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Supporting Information

Residual Dipolar Coupling Enhanced NMR Spectroscopy and Chiroptics: A Powerful Combination for the Complete Elucidation of Symmetrical Small Molecules

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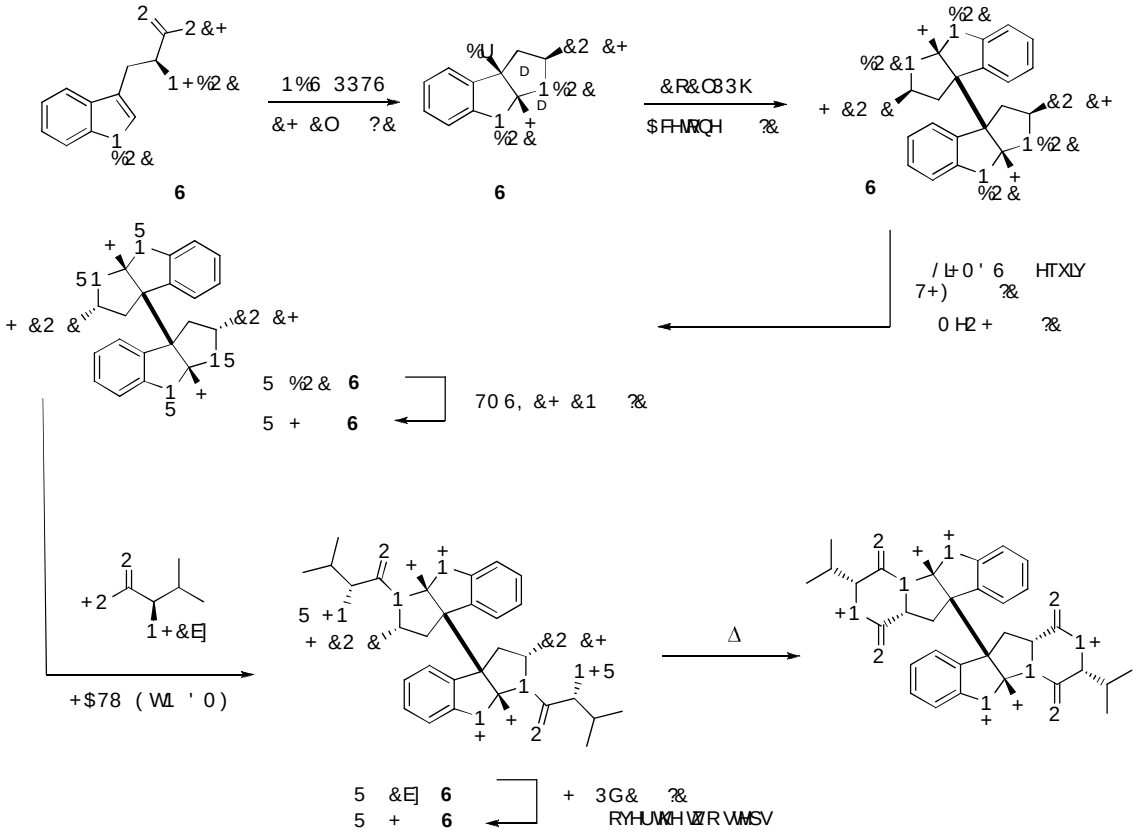
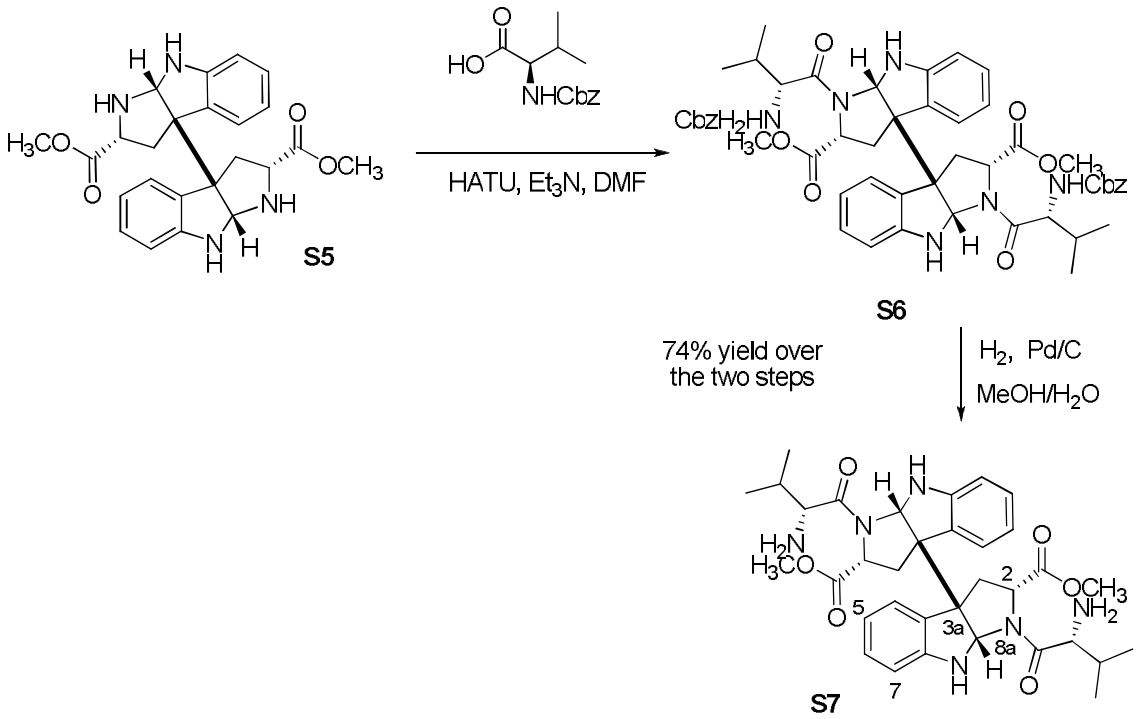
1. Synthesis of the Homodimer 6.

The general strategy for the preparation of bispyrrolidinoindoline diketopiperazines has been previously described.[1] The characterization of the intermediate **S7** and the final product **6** is herewith reported.



(2*R*,3a*S*,8a*S*,2'*R*,3'a*S*,8'a*S*)-1,1'-Bis-((*R*)-2-amino-3-methyl-butyryl)-2,3,8,8a,2',3',8',8'a-octahydro-1*H*,1'*H*-[3a,3'a]bi[pyrrolo[2,3-*b*]indolyl]-2,2'-dicarboxylic Acid Dimethyl Ester (S7)



N-Cbz-D-Valine[2] (100 mg, 0.40 mmol, 2.5 equiv) was added to a solution of tetraamine **S5** (69 mg, 0.16 mmol) in DMF (1.8 mL). The mixture was cooled down to 0 ºC and Et_3N (111 µL, 0.80 mmol, 5.0 equiv) was added, followed by HATU (152 mg, 0.40 mmol, 2.5 equiv). The cooling bath was removed and the mixture was stirred for 14 h at 25 ºC. A 5% aqueous LiCl solution (5 mL) was added and the resulting mixture was diluted with H_2O (10 mL) and extracted with EtOAc (3x 15 mL). The combined organic layers were washed with 5% aqueous LiCl solution (10 mL), dried over Na_2SO_4 and the solvents were removed under reduced pressure. The residue was purified by flash chromatography on silica gel (95:5 CH_2Cl_2/MeOH) to give the coupled tetra-peptide which was used directly in the next step.

To a solution of **S6** (115 mg) in a MeOH/H_2O mixture (10 mL, 9:1 v/v) was added 10% Pd/C (15 mg) and the vessel was purged several times with H_2. The mixture was stirred under 1 atm of H_2 for 4 h and then filtered over a pad of Celite®. After washing the

solids with a CH_2Cl_2/MeOH mixture (15 mL, 1:1 v/v), the filtrates were concentrated *in vacuo*. The residue was purified by flash chromatography on silica gel (90:10 CH_2Cl_2/MeOH) to give 76 mg (74% combined yield over the two steps) of the title compound as white foam.

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.11 (t, *J* = 7.6 Hz, 2H, ArH), 6.96 (d, *J* = 7.5 Hz, 2H, ArH), 6.67 (t, *J* = 7.6 Hz, 2H, ArH), 6.61 (d, *J* = 7.6 Hz, 2H, ArH), 5.46 (s, 2H), 5.38 (s, 2H), 4.43 (d, *J* = 8.5 Hz, 2H, C<u>H</u>NH_2), 3.14 (s, 6H, 2x CO_2CH_3), 2.93 (dd, *J* = 13.3, 8.7 Hz, 2H, H3A/H3A'), 2.82 (d, *J* = 8.5 Hz, 2H, H2/H2'), 2.50 (d, *J* = 13.3 Hz, 2H, H3B/H3B'), 1.8-1.7 (m, 2H, C<u>H</u>$(CH_3)_2$), 1.59 (br s, 4H, N<u>H</u>$_2$), 0.94 (d, *J* = 6.7 Hz, 6H, CH(C<u>H</u>$_3$)$_2$), 0.88 (d, *J* = 6.7 Hz, 6H, CH(C<u>H</u>$_3$)$_2$) ppm.

^{13}C NMR (100 MHz, $CDCl_3$) δ 177.1 (s, 2x <u>C</u>ON), 171.2 (s, <u>C</u>O_2CH_3), 151.6 (s, 2x), 130.2 (d, 2x), 126.6 (d, 2x), 126.3 (s, 2x), 118.2 (d, 2x), 110.2 (d, 2x), 80.2 (d, C8a/C8a'), 59.8 (d, 2x), 58.9 (s, C3a/C3a'), 58.7 (d, 2x), 52.8 (q, 2x OCH_3), 35.7 (t, C3/C3'), 32.2 (d, 2x), 20.1 (q, 2x), 18.2 (q, 2x) ppm.

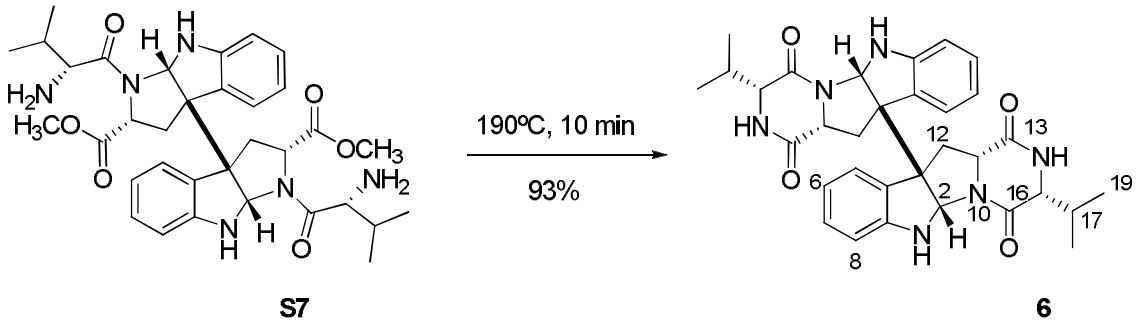
IR (NaCl) *n* 3356 (m, NH), 3050 (w), 2957 (w, C–H), 2872 (w, C-H), 1738 (s, CO), 1639 (s, CO), 1607 (m), 1469 (m), 1433 (s), 1317 (m), 1236 (s), 1209 (m), 1168 (m), 916 (m), 737 (s) cm^{-1}.

MS (ESI^+) *m/z* (%) 633 ($[M+1]^+$, 37), 601 ($[M-OCH_3]^+$, 84), 447 (46), 391 (100).

HRMS (ESI^+) calcd for $C_{34}H_{45}N_6O_6$, 633.3395; found 633.3391.

$[a]_D^{25}$ -515º (*c* 0.20, MeOH).

(3*R*,5a*S*,10b*S*,11a*R*, 3'*R*,5'a*S*,10'b*S*,11'a*R*)-3,3'-Diisopropyl-2,3,5a,6,11,11a,2',3',-5'a,6',11',11'a-dodecahydro-[10b,10'b]bi[pyrazino[1',2':1,5]pyrrolo[2,3-*b*]indolyl]-1,4,1',4'-tetraone (6)



S7 **6**

The tetra-peptide **S7** (38 mg, 0.06 mmol) was heated neat at 190 ºC for 10 min. The residue was purified by flash chromatography on silica gel (95:5 CH_2Cl_2/MeOH) to afford 31 mg (93% yield) of the title compound as a white solid.

^{1}H NMR (400 MHz, CD_3OD) δ 7.44 (d, *J* = 7.4 Hz, 2H, H5), 7.17 (t, *J* = 7.6 Hz, 2H, H7), 6.85 (t, *J* = 7.4 Hz, 2H, H6), 6.70 (d, *J* = 7.6 Hz, 2H, H8), 4.99 (s, 2H, H2), 4.21 (t, *J* = 8.1 Hz, 2H, H11), 3.90 (s, 2H, H15), 3.26 (dd, *J* = 13.7, 8.1 Hz, 2H, H12), 2.78 (dd, *J* = 13.7, 8.1 Hz, 2H, H12), 2.4-2.2 (m, 2H, H17), 0.96 (d, *J* = 7.2 Hz, 6H, H18), 0.81 (d, *J* = 7.0 Hz, 6H, H19) ppm.

^{13}C NMR (100 MHz, CD_3OD) δ 172.2 (s, C13), 169.9 (s, C16), 150.6 (s, C9), 131.9 (s, C4), 130.6 (d, C7), 126.4 (d, C5), 120.6 (d, C6), 110.6 (d, C8), 81.2 (d, C2), 62.0 (d, C15), 61.4 (s, C3), 58.2 (d, C11), 37.6 (t, C12), 30.4 (d, C17), 18.9 (q, C18), 16.5 (q, C19) ppm.

IR (NaCl) *n* 3362 (w, N-H), 3252 (w, N-H), 3053 (w, C-H), 2964 (m, C-H), 2875 (w, C-H), 1668 (s, CO), 1606 (m), 1467 (m), 1416 (m), 1346 (m), 1193 (m), 1095 (m), 743 (m) cm^{-1}.

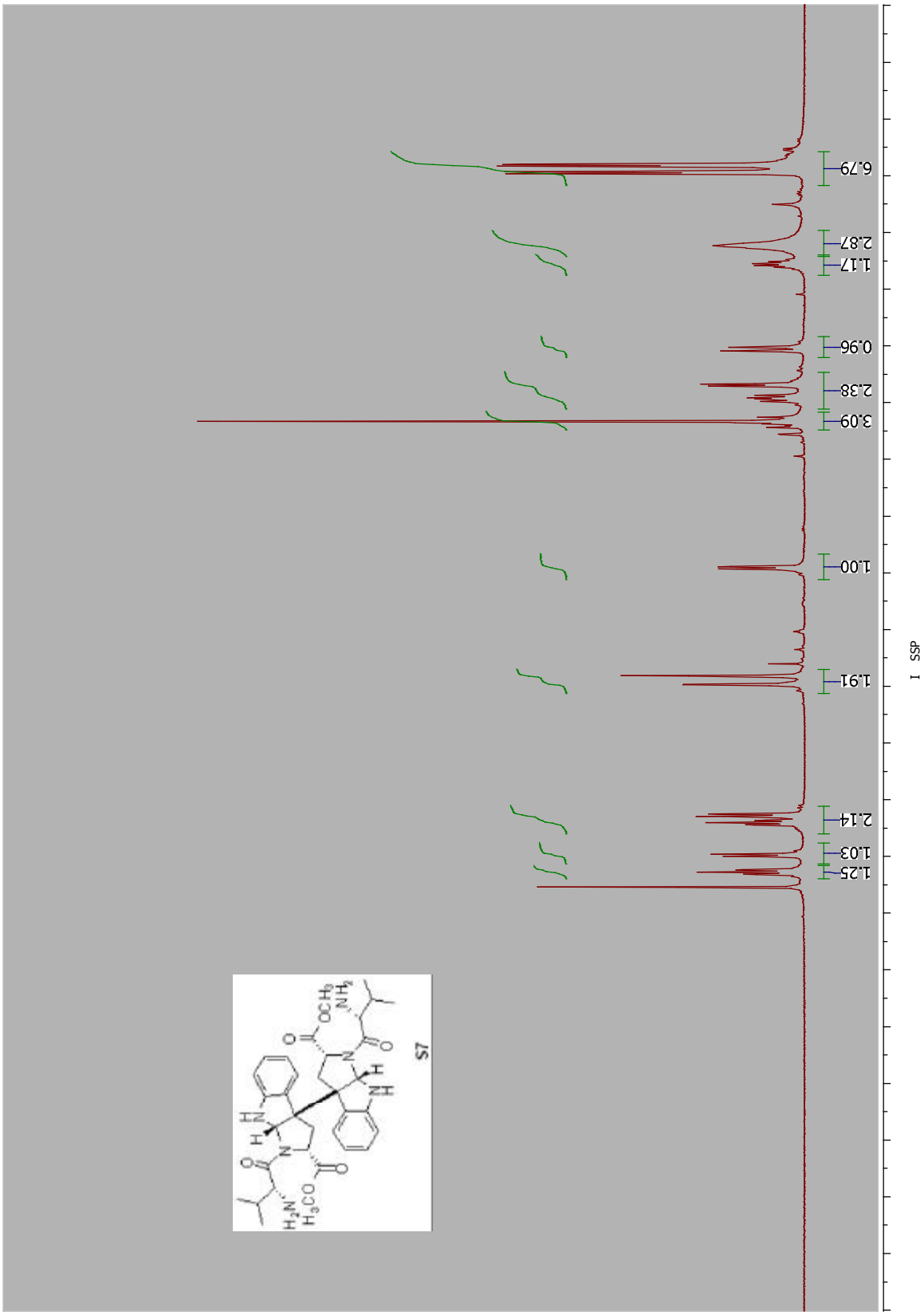
MS (ESI^+) *m/z* (%) 591 ($[M+Na]^+$, 22), (569 ($[M+H]^+$, 100), 413 (33), 201 (44).

HRMS (ESI^+) calcd for $C_{32}H_{37}N_6O_4$, 569.2871; found 569.2893.

