-0.36148
H	-6.16306	-1.97898	0.12877
H	-5.16116	-1.84880	-1.30731

C	-6.07983	-0.05515	-0.70388
O	-6.77841	0.11891	-1.68208
O	-3.00925	-0.10584	-1.22808
O	-5.88042	0.90545	0.21931
H	-6.36667	1.69537	-0.06897

Conformer 9: ΔH° = 1.3 kcal/mol, weight = 2.4%

O	-2.33967	0.58988	1.46249
O	-1.93679	1.93803	1.12395
C	-2.33570	2.22824	-0.19808
C	-3.80556	1.85375	-0.44839
C	-3.99853	0.45961	-1.04522
C	-3.39933	-0.71312	-0.25015
C	-2.03493	-0.35716	0.40164
C	-3.36758	-2.00774	-1.09206
C	-2.76999	-3.15782	-0.28090
C	-1.38068	-2.82198	0.24637
C	-1.39249	-1.56193	1.12557
C	-1.04277	0.27744	-0.59259
C	-0.00704	-1.17833	1.69503
O	0.22621	0.52465	-0.00175
O	-1.48753	1.49665	-1.10218
C	0.68832	-2.32794	2.42329
C	-4.75508	-2.38848	-1.61750
C	-2.03404	3.70146	-0.38403
H	-4.22841	2.58456	-1.14647
H	-4.34554	1.96494	0.49770
H	-3.57557	0.45683	-2.05724
H	-5.07396	0.29150	-1.16078
H	-4.05361	-0.90917	0.61360
H	-2.71567	-1.83486	-1.96352
H	-3.43875	-3.39146	0.56103
H	-2.72319	-4.06080	-0.90189
H	-0.99477	-3.66098	0.83431
H	-0.69431	-2.70265	-0.60249
H	-2.04704	-1.77292	1.98403
H	-0.91311	-0.39687	-1.45109
H	-0.16423	-0.35511	2.40208
H	1.02277	-3.11213	1.73592
H	1.56501	-1.96375	2.96521
H	0.01004	-2.78599	3.15103
H	-4.71349	-3.35494	-2.13161
H	-5.47231	-2.48082	-0.79217
H	-5.15008	-1.65687	-2.32772
H	-2.13017	3.95061	-1.44371
H	-2.73914	4.30811	0.18971
H	-1.01376	3.92063	-0.06098
C	0.83962	-0.60914	0.56703
H	1.06523	-1.35268	-0.20910
O	2.06883	-0.13553	1.10498
C	3.15425	-0.13719	0.29675
C	4.34015	0.47301	0.99972
H	4.08669	1.51033	1.24270
H	4.46973	-0.03991	1.95884
C	5.62295	0.38825	0.18191
H	5.88186	-0.64642	-0.05230
H	6.44963	0.79532	0.77773
C	5.62683	1.14908	-1.12074
O	6.28826	0.84451	-2.09307
O	3.16352	-0.58035	-0.83150
O	4.86148	2.25553	-1.08467
H	4.93241	2.69282	-1.94890

Conformer 10: ΔH° = 1.32 kcal/mol, weight = 2.3%

O	1.78819	0.47025	-1.63544

O	1.64210	1.88122	-1.34771
C	2.50992	2.23461	-0.29276
C	3.93648	1.70918	-0.52479
C	4.21736	0.36024	0.13681
C	3.27968	-0.79683	-0.24785
C	1.80682	-0.33776	-0.42637
C	3.44473	-1.99894	0.70796
C	2.50281	-3.13475	0.30684
C	1.05013	-2.67928	0.25579
C	0.85342	-1.51535	-0.72750
C	1.28766	0.49449	0.76182
C	-0.60611	-1.01847	-0.83623
O	-0.08265	0.84098	0.61598
O	1.98358	1.69155	0.93189
C	-1.60190	-2.13883	-1.13486
C	4.89159	-2.49827	0.76262
C	2.41718	3.74413	-0.19762
H	4.63997	2.44254	-0.11566
H	4.10712	1.67002	-1.60572
H	4.18603	0.49733	1.22463
H	5.24552	0.07538	-0.10795
H	3.56362	-1.14634	-1.25274
H	3.16597	-1.67159	1.72255
H	2.80377	-3.52200	-0.67817
H	2.60725	-3.96647	1.01430
H	0.41054	-3.51351	-0.04930
H	0.72570	-2.40040	1.26726
H	1.14290	-1.88232	-1.72331
H	1.41601	-0.08064	1.68959
H	-0.63743	-0.28874	-1.65378
H	-1.73623	-2.81280	-0.28258
H	-2.58182	-1.72615	-1.38598
H	-1.26020	-2.73660	-1.98672
H	4.95840	-3.39772	1.38446
H	5.25197	-2.75932	-0.24040
H	5.57561	-1.75682	1.18485
H	2.90868	4.07118	0.72197
H	2.91554	4.20859	-1.05220
H	1.37065	4.05627	-0.16874
C	-0.95711	-0.24993	0.42781
H	-0.97505	-0.88707	1.32199
O	-2.24295	0.33973	0.27022
C	-2.95477	0.60185	1.39248
C	-4.20607	1.39612	1.10198
H	-4.92913	1.14494	1.88116
H	-3.93125	2.44757	1.25370
C	-4.81076	1.24429	-0.28672
H	-4.08677	1.48037	-1.07263
H	-5.63537	1.95571	-0.41225
C	-5.36046	-0.13327	-0.54737
O	-5.36963	-1.05308	0.24594
O	-2.60344	0.27884	2.50642
O	-5.86648	-0.24258	-1.79035
H	-6.21235	-1.14463	-1.89215

Conformer 11: ΔH° = 1.32 kcal/mol, weight = 2.3%

O	-1.44125	1.45385	0.91041
O	-2.58737	0.57000	0.88752
C	-2.52549	-0.30671	1.99126
C	-2.24957	0.44273	3.30499
C	-0.77111	0.50150	3.68784
C	0.17966	1.11839	2.64807
C	-0.20375	0.74270	1.19082
C	1.65711	0.83058	2.99475
C	2.58386	1.45238	1.94950

C	2.25617	0.97554	0.54000
C	0.80290	1.28922	0.15428
C	-0.41957	-0.77081	0.99823
C	0.41796	0.83295	-1.27222
O	-0.69104	-1.10606	-0.35575
O	-1.48236	-1.26894	1.75187
C	1.37695	1.34544	-2.34603
C	2.02795	1.32195	4.39730
C	-3.84463	-1.05216	1.97315
H	-2.78914	-0.07067	4.10841
H	-2.68337	1.44439	3.21777
H	-0.43486	-0.51711	3.91732
H	-0.68917	1.06984	4.61976
H	0.05153	2.21174	2.67450
H	1.80819	-0.26078	2.97372
H	2.49834	2.54830	1.99856
H	3.62605	1.20986	2.19079
H	2.92633	1.45795	-0.17857
H	2.45838	-0.10141	0.46961
H	0.69004	2.38310	0.18332
H	0.48110	-1.30821	1.32762
H	-0.58510	1.22529	-1.47690
H	2.35565	0.85709	-2.29678
H	0.96870	1.16678	-3.34351
H	1.53229	2.42407	-2.23535
H	3.09850	1.17606	4.57825
H	1.81523	2.39302	4.50493
H	1.48717	0.78940	5.18442
H	-4.65892	-0.38811	2.27367
H	-4.04135	-1.44476	0.97292
H	-3.78838	-1.88715	2.67584
C	0.28858	-0.68250	-1.27793
H	1.24292	-1.19034	-1.08437
O	-0.19429	-1.10709	-2.54736
C	0.07896	-2.38045	-2.92251
C	-0.63366	-2.76220	-4.19764
H	-0.05326	-3.56496	-4.65733
H	-1.59017	-3.20038	-3.88573
C	-0.91081	-1.63987	-5.18847
H	-1.48999	-0.83088	-4.73220
H	-1.52018	-2.01711	-6.01769
C	0.34228	-1.04726	-5.77709
O	1.47753	-1.39102	-5.51520
O	0.77332	-3.13855	-2.28115
O	0.06589	-0.06690	-6.65757
H	0.90926	0.26815	-7.00408

