Supporting Information for

Application of Residual Dipolar Couplings in Structural Analysis of Thiacalix[4]arene Derivatives

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NMR SECTION

USED CHEMICALS

Chloroform-d_1 ($CDCl_3$) – degree of deuteration min. 99.8 % and dimethylsulfoxide-d_6 (DMSO) – degree of deuteration min. 99.8 % were purchased from Merck, Germany. Poly(γ-ethyl-L-glutamate) – M > 100 000 g/mol (medium A) and poly(γ-benzyl-L-glutamate) – 150 000 < M < 350 000 g/mol (medium B) were purchased from Sigma-Aldrich.

MEASUREMENTS CONDITIONS

All NMR data were acquired on Bruker Avance^{III} 600 MHz (proton frequency) NMR spectrometer equipped with triple resonance cryo-probe. Scalar coupling constants ($^1J_{C\text{-}H}$) and total splitting ($^1T_{C\text{-}H}$) were measured using heteronuclear (^{1}H-^{13}C) CLIP-HSQC pulse sequence without proton decoupling in direct (F2) domain. Nine heteronuclear one bond RDCs were sufficient to obtain structural information, so it was unnecessary to measure any other type of RDCs.

1D | ^{1}H NMR spectra

π/2 pulse for ^{1}H nuclei was approximately 9 μs. Spectral width: 7 kHz, size of fid: 32k data points, relaxation period: 10 s, number of scans: 8.

1D | ^{2}H NMR spectra

π/2 pulse for ^{2}H nuclei was approximately 68 μs. Spectral width: 4 kHz, size of fid: 16k data points, relaxation period: 10 s, number of scans: 8.

1D | ^{13}C-APT NMR spectra

^{13}C NMR spectra with proton decoupling - *waltz16* (decoupling pulse 100 μs, power level 23.6 dB). π/2 pulse for ^{13}C nuclei was approximately 12 μs. Spectral width: 31.5 kHz, size of fid: 64k data points, polarization transfer: 7 ms, relaxation period: 2.0 s, number of scans: 20 000.

1D | ^{13}C (de)coupled NMR spectra (Z-Restored)

Modified version of classical 1D ^{13}C NMR experiment with straight baseline free of distortions. Spectral width: 19.5 kHz, size of fid: 64k data points, relaxation period: 1 s, number of scans: 4k - 16k.

For pulse sequence details see ref.: Y. Xia, S. Moran, E. P. Nikonowiczb, X. Gaoa, *Magn. Res. Chem.*, **2007**, *46*, 432.

2D | ^{1}H-^{1}H COSY spectra

Spectral width: 3.8 kHz in both domains, size of fid: 1024 (F2) a 256 (F1) data points, relaxation period: 1.0 s, number of scans: 12.

2D | ^{1}H-^{13}C HMQC spectra

Spectral width: 4.0 kHz (F2) a 21.4 kHz (F1), size of fid: 2048 (F2) a 256 (F1) data points, polarization transfer: 3.5 ms, relaxation period: 1.0 s, number of scans: 16.

2D | CLIP ^{1}H-^{13}C HSQC spectra

2D ^{1}H-^{13}C CLIP HSQC is a modification of classical F2-coupled HSQC experiment providing clear spectra without antiphase artefacts and other spectral distortions. Residual dipolar coupling constants were measured from splitting in the direct domain (F2). Spectral width: 4.7 kHz (F2) a 19.6 kHz (F1), size of fid: 8k (F2) a 256 (F1) data points, polarization transfer: 3,125 ms, relaxation period: 0.1 s, number of scans: 16.

For pulse sequence details see ref.: A. Enthart, J. C. Freudenberger, J. Furrer, H. Kessler, B. Luy, *J. Magn. Reson.*, **2008**, *192*, 314.

2D | ^{1}H-^{13}C HMBC spectra

Spectral width: 4,0 kHz (F2) a 27,7 kHz (F1), size of fid: 2k (F2) a 256 (F1) data points, polarization transfer: 70 ms, relaxation period: 1,0 s, number of scans: 64.

1D | ^{1}H DPFGSE – NOE spectra

Nuclear Overhauser effect (NOE) based experiment with selective inversion – DPFGSE sequence. Selective inversion was performed via 80ms *q3-gaussian cascade.* Spectral width: 12.0 kHz, size of fid: 32k data points, mixing time: 0.2-1.6 s, relaxation period: 2.0 s, number of scans: 128.

NMR CHARACTERIZATION

FIGURE 1: ^{1}H NMR SPECTRUM OF 5C (600 MHZ, $CDCl_3$)

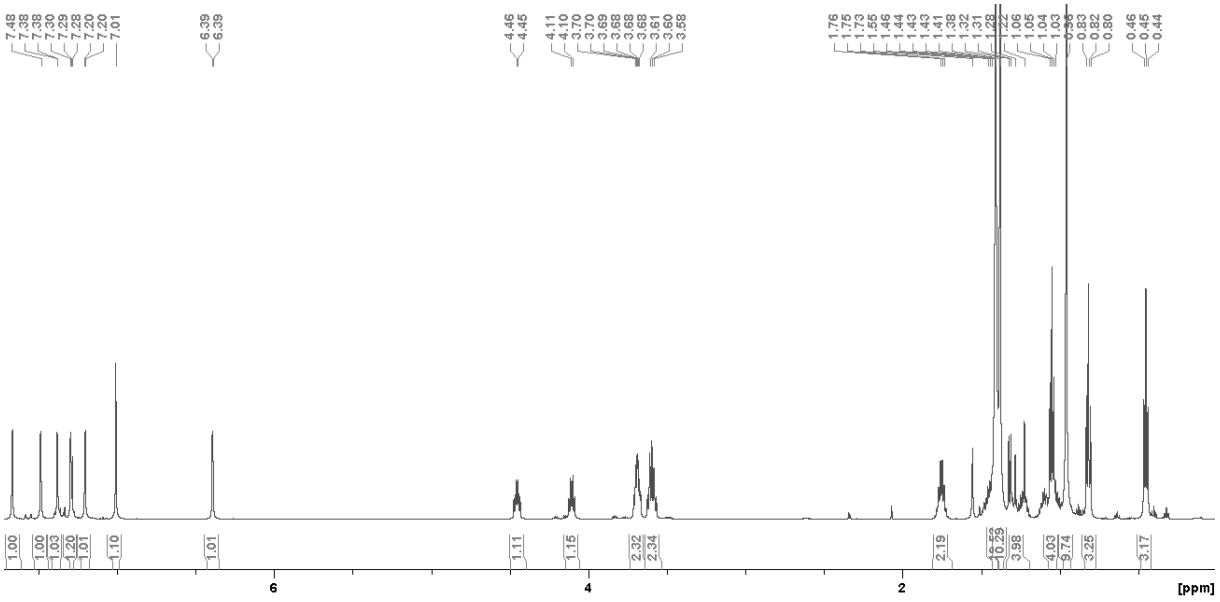


FIGURE 2: ^{13}C NMR SPECTRUM OF 5C (600 MHZ, $CDCl_3$)

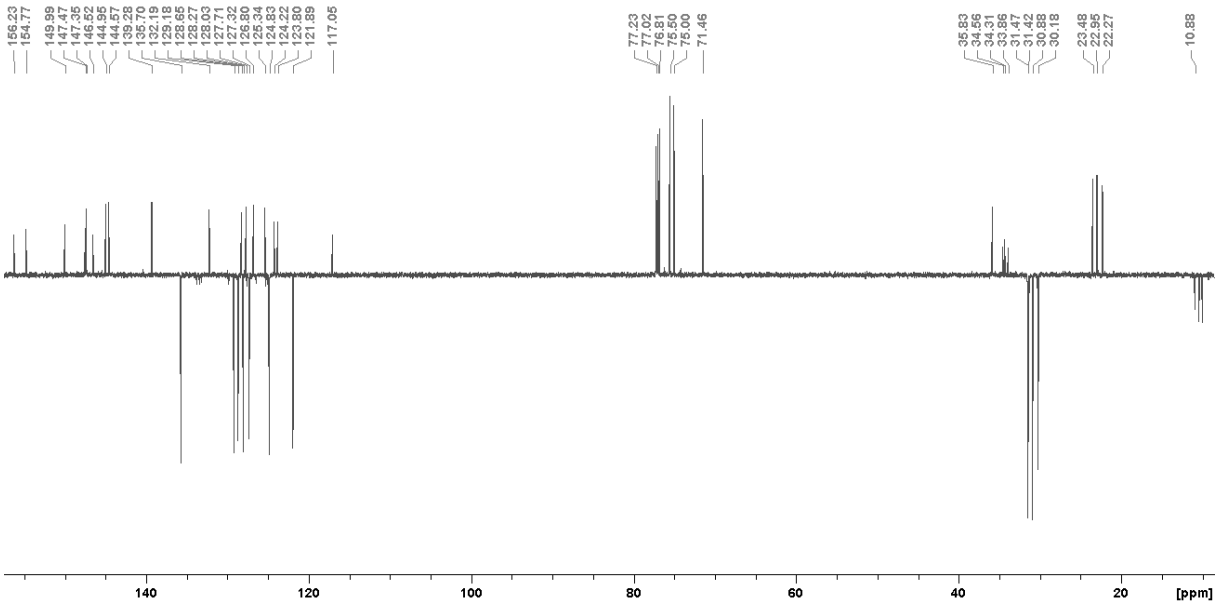


FIGURE 3: ^{1}H-^{1}H COSY SPECTRUM OF 5C (600 MHZ, $CDCl_3$)

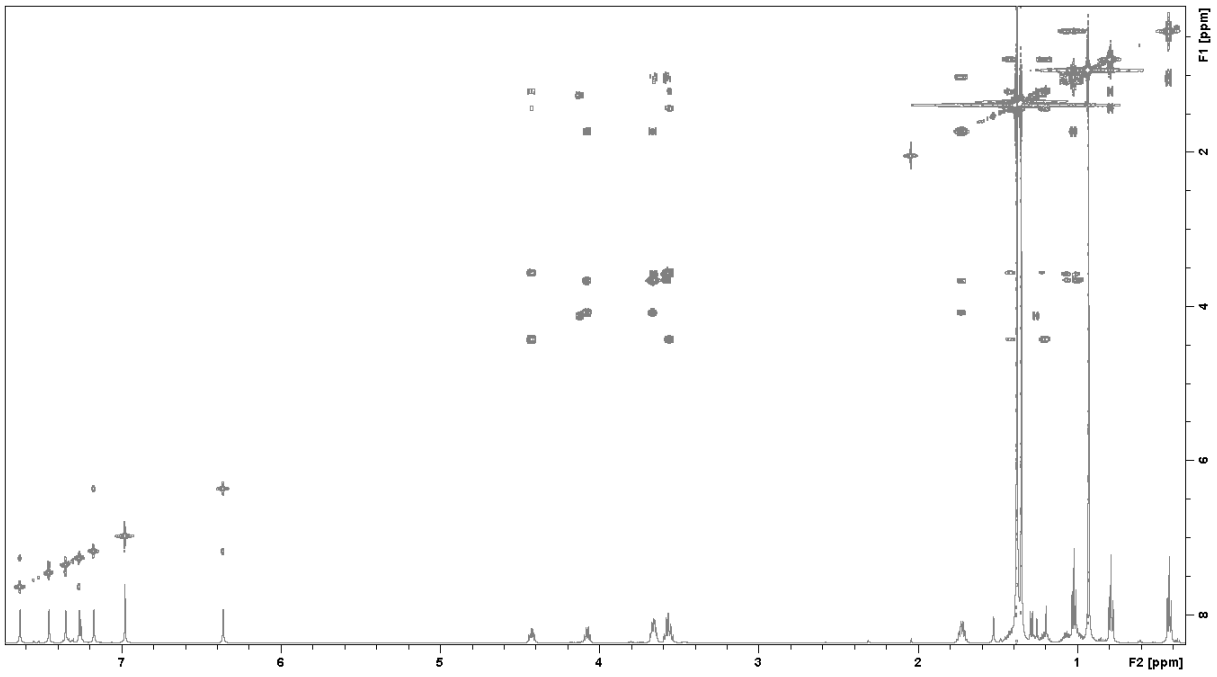


FIGURE 4: ^{1}H-^{13}C HMQC SPECTRUM OF 5C (600 MHZ, $CDCl_3$)

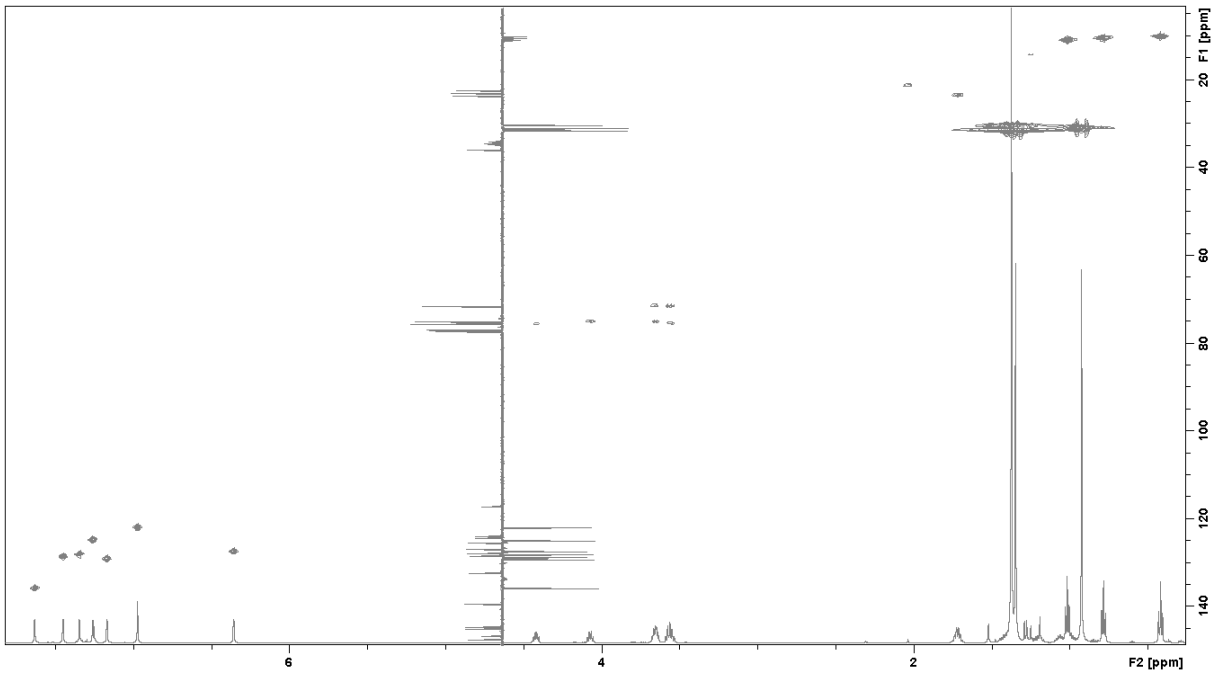


FIGURE 5: ^{1}H-^{13}C HMBC SPECTRUM OF 5C (600 MHZ, $CDCl_3$)

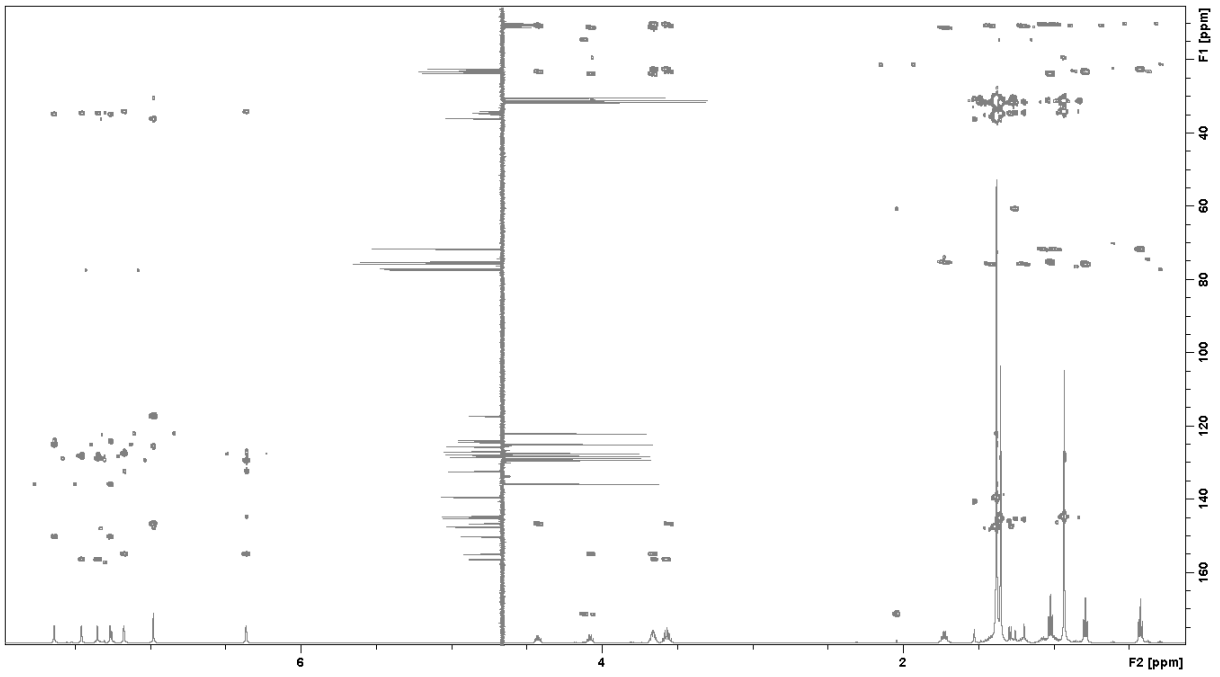


FIGURE 6: 1D ^{1}H-DPFGSE NOE EXPERIMENTS OF 5C (600 MHZ, $CDCl_3$)

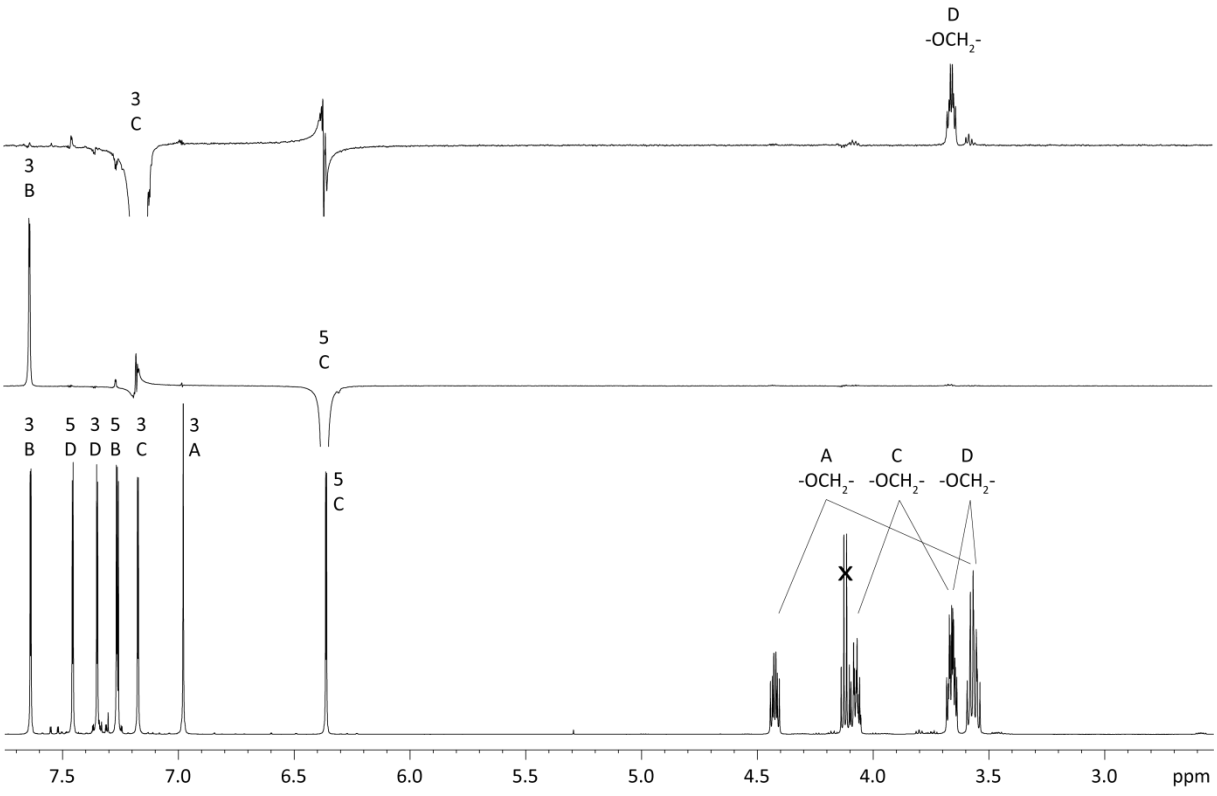


FIGURE 7: ^{1}H NMR SPECTRUM OF 5D (600 MHZ, $CDCl_3$)

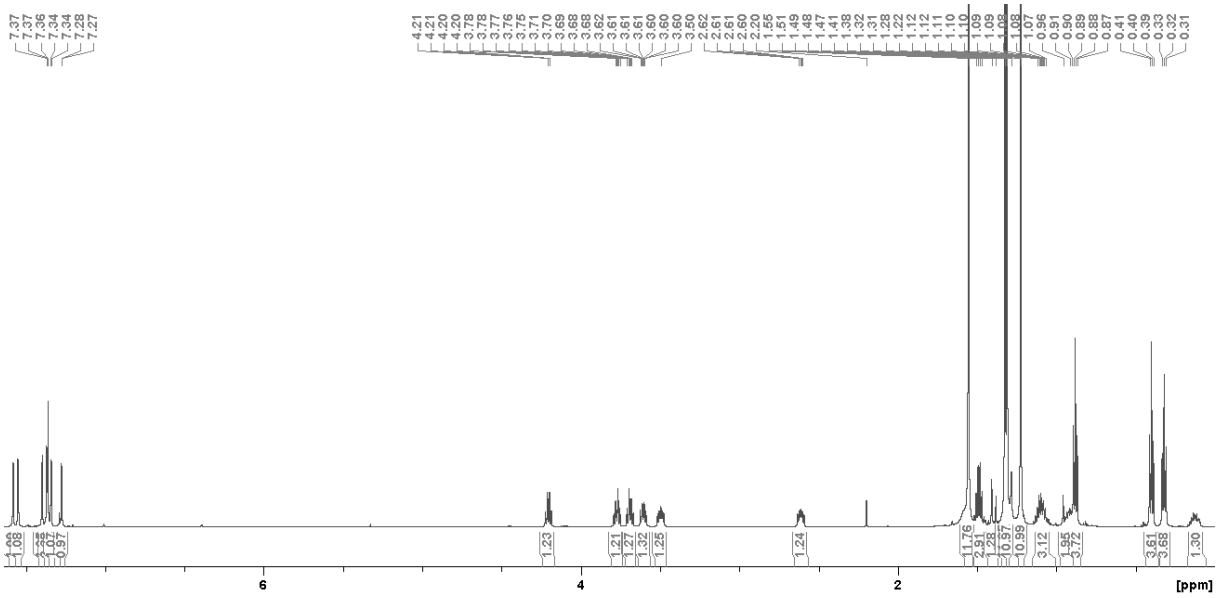


FIGURE 8: ^{13}C NMR SPECTRUM OF 5D (600 MHZ, $CDCl_3$)