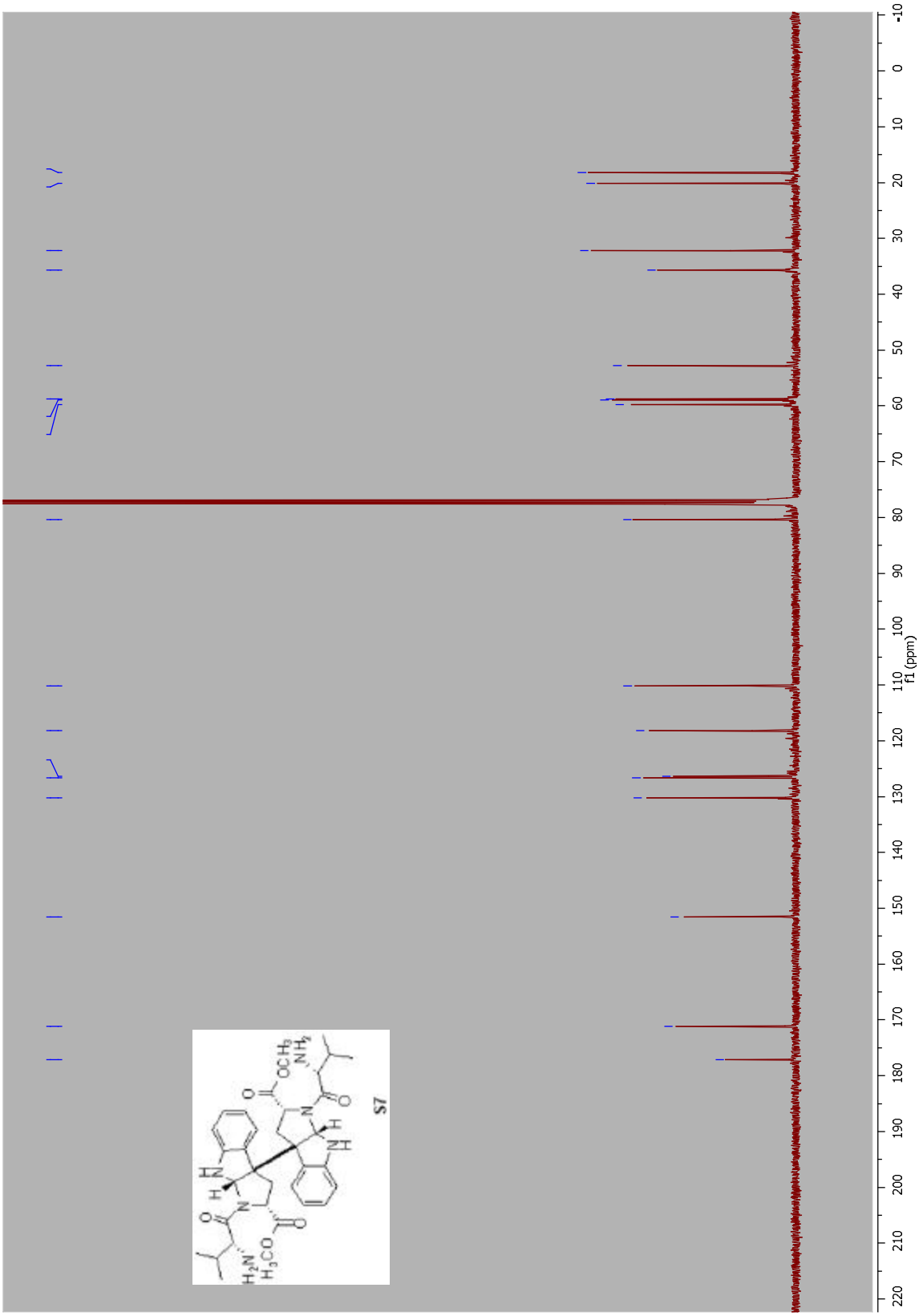
$[a]_D^{22}$ - 273º (*c* 0.11, MeOH).

M. p. (MeOH): 185-188 ºC.

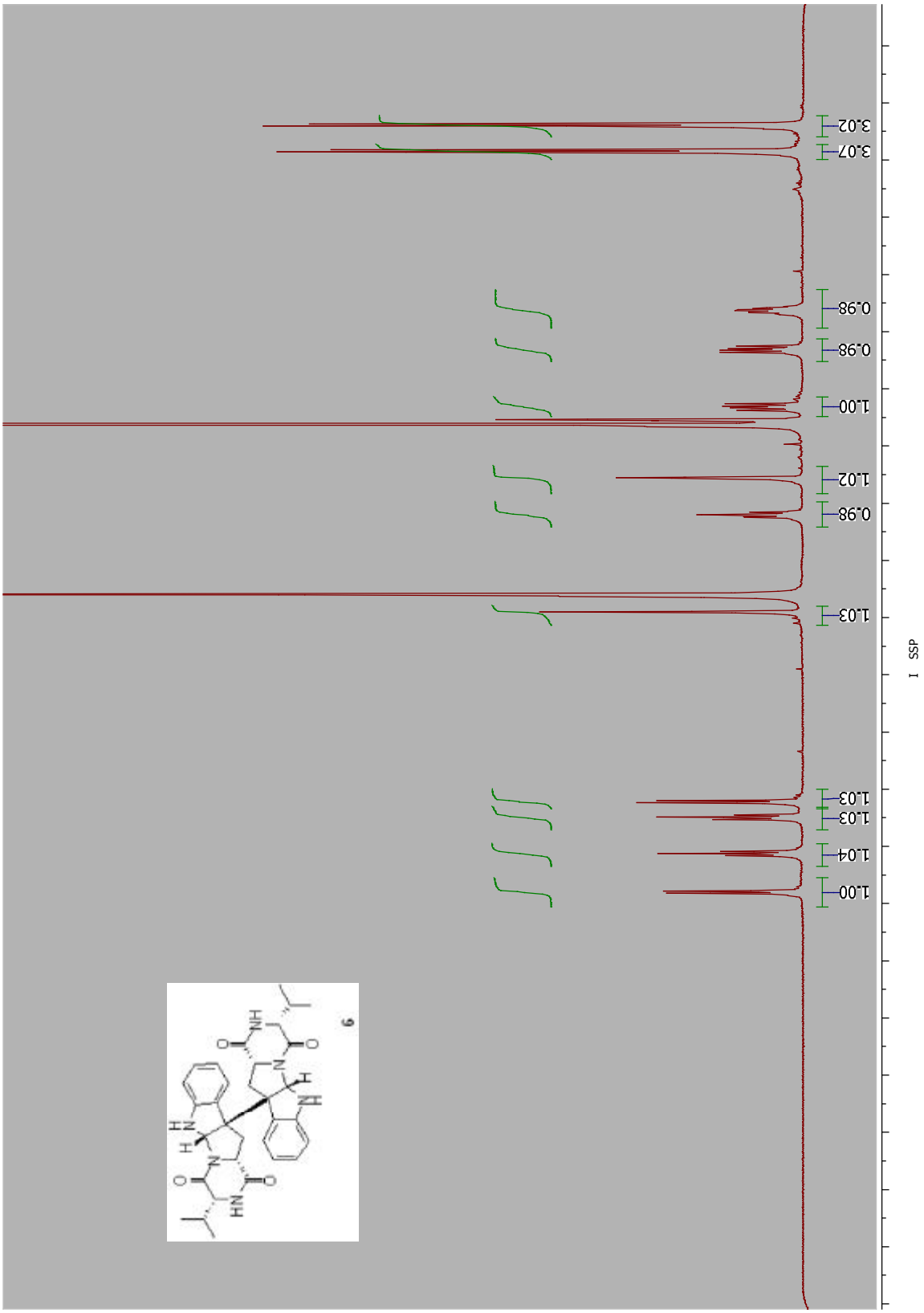
^{1}H NMR (400 MHz, CD_3OD)



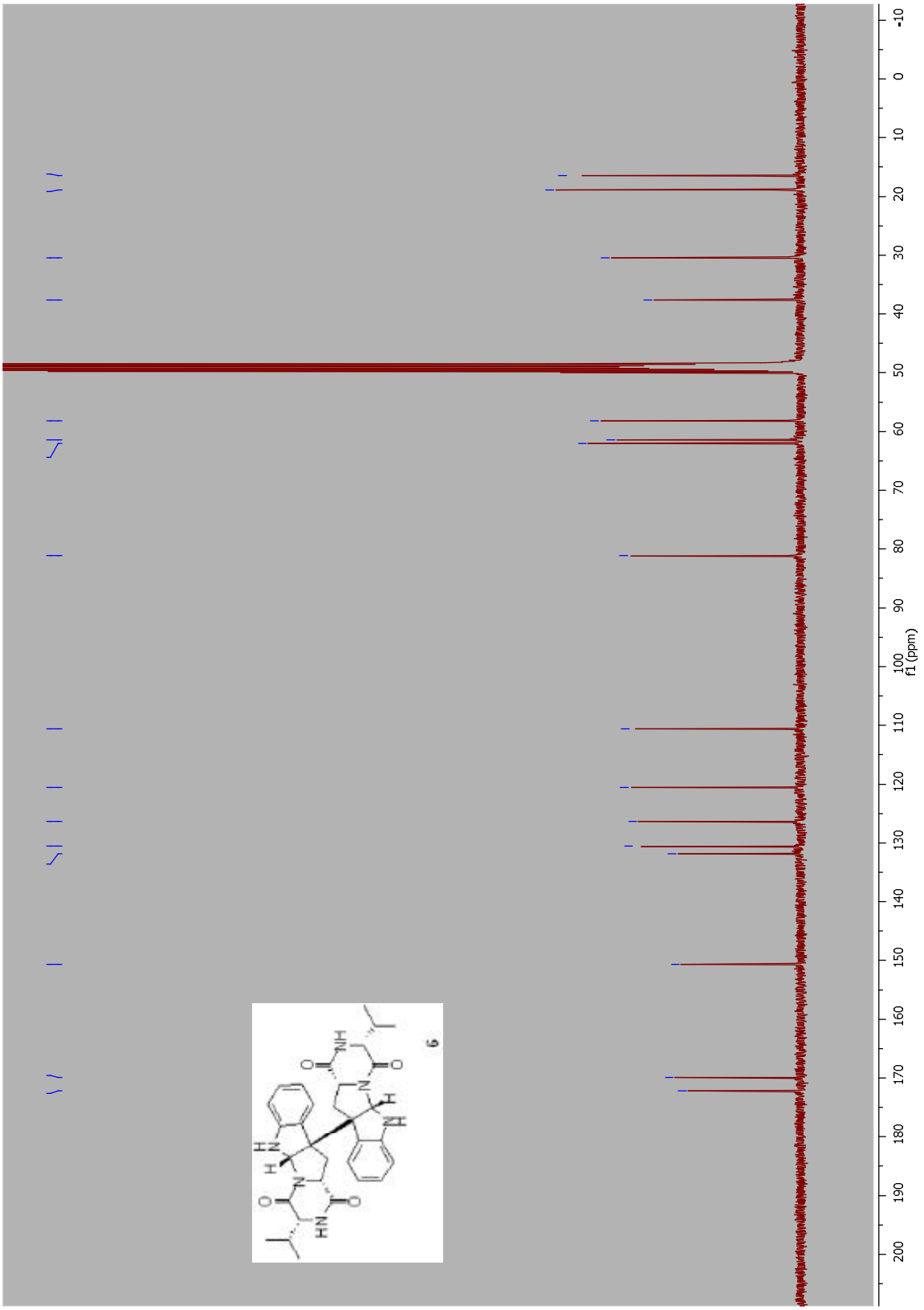
^{13}C NMR (100 MHz, $CDCl_3$)



^{1}H NMR (400 MHz, CD_3OD)

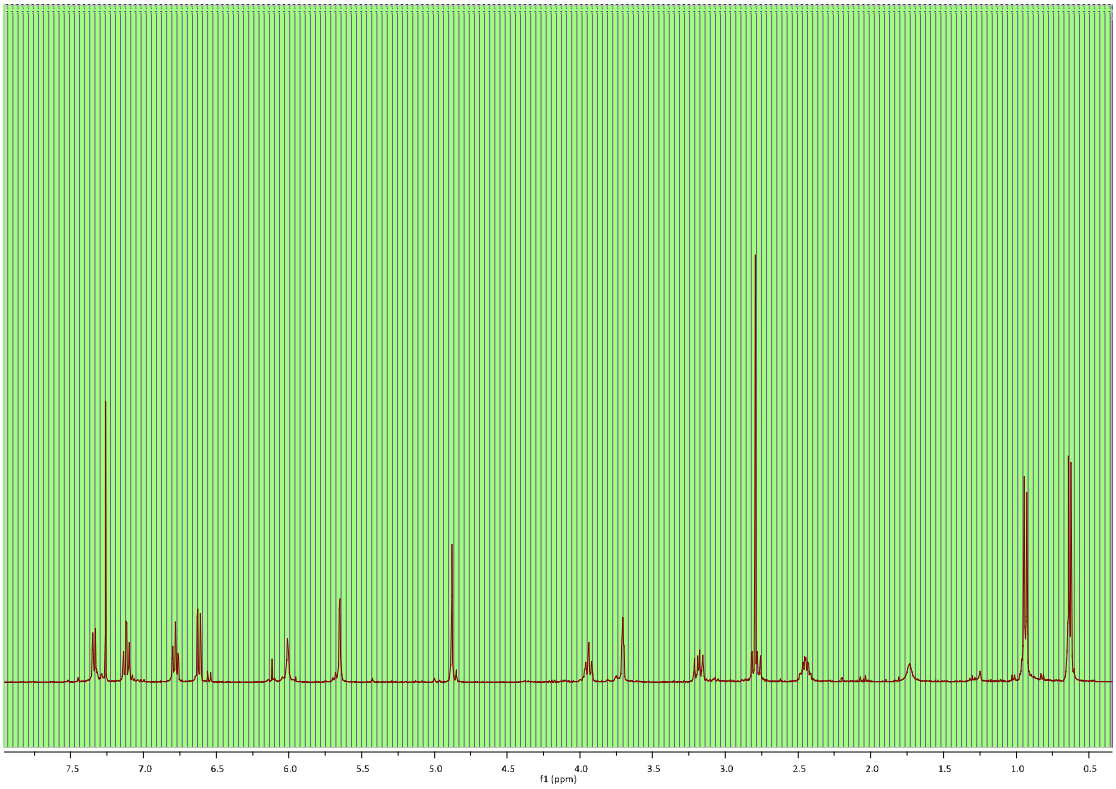


^{13}C NMR (100 MHz, CD_3OD)

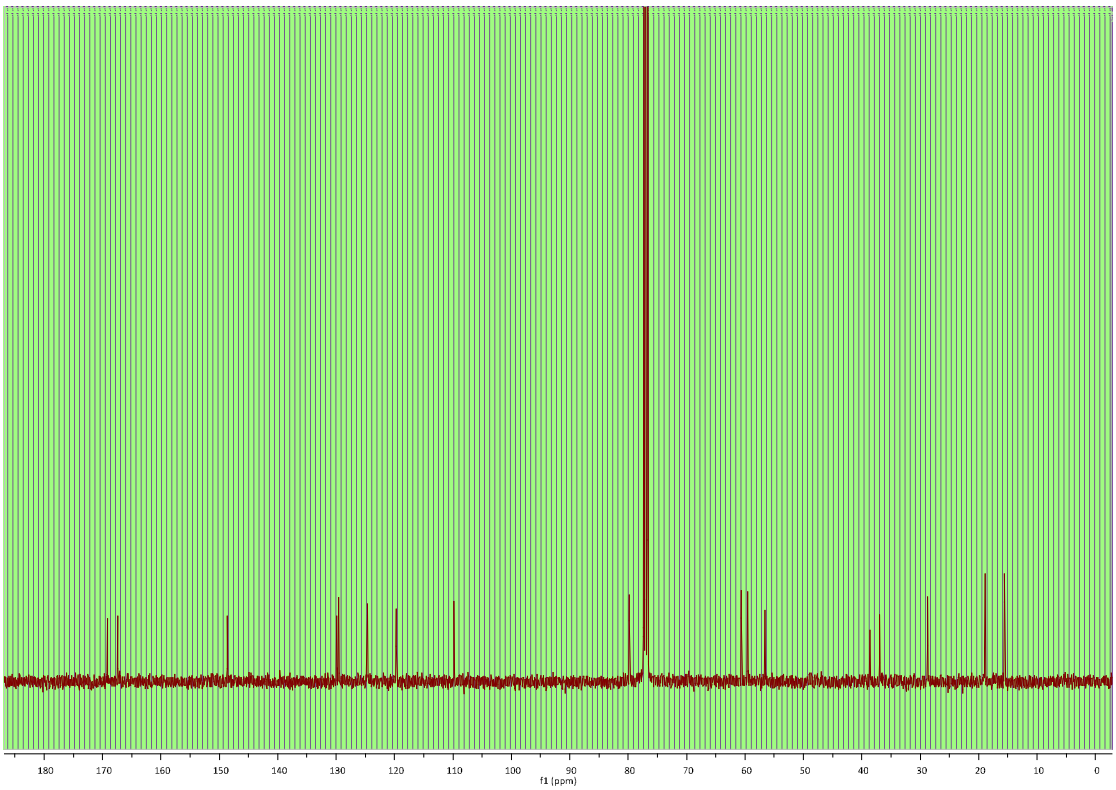


2. 2D spectra in non-aligned an aligned conditions

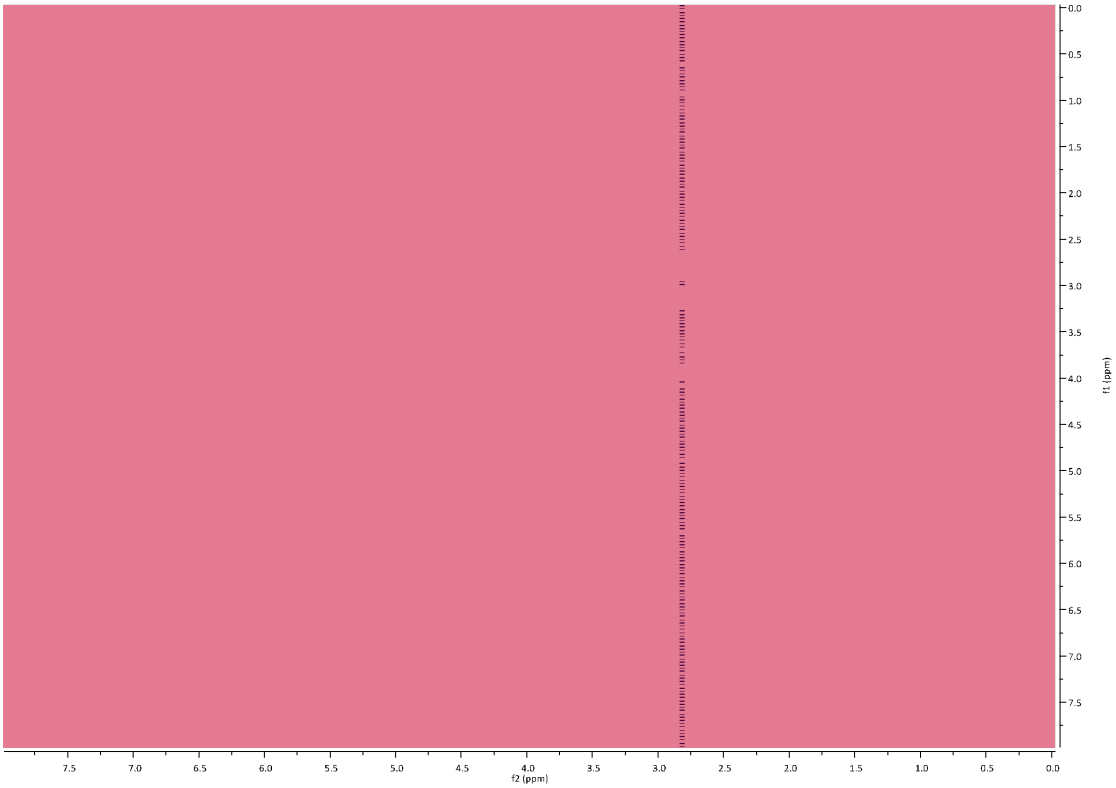
Spectra of homodimer 6 in $CDCl_3$ (Spectrometer ^1H frequency 400.2 MHz)
^1H 400.13 MHz



