Supporting Information

O,S-Chelated bis(pentafluorophenyl)boron and diphenylboron-β-thioketonates: Synthesis, photophysical, electrochemical and NLO properties

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General information:

All the reactions were carried out under N_2 atmosphere using standard glove box, Schlenk line and vacuum line techniques. Dry solvents used for the reactions were dried according to the standard procedures. All the reactions were monitored by thin-layer chromatography. Nuclear magnetic resonance spectra were recorded on a 400 MHz or 700 MHz Fourier transform NMR spectrometer (JEOL or Bruker) with $CDCl_3$ as a solvent. ^{11}B and ^{19}F NMR spectra were externally referenced to $BF_3.Et_2O$ in $CDCl_3$ (δ=0 ppm) and α,α,α-trifluoro toluene in $CDCl_3$ (δ=-63.73 ppm), respectively. Chemical shifts are reported in δ ppm (parts per million) using residual solvent protons as the internal standard (δ 7.26 for $CDCl_3$ in ^1H NMR, δ 77.16 for $CDCl_3$ in ^{13}C NMR). Coupling constants are reported as J values in hertz (Hz). Splitting patterns are designated as s(singlet), d(doublet), t(triplet), q(quartet), dd(doublet of doublet), dt(doublet of triplet), m(multiplet) and br(broad). HRMS were recorded using Waters XEVO G2-XS QTOF mass spectrometer. UV – Visible spectra were recorded on Agilent Technologies Cary 60 UV/Visible spectrometer. Fluorescence spectra and absolute quantum yield were measured using Edinburgh spectrofluorimeter instrument FS5. For the measurement of absolute quantum yield, the concentration of the boron compounds was such as to give an absorbance of around 0.1 at excitation wavelength. Absolute total quantum yields were measured using an integrating sphere (Edinburgh instrument FS5) mounted in SC-30 compartment of the spectrofluorimeter. A Rigaku Super Nova fine-focused dual diffractometer, fitted with a PILATUS200K, was utilised to gather single crystal X-ray diffraction data using Cu Kα radiation (λ = 1.54178 Å). The structures were solved using Olex2 and the ShelXS structure solution program using Direct Methods. The ShelXL refinement tool

was then used to refine the structures using Least Squares minimization. Anisotropic displacement coefficients were utilised in the refinement of all non-hydrogen atoms. The H atoms were placed at calculated positions and were refined as riding atoms. The standard three electrode arrangement used for cyclic voltammetry included an Ag wire serving as the reference electrode, a Pt wire serving as the secondary electrode, and a glassy carbon working electrode. About 1.0 x 10^{-3} M solution in CH_2Cl_2 with $[Bu_4N][PF_6]$ (0.1 M) as a supporting electrolyte was used to record the voltammogram. The scans were referenced with a small amount of ferrocene as an internal standard. Starting materials: methyl benzodithioate was prepared according to the literature procedure.[1] Commercially available 4-methoxy acetophenone, 4-methyl acetophenone, acetophenone, 2-acetyl naphthalene, tris(pentafluorophenyl)borane, triphenylborane were purchased from Sigma-Aldrich, Spectrochem, Alfa-Aaser.

Z-Scan measurements

The nonlinear optical characteristics were measured using an in-house developed single-beam Z-scan setup. A femtosecond Yb-doped fiber laser (Cazadero, M/S Calmar Inc., USA) is used as an excitation source for the nonlinear absorption (NLA) measurements. The laser delivers linearly polarized ultrashort pulses of width 370 fs at a central wavelength of 1030 nm. The pump laser is about 4 mm wide in the form of a symmetric Gaussian (TEM_{00}) mode profile ($M^2 < 1.05$). The Z-scan transmission measurements were carried out at a laser repetition rate fixed at 1 MHz. A plano-convex lens with a focal length of 100 mm is employed to focus the laser beam to a 32 μm beam waist. The sample is moved symmetrically through the lens focus over a 50 mm distance using a motorized translation stage. A combination of half-wave plate and a cube beam splitter is positioned in front of the lens which controls the incident optical power on the prepared sample. The Z-scan measurements are carried out with the solution form of the prepared sample. A reference photodetector (D_1) is records the variations in the excitation beam. In order to measure the open-aperture (OA) transmission, a second photodetector (D_2) is used. The measurements from both the detectors are synchronised through a data-logger algorithm. The standard CS_2 solvent is used to calibrate the OA Z-scan transmission measurements.

Figure S1 displays the OA Z-scan normalized transmittance curves for the compounds **2-8**. The red solid lines represent the theoretical fit to the observed experimental measurements. The black dots represent the experimental measurements. In order to ascertain the NLA coefficient

(β), we note that the normalized transmittance (T) depends on the samples translation distance (z) through the relation,

$$T(x) = 1 - \frac{\beta I_0 L_{eff}}{2^{\frac{3}{2}}(x^2+1)} \qquad \text{..... Eq. (S6)}$$

where I_0 is the on-axis peak intensity at the focal point, α is the membrane's linear absorption coefficient, and $L_{eff} = \frac{(1-e^{-aL})}{a}$ is the effective membrane thickness. The normalized propagation distance represented by $x=z/z_0$ in the x-axis of the curve, where z_0 is the Rayleigh range of the laser beam. It is important to note that Eq. S6 assumes that the translation length (z) is significantly longer as compared to the Rayleigh range of the Gaussian beam (> 10 times). In the present experimental set-up, the selection of excitation laser beam waist is governed by the constraint imposed by this assumption.

Additionally, we have performed the closed-aperture (CA) Z-scan experiment for ascertaining the applicability of the complexes for photonic switching applications. Figure S2 presents the measured normalized transmittance in CA Z-scan for compounds **2**-**8** (black dots). We adopt the following relation for analayzing the experimental measurements. A theoretical fitting to the experimental measurements[2] yields us a quantitative estimation of n_2 which is tabulated in Table 5.

$$T(x) = 1 - \frac{4\ {}_0x}{(x^2+9)(x^2+1)} - \frac{2(x^2+3)\ {}_0}{(x^2+9)(x^2+1)} \qquad \text{..... Eq. (S7)}$$

Table S1. Crystal data and structure refinement for Compound 1-3.

	1	**2**	**3**
Empirical formula	$C_{28}H_{13}BF_{10}O_2S$	$C_{28}H_{13}BF_{10}OS$	$C_{27}H_{11}BF_{10}OS$
Formula weight	614.25	598.25	584.23
Temperature/K	100.00(10)	100.00(10)	100.00(10)
Crystal system	triclinic	triclinic	triclinic
Space group	P-1	P-1	P-1
a/Å	8.88200(10)	9.0473(3)	9.3857(2)
b/Å	11.7045(2)	11.9367(3)	10.9581(4)
c/Å	14.6627(3)	12.7968(5)	12.3752(4)
α/°	71.659(2)	112.846(3)	72.326(3)
β/°	81.2320(10)	104.805(4)	70.919(2)
γ/°	76.3720(10)	93.529(3)	76.257(3)
Volume/Å^3	1401.08(4)	1211.08(8)	1132.48(7)
Z	2	2	2
ρ_{calc}g/cm^3	1.456	1.641	1.713
μ/mm^{-1}	1.874	2.117	2.248
F(000)	616.0	600.0	584.0
Crystal size/mm^3	0.12 × 0.1 × 0.09	0.12 × 0.11 × 0.1	0.12 × 0.11 × 0.1
Radiation	CuKα (λ = 1.54184)	CuKα (λ = 1.54184)	CuKα (λ = 1.54184)
2Θ range for data collection/°	8.122 to 156.224	7.868 to 157.426	7.8 to 156.122
Index ranges	-11 ≤ h ≤ 8, -14 ≤ k ≤ 14, -18 ≤ l ≤ 17	-11 ≤ h ≤ 10, -15 ≤ k ≤ 14, -16 ≤ l ≤ 15	-11 ≤ h ≤ 10, -13 ≤ k ≤ 13, -15 ≤ l ≤ 15
Reflections collected	22444	18134	18114
Independent reflections	5864 [R_{int} = 0.0424, R_{sigma} = 0.0264]	5052 [R_{int} = 0.0496, R_{sigma} = 0.0271]	4725 [R_{int} = 0.0287, R_{sigma} = 0.0199]
Data/restraints/parameters	5864/0/380	5052/0/372	4725/0/362
Goodness-of-fit on F^2	1.085	1.038	1.043
Final R indexes [I>=2σ (I)]	R_1 = 0.0398, wR_2 = 0.1133	R_1 = 0.0558, wR_2 = 0.1540	R_1 = 0.0348, wR_2 = 0.0905
Final R indexes [all data]	R_1 = 0.0411, wR_2 = 0.1145	R_1 = 0.0578, wR_2 = 0.1564	R_1 = 0.0358, wR_2 = 0.0916
Largest diff. peak/hole / e Å^{-3}	0.37/-0.52	0.52/-0.48	0.43/-0.27

Table S2. Crystal data and structure refinement for Compound 4 and 5.

	4	**5**
Empirical formula	$C_{31}H_{13}BF_{10}OS$	$C_{28}H_{23}BO_2S$
Formula weight	634.28	434.33
Temperature/K	109(13)	100.01(10)
Crystal system	triclinic	monoclinic
Space group	P-1	$P2_1/c$
a/Å	8.9743(4)	8.3139(2)
b/Å	11.7030(4)	19.4235(6)
c/Å	15.0237(4)	13.8886(4)
α/°	74.848(3)	90
β/°	82.963(3)	98.258(3)
γ/°	71.503(4)	90
Volume/$Å^3$	1443.00(10)	2219.55(11)
Z	2	4
$\rho_{calc}g/cm^3$	1.460	1.300
μ/mm^{-1}	1.814	1.469
F(000)	636.0	912.0
Crystal size/mm^3	0.14 × 0.12 × 0.11	0.12 × 0.1 × 0.09
Radiation	CuKα (λ = 1.54184)	CuKα (λ = 1.54184)
2Θ range for data collection/°	8.198 to 152.024	7.88 to 156.492
Index ranges	$-11 \leq h \leq 11$, $-14 \leq k \leq 14$, $-18 \leq l \leq 14$	$-10 \leq h \leq 10$, $-24 \leq k \leq 23$, $-17 \leq l \leq 17$
Reflections collected	19128	17918
Independent reflections	5833 [R_{int} = 0.0991, R_{sigma} = 0.0570]	4652 [R_{int} = 0.0448, R_{sigma} = 0.0366]
Data/restraints/parameters	5833/0/397	4652/0/290
Goodness-of-fit on F^2	1.096	1.067
Final R indexes [I>=2σ (I)]	R_1 = 0.0893, wR_2 = 0.2742	R_1 = 0.0396, wR_2 = 0.1015
Final R indexes [all data]	R_1 = 0.0978, wR_2 = 0.2816	R_1 = 0.0480, wR_2 = 0.1052
Largest diff. peak/hole / e $Å^{-3}$	0.65/-0.84	0.38/-0.31

Table S3. Comparison of bond lengths, bond angles, and other structural data for compounds **1-4** (DFT optimized).

	1	**2**	**3**	**4**
S-C1 (Å)	1.729	1.726	1.724	1.726
O-C3 (Å)	1.307	1.305	1.304	1.304
B-S (Å)	1.971	1.973	1.973	1.972
B-O (Å)	1.497	1.498	1.499	1.499
B-C4 (Å)	1.644	1.643	1.642	1.643
B-C5 (Å)	1.627	1.627	1.626	1.627
C1-C2 (Å)	1.389	1.392	1.394	1.392
C2-C3 (Å)	1.412	1.408	1.406	1.407
S-B-O (deg)	105.28	105.25	105.30	105.35
S-B-C4 (deg)	115.18	115.14	115.18	115.22
O-B-C5 (deg)	110.35	110.38	110.44	110.42
C4-B-C5 (deg)	110.69	110.80	110.90	110.89
C1-C2-C3 (deg)	124.0	123.91	123.88	123.89
Deviation of B from C_3SOB plane (Å)	0.347	0.344	0.340	0.342

Table S4. Comparison of bond lengths, bond angles, and other structural data for compounds 5-8 (DFT optimized).

	5	**6**	**7**	**8**
S-C1 (Å)	1.729	1.726	1.724	1.726
O-C3 (Å)	1.303	1.302	1.301	1.301
B-S (Å)	2.007	2.010	2.010	2.010
B-O (Å)	1.517	1.518	1.518	1.519
B-C4 (Å)	1.617	1.616	1.616	1.616
B-C5 (Å)	1.612	1.612	1.612	1.612
C1-C2 (Å)	1.390	1.393	1.395	1.394
C2-C3 (Å)	1.413	1.410	1.408	1.409
S-B-O (deg)	104.59	104.49	104.42	104.47
S-B-C4 (deg)	110.58	110.40	110.36	110.41
O-B-C5 (deg)	108.12	108.08	108.14	108.10
C4-B-C5 (deg)	116.00	116.27	116.30	116.28
C1-C2-C3 (deg)	124.66	124.57	124.50	124.49
Deviation of B from C_3SOB plane (Å)	0.343	0.340	0.340	0.341

Table S5. Photophysical data of compounds 1-8 at 298K

Complexes	Solvent	$\lambda_{abs}{}^{a}$ /nm (ε x 10^4/M^{-1} cm^{-1})	$\lambda_{ems}{}^{b}$ (nm)	Stokes Shift (cm^{-1})	$\phi_F{}^{c}$ (%)	τ^{d} (ns)
1	Toluene	356(1.3), 461(2.6)	538	3104	-	-
	THF	355(1.5), 461(3.0)	533	2930	-	-
	CH_2Cl_2	353(1.5), 458(3.0)	534	3108	0.12	0.23
	CH_3CN	351(1.8), 457(3.4)	542	3431	-	-
	Solid	-	564	-	-	-
2	Toluene	347(1.7), 451(2.1)	568	4567	-	-
	THF	347(1.9), 450(2.2)	553	4139	-	-
	CH_2Cl_2	345(1.8), 448(2.2)	551	4173	0.11	0.41
	CH_3CN	344(1.9), 446(2.3)	521	3228	-	-
	Solid	-	554	-	-	-
3	Toluene	346(1.6), 448(1.7)	569	4747	-	-
	THF	346(1.8), 446(1.8)	560	4564	-	-
	CH_2Cl_2	344(1.9), 445(1.9)	557	4518	0.10	0.59
	CH_3CN	341(1.9), 442(1.9)	551	4476	-	-
	Solid	-	614	-	-	-
4	Toluene	349(1.5), 465(2.3)	555	3487	-	-
	THF	350(2.0), 466(2.8)	537	2838	-	-
	CH_2Cl_2	348(1.8), 463(2.7)	549	3384	0.14	0.35
	CH_3CN	346(2.1), 462(3.0)	531	2813	-	-
	Solid	-	617	-	-	-
5	Toluene	348(1.5), 468(1.8)	-	-	-	-
	THF	347(1.7), 464(2.0)	-	-	-	-
	CH_2Cl_2	346(1.6), 465(2.1)	-	-	-	-
	CH_3CN	341(1.4), 457(1.8)	-	-	-	-
6	Toluene	335(1.5), 463(1.6)	-	-	-	-
	THF	335(1.7), 455(1.2)	-	-	-	-
	CH_2Cl_2	336(1.7), 455(1.3)	-	-	-	-
	CH_3CN	332(1.6), 432(1.3)	-	-	-	-
7	Toluene	333(1.5), 461(1.0)	-	-	-	-
	THF	332(1.5), 419(1.1)	-	-	-	-
	CH_2Cl_2	334(1.5), 455(1.0)	-	-	-	-

	CH_3CN	329(1.4), 413(1.4)	-	-	-	-
8	Toluene	339(1.7), 472(1.6)	-	-	-	-
	THF	336(1.7), 447(1.5)	-	-	-	-
	CH_2Cl_2	337(1.6), 467(1.6)	-	-	-	-
	CH_3CN	334(1.5), 431(1.6)	-	-	-	-

[a]Absorption maximum (concentration = 3.5 x 10^{-5} M), [b]excited at λ_{max}, [c]relative quantum yield using integrating sphere module, [d]emission lifetime.

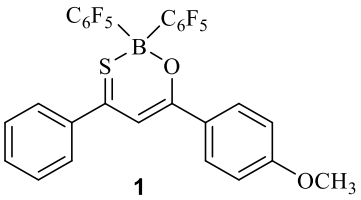
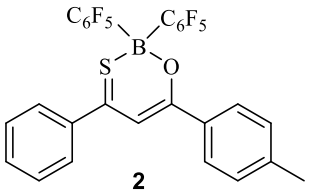
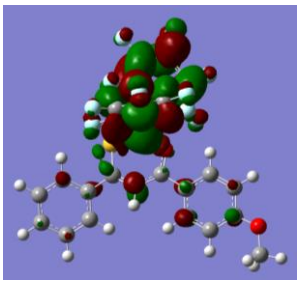
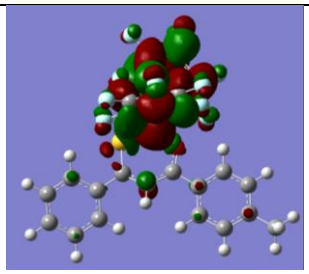
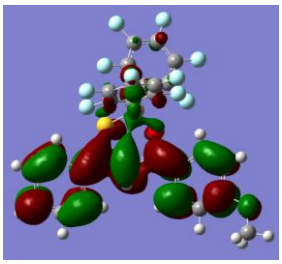
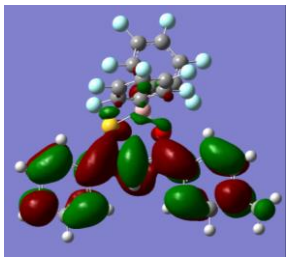
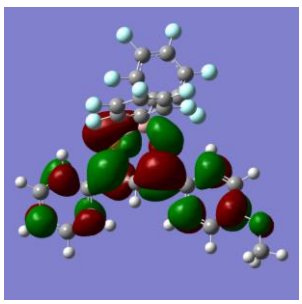
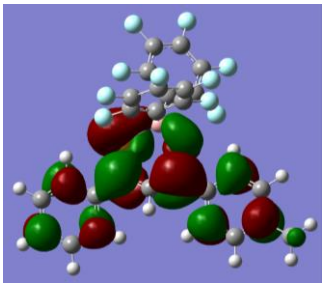
Table S6. Calculated electronic transitions for compounds **1-8** from TD-DFT (B3LYP (6-31G(d,p)) calculations

Compounds	Transition	MO contributions	Energy gap eV (nm)	Oscillator strength/f
1	$S_0 \rightarrow S_1$	HOMO→LUMO	2.92 (424)	0.6505
	$S_0 \rightarrow S_2$	HOMO-2→LUMO	3.21 (385)	0.0010
		HOMO-1→LUMO		
	$S_0 \rightarrow S_3$	HOMO-3→LUMO	3.29 (376)	0.0013
		HOMO-2→LUMO		
2	$S_0 \rightarrow S_1$	HOMO→LUMO	3.01 (411)	0.4975
	$S_0 \rightarrow S_2$	HOMO-2→LUMO	3.14 (394)	0.0059
		HOMO-1→LUMO		
	$S_0 \rightarrow S_3$	HOMO-3→LUMO	3.21 (385)	0.0012
		HOMO-2→LUMO		
		HOMO-1→LUMO		
3	$S_0 \rightarrow S_1$	HOMO→LUMO	3.05 (406)	0.3532
		HOMO-1→LUMO		

	$S_0 \rightarrow S_2$	HOMO-2→LUMO HOMO-1→LUMO HOMO→LUMO	3.10 (399)	0.0414
	$S_0 \rightarrow S_3$	HOMO-3→LUMO HOMO-2→LUMO HOMO-1→LUMO	3.16 (391)	0.0011
4	S0→S1	HOMO→LUMO	2.70 (459)	0.3147
	S0→S2	HOMO-1→LUMO	3.06 (404)	0.2948
	S0→S3	HOMO-3→LUMO HOMO-2→LUMO	3.10 (399)	0.0375
5	S0→S1	HOMO-2→LUMO HOMO-1→LUMO HOMO→LUMO	2.88 (430)	0.1595
	S0→S2	HOMO-2→LUMO HOMO→LUMO	2.92 (424)	0.3601
	S0→S3	HOMO-2→LUMO HOMO-1→LUMO	2.94 (420)	0.0188
6	S0→S1	HOMO-2→LUMO HOMO-1→LUMO HOMO →LUMO	2.81 (440)	0.0129
	S0→S2	HOMO-2→LUMO HOMO-1→LUMO HOMO→LUMO	2.88 (429)	0.0044
	S0→S3	HOMO-2→LUMO	2.95 (419)	0.3217

		HOMO-1→LUMO HOMO→LUMO		
7	S0→S1	HOMO-2→LUMO HOMO →LUMO	2.78 (445)	0.0075
	S0→S2	HOMO-2→LUMO HOMO-1→LUMO HOMO→LUMO	2.84 (436)	0.0034
	S0→S3	HOMO-4→LUMO HOMO-2→LUMO HOMO-1→LUMO HOMO→ LUMO	2.96 (418)	0.2198
8	S0→S1	HOMO-2→LUMO HOMO→ LUMO	2.74 (452)	0.3270
	S0→S2	HOMO-2→LUMO HOMO-1→LUMO HOMO→LUMO	2.79 (443)	0.0488
	S0→S3	HOMO-2→LUMO HOMO-1→LUMO	2.84 (435)	0.0037

Table S7. Computed orbitals for compounds **1** and **2**.

