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Supporting Information

for

B-N coordinated triaryl pyrazole: Effect of dimerization, optical and NLO properties

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General Information

All reagents and starting materials were purchased from Sigma-Aldrich, Alfa Aesar and Spectrochem chemical companies and used as received unless otherwise noted. Tetrahydrofuran and toluene were distilled from Na/benzophenone prior to use. Dichloromethane, N,N-dimethylformamide and acetonitrile were distilled from CaH_2. 2,7-Dibromo-9,9-dihexyl-9H-fluorene, 1,4-dibromo-2,5-bis(hexyloxy)benzene, 2,7-dibromo-9-hexyl-9H-carbazole, 2,5-bis(tributylstannyl)thiophene and 5,5'-bis(tributylstannyl)-2,2'-bithiophene were prepared by following literature reported methods.[1-4] All 400 MHz ^{1}H, 100 MHz ^{13}C and 128 MHz ^{11}B NMR spectra were recorded on a Bruker ARX 400 spectrometer operating at 400 MHz. All ^{1}H and ^{13}CNMR spectra were referenced internally to solvent signals. ^{11}B NMR spectra were referenced externally to $BF_3 \cdot Et_2O$ in $CDCl_3$ ($\delta = 0$). ESI mass spectra were recorded using a Bruker microTOF-QII mass spectrometer. The absorbance spectra were recorded with a JASCO V-730 UV-Visible spectrometer. The fluorescence spectra were recorded using Edinburgh FS5 spectrofluorometer. Absolute fluorescence quantum yields of compounds **4** and **7-11** in solution and solid state were measured by integrating sphere method using Edinburgh FS5 spectrofluorometer. Single-crystal X-ray diffraction data were collected on a Bruker APEX-II diffractometer equipped with an Oxford Instruments low-temperature attachment. The data were collected at 100 K using Mo-Kα radiation (0.71073 Å). SADABS absorption corrections were applied. The structures were solved and refined with SHELX suite of programs. All non-hydrogen atoms were refined with anisotropic displacement coefficients. The H atoms were placed at calculated positions and were refined as riding atoms. Crystallographic data for compounds **4**, **8**, **10** & **11** has been deposited with the Cambridge Crystallographic Data Center as supplementary publication no. CCDC- 1936275-1936278. Copies of the data can be obtained free of charge on application to CCDC, 12 Union Road, Cambridge CB2 1EZ, UK (fax: (+44) 1223-336-033; email: deposit@ccdc.cam.ac.uk). DFT calculations were performed with the Gaussian09 program.[5] The structures were optimized using 6-31G(d) (B3LYP) as the basis set. Excitation data were determined using TD-DFT (B3LYP) calculations.

The NLO coefficients, namely, nonlinear refractive index (n_2) and nonlinear absorption (β) is estimated using closed-aperture (CA) and open-aperture (OA) single-beam Z-scan technique. The experimental set-up, shown in Fig. S1, comprises a frequency-doubled pulsed Yb-doped fiber laser (Model: Cazadero,M/S Calmar Inc., USA) which emits Fourier-transform limited (FTL) ultrashort pulses ($\Delta\tau \approx 300$ fs) at an operating wavelength of $\lambda = 1030$ nm. The

Yb-fiber laser system delivers fixed pulse energy of ≈ 30 μJ across a broad range of pulse repetition rate (RR), ranging from 780 Hz to 200 kHz. In the preliminary investigation, we fix the repetition rate at 1 kHz so as to minimize the thermally-induced manifestations during the NLO measurements. An optimally focused single-pass frequency-doubling of Yb-fiber laser is carried out using an LiB_3O_6 (LBO) crystal of length L = 4 mm, which generates transform-limited green ultrashort ($\Delta\tau \lesssim 300$ fs) pulses at $\lambda = 515$ nm. The choice of length for LBO crystal is governed by the onset of group-velocity mismatch between the interacting waves which could degrade the pulse-shape and consequently, adversely affect the pulse energy. The green ultrashort pulses have maximum energy of 3 μJ at the repetition rate of 1 kHz. A combination of half-wave plate (HWP) and a polarizing beam-splitter (PBS) is employed for incidence of optimum laser fluence on the samples. A convex lens (f = 150 mm) is used to focus the beam at the sample (z = 0). The green beam spot-size at (z = 0) is measured to be w_o = 50 μm which results in a Rayleigh-length of ≈ 3 cm. Since, we translate the sample to more than 10 cm, the experimental configuration allowed us to apply thin-sample approximation for estimating the NLO coefficients. The closed-aperture (CA) as well as open-aperture (OA) transmitted pulse energy was recorded using a pyroelectric energy meter (Model: PE9-ES-C, M/S Ophir Inc., USA). In order to observe the impact of thermal effects on NLO properties of dimers, we measured the OA and CA Z-scan transmittance at 80 MHz RR as well. The optical pulses at 80 MHz RR were derived through a frequency-doubled Yb-fiber laser (FP-1060-5-FS, Fianium, UK) which delivered FTL ultrashort pulses of 200 fs (approximately) at 532 nm wavelength.