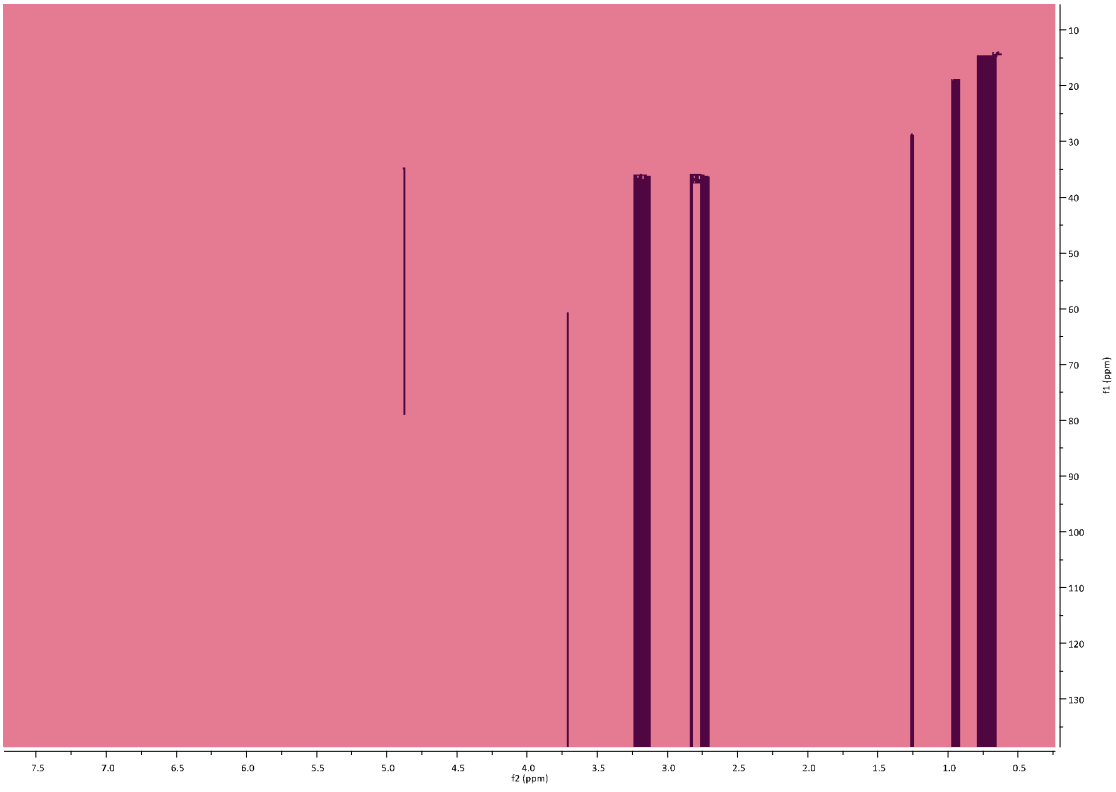
^{13}C gated decoupled 100.92 MHz



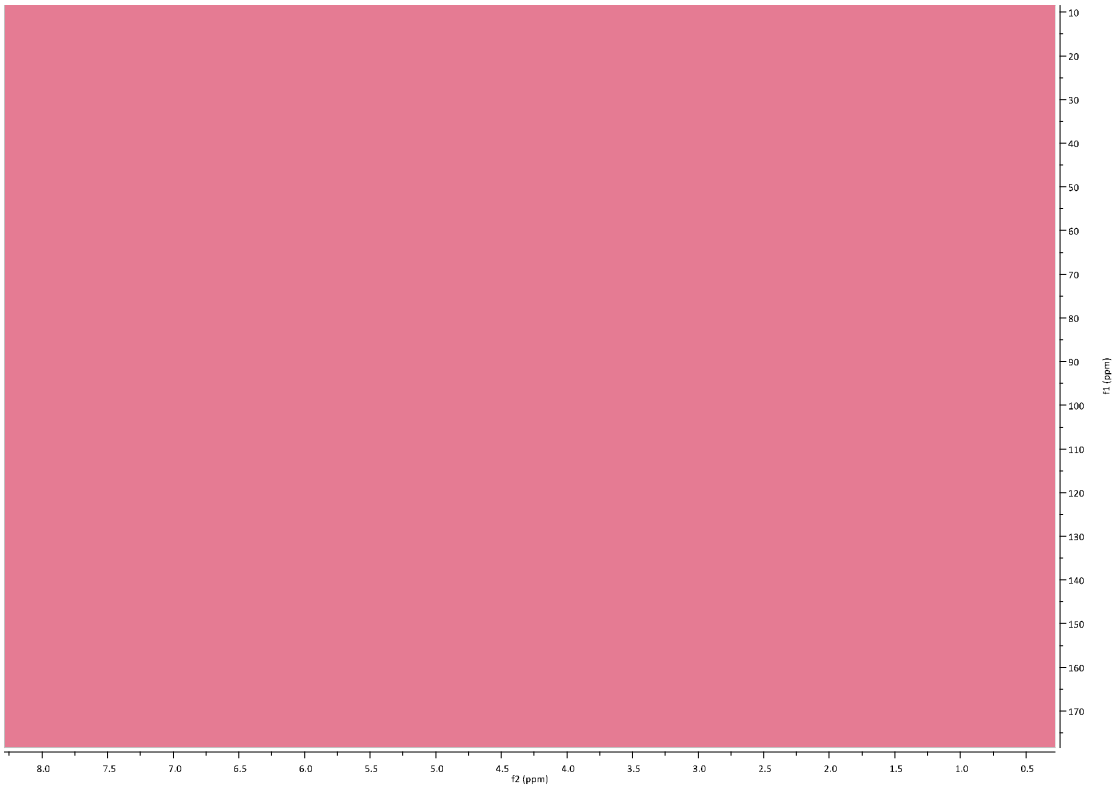
COSY-90 (cosygdfqf) 400.13 MHz



HSQC (hsqcedtgp) 400.13 MHz

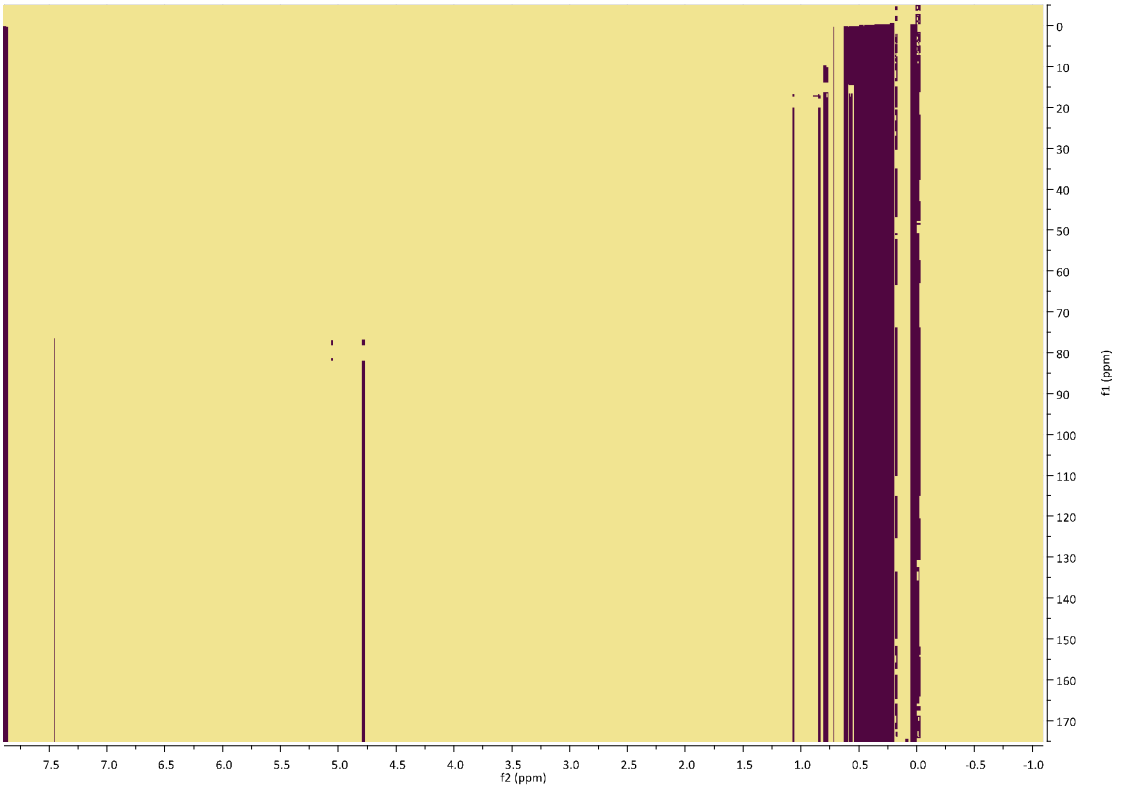


HMBC (hmbcgpldnqf) 400.13 MHz

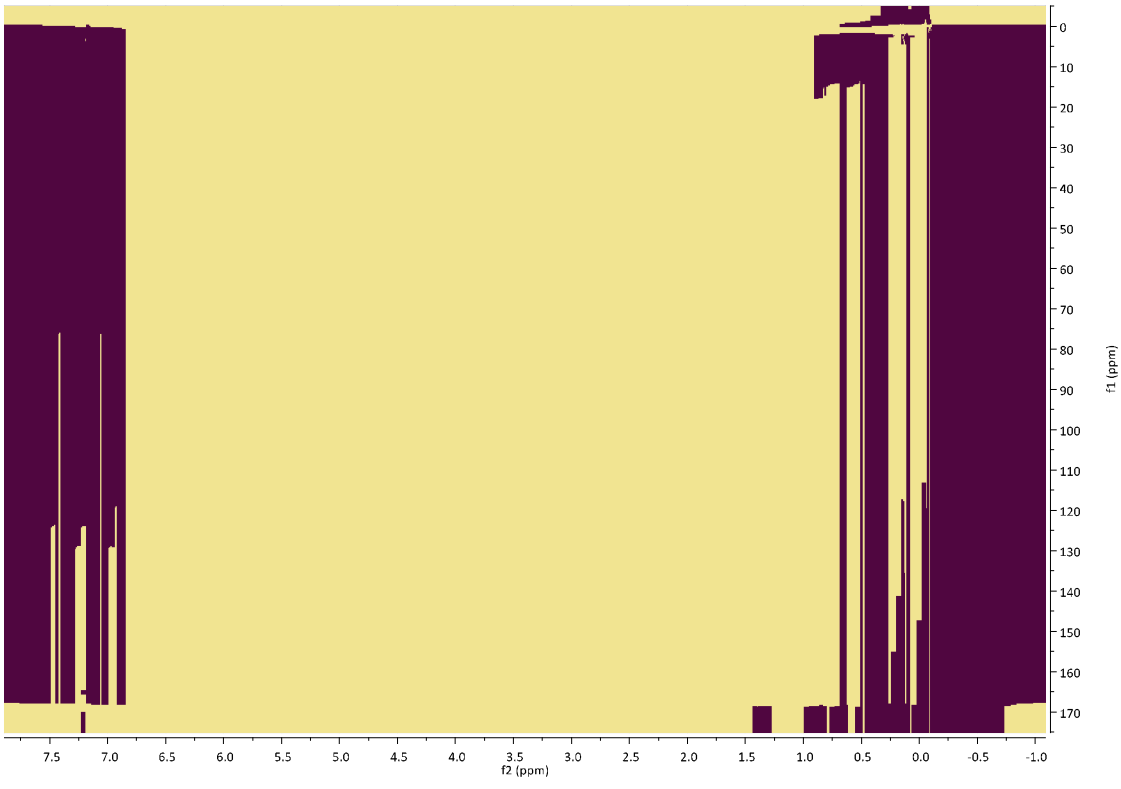


NOESY-800 ms mixing time 400.13 MHz

CLIP-HSQC non aligned conditions 600.13 MHz



CLIP-HSQC (PDMS/CDCl3) 600.13 MHz



3. DFT General Computational details

Anti, *syn* and +synclinal conformations of (11*R*,15*R*)-**6** were optimized in vacuo using the OPBE functional[3] and the 6-31G* basis set. The reported energy gap (ΔE=1.6 kcal/mol) between the two conformations was computed by single point computations at the PCM[4] (CHCl3)/CAM-B3LYP[5]/6-31+G** on the OPBE geometries. All DFT computations were done with the Gaussian09 rev A.02 package.[6]

4. DFT computed structures and energies

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Homodimer 6 RR configuration anti conformation OPBE/6-31G* geometry
E(SCF) OPBE/6-31G* = -1869.77690
E(SCF) CAM-B3LYP = -1869.78258

78
Homodimer 6 RR
C   -4.206858  0.502067  0.768514
C   -4.515613  0.990783 -0.505301
C   -3.507498  1.367202 -1.398285
C   -2.175504  1.229364 -0.988853
C   -1.844585  0.715590  0.282245
C   -2.867392  0.372821  1.166133
N   -1.027050  1.501942 -1.710985
C    0.094689  1.552416 -0.816070
C   -0.324022  0.720325  0.446758
N    0.377220  2.892438 -0.267384
C    0.867148  2.783769  1.096847
C    0.105148  1.585302  1.667717
C    0.505017  3.994697 -1.047717
C    0.910029  5.285955 -0.313304
N    0.697431  5.197347  1.119462
C    0.701339  4.075150  1.889473
C    0.203853  6.517336 -0.929086
C    0.867148  7.830526 -0.500139
C   -1.306501  6.530382 -0.680488
O    0.607279  4.090083  3.113218
O    0.319687  3.990752 -2.268769
C    4.206858 -0.502067  0.768514
C    4.515613 -0.990783 -0.505301
C    3.507498 -1.367202 -1.398285
C    2.175504 -1.229364 -0.988853
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C   -0.105148 -1.585302  1.667717
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C   -0.867148 -7.830526 -0.500139
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O   -0.319687 -3.990752 -2.268769
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```

```
H   -0.719731 -1.042447  2.390077
H   -1.993344 -5.400594 -0.522475
H   -0.661274 -6.063732  1.644556
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H    1.766870 -7.378808 -1.205375

Homodimer 6 RR configuration syn conformation OPBE/6-31G* geometry
E(SCF) OPBE/6-31G* = -1869.77440
E(SCF) CAM-B3LYP = -1869.78008

78
title
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C   -0.795545  1.434317  1.618261
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C   -0.691261  1.421613 -0.736408
C    0.030281  0.791200  0.503786
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C    1.481389  1.333166  0.456355
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C    2.640273 -2.771216  3.235989
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Homodimer 6 RR configuration +synclinal) conformation OPBE/6-31G* geometry
E(SCF) OPBE/6-31G* = -1869.77102
E(SCF) CAM-B3LYP = -1869.77854
78 title
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C      2.108259    1.060965    2.036501
N     -1.293832    2.122989    1.520301
C     -1.062888    1.703478    0.168917
C      0.193915    0.765636    0.215242
N     -0.633797    2.796039   -0.727969
C      0.349345    2.348070   -1.697070
C      1.038421    1.149458   -1.035108
C     -1.276965    3.989227   -0.798305
C     -0.678879    5.000265   -1.796604
N      0.704518    4.697836   -2.115562
C      1.293832    3.472409   -2.123387
C     -0.851853    6.450452   -1.287231
C     -0.643122    7.476976   -2.405840
C      0.003270    6.763584   -0.056407
O      2.453821    3.272766   -2.469675
O     -2.275540    4.266853   -0.127282
C     -2.456742   -1.667039    3.251888
C     -1.529476   -2.463653    3.931722
C     -0.246589   -2.678131    3.417346
C      0.085234   -2.067654    2.204034
C     -0.831869   -1.253734    1.514453
C     -2.108259   -1.060965    2.036501
N      1.293832   -2.122989    1.520301
C      1.062888   -1.703478    0.168917
C     -0.193915   -0.765636    0.215242
N      0.633797   -2.796039   -0.727969
C     -0.349345   -2.348070   -1.697070
C     -1.038421   -1.149458   -1.035108
C      1.276965   -3.989227   -0.798305
C      0.678879   -5.000265   -1.796604
N     -0.704518   -4.697836   -2.115562
C     -1.293832   -3.472409   -2.123387
C      0.851853   -6.450452   -1.287231
C      0.643122   -7.476976   -2.405840
C     -0.003270   -6.763584   -0.056407
O     -2.453821   -3.272766   -2.469675
O      2.275540   -4.266853   -0.127282
H      3.455106    1.517720    3.663936
H      1.810101    2.935706    4.874905
H     -0.470746    3.309918    3.942783
H      2.841411    0.447060    1.514259
H     -1.883896    2.943759    1.610868
H     -1.965996    1.238303   -0.251089
H     -0.164788    2.017097   -2.621682
H      2.060292    1.423324   -0.753757
H      1.119779    0.326556   -1.753914
H     -1.301387    4.905363   -2.710105
H      1.290122    5.451926   -2.455396
H     -1.907579    6.495691   -0.981599
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H	0.400516	7.526453	-2.752587
H	-0.900908	8.483031	-2.047309
H	-1.277373	7.263763	-3.278370
H	-0.231355	7.770250	0.315970
H	-0.190235	6.055441	0.758784
H	1.079264	6.737395	-0.278337
H	-3.455106	-1.517720	3.663936
H	-1.810101	-2.935706	4.874905
H	0.470746	-3.309918	3.942783
H	-2.841411	-0.447060	1.514259
H	1.883896	-2.943759	1.610868
H	1.965996	-1.238303	-0.251089
H	0.164788	-2.017097	-2.621682
H	-2.060292	-1.423324	-0.753757
H	-1.119779	-0.326556	-1.753914
H	1.301387	-4.905363	-2.710105
H	-1.290122	-5.451926	-2.455396
H	1.907579	-6.495691	-0.981599
H	-0.400516	-7.526453	-2.752587
H	1.277373	-7.263763	-3.278370
H	0.900908	-8.483031	-2.047309
H	-1.079264	-6.737395	-0.278337
H	0.190235	-6.055441	0.758784
H	0.231355	-7.770250	0.315970

5. RDC analysis details

RDC experimental data

^{1}H-^{13}C couplings were recorded by means of F2-coupled CLIP-HSQC[7] experiments in echo-antiecho mode with time domains of 8k and 256 real points in F2 and F1 respectively. RDCs (*D*) were collected as the difference $D = T - J$ between the measured splitting in aligned (*T*) and non-aligned (*J*) conditions by superimposing visually the two components of the CH doublet. corresponds to a definition of the residual dipolar coupling between proton and carbon nuclei as,[8]

$$^1D_{CH} = -\frac{3g_C g_H m_0 \hbar}{8p^2 R_{CH}^3}(A'_x r_x^2 + A'_y r_y^2 + A'_z r_z^2)$$

being ?$_C$ and ?$_H$ the corresponding gyromagnetic ratios, μ_0 the vacuum magnetic permeability, R_{CH} the internuclear CH distance, A'_i the matrix elements of the alignment tensor in the principal frame orientation, and r^2_i the director cosines of the $\mathbf{r}_{CH}$ internuclear vector.

	$^1J_{CH}$	$^1T_{CH}$	$^1D_{CH}$
C17H17	132.09	132.49	0.4
C12H12a	136.27	143.92	7.65
C12H12ß	134.13	136.73	2.6
C16H16	139.42	149.08	9.66
C11H11	140.05	154.18	14.13
C2H2	166.28	173.03	6.75
C8H8	160.34	160.5	0.16
C6H6	161.69	168.54	6.85
Me(C17)-proR[a,b]	125.57	127.62	2.05
Me(C17)-proS[a,b]	126.29	123.9	-2.39

a) Temptavively assigned by chemical shift computation analysis (see below) b) Not used for later RDC structural fitting

RDC Analysis on MMFF94 ensemble

$^1D_{CH}$ RDCs from methylene groups are averaged

11R,15R configuration

