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Supporting Information

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Structural Discrimination in Small Molecules by Accurate Measurement of Long-Range Proton–Carbon NMR Residual Dipolar Couplings**

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Experimental Procedures

Materials

The sample of 10-epi-8-deoxycumambrin B (**1**) was reisolated from *Stevia yaconensis var. subeglandulosa*[1] by Dr. Viviana E. Nicotra from Córdoba National University, Córdoba, Argentina.

NMR experiments

All NMR experiments were carried out at 298 K on a Bruker Avance III NMR spectrometer operating at 747.33 MHz ^{1}H frequency and equipped with a triple resonance room temperature TXI probehead, containing a three-axis pulsed field gradient accessory. Spectra were acquired as a 512* (^{13}C) × 800* (^{1}H) data matrices, where N* refers to N complex pairs, with acquisition time of 22.5 ms (^{13}C) and 89.2 ms (^{1}H), using 4 transients per FID and a 1.5 s delay between scans. The total measurement time was approximately 1.8 h per spectrum.

Alignment of Compound 1 Using Reversible Compression / Relaxation of PMMA Gels

A 25 mm length PMMA gel was swollen and washed in $CDCl_3$ following the protocol of Gil and coworkers.[2] The maximum ^{2}H quadrupolar splitting achievable for $CDCl_3$with this gel was about 27 Hz. Compound **1** (3 mg) was dissolved in $CDCl_3$ (200 μL), and added to the NMR tube containing the clean and fully relaxed swollen PMMA gel stick. The Shigemi plunger was subsequently inserted and the gel was compressed and relaxed several times by gently pumping it with the Shigemi plunger. Once the gel was equilibrated with the compound **1** solution, the gel was compressed to its maximum extent, and the tube was sealed with Teflon tape for holding the position of the plunger and avoiding solvent evaporation. [2] In the current work, all anisotropic NMR measurements were conducted with the gel fully compressed, resulting in a $CDCl_3$ ^{2}H quadrupolar splitting of 27 Hz.

A separate sample of 3 mg of **1** in 500 μL of $CDCl_3$ was prepared to collect the NMR data in isotropic conditions.

Computational details

The conformational space of the different configurations was explored by means of molecular mechanics using the MM3 force field[3] and the mixed torsional/low-mode sampling algorithm[4] as implemented in MacroModel. All conformers in the resulting ensembles were then minimized at the DFT level using the OPBE functional[5-6] and the 6-31G* basis set using the Gaussian09 program,[7] retaining only conformers with a relative energy below 2 kcal/mol. Twelve configurations yielded a single dominant conformation; the configurations *RSSSR*, *RSSSS* and *SRRSS* were found to have a nearly 1:1 ratio mixture of two conformers (<0.2 kcal/mol relative energy difference), and configuration *SRSSR* showed three conformers with a population ratio of ca. 6.5:2.0:1.5 based on the DFT energy differences.

Fitting RDCs to Structure Using Singular Value Decomposition (SVD)[8]

Alignment tensor determination, back computation of RDC values, and calculation of quality factors *Q* were conducted using an in-house modified version of the MSpin software suite (MestReLab research).[9] The goodness of fit between experimental and back-computed RDCs was expressed in terms of the Cornilescu quality factor *Q*.[10] To have comparable weights in the fitting process when using both one-bond and long-range couplings, experimental and computed long range RDCs were scaled by r_{CH}^3, where r_{CH} is the distance between the coupled nuclei.
Ensembles in which a single structure represented more than the 90% of population according to the computed DFT energies the SVD fit was performed was done using only the basal conformation. The configurations *RSSSR, RSSSS* and *SRRSS* were found to have a nearly 1:1 ratio mixture of two conformers (<0.2 kcal/mol relative energy difference) and populations were kept fixed at 1:1 ratio in the SVD fitting. For the configuration *SRSSR* three conformers with a population ratio of ca. 6.5:2.0:1.5 based on the computed ΔE DFT energy difference were employed in the fit. In all these multiconformational cases the single tensor approximation was used by visually superimposing conformations in order to minimize global rotational movement.[11-12]

Table S1. Experimental *J* couplings, total splittings (*T*), RDCs (*D*), and standard errors.[a]

Spins Pair	*J (Hz)*	*T=J+D (Hz)*	*D (Hz)*	Exp. Error
C1-H1	127.4	120.0	-7.5	1.0
C3-H3	159.3	171.3	12.0	0.6
C5-H5	129.5	103.2	-26.3	1.1
C6-H6	153.9	121.1	-32.8	0.8
C7-H7	127.6	100.8	-26.9	1.5
C13-H13a	163.1	186.5	23.4	0.3
C13-H13b	160.2	164.6	4.4	0.3
H13a-H13b	≤2; ≥-2	11.0	11.0	2
H2α-C1	≤0.5; ≥-0.5	1.9	1.9	0.5
H2α-C3	-5.99	-4.46	1.53	0.05
H3-C1	6.88	7.16	0.28	0.09
H3-C2	7.82	8.24	0.42	0.05
H3-C5	8.96	9.29	0.33	0.03
H3-C15	3.80	4.11	0.31	0.01
H5-C1	-2.86	-4.41	-1.55	0.12
H5-C2	-	-	0.1[b]	0.1
H5-C3	4.47	4.41	-0.06	0.03
H5-C6	-7.77	-8.99	-1.22	0.03
H5-C7	3.80	4.22	0.42	0.14
H5-C15	-	-	0.9[c]	0.5
H6-C5	-0.6	-1.6	-1.0	0.2
H6-C8	2.74	3.36	0.62	0.07
H13b-C7	3.71	4.85	1.14	0.08

Methylene Sum Splittings

Methylene Group	Isotropic Sum Splitting (Hz)[d]	Anisotropic Sum Splitting (Hz)[d]	Difference (Hz)	Exp. Error
C2-H2	258.5	250.9	-7.6	0.8
C8-H8	254.6	241.7	-12.9	1.2
C9-H9	248.3	222.1	-26.2	2.1

Methyl Splittings

Methyl Group	Isotropic Splitting (Hz)	Anisotropic Splitting (Hz)	Average RDC (Hz)	Exp. Error
C14H14	125.7	120.2	-5.5	0.3
C15H15	125.8	126.9	1.1	0.4

[a]Standard errors determined by LW/SN, where LW is the line width (down scaled by κ=20 for ${}^{n}D_{CH}$) and SN is the signal-to-noise ratio in the weaker of the two 2D spectra (usually the one acquired for the aligned sample).[13]
[b]Average value from the cross-peaks C2-H2α and C2-H2β and has much larger error than for most other couplings.
[c]This RDC was measured manually and has a much larger error than for most other couplings (See Figure S4).
[d] Methylene sum splitting is defined as ${}^{1}J_{CHa}+{}^{1}J_{CHb}$ (or ${}^{1}T_{CHa}+{}^{1}T_{CHb}$).

Table S2. Cornilescu Quality factors (*Q*) obtained from the SVD fittings of RDC data to each of the possible configurational isomers of compound **1,** evaluating the impact of long-range (LR) RDCs in two different scenarios, as well as discrimination using only LR RDCs.

Isomer	Scenario #1 No LR RDCs	Scenario #1 With LR RDCs	Scenario #2 No LR RDCs	Scenario #2 With LR RDCs	LR RDCs only
RRRSR	0.482	0.763	0.623	0.805	0.259
RRRSS	0.347	0.576	0.424	0.560	0.270
RRSSR	0.099	0.128	0.155	0.178	0.149
RSRSR	0.242	0.360	0.327	0.435	0.249
RRSSS 10-Epi	**0.039**	**0.060**	**0.078**	**0.085**	**0.084**
RSRSS	0.270	0.391	0.293	0.412	0.219
RSSSR	0.246	0.392	0.330	0.453	0.306
RSSSS	0.205	0.381	0.252	0.405	0.250
SRRSR	0.532	0.703	0.622	0.774	0.239
SRRSS	0.307	0.636	0.344	0.640	0.234
SRSSR	0.237	0.335	0.259	0.352	0.156
SRSSS	0.057	0.228	0.146	0.278	0.124
SSRSR	0.166	0.439	0.192	0.437	0.303
SSRSS	0.135	0.661	0.232	0.654	0.291
SSSSR	0.506	0.813	0.614	0.824	0.409
SSSSS	0.507	0.822	0.556	0.819	0.495

Scenario #1: RDCs from C1H1, C3H3, C5H5, C6H6, C7H7, C13Ha, C13Hb and H13aH13b.
Scenario #2: RDCs from C1H1, C3H3, C5H5, C6H6, C7H7, C13Ha, C13Hb and H13aH13b, the CH_2 Sum Splitting of C2H2, C8H8, C9H9, and the average $^1D_{CH}$ of methyl groups 14 and 15.
The fit to CH_2 sums and average methyls $^1D_{CH}$ is currently implemented in the development version of MSpin. The SVD fits include the individual error of each RDC.