Compound	 **1**	 **2**
LUMO+2	 -0.7210 eV	 -0.7376 eV
LUMO+1	 -0.9987 eV	 -1.067 eV
LUMO	 -2.913 eV	 -2.998 eV

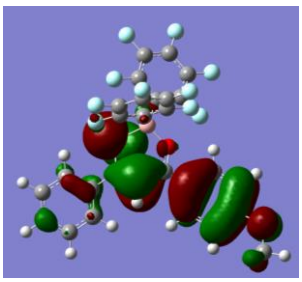
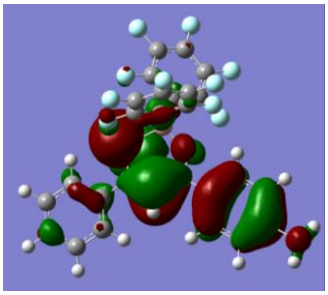
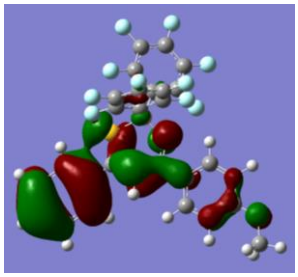
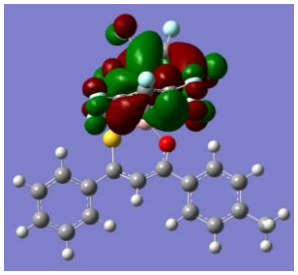
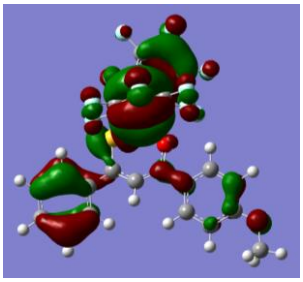
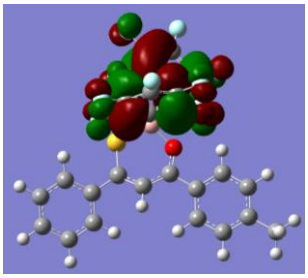
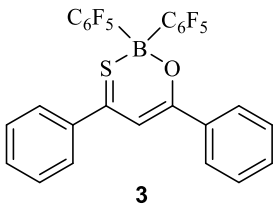
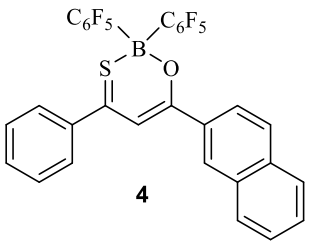
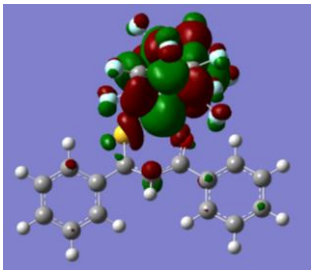
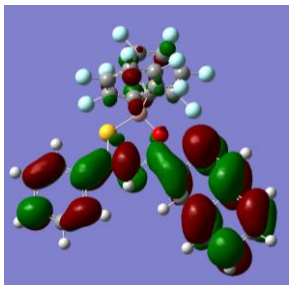
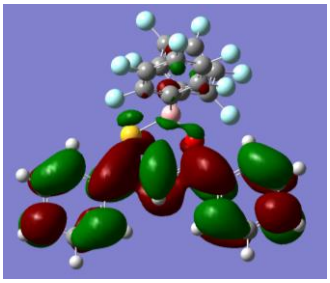
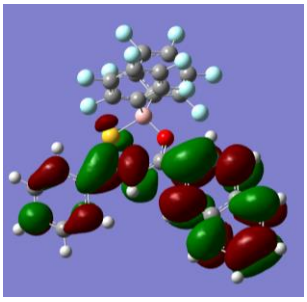
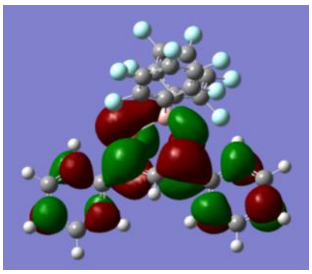
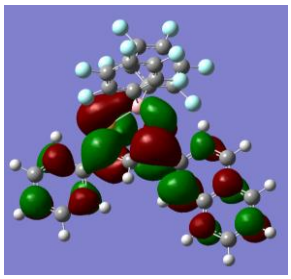
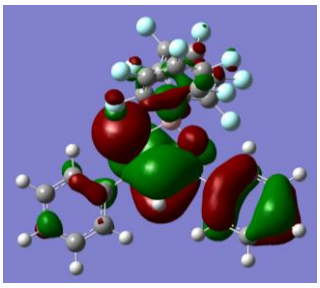
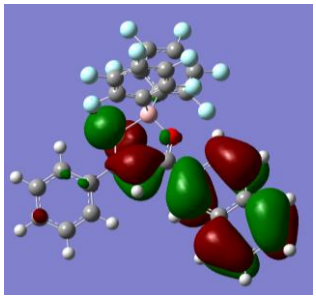
HOMO	 -6.212 eV	 -6.442 eV
HOMO-1	 -6.6822 eV	 -6.694 eV
HOMO-2	 -6.7366 eV	 -6.747 eV

Table S8. Computed orbitals for compounds **3** and **4**.

Compound		
	 **3**	 **4**

LUMO+2	 -0.745 eV	 -0.893 eV
LUMO+1	-1.112 eV 	 -1.502 eV
LUMO	 -3.046 eV	 -3.056 eV
HOMO	 -6.539 eV	 -6.187 eV

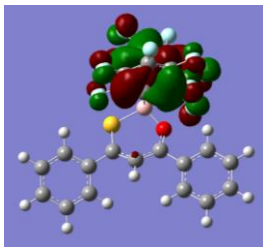
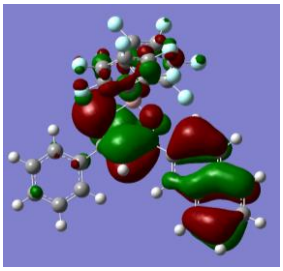
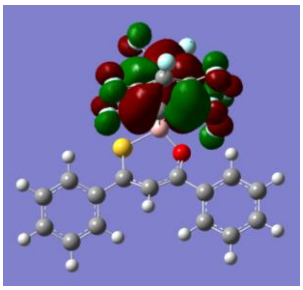
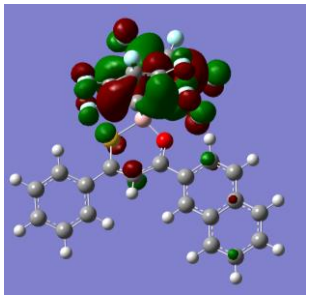
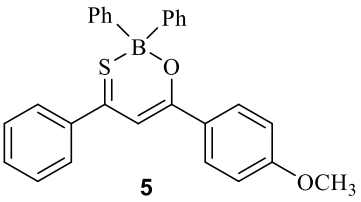
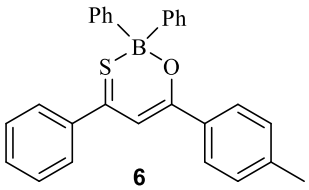
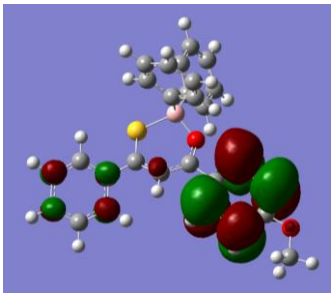
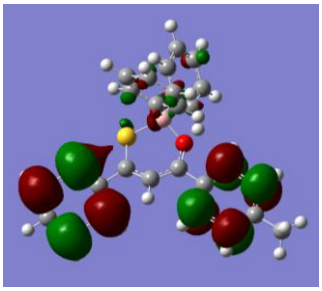
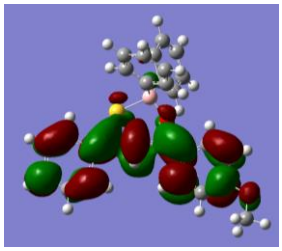
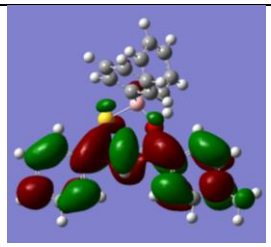
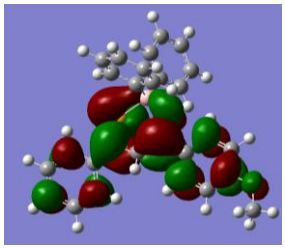
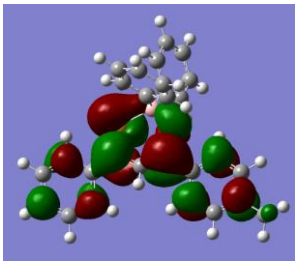
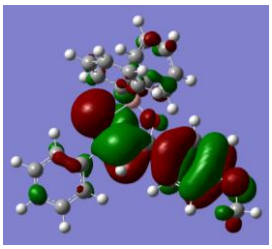
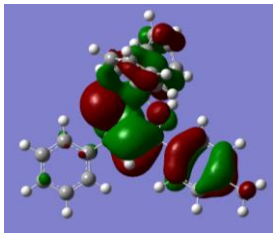
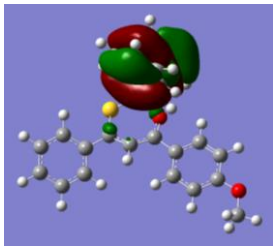
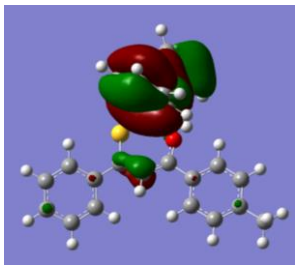
HOMO-1	 -6.700 eV	 -6.636 eV
HOMO-2	 -6.756 eV	 -6.699 eV

Table S9. Computed orbitals for compounds **5** and **6**.

Compound	 **5**	 **6**
LUMO+2	 -0.472 eV	 -0.419 eV

LUMO+1	 -0.937 eV	 -1.010 eV
LUMO	 -2.811 eV	 -2.892 eV
HOMO	 -6.132 eV	 -6.302 eV
HOMO-1	 -6.351 eV	 -6.380 eV

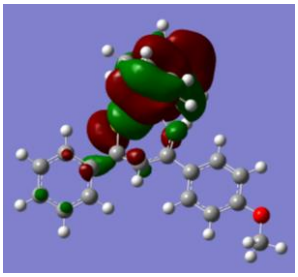
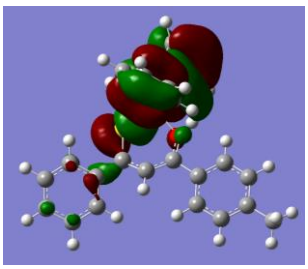
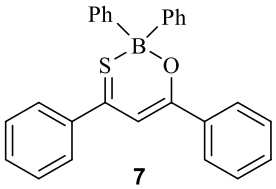
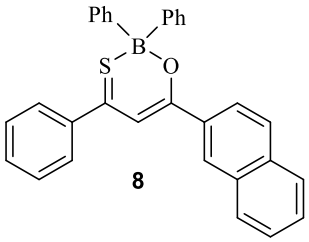
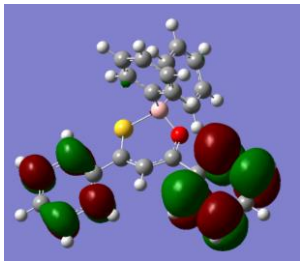
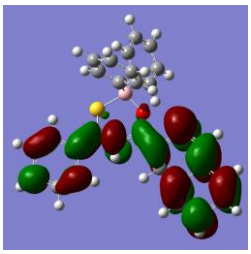
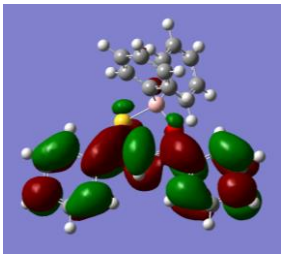
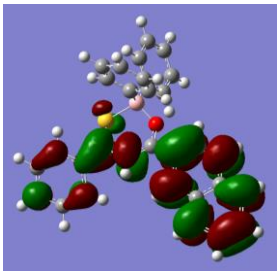
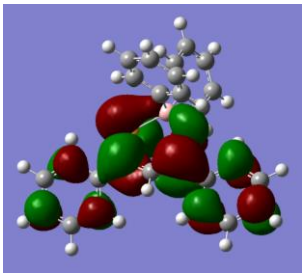
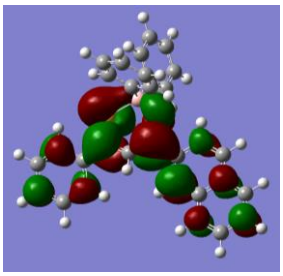
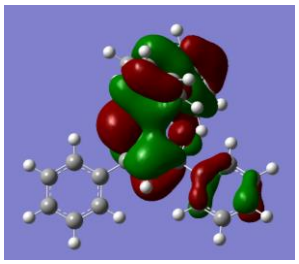
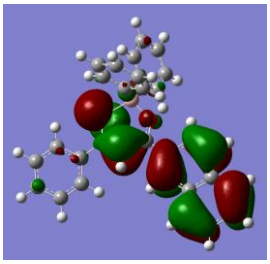
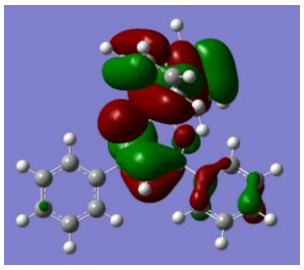
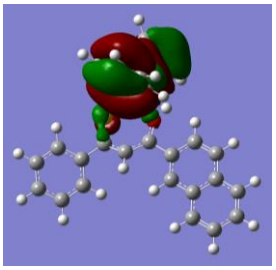
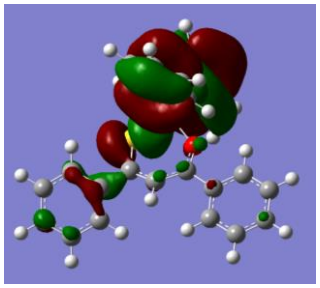
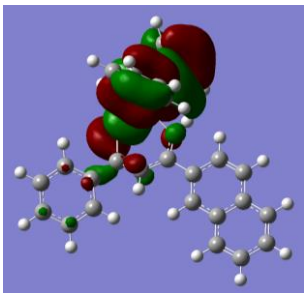
HOMO-2	 -6.392 eV	 -6.404 eV

Table S10. Computed orbitals for compounds **7** and **8**.

Compound	 **7**	 **8**
LUMO+2	 -0.442 eV	 -0.864 eV
LUMO+1	 -1.055 eV	 -1.476 eV

LUMO	 -2.941 eV	 -2.947 eV
HOMO	 -6.361 eV	 -6.130 eV
HOMO-1	 -6.394 eV	 -6.377 eV
HOMO-2	 -6.421 eV	 -6.410 eV

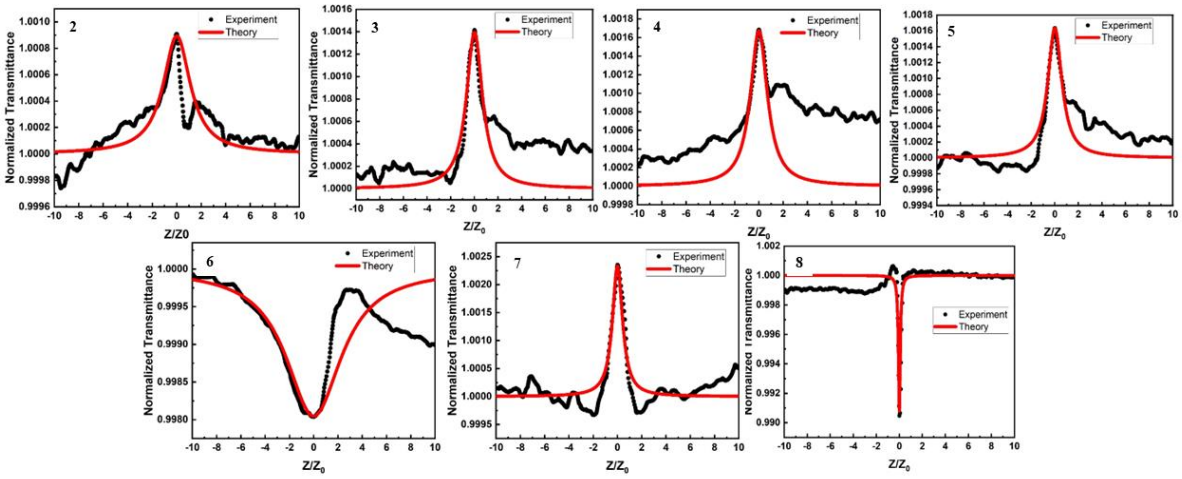


Figure S1. Measured normalized transmittance (black dotted curve) as a function of sample position (*z*) for open-aperture Z-scan experiment for compounds 2-8. The red solid-curves are theoretical fits as per Eq. (S6)

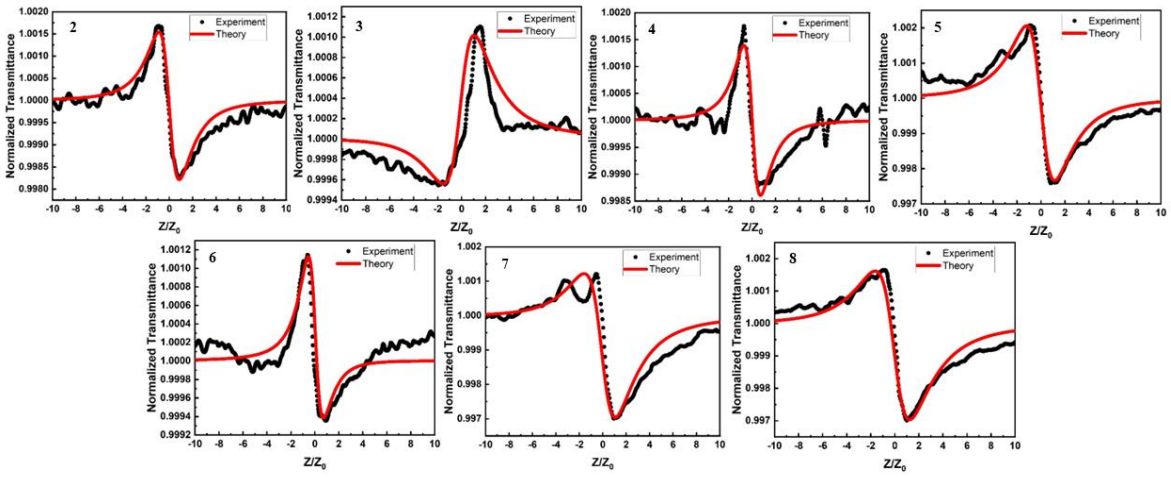


Figure S2. Measured normalized transmittance (black dotted curve) as a function of sample position for closed-aperture Z-scan experiment for the compounds 2-8. The red solid-curves are theoretical fits as per Eq. (S7)