```
Anti conformation
78
Structure #1 E=0.176
C      2.114642    7.479281   -7.186896
C      1.289177    7.464890   -6.055811
C      0.047920    6.829125   -6.096797
C     -0.349872    6.223328   -7.274762
```

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C      0.489118    6.189659   -8.389157
C      1.715632    6.843103   -8.364697
N     -1.535553    5.503397   -7.452331
C     -1.627593    5.221931   -8.874266
C     -0.203363    5.440567   -9.521903
N     -2.483123    6.195112   -9.502246
C     -1.967838    6.548663  -10.810039
C     -0.453613    6.436471  -10.687192
C     -3.846025    6.270393   -9.263505
C     -4.596703    7.211777  -10.251956
N     -3.703072    8.266964  -10.737906
C     -2.453063    7.941572  -11.221087
C     -5.898364    7.766899   -9.633390
C     -6.794533    8.407891  -10.697481
C     -5.636546    8.763365   -8.499422
O     -1.865986    8.672544  -12.010324
O     -4.416940    5.599592   -8.409294
C     -1.441599    2.433086  -12.835852
C     -1.841031    1.278461  -12.151564
C     -1.469916    1.083571  -10.820815
C     -0.697164    2.047088  -10.198468
C     -0.339060    3.223248  -10.858256
C     -0.682403    3.412805  -12.191710
N     -0.295151    2.018979   -8.859337
C      0.647492    3.112142   -8.698035
C      0.485619    4.098459   -9.921401
N      1.991850    2.605485   -8.794794
C      2.835523    3.548976   -9.501116
C      1.917733    4.230649  -10.507869
C      2.553853    1.765651   -7.846649
C      4.089779    1.573686   -8.022162
N      4.472225    1.736599   -9.427631
C      4.028361    2.831480  -10.139056
C      4.569161    0.233754   -7.422240
C      6.094759    0.193344   -7.291075
C      4.079380   -0.980009   -8.218648
O      4.636372    3.241218  -11.121049
O      1.918641    1.285170   -6.913242
H      3.070236    7.997415   -7.146864
H      1.613487    7.955829   -5.141560
H     -0.590805    6.808814   -5.219767
H      2.357918    6.895921   -9.236610
H     -2.367901    5.939028   -7.066196
H     -2.065185    4.234537   -9.041475
H     -2.358143    5.826126  -11.537335
H     -0.022048    7.424081  -10.477820
H     -0.002473    6.126040  -11.632742
H     -4.847854    6.587749  -11.120590
H     -4.090668    9.103691  -11.156405
H     -6.462961    6.926875   -9.207690
H     -6.334499    9.299325  -11.135502
H     -7.753366    8.708995  -10.261642
H     -7.005450    7.700284  -11.506144
H     -6.580324    9.076229   -8.039489
H     -5.019140    8.317932   -7.713053
H     -5.129839    9.664418   -8.860445
H     -1.720105    2.561331  -13.879497
H     -2.439157    0.526345  -12.660113
H     -1.784565    0.193999  -10.284883
H     -0.358158    4.282419  -12.752240
H      0.055640    1.123806   -8.531816
H      0.533999    3.573377   -7.713769
H      3.224962    4.270513   -8.772367
H      2.004087    3.737599  -11.485055
H      2.224343    5.264334  -10.685227
H      4.555567    2.402419   -7.471478
H      5.361891    1.379046   -9.753432
H      4.161316    0.145603   -6.406596
H      6.589065    0.212823   -8.267519
H      6.457797    1.045968   -6.707675
H      6.412058   -0.720067   -6.776303
H      4.498581   -0.997293   -9.230062
H      2.988109   -0.986695   -8.302644
H      4.377011   -1.909541   -7.721128

Distribution size=512
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Distribution type=Gaussian
RDC general Std.Dev=1 Hz
Alignment tensor
<Axx>=-1.5736e-05 stdved=8.25619e-06
 <Ayy>=-0.000181988 stdved=7.84599e-05
 <Azz>=0.000197724 stdved=8.25369e-05
Quality factors statistic
<Q>=0.175661
StdDev(Q)=0.00767921
Highest Q=0.207698
Lowest Q=0.163474

     Exp [Std.Dev]  Hz Comp [Std.Dev] Hz*
C35,H70  9.66[1.00]    11.62[0.40]
C14,H52  9.66[1.00]    11.65[0.40]
C38,H72  0.40[1.00]    2.55[0.53]
C17,H54  0.40[1.00]    2.49[0.52]
C32,H67  14.13[1.00]   12.45[0.38]
C11,H49  14.13[1.00]   12.45[0.38]
C33,H68  5.20[1.00]    4.13[0.38]
C33,H69  5.20[1.00]    4.13[0.38]
C12,H51  5.20[1.00]    4.13[0.38]
C12,H50  5.20[1.00]    4.13[0.38]
C29,H66  6.75[1.00]    6.93[0.50]
C8,H48   6.75[1.00]    6.86[0.50]
C24,H63  0.16[1.00]    -0.55[0.58]
C3,H45   0.16[1.00]    -0.52[0.58]
C23,H62  13.29[1.00]   12.84[0.47]
C2,H44   13.29[1.00]   12.89[0.46]
C22,H61  6.85[1.00]    6.49[0.82]
C1,H43   6.85[1.00]    6.41[0.84]
C27,H64  1.14[1.00]    -0.45[0.58]
C6,H46   1.14[1.00]    -0.42[0.58]

Syn conformation
78
Structure #19 E=3.9 kcal/mol
C       1.312569    8.859573  -11.228414
C       1.322961    9.535658  -10.001427
C       0.834065    8.916325   -8.850341
C       0.339595    7.628372   -8.950934
C       0.385047    6.926980  -10.156154
C       0.835492    7.549762  -11.312081
N      -0.169379    6.868237   -7.883454
C      -0.793832    5.717114   -8.513851
C      -0.196030    5.536929   -9.962784
N      -2.194110    5.967388   -8.694353
C      -2.664217    5.434028   -9.957755
C      -1.448506    5.362713  -10.873585
C      -3.090211    6.126034   -7.651402
C      -4.570327    6.242015   -8.124208
N      -4.627490    6.804767   -9.477345
C      -3.826394    6.287503  -10.477620
C      -5.429644    7.027279   -7.110183
C      -6.924678    6.858755   -7.396428
C      -5.069961    8.515635   -7.056635
O      -4.129642    6.411996  -11.657739
O      -2.751727    6.094319   -6.472672
C       2.556026    4.076430  -13.459111
C       1.969510    2.867009  -13.854115
C       1.088036    2.199249  -13.003029
C       0.812226    2.756063  -11.767293
C       1.343255    3.991127  -11.393749
C       2.249540    4.641874  -12.219378
N      -0.063440    2.214297  -10.809603
C       0.183331    2.989970   -9.605438
C       0.846964    4.363463  -10.007222
N       1.146810    2.313346   -8.786804
C       2.057784    3.252099   -8.162233
C       2.057652    4.500811   -9.035929
C       0.927577    1.084180   -8.190122
C       2.084012    0.644984   -7.242942
N       3.351425    1.236911   -7.683932
C       3.425290    2.588556   -7.963155
C       2.153119   -0.891099   -7.106590
C       3.050965   -1.308356   -5.938246
C       2.615637   -1.579321   -8.394959
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O      4.492582    3.186979   -7.912887
O     -0.113155    0.450415   -8.335330
H      1.675455    9.361053  -12.122622
H      1.706308   10.551504   -9.947289
H      0.839111    9.438407   -7.899492
H      0.806671    7.047793  -12.274157
H     -0.805757    7.393878   -7.288815
H     -0.685024    4.843776   -7.864561
H     -3.052241    4.423472   -9.772197
H     -1.498919    6.127154  -11.657827
H     -1.467898    4.407240  -11.403349
H     -4.942646    5.210896   -8.194167
H     -5.490063    7.207056   -9.823768
H     -5.249240    6.610506   -6.110428
H     -7.209000    7.302780   -8.355687
H     -7.522451    7.342247   -6.616051
H     -7.199529    5.798867   -7.415839
H     -5.647584    9.020906   -6.274803
H     -4.009486    8.660830   -6.827521
H     -5.285304    9.019619   -8.004610
H      3.257997    4.576242  -14.122654
H      2.208738    2.442094  -14.825722
H      0.635087    1.261067  -13.304740
H      2.732949    5.564760  -11.914371
H      0.066289    1.214310  -10.674450
H     -0.744525    3.081322   -9.033887
H      1.659954    3.493430   -7.167405
H      3.007778    4.611613   -9.571291
H      1.990399    5.376782   -8.386039
H      1.851843    1.086260   -6.264070
H      4.231287    0.844138   -7.371632
H      1.144724   -1.262294   -6.880288
H      4.095420   -1.027383   -6.106320
H      2.717557   -0.841458   -5.005610
H      3.017402   -2.393969   -5.796362
H      3.644700   -1.307743   -8.652543
H      1.972466   -1.315311   -9.240270
H      2.579425   -2.668163   -8.281210
Distribution size=512
Distribution type=Gaussian
RDC general Std.Dev=1 Hz
Alignment tensor
<Axx>=-0.000170255 stdved=8.50351e-06
 <Ayy>=-0.00021637 stdved=1.54785e-05
 <Azz>=0.000386625 stdved=1.54816e-05
Quality factors statistic
<Q>=0.371901
StdDev(Q)=0.00405132
Highest Q=0.390841
Lowest Q=0.36588
     Exp [Std.Dev]  Hz Comp [Std.Dev] Hz*
C35,H70  9.66[1.00]    8.73[0.45]
C14,H52  9.66[1.00]    9.02[0.45]
C38,H72  0.40[1.00]    -4.11[0.66]
C17,H54  0.40[1.00]    -4.17[0.66]
C32,H67  14.13[1.00]  10.92[0.47]
C11,H49  14.13[1.00]  11.17[0.49]
C33,H68  5.20[1.00]    7.87[0.40]
C33,H69  5.20[1.00]    7.87[0.40]
C12,H51  5.20[1.00]    7.96[0.40]
C12,H50  5.20[1.00]    7.96[0.40]
C29,H66  6.75[1.00]    6.66[0.62]
C8,H48   6.75[1.00]    6.53[0.60]
C24,H63  0.16[1.00]    2.97[0.47]
C3,H45   0.16[1.00]    3.22[0.48]
C23,H62  13.29[1.00]  9.14[0.46]
C2,H44   13.29[1.00]  9.16[0.46]
C22,H61  6.85[1.00]    10.60[0.62]
C1,H43   6.85[1.00]    10.72[0.62]
C27,H64  1.14[1.00]    1.86[0.50]
C6,H46   1.14[1.00]    2.16[0.50]
```

11R,15S configuration

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Anti conformation
78
Structure #30 E=3.6 kcal/mol
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C	-3.895939	2.791019	-0.595107
C	-3.454459	4.086329	-0.297004
C	-2.094740	4.396457	-0.342296
C	-1.197304	3.399496	-0.678319
C	-1.635478	2.121466	-1.029156
C	-2.984977	1.797130	-0.959946
N	0.184290	3.567492	-0.818889
C	0.737766	2.232098	-0.964598
C	-0.433169	1.252969	-1.380153
N	1.178350	1.753596	0.323610
C	0.973612	0.324443	0.380874
C	-0.341894	0.093403	-0.349970
C	2.272614	2.290078	0.983397
C	2.461043	1.700067	2.416497
N	2.061150	0.291354	2.547832
C	1.017752	-0.216301	1.804657
C	3.876632	1.892685	3.008029
C	4.181981	3.351925	3.354875
C	4.975206	1.307900	2.116075
O	0.364035	-1.172740	2.204218
O	2.863173	3.286470	0.578876
C	2.731570	-1.415785	-3.484561
C	3.420634	-0.547045	-4.340162
C	2.866474	0.684475	-4.691279
C	1.624854	1.022341	-4.184827
C	0.957926	0.184995	-3.289017
C	1.490205	-1.054714	-2.955948
N	0.965849	2.237323	-4.400533
C	-0.374097	2.066905	-3.865707
C	-0.361239	0.829574	-2.880132
N	-1.268408	1.680428	-4.929897
C	-2.273624	0.792281	-4.392240
C	-1.527143	-0.067332	-3.381222
C	-1.630079	2.542970	-5.950602
C	-2.502276	1.854001	-7.043775
N	-3.383514	0.791229	-6.550867
C	-3.007768	0.012476	-5.477375
C	-3.268775	2.896344	-7.891183
C	-4.396369	3.570504	-7.102881
C	-3.824529	2.283150	-9.180191
O	-3.442535	-1.125126	-5.340090
O	-1.121923	3.650165	-6.101795
H	-4.957214	2.559267	-0.537371
H	-4.174128	4.854759	-0.025495
H	-1.750702	5.401557	-0.121306
H	-3.347455	0.794787	-1.159840
H	0.632318	4.122355	-0.096428
H	1.599141	2.238734	-1.637472
H	1.801538	-0.149520	-0.163219
H	-1.172827	0.118129	0.367332
H	-0.380571	-0.900789	-0.801548
H	1.742407	2.246855	3.043183
H	2.073031	-0.095758	3.484382
H	3.912889	1.341007	3.958344
H	4.295931	3.976952	2.465226
H	5.117661	3.419547	3.921054
H	3.388612	3.780000	3.976271
H	5.947376	1.368538	2.617434
H	4.783972	0.253080	1.893960
H	5.060046	1.845528	1.166661
H	3.167521	-2.380597	-3.234736
H	4.391558	-0.834149	-4.736371
H	3.402252	1.363696	-5.346270
H	0.963119	-1.755152	-2.317531
H	0.987728	2.581710	-5.355281
H	-0.743045	3.001178	-3.434735
H	-3.024949	1.412674	-3.885547
H	-1.159682	-0.978947	-3.870633
H	-2.188870	-0.414894	-2.584229
H	-1.773852	1.344266	-7.690379
H	-3.875727	0.246058	-7.248672
H	-2.564782	3.682800	-8.193458
H	-5.173264	2.854461	-6.815136
H	-4.015956	4.043485	-6.192000
H	-4.871911	4.351491	-7.706167
H	-4.599706	1.537579	-8.976292
H	-3.028413	1.800683	-9.756741

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H     -4.269579    3.058708   -9.813039

Distribution size=512
Distribution type=Gaussian
RDC general Std.Dev=1 Hz
Alignment tensor
<Axx>=-2.30004e-05 stdved=8.25958e-06
 <Ayy>=-0.000195389 stdved=7.41e-06
 <Azz>=0.00021839 stdved=1.0955e-05
Quality factors statistic
<Q>=0.260625
StdDev(Q)=0.00506574
Highest Q=0.282534
Lowest Q=0.252762
     Exp [Std.Dev]  Hz Comp [Std.Dev] Hz*
C35,H70  9.66[1.00]    10.04[0.43]
C14,H52  9.66[1.00]    10.26[0.42]
C38,H72  0.40[1.00]    1.31[0.53]
C17,H54  0.40[1.00]    -5.51[0.61]
C32,H67  14.13[1.00]   11.88[0.38]
C11,H49  14.13[1.00]   11.83[0.38]
C33,H68  5.20[1.00]    4.94[0.36]
C33,H69  5.20[1.00]    4.94[0.36]
C12,H51  5.20[1.00]    3.96[0.35]
C12,H50  5.20[1.00]    3.96[0.35]
C29,H66  6.75[1.00]    7.70[0.50]
C8,H48   6.75[1.00]    8.15[0.49]
C24,H63  0.16[1.00]    1.56[0.57]
C3,H45   0.16[1.00]    -1.67[0.56]
C23,H62  13.29[1.00]   12.43[0.50]
C2,H44   13.29[1.00]   13.18[0.51]
C22,H61  6.85[1.00]    7.91[0.82]
C1,H43   6.85[1.00]    3.84[0.74]
C27,H64  1.14[1.00]    1.55[0.57]
C6,H46   1.14[1.00]    -1.65[0.56]

