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Supporting Information

Residual-Chemical-Shift-Anisotropy-Based Enantiodifferentiation in Lyotropic Liquid Crystalline Phases Based on Helically Chiral Polyacetylenes

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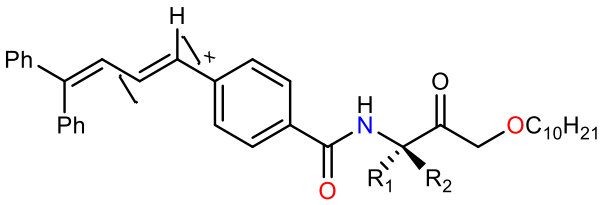
S1. Preparation of NMR sample:

The anisotropic samples of enantiomers were prepared in the lyotropic liquid crystalline phase of polyacetylene dissolved in $CDCl_3$. A total amount of 139-155 mg of the polymer (either PPA-L-Val_{dec} or PPA-D-Val_{dec}) was weighted directly into a 5 mm NMR tube.



R_1 = *i*Pr; R_2=H; x = 750: *PPA-L-Val* $_{dec}$
R_1 = H; R_2= *i*Pr; x = 1000: *PPA-D-Val* $_{dec}$

A stock solution of the analyte in $CDCl_3$ was added in such a way that the polymer concentration was approximately 17 % $w_{PPA\text{-}L\text{-}Valdec}$. Polymer concentration in the sample was computed using the equation bellow. The NMR-tube was fire sealed and the polymer was allowed to dissolve overnight. The sample was centrifuged back and forth (1000 rpm) until the ^2H signals of the solvent were sharp and the line widths constant. For both the chiral molecules, separate enantiomeric samples of the individual enantiomers are prepared. The sample concentrations of both enantiomers were the same. For the liquid crystal sample preparation, 7 mg of (+)-IPC and 7 mg of (-)-IPC were used in two 5 mm NMR tubes to prepare two separate samples. For the enantiomeric samples of indanol, 10 mg of *R*-indanol and 10 mg of *S*-indanol were used in two 3 mm NMR tube to prepare separate samples. Mass of polyacetylene and $CDCl_3$ were proportionally adjusted in the samples prepared into 3 mm NMR tubes to a concentration of approximately 17 % $w_{PPA\text{-}X\text{-}Valdec}$ (where X is either L or D) (See table below).

Table S1: Mass of chemicals used in the sample preparation of indanol enantiomers.

Enantiomer	Analyte (mg)	Lyotropic liquid crystal (mg)	$CDCl_3$ (mg)	Mass percent of lyotropic liquid crystal concentration (100 w $_{PPA\text{-}X\text{-}Valdec}$)*
S-indanol	10.2	55.1	252.0	17.4
R-indanol	10.5	55.1	251.0	17.4

* Either PPA-L-Val_{dec} or PPA-D-Val_{dec}. Sample was prepared in an 3 mm NMR tube.

Lyotropic liquid crystal mass precent in the sample was computed using the following equation:

$$w_{\mathrm{PPA-X-Valdec}} = \frac{polymer\ mass\ (mg)}{polymer\ mass\ (mg) + analyte\ mass\ (mg) + solvent\ mass\ (mg)} * 100\ (\%)$$

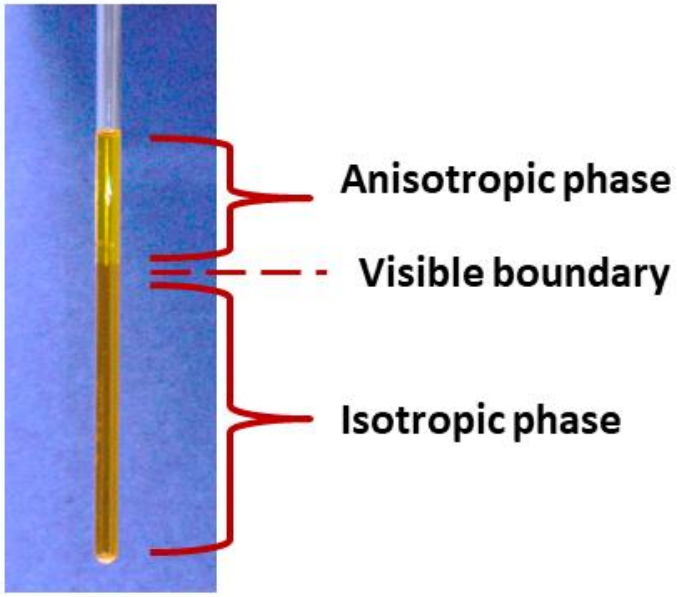


Figure S1: The photographic image of a sample in the NMR tube embedded in the biphasic PLA liquid crystal. The light-yellow phase on the top corresponds to the anisotropic phase while dark-brownish phase in the lower half of the 3 mm tube corresponds to the isotropic phase.

S2. Experimental details:

All the NMR spectra were measured in a Bruker NEO 800 MHz spectrometer with a nominal ^{13}C NMR frequency of 201.29 MHz for the anisotropic samples of *R*-indanol, *S*-indanol, (+)-IPC and (-)-IPC. A standard Bruker pulse sequence "zgdc30" was used for recording one dimensional ^{13}C-{^{1}H} NMR spectrum at 295 K. For indanol samples, one dimensional ^{13}C-{^{1}H} NMR spectra were acquired using 26 K data points for the spectral width of 32.7 kHz.

The number of scans used was 3072 scans with relaxation delay of 2 s between transients, and acquisition time is 1 s.

S3. NMR data tables

Table S2: Experimental ^{13}C RCSA values for the enantiomers of indanol from L-valine derived polyacetylene LLC, which were collected on an 800 MHz spectrometer when C7a is taken as reference.

Atom	*R*-indanol ΔRCSA(Hz)	*S*-indanol ΔRCSA(Hz)
C1	36.3	-11.6
C2	22.2	-6.4
C3	57.5	8.9
C3a	44.3	-6.3
C4	40.0	23.5
C5	-3.9	-4.9
C6	47.1	-4.9
C7	37.4	18.6
C7a	reference	reference

Table S3: Experimental ^{13}C RCSA values for the enantiomers of indanol from L-valine derived polyacetylene LLC which were collected on an 800 MHz spectrometer when C7a is taken as reference, in which RCSA data of R-indanol was normalised.

Atom	*R*-indanol ΔRCSA(Hz)	*S*-indanol ΔRCSA(Hz)
C1	31.4	-11.6
C2	19.2	-6.4
C3	49.6	8.9
C3a	38.3	-6.3
C4	34.5	23.5
C5	-3.4	-4.9
C6	40.7	-4.9
C7	32.3	18.6
C7a	reference	reference

[a] The concentration of isotropic and anisotropic phases in the two samples may not be identical and thus the RCSA data was normalised by the ratio of quadrupolar splitting of the two samples in Hz [$^{1}\delta_{(R),\mathrm{norm}} = {}^{1}\delta_{(R),\mathrm{meas}} * (57/66)$]

Table S4: Experimental ^{13}C RCSA values for the enantiomers of IPC molecule from L-valine derived polyacetylene LLC which were collected on an 800 MHz spectrometer when C2 is taken as reference.

Atom	(+)-IPC ΔRCSA(Hz)	(-)-IPC ΔRCSA(Hz)
C1	1.3	-3.2
C2	reference	reference
C3	1.3	2.7
C4	6.1	-0.1
C5	7.6	-2.7
C6	9.3	-5.1
C7	1.1	2.3
C8	3.2	0.8
C9	9.5	-7.9
C10	6.8	-4.3

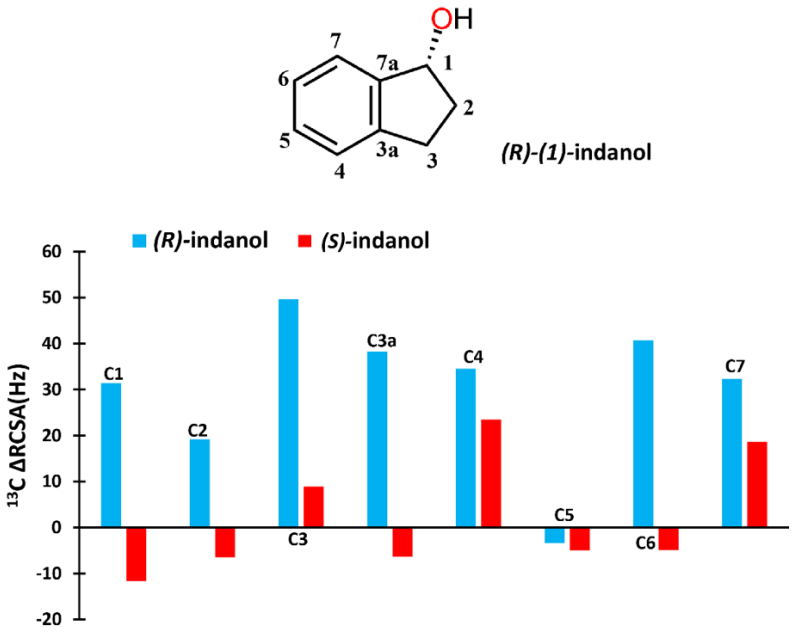


Figure S2: The carbon residual chemical shift anisotropy (^{13}C ΔRCSA) values in Hz for *R*-indanol (blue bar) and *S*-indanol (red bar) aligned in the LLC phase of L-valine derived polyacetylene. The C7a is taken as a reference to extract the RCSA values.