Annotated ^{1}H NMR Spectra of 10-Epi (1) in Isotropic Solution ($CDCl_3$)

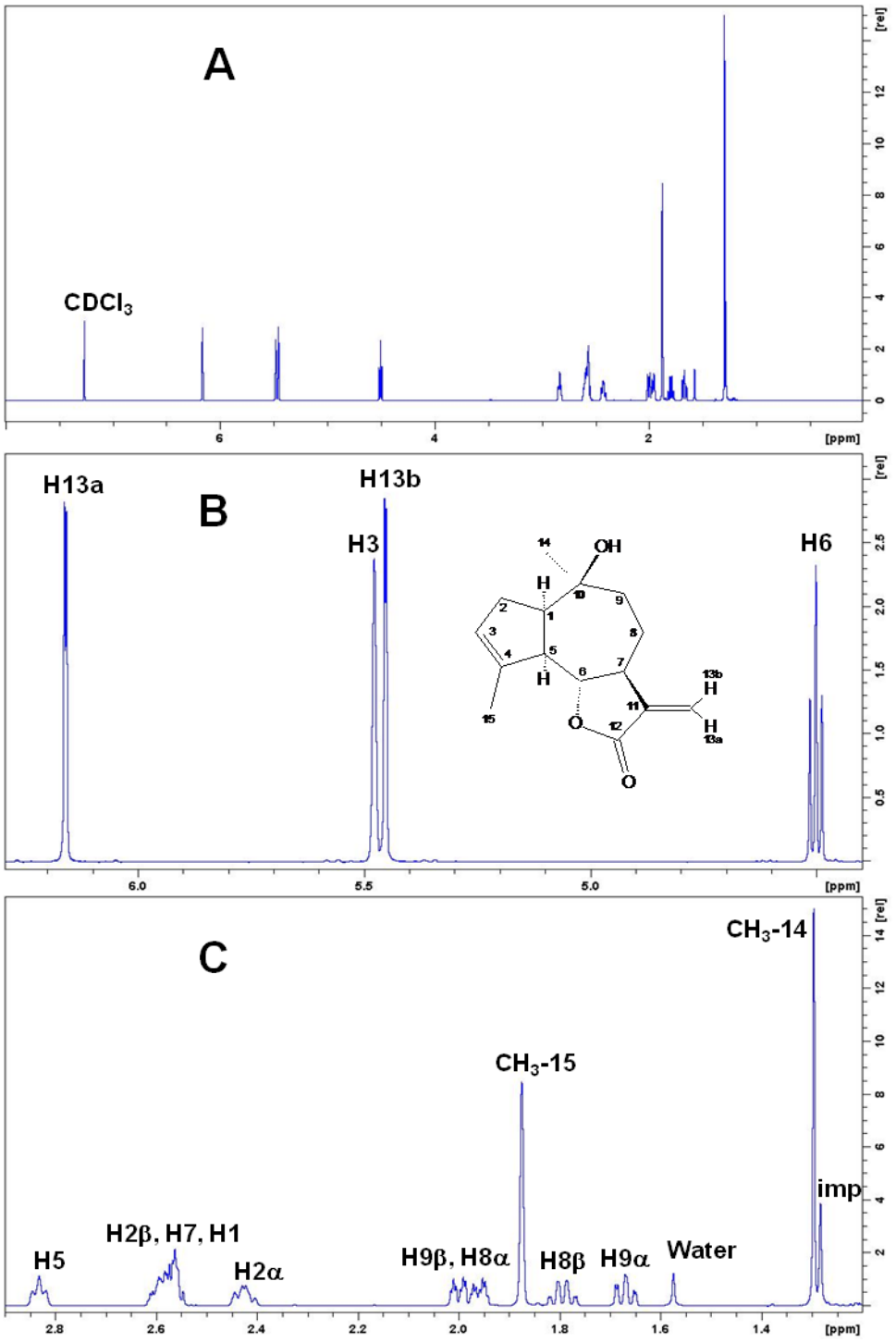

Figure S1. 1D ^{1}H NMR spectrum of 10-Epi (750MHz, $CDCl_3$). Full spectrum (**A**), 6.3-4.4 ppm expansion (**B**), and 2.9-1.2 ppm expansion (**C**).

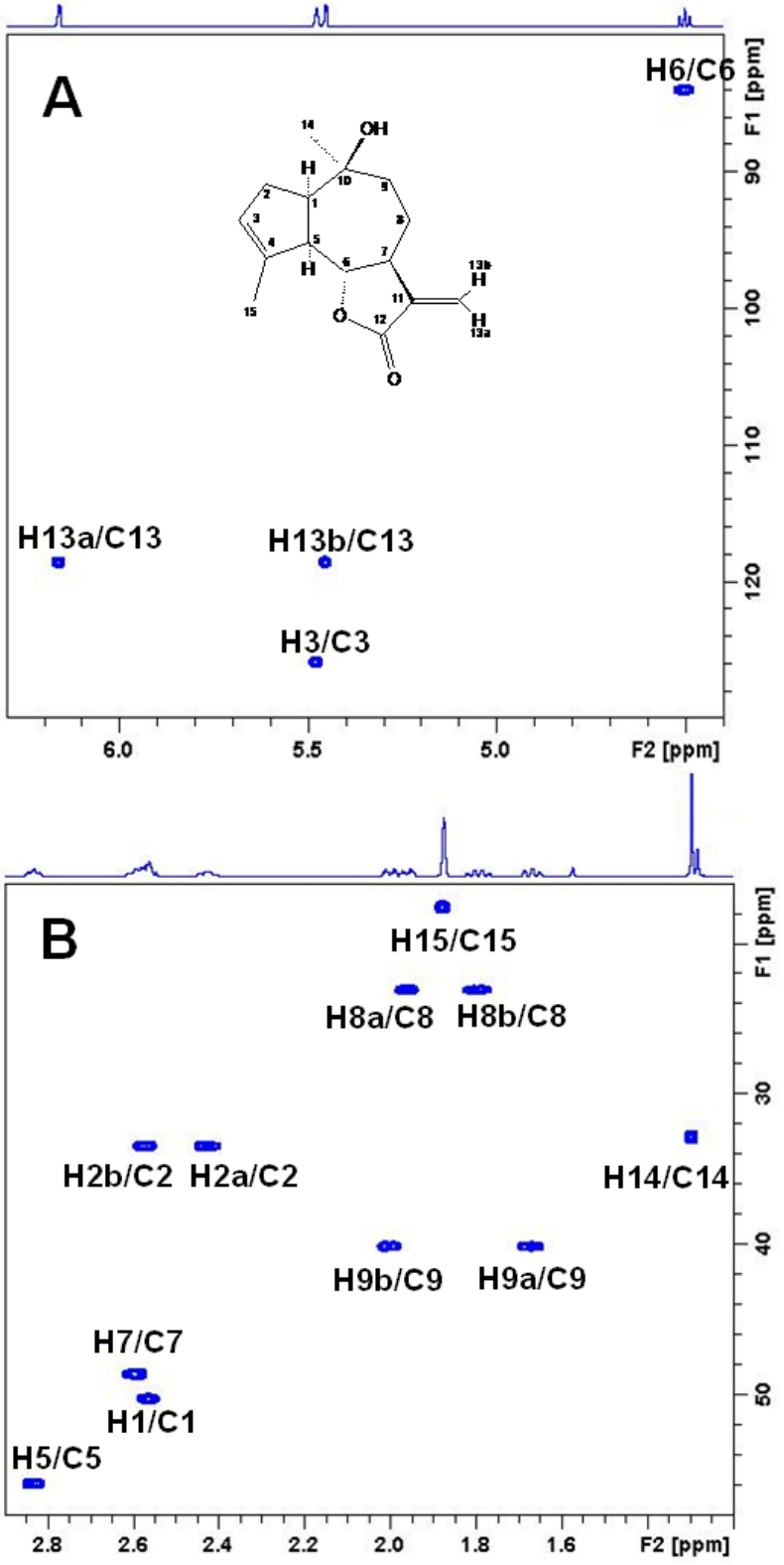

Figure S2. Two expansions of the standard $^{1}H,^{13}C$-HSQC spectrum of 10-Epi (750MHz, $CDCl_3$).

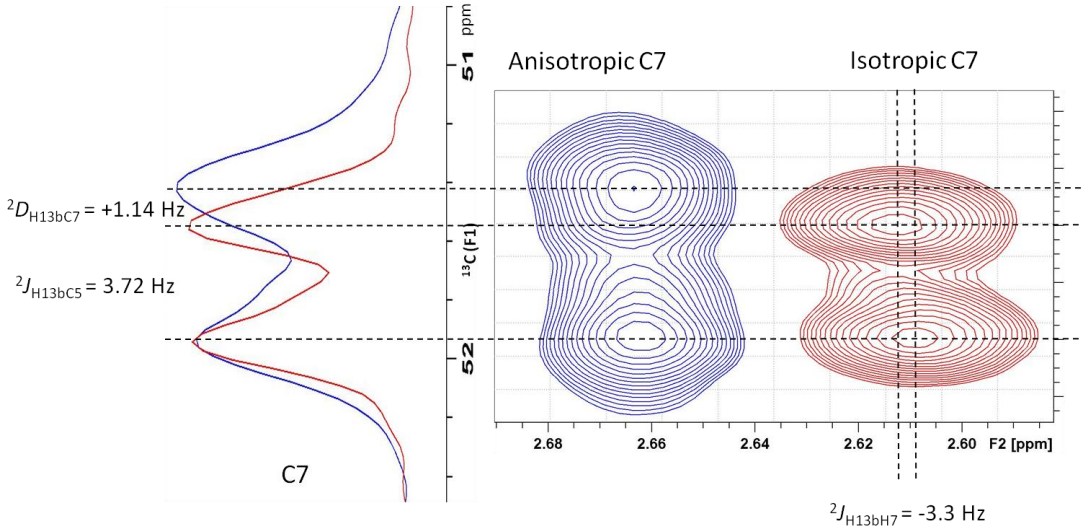

Figure S3. Extraction of long-range CH couplings ($^nJ_{CH}$ and $^nD_{CH}$) from the experimental data collected with the SJS-HSQC experiment. Expanded regions showing the C7-H7 cross-peak in the SJS-HSQC spectrum where H13b is selectively inverted, with the isotropic spectrum shown in red, and the anisotropic spectrum in blue, with F1 slices shown to the left of the figure.

