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Supporting Information

Noncovalent Interactions between Stacked Arenes in 1,8-Bis-(1-naphthyl)-naphthalenes

Michel Chiarucci, Andrea Mazzanti, Paolo Righi, Giorgio Bencivenni, and Michele Mancinelli*

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Table S1. Comparison among several DFT approaches for the geometry optimization of the *anti* and *syn* isomers of compound **2**. The experimental free energy difference from NMR is 1.00 kcal/mol, being the *anti* isomer the more stable. Calculations included the solvent with the IEFPCM approach (chloroform).

Method	Anti (a.u)	Syn (a.u)	ΔG° (kcal/mol)
B3LYP-D3/6-31+G(d,p)	-1949.001297	-1948.998094	2.01
wB97-XD/6-31+G(d,p)	-1948.333285	-1948.330679	1.64
PBE0-D3/6-31+G(d,p)	-1946.906057	-1946.902863	2.00
PBE0-D3/def2-TZVPP	-1947.553060	-1947.550149	1.83
B97-D3/6-31+G(d,p)	-1947.807449	-1947.804136	2.08
B97-D3/def2-TZVPP	-1948.479097	-1948.476013	1.94
M06-2X/6-31+G(d,p)	-1948.217431	-1948.215195	1.40

Table S2. Geometric parameters and relative free energies of the various conformations of compounds **1-6**. Calculations at the PCM-M06-2X/6-311++G(2d,p)//PCM-M06-2X/6-31+G(d,p) in DMSO. Energies in kcal/mol.

Conf.	ϕ_1	ϕ_2	φ	α_1	α_2	β_1	β_2	Calcd. Dipole (D)	G° $CHCl_3$[a]	G° DMSO[a]
1-*anti* (X-ray)	80.1	80.1	-1.8	124.7	124.7	121.1	121.1	-	-	-
1-*anti*-in	67.6	67.6	9.7	124.6	124.6	121.3	121.3	0.86	**0.00**	**0.00**
1-*anti*-out	99.6	99.6	-19.6	123.1	123.1	122.5	122.5	0.95	0.21	0.25
1-*syn*	99.4	-82.7	-22.8	122.6	123.4	122.5	118.8	0.99	1.06	1.15
2-*anti*-in	80.4	80.4	-5.4	124.5	124.5	123.8	123.8	1.86	**0.00**	**0.00**
2-*syn*	94.5	-86.5	-18.1	123.2	123.7	124.0	121.1	8.87	0.93	0.70
3-*anti*-in	78.7	77.2	-2.5	125.4	123.6	124.1	121.5	4.58	**0.00**	**0.00**
3-*syn*-in	80.6	-101.7	-6.5	124.9	124.2	123.8	120.1	4.20	0.11	0.12
3-*syn*-out	83.2	-98.9	21.7	123.5	122.5	120.7	122.5	4.74	1.45	1.48
4-*anti*-in	80.1	78.8	-4.2	125.2	123.7	124.1	121.6	3.00	**0.00**	**0.00**
4-*syn*-in	80.2	102.1	-6.7	125.0	124.1	123.8	120.1	5.73	0.46	0.34
4-*syn*-out	113.6	-72.0	-1.2	125.5	123.6	122.0	121.3	6.29	1.71	1.77
5-*anti*-in	76.4	74.9	-0.7	125.3	124.0	124.0	121.0	6.24	0.16	0.12
5-*syn*-in	82.2	-98.6	-8.6	124.2	124.6	123.7	119.4	2.50	**0.00**	**0.00**
5-*syn*-out	117.9	-67.7	-5.6	125.2	123.9	122.6	120.7	2.96	1.59	1.64
6-*anti*-in	67.0	67.0	8.3	124.6	124.6	121.0	121.0	1.45	**0.00**	**0.00**
6-*syn*	99.8	-81.5	-23.0	122.7	123.3	122.0	118.4	3.59	0.32	0.61

[a] energies relative to the best conformer within the same compound (in bold).

Table S3. Comparison between the DFT results with PCM-M06-2X/6-311++G(2d,p)//PCM-M06-2X/6-31+G(d,p) and ωB97X-X/6-311++G(2d,p)//M06-2X/6-31+G(d,p).

		M06-2X		ωB97X-D
Conf.	EXP G°	G° $CHCl_3$[b]	G° DMSO[b]	G° $CHCl_3$[b]
1-*anti*-in	**0.00**	**0.00**	**0.00**	**0.00**
1-*anti*-out		0.21	0.25	0.54
1-*syn*	0.88	1.06	1.15	1.33
2-*anti*-in	**0.00**	**0.00**	**0.00**	**0.00**
2-*syn*	1.00	0.93	0.70	1.56
3-*anti*-in	**0.00**	**0.00**	**0.00**	**0.00**
3-*syn*-in	0.35	0.11	0.12	0.48
3-*syn*-out		1.45	1.48	2.88
4-*anti*-in	**0.00**	**0.00**	**0.00**	**0.00**
4-*syn*-in	0.60	0.46	0.34	0.75
4-*syn*-out		1.71	1.77	1.87
5-*anti*-in	**0.00**	0.16	0.12	0.00
5-*syn*-in	0.13	**0.00**	**0.00**	**0.45**
5-*syn*-out		1.59	1.64	1.83
6-*anti*-in	**0.00**	**0.00**	**0.00**	**0.00**
6-*syn*	0.78	0.32	0.61	0.02

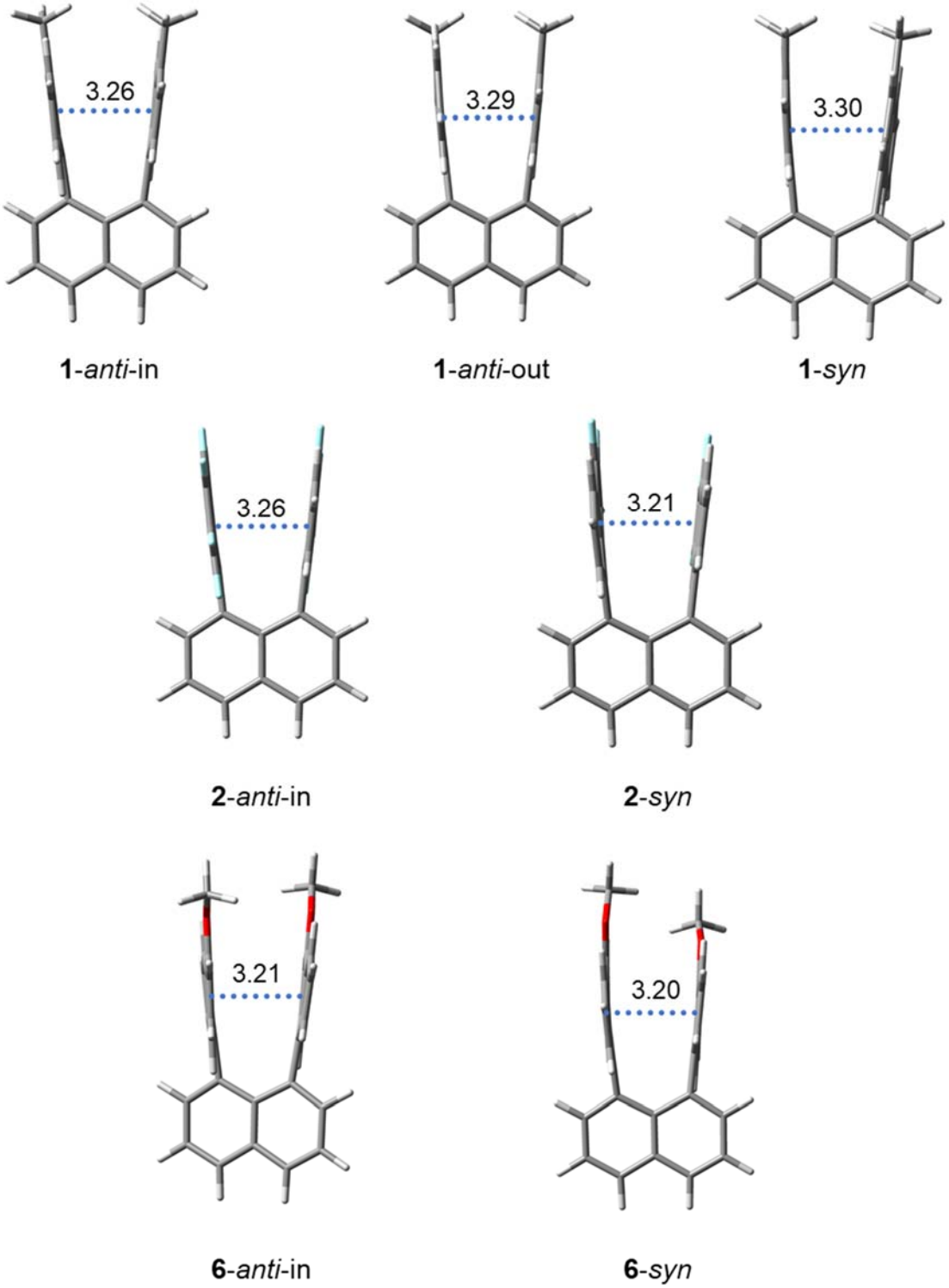


Figure S1. Intra-ring distances for the isomers and conformations of compounds **1,2,6**. Data for the optimized structures using chloroform as the solvent for IEFPCM.

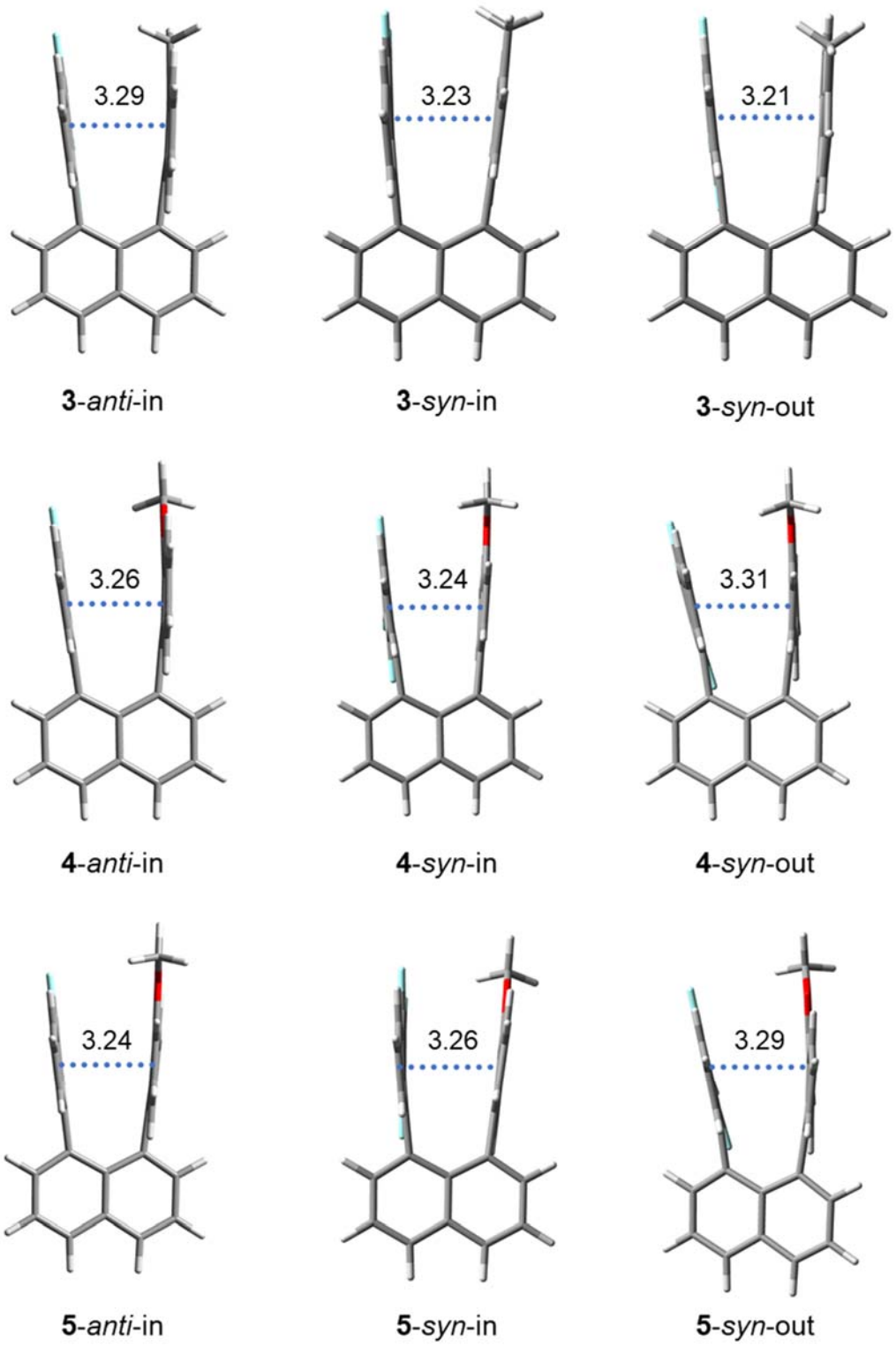


Figure S2. Intra-ring distances for the isomers and conformations of compounds **3-5**. Data for the optimized structures using chloroform as the solvent for IEFPCM.

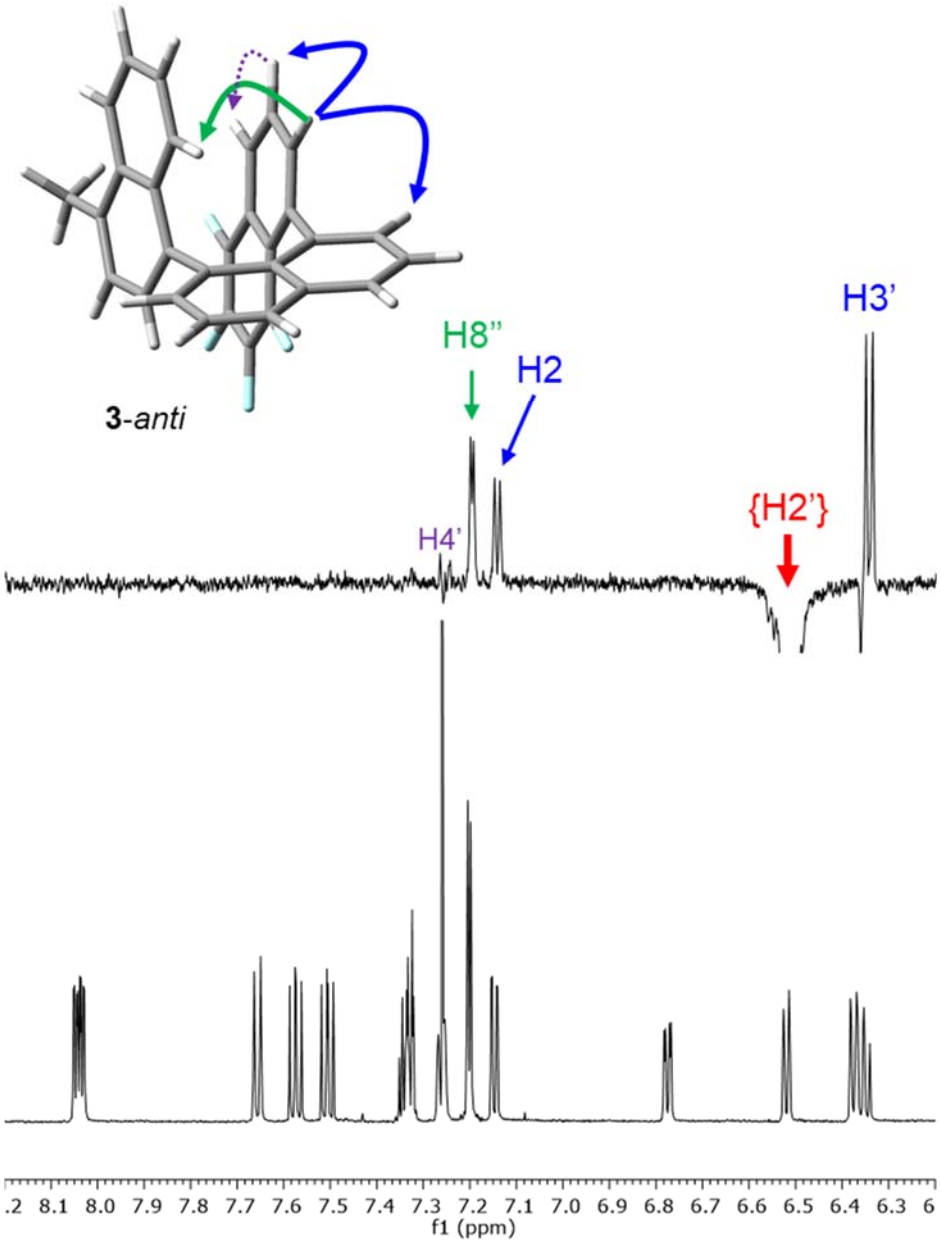


Figure S3. Bottom: ^{1}H spectrum of **3**-*anti* (600 MHz in $CDCl_3$). Top: DPFGSE-NOE spectrum. The signal of H-2' was assigned by means of HMBC and COSY spectra. Blue labels (top) represent control NOEs. Green labels indicate diagnostic NOEs. The NOE signal on H3' is not a triplet due to zero-quantum coherence effect with the saturated signal of H2'.

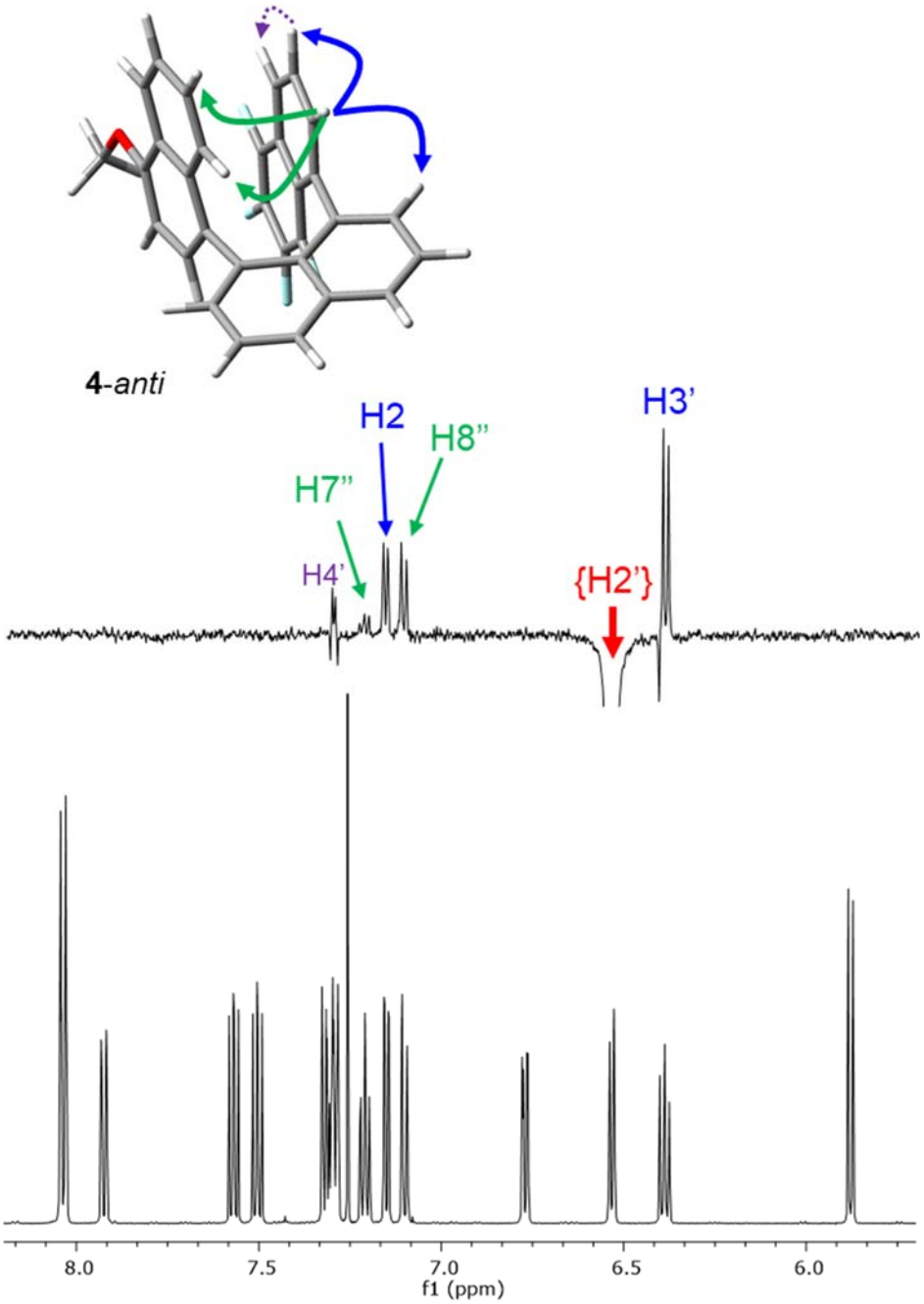


Figure S4. Bottom: ^{1}H spectrum of **4**-*anti* (600 MHz in $CDCl_3$). Top: DPFGSE-NOE spectrum. The signal of H-2' was assigned by means of HMBC and COSY spectra. Blue labels (top) represent control NOEs. Green labels indicate diagnostic NOEs. The NOE signal on H3' is not a triplet due to zero-quantum coherence effect with the saturated signal of H2'.

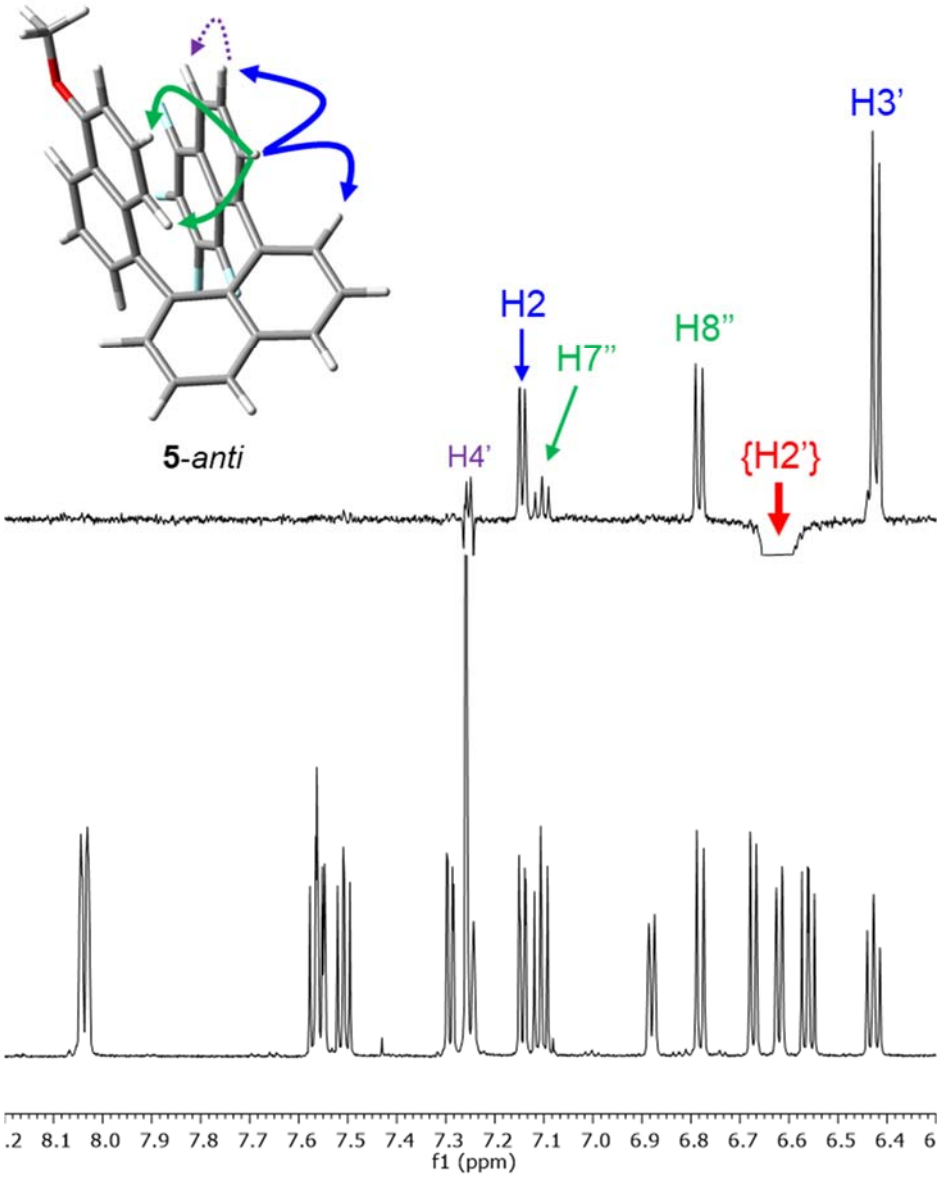


Figure S5. Bottom: ^{1}H spectrum of **5**-*anti* (600 MHz in $CDCl_3$). Top: DPFGSE-NOE spectrum. The signal of H-2' was assigned by means of HMBC and COSY spectra. Blue labels (top) represent control NOEs. Green labels indicate diagnostic NOEs. The NOE signal on H3' is not a triplet due to zero-quantum coherence effect with the saturated signal of H2'.

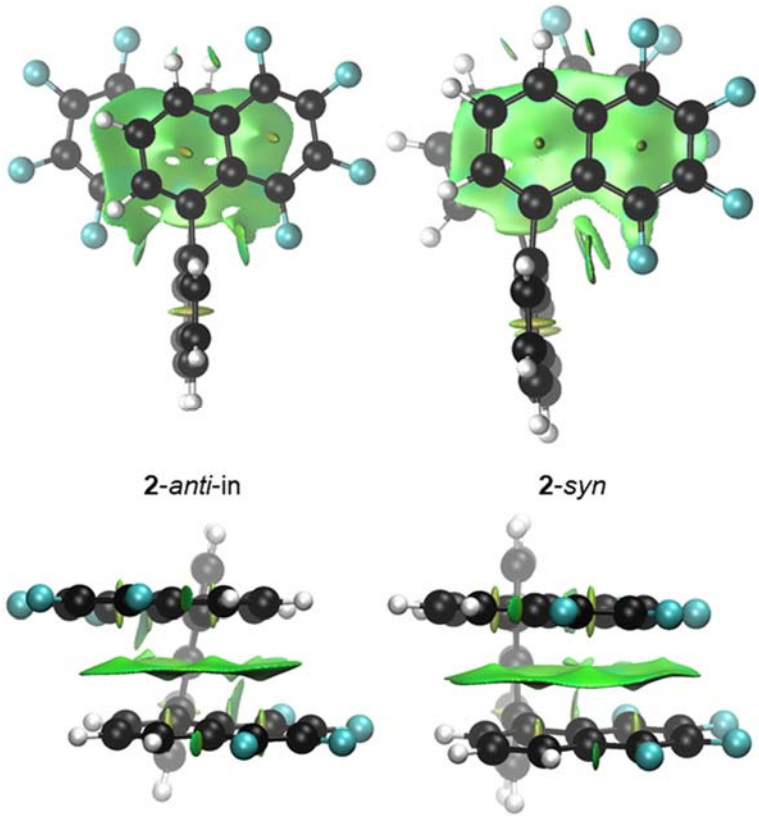


Figure S6. Plots of the noncovalent interactions of compound **2.** 3D representation obtained with VMD software.

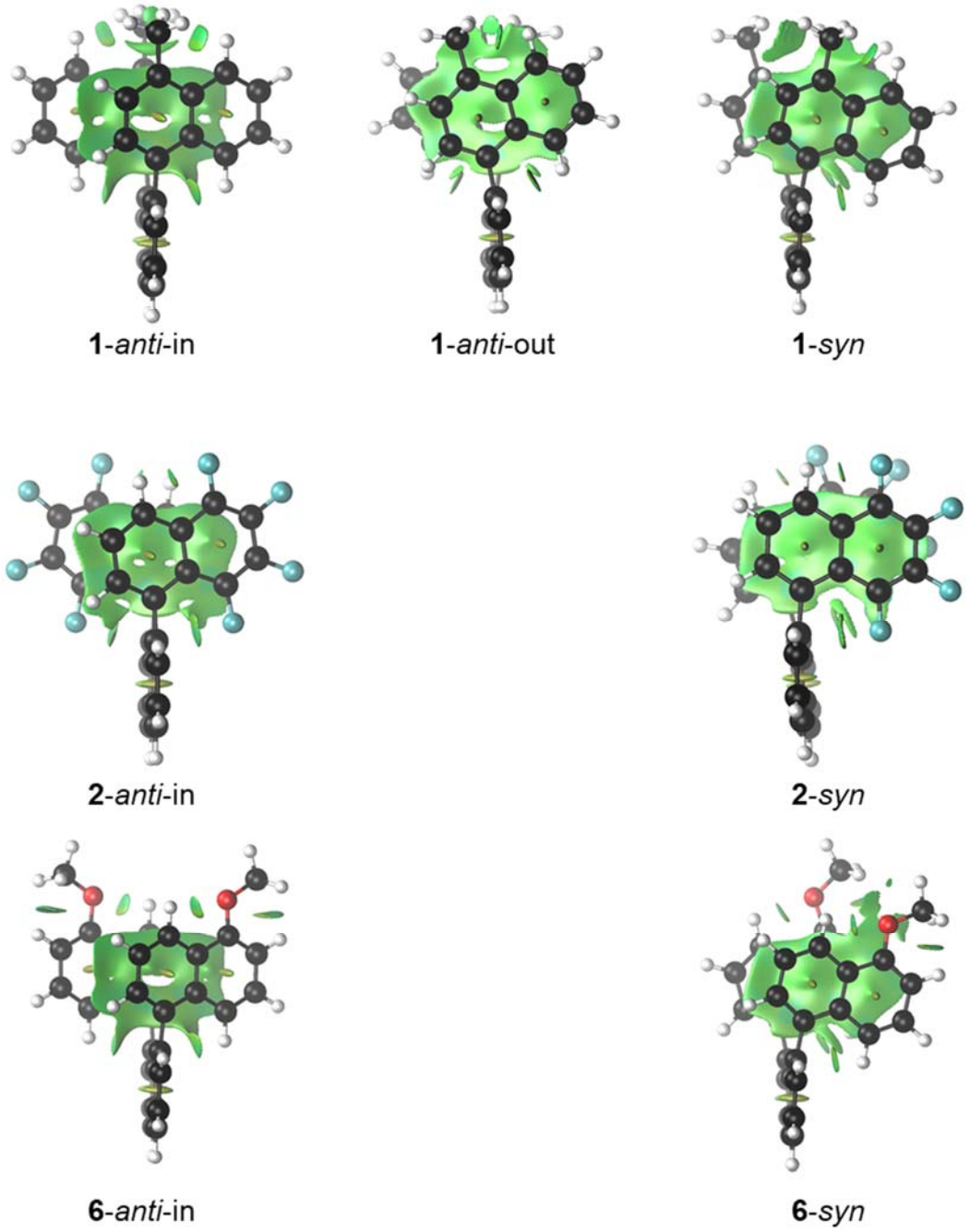


Figure S7. Plots of the noncovalent interactions of compounds **1,2,6.** 3D representation obtained with VMD software.

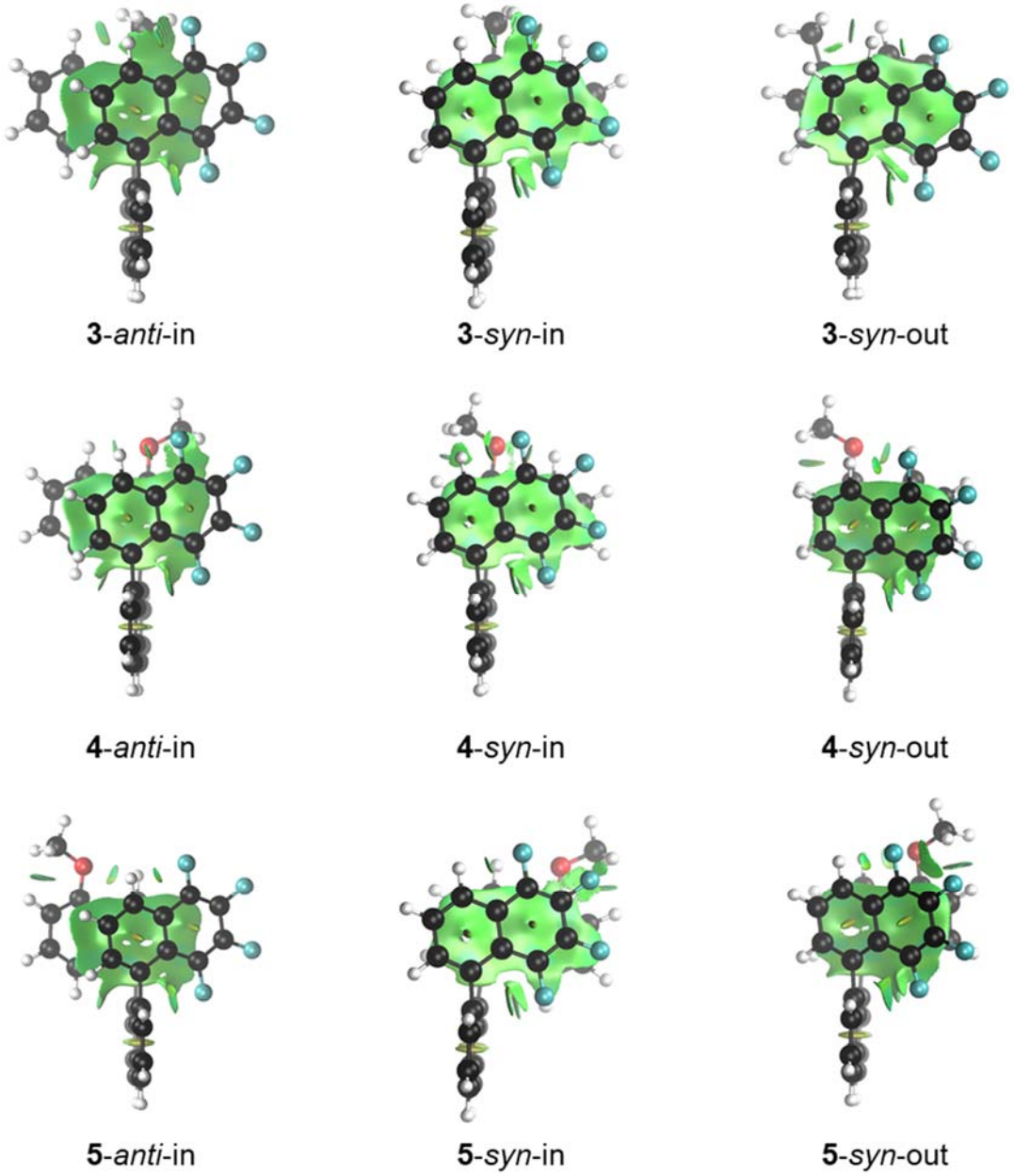


Figure S8. Plots of the noncovalent interactions of compounds **3-5.** 3D representation obtained with VMD software.

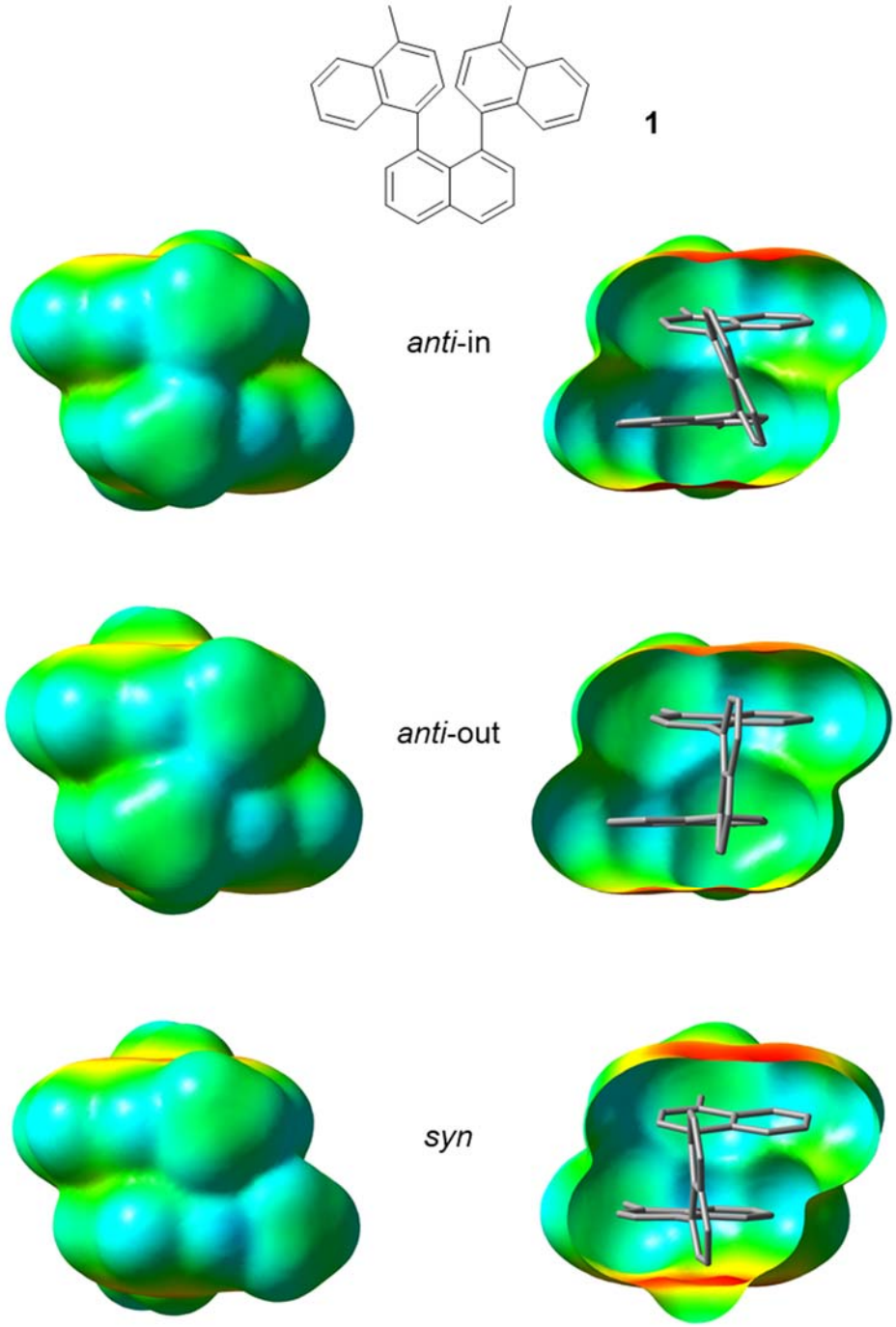


Figure S9. Electrostatic surfaces for the three conformations of compound **1** (Isovalues at 10^{-4} e^-/au^3). Hydrogens were removed for clarity.

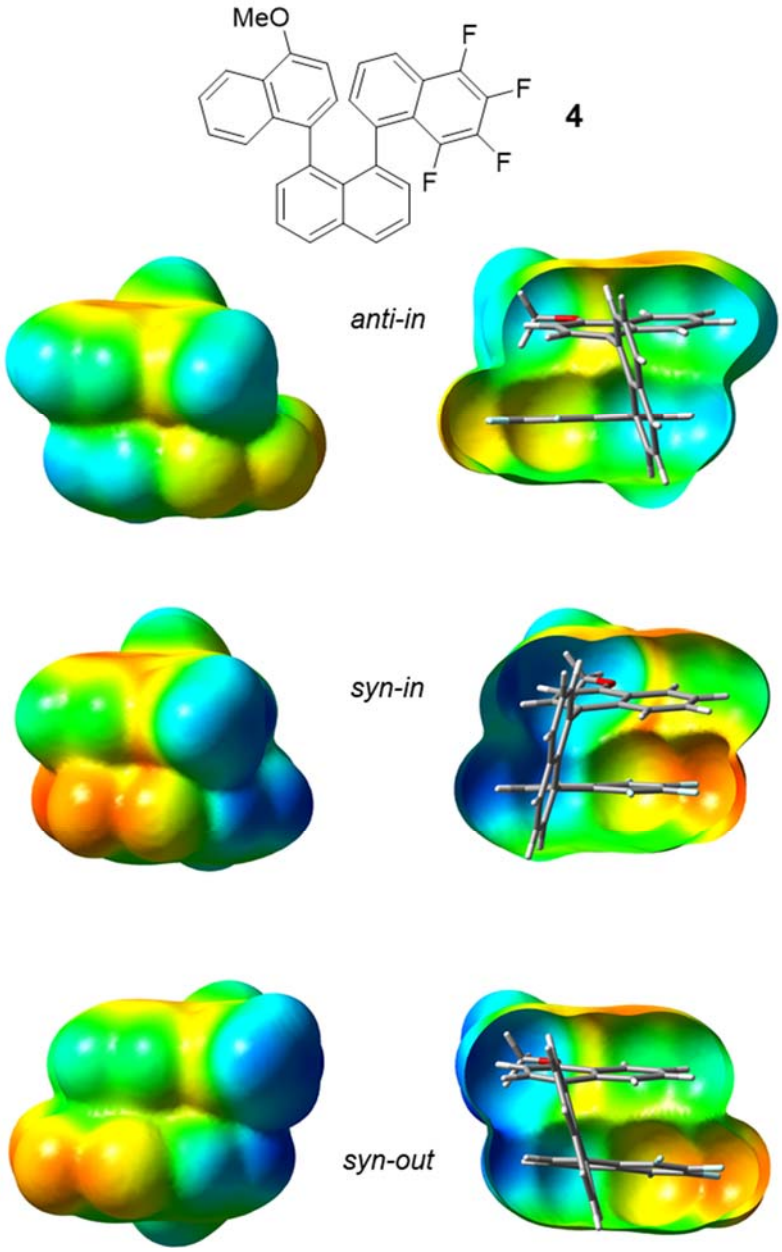


Figure S10. Electrostatic surfaces for the three conformations of compound **4** (Isovalues at 10^{-4} e^-/au^3).

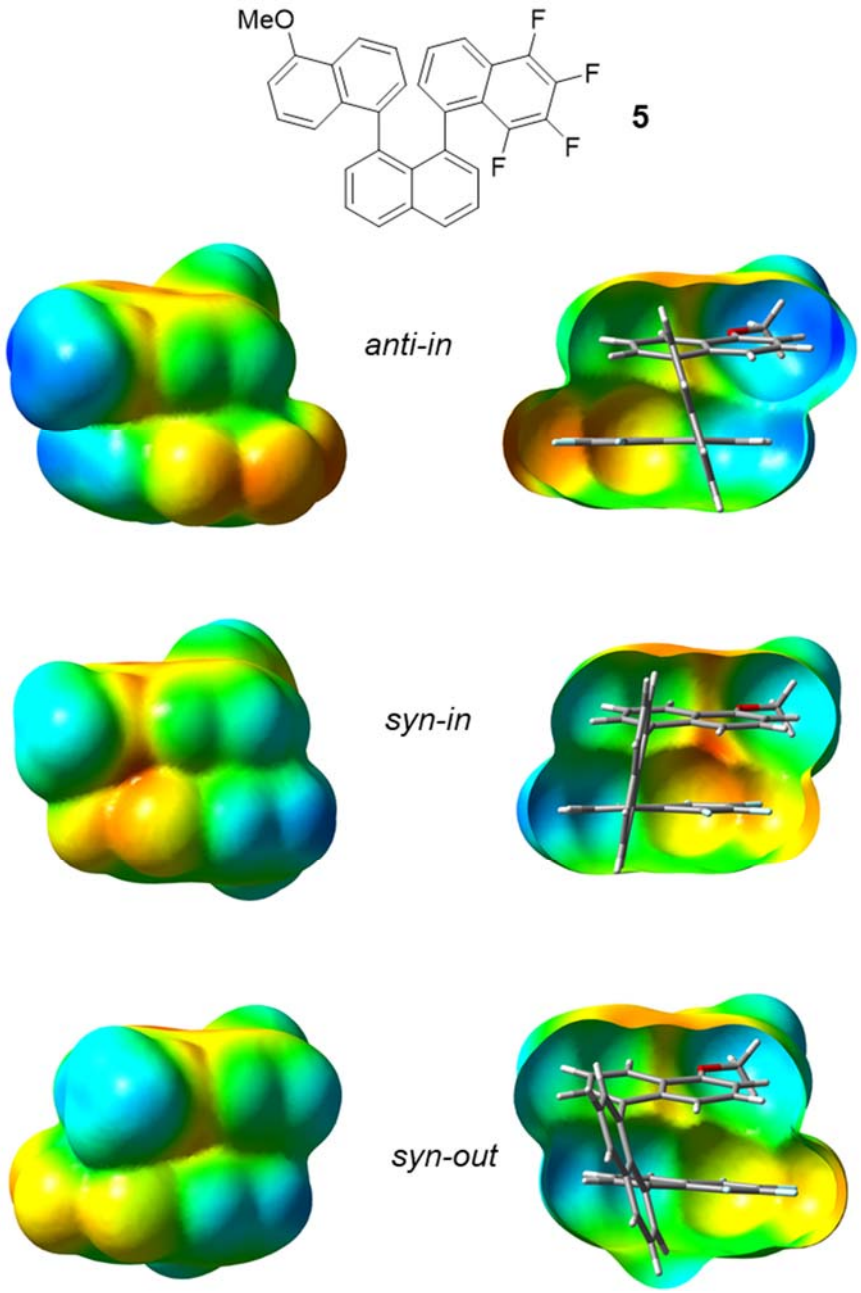


Figure S11. Electrostatic surfaces for the three conformations of compound **5** (Isovalues at 10^{-4} e^-/au^3).

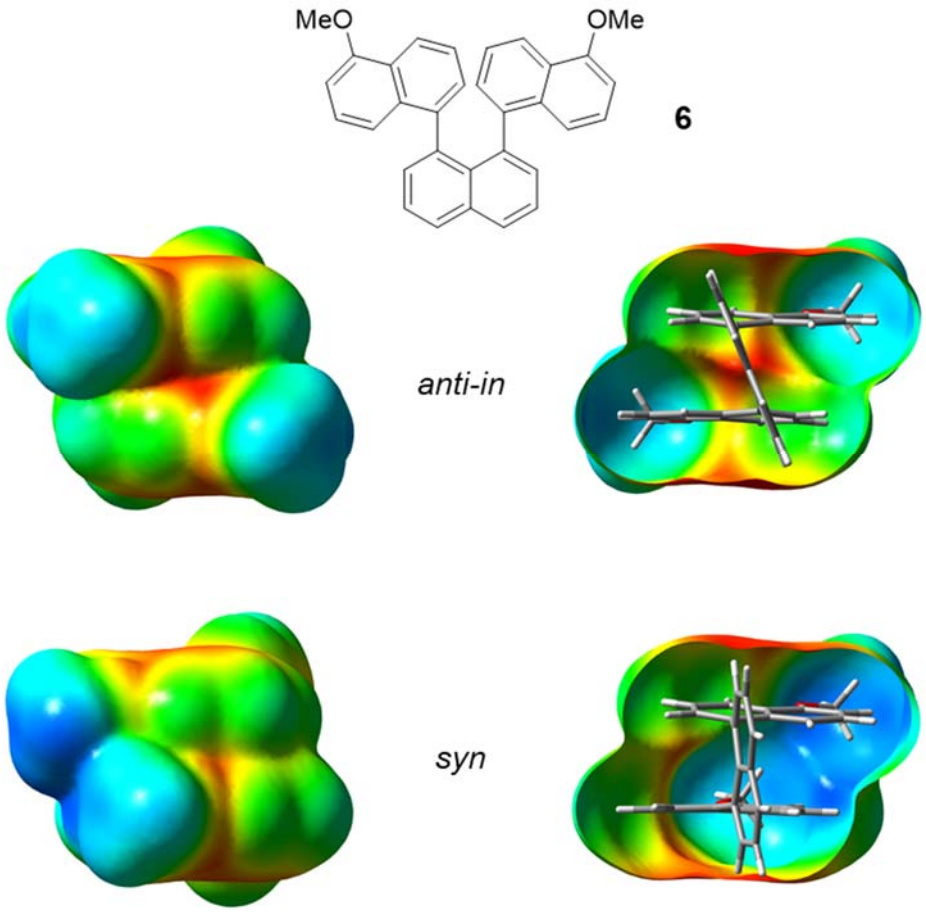


Figure S12. Electrostatic surfaces for the two conformations of compound **6** (Isovalues at 10^{-4} e^-/au^3).

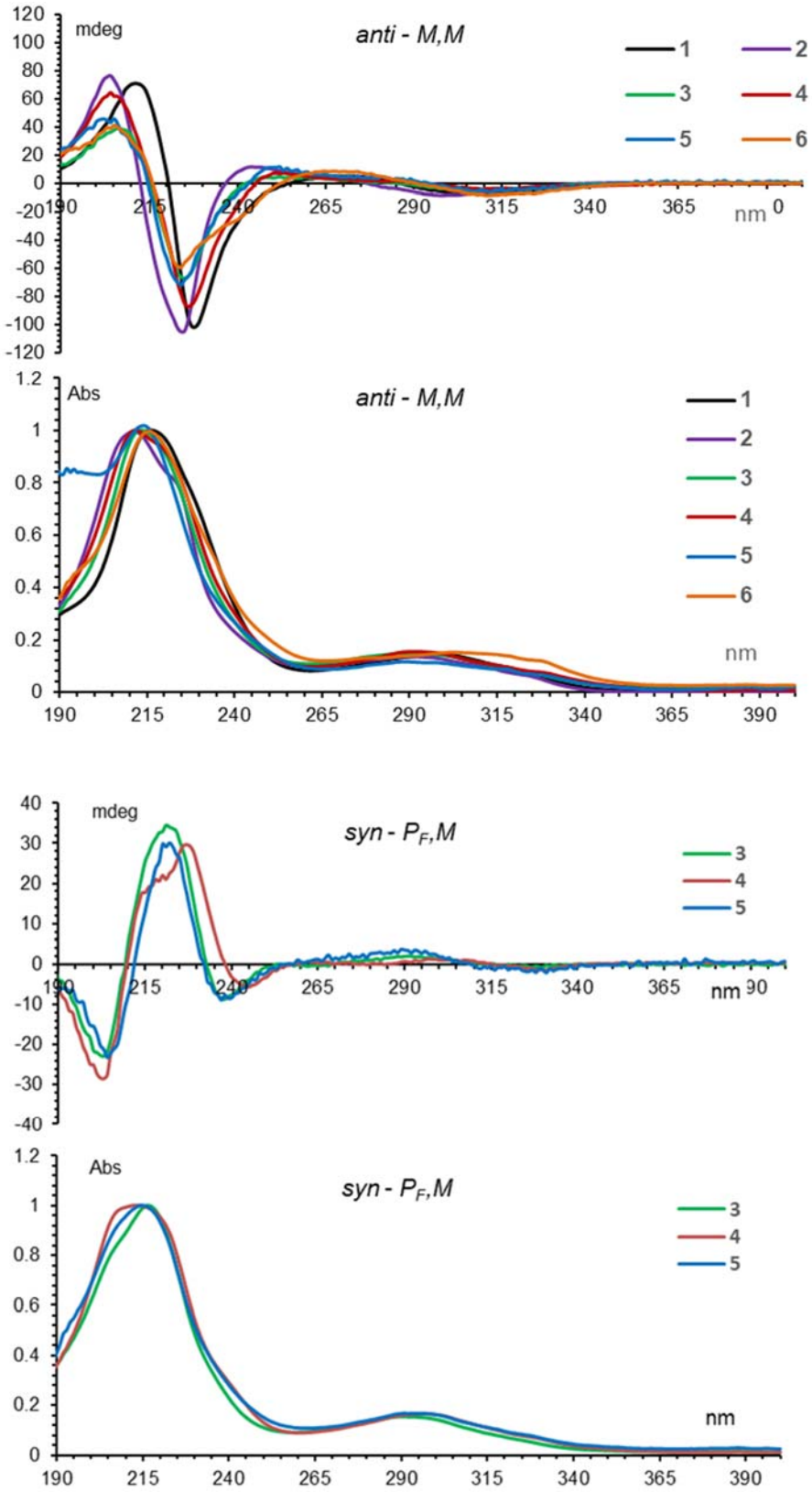


Figure S13. UV and ECD spectra for compounds **1-6**.

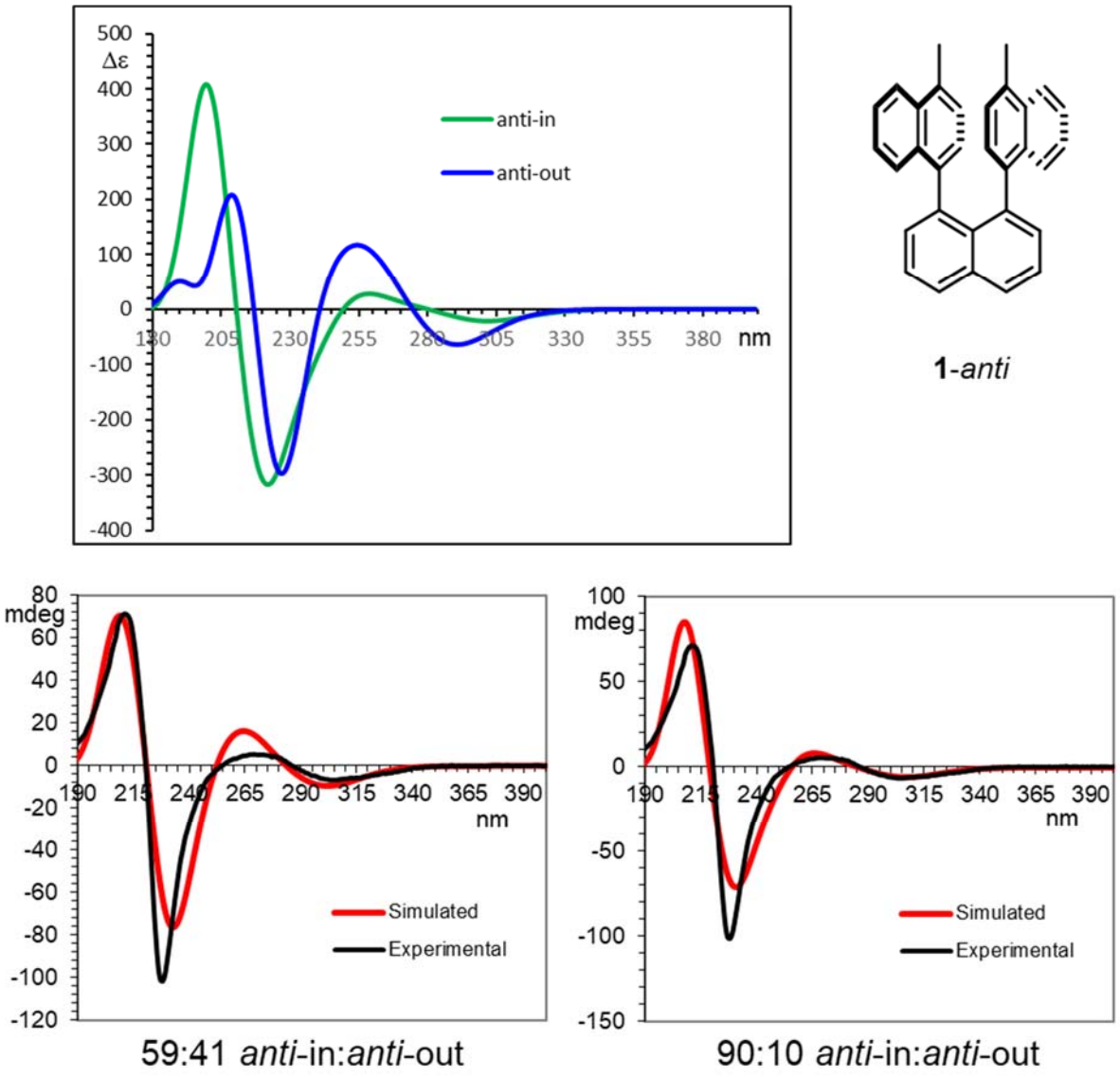


Figure S14. Top: TD-DFT simulations of the **1**-*anti*-in and **1**-*anti*-out conformations, at the CAM-B3LYP/6-311++G(2d,p) level. Bottom: Simulations of the experimental ECD spectrum (black line) using two different conformational ratios.

Summary of chiral resolution on CSP-HPLC

compound	CSP Column	1° eluted *anti*	1°eluted *syn*	
1-*anti*	Chiralcel OG	*M, M*		
2-*anti*	Lux Cellulose 2	*P, P*		
3-*anti*	Chiralcel OG	*M, M*		
3-*syn*	Chiralcel OG		P_F, *M*	
4-*anti*	Chiralcel OD-H	*P, P*		
4-*syn*	Chiralcel OD-H		P_F, *M*	
5-*anti*	Chiralcel OD-H	*M, M*		
5-*syn*	Chiralcel OD-H		M_F, *P*	
6-*anti*	Chiralcel OD-H	*M, M*		

Absolute configuration assignment.

The absolute configuration of the optically active stereoisomers was assigned by the simulation of ECD spectra based on time-dependent density functional theory (TD-DFT).[1] The theoretical ECD spectra of the ground state conformations were obtained with four different functionals (CAM-B3LYP,[2] ωB97X-D,[3] BH&HLYP[4] and M06-2x[5]) with the same 6-311++G(2d,p) basis set, in order to have data redundancy, and to enhance reliability.

For each conformation 70 discrete transitions were calculated, and the ECD spectrum was obtained by convolution of Gaussian shaped lines (0.5 eV half-height line width). The simulated spectra resulting from the Boltzmann averaged sum of the conformations were vertically scaled and red-shifted by 6-12 nm to get the best simulations with the experimental spectra.

[1] a) Laurent, A. D.; Jacquemin, D. *Int. J. Quantum Chem.* **2013**, *113*, 2019–2039. b) Jacquemin, D.; Wathelet, V.; Perpète, E. A.; Adamo, C. *J. Chem. Theory Comput.* **2009**, *5*, 2420–2435

[2] Yanai, T.; Tew, D.; Handy, N. *Chem. Phys. Lett.* **2004**, *393*, 51–57.

[3] a) Chai, J-D.; Head-Gordon, M. *Phys. Chem. Chem. Phys.* **2008**, *10*, 6615–6620.

[4] In Gaussian 16 the BH&HLYP functional has the form: $0.5*^{EXHF} + 0.5*^{EXLSDA} + 0.5*\Delta EX^{Becke88} + EC^{LYP}$

[5] Zhao, Y.; Truhlar, D. G.. *Theor. Chem. Acc.* **2008**, *120*, 215–241.

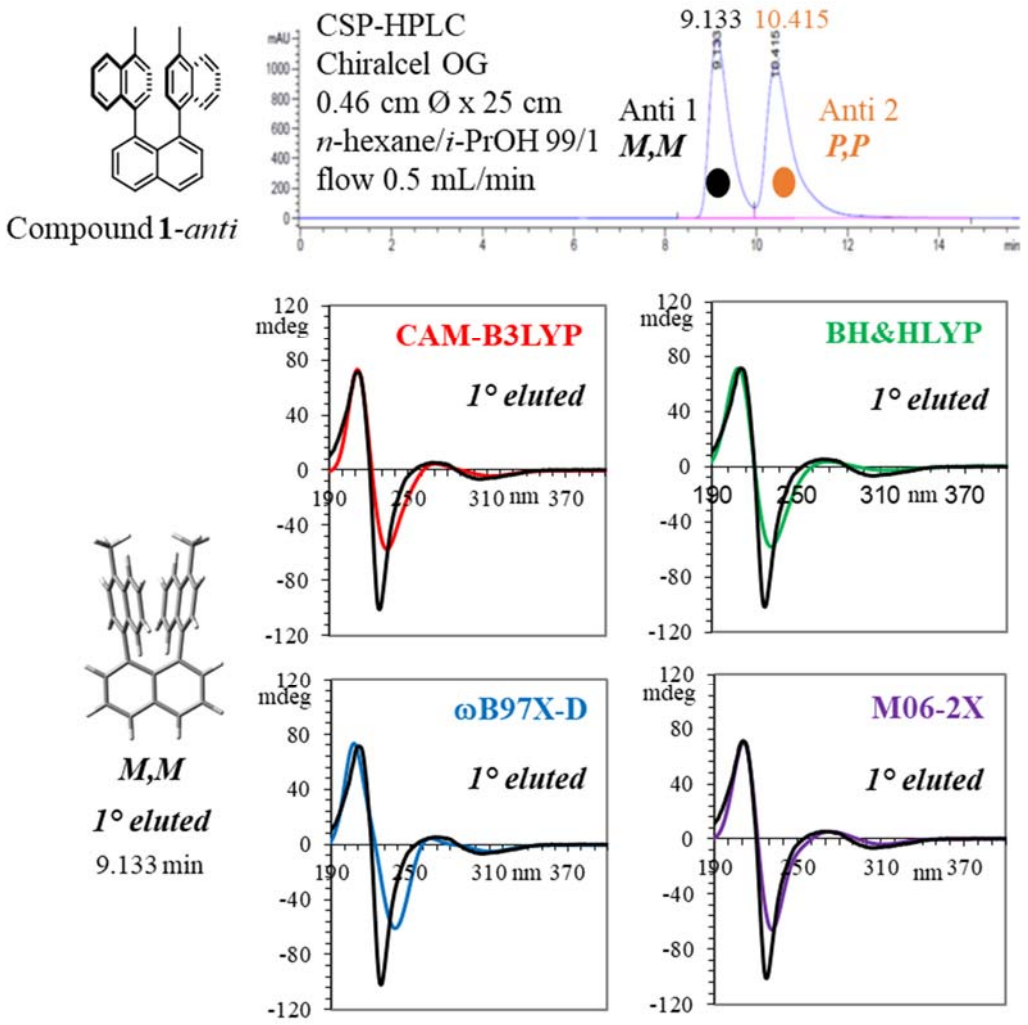


Figure S15. Experimental and calculated ECD of compound **1**-*anti*. The calculated spectra have been red shifted by 12, 12, 12 and 10 nm and multiplied by a scale factor of 0.18, 0.20, 0.23, and 0.16 for CAM-B3LYP, BH&HLYP, ωB97X-D and M06-2X, respectively.

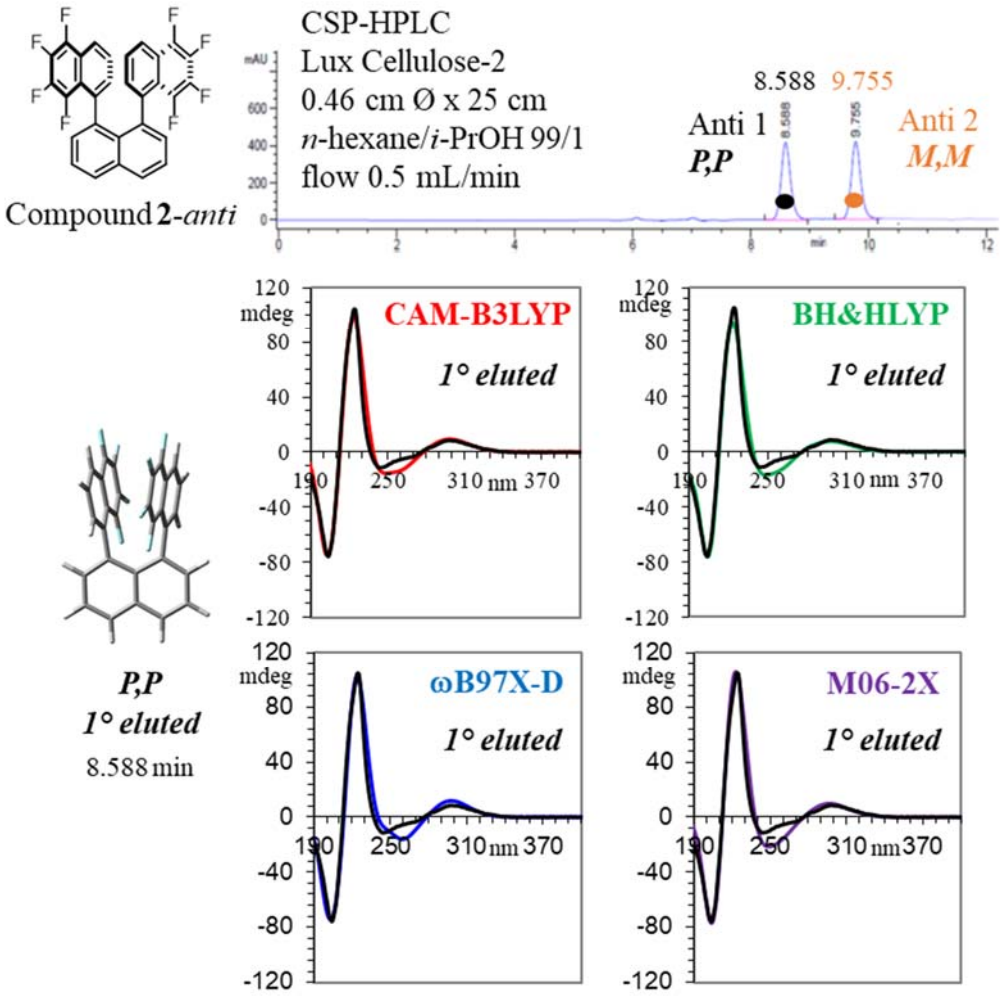


Figure S16. Experimental and calculated ECD of compound **2**-*anti*. The calculated spectra have been red shifted by 8, 12, 10 and 8 nm and multiplied by a scale factor of 0.23, 0.21, 0.27, and 0.22 for CAM-B3LYP, BH&HLYP, ωB97X-D and M06-2X, respectively.