Syn conformation
78
Structure #25 E=2.9 kcal/mol
C     -2.605083   -0.923436    0.842909
C     -3.464528    0.177528    0.960648
C     -3.187289    1.364451    0.283003
C     -2.050851    1.420471   -0.501775
C     -1.235882    0.298872   -0.694331
C     -1.478188   -0.864300    0.018226
N     -1.610825    2.550844   -1.225582
C     -0.226020    2.229402   -1.544358
C     -0.120678    0.660331   -1.664230
N      0.624120    2.570634   -0.430514
C      1.615902    1.546829   -0.160992
C      1.278728    0.363728   -1.065517
C      0.641171    3.776346    0.234179
C      1.503659    3.775566    1.527915
N      1.473583    2.419432    2.107838
C      1.649113    1.280754    1.344926
C      2.940727    4.295760    1.299128
C      3.760653    4.248744    2.594868
C      2.940778    5.732613    0.765099
O      1.933658    0.205783    1.857883
O      0.039351    4.768843   -0.166726
C      0.619682   -3.626952   -3.276384
C      1.473163   -3.558018   -4.384273
C      1.683164   -2.342705   -5.035267
C      1.070271   -1.207538   -4.533851
C      0.234879   -1.265139   -3.413457
C     -0.019898   -2.480086   -2.797951
N      1.062292    0.048297   -5.166363
C      0.529081    0.950340   -4.159079
C     -0.325614    0.115034   -3.131500
N     -0.387254    1.824060   -4.821700
C     -1.770785    1.580976   -4.446228
C     -1.755048    0.232546   -3.741852
C     -0.013927    2.903898   -5.586605
C     -1.197630    3.610819   -6.301173
N     -2.222481    2.601633   -6.619001
C     -2.647427    1.662722   -5.698261
C     -1.768954    4.795563   -5.487431
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C     -2.939579    5.459194   -6.224263
C     -0.699482    5.855506   -5.200827
O     -3.704615    1.062084   -5.851182
O      1.142938    3.315066   -5.636733
H     -2.816594   -1.831689    1.403000
H     -4.343318    0.110841    1.597198
H     -3.839517    2.224818    0.385743
H     -0.807791   -1.714655   -0.025227
H     -1.693902    3.411747   -0.683966
H      0.124383    2.805321   -2.402365
H      2.602296    1.934344   -0.440140
H      1.328447   -0.597646   -0.544554
H      2.034992    0.327081   -1.858634
H      0.982910    4.409275    2.256476
H      1.590070    2.294189    3.106000
H      3.456679    3.672506    0.560918
H      3.282663    4.834106    3.387736
H      4.765337    4.654852    2.434435
H      3.881027    3.221579    2.953464
H      3.963734    6.113887    0.673311
H      2.488219    5.787541   -0.229576
H      2.389103    6.404233    1.431563
H      0.430835   -4.587832   -2.802833
H      1.943565   -4.462485   -4.761627
H      2.292565   -2.297746   -5.931585
H     -0.730167   -2.572822   -1.988327
H      1.958839    0.320917   -5.556042
H      1.354924    1.515069   -3.711868
H     -2.092030    2.372917   -3.766103
H     -1.936875   -0.565582   -4.475464
H     -2.563253    0.143508   -3.011299
H     -0.823141    3.959419   -7.271395
H     -2.846618    2.745164   -7.402837
H     -2.146420    4.443355   -4.521091
H     -2.634428    5.813473   -7.214780
H     -3.775656    4.764420   -6.352306
H     -3.317358    6.318748   -5.659895
H     -0.229524    6.206109   -6.125854
H      0.082998    5.463649   -4.543926
H     -1.136661    6.723082   -4.694471

Distribution size=512
Distribution type=Gaussian
RDC general Std.Dev=1 Hz
Alignment tensor
<Axx>=-8.81601e-05 stdved=6.49096e-06
 <Ayy>=-0.000300275 stdved=1.49574e-05
 <Azz>=0.000388435 stdved=1.44456e-05
Quality factors statistic
<Q>=0.550653
StdDev(Q)=0.00248798
Highest Q=0.560968
Lowest Q=0.546505
     Exp [Std.Dev]  Hz Comp [Std.Dev] Hz*
C35,H70  9.66[1.00]    -0.42[0.47]
C14,H52  9.66[1.00]    7.08[0.45]
C38,H72  0.40[1.00]    -0.26[0.47]
C17,H54  0.40[1.00]    7.02[0.46]
C32,H67  14.13[1.00]   9.43[0.59]
C11,H49  14.13[1.00]   11.77[0.73]
C33,H68  5.20[1.00]    8.30[0.39]
C33,H69  5.20[1.00]    8.30[0.39]
C12,H51  5.20[1.00]    4.50[0.28]
C12,H50  5.20[1.00]    4.50[0.28]
C29,H66  6.75[1.00]    2.63[0.61]
C8,H48   6.75[1.00]    2.54[0.43]
C24,H63  0.16[1.00]    4.95[0.43]
C3,H45   0.16[1.00]    0.16[0.57]
C23,H62  13.29[1.00]   8.64[0.50]
C2,H44   13.29[1.00]   9.10[0.57]
C22,H61  6.85[1.00]    10.48[0.66]
C1,H43   6.85[1.00]    8.60[0.60]
C27,H64  1.14[1.00]    7.56[0.44]
C6,H46   1.14[1.00]    -1.79[0.61]
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11S,15R configuration

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Anti conformation
78
Structure #38 E=6.8 kcal/mol
C     -8.123897    7.245693    0.049687
C     -8.285406    5.867696    0.243646
C     -7.655821    4.956841   -0.605157
C     -6.879783    5.444219   -1.639992
C     -6.664391    6.815291   -1.801457
C     -7.313816    7.728497   -0.980945
N     -6.160767    4.665721   -2.553687
C     -5.722337    5.580436   -3.598037
C     -5.742280    7.041020   -2.999089
N     -6.697980    5.593405   -4.672359
C     -7.450922    6.831461   -4.699302
C     -6.502066    7.851729   -4.074732
C     -7.068198    4.491613   -5.406258
C     -7.787059    4.829381   -6.745136
N     -8.446711    6.136211   -6.801105
C     -7.924736    7.201321   -6.099905
C     -8.733558    3.682924   -7.172722
C     -9.160050    3.812268   -8.638145
C     -9.969750    3.587460   -6.272699
O     -8.050857    8.349854   -6.508627
O     -6.694817    3.354228   -5.127745
C     -2.114495    7.910395   -5.789936
C     -1.191560    6.905725   -5.471511
C     -1.303849    6.197700   -4.274603
C     -2.336969    6.514781   -3.412764
C     -3.296459    7.472165   -3.752034
C     -3.172575    8.203579   -4.926195
N     -2.604183    5.879458   -2.195055
C     -3.598705    6.704947   -1.524912
C     -4.323524    7.574879   -2.625033
N     -2.932399    7.659931   -0.658749
C     -3.005680    9.007240   -1.187749
C     -4.278845    9.001828   -2.030582
C     -2.102658    7.323744    0.384374
C     -1.859850    8.475745    1.402889
N     -2.051622    9.832994    0.885999
C     -2.989697   10.069729   -0.095111
C     -0.494757    8.312436    2.112046
C     -0.391420    9.194501    3.359995
C      0.682360    8.592573    1.172239
O     -3.574269   11.144693   -0.164445
O     -1.743264    6.168132    0.598935
H     -8.635462    7.944008    0.708564
H     -8.908444    5.504778    1.057433
H     -7.775534    3.888724   -0.456221
H     -7.224426    8.799956   -1.125852
H     -6.647167    3.846664   -2.911204
H     -4.773263    5.249453   -4.025059
H     -8.347146    6.692400   -4.080849
H     -7.042303    8.717161   -3.676251
H     -5.832246    8.227116   -4.849572
H     -6.968623    4.896773   -7.476213
H     -8.781108    6.429098   -7.711490
H     -8.190657    2.732720   -7.084247
H     -9.783680    4.696320   -8.805244
H     -9.739365    2.935525   -8.947653
H     -8.285642    3.880806   -9.293624
H    -10.585303    2.726922   -6.556616
H     -9.686699    3.458383   -5.223161
H    -10.595609    4.482794   -6.348480
H     -2.003683    8.466239   -6.718484
H     -0.379931    6.678563   -6.158393
H     -0.593139    5.416419   -4.025834
H     -3.859730    9.002694   -5.183543
H     -1.791204    5.676702   -1.617786
H     -4.245863    6.091218   -0.894724
H     -2.117441    9.171366   -1.811554
H     -4.268675    9.795058   -2.785775
H     -5.131214    9.197633   -1.378594
H     -2.657684    8.343985    2.147837
H     -2.048683   10.577244    1.573382
H     -0.401654    7.272459    2.451514
H     -0.390793   10.259796    3.107957
H     -1.226841    9.004092    4.041727
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H      0.535823    8.982642    3.903509
H      0.689456    9.633231    0.831608
H      0.647087    7.946171    0.289499
H      1.633416    8.403399    1.681870
Distribution size=512
Distribution type=Gaussian
RDC general Std.Dev=1 Hz
Alignment tensor
<Axx>=-1.05959e-05 stdved=7.0186e-06
 <Ayy>=-0.000153907 stdved=9.62539e-05
 <Azz>=0.000164503 stdved=0.000100306
Quality factors statistic
<Q>=0.241523
StdDev(Q)=0.00576065
Highest Q=0.264612
Lowest Q=0.232289
     Exp [Std.Dev]  Hz Comp [Std.Dev] Hz*
C35,H70  9.66[1.00]    12.11[0.37]
C14,H52  9.66[1.00]    12.10[0.37]
C38,H72  0.40[1.00]    1.23[0.50]
C17,H54  0.40[1.00]    1.20[0.49]
C32,H67  14.13[1.00]   11.05[0.44]
C11,H49  14.13[1.00]   11.05[0.44]
C33,H68  5.20[1.00]    7.71[0.33]
C33,H69  5.20[1.00]    7.71[0.33]
C12,H51  5.20[1.00]    7.70[0.34]
C12,H50  5.20[1.00]    7.70[0.34]
C29,H66  6.75[1.00]    8.76[0.53]
C8,H48   6.75[1.00]    8.71[0.51]
C24,H63  0.16[1.00]    -0.22[0.59]
C3,H45   0.16[1.00]    -0.20[0.61]
C23,H62  13.29[1.00]   11.71[0.47]
C2,H44   13.29[1.00]   11.75[0.45]
C22,H61  6.85[1.00]    5.77[0.78]
C1,H43   6.85[1.00]    5.70[0.84]
C27,H64  1.14[1.00]    -0.20[0.58]
C6,H46   1.14[1.00]    -0.17[0.60]

Syn conformation
78
Structure #4 E=1.3 kcal/mol
C     -3.494019   11.284684   -3.689648
C     -2.298582   10.925709   -4.327607
C     -1.855690    9.602167   -4.307506
C     -2.620075    8.661470   -3.643515
C     -3.848023    8.999975   -3.070527
C     -4.273955   10.319860   -3.048612
N     -2.313866    7.295442   -3.522573
C     -3.224599    6.798706   -2.499586
C     -4.473264    7.758985   -2.453005
N     -2.593177    6.911964   -1.205505
C     -3.279274    7.860525   -0.336866
C     -4.685565    7.946764   -0.930490
C     -1.449744    6.244987   -0.829055
C     -1.000926    6.505432    0.628565
N     -2.202801    6.597911    1.465552
C     -3.276835    7.386200    1.119697
C     -0.092651    7.750676    0.754607
C      1.173358    7.613439   -0.098758
C      0.315418    7.994314    2.212982
O     -4.093607    7.741072    1.961633
O     -0.784534    5.570827   -1.611847
C     -8.616478    9.729235   -3.310282
C     -9.475839    9.036590   -2.446183
C     -9.100895    7.801025   -1.915978
C     -7.869432    7.280176   -2.265681
C     -6.979725    8.000067   -3.066265
C     -7.361548    9.207745   -3.631704
N     -7.346401    6.051412   -1.828644
C     -6.198752    5.806808   -2.692214
C     -5.701081    7.196480   -3.244125
N     -6.626019    5.054720   -3.848922
C     -6.485940    5.814721   -5.084968
C     -5.448832    6.883701   -4.739760
C     -7.149793    3.782702   -3.808414
C     -7.489281    3.180152   -5.192469
N     -6.452477    3.604208   -6.140530
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C     -6.049616    4.916108   -6.246295
C     -8.913988    3.550894   -5.666012
C     -9.980567    3.064083   -4.678454
C     -9.210529    2.958278   -7.049345
O     -5.474868    5.318562   -7.251086
O     -7.415151    3.205670   -2.756569
H     -3.815716   12.323656   -3.695832
H     -1.707630   11.684555   -4.834614
H     -0.927591    9.322690   -4.794693
H     -5.187057   10.613639   -2.540557
H     -1.336128    7.105850   -3.312911
H     -3.449872    5.743999   -2.677315
H     -2.760451    8.823581   -0.394811
H     -5.175554    8.890308   -0.667621
H     -5.295845    7.138853   -0.513119
H     -0.472330    5.607963    0.972057
H     -2.142335    6.374760    2.451767
H     -0.626258    8.642993    0.407644
H      1.728778    6.705058    0.157953
H      1.839203    8.470221    0.051983
H      0.932399    7.578851   -1.165665
H      0.987565    8.855895    2.290037
H     -0.555694    8.207011    2.840685
H      0.833141    7.123875    2.630181
H     -8.931009   10.681096   -3.732204
H    -10.444715    9.460316   -2.193475
H     -9.766672    7.259664   -1.252280
H     -6.713563    9.743549   -4.318151
H     -8.019612    5.288104   -1.833394
H     -5.447795    5.216585   -2.160763
H     -7.455428    6.261855   -5.330269
H     -5.539690    7.757699   -5.393471
H     -4.447485    6.467915   -4.893990
H     -7.383236    2.091747   -5.108922
H     -6.259952    3.035718   -6.956511
H     -9.013461    4.639568   -5.745037
H     -9.900889    1.985155   -4.507820
H     -9.890909    3.572110   -3.713355
H    -10.986800    3.272424   -5.058238
H     -9.101768    1.868367   -7.044993
H     -8.537616    3.365774   -7.810410
H    -10.233436    3.194267   -7.362420

Distribution size=512
Distribution type=Gaussian
RDC general Std.Dev=1 Hz
Alignment tensor
<Axx>=-8.45825e-05 stdved=6.04273e-06
 <Ayy>=-0.00034618 stdved=1.67466e-05
 <Azz>=0.000430763 stdved=1.53055e-05
Quality factors statistic
<Q>=0.361207
StdDev(Q)=0.00361344
Highest Q=0.384417
Lowest Q=0.355815

     Exp [Std.Dev]  Hz Comp [Std.Dev] Hz*
C35,H70  9.66[1.00]   6.23[0.43]
C14,H52  9.66[1.00]   6.23[0.42]
C38,H72  0.40[1.00]   6.26[0.43]
C17,H54  0.40[1.00]   6.27[0.42]
C32,H67  14.13[1.00]  15.17[0.69]
C11,H49  14.13[1.00]  15.16[0.67]
C33,H68  5.20[1.00]   5.87[0.29]
C33,H69  5.20[1.00]   5.87[0.29]
C12,H51  5.20[1.00]   5.86[0.30]
C12,H50  5.20[1.00]   5.86[0.30]
C29,H66  6.75[1.00]   7.28[0.56]
C8,H48   6.75[1.00]   7.27[0.55]
C24,H63  0.16[1.00]   2.81[0.54]
C3,H45   0.16[1.00]   2.82[0.56]
C23,H62  13.29[1.00]  9.49[0.57]
C2,H44   13.29[1.00]  9.48[0.54]
C22,H61  6.85[1.00]   4.59[0.48]
C1,H43   6.85[1.00]   4.59[0.48]
C27,H64  1.14[1.00]   1.49[0.55]
C6,H46   1.14[1.00]   1.50[0.57]
```

```
+Synclinal conformation
78
Structure #23 E=4.1 kcal/mol
C     -6.370783    2.976834   -1.075141
C     -6.355534    2.132820   -2.194802
C     -6.062786    2.641155   -3.462048
C     -5.809962    3.993975   -3.588848
C     -5.800763    4.831603   -2.471453
C     -6.089612    4.337823   -1.207346
N     -5.436495    4.648111   -4.773584
C     -5.507059    6.069922   -4.468891
C     -5.464242    6.245654   -2.905635
N     -6.799421    6.558964   -4.890885
C     -7.653566    6.903779   -3.767210
C     -6.671494    7.181254   -2.631744
C     -7.230824    6.605358   -6.198187
C     -8.659728    7.171184   -6.386329
N     -8.852178    8.258026   -5.419015
C     -8.527261    8.119659   -4.089675
C     -9.748221    6.078356   -6.274105
C     -9.551235    4.976771   -7.321752
C    -11.152040    6.674307   -6.438359
O     -8.987411    8.877232   -3.243025
O     -6.577261    6.150218   -7.133540
C     -1.314162    4.190382   -2.946900
C     -0.991086    3.975339   -1.599446
C     -1.666621    4.663877   -0.589708
C     -2.642701    5.573730   -0.949623
C     -2.982633    5.771283   -2.289653
C     -2.318812    5.092533   -3.301515
N     -3.455730    6.294630   -0.060631
C     -4.152417    7.274260   -0.881828
C     -4.098292    6.795260   -2.379855
N     -3.412524    8.514177   -0.831627
C     -2.767708    8.824456   -2.096170
C     -3.593666    8.058428   -3.126592
C     -3.240204    9.278314    0.301385
C     -2.402990   10.563696    0.091413
N     -2.734046   11.114501   -1.228013
C     -2.764672   10.333187   -2.359607
C     -0.886397   10.317214    0.267055
C     -0.560551    9.782436    1.666224
C     -0.083986   11.602350    0.027470
O     -2.706349   10.834012   -3.476846
O     -3.636202    8.927373    1.410078
H     -6.584205    2.563710   -0.092113
H     -6.555625    1.071465   -2.072113
H     -6.022870    1.983932   -4.323727
H     -6.078160    4.975081   -0.328907
H     -5.964427    4.372462   -5.596076
H     -4.738213    6.617190   -5.020980
H     -8.298318    6.048128   -3.539615
H     -7.144963    7.012439   -1.658021
H     -6.368149    8.233911   -2.654112
H     -8.693912    7.647570   -7.373637
H     -9.515487    8.996053   -5.622589
H     -9.704644    5.603398   -5.287267
H     -9.526099    5.392108   -8.334880
H    -10.366352    4.246241   -7.276503
H     -8.619756    4.428082   -7.152106
H    -11.915235    5.889671   -6.394305
H    -11.377595    7.389406   -5.640937
H    -11.253383    7.190351   -7.399185
H     -0.790850    3.634779   -3.721505
H     -0.221048    3.253819   -1.338623
H     -1.436838    4.477071    0.453527
H     -2.577653    5.229750   -4.346533
H     -2.966819    6.692047    0.735736
H     -5.155184    7.459100   -0.487233
H     -1.734169    8.463508   -2.062146
H     -2.993850    7.832054   -4.015296
H     -4.431594    8.678645   -3.463970
H     -2.758099   11.305779    0.816729
H     -2.623966   12.107264   -1.396568
H     -0.539557    9.571568   -0.457560
H     -0.933811   10.455483    2.445459
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H     -1.000449    8.793392    1.826772
H      0.521607    9.677576    1.800697
H     -0.403132   12.400861    0.705894
H     -0.201231   11.960027   -1.000367
H      0.985483   11.429048    0.189449
     Exp [Std.Dev]  Hz Comp [Std.Dev] Hz*
C35,H70  9.66[1.00]    4.37[0.47]
C14,H52  9.66[1.00]    4.34[0.49]
C38,H72  0.40[1.00]    4.24[0.47]
C17,H54  0.40[1.00]    4.21[0.49]
C32,H67  14.13[1.00]   0.65[0.52]
C11,H49  14.13[1.00]   0.63[0.50]
C33,H68  5.20[1.00]    5.05[0.35]
C33,H69  5.20[1.00]    5.05[0.35]
C12,H51  5.20[1.00]    5.03[0.36]
C12,H50  5.20[1.00]    5.03[0.36]
C29,H66  6.75[1.00]    4.37[0.61]
C8,H48   6.75[1.00]    4.34[0.61]
C24,H63  0.16[1.00]    -4.90[0.46]
C3,H45   0.16[1.00]    -4.87[0.49]
C23,H62  13.29[1.00]   7.74[0.69]
C2,H44   13.29[1.00]   7.73[0.69]
C22,H61  6.85[1.00]    6.40[0.54]
C1,H43   6.85[1.00]    6.36[0.56]
C27,H64  1.14[1.00]    -6.49[0.48]
C6,H46   1.14[1.00]    -6.47[0.52]