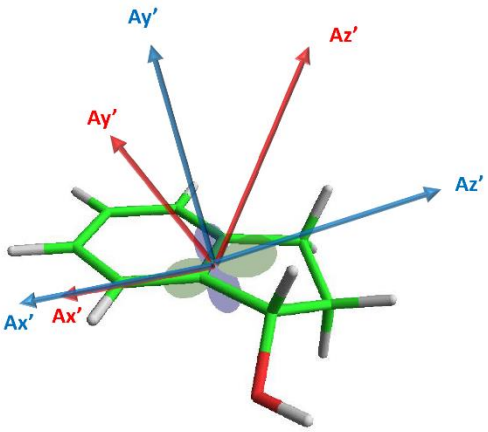


Figure S3: The RCSA data of *R* and *S* indanol enantiomers (which were measured in the polyacetylene liquid crystal with same configuration) were both SVD fitted into S-indanol. It should be noted that since the tensor is inversion symmetric, it does not matter which configuration one chooses. The principal axes of the alignment tensors obtained using RCSA data for *R*-enantiomer are shown as reddish solid arrow, and for *S*-indanol as blue solid arrow. The least ordered axes A_x have the same directions. For clarity, the pictorial representation of

the 3D surface of the alignment tensor obtained using *S*-indanol RCSA data is shown. As clearly seen here, the alignment tensors obtained from RCSA data for *R*- and *S*-indanol have different orientations relative to each other. The GCB value of 0.78 was reported in the main text.

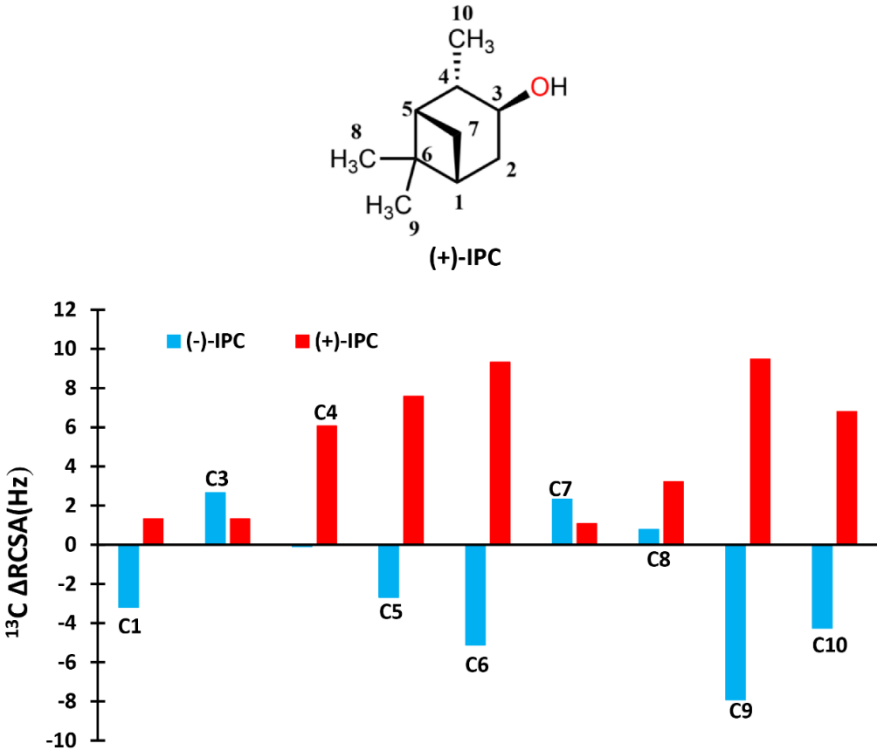


Figure S4: ^{13}C ΔRCSA values (in Hz) for (-)-IPC (blue bar) and (+)-IPC (red bar) aligned in the LLC phase of polyacetylene. The carbon C2 is taken as a reference to extract the RCSA values.

S4: Orientation properties of enantiomeric analytes

Table S5: Orientational properties of *R*-indanol and *S*-indanol aligned in the LLC phase of L-valine derived polyacetylene. $\Delta\nu_Q$ denotes the absolute value of the quadrupolar splitting of the solvent while *D*a represents the axial component of the alignment tensor. The angles α, β, and γ are the Euler angles relating the principal axis system and the initial molecular axis frame.

Analyte ***($\Delta\nu_Q$)***	***Da* [10^{-3}]**	***α* [°]**	***β* [°]**	***γ* [°]**
R-indanol (57 Hz)	7.94	-36.1	209.7	-54.2
S-indanol (66 Hz)	-4.03	-161.6	226.5	96.6

Table S6: Orientational properties of (+)-IPC and (-)-IPC aligned in the LLC phase of L-valine derived polyacetylene. $\Delta\upsilon_Q$ denotes the absolute value of the quadrupolar splitting of the solvent while D_a represents the axial component of the alignment tensor. The angles α, β, and γ are the Euler angles relating the principal axis system and the initial molecular axis frame.

Analyte	***Da* [10^{-3}]**	***α* [°]**	***β* [°]**	***γ* [°]**
(+)-IPC	-1.30	175.3	193.9	96.6
(-)-IPC	1.24	-147.2	191.4	136.4

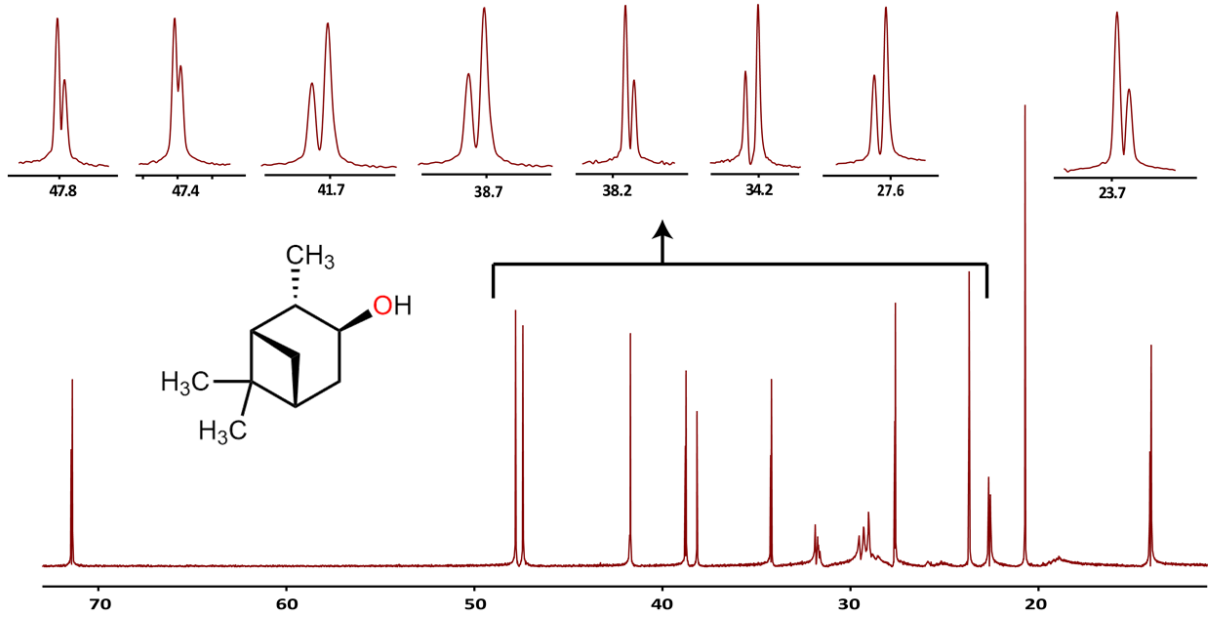


Figure S5: 1D ^{13}C-{^{1}H} NMR spectrum of (+)-IPC (201.29 MHz) aligned in PLA liquid crystal in $CDCl_3$. The inset from 23 until 50 ppm, which shows seven pairs of isotropic and anisotropic ^{13}C resonances of (+)-IPC sample, are depicted on the top.