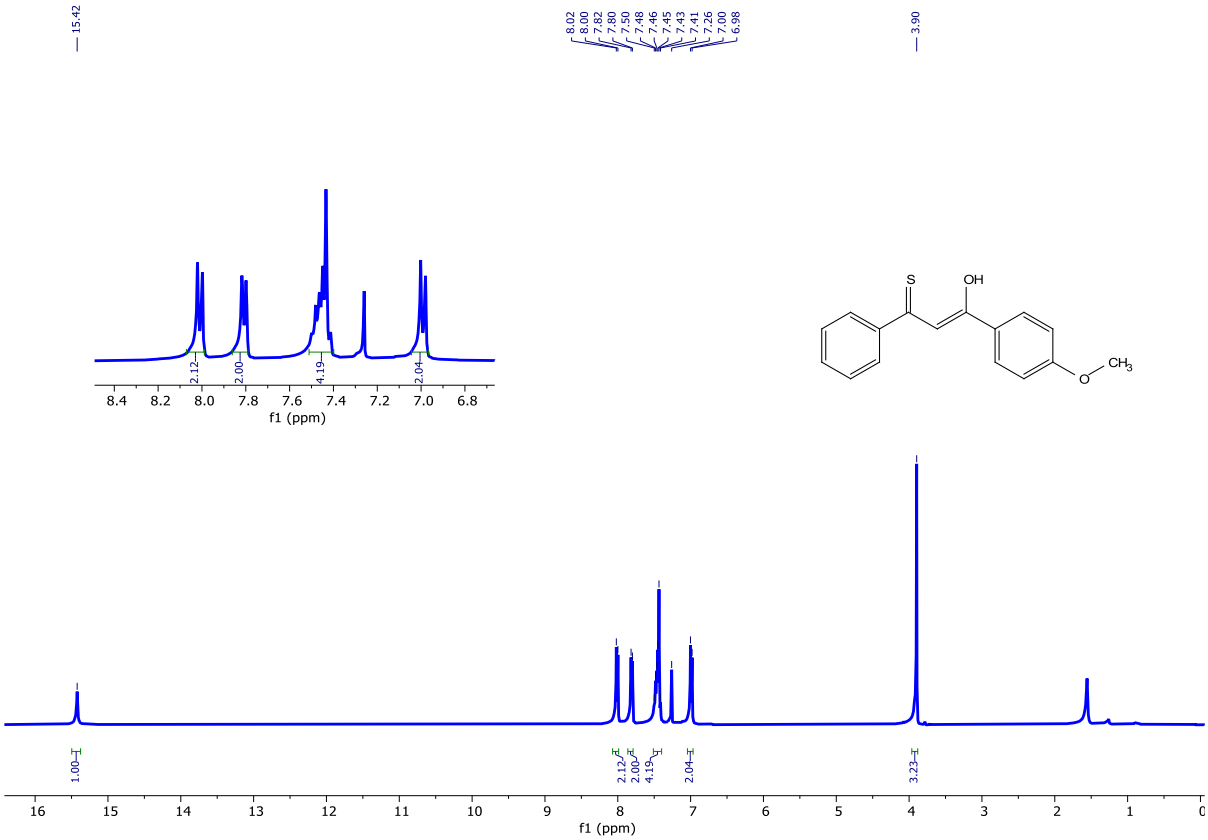


Figure S3. ^{1}H NMR (400 MHz) spectrum of **compound L1 in $CDCl_3$**

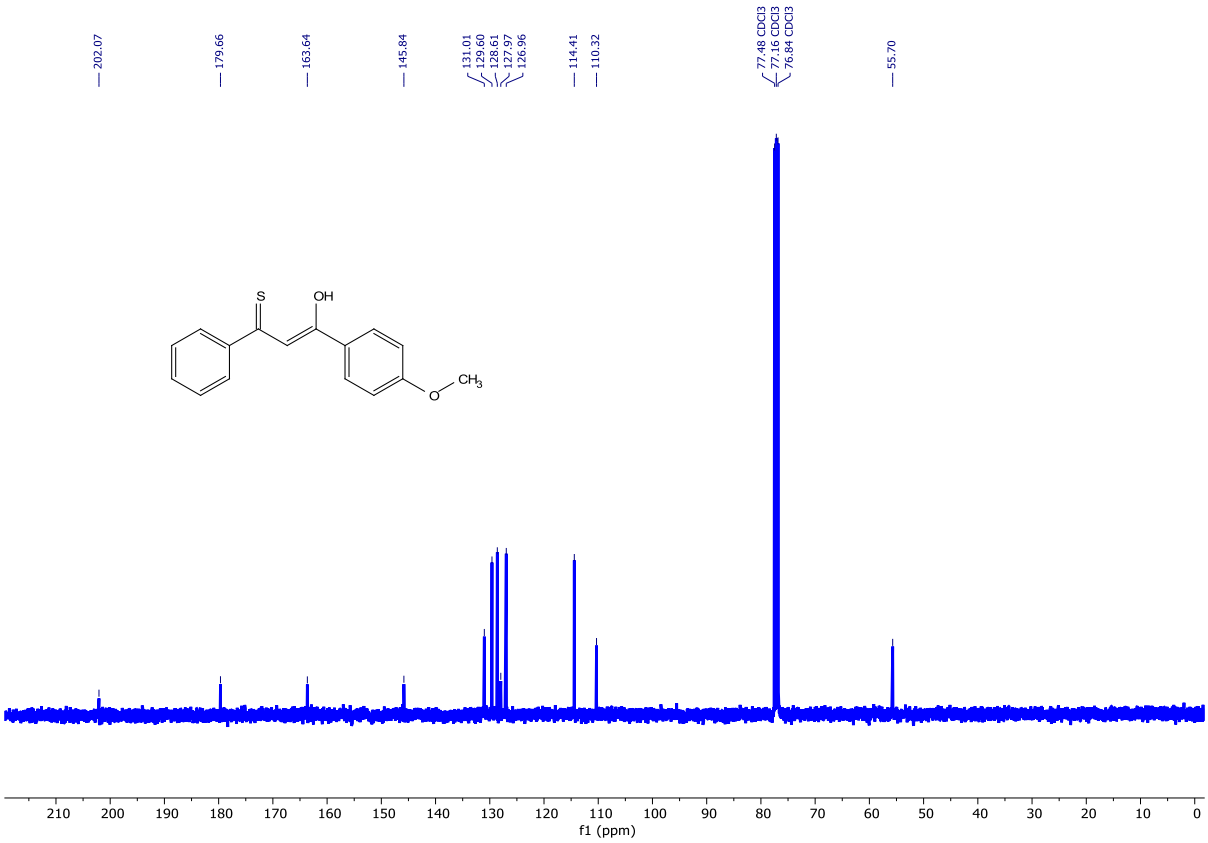


Figure S4. ^{13}C NMR (101 MHz) spectrum of **compound L1 in $CDCl_3$**

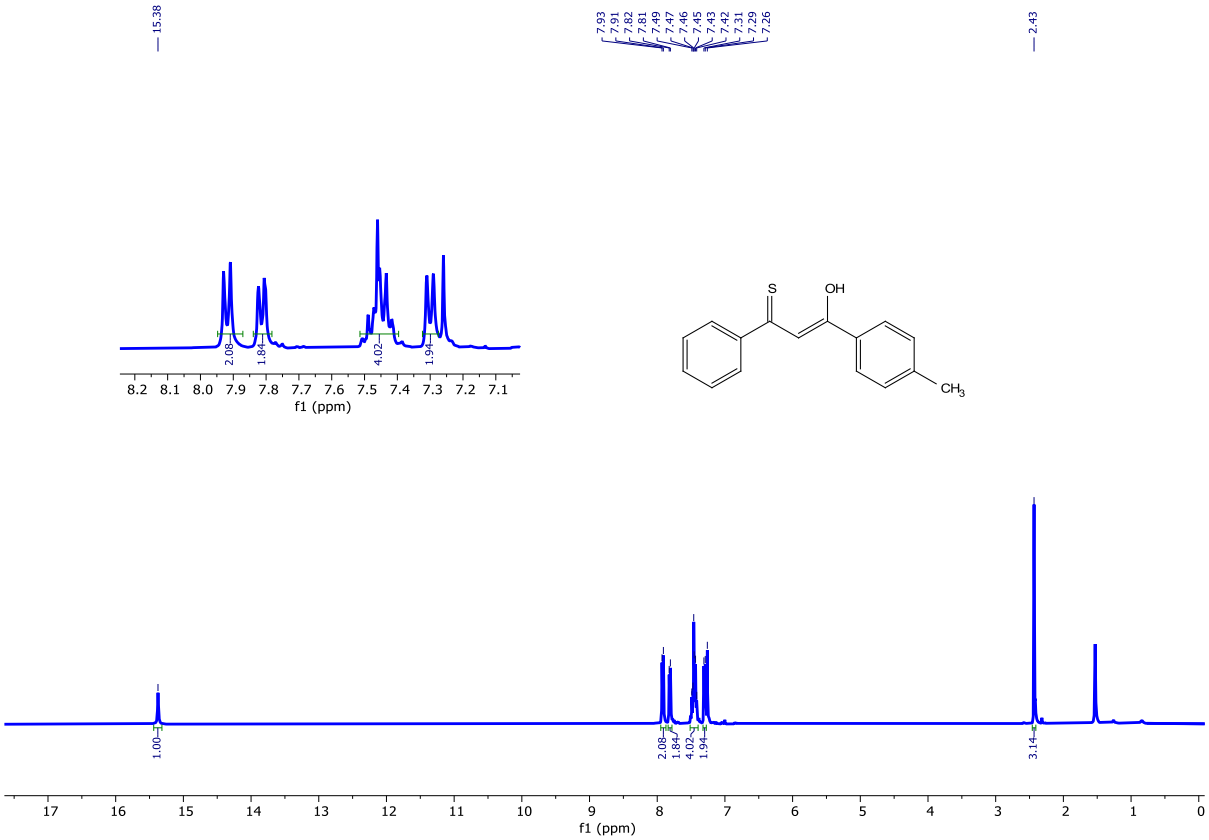


Figure S5. ^{1}H NMR (400 MHz) spectrum of **L2 in $CDCl_3$**

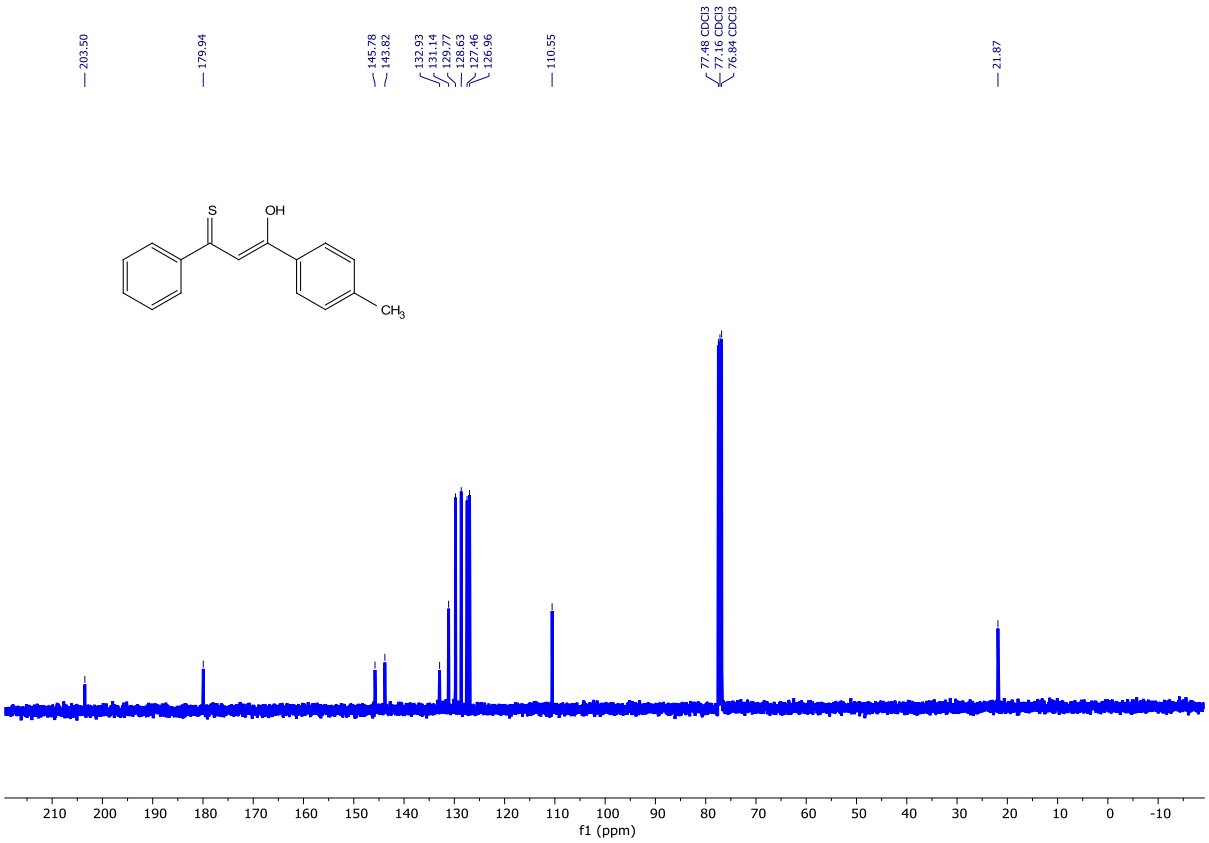


Figure S6. ^{13}C NMR (101 MHz) spectrum of **compound L2 in $CDCl_3$**

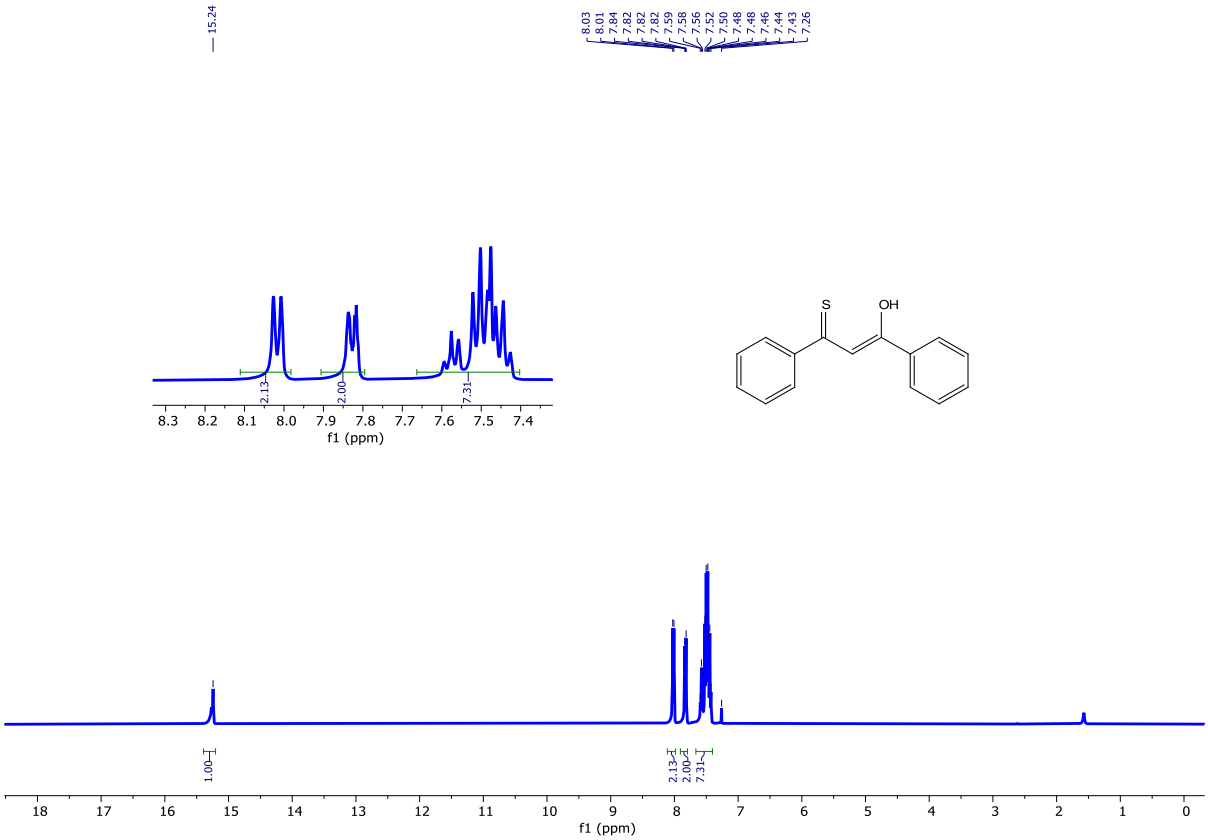


Figure S7. ^{1}H NMR (400 MHz) spectrum of **compound L3 in $CDCl_3$**

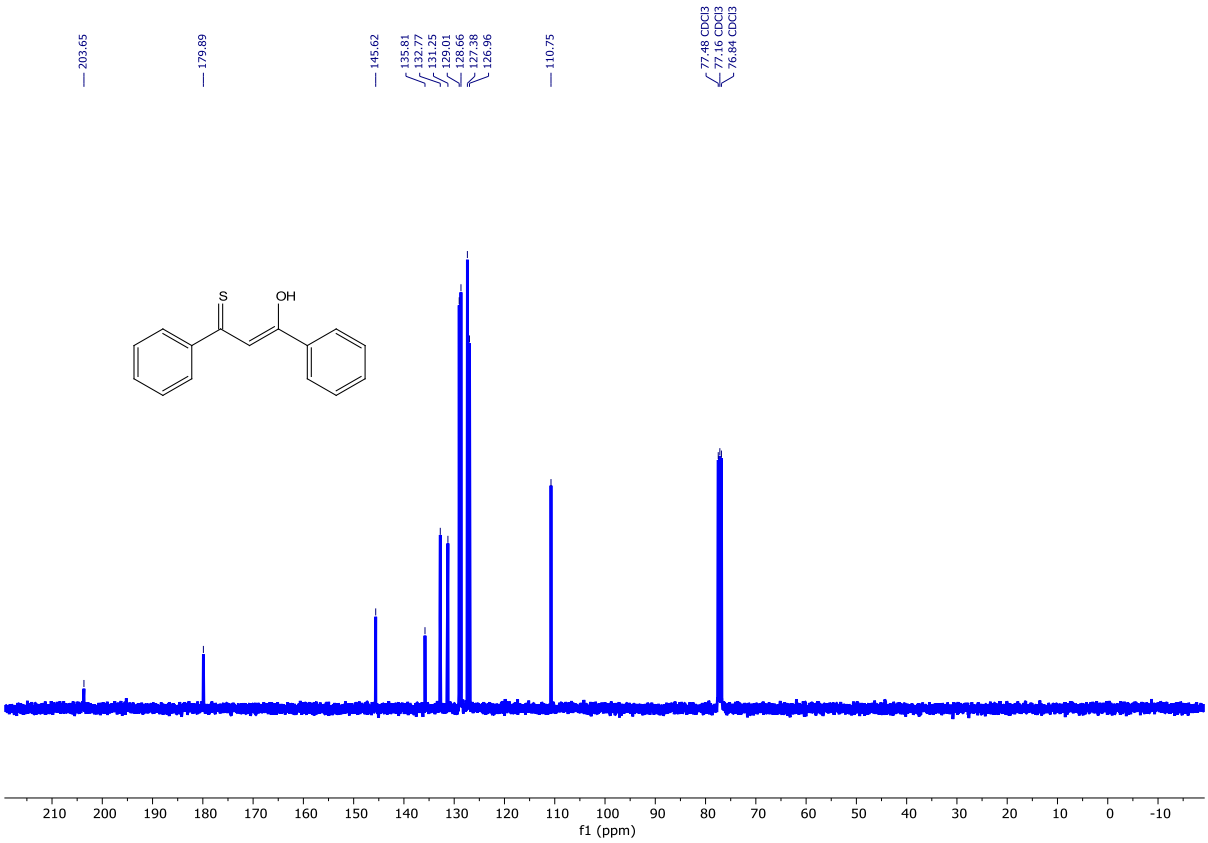


Figure S8. ^{13}C NMR (101 MHz) spectrum of **compound L3 in $CDCl_3$**

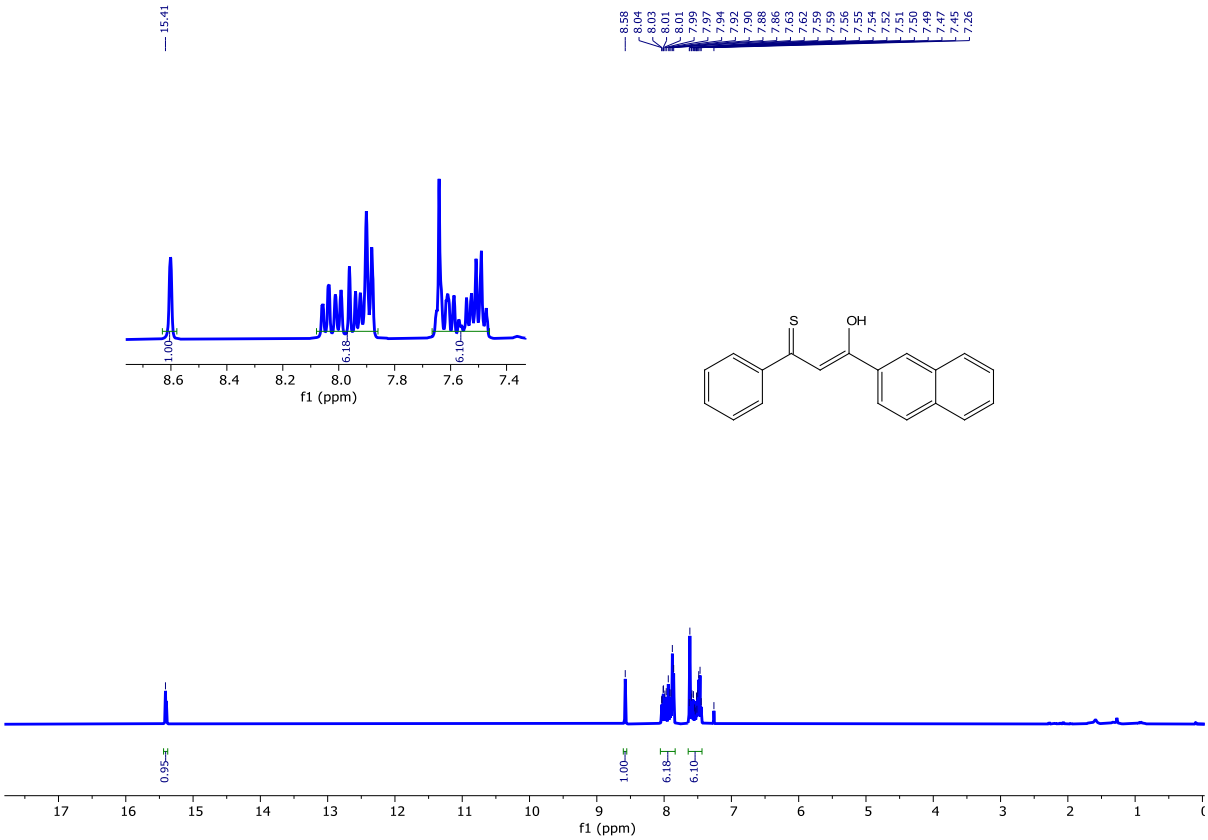


Figure S9. ^{1}H NMR (400 MHz) spectrum of **compound L4 in $CDCl_3$**

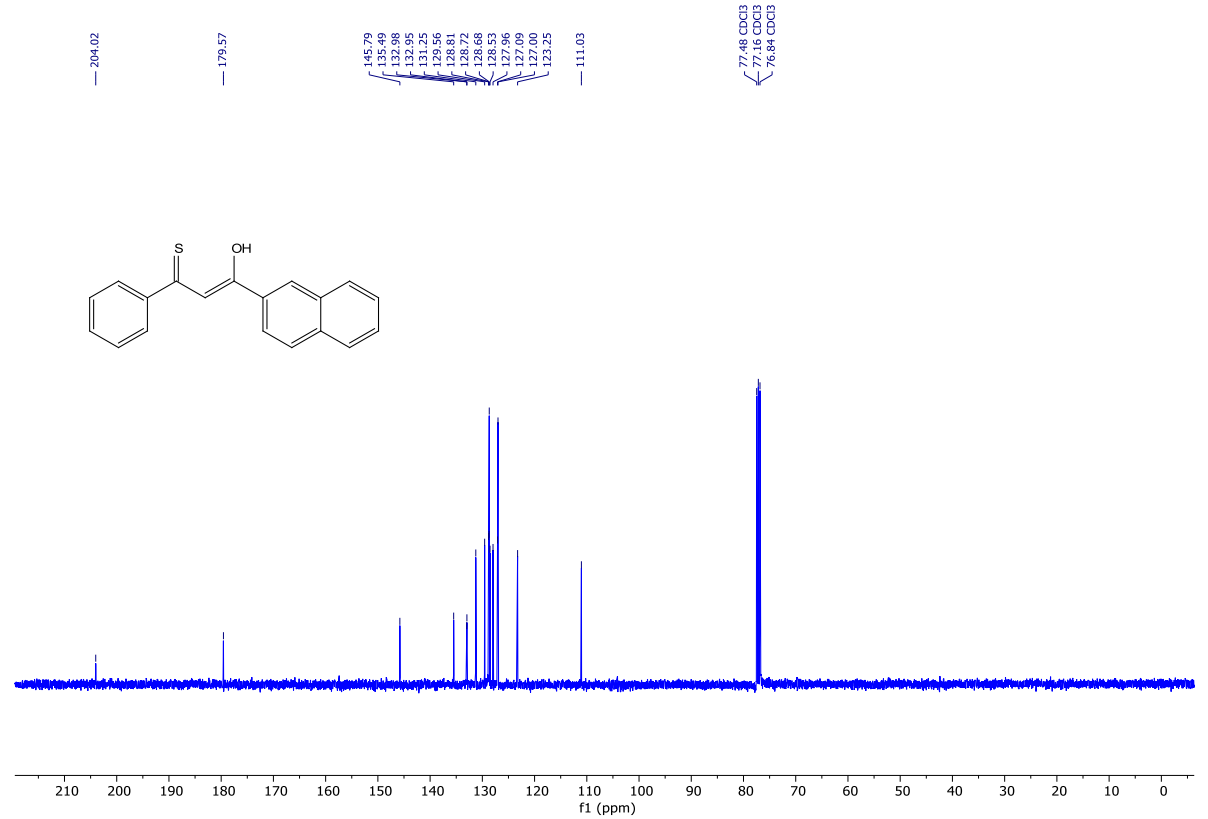