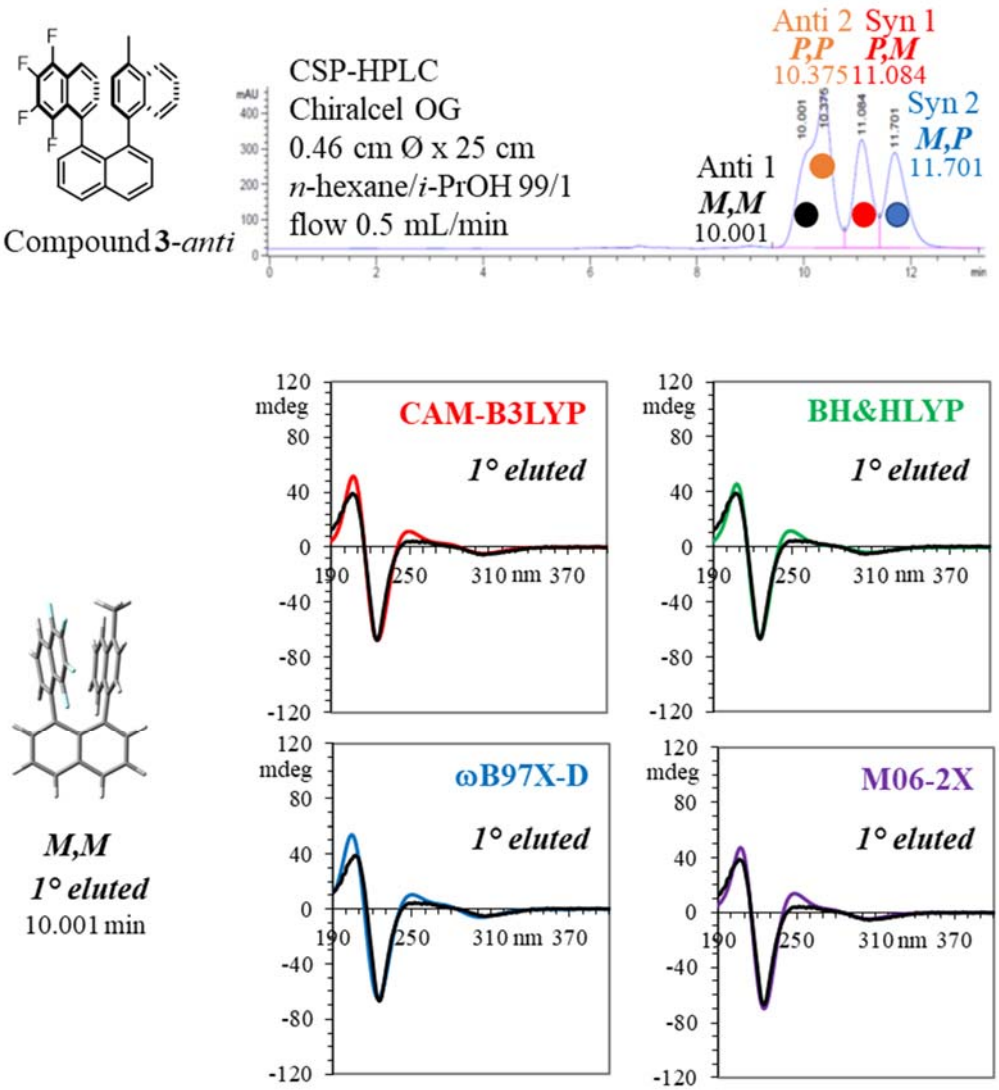


Figure S17. Experimental and calculated ECD of compound **3**-*anti*. The calculated spectra have been red shifted by 8, 12, 9 and 7 nm and multiplied by a scale factor of 0.13, 0.11, 0.16, and 0.12 for CAM-B3LYP, BH&HLYP, ωB97X-D and M06-2X, respectively.

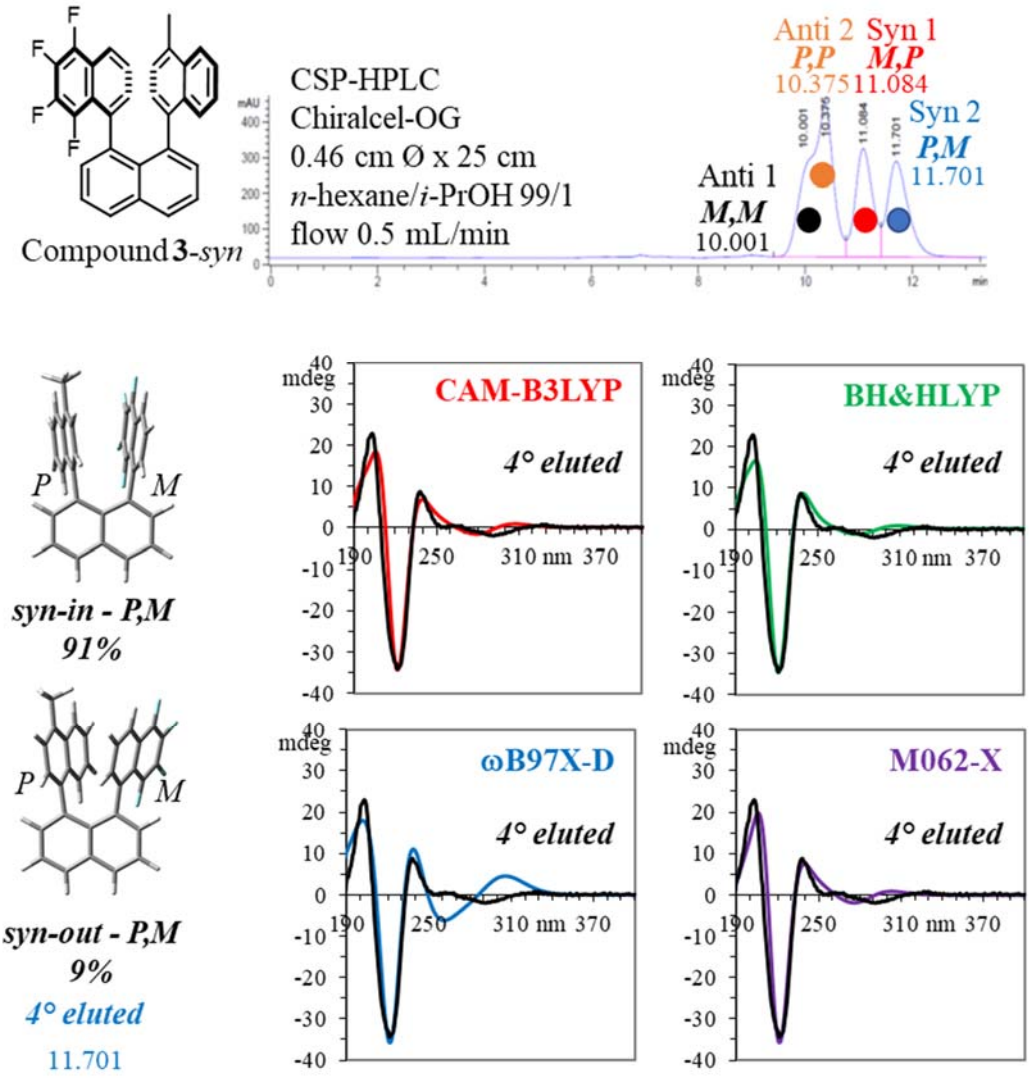


Figure S18. Experimental and calculated ECD of compound **3**-*syn*. The calculated spectra have been red shifted by 7, 10, 10 and 6 nm and multiplied by a scale factor of 0.15, 0.14, 0.18, and 0.13 for CAM-B3LYP, BH&HLYP, ωB97X-D and M06-2X, respectively.

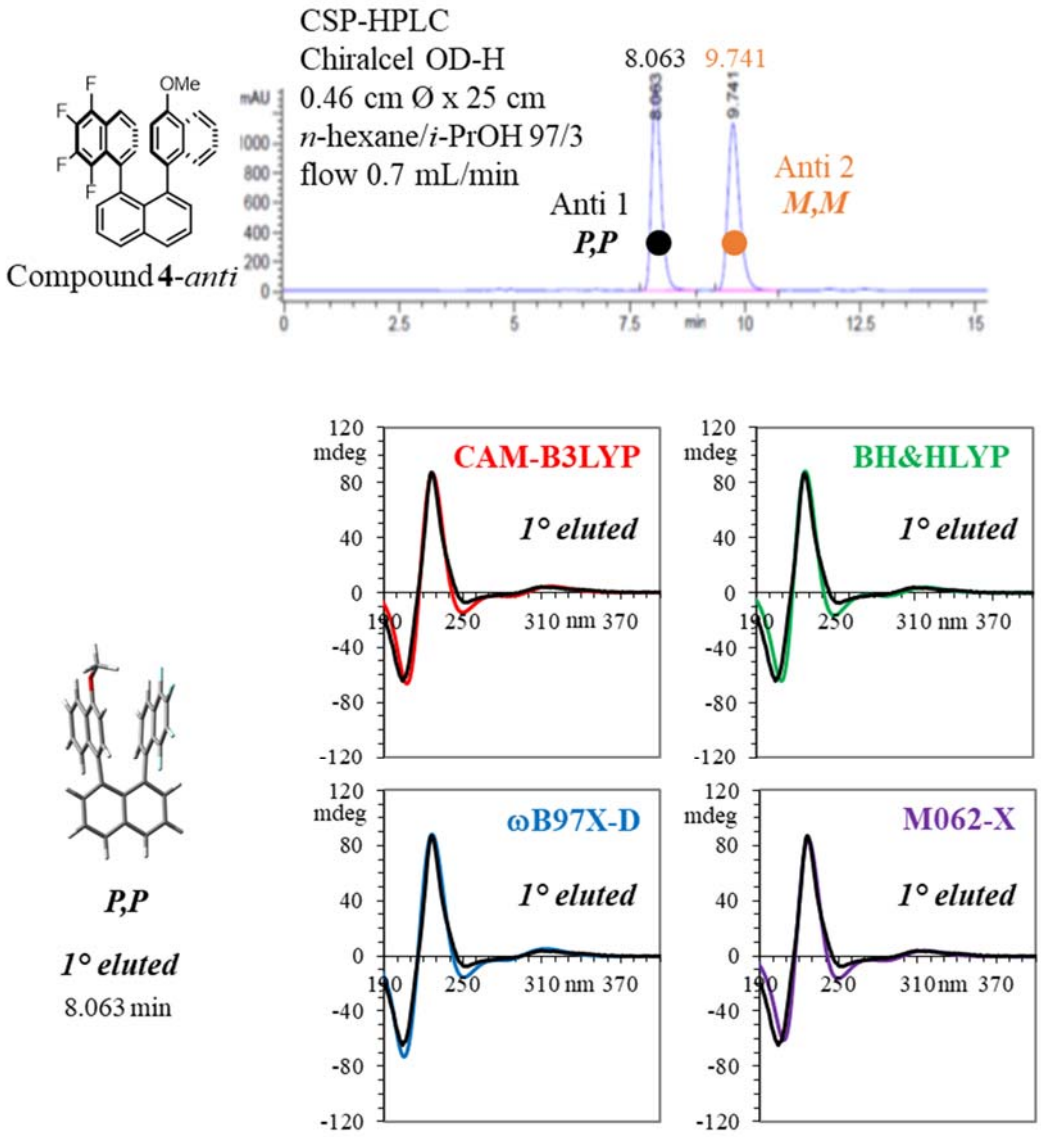


Figure S19. Experimental and calculated ECD of compound **4**-*anti*. The calculated spectra have been red shifted by 8, 12, 9 and 8 nm and multiplied by a scale factor of 0.18, 0.16, 0.22, and 0.16 for CAM-B3LYP, BH&HLYP, ωB97X-D and M06-2x, respectively.

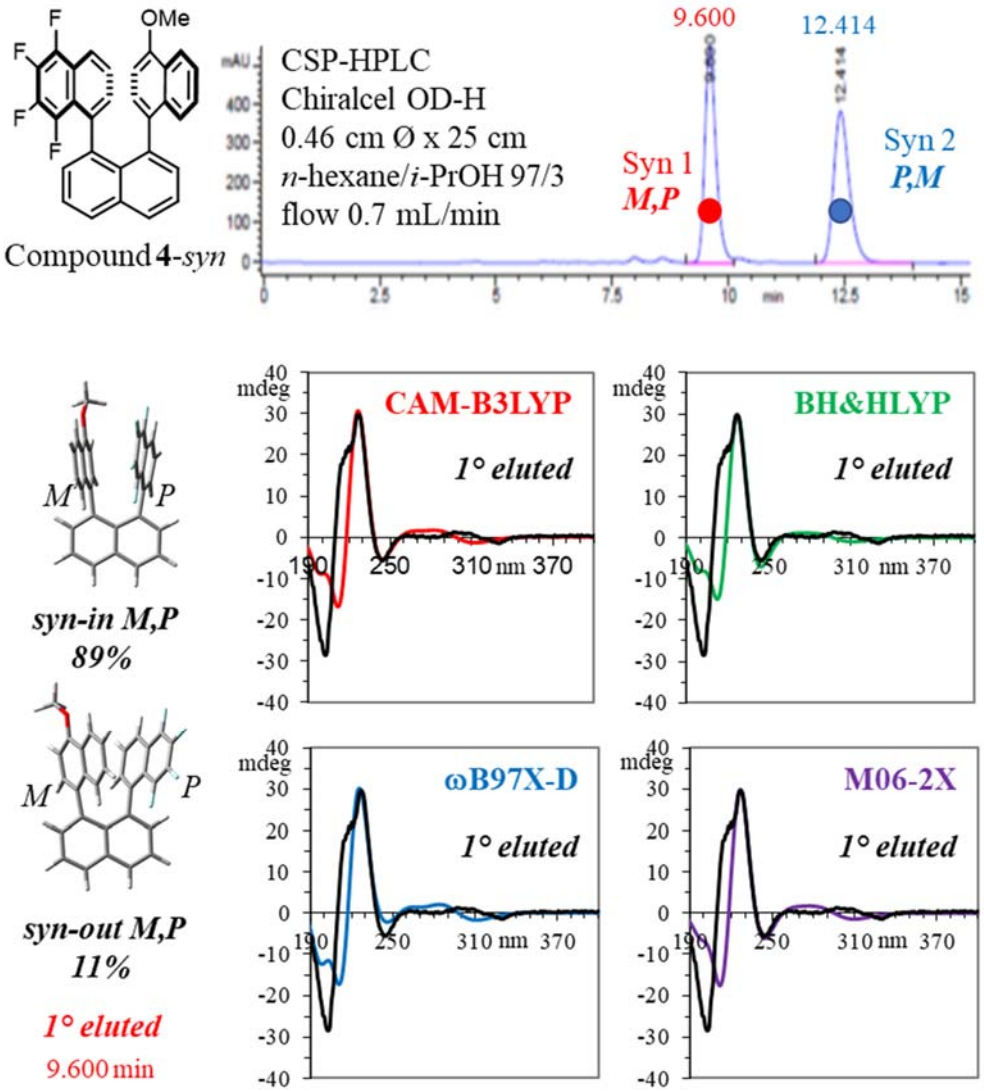


Figure S20. Experimental and calculated ECD of compound **4**-*syn*. The calculated spectra have been red shifted by 10, 14, 12 and 10 nm and multiplied by a scale factor of 0.16, 0.13, 0.24, and 0.14 for CAM-B3LYP, BH&HLYP, ωB97X-D and M06-2X, respectively.

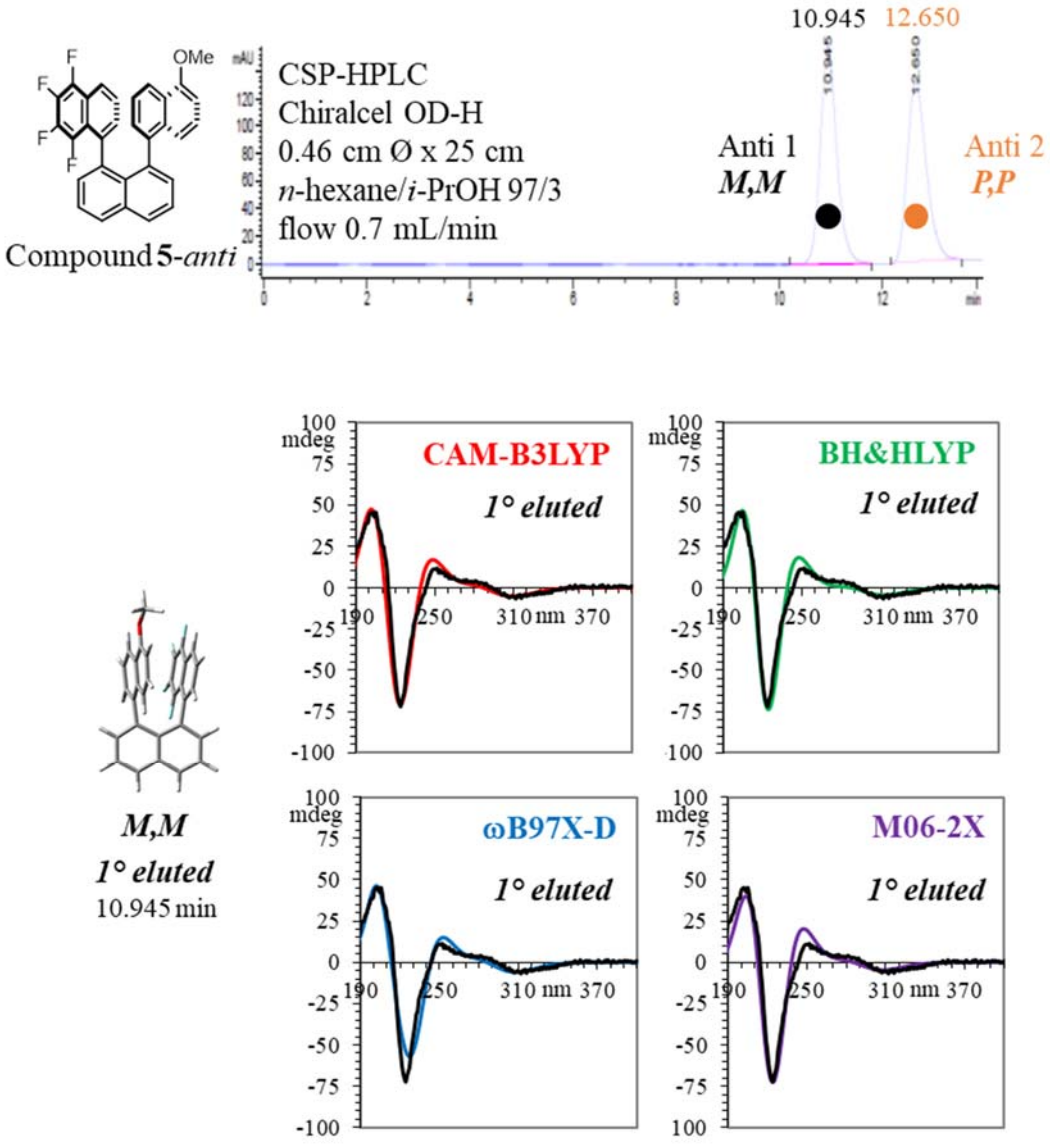


Figure S21. Experimental and calculated ECD of compound **5**-*anti*. The calculated spectra have been red shifted by 6, 10, 10 and 5 nm and multiplied by a scale factor of 0.17, 0.15, 0.18, and 0.15 for CAM-B3LYP, BH&HLYP, ωB97X-D and M06-2X, respectively.

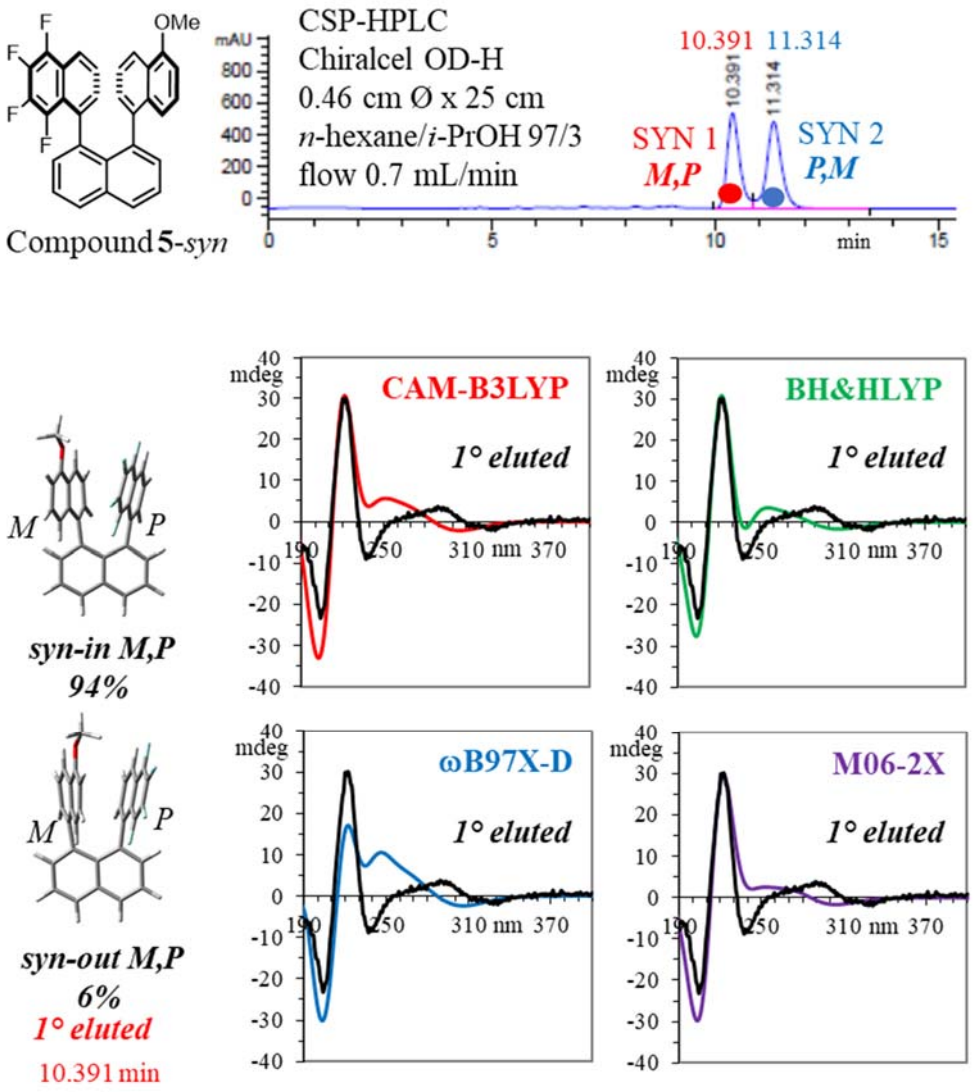


Figure S22. Experimental and calculated ECD of compound **5**-*syn*. The calculated spectra have been red shifted by 6, 9, 11 and 5 nm and multiplied by a scale factor of 0.14, 0.10, 0.15, and 0.11 for CAM-B3LYP, BH&HLYP, ωB97X-D and M06-2X, respectively.

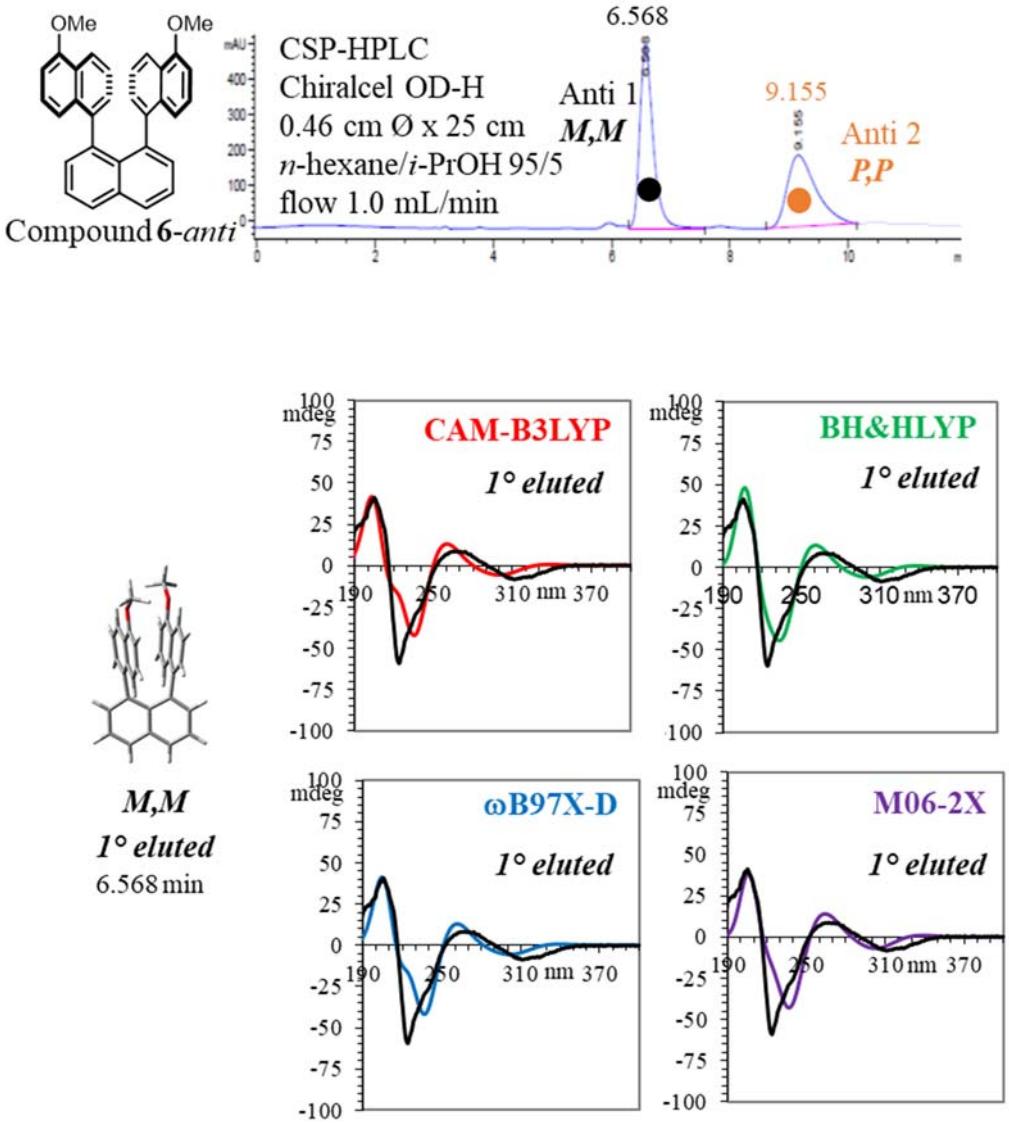
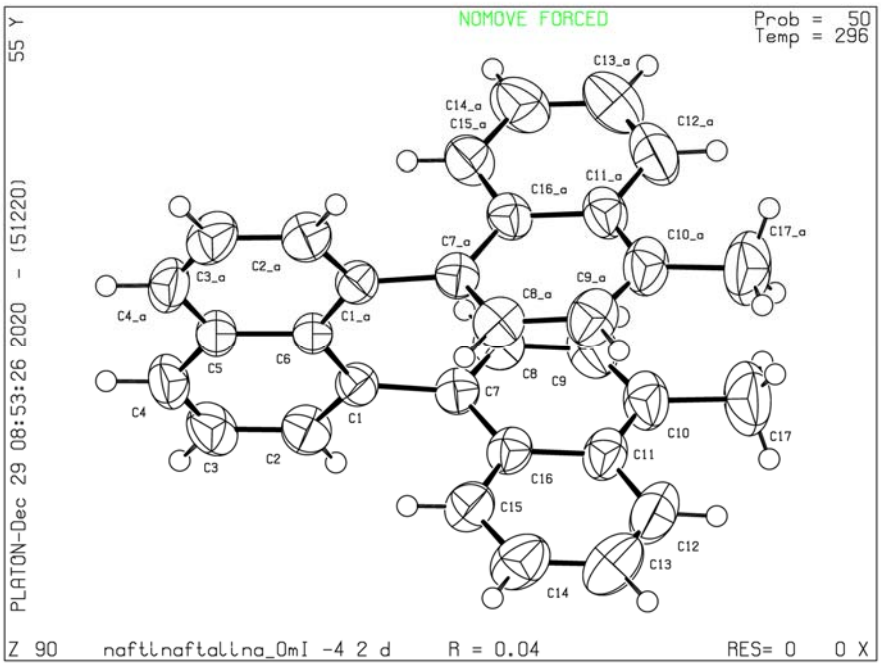


Figure S23. Experimental and calculated ECD of compound **6**-*anti*. The calculated spectra have been red shifted by 8, 12, 10 and 10 nm and multiplied by a scale factor of 0.15, 0.15, 0.15, and 0.15 for CAM-B3LYP, BH&HLYP, ωB97X-D and M06-2X, respectively

Crystal data for compound 1-*anti*



A specimen of $C_{32}H_{24}$, approximate dimensions 0.300 mm x 0.300 mm x 0.350 mm, was used for the X-ray crystallographic analysis. The X-ray intensity data were measured. The total exposure time was 3.33 hours. The frames were integrated with the Bruker SAINT software package using a narrow-frame algorithm. The integration of the data using a tetragonal unit cell yielded a total of 12753 reflections to a maximum θ angle of 27.50° (0.77 Å resolution), of which 2588 were independent (average redundancy 4.928, completeness = 99.5%, R_{int} = 1.93%, R_{sig} = 1.61%) and 2278 (88.02%) were greater than $2\sigma(F^2)$. The final cell constants of a = 12.307(2) Å, b = 12.307(2) Å, c = 29.808(6) Å, α = 90.00(3)°, β = 90.00(3)°, γ = 90.00(3)°, volume = 4514.8(17) $Å^3$, are based upon the refinement of the XYZ-centroids of 5806 reflections above 20 σ(I) with 5.269° < 2θ < 54.49°. Data were corrected for absorption effects using the Multi-Scan method (SADABS). The ratio of minimum to maximum apparent transmission was 0.951. The calculated minimum and maximum transmission coefficients (based on crystal size) are 0.9770 and 0.9800.

The structure was solved and refined using the Bruker SHELXTL Software Package, using the space group I -4 2 d, with Z = 8 for the formula unit, $C_{32}H_{24}$. The final anisotropic full-matrix least-squares refinement on F^2 with 148 variables converged at R1 = 3.69%, for the observed data and wR2 = 9.60% for all data. The goodness-of-fit was 1.059. The largest peak in the final difference electron density synthesis was 0.129 $e^-/Å^3$ and the largest hole was -0.141 $e^-/Å^3$ with an RMS deviation of 0.030 $e^-/Å^3$. On the basis of the final model, the calculated density was 1.202 g/cm^3 and F(000), 1728 e^-.

Xray data were deposited at CCD with code CCDC-2055991

Table 1. Sample and crystal data for 1-anti.

Identification code	1-anti	
Chemical formula	$C_{32}H_{24}$	
Formula weight	408.51 g/mol	
Temperature	296(2) K	
Wavelength	0.71073 Å	
Crystal size	0.300 x 0.300 x 0.350 mm	
Crystal system	Tetragonal	
Space group	I -4 2 d	
Unit cell dimensions	a = 12.307(2) Å	α = 90.00(3)°
	b = 12.307(2) Å	β = 90.00(3)°
	c = 29.808(6) Å	γ = 90.00(3)°
Volume	4514.8(17) $Å^3$	
Z	8	
Density (calculated)	1.202 g/cm^3	
Absorption coefficient	0.068 mm^{-1}	
F(000)	1728	

Table 2. Data collection and structure refinement for 1-anti.

Theta range for data collection	1.79 to 27.50°
Index ranges	-10<=h<=15, -15<=k<=15, -38<=l<=38
Reflections collected	12753
Independent reflections	2588 [R(int) = 0.0193]
Coverage of independent reflections	99.5%
Absorption correction	Multi-Scan
Max. and min. transmission	0.9800 and 0.9770
Structure solution technique	direct methods
Structure solution program	XT, VERSION 2014/5
Refinement method	Full-matrix least-squares on F^2
Refinement program	SHELXL-2014/7 (Sheldrick, 2014)
Function minimized	$\Sigma\, w(F_o^2 - F_c^2)^2$
Data / restraints / parameters	2588 / 0 / 148
Goodness-of-fit on F^2	1.059
Final R indices	2278 data; I>2σ(I) R1 = 0.0369, wR2 = 0.0910
	all data R1 = 0.0433, wR2 = 0.0960
Weighting scheme	$w=1/[\sigma^2(F_o^2)+(0.0468P)^2+0.8081P]$ where $P=(F_o^2+2F_c^2)/3$
Absolute structure parameter	3.4(10)
Extinction coefficient	0.0024(3)
Largest diff. peak and hole	0.129 and -0.141 $eÅ^{-3}$
R.M.S. deviation from mean	0.030 $eÅ^{-3}$

Table 3. Atomic coordinates and equivalent isotropic atomic displacement parameters ($Å^2$) for 1-anti.

U(eq) is defined as one third of the trace of the orthogonalized U_{ij} tensor.

	x/a	y/b	z/c	U(eq)
C6	0.25	0.44272(19)	0.375	0.0393(5)
C1	0.21694(14)	0.49615(15)	0.33414(6)	0.0428(4)
C7	0.21018(15)	0.61692(15)	0.32811(5)	0.0445(4)
C5	0.25	0.3266(2)	0.375	0.0482(6)
C15	0.40871(17)	0.63178(18)	0.31547(7)	0.0583(5)
C2	0.18628(17)	0.43522(17)	0.29775(7)	0.0548(5)
C16	0.30469(16)	0.68002(15)	0.31938(6)	0.0478(4)
C8	0.11086(18)	0.66712(16)	0.32786(6)	0.0544(5)
C4	0.21751(18)	0.26948(16)	0.33604(8)	0.0606(5)
C11	0.29512(18)	0.79523(16)	0.31444(7)	0.0556(5)
C3	0.18643(19)	0.32161(18)	0.29836(8)	0.0627(6)
C10	0.1911(2)	0.84452(17)	0.31687(8)	0.0654(6)
C9	0.1019(2)	0.78005(19)	0.32251(7)	0.0648(6)
C12	0.3928(3)	0.8545(2)	0.30710(9)	0.0801(8)
C14	0.4992(2)	0.6929(2)	0.30818(9)	0.0773(7)
C13	0.4906(3)	0.8049(3)	0.30428(10)	0.0884(8)
C17	0.1776(3)	0.9668(2)	0.31419(12)	0.1010(10)

Table 4. Bond lengths (Å) for 1-anti.

C6-C5	1.430(3)	C6-C1	1.443(2)
C6-C1	1.443(2)	C1-C2	1.372(3)
C1-C7	1.499(3)	C7-C8	1.370(3)
C7-C16	1.423(3)	C5-C4	1.415(3)
C5-C4	1.415(3)	C15-C14	1.362(3)
C15-C16	1.416(3)	C15-H15	0.93
C2-C3	1.398(3)	C2-H2	0.93
C16-C11	1.430(3)	C8-C9	1.403(3)
C8-H8	0.93	C4-C3	1.349(3)
C4-H4	0.93	C11-C10	1.419(3)
C11-C12	1.424(4)	C3-H3	0.93
C10-C9	1.365(4)	C10-C17	1.516(3)
C9-H9	0.93	C12-C13	1.352(4)
C12-H12	0.93	C14-C13	1.387(4)
C14-H14	0.93	C13-H13	0.93
C17-H17A	0.96	C17-H17B	0.96
C17-H17C	0.96		

Table 5. Bond angles (°) for 1-anti.

C5-C6-C1	117.12(11)	C5-C6-C1	117.12(11)
C1-C6-C1	125.8(2)	C2-C1-C6	119.74(17)
C2-C1-C7	115.57(16)	C6-C1-C7	124.67(15)
C8-C7-C16	118.84(17)	C8-C7-C1	119.82(17)
C16-C7-C1	121.18(17)	C4-C5-C4	120.5(3)

C4-C5-C6	119.77(13)	C4-C5-C6	119.77(13)
C14-C15-C16	121.4(2)	C14-C15-H15	119.3
C16-C15-H15	119.3	C1-C2-C3	122.4(2)
C1-C2-H2	118.8	C3-C2-H2	118.8
C15-C16-C7	121.69(17)	C15-C16-C11	118.79(19)
C7-C16-C11	119.52(18)	C7-C8-C9	121.2(2)
C7-C8-H8	119.4	C9-C8-H8	119.4
C3-C4-C5	121.83(18)	C3-C4-H4	119.1
C5-C4-H4	119.1	C10-C11-C12	123.4(2)
C10-C11-C16	119.53(19)	C12-C11-C16	117.0(2)
C4-C3-C2	119.13(19)	C4-C3-H3	120.4
C2-C3-H3	120.4	C9-C10-C11	118.93(18)
C9-C10-C17	119.7(3)	C11-C10-C17	121.4(3)
C10-C9-C8	121.8(2)	C10-C9-H9	119.1
C8-C9-H9	119.1	C13-C12-C11	122.0(2)
C13-C12-H12	119.0	C11-C12-H12	119.0
C15-C14-C13	120.0(3)	C15-C14-H14	120.0
C13-C14-H14	120.0	C12-C13-C14	120.8(2)
C12-C13-H13	119.6	C14-C13-H13	119.6
C10-C17-H17A	109.5	C10-C17-H17B	109.5
H17A-C17-H17B	109.5	C10-C17-H17C	109.5
H17A-C17-H17C	109.5	H17B-C17-H17C	109.5

Table 6. Torsion angles (°) for 1-anti.

C5-C6-C1-C2	0.7(2)	C1-C6-C1-C2	-179.3(2)
C5-C6-C1-C7	178.99(13)	C1-C6-C1-C7	-1.02(13)
C2-C1-C7-C8	73.8(2)	C6-C1-C7-C8	-104.53(19)
C2-C1-C7-C16	-101.6(2)	C6-C1-C7-C16	80.0(2)
C1-C6-C5-C4	-0.52(13)	C1-C6-C5-C4	179.48(13)
C1-C6-C5-C4	179.48(13)	C1-C6-C5-C4	-0.52(13)
C6-C1-C2-C3	-0.5(3)	C7-C1-C2-C3	-179.0(2)
C14-C15-C16-C7	-178.4(2)	C14-C15-C16-C11	1.5(3)
C8-C7-C16-C15	-174.70(17)	C1-C7-C16-C15	0.8(3)
C8-C7-C16-C11	5.4(2)	C1-C7-C16-C11	-179.15(15)
C16-C7-C8-C9	-4.8(3)	C1-C7-C8-C9	179.67(17)
C4-C5-C4-C3	-179.8(2)	C6-C5-C4-C3	0.2(2)
C15-C16-C11-C10	178.06(18)	C7-C16-C11-C10	-2.0(3)
C15-C16-C11-C12	-1.8(3)	C7-C16-C11-C12	178.14(19)
C5-C4-C3-C2	0.0(3)	C1-C2-C3-C4	0.2(4)
C12-C11-C10-C9	177.8(2)	C16-C11-C10-C9	-2.0(3)
C12-C11-C10-C17	-3.3(3)	C16-C11-C10-C17	176.8(2)
C11-C10-C9-C8	2.8(3)	C17-C10-C9-C8	-176.1(2)
C7-C8-C9-C10	0.7(3)	C10-C11-C12-C13	-179.0(3)
C16-C11-C12-C13	0.9(4)	C16-C15-C14-C13	-0.2(4)
C11-C12-C13-C14	0.4(5)	C15-C14-C13-C12	-0.8(5)

Table 7. Anisotropic atomic displacement parameters (Å^2) for 1-anti.

The anisotropic atomic displacement factor exponent takes the form: $-2\pi^2[h^2 a^{*2} U_{11} + ... + 2 h k a^* b^* U_{12}]$

	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
C6	0.0390(12)	0.0359(11)	0.0430(12)	0	0.0019(9)	0
C1	0.0446(9)	0.0424(9)	0.0414(8)	-0.0018(7)	-0.0012(7)	-0.0017(7)
C7	0.0539(10)	0.0442(9)	0.0354(8)	0.0020(7)	-0.0084(7)	0.0014(8)
C5	0.0487(15)	0.0371(13)	0.0590(16)	0	0.0051(12)	0
C15	0.0570(12)	0.0572(12)	0.0607(11)	0.0090(10)	0.0020(9)	-0.0014(9)
C2	0.0624(12)	0.0572(11)	0.0449(9)	-0.0047(9)	-0.0069(9)	-0.0038(10)
C16	0.0580(11)	0.0469(10)	0.0384(9)	0.0051(7)	-0.0066(8)	-0.0015(8)
C8	0.0515(11)	0.0609(12)	0.0507(10)	-0.0007(8)	-0.0098(9)	0.0049(9)
C4	0.0643(13)	0.0386(10)	0.0788(14)	-0.0123(9)	0.0049(11)	-0.0051(9)
C11	0.0741(14)	0.0455(10)	0.0472(10)	0.0068(8)	-0.0069(9)	-0.0038(9)
C3	0.0683(14)	0.0603(13)	0.0595(12)	-0.0222(10)	-0.0041(11)	-0.0079(10)
C10	0.0905(17)	0.0471(11)	0.0586(12)	0.0052(9)	-0.0122(12)	0.0116(11)
C9	0.0700(15)	0.0611(13)	0.0634(13)	0.0003(10)	-0.0150(11)	0.0179(11)
C12	0.101(2)	0.0564(13)	0.0824(16)	0.0152(12)	0.0000(16)	-0.0192(14)
C14	0.0598(13)	0.0830(17)	0.0891(16)	0.0143(14)	0.0080(13)	-0.0104(12)
C13	0.0798(18)	0.0853(19)	0.100(2)	0.0191(16)	0.0052(16)	-0.0274(15)
C17	0.142(3)	0.0508(14)	0.110(2)	0.0083(14)	-0.007(2)	0.0224(15)

Table 8. Hydrogen atomic coordinates and isotropic atomic displacement parameters (Å^2) for 1-anti.

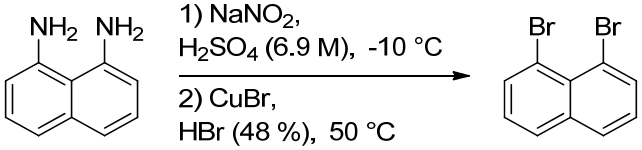
	x/a	y/b	z/c	U(eq)
H15	0.4154	0.5567	0.3179	0.07
H2	0.1646	0.4708	0.2717	0.066
H8	0.0483	0.6256	0.3313	0.065
H4	0.2176	0.1939	0.3364	0.073
H3	0.1654	0.2825	0.2731	0.075
H9	0.0333	0.8118	0.3228	0.078
H12	0.3893	0.9297	0.3042	0.096
H14	0.5668	0.6596	0.3058	0.093
H13	0.5528	0.8463	0.2997	0.106
H17A	0.1017	0.9847	0.3147	0.151
H17B	0.2094	0.9930	0.2868	0.151
H17C	0.2132	1.0001	0.3393	0.151

General Methods.

Chemicals were purchased by Sigma Aldrich and Alfa Aesar and used without further purification. 5,6,7,8-tetrafluoronaphthalen-1-ol was prepared according to known procedure. [6] Diethyl ether and THF have been dried by distillation on Na/benzophenone. Chromatography employed the following stationary phases: Silica gel 60 F254 for the TLC and silica gel 60 Å (230-400 mesh) for pre-purification. All the reactions were performed in dried glassware and under dry nitrogen atmosphere. Glassware was dried at +70 °C for at least 3 hours immediately before use. Semi-preparative HPLC purification was achieved using a Waters 600 pump with a Waters 2487 UV detector. Detection wavelength was 254 nm. Phenomenex Luna C8 (5 µm, 100 Å, 250×10.0 mm) semi-preparative column was used to purify the compounds using mixtures of CH_3CN and H_2O as eluent.

NMR spectra were recorded using a spectrometer operating at a field of 14.4 Tesla (600 MHz for ^{1}H, 150.8 for ^{13}C). Chemical shifts are given in ppm relative to the internal standards tetramethylsilane (^{1}H and ^{13}C) or relative to the residual peak of the solvents. 19F spectra were recorded on a 9.6 T spectrometer (376 MHz for ^{19}F), and chemical shifts are relative to the external standard $CFCl_3$. The standard 150.8 MHz ^{13}C spectra were acquired under proton decoupling conditions with a 38000 Hz spectral width, 4.2 µs (60° tip angle) pulse width, 1 s acquisition time and 1 s delay time. A line broadening function of 1–2 Hz was applied before the Fourier transformation. The $\{^{19}F\}$-^{13}C spectra were acquired at 150.8 MHz by broadband ^{19}F decoupling (50 ppm) obtained using a WURST40 modulated decoupling sequence, centred at -150 ppm in the ^{19}F spectrum.

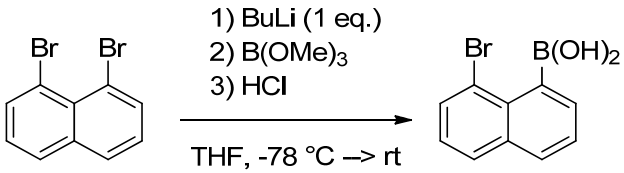
Intermediates



1,8-dibromonaphthalene[7]: In an oven-dried 500 mL three-necked round bottom flask equipped with a mechanical stirrer and a dropping funnel, 6.32 g (40 mmol, 1 eq.) of 1,8-diaminonaphthalene were suspended in 100 mL of 6.9 M aqueous H_2SO_4. The reaction mixture was cooled at -15 °C in an ice/NaCl bath and a solution of 8.29 g of $NaNO_2$ (120 mmol, 3 eq.) in 15 mL of water was added drop-wise. The dark red solution was stirred at -15 °C for 15 minutes, then 14.4 g of CuBr (120 mmol, 3 eq.) dissolved in 20 mL of 48% aqueous HBr were added in one portion and the dark solution was

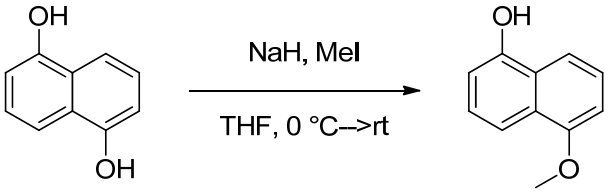
[6] Gribble G. W.; LeHoullier C. S.; Sibi M. P.; Allen R. W. *J. Org. Chem.* **1985**, *50*, 1611-1616.
[7] Seyferth D.; Vick S C. *J. Organomet. Chem.* **1977**, *141*, 173-187.

warmed at 60 °C for 2 hours. After the addition of CuBr, a great deal of gas evolution was observed with large production of foam which was controlled by the addition of a small portion of Et_2O. The black solution was then cooled at room temperature and filtered. The solid residue was filtered and washed with water (20-30 mL) and then extracted with ethyl acetate (5 x 20 mL). The organic phase was washed with brine, dried over Na_2SO_4 and the solvent was removed under reduced pressure. The residue was purified with silica-gel flash chromatography eluting with petrol ether, to afford the desired product as a white solid in 24% yield. ^{1}H-NMR agreed with literature data[8]: ***^{1}H-NMR*** (600 MHz, $CDCl_3$): δ 7.28 (t, J = 7.8 Hz, 2H), 7.84 (dd, J_1 = 7.8 Hz, J_2 = 1.2 Hz, 2H), 7.96 (dd, J_1 = 7.8 Hz, J_2 = 1.2 Hz, 2H). ***GC-MS*** (m/z): 288 (10), 286 (20), 284 (15) $[M]^+$, 205 (20) $[M\text{-}Br]^+$, 126 $[M\text{-}2Br]^+$.



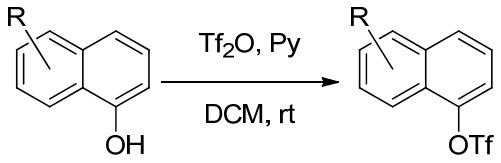
(8-bromonaphthalen-1-yl)boronic acid: In an oven-dried three-necked round bottom flask equipped with a thermometer and a dropping funnel 500 mg (1.75 mmol, 1 eq.) of 1,8-dibromonaphthalene were dissolved in 8 mL of anhydrous THF and the solution was cooled at -78 °C. 1.1 mL of BuLi (1.6 M solution in hexane, 1.75 mmol, 1 eq.) were added drop-wise and the reaction mixture was stirred at -78 °C for one hour and then trimethyl borate (390 µl, 3.5 mmol, 2 eq.) was added. The solution was stirred at -78 °C for one hour and then warmed at room temperature. After three hours the reaction was quenched with 1 M HCl (5 mL) and stirred overnight at room temperature. The solution was diluted with water and extracted with ethyl acetate (3 x 10 mL). The combined organic layers were dried over Na_2SO_4 and the volatiles were removed under reduced pressure. The solid was washed with petroleum ether (4 x 3 mL) affording the desired product as a white-grey solid in 81% yield. ***^{1}H-NMR*** (600 MHz, $CDCl_3$): δ 4.59 (s, 2H), 7.36 (t, J = 7.8 Hz, 1H), 7.52 (dd, J_1 = 8.4 Hz, J_2 = 7.2 Hz, 1H), 7.70 (d, J = 7.2 Hz, 1H), 7.83 (dd, J_1 = 7.8 Hz, J_2 = 1.2 Hz, 1H), 7.85 (d, J = 7.8 Hz, 1H), 7.88 (dd, J_1 = 8.4 Hz, J_2 = 1.2 Hz, 1H). ***^{13}C-NMR*** (150 MHz, DMSO-d_6): δ 123.1 (Cq), 125.9 (CH), 126.1 (CH), 128.3 (CH), 128.7 (CH), 130.4 (CH), 131.4 (CH), 133.0 (Cq), 134.7 (Cq). *Ipso*-carbon bound to boron was not detected under the acquisition conditions.[9]

[8] Vyskočil S.; Meca L.; Tišlerová I.; Císarŏvá I.; Polášek M.; Harutyunyan S. R.; Belokon Y. N.; Stead R. M. J.; Farrugia L.; Lockhart S. C.; Mitchell W. L.; Kocoeovsky P. *Chem. Eur. J.* **2002**, *8*, 4633-4648.
[9] Bruns S.; Sinnwell V.; Voss J. *Magn. Reson. Chem.* **2003**, *41*, 269-272.



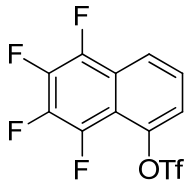
In an oven dried two-necked round bottom flask 1.0 g of 1,5-dihydroxynaphthalene (6.25 mmol, 1 eq.) was dissolved in 20 mL of anhydrous THF and the solution was cooled at 0 °C. 250 mg of NaH (60% in paraffin, 6.25 mmol, 1 eq.) were added portion-wise. After gas evolution stopped MeI (780 µl, 12.5 mmol, 2 eq.) was added and the reaction solution was stirred overnight at room temperature. The reaction was then quenched at 0°C with 1M HCl aqueous solution (15 mL) and the THF was removed under reduced pressure. The aqueous layer was extracted with ethyl acetate (3 x 20 mL) and the combined organic layers were dried over Na_2SO_4. The solvent was removed under vacuum and the crude product was purified with silica-gel flash chromatography (petroleum ether/AcOEt 95/5→90/10) to afford the desired product in 32% yield.[10]

General procedure for the synthesis of triflates.

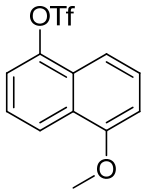


In an oven-dried two-necked round bottom flask the naphthol (2.5 mmol, 1 eq.) was dissolved in 15 mL of DCM and 403 µl of pyridine (5.0 mmol, 2 eq.) were added. The solution was cooled at 0 °C and 504 µl of Tf_2O (3.0 mmol, 1.2 eq.) were added. The reaction mixture was stirred at room temperature until complete consumption of the staring material (TLC, 2-4 hours) and then 10 mL of 1 M HCl was added at 0 °C. The aqueous phase was extracted with DCM (3 x 15 mL), the combined organic layers were washed with $NaHCO_3$ saturated solution and brine and then dried over Na_2SO_4. The solvent was removed under reduced pressure and the crude product was purified with silica-gel flash chromatography initially eluting with petrol ether and then with 90/10 mixture of petroleum ether/Et_2O. The desired product was isolated as a white solid.

[10] Ballantine M.; Menard M. L.; Tam W. *J. Org. Chem.* **2009**, *74*, 7570-7573.

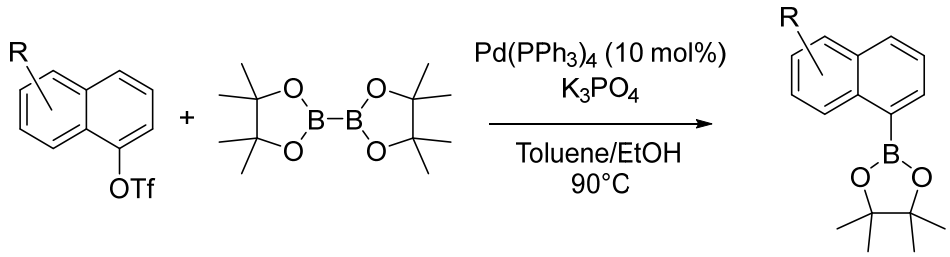


68 % yield white solid. ***^{1}H-NMR*** (400 MHz, $CDCl_3$): δ 7.57 (d, *J* = 8.0 Hz, 1H), 7.64 (t, *J* = 8.0 Hz, 1H), 8.13 (d, *J* = 8.0 Hz, 1H). ***^{13}C-NMR*** (150 MHz, $CDCl_3$)[11]: δ 113.4 (Cq), 118.7 (q, *J* = 320 Hz, CF_3), 120.6 (CH), 121.7 (CH), 121.8 (Cq), 126.9 (CH), 138.6 (CF), 139.7 (CF), 141.3 (CF), 142.0 (CF), 142.9 Cq). ***^{19}F-NMR*** (564 MHz, $CDCl_3$): δ -155.0 (t, J_1 = 19 Hz, 1F), -154.1 (t, J_1 = 19 Hz, 1F), -146.9 (t, *J* = 19 Hz, 1F), -144.4/-144.3 (m, 1F), -72.9 (d, *J* = 7 Hz, 3F). ***GC-MS*** (m/z): 348 (5) $[M]^+$, 215 (50) $[M\text{-}SO_2CF_3]^+$, 187 (100).



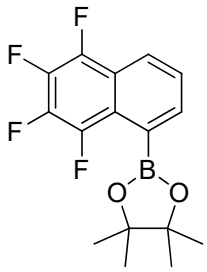
52 % yield, white solid. ***^{1}H-NMR*** (600 MHz, $CDCl_3$): δ 4.00 (s, 3H), 6.90 (d, *J* = 7.8 Hz, 1H), 7.45 (t, *J* = 7.8 Hz, 1H), 7.51 (dd, J_1 = 7.8 Hz, J_2 = 1.2 Hz, 1H), 7.55 (t, *J* = 7.8 Hz, 1H), 7.70 (d, *J* = 8.4 Hz, 1H), 8.33 (dd, J_1 = 8.4 Hz, J_2 = 1.2 Hz, 1H). ***^{13}C-NMR*** (150 MHz, $CDCl_3$): δ 55.5 (CH_3), 105.1 (CH), 112.6 (CH), 118.3 (CH), 118.8 (q, *J* = 321 Hz, CF_3), 122.8 (CH), 124.1 (CH), 127.2 (Cq), 127.4 (Cq), 128.1 (CH), 145.5 (Cq), 155.5 (Cq). ***GC-MS*** (m/z): 306 (70) $[M]^+$, 173 (100) $[M\text{-}SO_2CF_3]^+$, 145 (10), 115 (35).

General procedure for the synthesis of boronic ester from triflates

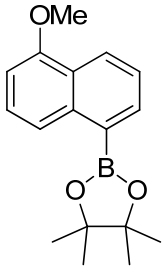


In a Schlenk tube the proper triflate (0.20 mmol, 1 eq.), bis(pinacolato)diboron (61 mg, 0.24 mmol, 1.2 eq.) and K_3PO_4 (85 mg, 0.40 mmol, 2 eq.) were suspended in 1.3 mL of toluene and 0.2 mL of ethanol. The solution was degased by nitrogen bubbling for 5-10 minutes and then $(Ph_3P)_4Pd$ (9 mg, 0.01 mmol, 0.05 eq.) was added. The reaction mixture was stirred overnight at 90 °C and then diluted with water (5 mL). The aqueous phase was extracted with ethyl acetate (3 x 5 mL) and the combined organic layers were washed brine, dried over Na_2SO_4 and concentrated under reduced pressure. The crude product was filtered throw a pad silica gel eluting with petroleum ether/ethyl acetate mixture affording a mixture of products that was employed in the Suzuki coupling without further purification.

[11] ^{13}C-NMR resonance frequencies were determined by examination of {^{1}H} decoupled spectra and {^{19}F} decoupled spectra.

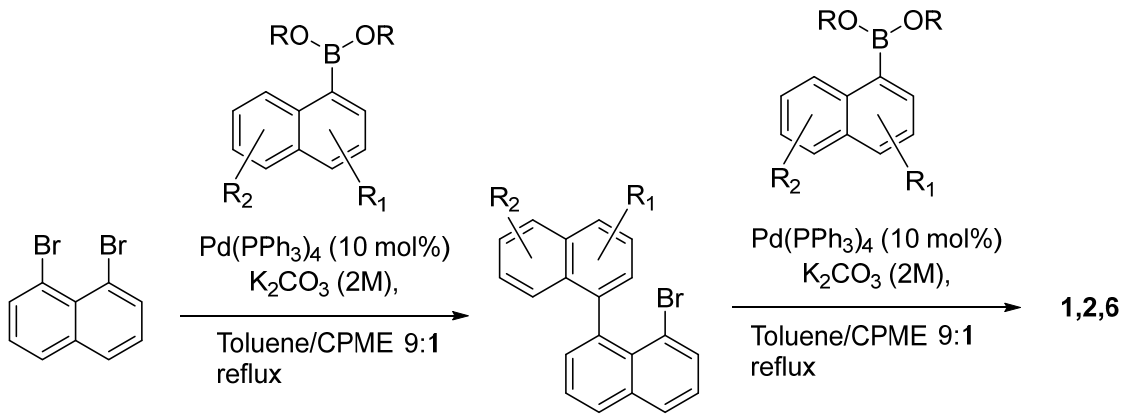


Yield ≈ 30%. ***¹H-NMR*** (600 MHz, $CDCl_3$): δ 1.45 (s, 12H), 7.58 (t, *J* = 7.8 Hz, 1H), 7.74 (d, *J* = 7.8 Hz, 1H), 8.08 (d, *J* = 7.8 Hz, 1H).



Yield ≈ 45%. ***¹H-NMR*** (600 MHz, $CDCl_3$): δ 1.44 (s, 12H), 4.02 (s, 3H), 6.97 (d, *J* = 8.4 Hz, 1H), 7.21 (t, *J* = 8.4 Hz, 1H), 7.45 (d, *J* = 8.4 Hz, 1H), 7.51 (dd, J_1 = 7.2 Hz, J_2 = 1.2 Hz, 1H), 7.60 (dd, J_1 = 8.4 Hz, J_1 = 7.2 Hz, 1H), 8.42 (d, *J* = 8.4 Hz, 1H).

General procedure for the synthesis of compounds 1, 2, 6.

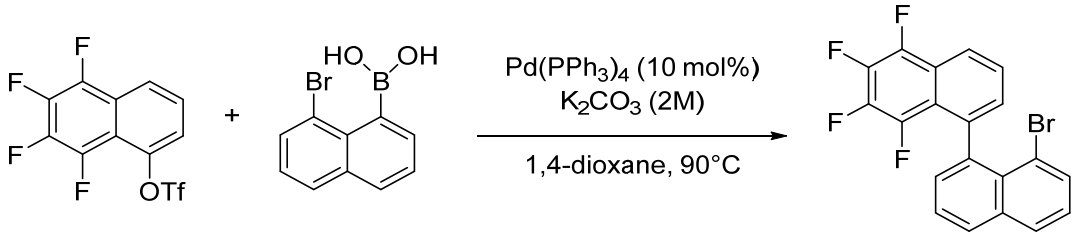


In an oven-dried two-necked round bottom flask equipped with a condenser, 1,8-dibromonaphthalene (200 mg, 0.70 mmol, 1.0 eq.) and the appropriate boronic acid or ester (1.4 mmol, 2.0 eq.) were dissolved in 5 mL of a mixture of toluene and ciclopenthylmethylether (CPME) and 0.8 mL of 2 M K_2CO_3 aqueous solution (1.6 mmol, 2.5 eq.) were added. The reaction mixture was degased by vacuum and nitrogen bubbling for 5-10 minutes and then $(Ph_3P)_4Pd$ (62 mg, 0.07 mmol, 0.1 eq.) was added. The reaction mixture was stirred at reflux for 3-4 hours, and then diluted with water (5 mL). The aqueous phase was extracted with ethyl acetate (3 x 10 mL) and the combined organic layers were dried over Na_2SO_4 and passed through a short silica-gel plug. After evaporation, the crude was again treated with a second amount of the same boronic acid or ester (1.4 mmol, 2.0 eq.) following the same procedure of the first step. After pre-purification of the crude by chromatography on silica-

gel, the pure syn and anti isomers of **1**,**2**,**6** were obtained by semi-preparative HPLC on reverse-phase C8 or C18 columns (40-60% of yields).

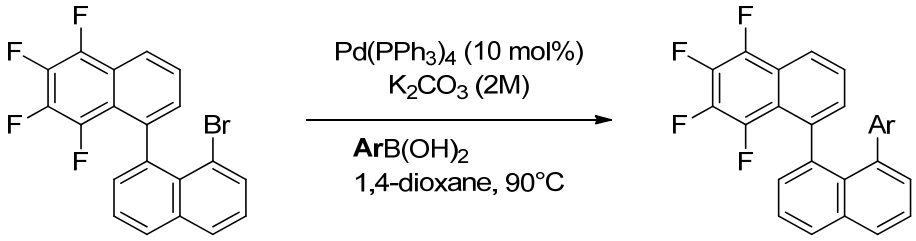
General procedure for the synthesis of compounds 3-5.

Step-1



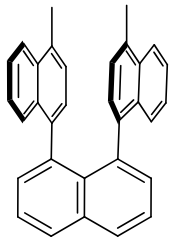
In an oven-dried two-necked round bottom flask equipped with a condenser, triflate **5** (252 mg, 0.724 mmol, 1 eq.) and (8-bromonaphthalen-1-yl)boronic acid (200 mg, 0.797 mmol, 1.1 eq.) were dissolved in 4 mL of 1,4-dioxane and 1.1 mL of 2M K_2CO_3 aqueous solution (2.2 mmol, 3 eq.) was added. The reaction mixture was degased by nitrogen bubbling for 5-10 minutes and then $(Ph_3P)_4Pd$ (32 mg, 0.036 mmol, 0.1 eq.) was added. The reaction mixture was stirred 3 hours at 90 °C and then diluted with water (10 mL). The aqueous phase was extracted with ethyl acetate (3 x 10 mL) and the combined organic layers were dried over Na_2SO_4 and concentrated under reduced pressure. The crude product was purified with silica-gel flash chromatography eluting with petroleoum ether, affording the desired product in 75% yield as a withe solid. ***^{1}H-NMR*** (400 MHz, $CDCl_3$): δ 7.31 (dd, J_1 = 8.0 Hz, J_2 = 7.6 Hz, 1H), 7.37-7.40 (m, 2H), 7.52 (dd, J_1 = 8.4 Hz, J_2 = 7.2 Hz, 1H), 7.59 (dd, J_1 = 8.4 Hz, J_2 = 7.2 Hz, 1H), 7.73 (dd, J_1 = 7.2 Hz, J_2 = 1.6 Hz, 1H), 7.93 (dd, J_1 = 8.4 Hz, J_2 = 1.6 Hz, 1H), 7.96 (dd, J_1 = 8.4 Hz, J_2 = 1.6 Hz, 1H), 8.12 (dm, J = 8.4 Hz, 1H). ***^{13}C-NMR*** (150 MHz, $CDCl_3$): δ 119.2 (m, CH), 119.7 (Cq), 119.9 (d, J = 13 Hz, Cq), 120.6 (d, J = 10 Hz, Cq), 125.0 (CH), 126.2 (CH), 126.3 (d, J = 2, CH), 129.2 (CH), 129.6 (CH), 130.0 (d, J = 4 Hz, Cq), 130.4 (d, J = 4 Hz, CH), 130.6 (CH), 133.6 (CH), 135.7 (Cq), 137.3 (Cq), 137.5 (dm, J = 253 Hz, CF), 138.5 (d, J = 3 Hz, Cq), 138.8 (dm, J = 253 Hz, CF), 141.9 (dm, J = 253 Hz, CF), 143.6 (dm, J = 253 Hz, CF). ***^{19}F-NMR*** (376 MHz, $CDCl_3$): δ -159.2/-159.0 (m, 2F), -150.1/-149.9 (m, 1F), -140.1/-140.0 (m, 1F). ***GC-MS*** (*m/z*): 406 (5), 404 (5) $[M]^+$, 325 (100) $[M\text{-}Br]^+$, 324 (45), 306 (40) $[M\text{-}Br\text{-}F]^+$, 275 (45), 153 (25), 138 (35).

Step-2

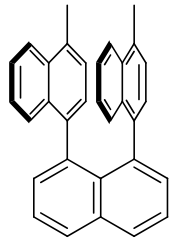


In a Schlenk tube the appropriate aryl bromide (0.1 mmol, 1.0 eq.), the proper aryl boronic acid or ester (0.15 mmol, 1.5 eq.) were dissolved in 1 mL of 1,4-dioxane and a 2M aqueous solution of K_2CO_3 was added (0.3 mmol, 3.0 eq.). The solution was degassed by nitrogen bubbling for 5-10 minutes and then $(Ph_3P)_4Pd$ (0.01 mmol, 0.1 eq.) was added. The reaction mixture was stirred at 90 °C until complete consumption of the starting material (2-8 hours, TLC) and then diluted with water (5 mL). The aqueous phase was extracted with ethyl acetate (3 x 5 mL) and the combined organic layers were washed with brine, dried over Na_2SO_4 and concentrated under reduced pressure. The crude product was purified with silica-gel chromatography eluting with petroleoum ether, affording the product as a mixture of anti:syn in overall 32-52 % yield which were separated with semi-preparative HPLC.

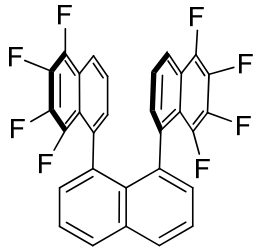
Spectroscopic data for compounds 1-6



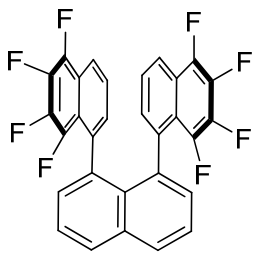
1-*anti***:** White solid. ***HPLC:*** Phenomenex Luna C8 (5 µm, 100 Å, 250×10.0 mm), MeCN/H_2O 95/5, 5 ml/min, λ = 254 nm. t_R = 10.6 min. Crystals of pure *anti* isomer were obtained by slow evaporation in MeCN. *anti* conformation was also confirmed by chiral HPLC analysis of the product which confirmed the presence of a racemic mixture of the two enantiomers (Chiralcel OG, 0.46 cm Ø x 25 cm, *n*-Hex/*i*-PrOH 99/1, flow = 0.5 ml/min, λ = 254 nm. t_R = 9.133 min, 10.415 min). ***^{1}H-NMR*** (600 MHz, $CDCl_3$): δ 2.35 (s, 6H), 6.11 (d, J = 7.2 Hz, 2H), 6.29 (d, J = 7.2 Hz, 2H), 7.20-7.24 (m, 4H), 7.27 (dd, J_1 = 6.0 Hz, J_1 = 1.2 Hz, 2H), 7.38 (ddd, J_1 = 8.4 Hz, J_2 = 6.0 Hz, J_3 = 2.4 Hz, 2H) 7.57 (dd, J_1 = 8.4 Hz, J_1 = 7.2 Hz, 2H), 7.73 (d, J = 8.4 Hz, 2H), 8.06 (dd, J_1 = 8.4 Hz, J_1 = 1.2 Hz, 2H). ***^{13}C-NMR*** (150 MHz, $CDCl_3$): δ 19.1 ($2CH_3$), 123.5 (2CH), 123.9 (2CH), 124.7 (2CH), 124.8 (2CH), 125.1 (2CH), 126.6 (2CH), 127.1 (2CH), 128.8 (2CH), 130.6 (2CH), 131.4 (2Cq), 132.0 (2Cq), 132.5 (Cq), 132.6 (2Cq), 134.8 (Cq), 137.6 (2Cq), 139.0 (2Cq). Elem. Anal. Calcd for $C_{32}H_{24}$: C, 94.08; H, 5.92%. Found C, 94.58; H, 6.01.