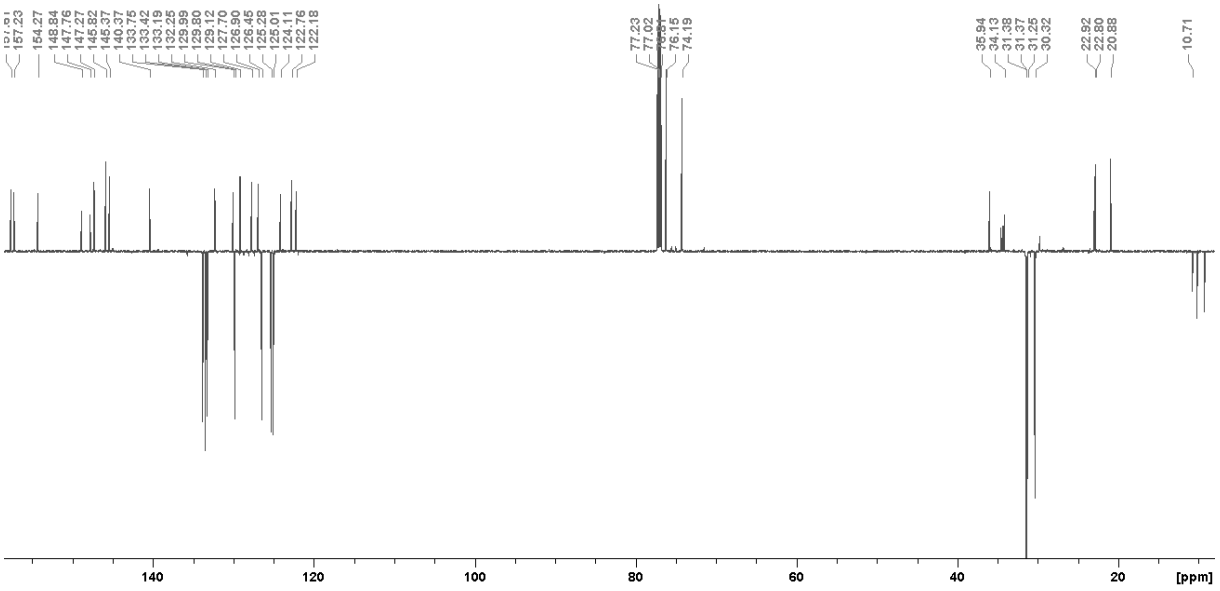


FIGURE 9: ^{1}H-^{1}H COSY SPECTRUM OF 5D (600 MHZ, $CDCl_3$)

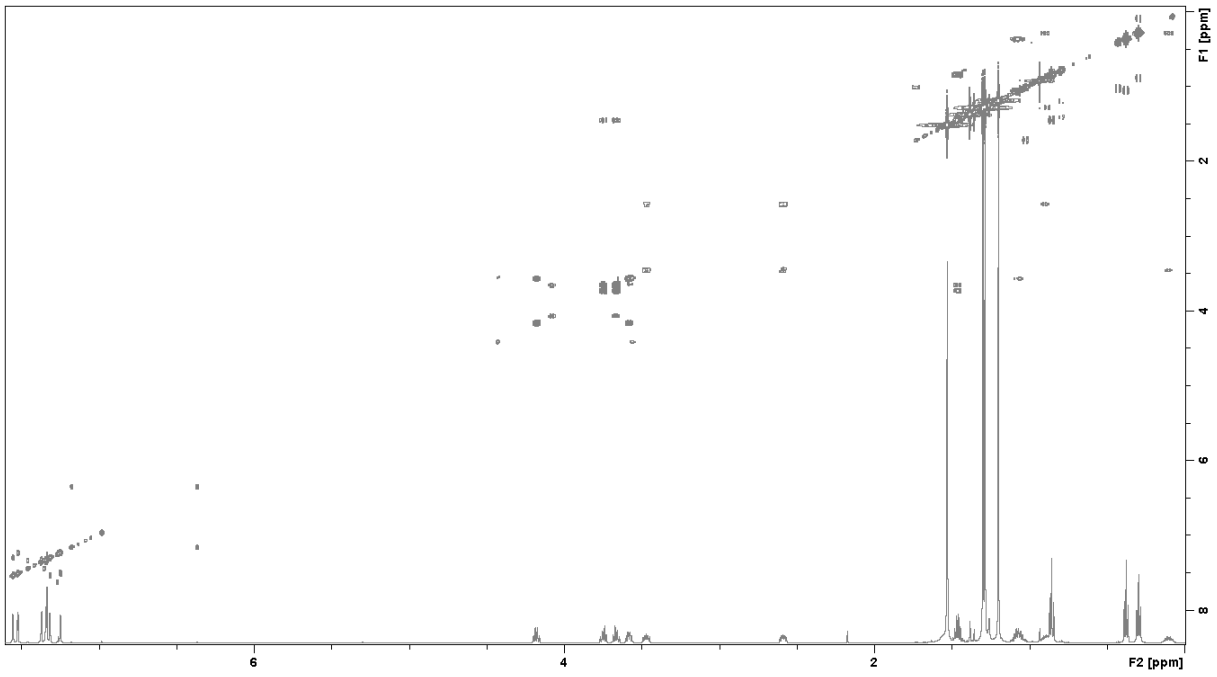


FIGURE 10: ^{1}H-^{13}C HMQC SPECTRUM OF 5D (600 MHZ, $CDCl_3$)

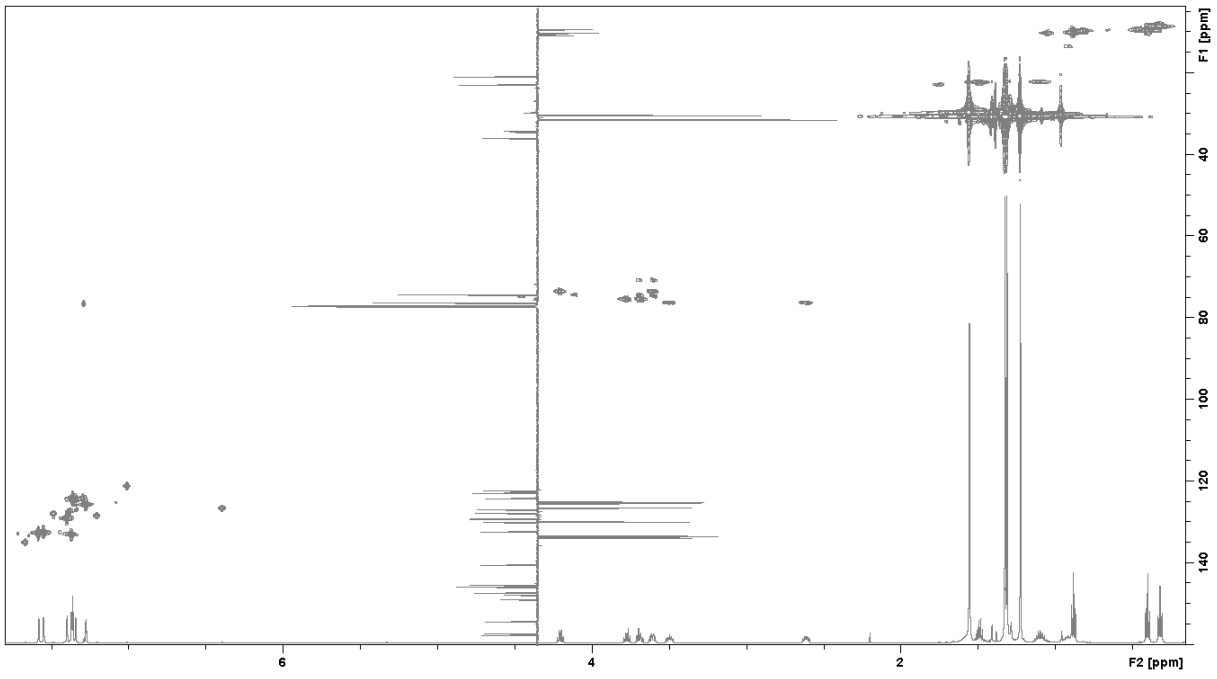


FIGURE 11: ^{1}H-^{13}C HMBC SPECTRUM OF 5D (600 MHZ, $CDCl_3$)

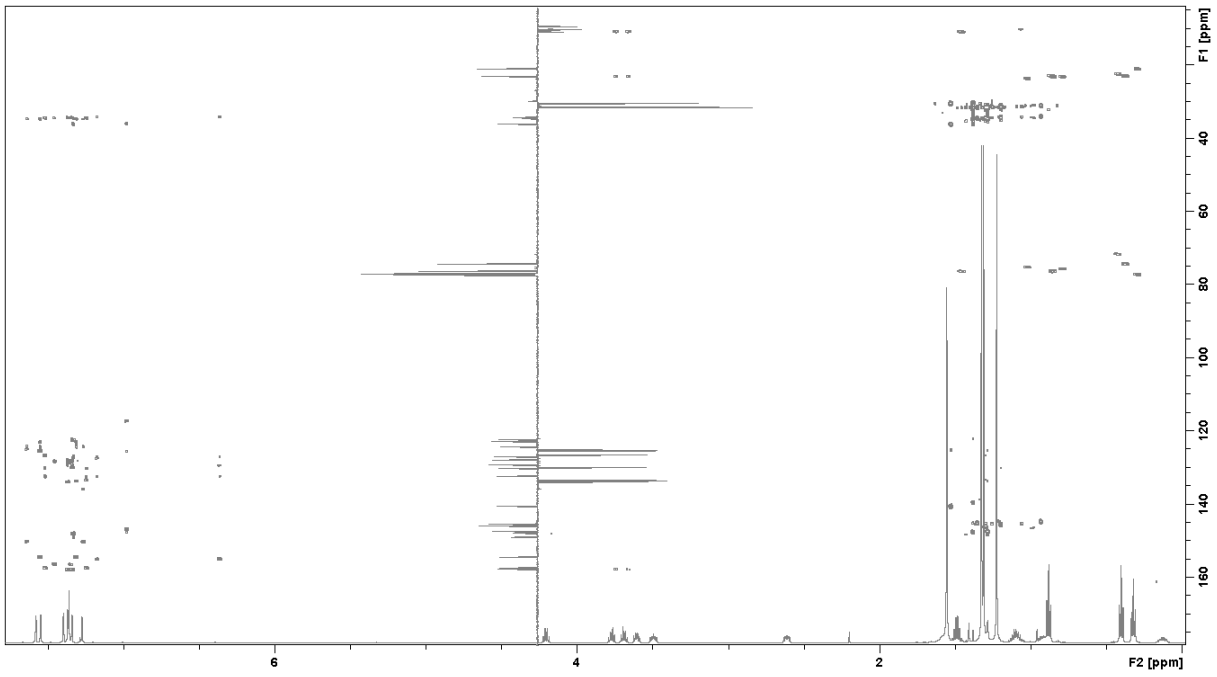


FIGURE 12: 1D ^{1}H-DPFGSE NOE EXPERIMENTS OF 5D (600 MHZ, $CDCl_3$)

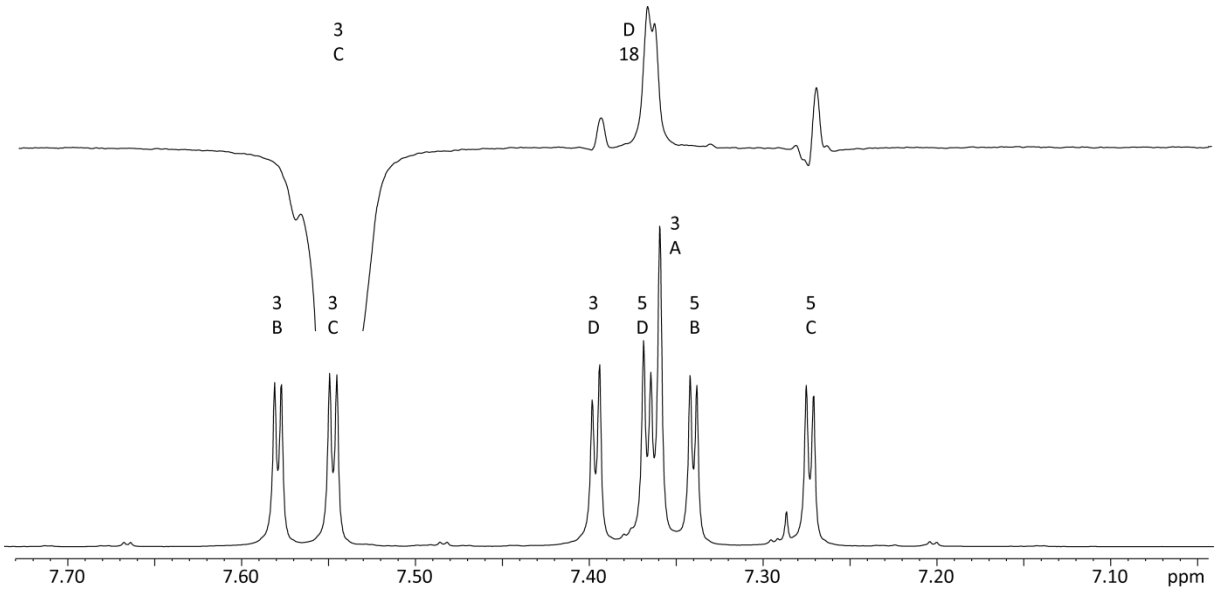


FIGURE 13: ^{1}H NMR SPECTRUM OF 7C (600 MHZ, $CDCl_3$)

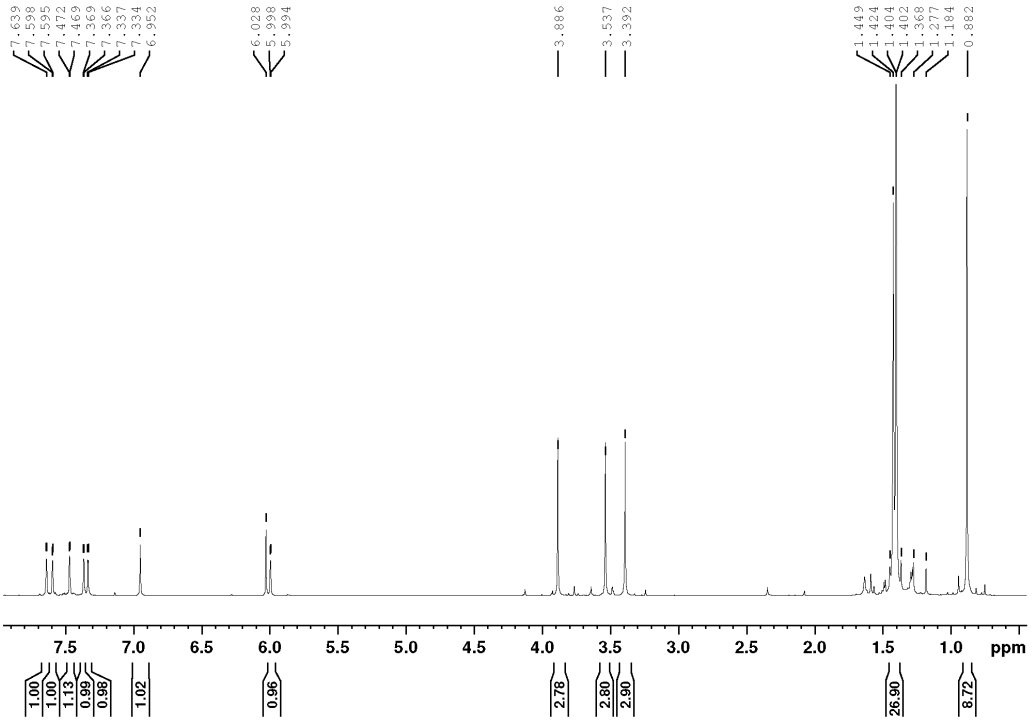


FIGURE 14: ^{13}C NMR SPECTRUM OF 7C (600 MHZ, $CDCl_3$)

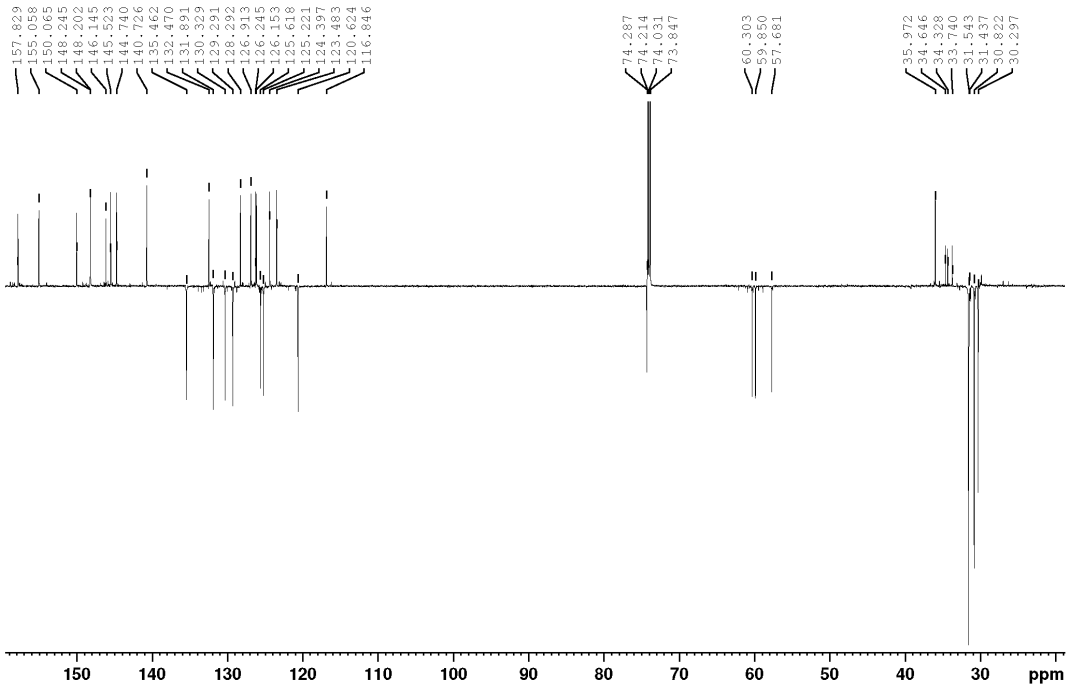


FIGURE 15: ^{1}H-^{1}H COSY SPECTRUM OF 7C (600 MHZ, $CDCl_3$)

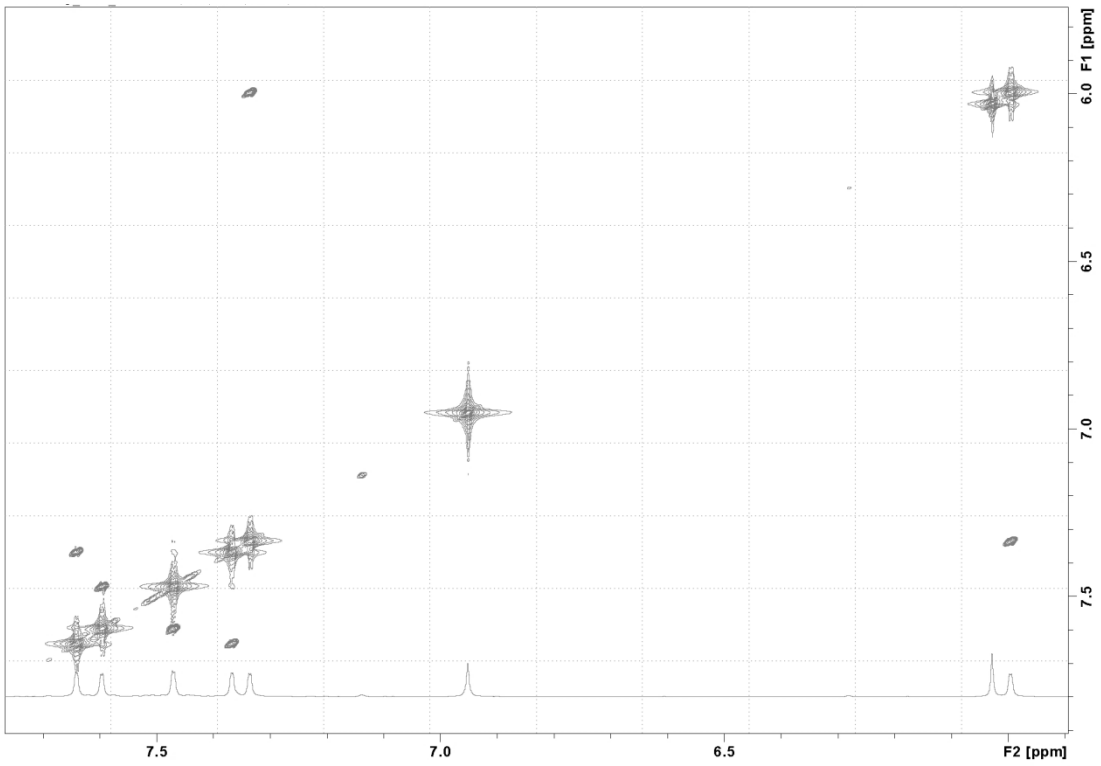


FIGURE 16: ^{1}H-^{13}C HMQC SPECTRUM OF 7C (600 MHZ, $CDCl_3$)

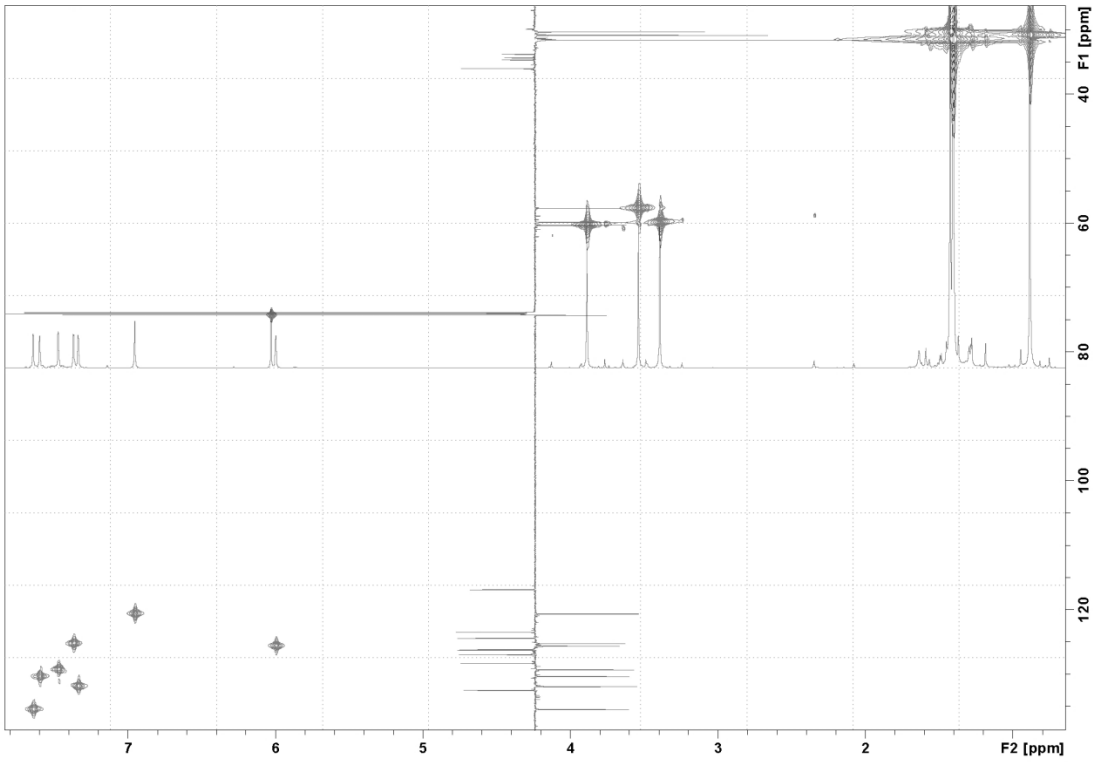


FIGURE 17: ^{1}H-^{13}C HMBC SPECTRUM OF 7C (600 MHZ, $CDCl_3$)