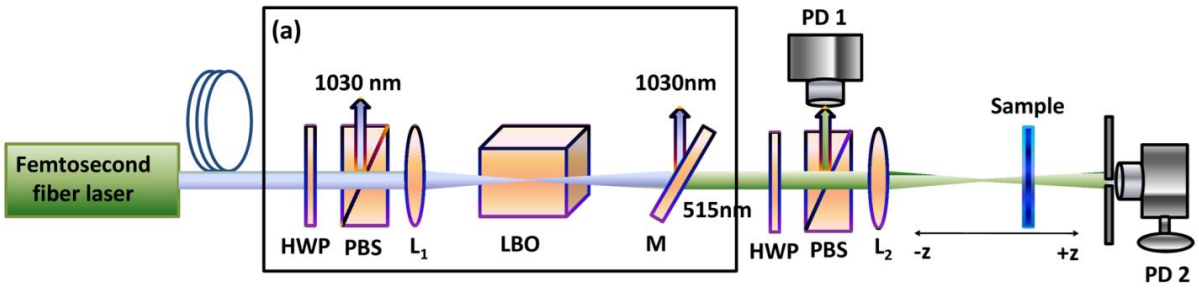
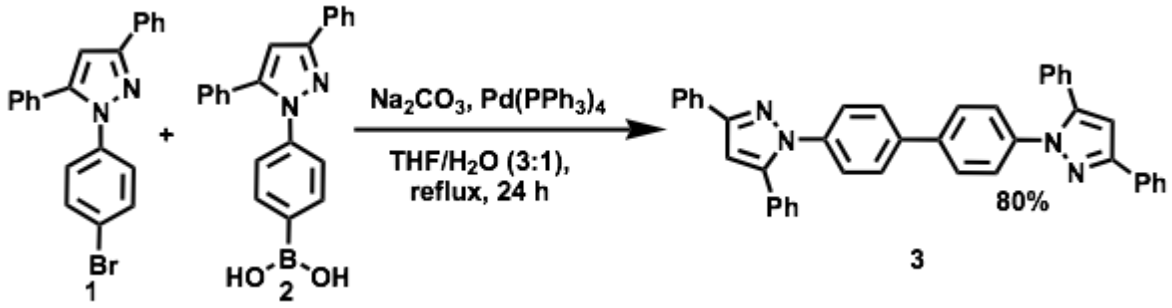


Figure S1: Schematic of closed aperture Z-Scan experimental setup. HWP: Half wave plate; PBS: polarizing beam splitter; L1: Convex Lens (100mm); L2: Convex Lens (150mm); PD1: Reference photodetector; PD2: Pyroelectric energy meter. (*Inset* (a) represents setup of second harmonic generation (SHG) of the pump beam).