1-*syn***:** White solid. ***HPLC:*** Phenomenex Luna C8 (5 µm, 100 Å, 250×10.0 mm), MeCN/H_2O 95/5, 5 ml/min, λ = 254 nm. t_R = 10.6 min. ***^{1}H-NMR*** (600 MHz, $CDCl_3$): δ 2.47 (s, 6H), 6.65 (ddd, J_1 = 8.4 Hz, J_2 = 6.6 Hz, J_3 = 1.2 Hz, 2H), 6.76 (d, J = 7.2 Hz, 2H), 6.82 (d, J = 7.2 Hz, 2H), 6.85 (d, J = 8.4 Hz, 2H), 7.01 (ddd, J_1 = 8.4 Hz, J_2 = 6.6 Hz, J_3 = 1.2 Hz, 2H), 7.31 (dd, J_1 = 7.2 Hz, J_2 = 1.2 Hz, 2H), 7.44 (d, J = 8.4 Hz, 2H), 7.57 (dd, J_1 = 8.4 Hz, J_2 = 7.2 Hz, 2H), 8.07 (dd, J_1 = 8.4 Hz, J_2 = 1.2 Hz, 2H). ***^{13}C-NMR*** (150 MHz, $CDCl_3$): δ 19.2 ($2CH_3$), 123.0 (2CH), 124.2 (2CH), 124.4 (2CH), 124.8 (2CH), 125.0 (2CH), 127.1 (2CH), 127.8 (2CH), 128.8 (2CH), 130.8 (2CH), 131.1 (2Cq), 131.6 (2Cq), 132.2 (2Cq), 133.0 (Cq), 135.0 (Cq), 138.4 (2Cq), 138.9 (2Cq). Elem. Anal. Calcd for $C_{32}H_{24}$: C, 94.08; H, 5.92%. Found C, 94.37; H, 6.12.

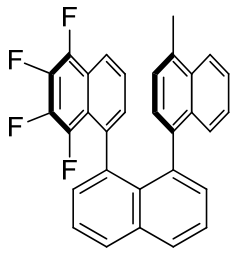


2-*anti***:** White solid. ***HPLC:*** Phenomenex Luna C8 (5 µm, 100 Å, 250×10.0 mm), MeCN/H_2O 90/10, 5 ml/min, λ = 254 nm. t_R = 15.5 min. *Anti* conformation was confirmed by chiral HPLC analysis of the product which confirmed the presence of a racemic mixture of the two enantiomers (LUX CELLULOSE-2, 0.46 cm Ø x 25 cm, *n*-Hex/*i*-PrOH 99/1, flow = 0.5 ml/min, λ = 254 nm. t_R = 8.59 min, 9.76 min). ***^{1}H-NMR*** (600 MHz, $CDCl_3$): δ 6.74 (dd, J_1 = 8.4 Hz, J_2 = 7.2 Hz, 2H), 6.98 (d, J = 6.6 Hz, 2H), 7.21 (dd, J_1 = 7.2 Hz, J_2 = 1.2 Hz, 2H), 7.38 (d, J = 7.8 Hz, 2H), 7.54 (dd, J_1 = 7.8 Hz, J_2 = 6.6 Hz, 2H), 8.05 (dd, J_1 = 8.4 Hz, J_2 = 1.2 Hz, 2H). ***^{13}C-NMR*** (150 MHz, $CDCl_3$): δ 117.8-117.9 (m, 2CH), 118.8 (2Cq), 118.9 (2Cq), 124.6 (2CH), 124.7 (2CH), 129.2 (d, J = 3 Hz, 2CH), 129.3 (2CH), 129.9 (2CH), 131.4 (t, J = 3 Hz, Cq), 134.1 (Cq), 136.6 (d, J = 4 Hz, 2Cq), 137.2 (dm, J = 253 Hz, 2CF), 138.4 (d, J = 3 Hz, 2Cq), 138.8 (dm, J = 253 Hz, 2CF), 141.7 (dm, J = 253 Hz, 2CF), 143.4 (dm, J = 253 Hz, 2CF). ***^{19}F-NMR*** (376 MHz, $CDCl_3$): δ -159.8/-159.6 (m, 2F), -150.1/-150.0 (m, 1F), -139.1/-138.0 (m, 1F). Elem. Anal. Calcd for $C_{30}H_{12}F_8$: C, 68.71; H, 2.31; F,28.98. Found C, 68.85; H, 2.65.

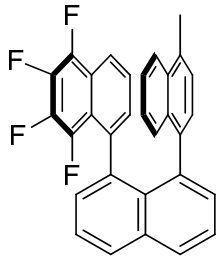


2-*syn***:** White solid. ***HPLC:*** Phenomenex Luna C8 (5 µm, 100 Å, 250×10.0 mm), MeCN/H_2O 90/10, 5 ml/min, λ = 254 nm. t_R = 13.67 min. ***^{1}H-NMR*** (600 MHz, $CDCl_3$): δ6.96 (d, J = 6.6 Hz, 2H), 7.12 (t, J = 7.8 Hz, 2H), 7.26 (dd, J_1 = 7.2 Hz, J_2 = 1.2 Hz, 2H), 7.52-7.56 (m, 4H), 8.07 (dd, J_1 = 7.8 Hz, J_2 = 1.2 Hz, 2H). ***^{13}C-NMR*** (150 MHz, $CDCl_3$): δ 118.0 (m, 2Cq), 118.3 (m, 2CH), 119.0 (d, J = 13 Hz, 2Cq), 124.6 (2CH), 125.5 (2CH), 129.4 (2CH), 129.5 (d, J = 3 Hz, 2CH), 130.8 (Cq), 131.4 (2CH), 134.4 (Cq), 136.6 (m, 2Cq), 136.9 (dm, J = 253 Hz, 2CF), 137.9 (2Cq), 139.5

(dm, J = 253 Hz, 2CF), 141.2 (dm, J = 253 Hz, 2CF), 143.1 (dm, J = 253 Hz, 2CF). ***^{19}F-NMR*** (376 MHz, $CDCl_3$): δ -162.3 (t, J_1 = 18 Hz, 1F), -160.2 (t, J_1 = 18 Hz, 1F), -151.8 (t, J_1 = 18 Hz, 1F), -139.2/-139.0 (m, 1F). Elem. Anal. Calcd for $C_{30}H_{12}F_8$: C, 68.71; H, 2.31; F,28.98. Found C, 68.98; H, 2.07.

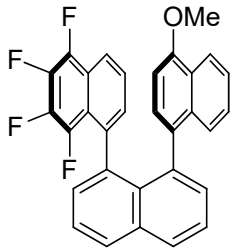


3-anti*:** White solid. HPLC Phenomenex Luna C8 (5 µm, 100 Å, 250×10.0 mm), MeCN/H_2O 90/10, 5 ml/min, λ = 254 nm. t_R = 18.2 min. *Anti* enantiomers was separated by chiral HPLC analysis (Chiralcel OG, 0.46 cm Ø x 25 cm, *n*-Hex/*i*-PrOH 99/1, flow = 0.5 ml/min, λ = 254 nm. t_R = 10.00 min, 10.37 min).^{1}H-NMR*** (600 MHz, $CDCl_3$): δ 2.35 (s, 3H), 6.36 (t, J = 7.2 Hz, 1H), 6.39 (d, J = 7.2 Hz, 1H), 6.53 (d, J = 7.2 Hz, 1H), 6.79 (dd, J_1 = 7.2 Hz, J_2 = 1.8 Hz, 1H), 7.16 (dd, J_1 = 7.2 Hz, J_2 = 1.2 Hz, 1H), 7.21 (*p*d, J_1 = 3.6 Hz, 2H), 7.27 (d, J = 7.2 Hz, 1H), 7.33-7.36 (m, 2H), 7.52 (dd, J_1 = 8.4 Hz, J_2 = 7.2 Hz, 1H), 7.59 (dd, J_1 = 8.4 Hz, J_2 = 7.2 Hz, 1H), 7.67 (d, J = 8.4 Hz, 1H), 8.05 (dd, J_1 = 8.4 Hz, J_2 = 1.2 Hz, 1H), 8.06 (dd, J_1 = 8.4 Hz, J_2 = 1.2 Hz, 1H). ***^{13}C-NMR*** (150 MHz, $CDCl_3$): δ 18.7 (CH_3), 116.5 (m, CH), 118.5 (dd, J_1 = 14.8 Hz, J_2 = 2.0 Hz, Cq), 118.7 (dd, J_1 = 7.6 Hz, J_2 = 3.6 Hz, Cq), 123.8 (CH), 124.0 (CH), 124.5 (CH), 124.6 (CH), 125.0 (CH), 125.1 (CH), 125.2 (CH), 126.7 (CH), 127.4 (CH), 129.0 (CH), 129.1 (CH), 129.3 (CH), 130.1 (CH), 130.4 (CH), 131.2 (Cq), 132.2 (Cq), 132.5 (Cq), 132.9 (Cq), 134.5 (Cq), 135.7-135.8 (m, Cq), 137.0 (dm, $J_{C\text{-}F}$ = 252 Hz, Cq), 138.1 (Cq), 138.2 (Cq), 138.5 (dm, $J_{C\text{-}F}$ = 252 Hz, Cq), 139.2 (d, J = 2.3 Hz, Cq), 141.8 (dm, $J_{C\text{-}F}$ = 252 Hz, Cq), 143.6 (dm, $J_{C\text{-}F}$ = 252 Hz, Cq). ***^{19}F-NMR*** (376 MHz, $CDCl_3$): δ -162.3(t, J = 18 Hz, 1F), -161.9 (t, J = 18 Hz, 1F), -152.7 (dd, J_1 = 18 Hz, J_2 = 16 Hz, 1F), -140.6 (t, J_1 = 16 Hz, 1F). Elem. Anal. Calcd for $C_{31}H_{18}F_4$: C, 79.82; H, 3.89; F,16.29. Found C, 80.06; H, 3.57.

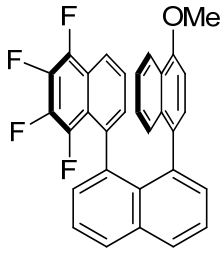


3-*syn***:** White solid. HPLC Phenomenex Luna C8 (5 µm, 100 Å, 250×10.0 mm), MeCN/H_2O 90/10, 5 ml/min, λ = 254 nm. t_R = 17.1 min. *Syn* enantiomers was separated by chiral HPLC analysis (Chiralcel OG, 0.46 cm Ø x 25 cm, *n*-Hex/*i*-PrOH 99/1, flow = 0.5 ml/min, λ = 254 nm. t_R = 11.08 min, 11.70 min). ***^{1}H-NMR*** (600 MHz, $CDCl_3$): δ 2.44 (s, 3H), 6.61 (d, J = 6.6 Hz, 1H), 6.64 (d, J = 6.6 Hz, 1H), 7.09-7.14 (m, 2H), 7.24-7.30 (m, 4H), 7.34 (dd, J_1 = 6.6 Hz, J_2 = 1.2 Hz, 1H), 7.54 (dd, J_1 = 7.8 Hz, J_2 = 7.2 Hz, 1H), 7.57-7.62 (m, 3H), 8.08 (d, J = 7.8 Hz, 2H). ***^{13}C-NMR*** (150 MHz, $CDCl_3$): δ 18.9 (CH_3), 117.6-117.7 (m, CH), 118.0 (dd, J_1 = 8 Hz, J_2 = 4 Hz, Cq), 119.0 (dd, J_1 = 13 Hz, J_2 = 2 Hz, Cq), 123.2 (CH), 124.5 (CH), 124.7 (CH), 124.8 (CH), 124.9 (CH), 125.0 (CH), 125.6 (CH), 126.6 (CH), 128.7 (CH) 129.1 (CH), 129.4 (2CH), 130.4 (CH), 130.8 (Cq), 131.2 (CH), 131.6 (Cq), 131.7 (Cq), 131.8 (Cq), 132.1 (Cq), 134.7 (Cq), 136.6 (dm, $J_{C\text{-}F}$ = 253 Hz, Cq), 136.9 (dm, $J_{C\text{-}F}$ = 253

Hz, Cq) 137.0 (Cq), 137.7 (Cq), 139.1(d, J = 3Hz, Cq), 141.0 (dm, $J_{C\text{-}F}$ = 253 Hz, Cq), 142.8 (dm, $J_{C\text{-}F}$ = 253 Hz, Cq). ***^{19}F-NMR*** (376 MHz, $CDCl_3$): δ -160.6 (t, J = 19 Hz, 1F), -158.0 (t, J = 19 Hz, 1F), -152.1 (dd, J_1 = 19 Hz, J_2 = 16 Hz, 1F), -136.9 (dd, J_1 = 19 Hz, J_2 = 16 Hz, 1F). Elem. Anal. Calcd for $C_{31}H_{18}F_4$: C, 79.82; H, 3.89; F,16.29. Found C, 80.15; H, 4.08.

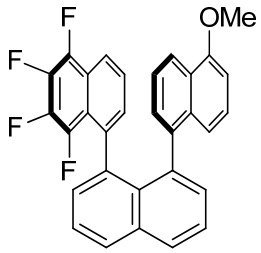


4-*anti***:** White solid. HPLC Phenomenex Luna C8 (5 µm, 100 Å, 250×10.0 mm), MeCN/H_2O 90/10, 5 ml/min, λ = 254 nm. t_R = 17.22 min. *Anti* enantiomers was separated by chiral HPLC analysis (Chiralcel OD-H, 0.46 cm Ø x 25 cm, *n*-Hex/*i*-PrOH 97/3, flow = 0.7 ml/min, λ = 254 nm. t_R = 8.06 min, 9.74 min). ***^{1}H-NMR*** (600 MHz, $CDCl_3$): δ 3.77 (s, 3H), 5.89 (d J = 7.8 Hz, 1H), 6.40 (t, J = 7.8 Hz, 1H), 6.55 (d, J = 7.8 Hz, 1H), 6.78 (d, J = 7.8 Hz, 1H), 7.11 (d, J = 7.8 Hz, 1H), 7.16 (dd, J_1 = 7.2 Hz, J_2 = 1.2 Hz, 1H), 7.22 (ddd, J_1 = 8.4 Hz, J_2 = 6.6 Hz, J_3 = 1.2 Hz, 1H), 7.29-7.34 (m, 3H), 7.52 (dd, J_1 = 8.4 Hz, J_2 = 7.2 Hz, 1H), 7.58 (dd, J_1 = 7.8 Hz, J_2 = 6.6 Hz, 1H), 7.94 (d, J = 8.4 Hz, 1H), 8.05 (dt, J_1 = 8.4 Hz, J_2 = 1.2 Hz, 2H). ***^{13}C-NMR*** (150 MHz, $CDCl_3$): δ 55.0 (CH_3), 101.2 (CH), 117.0 (m, CH), 118.7 (dd, J_1 = 14 Hz, J_1 = 2 Hz Cq), 119.0 (dd, J_1 = 7 Hz, J_1 = 2 Hz Cq), 121.7 (CH), 124.2 (Cq), , 124.4_8 (CH), 124.5_6 (CH), 124.6_0 (CH), 125.2 (CH), 126.0 (CH), 126.5 (CH), 126.8 (CH), 129.0 (CH), 129.2 (CH), 129.3 (d, J = 2 Hz, CH), 130.0 (CH), 130.7 (CH), 132.0 (Cq), 132.4 (Cq), 133.5 (Cq), 134.5 (Cq), 135.8 (m, Cq), 136.8 (dm, J = 253 Hz, CF), 138.0 (Cq), 138.5 (dm, J = 253 Hz, CF), 139.2 (d, J = 3 Hz, Cq), 141.8 (dm, J = 253 Hz, CF), 143.7 (dm, J = 253 Hz, CF), 153.9 (Cq). ***^{19}F-NMR*** (376 MHz, $CDCl_3$): δ -162.8 (t, J = 19 Hz, 1F), -162.2 (t, J = 19 Hz, 1F), -152.7 (dd, J_1 = 19 Hz, J_1 = 16 Hz, 1F), -140.7 (t, J = 16 Hz, 1F). Elem. Anal. Calcd for $C_{31}H_{18}F_4O$: C, 77.17; H, 3.76; F,15.75. Found C, 77.34; H, 4.01.

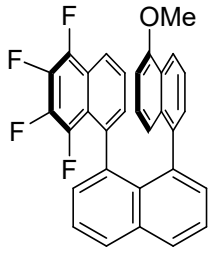


4-*syn***:** White solid. HPLC Phenomenex Luna C8 (5 µm, 100 Å, 250×10.0 mm), MeCN/H_2O 90/10, 5 ml/min, λ = 254 nm. t_R = 14.31 min. *Syn* enantiomers was separated by chiral HPLC analysis (Chiralcel OD-H, 0.46 cm Ø x 25 cm, *n*-Hex/*i*-PrOH 97/3, flow = 0.7 ml/min, λ = 254 nm. t_R = 9.60 min, 12.41 min). ***^{1}H-NMR*** (600 MHz, $CDCl_3$): δ 3.91 (s, 3H), 6.21 (d, J = 7.8 Hz, 1H), 6.67 (d, J = 7.2 Hz, 1H), 7.12 (m, 2H), 7.20-7.28 (m, 4H), 7.35 (dd, J_1 = 7.2 Hz, J_2 = 1.2 Hz, 1H), 7.53 (dd, J_1 = 8.4 Hz, J_2 = 7.2 Hz, 1H), 7.55 (m, 1H), 7.58 (dd, J_1 = 7.8 Hz, J_2 = 7.2 Hz, 1H), 7.89 (d, J = 8.4 Hz, 1H), 8.08 (dm, J = 8.4 Hz, 2H). ***^{13}C-NMR*** (150 MHz, $CDCl_3$): δ 55.3 (CH_3), 102.6 (CH), 118.0 (m, CH + Cq), 119.1 (d, J = 13 Hz, Cq), 121.0 (CH), 123.8 (Cq), 124.3 (CH), 124.4 (CH), 124.8 (CH), 125.5 (CH), 125.7 (CH), 128.9 (CH), 129.0 (CH), 129.4 (2CH), 129.5 (d, J = 2 Hz, CH), 130.3 (CH), 131.0 (Cq),

131.5 (CH), 131.8 (d, J = 3 Hz, Cq), 132.7 (Cq), 134.7 (Cq), 136.6 (CF), 137.0 (CF), 137.6 (Cq), 138.0 (Cq), 139.1 (Cq), 141.1 (CF), 142.7 (CF), 153.4 (Cq). ***^{19}F-NMR*** (564 MHz, $CDCl_3$): δ -160.5 (t, J = 19 Hz, 1F), -158.1 (t, J = 19 Hz, 1F), -151.8 (dd, J_1 = 19 Hz, J_2 = 16 Hz, 1F), -137.1 (t, J = 16 Hz, 1F). Elem. Anal. Calcd for $C_{31}H_{18}F_4O$: C, 77.17; H, 3.76; F,15.75. Found C, 76.93; H, 3.45.

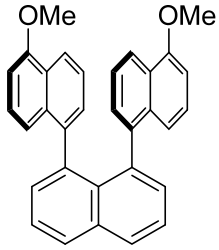


5-*anti***:** White solid. HPLC Phenomenex Polar-RP (4 µm, 80 Å, 250×21.2 mm), MeCN/H_2O 90/10, 20 ml/min, λ = 254 nm. t_R = 10.15 min. *Anti* enantiomers was separated by chiral HPLC analysis (Chiralcel OD-H, 0.46 cm Ø x 25 cm, *n*-Hex/*i*-PrOH 97/3, flow = 0.7 ml/min, λ = 254 nm. t_R = 10.94 min, 12.65 min). ***^{1}H-NMR*** (600 MHz, $CDCl_3$): δ 3.98 (s, 3H), 6.44 (t, J = 7.8 Hz, 1H), 6.57 (dd, J_1 = 8.4 Hz, J_2 = 7.2 Hz, 1H), 6.63 (d, J = 7.2 Hz, 1H), 6.68 (d, J = 7.2 Hz, 1H), 6.79 (d, J = 8.4 Hz, 1H), 6.89 (d, J = 7.2 Hz, 1H), 7.12 (dd, J_1 = 8.4 Hz, J_2 = 7.2 Hz, 1H), 7.16 (dd, J_1 = 7.2 Hz, J_2 = 1.2 Hz, 1H), 7.26 (d, J = 7.8 Hz, 1H), 7.30 (dd, J_1 = 7.2 Hz, J_2 = 1.2 Hz, 1H), 7.52 (dd, J_1 = 8.4 Hz, J_2 = 7.2 Hz, 1H), 7.56-7.59 (m, 2H), 8.05 (dt, J_1 = 8.4 Hz, J_2 = 1.2 Hz, 2H). ***^{13}C-NMR*** (150 MHz, $CDCl_3$): δ 55.7 (CH_3), 103.3 (CH), 117.5 (m, CH), 118.7 (m, Cq), 118.8 (m, Cq), 119.3 (CH), 120.7 (CH), 122.6 (CH), 124.2 (CH), 124.6 (CH + Cq), 125.1 (CH), 125.3 (CH), 127.2 (CH), 129.0 (d, J = 3 Hz, CH), 129.1 (CH), 129.3 (CH), 129.9 (CH), 130.4 (CH), 131.7 (d, J = 4 Hz, Cq), 133.5 (Cq), 134.4 (Cq), 135.6 (d, J_1 = 6 Hz, Cq), 136.9 (dm, J = 253 Hz, CF), 138.3 (Cq), 138.6 (dm, J = 253 Hz, CF), 139.2 (d, J_1 = 3 Hz, Cq), 139.3 (Cq), 141.8 (dm, J = 253 Hz, CF), 145.5 (dm, J = 253 Hz, CF), 155.5 (Cq). ***^{19}F-NMR*** (564 MHz, $CDCl_3$): δ -161.2 (t, J = 19 Hz, 1F), -160.9 (t, J = 19 Hz, 1F), -150.8 (dd, J_1 = 19 Hz, J_2 = 16 Hz, 1F), -139.9 (t, J = 16 Hz, 1F). Elem. Anal. Calcd for $C_{31}H_{18}F_4O$: C, 77.17; H, 3.76; F,15.75. Found C, 77.29; H, 3.91.



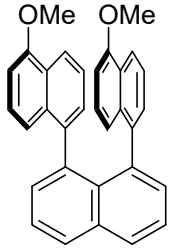
5-*syn***:** White solid. HPLC Phenomenex Polar-RP (4 µm, 80 Å, 250×21.2 mm), MeCN/H_2O 90/10, 20 ml/min, λ = 254 nm. t_R = 10.62 min. *Syn* enantiomers was separated by chiral HPLC analysis (Chiralcel OD-H, 0.46 cm Ø x 25 cm, *n*-Hex/*i*-PrOH 97/3, flow = 0.7 ml/min, λ = 254 nm. t_R = 10.39 min, 11.31 min). ***^{1}H-NMR*** (600 MHz, $CDCl_3$): δ 3.95 (s, 3H), 6.58. (d, J = 7.8 Hz, 1H), 6.75 (dd, J_1 = 7.2 Hz, J_2 = 1.2 Hz, 1H) 6.80-6.85 (m, 2H), 7.01 (t, J = 7.8 Hz, 1H), 7.10 (d, J = 7.2 Hz, 1H), 7.25 (t, J = 7.2 Hz, 1H), 7.27 (dd, J_1 = 6.6 Hz, J_2 = 1.2 Hz, 1H), 7.32 (dd, J_1 = 6.6 Hz, J_2 = 1.2 Hz, 1H), 7.53-7.59 (m, 3H), 7.66 (d, J = 8.4 Hz, 1H), 8.07 (dm, J = 8.4 Hz, 2H). ***^{13}C-NMR*** (150 MHz, $CDCl_3$): δ 55.5 (CH_3), 102.9 (CH), 118.1 (m, Cq), 118.6 (CH), 118.8 (CH), 119.2 (m, Cq), 120.2 (CH), 123.4 (CH), 123.9 (Cq), 124.5 (CH), 124.7 (CH), 124.8 (CH), 125.5 (CH), 129.1 (CH), 129.3 (2CH), 129.4 (CH), 130.4 (CH), 131.1 (CH), 131.3 (Cq), 132.7 (Cq), 134.6 (Cq), 136.4 (CF), 136.8 (CF), 137.4 (Cq),

137.9 (Cq), 138.3(Cq), 139.0 (Cq), 141.2 (CF), 142.9 (CF), 154.8 (Cq). ***^{19}F-NMR*** (564 MHz, $CDCl_3$): δ -161.4 (t, *J* = 19 Hz, 1F), -158.0 (t, *J* = 19 Hz, 1F), -151.9 (t, *J* = 18 Hz, 1F), -136.9 (t, *J* = 18 Hz, 1F). Elem. Anal. Calcd for $C_{31}H_{18}F_4O$: C, 77.17; H, 3.76; F,15.75. Found C, 76.84; H, 3.99.



6-*anti*: White solid, HPLC Phenomenex Luna C8 (5 µm, 100 Å, 250×10.0 mm), MeCN/H_2O 90/10, 5 ml/min, λ = 254 nm. tR = 12.55 min.*Anti* conformation was confirmed by chiral HPLC analysis of the product which confirmed the presence of a racemic mixture of the two enantiomers ((Chiralcel OD-H, 0.46 cm Ø x 25 cm, *n*-Hex/*i*-PrOH 95/5, flow = 1 ml/min, λ = 254 nm. t_R = 6.57 min, 9.16 min). ***^{1}H-NMR*** (600 MHz, $CDCl_3$): δ 8.05 (dd, J = 8.2, 1.4 Hz, 2H), 7.59 – 7.51 (m, 4H), 7.25 (dd, J = 6.9, 1.4 Hz, 2H), 7.11 (dd, J = 8.5, 7.5 Hz, 2H), 6.76 (d, J = 8.5 Hz, 2H), 6.69 (d, J = 7.5 Hz, 2H), 6.51 (dd, J = 6.9, 1.3 Hz, 2H), 6.36 (dd, J = 8.4, 6.9 Hz, 2H), 3.97 (s, 6H).***^{3}C-NMR*** (150 MHz, $CDCl_3$): δ 155.46 (Cq), 139.08 (Cq), 138.79 (Cq), 134.65 (Cq), 133.60 (Cq), 131.90 (Cq), 130.73 (CH), 128.81 (CH), 127.11 (CH), 125.11 (CH), 124.94 (CH), 124.68 (Cq), 122.51 (CH), 120.38 (CH), 119.04 (CH), 103.09 (CH), 55.68 (OCH_3).

Elem. Anal. Calcd for $C_{32}H_{24}O_2$: C, 87.25; H, 5.49; Found C, 86.94; H, 5.68.

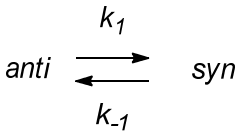


6-*syn*: White solid, HPLC Phenomenex Luna C8 (5 µm, 100 Å, 250×10.0 mm), MeCN/H_2O 90/10, 5 ml/min, λ = 254 nm. t_R = 12.99 min.

1H-NMR (600 MHz, $CDCl_3$): δ 8.06 (dd, J = 8.3, 1.4 Hz, 2H), 7.64 (dt, J = 8.4, 1.1 Hz, 2H), 7.56 (dd, J = 8.3, 6.9 Hz, 2H), 7.30 (dd, J = 6.9, 1.4 Hz, 2H), 6.95 (dd, J = 8.4, 6.9 Hz, 2H), 6.87 (dd, J = 6.9, 1.3 Hz, 2H), 6.55 (dd, J = 8.5, 7.5 Hz, 2H), 6.46 (dd, J = 8.5, 1.2 Hz, 2H), 6.34 (d, J = 7.3 Hz, 2H), 3.89 (s, 6H). 13C NMR (151 MHz, $CDCl_3$) δ 154.61 (Cq), 139.47 (Cq), 138.99 (Cq), 134.93 (Cq), 132.66 (Cq), 132.49 (Cq), 130.74 (CH), 128.81 (CH), 128.68 (CH), 124.85 (CH), 124.42 (Cq), 124.29 (CH), 123.28 (CH), 120.20 (CH), 119.32 (CH), 102.97 (CH), 55.44 (OCH_3).Elem. Anal. Calcd for $C_{32}H_{24}O_2$: C, 87.25; H, 5.49; Found C, 87.39; H, 5.77.

Kinetic measurements for *anti/syn* diastereomerization process

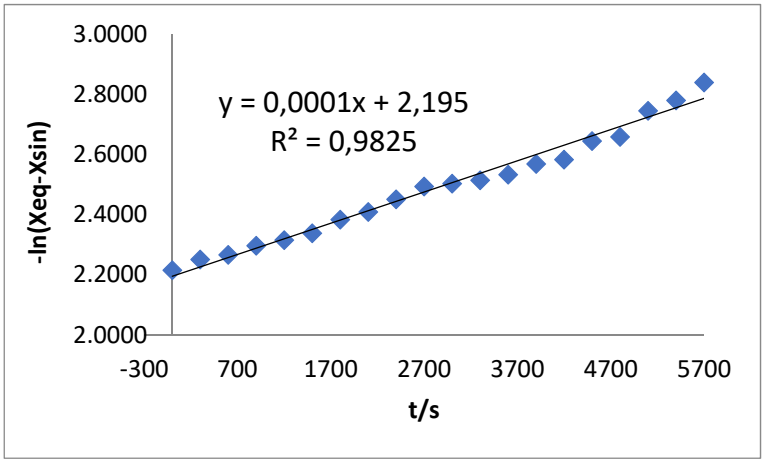
The diastereomerization barriers were determined by standard kinetic analysis using NMR samples of a single isomer in TCE-d_2. The sample was prepared using 0.7 mL of solvent, carefully degassed with argon and sealed by a torch to avoid evaporation and degradation of the compounds. Depending on the time required, the samples were heated within the NMR probe or into an oil bath at a fixed temperature, measuring by NMR integration the growth of the second isomer as a function of time, to determine the kinetic rate constant for diastereomerization. The rate constants were then determined by applying a first-order law at equilibrium. The ratio at the equilibrium was determined by heating the NMR sample at +125°C for 7 days. The diastereomerization $\Delta G^{\neq}$ was then derived by means of the Eyring equation.



Compound 1 @ 71 °C in TCE-d_2.

t (s)	X_{syn}	-ln (X_{eq} - X_{syn})	t (s)	X_{syn}	-ln (X_{eq} - X_{syn})
0	0,0996	2,2150	3000	0,1269	2,5028
300	0,1034	2,2504	3300	0,1278	2,5139
600	0,1050	2,2657	3600	0,1293	2,5326
900	0,1081	2,2961	3900	0,1321	2,5685
1200	0,1100	2,3151	4200	0,1332	2,5829
1500	0,1122	2,3377	4500	0,1377	2,6443
1800	0,1165	2,3832	4800	0,1387	2,6585
2100	0,1188	2,4085	5100	0,1445	2,7449
2400	0,1225	2,4505	5400	0,1467	2,7798
2700	0,1261	2,4931	5700	0,1503	2,8395

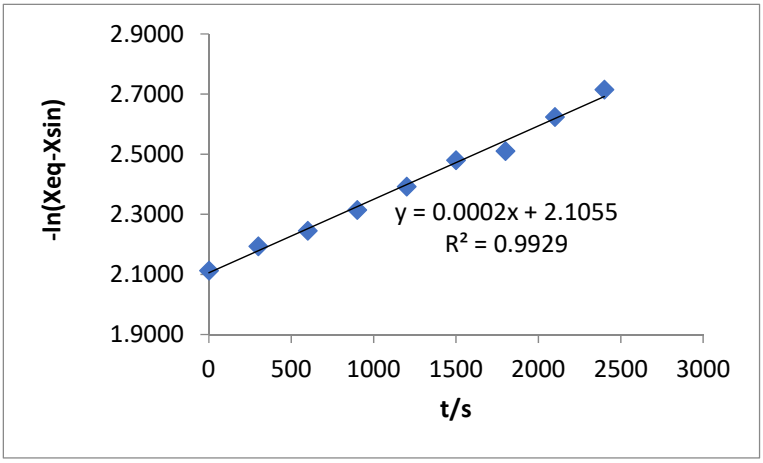
T (°C)	71
$k_1 + k_{-1}$ (s^{-1})	1.04 x 10^{-4}
k_1 (s^{-1})	2.17 x 10^{-5}
k_{-1} (s^{-1})	8.21 x 10^{-5}
$\Delta G^{\neq}$ (kcal/mol)	27.6



Compound 1 @ 82 °C in TCE-d_2.

t (s)	X_{syn}	-ln (X_{eq} - X_{syn})
0	0,0943	2,1126
300	0,1037	2,1936
600	0,1093	2,2451
900	0,1164	2,3145
1200	0,1238	2,3923
1500	0,1315	2,4803
1800	0,134	2,5106
2100	0,1427	2,6239
2400	0,149	2,7148

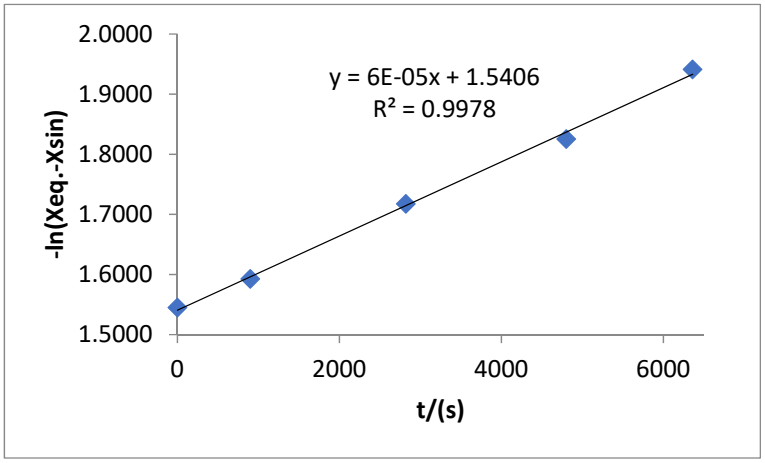
T (°C)	82
$k_1 + k_{-1}$ (s^{-1})	2.44 x 10^{-4}
k_1 (s^{-1})	5.26 x 10^{-5}
k_{-1} (s^{-1})	1.92 x 10^{-4}
$\Delta G^{\neq}$ (kcal/mol)	27.7



Compound 2 @ 113 °C in TCE-d_2.

t (min)	X_{syn}	-ln (X_{eq} - X_{syn})
0	0,000	1,5450
15	0,010	1,5925
47	0,034	1,7175
80	0,052	1,8252
106	0,070	1,9410

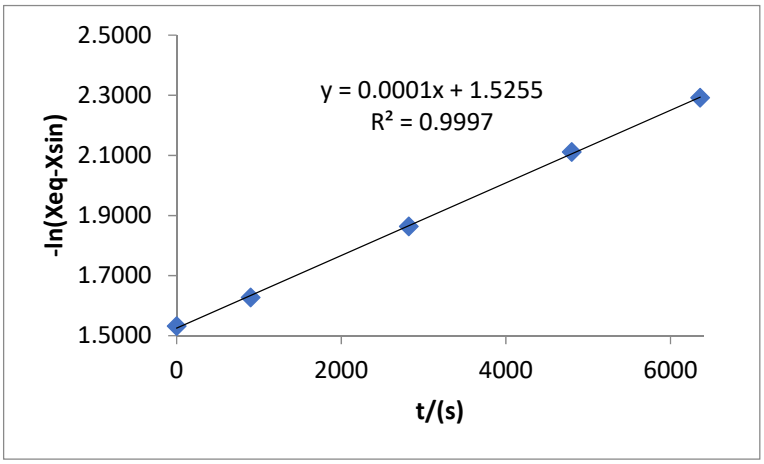
T (°C)	113
$k_1 + k_{-1}$ (s^{-1})	6.17 x 10^{-5}
k_1 (s^{-1})	1.32 x 10^{-5}
k_{-1} (s^{-1})	4.85 x 10^{-5}
$\Delta G^{\neq}$ (kcal/mol)	31.4



Compound 2 @ 118 °C in TCE-d_2.

t (min)	X_{syn}	-ln (X_{eq} - X_{syn})
0	0,000	1,5318
15	0,020	1,6269
47	0,061	1,8637
80	0,095	2,1110
106	0,115	2,2917

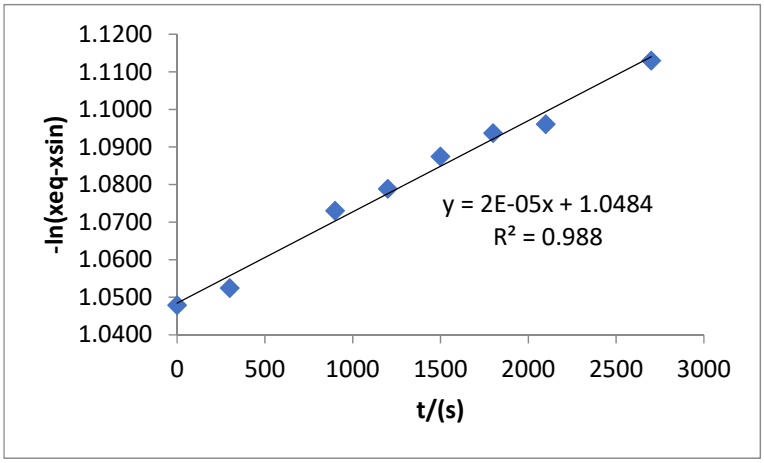
T (°C)	118
$k_1 + k_{-1}$ (s^{-1})	1.21 x 10^{-4}
k_1 (s^{-1})	2.61 x 10^{-5}
k_{-1} (s^{-1})	9.47 x 10^{-5}
$\Delta G^{\neq}$ (kcal/mol)	31.3



Compound 3 @ 92 °C in TCE-d_2.

t (s)	X_{syn}	-ln (X_{eq} - X_{syn})
0	0,041	1,0479
300	0,042	1,0525
900	0,049	1,0730
1200	0,051	1,0789
1500	0,054	1,0874
1800	0,056	1,0937
2100	0,057	1,0961
2700	0,063	1,1130

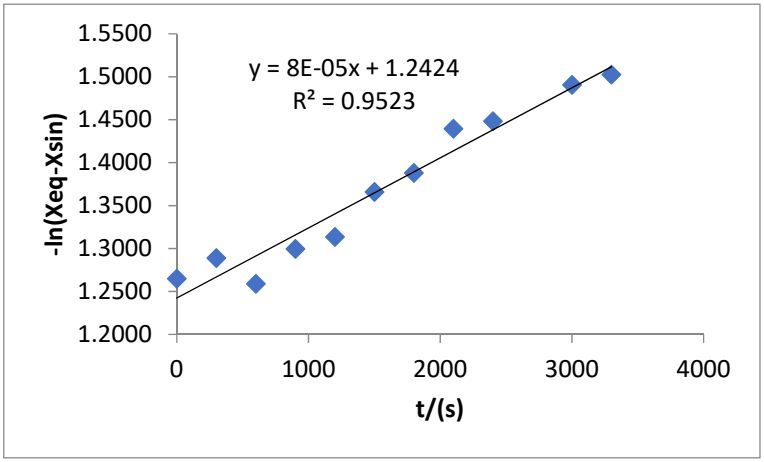
T (°C)	92
$k_1 + k_{-1}$ (s^{-1})	2.43 x 10^{-5}
k_1 (s^{-1})	9.49 x 10^{-6}
k_{-1} (s^{-1})	1.48 x 10^{-5}
$\Delta G^{\neq}$ (kcal/mol)	29.9



Compound 3 @ 102 °C in TCE-d_2.

t (s)	X_{syn}	-ln (X_{eq} - X_{syn})
0	0,112	1,2650
300	0,119	1,2890
600	0,110	1,2590
900	0,121	1,2996
1200	0,125	1,3136
1500	0,139	1,3659
1800	0,145	1,3881
2100	0,157	1,4395
2400	0,159	1,4484
3000	0,169	1,4906

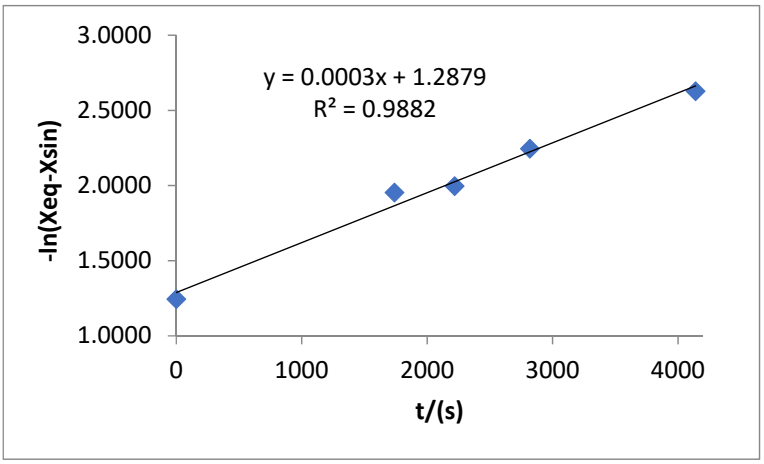
T (°C)	102
$k_1 + k_{-1}$ (s^{-1})	8.16 x 10^{-5}
k_1 (s^{-1})	3.22 x 10^{-5}
k_{-1} (s^{-1})	4.94 x 10^{-5}
$\Delta G^{\neq}$ (kcal/mol)	29.8



Compound 4 @ 111 °C in TCE-d_2.

t (s)	X_{syn}	-ln (X_{eq} - X_{syn})
0	0,026	1,2439
1740	0,172	1,9537
2220	0,178	1,9962
2820	0,208	2,2448
4140	0,242	2,6276

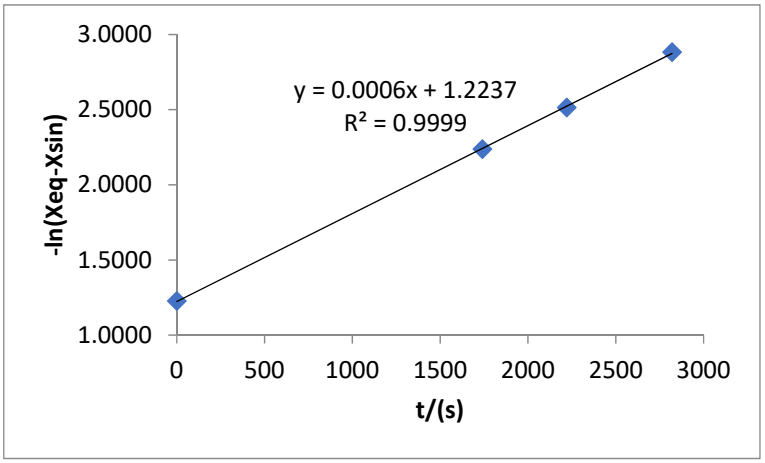
T (°C)	111
$k_1 + k_{-1}$ (s^{-1})	3.32 x 10^{-4}
k_1 (s^{-1})	1.04 x 10^{-4}
k_{-1} (s^{-1})	2.28 x 10^{-4}
$\Delta G^{\neq}$ (kcal/mol)	29.7



Compound 4 @ 111 °C in TCE-d_2.

t (s)	X_{syn}	-ln (X_{eq} - X_{syn})
0	0,024	1,2269
1740	0,211	2,2378
2220	0,237	2,5146
2820	0,262	2,8825
4140	0,300	4,0632

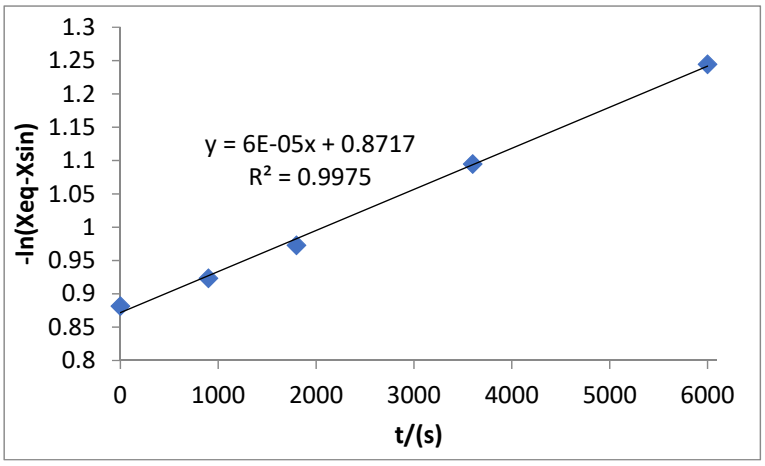
T (°C)	119
$k_1 + k_{-1}$ (s^{-1})	6,74 x 10^{-4}
k_1 (s^{-1})	2.14 x 10^{-4}
k_{-1} (s^{-1})	4.60 x 10^{-4}
$\Delta G^{\neq}$ (kcal/mol)	29.7



Compound 5 @ 96 °C in TCE-d_2.

t (s)	X_{syn}	-ln (X_{eq} - X_{syn})
0	0,0427	0,88147534
900	0,0597	0,923387311
1800	0,0788	0,972672167
3600	0,1223	1,094904918
6000	0,1688	1,244546854

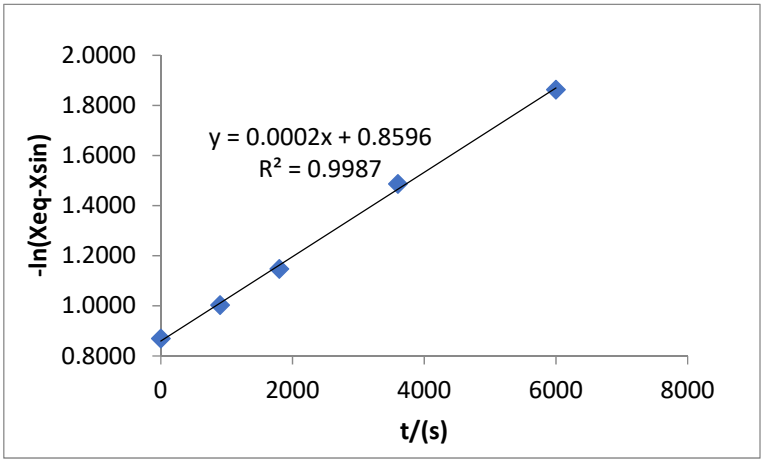
T (°C)	96
$k_1 + k_{-1}$ (s^{-1})	6,17 x 10^{-5}
k_1 (s^{-1})	2.82 x 10^{-5}
k_{-1} (s^{-1})	3.35 x 10^{-5}
$\Delta G^{\neq}$ (kcal/mol)	29.4



Compound 5 @ 108 °C in TCE-d_2.

t (s)	X_{syn}	-ln (X_{eq} - X_{syn})
0	0,039	0,8691
900	0,091	1,0029
1800	0,141	1,1472
3600	0,232	1,4862
6000	0,303	1,8629

T (°C)	108
$k_1 + k_{-1}$ (s^{-1})	1.68 x 10^{-4}
k_1 (s^{-1})	7.71 x 10^{-5}
k_{-1} (s^{-1})	9.11 x 10^{-5}
$\Delta G^{\neq}$ (kcal/mol)	29.6



Compound 6 @ 87 °C in TCE-d_2.

t (s)	X_{syn}	-ln (X_{eq} - X_{syn})
0	0,099	2.1258
150	0,103	2.1582
300	0,105	2.1721
450	0,108	2.1997
600	0,110	2.2170
750	0,112	2.2374
900	0,116	2.2785
1050	0,119	2.3012

T (°C)	87
$k_1 + k_{-1}$ (s^{-1})	1.35×10^{-4}
k_1 (s^{-1})	1.03×10^{-4}
k_{-1} (s^{-1})	3.61×10^{-5}
$\Delta G^{\neq}$ (kcal/mol)	28.6

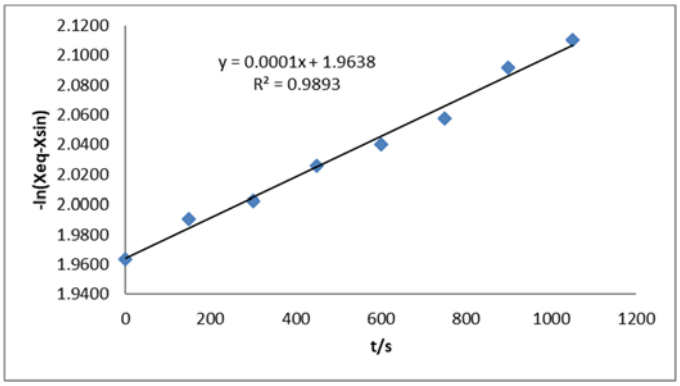


Table S4. Summary of calculations for compounds 1-6
(energies in a.u. except for the green columns, in kcal/mol)

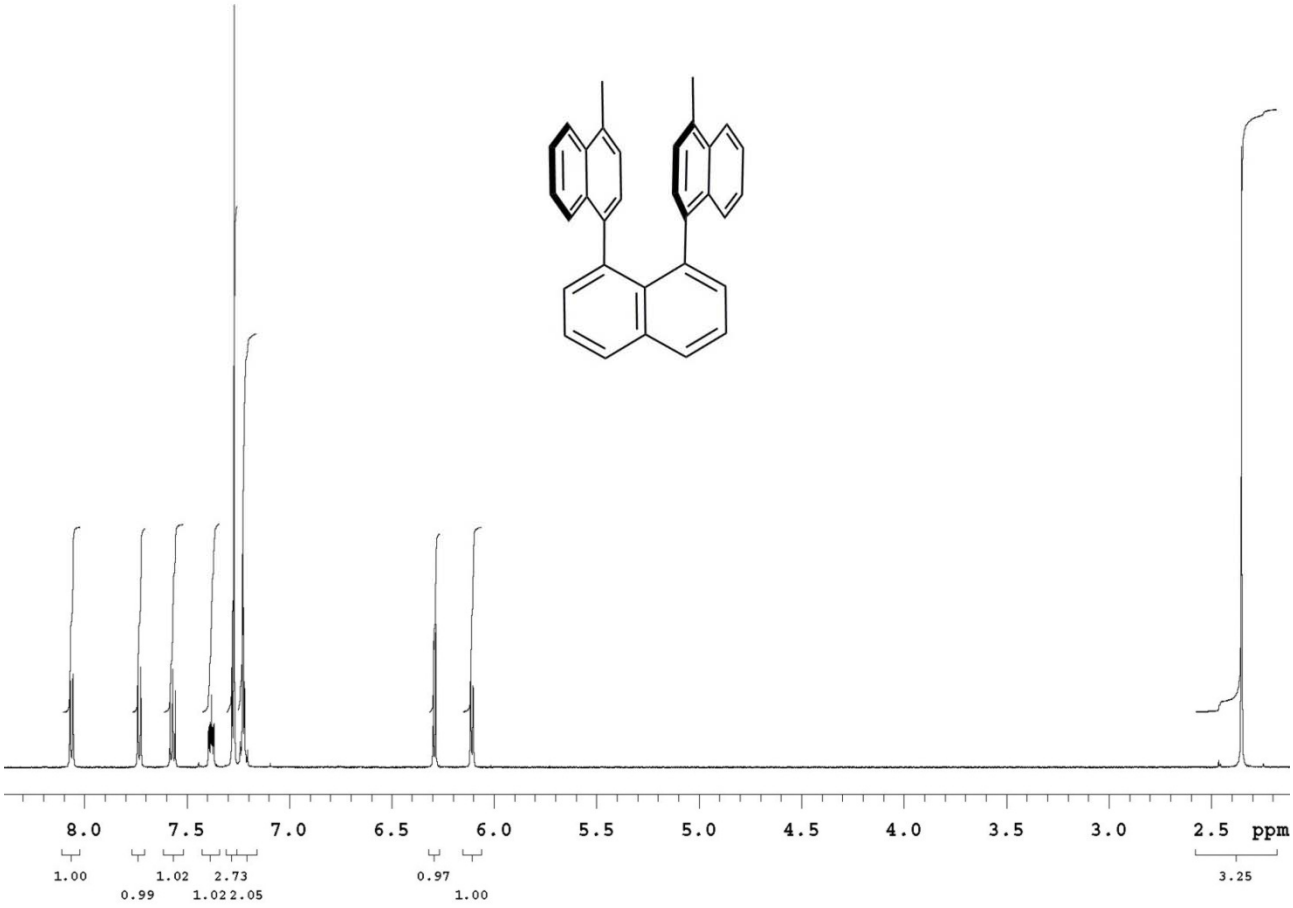
		Full opt M06-2X/6-31+G(d,p)									M06-2X/6-311++G(2d,p)		
	PCM solv.	EE	corr_H	corr_G	H°	G°	ΔH°	**ΔG°**	**qh-G° (th =100 cm^{-1})**	**ΔG°**	**singlepoint-EE**	**G° with qh-corr**	**Rel.G°**
Compound 1													
anti-in	$CHCl_3$	-1233.461591	0.487065	0.407788	-1232.974526	-1233.053803	0.27	**0.00**	-1233.065685	**0.00**	-1233.741311	-1233.345405	**0.00**
anti-out	$CHCl_3$	-1233.461981	0.487021	0.4093	-1232.97496	-1233.052681	0.00	**0.70**	-1233.065384	**0.19**	-1233.741670	-1233.345073	**0.21**
syn	$CHCl_3$	-1233.460989	0.487115	0.409762	-1232.973874	-1233.051227	0.68	**1.62**	-1233.064057	**1.02**	-1233.740643	-1233.343711	**1.06**
TS rotation	$CHCl_3$	-1233.414602	0.486579	0.410753	-1232.928023	-1233.003849	29.45	**31.35**	-1233.016960	**30.57**	-1233.694570	-1233.296928	**30.42**
anti-in	DMSO	-1233.464548	0.486954	0.407204	-1232.977594	-1233.057344	0.18	**0.00**	-1233.068905	**0.00**	-1233.744206	-1233.348563	**0.00**
anti-out	DMSO	-1233.464796	0.486912	0.408988	-1232.977884	-1233.055808	0.00	**0.96**	-1233.068400	**0.32**	-1233.744553	-1233.348157	**0.25**
syn	DMSO	-1233.463783	0.486976	0.409449	-1232.976807	-1233.054334	0.68	**1.89**	-1233.067081	**1.14**	-1233.743430	-1233.346728	**1.15**
Compound 2													
anti-in	$CHCl_3$	-1948.499717	0.370482	0.282286	-1948.129235	-1948.217431	0.00	**0.00**	-1948.224789	**0.00**	-1949.027510	-1948.752582	**0.00**
syn	$CHCl_3$	-1948.497705	0.370397	0.28251	-1948.127308	-1948.215195	1.21	**1.40**	-1948.222685	**1.32**	-1949.026112	-1948.751092	**0.93**
TS rotation	$CHCl_3$	-1948.446493	0.369197	0.283405	-1948.077296	-1948.163088	32.59	**34.10**	-1948.171248	**33.60**	-1948.973927	-1948.698682	**33.82**
anti-in	DMSO	-1948.502860	0.370352	0.282018	-1948.132508	-1948.220842	0.00	**0.00**	-1948.228135	**0.00**	-1949.030491	-1948.755766	**0.00**
syn	DMSO	-1948.501277	0.370276	0.282300	-1948.131001	-1948.218977	0.95	**1.17**	-1948.226435	**1.07**	-1949.029490	-1948.754648	**0.70**
Compound 3													
anti-in	$CHCl_3$	-1590.982249	0.428809	0.34591	-1590.55344	-1590.636339	0.00	**0.00**	-1590.646339	**0.00**	-1591.386013	-1591.050103	**0.00**
syn-in	$CHCl_3$	-1590.982103	0.428895	0.346629	-1590.553208	-1590.635474	0.15	**0.54**	-1590.645863	**0.30**	-1591.386163	-1591.049923	**0.11**
syn-out	$CHCl_3$	-1590.979216	0.427823	0.348189	-1590.551393	-1590.631027	1.28	**3.33**	-1590.642140	**2.63**	-1591.382869	-1591.045793	**2.70**
TS-rotation, 4Fnap	$CHCl_3$	-1590.930863	0.427847	0.347292	-1590.503016	-1590.583571	31.64	**33.11**	-1590.594338	**32.63**	-1591.334319	-1590.997794	**32.82**
TS-rotation, 4MeNap	$CHCl_3$	-1590.930895	0.427966	0.346982	-1590.502929	-1590.583913	31.70	**32.90**	-1590.594522	**32.52**	-1591.334753	-1590.998380	**32.46**
anti-in	DMSO	-1590.985154	0.428704	0.345789	-1590.55645	-1590.639365	0.00	**0.00**	-1590.649360	**0.00**	-1591.388821	-1591.053027	**0.00**
syn-in	DMSO	-1590.984947	0.428776	0.346396	-1590.556171	-1590.638551	0.18	**0.51**	-1590.648882	**0.30**	-1591.388901	-1591.052836	**0.12**
syn-out	DMSO	-1590.982778	0.428538	0.345788	-1590.55424	-1590.63699	1.39	**1.49**	-1590.647111	**1.41**	-1591.386337	-1591.050670	**1.48**
Compound 4													
anti-in	$CHCl_3$	-1666.168924	0.435073	0.350147	-1665.733851	-1665.818777	0.00	**0.00**	-1665.828861	**0.00**	-1666.596695	-1666.256632	**0.00**
syn-in	$CHCl_3$	-1666.168099	0.435142	0.350544	-1665.732957	-1665.817555	0.56	**0.77**	-1665.827817	**0.66**	-1666.596180	-1666.255898	**0.46**

syn-out	$CHCl_3$	-1666.165191	0.43492	0.348153	-1665.730271	-1665.817038	2.25	**1.09**	-1665.826239	**1.65**	-1666.592854	-1666.253902	**1.71**
TS-rotation, 4Fnap	$CHCl_3$	-1666.117103	0.434009	0.350887	-1665.683094	-1665.766216	31.85	**32.98**	-1665.776785	**32.68**	-1666.544581	-1666.204263	**32.86**
TS-rotation, 4OMeNap	$CHCl_3$	-1666.117582	0.434227	0.350719	-1665.683355	-1665.766863	31.69	**32.58**	-1665.777277	**32.37**	-1666.545496	-1666.205191	**32.28**
anti-in	DMSO	-1666.172094	0.434946	0.349777	-1665.737148	-1665.822317	0.00	**0.00**	-1665.832279	**0.00**	-1666.599738	-1666.259923	**0.00**
syn-in	DMSO	-1666.17155	0.435028	0.350282	-1665.736522	-1665.821268	0.39	**0.66**	-1665.831464	**0.51**	-1666.599467	-1666.259381	**0.34**
syn-out	DMSO	-1666.168603	0.434799	0.348495	-1665.733804	-1665.820108	2.10	**1.39**	-1665.829566	**1.70**	-1666.596132	-1666.257095	**1.77**
Compound 5													
anti-in	$CHCl_3$	-1666.167553	0.435014	0.349228	-1665.732539	-1665.818325	0.44	**0.00**	-1665.827955	**0.00**	-1666.595225	-1666.255627	**0.16**
syn-in	$CHCl_3$	-1666.168465	0.435224	0.351304	-1665.733241	-1665.817161	0.00	**0.73**	-1665.827731	**0.14**	-1666.596615	-1666.255881	**0.00**
syn-out	$CHCl_3$	-1666.165603	0.43503	0.350023	-1665.730573	-1665.815580	1.67	**1.72**	-1665.825594	**1.48**	-1666.593356	-1666.253347	**1.59**
TS-rotation, 4Fnap	$CHCl_3$	-1666.117005	0.433959	0.350720	-1665.683046	-1665.766285	31.50	**32.66**	-1665.776770	**32.12**	-1666.544448	-1666.204213	**32.42**
TS-rotation, 5OMeNap	$CHCl_3$	-1666.116343	0.434238	0.350936	-1665.682105	-1665.765407	32.09	**33.21**	-1665.775897	**32.67**	-1666.544165	-1666.203719	**32.73**
anti-in	DMSO	-1666.170971	0.434868	0.348968	-1665.736103	-1665.822003	0.32	**0.00**	-1665.831583	**0.00**	-1666.598497	-1666.259109	**0.12**
syn-in	DMSO	-1666.171670	0.435052	0.350779	-1665.736618	-1665.820891	0.00	**0.70**	-1665.831296	**0.18**	-1666.599681	-1666.259307	**0.00**
syn-out	DMSO	-1666.168791	0.434882	0.349639	-1665.733909	-1665.819152	1.70	**1.79**	-1665.829060	**1.58**	-1666.596423	-1666.256692	**1.64**
Compound 6													
anti-in	$CHCl_3$	-1383.833726	0.499498	0.416379	-1383.334228	-1383.417347	0.00	**0.00**	-1383.429329	**0.00**	-1384.161432	-1383.757035	**0.00**
syn	$CHCl_3$	-1383.833017	0.499387	0.416119	-1383.333630	-1383.416898	0.38	**0.28**	-1383.428822	**0.32**	-1384.160727	-1383.756532	**0.32**
TS-rotation	$CHCl_3$	-1383.786207	0.498976	0.418135	-1383.287231	-1383.368072	29.49	**30.92**	-1383.380826	**30.44**	-1384.114122	-1383.708741	**30.30**
anti-in	DMSO	-1383.837736	0.499361	0.415853	-1383.338375	-1383.421883	0.00	**0.00**	-1383.433687	**0.00**	-1384.165342	-1383.761293	**0.00**
syn	DMSO	-1383.836931	0.499311	0.416283	-1383.337620	-1383.420648	0.47	**0.77**	-1383.432717	**0.61**	-1384.164540	-1383.760326	**0.61**

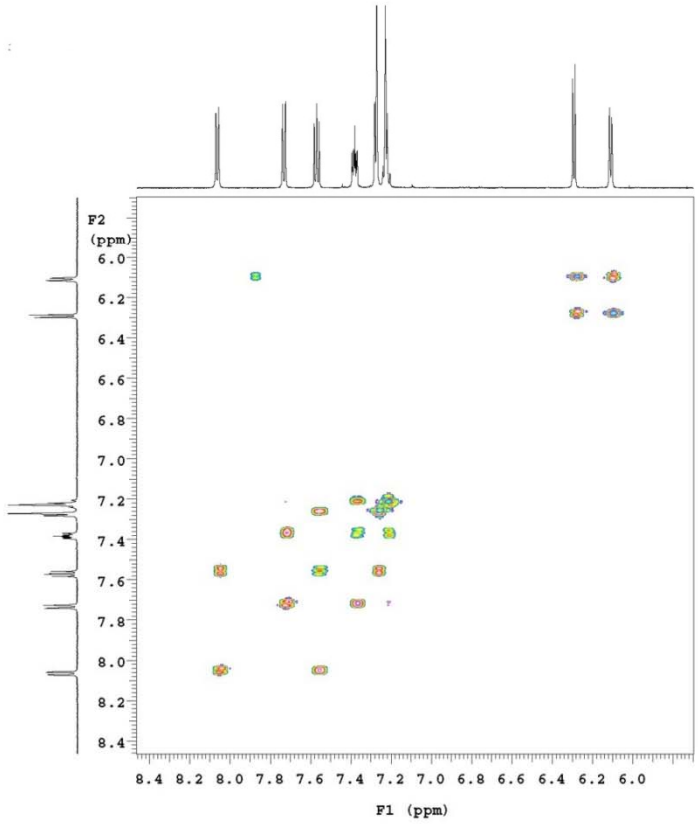
Table S5. Summary of calculations for compounds 1-6
(energies in a.u. except for the green columns, in kcal/mol)

		Full opt M06-2X/6-31+G(d,p)									ωB97X-D/6-311++G(2d,p)		
	PCM solv.	EE	corr_H	corr_G	H°	G°	ΔH°	**ΔG°**	**qh-G° (th =100 cm^{-1})**	**ΔG°**	**singlepoint-EE**	**G° with qh-corr**	**Rel.G°**
Compound 1													
anti-in	$CHCl_3$	-1233.461591	0.487065	0.407788	-1232.974526	-1233.053803	0.27	**0.00**	-1233.065685	**0.00**	-1233.818347	-1233.422441	**0.00**
anti-out	$CHCl_3$	-1233.461981	0.487021	0.4093	-1232.97496	-1233.052681	0.00	**0.70**	-1233.065384	**0.19**	-1233.818183	-1233.421586	**0.54**
syn	$CHCl_3$	-1233.460989	0.487115	0.409762	-1232.973874	-1233.051227	0.68	**1.62**	-1233.064057	**1.02**	-1233.817250	-1233.420318	**1.33**
TS rotation	$CHCl_3$	-1233.414602	0.486579	0.410753	-1232.928023	-1233.003849	29.45	**31.35**	-1233.016960	**30.57**	-1233.767854	-1233.370212	**32.77**
anti-in	DMSO	-1233.464548	0.486954	0.407204	-1232.977594	-1233.057344	0.18	**0.00**	-1233.068905	**0.00**	-1233.821083	-1233.425440	**0.00**
anti-out	DMSO	-1233.464796	0.486912	0.408988	-1232.977884	-1233.055808	0.00	**0.96**	-1233.068400	**0.32**	-1233.820778	-1233.424382	**0.66**
syn	DMSO	-1233.463783	0.486976	0.409449	-1232.976807	-1233.054334	0.68	**1.89**	-1233.067081	**1.14**	-1233.819866	-1233.423164	**1.43**
Compound 2													
anti-in	$CHCl_3$	-1948.499717	0.370482	0.282286	-1948.129235	-1948.217431	0.00	**0.00**	-1948.224789	**0.00**	-1949.086830	-1948.811902	**0.00**
syn	$CHCl_3$	-1948.497705	0.370397	0.28251	-1948.127308	-1948.215195	1.21	**1.40**	-1948.222685	**1.32**	-1949.084433	-1948.809413	**1.56**
TS rotation	$CHCl_3$	-1948.446493	0.369197	0.283405	-1948.077296	-1948.163088	32.59	**34.10**	-1948.171248	**33.60**	-1949.029076	-1948.753831	**36.44**
anti-in	DMSO	-1948.502860	0.370352	0.282018	-1948.132508	-1948.220842	0.00	**0.00**	-1948.228135	**0.00**	-1949.089706	-1948.814981	**0.00**
syn	DMSO	-1948.501277	0.370276	0.282300	-1948.131001	-1948.218977	0.95	**1.17**	-1948.226435	**1.07**	-1949.087654	-1948.812812	**1.36**
Compound 3													
anti-in	$CHCl_3$	-1590.982249	0.428809	0.34591	-1590.55344	-1590.636339	0.00	**0.00**	-1590.646339	**0.00**	-1591.453543	-1591.117633	**0.00**
syn-in	$CHCl_3$	-1590.982103	0.428895	0.346629	-1590.553208	-1590.635474	0.15	**0.54**	-1590.645863	**0.30**	-1591.453110	-1591.116870	**0.48**
syn-out	$CHCl_3$	-1590.979216	0.427823	0.348189	-1590.551393	-1590.631027	1.28	**3.33**	-1590.642140	**2.63**	-1591.450124	-1591.113048	**2.88**
TS-rotation, 4Fnap	$CHCl_3$	-1590.930863	0.427847	0.347292	-1590.503016	-1590.583571	31.64	**33.11**	-1590.594338	**32.63**	-1591.398247	-1591.061722	**35.08**
TS-rotation, 4MeNap	$CHCl_3$	-1590.930895	0.427966	0.346982	-1590.502929	-1590.583913	31.70	**32.90**	-1590.594522	**32.52**	-1591.399206	-1591.062833	**34.39**
anti-in	DMSO	-1590.985154	0.428704	0.345789	-1590.55645	-1590.639365	0.00	**0.00**	-1590.649360	**0.00**	-1591.456203	-1591.120409	**0.00**
syn-in	DMSO	-1590.984947	0.428776	0.346396	-1590.556171	-1590.638551	0.18	**0.51**	-1590.648882	**0.30**	-1591.455709	-1591.119644	**0.48**
syn-out	DMSO	-1590.982778	0.428538	0.345788	-1590.55424	-1590.63699	1.39	**1.49**	-1590.647111	**1.41**	-1591.455709	-1591.120042	**0.23**
Compound 4													
anti-in	$CHCl_3$	-1666.168924	0.435073	0.350147	-1665.733851	-1665.818777	0.00	**0.00**	-1665.828861	**0.00**	-1666.662636	-1666.322573	**0.00**