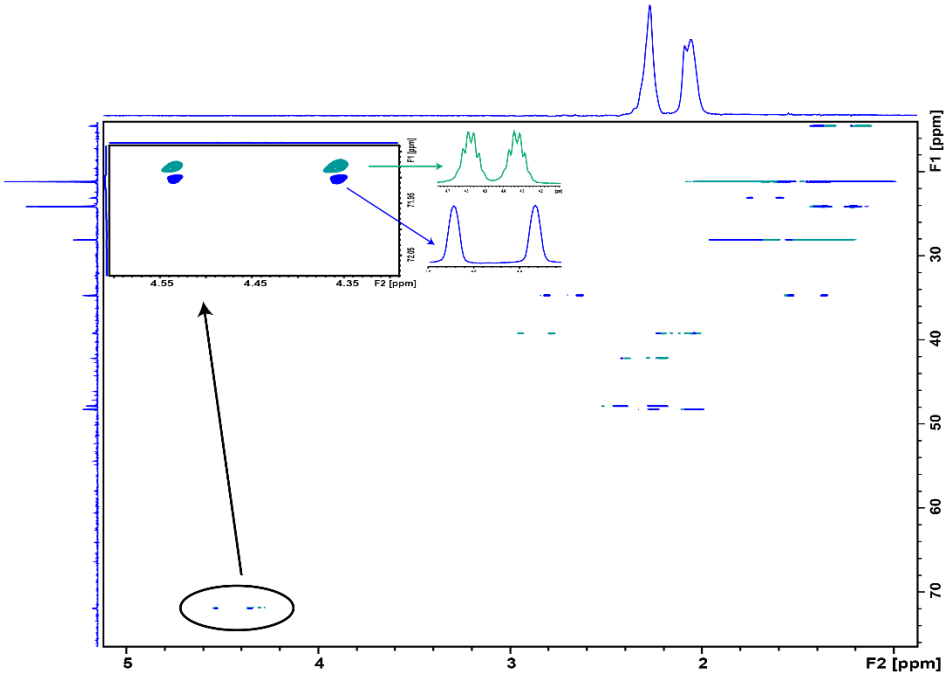
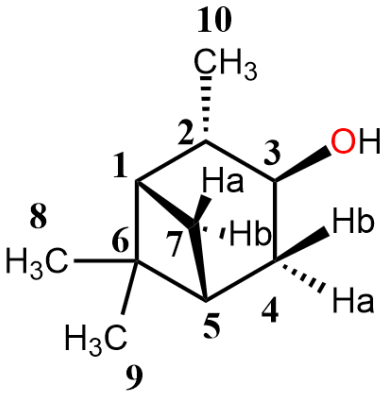


Figure S6: 800 MHz *F*2-coupled-HSQC spectrum of (+)-IPC aligned in the PLA liquid crystal in $CDCl_3$, where blue cross peaks correspond to isotropic signals and green cross peaks corresponds to anisotropic signals. The C3-H3 cross peak is zoomed in the inset and traces from the isotropic and anisotropic spectra are also shown.

S5: *F*2 traces for RDC data extraction of (+)-IPC sample

Residual dipolar couplings (RDCs) were extracted using the formula $T=J+D$; where, T is the total coupling measured in anisotropic spectrum, J is scalar coupling measured in isotropic spectrum and D is the RDC. F_2 slices (^{1}H dimension) were taken from the anisotropic (LLC phase of L-valine derived polyacetylene - blue traces) and isotropic ($CDCl_3$ alone - red traces) proton-coupled ^{1}H-^{13}C-HSQC spectra of (+)-IPC. The left submultiplet of each signal for the all carbons were stacked on top of one another so that size of the RDC can be visualized.



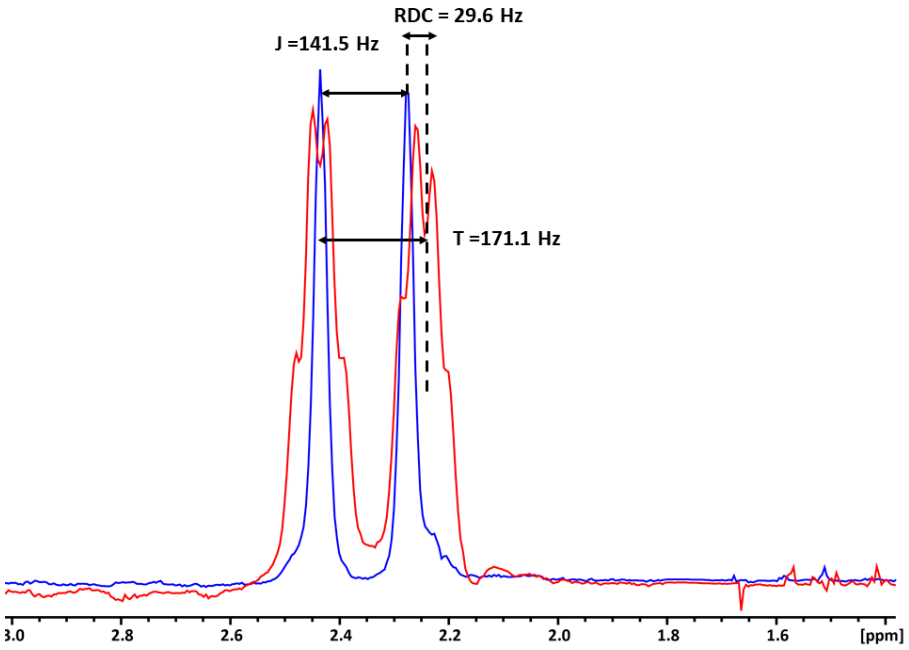


Figure S7.1: *F2* slice (^{1}H dimension) at the chemical shift of C1 (49.1 ppm)

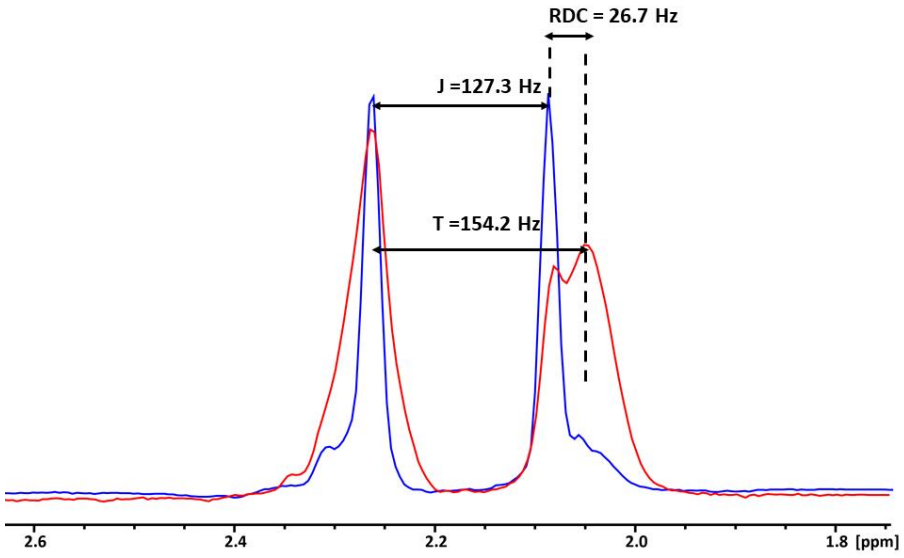


Figure S7.2: *F2* slice (^{1}H dimension) at the chemical shift of C2 (48.9 ppm)

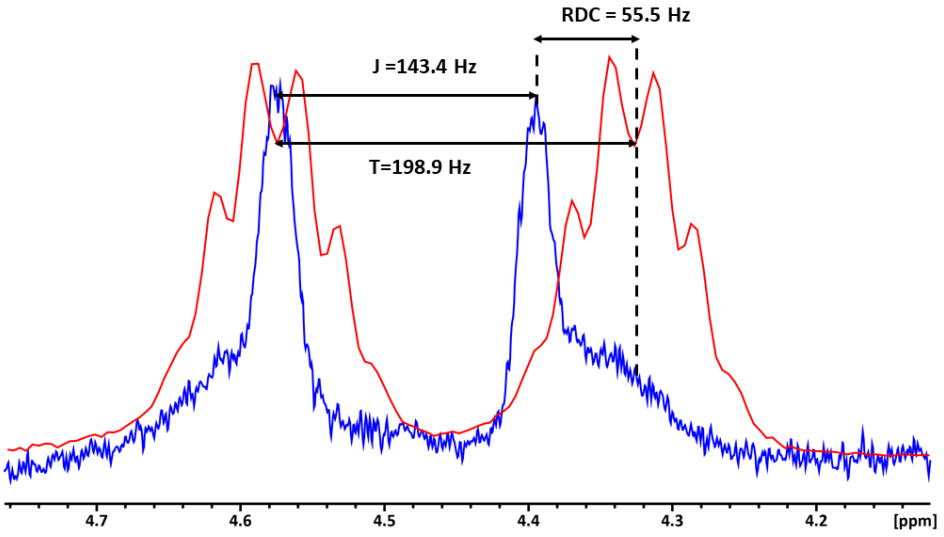


Figure S7.3: *F*2 slice (^{1}H dimension) at the chemical shift of C3 (71.9 ppm)