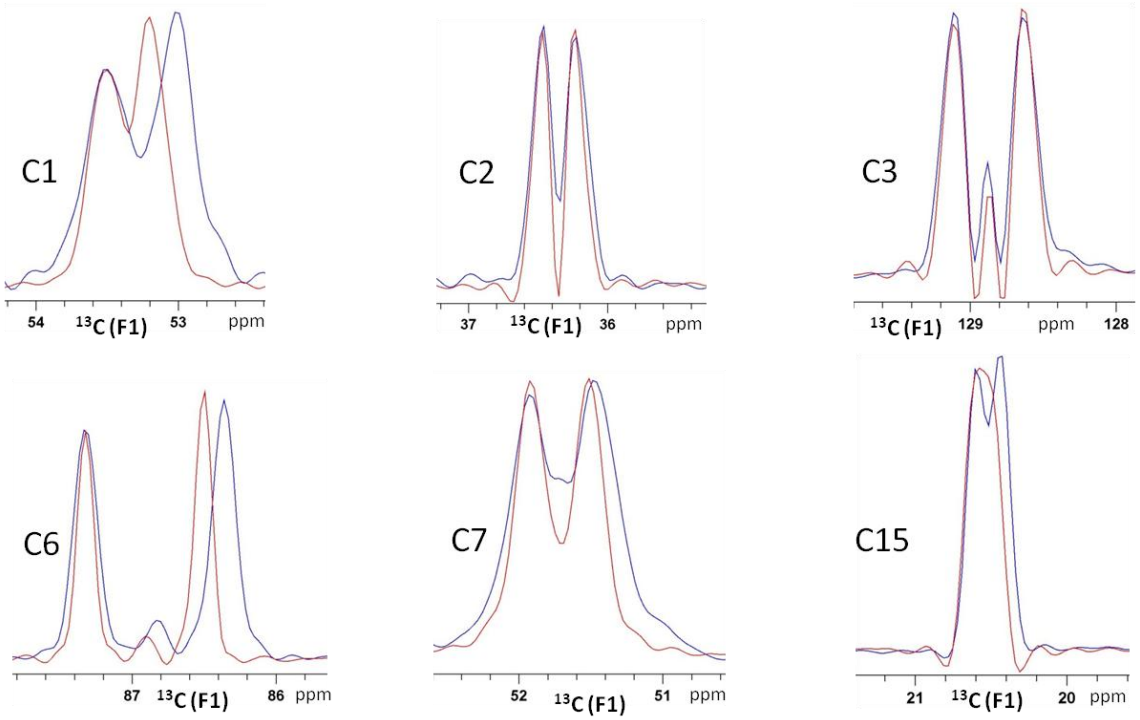

Figure S4. F1 slices upon selective inversion of H5. Isotropic spectrum (red), anisotropic spectrum (blue).

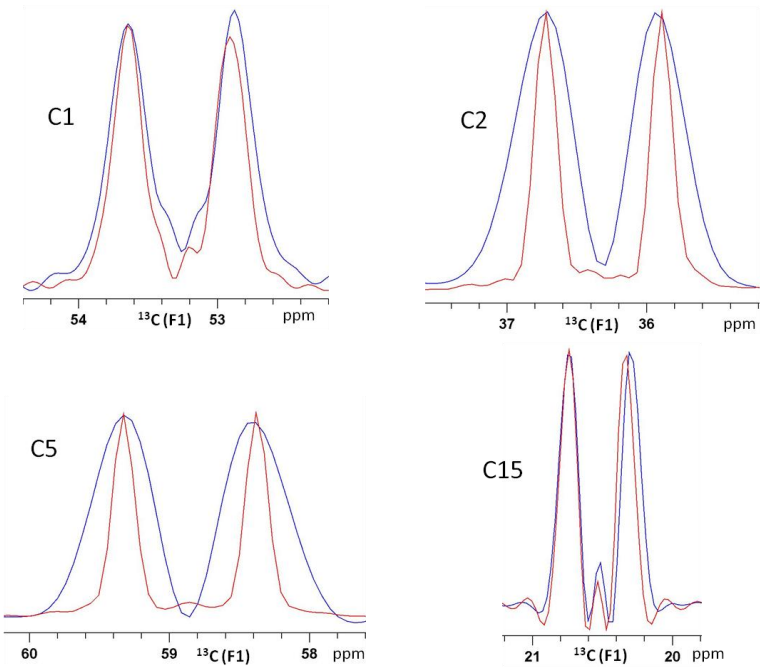

Figure S5. F1 slices upon selective inversion of H3. Isotropic spectrum (red), anisotropic spectrum (blue).

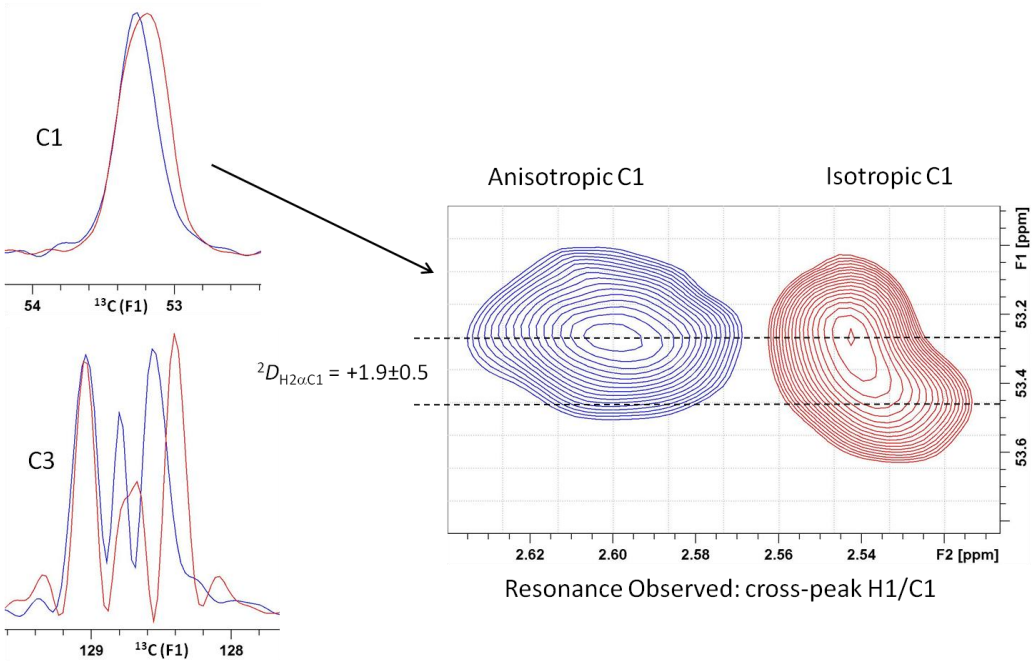

Figure S6. F1 slices upon selective inversion of H2α. Isotropic spectrum (red), anisotropic spectrum (blue). Carbon C1 resonance is not resolved but the E.COSY pattern in the 2D plot (right in red) helps to provide an estimate for it. Due to the splitting remaining unresolved in both the isotropic and aligned states, the estimated error in its value (±0.5 Hz) is much larger than for most other couplings.

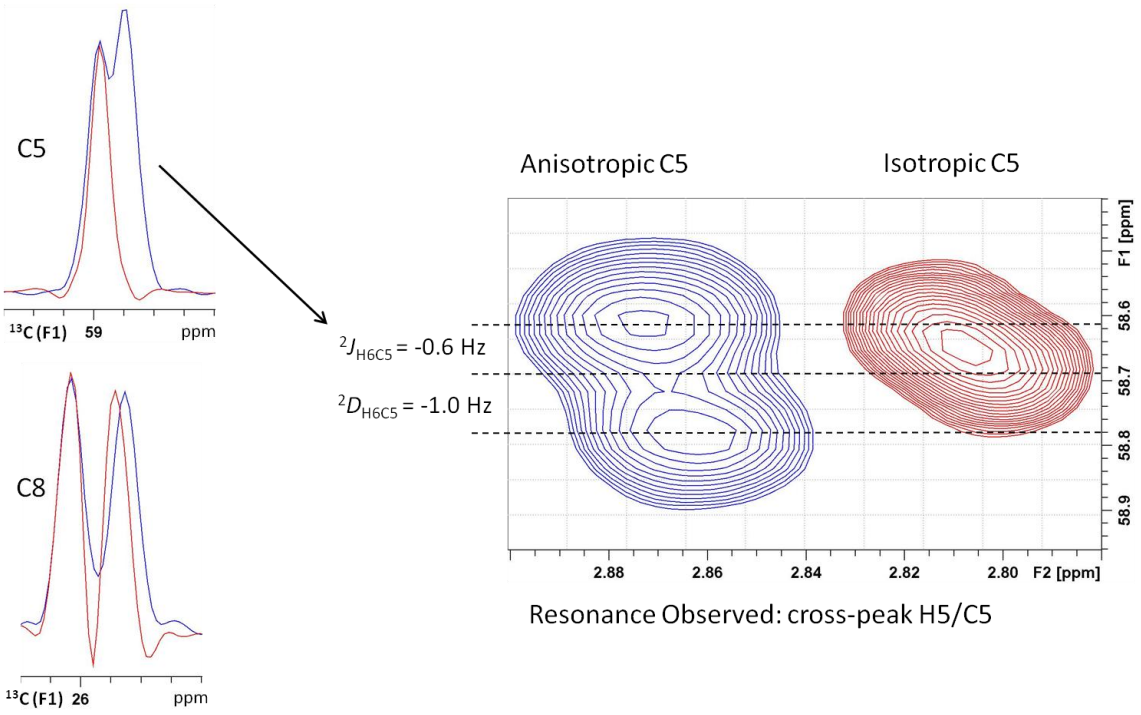

Figure S7. F1 slices upon selective inversion of H6. Isotropic spectrum (red), anisotropic spectrum (blue). As shown above in Figure S6, the C5 resonance is not resolved, but the E.COSY pattern in the 2D plot (right in red) helps to fit a coupling to it.