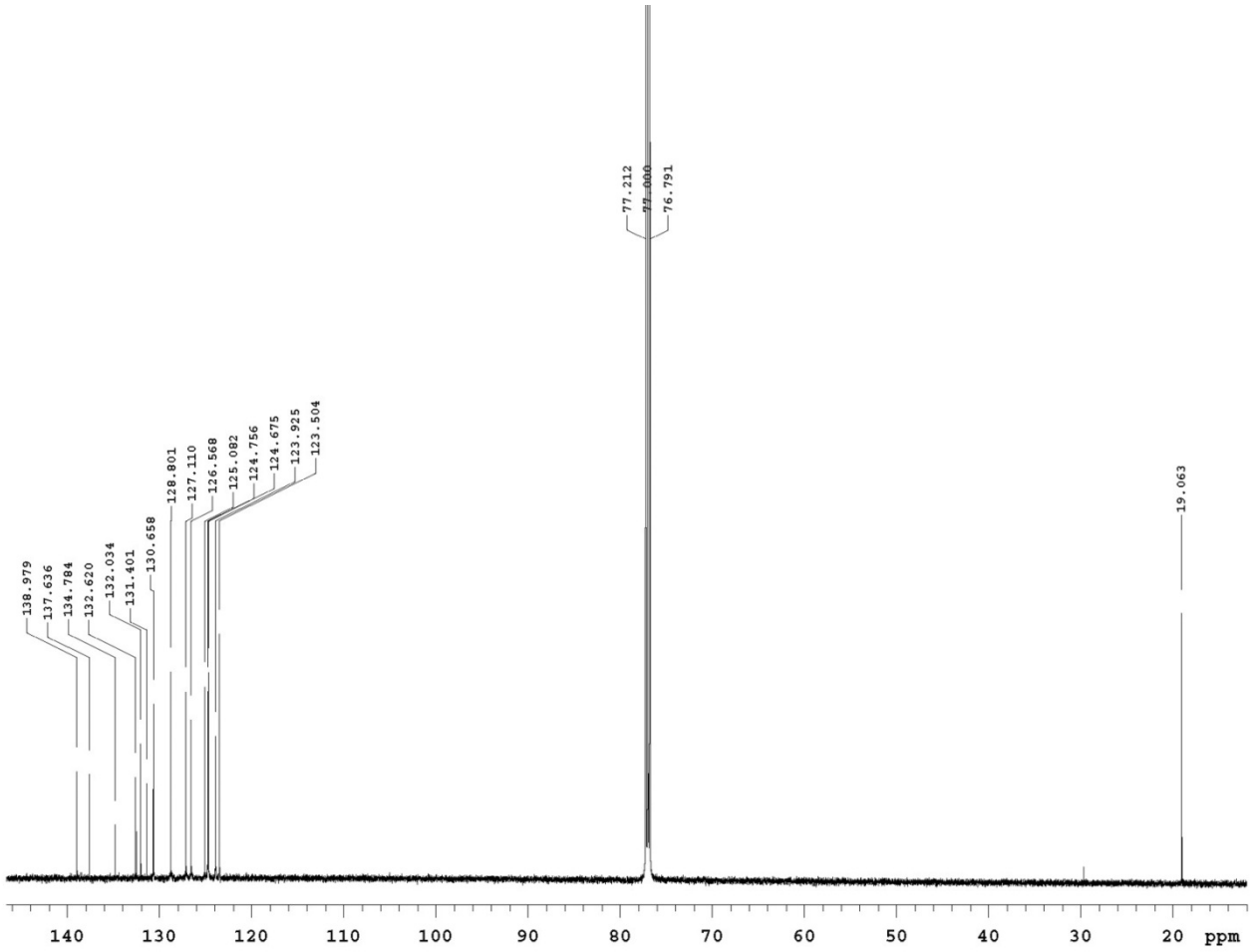
syn-in	$CHCl_3$	-1666.168099	0.435142	0.350544	-1665.732957	-1665.817555	0.56	**0.77**	-1665.827817	**0.66**	-1666.661661	-1666.321379	**0.75**
syn-out	$CHCl_3$	-1666.165191	0.43492	0.348153	-1665.730271	-1665.817038	2.25	**1.09**	-1665.826239	**1.65**	-1666.658541	-1666.319589	**1.87**
TS-rotation, 4Fnap	$CHCl_3$	-1666.117103	0.434009	0.350887	-1665.683094	-1665.766216	31.85	**32.98**	-1665.776785	**32.68**	-1666.606969	-1666.266651	**35.09**
TS-rotation, 4OMeNap	$CHCl_3$	-1666.117582	0.434227	0.350719	-1665.683355	-1665.766863	31.69	**32.58**	-1665.777277	**32.37**	-1666.608542	-1666.268237	**34.10**
anti-in	DMSO	-1666.172094	0.434946	0.349777	-1665.737148	-1665.822317	0.00	**0.00**	-1665.832279	**0.00**	-1666.665557	-1666.325742	**0.00**
syn-in	DMSO	-1666.17155	0.435028	0.350282	-1665.736522	-1665.821268	0.39	**0.66**	-1665.831464	**0.51**	-1666.664821	-1666.324735	**0.63**
syn-out	DMSO	-1666.168603	0.434799	0.348495	-1665.733804	-1665.820108	2.10	**1.39**	-1665.829566	**1.70**	-1666.661617	-1666.322580	**1.98**
Compound 5													
anti-in	$CHCl_3$	-1666.167553	0.435014	0.349228	-1665.732539	-1665.818325	0.44	**0.00**	-1665.827955	**0.00**	-1666.661198	-1666.321600	**0.00**
syn-in	$CHCl_3$	-1666.168465	0.435224	0.351304	-1665.733241	-1665.817161	0.00	**0.73**	-1665.827731	**0.14**	-1666.661613	-1666.320879	**0.45**
syn-out	$CHCl_3$	-1666.165603	0.43503	0.350023	-1665.730573	-1665.815580	1.67	**1.72**	-1665.825594	**1.48**	-1666.658687	-1666.318678	**1.83**
TS-rotation, 4Fnap	$CHCl_3$	-1666.117005	0.433959	0.350720	-1665.683046	-1665.766285	31.50	**32.66**	-1665.776770	**32.12**	-1666.606712	-1666.266477	**34.59**
TS-rotation, 5OMeNap	$CHCl_3$	-1666.116343	0.434238	0.350936	-1665.682105	-1665.765407	32.09	**33.21**	-1665.775897	**32.67**	-1666.606850	-1666.266404	**34.64**
anti-in	DMSO	-1666.170971	0.434868	0.348968	-1665.736103	-1665.822003	0.32	**0.00**	-1665.831583	**0.00**	-1666.664285	-1666.324897	**0.00**
syn-in	DMSO	-1666.171670	0.435052	0.350779	-1665.736618	-1665.820891	0.00	**0.70**	-1665.831296	**0.18**	-1666.664512	-1666.324138	**0.48**
syn-out	DMSO	-1666.168791	0.434882	0.349639	-1665.733909	-1665.819152	1.70	**1.79**	-1665.829060	**1.58**	-1666.661638	-1666.321907	**1.88**
Compound 6													
anti-in	$CHCl_3$	-1383.833726	0.499498	0.416379	-1383.334228	-1383.417347	0.00	**0.00**	-1383.429329	**0.00**	-1384.234086	-1383.829689	**0.00**
syn	$CHCl_3$	-1383.833017	0.499387	0.416119	-1383.333630	-1383.416898	0.38	**0.28**	-1383.428822	**0.32**	-1384.233847	-1383.829652	**0.02**
TS-rotation	$CHCl_3$	-1383.786207	0.498976	0.418135	-1383.287231	-1383.368072	29.49	**30.92**	-1383.380826	**30.44**	-1384.183922	-1383.778541	**32.10**
anti-in	DMSO	-1383.837736	0.499361	0.415853	-1383.338375	-1383.421883	0.00	**0.00**	-1383.433687	**0.00**	-1384.237767	-1383.833718	**0.00**
syn	DMSO	-1383.836931	0.499311	0.416283	-1383.337620	-1383.420648	0.47	**0.77**	-1383.432717	**0.61**	-1384.237543	-1383.833329	**0.24**

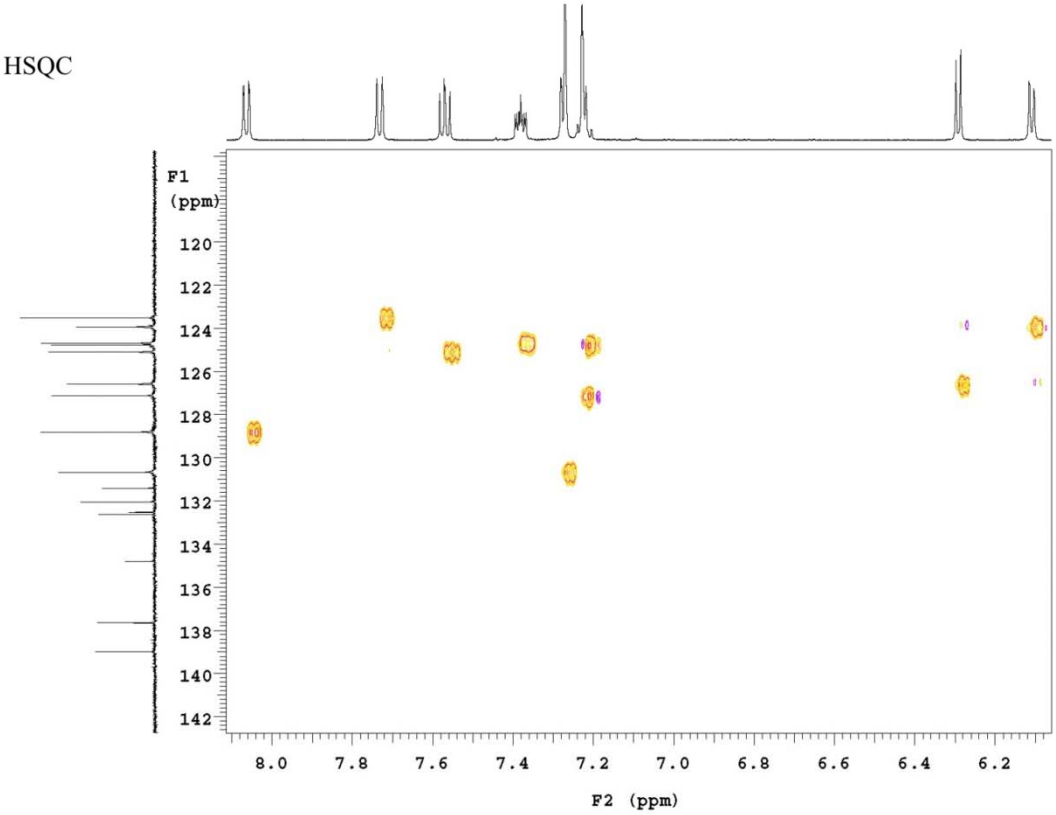


COSY

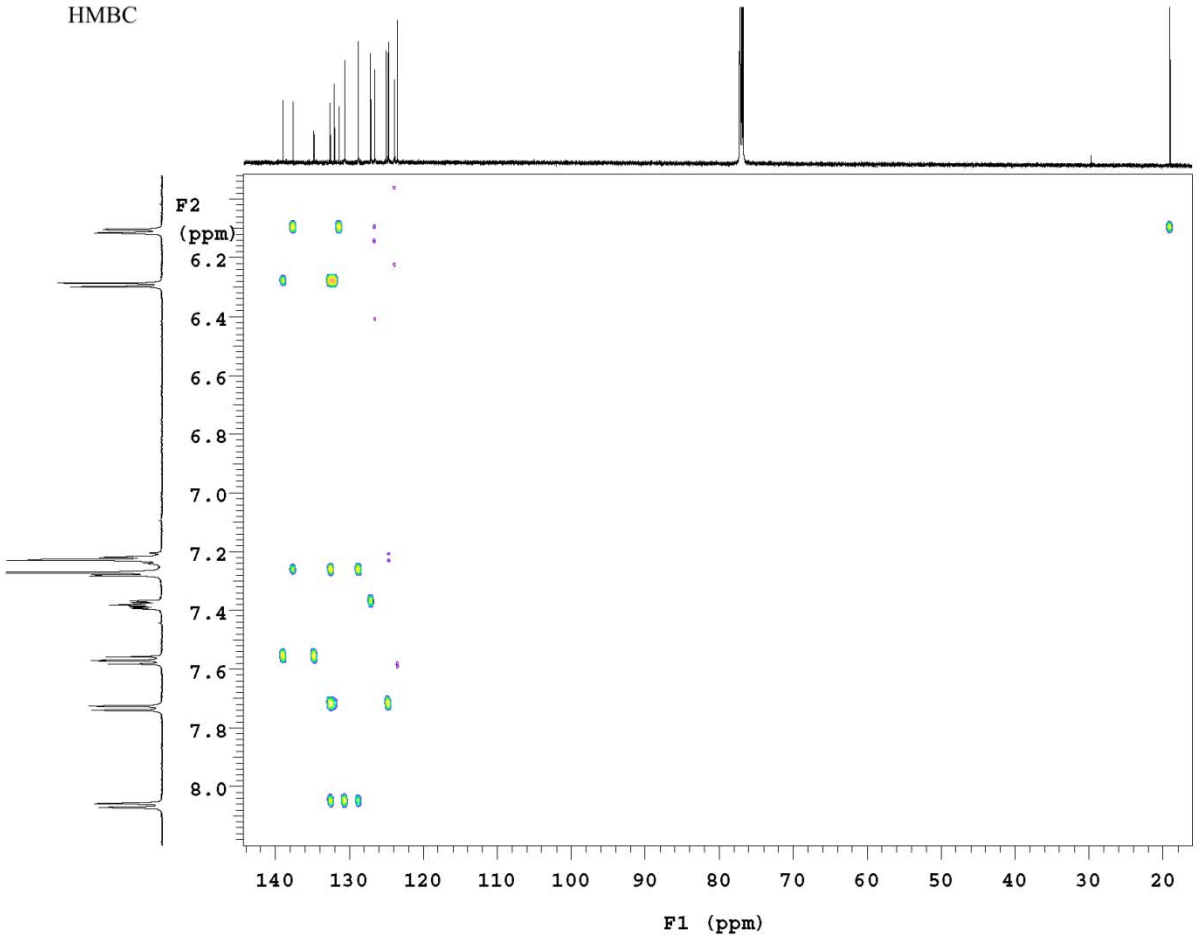


Compound **1**-*anti*

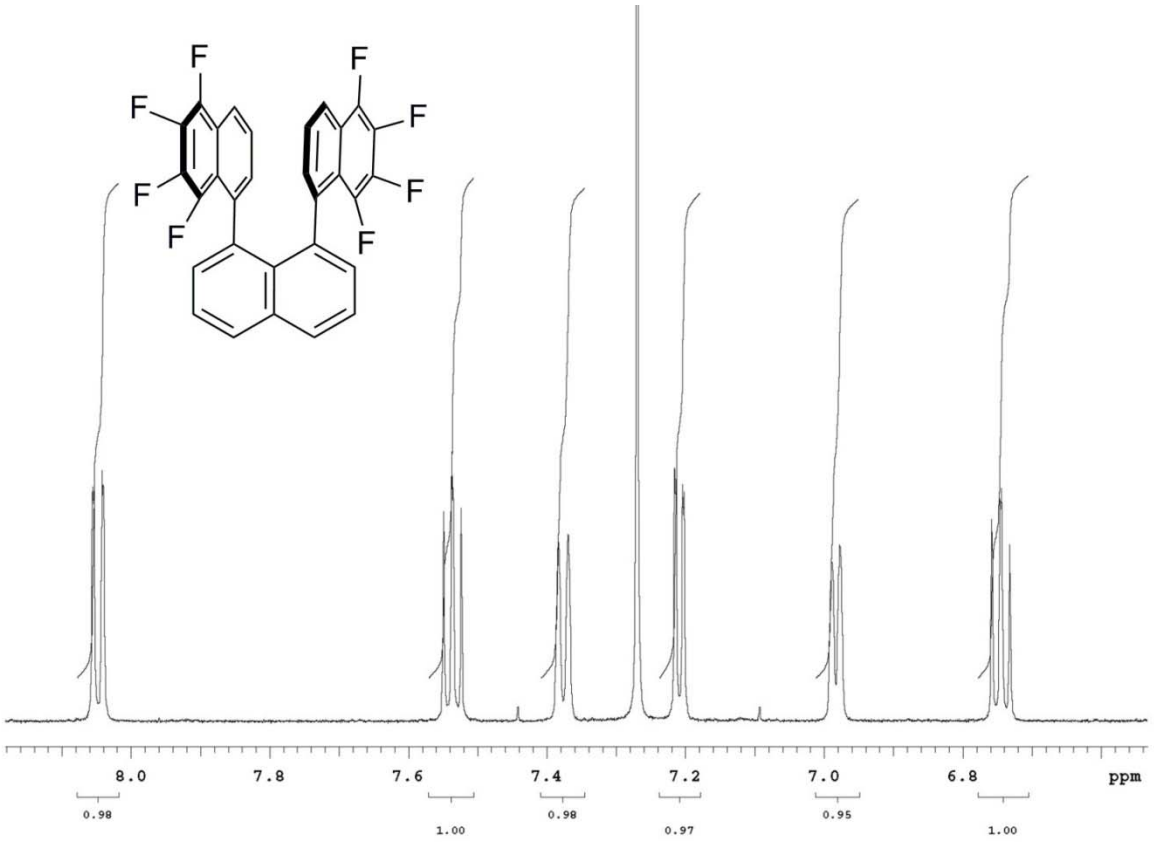




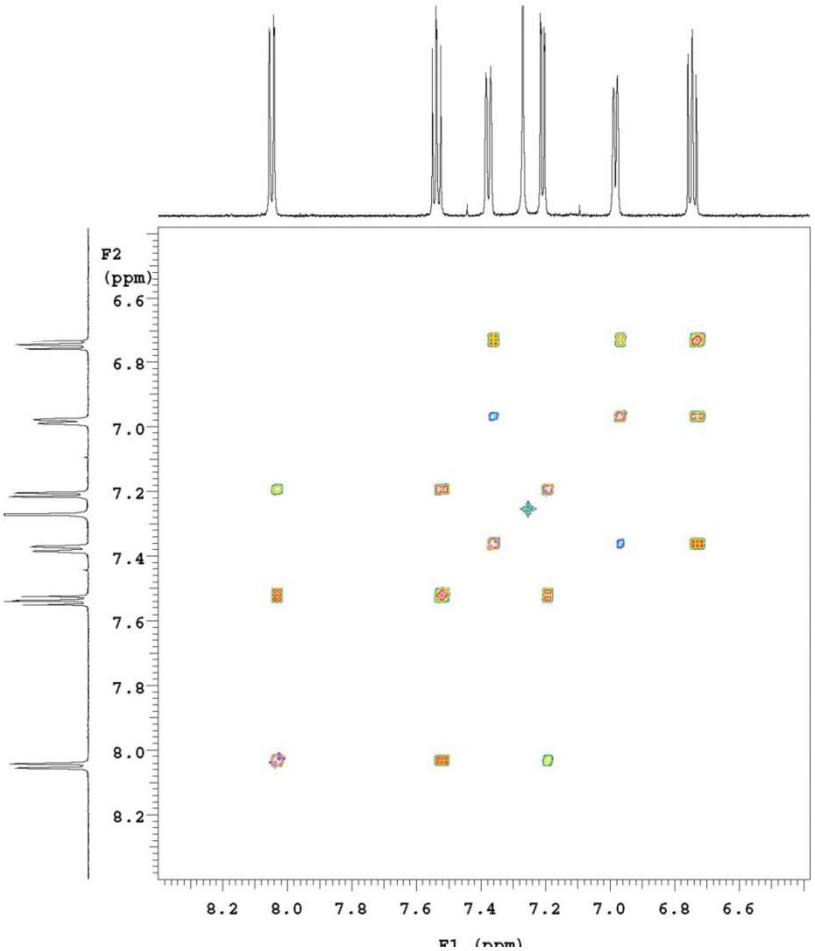
Compound **1**-*anti*



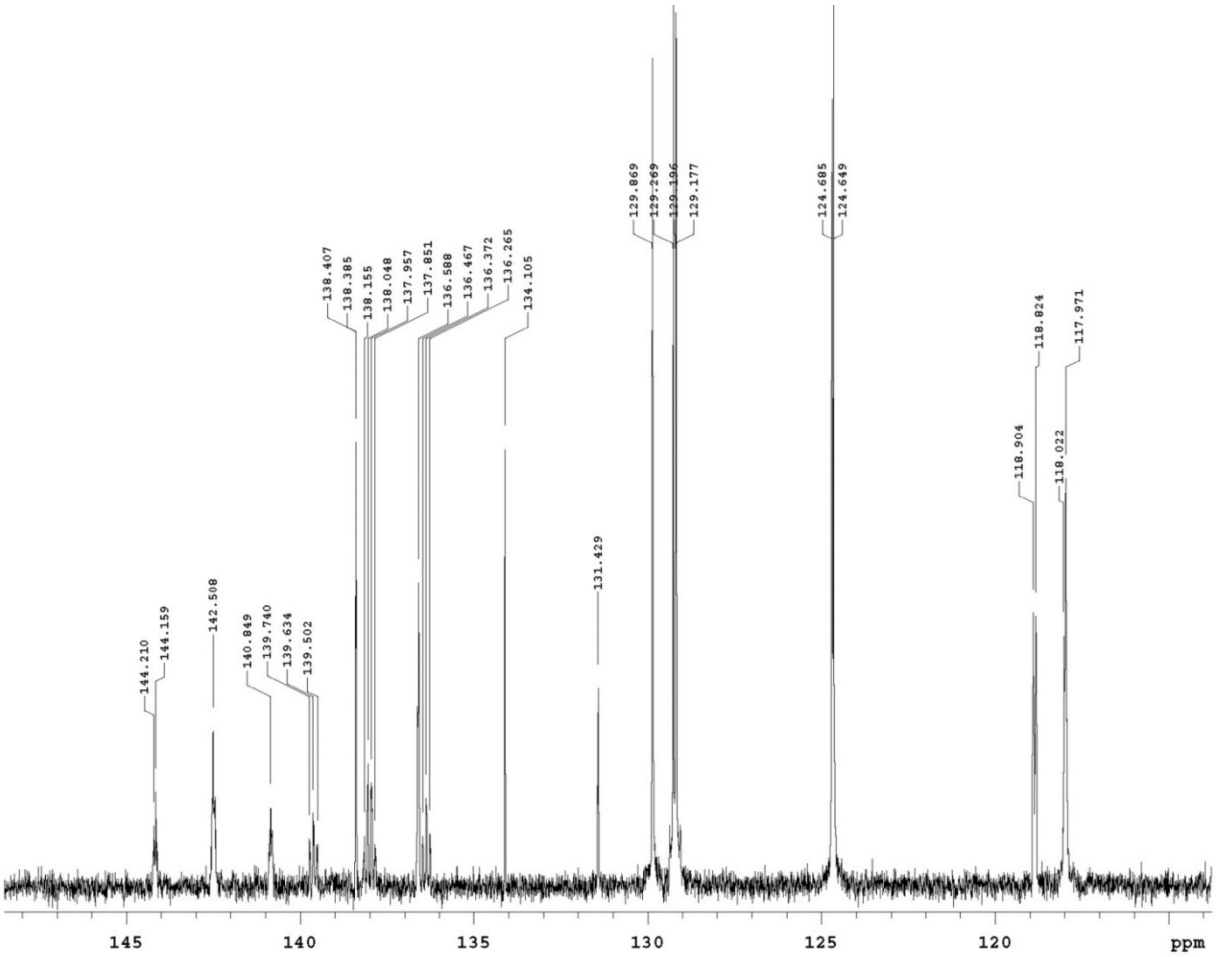
Compound **1**-*anti*

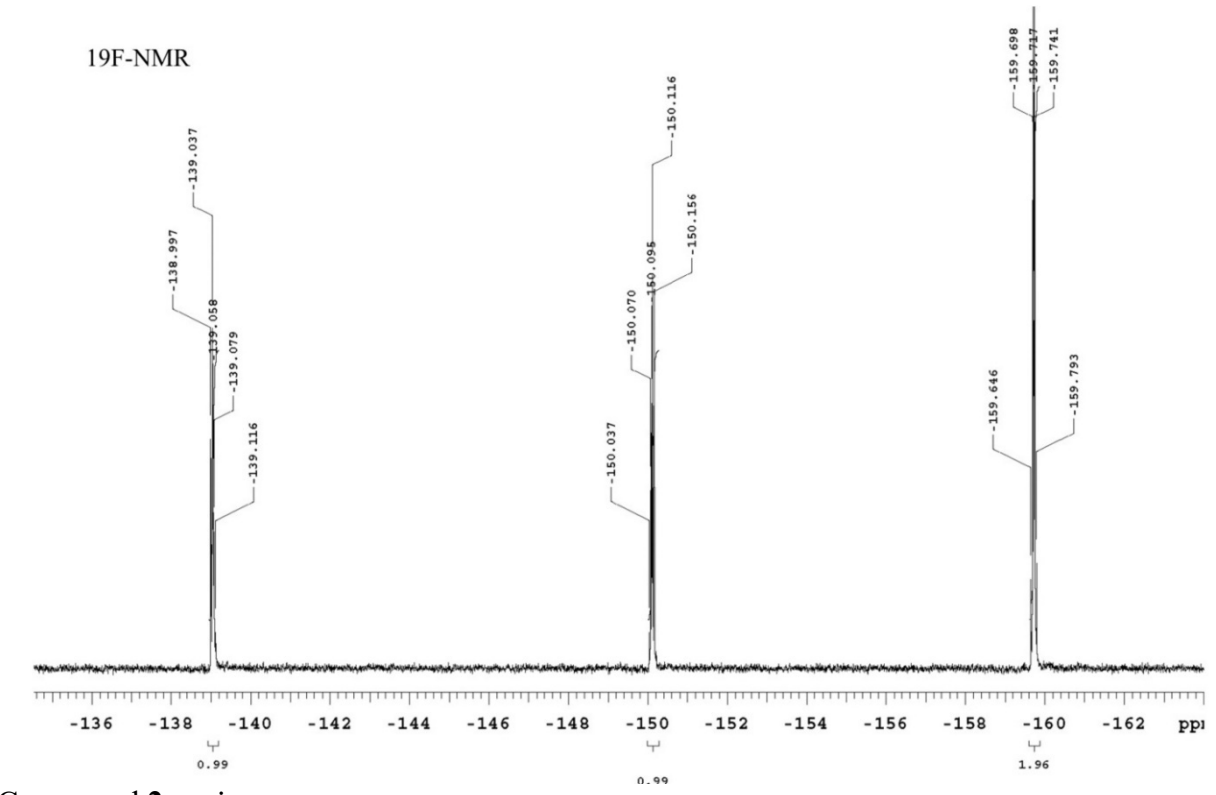


COSY

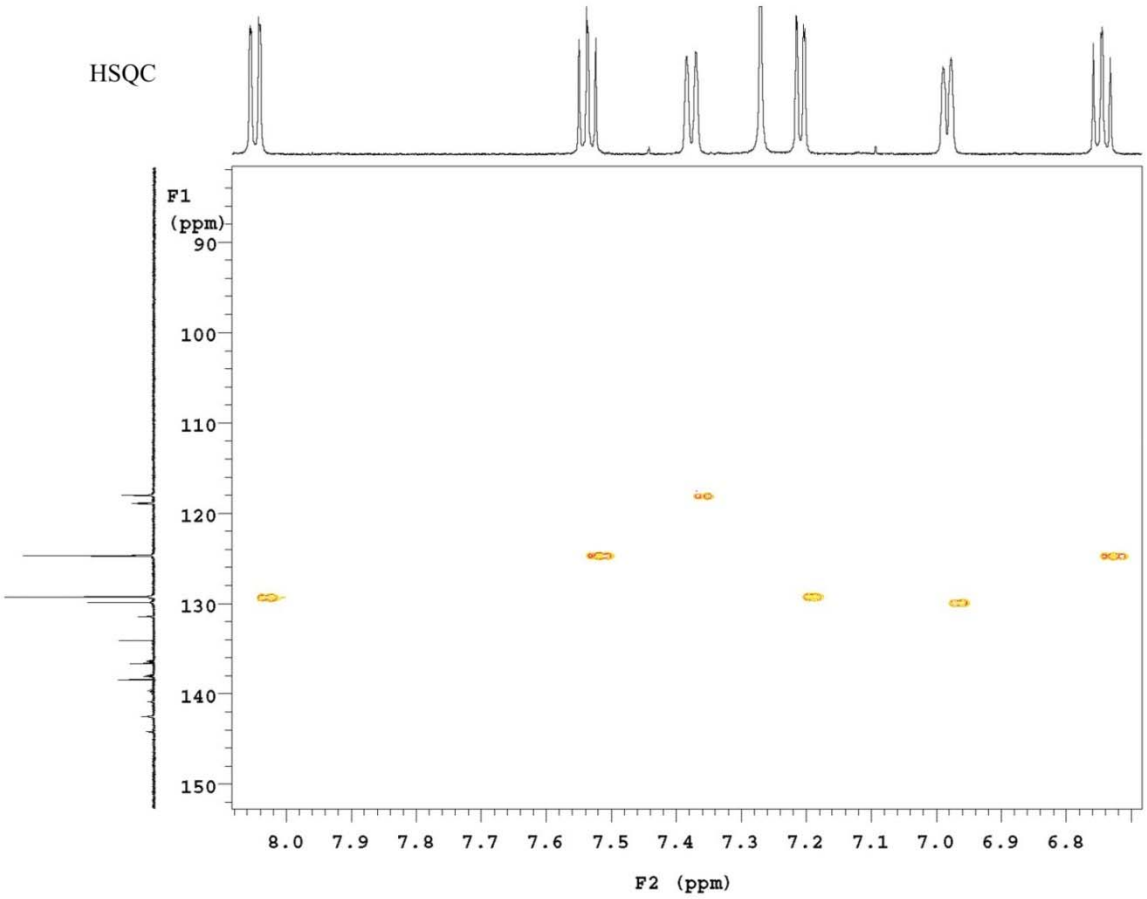


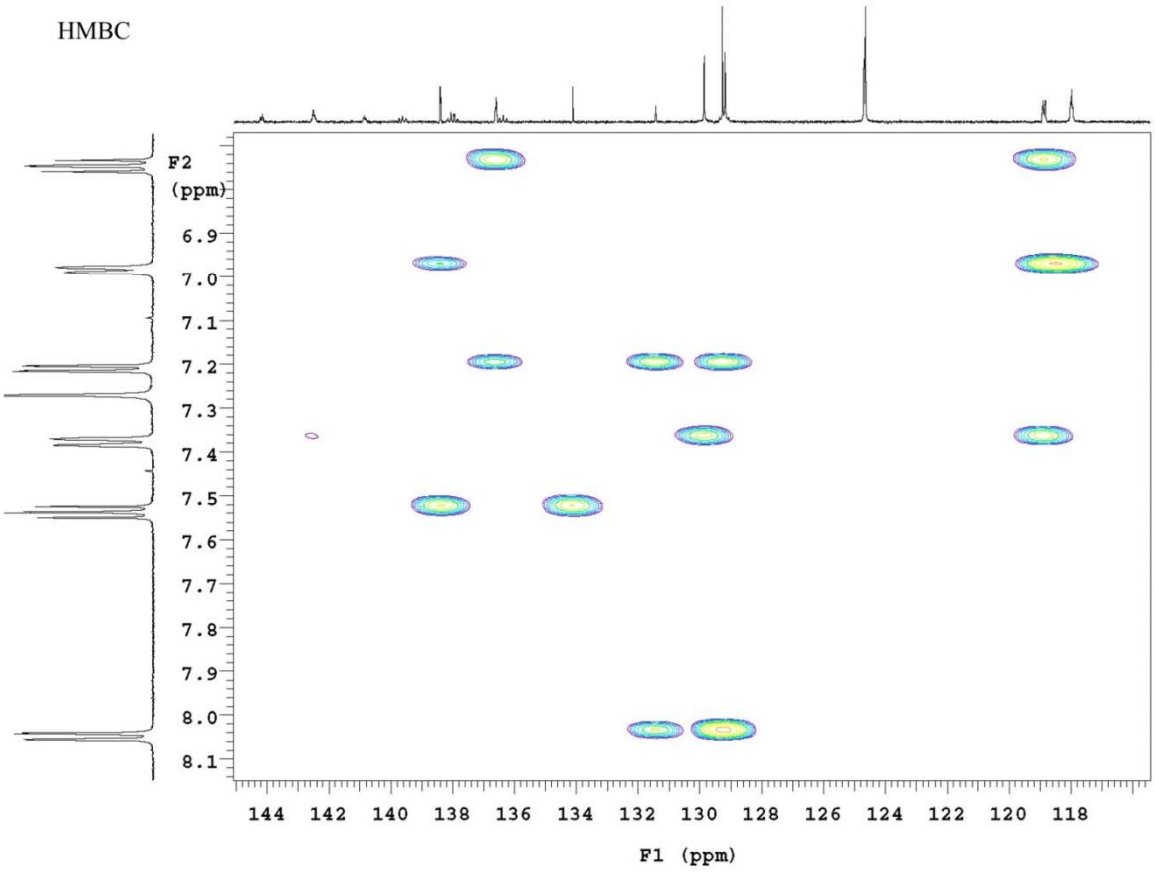
Compound **2**-*anti*



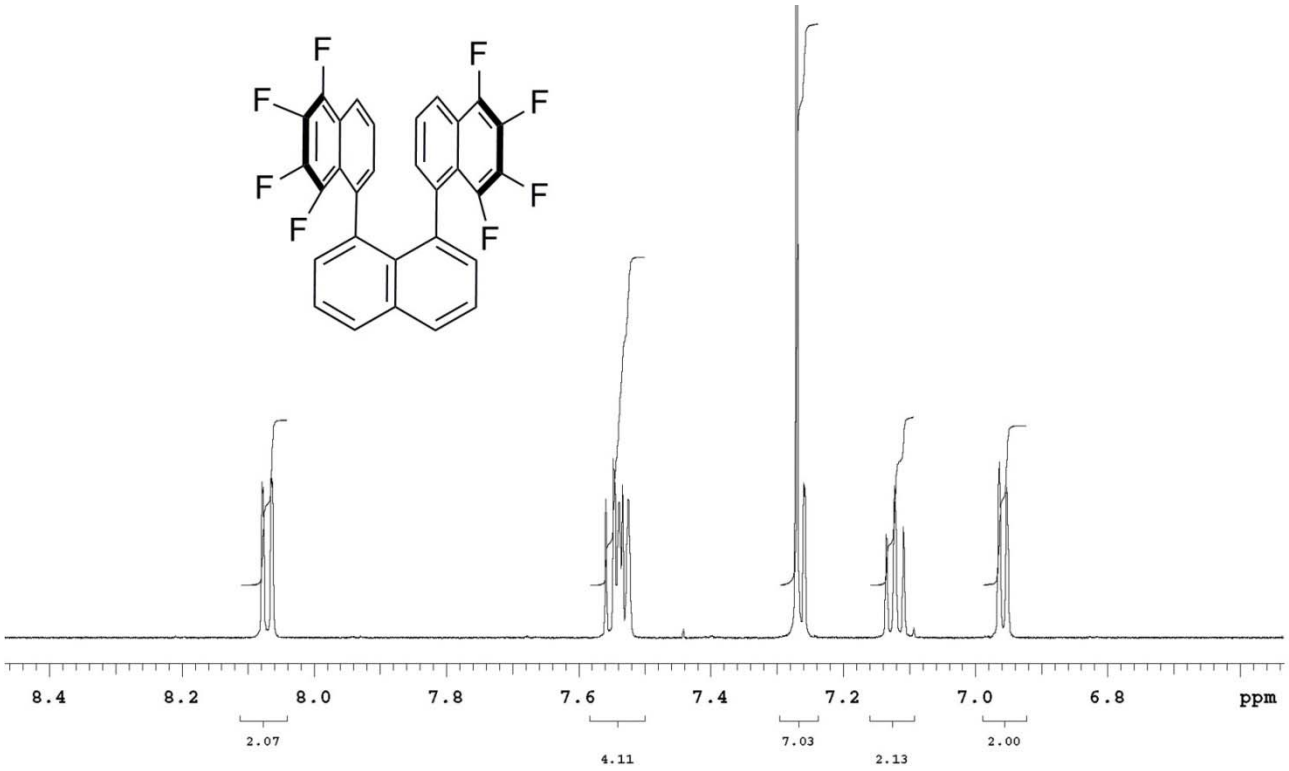


Compound **2**-*anti*

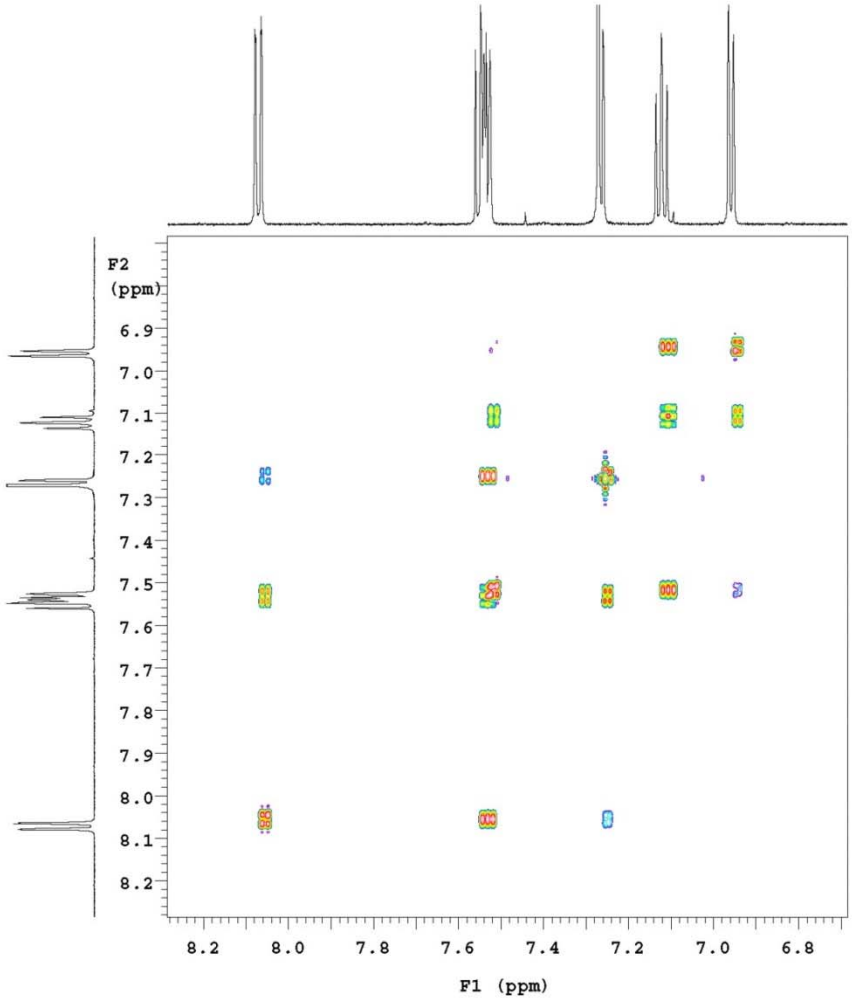




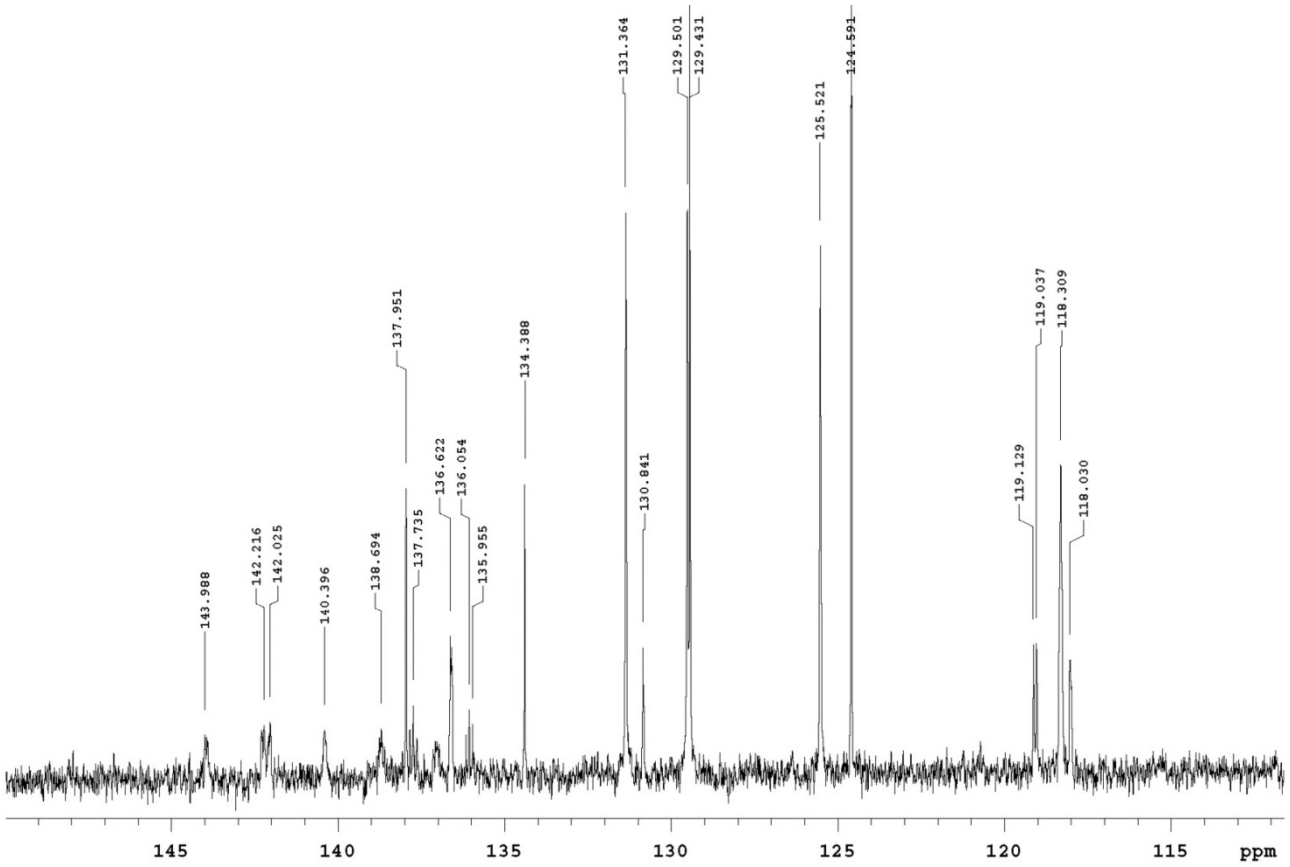
Compound **2**-*anti*



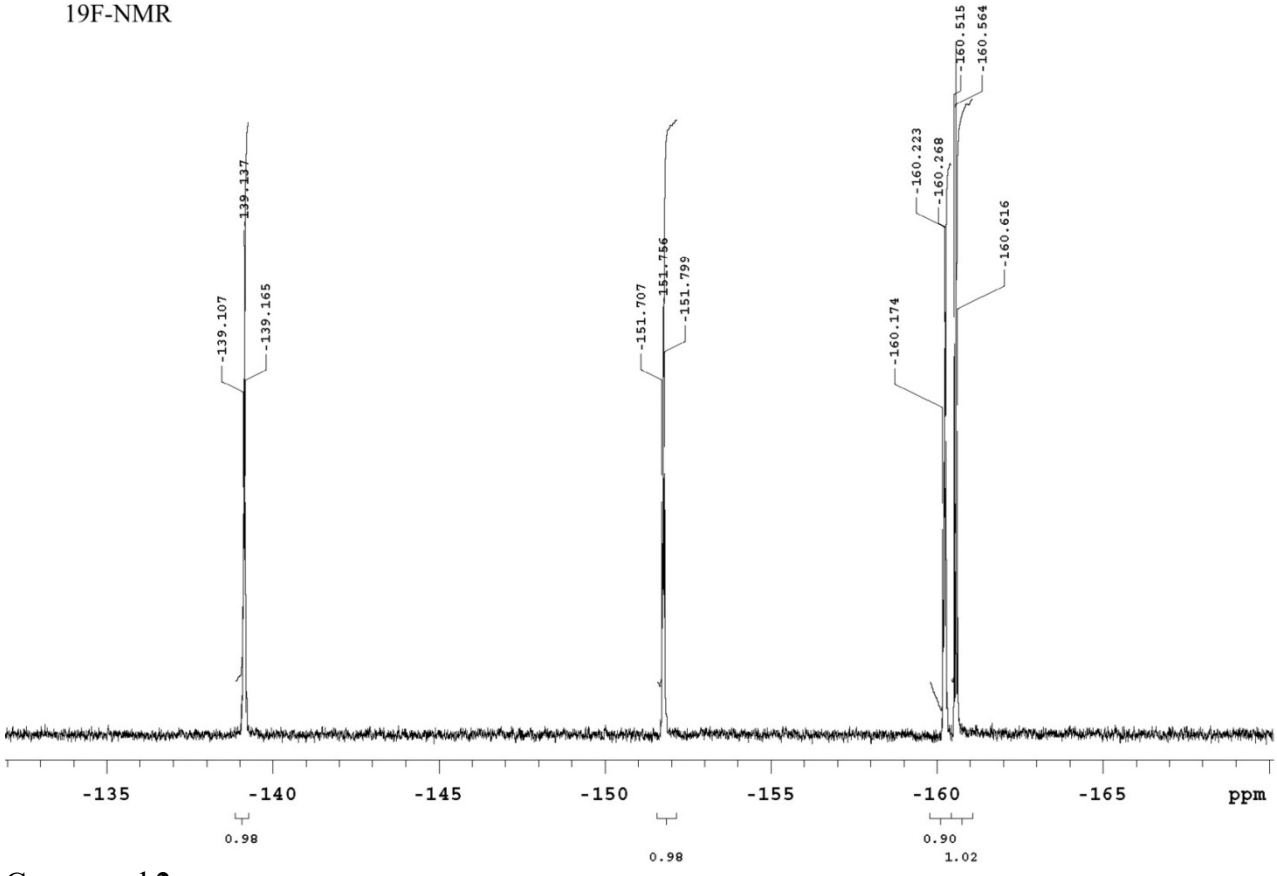
COSY



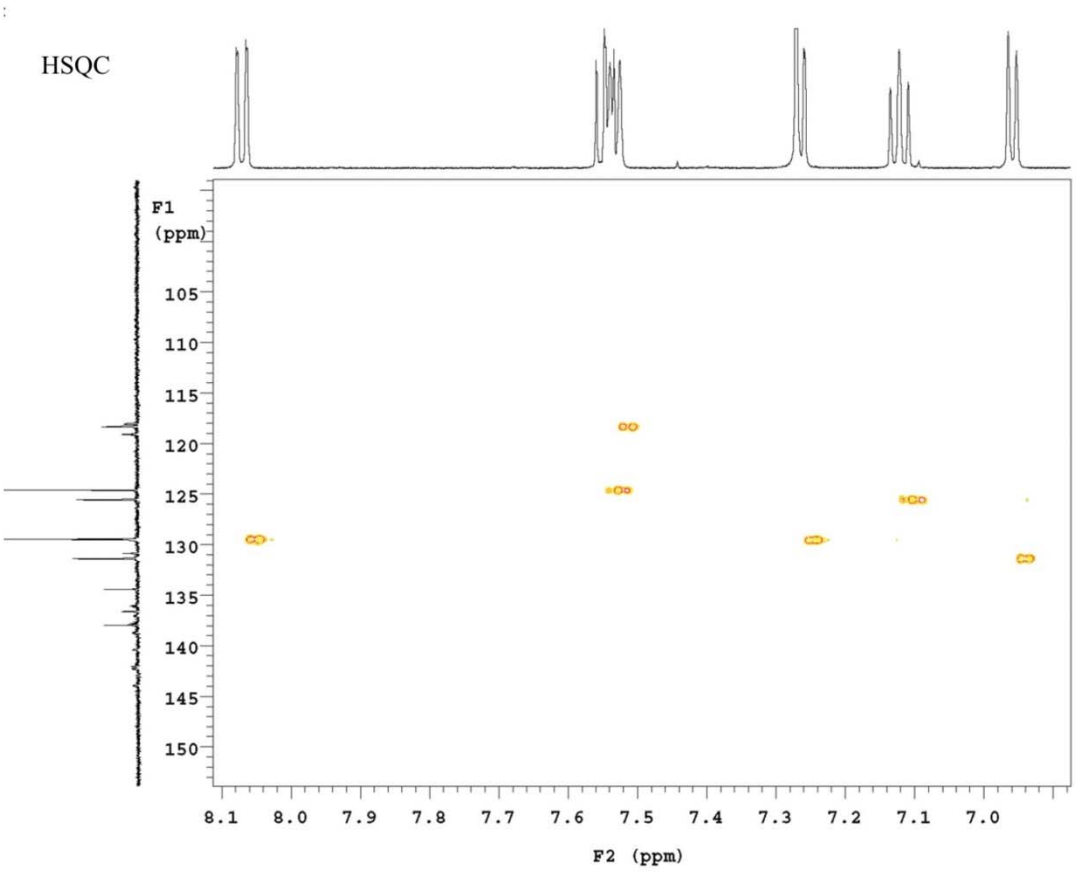
Compound **2**-*syn*

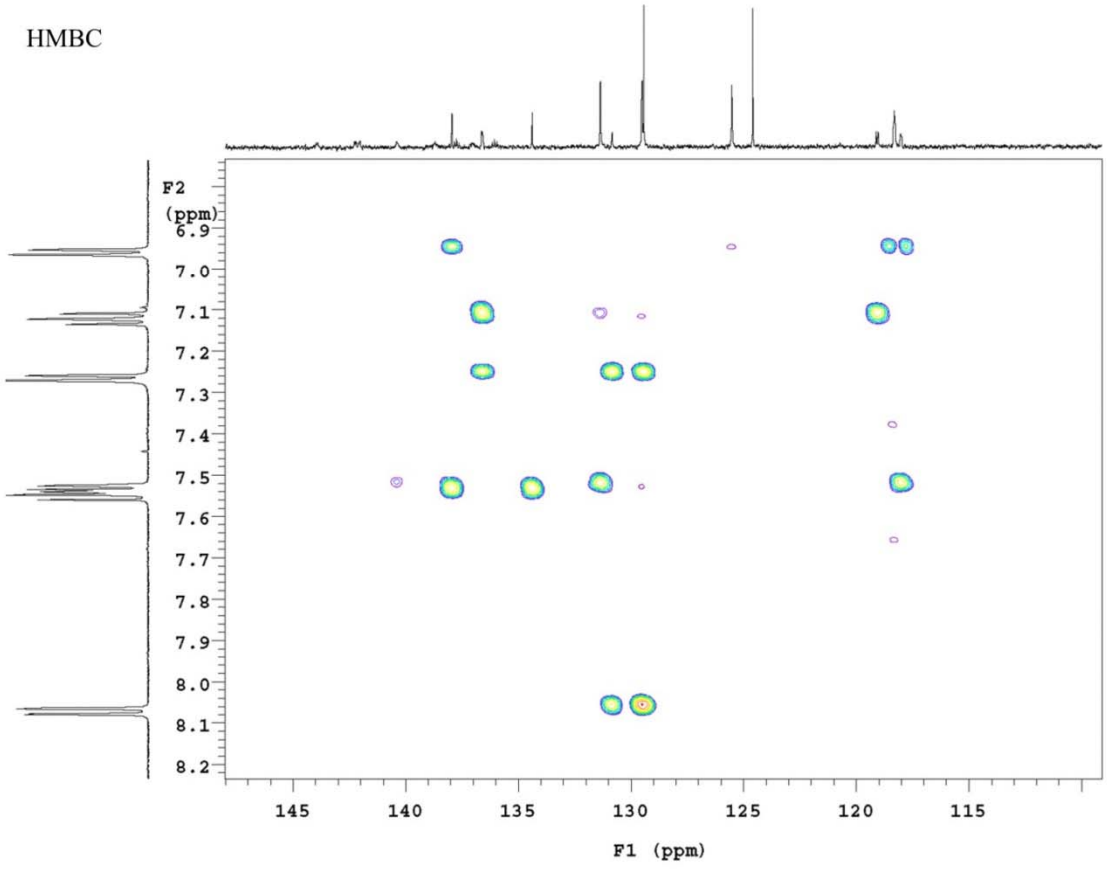


19F-NMR

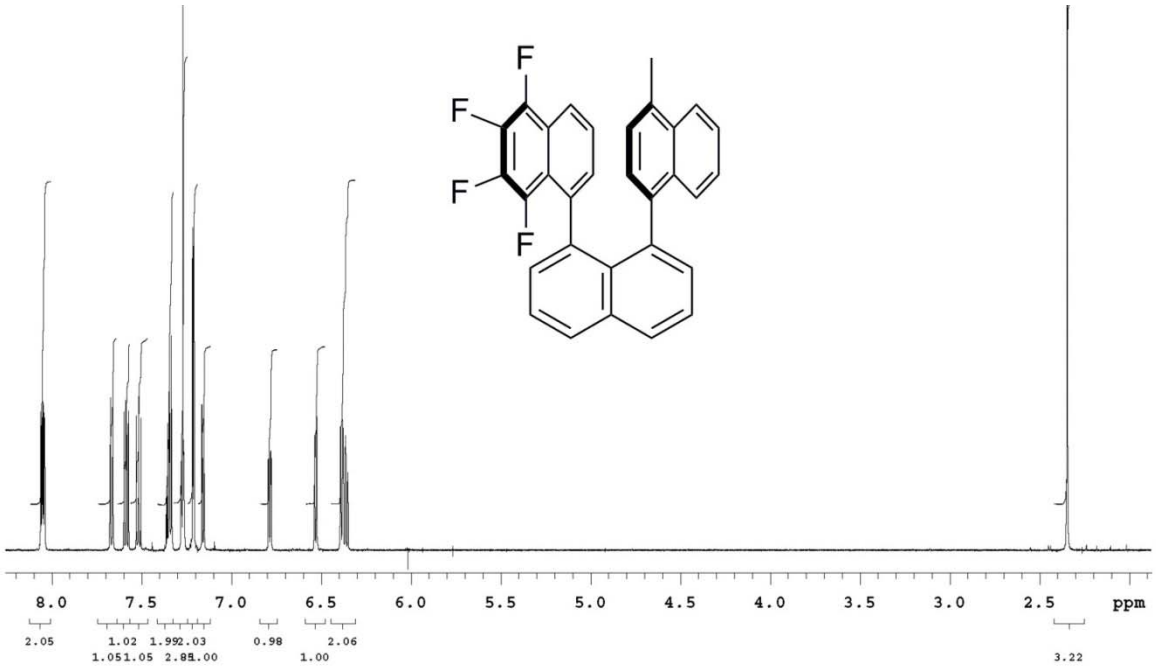


Compound **2**-*syn*





Compound **2**-*syn*



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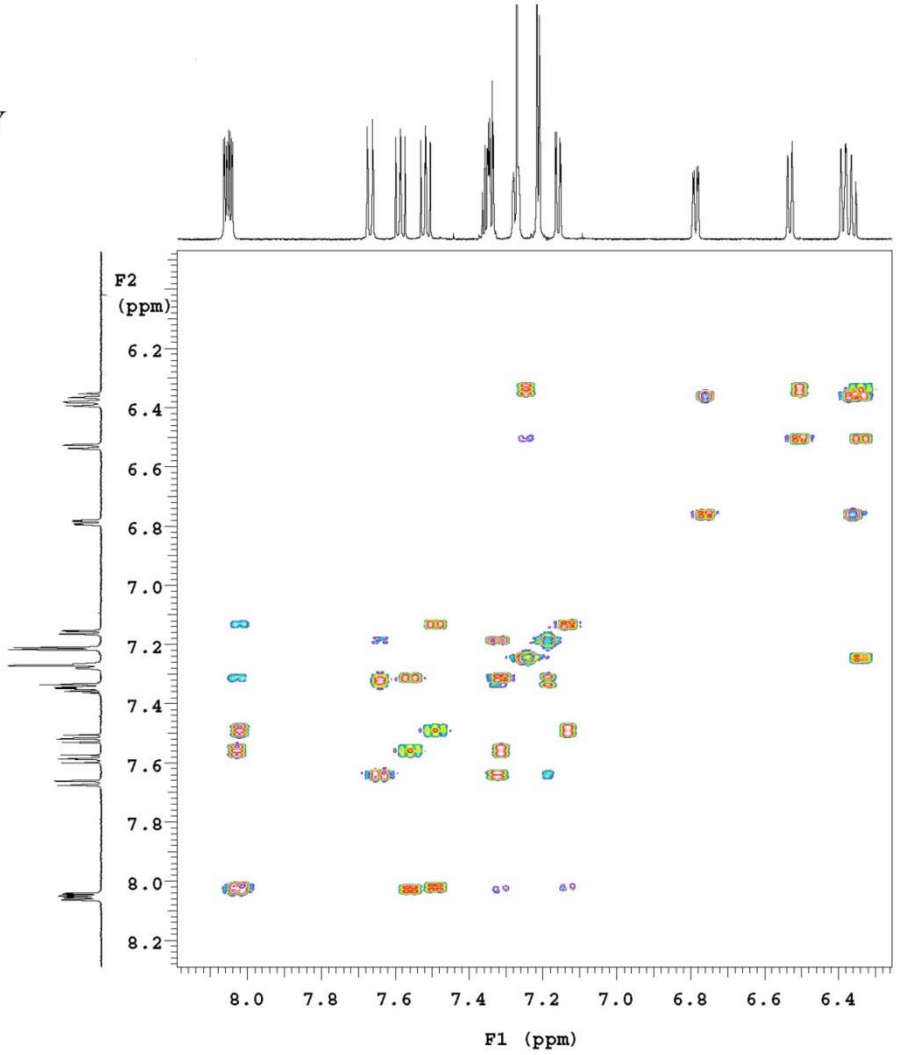
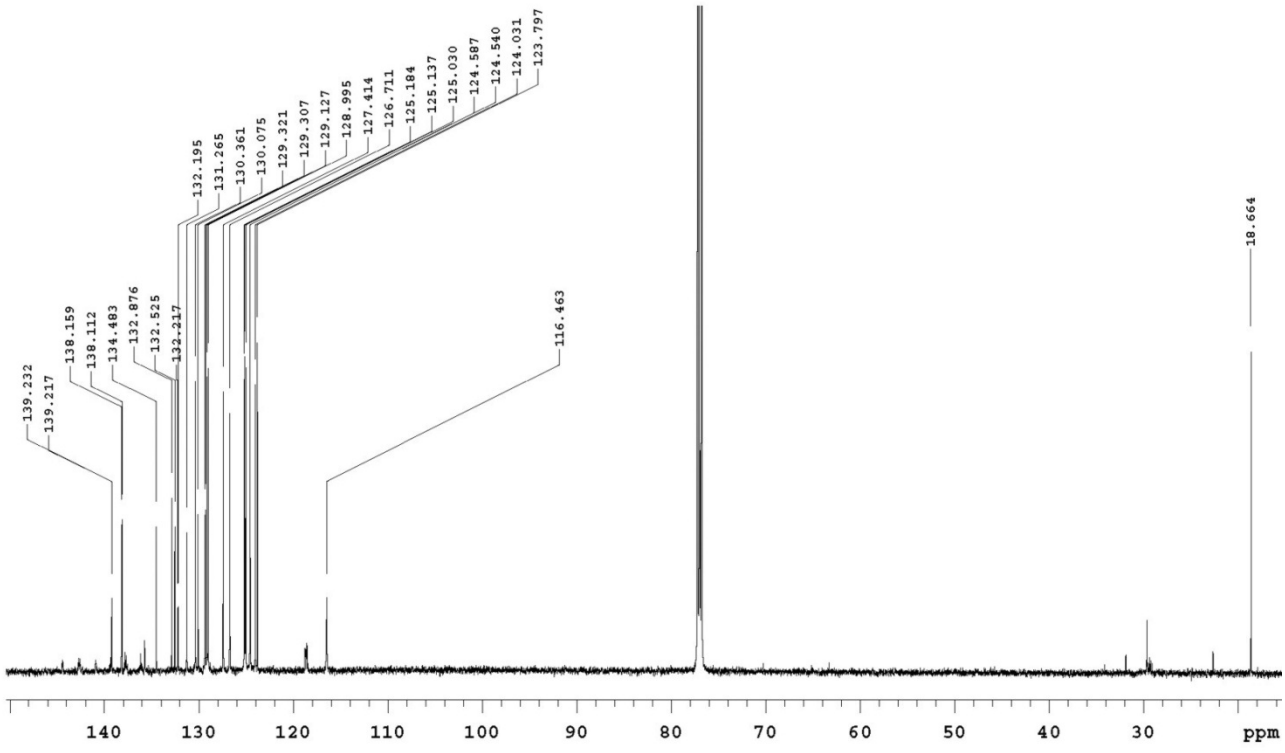
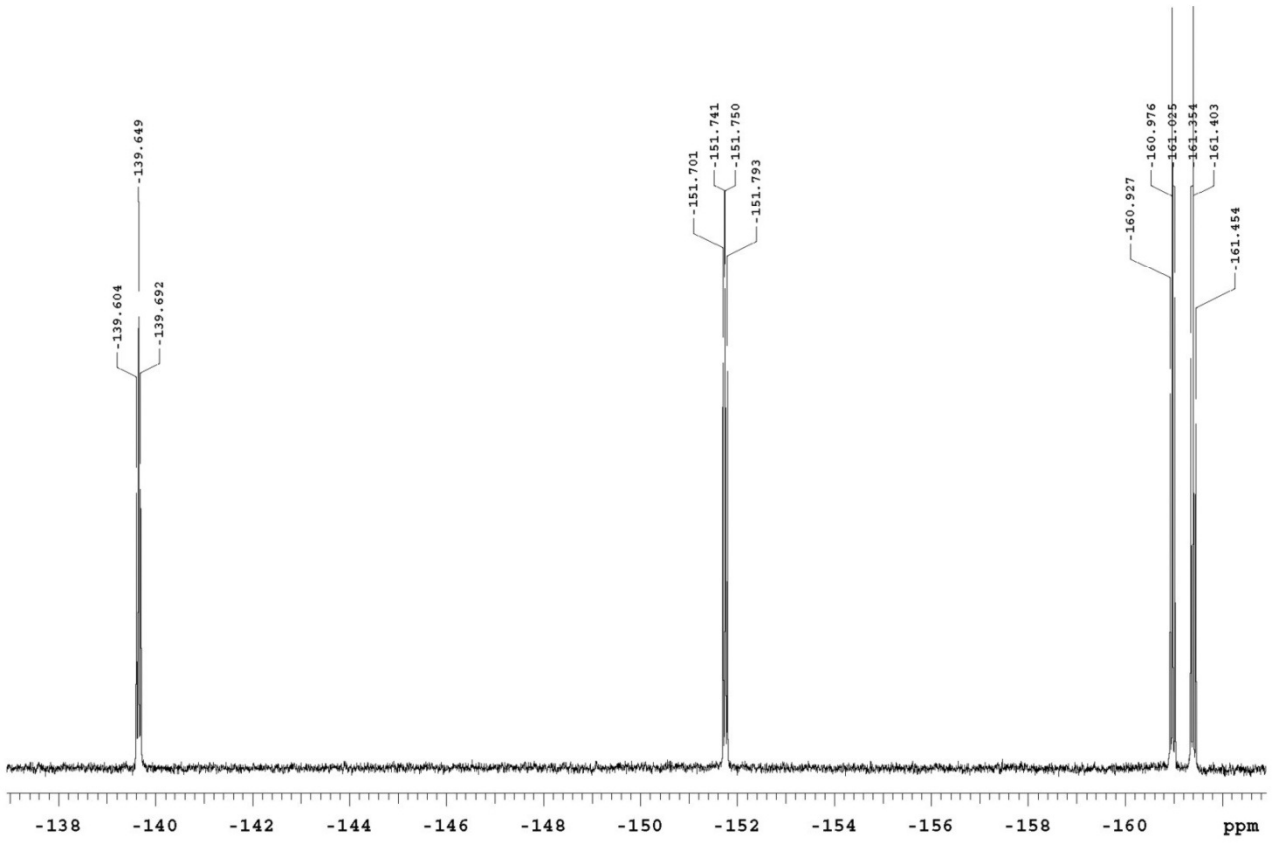