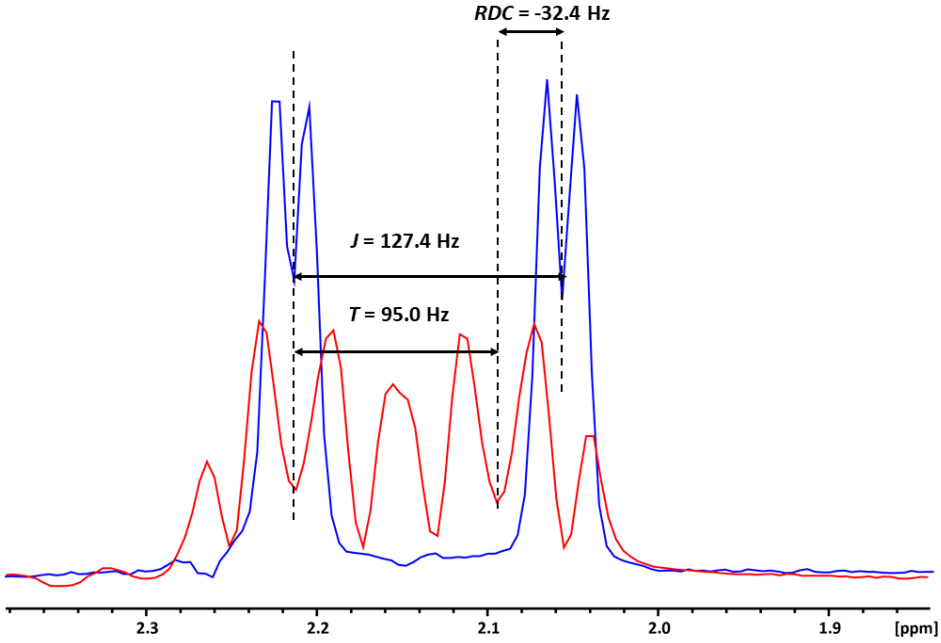


Figure S7.4: *F*2 slice (^{1}H dimension) at the chemical shift of C4-H4b (39.0 ppm)

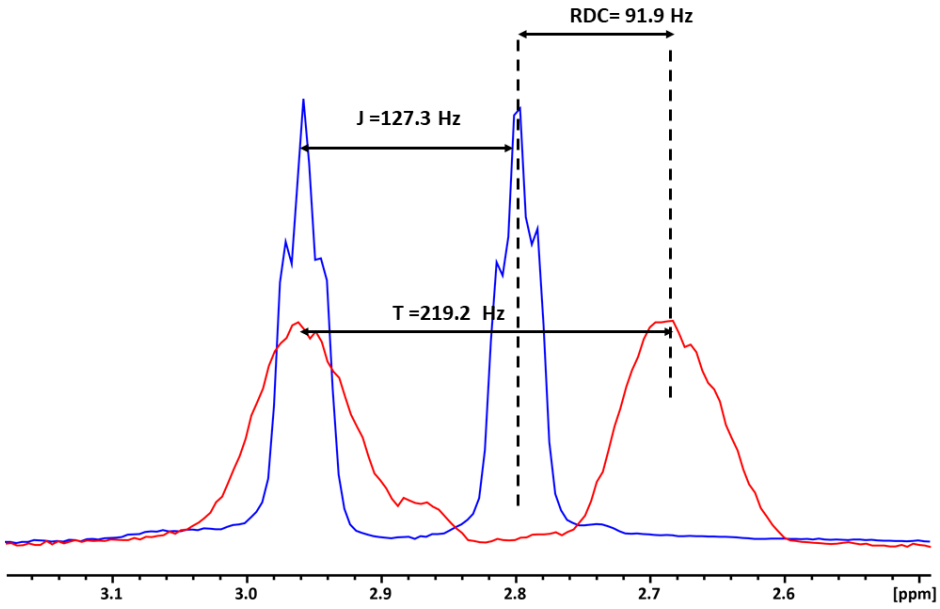


Figure S7.5: *F*2 slice (^{1}H dimension) at the chemical shift of C4-H4a (39.0 ppm)

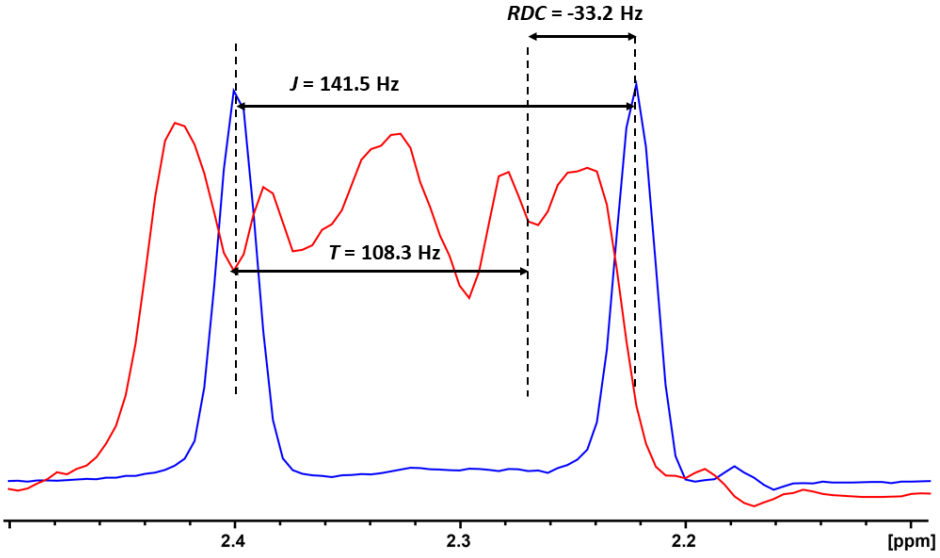


Figure S7.6: *F*2 slice (^{1}H dimension) at the chemical shift of C5 (41.9 ppm)

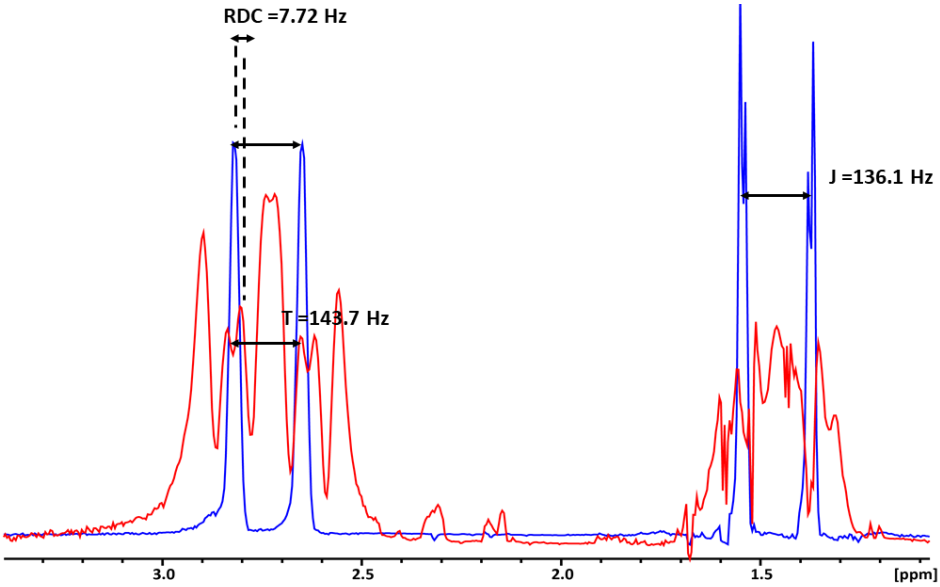


Figure S7.7: *F*2 slice (^{1}H dimension) at the chemical shift of C7-H7b (34.6 ppm) (on the left) and C7-H7a (on the right)

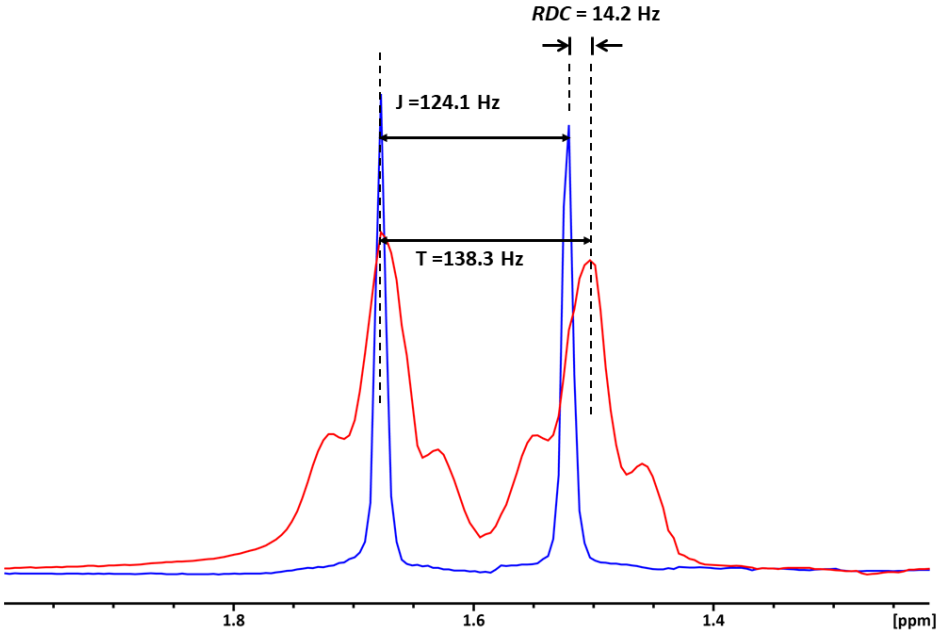


Figure S7.8: *F*2 slice (^{1}H dimension) at the chemical shift of C8 (27.9 ppm)