Figure S10. ^{13}C NMR (101 MHz) spectrum of **compound L4 in $CDCl_3$**

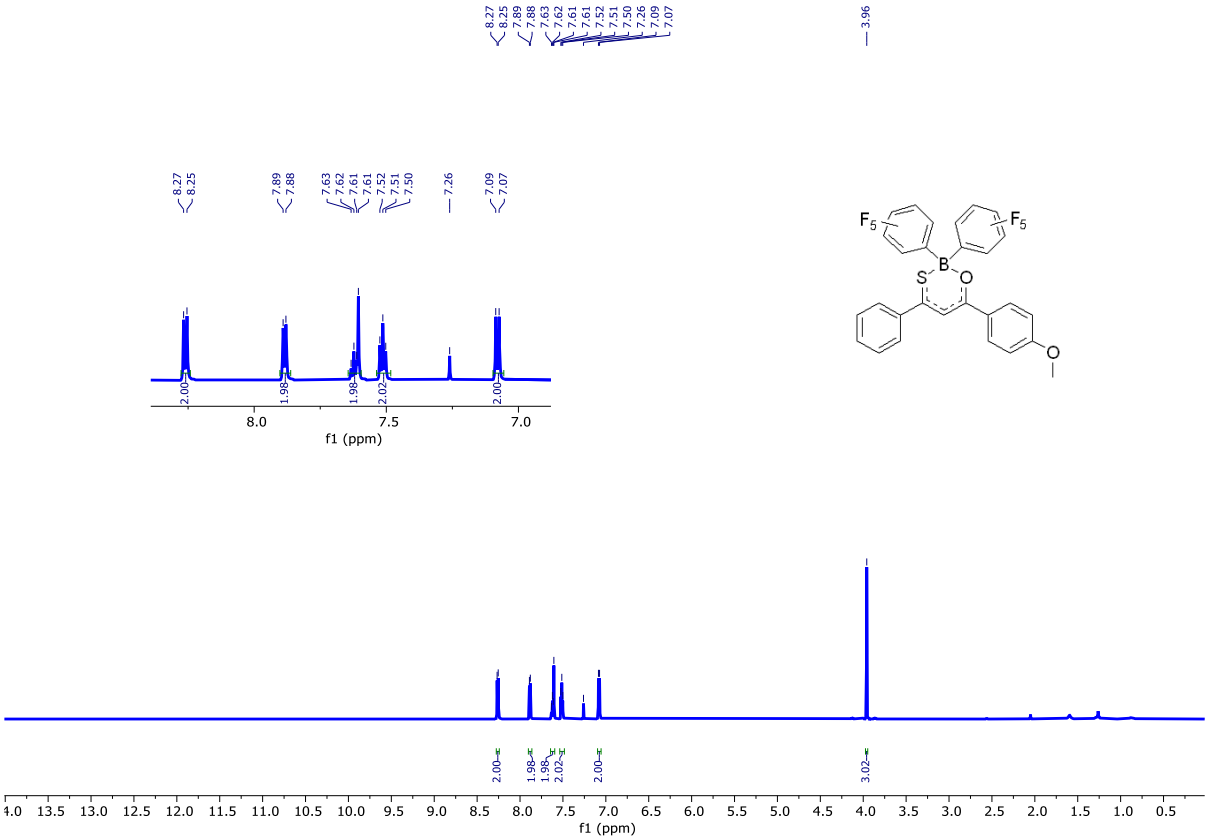


Figure S11. ^{1}H NMR (400 MHz) spectrum of **compound 1 in $CDCl_3$**

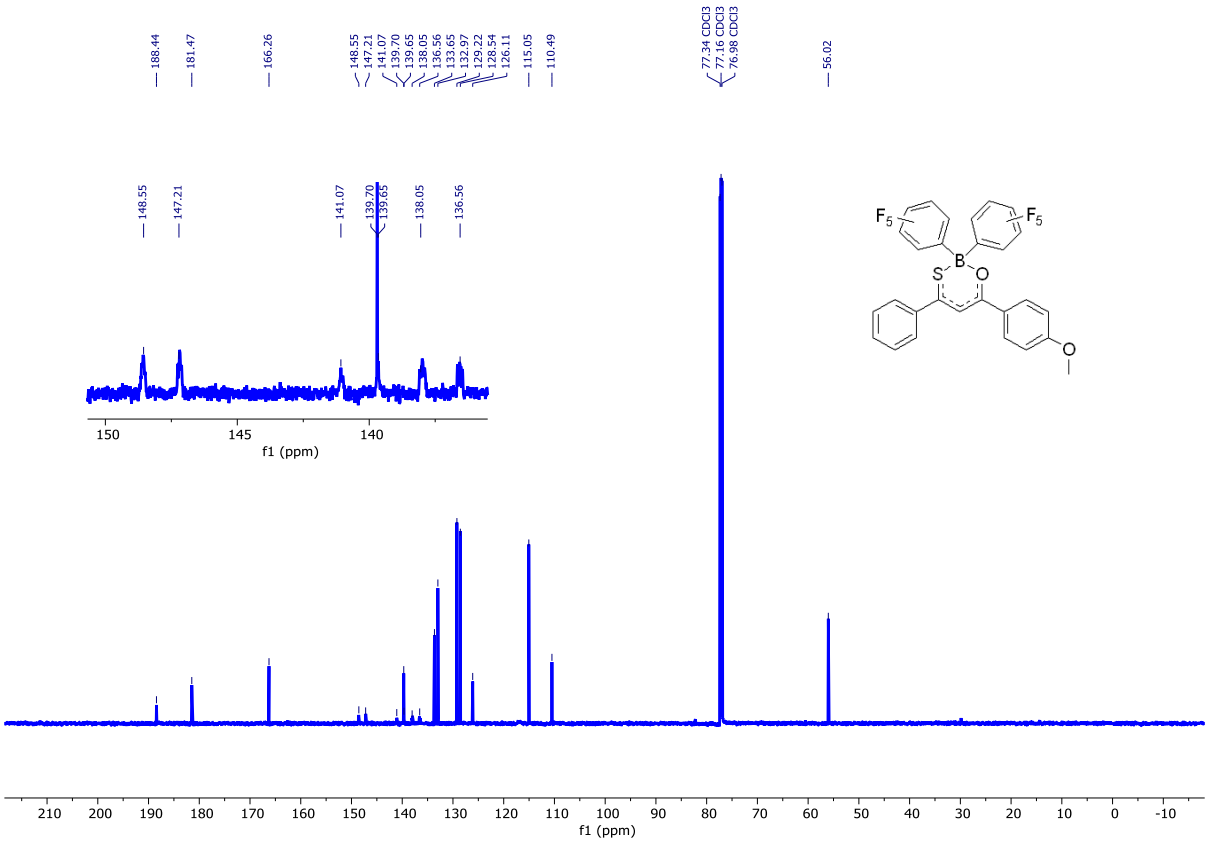


Figure S12. ^{13}C NMR (101 MHz) spectrum of **compound 1 in $CDCl_3$**

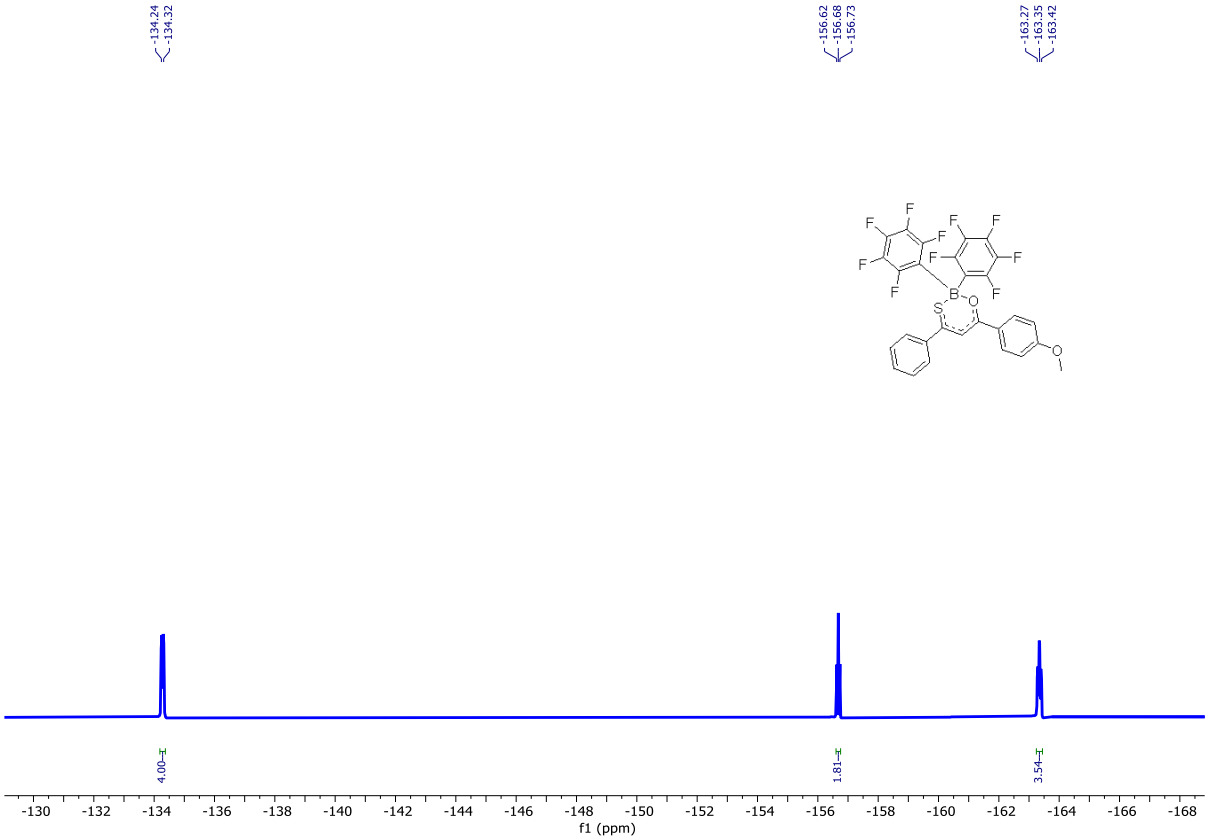


Figure S13. ^{19}F NMR (376 MHz) spectrum of **compound 1 in $CDCl_3$**

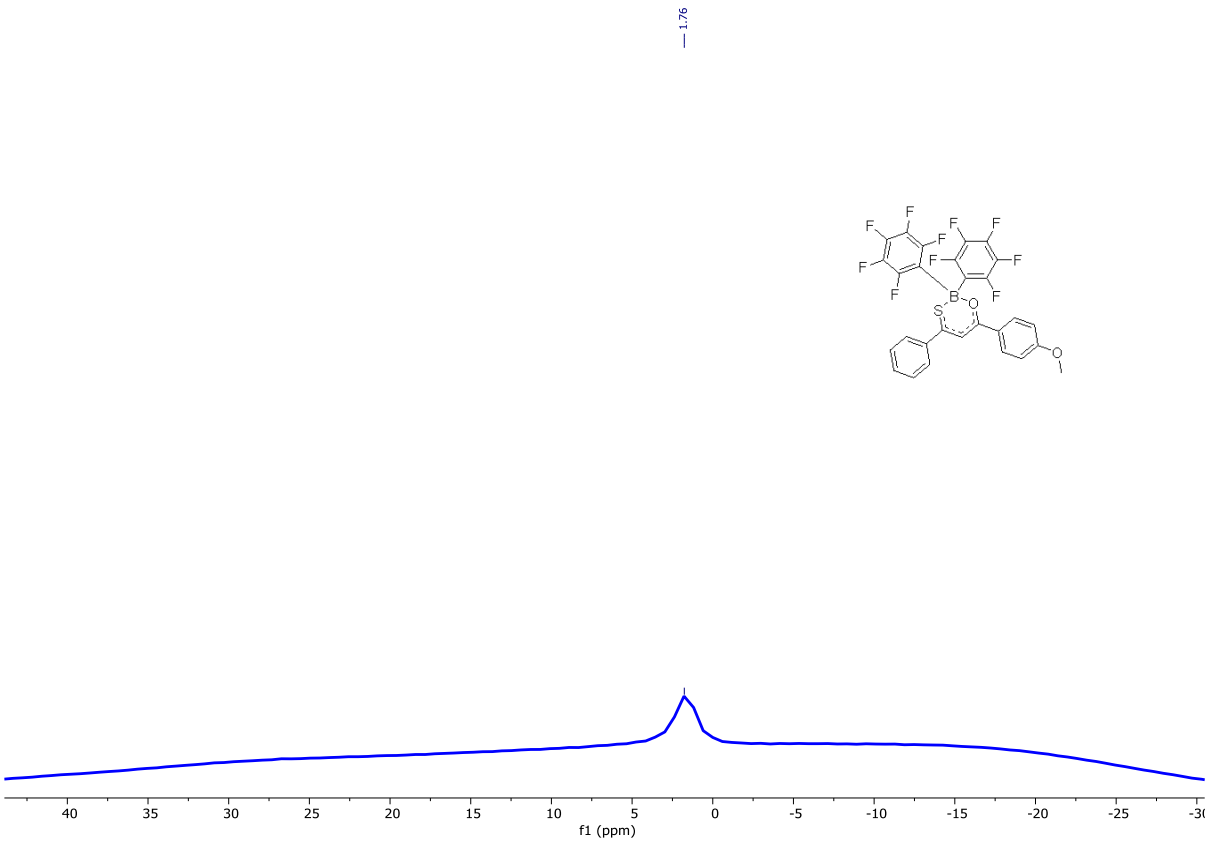


Figure S14. ^{11}B NMR (128 MHz) spectrum of **compound 1 in $CDCl_3$**

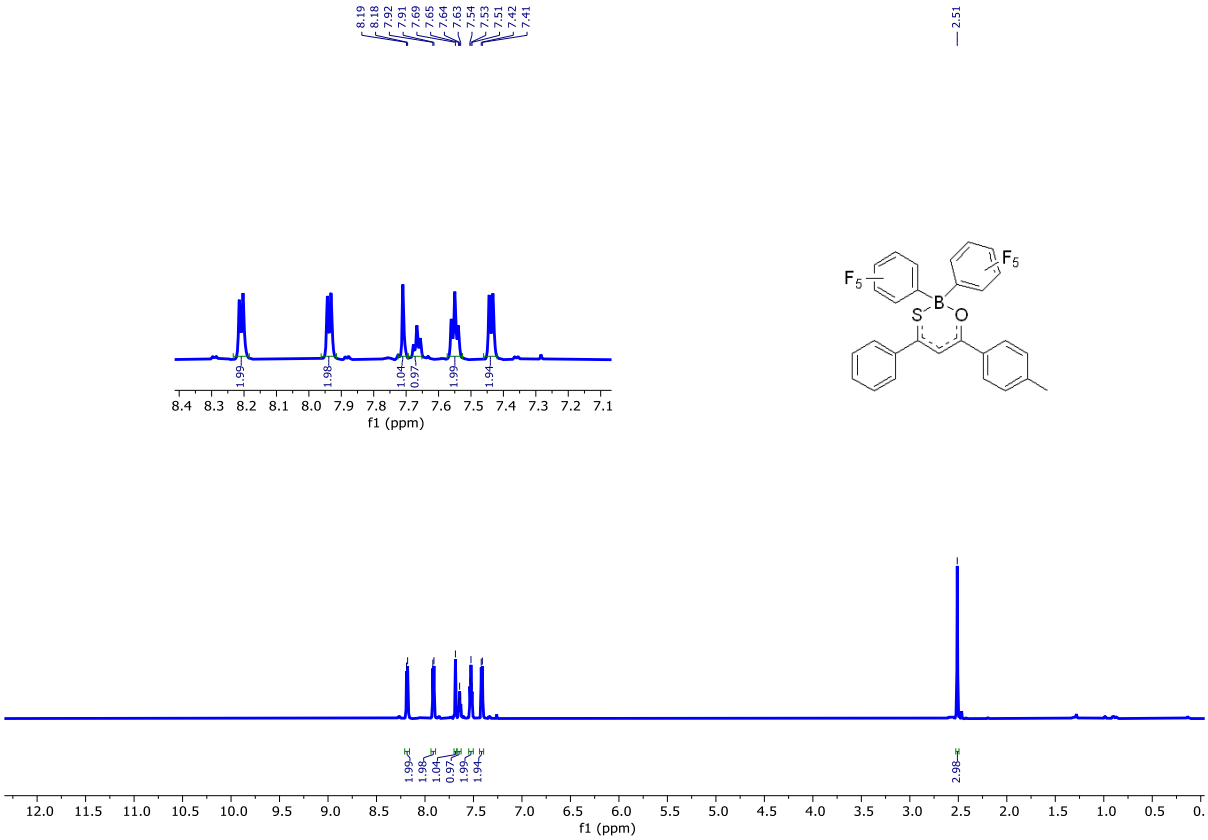


Figure S15. ^{1}H NMR (400 MHz) spectrum of **compound 2 in $CDCl_3$**

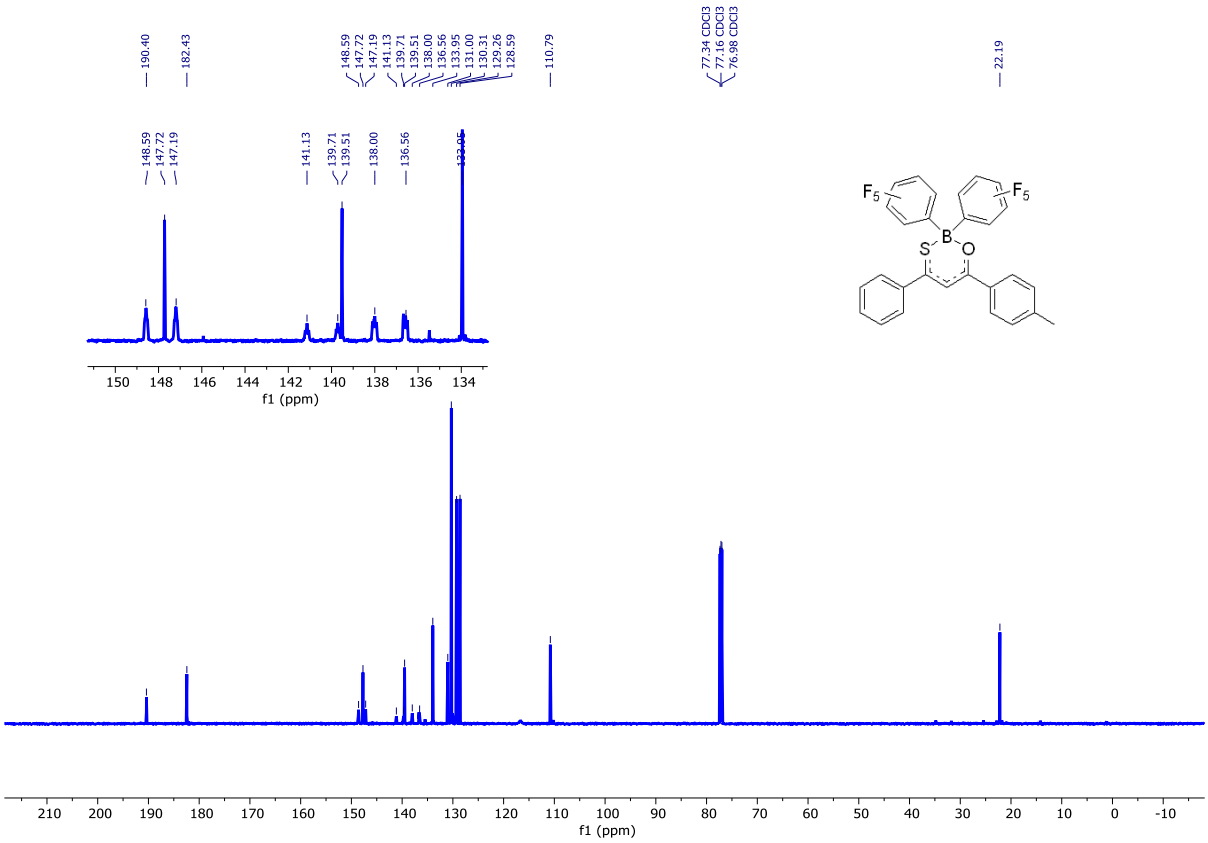


Figure S16. ^{13}C NMR (101 MHz) spectrum of **compound 2 in $CDCl_3$**

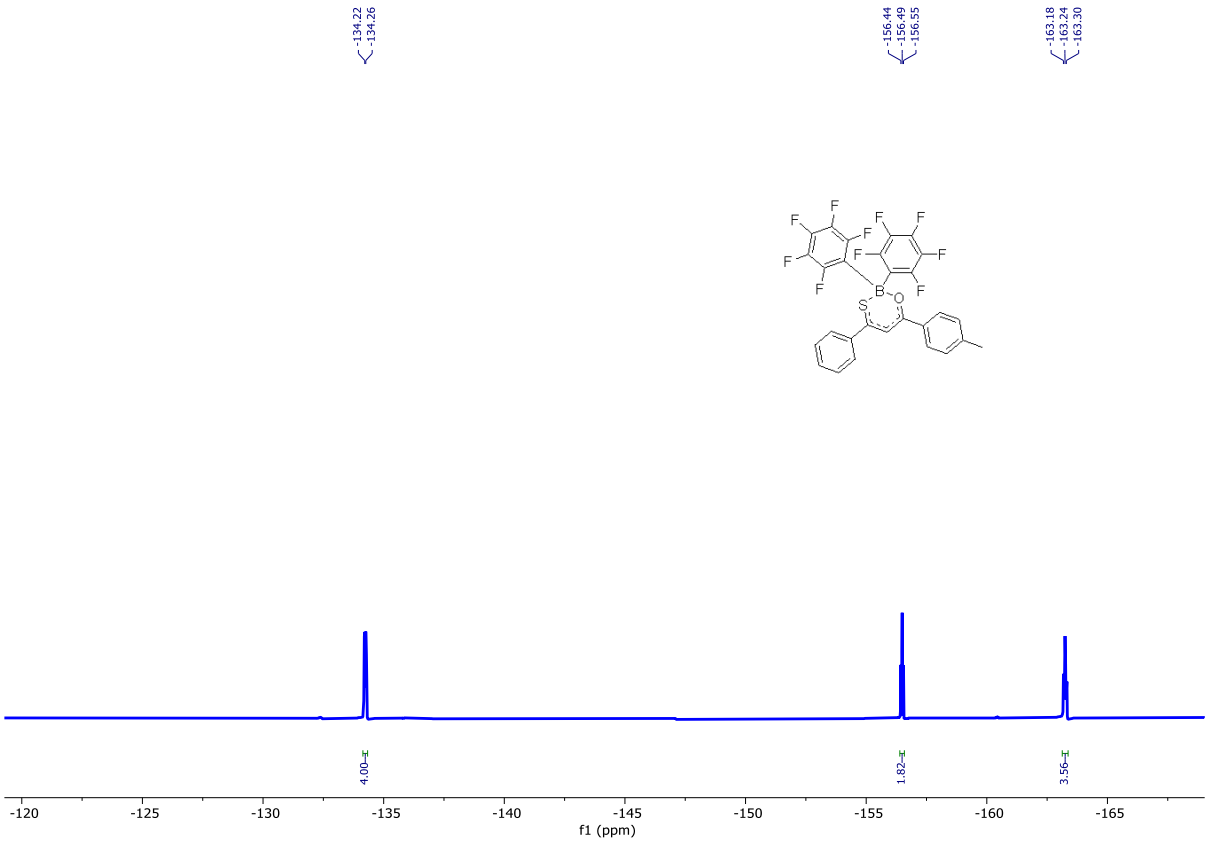


Figure S17. ^{19}F NMR (376 MHz) spectrum of **compound 2 in $CDCl_3$**