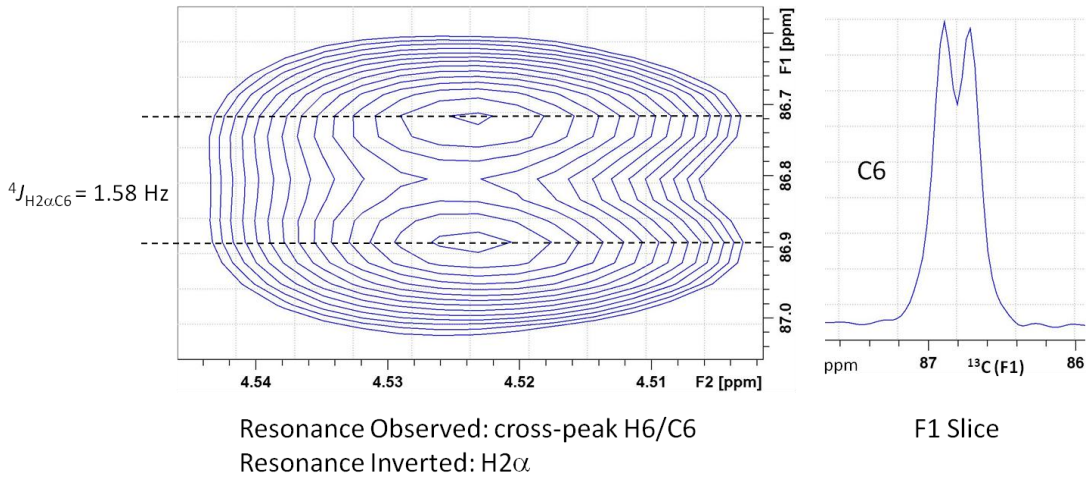

Figure S8. Example of a small $^{4}J_{CH}$ coupling in 10-Epi, observed in the SJS-HSQC spectrum with selective inversion of H2α.

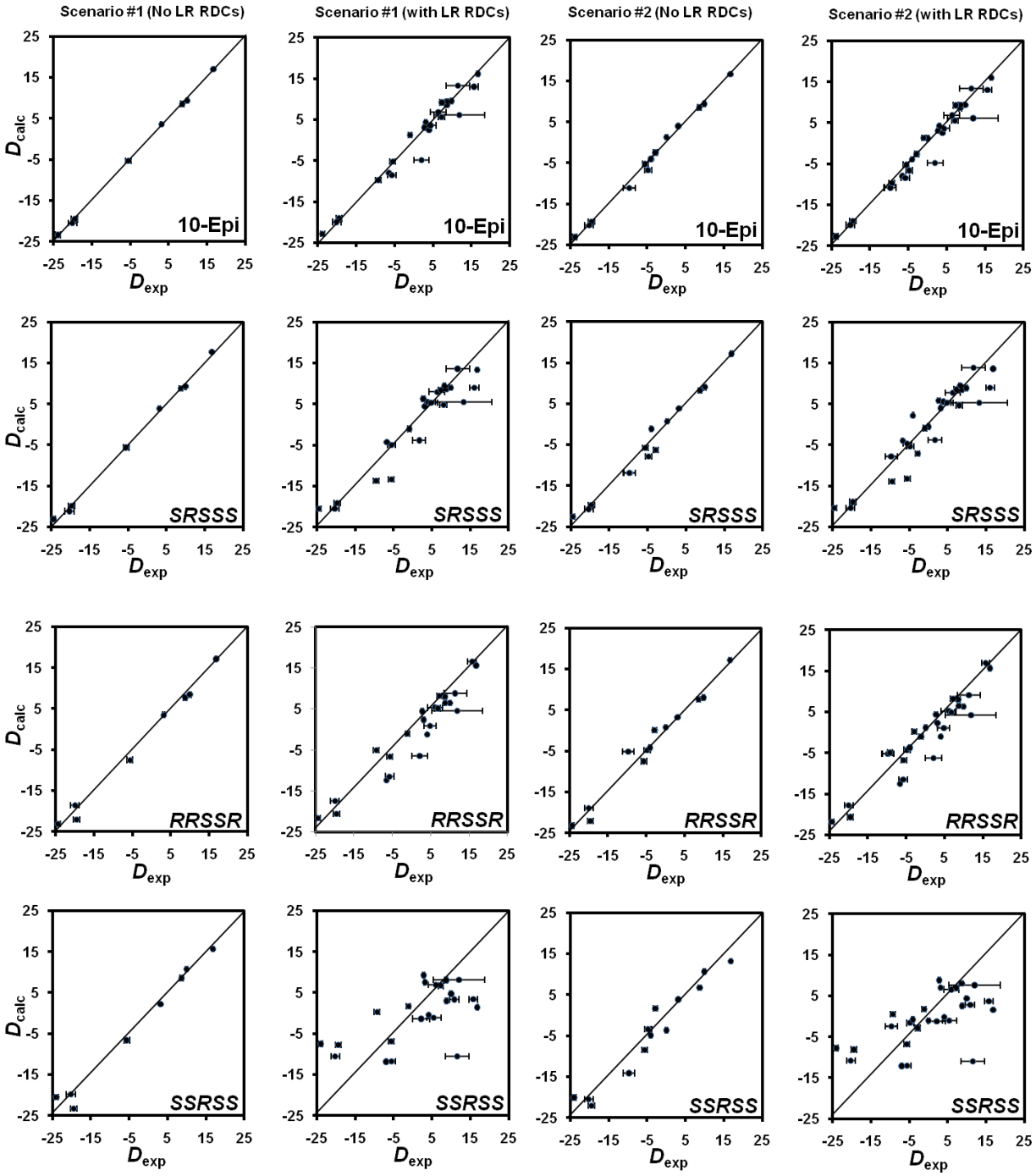

Figure S9. Plots of the normalized back-calculated (D_{calc}) *vs.* experimental (D_{exp}) RDCs for the four best fitting structures (10-Epi (1st), *SRSSS* (2nd), *RRSSR* (3rd), *SSRSS* (4th)) in both scenarios, with and without long-range (LR) RDCs. Note the similarities of the four plots for scenarios #1 without long-range RDCs and how the discrimination improves when LR RDCs are added to the fittings, particularly for *SSRSS*. Normalized RDCs are expressed in Hz×r_{CH}^3, where r is the internuclear distance for the pair of dipolar-coupled nuclei in Angstrom.

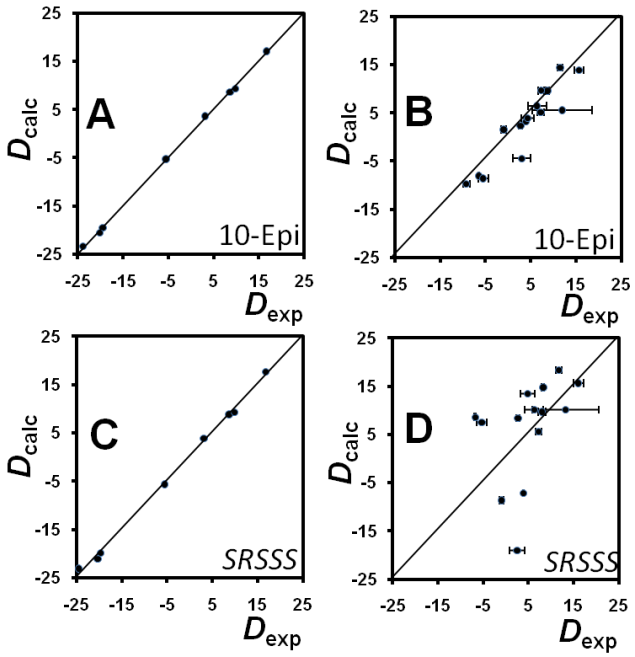

Figure S10. Based on scenario #1, experimental (D_{exp}) vs. back calculated (D_{calc}) normalized one-bond RDCs from SVD fits for 10-Epi and *SRSSS* isomer (**A** and **C**). Normalized predicted long-range RDCs from SVD fits **A** and **C** for 10-Epi and *SRSSS* (**B** and **D**). While the graphs **A** and **C** are almost identical, the structural discrimination of 10-Epi and *SRSSS* using long-range *D* couplings is strikingly revealing in **B** and **D**. Error bars in (B,D) are the lower limits for errors, based on the ratio of line width and signal-to-noise ratio.[13]

SJS-HSQC Pulse program in Bruker format

; SJS-HSQC for measurement of long range 1H-13C J and RDC. Selectively flips a selected proton by p6:sp10

; author: Jinfa Ying October 1, 2010
#include <Avance.incl>
#include <Grad.incl>
#include <Delay.incl>

"p2=p1*2"
"p4=p3*2"
"d4=1s/(cnst2*4)" ;cnst2 set to 155 Hz
"d11=30m"

"d0=3u"
"d29=0.85*p6/2 - p14/2"
"d30=0.15*p6/2"
"d28=0.85*p6/2 - p14/2"
"d3=d1*0.25"
"in0=inf1/2"
"p26=p16*0.251"
"DELTA1=p26+d16+8u"
"DELTA2=d4-larger(p2,p14)/2"
"DELTA=p16*0.2+50u-d0*2-p3*1.26-p1*2"
"DELTA4=d4*2-p14/2"

1 ze
  d11 pl12:f2
2 d1 do:f2
3 (p1 ph1)
  DELTA4 pl0:f2
  4u
  (center (p2 ph1) (p14:sp3 ph6):f2) ;500us hyperbolic secant for sp3
  4u
  DELTA4
  (p1 ph11)
  d3
  (p1 ph1)
  DELTA2 pl0:f2
  4u
  (center (p2 ph1) (p14:sp3 ph6):f2) ;500us hyperbolic secant for sp3
  4u
  DELTA2 pl2:f2
  (p1 ph2)
  3u pl2:f2
  3u pl0:f1