Conformer 12: ΔH° = 1.38 kcal/mol, weight = 2.1%

O	0.84524	1.97043	-0.30923
O	-0.26612	2.46117	-1.09726
C	-1.30681	2.86828	-0.23576
C	-0.79406	3.77934	0.89095
C	-0.46088	3.03775	2.18484
C	0.56444	1.89702	2.07385
C	0.41314	1.08323	0.75897
C	0.57222	1.02051	3.34521
C	1.59820	-0.10543	3.21297
C	1.35591	-0.95753	1.97284
C	1.38522	-0.11488	0.68846
C	-1.03594	0.62762	0.50215
C	1.15265	-0.92754	-0.60683
O	-1.14643	-0.18053	-0.66103
O	-1.91883	1.69358	0.32767
C	2.08460	-2.13131	-0.74003
C	0.83956	1.84031	4.61128

C	-2.33079	3.52533	-1.13909
H	-1.57266	4.51759	1.11204
H	0.07080	4.33147	0.50856
H	-1.39334	2.63859	2.60238
H	-0.09060	3.77244	2.90678
H	1.56645	2.34513	1.98619
H	-0.42334	0.55985	3.45042
H	2.60762	0.33059	3.17015
H	1.56933	-0.73761	4.10893
H	2.12220	-1.73616	1.90261
H	0.39693	-1.48255	2.07855
H	2.39040	0.32577	0.61458
H	-1.39462	0.05864	1.37169
H	1.32972	-0.24820	-1.44899
H	1.84869	-2.92172	-0.01997
H	2.01155	-2.56541	-1.73994
H	3.12468	-1.82819	-0.57892
H	0.92084	1.17832	5.48035
H	1.78297	2.39412	4.52545
H	0.04326	2.55964	4.82094
H	-3.24931	3.68936	-0.57014
H	-1.95749	4.48798	-1.49744
H	-2.55362	2.87855	-1.99066
C	-0.31466	-1.31895	-0.68061
H	-0.60618	-2.02240	0.11028
O	-0.57440	-1.92736	-1.94162
C	-1.60891	-2.79768	-2.01381
C	-1.92348	-3.20717	-3.43318
H	-2.23679	-4.25352	-3.39942
H	-2.81109	-2.62649	-3.71364
C	-0.83985	-2.98606	-4.47805
H	-0.49388	-1.94835	-4.49229
H	-1.24632	-3.18276	-5.47745
C	0.35447	-3.88615	-4.30068
O	0.45417	-4.77906	-3.48314
O	-2.24351	-3.17447	-1.05207
O	1.32960	-3.60072	-5.18439
H	2.05902	-4.22418	-5.03326

Conformer 13: ΔH° = 1.4 kcal/mol, weight = 2.0%

O	-1.83946	0.76513	1.44195
O	-1.23620	2.00749	1.00890
C	-1.86466	2.44461	-0.17640
C	-3.39717	2.41397	-0.05859
C	-4.03446	1.12830	-0.58539
C	-3.54347	-0.18564	0.04558
C	-2.01915	-0.17099	0.34354
C	-4.00277	-1.41191	-0.77394
C	-3.50203	-2.70491	-0.12951
C	-1.98855	-2.70851	0.04329
C	-1.51052	-1.52214	0.89406
C	-1.17632	0.28022	-0.86549
C	0.01861	-1.47778	1.11301
O	0.21931	0.21442	-0.60210
O	-1.44357	1.59172	-1.25711
C	0.59195	-2.78578	1.65760
C	-5.52397	-1.45466	-0.94643
C	-1.29351	3.82359	-0.43736
H	-3.79903	3.25434	-0.63518
H	-3.65710	2.59196	0.99016
H	-3.87303	1.08402	-1.66946
H	-5.11622	1.20620	-0.43786
H	-4.00009	-0.27724	1.04338
H	-3.55530	-1.33976	-1.77851
H	-3.98551	-2.82944	0.85112

H	-3.80869	-3.56323	-0.73976
H	-1.67356	-3.63955	0.52525
H	-1.51305	-2.70178	-0.94676
H	-1.97416	-1.62903	1.88586
H	-1.40893	-0.36170	-1.72711
H	0.21780	-0.67736	1.83539
H	0.57745	-3.58824	0.91247
H	1.62829	-2.64731	1.97656
H	0.01606	-3.12324	2.52592
H	-5.82096	-2.37571	-1.45977
H	-6.02812	-1.43942	0.02810
H	-5.90242	-0.61494	-1.53568
H	-1.58254	4.14145	-1.44218
H	-1.68540	4.53992	0.28903
H	-0.20319	3.79770	-0.37529
C	0.68503	-1.04874	-0.18527
H	0.56283	-1.78671	-0.98947
O	2.07656	-0.86920	0.05053
C	2.92482	-1.03981	-0.99255
C	4.34527	-0.73389	-0.58848
H	4.63393	-1.43135	0.20552
H	4.98322	-0.92869	-1.45201
C	4.51751	0.70170	-0.09360
H	3.84273	0.91378	0.74321
H	4.26821	1.42821	-0.87480
C	5.92229	0.97907	0.37351
O	6.81110	0.15852	0.48266
O	2.57719	-1.41130	-2.09268
O	6.09331	2.27887	0.67948
H	7.00745	2.39439	0.98696

Conformer 14: ΔH° = 1.47 kcal/mol, weight = 1.9%

O	1.44721	1.97558	-0.36644
O	0.50078	2.47787	-1.33988
C	-0.58449	3.08089	-0.67021
C	-0.11455	4.06140	0.41691
C	-0.01985	3.44431	1.81257
C	0.87657	2.20163	1.95242
C	0.79224	1.26295	0.71862
C	0.63656	1.48455	3.29903
C	1.53529	0.25247	3.41671
C	1.34503	-0.70603	2.24826
C	1.62617	-0.02524	0.90040
C	-0.65635	0.92353	0.31617
C	1.46209	-0.95465	-0.32287
O	-0.71245	0.00323	-0.76672
O	-1.38742	2.04409	-0.07566
C	2.26149	-2.25250	-0.20772
C	0.84830	2.41588	4.49624
C	-1.41161	3.72424	-1.76486
H	-0.82989	4.89015	0.45952
H	0.84415	4.48257	0.09644
H	-1.03382	3.18930	2.14445
H	0.34254	4.21812	2.49676
H	1.92584	2.53552	1.94967
H	-0.41079	1.14248	3.32432
H	2.58617	0.57554	3.46205
H	1.32755	-0.26633	4.36061
H	2.01718	-1.56286	2.35959
H	0.32519	-1.11221	2.27983
H	2.67594	0.30310	0.91700
H	-1.17842	0.49027	1.18095
H	1.81476	-0.40016	-1.20042
H	1.84489	-2.93130	0.54407
H	2.27387	-2.78215	-1.16388

H	3.29900	-2.03910	0.07070
H	0.75319	1.85542	5.43267
H	1.85203	2.85861	4.47385
H	0.12016	3.23111	4.52762
H	-2.37056	4.03753	-1.34491
H	-0.89492	4.60013	-2.16511
H	-1.59547	3.00760	-2.56864
C	-0.02027	-1.20566	-0.54909
H	-0.48411	-1.76942	0.27157
O	-0.18080	-1.94819	-1.75184
C	-1.25957	-2.75922	-1.85772
C	-1.28779	-3.41274	-3.21613
H	-1.28449	-2.61698	-3.96981
H	-0.34612	-3.95577	-3.34725
C	-2.49012	-4.33633	-3.38638
H	-3.42955	-3.78884	-3.29430
H	-2.48722	-5.09528	-2.59404
C	-2.52476	-5.07549	-4.69872
O	-3.52817	-5.28404	-5.35117
O	-2.06750	-2.93618	-0.97189
O	-1.31439	-5.53235	-5.07576
H	-1.42888	-6.02073	-5.90760

Conformer 15: ΔH° = 1.64 kcal/mol, weight = 1.3%

O	-0.58574	1.92823	-0.95635
O	-0.41877	2.65749	0.28306
C	0.94351	2.98071	0.45850
C	1.55353	3.60929	-0.80473
C	2.24772	2.60470	-1.72413
C	1.39213	1.42606	-2.21780
C	0.42263	0.89472	-1.12644
C	2.26536	0.32755	-2.86352
C	1.39746	-0.83692	-3.34038
C	0.54657	-1.41289	-2.21564
C	-0.36797	-0.34857	-1.59129
C	1.12197	0.62619	0.22068
C	-1.26773	-0.87986	-0.45122
O	0.23563	0.07009	1.18283
O	1.65812	1.77766	0.79559
C	-2.07730	-2.11482	-0.84450
C	3.11370	0.86789	-4.01868
C	0.97717	3.88596	1.67334
H	2.29482	4.35195	-0.48997
H	0.75884	4.15227	-1.32711
H	3.12698	2.21042	-1.20015
H	2.62616	3.15252	-2.59286
H	0.71601	1.80069	-3.00216
H	2.95527	-0.05835	-2.09561
H	0.74546	-0.49123	-4.15659
H	2.03585	-1.62250	-3.76281
H	-0.07096	-2.23029	-2.60150
H	1.20626	-1.85969	-1.45971
H	-1.03651	0.00935	-2.38814
H	1.95955	-0.06760	0.06085
H	-1.96044	-0.07298	-0.18473
H	-1.44781	-3.00265	-0.96646
H	-2.82698	-2.34099	-0.08188
H	-2.60259	-1.94321	-1.79009
H	3.65584	0.04942	-4.50481
H	2.48094	1.34469	-4.77790
H	3.85536	1.60036	-3.68840
H	2.01532	4.01351	1.98976
H	0.55710	4.86452	1.42774
H	0.41042	3.43893	2.49321
C	-0.40477	-1.11780	0.77796