Distribution size=512
Distribution type=Gaussian
RDC general Std.Dev=1 Hz
Alignment tensor
<Axx>=-0.000101398 stdved=1.04009e-05
<Ayy>=-0.000198504 stdved=1.27153e-05
<Azz>=0.000299903 stdved=1.33912e-05
Quality factors statistic
<Q>=0.767049
StdDev(Q)=0.0018615
Highest Q=0.781559
Lowest Q=0.764277
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11S,15S configuration

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Anti conformation
78
Structure #2 E=0.2
C     -5.128314   -1.576138   -3.423616
C     -4.140305   -1.989100   -4.327405
C     -3.043164   -1.170446   -4.597300
C     -2.960659    0.054015   -3.961861
C     -3.910308    0.445262   -3.013905
C     -5.020424   -0.350082   -2.762775
N     -1.912391    0.973640   -4.095294
C     -2.395123    2.205145   -3.484390
C     -3.523792    1.814444   -2.456069
N     -3.060859    3.000340   -4.497920
C     -4.488455    3.138264   -4.250173
C     -4.648149    2.827466   -2.762381
C     -2.464082    3.483079   -5.644226
C     -3.412942    4.358786   -6.508418
N     -4.283292    5.148951   -5.633943
C     -4.979246    4.544392   -4.610765
C     -2.637271    5.225634   -7.523946
C     -1.827621    6.343142   -6.857958
C     -3.575235    5.818607   -8.580070
O     -5.971732    5.072546   -4.121733
O     -1.335392    3.154370   -5.997724
C     -1.913872    5.316433    0.158118
C     -0.544295    5.041822    0.269323
C     -0.057030    3.761083    0.006595
C     -0.954569    2.774294   -0.354763
C     -2.312706    3.056062   -0.526838
C     -2.809468    4.320058   -0.237758
N     -0.625765    1.453070   -0.684329
C     -1.891279    0.731411   -0.707443
C     -3.033676    1.784424   -0.972267
N     -2.155249    0.207441    0.618663
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C     -3.316902    0.824856    1.241451
C     -4.107538    1.412502    0.073068
C     -1.347487   -0.684874    1.292803
C     -1.923644   -1.115206    2.670043
N     -3.381682   -1.226298    2.578741
C     -4.127470   -0.201392    2.040123
C     -1.256405   -2.402637    3.200740
C     -1.632606   -3.646977    2.389604
C     -1.579598   -2.627008    4.681270
O     -5.323285   -0.091135    2.287109
O     -0.233754   -1.010521    0.892163
H     -5.984544   -2.219760   -3.233612
H     -4.228898   -2.952835   -4.822866
H     -2.272583   -1.489220   -5.291402
H     -5.806814   -0.044776   -2.080522
H     -1.565458    1.105347   -5.042612
H     -1.567814    2.800050   -3.091813
H     -5.018646    2.413192   -4.879026
H     -5.652524    2.453789   -2.535586
H     -4.522954    3.750154   -2.193794
H     -4.058996    3.655733   -7.051721
H     -4.724378    5.990575   -5.984149
H     -1.927796    4.578854   -8.056912
H     -2.475504    7.072625   -6.360861
H     -1.234707    6.882634   -7.604690
H     -1.132748    5.942789   -6.113269
H     -3.003049    6.354142   -9.345426
H     -4.143549    5.029079   -9.082873
H     -4.287483    6.525142   -8.142156
H     -2.280244    6.316662    0.379035
H      0.143673    5.830786    0.563221
H      1.003502    3.545886    0.085069
H     -3.867363    4.552612   -0.299947
H      0.074072    1.016071   -0.089009
H     -1.847422   -0.117589   -1.392816
H     -2.965757    1.602341    1.930269
H     -4.725262    2.259201    0.391430
H     -4.792000    0.652829   -0.307358
H     -1.708703   -0.286128    3.357986
H     -3.890014   -1.790694    3.248501
H     -0.167571   -2.280357    3.128636
H     -2.700237   -3.876341    2.470228
H     -1.391388   -3.520152    1.329691
H     -1.078820   -4.520491    2.750807
H     -2.645987   -2.814848    4.841813
H     -1.293327   -1.754859    5.278408
H     -1.027580   -3.490097    5.068984

Distribution size=512
Distribution type=Gaussian
RDC general Std.Dev=1 Hz
Alignment tensor
<Axx>=2.60981e-06 stdved=7.30214e-06
 <Ayy>=4.38666e-05 stdved=0.000177799
 <Azz>=-4.64764e-05 stdved=0.000183476
Quality factors statistic
<Q>=0.259694
StdDev(Q)=0.00539412
Highest Q=0.283706
Lowest Q=0.250853
     Exp [Std.Dev]  Hz Comp [Std.Dev] Hz*
C35,H70  9.66[1.00]    10.90[0.43]
C14,H52  9.66[1.00]    10.91[0.43]
C38,H72  0.40[1.00]    2.30[0.50]
C17,H54  0.40[1.00]    2.28[0.52]
C32,H67  14.13[1.00]   10.94[0.45]
C11,H49  14.13[1.00]   10.94[0.45]
C33,H68  5.20[1.00]    7.56[0.33]
C33,H69  5.20[1.00]    7.56[0.33]
C12,H51  5.20[1.00]    7.56[0.35]
C12,H50  5.20[1.00]    7.56[0.35]
C29,H66  6.75[1.00]    9.66[0.45]
C8,H48   6.75[1.00]    9.68[0.45]
C24,H63  0.16[1.00]    -0.73[0.61]
C3,H45   0.16[1.00]    -0.75[0.62]
C23,H62  13.29[1.00]   11.95[0.49]
C2,H44   13.29[1.00]   11.94[0.46]
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C22,H61  6.85[1.00]    5.65[0.74]
C1,H43   6.85[1.00]    5.66[0.80]
C27,H64  1.14[1.00]    -0.80[0.60]
C6,H46   1.14[1.00]    -0.82[0.62]

Syn conformation
78
Structure #19 E=5.7 kcal/mol
C      -7.244749    0.735152   -4.016679
C      -6.720335   -0.176962   -4.942914
C      -5.340314   -0.348532   -5.063223
C      -4.509624    0.402121   -4.252962
C      -5.028639    1.256900   -3.278085
C      -6.396629    1.465224   -3.181336
N      -3.105670    0.355260   -4.252560
C      -2.692925    1.518243   -3.478493
C      -3.882568    1.909334   -2.520701
N      -2.512891    2.647149   -4.362705
C      -3.475263    3.710332   -4.103486
C      -3.931860    3.449917   -2.668665
C      -1.624806    2.692890   -5.417987
C      -1.630713    4.053456   -6.170312
N      -1.809666    5.135697   -5.194295
C      -2.841218    5.093293   -4.282133
C      -0.394357    4.319660   -7.055321
C      -0.364902    3.425778   -8.297496
C       0.930272    4.227428   -6.292527
O      -3.261834    6.118963   -3.759931
O      -0.990402    1.706761   -5.779692
C      -6.770862    2.139591    1.136894
C      -6.179255    3.127058    1.936868
C      -4.838860    3.473290    1.758148
C      -4.113836    2.818689    0.780478
C      -4.718123    1.888058   -0.067749
C      -6.037028    1.507323    0.130991
N      -2.760044    3.041613    0.477226
C      -2.381013    1.924261   -0.377595
C      -3.689277    1.373633   -1.062360
N      -1.882761    0.843770    0.441883
C      -2.725326   -0.341513    0.369356
C      -3.510463   -0.158439   -0.929049
C      -0.774299    0.915139    1.259789
C      -0.463338   -0.418412    2.004221
N      -0.673295   -1.504647    1.038606
C      -1.875970   -1.616372    0.372114
C       0.953655   -0.417310    2.630156
C       1.447073   -1.819404    3.011022
C       0.990608    0.455764    3.894315
O      -2.248990   -2.696203   -0.071295
O      -0.166539    1.965772    1.442027
H      -8.321438    0.873303   -3.948700
H      -7.392263   -0.748990   -5.578035
H      -4.931201   -1.048965   -5.783568
H      -6.813735    2.183227   -2.482276
H      -2.688435    0.327103   -5.181299
H      -1.738138    1.320821   -2.984490
H      -4.298004    3.611000   -4.821415
H      -4.921004    3.879376   -2.477378
H      -3.231157    3.935929   -1.981600
H      -2.530501    4.057257   -6.800345
H      -1.526179    6.078467   -5.434530
H      -0.475078    5.352844   -7.422241
H      -0.187640    2.375799   -8.049206
H       0.435841    3.741450   -8.975408
H      -1.309054    3.492290   -8.848124
H       1.762883    4.530586   -6.936934
H       0.932560    4.889105   -5.420479
H       1.136137    3.209614   -5.948184
H      -7.810620    1.866047    1.301359
H      -6.765833    3.621401    2.707364
H      -4.376693    4.232732    2.379847
H      -6.500586    0.730786   -0.469268
H      -2.160536    3.139079    1.294253
H      -1.584281    2.226769   -1.061944
H      -3.379483   -0.354021    1.248946
H      -4.455367   -0.711785   -0.908107
H      -2.920297   -0.560958   -1.759050
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H     -1.220174   -0.539948    2.790378
H     -0.239364   -2.407466    1.185526
H      1.667253   -0.000628    1.907397
H      0.717502   -2.339716    3.640751
H      1.638409   -2.430104    2.123307
H      2.391765   -1.764739    3.563476
H      0.313393    0.065462    4.662095
H      0.703891    1.490369    3.690382
H      2.000461    0.478851    4.318692
 Distribution size=512
Distribution type=Gaussian
RDC general Std.Dev=1 Hz
Alignment tensor
<Axx>=-9.38079e-05 stdved=8.17796e-06
 <Ayy>=-0.000139696 stdved=1.33076e-05
 <Azz>=0.000233504 stdved=1.05072e-05
Quality factors statistic
<Q>=0.64444
StdDev(Q)=0.00214917
Highest Q=0.652266
Lowest Q=0.641108
    Exp [Std.Dev]  Hz Comp [Std.Dev] Hz*
C35,H70  9.66[1.00]    6.66[0.45]
C14,H52  9.66[1.00]    7.36[0.50]
C38,H72  0.40[1.00]    2.77[0.50]
C17,H54  0.40[1.00]    -15.17[0.63]
C32,H67  14.13[1.00]  7.63[0.54]
C11,H49  14.13[1.00]  8.20[0.55]
C33,H68  5.20[1.00]    4.35[0.31]
C33,H69  5.20[1.00]    4.35[0.31]
C12,H51  5.20[1.00]    4.60[0.33]
C12,H50  5.20[1.00]    4.60[0.33]
C29,H66  6.75[1.00]    4.69[0.46]
C8,H48   6.75[1.00]    5.25[0.52]
C24,H63  0.16[1.00]    1.14[0.53]
C3,H45   0.16[1.00]    1.24[0.54]
C23,H62  13.29[1.00]  5.04[0.51]
C2,H44   13.29[1.00]  5.22[0.50]
C22,H61  6.85[1.00]    5.69[0.66]
C1,H43   6.85[1.00]    5.92[0.66]
C27,H64  1.14[1.00]    0.57[0.54]
C6,H46   1.14[1.00]    0.66[0.54]
```

RDC analysis of 11R,15R OPBE/6-31G* structures

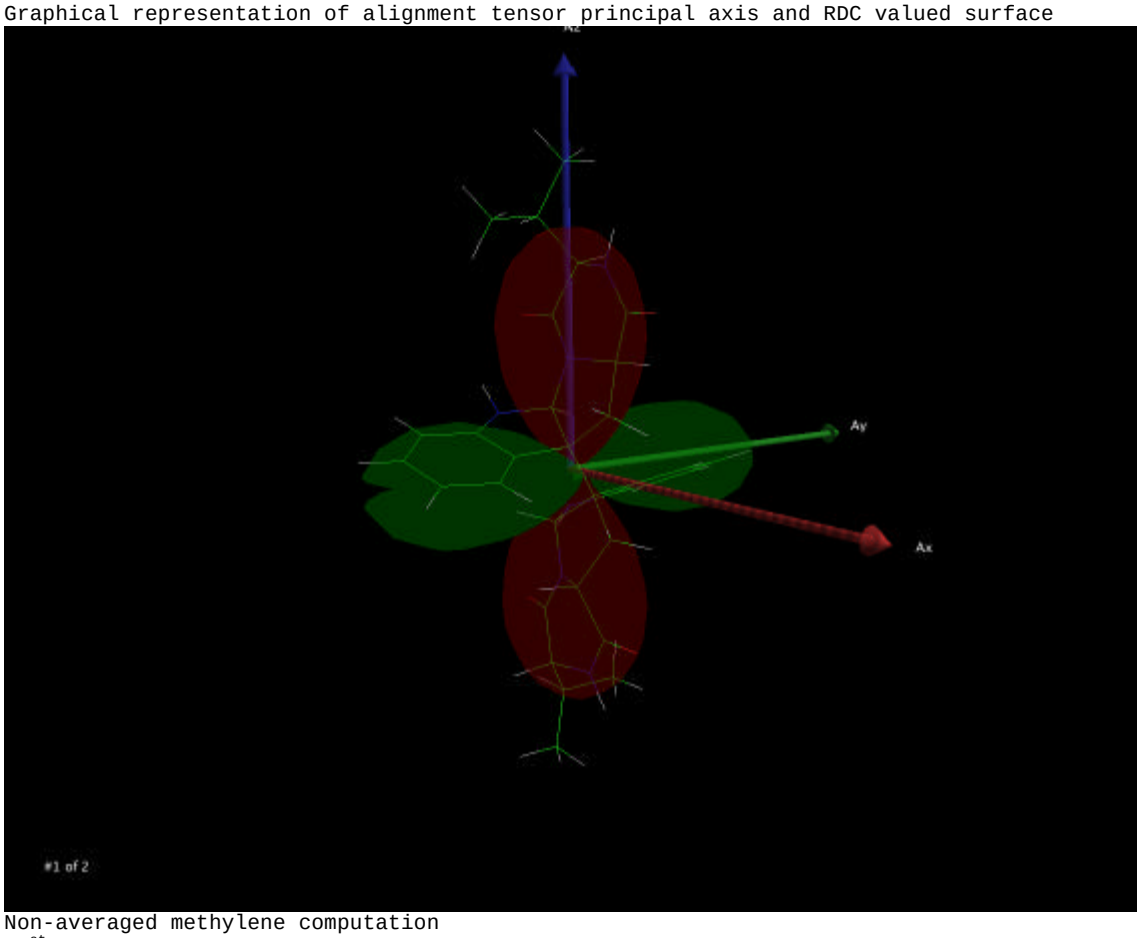
```
78
Anti conformation
C     -4.206858    0.502067    0.768514
C     -4.515613    0.990783   -0.505301
C     -3.507498    1.367202   -1.398285
C     -2.175504    1.229364   -0.988853
C     -1.844585    0.715590    0.282245
C     -2.867392    0.372821    1.166133
N     -1.027050    1.501942   -1.710985
C      0.094689    1.552416   -0.816070
C     -0.324022    0.720325    0.446758
N      0.377220    2.892438   -0.267384
C      0.867148    2.783769    1.096847
C      0.105148    1.585302    1.667717
C      0.505017    3.994697   -1.047717
C      0.910029    5.285955   -0.313304
N      0.697431    5.197347    1.119462
C      0.701339    4.075150    1.889473
C      0.203853    6.517336   -0.929086
C      0.867148    7.830526   -0.500139
C     -1.306501    6.530382   -0.680488
O      0.607279    4.090083    3.113218
O      0.319687    3.990752   -2.268769
C      4.206858   -0.502067    0.768514
C      4.515613   -0.990783   -0.505301
C      3.507498   -1.367202   -1.398285
C      2.175504   -1.229364   -0.988853
C      1.844585   -0.715590    0.282245
C      2.867392   -0.372821    1.166133
N      1.027050   -1.501942   -1.710985
```

```
C     -0.094689   -1.552416   -0.816070
C      0.324022   -0.720325    0.446758
N     -0.377220   -2.892438   -0.267384
C     -0.867148   -2.783769    1.096847
C     -0.105148   -1.585302    1.667717
C     -0.505017   -3.994697   -1.047717
C     -0.910029   -5.285955   -0.313304
N     -0.697431   -5.197347    1.119462
C     -0.701339   -4.075150    1.889473
C     -0.203853   -6.517336   -0.929086
C     -0.867148   -7.830526   -0.500139
C      1.306501   -6.530382   -0.680488
O     -0.607279   -4.090083    3.113218
O     -0.319687   -3.990752   -2.268769
H     -5.005142    0.234960    1.461388
H     -5.559240    1.097168   -0.806184
H     -3.751589    1.767926   -2.382960
H     -2.647073    0.029628    2.177338
H     -1.027431    2.203880   -2.443178
H      0.999499    1.177477   -1.311164
H      1.950624    2.558621    1.080830
H     -0.776608    1.944311    2.208663
H      0.719731    1.042447    2.390077
H      1.993344    5.400594   -0.522475
H      0.661274    6.063732    1.644556
H      0.365592    6.397543   -2.010597
H      0.723826    8.054067    0.568280
H      0.431538    8.672175   -1.056027
H      1.948253    7.825164   -0.700768
H     -1.766870    7.378808   -1.205375
H     -1.782078    5.614155   -1.052455
H     -1.551697    6.629277    0.386149
H      5.005142   -0.234960    1.461388
H      5.559240   -1.097168   -0.806184
H      3.751589   -1.767926   -2.382960
H      2.647073   -0.029628    2.177338
H      1.027431   -2.203880   -2.443178
H     -0.999499   -1.177477   -1.311164
H     -1.950624   -2.558621    1.080830
H      0.776608   -1.944311    2.208663
H     -0.719731   -1.042447    2.390077
H     -1.993344   -5.400594   -0.522475
H     -0.661274   -6.063732    1.644556
H     -0.365592   -6.397543   -2.010597
H     -0.723826   -8.054067    0.568280
H     -1.948253   -7.825164   -0.700768
H     -0.431538   -8.672175   -1.056027
H      1.551697   -6.629277    0.386149
H      1.782078   -5.614155   -1.052455
H      1.766870   -7.378808   -1.205375