  (d0*20 p6:sp10 ph8):f1 (d29 p3 ph3 3u pl0 d0*20 d30 p14:sp3 ph3 3u d30 d0*20 d29):f2   ;6.5-25ms center-lobe sinc pulse for sp10

  50u UNBLKGRAD
  p16*0.6:gp1*EA   ;for older Bruker spectrometers, assign a new pulse name to p16*0.6
  6u pl0:f2
  (p14:sp3 ph4):f2 ;500us hyperbolic secant for sp3
  6u
  p16*0.4:gp3*EA ;for older Bruker spectrometers, assign a new pulse name to p16*0.4

```
 DELTA pl2:f2
 d29
 d0 pl1:f1
 (p1*2 ph0):f1
 d0 pl2:f2
 (center (p1 ph1) (p3 ph4):f2 )
 d24
 (center (p2 ph1) (p4 ph1):f2 )
 d24
 (center (p1 ph2) (p3 ph5):f2 )
 DELTA2 pl0:f2
 (center (p2 ph1) (p14:sp3 ph1):f2 ) ;500us hyperbolic secant for sp3
 DELTA2
 (p1 ph1)
 DELTA1
 (p2 ph1)
 4u
 p26:gp2
 d16 pl12:f2
 4u BLKGRAD
 go=2 ph31 cpd2:f2
 d1 do:f2 mc #0 to 2
    F1EA(igrad EA & ip5*2, id0 & ip3*2 & ip6*2 & ip13*2 & ip31*2)
exit

ph0=0
ph1=0
ph2=1
ph3=0 2
ph13=0
ph4=0 0 2 2
ph14=1 1 3 3
ph5=1 1 3 3
ph6=0
ph7=0 0 2 2
ph8=0 0 0 0 2 2 2 2
ph11=2
ph31=0 2 2 0
```

DFT geometries for each configuration in xyz coordinates format

Configurations with a single conformation

RRRSR

C	1.353634	-1.746509	0.099862
C	1.728985	-0.246829	0.045081
C	1.982838	0.522994	1.357862
H	2.901364	0.186419	1.860675
H	1.161393	0.430971	2.086617
C	2.069342	-2.438220	1.270482
O	1.893314	-2.268207	-1.129325
H	1.690400	-2.105102	2.245275
H	3.149963	-2.249833	1.229561
H	1.917246	-3.527083	1.214193
H	1.708248	-3.221743	-1.119688
C	-0.603193	0.872422	-0.692374
C	0.926270	0.758970	-0.827664
H	1.109230	0.564347	-1.897733
C	-1.518615	-0.276519	-1.177925
O	-0.981997	1.133703	0.678657
H	-0.897825	1.772748	-1.257970
C	-2.703526	-0.087561	-0.267982
H	-1.804308	-0.087511	-2.223569
C	-2.249024	0.689451	0.921615
O	-2.829123	0.917377	1.961590
C	-3.973783	-0.492599	-0.417008
C	1.558307	2.076871	-0.378760
H	-4.311130	-1.046116	-1.294650
H	-4.710213	-0.267475	0.355354
C	2.092954	1.930088	0.847685
C	1.508258	3.327041	-1.197436
H	2.554304	2.734554	1.423314
H	1.986867	3.180533	-2.179357
H	2.023542	4.153134	-0.690708
H	0.476707	3.657307	-1.397348
C	-0.156942	-2.060541	0.163934
C	-0.926923	-1.693644	-1.107823
H	-0.597245	-1.603300	1.060311
H	-0.251549	-3.148701	0.320119
H	-1.760822	-2.397089	-1.250045
H	-0.250905	-1.836513	-1.962912
H	2.715696	-0.265014	-0.446101