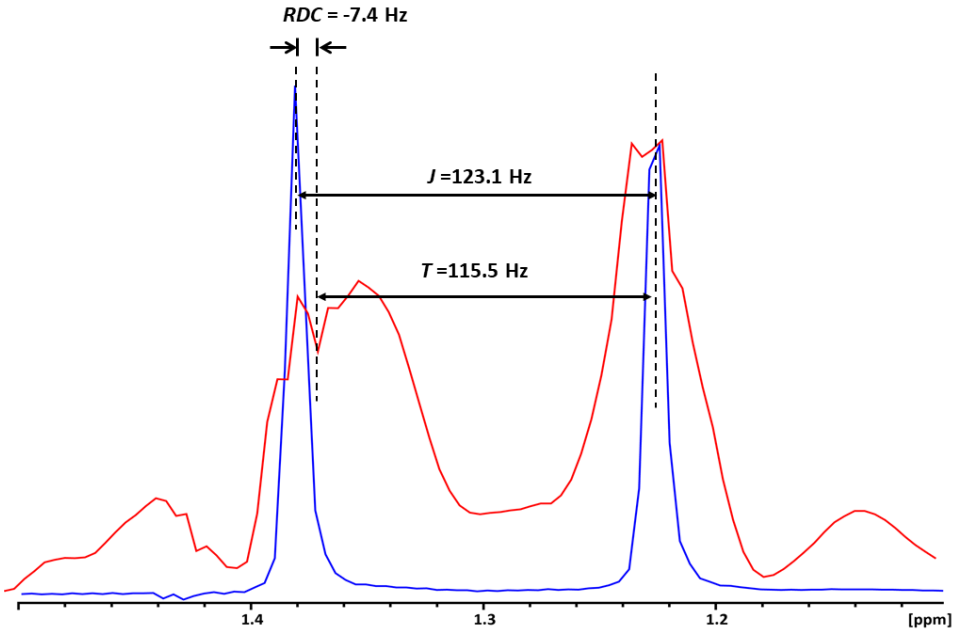


Figure S7.9: *F*2 slice (^{1}H dimension) at the chemical shift of C9-Me (23.9 ppm)

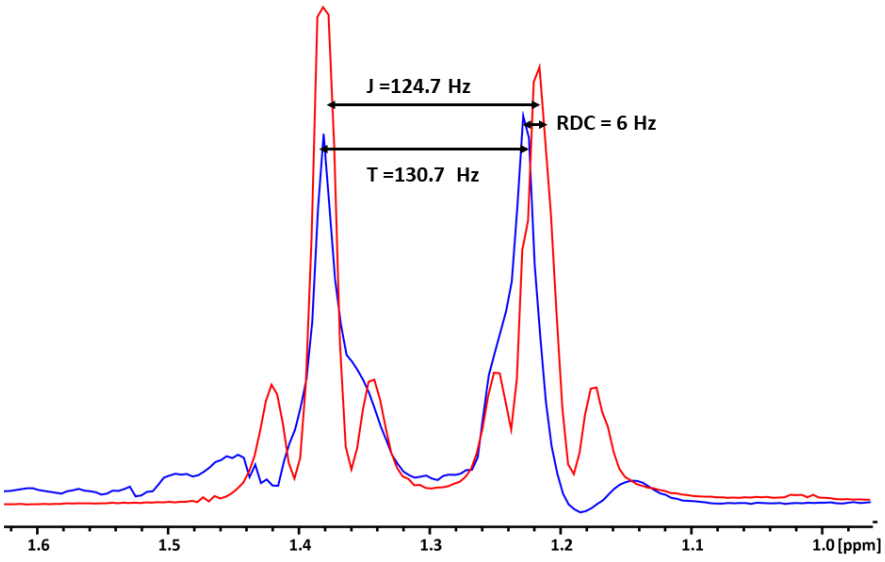


Figure S7.10: *F*2 slice (^{1}H dimension) at the chemical shift of C10-Me (20.9 ppm)

S6: Alignment tensors

Alignment tensor of Indanol	
***R*-indanol**	***S*-indanol**
Conformer 1 Alignment tensor A'x=-4.248e-04 A'y=-4.869e-03 A'z= 5.294e-03 Saupe tensor S'x=-6.372e-04 S'y=-7.303e-03 S'z= 7.941e-03 Alignment tensor eigenvectors e[x]=(-0.508, 0.826, 0.244) e[y]=(0.705, 0.236, 0.669) e[z]=(0.495, 0.512,-0.702) Alignment tensor in laboratory coordinates: [-1.229e-03,7.119e-04,-4.085e-03] [7.119e-04,8.261e-04,-2.754e-03] [-4.085e-03,-2.754e-03,4.030e-04] SVD condition number is 3.088e+01 Axial component Aa = 7.941e-03 Rhombic component Ar = 4.444e-03 rhombicity R = 0.560 Asimmetry parameter etha =8.395e-01 GDO = 1.066e-02 Euler Angles (degrees) Set 1 (143.9,-29.7,125.8) Set 2 (-36.1,209.7,-54.2)	Conformer 1 Alignment tensor A'x= 8.212e-04 A'y= 1.866e-03 A'z=-2.687e-03 Saupe tensor S'x= 1.232e-03 S'y= 2.799e-03 S'z=-4.031e-03 Alignment tensor eigenvectors e[x]=(0.080, 0.916,-0.393) e[y]=(-0.684, 0.337, 0.647) e[z]=(0.725, 0.218, 0.654) Alignment tensor in laboratory coordinates: [-5.334e-04,-7.947e-04,-2.124e-03] [-7.947e-04,7.739e-04,-2.712e-04] [-2.124e-03,-2.712e-04,-2.405e-04] SVD condition number is 3.088e+01 Axial component Aa = -4.031e-03 Rhombic component Ar = -1.045e-03 rhombicity R = 0.259 Asimmetry parameter etha =3.888e-01 GDO = 4.827e-03 Euler Angles (degrees) Set 1 (18.4,-46.5,-83.4) Set 2 (-161.6,226.5,96.6)

Alignment tensor of IPCs	
(+)-IPC	**(-)-IPC**
Conformer 1 Alignment tensor A'x= 2.532e-04 A'y= 6.153e-04 A'z=-8.685e-04 Saupe tensor S'x= 3.798e-04 S'y= 9.230e-04 S'z=-1.303e-03 Alignment tensor eigenvectors e[x]=(0.111, 0.992, 0.055) e[y]=(-0.964, 0.094, 0.247) e[z]=(0.240,-0.080, 0.967) Alignment tensor in laboratory coordinates: [5.252e-04,-1.137e-05,-3.470e-04] [-1.137e-05,2.492e-04,9.556e-05] [-3.470e-04,9.556e-05,-7.744e-04] SVD condition number is 6.634e+00 Axial component Aa = -1.303e-03 Rhombic component Ar = -3.621e-04 rhombicity R = 0.278 Asimmetry parameter etha =4.169e-01 GDO = 1.568e-03 Euler Angles (degrees) Set 1 (-4.7,-13.9,-83.4) Set 2 (175.3,193.9,96.6)	Conformer 1 Alignment tensor A'x=-1.341e-04 A'y=-6.964e-04 A'z= 8.305e-04 Saupe tensor S'x=-2.011e-04 S'y=-1.045e-03 S'z= 1.246e-03 Alignment tensor eigenvectors e[x]=(0.710, 0.502,-0.494) e[y]=(-0.676, 0.683,-0.278) e[z]=(0.198, 0.531, 0.824) Alignment tensor in laboratory coordinates: [-3.531e-04,3.608e-04,5.165e-05] [3.608e-04,-1.241e-04,5.287e-04] [5.165e-05,5.287e-04,4.772e-04] SVD condition number is 6.634e+00 Axial component Aa = 1.246e-03 Rhombic component Ar = 5.623e-04 rhombicity R = 0.451 Asimmetry parameter etha =6.772e-01 GDO = 1.595e-03 Euler Angles (degrees) Set 1 (32.8,-11.4,-43.6) Set 2 (-147.2,191.4,136.4)

S7. Z-matrices and CSA tensors:

***S*-indanol: Conformer A:**

Symbolic Z-matrix:
Charge = 0 Multiplicity = 1

C	-1.51908	-0.69817	-0.33916
C	-2.05651	0.73752	-0.56279
C	-1.02932	1.67414	0.11856
C	0.25115	0.86724	0.05709
C	1.56821	1.28585	0.24132
C	2.59847	0.34528	0.14983
C	2.31595	-0.99891	-0.11625
C	0.99538	-1.41895	-0.2958
C	-0.02764	-0.47741	-0.21494
O	-1.9734	-1.27762	0.8924
H	-1.7766	-1.3638	-1.17711
H	-3.07602	0.85601	-0.17897
H	-2.08149	0.94408	-1.64004
H	-0.95139	2.64697	-0.38014
H	-1.30651	1.87011	1.16303
H	1.7962	2.32885	0.449
H	3.62983	0.66203	0.28326
H	3.12798	-1.71797	-0.18527
H	0.77095	-2.46354	-0.4969
H	-2.92547	-1.44138	0.79672

SCF GIAO Magnetic shielding tensor (ppm):

1 C Isotropic = 118.3976 Anisotropy = 26.2014
XX= 115.6401 YX= -2.3567 ZX= -12.1349
XY= -2.2130 YY= 122.7375 ZY= -11.0804
XZ= -12.5946 YZ= -16.0346 ZZ= 116.8152
Eigenvalues: 98.3701 120.9574 135.8652

2 C Isotropic = 157.3152 Anisotropy = 30.8073
XX= 161.0515 YX= -3.7055 ZX= -2.7833
XY= -7.8412 YY= 175.6743 ZY= -7.4415
XZ= 2.3428 YZ= 1.5177 ZZ= 135.2199
Eigenvalues: 134.9880 159.1042 177.8534

3 C Isotropic = 162.4427 Anisotropy = 31.8196
XX= 181.5659 YX= -6.4394 ZX= 8.4814
XY= -4.3015 YY= 165.8324 ZY= 3.3804
XZ= 4.7649 YZ= 11.5344 ZZ= 139.9298
Eigenvalues: 136.5772 167.0952 183.6557

4 C Isotropic = 52.0171 Anisotropy = 160.8638
XX= -5.0614 YX= 28.2891 ZX= -7.7437
XY= 39.2494 YY= 4.3507 ZY= -24.3433
XZ= 3.7738 YZ= -13.1037 ZZ= 156.7621
Eigenvalues: -35.0695 31.8612 159.2597

5 C Isotropic = 73.0137 Anisotropy = 157.9427
XX= 57.8760 YX= -13.1244 ZX= -11.6498
XY= -14.1561 YY= -9.3511 ZY= -35.8699

XZ= -8.1388 YZ= -38.4565 ZZ= 170.5160
Eigenvalues: -19.7545 60.4866 178.3088
6 C Isotropic = 68.9161 Anisotropy = 168.5164
XX= -20.5621 YX= -22.0162 ZX= -19.3478
XY= -23.3474 YY= 53.3495 ZY= -25.1313
XZ= -25.2799 YZ= -29.1101 ZZ= 173.9610
Eigenvalues: -31.1140 56.6020 181.2604
7 C Isotropic = 71.3811 Anisotropy = 165.0835
XX= 14.9976 YX= 41.7983 ZX= -4.9317
XY= 46.7038 YY= 22.3950 ZY= -25.4356
XZ= -6.0375 YZ= -23.1661 ZZ= 176.7507
Eigenvalues: -26.4875 59.1940 181.4367
8 C Isotropic = 71.0987 Anisotropy = 163.3954
XX= 53.5895 YX= -13.8718 ZX= -11.7553
XY= -13.3819 YY= -13.7054 ZY= -35.7846
XZ= -6.1747 YZ= -33.9712 ZZ= 173.4120
Eigenvalues: -22.9434 56.2105 180.0289
9 C Isotropic = 54.4097 Anisotropy = 159.3258
XX= -24.8702 YX= -7.2488 ZX= -15.9701
XY= -24.4215 YY= 37.4748 ZY= -26.8544
XZ= -13.8617 YZ= -41.1812 ZZ= 150.6246
Eigenvalues: -31.6166 34.2188 160.6269
10 O Isotropic = 276.6841 Anisotropy = 94.5551
XX= 331.5631 YX= 11.2758 ZX= -17.6156
XY= -7.3222 YY= 248.5884 ZY= -12.8708
XZ= -33.3126 YZ= -36.0055 ZZ= 249.9008
Eigenvalues: 222.1758 268.1557 339.7208
11 H Isotropic = 26.2477 Anisotropy = 5.8642
XX= 23.4006 YX= 0.3484 ZX= -0.9585
XY= 0.5515 YY= 27.3336 ZY= 1.2536
XZ= 1.5904 YZ= 3.5871 ZZ= 28.0089
Eigenvalues: 23.3492 25.2367 30.1572
12 H Isotropic = 29.6419 Anisotropy = 8.1917
XX= 34.9605 YX= -0.4929 ZX= -0.6281
XY= -1.1427 YY= 28.4756 ZY= 0.7844
XZ= -0.5565 YZ= -0.1305 ZZ= 25.4897
Eigenvalues: 25.4273 28.3954 35.1031
13 H Isotropic = 29.3746 Anisotropy = 9.1616
XX= 26.2001 YX= 0.6027 ZX= 2.3253
XY= -0.6494 YY= 28.9437 ZY= -2.5028
XZ= 5.4537 YZ= -2.2547 ZZ= 32.9801
Eigenvalues: 24.2136 28.4279 35.4824
14 H Isotropic = 28.7131 Anisotropy = 9.3336
XX= 27.7006 YX= 0.6266 ZX= 0.8604
XY= 1.3904 YY= 34.1756 ZY= -1.9318
XZ= 1.4466 YZ= -3.4872 ZZ= 24.2632
Eigenvalues: 23.1559 28.0480 34.9356
15 H Isotropic = 28.2463 Anisotropy = 8.4024
XX= 27.7195 YX= -0.6664 ZX= -1.0272
XY= 0.2615 YY= 27.2737 ZY= 3.7237

XZ= -2.6878 YZ= 5.7961 ZZ= 29.7455
Eigenvalues: 23.3598 27.5311 33.8479
16 H Isotropic = 23.9101 Anisotropy = 6.3608
XX= 28.0656 YX= -0.1647 ZX= 0.6795
XY= -0.7996 YY= 23.4069 ZY= 0.5573
XZ= 0.4723 YZ= 0.3085 ZZ= 20.2578
Eigenvalues: 20.1481 23.4316 28.1506
17 H Isotropic = 23.9011 Anisotropy = 4.6864
XX= 24.4648 YX= -1.0156 ZX= 0.1906
XY= -1.1138 YY= 26.4602 ZY= 0.9758
XZ= -0.3779 YZ= 0.6951 ZZ= 20.7782
Eigenvalues: 20.6570 24.0209 27.0254
18 H Isotropic = 24.0008 Anisotropy = 4.5175
XX= 25.8686 YX= 1.1118 ZX= 0.6344
XY= 1.4208 YY= 25.1724 ZY= 0.9399
XZ= 0.4191 YZ= 1.0842 ZZ= 20.9613
Eigenvalues: 20.7194 24.2705 27.0124
19 H Isotropic = 23.7737 Anisotropy = 6.6022
XX= 27.6042 YX= -1.8197 ZX= 0.0700
XY= -1.4428 YY= 23.4213 ZY= 0.7670
XZ= -0.0886 YZ= 0.9002 ZZ= 20.2957
Eigenvalues: 20.0654 23.0806 28.1752
20 H Isotropic = 30.7088 Anisotropy = 19.6266
XX= 41.6378 YX= 5.5435 ZX= -0.2112
XY= 5.2497 YY= 25.5300 ZY= -2.7824
XZ= -4.4523 YZ= -3.1488 ZZ= 24.9586
Eigenvalues: 22.0176 26.3155 43.7932

_S_-indanol : Conformer B

Symbolic Z-matrix:
Charge = 0 Multiplicity = 1

C	-1.51908	-0.69817	-0.33916
C	-2.09634	0.57305	0.33227
C	-1.02932	1.67414	0.11856
C	0.25115	0.86724	0.05709
C	1.56821	1.28585	0.24132
C	2.59847	0.34528	0.14983
C	2.31595	-0.99891	-0.11625
C	0.99538	-1.41895	-0.2958
C	-0.02764	-0.47741	-0.21494
O	-1.83763	-1.90254	0.37284
H	-1.84377	-0.79209	-1.38668
H	-2.3413	0.40226	1.38658
H	-3.02305	0.85711	-0.18181
H	-1.20708	2.27188	-0.78271
H	-0.99964	2.37211	0.96598
H	1.7962	2.32885	0.449
H	3.62983	0.66203	0.28326
H	3.12798	-1.71797	-0.18527

H 0.77095 -2.46354 -0.4969
H -2.79082 -2.05301 0.26713

SCF GIAO Magnetic shielding tensor (ppm):