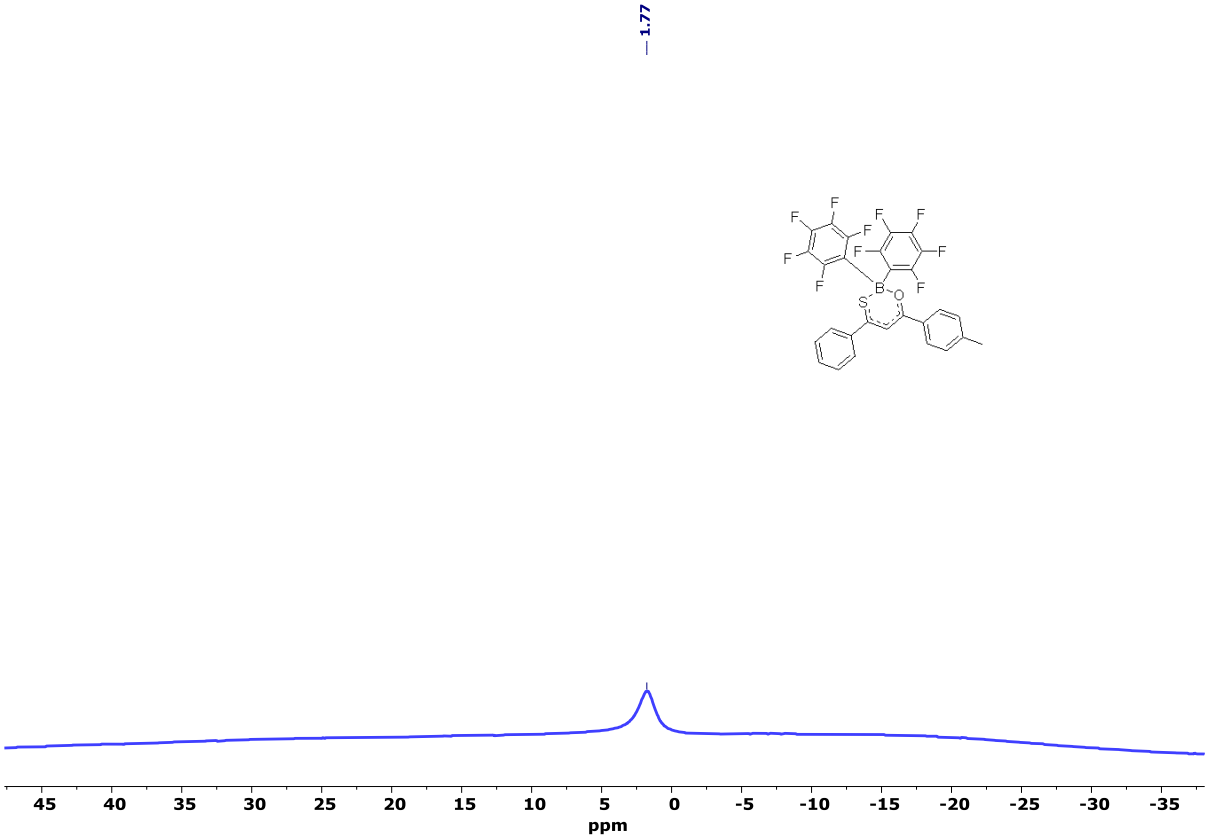


Figure S18. ^{11}B NMR (128 MHz) spectrum of **compound 2 in $CDCl_3$**

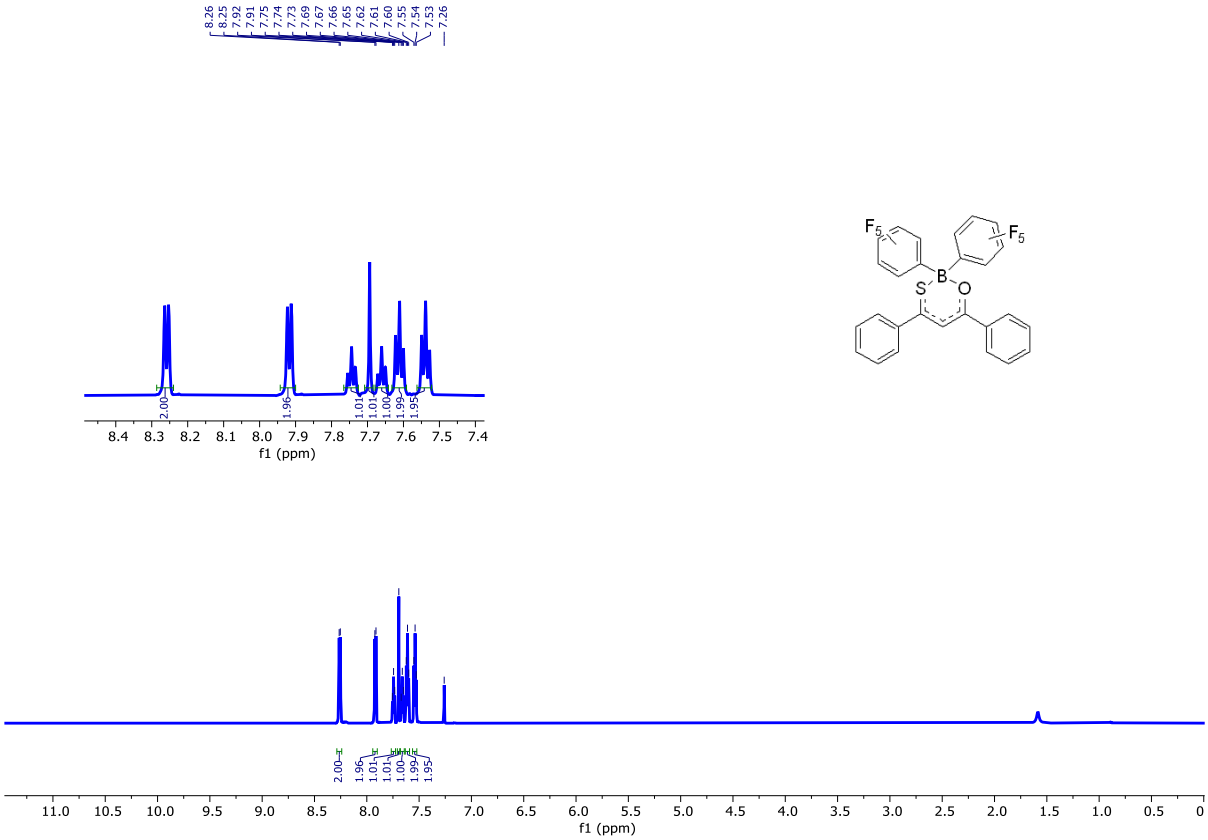


Figure S19. ^{1}H NMR (400 MHz) spectrum of **compound 3 in $CDCl_3$**

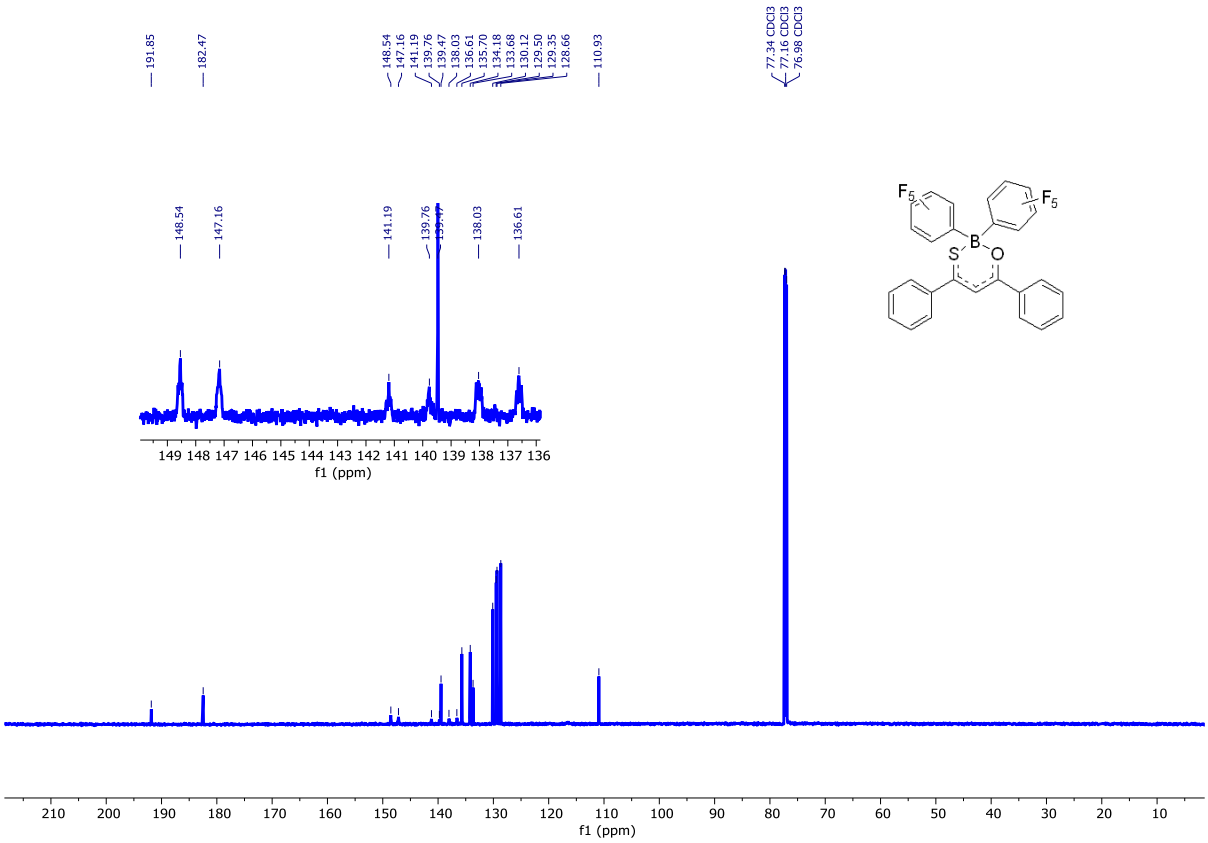


Figure S20. ^{13}C NMR (101 MHz) spectrum of **compound 3 in $CDCl_3$**

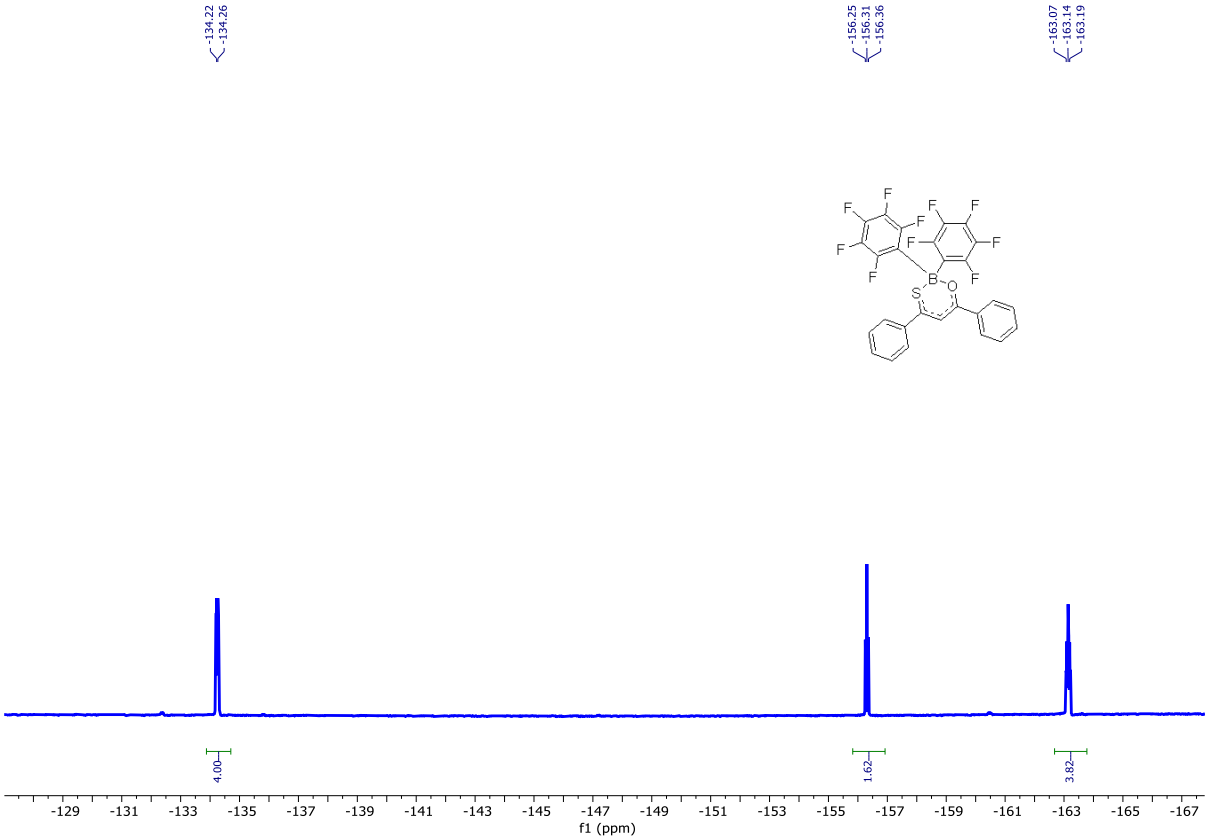


Figure S21. ^{19}F NMR (376 MHz) spectrum of **compound 3 in $CDCl_3$**

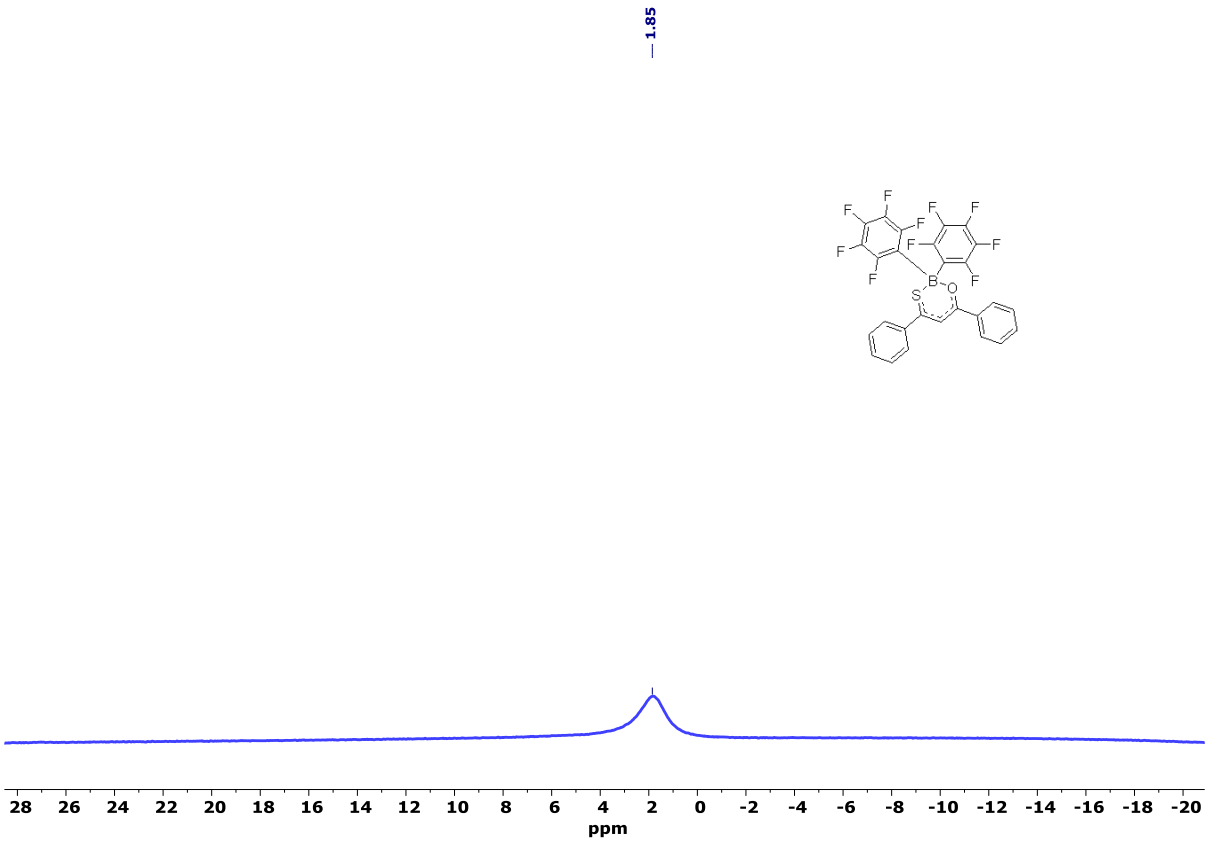


Figure S22. ^{11}B NMR (128 MHz) spectrum of **compound 3 in $CDCl_3$**

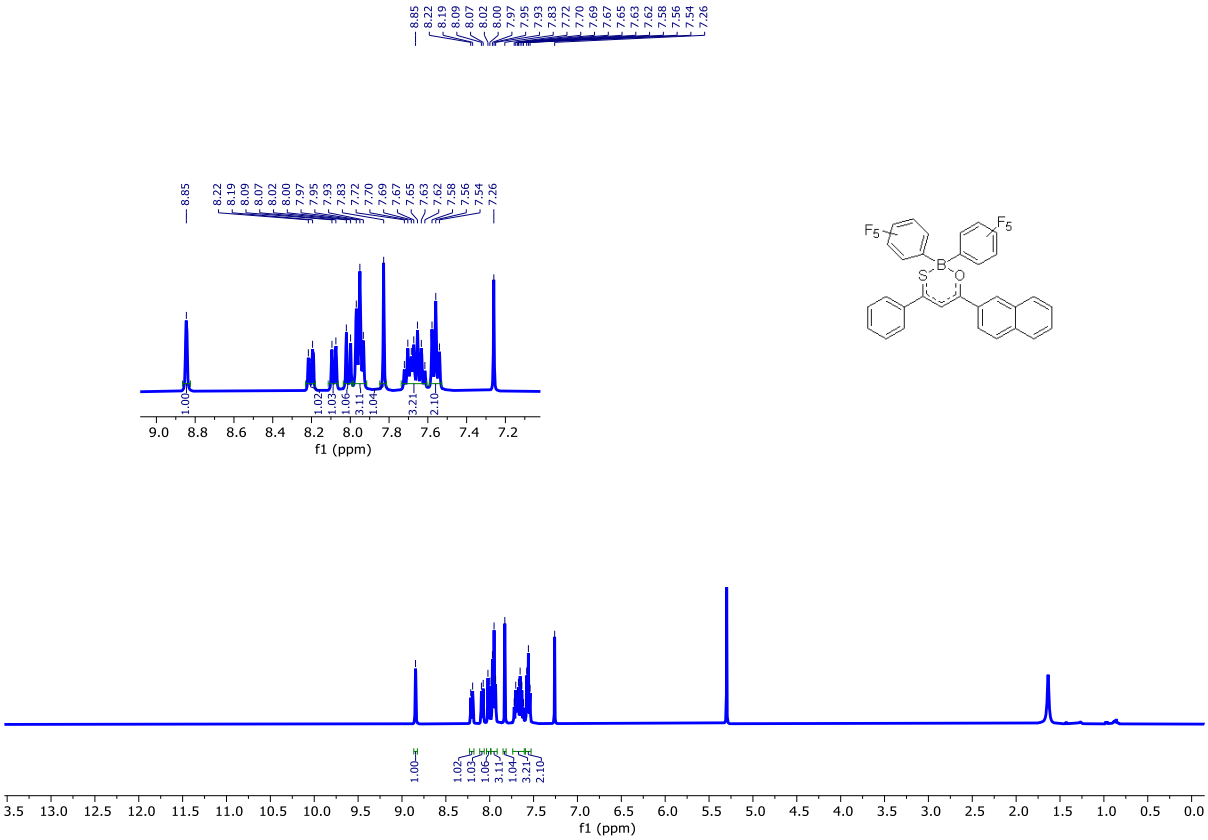


Figure S23. ^{1}H NMR (400 MHz) spectrum of **compound 4 in $CDCl_3$**

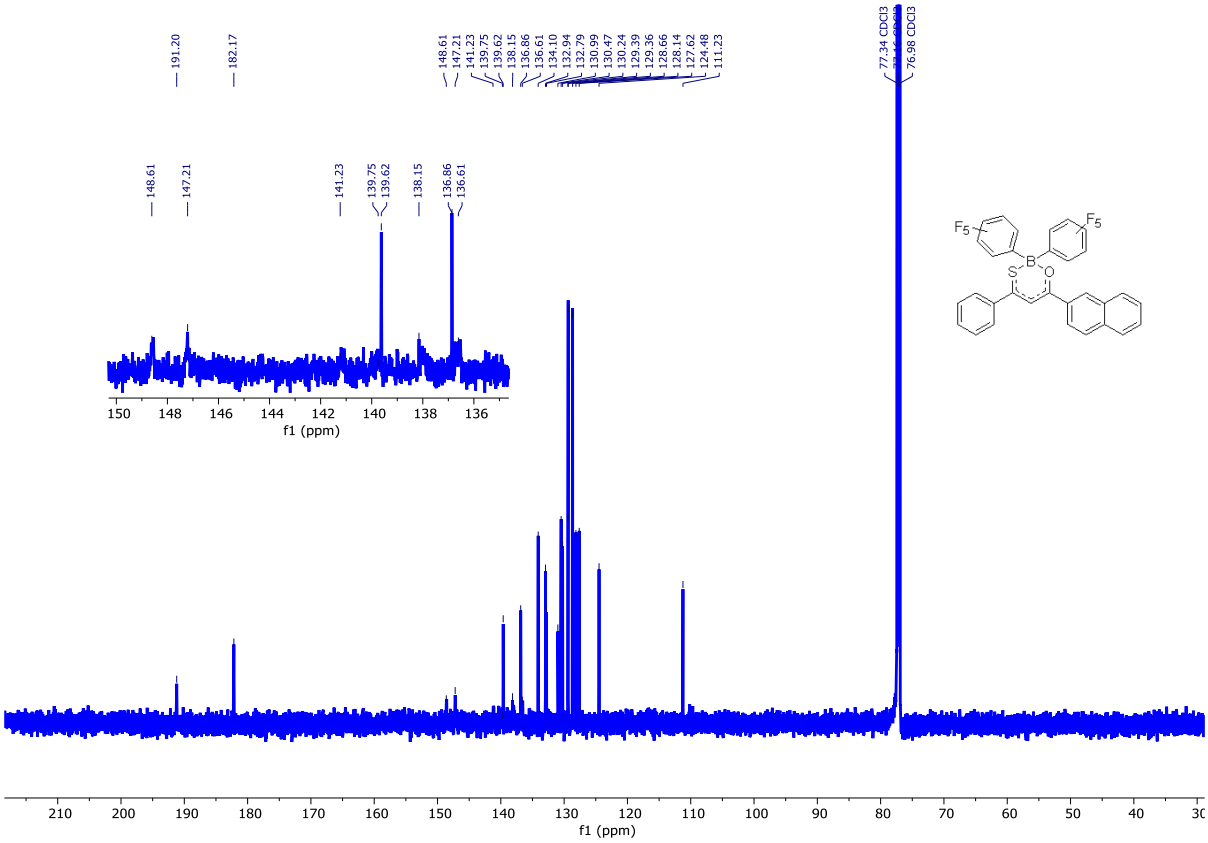


Figure S24. ^{13}C NMR (101 MHz) spectrum of **compound 4 in $CDCl_3$**