From a practical perspective, it is important to note that the non-resonant NLO responses occur at extremely short time-scales (< 1 ps) and therefore, ultrashort optical pulses are essentially required for appropriately characterizing NLO properties. Conventionally, the

measurement of NLO coefficients is carried out using ultrashort pulsed lasers in the visible or near-infrared band. However, such laser systems exhibit high repetition-rates (R> 1 MHz) which could result in unavoidable thermal lensing effect during the measurements. The thermal lensing effect is primarily due to accumulated thermal effects (ATE) in liquid as well as solid samples. In other words, the ATE comes into play when pulses are incident on the sample at a time-scale faster than the characteristic thermal lifetime $t_c = \frac{w_0^2}{4D}$ where w_0 is beam-spot size and D is thermal diffusivity of medium i.e. ATE would affect the NLO measurements for R ≥ $1/t_c$. This manifestation is dominant in case of liquids due to their small thermal diffusivities 10^{-7}-10^{-8} m^2/s as compared to solid dielectric or semiconducting materials such as quartz 10^{-4}-10^{-5} m^2/s. Typically, $1/t_c \approx 0.5$ kHz in case of liquid samples for tightly focused beams ($w_0 \approx$ 50 μm). This implies that the NLO measurements using ultrashort pulsed lasers with $R >> 1$ kHz are inevitably accompanied by thermal lensing induced manifestations. In order to elucidate this point, we also carried out OA as well as CA Z-scan measurements at 1 kHz as well as at 80 MHz of repetition rates of solutions of various boron-doped triaryl pyrazole dimers.

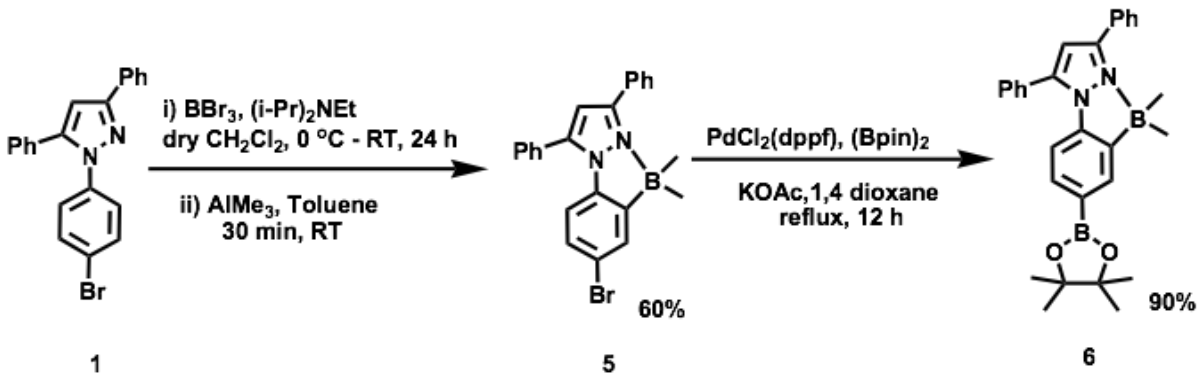
Synthetic procedure and spectral characterization



Scheme S1. Synthesis of compound **3**

Synthesis of compound 3

Compound **1** was synthesized using the literature reported method.[6] 4-Bromophenylhydrazine hydrochloride (5.48 g, 24.53 mmol), and 1,3-diphenylpropane-1,3-dione (5.00 g, 22.30 mmol) were dissolved in 40 mL of methanol and 40 mL of acetic acid . The reaction mixture was heated to reflux for 24 h and then poured into distilled water, extracted with ethyl acetate. The combined organic layers were washed with saturated $NaHCO_3$ solution, distilled water, brine and dried over Na_2SO_4. The solvent was removed under vacuum and the resulting residue was purified by silica gel column chromatography using ethyl acetate *n*-hexane as the eluent to yield compound **1** (yield = 75%). Compound **2** was synthesized following analogues literature reported method.[7] *n*-BuLi (7.00 mL, 11.19 mmol, 1.6 M in hexane) was added dropwise to a solution of compound **1** (3.50 g, 9.32 mmol) at -78 ^oC in anhydrous THF under nitrogen atmosphere. After being stirred at the same temperature for 0.5 h, $B(O^iPr)_3$ (11.19 mmol, 2.58 mL) was added dropwise *via* syringe. The reaction mixture was warmed to room temperature and stirred overnight at that temperature. 3 N HCl (75 mL) was added to the reaction mixture, stirred for 1 h and extracted with ethyl acetate. The combined organic layers were washed with brine, dried over Na_2SO_4 then concentrated. The resultant compound was washed with hot hexane and diethyl ether, to get compound **2** as a white powder and used without further purification. Synthesis of compound **3.** Degassed mixture of THF:H_2O (60:20 mL) was added to a mixture of compound **1** (3.30 g, 8.82 mmol), compound **2** (3.30 g, 9.70 mmol), Na_2CO_3 (4.69 g, 44.1 mmol) and $Pd(PPh_3)_4$ (305 mg, 0.26 mmol) under nitrogen atmosphere. The reaction mixture was refluxed for 24 h and cooled to room temperature. Distilled water was then added to the reaction mixture and extracted with ethyl acetate (3 × 25 mL). The combined organic layers were washed with brine solution, dried over Na_2SO_4 and concentrated. The residue was purified by silicagel column chromatography using *n*-hexane/ethylacetate mixture as the eluent. Yield: 4.16 g, (80%). mp: 280 ^oC. ^1H NMR (400 MHz, $CDCl_3$): δ = 7.96 – 7.94 (m, 4H), 7.58 – 7.56 (m, 4H), 7.47 – 7.43 (m, 8H), 7.38 – 7.33 (m, 12H), 6.85 (s, 2H) ppm. ^{13}C NMR (100 MHz, $CDCl_3$): δ = 152.28, 144.54, 139.68, 139.10, 133.12, 130.73, 128.96, 128.81, 128.73, 128.56, 128.21, 127.56, 125.97, 125.55, 105.64 ppm. HR-MS (ESI): calcd. for $C_{42}H_{31}N_4$ ($[M + H]^+$): 591.2543, found : 591.2514.