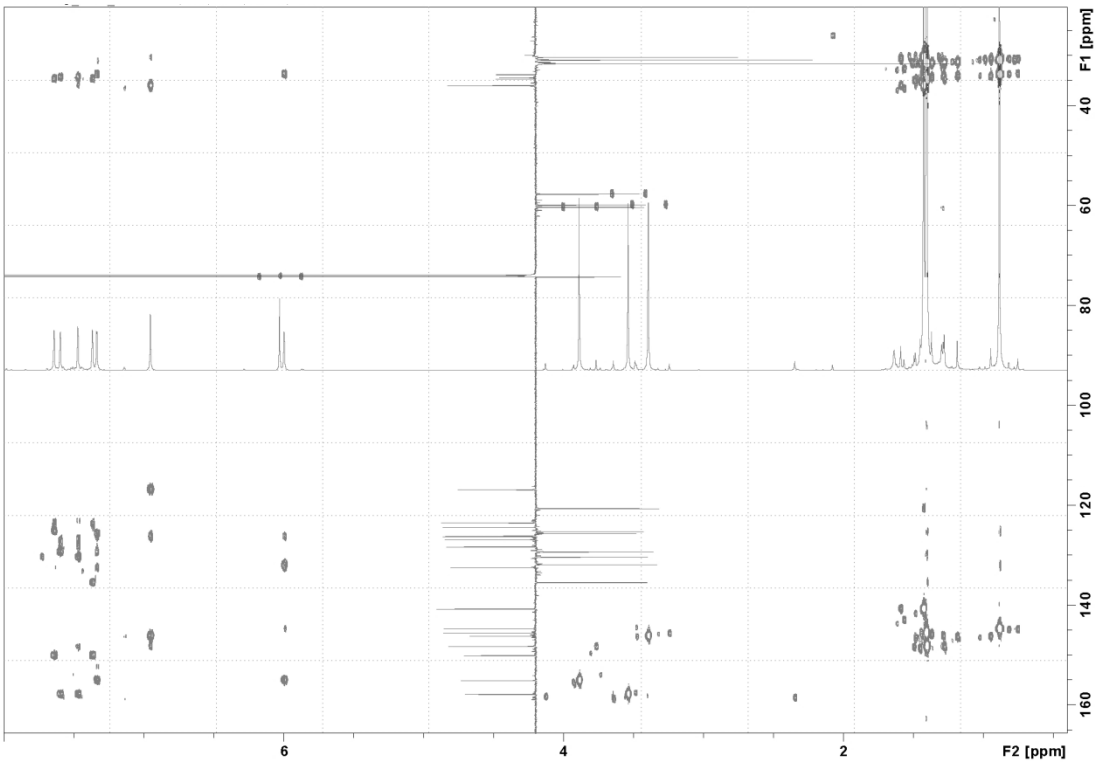


FIGURE 18: 1D ^{1}H-DPFGSE NOE EXPERIMENTS OF 7C (600 MHZ, $CDCl_3$, 273 K)

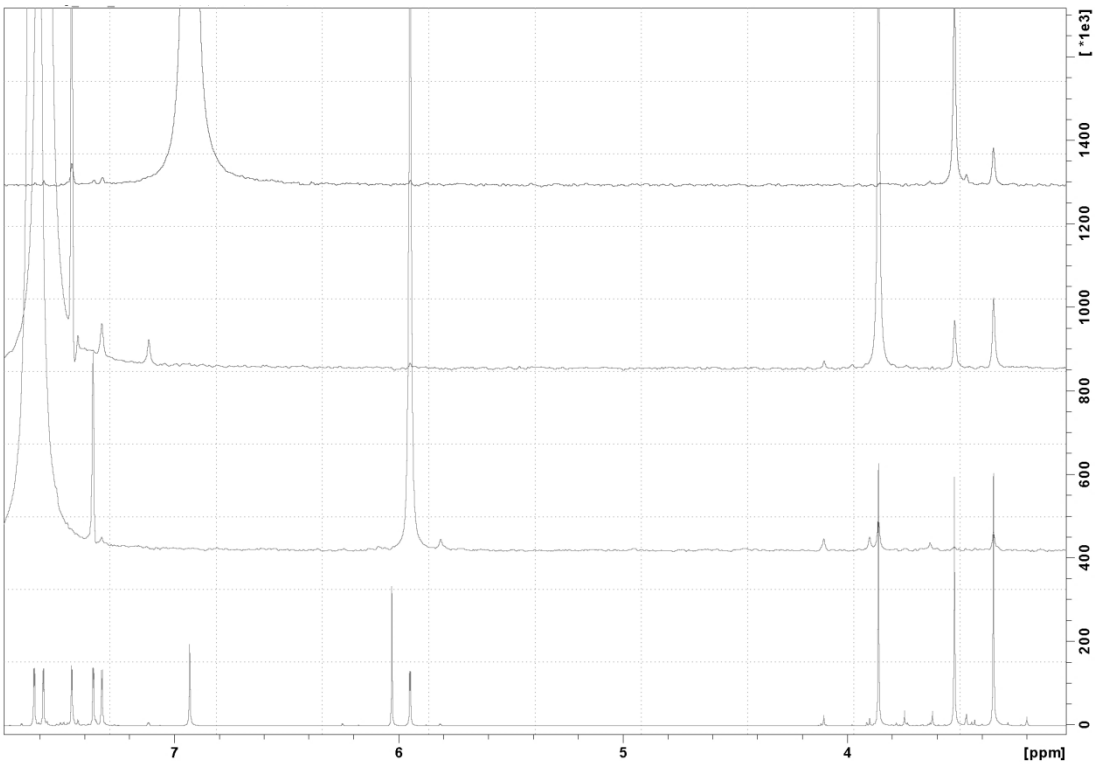


FIGURE 19: ^{1}H NMR SPECTRUM OF 7D (600 MHZ, $CDCl_3$)

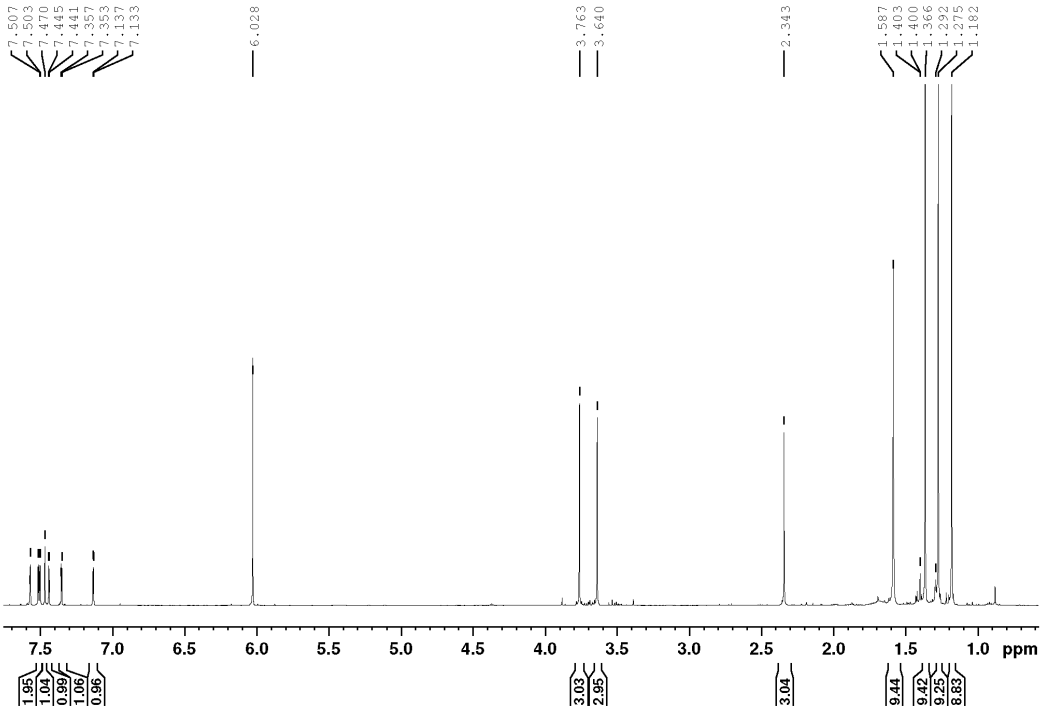


FIGURE 20: ^{13}C NMR SPECTRUM OF 7D (600 MHZ, $CDCl_3$)

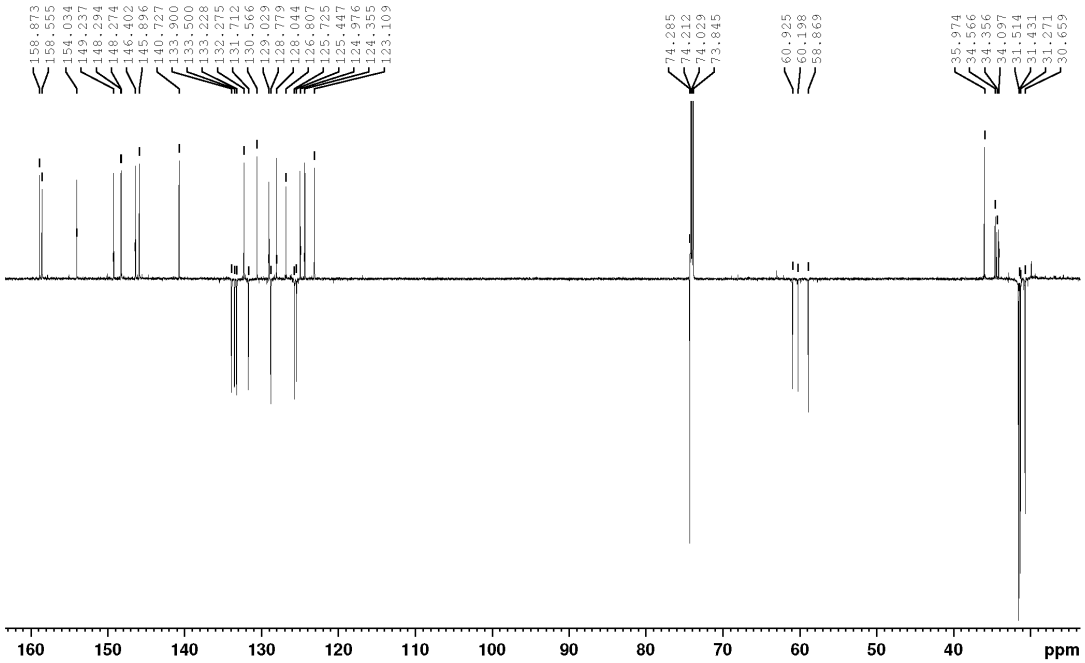


FIGURE 21: ^{1}H-^{1}H COSY SPECTRUM OF 7D (600 MHZ, $CDCl_3$)

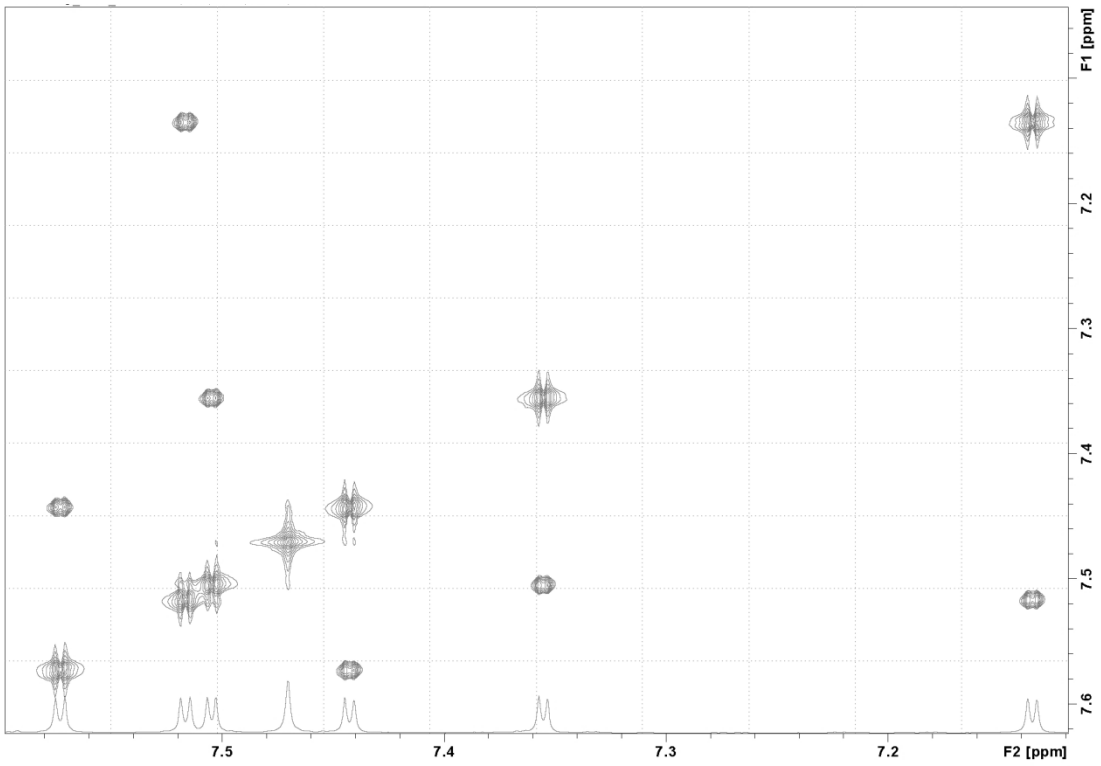


FIGURE 22: ^{1}H-^{13}C HMQC SPECTRUM OF 7D (600 MHZ, $CDCl_3$)

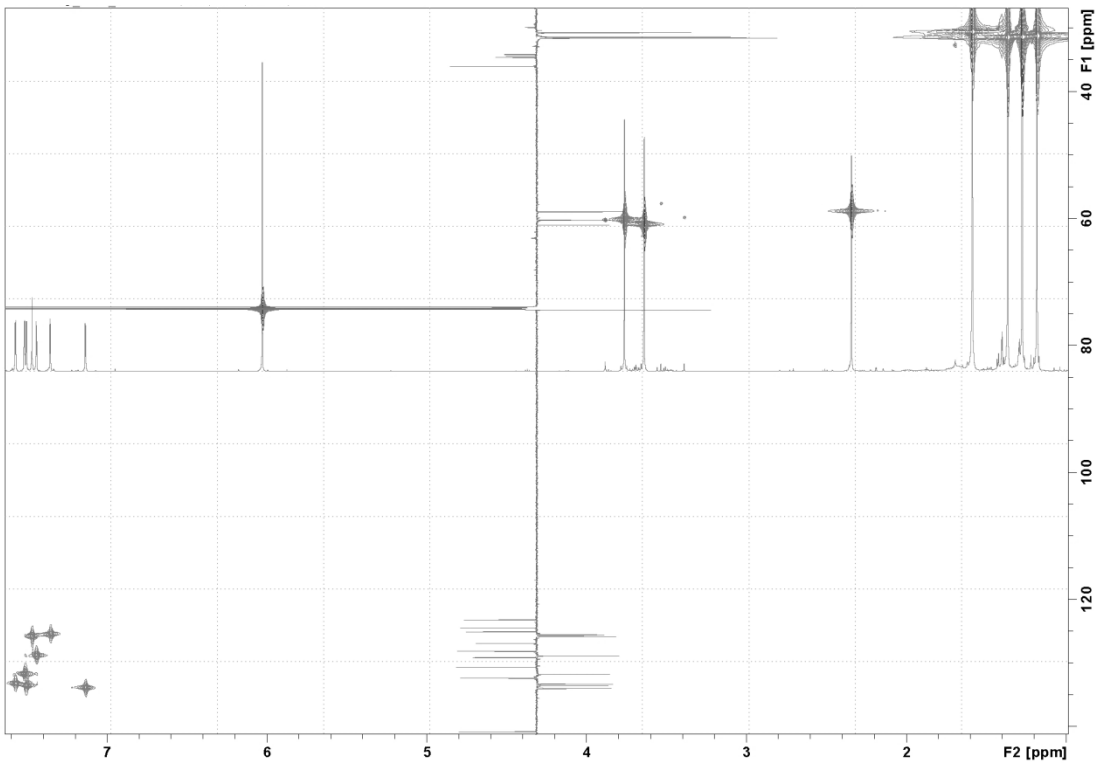


FIGURE 23: ^{1}H-^{13}C HMBC SPECTRUM OF 7D (600 MHZ, $CDCl_3$)

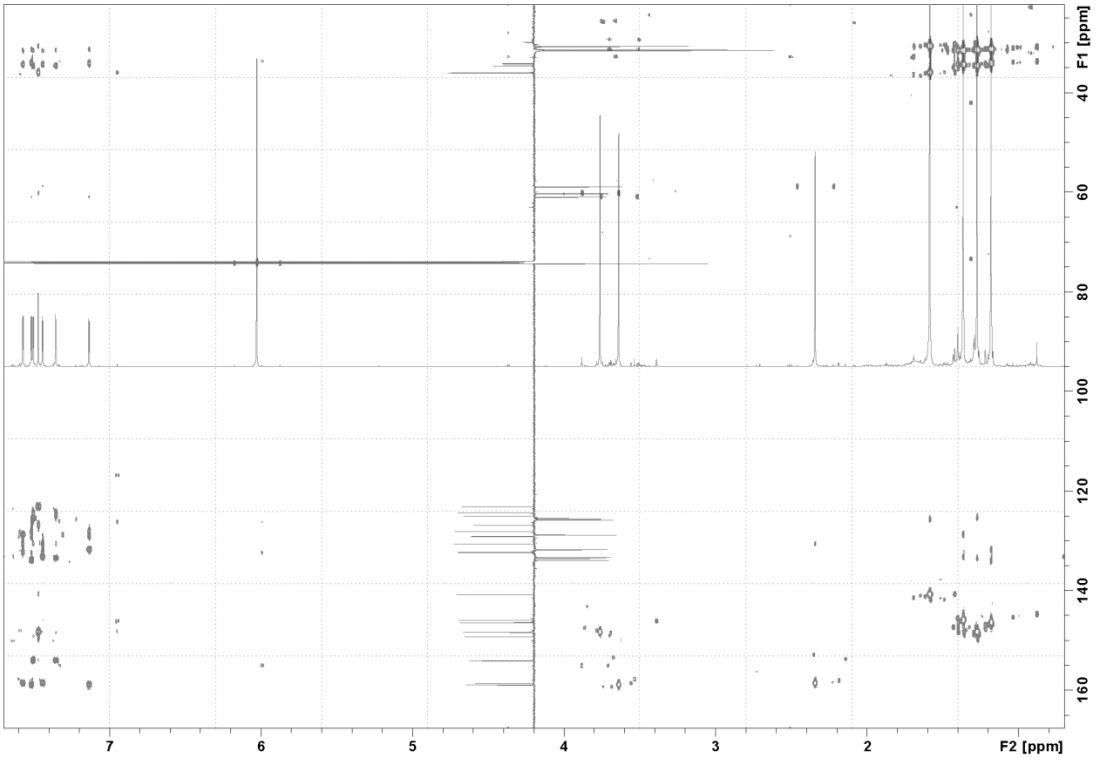
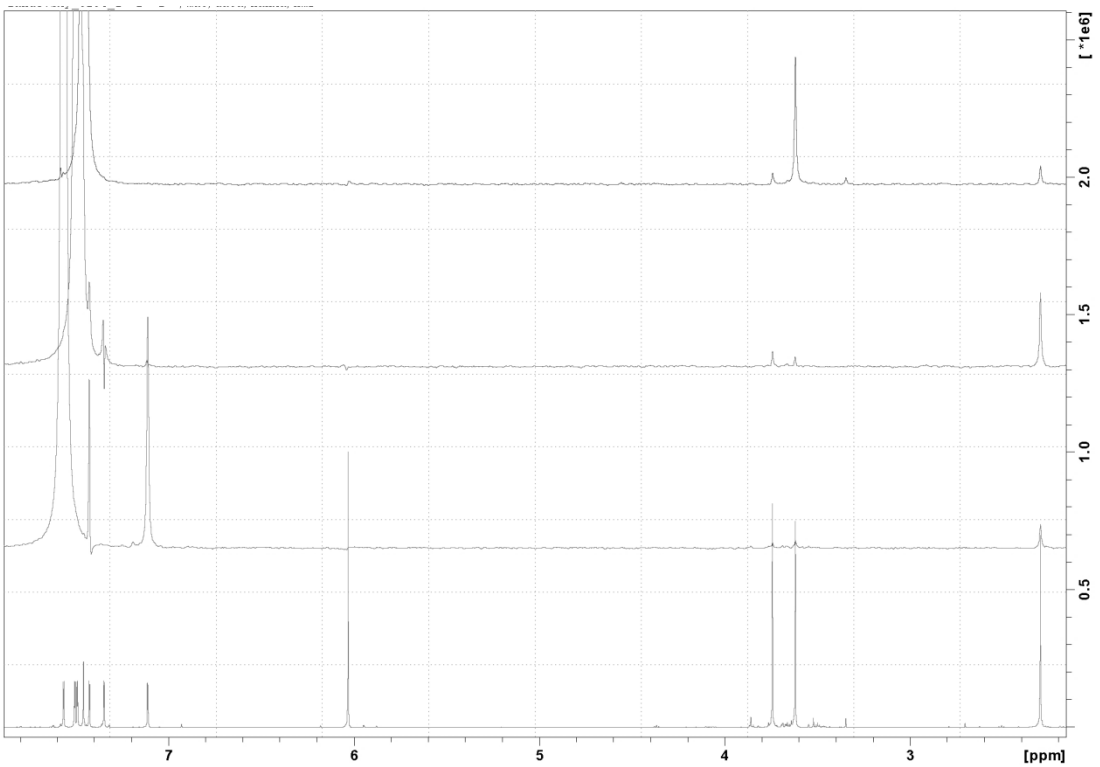


FIGURE 24: 1D ^{1}H-DPFGSE NOE EXPERIMENTS OF 7D (600 MHZ, $CDCl_3$, 273 K)



STATISTICAL FORMULAS

$$x_{\mathrm{rms}} = \sqrt{\frac{1}{n}\left({x_1}^2 + {x_2}^2 + \cdots + {x_n}^2\right)}$$

$$r_{xy} = \frac{\sum_{i=1}^{n}(x_i - \bar{x})(y_i - \bar{y})}{(n-1)s_x s_y} = \frac{\sum_{i=1}^{n}(x_i - \bar{x})(y_i - \bar{y})}{\sqrt{\sum_{i=1}^{n}(x_i - \bar{x})^2 \sum_{i=1}^{n}(y_i - \bar{y})^2}},$$

$$r_{xy} = \frac{\sum x_i y_i - n\bar{x}\bar{y}}{(n-1)s_x s_y} = \frac{n\sum x_i y_i - \sum x_i \sum y_i}{\sqrt{n\sum x_i^2 - (\sum x_i)^2}\ \sqrt{n\sum y_i^2 - (\sum y_i)^2}}.$$