H	0.33109	-1.91999	0.63155
O	-1.24305	-1.47408	1.87178
C	-0.69515	-2.21220	2.86706
C	-1.64241	-2.38282	4.02822
H	-1.27218	-3.21685	4.62768
H	-1.54396	-1.48254	4.64757
C	-3.10407	-2.58044	3.64219
H	-3.24672	-3.49254	3.05229
H	-3.46234	-1.75594	3.01635
C	-4.00694	-2.65775	4.84547
O	-3.67697	-2.46343	5.99790
O	0.43270	-2.65571	2.83431
O	-5.27046	-2.96574	4.49504
H	-5.80746	-2.98484	5.30429

Conformer 16: ΔH° = 1.64 kcal/mol, weight = 1.3%

O	-1.91576	0.70537	1.58117
O	-1.61373	2.03897	1.10622
C	-2.42940	2.33495	-0.00617
C	-3.90678	2.00336	0.26077
C	-4.32665	0.61445	-0.21924
C	-3.52825	-0.57243	0.34568
C	-2.01477	-0.25588	0.49428
C	-3.81662	-1.87123	-0.43914
C	-3.01514	-3.03524	0.14390
C	-1.52032	-2.74225	0.16831
C	-1.19888	-1.47647	0.97768
C	-1.40031	0.34302	-0.78594
C	0.30798	-1.13412	1.03821
O	-0.00020	0.55290	-0.66155
O	-1.95601	1.57411	-1.13310
C	1.17551	-2.30182	1.50697
C	-5.30989	-2.21035	-0.46819
C	-2.17181	3.79780	-0.30522
H	-4.52122	2.74493	-0.26142
H	-4.09120	2.13203	1.33247
H	-4.26576	0.59614	-1.31433
H	-5.38305	0.47800	0.03273
H	-3.85914	-0.74350	1.38189
H	-3.48832	-1.72324	-1.48081
H	-3.36868	-3.24005	1.16564
H	-3.20606	-3.94372	-0.44037
H	-0.98422	-3.58936	0.60822
H	-1.15515	-2.65338	-0.86376
H	-1.52903	-1.66040	2.01062
H	-1.58756	-0.33807	-1.62841
H	0.42199	-0.30321	1.74443
H	1.24097	-3.09789	0.75766
H	2.19226	-1.96291	1.72163
H	0.76723	-2.73781	2.42500
H	-5.46912	-3.17620	-0.95999
H	-5.71369	-2.28469	0.54945
H	-5.89794	-1.46558	-1.01141
H	-2.61574	4.04313	-1.27316
H	-2.62568	4.42720	0.46433
H	-1.09765	3.99066	-0.35047
C	0.73770	-0.59710	-0.31812
H	0.66602	-1.35048	-1.11412
O	2.08910	-0.15792	-0.23790
C	2.82084	-0.16117	-1.37853
C	4.17835	0.46129	-1.17024
H	4.77775	0.23711	-2.05439
H	4.03133	1.54802	-1.14928
C	4.88599	0.01715	0.10632
H	5.07885	-1.06150	0.10553

H	4.26889	0.21462	0.98949
C	6.20087	0.72452	0.30563
O	6.63372	1.62971	-0.37833
O	2.41702	-0.59121	-2.43761
O	6.86748	0.23592	1.36910
H	7.69498	0.73691	1.45724

β-artesunate

Conformer 1: ΔH° = 0.00 kcal/mol, weight = 11.1%

O	-0.28635	2.48582	-1.43144
O	-1.71061	2.49861	-1.68997
C	-2.40827	2.62471	-0.46974
C	-1.84659	3.76274	0.39814
C	-0.80573	3.30580	1.42013
C	0.41873	2.56395	0.85998
C	0.06084	1.61591	-0.31807
C	1.23249	1.88257	1.98257
C	2.45124	1.16752	1.39833
C	2.05177	0.15041	0.33773
C	1.28005	0.80720	-0.81546
C	-1.12262	0.68547	-0.00067
C	0.84696	-0.15162	-1.94224
O	-1.41647	-0.22974	-1.05919
O	-2.30831	1.37837	0.24438
C	1.98032	-0.99976	-2.51613
C	1.66030	2.87499	3.06803
C	-3.85911	2.80867	-0.86606
H	-2.68132	4.21901	0.94148
H	-1.44383	4.52949	-0.27202
H	-1.30541	2.66507	2.15704
H	-0.46006	4.18983	1.96517
H	1.08313	3.30796	0.39338
H	0.59164	1.12268	2.45865
H	3.13341	1.91432	0.96470
H	3.00574	0.66867	2.20296
H	1.45243	-0.64279	0.79760
H	2.94437	-0.33725	-0.06830
H	1.95391	1.54889	-1.27083
H	-0.89630	0.11387	0.90724
H	0.46557	0.48512	-2.75024
H	2.35720	-1.73084	-1.79615
H	1.63875	-1.54949	-3.39962
H	2.81515	-0.36183	-2.82483
H	2.30347	2.37817	3.80261
H	2.23113	3.70586	2.63431
H	0.80949	3.29691	3.61016
H	-4.48378	2.71250	0.02542
H	-4.01030	3.79958	-1.30149
H	-4.15256	2.04240	-1.58712
C	-0.36334	-0.99370	-1.55768
H	-0.76830	-1.52648	-2.41973
O	0.02278	-1.98782	-0.57174
C	-0.56833	-3.19966	-0.62531
C	-0.16564	-4.04004	0.56358
H	0.90575	-3.91056	0.73957
H	-0.67830	-3.61994	1.43743
C	-0.53174	-5.50642	0.41000
H	-1.58505	-5.63064	0.14240
H	-0.39089	-6.03125	1.36247
C	0.30969	-6.21970	-0.61677
O	1.31243	-5.77798	-1.14150
O	-1.33313	-3.55084	-1.49918
O	-0.16440	-7.45089	-0.88196

H	0.42760	-7.86381	-1.53201

Conformer 2: ΔH° = 0.03 kcal/mol, weight = 10.4%

O	2.61178	-0.39376	1.45592
O	2.93409	-1.67577	0.86574
C	3.34839	-1.48579	-0.46982
C	4.40581	-0.37634	-0.58977
C	3.82582	0.99806	-0.92278
C	2.75766	1.53884	0.04241
C	1.80460	0.42991	0.56883
C	2.02377	2.76072	-0.55321
C	0.97297	3.28330	0.42735
C	-0.02052	2.19859	0.82244
C	0.68316	0.99569	1.46665
C	1.21857	-0.44219	-0.55403
C	-0.24840	-0.14529	1.91982
O	0.29847	-1.42751	-0.07594
O	2.19542	-1.14334	-1.26133
C	-1.39503	0.30319	2.82407
C	2.99226	3.87969	-0.94831
C	3.82921	-2.84753	-0.92881
H	5.10241	-0.65550	-1.38792
H	4.97937	-0.35632	0.34286
H	3.40417	0.95736	-1.93461
H	4.65535	1.71108	-0.96315
H	3.26784	1.88697	0.95409
H	1.50007	2.43438	-1.46637
H	1.47874	3.67227	1.32398
H	0.44039	4.13051	-0.02238
H	-0.75101	2.60147	1.53185
H	-0.59158	1.88377	-0.05798
H	1.19200	1.36740	2.36923
H	0.70378	0.20017	-1.27834
H	0.37988	-0.83584	2.49584
H	-2.11848	0.93006	2.29635
H	-1.93369	-0.56407	3.22039
H	-1.00749	0.87100	3.67650
H	2.43504	4.76063	-1.28540
H	3.60795	4.18314	-0.09219
H	3.66380	3.58675	-1.76015
H	3.98011	-2.82232	-2.01089
H	4.77577	-3.09832	-0.44351
H	3.08319	-3.61028	-0.69417
C	-0.73478	-0.99962	0.75510
H	-1.22320	-1.90980	1.10708
O	-1.71026	-0.25739	-0.02455
C	-2.74551	-0.94171	-0.55453
C	-3.58755	-0.04546	-1.43151
H	-3.71212	0.91954	-0.93268
H	-3.00840	0.14614	-2.34288
C	-4.92794	-0.66220	-1.79431
H	-4.80676	-1.66309	-2.21839
H	-5.42485	-0.05793	-2.56275
C	-5.87084	-0.75043	-0.62179
O	-5.71568	-0.20672	0.45356
O	-2.95541	-2.12143	-0.36334
O	-6.95361	-1.49675	-0.90680
H	-7.52765	-1.49934	-0.12316