1 C Isotropic = 118.0082 Anisotropy = 47.8548
XX= 119.4476 YX= -11.6253 ZX= -20.4197
XY= -10.0643 YY= 141.1571 ZY= 13.2795
XZ= -13.0336 YZ= 5.2421 ZZ= 93.4199
Eigenvalues: 84.9962 119.1170 149.9114
2 C Isotropic = 155.6657 Anisotropy = 37.1863
XX= 154.6328 YX= 3.1468 ZX= -7.0623
XY= -1.6231 YY= 179.0639 ZY= -5.3775
XZ= -19.5180 YZ= -8.7029 ZZ= 133.3004
Eigenvalues: 126.2347 160.3058 180.4565
3 C Isotropic = 163.0379 Anisotropy = 28.6531
XX= 180.2256 YX= 4.2953 ZX= -4.2689
XY= 4.4529 YY= 168.4881 ZY= -1.6268
XZ= -4.4876 YZ= 0.0911 ZZ= 140.4000
Eigenvalues: 139.9213 167.0524 182.1400
4 C Isotropic = 55.1148 Anisotropy = 163.0114
XX= 7.4509 YX= -28.6183 ZX= -14.3474
XY= -41.4730 YY= 0.0916 ZY= 7.2061
XZ= -27.8308 YZ= 27.5977 ZZ= 157.8018
Eigenvalues: -31.4749 33.0301 163.7890
5 C Isotropic = 73.1374 Anisotropy = 156.8247
XX= 55.7262 YX= 23.0587 ZX= -14.6590
XY= 21.2567 YY= -11.4512 ZY= 14.6022
XZ= -16.8936 YZ= 10.5478 ZZ= 175.1373
Eigenvalues: -19.5252 61.2502 177.6872
6 C Isotropic = 70.1072 Anisotropy = 166.9402
XX= -23.3640 YX= 16.4125 ZX= -21.6439
XY= 17.3090 YY= 54.8114 ZY= 9.3945
XZ= -20.7501 YZ= 6.9939 ZZ= 178.8743
Eigenvalues: -29.2615 58.1825 181.4007
7 C Isotropic = 71.2478 Anisotropy = 166.8012
XX= 23.2574 YX= -42.5836 ZX= -13.4630
XY= -44.7476 YY= 10.1013 ZY= 5.5847
XZ= -11.5759 YZ= 13.8606 ZZ= 180.3846
Eigenvalues: -27.4821 58.7768 182.4486
8 C Isotropic = 73.1272 Anisotropy = 167.9453
XX= 51.0224 YX= 20.3924 ZX= -14.6348
XY= 21.7861 YY= -13.9424 ZY= 11.4812
XZ= -18.5141 YZ= 17.8037 ZZ= 182.3016
Eigenvalues: -21.9236 56.2144 185.0907
9 C Isotropic = 53.2766 Anisotropy = 158.0805
XX= -26.4155 YX= 8.0768 ZX= -20.2400
XY= 17.5437 YY= 29.5278 ZY= 10.9297
XZ= -15.9434 YZ= 1.1219 ZZ= 156.7174
Eigenvalues: -31.1238 32.2900 158.6636
10 O Isotropic = 287.0773 Anisotropy = 41.3972

XX= 307.0510 YX= -22.2444 ZX= -6.1497
XY= -5.7754 YY= 278.5405 ZY= 7.6774
XZ= -1.6180 YZ= 17.2965 ZZ= 275.6404
Eigenvalues: 263.4113 283.1452 314.6754
11 H Isotropic = 26.0258 Anisotropy = 3.9223
XX= 24.0021 YX= -1.1361 ZX= -0.8927
XY= -1.1773 YY= 26.2248 ZY= 0.7933
XZ= 3.6671 YZ= -1.8885 ZZ= 27.8505
Eigenvalues: 23.2465 26.1902 28.6406
12 H Isotropic = 29.7379 Anisotropy = 7.0745
XX= 28.5774 YX= -1.2548 ZX= -2.8838
XY= -0.9222 YY= 29.0263 ZY= -1.0164
XZ= -5.2677 YZ= -1.1002 ZZ= 31.6100
Eigenvalues: 25.1633 29.5962 34.4542
13 H Isotropic = 29.1756 Anisotropy = 8.1257
XX= 33.2563 YX= 1.7108 ZX= 2.4409
XY= 2.4302 YY= 28.8793 ZY= 0.8004
XZ= 1.6324 YZ= 0.7063 ZZ= 25.3911
Eigenvalues: 24.8781 28.0559 34.5927
14 H Isotropic = 28.6684 Anisotropy = 8.9948
XX= 27.6826 YX= -0.3875 ZX= 0.1528
XY= -0.2090 YY= 29.4993 ZY= 4.3302
XZ= 1.8710 YZ= 6.5907 ZZ= 28.8232
Eigenvalues: 23.4785 27.8617 34.6649
15 H Isotropic = 28.5802 Anisotropy = 9.4298
XX= 27.8148 YX= -0.4485 ZX= 0.1413
XY= -1.6000 YY= 32.4690 ZY= -4.0497
XZ= -0.2677 YZ= -5.1689 ZZ= 25.4568
Eigenvalues: 23.1151 27.7588 34.8667
16 H Isotropic = 23.9877 Anisotropy = 6.1574
XX= 27.8573 YX= 0.6310 ZX= 0.6933
XY= 1.1924 YY= 23.6697 ZY= -0.0462
XZ= 0.5751 YZ= -0.2646 ZZ= 20.4360
Eigenvalues: 20.3654 23.5050 28.0926
17 H Isotropic = 23.9948 Anisotropy = 4.5415
XX= 24.3893 YX= 0.6968 ZX= 0.2041
XY= 0.8340 YY= 26.7904 ZY= -0.2854
XZ= 0.3683 YZ= -0.3663 ZZ= 20.8046
Eigenvalues: 20.7566 24.2052 27.0224
18 H Isotropic = 23.9877 Anisotropy = 4.5831
XX= 26.0964 YX= -1.1637 ZX= 0.4997
XY= -1.3959 YY= 25.1109 ZY= -0.4523
XZ= 0.8106 YZ= 0.0529 ZZ= 20.7557
Eigenvalues: 20.6760 24.2439 27.0431
19 H Isotropic = 23.7555 Anisotropy = 7.3537
XX= 27.8561 YX= 2.2798 ZX= 0.1424
XY= 1.8008 YY= 23.4374 ZY= -0.4231
XZ= -0.3133 YZ= -0.1455 ZZ= 19.9731
Eigenvalues: 19.9489 22.6597 28. 6580
20 H Isotropic = 30.1129 Anisotropy = 19.0400

XX= 40.4110 YX= -5.2878 ZX= 4.1381
XY= -5.7980 YY= 27.4493 ZY= 1.4678
XZ= 2.5607 YZ= 1.4517 ZZ= 22.4784
Eigenvalues: 20.7750 26.7575 42.8062

(-)-IPC

Symbolic Z-matrix:
Charge = 0 Multiplicity = 1

C	0.122	-0.178	0.118
H	0.413	-0.194	-0.937
H	1.04	-0.194	0.712
H	-0.427	-1.102	0.322
C	-0.75	1.046	0.423
C	-1.326	1.008	1.865
H	-1.624	0.986	-0.236
C	-1.384	2.392	2.584
H	-0.701	0.336	2.464
O	-2.628	0.404	1.761
C	-0.628	3.5	1.839
H	-1.004	2.29	3.607
H	-2.436	2.687	2.669
C	-1.123	3.513	0.369
H	-0.642	4.439	2.403
C	-0.073	2.395	0.114
H	-0.913	4.444	-0.156
H	-2.17	3.246	0.2
H	0.421	2.366	-0.864
H	-2.955	0.204	2.647
C	0.761	3.004	1.306
C	1.631	2.121	2.205
C	1.638	4.171	0.825
H	2.501	3.797	0.265
H	2.024	4.739	1.678
H	1.11	4.874	0.178
H	2.017	2.709	3.046
H	2.499	1.741	1.656
H	1.112	1.262	2.627

SCF GIAO Magnetic shielding tensor (ppm):
1 C Isotropic = 161.2144 Anisotropy = 33.7035
XX= 147.8382 YX= 6.8248 ZX= 7.4696
XY= 9.4439 YY= 181.2851 ZY= -0.3907
XZ= 9.9385 YZ= 4.1714 ZZ= 154.5199
Eigenvalues: 141.0276 158.9322 183.6834
2 H Isotropic = 31.0281 Anisotropy = 9.8659
XX= 27.6628 YX= 1.0116 ZX= 0.4177
XY= 0.5412 YY= 34.7127 ZY= -4.9471
XZ= 0.1867 YZ= -3.9330 ZZ= 30.7088
Eigenvalues: 27.0577 28.4213 37.6054