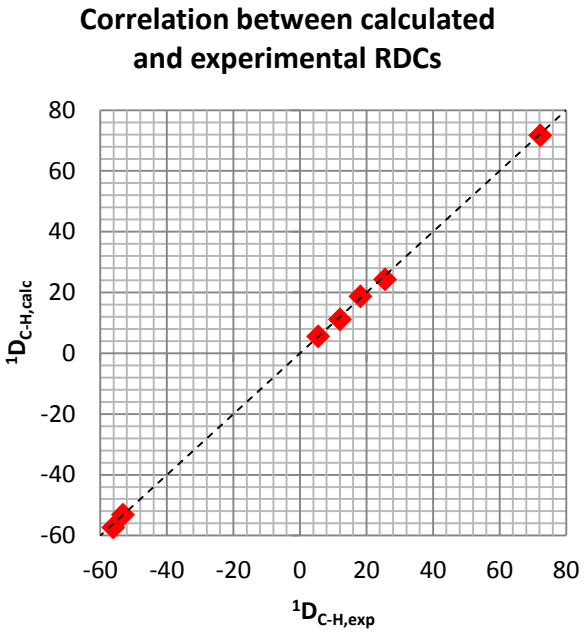
5C (D-*PACO*) @ POLY(γ-ETHYL-L-GLUTAMATE), MEDIUM A

EVALUATION OF RDCs

	$^1J_{C\text{-}H}$ [Hz]	$^1T_{C\text{-}H}$ [Hz]	RDC [Hz]	$^1D_{C\text{-}H}$ [Hz]
CH-A3	159.8	184.0	24.1	12.1
CH-B8	160.3	48.4	-111.9	-56.0
CH-B10	161.1	197.4	36.3	18.2
CH-C13	157.0	50.8	-106.2	-53.1
CH-C15	159.7	304.4	144.7	72.3
CH-D18	159.4	170.4	11.1	5.5
CH-D20	158.0	209.3	51.3	25.6

FITTING RESULTS

$^1D_{C\text{-}H}$	$^1D_{C\text{-}H.exp}$	$^1D_{C\text{-}H.calc}$
CH-A3	12.1	11.2
CH-B8	-56.0	-57.3
CH-B10	18.2	18.7
CH-C13	-53.1	-53.2
CH-C15	72.3	71.6
CH-D18	5.5	5.5
CH-D20	25.6	24.3



n =	7
RMS =	0,9
R(xy) =	1,000
R^2 =	99,98%

PALES output file (fitting procedure results)

```
REMARK Molecular Alignment Simulation.

REMARK Simulation parameters.

DATA PALES_MODE DC

DATA TENSOR_MODE SVD (Order Matrix Method)


REMARK Order matrix.

DATA SAUPE_MATRIX     S(zz)       S(xx-yy)      S(xy)      S(xz)      S(yz)
DATA SAUPE         1.2979e-003 -2.1603e-003  3.3227e-005 -9.8188e-004 -6.7164e-004

DATA IRREDUCIBLE_REP    A0          A1R          A1I         A2R         A2I
DATA IRREDUCIBLE     2.0577e-003  1.2710e-003 -8.6938e-004 -1.3981e-003 -4.3009e-
005
DATA IRREDUCIBLE GENERAL_MAGNITUDE   3.5902e-003


REMARK Mapping of coordinates.

DATA MAPPING_COOR   Szz_d(x)  Szz_d(y)  Syy_d(x)  Syy_d(y)  Sxx_d(x)  Sxx_d(y)
DATA MAPPING        0.06763   0.29927  -1.00494   1.07262   1.63742   0.38551
DATA MAPPING INV   -2.93433  -0.29927   0.49620  -1.07262  -1.27360  -0.38551


REMARK Eigensystem & Euler angles for clockwise rotation about z, y', z''.

DATA EIGENVALUES (Sxx_d,Syy_d,Szz_d)    1.4665e-004  1.8838e-003 -2.0304e-003
DATA EIGENVECTORS           (x_coor      y_coor      z_coor)
DATA EIGENVECTORS X_AXIS -1.8074e-001  9.0881e-001  3.7603e-001
DATA EIGENVECTORS Y_AXIS -2.4252e-001 -4.1170e-001  8.7845e-001
DATA EIGENVECTORS Z_AXIS  9.5316e-001  6.7575e-002  2.9482e-001

DATA Q_EULER_SOLUTIONS    ALPHA     BETA    GAMMA
DATA Q_EULER_ANGLES  1    66.83    72.85   175.94
DATA Q_EULER_ANGLES  2   246.83    72.85   175.94
DATA Q_EULER_ANGLES  3   113.17   107.15   355.94
DATA Q_EULER_ANGLES  4   293.17   107.15   355.94


REMARK Euler angles (psi/theta/phi) for rotation about x, y, z.

DATA EULER_SOLUTIONS 2
DATA EULER_ANGLES   12.91  -72.39   53.31
DATA EULER_ANGLES  192.91  252.39  233.31

DATA Da -1.015225e-003
DATA Dr -5.790510e-004


DATA Aa -2.030449e-003
DATA Ar -1.158102e-003


DATA Da_HN      -2.191383e+001
DATA Rhombicity  5.703673e-001


REMARK Dipolar couplings.

DATA N                    7
DATA RMS                  0.854
```

```
DATA Chi2                 5.103
DATA CORR R               1.000
DATA Q SAUPE              0.012
DATA REGRESSION OFFSET    -0.544 +/- 0.296 [Hz]
DATA REGRESSION SLOPE     1.001 +/- 0.007 [Hz]
DATA REGRESSION BAX SLOPE 1.001 +/- 0.005 [Hz]

VARS    RESID_I RESNAME_I ATOMNAME_I RESID_J RESNAME_J ATOMNAME_J DI D_OBS D D_DIFF
DD W
FORMAT  %4d %4s %4s %4d %4s %4s %9.2f %9.3f %9.3f %9.3f %.2f %.2f

    1  CAL   C7    1  CAL   H6  47734.91   12.1000   11.1586    0.9414  1.0000 1.00
    1  CAL   C5    1  CAL   H1  47198.19  -56.0000  -57.3349    1.3349  1.0000 1.00
    1  CAL   C6    1  CAL   H5  47580.15   18.2000   18.7039   -0.5039  1.0000 1.00
    1  CAL   C4    1  CAL   H3  47355.66  -53.1000  -53.1602    0.0602  1.0000 1.00
    1  CAL   C3    1  CAL   H4  47434.36   72.3000   71.6497    0.6503  1.0000 1.00
    1  CAL   C2    1  CAL   H2  47449.07    5.5000    5.5168   -0.0168  1.0000 1.00
    1  CAL   C1    1  CAL   H7  47166.41   25.6000   24.2754    1.3246  1.0000 1.00
```

5B (C-*PACO*) @ POLY(γ-ETHYL-L-GLUTAMATE), MEDIUM A

EVALUATION OF RDCs

	$^1J_{C\text{-}H}$ [Hz]	$^1T_{C\text{-}H}$ [Hz]	RDC [Hz]	$^1D_{C\text{-}H}$ [Hz]
CH-A3	159.8	184.0	24.1	12.1
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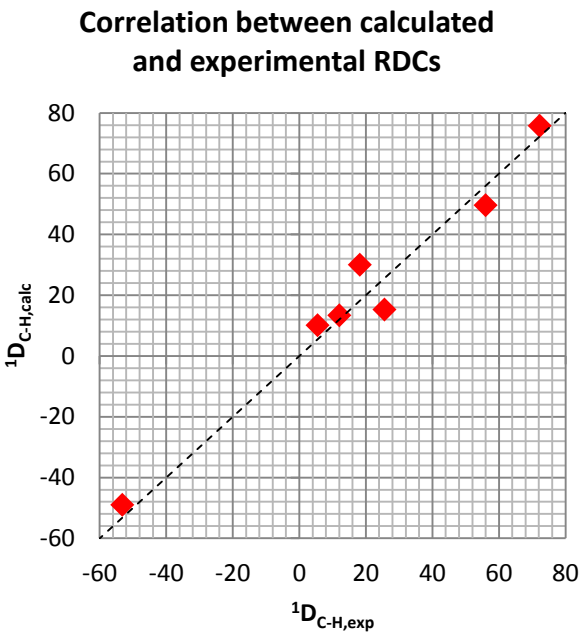
CH-B10	161.1	197.4	36.3	18.2
CH-C13	157.0	50.8	-106.2	-53.1
CH-C15	159.7	304.4	144.7	72.3
CH-D18	159.4	170.4	11.1	5.5
CH-D20	158.0	209.3	51.3	25.6

FITTING RESULTS

$^1D_{C\text{-}H}$	$^1D_{C\text{-}H.exp}$	$^1D_{C\text{-}H.calc}$
CH-A3	12.1	13.4
CH-B8	56.0	49.6
CH-B10	18.2	29.9
CH-C13	-53.1	-49.0
CH-C15	72.3	75.7
CH-D18	5.5	10.0
CH-D20	25.6	15.3

n =	7
RMS =	6,9
R(xy) =	0,983
R^2 =	96,67%



5C (D-*PACO*) @ POLY(γ-BENZYL-L-GLUTAMATE), MEDIUM B

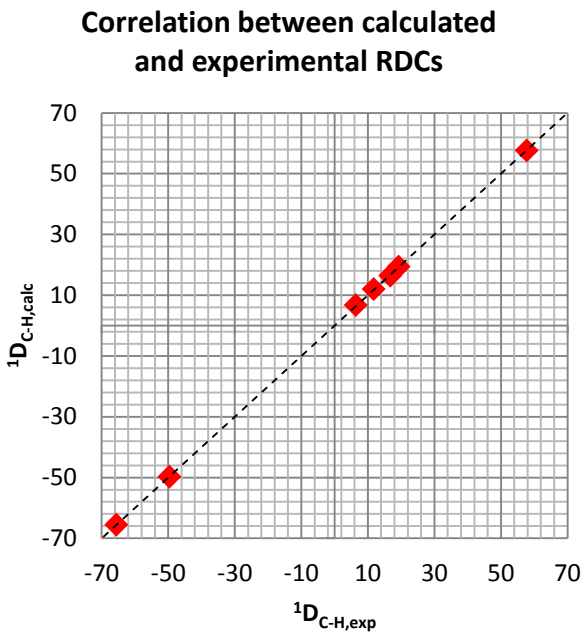
EVALUATION OF RDCs

	$^1J_{C\text{-}H}$ [Hz]	$^1T_{C\text{-}H}$ [Hz]	RDC [Hz]	$^1D_{C\text{-}H}$ [Hz]
CH-A3	159.8	183.5	23.7	11.8
CH-B8	160.3	61.1	-99.2	-49.6
CH-B10	161.1	194.7	33.6	16.8
CH-C13	157.0	26.1	-130.9	-65.5
CH-C15	159.7	275.2	115.5	57.8
CH-D18	159.4	172.2	12.8	6.4
CH-D20	158.0	196.5	38.5	19.3

FITTING RESULTS

$^1D_{C\text{-}H}$	$^1D_{C\text{-}H.exp}$	$^1D_{C\text{-}H.calc}$
CH-A3	11.8	12.0
CH-B8	-49.6	-49.8
CH-B10	16.8	16.4
CH-C13	-65.5	-65.6
CH-C15	57.8	57.6
CH-D18	6.4	6.7
CH-D20	19.3	19.3

n =	7
RMS =	0.2
R(xy) =	1.000
R^2 =	100.00%



PALES output file (fitting procedure results)

```
REMARK Molecular Alignment Simulation.

REMARK Simulation parameters.

DATA PALES_MODE DC

DATA TENSOR_MODE SVD (Order Matrix Method)


REMARK Order matrix.

DATA SAUPE_MATRIX     S(zz)       S(xx-yy)      S(xy)      S(xz)      S(yz)
DATA SAUPE         1.0384e-003 -2.5764e-003  2.1279e-004 -4.7530e-004 -6.7312e-004

DATA IRREDUCIBLE_REP    A0          A1R          A1I         A2R         A2I
DATA IRREDUCIBLE     1.6462e-003  6.1523e-004 -8.7129e-004 -1.6675e-003 -2.7544e-
004
DATA IRREDUCIBLE GENERAL_MAGNITUDE   3.2708e-003


REMARK Mapping of coordinates.

DATA MAPPING_COOR   Szz_d(x)  Szz_d(y)  Syy_d(x)  Syy_d(y)  Sxx_d(x)  Sxx_d(y)
DATA MAPPING       -0.04085   0.15156  -1.13990   0.88494   1.30011   0.66248
DATA MAPPING INV    3.06473  -0.15156   0.84977  -0.88494  -1.17694  -0.66248


REMARK Eigensystem & Euler angles for clockwise rotation about z, y', z''.

DATA EIGENVALUES (Sxx_d,Syy_d,Szz_d)    2.2567e-004  1.6632e-003 -1.8889e-003
DATA EIGENVECTORS           (x_coor      y_coor      z_coor)
DATA EIGENVECTORS X_AXIS -6.1522e-002  7.8607e-001  6.1507e-001
DATA EIGENVECTORS Y_AXIS -1.4380e-001 -6.1679e-001  7.7388e-001
DATA EIGENVECTORS Z_AXIS  9.8769e-001 -4.0837e-002  1.5098e-001

DATA Q_EULER_SOLUTIONS    ALPHA     BETA    GAMMA
DATA Q_EULER_ANGLES  1    51.52    81.32   182.37
DATA Q_EULER_ANGLES  2   231.52    81.32   182.37
DATA Q_EULER_ANGLES  3   128.48    98.68     2.37
DATA Q_EULER_ANGLES  4   308.48    98.68     2.37


REMARK Euler angles (psi/theta/phi) for rotation about x, y, z.

DATA EULER_SOLUTIONS 2
DATA EULER_ANGLES  -15.13  -81.00   66.84
DATA EULER_ANGLES  164.87  261.00  246.84

DATA Da -9.444267e-004
DATA Dr -4.791692e-004


DATA Aa -1.888853e-003
DATA Ar -9.583384e-004


DATA Da_HN      -2.038564e+001
DATA Rhombicity  5.073652e-001


REMARK Dipolar couplings.

DATA N                    7
DATA RMS                  0.221
DATA Chi2                 0.343
```

```
DATA CORR R               1.000
DATA Q SAUPE              0.004
DATA REGRESSION OFFSET    -0.052 +/- 0.096 [Hz]
DATA REGRESSION SLOPE     1.000 +/- 0.002 [Hz]
DATA REGRESSION BAX SLOPE 1.000 +/- 0.002 [Hz]

VARS    RESID_I RESNAME_I ATOMNAME_I RESID_J RESNAME_J ATOMNAME_J DI D_OBS D D_DIFF
DD W
FORMAT  %4d %4s %4s %4d %4s %4s %9.2f %9.3f %9.3f %9.3f %.2f %.2f

    1  CAL   C1    1  CAL   H7  47758.57   11.8000   12.0062   -0.2062  1.0000 1.00
    1  CAL  C29    1  CAL  H33  47176.79  -49.6000  -49.7862    0.1862  1.0000 1.00
    1  CAL  C27    1  CAL  H54  47536.98   16.8000   16.4300    0.3700  1.0000 1.00
    1  CAL  C83    1  CAL  H87  47668.52  -65.5000  -65.5755    0.0755  1.0000 1.00
    1  CAL  C81    1  CAL  H85  47711.00   57.8000   57.5835    0.2165  1.0000 1.00
    1  CAL  C95    1  CAL  H97  47612.93    6.4000    6.6769   -0.2769  1.0000 1.00
    1  CAL  C93    1  CAL  H96  47258.25   19.3000   19.3005   -0.0005  1.0000 1.00
```

5B (C-*PACO*) @ POLY(γ-BENZYL-L-GLUTAMATE), MEDIUM B

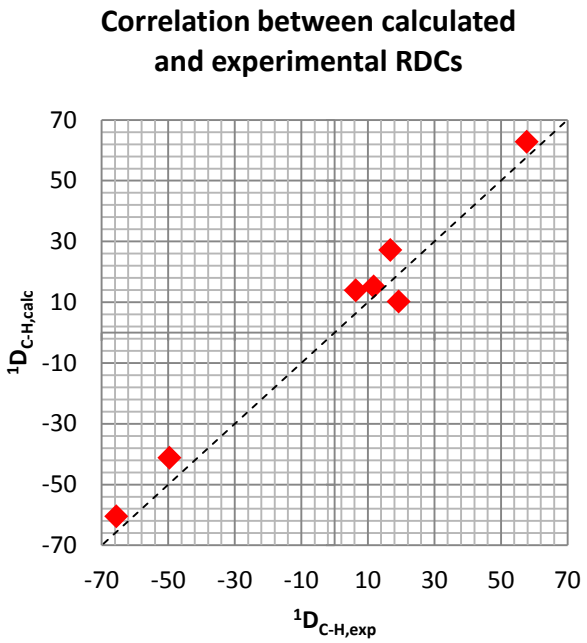
EVALUATION OF RDCs

	$^1J_{C\text{-}H}$ [Hz]	$^1T_{C\text{-}H}$ [Hz]	RDC [Hz]	$^1D_{C\text{-}H}$ [Hz]
CH-A3	159.8	183.5	23.7	11.8
CH-B8	160.3	61.1	-99.2	-49.6
CH-B10	161.1	194.7	33.6	16.8
CH-C13	157.0	26.1	-130.9	-65.5
CH-C15	159.7	275.2	115.5	57.8
CH-D18	159.4	172.2	12.8	6.4
CH-D20	158.0	196.5	38.5	19.3

FITTING RESULTS

$^1D_{C\text{-}H}$	$^1D_{C\text{-}H.exp}$	$^1D_{C\text{-}H.calc}$
CH-A3	11.8	15.1
CH-B8	-49.6	-41.2
CH-B10	16.8	27.1
CH-C13	-65.5	-60.5
CH-C15	57.8	62.7
CH-D18	6.4	13.8
CH-D20	19.3	10.2

n =	7
RMS =	7.3
R(xy) =	0.989
R^2 =	97.78%



5D (1,2-*ALT*) @ POLY(γ-ETHYL-L-GLUTAMATE), MEDIUM A

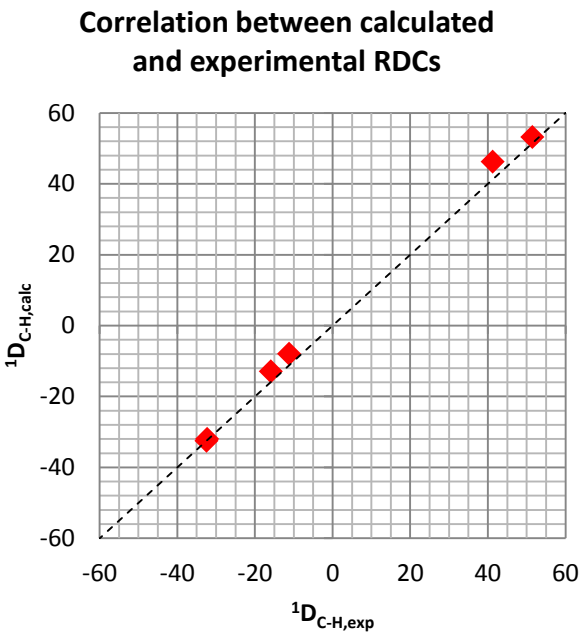
EVALUATION OF RDCs

	$^1J_{C\text{-}H}$ [Hz]	$^1T_{C\text{-}H}$ [Hz]	RDC [Hz]	$^1D_{C\text{-}H}$ [Hz]
CH-A3	160.4	138.0	-22.4	-11.2
CH-B8	159.3	32.0	-127.3	-63.6
CH-B10	160.8	96.0	-64.8	-32.4
CH-C13	157.0	260.0	103.0	51.5
CH-C15	159.8	128.0	-31.8	-15.9
CH-D18	158.6	82.0	-76.6	-38.3
CH-D20	158.3	241.0	82.7	41.3

FITTING RESULTS

$^1D_{C\text{-}H}$	$^1D_{C\text{-}H.exp}$	$^1D_{C\text{-}H.calc}$
CH-A3	-11.2	-8.0
CH-B8	-63.6	-59.5
CH-B10	-32.4	-32.6
CH-C13	51.5	53.1
CH-C15	-15.9	-13.0
CH-D18	-32.3	-32.0
CH-D20	41.3	46.2

n =	7
RMS =	3.0
R(xy) =	0.999
R^2 =	99.80%



PALES output file (fitting procedure results)

```
REMARK Molecular Alignment Simulation.

REMARK Simulation parameters.

DATA PALES_MODE DC

DATA TENSOR_MODE SVD (Order Matrix Method)


REMARK Order matrix.

DATA SAUPE_MATRIX     S(zz)       S(xx-yy)      S(xy)      S(xz)      S(yz)
DATA SAUPE         3.2052e-03 -9.9240e-04  7.8311e-04 -2.1170e-04 -1.0380e-04

DATA IRREDUCIBLE_REP    A0          A1R          A1I         A2R         A2I
DATA IRREDUCIBLE     5.0812e-03  2.7403e-04 -1.3436e-04 -6.4229e-04 -1.0137e-03
DATA IRREDUCIBLE GENERAL_MAGNITUDE   5.3745e-03


REMARK Mapping of coordinates.

DATA MAPPING_COOR   Szz_d(x)  Szz_d(y)  Syy_d(x)  Syy_d(y)  Sxx_d(x)  Sxx_d(y)
DATA MAPPING       -0.13797   1.51597  -0.50041   0.02368   1.07011   0.04944
DATA MAPPING INV    0.03420  -1.51597   2.64030  -0.02368  -2.06764  -0.04944


REMARK Eigensystem & Euler angles for clockwise rotation about z, y', z''.

DATA EIGENVALUES (Sxx_d,Syy_d,Szz_d)   -6.8506e-04 -2.5329e-03  3.2179e-03
DATA EIGENVECTORS           (x_coor      y_coor      z_coor)
DATA EIGENVECTORS X_AXIS  4.7829e-01  8.7681e-01  4.9423e-02
DATA EIGENVECTORS Y_AXIS  8.7707e-01 -4.7977e-01  2.3680e-02
DATA EIGENVECTORS Z_AXIS -4.4475e-02 -3.2022e-02  9.9850e-01

DATA Q_EULER_SOLUTIONS    ALPHA     BETA    GAMMA
DATA Q_EULER_ANGLES  1   154.40     3.14   324.25
DATA Q_EULER_ANGLES  2   334.40     3.14   324.25
DATA Q_EULER_ANGLES  3    25.60   176.86   144.25
DATA Q_EULER_ANGLES  4   205.60   176.86   144.25


REMARK Euler angles (psi/theta/phi) for rotation about x, y, z.

DATA EULER_SOLUTIONS 2
DATA EULER_ANGLES   -1.84    2.55  118.60
DATA EULER_ANGLES  178.16  177.45  -61.40

DATA Da  1.608961e-03
DATA Dr  6.159366e-04


DATA Aa  3.217922e-03
DATA Ar  1.231873e-03


DATA Da_HN       3.472975e+01
DATA Rhombicity  3.828164e-01


REMARK Dipolar couplings.

DATA N                    7
DATA RMS                  3.000
DATA Chi2                 62.993
```

```
DATA CORR R               0.999
DATA Q SAUPE              0.029
DATA REGRESSION OFFSET    2.499 +/- 0.799 [Hz]
DATA REGRESSION SLOPE     1.009 +/- 0.020 [Hz]
DATA REGRESSION BAX SLOPE 1.010 +/- 0.014 [Hz]

VARS    RESID_I RESNAME_I ATOMNAME_I RESID_J RESNAME_J ATOMNAME_J DI D_OBS D D_DIFF
DD W
FORMAT  %4d %4s %4s %4d %4s %4s %9.2f %9.3f %9.3f %9.3f %.2f %.2f

    1  CAL  C14    1  CAL  H33  47786.71  -11.2000   -7.9838   -3.2162  1.0000 1.00
    1  CAL  C40    1  CAL  H37  47458.52  -63.6000  -59.4735   -4.1265  1.0000 1.00
    1  CAL  C13    1  CAL  H15  47274.22  -32.4000  -32.5502    0.1502  1.0000 1.00
    1  CAL  C12    1  CAL  H18  47421.91   51.5000   53.1087   -1.6087  1.0000 1.00
    1  CAL   C6    1  CAL  H20  47278.38  -15.9000  -12.9653   -2.9347  1.0000 1.00
    1  CAL  C21    1  CAL  H22  47586.48  -32.3000  -32.0141   -0.2859  1.0000 1.00
    1  CAL  C11    1  CAL  H26  47145.48   41.3000   46.2311   -4.9311  1.0000 1.00
```