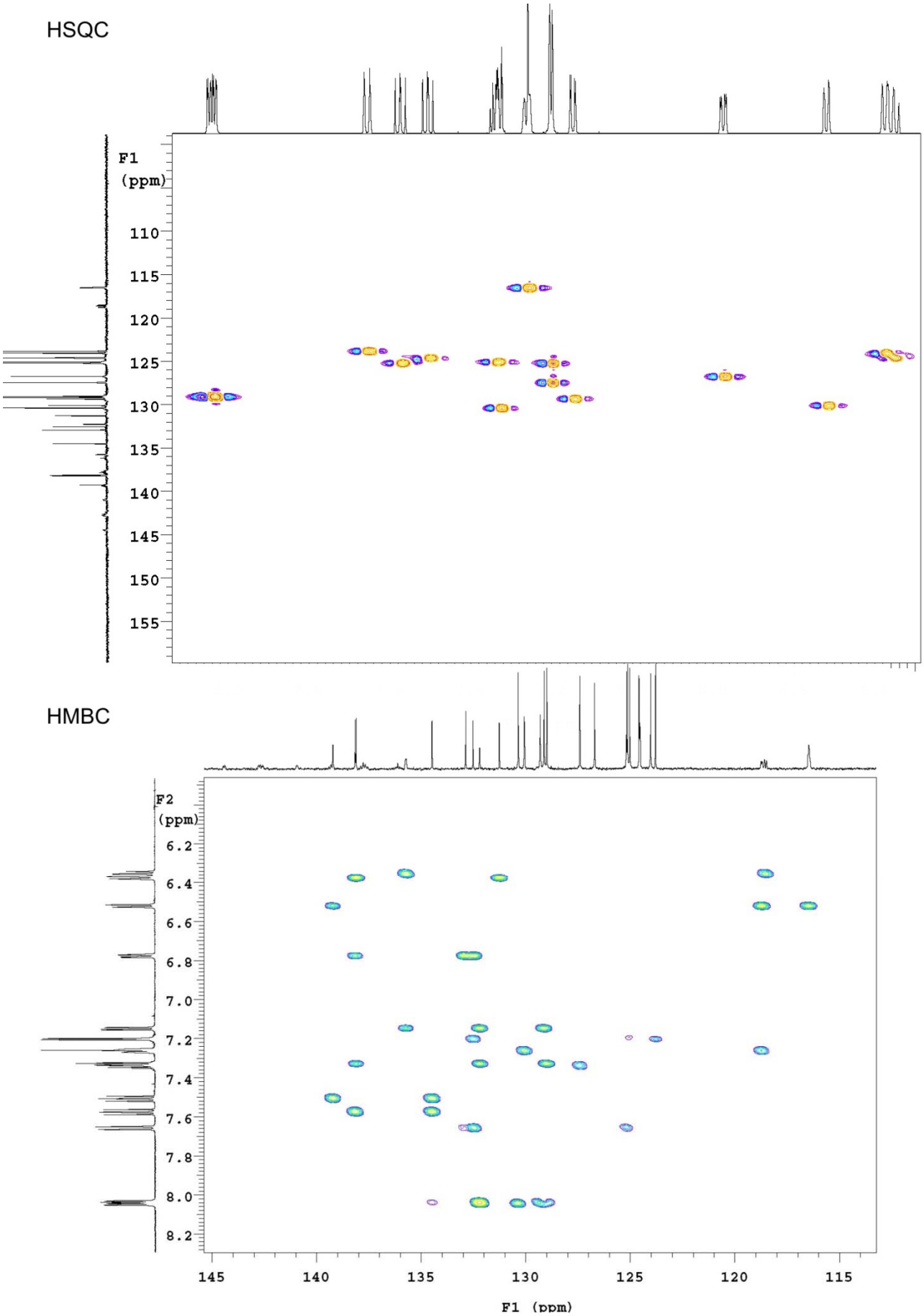
Compound **3**-*anti*



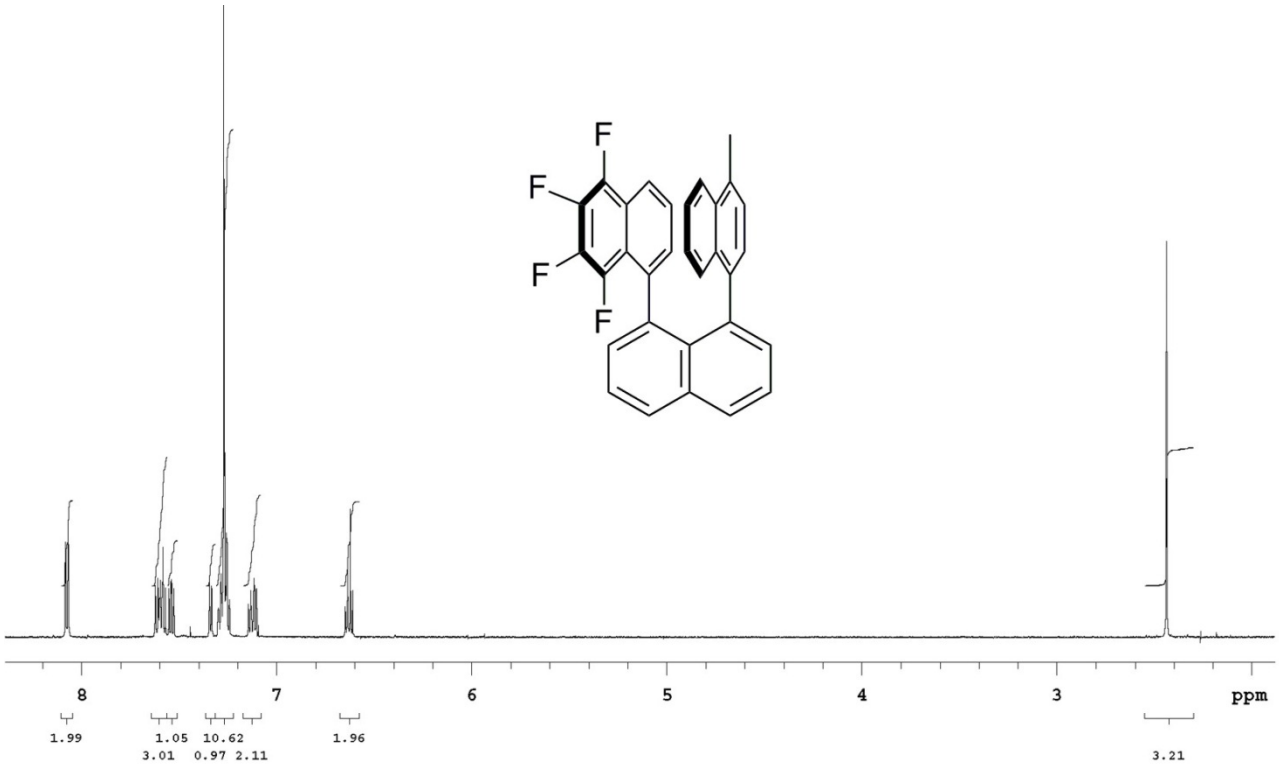
19F-NMR



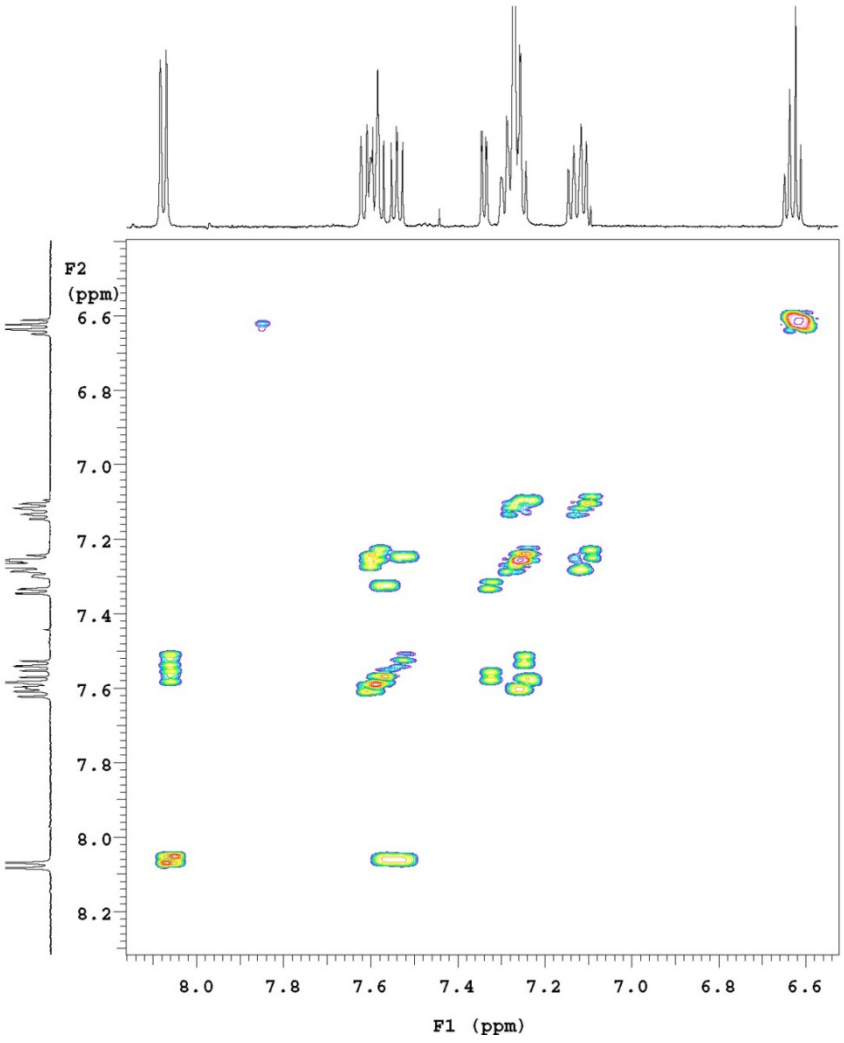
Compound **3**-*anti*



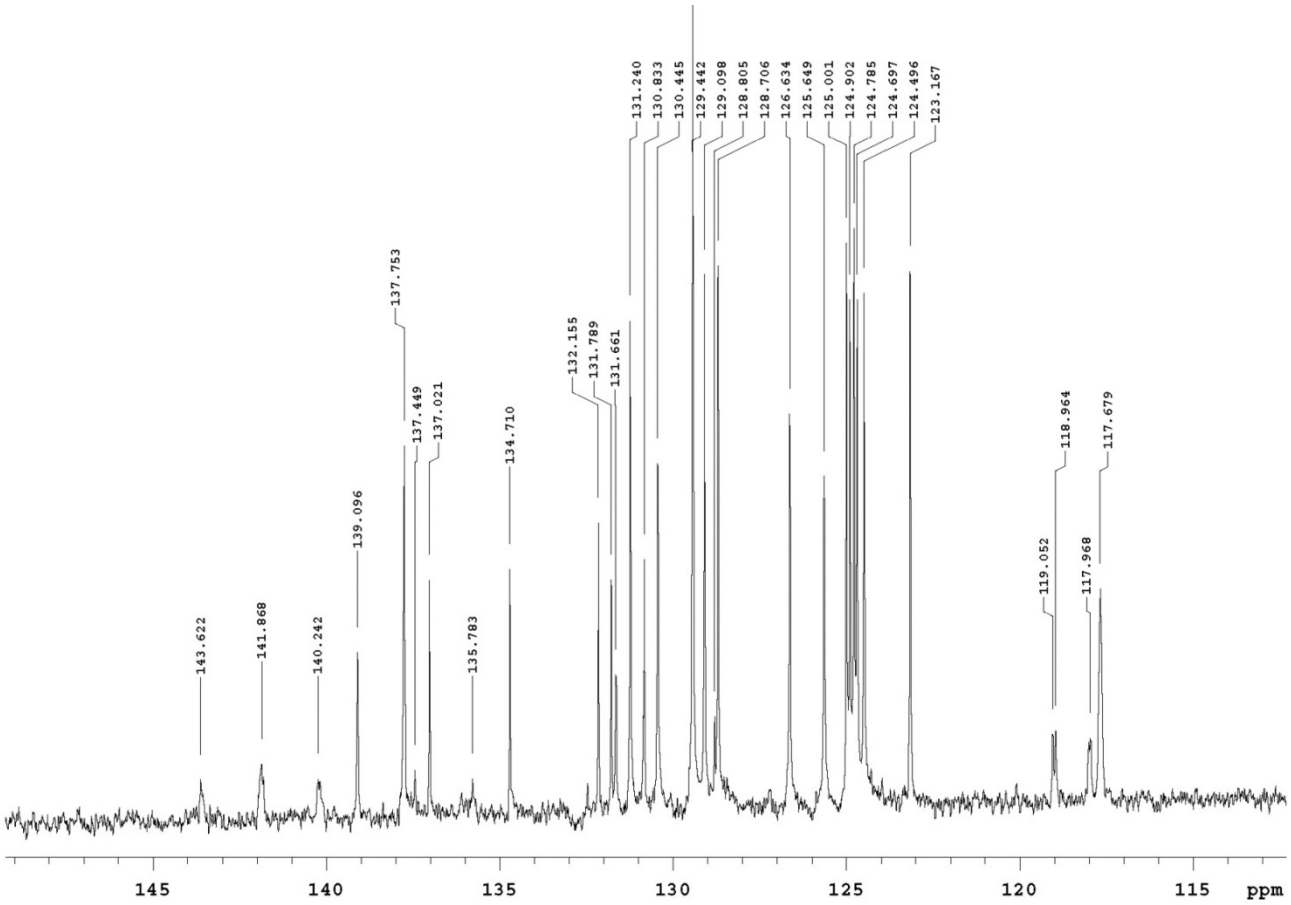
Compound **3**-*anti*



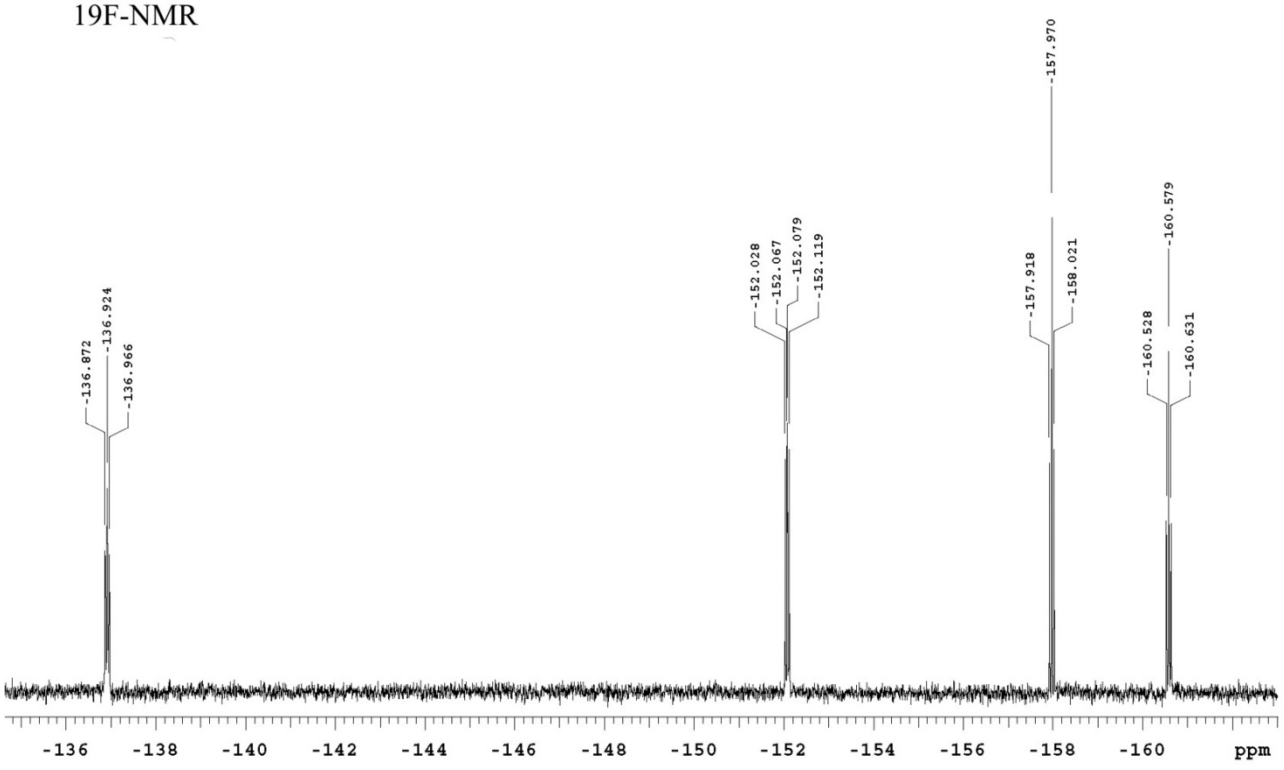
COSY



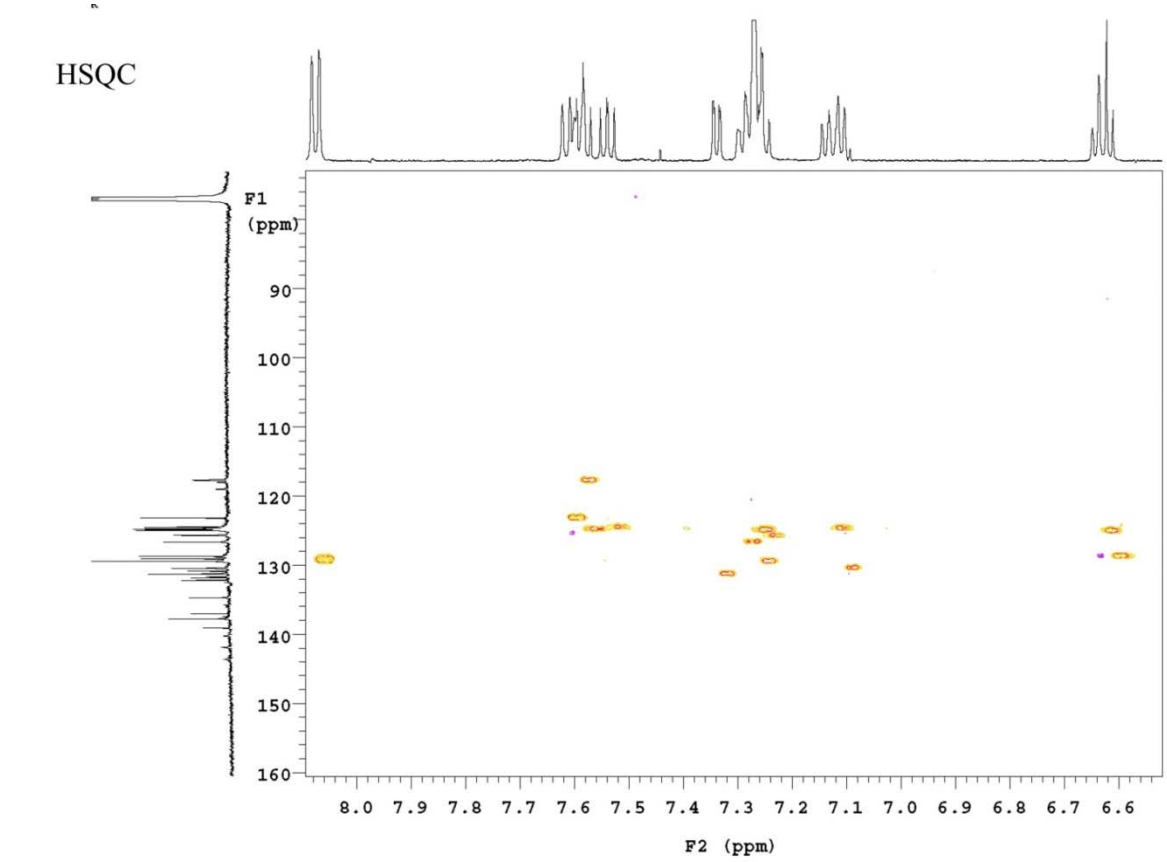
Compound **3**-*syn*

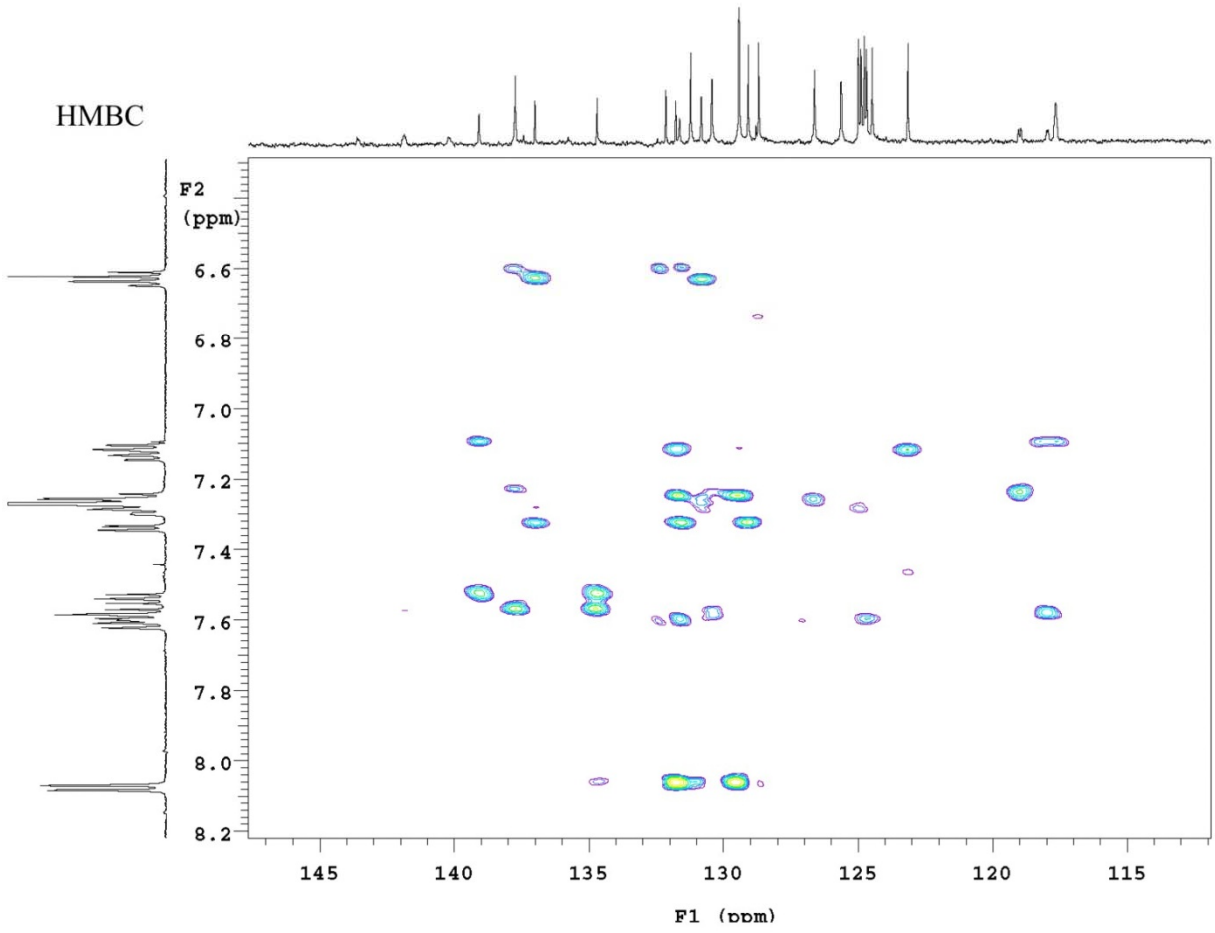


19F-NMR



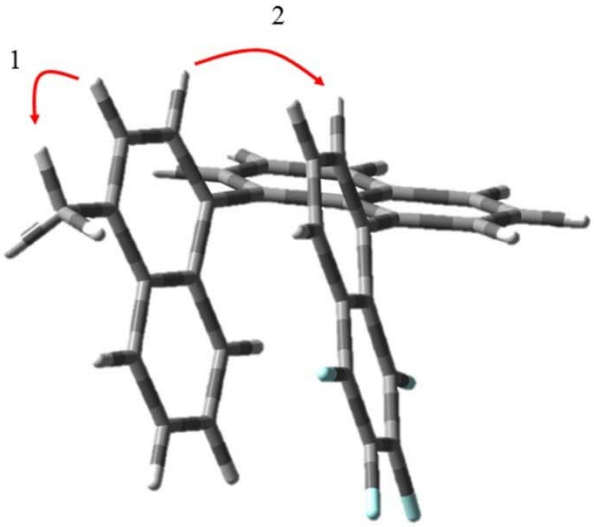
Compound **3**-*syn*





Compound **3**-*syn*

1D-NOE


2
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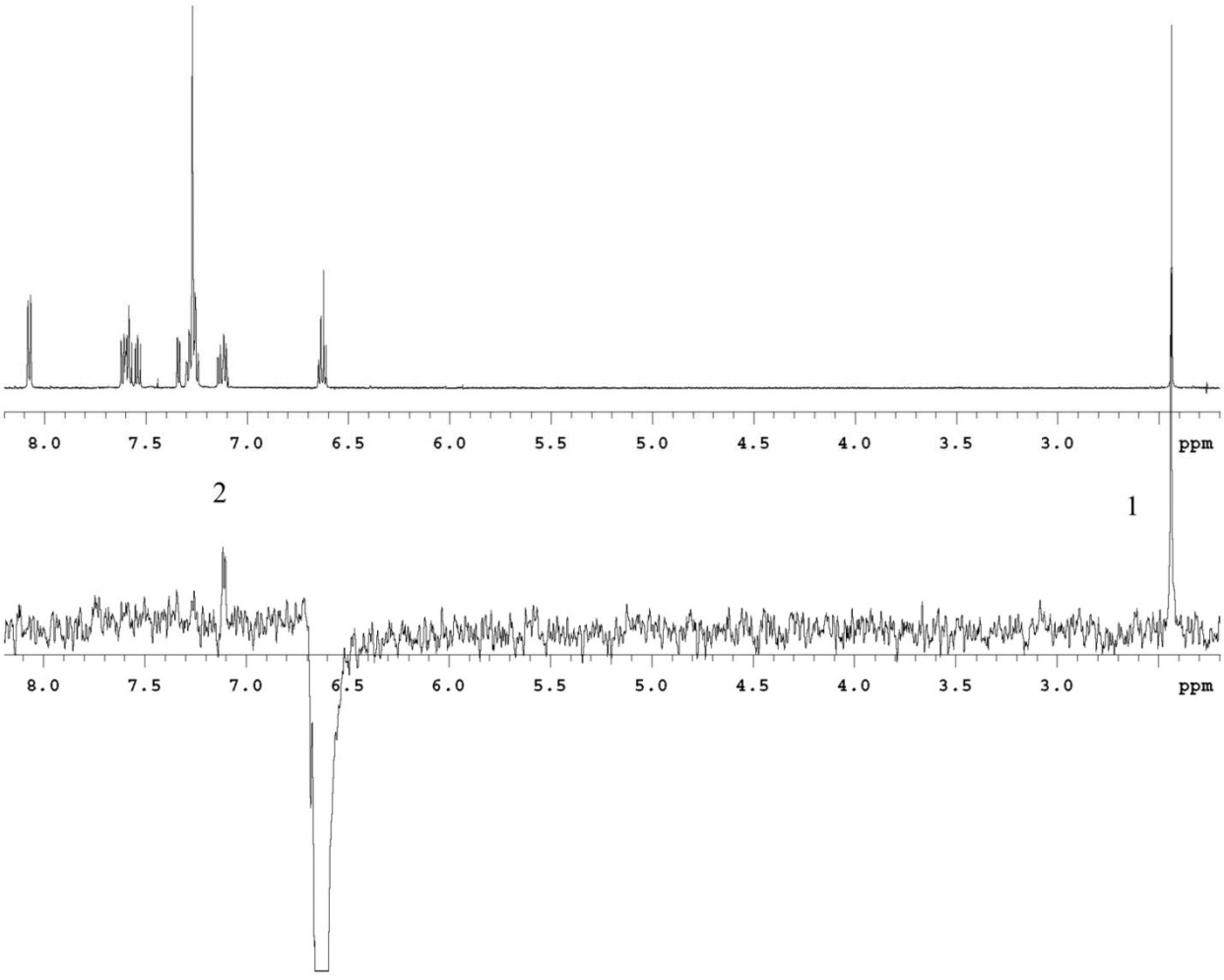
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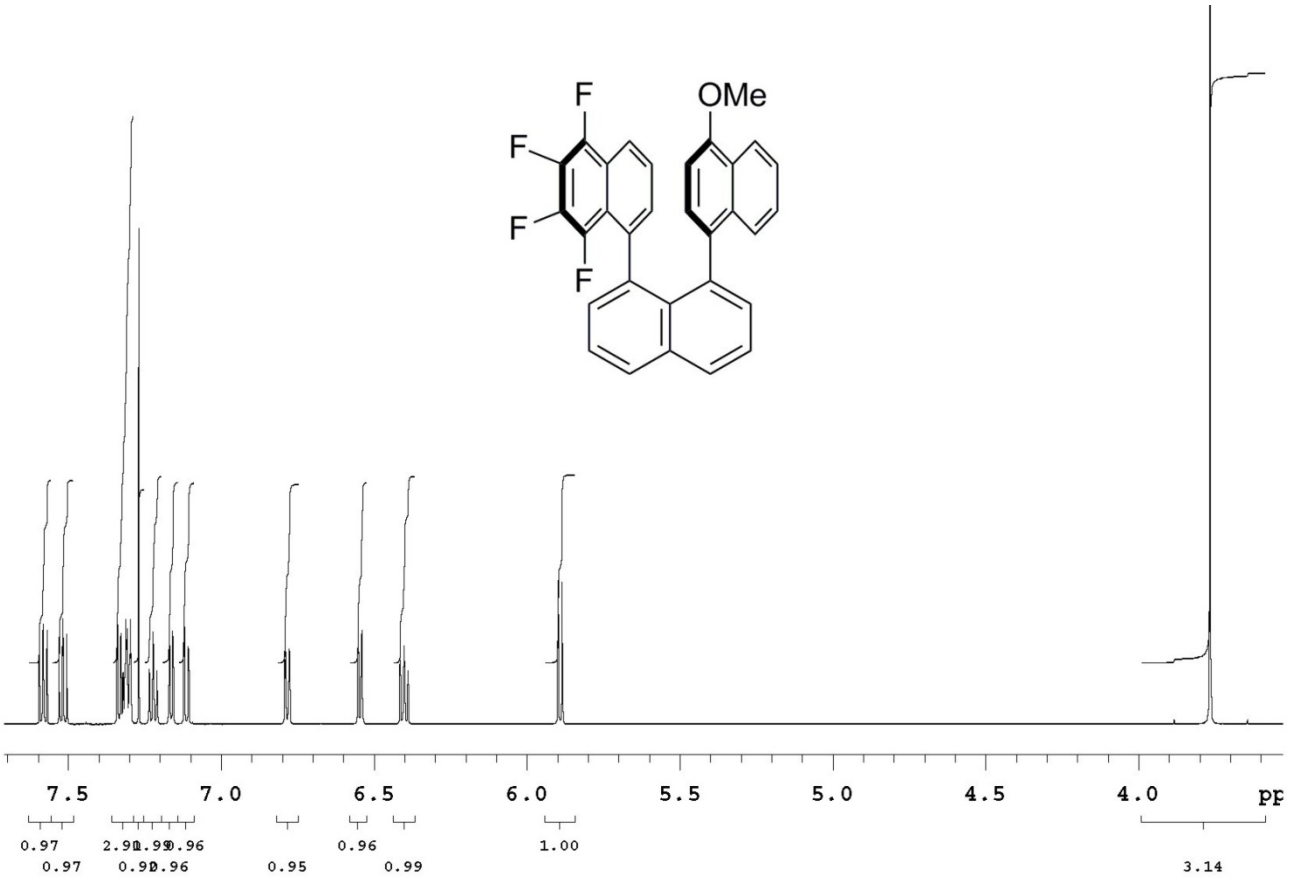
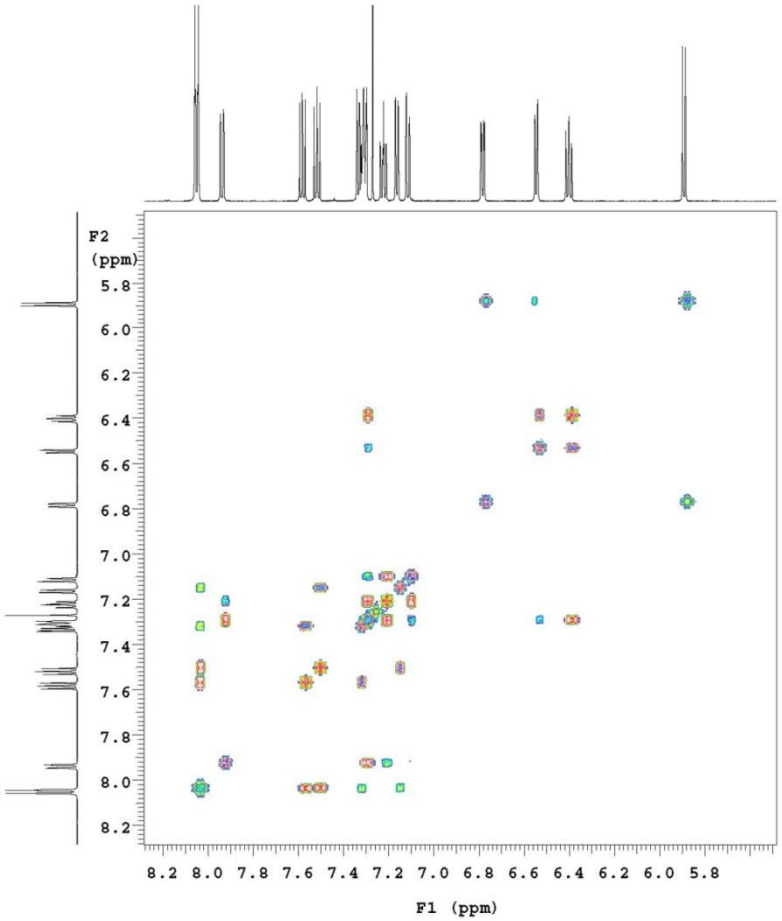
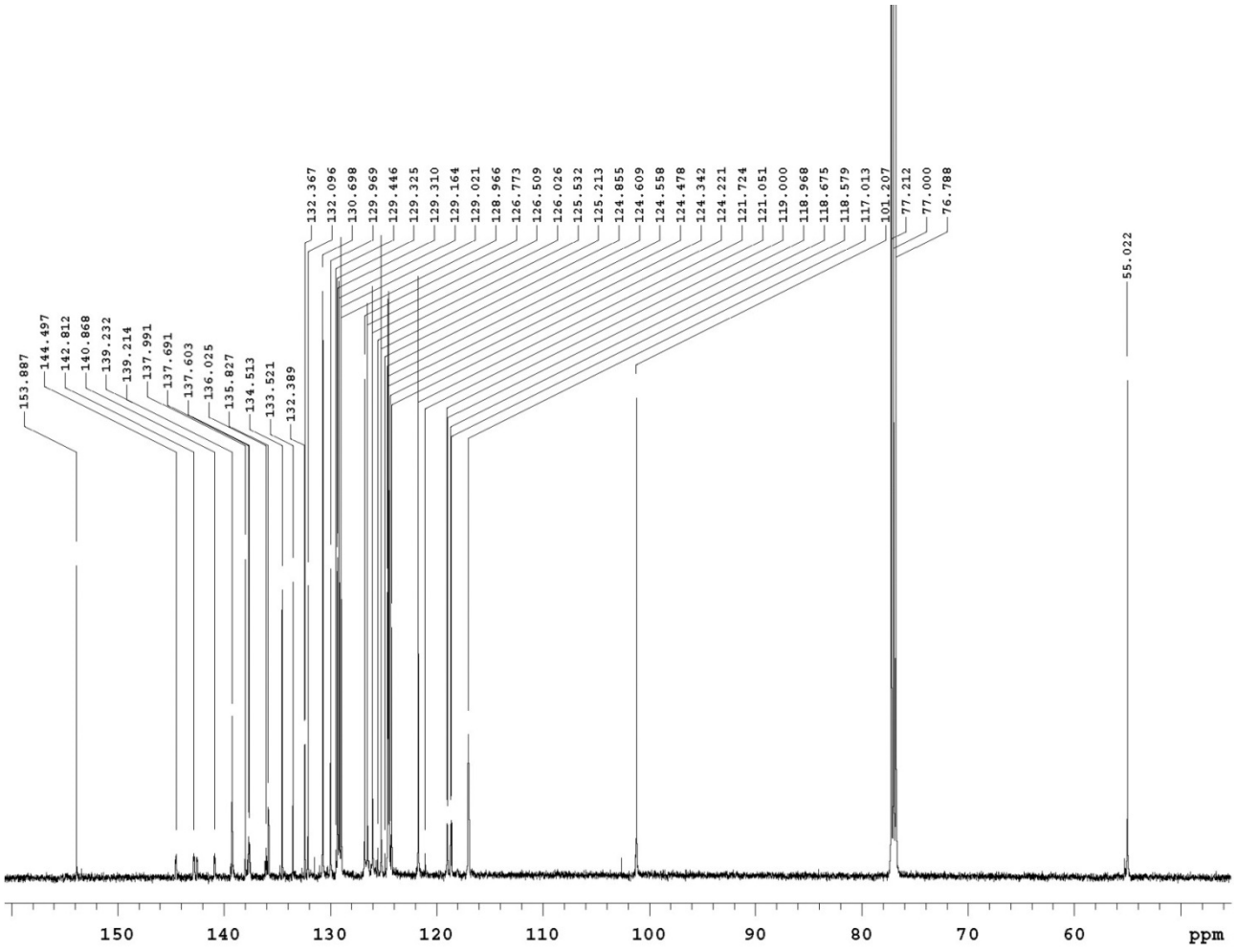