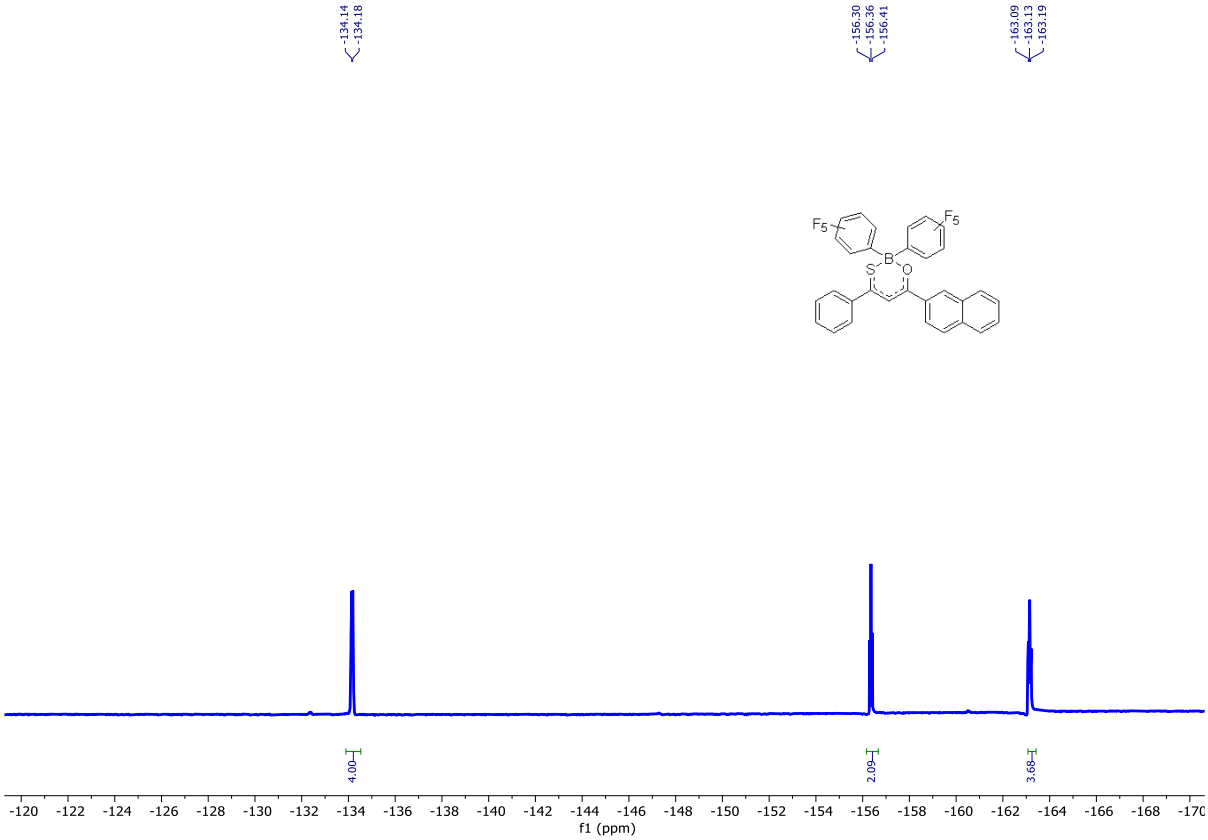


Figure S25. ^{19}F NMR (376 MHz) spectrum of **compound 4 in $CDCl_3$**

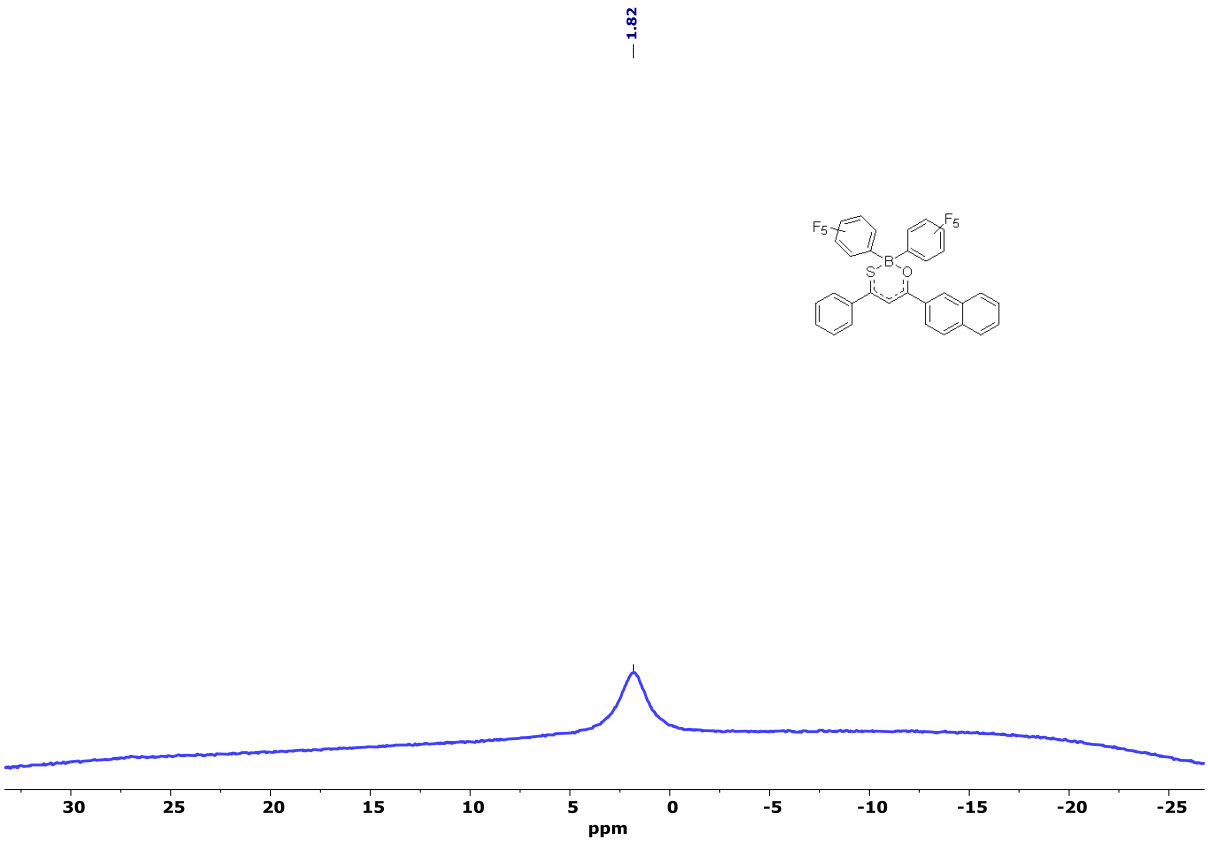


Figure S26. ^{11}B NMR (128 MHz) spectrum of **compound 4 in $CDCl_3$**

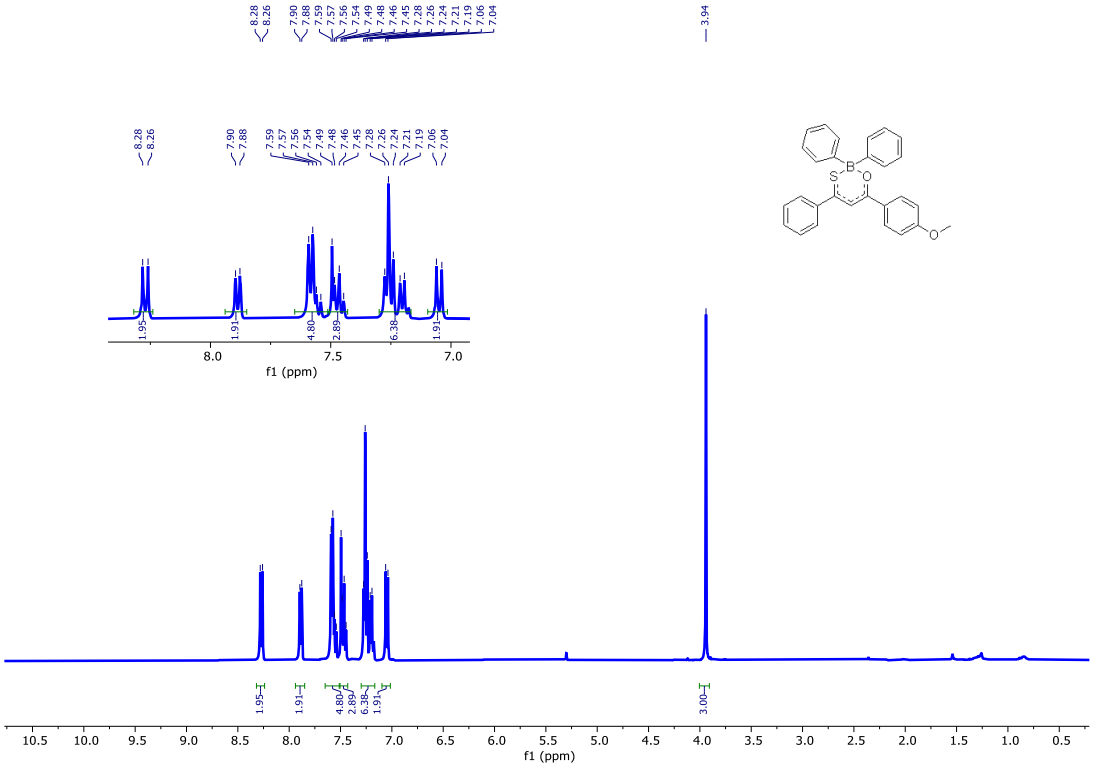


Figure S27. ^{1}H NMR (400 MHz) spectrum of **compound 5 in $CDCl_3$**

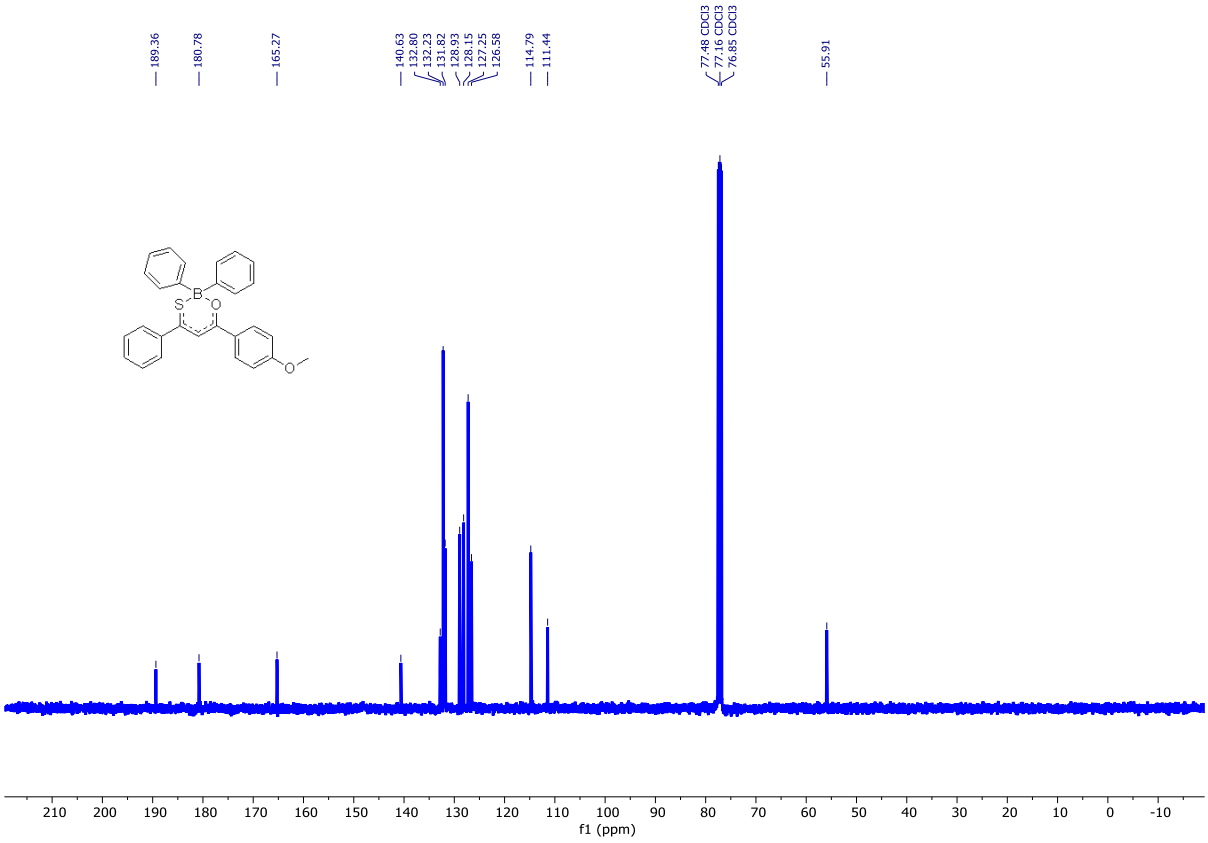


Figure S28. ^{13}C NMR (101 MHz) spectrum of **compound 5 in $CDCl_3$**

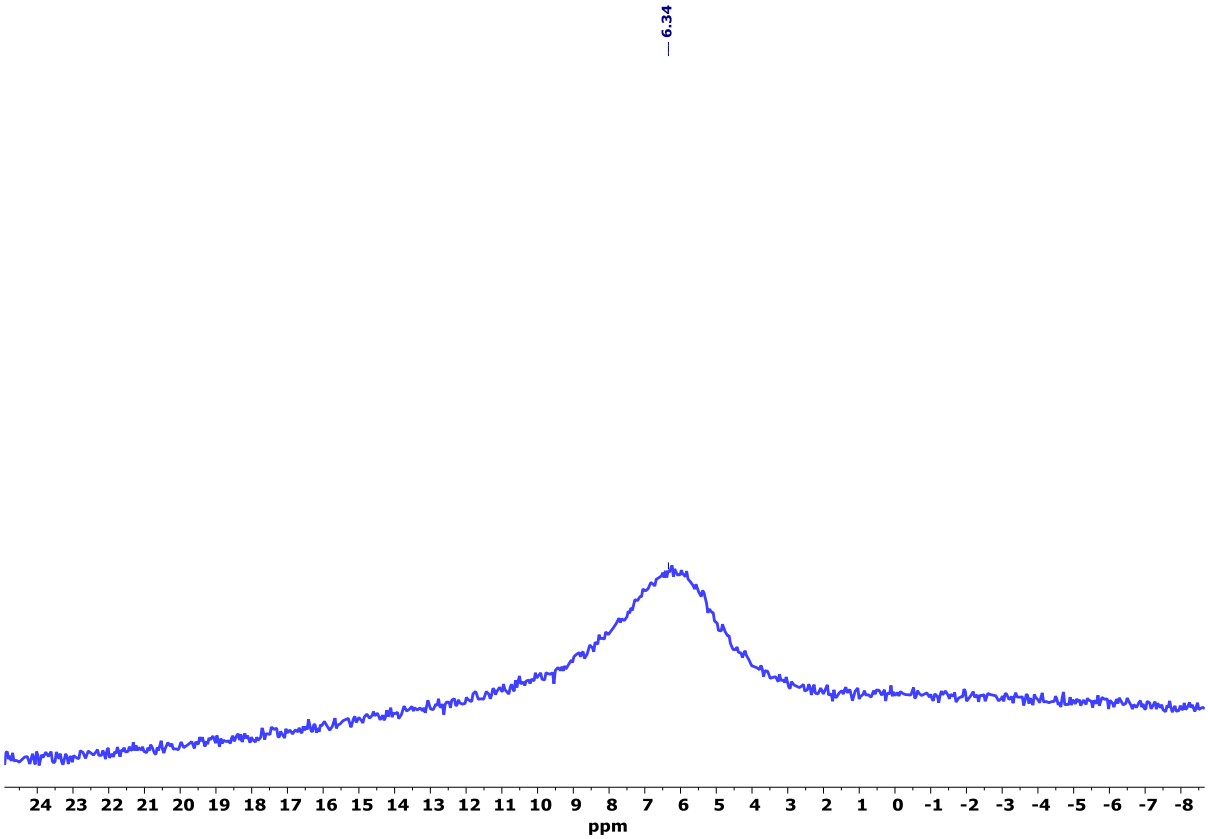


Figure S29. ^{11}B NMR (128 MHz) spectrum of **compound 5 in $CDCl_3$**

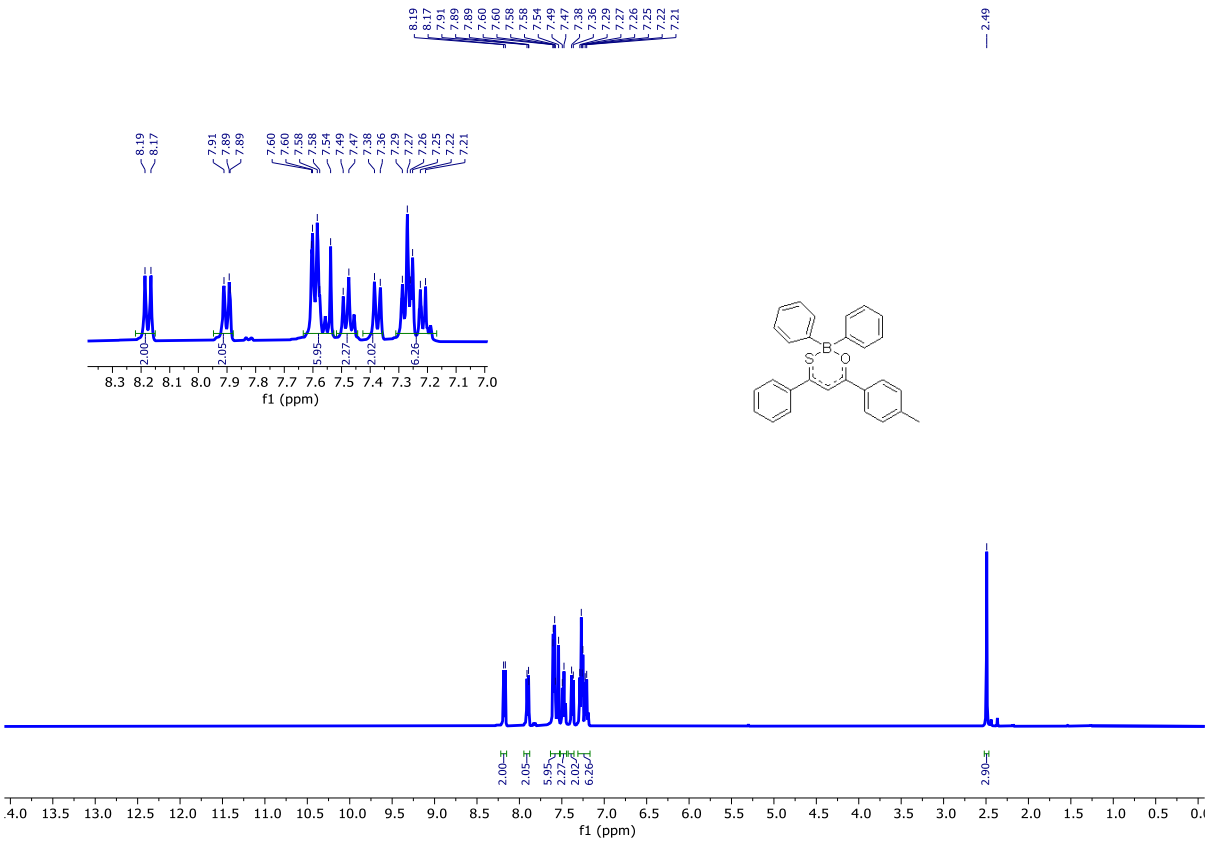


Figure S30. ^{1}H NMR (400 MHz) spectrum of **compound 6 in $CDCl_3$**

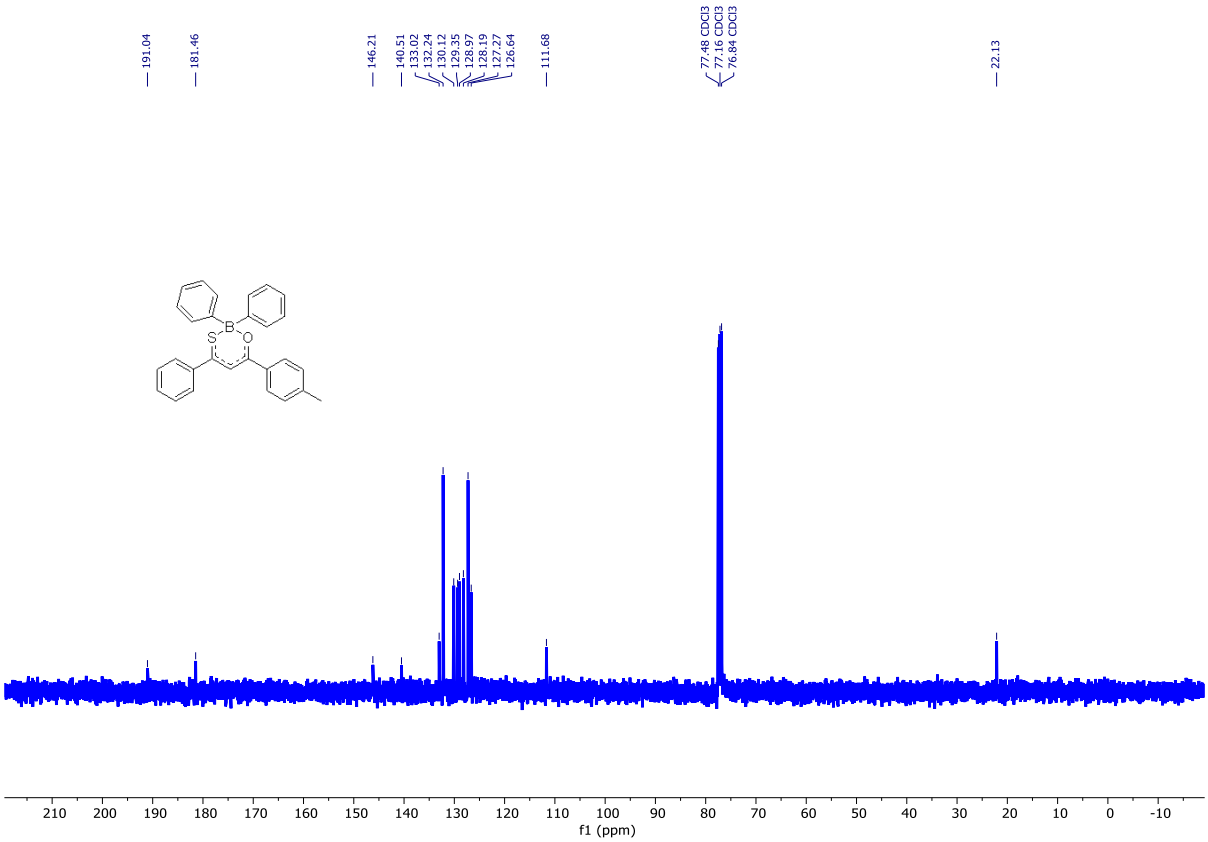


Figure S31. ^{13}C NMR (101 MHz) spectrum of **compound 6 in $CDCl_3$**

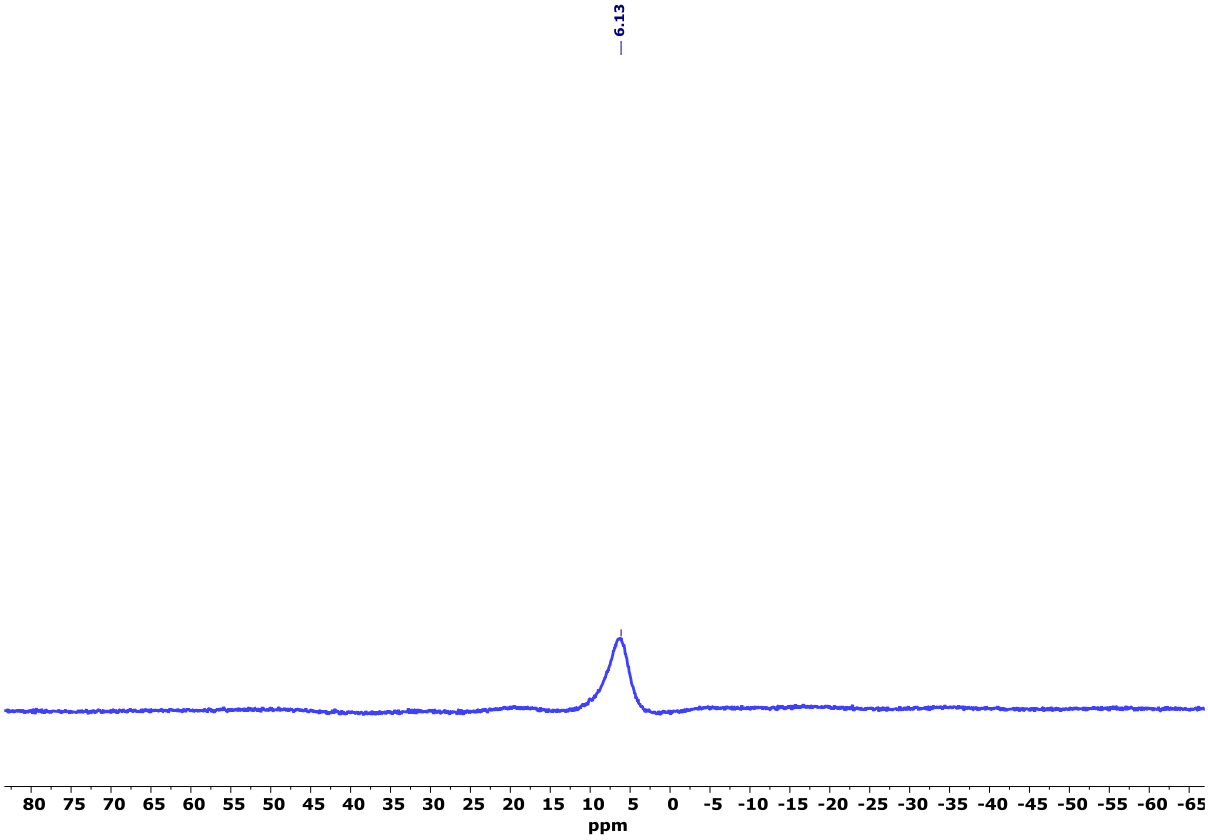