5A (*CONE*) @ POLY(γ-ETHYL-L-GLUTAMATE), MEDIUM A

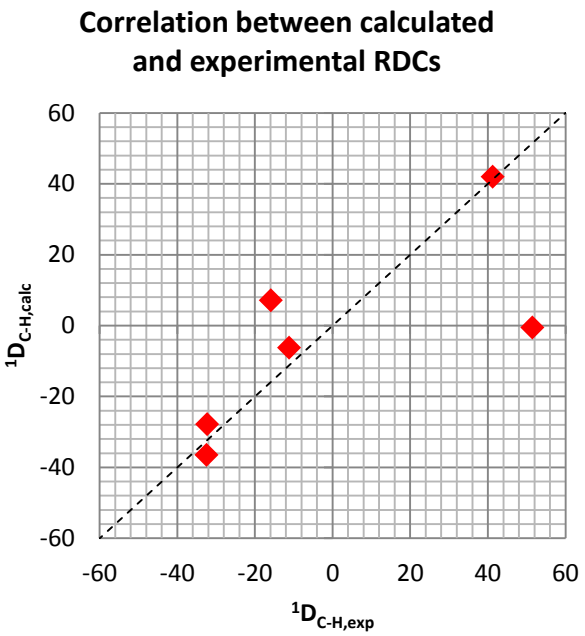
EVALUATION OF RDCs

	$^1J_{C\text{-}H}$ [Hz]	$^1T_{C\text{-}H}$ [Hz]	RDC [Hz]	$^1D_{C\text{-}H}$ [Hz]
CH-A3	160.4	138.0	-22.4	-11.2
CH-B8	159.3	32.0	-127.3	-63.6
CH-B10	160.8	96.0	-64.8	-32.4
CH-C13	157.0	260.0	103.0	51.5
CH-C15	159.8	128.0	-31.8	-15.9
CH-D18	158.6	82.0	-76.6	-38.3
CH-D20	158.3	241.0	82.7	41.3

FITTING RESULTS

$^1D_{C\text{-}H}$	$^1D_{C\text{-}H.exp}$	$^1D_{C\text{-}H.calc}$
CH-A3	-11.2	-6.3
CH-B8	-63.6	-60.0
CH-B10	-32.4	-36.5
CH-C13	51.5	-0.6
CH-C15	-15.9	7.0
CH-D18	-32.3	-27.8
CH-D20	41.3	41.9

n =	7
RMS =	21.8
R(xy) =	0.827
R^2 =	68.47%



5D (1,2-*ALT*) @ POLY(γ-BENZYL-L-GLUTAMATE), MEDIUM B

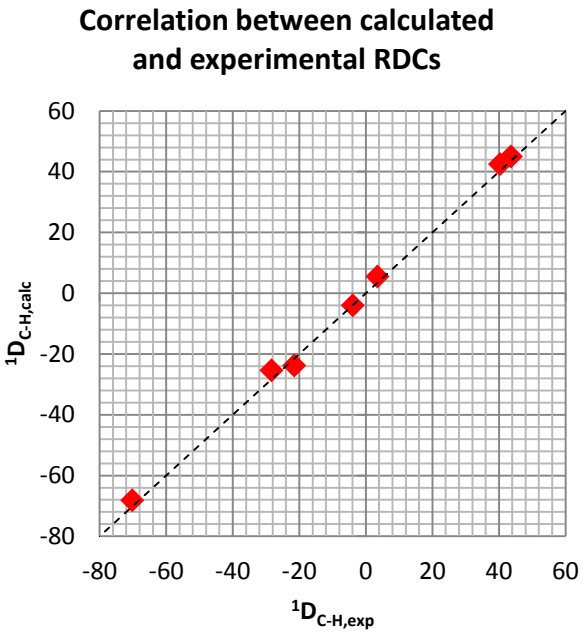
EVALUATION OF RDCs

	$^1J_{C\text{-}H}$ [Hz]	$^1T_{C\text{-}H}$ [Hz]	RDC [Hz]	$^1D_{C\text{-}H}$ [Hz]
CH-A3	160.4	152.5	-7.9	-3.9
CH-B8	159.3	18.8	-140.5	-70.2
CH-B10	160.8	104.1	-56.7	-28.3
CH-C13	157.0	244.3	87.3	43.6
CH-C15	159.8	166.9	7.1	3.5
CH-D18	158.6	115.6	-43.0	-21.5
CH-D20	158.3	239.2	80.9	40.4

FITTING RESULTS

$^1D_{C\text{-}H}$	$^1D_{C\text{-}H.exp}$	$^1D_{C\text{-}H.calc}$
CH-A3	-3.9	-4.0
CH-B8	-70.2	-68.2
CH-B10	-28.3	-25.4
CH-C13	43.6	44.9
CH-C15	3.5	5.4
CH-D18	-21.5	-23.9
CH-D20	40.4	42.4

n =	7
RMS =	2.0
R(xy) =	0.999
R^2 =	99.80%



PALES output file (fitting procedure results)

```
REMARK Molecular Alignment Simulation.

REMARK Simulation parameters.

DATA PALES_MODE DC

DATA TENSOR_MODE SVD (Order Matrix Method)


REMARK Order matrix.

DATA SAUPE_MATRIX     S(zz)       S(xx-yy)      S(xy)      S(xz)      S(yz)
DATA SAUPE         2.6191e-003 -1.1043e-003  5.0729e-004  2.6151e-004  2.1389e-005

DATA IRREDUCIBLE_REP    A0          A1R          A1I         A2R         A2I
DATA IRREDUCIBLE     4.1521e-003 -3.3851e-004  2.7687e-005 -7.1470e-004 -6.5665e-
004
DATA IRREDUCIBLE GENERAL_MAGNITUDE   4.3994e-003


REMARK Mapping of coordinates.

DATA MAPPING_COOR   Szz_d(x)  Szz_d(y)  Syy_d(x)  Syy_d(y)  Sxx_d(x)  Sxx_d(y)
DATA MAPPING        0.01539   1.50908  -0.36725  -0.05035   1.20411  -0.03566
DATA MAPPING INV   -0.17836  -1.50908   2.77036   0.05035  -1.93548   0.03566


REMARK Eigensystem & Euler angles for clockwise rotation about z, y', z''.

DATA EIGENVALUES (Sxx_d,Syy_d,Szz_d)   -5.6384e-004 -2.0712e-003  2.6351e-003
DATA EIGENVECTORS           (x_coor      y_coor      z_coor)
DATA EIGENVECTORS X_AXIS  3.5758e-001  9.3320e-001 -3.5650e-002
DATA EIGENVECTORS Y_AXIS  9.3197e-001 -3.5903e-001 -5.0325e-002
DATA EIGENVECTORS Z_AXIS  5.9763e-002  1.5230e-002  9.9810e-001

DATA Q_EULER_SOLUTIONS    ALPHA     BETA    GAMMA
DATA Q_EULER_ANGLES  1   305.31     3.54   165.70
DATA Q_EULER_ANGLES  2   125.31     3.54   165.70
DATA Q_EULER_ANGLES  3   234.69   176.46   345.70
DATA Q_EULER_ANGLES  4    54.69   176.46   345.70


REMARK Euler angles (psi/theta/phi) for rotation about x, y, z.

DATA EULER_SOLUTIONS 2
DATA EULER_ANGLES    0.87   -3.43  110.99
DATA EULER_ANGLES  180.87  183.43  -69.01

DATA Da  1.317540e-003
DATA Dr  5.024638e-004


DATA Aa  2.635081e-003
DATA Ar  1.004928e-003


DATA Da_HN       2.843937e+001
DATA Rhombicity  3.813650e-001


REMARK Dipolar couplings.

DATA N                    7
DATA RMS                  1.998
```

```
DATA Chi2                 27.946
DATA CORR R               0.999
DATA Q SAUPE              0.024
DATA REGRESSION OFFSET    1.101 +/- 0.755 [Hz]
DATA REGRESSION SLOPE     1.001 +/- 0.020 [Hz]
DATA REGRESSION BAX SLOPE 1.002 +/- 0.014 [Hz]

VARS    RESID_I RESNAME_I ATOMNAME_I RESID_J RESNAME_J ATOMNAME_J DI D_OBS D D_DIFF
DD W
FORMAT  %4d %4s %4s %4d %4s %4s %9.2f %9.3f %9.3f %9.3f %.2f %.2f

    1  CAL  C14    1  CAL  H33  47786.72   -3.9000   -4.0434    0.1434  1.0000 1.00
    1  CAL  C40    1  CAL  H37  47458.52  -70.2000  -68.1616   -2.0384  1.0000 1.00
    1  CAL  C13    1  CAL  H15  47274.22  -28.3000  -25.3818   -2.9182  1.0000 1.00
    1  CAL  C12    1  CAL  H18  47421.91   43.6000   44.9232   -1.3232  1.0000 1.00
    1  CAL   C6    1  CAL  H20  47278.38    3.5000    5.4229   -1.9229  1.0000 1.00
    1  CAL  C21    1  CAL  H22  47586.48  -21.5000  -23.9042    2.4042  1.0000 1.00
    1  CAL  C11    1  CAL  H26  47145.48   40.4000   42.4065   -2.0065  1.0000 1.00
```

5A (*CONE*) @ POLY(γ-BENZYL-L-GLUTAMATE), MEDIUM B

EVALUATION OF RDCs

	$^1J_{C\text{-}H}$ [Hz]	$^1T_{C\text{-}H}$ [Hz]	RDC [Hz]	$^1D_{C\text{-}H}$ [Hz]
CH-A3	160.4	152.5	-7.9	-3.9
CH-B8	159.3	18.8	-140.5	-70.2
CH-B10	160.8	104.1	-56.7	-28.3
CH-C13	157.0	244.3	87.3	43.6
CH-C15	159.8	166.9	7.1	3.5
CH-D18	158.6	115.6	-43.0	-21.5
CH-D20	158.3	239.2	80.9	40.4

FITTING RESULTS

$^1D_{C\text{-}H}$	$^1D_{C\text{-}H.exp}$	$^1D_{C\text{-}H.calc}$
CH-A3	-3.9	-2.4
CH-B8	-70.2	-69.1
CH-B10	-28.3	-29.6
CH-C13	43.6	-0.6
CH-C15	3.5	7.4
CH-D18	-21.5	-20.2
CH-D20	40.4	40.6

n =	7
RMS =	16.8
R(xy) =	0.904
R^2 =	81.65%

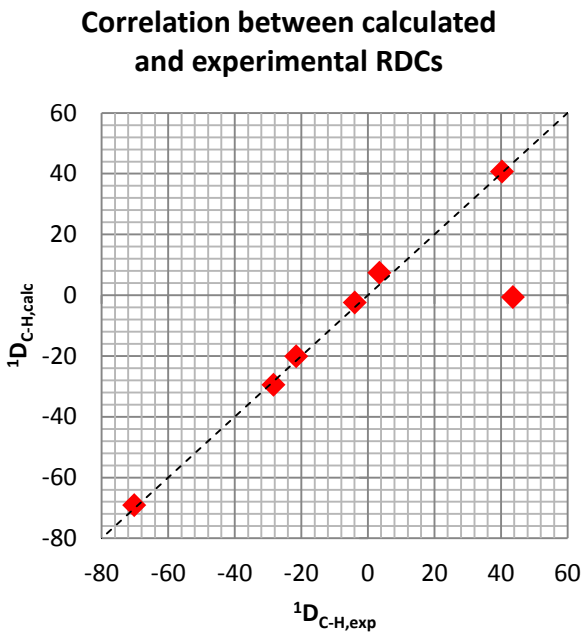


Table 1: Comparison of RDC values of structure 5c (D-*paco*) in various polypeptide alignment media.

	$^1J_{CH}$ ($CDCl_3$)	$^1D_{CH}$ (*PELG*)	$^1D_{CH}$ (*PBLG*)
CH-3A	159.8	12.1	11.8
CH-8B	160.3	-56.0	-49.6
CH-10B	161.1	18.2	16.8
CH-13C	157.0	-53.1	-65.5
CH-15C	159.7	72.3	57.8
CH-18D	159.4	5.5	6.4
CH-20D	158.0	25.6	19.3

Table 2: Comparison of RDC values of structure 5d (1,2-*alt*) in various polypeptide alignment media.

	$^1J_{CH}$ ($CDCl_3$)	$^1D_{CH}$ (*PELG*)	$^1D_{CH}$ (*PBLG*)
CH-3A	160.4	-11.2	-3.9
CH-8B	159.3	-63.6	-70.2
CH-10B	160.8	-32.4	-28.3
CH-13C	157.0	51.5	43.6
CH-15C	159.8	-15.9	3.5
CH-18D	158.6	-32.3	-21.5
CH-20D	158.3	41.3	40.4

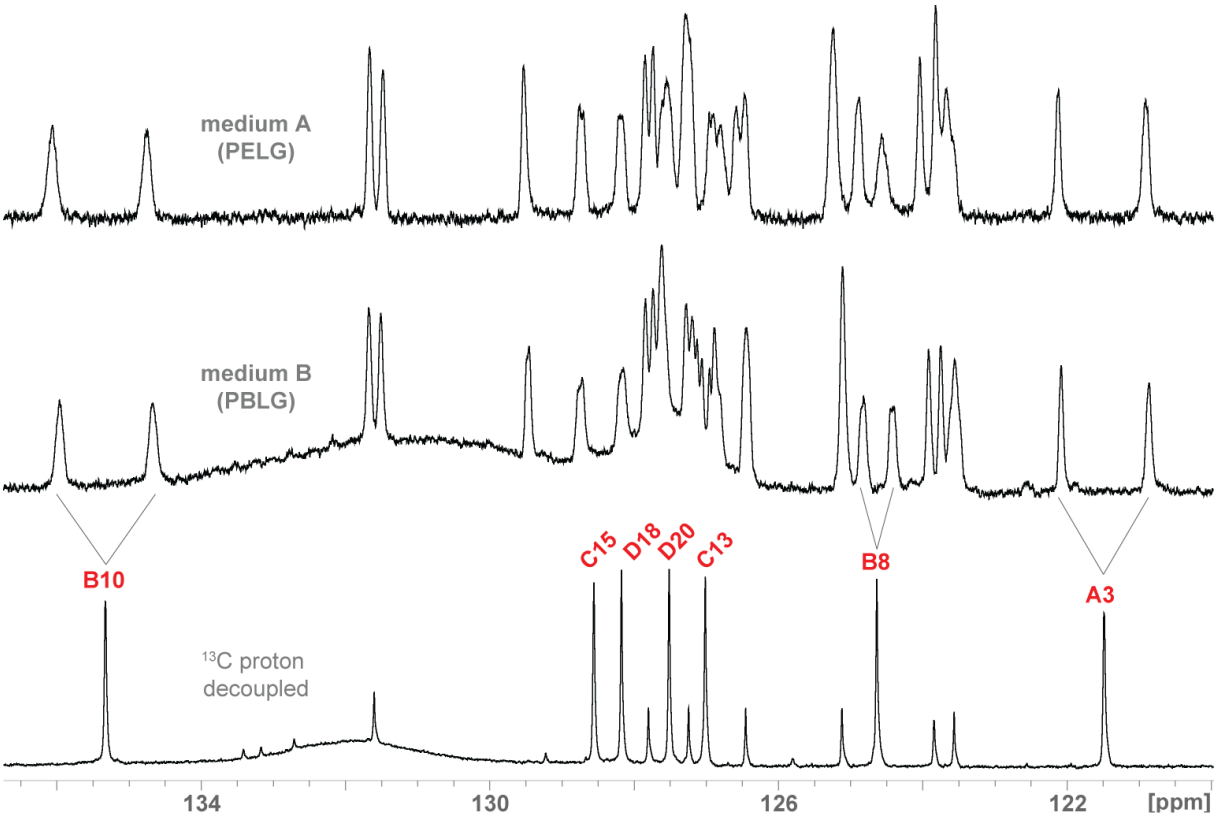


Figure 25: Comparison of selected region of ^{13}C Z-restored proton coupled spectra of 5c (D-*paco*) in polypeptide alignment media.

Table 3: Comparison of fitting quality of structures 5c (D-*paco*) and 5b (C-*paco*) in various alignment media.

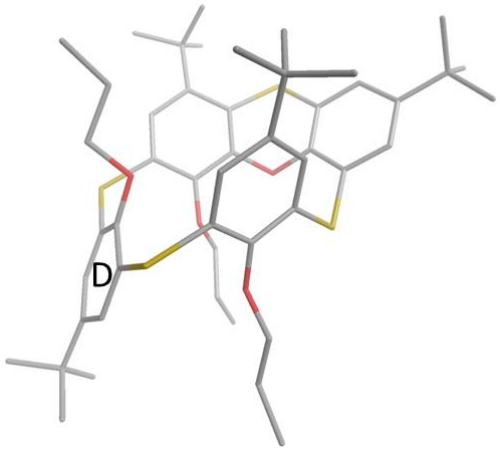
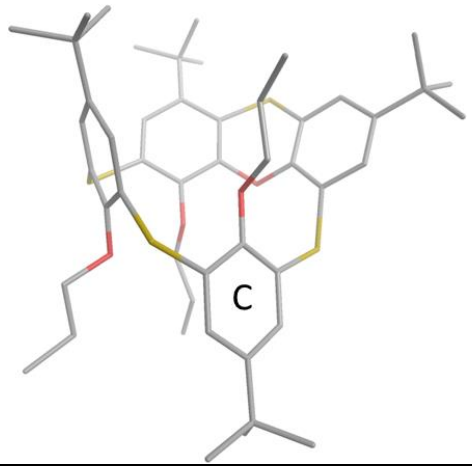
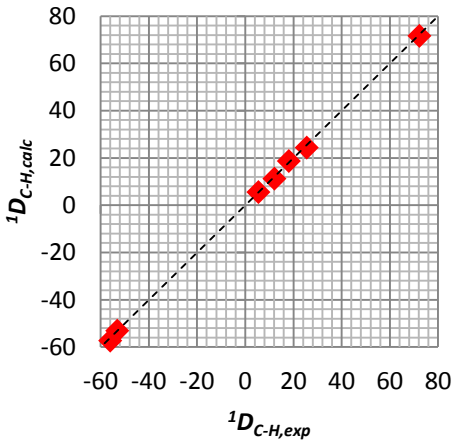
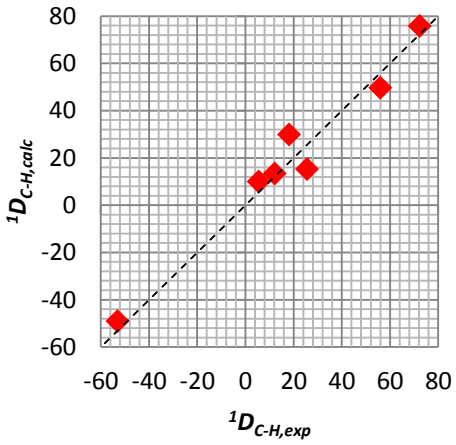
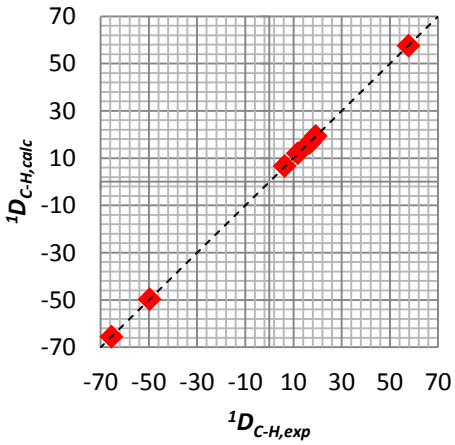
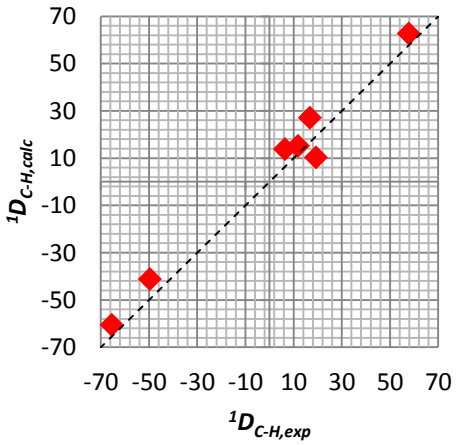
	5c (D-*paco*) – right conformer	5b (*C-paco*) – wrong conformer
input structures		
PELG		
PBLG		

Table 4: Comparison of fitting quality of structures K2(C*D_down*) and K2(*cone*) in various alignment media.