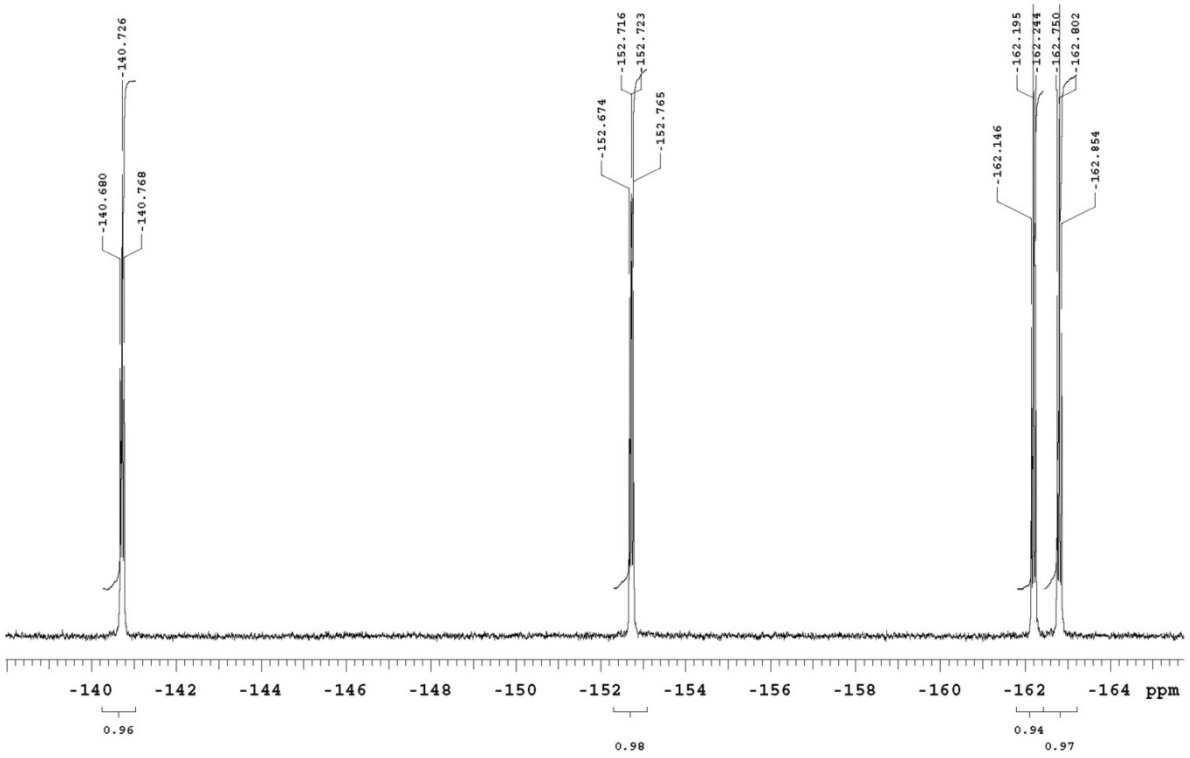
COSY



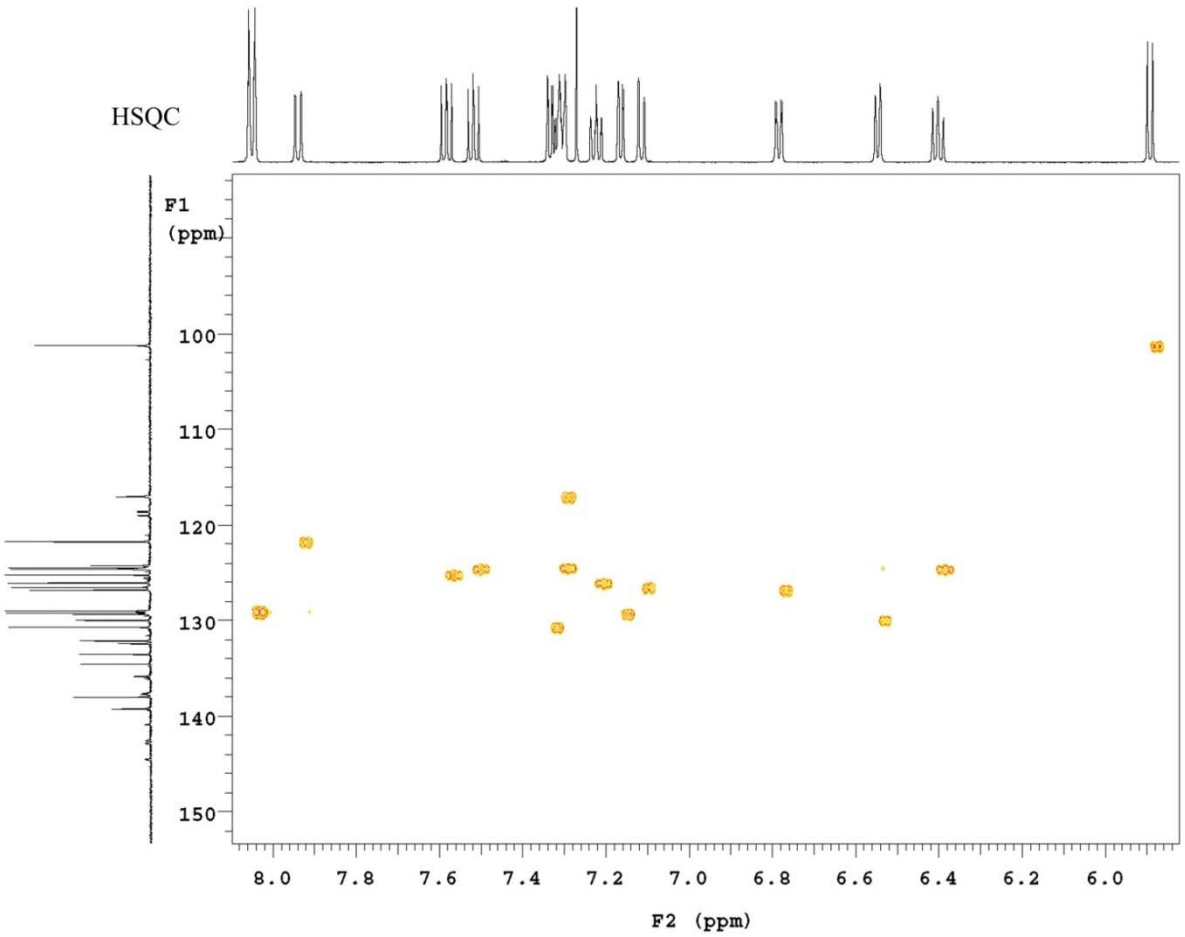
Compound **4**-*anti*

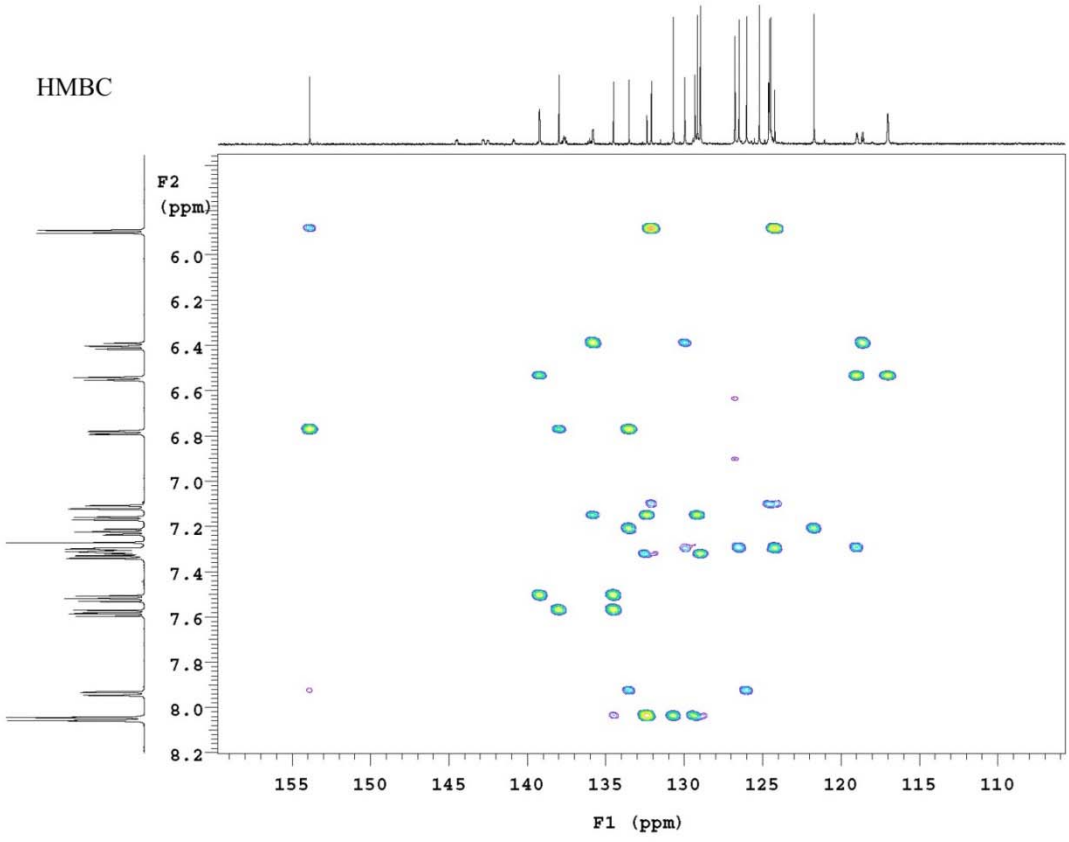


19F-NMR

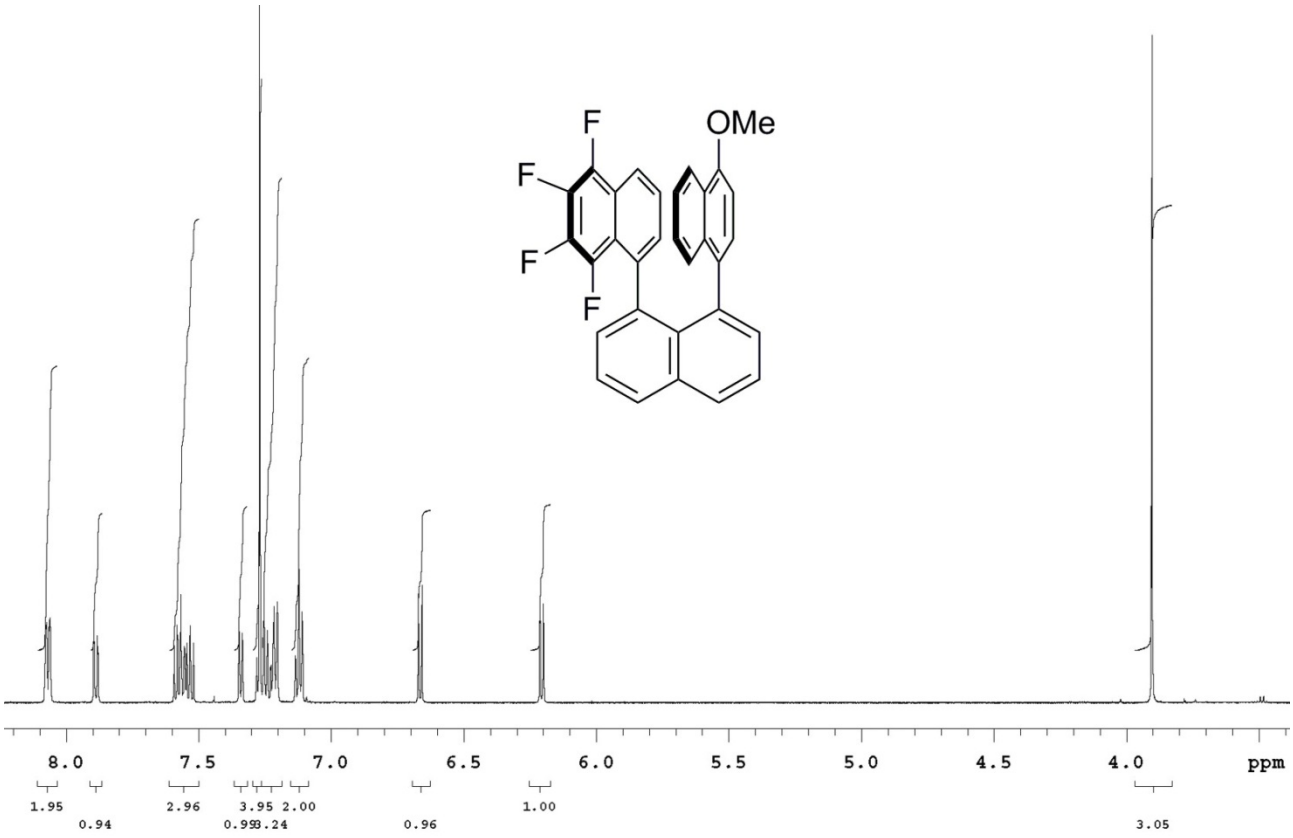


Compound **4**-*anti*

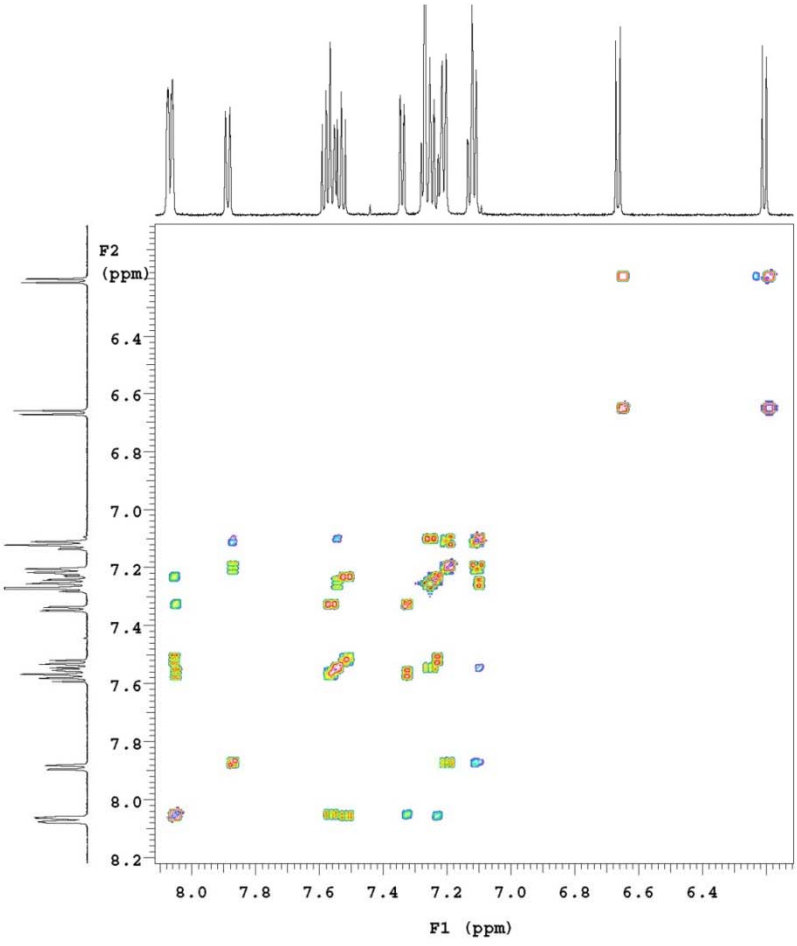




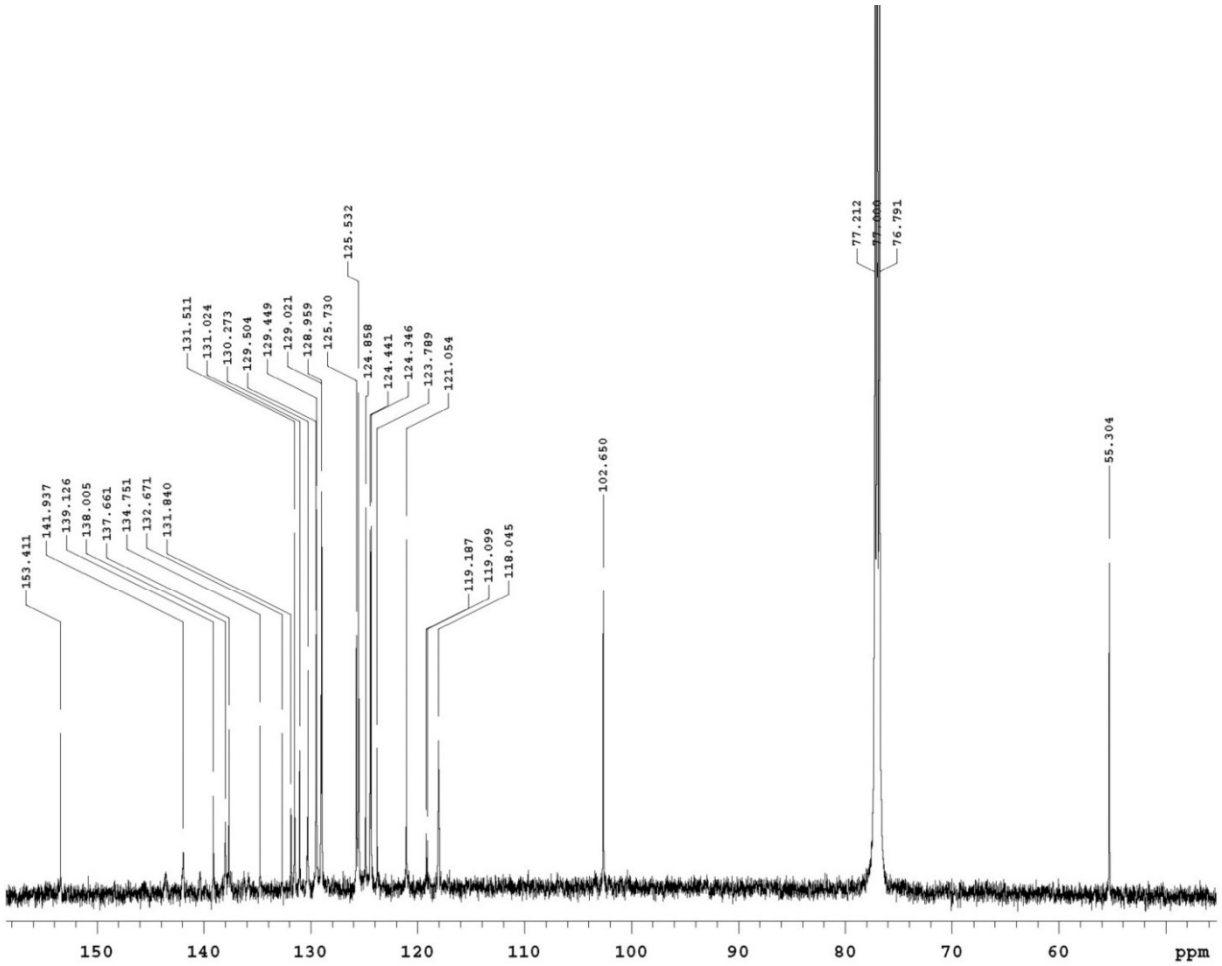
Compound **4**-*anti*

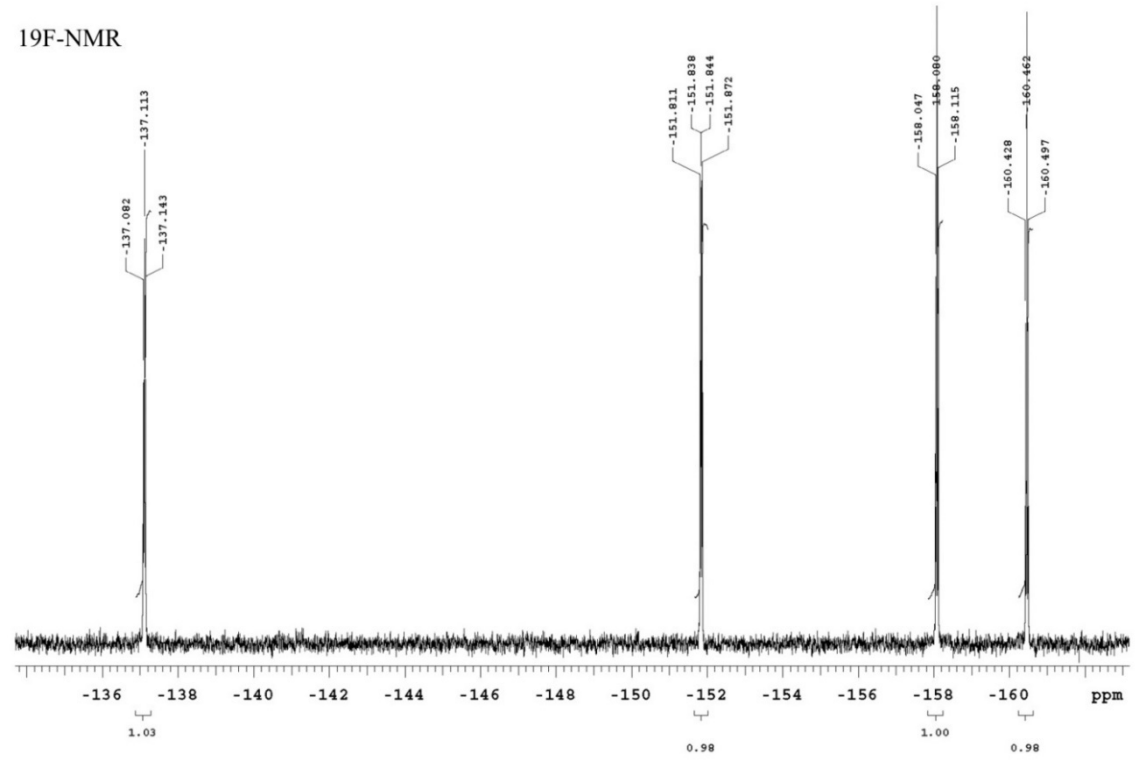


COSY

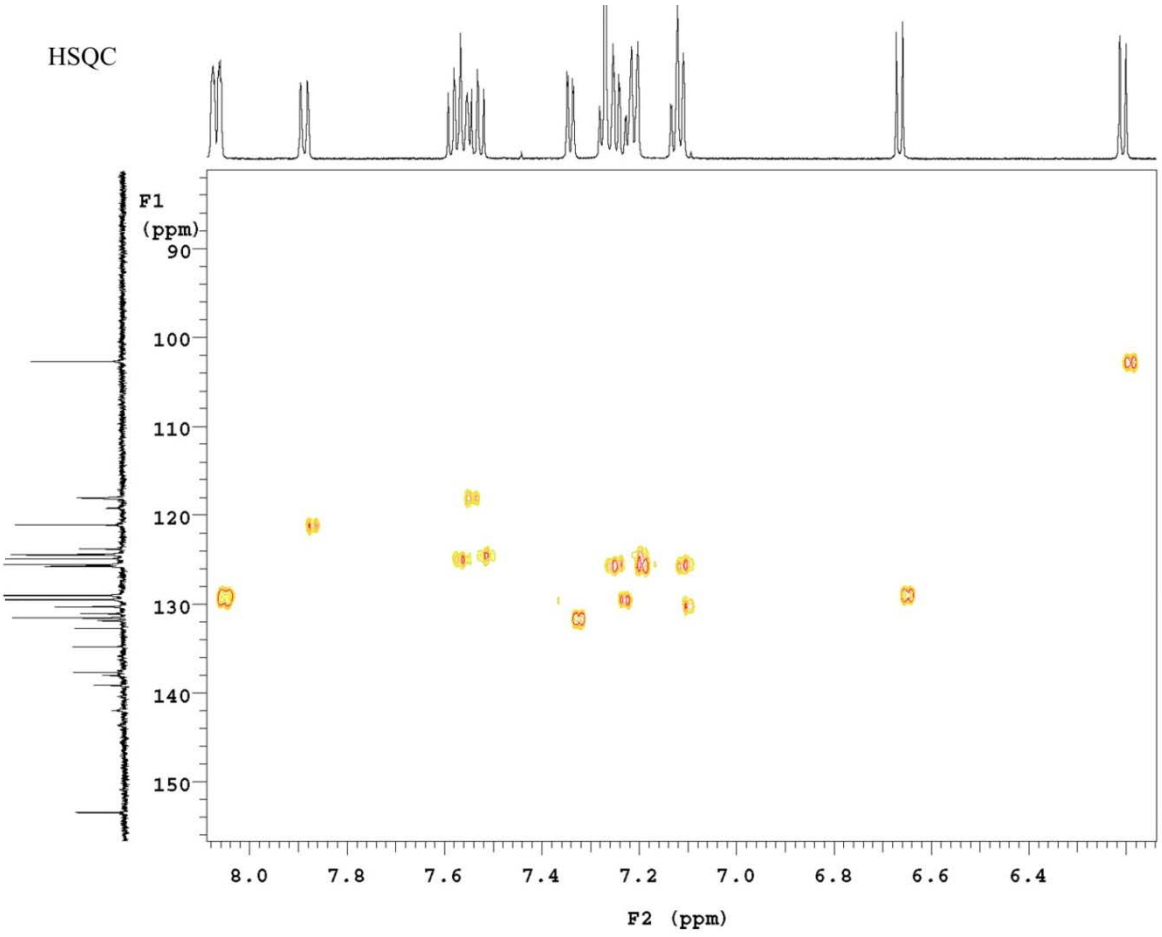


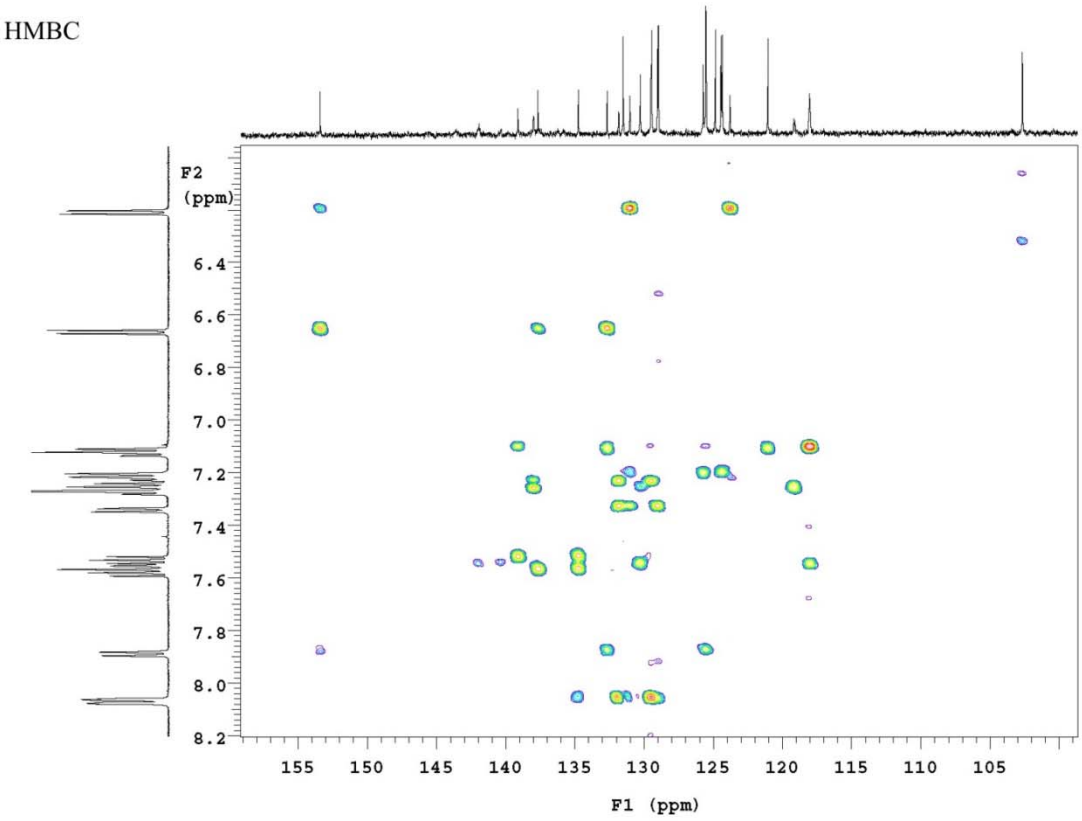
Compound **4**-*syn*



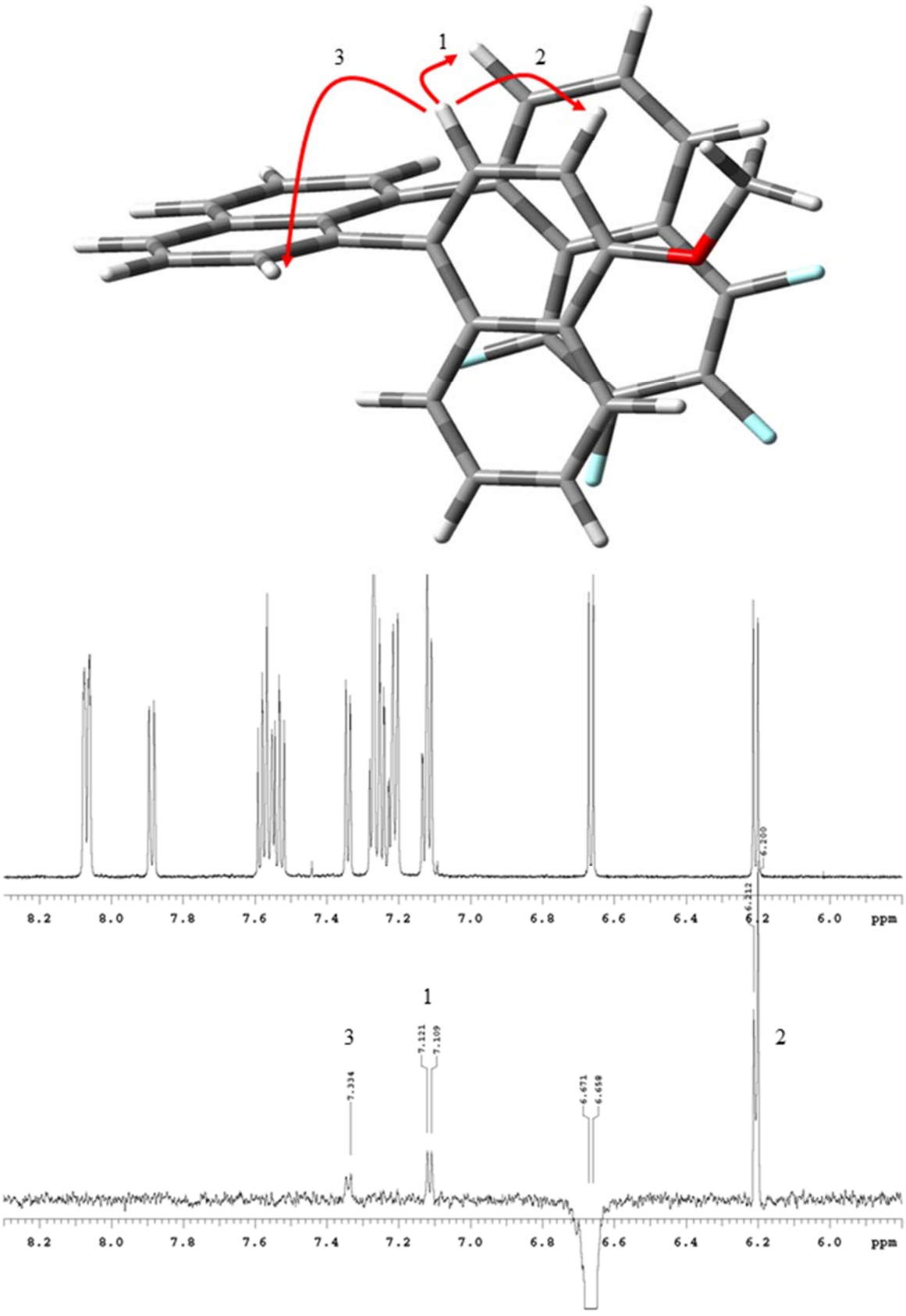


Compound **4**-*syn*





Compound **4**-*syn*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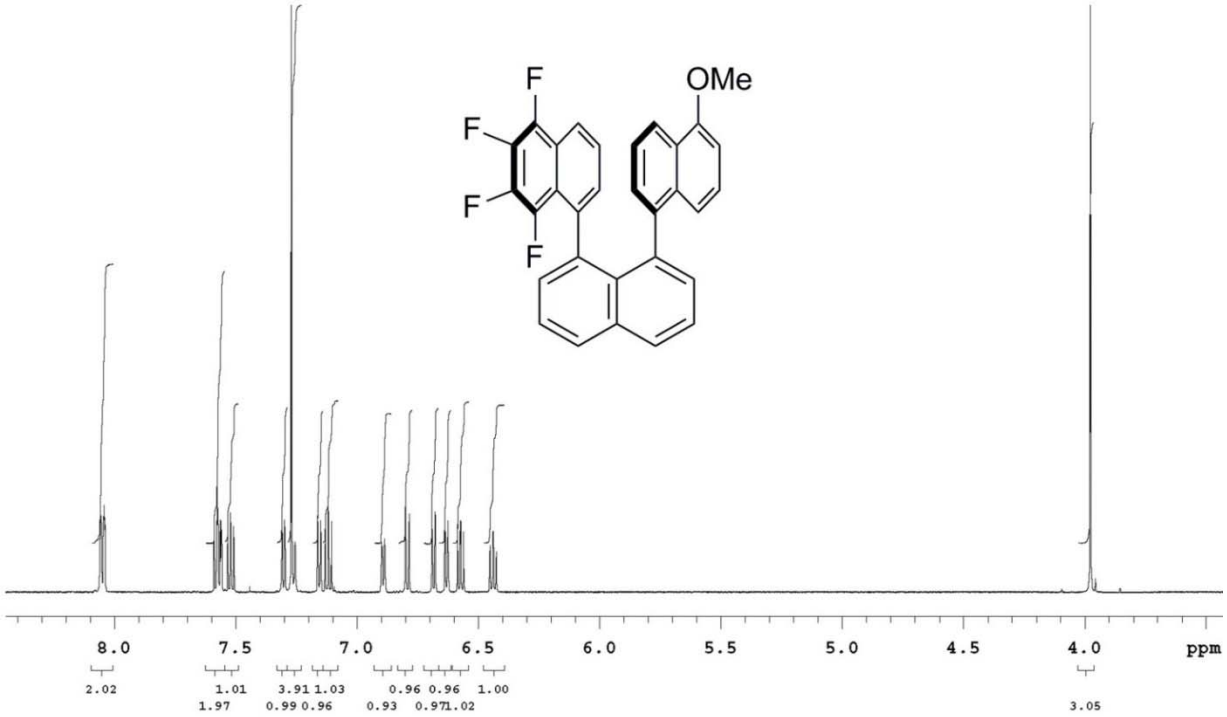
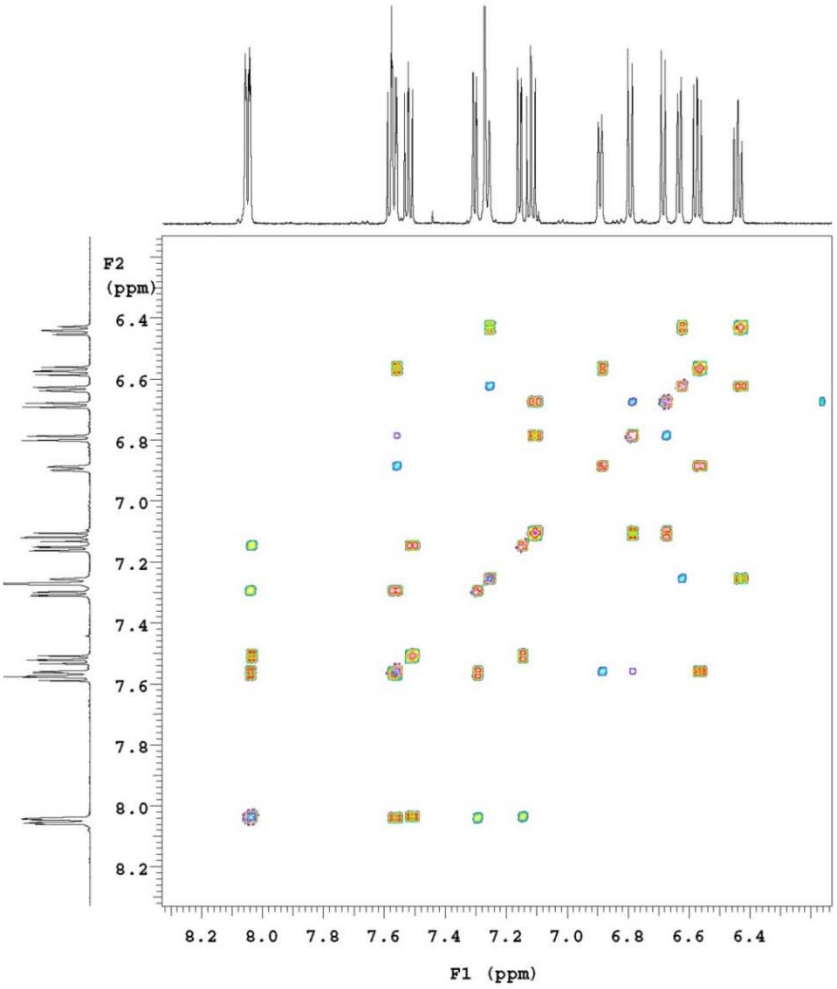
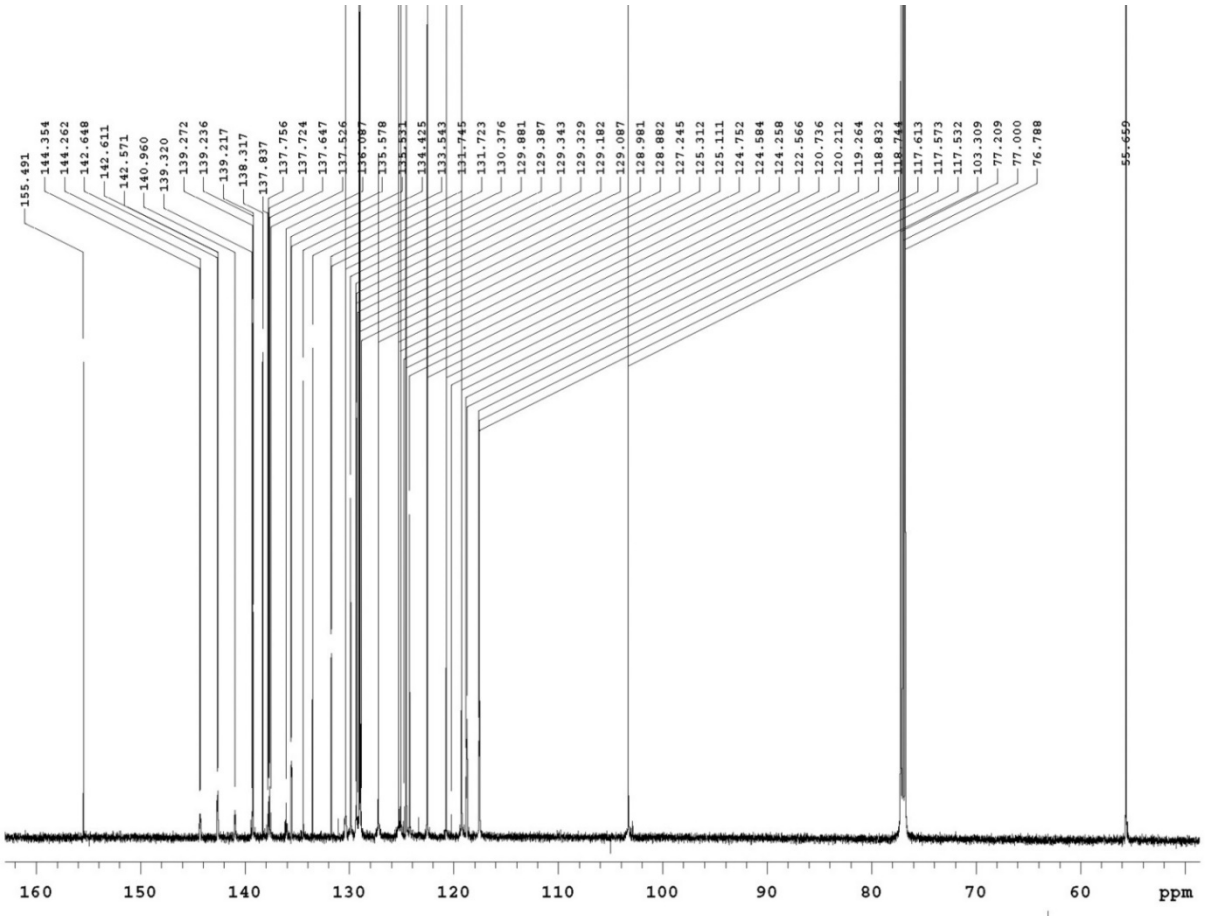
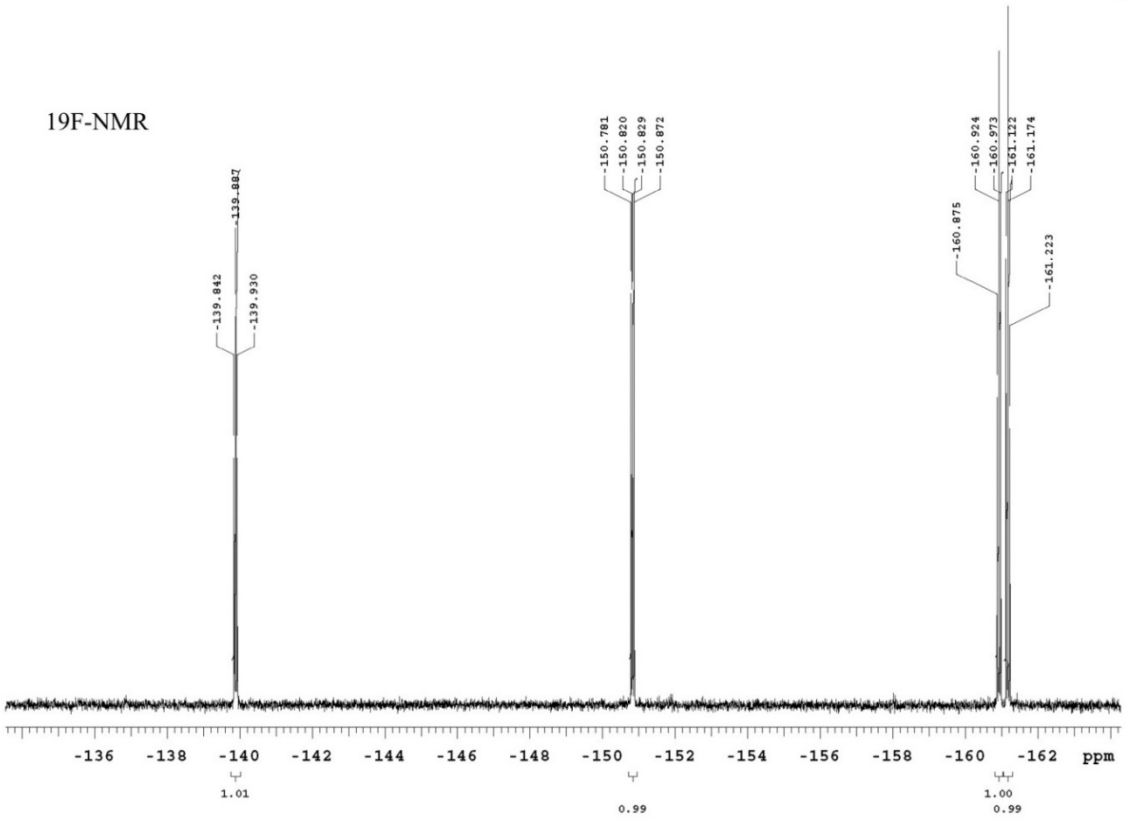
ppm



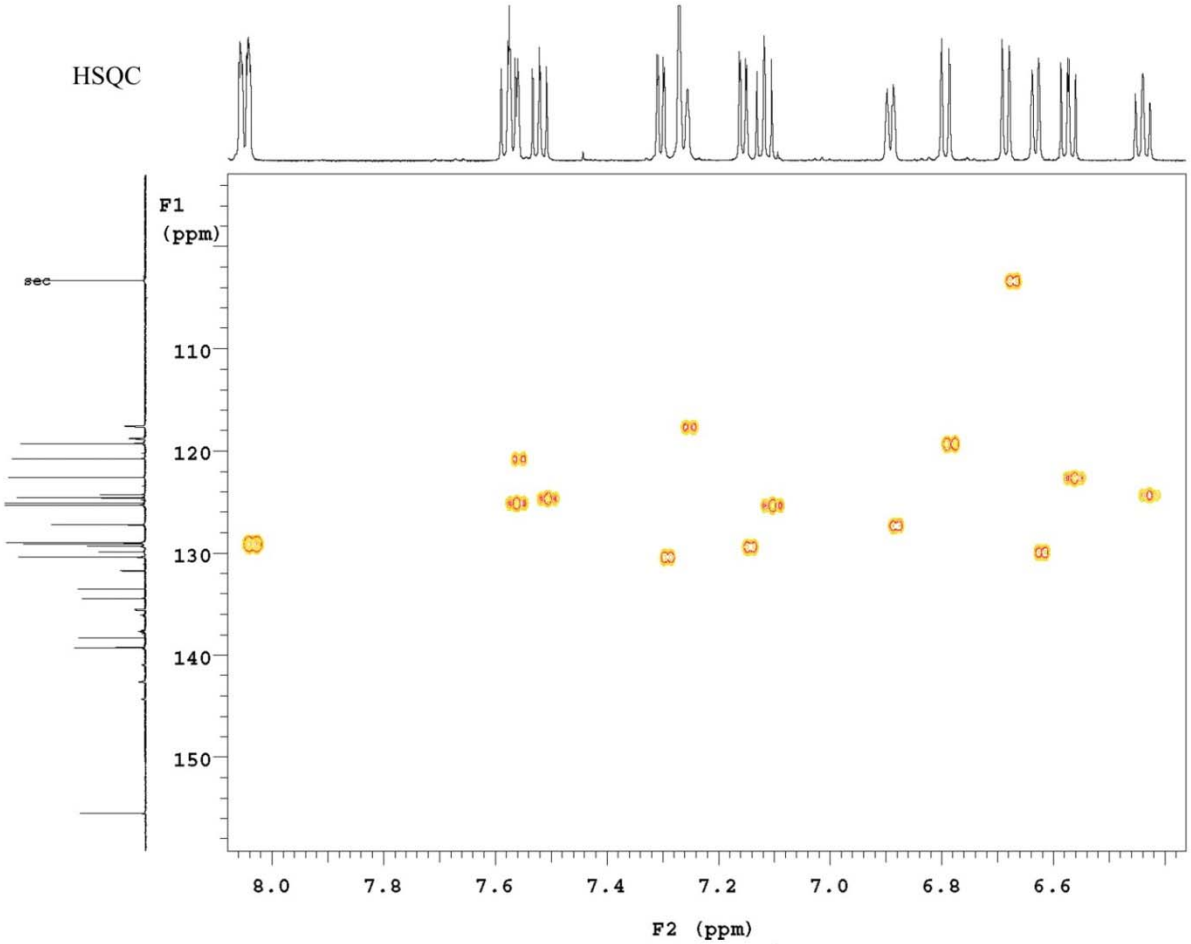


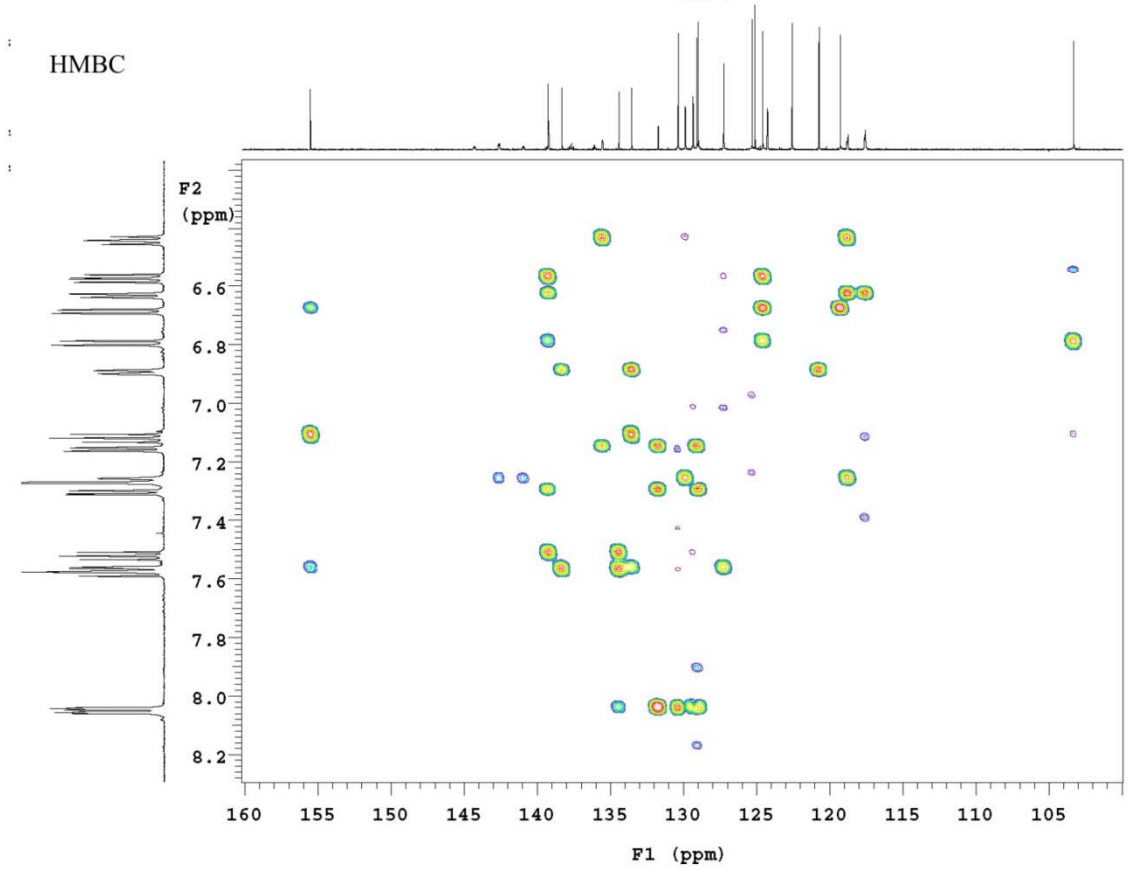
Compound **5**-*anti*



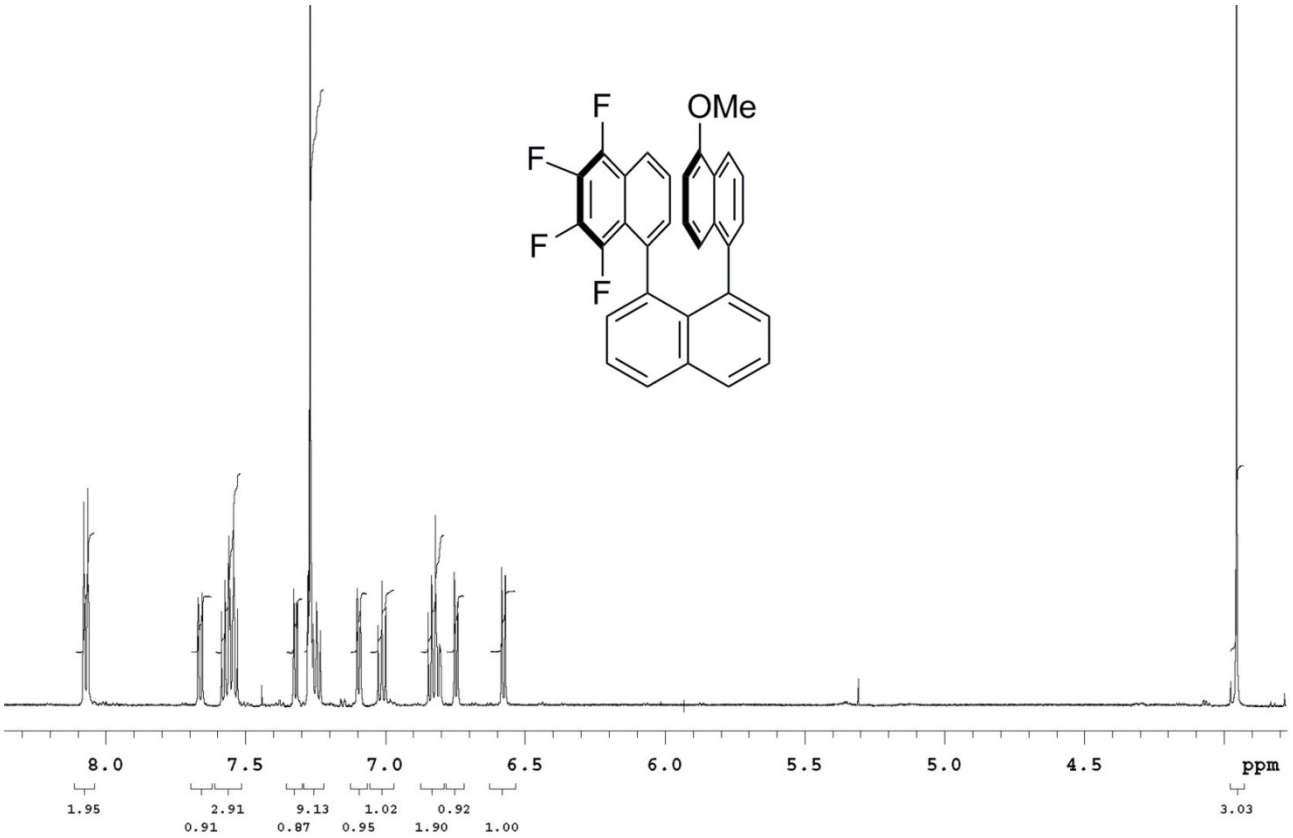


Compound **5**-*anti*

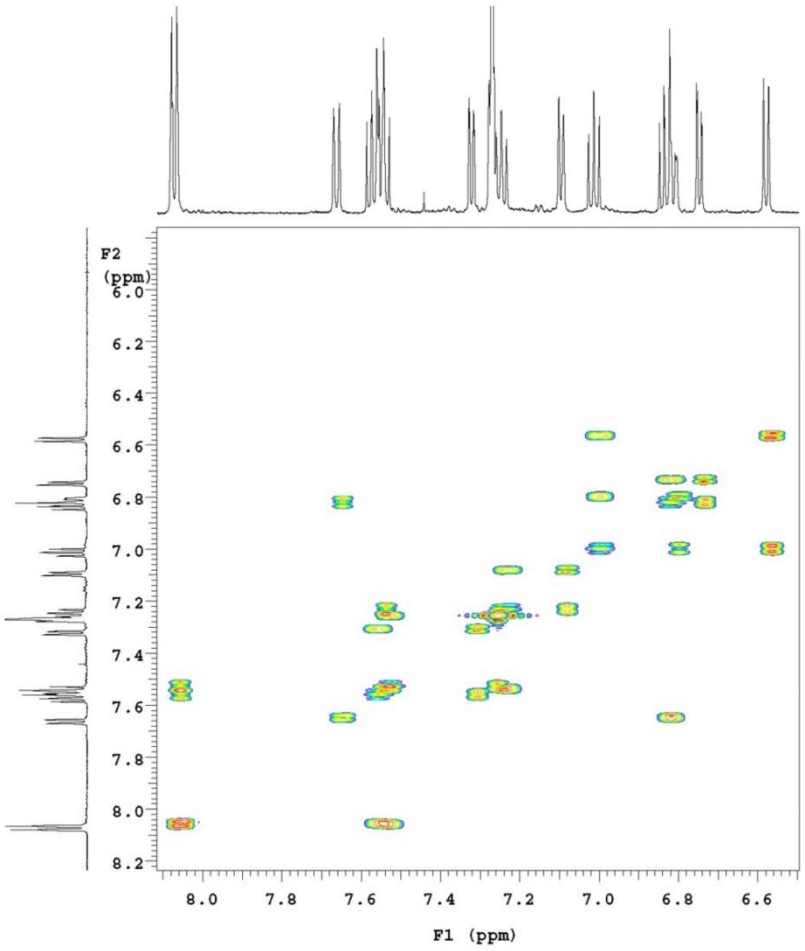




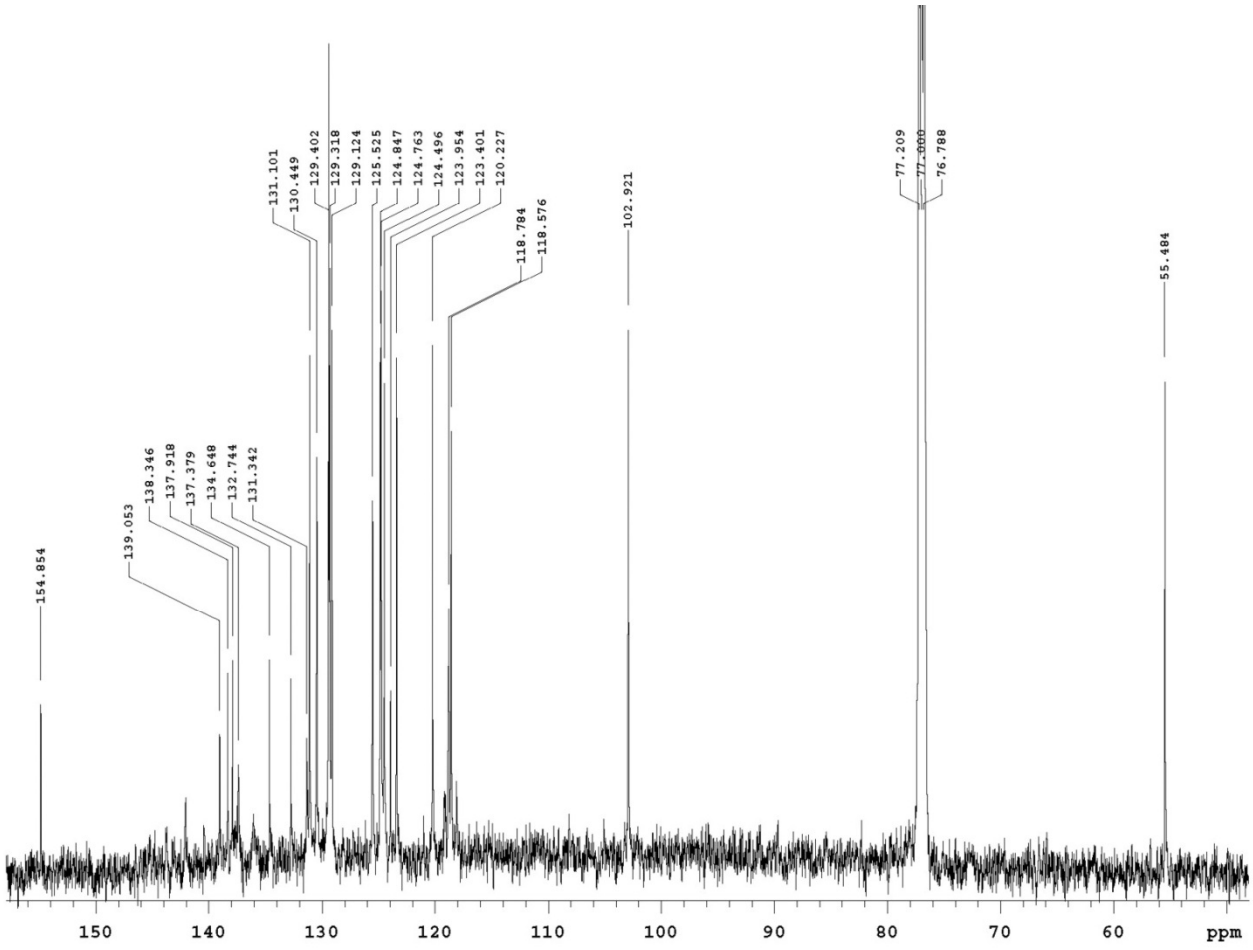
Compound **5**-*anti*



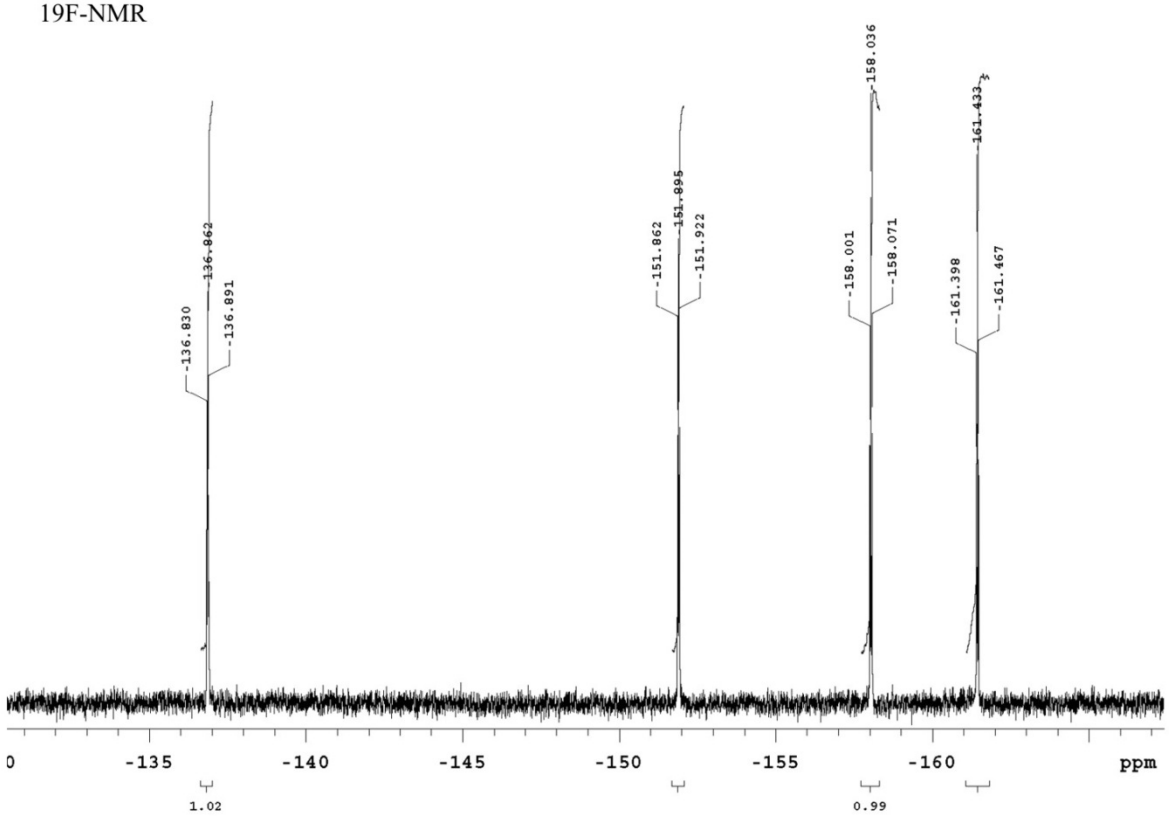
COSY



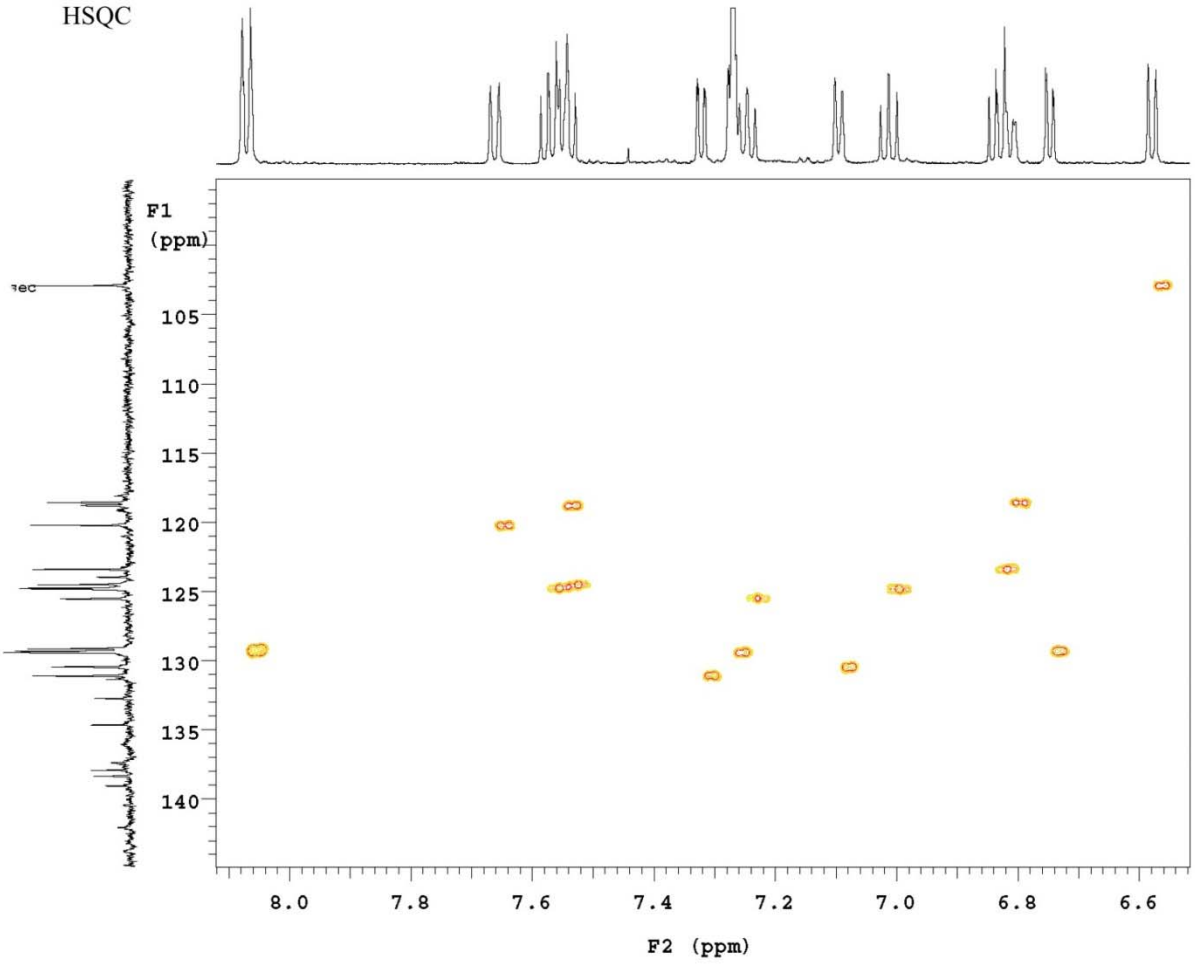
Compound **5**-*syn*

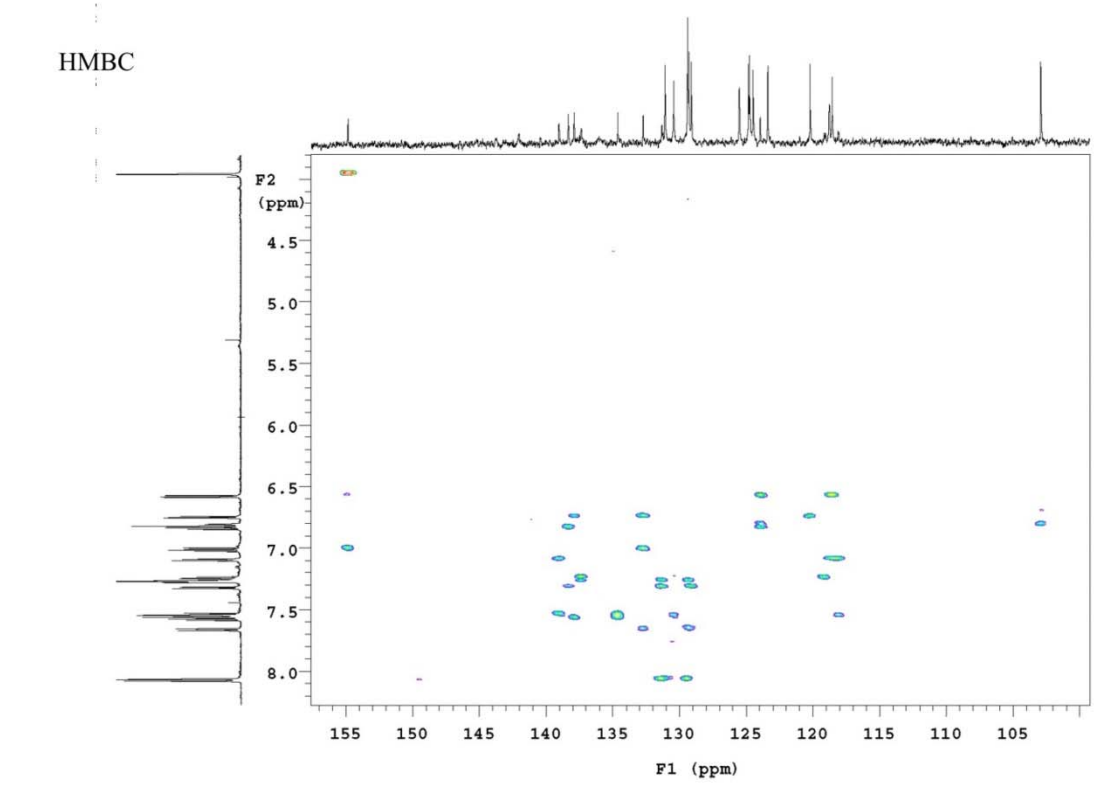


19F-NMR

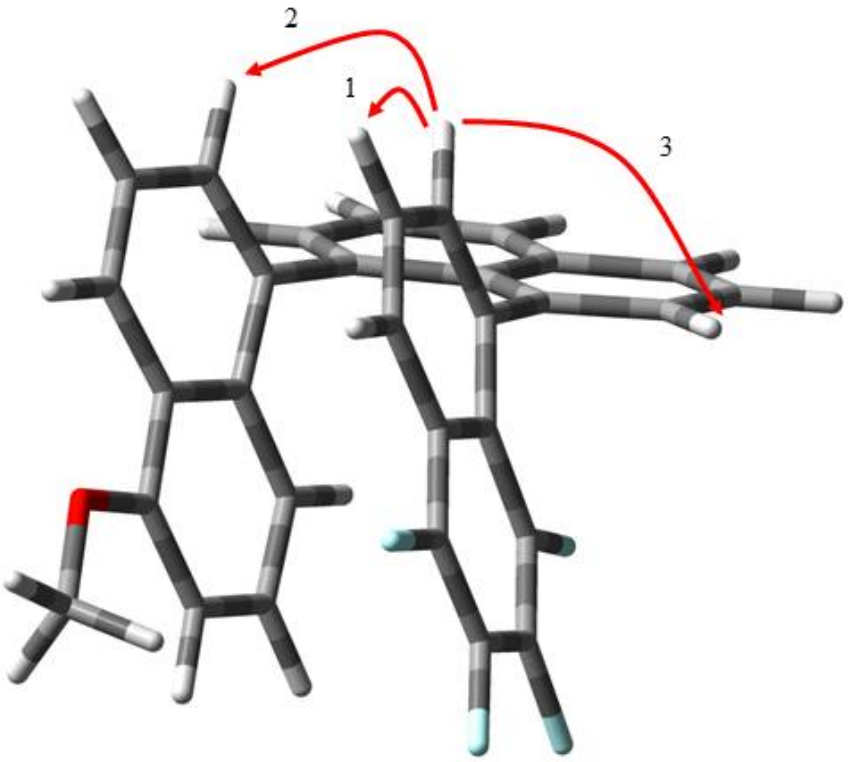


Compound **5**-*syn*

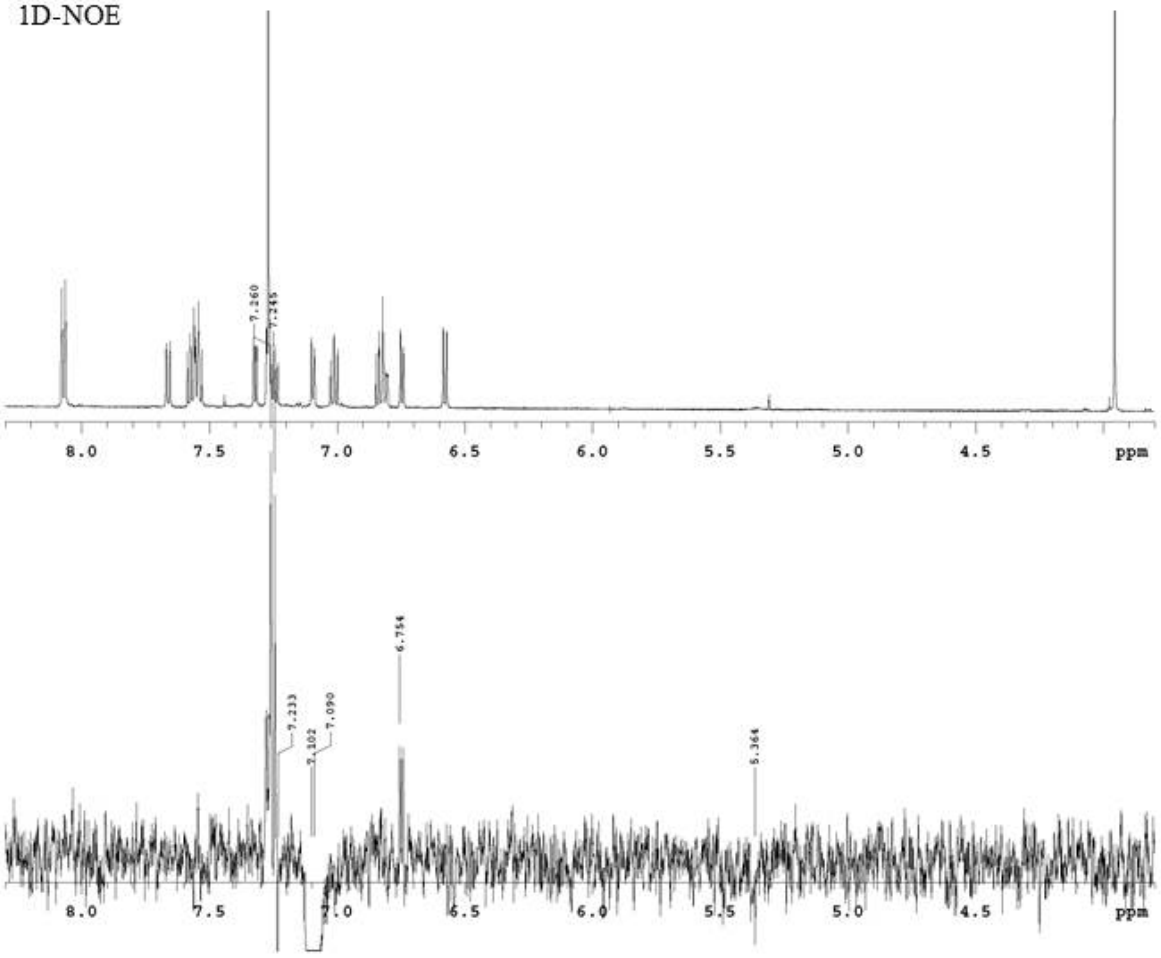




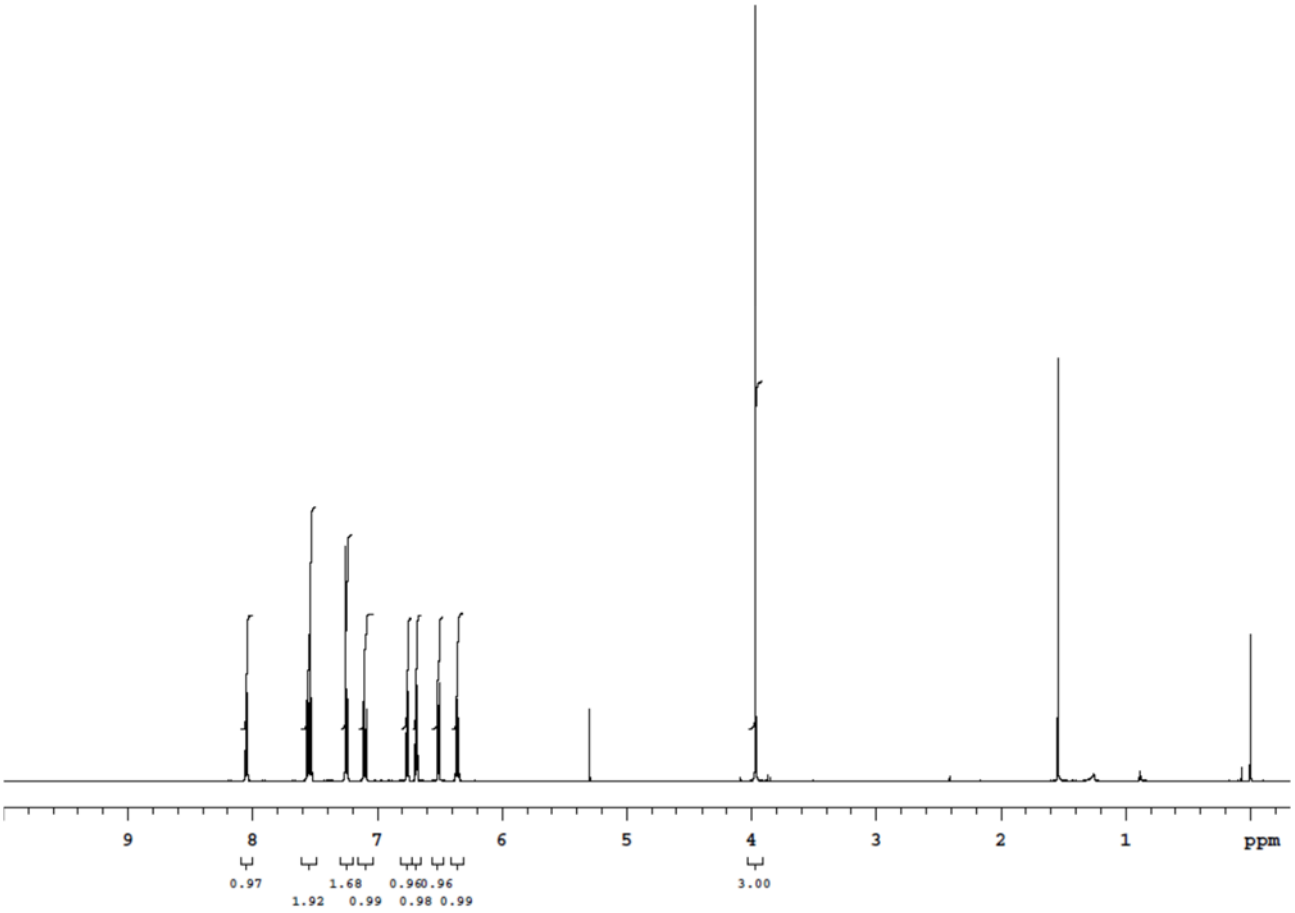
Compound **5**-*syn*

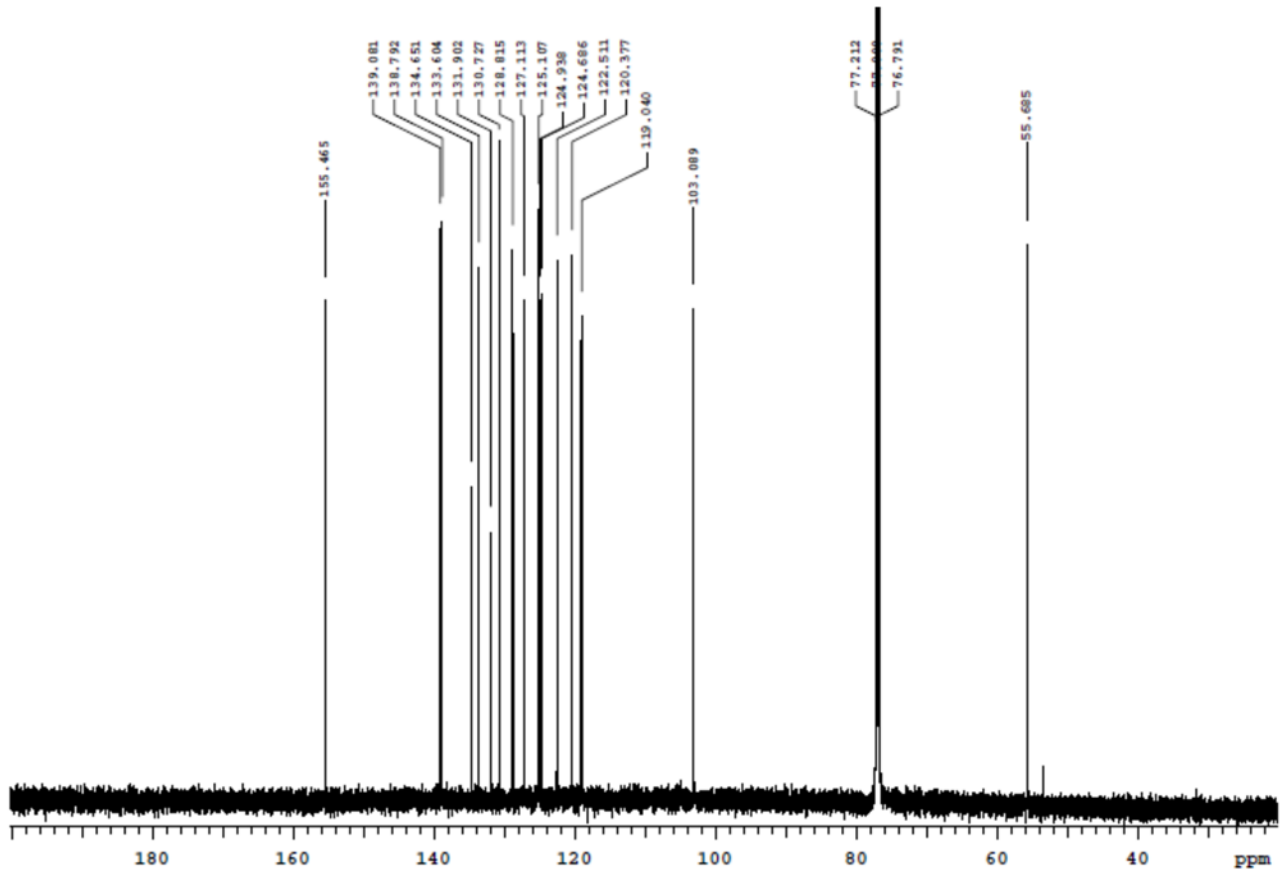

2
1
3

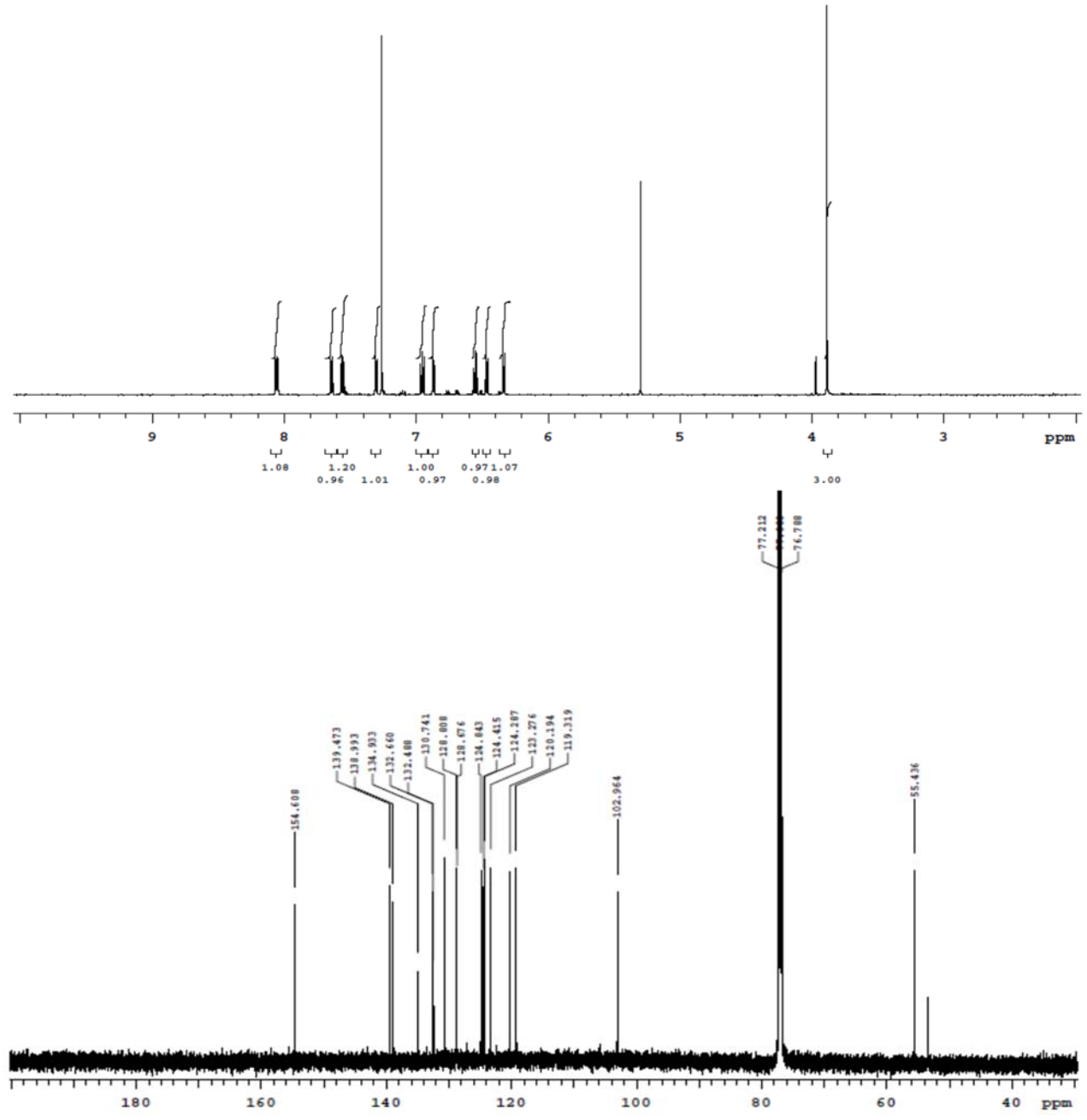
1D-NOE


7.260
7.245
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
ppm
6.754
7.233
7.102
7.090
5.364
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
ppm

Compound **6**-*anti*







Compound **6**-*syn*

Compound 1 anti-in GS1 $CHCl_3$

Method: m062x/6-31+g(d,p)
SCF Done: E(RM062X) = -1233.46159084 A.U. after 1 cycles
Lowest frequency = 10.4590

Zero-point correction= 0.461581
(Hartree/Particle)
Thermal correction to Energy= 0.486121
Thermal correction to Enthalpy= 0.487065
Thermal correction to Gibbs Free Energy= 0.407788
Sum of electronic and zero-point Energies= -1233.000009
Sum of electronic and thermal Energies= -1232.975470
Sum of electronic and thermal Enthalpies= -1232.974525
Sum of electronic and thermal Free Energies= -1233.053803

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.824410	0.752248	-1.039614
2	6	0	-2.579487	1.380795	-2.010735
3	6	0	-3.991007	1.342535	-2.017526
4	6	0	-4.645278	0.674645	-1.018836
5	6	0	-3.919471	-0.000059	0.000034
6	6	0	-4.645229	-0.674791	1.018920
7	6	0	-3.990911	-1.342625	2.017616
8	6	0	-2.579388	-1.380820	2.010799
9	6	0	-1.824359	-0.752260	1.039651
10	6	0	-2.485376	-0.000024	0.000021
11	6	0	-0.344242	0.920048	-1.161123
12	6	0	0.315562	0.335381	-2.216844
13	6	0	1.715361	0.456990	-2.367725
14	6	0	2.474926	1.170195	-1.470435
15	6	0	1.812965	1.836812	-0.389742
16	6	0	1.889969	3.284393	1.570190
17	6	0	0.481052	3.212085	1.684320
18	6	0	-0.243157	2.455339	0.796581
19	6	0	0.396852	1.735559	-0.249024
20	6	0	-0.344176	-0.920012	1.161103
21	6	0	0.315641	-0.335334	2.216809
22	6	0	1.813014	-1.836859	0.389766
23	6	0	2.534450	-2.618319	-0.555794
24	6	0	1.889976	-3.284610	-1.570049
25	6	0	0.481088	-3.212022	-1.684371
26	6	0	-0.243091	-2.455118	-0.796737
27	6	0	0.396918	-1.735467	0.248955
28	1	0	-2.059403	1.942199	-2.781583
29	1	0	-4.541916	1.855234	-2.799349
30	1	0	-5.730905	0.645493	-0.984791
31	1	0	-5.730858	-0.645699	0.984887
32	1	0	-4.541782	-1.855334	2.799459
33	1	0	-2.059261	-1.942180	2.781651
34	1	0	-0.244247	-0.271472	-2.922897

35	1	0	2.200887	-0.046914	-3.199419
36	1	0	-0.025409	3.753634	2.477398
37	1	0	-1.323561	2.390637	0.892110
38	1	0	-0.244164	0.271494	2.922883
39	6	0	1.715465	-0.456781	2.367577
40	6	0	2.534438	2.618072	0.555954
41	1	0	2.459681	3.876269	2.280009
42	1	0	3.613927	2.691668	0.469735
43	1	0	2.201006	0.047203	3.199215
44	6	0	2.475002	-1.170103	1.470360
45	1	0	3.613922	-2.692064	-0.469476
46	1	0	2.459665	-3.876624	-2.279771
47	1	0	-0.025378	-3.753510	-2.477487
48	1	0	-1.323477	-2.390257	-0.892366
49	6	0	3.969583	1.263114	-1.632268
50	1	0	4.298217	0.664493	-2.484432
51	1	0	4.292399	2.296788	-1.797942
52	1	0	4.492882	0.900538	-0.741329
53	6	0	3.969661	-1.263020	1.632179
54	1	0	4.298304	-0.664372	2.484320
55	1	0	4.292480	-2.296687	1.797883
56	1	0	4.492952	-0.900471	0.741223

Compound 1 anti-out GS2 $CHCl_3$

Method: m062x/6-31+g(d,p)
SCF Done: E(RM062X) = -1233.46198144 A.U. after 1 cycles
Lowest frequency = 17.3343

Zero-point correction= 0.461732
(Hartree/Particle)
Thermal correction to Energy= 0.486076
Thermal correction to Enthalpy= 0.487021
Thermal correction to Gibbs Free Energy= 0.409300
Sum of electronic and zero-point Energies= -1233.000249
Sum of electronic and thermal Energies= -1232.975905
Sum of electronic and thermal Enthalpies= -1232.974961
Sum of electronic and thermal Free Energies= -1233.052682

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.932650	1.056241	-0.718222
2	6	0	-2.675451	2.072915	-1.281574
3	6	0	-4.086936	2.100464	-1.211703
4	6	0	-4.749492	1.067722	-0.603948
5	6	0	-4.031611	-0.000023	-0.000004
6	6	0	-4.749476	-1.067788	0.603928
7	6	0	-4.086902	-2.100484	1.211737
8	6	0	-2.675419	-2.072878	1.281652
9	6	0	-1.932630	-1.056200	0.718286
10	6	0	-2.598968	0.000002	0.000016

11	6	0	-0.465442	1.045776	-1.015798
12	6	0	-0.023855	0.343948	-2.111468
13	6	0	1.351135	0.274738	-2.435396
14	6	0	2.300891	0.905631	-1.669098
15	6	0	1.870012	1.686595	-0.547284
16	6	0	2.377200	3.136370	1.345910
17	6	0	0.997512	3.241777	1.641292
18	6	0	0.076245	2.575615	0.870331
19	6	0	0.481617	1.777934	-0.233193
20	6	0	-0.465423	-1.045751	1.015863
21	6	0	-0.023786	-0.343970	2.111541
22	6	0	1.870008	-1.686618	0.547269
23	6	0	2.798295	-2.380126	-0.278099
24	6	0	2.377142	-3.136226	-1.346068
25	6	0	0.997442	-3.241613	-1.641405
26	6	0	0.076202	-2.575509	-0.870363
27	6	0	0.481603	-1.777903	0.233206
28	1	0	-2.151868	2.857952	-1.820632
29	1	0	-4.634010	2.919682	-1.667036
30	1	0	-5.835421	1.044178	-0.572317
31	1	0	-5.835405	-1.044289	0.572245
32	1	0	-4.633955	-2.919713	1.667077
33	1	0	-2.151831	-2.857883	1.820751
34	1	0	-0.741681	-0.201613	-2.718592
35	1	0	1.661203	-0.318247	-3.291914
36	1	0	0.669472	3.845174	2.482210
37	1	0	-0.982836	2.642804	1.103313
38	1	0	-0.741580	0.201574	2.718716
39	6	0	1.351210	-0.274840	2.435457
40	6	0	2.798323	2.380179	0.277992
41	1	0	3.103080	3.658389	1.961922
42	1	0	3.859028	2.311909	0.056821
43	1	0	1.661310	0.318108	3.291988
44	6	0	2.300932	-0.905749	1.669129
45	1	0	3.859007	-2.311847	-0.056967
46	1	0	3.103000	-3.658200	-1.962143
47	1	0	0.669367	-3.844936	-2.482364
48	1	0	-0.982881	-2.642670	-1.103340
49	6	0	3.764630	0.773480	-1.998228
50	1	0	3.900144	0.138696	-2.876539
51	1	0	4.224309	1.746007	-2.204293
52	1	0	4.317368	0.318592	-1.168457
53	6	0	3.764676	-0.773669	1.998264
54	1	0	3.900191	-0.139227	2.876821
55	1	0	4.224413	-1.746249	2.203934
56	1	0	4.317362	-0.318430	1.168647

Compound 1 syn GS1 $CHCl_3$

Method: m062x/6-31+g(d,p)
SCF Done: E(RM062X) = -1233.46098898 A.U. after 2 cycles
Lowest frequency = 19.7620

Zero-point correction= 0.461903
(Hartree/Particle)
Thermal correction to Energy= 0.486171
Thermal correction to Enthalpy= 0.487115
Thermal correction to Gibbs Free Energy= 0.409762
Sum of electronic and zero-point Energies= -1232.999086
Sum of electronic and thermal Energies= -1232.974818
Sum of electronic and thermal Enthalpies= -1232.973874
Sum of electronic and thermal Free Energies= -1233.051227

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.902877	0.647436	-1.117614
2	6	0	-2.686092	1.508975	-1.856661
3	6	0	-4.090924	1.566813	-1.704502
4	6	0	-4.696982	0.783481	-0.759395
5	6	0	-3.937910	-0.133802	0.018074
6	6	0	-4.592052	-0.925007	1.000727
7	6	0	-3.891503	-1.837234	1.744421
8	6	0	-2.515782	-2.032695	1.485823
9	6	0	-1.837851	-1.295399	0.537304
10	6	0	-2.527150	-0.262495	-0.190551
11	6	0	-0.421073	0.832167	-1.221292
12	6	0	0.322492	0.226585	-2.203991
13	6	0	1.722515	0.411666	-2.282208
14	6	0	2.395692	1.212583	-1.389657
15	6	0	1.643491	1.902099	-0.385533
16	6	0	1.543825	3.447320	1.497411
17	6	0	0.141604	3.277825	1.567587
18	6	0	-0.495485	2.433788	0.690635
19	6	0	0.230166	1.721759	-0.305356
20	6	0	-0.444730	-1.727866	0.202706
21	6	0	-0.268968	-2.629381	-0.820036
22	6	0	2.000778	-1.661266	0.506107
23	6	0	3.126024	-1.141123	1.204552
24	6	0	2.970000	-0.285408	2.268240
25	6	0	1.674830	0.093722	2.693256
26	6	0	0.568754	-0.383143	2.035039
27	6	0	0.697445	-1.260314	0.923702
28	1	0	-2.195194	2.195016	-2.541534
29	1	0	-4.670784	2.258314	-2.307249
30	1	0	-5.768321	0.844578	-0.587966
31	1	0	-5.660467	-0.790564	1.146021
32	1	0	-4.389128	-2.436539	2.500009
33	1	0	-1.976166	-2.809932	2.020322
34	1	0	-0.166652	-0.442196	-2.906828
35	1	0	2.279208	-0.115226	-3.053548
36	1	0	-0.431079	3.813792	2.318324
37	1	0	-1.571809	2.302153	0.752464
38	1	0	-1.137692	-2.998727	-1.359016
39	6	0	1.024113	-3.041272	-1.217918
40	6	0	2.271727	2.774284	0.545786

41	1	0	2.044137	4.110452	2.196610
42	1	0	3.347859	2.908849	0.501728
43	1	0	1.124894	-3.735399	-2.048449
44	6	0	2.153270	-2.558218	-0.599298
45	1	0	4.124902	-1.427387	0.890445
46	1	0	3.842417	0.103804	2.784781
47	1	0	1.557799	0.775572	3.529913
48	1	0	-0.426025	-0.079389	2.347539
49	6	0	3.524837	-2.946789	-1.084670
50	1	0	4.112750	-3.432693	-0.298971
51	1	0	3.450680	-3.636197	-1.928238
52	1	0	4.086555	-2.064850	-1.415160
53	6	0	3.892993	1.359433	-1.464660
54	1	0	4.294077	0.757553	-2.283348
55	1	0	4.190387	2.400194	-1.632303
56	1	0	4.366599	1.027681	-0.533720