RRRSS

C	1.323799	-1.682278	0.068726
C	1.868150	-0.273343	-0.273445
C	2.659175	0.418994	0.859488
H	3.716174	0.112083	0.864895
H	2.258382	0.165922	1.854595
C	2.493718	-2.668855	0.177904
O	0.699576	-1.723880	1.348048
H	2.118030	-3.640635	0.524599
H	3.238633	-2.320893	0.903558
H	2.986671	-2.813763	-0.792973
H	0.154039	-0.923115	1.427297

```
C     -0.611819    0.786037   -0.535324
C      0.891306    0.813601   -0.826665
H      0.910059    0.775127   -1.931759
C     -1.514686   -0.319820   -1.112018
O     -0.931457    0.812735    0.880742
H     -1.006212    1.730297   -0.949064
C     -2.753376   -0.012808   -0.309176
H     -1.651528   -0.150010   -2.189560
C     -2.273938    0.512806    1.009610
O     -2.871093    0.662240    2.049798
C     -4.053067   -0.143351   -0.612170
C      1.537298    2.114310   -0.364840
H     -4.387762   -0.517272   -1.580607
H     -4.816169    0.128170    0.118218
C      2.491990    1.872180    0.550535
C      1.127647    3.455236   -0.888442
H      3.083318    2.649556    1.038553
H      1.792084    4.243407   -0.512207
H      0.102454    3.726248   -0.590927
H      1.157625    3.485876   -1.989704
C      0.354329   -2.184206   -1.043004
C     -1.106728   -1.786968   -0.853644
H      0.378062   -3.284908   -1.036343
H      0.731997   -1.880224   -2.032493
H     -1.390425   -2.074514    0.168731
H     -1.737512   -2.404440   -1.511140
H      2.583069   -0.424895   -1.097575

RRSSR
C     -2.015593   -1.227867    0.242478
C     -1.863744    0.318433    0.287571
C     -2.491607    1.127414   -0.870990
H     -3.588474    1.172626   -0.795312
H     -2.270387    0.699377   -1.864629
C     -3.502781   -1.579608    0.055105
O     -1.566569   -1.797268    1.478789
H     -3.638581   -2.658702    0.206419
H     -3.871500   -1.324785   -0.947053
H     -4.133690   -1.050319    0.786110
H     -2.139553   -1.427943    2.169734
C      0.677178    0.349475   -0.299499
C     -0.469214    0.981671    0.505468
H     -0.175915    0.920140    1.566000
C      1.042934   -1.081596    0.138162
O      1.876038    1.134290   -0.116789
H      0.447722    0.385040   -1.376796
C      2.537483   -1.085399    0.006894
H      0.799915   -1.156214    1.210401
C      2.983593    0.338545   -0.022102
O      4.103115    0.798653    0.029219
C      3.409116   -2.102329   -0.072093
C     -0.752540    2.422822    0.090428
H      3.095788   -3.146446   -0.056545
H      4.476435   -1.893427   -0.152599
C     -1.846333    2.469505   -0.694243
C      0.085216    3.585877    0.517357
H     -2.238333    3.378234   -1.155055
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H	0.154931	3.635378	1.615707
H	-0.343727	4.532119	0.162723
H	1.114861	3.507739	0.144699
C	-1.198488	-1.916712	-0.868950
C	0.284239	-2.195483	-0.585002
H	-1.300883	-1.314886	-1.782542
H	-1.673064	-2.882179	-1.098930
H	0.779880	-2.410507	-1.544276
H	0.365751	-3.108731	0.019426
H	-2.438609	0.629595	1.179248

RSRSR

C	1.984919	-1.345966	0.215856
C	1.682833	-0.010029	-0.500285
C	2.895277	0.940282	-0.649807
H	3.404628	0.793423	-1.613859
H	3.666297	0.761214	0.116866
C	2.332815	-1.192969	1.704000
O	3.131153	-1.856642	-0.479075
H	1.481484	-0.866965	2.314427
H	3.153191	-0.481209	1.854270
H	2.658440	-2.164448	2.106843
H	3.357176	-2.695119	-0.045615
C	-0.825306	0.535307	-0.500536
C	0.542038	0.844823	0.116825
H	0.441115	0.659596	1.199464
C	-1.247650	-0.953006	-0.621928
O	-1.846649	1.170697	0.303021
H	-0.880078	0.994401	-1.502152
C	-2.733494	-0.841764	-0.410470
H	-1.027417	-1.313078	-1.637446
C	-3.002921	0.444576	0.294407
O	-4.026410	0.845720	0.803523
C	-3.715644	-1.685891	-0.760222
C	1.015861	2.279878	-0.076793
H	-3.523032	-2.619058	-1.291615
H	-4.750827	-1.445251	-0.515382
C	2.293843	2.299373	-0.496995
C	0.180086	3.477423	0.249860
H	2.866125	3.214499	-0.663846
H	0.756176	4.402684	0.120501
H	-0.183512	3.439687	1.287870
H	-0.717355	3.543141	-0.381735
C	0.829345	-2.353603	0.021778
C	-0.597674	-1.928787	0.380107
H	1.073427	-3.258208	0.605166
H	0.853246	-2.660579	-1.036004
H	-0.656910	-1.522542	1.400674
H	-1.222338	-2.834680	0.391131
H	1.379456	-0.283601	-1.524086

10-epi RRSSS

C	1.993742	-1.261098	0.042227
C	1.903452	0.222595	-0.435123
C	2.755929	1.201686	0.429695
H	3.783527	1.284116	0.052387
H	2.844027	0.878883	1.479604

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C      3.446749   -1.744723   -0.128951
O      1.614653   -1.403975    1.428539
H      3.735549   -1.764158   -1.186673
H      3.549348   -2.758126    0.273739
H      4.155940   -1.094454    0.397022
H      2.315600   -1.035055    1.987519
C     -0.644184    0.258135    0.161358
C      0.501691    0.932673   -0.606164
H      0.209668    0.912851   -1.667777
C     -1.193724   -1.015598   -0.520035
O     -1.803847    1.146124    0.235649
H     -0.345049    0.047418    1.192478
C     -2.634791   -0.997246   -0.074580
H     -1.186579   -0.816846   -1.606359
C     -2.963806    0.428311    0.238394
O     -4.041026    0.934158    0.452502
C     -3.521657   -1.985898    0.061967
C      0.792473    2.381353   -0.211871
H     -3.273868   -3.021923   -0.153302
H     -4.531382   -1.768156    0.400032
       2.008805    2.500923    0.336016
C     -0.154848    3.513523   -0.492800
H      2.431328    3.441943    0.681942
H     -1.070831    3.436574    0.100182
H     -0.464932    3.510857   -1.547121
H      0.322607    4.476767   -0.281186
C      1.064088   -2.226062   -0.733550
C     -0.397898   -2.292253   -0.263508
H      1.483953   -3.235263   -0.639283
H      1.108433   -1.970972   -1.802041
H     -0.426381   -2.540485    0.802494
H     -0.884588   -3.119176   -0.797524
H      2.349278    0.226834   -1.438107

RSRSS
C      1.991451   -1.322299    0.216253
C      1.708503    0.023910   -0.491170
C      2.909219    1.000076   -0.506180
H      3.548393    0.864591   -1.392575
H      3.550545    0.844950    0.377672
C      3.285127   -1.960668   -0.321120
O      2.148395   -1.008305    1.602458
H      3.244156   -2.112433   -1.408687
H      3.447427   -2.947404    0.140186
H      4.157143   -1.337648   -0.091728
H      2.406999   -1.834171    2.041194
C     -0.827289    0.513604   -0.515179
C      0.531182    0.848229    0.105621
H      0.455324    0.649926    1.187407
C     -1.237039   -0.978468   -0.613589
O     -1.858646    1.151816    0.274958
H     -0.884617    0.958538   -1.523332
C     -2.723388   -0.881854   -0.402466
H     -1.014191   -1.353625   -1.623499
C     -3.006265    0.414393    0.278863
O     -4.035230    0.813660    0.778990
C     -3.696048   -1.744286   -0.733201
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C	0.968303	2.295443	-0.089049
H	-3.493776	-2.685674	-1.246288
H	-4.733287	-1.511240	-0.489682
C	2.266356	2.347104	-0.437130
C	0.089097	3.476227	0.178881
H	2.827626	3.273110	-0.577202
H	-0.315267	3.446665	1.201703
H	-0.783098	3.509660	-0.489633
H	0.647948	4.413106	0.056514
C	0.849295	-2.345368	0.028502
C	-0.568182	-1.919262	0.406370
H	1.113433	-3.231003	0.632287
H	0.852245	-2.696031	-1.016755
H	-0.581346	-1.475077	1.411899
H	-1.189261	-2.825533	0.468056
H	1.465511	-0.208741	-1.541226

SRRSR

C	1.156136	-1.773992	0.152798
C	1.292292	-0.284142	0.519931
C	2.713179	0.160734	0.936497
H	3.483125	-0.415758	0.396075
H	2.898249	0.014101	2.011814
C	1.653166	-2.659085	1.308273
O	1.981091	-1.980851	-0.999494
H	1.086461	-2.477477	2.231908
H	2.715295	-2.479021	1.511720
H	1.534671	-3.724587	1.056234
H	1.977837	-2.936678	-1.166893
C	-0.625834	1.029707	-0.659167
C	0.871432	0.726977	-0.577691
H	1.153791	0.338672	-1.572980
C	-1.559156	-0.094627	-1.194709
O	-1.122206	1.415888	0.640227
H	-0.759889	1.914286	-1.300486
C	-2.708378	-0.038099	-0.224193
H	-1.916145	0.213721	-2.190117
C	-2.341785	0.867632	0.903526
O	-2.960328	1.119739	1.915137
C	-3.906927	-0.639169	-0.278338
C	1.750007	1.939025	-0.294380
H	-4.199147	-1.292881	-1.101291
H	-4.630344	-0.475173	0.521139
C	2.755867	1.599694	0.529923
C	1.540638	3.272586	-0.938593
H	3.558453	2.274472	0.833874
H	0.606414	3.747734	-0.600766
H	1.479287	3.189866	-2.036103
H	2.363729	3.958449	-0.701014
C	-0.307067	-2.165132	-0.163699
C	-0.945307	-1.494941	-1.381613
H	-0.929997	-2.015935	0.730913
H	-0.313277	-3.254088	-0.342453
H	-1.757285	-2.140875	-1.749590
H	-0.203543	-1.456295	-2.192785
H	0.634281	-0.103742	1.382463

SRSSS

C	-2.135049	-1.222069	0.180111
C	-1.619028	0.105815	-0.435366
C	-2.707059	1.155701	-0.777347
H	-3.586447	1.105438	-0.112448
H	-3.091937	1.026085	-1.802510
C	-3.001422	-1.036593	1.436237
O	-2.907014	-1.888851	-0.832245
H	-3.273154	-2.020620	1.841488
H	-3.937768	-0.506232	1.216974
H	-2.476947	-0.474642	2.221073
H	-3.637725	-1.290502	-1.054533
C	0.852348	0.363766	-0.239088
C	-0.482790	0.888921	0.292597
H	-0.500731	0.732361	1.386465
C	1.217640	-1.058125	0.213570
O	1.994733	1.149708	0.169948
H	0.824352	0.405305	-1.342294
C	2.685543	-1.051594	-0.105658
H	1.162479	-1.032818	1.320182
C	3.121322	0.368713	0.088303
O	4.236020	0.829152	0.187853
C	3.524477	-2.024438	-0.487687
C	-0.799953	2.348687	-0.000935
H	3.199579	-3.054752	-0.634068
H	4.575865	-1.795734	-0.664957
C	-2.005552	2.461231	-0.588045
C	0.076217	3.489701	0.412242
H	-2.470720	3.413996	-0.849067