Figure S32. ^{11}B NMR (128 MHz) spectrum of **compound 6 in $CDCl_3$**

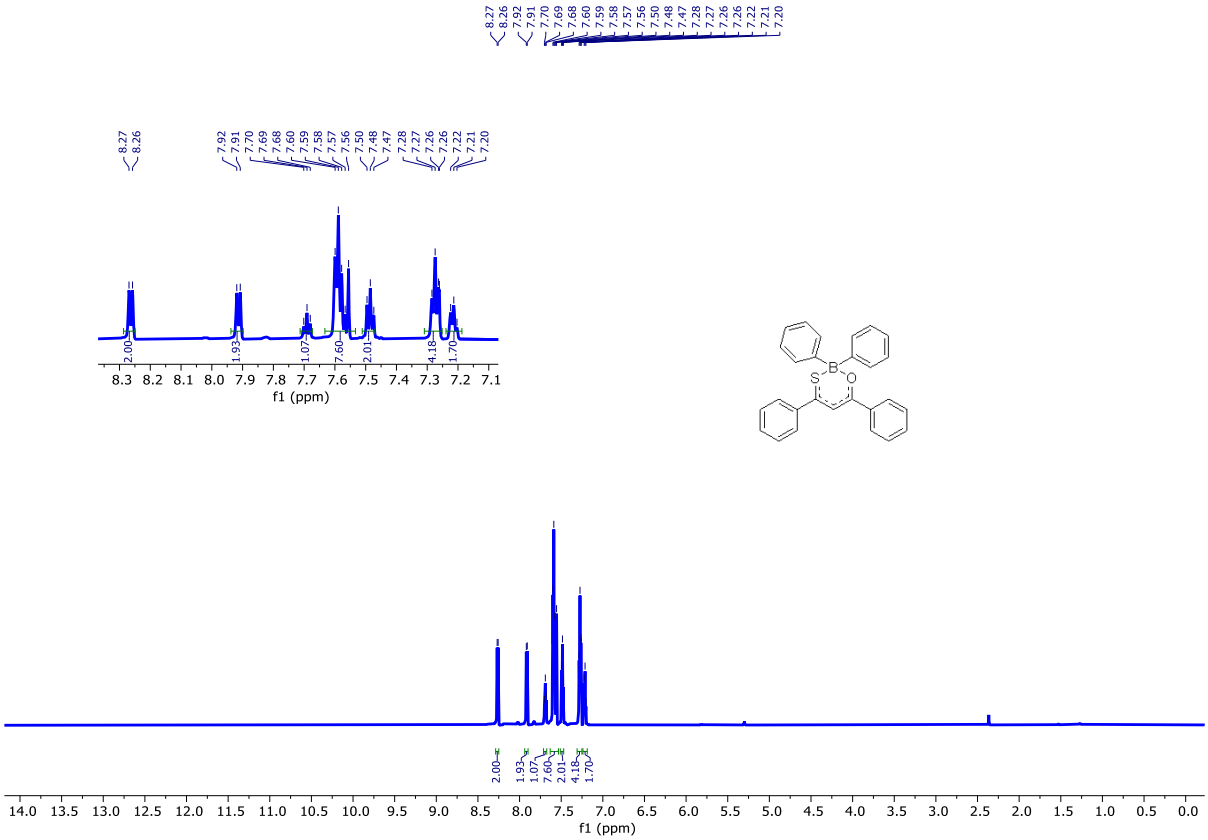


Figure S33. ^{1}H NMR (400 MHz) spectrum of **compound 7 in $CDCl_3$**

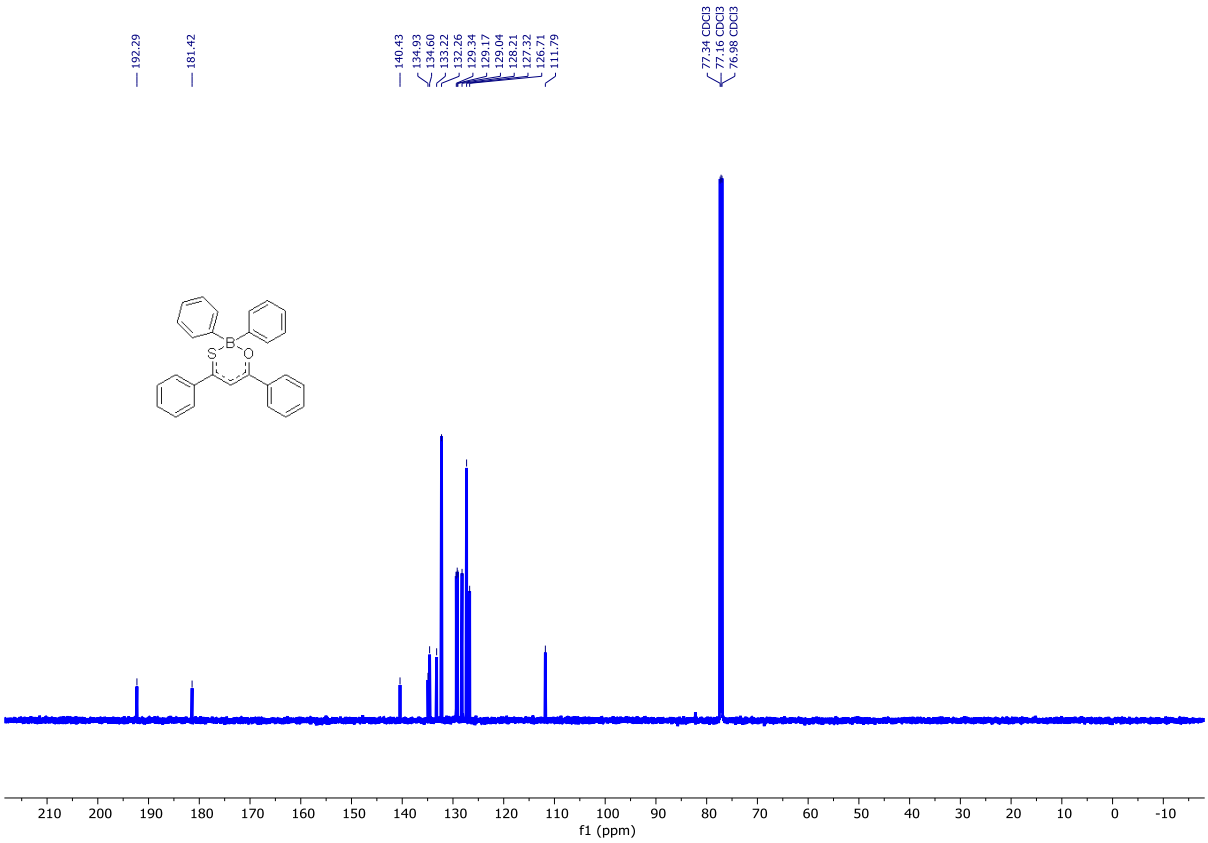


Figure S34. ^{13}C NMR (101 MHz) spectrum of **compound 7 in $CDCl_3$**

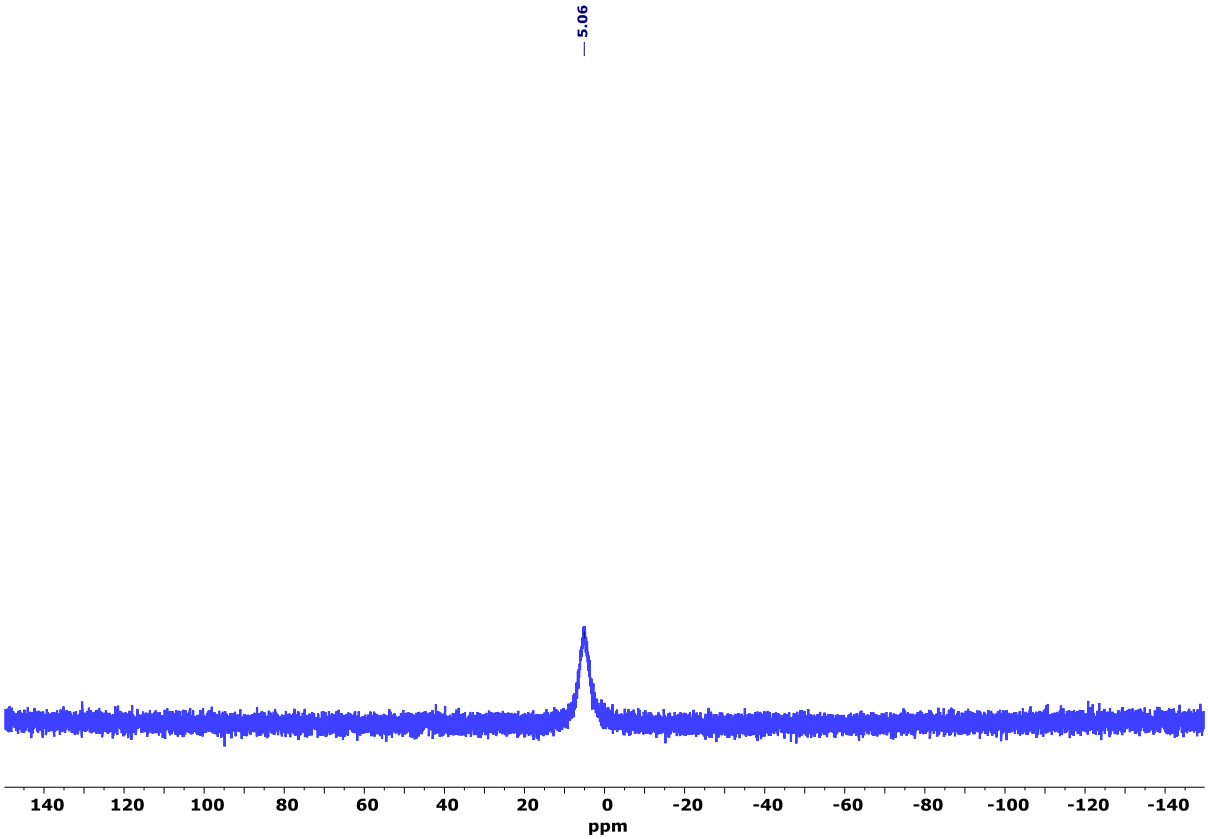


Figure S35. ^{11}B NMR (128 MHz) spectrum of **compound 7 in $CDCl_3$**

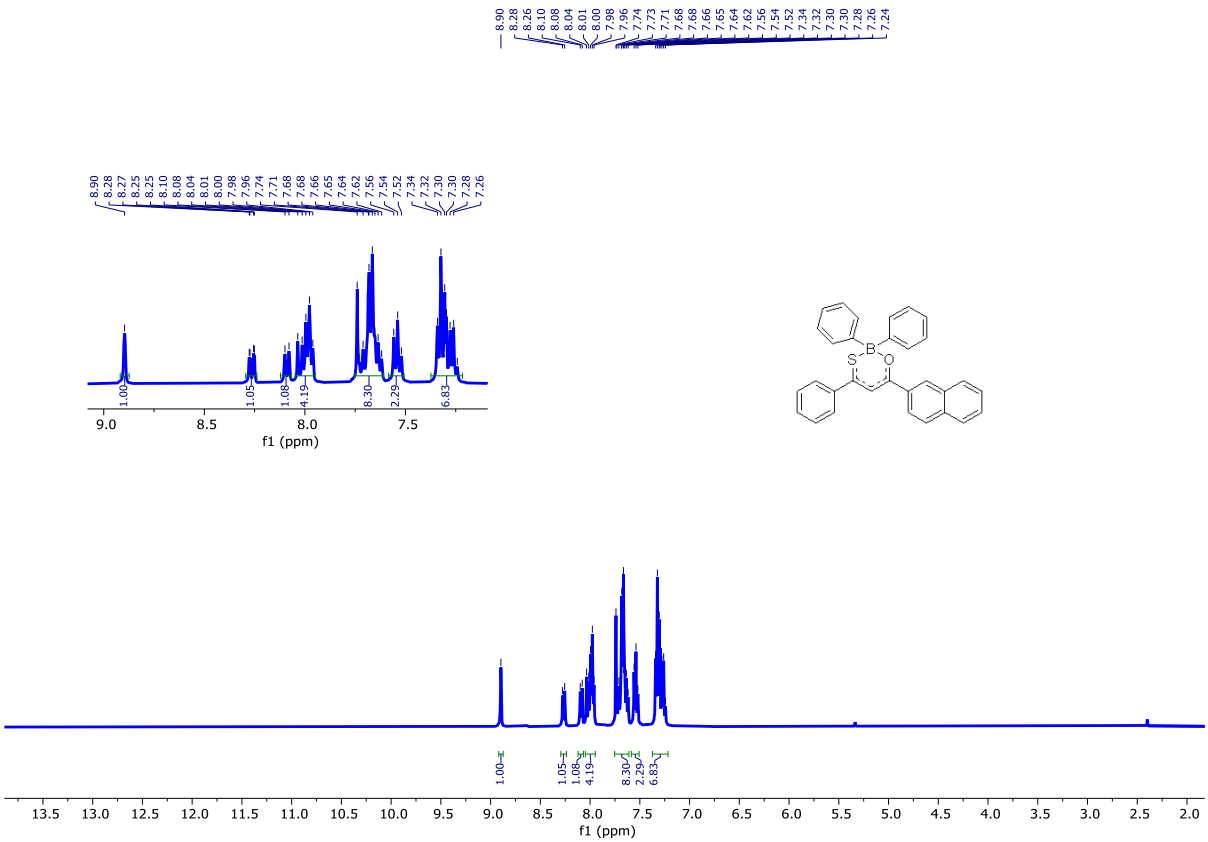


Figure S36. ^{1}H NMR (400 MHz) spectrum of **compound 8 in $CDCl_3$**

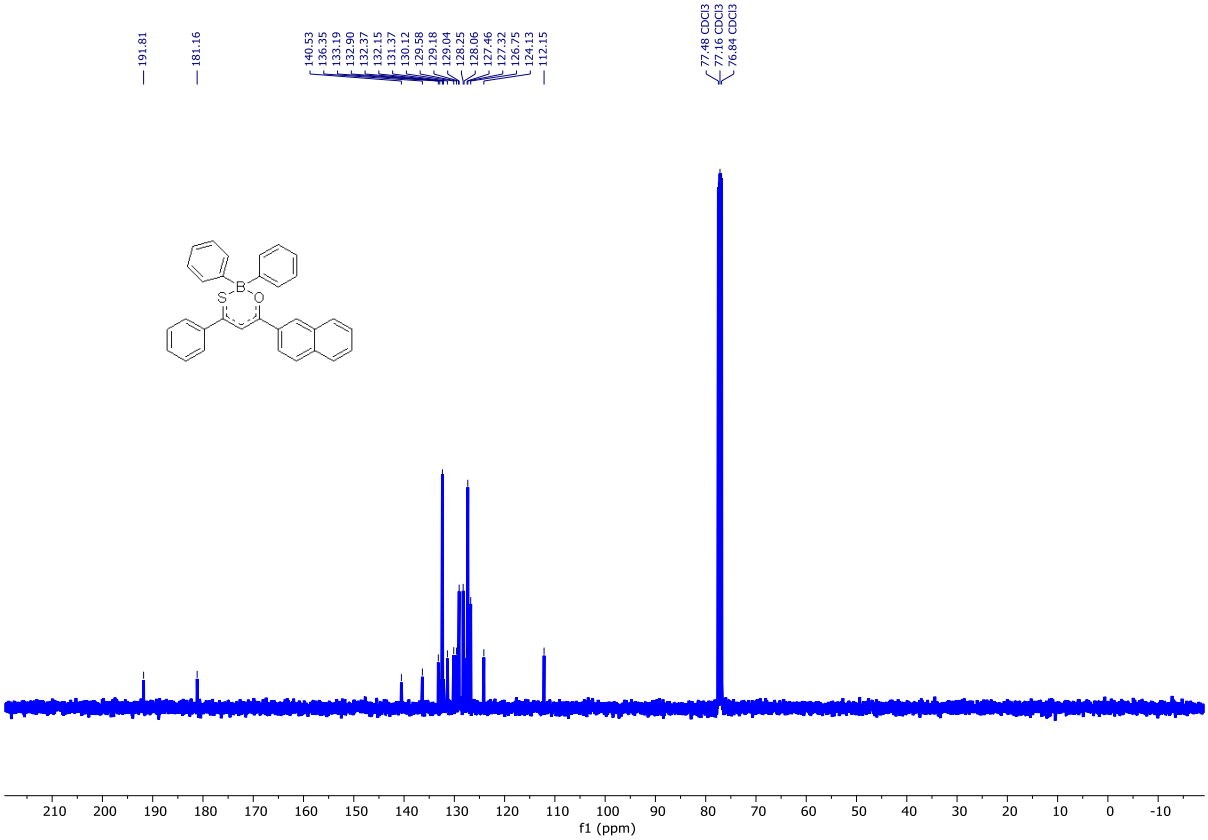


Figure S37. ^{13}C NMR (101 MHz) spectrum of **compound 8 in $CDCl_3$**

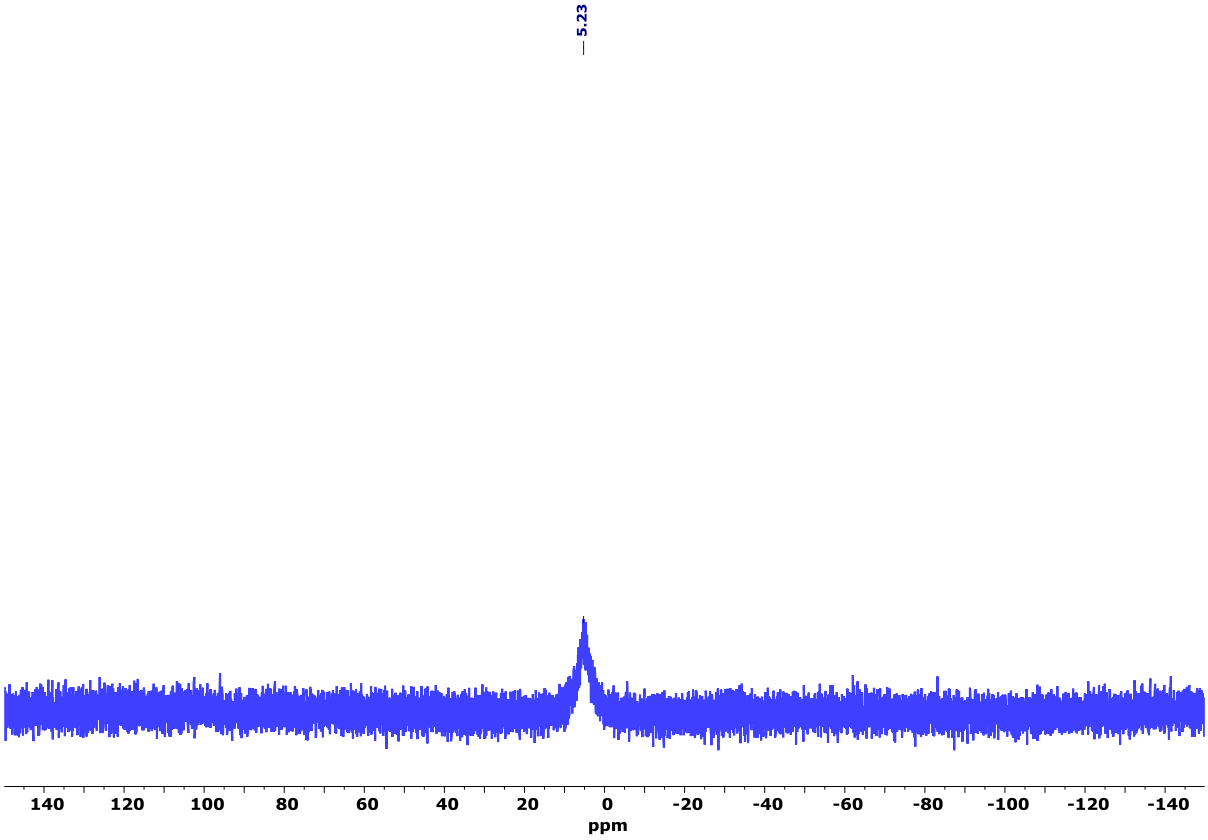


Figure S38. ^{11}B NMR (128 MHz) spectrum of **8 in $CDCl_3$**

Optimized x,y,z coordinates for compounds **1- 8** calculated on Gaussian 03 at the B3LYP//6-31g(d) level