Compound 1 TS rotation

Method: m062x/6-31+g(d,p)
SCF Done: E(RM062X) = -1233.41460208 A.U. after 11 cycles
Lowest frequency = -26.86

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.152792	1.870541	-0.322909
2	6	0	-2.018224	2.778873	-0.911028
3	6	0	-1.623653	4.090377	-1.241291
4	6	0	-0.396941	4.530504	-0.817157
5	6	0	0.512970	3.642602	-0.184230
6	6	0	1.657116	4.181840	0.469802
7	6	0	2.452461	3.359670	1.218615
8	6	0	2.294466	1.959842	1.100135
9	6	0	1.326090	1.369930	0.301243
10	6	0	0.225979	2.241130	-0.108776
11	6	0	-1.789427	0.707660	0.373009
12	6	0	-1.539835	0.540549	1.715907
13	6	0	-2.184009	-0.467535	2.469267
14	6	0	-3.095641	-1.322839	1.898691
15	6	0	-3.368801	-1.192883	0.497685
16	6	0	-4.494769	-1.992892	-1.512362
17	6	0	-3.808498	-1.026623	-2.282541
18	6	0	-2.943596	-0.147522	-1.675743
19	6	0	-2.713407	-0.184249	-0.271851
20	6	0	1.537128	-0.044774	-0.138605
21	6	0	0.521682	-0.813048	-0.671121
22	6	0	2.946102	-2.099819	-0.261488
23	6	0	4.216606	-2.731296	-0.146869
24	6	0	5.372749	-2.004054	-0.014308
25	6	0	5.302548	-0.595129	-0.039173
26	6	0	4.083840	0.040036	-0.083325
27	6	0	2.850240	-0.676874	-0.111880
28	1	0	-3.061291	2.499934	-1.030726

29	1	0	-2.325648	4.765846	-1.718794
30	1	0	-0.112858	5.574509	-0.916663
31	1	0	1.828057	5.253552	0.424807
32	1	0	3.256123	3.757789	1.829377
33	1	0	3.013952	1.326172	1.602466
34	1	0	-0.840895	1.207205	2.213421
35	1	0	-1.958096	-0.555358	3.528559
36	1	0	-3.960260	-0.982141	-3.356393
37	1	0	-2.409963	0.579969	-2.278913
38	1	0	-0.423274	-0.364413	-0.910463
39	6	0	0.637082	-2.200214	-0.896062
40	6	0	-4.272705	-2.073825	-0.158827
41	1	0	-5.185080	-2.678732	-1.993238
42	1	0	-4.787731	-2.831767	0.422039
43	1	0	-0.234544	-2.738593	-1.260563
44	6	0	1.795764	-2.877474	-0.612416
45	6	0	-3.782435	-2.379506	2.723699
46	1	0	-4.870504	-2.257064	2.706009
47	1	0	-3.559889	-3.385359	2.352350
48	1	0	-3.452750	-2.322848	3.762903
49	6	0	1.872507	-4.374393	-0.751345
50	1	0	2.589051	-4.671652	-1.524426
51	1	0	2.186885	-4.846768	0.185168
52	1	0	0.895130	-4.778109	-1.022686
53	1	0	4.269678	-3.813256	-0.202535
54	1	0	6.332910	-2.505063	0.056411
55	1	0	6.213560	-0.004891	-0.042335
56	1	0	4.073865	1.119412	-0.154251

Compound 2 anti-in GS1 $CHCl_3$

Method: m062x/6-31+g(d,p)
SCF Done: E(RM062X) = -1948.49971749 A.U. after 1 cycles
Lowest frequency = 17.9867

Zero-point correction= 0.340893
(Hartree/Particle)
Thermal correction to Energy= 0.369538
Thermal correction to Enthalpy= 0.370482
Thermal correction to Gibbs Free Energy= 0.282286
Sum of electronic and zero-point Energies= -1948.158825
Sum of electronic and thermal Energies= -1948.130179
Sum of electronic and thermal Enthalpies= -1948.129235
Sum of electronic and thermal Free Energies= -1948.217432

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.067479	0.435283	-1.204549
2	6	0	-2.813259	0.828905	-2.295809
3	6	0	-4.225377	0.841531	-2.275792
4	6	0	-4.881276	0.433553	-1.146800
5	6	0	-4.158451	0.005940	-0.000218

6	6	0	-4.882468	-0.419847	1.146310
7	6	0	-4.227771	-0.829115	2.275529
8	6	0	-2.815608	-0.819889	2.295781
9	6	0	-2.068856	-0.428461	1.204462
10	6	0	-2.726560	0.004156	-0.000148
11	6	0	-0.583670	0.411458	-1.414102
12	6	0	-0.064838	-0.616752	-2.172960
13	6	0	1.319391	-0.735354	-2.433181
14	6	0	2.196951	0.192320	-1.934980
15	6	0	1.703607	1.295254	-1.192011
16	6	0	2.143122	3.365122	0.000802
17	6	0	0.761686	3.507693	0.241838
18	6	0	-0.122296	2.568960	-0.213236
19	6	0	0.304615	1.427923	-0.940475
20	6	0	-0.584911	-0.408439	1.413153
21	6	0	-0.062370	0.619201	2.170130
22	6	0	1.699522	-1.299192	1.189841
23	6	0	2.583212	-2.288839	0.695472
24	6	0	2.131354	-3.373023	0.001162
25	6	0	0.749304	-3.511490	-0.238863
26	6	0	-0.131257	-2.568769	0.214600
27	6	0	0.299904	-1.427980	0.939712
28	1	0	-2.290772	1.142120	-3.195178
29	1	0	-4.774565	1.166924	-3.153080
30	1	0	-5.966836	0.425797	-1.104908
31	1	0	-5.968002	-0.409516	1.104221
32	1	0	-4.777904	-1.153017	3.152778
33	1	0	-2.293925	-1.134117	3.195265
34	1	0	-0.745587	-1.374853	-2.550646
35	1	0	1.684184	-1.574030	-3.017574
36	1	0	-0.740757	1.379149	2.548320
37	6	0	1.322587	0.734813	2.427736
38	6	0	2.590892	2.280880	-0.696046
39	1	0	3.264209	0.107937	-2.107321
40	1	0	1.690469	1.573585	3.010028
41	6	0	2.196877	-0.196317	1.930264
42	1	0	3.264590	-0.114605	2.101095
43	9	0	-1.425572	-2.743671	-0.081308
44	9	0	0.323408	-4.569025	-0.932540
45	9	0	2.964567	-4.305728	-0.461962
46	9	0	3.898756	-2.162092	0.917465
47	9	0	3.905880	2.150092	-0.918992
48	9	0	2.979729	4.293911	0.465665
49	9	0	0.339658	4.565157	0.938021
50	9	0	-1.415822	2.747740	0.083792

Compound 2 syn GS1 $CHCl_3$

Method: m062x/6-31+g(d,p)
SCF Done: E(RM062X) = -1948.49770469 A.U. after 2 cycles
Lowest frequency = 15.8823

Zero-point correction= 0.340825
(Hartree/Particle)

Thermal correction to Energy= 0.369453
Thermal correction to Enthalpy= 0.370397
Thermal correction to Gibbs Free Energy= 0.282510
Sum of electronic and zero-point Energies= -1948.156880
Sum of electronic and thermal Energies= -1948.128251
Sum of electronic and thermal Enthalpies= -1948.127307
Sum of electronic and thermal Free Energies= -1948.215195

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.347960	-0.471491	1.219227
2	6	0	-3.065750	-1.369014	1.979284
3	6	0	-4.355440	-1.804856	1.600710
4	6	0	-4.899348	-1.350339	0.429945
5	6	0	-4.211337	-0.399036	-0.371599
6	6	0	-4.812737	0.059066	-1.574435
7	6	0	-4.196767	1.004962	-2.349170
8	6	0	-2.970214	1.558595	-1.920678
9	6	0	-2.344356	1.139030	-0.766516
10	6	0	-2.932608	0.100039	0.034797
11	6	0	-0.936515	-0.220520	1.653640
12	6	0	-0.666959	0.746085	2.597957
13	6	0	0.645683	1.010128	3.046207
14	6	0	1.703333	0.292649	2.548195
15	6	0	1.470655	-0.733573	1.599511
16	6	0	2.366582	-2.472690	0.158909
17	6	0	1.058660	-2.768879	-0.276564
18	6	0	-0.013695	-2.068909	0.205325
19	6	0	0.142597	-1.016280	1.151400
20	6	0	-1.150338	1.934845	-0.331125
21	6	0	-1.387951	3.066440	0.420013
22	6	0	1.254635	2.429179	-0.177696
23	6	0	2.595229	2.076018	-0.468152
24	6	0	2.901854	0.994662	-1.242395
25	6	0	1.859108	0.207366	-1.774430
26	6	0	0.553766	0.512520	-1.504557
27	6	0	0.196159	1.617085	-0.686737
28	1	0	-2.601865	-1.784494	2.869608
29	1	0	-4.887555	-2.518247	2.221270
30	1	0	-5.871406	-1.701258	0.094789
31	1	0	-5.775631	-0.354477	-1.861039
32	1	0	-4.654117	1.354404	-3.268900
33	1	0	-2.511234	2.353462	-2.501978
34	1	0	-1.492024	1.339563	2.980808
35	1	0	0.813860	1.794466	3.776654
36	1	0	-2.415040	3.312037	0.674065
37	6	0	-0.339471	3.886772	0.891434
38	6	0	2.554531	-1.479839	1.075774
39	1	0	2.720112	0.493355	2.867107
40	1	0	-0.571815	4.764049	1.485908
41	6	0	0.965191	3.567199	0.615115
42	1	0	1.784709	4.171382	0.987612

43	9	0	-0.386052	-0.288209	-2.022841
44	9	0	2.174695	-0.849186	-2.526863
45	9	0	4.163375	0.657732	-1.508905
46	9	0	3.591110	2.823477	0.027060
47	9	0	3.800129	-1.196830	1.481954
48	9	0	3.387379	-3.166859	-0.342185
49	9	0	0.891301	-3.738882	-1.175815
50	9	0	-1.217184	-2.408746	-0.268653

Compound 2 TS rotation

Method: m062x/6-31+g(d,p)
SCF Done: E(RM062X) = -1948.44649347 A.U. after 1 cycles
Lowest frequency = -25.2608

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.289025	2.024717	-0.021131
2	6	0	-2.191429	2.934940	-0.545503
3	6	0	-1.808093	4.230704	-0.938040
4	6	0	-0.539005	4.655209	-0.638846
5	6	0	0.411772	3.761964	-0.080413
6	6	0	1.627867	4.288935	0.441272
7	6	0	2.490340	3.468236	1.112107
8	6	0	2.297009	2.071164	1.035605
9	6	0	1.229129	1.489509	0.374039
10	6	0	0.107213	2.369560	0.057607
11	6	0	-1.888519	0.914624	0.786618
12	6	0	-1.527080	0.837962	2.116377
13	6	0	-2.152277	-0.051758	3.017486
14	6	0	-3.171481	-0.863969	2.594632
15	6	0	-3.562773	-0.841016	1.231814
16	6	0	-4.940949	-1.762533	-0.545248
17	6	0	-4.262189	-0.952198	-1.475695
18	6	0	-3.274358	-0.098221	-1.063972
19	6	0	-2.909570	0.028445	0.304326
20	6	0	1.368312	0.053502	-0.015055
21	6	0	0.291500	-0.757960	-0.319535
22	6	0	2.734361	-2.018853	-0.032775
23	6	0	3.990711	-2.670231	0.001198
24	6	0	5.162182	-1.985607	-0.136740
25	6	0	5.106632	-0.599067	-0.360036
26	6	0	3.906913	0.064195	-0.368579
27	6	0	2.671449	-0.588821	-0.094425
28	1	0	-3.245043	2.670035	-0.572260
29	1	0	-2.539598	4.908824	-1.363949
30	1	0	-0.247512	5.691176	-0.786749
31	1	0	1.811133	5.356108	0.356067
32	1	0	3.367878	3.861407	1.613700
33	1	0	3.072289	1.432974	1.445208
34	1	0	-0.755274	1.507672	2.483573
35	1	0	-1.835771	-0.068728	4.054805
36	1	0	-0.669800	-0.313097	-0.488587
37	6	0	0.367969	-2.165846	-0.369360
38	6	0	-4.584750	-1.705019	0.771080
39	1	0	-0.537333	-2.735376	-0.553456

40	6	0	1.554039	-2.800711	-0.120710
41	1	0	-3.679738	-1.534561	3.277723
42	9	0	-5.209744	-2.503969	1.645860
43	9	0	-5.896840	-2.584128	-0.977406
44	9	0	-4.582449	-1.052323	-2.765828
45	9	0	-2.628460	0.583675	-2.019634
46	1	0	1.626219	-3.880624	-0.070224
47	9	0	4.030872	-4.005152	0.114688
48	9	0	6.344100	-2.602091	-0.135873
49	9	0	6.240245	0.052014	-0.627836
50	9	0	3.961961	1.346759	-0.756689

Compound 3 anti-in GS1 $CHCl_3$

Method: m062x/6-31+g(d,p)
SCF Done: E(RM062X) = -1590.98224853 A.U. after 1 cycles
Lowest frequency = 17.9244

Zero-point correction= 0.401394
(Hartree/Particle)
Thermal correction to Energy= 0.427864
Thermal correction to Enthalpy= 0.428809
Thermal correction to Gibbs Free Energy= 0.345910
Sum of electronic and zero-point Energies= -1590.580855
Sum of electronic and thermal Energies= -1590.554384
Sum of electronic and thermal Enthalpies= -1590.553440
Sum of electronic and thermal Free Energies= -1590.636339

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.118351	0.343446	-1.184894
2	6	0	-2.931980	0.545685	-2.281034
3	6	0	-4.286462	0.146095	-2.298169
4	6	0	-4.816086	-0.465040	-1.194498
5	6	0	-4.019628	-0.703947	-0.041742
6	6	0	-4.614391	-1.349640	1.076065
7	6	0	-3.886944	-1.599514	2.206934
8	6	0	-2.529793	-1.211408	2.253519
9	6	0	-1.900912	-0.592972	1.191919
10	6	0	-2.643965	-0.304016	-0.009907
11	6	0	-0.701072	0.795125	-1.316664
12	6	0	0.172467	0.065243	-2.087403
13	6	0	1.540866	0.415245	-2.174206
14	6	0	2.047686	1.501918	-1.501158
15	6	0	1.144317	2.337032	-0.765596
16	6	0	0.712386	4.318746	0.584950
17	6	0	-0.662877	3.990319	0.635656
18	6	0	-1.123192	2.854881	0.014283
19	6	0	-0.238093	1.996355	-0.691456
20	6	0	-0.471505	-0.210948	1.442969
21	6	0	-0.238702	0.840849	2.305967

22	6	0	1.968677	-0.473249	1.242771
23	6	0	3.084197	-1.153226	0.695037
24	6	0	2.937011	-2.238539	-0.117245
25	6	0	1.640022	-2.698651	-0.424623
26	6	0	0.541211	-2.061269	0.079143
27	6	0	0.651960	-0.923096	0.919953
28	1	0	-2.508679	1.036340	-3.152885
29	1	0	-4.892816	0.326957	-3.179684
30	1	0	-5.854873	-0.782965	-1.177888
31	1	0	-5.659775	-1.638172	1.009695
32	1	0	-4.337211	-2.091111	3.063052
33	1	0	-1.951198	-1.413472	3.150315
34	1	0	-0.182815	-0.831070	-2.590220
35	1	0	2.210044	-0.213814	-2.756320
36	1	0	-1.353398	4.637259	1.167891
37	1	0	-2.177450	2.595999	0.060584
38	1	0	-1.092745	1.371077	2.716111
39	6	0	1.064267	1.274186	2.631978
40	6	0	1.590105	3.511839	-0.098717
41	1	0	1.072324	5.213815	1.082780
42	1	0	2.641885	3.776862	-0.136647
43	1	0	1.194766	2.124343	3.293277
44	6	0	2.156583	0.638777	2.099997
45	1	0	3.165313	0.967041	2.325124
46	9	0	-0.660284	-2.532672	-0.279635
47	9	0	1.510560	-3.756185	-1.229949
48	9	0	3.989403	-2.879420	-0.630393
49	9	0	4.321658	-0.725115	0.988416
50	6	0	3.523283	1.799509	-1.519302
51	1	0	3.735639	2.785149	-1.946340
52	1	0	3.935722	1.787172	-0.503222
53	1	0	4.056712	1.050707	-2.108735

Compound 3 syn-in GS1 $CHCl_3$

Method: m062x/6-31+g(d,p)
SCF Done: E(RM062X) = -1590.98210253 A.U. after 1 cycles
Lowest frequency = 15.8636

Zero-point correction= 0.401565
(Hartree/Particle)
Thermal correction to Energy= 0.427950
Thermal correction to Enthalpy= 0.428895
Thermal correction to Gibbs Free Energy= 0.346629
Sum of electronic and zero-point Energies= -1590.580537
Sum of electronic and thermal Energies= -1590.554152
Sum of electronic and thermal Enthalpies= -1590.553208
Sum of electronic and thermal Free Energies= -1590.635474

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z

1	6	0	-2.153253	0.948980	-0.937683
2	6	0	-2.853453	2.082314	-1.300943
3	6	0	-4.195008	2.296755	-0.920266
4	6	0	-4.827935	1.357374	-0.151544
5	6	0	-4.156931	0.170212	0.245540
6	6	0	-4.862138	-0.776648	1.037866
7	6	0	-4.267540	-1.945127	1.425881
8	6	0	-2.939641	-2.209015	1.022804
9	6	0	-2.206762	-1.317181	0.268154
10	6	0	-2.799260	-0.070016	-0.150210
11	6	0	-0.725898	0.891846	-1.382039
12	6	0	-0.358084	0.151662	-2.479906
13	6	0	0.990877	0.072641	-2.893597
14	6	0	1.990751	0.735001	-2.219654
15	6	0	1.637175	1.553304	-1.099982
16	6	0	2.281670	3.052226	0.711783
17	6	0	0.927807	3.157130	1.110434
18	6	0	-0.048137	2.473361	0.428311
19	6	0	0.272957	1.649350	-0.688310
20	6	0	-0.845087	-1.797182	-0.136944
21	6	0	-0.776407	-2.762532	-1.118841
22	6	0	1.612219	-1.858168	-0.013836
23	6	0	2.817422	-1.380594	0.553291
24	6	0	2.822320	-0.484556	1.582590
25	6	0	1.597460	-0.025084	2.106248
26	6	0	0.413997	-0.451424	1.569424
27	6	0	0.368504	-1.360567	0.480593
28	1	0	-2.339695	2.836270	-1.891326
29	1	0	-4.707886	3.201467	-1.229961
30	1	0	-5.856886	1.499200	0.167226
31	1	0	-5.886115	-0.550466	1.322027
32	1	0	-4.803360	-2.671175	2.028395
33	1	0	-2.471664	-3.144283	1.316355
34	1	0	-1.114393	-0.413938	-3.017526
35	1	0	1.242989	-0.547859	-3.749590
36	1	0	0.663161	3.769669	1.966519
37	1	0	-1.082041	2.542164	0.750491
38	1	0	-1.701678	-3.105685	-1.572296
39	6	0	0.455728	-3.278824	-1.579207
40	6	0	2.622822	2.272762	-0.366856
41	1	0	3.050245	3.586286	1.261786
42	1	0	3.664191	2.197281	-0.663661
43	1	0	0.461885	-4.027648	-2.364348
44	6	0	1.636046	-2.820790	-1.054393
45	1	0	2.592388	-3.185056	-1.412843
46	9	0	-0.714776	0.027515	2.107341
47	9	0	1.619499	0.823820	3.135204
48	9	0	3.960660	-0.035891	2.113704
49	9	0	3.990601	-1.826551	0.075841
50	6	0	3.429189	0.586152	-2.640583
51	1	0	3.505461	-0.074023	-3.506992
52	1	0	3.875213	1.549986	-2.907255
53	1	0	4.035869	0.157587	-1.834562

Compound 3 syn-out GS2 $CHCl_3$

Method: opt freq 6-31+g
SCF Done: E(RM062X) = -1590.97921645 A.U. after 1 cycles
Lowest frequency = -3.9004

Zero-point correction= 0.401310
(Hartree/Particle)
Thermal correction to Energy= 0.426878
Thermal correction to Enthalpy= 0.427823
Thermal correction to Gibbs Free Energy= 0.348189
Sum of electronic and zero-point Energies= -1590.577907
Sum of electronic and thermal Energies= -1590.552338
Sum of electronic and thermal Enthalpies= -1590.551394
Sum of electronic and thermal Free Energies= -1590.631028

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.697716	0.855977	-0.430254
2	6	0	3.792895	1.305750	-1.138704
3	6	0	4.974981	0.543460	-1.269049
4	6	0	5.045460	-0.683764	-0.669906
5	6	0	3.951111	-1.191844	0.082901
6	6	0	4.086732	-2.463198	0.700127
7	6	0	3.070046	-2.989195	1.450789
8	6	0	1.876975	-2.254032	1.600328
9	6	0	1.688240	-1.019057	1.012220
10	6	0	2.741917	-0.431804	0.222846
11	6	0	1.529986	1.782386	-0.358977
12	6	0	1.617453	2.928856	0.393054
13	6	0	0.499043	3.779663	0.563687
14	6	0	-0.718760	3.486590	-0.002595
15	6	0	-0.822194	2.335953	-0.851253
16	6	0	-2.115666	0.909172	-2.344181
17	6	0	-0.967278	0.124202	-2.598889
18	6	0	0.218527	0.413414	-1.967169
19	6	0	0.317471	1.506109	-1.065427
20	6	0	0.366020	-0.377790	1.314186
21	6	0	0.315389	0.659634	2.219317
22	6	0	-2.095673	-0.312190	1.222596
23	6	0	-3.319319	-0.820257	0.723002
24	6	0	-3.360062	-1.856350	-0.161741
25	6	0	-2.150572	-2.423335	-0.609014
26	6	0	-0.949707	-1.951001	-0.158487
27	6	0	-0.864009	-0.895899	0.792084
28	1	0	3.729938	2.278262	-1.618425
29	1	0	5.809980	0.933340	-1.841934
30	1	0	5.939987	-1.294749	-0.753480
31	1	0	5.019197	-3.004633	0.566934
32	1	0	3.172658	-3.957238	1.929929
33	1	0	1.068721	-2.671981	2.194932
34	1	0	2.543981	3.153768	0.914904

35	1	0	0.598234	4.661571	1.191225
36	1	0	-1.028154	-0.718293	-3.281921
37	1	0	1.095088	-0.203717	-2.143482
38	1	0	1.248747	1.037267	2.625945
39	6	0	-0.903773	1.248460	2.619517
40	6	0	-2.040786	1.990320	-1.496633
41	1	0	-3.056125	0.662412	-2.827752
42	1	0	-2.925670	2.593959	-1.321673
43	1	0	-0.891652	2.077914	3.319166
44	6	0	-2.094483	0.771433	2.135296
45	1	0	-3.040415	1.205204	2.439585
46	9	0	0.148724	-2.490197	-0.704005
47	9	0	-2.200729	-3.396525	-1.523431
48	9	0	-4.513970	-2.332145	-0.635250
49	9	0	-4.472252	-0.265184	1.127125
50	6	0	-1.924255	4.345574	0.269446
51	1	0	-1.660168	5.178953	0.923579
52	1	0	-2.347312	4.756969	-0.652789
53	1	0	-2.713544	3.764024	0.760615

Compound 3 TS1 rotation

Method: m062x/6-31+g(d,p)
SCF Done: E(RM062X) = -1590.93086285 A.U. after 1 cycles
Lowest frequency = -22.6095

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.023981	1.702717	-0.234378
2	6	0	-3.001112	2.540383	-0.749016
3	6	0	-2.773712	3.910306	-0.982574
4	6	0	-1.602473	4.463879	-0.534326
5	6	0	-0.581536	3.648480	0.020489
6	6	0	0.503423	4.273586	0.699578
7	6	0	1.417696	3.507272	1.366218
8	6	0	1.430061	2.113286	1.139241
9	6	0	0.512077	1.469945	0.326819
10	6	0	-0.697180	2.221071	-0.004543
11	6	0	-2.509093	0.427287	0.381256
12	6	0	-2.225619	0.199949	1.708620
13	6	0	-2.730708	-0.930972	2.390396
14	6	0	-3.534852	-1.851745	1.762685
15	6	0	-3.838876	-1.658966	0.375169
16	6	0	-4.880108	-2.449567	-1.683480
17	6	0	-4.328373	-1.353617	-2.384999
18	6	0	-3.572243	-0.418145	-1.719859
19	6	0	-3.323348	-0.524709	-0.322777
20	6	0	0.881120	0.115125	-0.182475
21	6	0	-0.044557	-0.776816	-0.690611
22	6	0	2.495738	-1.768852	-0.237115
23	6	0	3.814868	-2.268510	-0.119174
24	6	0	4.897461	-1.441126	-0.057139
25	6	0	4.688572	-0.055095	-0.157805
26	6	0	3.421022	0.460202	-0.243274

27	6	0	2.257371	-0.357365	-0.172023
28	1	0	-4.004374	2.145917	-0.883104
29	1	0	-3.559745	4.528434	-1.403161
30	1	0	-1.448214	5.539058	-0.556985
31	1	0	0.539947	5.358616	0.734507
32	1	0	2.187965	3.956859	1.983439
33	1	0	2.250324	1.542568	1.560076
34	1	0	-1.609802	0.912743	2.250171
35	1	0	-2.484255	-1.063395	3.440385
36	1	0	-4.497905	-1.252767	-3.452315
37	1	0	-3.141544	0.411566	-2.271085
38	1	0	-1.034043	-0.434763	-0.925802
39	6	0	0.216187	-2.152768	-0.863094
40	6	0	-4.634032	-2.597292	-0.339714
41	1	0	-5.485691	-3.180421	-2.209909
42	1	0	-5.044644	-3.452170	0.187137
43	1	0	-0.586446	-2.798981	-1.204276
44	6	0	1.440167	-2.668888	-0.534991
45	1	0	1.643528	-3.732437	-0.575415
46	9	0	3.351695	1.773600	-0.508190
47	9	0	5.751414	0.748842	-0.234976
48	9	0	6.142445	-1.912359	0.022432
49	9	0	4.013914	-3.594344	-0.126098
50	6	0	-4.075759	-3.040728	2.512654
51	1	0	-5.170727	-3.052256	2.508091
52	1	0	-3.736497	-3.982748	2.069272
53	1	0	-3.742297	-3.017434	3.551882

Compound 3 TS2 rotation MeNp

Method: m062x/6-31+g(d,p)
SCF Done: E(RM062X) = -1590.93072716 A.U. after 14 cycles
Lowest frequency = -29.86

Entering Gaussian System, Link 0=g16
Input=/scripts/4FNp-MeNp-TS-4Me-in-M062X-chcl3-hansel-AM-M.gjf
Output=/scripts/4FNp-MeNp-TS-4Me-in-M062X-chcl3-hansel-AM-M.log
Initial command:
/g16/g16/l1.exe "/scratch/Gau-39141.inp" -scrdir="/scratch/"
Entering Link 1 = /g16/g16/l1.exe PID= 39142.

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.339152	2.056728	-0.115460
2	6	0	-1.101633	3.064582	-0.686304
3	6	0	-0.532937	4.261667	-1.158306
4	6	0	0.791848	4.504739	-0.897492
5	6	0	1.606725	3.513338	-0.290629
6	6	0	2.895225	3.879873	0.189351
7	6	0	3.625990	2.977429	0.913794
8	6	0	3.221033	1.624503	0.931278

9	6	0	2.075575	1.162853	0.292938
10	6	0	1.096674	2.189198	-0.066991
11	6	0	-1.090379	1.093922	0.755047
12	6	0	-0.725551	1.033259	2.087223
13	6	0	-1.473217	0.313244	3.043514
14	6	0	-2.619978	-0.343498	2.677236
15	6	0	-3.024842	-0.337682	1.318551
16	6	0	-4.567914	-1.121676	-0.391401
17	6	0	-3.782196	-0.488747	-1.374158
18	6	0	-2.658951	0.215276	-1.021354
19	6	0	-2.251245	0.358718	0.333351
20	6	0	1.996515	-0.292522	-0.046361
21	6	0	0.807549	-0.916896	-0.374567
22	6	0	3.039203	-2.560638	-0.178882
23	6	0	4.200860	-3.382834	-0.173111
24	6	0	5.463895	-2.848112	-0.244569
25	6	0	5.610655	-1.451432	-0.371217
26	6	0	4.509424	-0.627839	-0.314278
27	6	0	3.187030	-1.131770	-0.134108
28	1	0	-2.183233	2.963800	-0.688633
29	1	0	-1.161027	5.017943	-1.617950
30	1	0	1.233325	5.474545	-1.110861
31	1	0	3.239628	4.898842	0.036417
32	1	0	4.553863	3.264980	1.398327
33	1	0	3.878609	0.906228	1.404001
34	1	0	0.150679	1.586636	2.409807
35	1	0	-1.146566	0.305200	4.078405
36	1	0	-0.077113	-0.330545	-0.531022
37	6	0	0.675626	-2.313790	-0.499806
38	6	0	-4.182800	-1.047362	0.918463
39	1	0	-0.309746	-2.724805	-0.705555
40	6	0	1.744279	-3.156535	-0.316444
41	6	0	1.562597	-4.651754	-0.344898
42	1	0	2.113103	-5.112416	-1.173110
43	1	0	1.918885	-5.117745	0.580822
44	1	0	0.506023	-4.903728	-0.462710
45	1	0	4.078370	-4.460378	-0.149303
46	1	0	6.335582	-3.495456	-0.254724
47	1	0	6.593986	-1.019646	-0.532478
48	1	0	4.657001	0.432901	-0.466631
49	1	0	-3.220626	-0.879752	3.402737
50	9	0	-4.916050	-1.681729	1.846309
51	9	0	-5.655139	-1.799562	-0.765127
52	9	0	-4.137438	-0.608036	-2.655709
53	9	0	-1.926951	0.726655	-2.023250

Compound 4 anti-in GS1 $CHCl_3$

Method: m062x/6-31+g(d,p)
SCF Done: E(RM062X) = -1666.16892396 A.U. after 1 cycles
Lowest frequency = 18.5499

Zero-point correction= 0.406709
(Hartree/Particle)
Thermal correction to Energy= 0.434128
Thermal correction to Ent halpy= 0.435073
Thermal correction to Gibbs Free Energy= 0.350147

Sum of electronic and zero-point Energies= -1665.762215
Sum of electronic and thermal Energies= -1665.734795
Sum of electronic and thermal Enthalpies= -1665.733851
Sum of electronic and thermal Free Energies= -1665.818777

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.176729	0.467942	-1.221716
2	6	0	-2.916794	0.772836	-2.346077
3	6	0	-4.284747	0.441167	-2.462355
4	6	0	-4.904086	-0.208646	-1.429750
5	6	0	-4.187716	-0.550583	-0.250692
6	6	0	-4.873808	-1.233456	0.790006
7	6	0	-4.226328	-1.579700	1.943909
8	6	0	-2.861116	-1.250307	2.093851
9	6	0	-2.145922	-0.599472	1.109211
10	6	0	-2.800761	-0.215501	-0.116812
11	6	0	-0.731728	0.843132	-1.252937
12	6	0	0.146360	0.094066	-1.997318
13	6	0	1.539092	0.355035	-2.011164
14	6	0	2.041724	1.392550	-1.260763
15	6	0	1.157068	2.263312	-0.543677
16	6	0	0.784909	4.221858	0.837723
17	6	0	-0.607535	3.974017	0.807704
18	6	0	-1.104717	2.887222	0.128433
19	6	0	-0.239104	1.995841	-0.559351
20	6	0	-0.725053	-0.277257	1.468869
21	6	0	-0.517603	0.735463	2.383134
22	6	0	1.713876	-0.607686	1.413183
23	6	0	2.842005	-1.298945	0.907261
24	6	0	2.714844	-2.350595	0.048089
25	6	0	1.427633	-2.762258	-0.353641
26	6	0	0.317879	-2.110430	0.105797
27	6	0	0.408340	-1.006664	0.993535
28	1	0	-2.421180	1.289424	-3.163099
29	1	0	-4.830044	0.701758	-3.363627
30	1	0	-5.954703	-0.478828	-1.490928
31	1	0	-5.924062	-1.471753	0.646232
32	1	0	-4.746583	-2.100370	2.741159
33	1	0	-2.347370	-1.523184	3.011220
34	1	0	-0.227390	-0.762810	-2.552690
35	1	0	2.189489	-0.293530	-2.585920
36	1	0	-1.285571	4.645845	1.325164
37	1	0	-2.173585	2.692402	0.114026
38	1	0	-1.380460	1.278472	2.756718
39	6	0	0.773895	1.116093	2.807218
40	6	0	1.649286	3.383244	0.174312
41	1	0	1.169123	5.079372	1.381109
42	1	0	2.718023	3.566558	0.185276
43	1	0	0.886236	1.938676	3.505653
44	6	0	1.879202	0.467604	2.320678
45	1	0	2.880915	0.760269	2.614621

46	9	0	-0.871822	-2.530299	-0.344369
47	9	0	1.320003	-3.784584	-1.206447
48	9	0	3.780823	-2.996985	-0.430889
49	9	0	4.071265	-0.914987	1.284036
50	8	0	3.360769	1.681346	-1.133498
51	6	0	4.284249	0.856884	-1.825708
52	1	0	5.273000	1.241418	-1.581380
53	1	0	4.203807	-0.184993	-1.494862
54	1	0	4.122093	0.911592	-2.907375

Compound 4 syn-in GS1 $CHCl_3$

Method: m062x/6-31+g(d,p)
SCF Done: E(RM062X) = -1666.16809865 A.U. after 2 cycles
Lowest frequency = 15.6030

Zero-point correction= 0.406841
(Hartree/Particle)
Thermal correction to Energy= 0.434198
Thermal correction to Enthalpy= 0.435142
Thermal correction to Gibbs Free Energy= 0.350544
Sum of electronic and zero-point Energies= -1665.761258
Sum of electronic and thermal Energies= -1665.733901
Sum of electronic and thermal Enthalpies= -1665.732957
Sum of electronic and thermal Free Energies= -1665.817555

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.198847	0.816853	-1.121396
2	6	0	-2.878032	1.888731	-1.666169
3	6	0	-4.249871	2.116154	-1.427585
4	6	0	-4.936945	1.253519	-0.616628
5	6	0	-4.289614	0.131857	-0.033251
6	6	0	-5.050813	-0.735060	0.797744
7	6	0	-4.479179	-1.839873	1.365101
8	6	0	-3.118119	-2.118528	1.109985
9	6	0	-2.331677	-1.301573	0.324650
10	6	0	-2.899673	-0.121860	-0.281938
11	6	0	-0.737728	0.739306	-1.428684
12	6	0	-0.259334	-0.118440	-2.388230
13	6	0	1.120751	-0.238396	-2.675334
14	6	0	2.029109	0.524049	-1.977224
15	6	0	1.581567	1.475099	-1.006315
16	6	0	2.067113	3.184106	0.646665
17	6	0	0.682499	3.316514	0.907594
18	6	0	-0.230587	2.543254	0.232525
19	6	0	0.187344	1.593529	-0.742521
20	6	0	-0.934493	-1.798287	0.098598
21	6	0	-0.771507	-2.874256	-0.747921
22	6	0	1.503065	-1.798636	0.441425

23	6	0	2.650685	-1.229917	1.042855
24	6	0	2.557019	-0.219718	1.955722
25	6	0	1.286641	0.271603	2.317063
26	6	0	0.158242	-0.236864	1.734796
27	6	0	0.216422	-1.268621	0.762135
28	1	0	-2.323188	2.583343	-2.291168
29	1	0	-4.744033	2.970541	-1.878537
30	1	0	-5.991505	1.407787	-0.405374
31	1	0	-6.098079	-0.500034	0.966372
32	1	0	-5.057175	-2.505103	1.998104
33	1	0	-2.667039	-3.004589	1.547416
34	1	0	-0.957395	-0.757891	-2.921739
35	1	0	1.441065	-0.955706	-3.420829
36	1	0	0.341279	4.024881	1.656016
37	1	0	-1.288801	2.637737	0.452972
38	1	0	-1.650120	-3.286523	-1.235361
39	6	0	0.499913	-3.424634	-1.027424
40	6	0	2.506149	2.283089	-0.293543
41	1	0	2.781058	3.792237	1.193026
42	1	0	3.564712	2.169280	-0.500347
43	1	0	0.580209	-4.267229	-1.706323
44	6	0	1.625324	-2.885313	-0.461473
45	1	0	2.611758	-3.278822	-0.680444
46	9	0	-1.017714	0.279752	2.113498
47	9	0	1.210701	1.233999	3.237922
48	9	0	3.640320	0.312564	2.522973
49	9	0	3.863935	-1.702114	0.717854
50	8	0	3.375316	0.446236	-2.128504
51	6	0	3.879132	-0.507731	-3.048389
52	1	0	4.963943	-0.429078	-2.999166
53	1	0	3.569192	-1.520536	-2.767721
54	1	0	3.539069	-0.287731	-4.066098

Compound 4 syn-out GS2 $CHCl_3$

Method: m062x/6-31+g(d,p)
SCF Done: E(RM062X) = -1666.16519073 A.U. after 1 cycles
Lowest frequency = 5.4110

Zero-point correction= 0.406426
(Hartree/Particle)
Thermal correction to Energy= 0.433976
Thermal correction to Enthalpy= 0.434920
Thermal correction to Gibbs Free Energy= 0.348153
Sum of electronic and zero-point Energies= -1665.758765
Sum of electronic and thermal Energies= -1665.731215
Sum of electronic and thermal Enthalpies= -1665.730270
Sum of electronic and thermal Free Energies= -1665.817038

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z

1	6	0	-2.627628	1.055848	0.482732
2	6	0	-3.656995	1.622603	1.205908
3	6	0	-4.940985	1.038138	1.282172
4	6	0	-5.180821	-0.131761	0.616184
5	6	0	-4.159938	-0.755382	-0.152998
6	6	0	-4.470258	-1.958709	-0.839597
7	6	0	-3.530096	-2.587213	-1.610976
8	6	0	-2.240639	-2.027691	-1.711683
9	6	0	-1.882342	-0.867181	-1.054460
10	6	0	-2.850465	-0.174784	-0.241061
11	6	0	-1.334902	1.800007	0.470086
12	6	0	-1.233788	2.980299	-0.223161
13	6	0	-0.006125	3.676954	-0.352215
14	6	0	1.131698	3.157645	0.219852
15	6	0	1.064374	1.967709	1.016131
16	6	0	2.125544	0.313863	2.437651
17	6	0	0.873953	-0.312549	2.638728
18	6	0	-0.252522	0.170776	2.015289
19	6	0	-0.186583	1.309942	1.170874
20	6	0	-0.476021	-0.412239	-1.311513
21	6	0	-0.260340	0.651611	-2.159936
22	6	0	1.967234	-0.712787	-1.197417
23	6	0	3.095874	-1.420088	-0.716402
24	6	0	2.971229	-2.494223	0.113277
25	6	0	1.685134	-2.900079	0.520407
26	6	0	0.573038	-2.235258	0.085251
27	6	0	0.656963	-1.131166	-0.808277
28	1	0	-3.459371	2.547385	1.740292
29	1	0	-5.719482	1.516364	1.867612
30	1	0	-6.156761	-0.607461	0.657692
31	1	0	-5.473635	-2.364036	-0.742887
32	1	0	-3.765768	-3.502853	-2.143254
33	1	0	-1.493387	-2.526911	-2.323095
34	1	0	-2.107768	3.367246	-0.740582
35	1	0	0.021979	4.589048	-0.935478
36	1	0	0.805757	-1.189497	3.276336
37	1	0	-1.208837	-0.325696	2.153646
38	1	0	-1.122123	1.182723	-2.552807
39	6	0	1.037765	1.074967	-2.518849
40	6	0	2.217256	1.437189	1.647710
41	1	0	3.013252	-0.087638	2.916819
42	1	0	3.169661	1.934376	1.500217
43	1	0	1.157619	1.931884	-3.173948
44	6	0	2.138680	0.404918	-2.050863
45	1	0	3.142457	0.712470	-2.321247
46	9	0	-0.600860	-2.636306	0.591442
47	9	0	1.578602	-3.915725	1.382351
48	9	0	4.035907	-3.157732	0.569706
49	9	0	4.323345	-1.021802	-1.083457
50	8	0	2.370070	3.697198	0.100241
51	6	0	2.506278	4.855279	-0.705756
52	1	0	3.564542	5.110742	-0.689856
53	1	0	2.190131	4.651716	-1.735116
54	1	0	1.920821	5.686819	-0.299164

Compound 4 TS-rotation fluoro-naphthyl $CHCl_3$

Method: m062x/6-31+g(d,p)
SCF Done: E(RM062X) = -1666.11710295 A.U. after 1 cycles
Lowest frequency = -22.9824

Zero-point correction= 0.406451
(Hartree/Particle)
Thermal correction to Energy= 0.433065
Thermal correction to Enthalpy= 0.434009
Thermal correction to Gibbs Free Energy= 0.350887
Sum of electronic and zero-point Energies= -1665.710652
Sum of electronic and thermal Energies= -1665.684038
Sum of electronic and thermal Enthalpies= -1665.683094
Sum of electronic and thermal Free Energies= -1665.766216

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.775038	1.955031	-0.264640
2	6	0	-2.666884	2.900865	-0.746265
3	6	0	-2.335618	4.265170	-0.852655
4	6	0	-1.152142	4.694611	-0.309632
5	6	0	-0.217211	3.764852	0.215446
6	6	0	0.873268	4.251716	0.992269
7	6	0	1.700935	3.368934	1.626908
8	6	0	1.631280	2.001820	1.278171
9	6	0	0.711961	1.496034	0.375229
10	6	0	-0.427966	2.356342	0.061477
11	6	0	-2.367611	0.666934	0.211769
12	6	0	-2.156043	0.297206	1.519276
13	6	0	-2.743753	-0.856710	2.090576
14	6	0	-3.569293	-1.648452	1.327823
15	6	0	-3.814767	-1.321942	-0.046362
16	6	0	-4.819380	-1.873783	-2.185749
17	6	0	-4.184308	-0.752122	-2.764925
18	6	0	-3.402077	0.078734	-1.997047
19	6	0	-3.208213	-0.163062	-0.608646
20	6	0	1.016240	0.167203	-0.236513
21	6	0	0.059723	-0.616716	-0.854346
22	6	0	2.512791	-1.806712	-0.395329
23	6	0	3.792482	-2.399305	-0.272442
24	6	0	4.920264	-1.652352	-0.098087
25	6	0	4.801433	-0.252026	-0.084958
26	6	0	3.572843	0.349947	-0.171930
27	6	0	2.358925	-0.393326	-0.216010
28	1	0	-3.687482	2.592183	-0.954391
29	1	0	-3.056662	4.970893	-1.251351
30	1	0	-0.924176	5.754042	-0.232908

31	1	0	0.980368	5.324629	1.124016
32	1	0	2.469218	3.708781	2.312975
33	1	0	2.392194	1.341775	1.679542
34	1	0	-1.520783	0.915938	2.147145
35	1	0	-2.540669	-1.088293	3.128670
36	1	0	-0.896398	-0.192867	-1.093923
37	6	0	0.242396	-1.987307	-1.135595
38	6	0	-4.631195	-2.155132	-0.853418
39	1	0	-0.583354	-2.549096	-1.560754
40	6	0	1.417362	-2.607873	-0.808953
41	1	0	1.556201	-3.675213	-0.934128
42	9	0	3.909248	-3.730041	-0.387277
43	9	0	6.129420	-2.208450	-0.013228
44	9	0	5.914212	0.484680	-0.052012
45	9	0	3.596047	1.682788	-0.322736
46	1	0	-5.094047	-3.024296	-0.400088
47	1	0	-5.442506	-2.518947	-2.796649
48	1	0	-4.309894	-0.547113	-3.823446
49	1	0	-2.908364	0.927554	-2.458757
50	8	0	-4.193624	-2.765584	1.773868
51	6	0	-3.977668	-3.146059	3.123090
52	1	0	-4.557905	-4.054578	3.275244
53	1	0	-2.917243	-3.350218	3.305332
54	1	0	-4.326266	-2.366428	3.808620

Compound 4 TS rotation OMe-naphthyl $CHCl_3$

Method: m062x/6-31+g(d,p)
SCF Done: E(RM062X) = -1666.11758236 A.U. after 1 cycles
Lowest frequency = -30.9903

Zero-point correction= 0.406606
(Hartree/Particle)
Thermal correction to Energy= 0.433283
Thermal correction to Enthalpy= 0.434227
Thermal correction to Gibbs Free Energy= 0.350719
Sum of electronic and zero-point Energies= -1665.710976
Sum of electronic and thermal Energies= -1665.684300
Sum of electronic and thermal Enthalpies= -1665.683355
Sum of electronic and thermal Free Energies= -1665.766864

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.359963	2.221703	-0.149500
2	6	0	-1.121210	3.210445	-0.748294
3	6	0	-0.549769	4.396549	-1.246964
4	6	0	0.771630	4.647400	-0.981357
5	6	0	1.583439	3.671529	-0.344872
6	6	0	2.868895	4.050464	0.135884
7	6	0	3.592194	3.165565	0.886451

8	6	0	3.185174	1.812520	0.934208
9	6	0	2.045383	1.339172	0.300864
10	6	0	1.074009	2.356394	-0.094566
11	6	0	-1.109921	1.282887	0.745421
12	6	0	-0.750207	1.261328	2.077607
13	6	0	-1.493572	0.554560	3.048216
14	6	0	-2.628209	-0.126184	2.692509
15	6	0	-3.024585	-0.158108	1.331419
16	6	0	-4.540097	-1.010115	-0.366862
17	6	0	-3.756978	-0.390273	-1.359621
18	6	0	-2.650128	0.339348	-1.017574
19	6	0	-2.257494	0.523613	0.336553
20	6	0	1.966766	-0.123349	-0.003261
21	6	0	0.781809	-0.762216	-0.303750
22	6	0	3.026363	-2.378860	-0.113603
23	6	0	4.172545	-3.216173	-0.127681
24	6	0	5.434316	-2.683024	-0.215370
25	6	0	5.580046	-1.285659	-0.343234
26	6	0	4.484084	-0.456855	-0.278637
27	6	0	3.161884	-0.956522	-0.085217
28	1	0	-2.203013	3.106617	-0.754374
29	1	0	-1.174490	5.140061	-1.730176
30	1	0	1.214131	5.611568	-1.215767
31	1	0	3.214531	5.065137	-0.038957
32	1	0	4.517093	3.463112	1.369645
33	1	0	3.840971	1.104364	1.424934
34	1	0	0.118584	1.833205	2.389137
35	1	0	-1.172171	0.575332	4.083989
36	1	0	-0.107910	-0.183692	-0.458271
37	6	0	0.633981	-2.161207	-0.412550
38	6	0	-4.167741	-0.895850	0.941127
39	1	0	-0.352187	-2.565398	-0.607163
40	6	0	1.726604	-2.970458	-0.224633
41	1	0	4.024621	-4.289645	-0.104490
42	1	0	6.305208	-3.330024	-0.237370
43	1	0	6.562499	-0.856285	-0.513308
44	1	0	4.635845	0.602916	-0.432464
45	1	0	-3.224741	-0.653351	3.427927
46	9	0	-4.897106	-1.517218	1.877744
47	9	0	-5.611095	-1.714626	-0.732122
48	9	0	-4.099987	-0.550161	-2.638306
49	9	0	-1.919812	0.835604	-2.025203
50	8	0	1.692839	-4.322877	-0.203537
51	6	0	0.430073	-4.949984	-0.363702
52	1	0	-0.000263	-4.714190	-1.342625
53	1	0	0.615446	-6.020373	-0.293063
54	1	0	-0.260787	-4.640589	0.427612

Compound 5 anti-in GS1 $CHCl_3$

Method: m062x/6-31+g(d,p)
SCF Done: E(RM062X) = -1666.16755310 A.U. after 1 cycles
Lowest frequency = 16.2879

Zero-point correction=	0.406564
(Hartree/Particle)	
Thermal correction to Energy=	0.434070
Thermal correction to Enthalpy=	0.435014
Thermal correction to Gibbs Free Energy=	0.349228
Sum of electronic and zero-point Energies=	-1665.760989
Sum of electronic and thermal Energies=	-1665.733483
Sum of electronic and thermal Enthalpies=	-1665.732539
Sum of electronic and thermal Free Energies=	-1665.818325

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.077246	-0.799961	-1.175095
2	6	0	2.824709	-1.202664	-2.263305
3	6	0	4.233313	-1.291843	-2.219470
4	6	0	4.886392	-0.970405	-1.060992
5	6	0	4.165299	-0.540803	0.086009
6	6	0	4.891238	-0.211184	1.262794
7	6	0	4.240794	0.206215	2.391037
8	6	0	2.832886	0.316294	2.374063
9	6	0	2.081966	0.022739	1.253849
10	6	0	2.736220	-0.440126	0.054701
11	6	0	0.597627	-0.748143	-1.376363
12	6	0	0.059365	0.252800	-2.157323
13	6	0	-1.336794	0.363630	-2.345880
14	6	0	-2.186913	-0.532667	-1.743959
15	6	0	-1.663555	-1.605639	-0.978216
16	6	0	-2.010931	-3.629967	0.344813
17	6	0	-0.604734	-3.777322	0.453746
18	6	0	0.254656	-2.866138	-0.101130
19	6	0	-0.257919	-1.747658	-0.817649
20	6	0	0.599500	0.164310	1.432005
21	6	0	-0.035913	-0.763921	2.231331
22	6	0	-1.579510	1.269336	1.129376
23	6	0	-2.352790	2.315037	0.568917
24	6	0	-1.787110	3.309812	-0.172588
25	6	0	-0.394547	3.298767	-0.392186
26	6	0	0.380684	2.299200	0.124907
27	6	0	-0.171060	1.241790	0.894374
28	1	0	2.301535	-1.468449	-3.177474
29	1	0	4.782281	-1.616997	-3.097144
30	1	0	5.969009	-1.033917	-0.995124
31	1	0	5.973927	-0.299635	1.243208
32	1	0	4.790874	0.457100	3.292037
33	1	0	2.317009	0.657705	3.266885
34	1	0	0.723312	0.991750	-2.599369
35	1	0	-1.733852	1.174450	-2.949232
36	1	0	-0.212402	-4.630950	0.998080
37	1	0	1.328556	-2.982693	0.006256
38	1	0	0.553754	-1.571788	2.653323
39	6	0	-1.426799	-0.725702	2.470744

40	6	0	-2.529082	-2.563582	-0.355002
41	1	0	-2.657871	-4.362443	0.811532
42	1	0	-1.885024	-1.496119	3.082138
43	6	0	-2.195473	0.264494	1.915865
44	1	0	-3.268378	0.299006	2.068711
45	9	0	1.691756	2.336377	-0.148951
46	9	0	0.145242	4.274367	-1.127537
47	9	0	-2.517263	4.295518	-0.698880
48	9	0	-3.677946	2.332866	0.775258
49	1	0	-3.261839	-0.439855	-1.852520
50	8	0	-3.854318	-2.324258	-0.519107
51	6	0	-4.766369	-3.224253	0.086840
52	1	0	-4.631852	-3.242141	1.174086
53	1	0	-5.760934	-2.852142	-0.153600
54	1	0	-4.644041	-4.235659	-0.315219

Compound 5 syn-in GS1 $CHCl_3$

Method: m062x/6-31+g(d,p)
SCF Done: E(RM062X) = -1666.16846540 A.U. after 1 cycles
Lowest frequency = 17.8021

Zero-point correction= 0.407044
(Hartree/Particle)
Thermal correction to Energy= 0.434280
Thermal correction to Enthalpy= 0.435224
Thermal correction to Gibbs Free Energy= 0.351304
Sum of electronic and zero-point Energies= -1665.761421
Sum of electronic and thermal Energies= -1665.734185
Sum of electronic and thermal Enthalpies= -1665.733241
Sum of electronic and thermal Free Energies= -1665.817161

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.228944	-1.122236	-0.930646
2	6	0	2.781933	-2.333413	-1.295548
3	6	0	4.064822	-2.738275	-0.869082
4	6	0	4.785990	-1.913308	-0.048769
5	6	0	4.268997	-0.652011	0.350497
6	6	0	5.060855	0.171993	1.196165
7	6	0	4.618885	1.406812	1.583841
8	6	0	3.365258	1.865905	1.122454
9	6	0	2.552968	1.099050	0.314479
10	6	0	2.978207	-0.215663	-0.097859
11	6	0	0.830634	-0.879651	-1.409321
12	6	0	0.590696	-0.139541	-2.546653
13	6	0	-0.724030	0.087005	-3.008896
14	6	0	-1.797626	-0.428045	-2.322073
15	6	0	-1.587817	-1.215287	-1.163206
16	6	0	-2.486280	-2.523769	0.695266

17	6	0	-1.159681	-2.799916	1.115018
18	6	0	-0.076665	-2.293824	0.447002
19	6	0	-0.264637	-1.476906	-0.707927
20	6	0	1.302740	1.770157	-0.167691
21	6	0	1.427233	2.699315	-1.178229
22	6	0	-1.124553	2.165640	-0.202411
23	6	0	-2.417427	1.858138	0.284458
24	6	0	-2.603674	1.006879	1.334473
25	6	0	-1.484701	0.426669	1.965004
26	6	0	-0.222887	0.681737	1.503773
27	6	0	0.008470	1.530708	0.390059
28	1	0	2.192524	-3.000444	-1.918850
29	1	0	4.460911	-3.698972	-1.181519
30	1	0	5.769514	-2.204310	0.309652
31	1	0	6.028041	-0.201550	1.520949
32	1	0	5.222331	2.038839	2.227052
33	1	0	3.023024	2.856216	1.409014
34	1	0	1.430596	0.299481	-3.078241
35	1	0	-0.881695	0.686830	-3.899746
36	1	0	-1.011976	-3.411602	1.999520
37	1	0	0.928331	-2.494244	0.801432
38	1	0	2.415337	2.890906	-1.586378
39	6	0	0.307614	3.365548	-1.725264
40	6	0	-2.694771	-1.743550	-0.418921
41	1	0	-3.316154	-2.921924	1.265921
42	1	0	0.450209	4.081341	-2.528063
43	6	0	-0.953414	3.086071	-1.266779
44	1	0	-1.828280	3.558666	-1.699022
45	9	0	0.798816	0.097867	2.142748
46	9	0	-1.684528	-0.368097	3.017804
47	9	0	-3.823973	0.708440	1.785855
48	9	0	-3.488812	2.419202	-0.295991
49	1	0	-2.813038	-0.238501	-2.651872
50	8	0	-3.916659	-1.395379	-0.894935
51	6	0	-5.056337	-1.881068	-0.203546
52	1	0	-5.069153	-1.517245	0.829140
53	1	0	-5.920249	-1.492082	-0.740041
54	1	0	-5.079021	-2.976057	-0.211203

Compound 5 syn-out GS2 $CHCl_3$

Method: m062x/6-31+g(d,p)
SCF Done: E(RM062X) = -1666.16560282 A.U. after 1 cycles
Lowest frequency = 17.5147

Zero-point correction= 0.406682
(Hartree/Particle)
Thermal correction to Energy= 0.434086
Thermal correction to Enthalpy= 0.435030
Thermal correction to Gibbs Free Energy= 0.350023
Sum of electronic and zero-point Energies= -1665.758921
Sum of electronic and thermal Energies= -1665.731517
Sum of electronic and thermal Enthalpies= -1665.730573
Sum of electronic and thermal Free Energies= -1665.815580

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.824239	1.118383	-0.327549
2	6	0	3.870739	1.767663	-0.950268
3	6	0	5.105352	1.134806	-1.214577
4	6	0	5.274989	-0.171584	-0.848263
5	6	0	4.235876	-0.885697	-0.190228
6	6	0	4.473268	-2.236428	0.176772
7	6	0	3.514451	-2.963773	0.829251
8	6	0	2.285375	-2.350900	1.143232
9	6	0	1.999037	-1.043357	0.803327
10	6	0	2.981106	-0.253119	0.102168
11	6	0	1.578147	1.915519	-0.132536
12	6	0	1.585807	2.990574	0.729622
13	6	0	0.403501	3.714249	1.006343
14	6	0	-0.787699	3.331009	0.439928
15	6	0	-0.820680	2.258779	-0.488490
16	6	0	-2.052551	0.850334	-2.058855
17	6	0	-0.831226	0.244597	-2.446482
18	6	0	0.354010	0.579281	-1.846003
19	6	0	0.379558	1.579251	-0.833382
20	6	0	0.679140	-0.536484	1.302626
21	6	0	0.674526	0.376269	2.335368
22	6	0	-1.780313	-0.584887	1.446855
23	6	0	-3.028827	-1.078876	0.995431
24	6	0	-3.118685	-1.991557	-0.012836
25	6	0	-1.938081	-2.443648	-0.633679
26	6	0	-0.715469	-1.982673	-0.231343
27	6	0	-0.574532	-1.050750	0.834705
28	1	0	3.722466	2.797215	-1.263200
29	1	0	5.898234	1.682077	-1.713758
30	1	0	6.207899	-0.690702	-1.049737
31	1	0	5.436047	-2.676150	-0.068347
32	1	0	3.693681	-3.994959	1.115077
33	1	0	1.531012	-2.922548	1.677809
34	1	0	2.507926	3.249760	1.243309
35	1	0	0.435752	4.549085	1.699350
36	1	0	-0.851453	-0.520228	-3.217733
37	1	0	1.275059	0.080249	-2.129188
38	1	0	1.627526	0.750597	2.697715
39	6	0	-0.520696	0.842037	2.923510
40	6	0	-2.047849	1.834560	-1.094589
41	1	0	-2.974132	0.530674	-2.530285
42	1	0	-0.472717	1.574922	3.722105
43	6	0	-1.733016	0.370443	2.491387
44	1	0	-2.661415	0.716289	2.931310
45	9	0	0.343297	-2.412795	-0.929351
46	9	0	-2.040950	-3.294609	-1.659123
47	9	0	-4.296605	-2.448860	-0.444819
48	9	0	-4.156893	-0.634575	1.571554
49	1	0	-1.712101	3.842425	0.683802

50	8	0	-3.157740	2.472121	-0.645209
51	6	0	-4.408692	2.071045	-1.179566
52	1	0	-4.598286	1.011134	-0.974886
53	1	0	-5.159041	2.680004	-0.678086
54	1	0	-4.449003	2.250341	-2.259194

Compound 5 TS-rotation fluoro-naphthyl CHCl3

Method: m062x/6-31+g(d,p) SCF Done: E(RM062X) = -1666.11700486 A.U. after 1 cycles
Lowest frequency = -21.4903

Zero-point correction= 0.406403
(Hartree/Particle)
Thermal correction to Energy= 0.433015
Thermal correction to Enthalpy= 0.433959
Thermal correction to Gibbs Free Energy= 0.350720
Sum of electronic and zero-point Energies= -1665.710601
Sum of electronic and thermal Energies= -1665.683990
Sum of electronic and thermal Enthalpies= -1665.683046
Sum of electronic and thermal Free Energies= -1665.766284

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.460375	2.140936	-0.191586
2	6	0	-2.298155	3.110549	-0.719640
3	6	0	-1.850696	4.411501	-1.019892
4	6	0	-0.589187	4.775633	-0.626017
5	6	0	0.296781	3.821873	-0.059882
6	6	0	1.493104	4.280722	0.562322
7	6	0	2.285519	3.398311	1.241303
8	6	0	2.054402	2.014453	1.079616
9	6	0	1.015541	1.503503	0.320230
10	6	0	-0.058887	2.435161	-0.016389
11	6	0	-2.137541	0.993128	0.491651
12	6	0	-1.855315	0.780022	1.825674
13	6	0	-2.521893	-0.217179	2.570431
14	6	0	-3.481939	-0.998829	1.976622
15	6	0	-3.790365	-0.822134	0.603736
16	6	0	-5.018328	-1.531840	-1.387468
17	6	0	-4.304820	-0.569322	-2.142713
18	6	0	-3.384542	0.262384	-1.558884
19	6	0	-3.117577	0.172332	-0.161179
20	6	0	1.134259	0.085485	-0.134172
21	6	0	0.055955	-0.658865	-0.574576
22	6	0	2.409952	-2.043682	-0.142918
23	6	0	3.631147	-2.751877	-0.038590
24	6	0	4.837624	-2.115581	-0.046870
25	6	0	4.858425	-0.719583	-0.207115
26	6	0	3.691880	-0.003264	-0.280381
27	6	0	2.411953	-0.610846	-0.138182
28	1	0	-3.356827	2.885884	-0.813008
29	1	0	-2.534061	5.136523	-1.449034
30	1	0	-0.256360	5.807118	-0.700908
31	1	0	1.713981	5.344097	0.545182

32	1	0	3.140212	3.735471	1.817695
33	1	0	2.779041	1.330558	1.507235
34	1	0	-1.110997	1.402960	2.313897
35	1	0	-2.277419	-0.352995	3.619001
36	1	0	-0.869824	-0.166373	-0.802299
37	6	0	0.077751	-2.065263	-0.686938
38	6	0	-4.762205	-1.657525	-0.040832
39	1	0	-0.832773	-2.581461	-0.974437
40	6	0	1.209197	-2.765343	-0.367719
41	1	0	1.230609	-3.848692	-0.361927
42	9	0	3.606773	-4.091410	0.011924
43	9	0	5.989179	-2.784925	0.019016
44	9	0	6.036667	-0.109171	-0.352692
45	9	0	3.832159	1.291066	-0.604447
46	1	0	-5.744812	-2.163430	-1.883053
47	1	0	-4.495454	-0.498512	-3.209017
48	1	0	-2.843136	0.980815	-2.164032
49	8	0	-5.369544	-2.556168	0.772962
50	6	0	-6.334192	-3.421903	0.197632
51	1	0	-5.883625	-4.045556	-0.581846
52	1	0	-6.693707	-4.052035	1.009394
53	1	0	-7.168715	-2.851326	-0.223560
54	1	0	-4.007630	-1.761503	2.539184

Compound 5 TS-rotation 5OMe-naphthyl CHCl3

Method: m062x/6-31+g(d,p) SCF Done: E(RM062X) = -1666.11634292 A.U. after 1 cycles
Lowest frequency = -25.1612

Zero-point correction= 0.406673
(Hartree/Particle)
Thermal correction to Energy= 0.433294
Thermal correction to Enthalpy= 0.434238
Thermal correction to Gibbs Free Energy= 0.350936
Sum of electronic and zero-point Energies= -1665.709670
Sum of electronic and thermal Energies= -1665.683049
Sum of electronic and thermal Enthalpies= -1665.682105
Sum of electronic and thermal Free Energies= -1665.765406

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.124830	2.032200	-0.130858
2	6	0	-2.105876	2.816294	-0.712700
3	6	0	-1.842600	4.113990	-1.190630
4	6	0	-0.621559	4.675286	-0.918922
5	6	0	0.404894	3.915627	-0.298131
6	6	0	1.557382	4.588468	0.198478
7	6	0	2.474024	3.895111	0.939010
8	6	0	2.413265	2.482631	0.955979
9	6	0	1.425294	1.757752	0.307316
10	6	0	0.233108	2.511628	-0.073239
11	6	0	-1.618630	0.922409	0.746595

12	6	0	-1.256977	0.965141	2.077688
13	6	0	-1.800357	0.081232	3.035646
14	6	0	-2.737483	-0.848272	2.668403
15	6	0	-3.122576	-0.950565	1.307510
16	6	0	-4.397491	-2.113242	-0.404081
17	6	0	-3.794922	-1.303527	-1.385963
18	6	0	-2.895283	-0.334156	-1.031852
19	6	0	-2.549797	-0.085348	0.324694
20	6	0	1.708507	0.325166	-0.028654
21	6	0	0.704850	-0.569281	-0.356300
22	6	0	3.269301	-1.595661	-0.167256
23	6	0	4.601807	-2.131443	-0.168173
24	6	0	5.697598	-1.305864	-0.240500
25	6	0	5.486736	0.088507	-0.348406
26	6	0	4.232696	0.637435	-0.281309
27	6	0	3.071239	-0.180817	-0.114762
28	1	0	-3.129805	2.452321	-0.721205
29	1	0	-2.631440	4.690782	-1.661335
30	1	0	-0.428650	5.722465	-1.134606
31	1	0	1.643751	5.660149	0.044267
32	1	0	3.295778	4.401499	1.434453
33	1	0	3.223169	1.947272	1.434810
34	1	0	-0.552079	1.725697	2.399460
35	1	0	-1.487185	0.160539	4.071116
36	1	0	-0.293965	-0.211021	-0.511680
37	6	0	0.915830	-1.955134	-0.486330
38	6	0	-4.055362	-1.936092	0.905162
39	1	0	0.068438	-2.600506	-0.696943
40	6	0	2.169897	-2.477938	-0.308470
41	1	0	6.705489	-1.700392	-0.264773
42	1	0	6.344051	0.736362	-0.502392
43	1	0	4.129267	1.704333	-0.419629
44	1	0	-3.183282	-1.518529	3.394089
45	9	0	-4.606626	-2.732334	1.831028
46	9	0	-5.268653	-3.049103	-0.780693
47	9	0	-4.098657	-1.516710	-2.666761
48	9	0	-2.313413	0.343178	-2.030844
49	8	0	4.668103	-3.487133	-0.129011
50	6	0	5.952876	-4.084099	-0.172680
51	1	0	5.785851	-5.159422	-0.137015
52	1	0	6.474180	-3.821898	-1.099618
53	1	0	6.556323	-3.776651	0.688172
54	1	0	2.348060	-3.545847	-0.343234

Compound 6 anti-in GS1 CHCl3

Method: m062x/6-31+g(d,p)
SCF Done: E(RM062X) = -1383.83372569 A.U. after 1 cycles
Lowest frequency = 19.5030

Zero-point correction= 0.472208
(Hartree/Particle)
Thermal correction to Energy= 0.498554

Thermal correction to Enthalpy= 0.499498
Thermal correction to Gibbs Free Energy= 0.416379
Sum of electronic and zero-point Energies= -1383.361517
Sum of electronic and thermal Energies= -1383.335172
Sum of electronic and thermal Enthalpies= -1383.334228
Sum of electronic and thermal Free Energies= -1383.417346