H	-0.427236	4.450112	0.242354
H	1.029365	3.496719	-0.132816
H	0.336486	3.423206	1.479715
C	-1.009071	-2.228702	0.522742
C	0.309160	-2.187828	-0.259513
H	-1.471269	-3.219440	0.405354
H	-0.766421	-2.135823	1.592193
H	0.138258	-2.137057	-1.344998
H	0.825362	-3.142908	-0.078703
H	-1.201995	-0.201891	-1.406839

SSRSR

C	-2.011423	-1.221376	0.031897
C	-1.835371	0.240181	-0.433503
C	-2.701542	1.253146	0.353274
H	-2.802681	0.962800	1.411681
H	-3.721965	1.322534	-0.054505
C	-3.479142	-1.655071	-0.144026
O	-1.689433	-1.251381	1.429401
H	-3.599847	-2.715818	0.127056
H	-3.819729	-1.542983	-1.182367
H	-4.139318	-1.066883	0.504327
H	-1.908639	-2.145300	1.736581
C	0.610445	0.281548	0.521406
C	-0.402168	0.873659	-0.479777
H	0.035477	0.742494	-1.482618
C	1.046121	-1.197527	0.262953
O	1.815716	1.077384	0.474050

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H      0.218116    0.388536    1.539098
C      2.537687   -1.089401    0.103096
H      0.818384   -1.776358    1.168938
C      2.932390    0.341408    0.227508
O      4.032820    0.844399    0.143843
C      3.453523   -2.049662   -0.096675
C     -0.690843    2.355910   -0.262340
H      3.193036   -3.106000   -0.175463
H      4.506769   -1.779712   -0.180481
C     -1.943183    2.531005    0.197896
C      0.282102    3.447915   -0.581868
H     -2.376984    3.504298    0.435745
H     -0.192571    4.432974   -0.483468
H      0.655915    3.352793   -1.613625
H      1.165512    3.420766    0.068659
C     -1.119916   -2.221525   -0.740011
C      0.362674   -1.881987   -0.928985
H     -1.561705   -2.401144   -1.732454
H     -1.204470   -3.184409   -0.206723
H      0.502520   -1.267032   -1.828667
H      0.900087   -2.818752   -1.139036
H     -2.188867    0.264645   -1.476102

SSRSS
C      2.268567   -0.916883    0.224896
C      1.719176    0.533556    0.267470
C      2.166353    1.559117   -0.797921
H      2.017510    1.201107   -1.832829
H      3.233106    1.812416   -0.712017
C      3.757328   -0.907601   -0.159361
O      2.141523   -1.490850    1.534319
H      4.326617   -0.206263    0.469908
H      3.918543   -0.620261   -1.206813
H      4.175887   -1.911284   -0.007934
H      2.664634   -0.929063    2.127747
C     -0.687309    0.241580   -0.716351
C      0.197654    0.821193    0.413775
H     -0.186858    0.476841    1.385437
C     -0.987930   -1.278824   -0.727564
O     -1.991336    0.862663   -0.663827
H     -0.262138    0.557303   -1.677443
C     -2.319146   -1.341884   -0.036334
H     -1.178047   -1.518965   -1.790811
C     -2.933942    0.010847   -0.158124
O     -4.058191    0.378799    0.104043
C     -2.935194   -2.353753    0.592790
C      0.208563    2.348272    0.281946
H     -2.487154   -3.342410    0.692631
H     -3.923655   -2.198111    1.026425
C      1.272818    2.719433   -0.458860
C     -0.820308    3.247495    0.887685
H      1.493195    3.745696   -0.758149
H     -0.871754    3.098110    1.978306
H     -1.825194    3.046061    0.495031
H     -0.579272    4.302785    0.703931
C      1.512747   -1.894999   -0.690246
C      0.093356   -2.225828   -0.220583
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H      2.098990   -2.825383   -0.707157
H      1.515749   -1.511965   -1.721927
H      0.084999   -2.258181    0.875872
H     -0.167100   -3.239555   -0.559499
H      2.139574    0.945902    1.203693

SSSSR
C      2.351430   -0.726905    0.317524
C      1.801577    0.713588    0.151898
C      1.879016    1.278740   -1.287960
H      1.676672    0.528876   -2.069842
H      2.886194    1.663058   -1.503649
C      2.425803   -1.151658    1.792991
O      3.700985   -0.585495   -0.160842
H      1.447601   -1.286362    2.268132
H      2.987915   -0.403999    2.367722
H      2.958953   -2.111036    1.881544
H      4.110425   -1.461299   -0.072982
C     -0.643825   -0.018037    0.750166
C      0.390005    1.121216    0.691864
H      0.485606    1.480867    1.730174
C     -0.757088   -0.937635   -0.478442
O     -1.963596    0.506347    1.003180
H     -0.416626   -0.645018    1.625986
C     -2.228676   -1.252043   -0.490218
H     -0.532071   -0.347275   -1.382579
C     -2.915132   -0.239052    0.366966
O     -4.100072   -0.039623    0.521395
C     -2.912395   -2.219431   -1.119067
C      0.020170    2.295302   -0.208469
H     -2.430753   -2.968327   -1.748323
H     -3.996091   -2.271976   -1.009138
C      0.837957    2.350568   -1.276738
C     -1.048343    3.289877    0.126428
H      0.771442    3.112211   -2.056610
H     -0.896967    3.698479    1.138052
H     -2.053268    2.849510    0.120983
H     -1.035101    4.128888   -0.581441
C      1.674165   -1.800406   -0.568795
C      0.191179   -2.134733   -0.387536
H      2.241842   -2.736731   -0.427413
H      1.850738   -1.509655   -1.613912
H      0.018122   -2.647851    0.571450
H     -0.074402   -2.864630   -1.166963
H      2.506173    1.326082    0.735274

SSSSS
C      2.296923   -0.781221    0.346479
C      1.837298    0.697284    0.238117
C      2.051597    1.350169   -1.150236
H      1.973587    0.637434   -1.988602
H      3.055141    1.796809   -1.234260
C      3.821909   -0.832099    0.127554
O      2.017462   -1.157912    1.700032
H      4.198654   -1.853461    0.291975
H      4.332459   -0.167300    0.836600
H      4.108169   -0.541619   -0.891713
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H	2.384547	-2.048860	1.817333
C	-0.627213	-0.028831	0.742719
C	0.394211	1.117013	0.694244
H	0.448716	1.488852	1.730613
C	-0.777073	-0.885018	-0.526750
O	-1.940872	0.481921	1.061415
H	-0.346441	-0.682627	1.579885
C	-2.251917	-1.182132	-0.528032
H	-0.554179	-0.257767	-1.407592
C	-2.910287	-0.220317	0.408011
O	-4.091309	-0.028448	0.602663
C	-2.959153	-2.099979	-1.203419
C	0.063558	2.279265	-0.230501
H	-2.498886	-2.810232	-1.890932
H	-4.040649	-2.150313	-1.072392
C	0.973573	2.382805	-1.216954
C	-1.072675	3.227528	0.001051
H	0.952276	3.152883	-1.990983
H	-1.055813	3.614132	1.031684
H	-2.052734	2.751232	-0.128625
H	-1.013154	4.083048	-0.684329
C	1.642028	-1.769472	-0.651362
C	0.155197	-2.095118	-0.502456
H	2.195056	-2.721434	-0.574416
H	1.833984	-1.414985	-1.674943
H	-0.018271	-2.648837	0.432429
H	-0.114280	-2.781735	-1.319188
H	2.501705	1.231045	0.933775

Configurations with more than one conformation

RSSSR Conformer 1

C	1.343791	-1.488338	0.240566
C	0.827617	-0.109715	-0.239910
C	1.865981	1.005053	-0.447586
H	2.499459	0.820868	-1.324899
H	2.546642	1.101147	0.417778
C	1.553142	-1.590929	1.756537
O	2.613374	-1.636165	-0.410600
H	2.010594	-2.560717	2.006487
H	0.617699	-1.521232	2.325747
H	2.231022	-0.803235	2.108379
H	2.933637	-2.521572	-0.174517
C	-1.581044	-0.221079	0.719623
C	-0.280448	0.599333	0.575185
H	0.088967	0.745206	1.607401
C	-1.841557	-1.359902	-0.286129
O	-2.763694	0.602850	0.703050
H	-1.565777	-0.686836	1.719717
C	-3.343801	-1.439686	-0.234620
H	-1.573919	-1.012228	-1.299566
C	-3.837208	-0.117577	0.258895
O	-4.965753	0.320961	0.286479
C	-4.186100	-2.435071	-0.547370
C	-0.249198	2.004254	-0.042401
H	-3.845300	-3.407426	-0.903777
H	-5.261276	-2.281806	-0.448513
C	0.978421	2.207100	-0.562924
C	-1.308388	3.051985	0.096024
H	1.322227	3.163642	-0.961117
H	-1.641549	3.154946	1.139197
H	-2.208012	2.816274	-0.487855
H	-0.926123	4.024932	-0.240148
C	0.428523	-2.613193	-0.307392
C	-1.063561	-2.636709	0.043577
H	0.856975	-3.582269	0.003209
H	0.534447	-2.572943	-1.402919
H	-1.213776	-2.875836	1.108171
H	-1.506893	-3.476405	-0.512364
H	0.406893	-0.272283	-1.245515

RSSSR Conformer 2

C	1.369056	-1.480862	0.394991
C	0.814811	-0.149834	-0.150190
C	1.815758	0.944746	-0.554019
H	2.348608	0.690695	-1.480756
H	2.587081	1.120924	0.216710
C	2.319198	-1.324054	1.590026
O	2.088416	-2.015105	-0.726194
H	2.626684	-2.311611	1.968559
H	1.849804	-0.789197	2.426510
H	3.225982	-0.781317	1.297351
H	2.535355	-2.814129	-0.403913
C	-1.574977	-0.216978	0.797570
C	-0.270965	0.603161	0.658838

H	0.088741	0.783221	1.689679
C	-1.830585	-1.265033	-0.298046
O	-2.763390	0.597513	0.842566
H	-1.548959	-0.733147	1.769556
C	-3.327099	-1.380567	-0.239903
H	-1.608645	-0.776761	-1.263197
C	-3.833330	-0.105332	0.356362
O	-4.966891	0.314225	0.429195
C	-4.151324	-2.364434	-0.628883
C	-0.260224	1.974262	-0.025874
H	-3.787417	-3.293222	-1.069080
H	-5.228974	-2.247148	-0.510469
C	0.917806	2.138657	-0.661370
C	-1.294813	3.041758	0.151062
H	1.227257	3.071074	-1.137594
H	-1.547555	3.185161	1.212058
H	-2.238157	2.798376	-0.354990
H	-0.928981	3.997639	-0.246536
C	0.226017	-2.453428	0.783860
C	-0.980680	-2.548117	-0.161900
H	-0.115755	-2.224149	1.804028
H	0.671816	-3.459630	0.859382
H	-1.623332	-3.359533	0.210869
H	-0.629133	-2.862193	-1.154614
H	0.338047	-0.428842	-1.101667

RSSSR Conformer 1

C	1.343791	-1.488338	0.240566
C	0.827617	-0.109715	-0.239910
C	1.865981	1.005053	-0.447586
H	2.499459	0.820868	-1.324899
H	2.546642	1.101147	0.417778
C	1.553142	-1.590929	1.756537
O	2.613374	-1.636165	-0.410600
H	2.010594	-2.560717	2.006487
H	0.617699	-1.521232	2.325747
H	2.231022	-0.803235	2.108379
H	2.933637	-2.521572	-0.174517
C	-1.581044	-0.221079	0.719623
C	-0.280448	0.599333	0.575185
H	0.088967	0.745206	1.607401