Conformer 3: ΔH° = 0.11 kcal/mol, weight = 9.2%

O	2.96354	-0.67813	1.08849
O	3.13264	-1.83480	0.23371
C	3.24539	-1.41293	-1.10835
C	4.26509	-0.27355	-1.26690
C	3.64399	1.12254	-1.22731

C	2.81990	1.46753	0.02461
C	1.99213	0.26248	0.55189
C	1.98771	2.75292	-0.18206
C	1.18253	3.07674	1.07716
C	0.28671	1.91600	1.48939
C	1.10054	0.64138	1.75421
C	1.16316	-0.42368	-0.54657
C	0.27744	-0.58292	2.20076
O	0.36202	-1.50036	-0.05217
O	1.95167	-0.96995	-1.55866
C	-0.64096	-0.32068	3.39293
C	2.86019	3.94632	-0.58258
C	3.59520	-2.66614	-1.88493
H	4.76571	-0.39703	-2.23346
H	5.02955	-0.39673	-0.49256
H	3.01139	1.24301	-2.11522
H	4.45426	1.85203	-1.32535
H	3.52183	1.67143	0.84826
H	1.27329	2.57129	-1.00134
H	1.87651	3.32233	1.89519
H	0.57451	3.97323	0.90366
H	-0.26713	2.17596	2.39777
H	-0.46622	1.73818	0.71359
H	1.79810	0.87094	2.57412
H	0.50829	0.31702	-1.02072
H	1.00865	-1.34200	2.50466
H	-1.45659	0.36356	3.14450
H	-1.08624	-1.25652	3.74755
H	-0.07317	0.11156	4.22350
H	2.25277	4.85611	-0.64183
H	3.64817	4.12010	0.16104
H	3.33900	3.80814	-1.55597
H	3.50532	-2.45556	-2.95350
H	4.62167	-2.97215	-1.66777
H	2.90835	-3.47504	-1.62553
C	-0.45931	-1.24692	1.04332
H	-0.86348	-2.21790	1.33512
O	-1.57825	-0.41592	0.63445
C	-2.68153	-1.03873	0.16536
C	-3.69967	-0.03018	-0.30444
H	-3.88488	0.67834	0.50982
H	-3.24287	0.55853	-1.10774
C	-4.98988	-0.68196	-0.77312
H	-5.46055	-1.25862	0.03053
H	-4.79938	-1.40335	-1.57541
C	-5.99321	0.31913	-1.27897
O	-5.82708	1.52053	-1.35599
O	-2.82304	-2.24358	0.13520
O	-7.14048	-0.27716	-1.65574
H	-7.74372	0.41407	-1.97470

Conformer 4: ΔH° = 0.25 kcal/mol, weight = 7.3%

O	-2.55244	0.51357	-1.43219
O	-2.55749	-0.83763	-1.95155
C	-2.75478	-1.74607	-0.88911
C	-3.93898	-1.33682	0.00164
C	-3.53817	-0.50720	1.22220
C	-2.75529	0.78667	0.94157
C	-1.74445	0.63451	-0.22840
C	-2.13422	1.36335	2.23288
C	-1.36335	2.64873	1.92704
C	-0.29402	2.42854	0.86520
C	-0.90022	1.90908	-0.44617
C	-0.83905	-0.60048	-0.08586
C	0.10522	1.67978	-1.59104

O	0.12859	-0.70940	-1.13340
O	-1.55235	-1.79871	-0.10106
C	0.98698	2.88789	-1.90190
C	-3.18664	1.61583	3.31672
C	-2.92231	-3.09658	-1.55604
H	-4.42866	-2.25031	0.35635
H	-4.66420	-0.80730	-0.62513
H	-2.94527	-1.14344	1.89035
H	-4.45242	-0.25403	1.76847
H	-3.46537	1.53961	0.56538
H	-1.41635	0.62636	2.62750
H	-2.07077	3.42186	1.59099
H	-0.90170	3.02710	2.84755
H	0.23010	3.36904	0.66451
H	0.46230	1.73159	1.24275
H	-1.61092	2.67356	-0.79563
H	-0.31470	-0.55640	0.87589
H	-0.49789	1.47003	-2.48298
H	1.68045	3.11599	-1.08801
H	1.57946	2.70876	-2.80559
H	0.36905	3.77392	-2.08157
H	-2.72905	2.11020	4.18065
H	-3.98280	2.27113	2.94150
H	-3.65025	0.69299	3.67625
H	-2.88242	-3.87540	-0.79049
H	-3.88636	-3.14993	-2.06821
H	-2.11574	-3.26549	-2.27318
C	0.91815	0.40328	-1.40744
H	1.47179	0.15064	-2.31364
O	1.89047	0.59549	-0.34450
C	3.06798	-0.05508	-0.44886
C	3.95526	0.24915	0.73575
H	4.21332	1.31334	0.68616
H	3.37206	0.11330	1.65119
C	5.21920	-0.59415	0.75840
H	5.91403	-0.20642	1.51344
H	5.74606	-0.55480	-0.19871
C	4.95621	-2.03681	1.10817
O	3.93942	-2.46628	1.61531
O	3.37846	-0.76003	-1.38621
O	6.01245	-2.82104	0.82533
H	5.79024	-3.72717	1.09590

Conformer 5: ΔH° = 0.28 kcal/mol, weight = 6.7%

O	-2.37961	0.22218	-1.78111
O	-2.40895	-1.21388	-1.96051
C	-2.74355	-1.83147	-0.73577
C	-3.97611	-1.18267	-0.08505
C	-3.63661	-0.09667	0.93571
C	-2.76980	1.06725	0.42825
C	-1.67102	0.60824	-0.57045
C	-2.23420	1.92547	1.59548
C	-1.38281	3.07854	1.06262
C	-0.23601	2.57830	0.19422
C	-0.74960	1.76840	-1.00491
C	-0.84534	-0.58186	-0.05172
C	0.33691	1.23783	-1.96020
O	0.20250	-0.96873	-0.94512
O	-1.61586	-1.72676	0.15156
C	1.30146	2.30728	-2.46979
C	-3.36334	2.45726	2.48348
C	-2.92493	-3.29749	-1.07308
H	-4.54280	-1.96777	0.42744
H	-4.61556	-0.79744	-0.88619
H	-3.13385	-0.57078	1.78749

H	-4.57716	0.31001	1.32080
H	-3.40696	1.72477	-0.18388
H	-1.58752	1.28943	2.22136
H	-2.02247	3.76085	0.48260
H	-0.98672	3.66161	1.90344
H	0.34932	3.42559	-0.17877
H	0.44945	1.97676	0.80109
H	-1.38876	2.44277	-1.59531
H	-0.40352	-0.32144	0.91711
H	-0.19890	0.83156	-2.82685
H	1.93694	2.70410	-1.67361
H	1.95545	1.89665	-3.24663
H	0.74614	3.14158	-2.91105
H	-2.95917	3.12922	3.24856
H	-4.09029	3.02643	1.89043
H	-3.90153	1.65782	3.00018
H	-2.99189	-3.86762	-0.14325
H	-3.84345	-3.44326	-1.64712
H	-2.07062	-3.66067	-1.64888
C	1.06713	0.02379	-1.39647
H	1.68892	-0.45520	-2.15516
O	1.94572	0.44813	-0.31935
C	3.08713	-0.24561	-0.13016
C	3.88998	0.34240	1.00717
H	4.30877	1.28977	0.64673
H	3.21107	0.59336	1.82648
C	5.01069	-0.57081	1.47471
H	5.67972	-0.02964	2.15440
H	5.62703	-0.90887	0.63687
C	4.50848	-1.78143	2.21937
O	3.37384	-1.94372	2.62137
O	3.43614	-1.18645	-0.81219
O	5.48666	-2.68237	2.42547
H	5.10609	-3.42505	2.92269