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.117976	-0.345907	1.237043
2	6	0	-2.873047	-0.582470	2.369328
3	6	0	-4.284297	-0.533628	2.363906
4	6	0	-4.937909	-0.264935	1.192524
5	6	0	-4.211562	0.000369	-0.000230
6	6	0	-4.937600	0.265839	-1.193137
7	6	0	-4.283678	0.534398	-2.364373
8	6	0	-2.872413	0.582929	-2.369490
9	6	0	-2.117625	0.346187	-1.237055
10	6	0	-2.777925	0.000211	-0.000077
11	6	0	-0.639832	-0.495025	1.397726
12	6	0	0.043089	0.381561	2.215362
13	6	0	1.443873	0.300460	2.368912
14	6	0	2.156984	-0.663226	1.697010
15	6	0	1.481246	-1.613462	0.891441
16	6	0	1.534704	-3.585742	-0.550484
17	6	0	0.118279	-3.549493	-0.620766
18	6	0	-0.602851	-2.570310	0.008400
19	6	0	0.065538	-1.563342	0.763012
20	6	0	-0.639406	0.494980	-1.397496
21	6	0	0.043428	-0.381795	-2.215010
22	6	0	1.481845	1.613110	-0.891187
23	6	0	2.201355	2.636620	-0.191235
24	6	0	1.535535	3.585609	0.550432
25	6	0	0.119110	3.549493	0.620786
26	6	0	-0.602136	2.570323	-0.008263
27	6	0	0.066123	1.563198	-0.762788
28	1	0	-2.354145	-0.843282	3.287308
29	1	0	-4.835675	-0.731394	3.277385
30	1	0	-6.023494	-0.248165	1.149790
31	1	0	-6.023199	0.249300	-1.150633
32	1	0	-4.834811	0.732295	-3.277972
33	1	0	-2.353266	0.843632	-3.287362
34	1	0	-0.504825	1.180770	2.706125
35	1	0	1.956323	1.022750	2.996955
36	1	0	-0.393558	-4.315582	-1.195398
37	1	0	-1.685131	-2.547887	-0.070246
38	1	0	-0.504593	-1.180916	-2.705796
39	6	0	1.444243	-0.300989	-2.368417
40	6	0	2.200640	-2.636910	0.191283
41	1	0	2.071065	-4.365728	-1.076641
42	1	0	1.956618	-1.023485	-2.996289
43	6	0	2.157478	0.662657	-1.696590

44	1	0	2.071988	4.365635	1.076438
45	1	0	-0.392629	4.315687	1.195364
46	1	0	-1.684417	2.548037	0.070394
47	8	0	3.551016	2.580990	-0.330019
48	8	0	3.550314	-2.581369	0.329980
49	1	0	3.237250	-0.712844	1.774625
50	1	0	3.237756	0.712083	-1.774146
51	6	0	4.322877	3.552432	0.353662
52	1	0	4.163095	3.487093	1.435685
53	1	0	5.363119	3.328014	0.122810
54	1	0	4.078443	4.562461	0.007114
55	6	0	4.322101	-3.552680	-0.353970
56	1	0	4.162193	-3.487132	-1.435963
57	1	0	5.362369	-3.328302	-0.123195
58	1	0	4.077714	-4.562777	-0.007590

Compound 6 syn GS1 CHCl3

Method: m062x/6-31+g(d,p)
SCF Done: E(RM062X) = -1383.83301669 A.U. after 17 cycles
Lowest frequency = 14.9235

Zero-point correction= 0.472105
(Hartree/Particle)
Thermal correction to Energy= 0.498443
Thermal correction to Enthalpy= 0.499387
Thermal correction to Gibbs Free Energy= 0.416119
Sum of electronic and zero-point Energies= -1383.360911
Sum of electronic and thermal Energies= -1383.334574
Sum of electronic and thermal Enthalpies= -1383.333629
Sum of electronic and thermal Free Energies= -1383.416898

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.334490	-1.171365	-0.623483
2	6	0	2.976497	-1.824903	-1.654640
3	6	0	4.257671	-1.435487	-2.106681
4	6	0	4.909597	-0.410180	-1.474793
5	6	0	4.288059	0.300499	-0.412670
6	6	0	5.003871	1.339333	0.243499
7	6	0	4.428163	2.048821	1.262789
8	6	0	3.084416	1.787012	1.616906
9	6	0	2.342077	0.801022	1.001828
10	6	0	2.955861	-0.029802	-0.003804
11	6	0	1.078054	-1.794764	-0.100086
12	6	0	1.183435	-2.702457	0.932192
13	6	0	0.036133	-3.300949	1.497719
14	6	0	-1.214604	-2.966653	1.036393
15	6	0	-1.355851	-2.058232	-0.041767
16	6	0	-2.774037	-0.809834	-1.588824
17	6	0	-1.610381	-0.308025	-2.224775

18	6	0	-0.357713	-0.627873	-1.773933
19	6	0	-0.202705	-1.494686	-0.655055
20	6	0	0.880223	0.765888	1.323510
21	6	0	0.394261	0.075657	2.411749
22	6	0	-1.409820	1.466851	0.789440
23	6	0	-2.318524	2.172600	-0.064265
24	6	0	-1.855126	2.940313	-1.108132
25	6	0	-0.460552	3.016293	-1.352135
26	6	0	0.437962	2.324579	-0.583788
27	6	0	-0.016985	1.524336	0.505973
28	1	0	2.489585	-2.686081	-2.104353
29	1	0	4.728999	-1.974077	-2.922432
30	1	0	5.914577	-0.122445	-1.771185
31	1	0	6.018739	1.552916	-0.081101
32	1	0	4.977576	2.833438	1.772919
33	1	0	2.598947	2.408938	2.364008
34	1	0	2.166395	-2.932800	1.334956
35	1	0	0.146954	-4.007961	2.314064
36	1	0	-1.727332	0.366266	-3.067751
37	1	0	0.524210	-0.207434	-2.245678
38	1	0	1.084804	-0.489178	3.031956
39	6	0	-0.987639	0.048295	2.701679
40	6	0	-2.648970	-1.662540	-0.516408
41	1	0	-3.748320	-0.503602	-1.950335
42	1	0	-1.343776	-0.526112	3.551142
43	6	0	-1.878595	0.713042	1.893500
44	1	0	-2.536179	3.482406	-1.752721
45	1	0	-0.109200	3.629042	-2.176811
46	1	0	1.500194	2.381138	-0.798374
47	8	0	-3.631914	2.012707	0.245559
48	8	0	-3.697125	-2.185048	0.173256
49	1	0	-2.105796	-3.388533	1.487352
50	1	0	-2.944799	0.669321	2.086508
51	6	0	-4.585466	2.597679	-0.622117
52	1	0	-4.471309	2.210684	-1.641832
53	1	0	-5.562804	2.319286	-0.229559
54	1	0	-4.493505	3.689185	-0.633103
55	6	0	-4.994262	-1.732355	-0.172615
56	1	0	-5.251318	-2.019295	-1.198243
57	1	0	-5.678537	-2.215836	0.523154
58	1	0	-5.063035	-0.643232	-0.066332

Compound 6 TS-rotation 5OMe-naphthyl CHCl3

Method: m062x/6-31+g(d,p) SCF Done: E(RM062X) = -1383.78620667 A.U. after 1 cycles
Lowest frequency = -26.1550

Zero-point correction= 0.472536
(Hartree/Particle)
Thermal correction to Energy= 0.498031
Thermal correction to Enthalpy= 0.498976
Thermal correction to Gibbs Free Energy= 0.418135
Sum of electronic and zero-point Energies= -1383.313670
Sum of electronic and thermal Energies= -1383.288175

Sum of electronic and thermal Enthalpies= -1383.287231
Sum of electronic and thermal Free Energies= -1383.368071

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.311544	2.106575	-0.278128
2	6	0	-2.238840	2.951058	-0.866457
3	6	0	-1.925612	4.275229	-1.232317
4	6	0	-0.717907	4.792817	-0.842928
5	6	0	0.253476	3.971470	-0.211223
6	6	0	1.376804	4.587823	0.409609
7	6	0	2.230550	3.827712	1.159821
8	6	0	2.150922	2.419075	1.071061
9	6	0	1.203966	1.759280	0.302244
10	6	0	0.048326	2.558030	-0.101922
11	6	0	-1.869110	0.927488	0.458847
12	6	0	-1.580815	0.814745	1.803670
13	6	0	-2.148429	-0.205457	2.597295
14	6	0	-3.016378	-1.112575	2.041544
15	6	0	-3.326645	-1.041192	0.659684
16	6	0	-4.455628	-1.977183	-1.296493
17	6	0	-3.836855	-0.987310	-2.098805
18	6	0	-3.012923	-0.035923	-1.555613
19	6	0	-2.751296	-0.024624	-0.153952
20	6	0	1.487925	0.349381	-0.116046
21	6	0	0.497858	-0.479382	-0.614168
22	6	0	2.997302	-1.612525	-0.244818
23	6	0	4.306635	-2.195728	-0.155161
24	6	0	5.428824	-1.408743	-0.058970
25	6	0	5.271679	-0.003448	-0.085645
26	6	0	4.034047	0.585296	-0.101207
27	6	0	2.837198	-0.198371	-0.106718
28	1	0	-3.266191	2.610397	-0.958927
29	1	0	-2.674021	4.899406	-1.709053
30	1	0	-0.495909	5.848834	-0.969667
31	1	0	1.486503	5.666216	0.339788
32	1	0	3.020858	4.283086	1.747511
33	1	0	2.914464	1.837596	1.571060
34	1	0	-0.910537	1.536386	2.262178
35	1	0	-1.901334	-0.260245	3.652623
36	1	0	-0.470578	-0.077406	-0.841823
37	6	0	0.679035	-1.859764	-0.823723
38	6	0	-4.201363	-2.004593	0.055896
39	1	0	-0.163716	-2.454488	-1.163336
40	6	0	1.891345	-2.441119	-0.558216
41	1	0	6.421741	-1.837778	-0.013526
42	1	0	6.159018	0.621529	-0.108983
43	1	0	3.977508	1.662011	-0.174529
44	1	0	-3.465906	-1.895225	2.641370
45	8	0	4.328349	-3.552753	-0.210457
46	6	0	5.592502	-4.192108	-0.174141
47	1	0	5.390783	-5.260392	-0.234663
48	1	0	6.210692	-3.884210	-1.024393
49	1	0	6.117084	-3.969413	0.761292
50	1	0	2.039596	-3.510230	-0.650635
51	1	0	-2.541327	0.701261	-2.195786
52	1	0	-4.022442	-0.992900	-3.168355

53	1	0	-5.108461	-2.705312	-1.761302
54	8	0	-4.722763	-2.916465	0.914163
55	6	0	-5.585399	-3.907093	0.380829
56	1	0	-5.063518	-4.520785	-0.361182
57	1	0	-5.886911	-4.527542	1.223145
58	1	0	-6.469987	-3.450105	-0.075559

Compound 1 anti-in GS1 DMSO

Method: m062x/6-31+g(d,p)
SCF Done: E(RM062X) = -1233.46454814 A.U. after 1 cycles
Lowest frequency = 12.4451

Zero-point correction= 0.461399
(Hartree/Particle)
Thermal correction to Energy= 0.486009
Thermal correction to Enthalpy= 0.486954
Thermal correction to Gibbs Free Energy= 0.407204
Sum of electronic and zero-point Energies= -1233.003149
Sum of electronic and thermal Energies= -1232.978539
Sum of electronic and thermal Enthalpies= -1232.977595
Sum of electronic and thermal Free Energies= -1233.057344

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.790558	-0.645882	1.107947
2	6	0	-2.544076	-1.149663	2.150926
3	6	0	-3.955421	-1.093079	2.163444
4	6	0	-4.611729	-0.546859	1.093991
5	6	0	-3.886735	-0.000016	0.000010
6	6	0	-4.611747	0.546820	-1.093965
7	6	0	-3.955457	1.093045	-2.163426
8	6	0	-2.544112	1.149645	-2.150923
9	6	0	-1.790578	0.645875	-1.107951
10	6	0	-2.453180	-0.000008	0.000002
11	6	0	-0.314326	-0.851585	1.211547
12	6	0	0.390815	-0.232046	2.217259
13	6	0	1.789771	-0.393227	2.342710
14	6	0	2.503562	-1.179846	1.468829
15	6	0	1.792407	-1.884506	0.444547
16	6	0	1.775629	-3.443090	-1.430624
17	6	0	0.367443	-3.328955	-1.517644
18	6	0	-0.310379	-2.499209	-0.658367
19	6	0	0.377265	-1.742401	0.329906
20	6	0	-0.314349	0.851592	-1.211559
21	6	0	0.390794	0.232064	-2.217275
22	6	0	1.792378	1.884518	-0.444551
23	6	0	2.465266	2.742753	0.469923
24	6	0	1.775592	3.443087	1.430633
25	6	0	0.367406	3.328951	1.517645
26	6	0	-0.310413	2.499210	0.658361
27	6	0	0.377236	1.742408	-0.329913
28	1	0	-2.025623	-1.632695	2.974226
29	1	0	-4.505169	-1.505080	3.003416
30	1	0	-5.697345	-0.519073	1.060011
31	1	0	-5.697362	0.519022	-1.059973
32	1	0	-4.505218	1.505038	-3.003392
33	1	0	-2.025673	1.632682	-2.974229
34	1	0	-0.130132	0.433336	2.900074

35	1	0	2.312123	0.139038	3.133568
36	1	0	-0.175439	-3.896615	-2.267151
37	1	0	-1.390032	-2.406920	-0.734418
38	1	0	-0.130150	-0.433318	-2.900093
39	6	0	1.789749	0.393254	-2.342726
40	6	0	2.465299	-2.742749	-0.469917
41	1	0	2.308544	-4.093179	-2.117638
42	1	0	3.543365	-2.849031	-0.402771
43	1	0	2.312103	-0.138998	-3.133592
44	6	0	2.503536	1.179869	-1.468839
45	1	0	3.543333	2.849033	0.402784
46	1	0	2.308505	4.093166	2.117657
47	1	0	-0.175480	3.896610	2.267151
48	1	0	-1.390066	2.406921	0.734405
49	6	0	3.999128	-1.310091	1.594246
50	1	0	4.370156	-0.677212	2.403055
51	1	0	4.296568	-2.342804	1.806283
52	1	0	4.505215	-1.012379	0.669797
53	6	0	3.999102	1.310118	-1.594250
54	1	0	4.370130	0.677274	-2.403086
55	1	0	4.296542	2.342841	-1.806241
56	1	0	4.505188	1.012365	-0.669813

Compound 1 anti-out GS2 DMSO

Method: m062x/6-31+g(d,p)
SCF Done: E(RM062X) = -1233.46479591 A.U. after 1 cycles
Lowest frequency = 15.9093

Zero-point correction= 0.461594
(Hartree/Particle)
Thermal correction to Energy= 0.485968
Thermal correction to Enthalpy= 0.486912
Thermal correction to Gibbs Free Energy= 0.408988
Sum of electronic and zero-point Energies= -1233.003202
Sum of electronic and thermal Energies= -1232.978828
Sum of electronic and thermal Enthalpies= -1232.977884
Sum of electronic and thermal Free Energies= -1233.055808

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.933326	1.058476	-0.714734
2	6	0	-2.676392	2.077618	-1.273749
3	6	0	-4.088116	2.105689	-1.202945
4	6	0	-4.751029	1.070472	-0.599153
5	6	0	-4.032734	-0.000056	0.000185
6	6	0	-4.750939	-1.070639	0.599502
7	6	0	-4.087926	-2.106103	1.202791
8	6	0	-2.676200	-2.078138	1.273268
9	6	0	-1.933218	-1.058762	0.714550
10	6	0	-2.599855	-0.000053	0.000095

11	6	0	-0.466302	1.047338	-1.013811
12	6	0	-0.026045	0.345469	-2.110275
13	6	0	1.348577	0.277333	-2.437108
14	6	0	2.299834	0.908017	-1.671891
15	6	0	1.870208	1.688198	-0.548622
16	6	0	2.380578	3.139262	1.343156
17	6	0	1.001137	3.244074	1.641302
18	6	0	0.078544	2.576962	0.872363
19	6	0	0.482058	1.779275	-0.232172
20	6	0	-0.466192	-1.047465	1.013589
21	6	0	-0.026138	-0.345511	2.110092
22	6	0	1.870466	-1.688004	0.548691
23	6	0	2.800648	-2.382041	-0.274622
24	6	0	2.381259	-3.139116	-1.342942
25	6	0	1.001884	-3.244010	-1.641335
26	6	0	0.079107	-2.576951	-0.872560
27	6	0	0.482361	-1.779244	0.232048
28	1	0	-2.154045	2.865160	-1.810459
29	1	0	-4.634884	2.927031	-1.654687
30	1	0	-5.836899	1.047123	-0.567307
31	1	0	-5.836817	-1.047205	0.567998
32	1	0	-4.634640	-2.927582	1.654350
33	1	0	-2.153756	-2.865904	1.809557
34	1	0	-0.744116	-0.200691	-2.716715
35	1	0	1.656931	-0.313807	-3.295568
36	1	0	0.674731	3.846721	2.483357
37	1	0	-0.979826	2.643166	1.108840
38	1	0	-0.744354	0.200512	2.716483
39	6	0	1.348433	-0.277145	2.437060
40	6	0	2.800207	2.382272	0.274876
41	1	0	3.107347	3.661014	1.958278
42	1	0	3.860669	2.312984	0.052948
43	1	0	1.656593	0.314089	3.295525
44	6	0	2.299866	-0.907746	1.671983
45	1	0	3.861069	-2.312658	-0.052521
46	1	0	3.108176	-3.660872	-1.957884
47	1	0	0.675646	-3.846667	-2.483449
48	1	0	-0.979212	-2.643224	-1.109244
49	6	0	3.763182	0.776574	-2.003339
50	1	0	3.897116	0.147836	-2.886210
51	1	0	4.224252	1.749718	-2.202722
52	1	0	4.316119	0.315994	-1.176967
53	6	0	3.763153	-0.776146	2.003624
54	1	0	3.896909	-0.147236	2.886401
55	1	0	4.224262	-1.749221	2.203259
56	1	0	4.316188	-0.315686	1.177253

Compound 1 syn GS1 DMSO

Method: m062x/6-31+g(d,p)
SCF Done: E(RM062X) = -1233.46378324 A.U. after 1 cycles
Lowest frequency = 18.8033

Zero-point correction=	0.461733
(Hartree/Particle)	
Thermal correction to Energy=	0.486032
Thermal correction to Enthalpy=	0.486976
Thermal correction to Gibbs Free Energy=	0.409449
Sum of electronic and zero-point Energies=	-1233.002051
Sum of electronic and thermal Energies=	-1232.977752
Sum of electronic and thermal Enthalpies=	-1232.976807
Sum of electronic and thermal Free Energies=	-1233.054334

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.902274	0.641931	-1.121801
2	6	0	-2.685916	1.497821	-1.867331
3	6	0	-4.091210	1.555992	-1.716508
4	6	0	-4.697543	0.779198	-0.765842
5	6	0	-3.938068	-0.132858	0.017988
6	6	0	-4.592687	-0.917923	1.005706
7	6	0	-3.891765	-1.825355	1.755499
8	6	0	-2.515849	-2.022691	1.497754
9	6	0	-1.837728	-1.291730	0.544160
10	6	0	-2.527068	-0.262768	-0.189569
11	6	0	-0.420380	0.827733	-1.223820
12	6	0	0.325264	0.222486	-2.205485
13	6	0	1.725510	0.408577	-2.282097
14	6	0	2.397285	1.210112	-1.388563
15	6	0	1.642656	1.899993	-0.386036
16	6	0	1.539505	3.448478	1.494668
17	6	0	0.137024	3.278051	1.563302
18	6	0	-0.498278	2.431726	0.686825
19	6	0	0.229113	1.718518	-0.307454
20	6	0	-0.445422	-1.726516	0.208904
21	6	0	-0.271595	-2.628406	-0.814133
22	6	0	2.001210	-1.659114	0.506029
23	6	0	3.128499	-1.136830	1.200108
24	6	0	2.975103	-0.281281	2.264571
25	6	0	1.680625	0.095660	2.694624
26	6	0	0.572718	-0.381895	2.039497
27	6	0	0.698550	-1.258796	0.927323
28	1	0	-2.196282	2.179732	-2.557340
29	1	0	-4.670971	2.242905	-2.324525
30	1	0	-5.768802	0.841515	-0.594867
31	1	0	-5.661175	-0.782963	1.149824
32	1	0	-4.389273	-2.419776	2.514971
33	1	0	-1.977503	-2.797218	2.037620
34	1	0	-0.161703	-0.447277	-2.909032
35	1	0	2.283678	-0.118706	-3.052077
36	1	0	-0.436719	3.814254	2.313075
37	1	0	-1.574566	2.299033	0.748503
38	1	0	-1.140742	-2.997451	-1.352793
39	6	0	1.020647	-3.041208	-1.214571
40	6	0	2.269249	2.774178	0.544981

41	1	0	2.038422	4.112346	2.194106
42	1	0	3.345452	2.908992	0.502603
43	1	0	1.119124	-3.735042	-2.045545
44	6	0	2.151565	-2.557133	-0.599303
45	1	0	4.126770	-1.419448	0.880997
46	1	0	3.848935	0.110161	2.776940
47	1	0	1.566004	0.776443	3.532560
48	1	0	-0.421271	-0.078839	2.355315
49	6	0	3.521943	-2.944653	-1.088985
50	1	0	4.114798	-3.425476	-0.303933
51	1	0	3.445311	-3.637278	-1.929600
52	1	0	4.080134	-2.062742	-1.425114
53	6	0	3.894886	1.355930	-1.460298
54	1	0	4.296822	0.755244	-2.279280
55	1	0	4.193896	2.396822	-1.623989
56	1	0	4.366246	1.021420	-0.529278

Compound 2 anti-in GS1 DMSO

Method: m062x/6-31+g(d,p)
SCF Done: E(RM062X) = -1948.50285959 A.U. after 1 cycles
Lowest frequency = 17.8322

Zero-point correction= 0.340736
(Hartree/Particle)
Thermal correction to Energy= 0.369407
Thermal correction to Enthalpy= 0.370352
Thermal correction to Gibbs Free Energy= 0.282018
Sum of electronic and zero-point Energies= -1948.162124
Sum of electronic and thermal Energies= -1948.133452
Sum of electronic and thermal Enthalpies= -1948.132508
Sum of electronic and thermal Free Energies= -1948.220841

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.052963	0.402602	-1.215434
2	6	0	-2.800124	0.757419	-2.319556
3	6	0	-4.212608	0.761746	-2.301947
4	6	0	-4.867966	0.389228	-1.160070
5	6	0	-4.143740	0.000349	-0.000084
6	6	0	-4.868101	-0.388398	1.159863
7	6	0	-4.212880	-0.760983	2.301797
8	6	0	-2.800396	-0.756888	2.319499
9	6	0	-2.053110	-0.402241	1.215412
10	6	0	-2.711409	0.000231	-0.000037
11	6	0	-0.568274	0.395427	-1.418757
12	6	0	-0.032406	-0.630962	-2.168444
13	6	0	1.354821	-0.736105	-2.418039
14	6	0	2.218441	0.203875	-1.918349
15	6	0	1.707426	1.305695	-1.185826

16	6	0	2.115874	3.388409	-0.004238
17	6	0	0.731269	3.519912	0.222117
18	6	0	-0.138858	2.568989	-0.233271
19	6	0	0.304983	1.425317	-0.946032
20	6	0	-0.568430	-0.395333	1.418779
21	6	0	-0.032393	0.630962	2.168470
22	6	0	1.707124	-1.305961	1.185816
23	6	0	2.579646	-2.304134	0.688868
24	6	0	2.115241	-3.388761	0.004268
25	6	0	0.730613	-3.520075	-0.222034
26	6	0	-0.139370	-2.569019	0.233362
27	6	0	0.304657	-1.425382	0.946062
28	1	0	-2.278852	1.049077	-3.226771
29	1	0	-4.762312	1.055948	-3.189858
30	1	0	-5.953496	0.379954	-1.118059
31	1	0	-5.953627	-0.378956	1.117781
32	1	0	-4.762693	-1.055067	3.189679
33	1	0	-2.279227	-1.048605	3.226754
34	1	0	-0.700972	-1.398823	-2.548051
35	1	0	1.732816	-1.574379	-2.994270
36	1	0	-0.700829	1.398946	2.548058
37	6	0	1.354855	0.735885	2.418052
38	6	0	2.580104	2.303741	-0.688889
39	1	0	3.287768	0.128733	-2.081543
40	1	0	1.732988	1.574087	2.994298
41	6	0	2.218320	-0.204214	1.918329
42	1	0	3.287665	-0.129226	2.081481
43	9	0	-1.438679	-2.742008	-0.046851
44	9	0	0.290718	-4.581386	-0.902157
45	9	0	2.938888	-4.330337	-0.459862
46	9	0	3.898263	-2.186305	0.899493
47	9	0	3.898697	2.185733	-0.899565
48	9	0	2.939664	4.329862	0.459886
49	9	0	0.291549	4.581254	0.902307
50	9	0	-1.438133	2.742113	0.047015

Compound 2 syn GS1 DMSO

Method: m062x/6-31+g(d,p)
SCF Done: E(RM062X) = -1948.50127739 A.U. after 1 cycles
Lowest frequency = 16.1425

Zero-point correction= 0.340676
(Hartree/Particle)
Thermal correction to Energy= 0.369331
Thermal correction to Enthalpy= 0.370276
Thermal correction to Gibbs Free Energy= 0.282300
Sum of electronic and zero-point Energies= -1948.160602
Sum of electronic and thermal Energies= -1948.131946
Sum of electronic and thermal Enthalpies= -1948.131002
Sum of electronic and thermal Free Energies= -1948.218978

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.348108	-0.479443	1.216454
2	6	0	-3.064129	-1.381996	1.972594
3	6	0	-4.353511	-1.818365	1.592465
4	6	0	-4.899316	-1.358836	0.424108
5	6	0	-4.212909	-0.402289	-0.373253
6	6	0	-4.817158	0.061597	-1.572965
7	6	0	-4.203304	1.012898	-2.343363
8	6	0	-2.976014	1.565123	-1.913930
9	6	0	-2.347500	1.140003	-0.762926
10	6	0	-2.934033	0.096586	0.034536
11	6	0	-0.938151	-0.224888	1.653906
12	6	0	-0.673215	0.742511	2.598834
13	6	0	0.637816	1.010179	3.049825
14	6	0	1.698728	0.295754	2.554005
15	6	0	1.470789	-0.730679	1.604501
16	6	0	2.374839	-2.464159	0.162089
17	6	0	1.069082	-2.763904	-0.275713
18	6	0	-0.005949	-2.069107	0.206227
19	6	0	0.144216	-1.017172	1.153766
20	6	0	-1.152408	1.934045	-0.327010
21	6	0	-1.387986	3.063759	0.427575
22	6	0	1.253022	2.427729	-0.177876
23	6	0	2.592830	2.074802	-0.472535
24	6	0	2.897549	0.994433	-1.248385
25	6	0	1.853949	0.207723	-1.778270
26	6	0	0.549726	0.513022	-1.505346
27	6	0	0.193176	1.616389	-0.685773
28	1	0	-2.600338	-1.799952	2.861784
29	1	0	-4.884647	-2.534530	2.210660
30	1	0	-5.871872	-1.708228	0.088813
31	1	0	-5.780695	-0.350447	-1.859551
32	1	0	-4.663173	1.368422	-3.259502
33	1	0	-2.519311	2.363732	-2.491823
34	1	0	-1.499834	1.334464	2.980601
35	1	0	0.801956	1.795128	3.780359
36	1	0	-2.413794	3.309552	0.686300
37	6	0	-0.338231	3.882597	0.898946
38	6	0	2.557690	-1.472980	1.081247
39	1	0	2.713870	0.500403	2.875422
40	1	0	-0.569185	4.757041	1.497823
41	6	0	0.965795	3.563899	0.618407
42	1	0	1.785525	4.167030	0.991985
43	9	0	-0.390855	-0.289291	-2.023268
44	9	0	2.167648	-0.849596	-2.532737
45	9	0	4.159628	0.657286	-1.518298
46	9	0	3.591137	2.820893	0.020161
47	9	0	3.802709	-1.187444	1.488591
48	9	0	3.399997	-3.152835	-0.341190
49	9	0	0.906185	-3.731712	-1.180358
50	9	0	-1.207809	-2.413743	-0.272426

Compound 3 anti-in GS1 DMSO

Method: m062x/6-31+g(d,p)
SCF Done: E(RM062X) = -1590.98515357 A.U. after 1 cycles
Lowest frequency = 18.0055

Zero-point correction= 0.401280
(Hartree/Particle)
Thermal correction to Energy= 0.427760
Thermal correction to Enthalpy= 0.428704
Thermal correction to Gibbs Free Energy= 0.345789
Sum of electronic and zero-point Energies= -1590.583873
Sum of electronic and thermal Energies= -1590.557394
Sum of electronic and thermal Enthalpies= -1590.556449
Sum of electronic and thermal Free Energies= -1590.639364

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.110709	0.333117	-1.191479
2	6	0	-2.920156	0.520620	-2.293670
3	6	0	-4.274522	0.119601	-2.311905
4	6	0	-4.809042	-0.476873	-1.202253
5	6	0	-4.016688	-0.701245	-0.043257
6	6	0	-4.617012	-1.331962	1.080606
7	6	0	-3.893876	-1.568005	2.217590
8	6	0	-2.535564	-1.182784	2.263569
9	6	0	-1.901265	-0.579327	1.196178
10	6	0	-2.640509	-0.301889	-0.011120
11	6	0	-0.694485	0.788888	-1.321283
12	6	0	0.183863	0.059653	-2.087476
13	6	0	1.551579	0.413503	-2.171702
14	6	0	2.052828	1.504611	-1.501156
15	6	0	1.144421	2.339152	-0.770683
16	6	0	0.703032	4.323635	0.573215
17	6	0	-0.671283	3.990130	0.622874
18	6	0	-1.126487	2.851070	0.003943
19	6	0	-0.237127	1.993585	-0.698155
20	6	0	-0.470312	-0.202089	1.445601
21	6	0	-0.232813	0.851093	2.305787
22	6	0	1.968887	-0.472040	1.241869
23	6	0	3.081383	-1.157254	0.694410
24	6	0	2.930119	-2.245719	-0.112544
25	6	0	1.631766	-2.704382	-0.414188
26	6	0	0.536031	-2.062073	0.089063
27	6	0	0.650135	-0.919736	0.923444
28	1	0	-2.494702	1.001272	-3.170080
29	1	0	-4.877111	0.289427	-3.198146
30	1	0	-5.848170	-0.793499	-1.185335
31	1	0	-5.662702	-1.619309	1.014283
32	1	0	-4.348193	-2.046692	3.078833
33	1	0	-1.961082	-1.375487	3.165021
34	1	0	-0.165958	-0.839533	-2.589029

35	1	0	2.224349	-0.216390	-2.748584
36	1	0	-1.364555	4.634940	1.154018
37	1	0	-2.179757	2.588341	0.051716
38	1	0	-1.083982	1.385125	2.716971
39	6	0	1.072102	1.281127	2.628876
40	6	0	1.585029	3.517820	-0.106674
41	1	0	1.058973	5.220524	1.070507
42	1	0	2.636086	3.785958	-0.142240
43	1	0	1.206244	2.131352	3.289297
44	6	0	2.161757	0.641951	2.095575
45	1	0	3.171495	0.968957	2.317983
46	9	0	-0.667655	-2.536015	-0.263919
47	9	0	1.497269	-3.767550	-1.212396
48	9	0	3.980345	-2.892343	-0.624420
49	9	0	4.320993	-0.732016	0.983282
50	6	0	3.527500	1.806900	-1.515759
51	1	0	3.738449	2.791295	-1.946248
52	1	0	3.935748	1.801995	-0.497992
53	1	0	4.064825	1.056603	-2.099683

Compound 3 syn-in GS1 DMSO

Method: m062x/6-31+g(d,p)
SCF Done: E(RM062X) = -1590.98494660 A.U. after 1 cycles
Lowest frequency = 15.6419

Zero-point correction= 0.401422
(Hartree/Particle)
Thermal correction to Energy= 0.427832
Thermal correction to Enthalpy= 0.428776
Thermal correction to Gibbs Free Energy= 0.346396
Sum of electronic and zero-point Energies= -1590.583524
Sum of electronic and thermal Energies= -1590.557114
Sum of electronic and thermal Enthalpies= -1590.556170
Sum of electronic and thermal Free Energies= -1590.638551

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.152805	0.950054	-0.935291
2	6	0	-2.852489	2.084695	-1.296258
3	6	0	-4.194181	2.299587	-0.915410
4	6	0	-4.828198	1.358804	-0.148864
5	6	0	-4.157612	0.170245	0.246073
6	6	0	-4.864636	-0.777921	1.035900
7	6	0	-4.270833	-1.947828	1.421936
8	6	0	-2.942068	-2.211204	1.020243
9	6	0	-2.207448	-1.318152	0.268225
10	6	0	-2.799492	-0.070140	-0.149349
11	6	0	-0.726214	0.890543	-1.381842
12	6	0	-0.360588	0.143163	-2.475836
13	6	0	0.987860	0.059364	-2.890783

14	6	0	1.989877	0.723671	-2.221426
15	6	0	1.638589	1.549724	-1.106454
16	6	0	2.288063	3.062326	0.692780
17	6	0	0.934495	3.172877	1.092022
18	6	0	-0.043297	2.484294	0.416900
19	6	0	0.274733	1.650947	-0.693956
20	6	0	-0.844936	-1.798252	-0.134381
21	6	0	-0.774664	-2.766638	-1.113268
22	6	0	1.612360	-1.859545	-0.007232
23	6	0	2.816867	-1.381230	0.561079
24	6	0	2.820594	-0.481761	1.587077
25	6	0	1.595337	-0.019227	2.106051
26	6	0	0.412918	-0.446169	1.568386
27	6	0	0.367818	-1.359290	0.483080
28	1	0	-2.339388	2.839835	-1.885791
29	1	0	-4.706338	3.205130	-1.223714
30	1	0	-5.857331	1.500297	0.169331
31	1	0	-5.888958	-0.551963	1.318860
32	1	0	-4.807883	-2.675530	2.021314
33	1	0	-2.475671	-3.147652	1.312408
34	1	0	-1.117513	-0.425807	-3.009066
35	1	0	1.237644	-0.567337	-3.742862
36	1	0	0.671605	3.795204	1.941689
37	1	0	-1.076910	2.559269	0.738736
38	1	0	-1.698502	-3.111847	-1.567925
39	6	0	0.458139	-3.284374	-1.570426
40	6	0	2.626618	2.272945	-0.379728
41	1	0	3.057912	3.601263	1.236282
42	1	0	3.667428	2.193547	-0.677518
43	1	0	0.465182	-4.034596	-2.354058
44	6	0	1.637861	-2.825393	-1.044795
45	1	0	2.594214	-3.191209	-1.401575
46	9	0	-0.716484	0.037307	2.103971
47	9	0	1.615754	0.833448	3.133247
48	9	0	3.958668	-0.032428	2.120177
49	9	0	3.990991	-1.830454	0.089164
50	6	0	3.427737	0.568211	-2.641881
51	1	0	3.501795	-0.098681	-3.503173
52	1	0	3.876795	1.528776	-2.914956
53	1	0	4.033151	0.144496	-1.832435

Compound 3 syn-out GS2 DMSO

Method: m062x/6-31+g(d,p)
SCF Done: E(RM062X) = -1590.98277754 A.U. after 1 cycles
Lowest frequency = 19.0822

Zero-point correction= 0.401110
(Hartree/Particle)
Thermal correction to Energy= 0.427594
Thermal correction to Enthalpy= 0.428538
Thermal correction to Gibbs Free Energy= 0.345788
Sum of electronic and zero-point Energies= -1590.581668

Sum of electronic and thermal Energies= -1590.555184
Sum of electronic and thermal Enthalpies= -1590.554240
Sum of electronic and thermal Free Energies= -1590.636990

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.141457	1.026150	-0.868256
2	6	0	2.848372	1.294236	-2.022277
3	6	0	4.109775	0.710916	-2.279605
4	6	0	4.677472	-0.106565	-1.337716
5	6	0	3.984703	-0.421621	-0.137587
6	6	0	4.611016	-1.247583	0.836772
7	6	0	3.965448	-1.569147	2.000491
8	6	0	2.632987	-1.137247	2.197379
9	6	0	1.975734	-0.359810	1.269001
10	6	0	2.669688	0.093662	0.091412
11	6	0	0.925657	1.855077	-0.596345
12	6	0	1.070231	3.002516	0.147395
13	6	0	-0.046581	3.799630	0.489271
14	6	0	-1.320171	3.458020	0.096705
15	6	0	-1.497549	2.296715	-0.721911
16	6	0	-2.948007	0.780512	-1.963018
17	6	0	-1.822998	0.014950	-2.352932
18	6	0	-0.566848	0.370124	-1.924599
19	6	0	-0.368904	1.506004	-1.092164
20	6	0	0.512551	-0.137404	1.503234
21	6	0	0.087718	0.869690	2.341073
22	6	0	-1.847465	-0.757118	1.173691
23	6	0	-2.824098	-1.589339	0.577491
24	6	0	-2.483392	-2.646814	-0.213313
25	6	0	-1.122412	-2.914761	-0.451836
26	6	0	-0.150498	-2.120565	0.090582
27	6	0	-0.463549	-1.009750	0.921568
28	1	0	2.433788	2.005104	-2.732076
29	1	0	4.635229	0.945691	-3.199537
30	1	0	5.667920	-0.526779	-1.489362
31	1	0	5.616039	-1.610071	0.638951
32	1	0	4.449222	-2.183871	2.752449
33	1	0	2.090092	-1.468226	3.078403
34	1	0	2.055330	3.278272	0.514894
35	1	0	0.105028	4.686005	1.099691
36	1	0	-1.956265	-0.858613	-2.984545
37	1	0	0.297024	-0.223093	-2.213300
38	1	0	0.832649	1.522337	2.786496
39	6	0	-1.281557	1.105351	2.595786
40	6	0	-2.786280	1.892272	-1.170968
41	1	0	-3.940078	0.487250	-2.292751
42	1	0	-3.656158	2.473541	-0.882800
43	1	0	-1.570829	1.927293	3.242582
44	6	0	-2.239036	0.316595	2.011895
45	1	0	-3.295055	0.496128	2.180160
46	9	0	1.117904	-2.432324	-0.216560

47	9	0	-0.801116	-3.947627	-1.237181
48	9	0	-3.407921	-3.428619	-0.777023
49	9	0	-4.123313	-1.335803	0.794363
50	6	0	-2.507039	4.274422	0.534250
51	1	0	-2.183832	5.122962	1.140422
52	1	0	-3.072170	4.660849	-0.320100
53	1	0	-3.196471	3.669870	1.135225

Compound 4 anti-in GS1 DMSO

Method: m062x/6-31+g(d,p)
SCF Done: E(RM062X) = -1666.17209352 A.U. after 1 cycles
Lowest frequency = 17.8299

Zero-point correction= 0.406542
(Hartree/Particle)
Thermal correction to Energy= 0.434002
Thermal correction to Enthalpy= 0.434946
Thermal correction to Gibbs Free Energy= 0.349777
Sum of electronic and zero-point Energies= -1665.765552
Sum of electronic and thermal Energies= -1665.738092
Sum of electronic and thermal Enthalpies= -1665.737148
Sum of electronic and thermal Free Energies= -1665.822317

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.170661	0.465237	-1.226181
2	6	0	-2.907144	0.762500	-2.355283
3	6	0	-4.275186	0.430836	-2.473990
4	6	0	-4.898843	-0.210788	-1.438493
5	6	0	-4.185954	-0.545659	-0.254804
6	6	0	-4.876657	-1.220473	0.788670
7	6	0	-4.232572	-1.560255	1.946776
8	6	0	-2.866452	-1.233818	2.097613
9	6	0	-2.146900	-0.591121	1.110432
10	6	0	-2.798481	-0.211832	-0.119105
11	6	0	-0.726090	0.842591	-1.254342
12	6	0	0.154514	0.096243	-1.998899
13	6	0	1.546635	0.360368	-2.012435
14	6	0	2.046242	1.399387	-1.261829
15	6	0	1.159252	2.267016	-0.543345
16	6	0	0.781443	4.223412	0.841050
17	6	0	-0.610366	3.970971	0.811993
18	6	0	-1.104284	2.883465	0.131197
19	6	0	-0.236466	1.995407	-0.558576
20	6	0	-0.724928	-0.274083	1.470320
21	6	0	-0.513991	0.736157	2.386656
22	6	0	1.712967	-0.612530	1.413303
23	6	0	2.838409	-1.308103	0.907271
24	6	0	2.708092	-2.360247	0.049465
25	6	0	1.419550	-2.767827	-0.351150

26	6	0	0.312586	-2.111481	0.107680
27	6	0	0.405844	-1.006920	0.993850
28	1	0	-2.409662	1.273419	-3.174780
29	1	0	-4.817249	0.685935	-3.378734
30	1	0	-5.949799	-0.479187	-1.500902
31	1	0	-5.927169	-1.457026	0.644238
32	1	0	-4.756013	-2.073527	2.746680
33	1	0	-2.356217	-1.502659	3.018073
34	1	0	-0.215727	-0.760668	-2.556499
35	1	0	2.198277	-0.286635	-2.587442
36	1	0	-1.289852	4.638538	1.332858
37	1	0	-2.172511	2.684898	0.119681
38	1	0	-1.374458	1.281103	2.762869
39	6	0	0.778875	1.111169	2.811909
40	6	0	1.647961	3.388233	0.175673
41	1	0	1.163379	5.080478	1.386622
42	1	0	2.715990	3.575997	0.187689
43	1	0	0.893802	1.929923	3.514359
44	6	0	1.882029	0.460252	2.323281
45	1	0	2.884256	0.747867	2.620656
46	9	0	-0.879279	-2.531181	-0.340591
47	9	0	1.307199	-3.793271	-1.200292
48	9	0	3.771759	-3.012818	-0.426609
49	9	0	4.069381	-0.928252	1.283890
50	8	0	3.364606	1.692627	-1.136556
51	6	0	4.290311	0.871196	-1.832675
52	1	0	5.278179	1.258938	-1.590329
53	1	0	4.212943	-0.170989	-1.502879
54	1	0	4.125041	0.926493	-2.913493

Compound 4 syn-in GS1 DMSO

Method: m062x/6-31+g(d,p)
SCF Done: E(RM062X) = -1666.17155038 A.U. after 1 cycles
Lowest frequency = 15.4324

Zero-point correction= 0.406684
(Hartree/Particle)
Thermal correction to Energy= 0.434073
Thermal correction to Enthalpy= 0.435017
Thermal correction to Gibbs Free Energy= 0.350282
Sum of electronic and zero-point Energies= -1665.764866
Sum of electronic and thermal Energies= -1665.737477
Sum of electronic and thermal Enthalpies= -1665.736533
Sum of electronic and thermal Free Energies= -1665.821269

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.194810	0.817148	-1.119880
2	6	0	-2.871242	1.891478	-1.663827

3	6	0	-4.243147	2.121817	-1.427092
4	6	0	-4.933708	1.258873	-0.619012
5	6	0	-4.289260	0.134695	-0.036427
6	6	0	-5.054835	-0.732504	0.790930
7	6	0	-4.486612	-1.839926	1.357365
8	6	0	-3.124765	-2.120004	1.106181
9	6	0	-2.334149	-1.302670	0.324959
10	6	0	-2.898920	-0.121380	-0.282376
11	6	0	-0.734168	0.734336	-1.428517
12	6	0	-0.259092	-0.133113	-2.381482
13	6	0	1.120053	-0.259124	-2.670262
14	6	0	2.031949	0.506499	-1.979915
15	6	0	1.588268	1.467091	-1.016198
16	6	0	2.080944	3.193743	0.617860
17	6	0	0.696806	3.332738	0.879336
18	6	0	-0.218980	2.553386	0.214573
19	6	0	0.194406	1.591896	-0.751266
20	6	0	-0.936114	-1.799854	0.105345
21	6	0	-0.769633	-2.879611	-0.735719
22	6	0	1.500507	-1.797445	0.455465
23	6	0	2.645689	-1.225186	1.058322
24	6	0	2.549027	-0.210476	1.965487
25	6	0	1.277847	0.282705	2.319447
26	6	0	0.151992	-0.228854	1.735864
27	6	0	0.212536	-1.265996	0.769325
28	1	0	-2.315275	2.585938	-2.288094
29	1	0	-4.734605	2.977787	-1.877887
30	1	0	-5.988489	1.414405	-0.410074
31	1	0	-6.102247	-0.496187	0.956634
32	1	0	-5.067746	-2.506171	1.986374
33	1	0	-2.677240	-3.007957	1.543355
34	1	0	-0.958614	-0.776360	-2.908484
35	1	0	1.436557	-0.983874	-3.410123
36	1	0	0.358379	4.052461	1.618220
37	1	0	-1.276742	2.654751	0.434267
38	1	0	-1.645596	-3.295384	-1.224786
39	6	0	0.503075	-3.429958	-1.009679
40	6	0	2.515729	2.280553	-0.312840
41	1	0	2.797248	3.807774	1.154518
42	1	0	3.573900	2.163253	-0.520007
43	1	0	0.586014	-4.273831	-1.686389
44	6	0	1.626642	-2.887679	-0.442663
45	1	0	2.613597	-3.280880	-0.659561
46	9	0	-1.025262	0.292179	2.108608
47	9	0	1.198180	1.250694	3.235662
48	9	0	3.631247	0.325436	2.533835
49	9	0	3.861169	-1.697186	0.740348
50	8	0	3.377435	0.424085	-2.134083
51	6	0	3.876369	-0.538847	-3.050838
52	1	0	4.961372	-0.461552	-3.006656
53	1	0	3.565304	-1.548359	-2.761523
54	1	0	3.532290	-0.324617	-4.067998

Compound 4 syn-out GS2 DMSO

Method: m062x/6-31+g(d,p)
SCF Done: E(RM062X) = -1666.16860320 A.U. after 1 cycles
Lowest frequency = 7.9997

Zero-point correction= 0.406306
(Hartree/Particle)
Thermal correction to Energy= 0.433855
Thermal correction to Enthalpy= 0.434799
Thermal correction to Gibbs Free Energy= 0.348495
Sum of electronic and zero-point Energies= -1665.762297
Sum of electronic and thermal Energies= -1665.734749
Sum of electronic and thermal Enthalpies= -1665.733804
Sum of electronic and thermal Free Energies= -1665.820108

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.644043	1.046695	0.472259
2	6	0	-3.684629	1.614458	1.178787
3	6	0	-4.966234	1.023156	1.247465
4	6	0	-5.191956	-0.155842	0.592123
5	6	0	-4.159311	-0.780280	-0.161233
6	6	0	-4.455676	-1.992997	-0.838151
7	6	0	-3.504305	-2.622359	-1.595629
8	6	0	-2.218480	-2.053203	-1.693156
9	6	0	-1.873853	-0.882840	-1.045469
10	6	0	-2.852942	-0.191099	-0.244101
11	6	0	-1.353464	1.794353	0.469819
12	6	0	-1.248567	2.974421	-0.223880
13	6	0	-0.020594	3.671310	-0.346647
14	6	0	1.114466	3.152282	0.231569
15	6	0	1.042696	1.963306	1.029386
16	6	0	2.097121	0.308485	2.456515
17	6	0	0.844125	-0.317279	2.652240
18	6	0	-0.279030	0.166519	2.023001
19	6	0	-0.209226	1.305327	1.177833
20	6	0	-0.472619	-0.414017	-1.305936
21	6	0	-0.270808	0.650894	-2.156700
22	6	0	1.974012	-0.691882	-1.203951
23	6	0	3.111301	-1.388239	-0.727389
24	6	0	3.001268	-2.461138	0.105591
25	6	0	1.721559	-2.877251	0.520881
26	6	0	0.601464	-2.223631	0.090117
27	6	0	0.669545	-1.121080	-0.806378
28	1	0	-3.499283	2.545826	1.706159
29	1	0	-5.753646	1.503062	1.819383
30	1	0	-6.165075	-0.637529	0.629514
31	1	0	-5.457168	-2.404035	-0.746532
32	1	0	-3.729045	-3.544568	-2.121229
33	1	0	-1.464161	-2.551969	-2.296237
34	1	0	-2.118383	3.360428	-0.748799

35	1	0	0.010925	4.580945	-0.933442
36	1	0	0.773200	-1.194273	3.289409
37	1	0	-1.235914	-0.330070	2.156969
38	1	0	-1.138684	1.173986	-2.547019
39	6	0	1.021528	1.085354	-2.523786
40	6	0	2.192367	1.431840	1.666796
41	1	0	2.982625	-0.094117	2.938691
42	1	0	3.146384	1.927472	1.523857
43	1	0	1.130110	1.941943	-3.181118
44	6	0	2.130891	0.425072	-2.061450
45	1	0	3.129841	0.740315	-2.340909
46	9	0	-0.566115	-2.636642	0.603722
47	9	0	1.628325	-3.893018	1.385310
48	9	0	4.074985	-3.114576	0.557210
49	9	0	4.333927	-0.980532	-1.101915
50	8	0	2.353361	3.691025	0.116379
51	6	0	2.495660	4.840274	-0.705124
52	1	0	3.554567	5.092375	-0.688934
53	1	0	2.181647	4.623391	-1.731869
54	1	0	1.911480	5.677871	-0.310277

Compound 5 anti-in GS1 DMSO

Method: m062x/6-31+g(d,p)
SCF Done: E(RM062X) = -1666.17097067 A.U. after 1 cycles
Lowest frequency = 15.9310

Zero-point correction= 0.406394
(Hartree/Particle)
Thermal correction to Energy= 0.433924
Thermal correction to Enthalpy= 0.434868
Thermal correction to Gibbs Free Energy= 0.348968
Sum of electronic and zero-point Energies= -1665.764577
Sum of electronic and thermal Energies= -1665.737047
Sum of electronic and thermal Enthalpies= -1665.736102
Sum of electronic and thermal Free Energies= -1665.822003

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.073909	-0.783441	-1.183357
2	6	0	2.824927	-1.163277	-2.277713
3	6	0	4.233845	-1.251485	-2.232489
4	6	0	4.883770	-0.954144	-1.065508
5	6	0	4.158940	-0.547315	0.087944
6	6	0	4.882313	-0.242421	1.273415
7	6	0	4.228741	0.153747	2.407870
8	6	0	2.821048	0.269486	2.387835
9	6	0	2.072713	0.000067	1.259438
10	6	0	2.729743	-0.444526	0.054514
11	6	0	0.594287	-0.735622	-1.385300
12	6	0	0.052438	0.267497	-2.161255

13	6	0	-1.344251	0.375310	-2.348335
14	6	0	-2.191016	-0.526720	-1.749887
15	6	0	-1.664317	-1.602256	-0.989579
16	6	0	-2.004944	-3.632559	0.326805
17	6	0	-0.598292	-3.776822	0.432987
18	6	0	0.258373	-2.861308	-0.119827
19	6	0	-0.257778	-1.740917	-0.830889
20	6	0	0.590568	0.149469	1.433944
21	6	0	-0.053026	-0.779223	2.226491
22	6	0	-1.581452	1.267845	1.129118
23	6	0	-2.346767	2.320719	0.571148
24	6	0	-1.773428	3.317474	-0.161268
25	6	0	-0.380207	3.301661	-0.373624
26	6	0	0.387405	2.295154	0.140449
27	6	0	-0.171951	1.234402	0.899651
28	1	0	2.305248	-1.412606	-3.198512
29	1	0	4.785122	-1.558686	-3.115128
30	1	0	5.966074	-1.019934	-0.997536
31	1	0	5.964787	-0.333364	1.255686
32	1	0	4.776070	0.384288	3.315900
33	1	0	2.304019	0.596100	3.285469
34	1	0	0.712696	1.011338	-2.600557
35	1	0	-1.744001	1.188851	-2.946072
36	1	0	-0.203497	-4.630328	0.975588
37	1	0	1.332460	-2.975106	-0.011257
38	1	0	0.529958	-1.592340	2.647616
39	6	0	-1.444527	-0.734576	2.461483
40	6	0	-2.526762	-2.564654	-0.368292
41	1	0	-2.649128	-4.367004	0.794132
42	1	0	-1.909109	-1.504699	3.068334
43	6	0	-2.205864	0.262512	1.908407
44	1	0	-3.278870	0.301846	2.059685
45	9	0	1.701259	2.331078	-0.126215
46	9	0	0.168760	4.280991	-1.098302
47	9	0	-2.496903	4.310634	-0.684300
48	9	0	-3.673304	2.343980	0.770585
49	1	0	-3.266208	-0.434752	-1.857093
50	8	0	-3.852775	-2.327871	-0.528600
51	6	0	-4.762159	-3.224788	0.090909
52	1	0	-4.617019	-3.236494	1.176402
53	1	0	-5.757959	-2.852198	-0.142940
54	1	0	-4.644420	-4.237840	-0.307337

Compound 5 syn-in GS1 DMSO

Method: m062x/6-31+g(d,p)
SCF Done: E(RM062X) = -1666.17167039 A.U. after 1 cycles
Lowest frequency = 17.2954

Zero-point correction= 0.406799
(Hartree/Particle)
Thermal correction to Energy= 0.434108
Thermal correction to Enthalpy= 0.435052
Thermal correction to Gibbs Free Energy= 0.350779

Sum of electronic and zero-point Energies= -1665.764871
Sum of electronic and thermal Energies= -1665.737562
Sum of electronic and thermal Enthalpies= -1665.736618
Sum of electronic and thermal Free Energies= -1665.820891

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.221158	-1.128430	-0.926906
2	6	0	2.766690	-2.344714	-1.286846
3	6	0	4.048786	-2.754717	-0.862239
4	6	0	4.777641	-1.928799	-0.049285
5	6	0	4.268518	-0.662210	0.344520
6	6	0	5.069458	0.162672	1.181413
7	6	0	4.635984	1.402646	1.563299
8	6	0	3.381640	1.865151	1.106337
9	6	0	2.560438	1.097424	0.307727
10	6	0	2.977761	-0.221444	-0.100778
11	6	0	0.824405	-0.878821	-1.406907
12	6	0	0.589666	-0.131887	-2.541113
13	6	0	-0.723367	0.102151	-3.004815
14	6	0	-1.800397	-0.411689	-2.322099
15	6	0	-1.596491	-1.205440	-1.166337
16	6	0	-2.504101	-2.522662	0.682449
17	6	0	-1.179180	-2.807424	1.102206
18	6	0	-0.092788	-2.300630	0.439626
19	6	0	-0.274828	-1.475194	-0.710453
20	6	0	1.309103	1.771330	-0.167567
21	6	0	1.430420	2.703891	-1.175463
22	6	0	-1.118057	2.169487	-0.191786
23	6	0	-2.409126	1.860502	0.298763
24	6	0	-2.593071	1.005955	1.346264
25	6	0	-1.472547	0.422892	1.970493
26	6	0	-0.212651	0.678574	1.505327
27	6	0	0.016666	1.531112	0.394137
28	1	0	2.173193	-3.012043	-1.906041
29	1	0	4.438458	-3.719116	-1.171190
30	1	0	5.761190	-2.222629	0.306602
31	1	0	6.036492	-0.213820	1.503131
32	1	0	5.246460	2.036061	2.198413
33	1	0	3.046717	2.858982	1.389263
34	1	0	1.431623	0.307437	-3.069148
35	1	0	-0.876824	0.707116	-3.892861
36	1	0	-1.035834	-3.428146	1.981213
37	1	0	0.910698	-2.509738	0.793363
38	1	0	2.416439	2.896525	-1.587938
39	6	0	0.309397	3.373332	-1.715876
40	6	0	-2.707140	-1.733490	-0.426673
41	1	0	-3.336502	-2.923202	1.247773
42	1	0	0.449806	4.091199	-2.517026
43	6	0	-0.950291	3.093704	-1.253492
44	1	0	-1.825620	3.569344	-1.681422
45	9	0	0.810292	0.089080	2.139570

46	9	0	-1.668520	-0.376323	3.021637
47	9	0	-3.812761	0.706238	1.799752
48	9	0	-3.483510	2.421911	-0.277104
49	1	0	-2.813808	-0.215179	-2.654129
50	8	0	-3.927051	-1.377637	-0.902128
51	6	0	-5.070871	-1.869279	-0.218173
52	1	0	-5.086771	-1.514054	0.817227
53	1	0	-5.932574	-1.475975	-0.754800
54	1	0	-5.093205	-2.963780	-0.234625

Compound 5 syn-out GS2 DMSO

Method: m062x/6-31+g(d,p)
SCF Done: E(RM062X) = -1666.16879086 A.U. after 1 cycles
Lowest frequency = 16.6377

Zero-point correction= 0.406489
(Hartree/Particle)
Thermal correction to Energy= 0.433937
Thermal correction to Enthalpy= 0.434882
Thermal correction to Gibbs Free Energy= 0.349639
Sum of electronic and zero-point Energies= -1665.762302
Sum of electronic and thermal Energies= -1665.734854
Sum of electronic and thermal Enthalpies= -1665.733909
Sum of electronic and thermal Free Energies= -1665.819152

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.824643	1.118599	-0.324372
2	6	0	3.872265	1.769263	-0.944127
3	6	0	5.106509	1.135981	-1.210911
4	6	0	5.274971	-0.172263	-0.849728
5	6	0	4.234765	-0.887550	-0.193922
6	6	0	4.471556	-2.239693	0.169586
7	6	0	3.512186	-2.967839	0.821151
8	6	0	2.283279	-2.354723	1.136897
9	6	0	1.997695	-1.045933	0.799931
10	6	0	2.980349	-0.254636	0.100634
11	6	0	1.579056	1.916052	-0.126181
12	6	0	1.587710	2.987179	0.740993
13	6	0	0.406274	3.711816	1.019485
14	6	0	-0.784859	3.333897	0.448909
15	6	0	-0.819281	2.265283	-0.484078
16	6	0	-2.052580	0.863731	-2.060552
17	6	0	-0.831971	0.256527	-2.448088
18	6	0	0.353548	0.587689	-1.845564
19	6	0	0.380357	1.584238	-0.829421
20	6	0	0.678103	-0.539804	1.301007
21	6	0	0.673687	0.367946	2.338254
22	6	0	-1.781088	-0.593537	1.448579
23	6	0	-3.029108	-1.088489	0.996777

24	6	0	-3.118987	-1.995994	-0.015961
25	6	0	-1.938616	-2.441709	-0.641159
26	6	0	-0.716701	-1.979953	-0.238618
27	6	0	-0.575345	-1.053155	0.831557
28	1	0	3.727095	2.800959	-1.251458
29	1	0	5.900188	1.684765	-1.707050
30	1	0	6.207548	-0.691327	-1.052662
31	1	0	5.434148	-2.679295	-0.076230
32	1	0	3.691111	-3.999455	1.105553
33	1	0	1.529168	-2.927568	1.670544
34	1	0	2.508881	3.242669	1.257975
35	1	0	0.439055	4.542228	1.717626
36	1	0	-0.853595	-0.506161	-3.221405
37	1	0	1.273867	0.087557	-2.129379
38	1	0	1.626047	0.742421	2.702175
39	6	0	-0.521540	0.827377	2.931817
40	6	0	-2.046621	1.845988	-1.094062
41	1	0	-2.974199	0.546530	-2.533374
42	1	0	-0.473354	1.554309	3.735766
43	6	0	-1.733723	0.354921	2.499647
44	1	0	-2.661336	0.694314	2.946382
45	9	0	0.341979	-2.406202	-0.941006
46	9	0	-2.040573	-3.289945	-1.669649
47	9	0	-4.296543	-2.456661	-0.445970
48	9	0	-4.157338	-0.651490	1.578596
49	1	0	-1.707736	3.847141	0.695063
50	8	0	-3.155705	2.486186	-0.646561
51	6	0	-4.407824	2.090046	-1.186487
52	1	0	-4.600034	1.030181	-0.985746
53	1	0	-5.157537	2.699990	-0.685567
54	1	0	-4.443647	2.272400	-2.265416

Compound 6 anti-in GS1 DMSO

Method: m062x/6-31+g(d,p)
SCF Done: E(RM062X) = -1383.83773626 A.U. after 1 cycles
Lowest frequency = 18.2473

Zero-point correction= 0.472008
(Hartree/Particle)
Thermal correction to Energy= 0.498417
Thermal correction to Enthalpy= 0.499361
Thermal correction to Gibbs Free Energy= 0.415853
Sum of electronic and zero-point Energies= -1383.365728
Sum of electronic and thermal Energies= -1383.339319
Sum of electronic and thermal Enthalpies= -1383.338375
Sum of electronic and thermal Free Energies= -1383.421883

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.113129	0.332622	1.240749

2	6	0	2.868049	0.552277	2.376853
3	6	0	4.279481	0.500781	2.371745
4	6	0	4.933663	0.248272	1.196744
5	6	0	4.207191	0.000007	0.000002
6	6	0	4.933676	-0.248253	-1.196731
7	6	0	4.279506	-0.500767	-2.371739
8	6	0	2.868076	-0.552280	-2.376859
9	6	0	2.113142	-0.332631	-1.240761
10	6	0	2.773446	0.000003	-0.000005
11	6	0	0.635421	0.487005	1.400946
12	6	0	-0.051302	-0.388317	2.217106
13	6	0	-1.451504	-0.299900	2.373311
14	6	0	-2.160229	0.669412	1.704340
15	6	0	-1.481100	1.617209	0.898095
16	6	0	-1.526224	3.594213	-0.538608
17	6	0	-0.109954	3.551860	-0.608866
18	6	0	0.607067	2.567025	0.016999
19	6	0	-0.065352	1.560377	0.768710
20	6	0	0.635440	-0.487032	-1.400970
21	6	0	-0.051283	0.388267	-2.217153
22	6	0	-1.481082	-1.617226	-0.898099
23	6	0	-2.196325	-2.645630	-0.200069
24	6	0	-1.526210	-3.594189	0.538658
25	6	0	-0.109941	-3.551825	0.608932
26	6	0	0.607080	-2.567001	-0.016951
27	6	0	-0.065337	-1.560384	-0.768703
28	1	0	2.350243	0.801161	3.298794
29	1	0	4.830360	0.684383	3.288402
30	1	0	6.019194	0.231293	1.154435
31	1	0	6.019208	-0.231266	-1.154414
32	1	0	4.830395	-0.684365	-3.288391
33	1	0	2.350282	-0.801172	-3.298804
34	1	0	0.492652	-1.190695	2.707072
35	1	0	-1.966860	-1.019213	3.002406
36	1	0	0.404788	4.316937	-1.182150
37	1	0	1.689087	2.539897	-0.063828
38	1	0	0.492671	1.190632	-2.707141
39	6	0	-1.451487	0.299855	-2.373350
40	6	0	-2.196339	2.645634	0.200088
41	1	0	-2.059170	4.377152	-1.063754
42	1	0	-1.966838	1.019162	-3.002456
43	6	0	-2.160213	-0.669444	-1.704363
44	1	0	-2.059152	-4.377117	1.063820
45	1	0	0.404801	-4.316884	1.182240
46	1	0	1.689099	-2.539859	0.063891
47	8	0	-3.546239	-2.594413	-0.336608
48	8	0	-3.546250	2.594437	0.336620
49	1	0	-3.239890	0.725668	1.787711
50	1	0	-3.239874	-0.725700	-1.787727
51	6	0	-4.314613	-3.573728	0.344843
52	1	0	-4.153430	-3.511632	1.426372
53	1	0	-5.355667	-3.352471	0.115516
54	1	0	-4.065392	-4.580421	-0.006658
55	6	0	-4.314580	3.573743	-0.344893
56	1	0	-4.153331	3.511625	-1.426412

57	1	0	-5.355648	3.352496	-0.115621
58	1	0	-4.065371	4.580441	0.006603

Compound 6 syn GS1 DMSO

Method: m062x/6-31+g(d,p)
SCF Done: E(RM062X) = -1383.83693099 A.U. after 1 cycles
Lowest frequency = 16.5055

Zero-point correction= 0.472029
(Hartree/Particle)
Thermal correction to Energy= 0.498367
Thermal correction to Enthalpy= 0.499311
Thermal correction to Gibbs Free Energy= 0.416283
Sum of electronic and zero-point Energies= -1383.364902
Sum of electronic and thermal Energies= -1383.338564
Sum of electronic and thermal Enthalpies= -1383.337620
Sum of electronic and thermal Free Energies= -1383.420648

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.304175	-1.176431	-0.637678
2	6	0	2.921715	-1.825169	-1.686949
3	6	0	4.204304	-1.451113	-2.148886
4	6	0	4.883349	-0.448337	-1.508488
5	6	0	4.286614	0.257542	-0.428716
6	6	0	5.027931	1.272992	0.236601
7	6	0	4.474427	1.977178	1.272135
8	6	0	3.127782	1.737378	1.632777
9	6	0	2.361720	0.775393	1.008805
10	6	0	2.952744	-0.054136	-0.011246
11	6	0	1.048808	-1.789118	-0.098683
12	6	0	1.160286	-2.688819	0.940329
13	6	0	0.016590	-3.282420	1.518179
14	6	0	-1.237056	-2.953290	1.060219
15	6	0	-1.385613	-2.052172	-0.023480
16	6	0	-2.814707	-0.818367	-1.573786
17	6	0	-1.654544	-0.311844	-2.213063
18	6	0	-0.398725	-0.627410	-1.766841
19	6	0	-0.235927	-1.489958	-0.645626
20	6	0	0.899860	0.766614	1.331078
21	6	0	0.402864	0.094742	2.425908
22	6	0	-1.378278	1.502405	0.790378
23	6	0	-2.275685	2.215880	-0.069674
24	6	0	-1.799344	2.962344	-1.123700
25	6	0	-0.404055	3.010145	-1.369685
26	6	0	0.483330	2.311770	-0.593463
27	6	0	0.015305	1.531455	0.505141
28	1	0	2.416408	-2.672254	-2.143317
29	1	0	4.656008	-1.985420	-2.978378
30	1	0	5.890459	-0.175570	-1.811685

31	1	0	6.043462	1.473055	-0.094096
32	1	0	5.043099	2.743057	1.789494
33	1	0	2.661242	2.359330	2.391900
34	1	0	2.145310	-2.917885	1.338799
35	1	0	0.132507	-3.982305	2.339858
36	1	0	-1.777855	0.359261	-3.057668
37	1	0	0.479952	-0.207073	-2.244573
38	1	0	1.083468	-0.476094	3.051644
39	6	0	-0.979370	0.094394	2.716846
40	6	0	-2.682415	-1.667508	-0.498989
41	1	0	-3.790975	-0.520990	-1.937205
42	1	0	-1.344742	-0.464098	3.573057
43	6	0	-1.858805	0.768179	1.903074
44	1	0	-2.471322	3.508085	-1.774620
45	1	0	-0.043164	3.606349	-2.202326
46	1	0	1.546148	2.347305	-0.810065
47	8	0	-3.590050	2.087411	0.245652
48	8	0	-3.725893	-2.199003	0.190927
49	1	0	-2.124327	-3.374974	1.519220
50	1	0	-2.925123	0.747801	2.099901
51	6	0	-4.536723	2.668509	-0.636128
52	1	0	-4.423811	2.261369	-1.647332
53	1	0	-5.517234	2.406982	-0.240956
54	1	0	-4.431319	3.758130	-0.665231
55	6	0	-5.032093	-1.783863	-0.176406
56	1	0	-5.264678	-2.082876	-1.203918
57	1	0	-5.711924	-2.282935	0.512313
58	1	0	-5.134845	-0.697294	-0.077354