Averaged methylene:
Distribution size=512
Distribution type=Gaussian
RDC general Std.Dev=1 Hz
Alignment tensor
<Axx>=-1.60565e-05 stdved=7.19343e-06
 <Ayy>=-0.000185268 stdved=5.09634e-05
 <Azz>=0.000201324 stdved=5.36099e-05
Quality factors statistic
<Q>=0.16033
StdDev(Q)=0.00791965
Highest Q=0.189794
Lowest Q=0.146754
     Exp [Std.Dev]  Hz Comp [Std.Dev] Hz*
C35,H70  9.66[1.00]   11.47[0.49]
C14,H52  9.66[1.00]   11.46[0.51]
C38,H72  0.40[1.00]   1.23[0.50]
C17,H54  0.40[1.00]   1.21[0.49]
C32,H67  14.13[1.00]  12.36[0.39]
C11,H49  14.13[1.00]  12.36[0.39]
C33,H68  5.20[1.00]   5.31[0.38]
C33,H69  5.20[1.00]   5.31[0.38]
C12,H51  5.20[1.00]   5.31[0.39]
C12,H50  5.20[1.00]   5.31[0.39]
C29,H66  6.75[1.00]   8.58[0.53]
```

C8,H48	6.75[1.00]	8.55[0.52]
C24,H63	0.16[1.00]	-0.03[0.57]
C3,H45	0.16[1.00]	-0.01[0.59]
C23,H62	13.29[1.00]	12.39[0.46]
C2,H44	13.29[1.00]	12.42[0.44]
C22,H61	6.85[1.00]	5.93[0.75]
C1,H43	6.85[1.00]	5.90[0.76]
C27,H64	1.14[1.00]	0.33[0.55]
C6,H46	1.14[1.00]	0.35[0.57]

Graphical representation of alignment tensor principal axis and RDC valued surface



Non-averaged methylene computation
#1st assignment
C12-H12beta= 2.60
C12-H12alfa= 7.65

Distribution size=512
Distribution type=Gaussian
RDC general Std.Dev=1 Hz
Alignment tensor
<Axx>=-1.62083e-05 stdved=7.15925e-06
<Ayy>=-0.000184696 stdved=4.7698e-05
<Azz>=0.000200905 stdved=5.02463e-05
Quality factors statistic
<Q>=0.157709
StdDev(Q)=0.00749792
Highest Q=0.190629
Lowest Q=0.1461

Exp [Std.Dev] Hz	Comp [Std.Dev] Hz*
C35,H70 9.66[1.00]	11.41[0.49]
C14,H52 9.66[1.00]	11.40[0.50]
C38,H72 0.40[1.00]	1.23[0.48]
C17,H54 0.40[1.00]	1.22[0.48]
C32,H67 14.13[1.00]	12.27[0.37]
C11,H49 14.13[1.00]	12.27[0.37]
C33,H68 7.65[1.00]	8.26[0.43]
C33,H69 2.60[1.00]	2.26[0.51]
C12,H51 2.60[1.00]	2.27[0.51]
C12,H50 7.65[1.00]	8.24[0.44]
C29,H66 6.75[1.00]	8.50[0.43]

```
C8,H48   6.75[1.00]   8.49[0.44]
C24,H63  0.16[1.00]   -0.02[0.52]
C3,H45   0.16[1.00]   -0.02[0.52]
C23,H62  13.29[1.00]  12.31[0.43]
C2,H44   13.29[1.00]  12.33[0.42]
C22,H61  6.85[1.00]   5.92[0.72]
C1,H43   6.85[1.00]   5.88[0.73]
C27,H64  1.14[1.00]   0.35[0.51]
C6,H46   1.14[1.00]   0.35[0.51]

#2nd assignment
C12-H12beta= 7.65
C12-H12alfa= 2.60
Distribution size=512
Distribution type=Gaussian
RDC general Std.Dev=1 Hz
Alignment tensor
<Axx>=-1.8112e-05 stdved=7.16293e-06
<Ayy>=-0.000178715 stdved=2.34133e-05
<Azz>=0.000196827 stdved=2.53097e-05
Quality factors statistic
<Q>=0.343248
StdDev(Q)=0.00372271
Highest Q=0.360848
Lowest Q=0.337962

     Exp [Std.Dev]  Hz Comp [Std.Dev] Hz*
C35,H70  9.66[1.00]   10.54[0.47]
C14,H52  9.66[1.00]   10.52[0.49]
C38,H72  0.40[1.00]   1.37[0.49]
C17,H54  0.40[1.00]   1.36[0.48]
C32,H67  14.13[1.00]  11.74[0.36]
C11,H49  14.13[1.00]  11.74[0.37]
C33,H69  7.65[1.00]   2.55[0.48]
C33,H68  2.60[1.00]   8.13[0.45]
C12,H50  2.60[1.00]   8.11[0.44]
C12,H51  7.65[1.00]   2.57[0.54]
C29,H66  6.75[1.00]   8.37[0.45]
C8,H48   6.75[1.00]   8.35[0.44]
C24,H63  0.16[1.00]   0.24[0.50]
C3,H45   0.16[1.00]   0.24[0.53]
C23,H62  13.29[1.00]  11.66[0.44]
C2,H44   13.29[1.00]  11.68[0.41]
C22,H61  6.85[1.00]   5.35[0.72]
C1,H43   6.85[1.00]   5.31[0.73]
C27,H64  1.14[1.00]   0.57[0.49]
C6,H46   1.14[1.00]   0.57[0.52]
Anti conformation
78
title
C     -1.462613    2.258294    3.789085
C     -2.640273    2.771216    3.235989
C     -2.907530    2.649866    1.867734
C     -1.969418    1.986628    1.071851
C     -0.795545    1.434317    1.618261
C     -0.531795    1.593368    2.977024
N     -2.027199    1.739985   -0.299566
C     -0.691261    1.421613   -0.736408
C      0.030281    0.791200    0.503786
N      0.129276    2.607926   -1.030545
C      1.486924    2.519231   -0.511547
C      1.481389    1.333166    0.456355
C     -0.318113    3.651908   -1.772660
C      0.671243    4.834546   -1.846995
N      1.462613    4.917970   -0.631732
C      1.933130    3.860072    0.085412
C     -0.047662    6.162032   -2.169267
C      0.933984    7.238447   -2.646796
C     -0.937614    6.667270   -1.029712
O      2.660312    3.964426    1.066463
O     -1.410103    3.662815   -2.350222
C      1.462613   -2.258294    3.789085
C      2.640273   -2.771216    3.235989
C      2.907530   -2.649866    1.867734
C      1.969418   -1.986628    1.071851
C      0.795545   -1.434317    1.618261
C      0.531795   -1.593368    2.977024
```

```
N      2.027199   -1.739985   -0.299566
C      0.691261   -1.421613   -0.736408
C     -0.030281   -0.791200    0.503786
N     -0.129276   -2.607926   -1.030545
C     -1.486924   -2.519231   -0.511547
C     -1.481389   -1.333166    0.456355
C      0.318113   -3.651908   -1.772660
C     -0.671243   -4.834546   -1.846995
N     -1.462613   -4.917970   -0.631732
C     -1.933130   -3.860072    0.085412
C      0.047662   -6.162032   -2.169267
C     -0.933984   -7.238447   -2.646796
C      0.937614   -6.667270   -1.029712
O     -2.660312   -3.964426    1.066463
O      1.410103   -3.662815   -2.350222
H     -1.257690    2.386612    4.852313
H     -3.356409    3.292209    3.873730
H     -3.813681    3.074269    1.433228
H      0.396749    1.223584    3.410002
H     -2.502849    2.410439   -0.897279
H     -0.732811    0.780438   -1.628289
H      2.186879    2.316338   -1.345589
H      1.824895    1.661334    1.442480
H      2.177452    0.563617    0.109850
H      1.334159    4.611287   -2.709243
H      1.782794    5.828432   -0.325055
H     -0.706075    5.907238   -3.013036
H      1.618306    7.573590   -1.852715
H      0.384484    8.127501   -2.985681
H      1.546965    6.886094   -3.488814
H     -1.490385    7.559032   -1.355848
H     -1.673000    5.910748   -0.731327
H     -0.359577    6.949426   -0.138417
H      1.257690   -2.386612    4.852313
H      3.356409   -3.292209    3.873730
H      3.813681   -3.074269    1.433228
H     -0.396749   -1.223584    3.410002
H      2.502849   -2.410439   -0.897279
H      0.732811   -0.780438   -1.628289
H     -2.186879   -2.316338   -1.345589
H     -1.824895   -1.661334    1.442480
H     -2.177452   -0.563617    0.109850
H     -1.334159   -4.611287   -2.709243
H     -1.782794   -5.828432   -0.325055
H      0.706075   -5.907238   -3.013036
H     -1.618306   -7.573590   -1.852715
H     -1.546965   -6.886094   -3.488814
H     -0.384484   -8.127501   -2.985681
H      0.359577   -6.949426   -0.138417
H      1.673000   -5.910748   -0.731327
H      1.490385   -7.559032   -1.355848
```

Methylene couplings averaged

```
Distribution size=512
Distribution type=Gaussian
RDC general Std.Dev=1 Hz
Alignment tensor
<Axx>=-0.000120834 stdved=1.29771e-05
 <Ayy>=-0.000199113 stdved=7.91648e-06
 <Azz>=0.000319947 stdved=1.44027e-05
Quality factors statistic
<Q>=0.477439
StdDev(Q)=0.0032864
Highest Q=0.491854
Lowest Q=0.472213
     Exp [Std.Dev]  Hz Comp [Std.Dev] Hz*
C35,H70  9.66[1.00]   8.02[0.42]
C14,H52  9.66[1.00]   8.05[0.44]
C38,H72  0.40[1.00]   0.36[0.64]
C17,H54  0.40[1.00]   0.30[0.62]
C32,H67  14.13[1.00]  7.12[0.43]
C11,H49  14.13[1.00]  7.16[0.45]
C33,H68  5.20[1.00]   7.96[0.43]
C33,H69  5.20[1.00]   7.96[0.43]
C12,H51  5.20[1.00]   7.93[0.45]
C12,H50  5.20[1.00]   7.93[0.45]
C29,H66  6.75[1.00]   6.79[0.63]
```

```
C8,H48   6.75[1.00]    6.75[0.65]
C24,H63  0.16[1.00]    4.86[0.47]
C3,H45   0.16[1.00]    4.83[0.48]
C23,H62  13.29[1.00]   9.16[0.53]
C2,H44   13.29[1.00]   9.17[0.53]
C22,H61  6.85[1.00]    12.15[0.55]
C1,H43   6.85[1.00]    12.12[0.55]
C27,H64  1.14[1.00]    3.66[0.48]
C6,H46   1.14[1.00]    3.63[0.49]


+Synclinal conformation
78 title
C      2.456742    1.667039    3.251888
C      1.529476    2.463653    3.931722
C      0.246589    2.678131    3.417346
C     -0.085234    2.067654    2.204034
C      0.831869    1.253734    1.514453
C      2.108259    1.060965    2.036501
N     -1.293832    2.122989    1.520301
C     -1.062888    1.703478    0.168917
C      0.193915    0.765636    0.215242
N     -0.633797    2.796039   -0.727969
C      0.349345    2.348070   -1.697070
C      1.038421    1.149458   -1.035108
C     -1.276965    3.989227   -0.798305
C     -0.678879    5.000265   -1.796604
N      0.704518    4.697836   -2.115562
C      1.293832    3.472409   -2.123387
C     -0.851853    6.450452   -1.287231
C     -0.643122    7.476976   -2.405840
C      0.003270    6.763584   -0.056407
O      2.453821    3.272766   -2.469675
O     -2.275540    4.266853   -0.127282
C     -2.456742   -1.667039    3.251888
C     -1.529476   -2.463653    3.931722
C     -0.246589   -2.678131    3.417346
C      0.085234   -2.067654    2.204034
C     -0.831869   -1.253734    1.514453
C     -2.108259   -1.060965    2.036501
N      1.293832   -2.122989    1.520301
C      1.062888   -1.703478    0.168917
C     -0.193915   -0.765636    0.215242
N      0.633797   -2.796039   -0.727969
C     -0.349345   -2.348070   -1.697070
C     -1.038421   -1.149458   -1.035108
C      1.276965   -3.989227   -0.798305
C      0.678879   -5.000265   -1.796604
N     -0.704518   -4.697836   -2.115562
C     -1.293832   -3.472409   -2.123387
C      0.851853   -6.450452   -1.287231
C      0.643122   -7.476976   -2.405840
C     -0.003270   -6.763584   -0.056407
O     -2.453821   -3.272766   -2.469675
O      2.275540   -4.266853   -0.127282
H      3.455106    1.517720    3.663936
H      1.810101    2.935706    4.874905
H     -0.470746    3.309918    3.942783
H      2.841411    0.447060    1.514259
H     -1.883896    2.943759    1.610868
H     -1.965996    1.238303   -0.251089
H     -0.164788    2.017097   -2.621682
H      2.060292    1.423324   -0.753757
H      1.119779    0.326556   -1.753914
H     -1.301387    4.905363   -2.710105
H      1.290122    5.451926   -2.455396
H     -1.907579    6.495691   -0.981599
H      0.400516    7.526453   -2.752587
H     -0.900908    8.483031   -2.047309
H     -1.277373    7.263763   -3.278370
H     -0.231355    7.770250    0.315970
H     -0.190235    6.055441    0.758784
H      1.079264    6.737395   -0.278337
H     -3.455106   -1.517720    3.663936
H     -1.810101   -2.935706    4.874905
H      0.470746   -3.309918    3.942783
H     -2.841411   -0.447060    1.514259
```

```
H      1.883896   -2.943759    1.610868
H      1.965996   -1.238303   -0.251089
H      0.164788   -2.017097   -2.621682
H     -2.060292   -1.423324   -0.753757
H     -1.119779   -0.326556   -1.753914
H      1.301387   -4.905363   -2.710105
H     -1.290122   -5.451926   -2.455396
H      1.907579   -6.495691   -0.981599
H     -0.400516   -7.526453   -2.752587
H      1.277373   -7.263763   -3.278370
H      0.900908   -8.483031   -2.047309
H     -1.079264   -6.737395   -0.278337
H      0.190235   -6.055441    0.758784
H      0.231355   -7.770250    0.315970

Exp [Std.Dev]  Hz Comp [Std.Dev] Hz*
C35,H70  9.66[1.00]    12.99[0.54]
C14,H52  9.66[1.00]    13.00[0.56]
C38,H72  0.40[1.00]    4.49[0.52]
C17,H54  0.40[1.00]    4.48[0.50]
C32,H67  14.13[1.00]   11.52[0.53]
C11,H49  14.13[1.00]   11.54[0.53]
C33,H68  5.20[1.00]    -0.49[0.34]
C33,H69  5.20[1.00]    -0.49[0.34]
C12,H51  5.20[1.00]    -0.48[0.33]
C12,H50  5.20[1.00]    -0.48[0.33]
C29,H66  6.75[1.00]    2.13[0.56]
C8,H48   6.75[1.00]    2.14[0.56]
C24,H63  0.16[1.00]    -2.67[0.54]
C3,H45   0.16[1.00]    -2.67[0.58]
C23,H62  13.29[1.00]   10.23[0.59]
C2,H44   13.29[1.00]   10.25[0.58]
C22,H61  6.85[1.00]    4.90[0.51]
C1,H43   6.85[1.00]    4.91[0.52]
C27,H64  1.14[1.00]    -2.24[0.54]
C6,H46   1.14[1.00]    -2.25[0.58]

Methylenes averaged
Distribution size=512
Distribution type=Gaussian
RDC general Std.Dev=1 Hz
Alignment tensor
<Axx>=-5.28717e-05 stdved=7.89546e-06
<Ayy>=-0.000265641 stdved=1.04601e-05
<Azz>=0.000318513 stdved=1.092e-05
Quality factors statistic
<Q>=0.456947
StdDev(Q)=0.00344358
Highest Q=0.482407
Lowest Q=0.452223


Multitensor analysis:
SVD fitting of alignment tensors was done using a reported procedure[9] and implemented
in python. Program is available upon request from the authors. We scanned the population
of anti conformation from 0 to 1,with a 0.01 stepsize, and the final population was
extracted when the general degree of order of the tensors are equal
Computation results without including Gaussian error for illustration purposes

Anti form, population=0.7
Alignment tensor eigenvalues and eigenvectors
Axx= 1.876e-5 ( 0.000, 0.000, 1.000)
Ayy= 1.530e-4 (-0.114,-0.993, 0.000 )
Azz=-1.718e-4 (-0.993, 0.114, 0.000 )


Syn form, population=0.3

Alignment tensor eigenvalues and eigenvectors
Axx=-8.190e-5 (-0.935, 0.355, 1.000)
Ayy=-8.793e-5 ( 0.114, 0.000, 1.000 )
Azz= 1.698e-4 (-0.355,-0.935, 0.000 )


Atom-1 Atom-2 RDC-expt RDC-calc.

rdc ['35', '70', '9.66', 11.84 ]
```

```
rdc ['14', '52', '9.66', 11.84 ]
rdc ['38', '72', '0.40', 0.11 ]
rdc ['17', '54', '0.40', 0.11 ]
rdc ['32', '67', '14.13', 13.0 ]
rdc ['11', '49', '14.13', 13.0 ]
rdc ['33', '68', '7.65', 8.13 ]
rdc ['33', '69', '2.60', 2.78 ]
rdc ['12', '51', '2.60', 2.78 ]
rdc ['12', '50', '7.65', 8.13 ]
rdc ['29', '66', '6.75', 7.40 ]
rdc ['8', '48', '6.75', 7.40 ]
rdc ['24', '63', '0.16', 0.89 ]
rdc ['3', '45', '0.16', 0.89 ]
rdc ['23', '62', '13.29', 11.95 ]
rdc ['2', '44', '13.29', 11.95 ]
rdc ['22', '61', '6.85', 5.98 ]
rdc ['1', '43', '6.85', 5.98 ]
rdc ['27', '64', '1.14', 1.02 ]
rdc ['6', '46', '1.14', 1.02 ]