Conformer 6: ΔH° = 0.30 kcal/mol, weight = 6.7%

O	-2.54273	0.88014	-0.97061
O	-3.21513	-0.39968	-0.89376
C	-3.27080	-0.81769	0.45328
C	-3.78250	0.29815	1.37888
C	-2.67087	1.12340	2.02724
C	-1.67613	1.79894	1.06802
C	-1.33356	0.91324	-0.16164
C	-0.43706	2.33075	1.82118
C	0.53711	2.99581	0.84765
C	0.94804	2.05378	-0.27657
C	-0.26786	1.55944	-1.07293
C	-0.92848	-0.52032	0.22056
C	0.05555	0.61750	-2.24906
O	-0.56085	-1.31677	-0.90891
O	-1.95101	-1.21893	0.86230
C	1.09754	1.16561	-3.22208
C	-0.81554	3.30173	2.94375
C	-4.14291	-2.05692	0.44309
H	-4.37224	-0.16600	2.17701
H	-4.46662	0.92765	0.80028
H	-2.11667	0.47230	2.71420
H	-3.14347	1.89373	2.64492
H	-2.17582	2.67177	0.61936
H	0.07877	1.47263	2.28150
H	0.06699	3.89751	0.42695
H	1.42657	3.33403	1.39364
H	1.50766	1.20810	0.13817
H	1.63289	2.56698	-0.96003
H	-0.75299	2.44943	-1.50226

H	-0.08391	-0.48490	0.91872
H	-0.88354	0.49355	-2.80228
H	2.08822	1.24494	-2.76645
H	1.18356	0.51536	-4.09928
H	0.80380	2.15987	-3.57466
H	0.08721	3.72661	3.39635
H	-1.41520	4.13395	2.55397
H	-1.38524	2.81984	3.74302
H	-4.06617	-2.55008	1.41524
H	-5.18586	-1.78424	0.26307
H	-3.80589	-2.74969	-0.33130
C	0.38331	-0.79866	-1.79025
H	0.40822	-1.49266	-2.63227
O	1.69778	-0.81960	-1.17126
C	2.46533	-1.91377	-1.35698
C	3.77822	-1.77683	-0.62269
H	4.31679	-0.93018	-1.06350
H	3.56583	-1.50274	0.41512
C	4.62802	-3.03456	-0.69665
H	5.63067	-2.83016	-0.30130
H	4.76219	-3.36981	-1.72839
C	4.06439	-4.17313	0.11512
O	3.24227	-4.06790	1.00306
O	2.15056	-2.86202	-2.04539
O	4.61214	-5.35287	-0.22958
H	4.22912	-6.03674	0.34426

Conformer 7: ΔH° = 0.30 kcal/mol, weight = 6.6%

O	2.72885	-0.57739	1.37882
O	2.68833	-1.96539	0.97008
C	2.94390	-2.05234	-0.41499
C	4.18071	-1.23613	-0.82308
C	3.85971	0.17930	-1.30453
C	3.06997	1.06996	-0.32997
C	1.99304	0.28279	0.46512
C	2.52534	2.33342	-1.03243
C	1.74780	3.20338	-0.04331
C	0.62001	2.43008	0.62761
C	1.14947	1.19871	1.37653
C	1.08944	-0.57409	-0.43490
C	0.08304	0.36462	2.11118
O	0.05819	-1.25696	0.29287
O	1.78694	-1.56325	-1.12231
C	-0.80811	1.17264	3.05300
C	3.63865	3.14586	-1.70039
C	3.05965	-3.53571	-0.70038
H	4.68420	-1.76705	-1.63835
H	4.87129	-1.22658	0.02668
H	3.30449	0.10347	-2.24742
H	4.80602	0.67449	-1.54363
H	3.76222	1.41353	0.45449
H	1.82593	2.01193	-1.82114
H	2.44048	3.59034	0.71894
H	1.33993	4.07754	-0.56573
H	0.09567	3.07749	1.33828
H	-0.12224	2.13776	-0.12358
H	1.84625	1.56718	2.14459
H	0.61821	0.06475	-1.19083
H	0.63571	-0.36178	2.71976
H	-1.45760	1.86944	2.51642
H	-1.44615	0.50782	3.64482
H	-0.19397	1.74998	3.75166
H	3.23259	4.07477	-2.11539
H	4.41340	3.41722	-0.97237
H	4.11993	2.60426	-2.51945

H	3.05791	-3.68838	-1.78239
H	3.99180	-3.92895	-0.28715
H	2.21194	-4.07108	-0.26669
C	-0.72200	-0.51881	1.16802
H	-1.32568	-1.24403	1.71581
O	-1.65335	0.32060	0.40160
C	-2.81171	-0.21276	0.02237
C	-3.65845	0.76153	-0.75775
H	-4.15160	1.41919	-0.02984
H	-2.98828	1.40470	-1.33425
C	-4.68461	0.11463	-1.70139
H	-4.20655	-0.69421	-2.26785
H	-5.01564	0.86323	-2.42261
C	-5.94394	-0.44274	-1.05269
O	-7.06031	-0.09609	-1.38826
O	-3.15443	-1.35724	0.29584
O	-5.77627	-1.36418	-0.10145
H	-4.80896	-1.51656	0.06102

Conformer 8: ΔH° = 0.31 kcal/mol, weight = 6.6%

O	2.71966	-0.45316	1.38890
O	2.57741	-1.87377	1.14825
C	2.64414	-2.12388	-0.23980
C	3.84987	-1.42748	-0.89106
C	3.52400	-0.06004	-1.48995
C	2.91590	0.97388	-0.52854
C	1.91207	0.34299	0.47626
C	2.35477	2.19379	-1.29234
C	1.76113	3.20842	-0.31498
C	0.68530	2.58299	0.56353
C	1.23446	1.40059	1.37435
C	0.86325	-0.55648	-0.19965
C	0.21776	0.71911	2.31288
O	-0.08631	-1.09427	0.72382
O	1.42789	-1.65493	-0.84785
C	-0.51234	1.67835	3.25088
C	3.41443	2.85832	-2.17651
C	2.66373	-3.63390	-0.36502
H	4.22116	-2.07253	-1.69489
H	4.64538	-1.35988	-0.14144
H	2.83942	-0.20707	-2.33407
H	4.44728	0.35195	-1.90940
H	3.72198	1.34822	0.12195
H	1.54238	1.84391	-1.94970
H	2.56652	3.61850	0.31298
H	1.34045	4.05370	-0.87377
H	0.28721	3.33078	1.25774
H	-0.15798	2.26387	-0.05899
H	2.03891	1.79633	2.01312
H	0.32635	0.01900	-0.96280
H	0.80004	0.02582	2.93230
H	-1.18533	2.35176	2.71342
H	-1.10991	1.12099	3.98033
H	0.20666	2.28794	3.80822
H	3.00922	3.76846	-2.63236
H	4.29270	3.14582	-1.58473
H	3.75231	2.20867	-2.98862
H	2.51970	-3.90221	-1.41458
H	3.62392	-4.03026	-0.02518
H	1.85546	-4.07184	0.22512
C	-0.74103	-0.20195	1.56651
H	-1.31456	-0.82251	2.25776
O	-1.68990	0.59521	0.80780
C	-2.90953	0.06290	0.58345
C	-3.77243	1.01181	-0.21541

H	-4.05738	1.83044	0.45636
H	-3.16673	1.45592	-1.00972
C	-5.01886	0.34622	-0.77486
H	-5.70003	1.10296	-1.18210
H	-5.57409	-0.18385	0.00413
C	-4.71465	-0.62133	-1.89032
O	-3.65182	-0.71941	-2.47018
O	-3.27079	-1.01644	1.00355
O	-5.78586	-1.37116	-2.20813
H	-5.53137	-1.95687	-2.94020