3 H Isotropic = 30.9280 Anisotropy = 5.7310
XX= 29.5667 YX= 0.6480 ZX= -2.3846
XY= 0.8517 YY= 32.7584 ZY= 3.2174
XZ= -3.0854 YZ= 2.2027 ZZ= 30.4590
Eigenvalues: 26.3436 31.6917 34.7487
4 H Isotropic = 30.4659 Anisotropy = 9.4049
XX= 34.1129 YX= 3.0294 ZX= 1.0596
XY= 4.2012 YY= 31.1656 ZY= 0.7718
XZ= 1.7116 YZ= 0.2270 ZZ= 26.1193
Eigenvalues: 25.8828 28.7791 36.7359
5 C Isotropic = 131.3693 Anisotropy = 20.2305
XX= 142.0387 YX= -3.7516 ZX= 1.1326
XY= -11.4453 YY= 121.2354 ZY= -8.6718
XZ= 1.4439 YZ= 2.6524 ZZ= 130.8338
Eigenvalues: 118.2666 130.9850 144.8563
6 C Isotropic = 105.7890 Anisotropy = 42.6746
XX= 119.7031 YX= -19.0200 ZX= -9.5731
XY= -15.7323 YY= 107.4764 ZY= -1.7185
XZ= -13.7893 YZ= 2.6110 ZZ= 90.1875
Eigenvalues: 84.3899 98.7384 134.2387
7 H Isotropic = 29.8891 Anisotropy = 4.7777
XX= 30.3271 YX= -0.0795 ZX= -2.2833
XY= 1.1860 YY= 28.8324 ZY= 0.6532
XZ= -3.0246 YZ= 0.6172 ZZ= 30.5079
Eigenvalues: 27.3016 29.2916 33.0742
8 C Isotropic = 138.8108 Anisotropy = 32.2019
XX= 155.5693 YX= 7.8767 ZX= 0.7988
XY= 8.0313 YY= 146.3081 ZY= 4.6602
XZ= -6.9463 YZ= -3.9683 ZZ= 114.5550
Eigenvalues: 114.2972 141.8564 160.2788
9 H Isotropic = 27.7636 Anisotropy = 3.0830
XX= 29.1656 YX= -1.0686 ZX= -0.8032
XY= -0.2641 YY= 26.2038 ZY= 1.9603
XZ= 0.0545 YZ= 1.7217 ZZ= 27.9214
Eigenvalues: 24.9990 28.4728 29.8190
10 O Isotropic = 243.6187 Anisotropy = 57.7401
XX= 258.5779 YX= -16.0256 ZX= -2.6084
XY= -34.2247 YY= 242.4637 ZY= -21.1975
XZ= 2.6417 YZ= -30.5630 ZZ= 229.8147
Eigenvalues: 204.4325 244.3116 282.1121
11 C Isotropic = 135.5171 Anisotropy = 16.7873
XX= 138.2595 YX= 5.4358 ZX= -8.3547
XY= -2.8611 YY= 142.9157 ZY= 6.7699
XZ= -5.3610 YZ= 10.3807 ZZ= 125.3759
Eigenvalues: 119.3934 140.4492 146.7086
12 H Isotropic = 29.4914 Anisotropy = 6.7827
XX= 27.9339 YX= 0.5542 ZX= 0.1919
XY= -0.5949 YY= 28.3710 ZY= -3.4404
XZ= 0.7080 YZ= -2.9489 ZZ= 32.1694
Eigenvalues: 26.5235 27.9376 34.0132

13 H Isotropic = 30.1993 Anisotropy = 7.1911
XX= 30.5527 YX= -1.4048 ZX= 0.5059
XY= -3.1861 YY= 33.7182 ZY= -0.2975
XZ= 1.1502 YZ= -0.5837 ZZ= 26.3270
Eigenvalues: 26.1705 29.4340 34.9934
14 C Isotropic = 146.6358 Anisotropy = 19.5921
XX= 156.3136 YX= -5.9516 ZX= -12.0277
XY= -2.4007 YY= 149.9487 ZY= -5.5589
XZ= -5.3434 YZ= -7.5725 ZZ= 133.6450
Eigenvalues: 128.0745 152.1357 159.6972
15 H Isotropic = 29.9855 Anisotropy = 8.1645
XX= 30.4283 YX= 3.0436 ZX= 0.1110
XY= 3.3745 YY= 32.7209 ZY= -2.3279
XZ= 0.1372 YZ= -2.5579 ZZ= 26.8072
Eigenvalues: 25.5460 28.9819 35.4285
16 C Isotropic = 130.5181 Anisotropy = 9.7814
XX= 132.0973 YX= -5.1273 ZX= 1.9810
XY= -3.1643 YY= 123.5246 ZY= 1.4394
XZ= -6.0890 YZ= -8.0723 ZZ= 135.9323
Eigenvalues: 120.8645 133.6507 137.0390
17 H Isotropic = 29.5994 Anisotropy = 7.3367
XX= 30.4158 YX= 0.1289 ZX= 2.0046
XY= 0.5673 YY= 27.1192 ZY= 3.8092
XZ= 2.3263 YZ= 3.6299 ZZ= 31.2632
Eigenvalues: 24.8095 29.4982 34.4906
18 H Isotropic = 30.8374 Anisotropy = 7.7251
XX= 30.6114 YX= -1.3946 ZX= -1.3312
XY= -1.7290 YY= 29.5235 ZY= 3.8456
XZ= -1.6850 YZ= 4.0315 ZZ= 32.3774
Eigenvalues: 26.7107 29.8141 35.9875
19 H Isotropic = 30.1027 Anisotropy = 6.4421
XX= 29.4803 YX= 0.4055 ZX= 1.4588
XY= 0.6567 YY= 30.5755 ZY= -3.6992
XZ= 2.0451 YZ= -3.9608 ZZ= 30.2522
Eigenvalues: 25.8333 30.0774 34.3975
20 H Isotropic = 31.4481 Anisotropy = 17.3066
XX= 35.1868 YX= -6.5665 ZX= 5.0673
XY= -5.8438 YY= 27.4566 ZY= -6.2569
XZ= 4.7811 YZ= -4.5194 ZZ= 31.7008
Eigenvalues: 23.0466 28.3118 42.9858
21 C Isotropic = 137.6975 Anisotropy = 18.5475
XX= 128.9741 YX= 9.6893 ZX= 9.2438
XY= 6.4668 YY= 139.3833 ZY= 2.0581
XZ= 3.8705 YZ= 2.9069 ZZ= 144.7352
Eigenvalues: 123.5164 139.5137 150.0625
22 C Isotropic = 158.1578 Anisotropy = 33.8120
XX= 153.2877 YX= -0.0357 ZX= -0.1799
XY= 2.8760 YY= 149.1586 ZY= 15.1483
XZ= 6.4904 YZ= 16.8639 ZZ= 172.0271
Eigenvalues: 140.9194 152.8548 180.6991

23 C Isotropic = 154.8102 Anisotropy = 45.9345
XX= 182.3081 YX= 0.9656 ZX= 12.7291
XY= -0.6318 YY= 140.0760 ZY= -4.3105
XZ= 10.5039 YZ= -3.0464 ZZ= 142.0464
Eigenvalues: 135.8589 143.1383 185.4332
24 H Isotropic = 30.9443 Anisotropy = 8.6753
XX= 32.7980 YX= -4.3424 ZX= 1.5502
XY= -3.4529 YY= 32.2284 ZY= -0.5330
XZ= 1.4304 YZ= -1.1129 ZZ= 27.8065
Eigenvalues: 27.3680 28.7371 36.7278
25 H Isotropic = 31.0100 Anisotropy = 9.1042
XX= 35.3009 YX= 2.4640 ZX= -3.0455
XY= 2.2114 YY= 28.2061 ZY= -1.2759
XZ= -2.2544 YZ= -0.9076 ZZ= 29.5229
Eigenvalues: 27.4340 28.5164 37.0794
26 H Isotropic = 30.2769 Anisotropy = 8.0724
XX= 32.7217 YX= 0.8227 ZX= 3.9386
XY= -0.0546 YY= 26.8635 ZY= 2.7212
XZ= 2.1488 YZ= 3.1176 ZZ= 31.2454
Eigenvalues: 25.2416 29.9305 35.6585
27 H Isotropic = 31.1398 Anisotropy = 9.2247
XX= 30.6963 YX= 0.7773 ZX= -3.1689
XY= 0.3246 YY= 27.3609 ZY= -0.2236
XZ= -3.8656 YZ= -0.6106 ZZ= 35.3621
Eigenvalues: 27.2675 28.8623 37.2895
28 H Isotropic = 31.0448 Anisotropy = 8.2063
XX= 29.5732 YX= -1.6598 ZX= -0.5606
XY= -1.7038 YY= 34.5303 ZY= 2.6485
XZ= -1.4295 YZ= 3.6769 ZZ= 29.0308
Eigenvalues: 27.5619 29.0568 36.5157
29 H Isotropic = 30.9140 Anisotropy = 4.8468
XX= 33.4618 YX= -0.6281 ZX= -0.1193
XY= 0.5200 YY= 27.3690 ZY= 2.6844
XZ= 2.0925 YZ= 2.1551 ZZ= 31.9112
Eigenvalues: 26.2939 32.3030 34.1453