C	-1.841557	-1.359902	-0.286129
O	-2.763694	0.602850	0.703050
H	-1.565777	-0.686836	1.719717
C	-3.343801	-1.439686	-0.234620
H	-1.573919	-1.012228	-1.299566
C	-3.837208	-0.117577	0.258895
O	-4.965753	0.320961	0.286479
C	-4.186100	-2.435071	-0.547370
C	-0.249198	2.004254	-0.042401
H	-3.845300	-3.407426	-0.903777
H	-5.261276	-2.281806	-0.448513
C	0.978421	2.207100	-0.562924
C	-1.308388	3.051985	0.096024
H	1.322227	3.163642	-0.961117
H	-1.641549	3.154946	1.139197
H	-2.208012	2.816274	-0.487855

H	-0.926123	4.024932	-0.240148
C	0.428523	-2.613193	-0.307392
C	-1.063561	-2.636709	0.043577
H	0.856975	-3.582269	0.003209
H	0.534447	-2.572943	-1.402919
H	-1.213776	-2.875836	1.108171
H	-1.506893	-3.476405	-0.512364
H	0.406893	-0.272283	-1.245515

RSSSR Conformer 2

C	1.369056	-1.480862	0.394991
C	0.814811	-0.149834	-0.150190
C	1.815758	0.944746	-0.554019
H	2.348608	0.690695	-1.480756
H	2.587081	1.120924	0.216710
C	2.319198	-1.324054	1.590026
O	2.088416	-2.015105	-0.726194
H	2.626684	-2.311611	1.968559
H	1.849804	-0.789197	2.426510
H	3.225982	-0.781317	1.297351
H	2.535355	-2.814129	-0.403913
C	-1.574977	-0.216978	0.797570
C	-0.270965	0.603161	0.658838
H	0.088741	0.783221	1.689679
C	-1.830585	-1.265033	-0.298046
O	-2.763390	0.597513	0.842566
H	-1.548959	-0.733147	1.769556
C	-3.327099	-1.380567	-0.239903
H	-1.608645	-0.776761	-1.263197
C	-3.833330	-0.105332	0.356362
O	-4.966891	0.314225	0.429195
C	-4.151324	-2.364434	-0.628883
C	-0.260224	1.974262	-0.025874
H	-3.787417	-3.293222	-1.069080
H	-5.228974	-2.247148	-0.510469
C	0.917806	2.138657	-0.661370
C	-1.294813	3.041758	0.151062
H	1.227257	3.071074	-1.137594
H	-1.547555	3.185161	1.212058
H	-2.238157	2.798376	-0.354990
H	-0.928981	3.997639	-0.246536
C	0.226017	-2.453428	0.783860
C	-0.980680	-2.548117	-0.161900
H	-0.115755	-2.224149	1.804028
H	0.671816	-3.459630	0.859382
H	-1.623332	-3.359533	0.210869
H	-0.629133	-2.862193	-1.154614
H	0.338047	-0.428842	-1.101667

RSSSS Conformer 1

C	1.988533	-1.262385	0.098486
C	1.523992	0.076837	-0.530492
C	2.556767	1.156205	-0.897575
H	3.179343	0.881603	-1.761693
H	3.241611	1.365347	-0.055042
C	3.414925	-1.629823	-0.343558
O	1.961695	-1.095720	1.518370

H	4.135772	-0.886279	0.016015
H	3.503782	-1.701439	-1.436030
H	3.703313	-2.608646	0.070600
H	2.324580	-1.913323	1.895130
C	-0.803810	0.104160	0.594336
C	0.468848	0.897447	0.251441
H	0.916172	1.163015	1.225746
C	-1.189029	-1.078444	-0.315285
O	-1.971800	0.947910	0.680898
H	-0.656398	-0.306730	1.604707
C	-2.683541	-1.103969	-0.138403
H	-0.990635	-0.810581	-1.368335
C	-3.096145	0.243573	0.362079
O	-4.208612	0.708509	0.483580
C	-3.578667	-2.077710	-0.359608
C	0.458151	2.201897	-0.552822
H	-3.297012	-3.067498	-0.720079
H	-4.636970	-1.888102	-0.176881
C	1.661102	2.333934	-1.148872
C	-0.608103	3.250339	-0.525073
H	1.986733	3.224683	-1.689101
H	-0.882815	3.519276	0.505175
H	-1.535638	2.912926	-1.007014
H	-0.264843	4.157943	-1.039230
C	1.045318	-2.409744	-0.354006
C	-0.431830	-2.358464	0.050317
H	1.456252	-3.360229	0.027970
H	1.116480	-2.481904	-1.451357
H	-0.528473	-2.517243	1.134976
H	-0.925760	-3.218384	-0.426597
H	1.055074	-0.183012	-1.493045

RSSSS Conformer 2

C	2.055844	-1.248924	-0.058449
C	1.468415	0.089165	-0.604304
C	2.478134	1.157715	-1.071772
H	2.790119	1.019991	-2.118940
H	3.400259	1.152444	-0.462778
C	2.579909	-2.115066	-1.212824
O	3.112782	-1.001331	0.875629
H	3.330756	-1.574591	-1.808675
H	1.777622	-2.415258	-1.900325
H	3.052158	-3.024174	-0.816636
H	3.876273	-0.705370	0.356417
C	-0.886704	0.200149	0.493494
C	0.530025	0.830615	0.378126
H	0.972070	0.754412	1.388172
C	-1.111736	-1.119928	-0.267315
O	-1.939990	1.057257	-0.004265
H	-1.112847	0.033142	1.560113
C	-2.610193	-1.140363	-0.337063
H	-0.789521	-0.929110	-1.305149
C	-3.028100	0.296874	-0.346201
O	-4.102021	0.788262	-0.611967
C	-3.486014	-2.154151	-0.388853
C	0.667734	2.293586	-0.027636
H	-3.173402	-3.198549	-0.381425

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H     -4.554906   -1.944806   -0.441089
C      1.743134    2.439488   -0.824745
C     -0.145081    3.410365    0.548563
H      2.116849    3.403019   -1.176780
H     -1.194627    3.365057    0.233282
H      0.266408    4.383876    0.252290
H     -0.144429    3.366830    1.649691
C      1.043006   -2.026813    0.812331
C     -0.356003   -2.334545    0.266773
H      0.942518   -1.459941    1.749342
H      1.525284   -2.972471    1.100764
H     -0.933118   -2.786744    1.088188
H     -0.306121   -3.098980   -0.523018
H      0.879992   -0.148390   -1.501740

SRSSR Conformer 1
C     -1.933575   -1.327646    0.237909
C     -1.730184    0.093930   -0.367133
C     -2.922067    1.071295   -0.248240
H     -3.431576    0.990731    0.731423
H     -3.694514    0.886099   -1.009199
C     -3.377696   -1.821856    0.032090
O     -1.644827   -1.337866    1.643454
H     -3.465391   -2.856230    0.391004
H     -3.671684   -1.798270   -1.026573
H     -4.100405   -1.214245    0.593562
H     -2.256026   -0.705224    2.053997
C      0.803852    0.436246   -0.350878
C     -0.534511    0.923495    0.183306
H     -0.490837    0.817809    1.282357
C      1.148990   -1.022842   -0.002309
O      1.894797    1.213883    0.189778
H      0.834026    0.564375   -1.448110
C      2.650065   -0.968222   -0.056059
H      0.871148   -1.177438    1.055314
C      3.028890    0.447785    0.243462
O      4.112896    0.916606    0.510303
C      3.568477   -1.915434   -0.293626
C     -0.939727    2.358063   -0.142229
H      3.304615   -2.950030   -0.514353
H      4.628082   -1.659296   -0.266497
C     -2.266013    2.411196   -0.367125
C     -0.014744    3.532010   -0.089228
H     -2.827091    3.331071   -0.541965
H     -0.562776    4.466864   -0.264482
H      0.788269    3.459364   -0.836154
H      0.487534    3.601963    0.886864
C     -1.000761   -2.405842   -0.375236
C      0.408660   -2.039936   -0.863482
H     -1.526645   -2.873742   -1.220411
H     -0.924920   -3.183042    0.399542
H      0.374384   -1.667336   -1.899528
H      0.984076   -2.975947   -0.911975
H     -1.561134   -0.031931   -1.450437

SRSSR Conformer 2
C     -2.143203   -1.192031    0.184415
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C     -1.631106    0.123013   -0.445990
C     -2.733614    1.179083   -0.697707
H     -3.550482    1.083309    0.035345
H     -3.187156    1.073497   -1.695835
C     -3.076062   -1.901949   -0.813665
O     -2.887287   -0.817786    1.348690
H     -2.536852   -2.223372   -1.716153
H     -3.904138   -1.251324   -1.119482
H     -3.510490   -2.804099   -0.355632
H     -3.271739   -1.636175    1.700707
C      0.851137    0.344408   -0.251139
C     -0.477724    0.882683    0.281737
H     -0.514343    0.713669    1.372574
C      1.228645   -1.057320    0.250637
O      2.003066    1.143763    0.105876
H      0.808255    0.344007   -1.354921
C      2.688899   -1.067180   -0.097700
H      1.194097   -0.985373    1.355665
C      3.126919    0.360585    0.030974
O      4.244223    0.822314    0.089081
C      3.520835   -2.055732   -0.453811
C     -0.786287    2.349009    0.008191
H      3.194416   -3.091664   -0.549021
H      4.568654   -1.835070   -0.660123
C     -2.016052    2.476624   -0.523011
C      0.110882    3.479365    0.406041
H     -2.486702    3.436915   -0.744147
H     -0.396147    4.443604    0.271176
H      1.042796    3.494539   -0.174678
H      0.410711    3.395598    1.461911
C     -1.013910   -2.168573    0.624487
C      0.309711   -2.203902   -0.153486
H     -1.442000   -3.184031    0.641588
H     -0.781830   -1.925737    1.672461
H      0.150247   -2.218127   -1.242502
H      0.815328   -3.151099    0.088855
H     -1.237063   -0.153890   -1.436802

SRSSR Conformer 3
C     -1.960087   -1.315777    0.054680
C     -1.796791    0.183416   -0.296222
C     -2.923365    1.146906    0.121117
H     -3.234048    0.970021    1.166554
H     -3.821602    1.046130   -0.505656
C     -3.395890   -1.773715   -0.256555
O     -1.710408   -1.456032    1.454976
H     -3.509189   -2.847936   -0.042449
H     -3.653284   -1.624201   -1.314390
H     -4.123019   -1.230365    0.357921
H     -1.943212   -2.369588    1.684768
C      0.751006    0.346821   -0.434833
C     -0.520819    0.915225    0.190641
H     -0.421838    0.772985    1.282803
C      1.145366   -1.016706    0.174563
O      1.880859    1.209093   -0.178822
H      0.650689    0.280146   -1.532123
C      2.643781   -0.959059    0.124024
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H	0.856912	-0.954402	1.237842
C	3.018500	0.483823	0.041715
O	4.106051	1.006298	0.147674
C	3.565483	-1.933417	0.146921
C	-0.905796	2.379842	-0.025853
H	3.303157	-2.990059	0.203430
H	4.624386	-1.675177	0.111405
C	-2.249776	2.478006	-0.020036
C	0.048068	3.530735	-0.068198
H	-2.798749	3.420994	-0.051636
H	-0.498834	4.481742	-0.113496
H	0.721329	3.478735	-0.935113
H	0.698800	3.547360	0.818327
C	-0.994064	-2.181305	-0.801771
C	0.489396	-2.269684	-0.405979
H	-1.075653	-1.826399	-1.840525
H	-1.379777	-3.213806	-0.825313
H	1.052584	-2.592786	-1.294992
H	0.617128	-3.072230	0.335133
H	-1.767859	0.233294	-1.398392

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