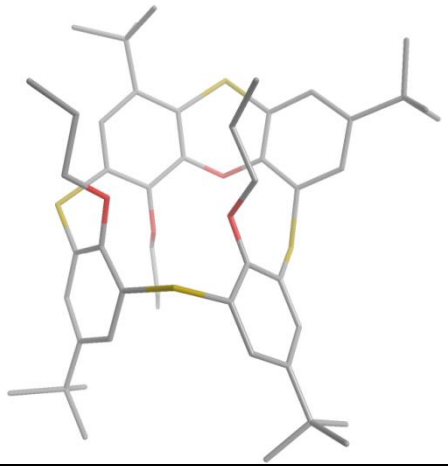
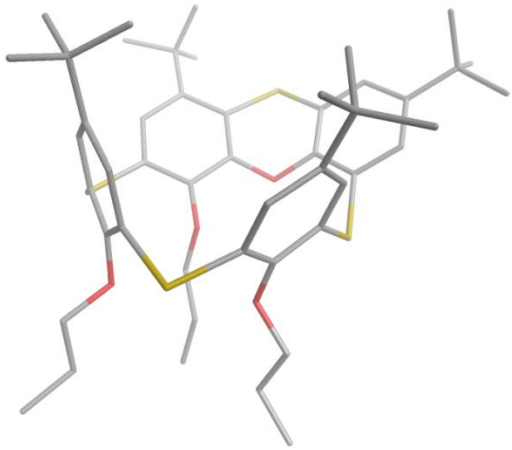
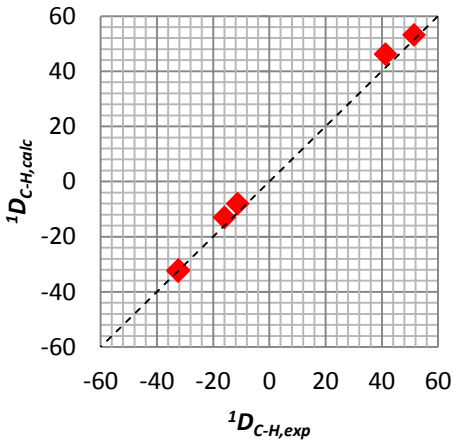
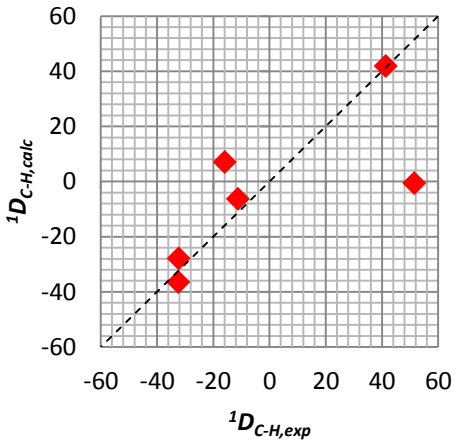
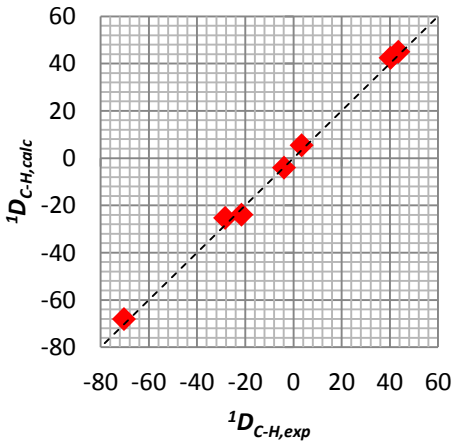
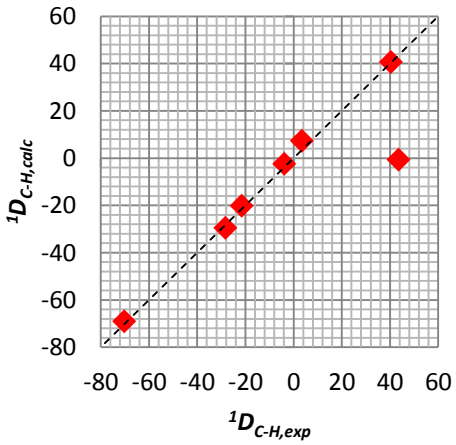
	5d (1,2-*alt*) – right conformer	5a (*cone*) – wrong conformer
input structures		
PELG		
PBLG		

Table 5: Comparison of molecular orientations of 5c (D-*paco*) within the magnetic field.

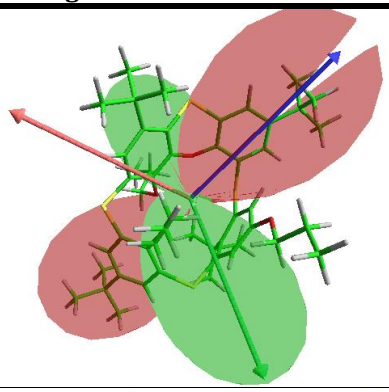
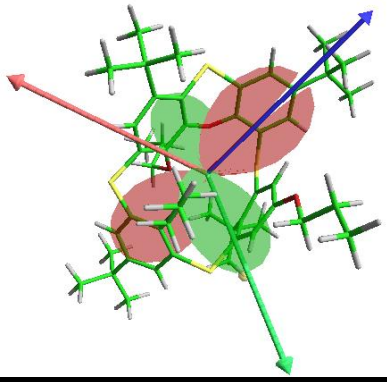
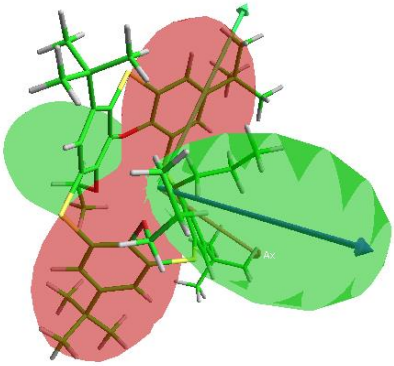
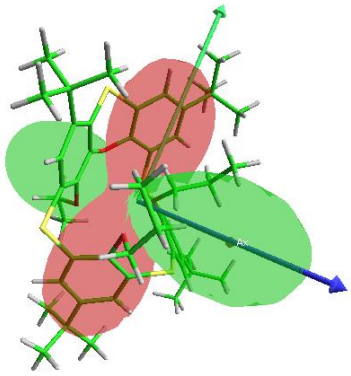
Alignment medium	**Orientation of 5c (D-*paco*) within the magnetic field**
PELG (medium A)	
PBLG (medium B)	

Table 6: Comparison of molecular orientations of 5d (1,2-*alt*) within the magnetic field.

Alignment medium	**Orientation of 5d (1,2-*alt*) within the magnetic field**
PELG (medium A)	
PBLG (medium B)	

DFT OPTIMIZATION OF CONFORMERS

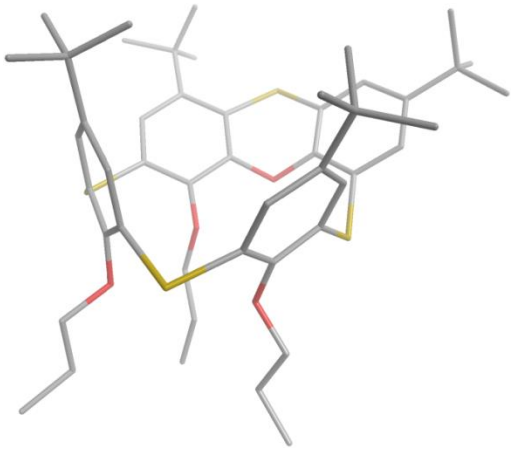
Ab initio **geometry optimizations were performer by program Gaussian03** (M. J. Frisch, H. B. Schlegel, G. E. Scuseria, M. A. Robb, J. R. Cheeseman, J. A. Montgomery, Jr., T. Vreven, K. N. Kudin, J. C. Burant, J. M. Millam, S. S. Iyengar, J. Tomasi, V. Barone, B. Mennucci, M. Cossi, G. Scalmani, N. Rega, G. A. Petersson, H. Nakatsuji, M. Hada, M. Ehara, K. Toyota, R. Fukuda, J. Hasegawa, M. Ishida, T. Nakajima, Y. Honda, O. Kitao, H. Nakai, M. Klene, X. Li, J. E. Knox, H. P. Hratchian, J. B. Cross, V. Bakken, C. Adamo, J. Jaramillo, R. Gomperts, R. E. Stratmann, O. Yazyev, A. J. Austin, R. Cammi, C. Pomelli, J. W. Ochterski, P. Y. Ayala, K. Morokuma, G. A. Voth, P. Salvador, J. J. Dannenberg, V. G. Zakrzewski, S. Dapprich, A. D. Daniels, M. C. Strain, O. Farkas, D. K. Malick, A. D. Rabuck, K. Raghavachari, J. B. Foresman, J. V. Ortiz, Q. Cui, A. G. Baboul, S. Clifford, J. Cioslowski, B. B. Stefanov, G. Liu, A. Liashenko, P. Piskorz, I. Komaromi, R. L. Martin, D. J. Fox, T. Keith, M. A. Al-Laham, C. Y. Peng, A. Nanayakkara, M. Challacombe, P. M. W. Gill, B. Johnson, W. Chen, M. W. Wong, C. Gonzalez, and J. A. Pople, Gaussian, Inc., Wallingford CT, **2004**.)

Table 7: Sums of electronic and thermal free energies (on computational level RB3LYP/6-31G*) of conformers 5a, 5b, 5c and 5d. 5c (D-*paco*) was selected due to the lowest energy state as the reference.

structure	GFE [Hartree]	GFE [kJ/mol]	ΔE [kJ/mol]	population
5a (*cone*)	-3798,460693	-9972858,55	29,78	6,06E-06
5b (*C-paco*)	-3798,460455	-9972857,92	30,40	4,71E-06
5c (*D-paco*)	-3798,472035	-9972888,33	0,00	1,00E+00
5d (1,2-*alt*)	-3798,462869	-9972864,26	24,07	6,08E-05

FINAL GEOMETRY OF 5A (*CONE*)

DFT method: RB3LYP/6-31G*



Created by GaussView 3.09

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   -0.5625    1.8442   -1.5323 C   0  0  0  0  0  0  0  0  0  0  0  0
   -2.9334    1.8114    0.7937 C   0  0  0  0  0  0  0  0  0  0  0  0
   -1.1344    2.9569   -0.8960 C   0  0  0  0  0  0  0  0  0  0  0  0
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    0.8370    1.8119   -1.6494 C   0  0  0  0  0  0  0  0  0  0  0  0
    4.7793    0.4052   -0.9070 C   0  0  0  0  0  0  0  0  0  0  0  0
    2.6310   -1.2779   -1.5255 C   0  0  0  0  0  0  0  0  0  0  0  0
    3.8753   -1.7994   -1.1335 C   0  0  0  0  0  0  0  0  0  0  0  0
   -1.5224   -2.6089    1.0740 C   0  0  0  0  0  0  0  0  0  0  0  0
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    4.9666   -0.9834   -0.8135 C   0  0  0  0  0  0  0  0  0  0  0  0
    2.5028    0.1101   -1.6787 C   0  0  0  0  0  0  0  0  0  0  0  0
   -3.3458    0.4818    0.5952 C   0  0  0  0  0  0  0  0  0  0  0  0
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   -2.6131   -0.0151    2.8605 C   0  0  0  0  0  0  0  0  0  0  0  0
   -3.0989   -0.4496    1.6262 C   0  0  0  0  0  0  0  0  0  0  0  0
   -1.9126   -4.2741   -2.7872 C   0  0  0  0  0  0  0  0  0  0  0  0
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   -2.9052    3.0060   -0.5635 S   0  0  0  0  0  0  0  0  0  0  0  0
    0.6532   -3.0213    2.1180 C   0  0  0  0  0  0  0  0  0  0  0  0
   -0.4795    0.9968    4.8300 C   0  0  0  0  0  0  0  0  0  0  0  0
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   -3.9435    0.0964   -0.5711 O   0  0  0  0  0  0  0  0  0  0  0  0
   -1.6488   -2.3138   -1.3362 O   0  0  0  0  0  0  0  0  0  0  0  0
    0.7210   -3.5255    4.6244 C   0  0  0  0  0  0  0  0  0  0  0  0
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    2.3310   -4.6418    3.0742 C   0  0  0  0  0  0  0  0  0  0  0  0
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3.5670	4.1232	0.6576	H	0	0	0	0	0	0	0	0	0	0	0	0
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-3.1205	1.1311	-3.8939	H	0	0	0	0	0	0	0	0	0	0	0	0
-3.1620	-0.4942	-3.2273	H	0	0	0	0	0	0	0	0	0	0	0	0
-7.8721	0.6961	-1.6429	H	0	0	0	0	0	0	0	0	0	0	0	0
-7.8754	-1.0020	-1.1399	H	0	0	0	0	0	0	0	0	0	0	0	0

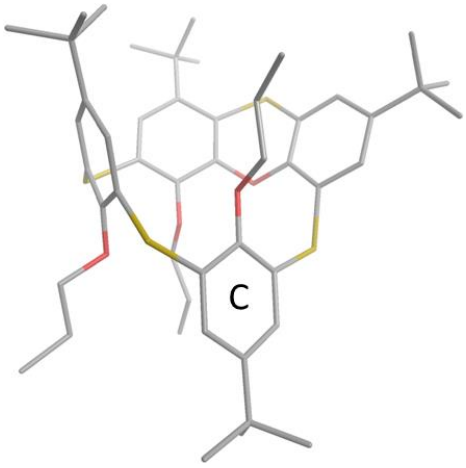
```
  -7.8501   -0.5873   -2.8596 H   0  0  0  0  0  0  0  0  0  0  0  0
   1.9994    6.1711   -2.1977 H   0  0  0  0  0  0  0  0  0  0  0  0
   3.4346    5.2188   -1.7938 H   0  0  0  0  0  0  0  0  0  0  0  0
   3.1974    6.7968   -1.0492 H   0  0  0  0  0  0  0  0  0  0  0  0
  -0.6321    1.0798   -3.8932 H   0  0  0  0  0  0  0  0  0  0  0  0
  -0.6562   -0.5911   -3.2870 H   0  0  0  0  0  0  0  0  0  0  0  0
   2.3142   -2.9011    0.7535 H   0  0  0  0  0  0  0  0  0  0  0  0
   3.1793   -2.0102    2.6891 H   0  0  0  0  0  0  0  0  0  0  0  0
   2.0067   -1.2365    3.7634 H   0  0  0  0  0  0  0  0  0  0  0  0
   3.1870   -2.3890    4.4195 H   0  0  0  0  0  0  0  0  0  0  0  0
   5.9097   -1.3387    1.7738 H   0  0  0  0  0  0  0  0  0  0  0  0
   7.6379   -1.4099    1.3764 H   0  0  0  0  0  0  0  0  0  0  0  0
   6.7197    0.0723    1.0773 H   0  0  0  0  0  0  0  0  0  0  0  0
 1  6  4  0  0  0  0
 1 20  4  0  0  0  0
 1 27  1  0  0  0  0
 2  4  4  0  0  0  0
 2  8  4  0  0  0  0
 2 57  1  0  0  0  0
 3  6  4  0  0  0  0
 3 18  4  0  0  0  0
 3 24  1  0  0  0  0
 4 14  4  0  0  0  0
 4 24  1  0  0  0  0
 5  8  4  0  0  0  0
 5 19  4  0  0  0  0
 5 46  1  0  0  0  0
 6 58  1  0  0  0  0
 7  9  4  0  0  0  0
 7 17  4  0  0  0  0
 7 46  1  0  0  0  0
 8 45  1  0  0  0  0
 9 16  4  0  0  0  0
 9 59  1  0  0  0  0
10 11  4  0  0  0  0
10 17  4  0  0  0  0
10 31  1  0  0  0  0
11 16  4  0  0  0  0
11 60  1  0  0  0  0
12 13  4  0  0  0  0
12 30  1  0  0  0  0
12 43  4  0  0  0  0
13 15  4  0  0  0  0
13 34  1  0  0  0  0
14 19  4  0  0  0  0
14 61  1  0  0  0  0
15 31  1  0  0  0  0
15 54  4  0  0  0  0
16 44  1  0  0  0  0
17 45  1  0  0  0  0
18 21  4  0  0  0  0
18 33  1  0  0  0  0
19 36  1  0  0  0  0
20 21  4  0  0  0  0
20 62  1  0  0  0  0
21 30  1  0  0  0  0
22 39  1  0  0  0  0
22 47  1  0  0  0  0
22 63  1  0  0  0  0
22 64  1  0  0  0  0
23 36  1  0  0  0  0
23 65  1  0  0  0  0
23 66  1  0  0  0  0
23 67  1  0  0  0  0
25 29  1  0  0  0  0
25 43  4  0  0  0  0
```

```
25 54  4  0  0  0  0
26 27  1  0  0  0  0
26 68  1  0  0  0  0
26 69  1  0  0  0  0
26 70  1  0  0  0  0
27 38  1  0  0  0  0
27 40  1  0  0  0  0
28 44  1  0  0  0  0
28 71  1  0  0  0  0
28 72  1  0  0  0  0
28 73  1  0  0  0  0
29 35  1  0  0  0  0
29 42  1  0  0  0  0
29 55  1  0  0  0  0
32 50  1  0  0  0  0
32 74  1  0  0  0  0
32 75  1  0  0  0  0
32 76  1  0  0  0  0
33 37  1  0  0  0  0
34 47  1  0  0  0  0
35 77  1  0  0  0  0
35 78  1  0  0  0  0
35 79  1  0  0  0  0
36 49  1  0  0  0  0
36 52  1  0  0  0  0
37 48  1  0  0  0  0
37 80  1  0  0  0  0
37 81  1  0  0  0  0
38 82  1  0  0  0  0
38 83  1  0  0  0  0
38 84  1  0  0  0  0
39 85  1  0  0  0  0
39 86  1  0  0  0  0
39 87  1  0  0  0  0
40 88  1  0  0  0  0
40 89  1  0  0  0  0
40 90  1  0  0  0  0
41 44  1  0  0  0  0
41 91  1  0  0  0  0
41 92  1  0  0  0  0
41 93  1  0  0  0  0
42 94  1  0  0  0  0
42 95  1  0  0  0  0
42 96  1  0  0  0  0
43 97  1  0  0  0  0
44 56  1  0  0  0  0
47 98  1  0  0  0  0
47 99  1  0  0  0  0
48 51  1  0  0  0  0
48100  1  0  0  0  0
48101  1  0  0  0  0
49102  1  0  0  0  0
49103  1  0  0  0  0
49104  1  0  0  0  0
50 53  1  0  0  0  0
50105  1  0  0  0  0
50106  1  0  0  0  0
51107  1  0  0  0  0
51108  1  0  0  0  0
51109  1  0  0  0  0
52110  1  0  0  0  0
52111  1  0  0  0  0
52112  1  0  0  0  0
53 57  1  0  0  0  0
53113  1  0  0  0  0
53114  1  0  0  0  0
```

```
54115  1  0  0  0  0
55116  1  0  0  0  0
55117  1  0  0  0  0
55118  1  0  0  0  0
56119  1  0  0  0  0
56120  1  0  0  0  0
56121  1  0  0  0  0
```

FINAL GEOMETRY OF 5B (C-*PACO)*

DFT method: RB3LYP/6-31G*



Created by GaussView 3.09

```
121126  0  0  0  0  0  0  0  0  0     0
   -1.5900    3.9534    0.2001 C    0  0  0  0  0  0  0  0  0  0  0  0
    1.4947   -1.9190    1.9781 C    0  0  0  0  0  0  0  0  0  0  0  0
   -3.7184    4.9815    1.2424 C    0  0  0  0  0  0  0  0  0  0  0  0
   -3.7063    2.9479   -0.2966 C    0  0  0  0  0  0  0  0  0  0  0  0
   -3.2302   -1.8762   -2.0626 C    0  0  0  0  0  0  0  0  0  0  0  0
   -2.7464    5.9120    1.9928 C    0  0  0  0  0  0  0  0  0  0  0  0
   -2.8520   -0.5092   -2.0782 C    0  0  0  0  0  0  0  0  0  0  0  0
    0.5708   -3.2930    0.2249 C    0  0  0  0  0  0  0  0  0  0  0  0
   -0.9241    3.0176   -0.6091 C    0  0  0  0  0  0  0  0  0  0  0  0
   -4.6121    5.8504    0.3248 C    0  0  0  0  0  0  0  0  0  0  0  0
    1.5324   -0.7499   -3.2098 C    0  0  0  0  0  0  0  0  0  0  0  0
   -1.4980   -0.1512   -2.0758 C    0  0  0  0  0  0  0  0  0  0  0  0
   -4.6057    4.2697    2.2902 C    0  0  0  0  0  0  0  0  0  0  0  0
   -0.8328   -2.4501   -1.9048 C    0  0  0  0  0  0  0  0  0  0  0  0
    3.2705    2.7394   -0.2703 C    0  0  0  0  0  0  0  0  0  0  0  0
    4.3680    2.1046    0.3172 C    0  0  0  0  0  0  0  0  0  0  0  0
   -0.4110   -3.7400    1.1119 C    0  0  0  0  0  0  0  0  0  0  0  0
   -0.4705   -1.1010   -2.0021 C    0  0  0  0  0  0  0  0  0  0  0  0
   -5.4133   -1.8175   -3.3734 C    0  0  0  0  0  0  0  0  0  0  0  0
    0.4901   -2.3699    2.8447 C    0  0  0  0  0  0  0  0  0  0  0  0
    1.9490    2.3362   -0.0341 C    0  0  0  0  0  0  0  0  0  0  0  0
   -4.6972   -2.3720   -2.1173 C    0  0  0  0  0  0  0  0  0  0  0  0
    1.6889    1.2712    0.8476 C    0  0  0  0  0  0  0  0  0  0  0  0
    4.0996    1.0159    1.1520 C    0  0  0  0  0  0  0  0  0  0  0  0
    2.7901    0.6004    1.4210 C    0  0  0  0  0  0  0  0  0  0  0  0
   -4.7811   -3.9114   -2.2132 C    0  0  0  0  0  0  0  0  0  0  0  0
   -2.9787    3.9402    0.3807 C    0  0  0  0  0  0  0  0  0  0  0  0
   -5.4555   -1.9599   -0.8313 C    0  0  0  0  0  0  0  0  0  0  0  0
   -0.4547   -3.3229    2.4498 C    0  0  0  0  0  0  0  0  0  0  0  0
   -2.1837   -2.8058   -1.9694 C    0  0  0  0  0  0  0  0  0  0  0  0
   -1.6824    2.0535   -1.2847 C    0  0  0  0  0  0  0  0  0  0  0  0
    1.5972   -2.4433    0.6788 C    0  0  0  0  0  0  0  0  0  0  0  0
   -3.0707    2.0291   -1.1295 C    0  0  0  0  0  0  0  0  0  0  0  0
    3.7586   -3.0210   -0.0240 C    0  0  0  0  0  0  0  0  0  0  0  0
   -0.1394    1.3638    2.3541 C    0  0  0  0  0  0  0  0  0  0  0  0
    6.0931   -3.4605   -0.8991 C    0  0  0  0  0  0  0  0  0  0  0  0
   -1.5499    0.8157    2.5063 C    0  0  0  0  0  0  0  0  0  0  0  0
    6.8669    1.7629    0.7417 C    0  0  0  0  0  0  0  0  0  0  0  0
    5.7947    2.6087    0.0289 C    0  0  0  0  0  0  0  0  0  0  0  0
    0.8141   -0.6613   -1.9623 O    0  0  0  0  0  0  0  0  0  0  0  0
    0.4089   -3.7062   -1.5295 S    0  0  0  0  0  0  0  0  0  0  0  0
```