Compound **1**

S 0.60917200S 1.85688800 -1.29591400

F 0.73723100 -2.56331200 -1.84964700
F 3.44067800 1.03966000 -0.30552600
O -0.55972700 -0.57885600 -0.67836400
F 0.62701700 -2.16195600 1.30646600
F 2.90375200 -3.75549200 -2.81688300
F 5.37007900 -2.60637600 -2.56547100
F 1.23429400 2.56411900 1.51922500
F 5.61460800 -0.19160500 -1.29344300
F 0.88345700 -2.29246300 3.96571800
F 1.32461600 -0.01757200 5.42632400
F 1.49656600 2.39281300 4.14774700
C 0.89114600 0.20557600 1.26126600
C -1.43051300 3.67302200 -1.14595600
C -1.74683200 -0.06006100 -0.50892500
C -1.95944100 1.33515500 -0.48759500
H -2.94430200 1.69328100 -0.22143100
C -1.02782100 2.26968600 -0.92172700
C -2.82993700 -1.03046900 -0.39708200
C -2.71580800 3.98027500 -1.63477000
H -3.40364100 3.17939000 -1.88412700
C 1.90966300 -1.91912700 -1.68369700
C 1.97899900 -0.68445400 -1.03321200
C 3.03061000 -2.56956100 -2.19952800
C 0.82401400 -0.99948900 1.97131700
C 4.28739200 -1.99108500 -2.07207000
C 3.26622000 -0.15128300 -0.92499500
C -3.09382100 5.30365000 -1.84375700
H -4.08183300 5.52470000 -2.23495100
C 1.13017400 1.32954800 2.05491300
C -0.53916500 4.72790800 -0.87138300
H 0.44154200 4.50364900 -0.46695500
C 4.40831600 -0.76494500 -1.42697100
C -4.18747700 -0.66330000 -0.48467000
H -4.46900000 0.36787400 -0.66294600
C -5.19975900 -1.60641900 -0.37460800
H -6.23163200 -1.28915800 -0.45265400
C -2.20214400 6.34224400 -1.56091500
H -2.50064200 7.37361700 -1.72133000
C -2.51774600 -2.39784300 -0.20414600
H -1.47848700 -2.69333400 -0.13255800

C 0.96097600 -1.10138800 3.35132200
C -4.87032300 -2.95885300 -0.17562900
C -0.92648900 6.05055800 -1.07225000
H -0.23418500 6.85392800 -0.84120500
C 1.18874800 0.05084700 4.09580800
B 0.72809800 0.11950700 -0.37210300
C 1.27514800 1.27241400 3.44127500
C -3.51701300 -3.34349600 -0.09308900
H -3.28415700 -4.39114700 0.06379200
O -5.77046400 -3.95556500 -0.05459500
C -7.16704800 -3.64349300 -0.12312200
H -7.68673900 -4.59239900 0.00386500
H -7.45696400 -2.95645200 0.67810500
H -7.42678300 -3.21036400 -1.09422100

Compound **2**

S 0.41801700 -1.79775700 -1.24887700

F -1.68573500 2.08321700 -1.88890300
F -2.47415500 -2.32036400 -0.26038900
O 0.36758000 0.91965500 -0.69884400
F -1.42094600 1.84282500 1.26147800
F -4.15538700 2.14969200 -2.86450600
F -5.83703800 0.01573000 -2.57537900
F 0.19178400 -2.63383700 1.58592200
F -4.96807100 -2.22350000 -1.25671100
F -1.70954500 1.90832000 3.92010900
F -1.06522200 -0.28040000 5.43577200
F -0.12000800 -2.53558500 4.21320900
C -0.57787900 -0.38549300 1.27246400
C 3.05574400 -2.49576700 -1.10666700
C 1.66081600 0.98968400 -0.53933700
C 2.47895100 -0.15496700 -0.49388500
H 3.52108000 -0.02133500 -0.23878000
C 2.06526300 -1.42172700 -0.89654000
C 2.19745500 2.35184600 -0.45910400
C 4.34098000 -2.19874800 -1.60252500
H 4.59434800 -1.17806800 -1.86777500
C -2.44160200 0.98297800 -1.70439100
C -1.94763900 -0.13718900 -1.03088900
C -3.73428300 1.04675700 -2.22448500
C -1.06755700 0.73506900 1.95459300
C -4.59451400 -0.03442500 -2.07779600
C -2.85547400 -1.19186500 -0.90352500
C 5.27319300 -3.21341800 -1.79920600
H 6.25406600 -2.97215100 -2.19622400
C -0.27827800 -1.47479200 2.09342800

C 2.73483600 -3.83500400 -0.81166500
H 1.75955700 -4.07037000 -0.40049500
C -4.15038900 -1.17012900 -1.40907100
C 3.56996800 2.63035100 -0.61413400
H 4.27437300 1.83503800 -0.82917800
C 4.03689800 3.93544600 -0.52931400
H 5.09694200 4.13100500 -0.66137100
C 4.94457100 -4.53792400 -1.49642800
H 5.67492600 -5.32686000 -1.64694800
C 1.31368900 3.42609800 -0.22961100
H 0.25701100 3.22143700 -0.10919600
C -1.23591600 0.79786000 3.33338000
C 3.16185300 5.00722500 -0.28819400
C 3.67532300 -4.84454200 -1.00017900
H 3.41936300 -5.86999100 -0.75338000
C -0.91322400 -0.31264500 4.10580000
B -0.47074300 -0.27556500 -0.36322700
C -0.43334300 -1.45541800 3.47971100
C 1.79329100 4.72629900 -0.14531700
H 1.09797700 5.54067700 0.03719100
C 3.68066500 6.41607900 -0.16389000
H 4.58665900 6.56235500 -0.75802700
H 3.93489600 6.64117600 0.87937200
H 2.93212100 7.14706400 -0.48102400

Compound **3**

S 0.90865400 -1.49689800 -1.16904000
F -2.07324300 1.71232100 -1.98884000
F -1.77030900 -2.66463600 -0.14272800
O 0.19087700 1.15052000 -0.74612300
F -1.81182400 1.67809700 1.16848900
F -4.47396100 1.12107200 -2.96221300
F -5.58252400 -1.34384200 -2.56145200
F 0.90550100 -2.20399200 1.70824500
F -4.20281700 -3.23303900 -1.13476200
F -2.13248800 1.79585400 3.82205000
F -0.95595200 -0.07362200 5.44159900
F 0.55443300 -2.06202900 4.32896200
C -0.42116700 -0.25271500 1.28702700
C 3.63572100 -1.51654700 -1.03558900
C 1.42751600 1.53940000 -0.60412900
C 2.50132600 0.63662800 -0.51768300
H 3.47844800 1.03491800 -0.28188600
C 2.41174500 -0.71211600 -0.85765000
C 1.61412500 2.99816600 -0.58721400
C 4.80615300 -0.93411700 -1.56204500

H 4.79903800 0.10446900 -1.87441500
C -2.53783200 0.47063000 -1.74886600
C -1.79070000 -0.45922700 -1.02126900
C -3.80108100 0.18859200 -2.26863400
C -1.19056200 0.73455200 1.91469500
C -4.37068800 -1.06236200 -2.06540200
C -2.41211500 -1.69748600 -0.83942300
C 5.95890200 -1.69571400 -1.72957500
H 6.84842400 -1.23831300 -2.15076800
C 0.14484000 -1.18445800 2.15978200
C 3.65608100 -2.87920800 -0.67962800
H 2.77062500 -3.32904000 -0.24458300
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C 2.87211100 3.59135800 -0.81063700
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C 5.96824300 -3.04550800 -1.36622100
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C 0.49803200 3.82459000 -0.34682500
H -0.46726100 3.36654100 -0.17012600
C -1.38179400 0.81918000 3.28924500
C 1.89737300 5.78624100 -0.53471900
C 4.81584000 -3.63314800 -0.83894100
H 4.82193300 -4.67791300 -0.54516100
C -0.78882100 -0.13034500 4.11438700
B -0.33185900 -0.19780000 -0.35183400
C -0.02249300 -1.13814000 3.54397900
C 0.64339200 5.20767200 -0.31816900
H -0.21965200 5.83619000 -0.12335800
H 2.00837300 6.86595300 -0.51287600

Compound **4**

S 0.94953500 1.82276100 -1.28382100
F 0.70666000 -2.59179900 -1.83266600
F 3.73737200 0.79002600 -0.40443800
O -0.38927600 -0.51563500 -0.61807100
F 0.79582800 -2.20024700 1.31102700
F 2.73526200 -3.94617700 -2.88495400
F 5.29036700 -2.99034100 -2.73302300
F 1.65897400 2.48608100 1.51718900
F 5.77012100 -0.60355300 -1.47517000
F 1.13669300 -2.35717700 3.95969800
F 1.74786500 -0.11594200 5.41084700
F 2.00302100 2.28818200 4.13452800
C 1.18839300 0.14923200 1.26384500
C -0.93556300 3.79157500 -1.09772000

C -1.52273800 0.10090100 -0.42878200
C -1.62831300 1.50396900 -0.40793800
H -2.57625700 1.93504800 -0.11689200
C -0.63649500 2.36419000 -0.87189100
C -2.21064800 4.19520600 -1.54201800
H -2.96861000 3.44953200 -1.75583900
C 1.93076200 -2.04104300 -1.71578100
C 2.12089200 -0.81658800 -1.07008300
C 2.97712000 -2.77458400 -2.27480900
C 1.08015100 -1.05372100 1.97237300
C 4.27872600 -2.29450400 -2.19797000
C 3.44832900 -0.38360100 -1.01395300
C -2.49014800 5.54200000 -1.75427500
H -3.47162800 5.83719400 -2.11132800
C 1.51117400 1.25575500 2.05238500
C 0.04666000 4.77501900 -0.87002100
H 1.02107500 4.47806200 -0.49862300
C 4.51913100 -1.08233800 -1.55992100
C -1.50859900 6.50893100 -1.51844700
H -1.73055400 7.55909300 -1.68091500
C 1.25739700 -1.16932700 3.34655600
C -0.24220300 6.12191700 -1.07369700
H 0.51950100 6.87008300 -0.87882400
C 1.57121200 -0.03414900 4.08612500
B 0.96292300 0.07955000 -0.36171800
C 1.69971300 1.18439400 3.43280300
C -2.68314400 -0.78699600 -0.28220800
C -3.98466700 -0.32201400 -0.43434300
C -2.46277100 -2.16909300 0.00833700
C -5.09361100 -1.18778400 -0.29102400
H -4.17861100 0.71316000 -0.69350600
C -3.52301200 -3.02620700 0.15431600
H -1.44520600 -2.51965200 0.12536600
C -6.43024500 -0.72349300 -0.44466800
C -4.86428300 -2.57089300 0.01251900
H -3.34872100 -4.07298200 0.38617600
C -7.49122000 -1.58753500 -0.29792800
H -6.59791400 0.32434900 -0.67680800
C -5.98026900 -3.43434600 0.15770000
C -7.26333000 -2.95328700 0.00620100
H -8.50826700 -1.22679100 -0.41435800
H -5.80769900 -4.48135900 0.38951500
H -8.10994200 -3.62355600 0.11888700

Compoun **5**

S 2.10262500 0.60529600 -0.87042400

O -0.23497300 -0.88493300 -0.44560800

C 1.47048400 -1.15291000 1.46108500
C 1.34786200 3.20856600 -0.43964700
C -0.94018100 0.17849400 -0.17991800
C -0.35629500 1.45330000 -0.00490800
H -0.99818800 2.25396100 0.33500900
C 0.94028300 1.78737000 -0.37983700
C -2.38806600 -0.03281700 -0.13211300
C 0.42064600 4.20808500 -0.79609300
H -0.59324100 3.93254600 -1.06516400
C 1.16785600 -2.67777700 -2.20655300
C 1.79916700 -2.28751600 -1.00980200
C 1.65221900 -3.73032000 -2.98602700
C 0.47242400 -1.69240000 2.29527100
C 2.80000600 -4.42289800 -2.59196700
C 2.94839300 -3.00668800 -0.63431000
C 0.80543000 5.54510900 -0.85076600
H 0.08169800 6.30053800 -1.14018400
C 2.68072600 -0.78977800 2.08116200
C 2.67038300 3.59146200 -0.14514700
H 3.39061100 2.83497300 0.14631200
C 3.44864600 -4.05496100 -1.41139200
C -3.31052800 1.03065600 -0.08672300
H -2.96894300 2.05859200 -0.10728500
C -4.67951000 0.80231100 -0.03949300
H -5.35717600 1.64574100 -0.00941500
C 2.11890200 5.91170600 -0.54542100
H 2.41604800 6.95513300 -0.58534500
C -2.89876300 -1.35214800 -0.14578200
H -2.20668400 -2.18431300 -0.18887700
C 0.66488900 -1.85613500 3.66944200
C -5.16519900 -0.51639700 -0.04319800
C 3.04863400 4.93104400 -0.19166800
H 4.06874300 5.20977500 0.05318300
C 1.87740900 -1.48748300 4.25588000
B 1.24077000 -1.05245900 -0.13626900
C 2.88812100 -0.95407200 3.45315100
C -4.25776800 -1.59233500 -0.10001400
H -4.64980800 -2.60360700 -0.10311600
O -6.47154000 -0.85192100 0.00142300
C -7.45264200 0.18958800 0.06546100
H -8.41686300 -0.31617600 0.10005600
H -7.32462500 0.79696800 0.96706500
H -7.40661800 0.83009200 -0.82106500
H 3.47860700 -0.35829200 1.48137500
H 3.83640600 -0.66011100 3.89580300
H -0.47984800 -1.99120800 1.86457900
H -0.13173700 -2.27096200 4.28182900
H 2.03223100 -1.61259200 5.32397100

H 0.27599300 -2.14808200 -2.53080900
H 1.13625000 -4.00937000 -3.90128500
H 3.18195500 -5.24106400 -3.19641200
H 4.34030300 -4.58834300 -1.09189400
H 3.45996400 -2.74815700 0.28924100

Compound **6**

S -1.94250000 -0.08690600 -0.85245500

O 0.72026600 0.69605100 -0.44509500
C -0.83720000 1.44155500 1.46193600
C -1.93664800 -2.79544900 -0.42745700
C 1.09951400 -0.52002100 -0.17619200
C 0.18919700 -1.58100100 0.00434800
H 0.58629700 -2.52822000 0.34120500
C -1.15316400 -1.54255400 -0.36644000
C 2.55672300 -0.71965100 -0.12888500
C -1.32159200 -4.01177600 -0.78595700
H -0.27139300 -4.02708800 -1.05613100
C -0.17507900 2.76381100 -2.24997100
C -0.84329800 2.60580000 -1.02025700
C -0.34660900 3.90152600 -3.04096400
C 0.27406700 1.65981800 2.29864300
C -1.20854800 4.91976600 -2.62505700
C -1.69963700 3.64892700 -0.62412800
C -2.06128100 -5.18990300 -0.84261600
H -1.57500900 -6.11548300 -1.13411200
C -2.10250000 1.45461300 2.07859300
C -3.31346900 -2.79796700 -0.13191900
H -3.79611200 -1.87258200 0.16241200
C -1.88710300 4.78799900 -1.41197700
C 3.14541800 -1.99906700 -0.09531100
H 2.53269600 -2.89201500 -0.12890800
C 4.52660900 -2.14090500 -0.04836800
H 4.95770500 -3.13758300 -0.02963100
C -3.42470600 -5.17933500 -0.53623900
H -3.99871900 -6.09988400 -0.57717900
C 3.40644800 0.40464200 -0.13076400
H 2.97040500 1.39571700 -0.16853100
C 0.13519000 1.87272500 3.67261700
C 5.37417400 -1.02176100 -0.03634700
C -4.04714900 -3.98060200 -0.17987600
H -5.10422900 -3.96713800 0.06618500
C -1.13350500 1.88061700 4.25574200
B -0.64898800 1.27310900 -0.13425200
C -2.25524300 1.67236900 3.45013300
C 4.78594800 0.25212300 -0.08477600

H 5.42048300 1.13376900 -0.08511000
C 6.86981500 -1.18310100 0.04729600
H 7.19715300 -2.11965400 -0.41204200
H 7.19695500 -1.20158900 1.09433400
H 7.38901800 -0.35399100 -0.44085300
H 1.27322900 1.66232600 1.87071700
H 1.01749100 2.03174800 4.28737100
H -1.24680800 2.04540800 5.32364600
H -3.24914900 1.67355400 3.89022200
H -2.99120700 1.28065800 1.47644300
H 0.49655100 1.98047200 -2.59147700
H 0.18979000 3.99381100 -3.98197100
H -1.34691000 5.80604700 -3.23824200
H -2.55761000 5.57469700 -1.07563500
H -2.22605200 3.57438000 0.32375400

Compound **7**

S 0.47800300 -1.60385600 -0.85874100

O -0.84137600 0.83503400 -0.43671800
C -1.24842900 -0.85597500 1.45938400
C 3.12505100 -1.03860600 -0.43063700
C 0.26961900 1.45499100 -0.16362600
C 1.49493900 0.78574400 0.01492500
H 2.33875300 1.36924700 0.35522900
C 1.73688900 -0.53428900 -0.36529900
C 0.16170400 2.92595800 -0.10978300
C 4.18684300 -0.18008000 -0.77990900
H 3.98320000 0.85267000 -1.04050800
C -2.69847500 -0.43906300 -2.23442700
C -2.38440100 -1.08821900 -1.02475000
C -3.77469800 -0.84088600 -3.02814500
C -1.70062800 0.17758200 2.30195700
C -4.56905600 -1.92138100 -2.63568700
C -3.20470600 -2.16821400 -0.65142900
C 5.49311700 -0.65758400 -0.84026700
H 6.29739800 0.01350700 -1.12456400
C -0.99129300 -2.09859900 2.06859200
C 3.41390000 -2.38767600 -0.14785400
H 2.60923000 -3.05514200 0.14005100
C -4.27818100 -2.58602800 -1.44268900
C 1.29524400 3.76179900 -0.08749200
H 2.29300000 3.34237700 -0.13437300
C 1.15000000 5.14464200 -0.03120300
H 2.03212700 5.77640600 -0.01706300
C 5.76637400 -1.99624200 -0.54644900
H 6.78636100 -2.36542100 -0.58973800

C -1.11738600 3.51669600 -0.09107900
H -1.99314200 2.87966600 -0.11725500
C -1.88077600 -0.01218100 3.67450000
C -0.12440300 5.71764800 -0.00292800
C 4.72339900 -2.85828500 -0.19922900
H 4.93037400 -3.89720500 0.03718000
C -1.61784100 -1.25683000 4.25021500
B -1.12274900 -0.62608500 -0.13510400
C -1.17331600 -2.30292700 3.43865000
C -1.25711700 4.89966200 -0.03612900
H -2.24864600 5.34042800 -0.01662700
H -0.23362500 6.79682300 0.04100700
H -3.00638500 -2.69008800 0.28108100
H -4.89085000 -3.42565300 -1.12456600
H -5.40614100 -2.23908700 -3.25127600
H -3.99300500 -0.31326300 -3.95315500
H -2.08956300 0.40110000 -2.55779100
H -0.63003200 -2.92590800 1.46221800
H -0.96234500 -3.27677900 3.87290200
H -1.75597200 -1.40946600 5.31698400
H -2.22571600 0.81185100 4.29383800
H -1.91655100 1.15583900 1.88027900

Compound **8**

S 2.24756500 0.88677600 -0.86631000

O 0.18758500 -0.96746800 -0.43162300
C 1.93298100 -0.96075100 1.45807700
C 1.08047700 3.32919000 -0.42930700
C -0.67549500 -0.03148500 -0.16227100
C -0.31027200 1.31747600 0.01712000
H -1.07334300 2.00001100 0.36413400
C 0.91406100 1.86130800 -0.36625900
C -0.00387500 4.16178500 -0.77188500
H -0.96193400 3.72289300 -1.02799800
C 1.86399400 -2.46395700 -2.24066500
C 2.41731100 -2.01727300 -1.02500100
C 2.50234500 -3.41969700 -3.03353200
C 1.03404700 -1.63522900 2.30633900
C 3.73054800 -3.95329900 -2.63428000
C 3.65115000 -2.57581400 -0.64534200
C 0.15498100 5.54361500 -0.83078800
H -0.68689500 6.16929800 -1.10984300
C 3.08555600 -0.42284800 2.06116300
C 2.32611300 3.92474300 -0.15202700
H 3.16462800 3.29768000 0.13009600
C 4.30457100 -3.52537000 -1.43560500

C 1.39432500 6.12154300 -0.54265100
H 1.51497900 7.19958700 -0.58522300
C 1.26520700 -1.76207200 3.67853300
C 2.47776300 5.30806300 -0.20223400
H 3.44092600 5.75152400 0.02966500
C 2.41830500 -1.21832100 4.24805100
B 1.67564900 -0.89594800 -0.13603000
C 3.33137500 -0.54828900 3.43073500
C -2.07732500 -0.48219700 -0.11177500
C -3.14067100 0.41307300 -0.10973500
C -2.35241400 -1.88425300 -0.08216400
C -4.48125300 -0.03596800 -0.05711500
H -2.96970700 1.48205700 -0.17001600
C -3.64305200 -2.34482100 -0.03117700
H -1.52193900 -2.57904500 -0.09780800
C -5.57506900 0.87447600 -0.05103700
C -4.74524900 -1.44481700 -0.01372600
H -3.83895300 -3.41276400 -0.00168800
C -6.86993400 0.41115300 0.00142700
H -5.37014700 1.94067200 -0.08597400
C -6.09134700 -1.88920100 0.04005200
C -7.12913400 -0.98178300 0.04782700
H -7.69941700 1.11118800 0.00759500
H -6.29142300 -2.95629900 0.07408200
H -8.15566100 -1.33293100 0.08859100
H 3.80535600 0.11644900 1.44990300
H 4.23236700 -0.11780200 3.86014400
H 2.60253000 -1.31397900 5.31449100
H 0.54480000 -2.28490100 4.30245400
H 0.13025000 -2.07200500 1.88933900
H 4.10854800 -2.26897000 0.29157000
H 0.91112500 -2.05742300 -2.56936200
H 2.04374700 -3.74708200 -3.96316400
H 4.23215100 -4.69558800 -3.24911100
H 5.25794000 -3.93538300 -1.11227300

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