Q-factor=1.525
```

6. ^{1}H chemical shift computation details

Shielding tensors were computed at the OPBE/pcS[10]-1/PCM(CHCl3)//OPBE/6-31G* level using the GIAO method.

Shifts were referenced to TMS shieldings computed at the same level of theory using the expression

$$d_{calc} \simeq s_{ref} - s_{calc}$$

	d ppm		
#	Anti	Syn	Experimental
H5	7.51	7.25	7.34
H6	6.98	7.02	6.78
H7	7.31	7.34	7.11
H8	6.75	6.83	6.62
H2	4.71	5.62	4.88
H12ß	3.14	3.20	3.18
H12a	2.68	2.49	2.79
H11	3.73	3.83	3.70
H17	2.58	2.63	2.45
Me(C17)-proR	0.95	0.96	0.94 [b]
Me(C17)-proS	0.66	0.62	0.63 [b]

a) Referenced to CHCl3 residual signal at 7.26 ppm b) Assigned according to computed shifts

7. ECD computation details

CAM-B3LYP/PCM(CHCl3)/6-31G+G**//OPBE/6-31G* electronic circular dichroism computations.
Computation were performed over 50 singlet states.

Anti conformation

Excited State	1:	Singlet-B	4.6242 eV	268.12 nm	f=0.1642	<S**2>=0.000
Excited State	2:	Singlet-A	4.6386 eV	267.29 nm	f=0.0324	<S**2>=0.000
Excited State	3:	Singlet-B	5.3890 eV	230.07 nm	f=0.1887	<S**2>=0.000
Excited State	4:	Singlet-A	5.4432 eV	227.78 nm	f=0.0533	<S**2>=0.000
Excited State	5:	Singlet-B	5.4686 eV	226.72 nm	f=0.0032	<S**2>=0.000
Excited State	6:	Singlet-A	5.4868 eV	225.97 nm	f=0.0095	<S**2>=0.000
Excited State	7:	Singlet-B	5.6249 eV	220.42 nm	f=0.0240	<S**2>=0.000
Excited State	8:	Singlet-A	5.6380 eV	219.91 nm	f=0.0010	<S**2>=0.000
Excited State	9:	Singlet-A	5.7519 eV	215.55 nm	f=0.0009	<S**2>=0.000
Excited State	10:	Singlet-B	5.7522 eV	215.54 nm	f=0.0015	<S**2>=0.000
Excited State	11:	Singlet-A	5.9341 eV	208.94 nm	f=0.0087	<S**2>=0.000
Excited State	12:	Singlet-B	5.9363 eV	208.86 nm	f=0.0519	<S**2>=0.000
Excited State	13:	Singlet-B	6.0094 eV	206.32 nm	f=0.0721	<S**2>=0.000
Excited State	14:	Singlet-A	6.0287 eV	205.66 nm	f=0.0051	<S**2>=0.000
Excited State	15:	Singlet-A	6.1347 eV	202.10 nm	f=0.0071	<S**2>=0.000
Excited State	16:	Singlet-B	6.1402 eV	201.92 nm	f=0.0162	<S**2>=0.000
Excited State	17:	Singlet-B	6.2298 eV	199.02 nm	f=0.3178	<S**2>=0.000
Excited State	18:	Singlet-A	6.2385 eV	198.74 nm	f=0.0662	<S**2>=0.000
Excited State	19:	Singlet-B	6.2963 eV	196.92 nm	f=0.3147	<S**2>=0.000
Excited State	20:	Singlet-B	6.3072 eV	196.58 nm	f=0.2648	<S**2>=0.000
Excited State	21:	Singlet-A	6.3130 eV	196.40 nm	f=0.0414	<S**2>=0.000
Excited State	22:	Singlet-A	6.3723 eV	194.57 nm	f=0.1525	<S**2>=0.000
Excited State	23:	Singlet-B	6.4354 eV	192.66 nm	f=0.2780	<S**2>=0.000
Excited State	24:	Singlet-A	6.4849 eV	191.19 nm	f=0.0000	<S**2>=0.000
Excited State	25:	Singlet-B	6.5127 eV	190.37 nm	f=0.0540	<S**2>=0.000
Excited State	26:	Singlet-A	6.5221 eV	190.10 nm	f=0.0002	<S**2>=0.000
Excited State	27:	Singlet-A	6.5615 eV	188.96 nm	f=0.0453	<S**2>=0.000
Excited State	28:	Singlet-B	6.5637 eV	188.89 nm	f=0.1132	<S**2>=0.000
Excited State	29:	Singlet-B	6.6064 eV	187.67 nm	f=0.0899	<S**2>=0.000
Excited State	30:	Singlet-A	6.6129 eV	187.49 nm	f=0.0182	<S**2>=0.000
Excited State	31:	Singlet-B	6.6340 eV	186.89 nm	f=0.1047	<S**2>=0.000
Excited State	32:	Singlet-A	6.6400 eV	186.72 nm	f=0.0181	<S**2>=0.000
Excited State	33:	Singlet-B	6.6741 eV	185.77 nm	f=0.0322	<S**2>=0.000
Excited State	34:	Singlet-A	6.6930 eV	185.24 nm	f=0.0271	<S**2>=0.000
Excited State	35:	Singlet-B	6.7039 eV	184.94 nm	f=0.0444	<S**2>=0.000
Excited State	36:	Singlet-A	6.7250 eV	184.36 nm	f=0.0369	<S**2>=0.000
Excited State	37:	Singlet-A	6.7876 eV	182.66 nm	f=0.0015	<S**2>=0.000
Excited State	38:	Singlet-B	6.8029 eV	182.25 nm	f=0.0109	<S**2>=0.000
Excited State	39:	Singlet-B	6.8220 eV	181.74 nm	f=0.0018	<S**2>=0.000
Excited State	40:	Singlet-A	6.8222 eV	181.74 nm	f=0.0636	<S**2>=0.000
Excited State	41:	Singlet-B	6.8509 eV	180.97 nm	f=0.0185	<S**2>=0.000
Excited State	42:	Singlet-A	6.8607 eV	180.72 nm	f=0.0000	<S**2>=0.000
Excited State	43:	Singlet-A	6.8836 eV	180.12 nm	f=0.0149	<S**2>=0.000
Excited State	44:	Singlet-B	6.8913 eV	179.91 nm	f=0.0046	<S**2>=0.000
Excited State	45:	Singlet-B	6.9533 eV	178.31 nm	f=0.0533	<S**2>=0.000
Excited State	46:	Singlet-A	6.9776 eV	177.69 nm	f=0.0085	<S**2>=0.000
Excited State	47:	Singlet-A	6.9978 eV	177.17 nm	f=0.0515	<S**2>=0.000
Excited State	48:	Singlet-B	7.0017 eV	177.08 nm	f=0.1005	<S**2>=0.000
Excited State	49:	Singlet-B	7.0160 eV	176.72 nm	f=0.0783	<S**2>=0.000
Excited State	50:	Singlet-A	7.0187 eV	176.65 nm	f=0.1893	<S**2>=0.000

Rotatory Strengths (R) in cgs (10**-40 erg-esu-cm/Gauss)

state	XX	YY	ZZ	R(length)	R(au)
1	125.0663	-402.3225	0.0000	-92.4187	-0.1960
2	0.0000	0.0000	125.8009	41.9336	0.0889
3	-90.0925	-584.7289	0.0000	-224.9405	-0.4771
4	0.0000	0.0000	271.5271	90.5090	0.1920
5	19.5478	-7.1694	0.0000	4.1261	0.0088
6	0.0000	0.0000	209.9140	69.9713	0.1484
7	-88.6954	-48.4715	0.0000	-45.7223	-0.0970
8	0.0000	0.0000	70.9881	23.6627	0.0502
9	0.0000	0.0000	-68.0743	-22.6914	-0.0481
10	0.1565	-12.4666	0.0000	-4.1034	-0.0087
11	0.0000	0.0000	3.4022	1.1341	0.0024
12	-156.3734	-57.7443	0.0000	-71.3726	-0.1514
13	213.7100	26.5632	0.0000	80.0911	0.1699
14	0.0000	0.0000	29.0638	9.6879	0.0205
15	0.0000	0.0000	182.1688	60.7229	0.1288
16	-79.5499	-37.3437	0.0000	-38.9645	-0.0826
17	-291.4472	-798.8967	0.0000	-363.4480	-0.7709
18	0.0000	0.0000	229.2637	76.4212	0.1621
19	-265.7031	-490.8670	0.0000	-252.1900	-0.5349

20	-96.9365	-9.2718	0.0000	-35.4028	-0.0751
21	0.0000	0.0000	430.0305	143.3435	0.3041
22	0.0000	0.0000	1179.4450	393.1483	0.8339
23	217.2657	-973.2157	0.0000	-251.9833	-0.5345
24	0.0000	0.0000	-0.0033	-0.0011	0.0000
25	223.4616	-13.0623	0.0000	70.1331	0.1488
26	0.0000	0.0000	-2.2032	-0.7344	-0.0016
27	0.0000	0.0000	146.4569	48.8190	0.1036
28	153.1911	-331.1075	0.0000	-59.3054	-0.1258
29	-32.9359	485.0153	0.0000	150.6931	0.3196
30	0.0000	0.0000	54.4571	18.1524	0.0385
31	586.1180	-164.6312	0.0000	140.4956	0.2980
32	0.0000	0.0000	-118.6551	-39.5517	-0.0839
33	2.9034	-73.4600	0.0000	-23.5189	-0.0499
34	0.0000	0.0000	-155.6233	-51.8744	-0.1100
35	-53.0823	192.7014	0.0000	46.5397	0.0987
36	0.0000	0.0000	117.8356	39.2785	0.0833
37	0.0000	0.0000	-30.8732	-10.2911	-0.0218
38	-170.5744	34.9039	0.0000	-45.2235	-0.0959
39	-123.5912	-4.8395	0.0000	-42.8102	-0.0908
40	0.0000	0.0000	88.5174	29.5058	0.0626
41	72.1910	12.4768	0.0000	28.2226	0.0599
42	0.0000	0.0000	2.0339	0.6780	0.0014
43	0.0000	0.0000	-88.1518	-29.3839	-0.0623
44	-1.5441	-6.5359	0.0000	-2.6933	-0.0057
45	-370.3314	42.0297	0.0000	-109.4339	-0.2321
46	0.0000	0.0000	-50.7830	-16.9277	-0.0359
47	0.0000	0.0000	-0.1960	-0.0653	-0.0001
48	-222.3767	178.0284	0.0000	-14.7828	-0.0314
49	113.9515	99.7224	0.0000	71.2246	0.1511
50	0.0000	0.0000	17.4276	5.8092	0.0123

Syn conformation

Excited State	1:	Singlet-B	4.7250 eV	262.40 nm	f=0.1599	<S**2>=0.000
Excited State	2:	Singlet-A	4.7562 eV	260.68 nm	f=0.0148	<S**2>=0.000
Excited State	3:	Singlet-B	5.3932 eV	229.89 nm	f=0.0001	<S**2>=0.000
Excited State	4:	Singlet-A	5.4087 eV	229.23 nm	f=0.1519	<S**2>=0.000
Excited State	5:	Singlet-A	5.4912 eV	225.79 nm	f=0.0747	<S**2>=0.000
Excited State	6:	Singlet-B	5.4931 eV	225.71 nm	f=0.0061	<S**2>=0.000
Excited State	7:	Singlet-B	5.6852 eV	218.08 nm	f=0.0043	<S**2>=0.000
Excited State	8:	Singlet-A	5.6878 eV	217.98 nm	f=0.0000	<S**2>=0.000
Excited State	9:	Singlet-A	5.7250 eV	216.57 nm	f=0.0026	<S**2>=0.000
Excited State	10:	Singlet-B	5.7442 eV	215.84 nm	f=0.0057	<S**2>=0.000
Excited State	11:	Singlet-A	5.9558 eV	208.17 nm	f=0.0008	<S**2>=0.000
Excited State	12:	Singlet-B	5.9682 eV	207.74 nm	f=0.0036	<S**2>=0.000
Excited State	13:	Singlet-A	6.0163 eV	206.08 nm	f=0.0080	<S**2>=0.000
Excited State	14:	Singlet-B	6.0423 eV	205.19 nm	f=0.0236	<S**2>=0.000
Excited State	15:	Singlet-B	6.1606 eV	201.25 nm	f=0.0060	<S**2>=0.000
Excited State	16:	Singlet-A	6.1725 eV	200.87 nm	f=0.0006	<S**2>=0.000
Excited State	17:	Singlet-B	6.2412 eV	198.66 nm	f=0.0097	<S**2>=0.000
Excited State	18:	Singlet-B	6.2757 eV	197.56 nm	f=0.0103	<S**2>=0.000
Excited State	19:	Singlet-A	6.2875 eV	197.19 nm	f=0.0178	<S**2>=0.000
Excited State	20:	Singlet-A	6.3554 eV	195.09 nm	f=0.4026	<S**2>=0.000
Excited State	21:	Singlet-A	6.3701 eV	194.64 nm	f=0.5088	<S**2>=0.000
Excited State	22:	Singlet-B	6.3711 eV	194.60 nm	f=0.2971	<S**2>=0.000
Excited State	23:	Singlet-B	6.4488 eV	192.26 nm	f=0.3757	<S**2>=0.000
Excited State	24:	Singlet-B	6.4954 eV	190.88 nm	f=0.0548	<S**2>=0.000
Excited State	25:	Singlet-A	6.5123 eV	190.38 nm	f=0.0429	<S**2>=0.000
Excited State	26:	Singlet-A	6.5694 eV	188.73 nm	f=0.1685	<S**2>=0.000
Excited State	27:	Singlet-B	6.5720 eV	188.66 nm	f=0.0781	<S**2>=0.000
Excited State	28:	Singlet-A	6.6149 eV	187.43 nm	f=0.0173	<S**2>=0.000
Excited State	29:	Singlet-B	6.6596 eV	186.17 nm	f=0.0819	<S**2>=0.000
Excited State	30:	Singlet-A	6.6656 eV	186.01 nm	f=0.0017	<S**2>=0.000
Excited State	31:	Singlet-B	6.6962 eV	185.16 nm	f=0.0424	<S**2>=0.000
Excited State	32:	Singlet-A	6.7049 eV	184.92 nm	f=0.0394	<S**2>=0.000
Excited State	33:	Singlet-B	6.7197 eV	184.51 nm	f=0.0120	<S**2>=0.000
Excited State	34:	Singlet-A	6.7243 eV	184.38 nm	f=0.0123	<S**2>=0.000
Excited State	35:	Singlet-A	6.7906 eV	182.58 nm	f=0.0003	<S**2>=0.000
Excited State	36:	Singlet-B	6.7985 eV	182.37 nm	f=0.0114	<S**2>=0.000
Excited State	37:	Singlet-B	6.8107 eV	182.04 nm	f=0.0169	<S**2>=0.000
Excited State	38:	Singlet-A	6.8343 eV	181.41 nm	f=0.1020	<S**2>=0.000
Excited State	39:	Singlet-B	6.8358 eV	181.38 nm	f=0.0338	<S**2>=0.000
Excited State	40:	Singlet-A	6.8438 eV	181.16 nm	f=0.0007	<S**2>=0.000
Excited State	41:	Singlet-B	6.8487 eV	181.03 nm	f=0.0310	<S**2>=0.000
Excited State	42:	Singlet-A	6.8736 eV	180.38 nm	f=0.0098	<S**2>=0.000
Excited State	43:	Singlet-B	6.8978 eV	179.75 nm	f=0.0402	<S**2>=0.000

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 Excited State  44:      Singlet-A      6.9256 eV  179.02 nm  f=0.0036  <S**2>=0.000
 Excited State  45:      Singlet-B      6.9448 eV  178.53 nm  f=0.1957  <S**2>=0.000
 Excited State  46:      Singlet-A      6.9481 eV  178.44 nm  f=0.1230  <S**2>=0.000
 Excited State  47:      Singlet-A      6.9668 eV  177.97 nm  f=0.0291  <S**2>=0.000
 Excited State  48:      Singlet-B      6.9932 eV  177.29 nm  f=0.0120  <S**2>=0.000
 Excited State  49:      Singlet-B      7.0710 eV  175.34 nm  f=0.0060  <S**2>=0.000
 Excited State  50:      Singlet-A      7.0822 eV  175.06 nm  f=0.0510  <S**2>=0.000
Rotatory Strengths (R) in cgs (10**-40 erg-esu-cm/Gauss)
       state          XX          YY          ZZ     R(length)     R(au)
         1       350.4401   -736.9248      0.0000   -128.8282     -0.2733
         2         0.0000      0.0000    103.6036     34.5345      0.0733
         3        -6.6579      5.2800      0.0000     -0.4593     -0.0010
         4         0.0000      0.0000   -372.6461   -124.2154     -0.2635
         5         0.0000      0.0000    -78.5866    -26.1955     -0.0556
         6       202.7481     63.0560      0.0000     88.6014      0.1879
         7        33.2825     -0.5128      0.0000     10.9232      0.0232
         8         0.0000      0.0000     -0.4898     -0.1633     -0.0003
         9         0.0000      0.0000     70.6755     23.5585      0.0500
        10       -71.5952    -28.8179      0.0000    -33.4710     -0.0710
        11         0.0000      0.0000    -14.5203     -4.8401     -0.0103
        12        -5.2626      0.1899      0.0000     -1.6909     -0.0036
        13         0.0000      0.0000    -64.0034    -21.3345     -0.0453
        14       -58.2625    252.1560      0.0000     64.6312      0.1371
        15      -142.5703    175.3897      0.0000     10.9398      0.0232
        16         0.0000      0.0000     -2.3875     -0.7958     -0.0017
        17       165.8395     64.6733      0.0000     76.8376      0.1630
        18      -135.7907    159.4934      0.0000      7.9009      0.0168
        19         0.0000      0.0000     23.5244      7.8415      0.0166
        20         0.0000      0.0000     23.7921      7.9307      0.0168
        21         0.0000      0.0000   -558.9273   -186.3091     -0.3952
        22       810.9623   -744.9502      0.0000     22.0040      0.0467
        23         2.5605   -940.6403      0.0000   -312.6933     -0.6633
        24        42.9139    695.5024      0.0000    246.1388      0.5221
        25         0.0000      0.0000    265.4920     88.4973      0.1877
        26         0.0000      0.0000    -17.2826     -5.7609     -0.0122
        27       324.3851   -194.4707      0.0000     43.3048      0.0919
        28         0.0000      0.0000     89.5623     29.8541      0.0633
        29       290.9703    -69.7960      0.0000     73.7248      0.1564
        30         0.0000      0.0000     19.1179      6.3726      0.0135
        31       -88.0094   -165.2873      0.0000    -84.4323     -0.1791
        32         0.0000      0.0000    -51.1345    -17.0448     -0.0362
        33        58.4546     12.1587      0.0000     23.5377      0.0499
        34         0.0000      0.0000    103.3739     34.4580      0.0731
        35         0.0000      0.0000     -9.5404     -3.1801     -0.0067
        36        27.1376     19.4249      0.0000     15.5208      0.0329
        37       -24.9521      8.4646      0.0000     -5.4958     -0.0117
        38         0.0000      0.0000   -998.7879   -332.9293     -0.7062
        39       174.8003    114.1264      0.0000     96.3089      0.2043
        40         0.0000      0.0000    -59.4813    -19.8271     -0.0421
        41         1.0336      5.3054      0.0000      2.1130      0.0045
        42         0.0000      0.0000    -82.4070    -27.4690     -0.0583
        43       268.9592    121.0070      0.0000    129.9887      0.2757
        44         0.0000      0.0000     14.4825      4.8275      0.0102
        45       727.8930    396.9687      0.0000    374.9539      0.7953
        46         0.0000      0.0000  -1153.3591   -384.4530     -0.8155
        47         0.0000      0.0000    -67.5841    -22.5280     -0.0478
        48       -62.9210     42.0060      0.0000     -6.9717     -0.0148
        49       -19.2927    -20.9227      0.0000    -13.4051     -0.0284
        50         0.0000      0.0000    129.9349     43.3116      0.0919
```

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