-1.5301	-3.8844	3.3981	C	0	0	0	0	0	0	0	0	0	0	0	0
4.8646	-2.5461	-0.9535	C	0	0	0	0	0	0	0	0	0	0	0	0
-1.4311	-3.2865	4.8142	C	0	0	0	0	0	0	0	0	0	0	0	0
-2.1584	1.1742	3.8663	C	0	0	0	0	0	0	0	0	0	0	0	0
0.7946	3.3127	-1.0151	S	0	0	0	0	0	0	0	0	0	0	0	0
2.6511	-2.1075	-0.1257	O	0	0	0	0	0	0	0	0	0	0	0	0
0.3976	0.8849	1.1048	O	0	0	0	0	0	0	0	0	0	0	0	0
2.6619	-0.7266	2.6308	S	0	0	0	0	0	0	0	0	0	0	0	0
6.0726	2.5548	-1.4917	C	0	0	0	0	0	0	0	0	0	0	0	0
-1.3538	-5.4178	3.5084	C	0	0	0	0	0	0	0	0	0	0	0	0
5.9283	4.0697	0.5212	C	0	0	0	0	0	0	0	0	0	0	0	0
-1.0865	1.1708	-2.1471	O	0	0	0	0	0	0	0	0	0	0	0	0
-2.9387	-3.5715	2.8399	C	0	0	0	0	0	0	0	0	0	0	0	0
-4.0057	0.8725	-2.1144	S	0	0	0	0	0	0	0	0	0	0	0	0
2.7534	0.1511	-3.1243	C	0	0	0	0	0	0	0	0	0	0	0	0
3.6227	0.0568	-4.3826	C	0	0	0	0	0	0	0	0	0	0	0	0
-0.9818	4.7106	0.6790	H	0	0	0	0	0	0	0	0	0	0	0	0
-4.7867	2.8966	-0.2012	H	0	0	0	0	0	0	0	0	0	0	0	0
-2.0767	5.3521	2.6558	H	0	0	0	0	0	0	0	0	0	0	0	0
-2.1316	6.5041	1.3060	H	0	0	0	0	0	0	0	0	0	0	0	0
-3.3144	6.6147	2.6127	H	0	0	0	0	0	0	0	0	0	0	0	0
-5.3544	5.2462	-0.2079	H	0	0	0	0	0	0	0	0	0	0	0	0
-4.0098	6.3769	-0.4240	H	0	0	0	0	0	0	0	0	0	0	0	0
-5.1525	6.5998	0.9160	H	0	0	0	0	0	0	0	0	0	0	0	0
1.8205	-1.7948	-3.3843	H	0	0	0	0	0	0	0	0	0	0	0	0
0.8727	-0.4310	-4.0286	H	0	0	0	0	0	0	0	0	0	0	0	0
-5.3599	3.6272	1.8239	H	0	0	0	0	0	0	0	0	0	0	0	0
-4.0038	3.6466	2.9609	H	0	0	0	0	0	0	0	0	0	0	0	0
-5.1366	5.0101	2.9006	H	0	0	0	0	0	0	0	0	0	0	0	0
3.4339	3.5794	-0.9403	H	0	0	0	0	0	0	0	0	0	0	0	0
-1.1670	-4.4171	0.7278	H	0	0	0	0	0	0	0	0	0	0	0	0
-4.8850	-2.1180	-4.2853	H	0	0	0	0	0	0	0	0	0	0	0	0
-5.4943	-0.7277	-3.3776	H	0	0	0	0	0	0	0	0	0	0	0	0
-6.4333	-2.2168	-3.4260	H	0	0	0	0	0	0	0	0	0	0	0	0
0.4626	-1.9499	3.8435	H	0	0	0	0	0	0	0	0	0	0	0	0
4.9082	0.4617	1.6127	H	0	0	0	0	0	0	0	0	0	0	0	0
-4.2626	-4.2997	-3.0969	H	0	0	0	0	0	0	0	0	0	0	0	0
-4.3712	-4.4063	-1.3260	H	0	0	0	0	0	0	0	0	0	0	0	0
-5.8333	-4.2060	-2.2902	H	0	0	0	0	0	0	0	0	0	0	0	0
-5.4881	-0.8771	-0.6958	H	0	0	0	0	0	0	0	0	0	0	0	0
-6.4885	-2.3266	-0.8746	H	0	0	0	0	0	0	0	0	0	0	0	0
-4.9776	-2.3994	0.0518	H	0	0	0	0	0	0	0	0	0	0	0	0
-2.4109	-3.8615	-1.9130	H	0	0	0	0	0	0	0	0	0	0	0	0
3.4248	-4.0312	-0.3026	H	0	0	0	0	0	0	0	0	0	0	0	0
4.1106	-3.0519	1.0168	H	0	0	0	0	0	0	0	0	0	0	0	0
-0.1445	2.4629	2.3482	H	0	0	0	0	0	0	0	0	0	0	0	0
0.5004	1.0295	3.1804	H	0	0	0	0	0	0	0	0	0	0	0	0
6.8761	-3.1039	-1.5767	H	0	0	0	0	0	0	0	0	0	0	0	0
6.5196	-3.4997	0.1106	H	0	0	0	0	0	0	0	0	0	0	0	0
5.8416	-4.4865	-1.1940	H	0	0	0	0	0	0	0	0	0	0	0	0
-2.1756	1.2065	1.6964	H	0	0	0	0	0	0	0	0	0	0	0	0
-1.5104	-0.2727	2.3830	H	0	0	0	0	0	0	0	0	0	0	0	0
6.7452	1.7821	1.8306	H	0	0	0	0	0	0	0	0	0	0	0	0
6.8476	0.7173	0.4133	H	0	0	0	0	0	0	0	0	0	0	0	0
7.8619	2.1618	0.5138	H	0	0	0	0	0	0	0	0	0	0	0	0
5.1387	-1.5213	-0.6746	H	0	0	0	0	0	0	0	0	0	0	0	0
4.4695	-2.5029	-1.9756	H	0	0	0	0	0	0	0	0	0	0	0	0
-0.4591	-3.4918	5.2768	H	0	0	0	0	0	0	0	0	0	0	0	0
-1.5880	-2.2018	4.8126	H	0	0	0	0	0	0	0	0	0	0	0	0
-2.2018	-3.7289	5.4553	H	0	0	0	0	0	0	0	0	0	0	0	0
-2.1982	2.2604	4.0161	H	0	0	0	0	0	0	0	0	0	0	0	0
-3.1813	0.7917	3.9521	H	0	0	0	0	0	0	0	0	0	0	0	0
-1.5737	0.7508	4.6926	H	0	0	0	0	0	0	0	0	0	0	0	0
5.3724	3.1771	-2.0584	H	0	0	0	0	0	0	0	0	0	0	0	0
5.9892	1.5290	-1.8683	H	0	0	0	0	0	0	0	0	0	0	0	0
7.0862	2.9156	-1.7058	H	0	0	0	0	0	0	0	0	0	0	0	0

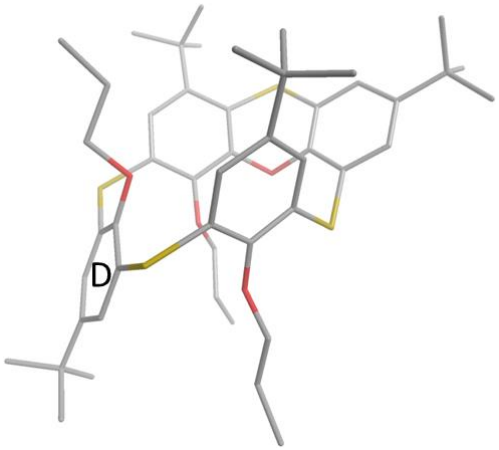
```
  -1.4443   -5.9086    2.5336 H   0  0  0  0  0  0  0  0  0  0  0  0
  -0.3695   -5.6704    3.9190 H   0  0  0  0  0  0  0  0  0  0  0  0
  -2.1180   -5.8437    4.1702 H   0  0  0  0  0  0  0  0  0  0  0  0
   5.2142    4.7337    0.0230 H   0  0  0  0  0  0  0  0  0  0  0  0
   5.7507    4.1374    1.6005 H   0  0  0  0  0  0  0  0  0  0  0  0
   6.9369    4.4499    0.3175 H   0  0  0  0  0  0  0  0  0  0  0  0
  -3.0927   -4.0102    1.8483 H   0  0  0  0  0  0  0  0  0  0  0  0
  -3.0965   -2.4904    2.7539 H   0  0  0  0  0  0  0  0  0  0  0  0
  -3.7105   -3.9765    3.5057 H   0  0  0  0  0  0  0  0  0  0  0  0
   2.4157    1.1816   -2.9690 H   0  0  0  0  0  0  0  0  0  0  0  0
   3.3293   -0.1317   -2.2369 H   0  0  0  0  0  0  0  0  0  0  0  0
   3.0664    0.3542   -5.2803 H   0  0  0  0  0  0  0  0  0  0  0  0
   4.4959    0.7136   -4.3033 H   0  0  0  0  0  0  0  0  0  0  0  0
   3.9892   -0.9648   -4.5438 H   0  0  0  0  0  0  0  0  0  0  0  0
 1  9  4  0  0  0  0
 1 27  4  0  0  0  0
 1 58  1  0  0  0  0
 2 20  4  0  0  0  0
 2 32  4  0  0  0  0
 2 49  1  0  0  0  0
 3  6  1  0  0  0  0
 3 10  1  0  0  0  0
 3 13  1  0  0  0  0
 3 27  1  0  0  0  0
 4 27  4  0  0  0  0
 4 33  4  0  0  0  0
 4 59  1  0  0  0  0
 5  7  4  0  0  0  0
 5 22  1  0  0  0  0
 5 30  4  0  0  0  0
 6 60  1  0  0  0  0
 6 61  1  0  0  0  0
 6 62  1  0  0  0  0
 7 12  4  0  0  0  0
 7 55  1  0  0  0  0
 8 17  4  0  0  0  0
 8 32  4  0  0  0  0
 8 41  1  0  0  0  0
 9 31  4  0  0  0  0
 9 46  1  0  0  0  0
10 63  1  0  0  0  0
10 64  1  0  0  0  0
10 65  1  0  0  0  0
11 40  1  0  0  0  0
11 56  1  0  0  0  0
11 66  1  0  0  0  0
11 67  1  0  0  0  0
12 18  4  0  0  0  0
12 53  1  0  0  0  0
13 68  1  0  0  0  0
13 69  1  0  0  0  0
13 70  1  0  0  0  0
14 18  4  0  0  0  0
14 30  4  0  0  0  0
14 41  1  0  0  0  0
15 16  4  0  0  0  0
15 21  4  0  0  0  0
15 71  1  0  0  0  0
16 24  4  0  0  0  0
16 39  1  0  0  0  0
17 29  4  0  0  0  0
17 72  1  0  0  0  0
18 40  1  0  0  0  0
19 22  1  0  0  0  0
19 73  1  0  0  0  0
19 74  1  0  0  0  0
```

```
19 75  1  0  0  0  0
20 29  4  0  0  0  0
20 76  1  0  0  0  0
21 23  4  0  0  0  0
21 46  1  0  0  0  0
22 26  1  0  0  0  0
22 28  1  0  0  0  0
23 25  4  0  0  0  0
23 48  1  0  0  0  0
24 25  4  0  0  0  0
24 77  1  0  0  0  0
25 49  1  0  0  0  0
26 78  1  0  0  0  0
26 79  1  0  0  0  0
26 80  1  0  0  0  0
28 81  1  0  0  0  0
28 82  1  0  0  0  0
28 83  1  0  0  0  0
29 42  1  0  0  0  0
30 84  1  0  0  0  0
31 33  4  0  0  0  0
31 53  1  0  0  0  0
32 47  1  0  0  0  0
33 55  1  0  0  0  0
34 43  1  0  0  0  0
34 47  1  0  0  0  0
34 85  1  0  0  0  0
34 86  1  0  0  0  0
35 37  1  0  0  0  0
35 48  1  0  0  0  0
35 87  1  0  0  0  0
35 88  1  0  0  0  0
36 43  1  0  0  0  0
36 89  1  0  0  0  0
36 90  1  0  0  0  0
36 91  1  0  0  0  0
37 45  1  0  0  0  0
37 92  1  0  0  0  0
37 93  1  0  0  0  0
38 39  1  0  0  0  0
38 94  1  0  0  0  0
38 95  1  0  0  0  0
38 96  1  0  0  0  0
39 50  1  0  0  0  0
39 52  1  0  0  0  0
42 44  1  0  0  0  0
42 51  1  0  0  0  0
42 54  1  0  0  0  0
43 97  1  0  0  0  0
43 98  1  0  0  0  0
44 99  1  0  0  0  0
44100  1  0  0  0  0
44101  1  0  0  0  0
45102  1  0  0  0  0
45103  1  0  0  0  0
45104  1  0  0  0  0
50105  1  0  0  0  0
50106  1  0  0  0  0
50107  1  0  0  0  0
51108  1  0  0  0  0
51109  1  0  0  0  0
51110  1  0  0  0  0
52111  1  0  0  0  0
52112  1  0  0  0  0
52113  1  0  0  0  0
54114  1  0  0  0  0
```

```
54115  1  0  0  0  0
54116  1  0  0  0  0
56 57  1  0  0  0  0
56117  1  0  0  0  0
56118  1  0  0  0  0
57119  1  0  0  0  0
57120  1  0  0  0  0
57121  1  0  0  0  0
```

FINAL GEOMETRY OF 5C (D-PACO)

DFT method: RB3LYP/6-31G*



Created by GaussView 3.09

```
121126  0  0  0  0  0  0  0  0  0  0     0
   -4.5839    1.4321   -0.3617 C   0  0  0  0  0  0  0  0  0  0  0  0
    7.3160   -1.8173   -2.3143 C   0  0  0  0  0  0  0  0  0  0  0  0
    3.1063    5.4884   -1.4578 C   0  0  0  0  0  0  0  0  0  0  0  0
    2.4490    4.8902   -0.1892 C   0  0  0  0  0  0  0  0  0  0  0  0
    2.3486   -1.7635    3.6940 C   0  0  0  0  0  0  0  0  0  0  0  0
   -2.5166   -0.5374   -3.2269 C   0  0  0  0  0  0  0  0  0  0  0  0
    1.2403   -1.8989    2.6325 C   0  0  0  0  0  0  0  0  0  0  0  0
   -0.3661    3.0358    4.7072 C   0  0  0  0  0  0  0  0  0  0  0  0
   -2.8159   -1.7223    2.4423 S   0  0  0  0  0  0  0  0  0  0  0  0
   -0.3295    2.1914    3.4290 C   0  0  0  0  0  0  0  0  0  0  0  0
   -2.5244    3.2161   -0.2380 S   0  0  0  0  0  0  0  0  0  0  0  0
    3.2939   -0.5990    3.3153 C   0  0  0  0  0  0  0  0  0  0  0  0
    6.3323   -3.7010   -0.9963 C   0  0  0  0  0  0  0  0  0  0  0  0
    4.9251   -0.1226   -1.4024 C   0  0  0  0  0  0  0  0  0  0  0  0
   -3.1984   -4.0715   -1.4098 C   0  0  0  0  0  0  0  0  0  0  0  0
    0.6263   -2.3294    0.3009 C   0  0  0  0  0  0  0  0  0  0  0  0
    2.5323   -0.2695   -1.7265 C   0  0  0  0  0  0  0  0  0  0  0  0
   -0.3869    1.6747   -1.2396 C   0  0  0  0  0  0  0  0  0  0  0  0
   -1.7253    1.8335    2.9415 C   0  0  0  0  0  0  0  0  0  0  0  0
    6.4166   -2.1669   -1.1047 C   0  0  0  0  0  0  0  0  0  0  0  0
   -1.1019   -1.9281    1.9438 C   0  0  0  0  0  0  0  0  0  0  0  0
   -4.7080   -0.6761    0.7600 C   0  0  0  0  0  0  0  0  0  0  0  0
   -6.6537    0.1234   -2.2091 C   0  0  0  0  0  0  0  0  0  0  0  0
    1.3427    0.3208   -2.0686 O   0  0  0  0  0  0  0  0  0  0  0  0
   -0.1188   -1.7554    2.9253 C   0  0  0  0  0  0  0  0  0  0  0  0
   -1.6883   -2.5470   -0.3229 O   0  0  0  0  0  0  0  0  0  0  0  0
   -0.8087    2.8352   -0.5846 C   0  0  0  0  0  0  0  0  0  0  0  0
   -1.5953    1.0327    1.7499 O   0  0  0  0  0  0  0  0  0  0  0  0
   -3.3303    1.6740    0.2028 C   0  0  0  0  0  0  0  0  0  0  0  0
   -3.4538   -0.4509    1.3443 C   0  0  0  0  0  0  0  0  0  0  0  0
    3.8447   -2.2595   -1.3425 C   0  0  0  0  0  0  0  0  0  0  0  0
    1.4983    3.7243   -0.5639 C   0  0  0  0  0  0  0  0  0  0  0  0
    3.1595   -3.0802    3.7553 C   0  0  0  0  0  0  0  0  0  0  0  0
   -7.6460    1.2168   -0.1634 C   0  0  0  0  0  0  0  0  0  0  0  0
    1.9167    2.5360   -1.2170 C   0  0  0  0  0  0  0  0  0  0  0  0
   -2.1381   -3.9167   -0.3305 C   0  0  0  0  0  0  0  0  0  0  0  0
    3.5817    2.2573   -1.8535 S   0  0  0  0  0  0  0  0  0  0  0  0
   -6.7241    0.0792   -0.6647 C   0  0  0  0  0  0  0  0  0  0  0  0
    5.0327   -1.5190   -1.2966 C   0  0  0  0  0  0  0  0  0  0  0  0
    7.0665   -1.6266    0.1911 C   0  0  0  0  0  0  0  0  0  0  0  0
    1.7811   -1.4886    5.0995 C   0  0  0  0  0  0  0  0  0  0  0  0
    1.0910   -2.6382   -1.4182 S   0  0  0  0  0  0  0  0  0  0  0  0
```

-7.3532	-1.2652	-0.2525	C	0	0	0	0	0	0	0	0	0	0	0	0
1.5866	-2.1614	1.3002	C	0	0	0	0	0	0	0	0	0	0	0	0
-2.7990	-0.7848	-4.7123	C	0	0	0	0	0	0	0	0	0	0	0	0
3.6962	0.4947	-1.6279	C	0	0	0	0	0	0	0	0	0	0	0	0
1.6976	6.0514	0.4988	C	0	0	0	0	0	0	0	0	0	0	0	0
0.1347	3.8125	-0.2455	C	0	0	0	0	0	0	0	0	0	0	0	0
2.5900	-1.6534	-1.5121	C	0	0	0	0	0	0	0	0	0	0	0	0
-5.3189	0.2738	-0.0645	C	0	0	0	0	0	0	0	0	0	0	0	0
3.5293	4.4045	0.8082	C	0	0	0	0	0	0	0	0	0	0	0	0
-1.4866	0.5600	-3.0214	C	0	0	0	0	0	0	0	0	0	0	0	0
-3.7574	-5.4973	-1.4645	C	0	0	0	0	0	0	0	0	0	0	0	0
0.9858	1.5250	-1.4853	C	0	0	0	0	0	0	0	0	0	0	0	0
-2.7841	0.7622	1.1252	C	0	0	0	0	0	0	0	0	0	0	0	0
-0.7406	-2.2805	0.6330	C	0	0	0	0	0	0	0	0	0	0	0	0
-1.2678	0.7024	-1.6000	O	0	0	0	0	0	0	0	0	0	0	0	0
-4.9780	2.1638	-1.0605	H	0	0	0	0	0	0	0	0	0	0	0	0
7.4500	-0.7359	-2.4243	H	0	0	0	0	0	0	0	0	0	0	0	0
6.8835	-2.1969	-3.2470	H	0	0	0	0	0	0	0	0	0	0	0	0
8.3095	-2.2656	-2.1925	H	0	0	0	0	0	0	0	0	0	0	0	0
2.3421	5.8398	-2.1605	H	0	0	0	0	0	0	0	0	0	0	0	0
3.7472	4.7787	-1.9861	H	0	0	0	0	0	0	0	0	0	0	0	0
3.7322	6.3457	-1.1820	H	0	0	0	0	0	0	0	0	0	0	0	0
-3.4383	-0.2581	-2.7034	H	0	0	0	0	0	0	0	0	0	0	0	0
-2.1435	-1.4459	-2.7444	H	0	0	0	0	0	0	0	0	0	0	0	0
0.6468	3.2834	5.0426	H	0	0	0	0	0	0	0	0	0	0	0	0
-0.8660	2.5039	5.5260	H	0	0	0	0	0	0	0	0	0	0	0	0
-0.9029	3.9791	4.5487	H	0	0	0	0	0	0	0	0	0	0	0	0
0.1907	2.7309	2.6285	H	0	0	0	0	0	0	0	0	0	0	0	0
0.2308	1.2645	3.5999	H	0	0	0	0	0	0	0	0	0	0	0	0
3.7730	-0.7605	2.3439	H	0	0	0	0	0	0	0	0	0	0	0	0
2.7465	0.3487	3.2606	H	0	0	0	0	0	0	0	0	0	0	0	0
4.0874	-0.4918	4.0654	H	0	0	0	0	0	0	0	0	0	0	0	0
5.7360	-4.0180	-0.1331	H	0	0	0	0	0	0	0	0	0	0	0	0
5.8991	-4.1511	-1.8966	H	0	0	0	0	0	0	0	0	0	0	0	0
7.3384	-4.1161	-0.8705	H	0	0	0	0	0	0	0	0	0	0	0	0
5.8093	0.5031	-1.3239	H	0	0	0	0	0	0	0	0	0	0	0	0
-2.7621	-3.7997	-2.3785	H	0	0	0	0	0	0	0	0	0	0	0	0
-4.0027	-3.3526	-1.2117	H	0	0	0	0	0	0	0	0	0	0	0	0
-2.2982	2.7412	2.7107	H	0	0	0	0	0	0	0	0	0	0	0	0
-2.2756	1.2620	3.7021	H	0	0	0	0	0	0	0	0	0	0	0	0
-5.1970	-1.6208	0.9664	H	0	0	0	0	0	0	0	0	0	0	0	0
-6.0139	-0.6779	-2.5954	H	0	0	0	0	0	0	0	0	0	0	0	0
-6.2548	1.0755	-2.5742	H	0	0	0	0	0	0	0	0	0	0	0	0
-7.6546	-0.0037	-2.6395	H	0	0	0	0	0	0	0	0	0	0	0	0
-0.4457	-1.4922	3.9239	H	0	0	0	0	0	0	0	0	0	0	0	0
3.8610	-3.3353	-1.2174	H	0	0	0	0	0	0	0	0	0	0	0	0
3.6281	-3.3148	2.7937	H	0	0	0	0	0	0	0	0	0	0	0	0
2.5166	-3.9248	4.0280	H	0	0	0	0	0	0	0	0	0	0	0	0
3.9564	-3.0029	4.5052	H	0	0	0	0	0	0	0	0	0	0	0	0
-7.7255	1.2036	0.9296	H	0	0	0	0	0	0	0	0	0	0	0	0
-7.2711	2.2024	-0.4588	H	0	0	0	0	0	0	0	0	0	0	0	0
-8.6545	1.1036	-0.5797	H	0	0	0	0	0	0	0	0	0	0	0	0
-1.2826	-4.5799	-0.5255	H	0	0	0	0	0	0	0	0	0	0	0	0
-2.5491	-4.1695	0.6558	H	0	0	0	0	0	0	0	0	0	0	0	0
6.4535	-1.8669	1.0675	H	0	0	0	0	0	0	0	0	0	0	0	0
7.1958	-0.5396	0.1624	H	0	0	0	0	0	0	0	0	0	0	0	0
8.0568	-2.0751	0.3360	H	0	0	0	0	0	0	0	0	0	0	0	0
1.1083	-2.2879	5.4305	H	0	0	0	0	0	0	0	0	0	0	0	0
1.2328	-0.5406	5.1432	H	0	0	0	0	0	0	0	0	0	0	0	0
2.6021	-1.4264	5.8227	H	0	0	0	0	0	0	0	0	0	0	0	0
-7.4606	-1.3493	0.8348	H	0	0	0	0	0	0	0	0	0	0	0	0
-6.7618	-2.1181	-0.6049	H	0	0	0	0	0	0	0	0	0	0	0	0
-8.3534	-1.3542	-0.6912	H	0	0	0	0	0	0	0	0	0	0	0	0
2.6324	-2.2343	1.0258	H	0	0	0	0	0	0	0	0	0	0	0	0
-1.8916	-1.0903	-5.2476	H	0	0	0	0	0	0	0	0	0	0	0	0
-3.1881	0.1149	-5.2054	H	0	0	0	0	0	0	0	0	0	0	0	0