Conformer 9: ΔH° = 0.33 kcal/mol, weight = 6.3%

O	2.73347	-0.59366	1.36767
O	2.68409	-1.95981	0.89069
C	2.90709	-1.97780	-0.50275
C	4.13458	-1.14203	-0.89870
C	3.80280	0.29418	-1.30390
C	3.03845	1.13575	-0.26786
C	1.97943	0.31027	0.51391
C	2.47901	2.43222	-0.89339
C	1.72940	3.25401	0.15619
C	0.61507	2.45062	0.81411
C	1.15802	1.18190	1.48771
C	1.05428	-0.50094	-0.40662
C	0.10346	0.31503	2.20309
O	0.03898	-1.21880	0.31072
O	1.73427	-1.45549	-1.15739
C	-0.76965	1.07944	3.19666
C	3.57686	3.27574	-1.54864
C	3.01597	-3.44485	-0.86478
H	4.61962	-1.63281	-1.74953
H	4.84405	-1.17239	-0.06518
H	3.22456	0.26378	-2.23547
H	4.74340	0.80085	-1.54185
H	3.75041	1.44005	0.51506
H	1.75914	2.15051	-1.67876
H	2.44136	3.60009	0.92037
H	1.31255	4.15431	-0.31189
H	0.11067	3.06250	1.56936
H	-0.14594	2.19748	0.06755
H	1.87220	1.51036	2.25778
H	0.56707	0.17577	-1.11797
H	0.66502	-0.43994	2.76716
H	-1.42173	1.80488	2.70322
H	-1.40355	0.38896	3.76298
H	-0.14292	1.61819	3.91463
H	3.16406	4.22827	-1.89830
H	4.37479	3.50253	-0.83043
H	4.02992	2.77916	-2.41111
H	2.98802	-3.54244	-1.95284
H	3.95802	-3.85703	-0.49472
H	2.17909	-4.00291	-0.43880
C	-0.72147	-0.52206	1.23507
H	-1.31671	-1.27053	1.76015
O	-1.66476	0.35419	0.52584
C	-2.83658	-0.15329	0.15165
C	-3.63430	0.81606	-0.68326
H	-3.40094	1.82823	-0.34234
H	-3.24935	0.74833	-1.70942
C	-5.15542	0.60167	-0.64967
H	-5.64310	1.50520	-1.01826
H	-5.48522	0.45440	0.38633
C	-5.69949	-0.54862	-1.48548
O	-6.55945	-0.39044	-2.33080
O	-3.21622	-1.27963	0.45004

O	-5.21187	-1.76529	-1.23301
H	-4.50930	-1.71659	-0.53424

Conformer 10: ΔH° = 0.38 kcal/mol, weight = 5.8%

O	2.67303	-0.51395	1.43138
O	2.85775	-1.82079	0.83619
C	3.20834	-1.67095	-0.52234
C	4.33943	-0.64852	-0.71540
C	3.85145	0.76621	-1.02620
C	2.88570	1.39421	-0.00710
C	1.88249	0.36602	0.58455
C	2.21438	2.66546	-0.57242
C	1.26624	3.27421	0.46155
C	0.21733	2.27252	0.92706
C	0.86427	1.02296	1.54015
C	1.16759	-0.46196	-0.49475
C	-0.12048	-0.04051	2.06269
O	0.19594	-1.37030	0.04581
O	2.03928	-1.24259	-1.24877
C	-1.17404	0.50017	3.02775
C	3.24202	3.70343	-1.03322
C	3.55138	-3.06852	-0.99532
H	4.96287	-0.98521	-1.55087
H	4.96774	-0.67001	0.18122
H	3.37173	0.75558	-2.01256
H	4.73127	1.41059	-1.11843
H	3.47289	1.70692	0.87017
H	1.61508	2.37548	-1.45088
H	1.85185	3.62982	1.32256
H	0.77408	4.15637	0.03386
H	-0.43460	2.73508	1.67566
H	-0.42952	2.00011	0.08570
H	1.45359	1.36069	2.40601
H	0.65995	0.21337	-1.19295
H	0.48840	-0.77221	2.60780
H	-1.87640	1.17877	2.53651
H	-1.75130	-0.31946	3.46853
H	-0.69281	1.04378	3.84719
H	2.73616	4.62124	-1.35227
H	3.92390	3.96674	-0.21480
H	3.84488	3.35205	-1.87515
H	3.63971	-3.06116	-2.08448
H	4.50178	-3.39164	-0.56329
H	2.76209	-3.76719	-0.70934
C	-0.73413	-0.86925	0.94229
H	-1.27314	-1.73416	1.33140
O	-1.71095	-0.04708	0.21432
C	-2.80675	-0.63510	-0.25853
C	-3.70118	0.33807	-0.98552
H	-4.22240	0.93415	-0.22517
H	-3.06050	1.04136	-1.52495
C	-4.69580	-0.30105	-1.96623
H	-4.17637	-1.03971	-2.58912
H	-5.07571	0.47546	-2.63171
C	-5.91510	-0.97259	-1.35003
O	-7.05304	-0.65220	-1.63495
O	-3.06322	-1.82318	-0.10154
O	-5.68521	-1.96580	-0.48759
H	-4.70947	-2.07833	-0.34953

Conformer 11: ΔH° = 0.39 kcal/mol, weight = 5.8%

O	-2.26491	-0.60743	-1.57288
O	-2.49427	-1.96128	-1.11563
C	-2.89540	-1.93440	0.23687
C	-4.01209	-0.90729	0.48297

C	-3.50862	0.45939	0.94735
C	-2.48523	1.15831	0.03483
C	-1.48611	0.16455	-0.61845
C	-1.80451	2.34310	0.75374
C	-0.78746	3.01904	-0.16867
C	0.24803	2.03187	-0.69337
C	-0.41451	0.88162	-1.46506
C	-0.83064	-0.77982	0.40115
C	0.54923	-0.15762	-2.06606
O	0.13943	-1.65951	-0.18827
O	-1.74823	-1.60561	1.04513
C	1.64588	0.43771	-2.94751
C	-2.82094	3.36646	1.26929
C	-3.28672	-3.36191	0.55948
H	-4.67623	-1.30646	1.25744
H	-4.60350	-0.82837	-0.43511
H	-3.07223	0.34258	1.94699
H	-4.37824	1.11348	1.06575
H	-3.02619	1.57601	-0.82844
H	-1.25888	1.94724	1.62549
H	-1.31940	3.48473	-1.01165
H	-0.28628	3.83202	0.37105
H	0.95086	2.54579	-1.35739
H	0.84243	1.64635	0.14277
H	-0.95906	1.33266	-2.30840
H	-0.33569	-0.18600	1.17817
H	-0.06808	-0.80871	-2.69742
H	2.35180	1.04804	-2.37809
H	2.21365	-0.35500	-3.44617
H	1.20383	1.06704	-3.72671
H	-2.30257	4.23201	1.69606
H	-3.45760	3.72949	0.45282
H	-3.47005	2.95707	2.04805
H	-3.41335	-3.45788	1.64065
H	-4.22845	-3.61621	0.06682
H	-2.50449	-4.05100	0.23306
C	1.10386	-1.11572	-1.02100
H	1.61184	-1.96231	-1.48476
O	2.10562	-0.41273	-0.20649
C	3.19841	-1.07474	0.16449
C	4.13731	-0.21135	0.96894
H	4.64798	0.45775	0.26410
H	3.53212	0.43755	1.60824
C	5.14741	-0.98154	1.83209
H	4.63213	-1.78204	2.37723
H	5.56419	-0.29907	2.57409
C	6.33306	-1.59250	1.09857
O	7.48554	-1.32481	1.37911
O	3.42232	-2.24202	-0.13471
O	6.05710	-2.47221	0.13210
H	5.07601	-2.55642	0.01745

Conformer 12: ΔH° = 0.44 kcal/mol, weight = 5.3%

O	-2.76350	0.41114	1.33653
O	-2.60047	1.84812	1.28422
C	-2.73132	2.28444	-0.05144
C	-3.97694	1.69177	-0.72984
C	-3.70430	0.41149	-1.52003
C	-3.05632	-0.74779	-0.74342
C	-2.00636	-0.26220	0.29351
C	-2.52755	-1.84303	-1.69536
C	-1.88847	-2.98294	-0.89957
C	-0.78025	-2.48385	0.01879
C	-1.30228	-1.43381	1.00911
C	-0.97760	0.70817	-0.30756