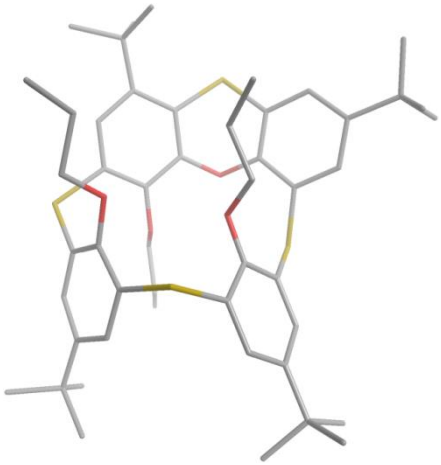
```
  -3.5422   -1.5793   -4.8422 H   0  0  0  0  0  0  0  0  0  0  0  0
   1.2298    5.7427    1.4401 H   0  0  0  0  0  0  0  0  0  0  0  0
   0.9260    6.4860   -0.1462 H   0  0  0  0  0  0  0  0  0  0  0  0
   2.4136    6.8458    0.7359 H   0  0  0  0  0  0  0  0  0  0  0  0
  -0.2327    4.6859    0.2762 H   0  0  0  0  0  0  0  0  0  0  0  0
   3.0621    4.0324    1.7273 H   0  0  0  0  0  0  0  0  0  0  0  0
   4.1490    3.6062    0.3954 H   0  0  0  0  0  0  0  0  0  0  0  0
   4.1888    5.2385    1.0784 H   0  0  0  0  0  0  0  0  0  0  0  0
  -1.8415    1.5200   -3.4229 H   0  0  0  0  0  0  0  0  0  0  0  0
  -0.5420    0.3036   -3.5133 H   0  0  0  0  0  0  0  0  0  0  0  0
  -4.2228   -5.7820   -0.5130 H   0  0  0  0  0  0  0  0  0  0  0  0
  -2.9693   -6.2286   -1.6812 H   0  0  0  0  0  0  0  0  0  0  0  0
  -4.5181   -5.5893   -2.2470 H   0  0  0  0  0  0  0  0  0  0  0  0
 1 29  4  0  0  0  0
 1 50  4  0  0  0  0
 1 58  1  0  0  0  0
 2 20  1  0  0  0  0
 2 59  1  0  0  0  0
 2 60  1  0  0  0  0
 2 61  1  0  0  0  0
 3  4  1  0  0  0  0
 3 62  1  0  0  0  0
 3 63  1  0  0  0  0
 3 64  1  0  0  0  0
 4 32  1  0  0  0  0
 4 47  1  0  0  0  0
 4 51  1  0  0  0  0
 5  7  1  0  0  0  0
 5 12  1  0  0  0  0
 5 33  1  0  0  0  0
 5 41  1  0  0  0  0
 6 45  1  0  0  0  0
 6 52  1  0  0  0  0
 6 65  1  0  0  0  0
 6 66  1  0  0  0  0
 7 25  4  0  0  0  0
 7 44  4  0  0  0  0
 8 10  1  0  0  0  0
 8 67  1  0  0  0  0
 8 68  1  0  0  0  0
 8 69  1  0  0  0  0
 9 21  1  0  0  0  0
 9 30  1  0  0  0  0
10 19  1  0  0  0  0
10 70  1  0  0  0  0
10 71  1  0  0  0  0
11 27  1  0  0  0  0
11 29  1  0  0  0  0
12 72  1  0  0  0  0
12 73  1  0  0  0  0
12 74  1  0  0  0  0
13 20  1  0  0  0  0
13 75  1  0  0  0  0
13 76  1  0  0  0  0
13 77  1  0  0  0  0
14 39  4  0  0  0  0
14 46  4  0  0  0  0
14 78  1  0  0  0  0
15 36  1  0  0  0  0
15 53  1  0  0  0  0
15 79  1  0  0  0  0
15 80  1  0  0  0  0
16 42  1  0  0  0  0
16 44  4  0  0  0  0
16 56  4  0  0  0  0
17 24  1  0  0  0  0
```

```
17 46  4  0  0  0  0
17 49  4  0  0  0  0
18 27  4  0  0  0  0
18 54  4  0  0  0  0
18 57  1  0  0  0  0
19 28  1  0  0  0  0
19 81  1  0  0  0  0
19 82  1  0  0  0  0
20 39  1  0  0  0  0
20 40  1  0  0  0  0
21 25  4  0  0  0  0
21 56  4  0  0  0  0
22 30  4  0  0  0  0
22 50  4  0  0  0  0
22 83  1  0  0  0  0
23 38  1  0  0  0  0
23 84  1  0  0  0  0
23 85  1  0  0  0  0
23 86  1  0  0  0  0
24 54  1  0  0  0  0
25 87  1  0  0  0  0
26 36  1  0  0  0  0
26 56  1  0  0  0  0
27 48  4  0  0  0  0
28 55  1  0  0  0  0
29 55  4  0  0  0  0
30 55  4  0  0  0  0
31 39  4  0  0  0  0
31 49  4  0  0  0  0
31 88  1  0  0  0  0
32 35  4  0  0  0  0
32 48  4  0  0  0  0
33 89  1  0  0  0  0
33 90  1  0  0  0  0
33 91  1  0  0  0  0
34 38  1  0  0  0  0
34 92  1  0  0  0  0
34 93  1  0  0  0  0
34 94  1  0  0  0  0
35 37  1  0  0  0  0
35 54  4  0  0  0  0
36 95  1  0  0  0  0
36 96  1  0  0  0  0
37 46  1  0  0  0  0
38 43  1  0  0  0  0
38 50  1  0  0  0  0
40 97  1  0  0  0  0
40 98  1  0  0  0  0
40 99  1  0  0  0  0
41100  1  0  0  0  0
41101  1  0  0  0  0
41102  1  0  0  0  0
42 49  1  0  0  0  0
43103  1  0  0  0  0
43104  1  0  0  0  0
43105  1  0  0  0  0
44106  1  0  0  0  0
45107  1  0  0  0  0
45108  1  0  0  0  0
45109  1  0  0  0  0
47110  1  0  0  0  0
47111  1  0  0  0  0
47112  1  0  0  0  0
48113  1  0  0  0  0
51114  1  0  0  0  0
51115  1  0  0  0  0
```

```
51116  1  0  0  0  0
52 57  1  0  0  0  0
52117  1  0  0  0  0
52118  1  0  0  0  0
53119  1  0  0  0  0
53120  1  0  0  0  0
53121  1  0  0  0  0
```

FINAL GEOMETRY OF 5D (1,2-*ALT*)

DFT method: RB3LYP/6-31G*



Created by GaussView 3.09

```
121126  0  0  0  0  0  0  0  0  0     0
   -4.1313    4.7334    1.7829 C    0  0  0  0  0  0  0  0  0  0  0  0
   -3.9651    3.2153   -0.2235 C    0  0  0  0  0  0  0  0  0  0  0  0
    1.7414   -2.0955    1.1364 C    0  0  0  0  0  0  0  0  0  0  0  0
   -3.7462    0.9747   -1.1519 C    0  0  0  0  0  0  0  0  0  0  0  0
   -0.5680   -1.7627   -1.4761 C    0  0  0  0  0  0  0  0  0  0  0  0
    3.1480    2.4532    1.4625 C    0  0  0  0  0  0  0  0  0  0  0  0
    2.0816    1.5583    1.5617 C    0  0  0  0  0  0  0  0  0  0  0  0
   -5.0955   -2.9709    0.7809 C    0  0  0  0  0  0  0  0  0  0  0  0
   -4.3957   -3.6877   -0.4000 C    0  0  0  0  0  0  0  0  0  0  0  0
    3.3261   -2.8871   -0.5246 C    0  0  0  0  0  0  0  0  0  0  0  0
    2.0655    3.5743   -0.3452 C    0  0  0  0  0  0  0  0  0  0  0  0
   -2.6141    3.4242   -0.5463 C    0  0  0  0  0  0  0  0  0  0  0  0
   -1.8499   -3.6069   -0.5816 C    0  0  0  0  0  0  0  0  0  0  0  0
   -0.6129   -3.0448   -0.9166 C    0  0  0  0  0  0  0  0  0  0  0  0
   -3.0169   -1.6407   -1.2879 C    0  0  0  0  0  0  0  0  0  0  0  0
    3.1565    3.4947    0.5231 C    0  0  0  0  0  0  0  0  0  0  0  0
    3.9505   -1.1061    0.9385 C    0  0  0  0  0  0  0  0  0  0  0  0
    0.9469    1.7015    0.7310 C    0  0  0  0  0  0  0  0  0  0  0  0
    2.0515   -2.9248    0.0411 C    0  0  0  0  0  0  0  0  0  0  0  0
   -6.2389    3.9305    0.7035 C    0  0  0  0  0  0  0  0  0  0  0  0
    0.9775    2.6882   -0.2708 C    0  0  0  0  0  0  0  0  0  0  0  0
   -4.7946    5.5785   -0.5012 C    0  0  0  0  0  0  0  0  0  0  0  0
    2.6734   -1.1185    1.5161 C    0  0  0  0  0  0  0  0  0  0  0  0
   -5.3382   -3.7636   -1.6268 C    0  0  0  0  0  0  0  0  0  0  0  0
    0.8046   -0.9875   -3.2524 C    0  0  0  0  0  0  0  0  0  0  0  0
   -4.1448   -5.1453    0.0452 C    0  0  0  0  0  0  0  0  0  0  0  0
   -3.0787   -2.9599   -0.7702 C    0  0  0  0  0  0  0  0  0  0  0  0
   -4.7802    4.3453    0.4333 C    0  0  0  0  0  0  0  0  0  0  0  0
    4.3215   -2.0150   -0.0565 C    0  0  0  0  0  0  0  0  0  0  0  0
   -1.8184    2.4361   -1.1362 C    0  0  0  0  0  0  0  0  0  0  0  0
   -2.4060    1.2026   -1.4570 C    0  0  0  0  0  0  0  0  0  0  0  0
   -4.5131    1.9633   -0.5286 C    0  0  0  0  0  0  0  0  0  0  0  0
   -1.7798   -1.0672   -1.6050 C    0  0  0  0  0  0  0  0  0  0  0  0
    6.6763   -1.0173   -0.0295 C    0  0  0  0  0  0  0  0  0  0  0  0
   -0.9590    1.1893    2.0160 C    0  0  0  0  0  0  0  0  0  0  0  0
    5.7449   -2.0805   -0.6420 C    0  0  0  0  0  0  0  0  0  0  0  0
    0.5454   -2.2373    1.7905 O    0  0  0  0  0  0  0  0  0  0  0  0
   -2.0538    0.1434    2.1351 C    0  0  0  0  0  0  0  0  0  0  0  0
   -0.7564   -4.3317    4.6605 C    0  0  0  0  0  0  0  0  0  0  0  0
   -0.1504    2.8213   -1.6671 S    0  0  0  0  0  0  0  0  0  0  0  0
    4.3427    4.4757    0.4690 C    0  0  0  0  0  0  0  0  0  0  0  0
```

2.1136	-0.2398	-3.4459	C	0	0	0	0	0	0	0	0	0	0	0	0
6.3422	-3.4768	-0.3434	C	0	0	0	0	0	0	0	0	0	0	0	0
-0.7604	-3.3270	3.5032	C	0	0	0	0	0	0	0	0	0	0	0	0
0.6106	-1.1826	-1.8351	O	0	0	0	0	0	0	0	0	0	0	0	0
2.2357	0.1668	2.7086	S	0	0	0	0	0	0	0	0	0	0	0	0
5.6461	3.6944	0.1773	C	0	0	0	0	0	0	0	0	0	0	0	0
0.8477	-4.0553	-0.6616	S	0	0	0	0	0	0	0	0	0	0	0	0
4.1690	5.5445	-0.6263	C	0	0	0	0	0	0	0	0	0	0	0	0
5.7080	-1.8604	-2.1719	C	0	0	0	0	0	0	0	0	0	0	0	0
0.6265	-3.1457	2.9063	C	0	0	0	0	0	0	0	0	0	0	0	0
-4.4516	-0.5966	-1.6114	S	0	0	0	0	0	0	0	0	0	0	0	0
-0.1414	0.8855	0.8617	O	0	0	0	0	0	0	0	0	0	0	0	0
2.4225	0.0006	-4.9273	C	0	0	0	0	0	0	0	0	0	0	0	0
-2.8825	0.3335	3.4102	C	0	0	0	0	0	0	0	0	0	0	0	0
4.4725	5.1974	1.8312	C	0	0	0	0	0	0	0	0	0	0	0	0
-1.6816	0.2270	-2.0983	O	0	0	0	0	0	0	0	0	0	0	0	0
-3.0995	5.0775	1.6564	H	0	0	0	0	0	0	0	0	0	0	0	0
-4.1178	3.8804	2.4713	H	0	0	0	0	0	0	0	0	0	0	0	0
-4.6967	5.5439	2.2585	H	0	0	0	0	0	0	0	0	0	0	0	0
3.9897	2.3121	2.1326	H	0	0	0	0	0	0	0	0	0	0	0	0
-4.4494	-2.9732	1.6665	H	0	0	0	0	0	0	0	0	0	0	0	0
-5.3479	-1.9349	0.5469	H	0	0	0	0	0	0	0	0	0	0	0	0
-6.0237	-3.4959	1.0388	H	0	0	0	0	0	0	0	0	0	0	0	0
3.5322	-3.5526	-1.3575	H	0	0	0	0	0	0	0	0	0	0	0	0
2.0346	4.3416	-1.1102	H	0	0	0	0	0	0	0	0	0	0	0	0
-2.1488	4.3825	-0.3405	H	0	0	0	0	0	0	0	0	0	0	0	0
-1.8328	-4.6004	-0.1543	H	0	0	0	0	0	0	0	0	0	0	0	0
4.6503	-0.3564	1.2864	H	0	0	0	0	0	0	0	0	0	0	0	0
-6.7678	3.6710	-0.2207	H	0	0	0	0	0	0	0	0	0	0	0	0
-6.3015	3.0757	1.3865	H	0	0	0	0	0	0	0	0	0	0	0	0
-6.7781	4.7633	1.1684	H	0	0	0	0	0	0	0	0	0	0	0	0
-5.2538	5.3349	-1.4658	H	0	0	0	0	0	0	0	0	0	0	0	0
-3.7848	5.9541	-0.6971	H	0	0	0	0	0	0	0	0	0	0	0	0
-5.3704	6.3936	-0.0461	H	0	0	0	0	0	0	0	0	0	0	0	0
-4.8450	-4.2715	-2.4634	H	0	0	0	0	0	0	0	0	0	0	0	0
-5.6683	-2.7827	-1.9772	H	0	0	0	0	0	0	0	0	0	0	0	0
-6.2392	-4.3337	-1.3691	H	0	0	0	0	0	0	0	0	0	0	0	0
-0.0318	-0.4143	-3.6655	H	0	0	0	0	0	0	0	0	0	0	0	0
0.8334	-1.9706	-3.7441	H	0	0	0	0	0	0	0	0	0	0	0	0
-3.6568	-5.7384	-0.7362	H	0	0	0	0	0	0	0	0	0	0	0	0
-3.5374	-5.2044	0.9549	H	0	0	0	0	0	0	0	0	0	0	0	0
-5.1071	-5.6191	0.2671	H	0	0	0	0	0	0	0	0	0	0	0	0
-5.5474	1.7383	-0.2955	H	0	0	0	0	0	0	0	0	0	0	0	0
6.7796	-1.1404	1.0545	H	0	0	0	0	0	0	0	0	0	0	0	0
6.3194	0.0002	-0.2269	H	0	0	0	0	0	0	0	0	0	0	0	0
7.6763	-1.1071	-0.4686	H	0	0	0	0	0	0	0	0	0	0	0	0
-1.3806	2.1966	1.8921	H	0	0	0	0	0	0	0	0	0	0	0	0
-0.3303	1.1838	2.9135	H	0	0	0	0	0	0	0	0	0	0	0	0
-2.7059	0.1973	1.2585	H	0	0	0	0	0	0	0	0	0	0	0	0
-1.5798	-0.8417	2.1234	H	0	0	0	0	0	0	0	0	0	0	0	0
-1.7605	-4.4448	5.0830	H	0	0	0	0	0	0	0	0	0	0	0	0
-0.4210	-5.3222	4.3302	H	0	0	0	0	0	0	0	0	0	0	0	0
-0.0910	-4.0077	5.4700	H	0	0	0	0	0	0	0	0	0	0	0	0
2.9198	-0.8144	-2.9761	H	0	0	0	0	0	0	0	0	0	0	0	0
2.0467	0.7143	-2.9107	H	0	0	0	0	0	0	0	0	0	0	0	0
5.7422	-4.2775	-0.7890	H	0	0	0	0	0	0	0	0	0	0	0	0
6.3931	-3.6587	0.7362	H	0	0	0	0	0	0	0	0	0	0	0	0
7.3582	-3.5535	-0.7500	H	0	0	0	0	0	0	0	0	0	0	0	0
-1.1291	-2.3551	3.8512	H	0	0	0	0	0	0	0	0	0	0	0	0
-1.4410	-3.6608	2.7104	H	0	0	0	0	0	0	0	0	0	0	0	0
5.8581	2.9506	0.9527	H	0	0	0	0	0	0	0	0	0	0	0	0
5.5813	3.1697	-0.7828	H	0	0	0	0	0	0	0	0	0	0	0	0
6.5007	4.3807	0.1329	H	0	0	0	0	0	0	0	0	0	0	0	0
3.2697	6.1498	-0.4659	H	0	0	0	0	0	0	0	0	0	0	0	0
4.1091	5.0998	-1.6261	H	0	0	0	0	0	0	0	0	0	0	0	0
5.0294	6.2230	-0.6184	H	0	0	0	0	0	0	0	0	0	0	0	0

```
    5.0936   -2.6107   -2.6805 H   0  0  0  0  0  0  0  0  0  0  0  0
    5.3026   -0.8722   -2.4163 H   0  0  0  0  0  0  0  0  0  0  0  0
    6.7204   -1.9244   -2.5892 H   0  0  0  0  0  0  0  0  0  0  0  0
    1.0262   -4.1093    2.5607 H   0  0  0  0  0  0  0  0  0  0  0  0
    1.3218   -2.7380    3.6546 H   0  0  0  0  0  0  0  0  0  0  0  0
    1.6367    0.5960   -5.4076 H   0  0  0  0  0  0  0  0  0  0  0  0
    2.5092   -0.9436   -5.4793 H   0  0  0  0  0  0  0  0  0  0  0  0
    3.3674    0.5417   -5.0469 H   0  0  0  0  0  0  0  0  0  0  0  0
   -2.2626    0.2453    4.3112 H   0  0  0  0  0  0  0  0  0  0  0  0
   -3.3638    1.3197    3.4359 H   0  0  0  0  0  0  0  0  0  0  0  0
   -3.6749   -0.4202    3.4761 H   0  0  0  0  0  0  0  0  0  0  0  0
    4.6352    4.4916    2.6525 H   0  0  0  0  0  0  0  0  0  0  0  0
    3.5666    5.7710    2.0581 H   0  0  0  0  0  0  0  0  0  0  0  0
    5.3205    5.8930    1.8156 H   0  0  0  0  0  0  0  0  0  0  0  0
 1 28  1  0  0  0  0
 1 58  1  0  0  0  0
 1 59  1  0  0  0  0
 1 60  1  0  0  0  0
 2 12  4  0  0  0  0
 2 28  1  0  0  0  0
 2 32  4  0  0  0  0
 3 19  4  0  0  0  0
 3 23  4  0  0  0  0
 3 37  1  0  0  0  0
 4 31  4  0  0  0  0
 4 32  4  0  0  0  0
 4 52  1  0  0  0  0
 5 14  4  0  0  0  0
 5 33  4  0  0  0  0
 5 45  1  0  0  0  0
 6  7  4  0  0  0  0
 6 16  4  0  0  0  0
 6 61  1  0  0  0  0
 7 18  4  0  0  0  0
 7 46  1  0  0  0  0
 8  9  1  0  0  0  0
 8 62  1  0  0  0  0
 8 63  1  0  0  0  0
 8 64  1  0  0  0  0
 9 24  1  0  0  0  0
 9 26  1  0  0  0  0
 9 27  1  0  0  0  0
10 19  4  0  0  0  0
10 29  4  0  0  0  0
10 65  1  0  0  0  0
11 16  4  0  0  0  0
11 21  4  0  0  0  0
11 66  1  0  0  0  0
12 30  4  0  0  0  0
12 67  1  0  0  0  0
13 14  4  0  0  0  0
13 27  4  0  0  0  0
13 68  1  0  0  0  0
14 48  1  0  0  0  0
15 27  4  0  0  0  0
15 33  4  0  0  0  0
15 52  1  0  0  0  0
16 41  1  0  0  0  0
17 23  4  0  0  0  0
17 29  4  0  0  0  0
17 69  1  0  0  0  0
18 21  4  0  0  0  0
18 53  1  0  0  0  0
19 48  1  0  0  0  0
20 28  1  0  0  0  0
20 70  1  0  0  0  0
```

```
20 71  1  0  0  0  0
20 72  1  0  0  0  0
21 40  1  0  0  0  0
22 28  1  0  0  0  0
22 73  1  0  0  0  0
22 74  1  0  0  0  0
22 75  1  0  0  0  0
23 46  1  0  0  0  0
24 76  1  0  0  0  0
24 77  1  0  0  0  0
24 78  1  0  0  0  0
25 42  1  0  0  0  0
25 45  1  0  0  0  0
25 79  1  0  0  0  0
25 80  1  0  0  0  0
26 81  1  0  0  0  0
26 82  1  0  0  0  0
26 83  1  0  0  0  0
29 36  1  0  0  0  0
30 31  4  0  0  0  0
30 40  1  0  0  0  0
31 57  1  0  0  0  0
32 84  1  0  0  0  0
33 57  1  0  0  0  0
34 36  1  0  0  0  0
34 85  1  0  0  0  0
34 86  1  0  0  0  0
34 87  1  0  0  0  0
35 38  1  0  0  0  0
35 53  1  0  0  0  0
35 88  1  0  0  0  0
35 89  1  0  0  0  0
36 43  1  0  0  0  0
36 50  1  0  0  0  0
37 51  1  0  0  0  0
38 55  1  0  0  0  0
38 90  1  0  0  0  0
38 91  1  0  0  0  0
39 44  1  0  0  0  0
39 92  1  0  0  0  0
39 93  1  0  0  0  0
39 94  1  0  0  0  0
41 47  1  0  0  0  0
41 49  1  0  0  0  0
41 56  1  0  0  0  0
42 54  1  0  0  0  0
42 95  1  0  0  0  0
42 96  1  0  0  0  0
43 97  1  0  0  0  0
43 98  1  0  0  0  0
43 99  1  0  0  0  0
44 51  1  0  0  0  0
44100  1  0  0  0  0
44101  1  0  0  0  0
47102  1  0  0  0  0
47103  1  0  0  0  0
47104  1  0  0  0  0
49105  1  0  0  0  0
49106  1  0  0  0  0
49107  1  0  0  0  0
50108  1  0  0  0  0
50109  1  0  0  0  0
50110  1  0  0  0  0
51111  1  0  0  0  0
51112  1  0  0  0  0
54113  1  0  0  0  0
```

```
54114  1  0  0  0  0
54115  1  0  0  0  0
55116  1  0  0  0  0
55117  1  0  0  0  0
55118  1  0  0  0  0
56119  1  0  0  0  0
56120  1  0  0  0  0
56121  1  0  0  0  0
```