C	-0.25828	-0.88496	1.99989
O	0.03116	1.11146	0.63218
O	-1.55067	1.88668	-0.77648
C	0.49613	-1.96229	2.77706
C	-3.62425	-2.38492	-2.61713
C	-2.72979	3.79729	0.02739
H	-4.37533	2.44116	-1.42247
H	-4.73672	1.53435	0.04280
H	-3.06767	0.66591	-2.37638
H	-4.65607	0.06645	-1.93605
H	-3.83201	-1.21553	-0.11758
H	-1.74722	-1.39551	-2.33209
H	-2.66538	-3.48637	-0.30472
H	-1.48882	-3.73466	-1.59128
H	-0.35801	-3.32340	0.58104
H	0.03946	-2.07455	-0.58166
H	-2.08363	-1.92132	1.61142
H	-0.48471	0.23186	-1.16279
H	-0.81814	-0.28154	2.72506
H	1.14173	-2.56368	2.13149
H	1.12349	-1.51098	3.55299
H	-0.21027	-2.63573	3.27310
H	-3.23739	-3.21515	-3.21792
H	-4.47242	-2.76383	-2.03315
H	-4.00218	-1.62801	-3.30990
H	-2.62550	4.20368	-0.98158
H	-3.66766	4.15446	0.45989
H	-1.89056	4.14295	0.63528
C	0.68089	0.12709	1.35774
H	1.28163	0.64803	2.10427
O	1.61851	-0.58028	0.47150
C	2.88388	-0.17389	0.42644
C	3.68035	-0.90463	-0.62473
H	3.24637	-1.89982	-0.75040
H	3.51297	-0.38014	-1.57501
C	5.18238	-1.03483	-0.32535
H	5.59615	-1.82261	-0.95647
H	5.32660	-1.34648	0.71684
C	6.03923	0.20027	-0.56806
O	7.03004	0.17629	-1.27309
O	3.34578	0.69783	1.15448
O	5.67664	1.32335	0.05483
H	4.84433	1.17710	0.57586

Conformer 13: ΔH° = 0.47 kcal/mol, weight = 5.0%

O	2.70150	-0.39074	1.40228
O	2.84974	-1.71368	0.83369
C	3.12481	-1.60074	-0.54620
C	4.24818	-0.58895	-0.82583
C	3.74919	0.82093	-1.14361
C	2.83867	1.47822	-0.09197
C	1.86631	0.46895	0.57717
C	2.14085	2.73624	-0.65537
C	1.24391	3.37204	0.40832
C	0.22165	2.38330	0.95415
C	0.90118	1.15200	1.56951
C	1.09062	-0.38378	-0.44003
C	-0.05207	0.10308	2.17190
O	0.15278	-1.27272	0.17400
O	1.92221	-1.18698	-1.22013
C	-1.04449	0.66930	3.18561
C	3.14510	3.76049	-1.19236
C	3.43841	-3.01230	-0.99893
H	4.82268	-0.94862	-1.68658
H	4.92567	-0.59303	0.03455

H	3.21946	0.78915	-2.10358
H	4.62554	1.45866	-1.29678
H	3.47151	1.81255	0.74492
H	1.49950	2.42531	-1.49592
H	1.87120	3.75236	1.22855
H	0.72922	4.24165	-0.01899
H	-0.39262	2.86730	1.72097
H	-0.46619	2.08628	0.15465
H	1.53600	1.51425	2.39268
H	0.55203	0.27637	-1.12968
H	0.58766	-0.61647	2.69727
H	-1.77428	1.33795	2.72113
H	-1.59626	-0.13876	3.67769
H	-0.51565	1.23051	3.96309
H	2.62458	4.67002	-1.51182
H	3.86551	4.04450	-0.41498
H	3.70656	3.38539	-2.05253
H	3.46759	-3.03468	-2.09106
H	4.40953	-3.32861	-0.60985
H	2.66292	-3.69949	-0.65312
C	-0.73619	-0.74474	1.10580
H	-1.24313	-1.60429	1.54742
O	-1.74558	0.04723	0.42144
C	-2.93480	-0.53036	0.15412
C	-3.83528	0.42422	-0.59344
H	-3.92989	1.33675	0.00480
H	-3.32821	0.71236	-1.52025
C	-5.20633	-0.16450	-0.88302
H	-5.86869	0.61877	-1.27248
H	-5.67920	-0.55169	0.02295
C	-5.17254	-1.25477	-1.92372
O	-4.30255	-1.40656	-2.75772
O	-3.24282	-1.65502	0.49037
O	-6.26319	-2.04040	-1.86255
H	-6.19600	-2.69697	-2.57535

Conformer 14: ΔH° = 1.16 kcal/mol, weight = 1.6%

O	2.61736	-0.40627	1.47686
O	2.87465	-1.71955	0.92377
C	3.27550	-1.59153	-0.42323
C	4.37935	-0.53602	-0.59582
C	3.85659	0.85118	-0.96552
C	2.83025	1.47064	-0.00248
C	1.83565	0.42411	0.57389
C	2.14445	2.70571	-0.62705
C	1.13431	3.30747	0.35011
C	0.09756	2.28301	0.79277
C	0.75427	1.07055	1.46673
C	1.19312	-0.45750	-0.51001
C	-0.22364	-0.01026	1.96963
O	0.23938	-1.38510	0.01588
O	2.12613	-1.22364	-1.20849
C	-1.33729	0.52289	2.86917
C	3.15763	3.76576	-1.06979
C	3.68840	-2.98761	-0.84297
H	5.04954	-0.87232	-1.39449
H	4.96837	-0.51180	0.32702
H	3.41560	0.79679	-1.96832
H	4.71643	1.52414	-1.04216
H	3.37060	1.82358	0.88971
H	1.59271	2.37589	-1.52223
H	1.67140	3.69939	1.22706
H	0.63498	4.16460	-0.11856
H	-0.60360	2.74109	1.49846
H	-0.49952	1.96616	-0.06935

H	1.29247	1.44777	2.34968
H	0.69329	0.18286	-1.24647
H	0.37922	-0.70910	2.56260
H	-2.03450	1.16653	2.32635
H	-1.91208	-0.30362	3.30055
H	-0.91348	1.09992	3.69778
H	2.63672	4.65998	-1.42931
H	3.79713	4.06846	-0.23091
H	3.80507	3.41616	-1.87870
H	3.82331	-3.00506	-1.92729
H	4.63045	-3.26373	-0.36274
H	2.91314	-3.70744	-0.57142
C	-0.76287	-0.88185	0.84102
H	-1.28809	-1.75599	1.22972
O	-1.71360	-0.12111	0.04748
C	-2.74499	-0.79166	-0.50784
C	-3.57609	0.12551	-1.37242
H	-3.86121	0.99766	-0.77613
H	-2.92887	0.50280	-2.17256
C	-4.79160	-0.56379	-1.97786
H	-4.50185	-1.41948	-2.59147
H	-5.30672	0.14099	-2.64267
C	-5.83043	-1.05635	-1.00130
O	-6.61170	-1.95837	-1.22705
O	-2.96964	-1.97076	-0.33156
O	-5.85350	-0.35295	0.14731
H	-6.55926	-0.72157	0.70360

Conformer 15: ΔH° = 1.22 kcal/mol, weight = 1.4%

O	-1.74449	1.80794	-1.31230
O	-2.89712	0.95617	-1.51847
C	-3.47778	0.64361	-0.27077
C	-3.68208	1.89610	0.59666
C	-2.53510	2.16801	1.56943
C	-1.13381	2.30837	0.95133
C	-0.89625	1.32951	-0.23130
C	-0.03185	2.25820	2.03320
C	1.35110	2.40239	1.39621
C	1.59655	1.34691	0.32583
C	0.54135	1.41566	-0.78768
C	-1.26476	-0.12430	0.10809
C	0.71991	0.39586	-1.92925
O	-0.99824	-1.03325	-0.96349
O	-2.61573	-0.28327	0.41565
C	2.10977	0.40103	-2.56304
C	-0.23635	3.32259	3.11513
C	-4.75978	-0.09030	-0.60822
H	-4.59941	1.76000	1.17981
H	-3.85203	2.74531	-0.07351
H	-2.51705	1.36285	2.31414
H	-2.77078	3.08686	2.11567
H	-1.06968	3.29950	0.47550
H	-0.07725	1.27132	2.52167
H	1.44264	3.40739	0.95744
H	2.12229	2.33062	2.17326
H	1.60835	0.35166	0.78387
H	2.58726	1.48982	-0.11851
H	0.61915	2.41570	-1.24091
H	-0.70042	-0.44367	0.99230
H	-0.00024	0.68524	-2.70453
H	2.88125	0.04884	-1.87319
H	2.13185	-0.24509	-3.44723
H	2.37642	1.41286	-2.88598
H	0.60385	3.31355	3.81815
H	-0.28776	4.32459	2.67092

H	-1.14965	3.16233	3.69461
H	-5.16270	-0.53492	0.30513
H	-5.49640	0.60337	-1.02128
H	-4.55958	-0.88602	-1.32947
C	0.26926	-1.00691	-1.53878
H	0.20714	-1.65982	-2.41109
O	1.23390	-1.59639	-0.62532
C	1.44731	-2.92605	-0.71242
C	2.40739	-3.38618	0.35768
H	3.28955	-2.73951	0.33320
H	1.92781	-3.21045	1.32780
C	2.78086	-4.85715	0.22952
H	1.89983	-5.49982	0.28646
H	3.42968	-5.13556	1.06941
C	3.52487	-5.24545	-1.02392
O	3.53452	-6.36360	-1.49783
O	0.93567	-3.64972	-1.54108
O	4.23894	-4.23245	-1.55203
H	4.69790	-4.57439	-2.33685

Conformer 16: ΔH° = 1.23 kcal/mol, weight = 1.4%

O	2.68101	-0.45287	1.42241
O	2.53931	-1.87457	1.18677
C	2.65047	-2.13531	-0.19602
C	3.87995	-1.44913	-0.81239
C	3.58065	-0.08460	-1.43121
C	2.94571	0.95918	-0.49840
C	1.90754	0.34064	0.47869
C	2.41509	2.17526	-1.28971
C	1.79257	3.20014	-0.34153
C	0.68747	2.58567	0.50815
C	1.20572	1.40847	1.34592
C	0.87656	-0.55960	-0.22314
C	0.15632	0.73877	2.25708
O	-0.10356	-1.08722	0.67378
O	1.45616	-1.66435	-0.84701
C	-0.60083	1.70882	3.16187
C	3.50600	2.82891	-2.14363
C	2.66675	-3.64615	-0.31031
H	4.27456	-2.10155	-1.59896
H	4.65069	-1.37989	-0.03753
H	2.92413	-0.23477	-2.29680
H	4.51962	0.31969	-1.82227
H	3.73168	1.33543	0.17517
H	1.62383	1.82338	-1.97155
H	2.57815	3.61514	0.30788
H	1.39189	4.04075	-0.92161
H	0.27084	3.34097	1.18304
H	-0.13748	2.26485	-0.13786
H	1.99054	1.80670	2.00719
H	0.36644	0.01321	-1.00663
H	0.71562	0.04952	2.90160
H	-1.25217	2.38071	2.59657
H	-1.22519	1.15995	3.87509
H	0.10170	2.31978	3.73822
H	3.11971	3.73703	-2.61947
H	4.36549	3.11772	-1.52560
H	3.86790	2.17162	-2.93906
H	2.55647	-3.92099	-1.36227
H	3.61348	-4.04421	0.06348
H	1.83781	-4.07682	0.25596
C	-0.78109	-0.18596	1.48899
H	-1.37788	-0.79866	2.16724
O	-1.70313	0.60435	0.69092
C	-2.92035	0.07601	0.44292

C	-3.72901	0.98565	-0.45062
H	-3.89750	1.92162	0.09490
H	-3.11937	1.24639	-1.32072
C	-5.06578	0.38201	-0.86138
H	-5.62310	1.11815	-1.45416
H	-5.68330	0.14654	0.00796
C	-4.99624	-0.86987	-1.70119
O	-5.88047	-1.69960	-1.77055
O	-3.31271	-0.97924	0.89466
O	-3.86424	-0.95888	-2.42476
H	-3.90655	-1.78140	-2.93973

Conformer 17: ΔH° = 1.25 kcal/mol, weight = 1.3%

O	-2.17431	-0.20075	-1.81519
O	-2.45749	-1.60387	-1.60072
C	-2.80159	-1.81127	-0.24771
C	-3.85624	-0.80338	0.23760
C	-3.26537	0.42926	0.92153
C	-2.25854	1.24690	0.09641
C	-1.32710	0.35400	-0.77008
C	-1.50089	2.26867	0.97163
C	-0.52448	3.07919	0.11903
C	0.45932	2.18137	-0.61945
C	-0.26025	1.17445	-1.52826
C	-0.67771	-0.78911	0.02952
C	0.66897	0.22828	-2.31605
O	0.22630	-1.57536	-0.75112
O	-1.61032	-1.68552	0.55083
C	1.76494	0.93974	-3.10748
C	-2.45316	3.19983	1.72815
C	-3.25099	-3.25660	-0.17571
H	-4.50802	-1.31324	0.95539
H	-4.47840	-0.52793	-0.62044
H	-2.78683	0.10950	1.85506
H	-4.09588	1.08193	1.20896
H	-2.82353	1.82497	-0.65144
H	-0.91326	1.71063	1.71847
H	-1.09314	3.68602	-0.60175
H	0.02265	3.78431	0.75701
H	1.13139	2.79181	-1.23204
H	1.09509	1.65866	0.10307
H	-0.82208	1.75948	-2.27226
H	-0.13204	-0.36883	0.88289
H	0.02734	-0.29670	-3.03452
H	2.50387	1.41646	-2.45786
H	2.29556	0.22946	-3.75067
H	1.33076	1.71065	-3.75256
H	-1.88504	3.96705	2.26545
H	-3.13050	3.71296	1.03379
H	-3.06338	2.66961	2.46467
H	-3.34300	-3.54604	0.87402
H	-4.22156	-3.37544	-0.66391
H	-2.51639	-3.90565	-0.65780
C	1.22075	-0.89905	-1.45126
H	1.72117	-1.65826	-2.05531
O	2.20140	-0.36265	-0.52219
C	3.19356	-1.18154	-0.11434
C	4.08229	-0.48615	0.88972
H	4.58579	0.33696	0.36876
H	3.44891	-0.02180	1.65104
C	5.12106	-1.41126	1.50976
H	5.77193	-0.82623	2.17153
H	5.76610	-1.85618	0.74908
C	4.58213	-2.54643	2.34527
O	5.18795	-3.57274	2.57922

O	3.35616	-2.31360	-0.51848
O	3.36519	-2.29219	2.86214
H	3.10067	-3.06413	3.38912

Conformer 18: ΔH° = 1.27 kcal/mol, weight = 1.3%

O	2.59216	-0.06434	-1.50407
O	2.37003	1.30127	-1.92932
C	2.48261	2.16246	-0.81689
C	3.75452	1.88252	0.00033
C	3.53804	0.93012	1.17605
C	2.94665	-0.44776	0.83710
C	1.87005	-0.38150	-0.28173
C	2.47975	-1.19084	2.10877
C	1.90429	-2.56018	1.74646
C	0.76529	-2.44502	0.74198
C	1.21949	-1.75523	-0.55214
C	0.79878	0.69071	-0.02216
C	0.13465	-1.61370	-1.63712
O	-0.22378	0.71368	-1.02313
O	1.32293	1.98270	0.01747
C	-0.57200	-2.92049	-1.99169
C	3.60410	-1.33593	3.13865
C	2.41722	3.56088	-1.39646
H	4.12013	2.83615	0.39666
H	4.51980	1.50720	-0.68714
H	2.88745	1.42757	1.90582
H	4.50282	0.78495	1.67216
H	3.74334	-1.05889	0.38492
H	1.67497	-0.59935	2.57484
H	2.70618	-3.19073	1.33361
H	1.54977	-3.06186	2.65549
H	0.38326	-3.44156	0.49597
H	-0.07018	-1.90028	1.19535
H	2.01945	-2.37659	-0.98306
H	0.33241	0.50853	0.95315
H	0.65347	-1.26032	-2.53673
H	-1.18586	-3.29535	-1.16835
H	-1.22545	-2.78178	-2.85959
H	0.16124	-3.69211	-2.24883
H	3.26170	-1.93449	3.98987
H	4.47139	-1.84595	2.70086
H	3.94108	-0.37243	3.53097
H	2.29968	4.27698	-0.57943
H	3.33782	3.78850	-1.93967
H	1.56212	3.65058	-2.07019
C	-0.85028	-0.48985	-1.33491
H	-1.48589	-0.27511	-2.19570
O	-1.72099	-0.88245	-0.23882
C	-3.01121	-0.49016	-0.28408
C	-3.73972	-0.90130	0.97274
H	-3.63606	-1.98637	1.08421
H	-3.21791	-0.45709	1.82646
C	-5.21418	-0.51923	0.95973
H	-5.68667	-0.89577	1.87574
H	-5.74024	-0.98020	0.12125
C	-5.51346	0.95851	0.90705
O	-6.52635	1.43820	0.43896
O	-3.51608	0.10222	-1.21488
O	-4.56257	1.70991	1.49374
H	-4.83834	2.63886	1.42814

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