Scheme S2. Synthesis of compound **5** and **6**

Synthesis of compound 5

To a stirred solution of compound **1** (10.00 g, 26.65 mmol), and N,N-diisopropylethylamine ($^{i}Pr_2NEt$ (4.62 mL, 26.65 mmol) in 150 mL of dichloromethane at 0 ^{o}C was added BBr_3 (1.0 M in dichloromethane, 79.95 mL, 79.95 mmol), under nitrogen. After being stirred at room temperature for 24 h, saturated K_2CO_3 aqueous solution was added to the reaction mixture and extracted with CH_2Cl_2. The combined organic layers were washed with water, dried over $MgSO_4$ and concentrated under vacuum to afford crude product. Under nitrogen atmosphere a mixture of CH_2Cl_2 and toluene (100 mL: 100 mL) and Me_3Al (1.0 M in toluene, 53.3 mL, 53.3 mmol) were added to the crude product at room temperature. After being stirred at this temperature for 0.5 h, the reaction was quenched by adding water and extracted with CH_2Cl_2. The combined organic layers were washed with water, brine, dried over sodium sulphate and concentrated. The residue was purified by silica-gel column chromatography using *n*-hexane/dichloromethane mixture as the eluent. Yield: 6.65 g, (60%). ^{1}H NMR (400 MHz, $CDCl_3$): δ = 7.81 – 7.79 (m, 2H), 7.64 – 7.50 (m, 9H), 7.05 (dd, *J* = 8.5, 2.1 Hz, 1H), 6.63 (d, *J* = 8.5 Hz, 1H), 6.60 (s, 1H), 0.12 (s, 6H) ppm. ^{13}C NMR (100 MHz, $CDCl_3$): δ = 159.40, 148.76, 140.27, 137.15, 132.67, 130.57, 129.72, 129.64, 129.42, 129.25, 129.05, 128.52, 128.44, 127.71, 121.15, 113.35, 111.02, 9.10 ppm. ^{11}B NMR (128 MHz, $CDCl_3$): δ = 0.30 ppm. HR-MS (ESI): calcd. for $C_{23}H_{21}B_1Br_1N_2$ ($[M + H]^+$): 415.0980, found : 415.0957.

Synthesis of compound 6

Degassed 1,4 dioxane was added to a mixture of compound **5** (5.00 g, 12.04 mmol), potassium acetate (3.54 g, 36.12 mmol), bis(pinacolato)diboron (3.36 g, 13.24 mmol), $Pd(dppf)Cl_2$ (264 mg, 0.36 mmol) under nitrogen atmosphere. After being stirred at 100 ^{o}C temperature for 12 h, the reaction mixture was poured into water, extracted with CH_2Cl_2. The combined organic

layers were washed with brine solution, dried over sodium sulfate and concentrated. The residue was purified by silica-gel column chromatography using *n*-hexane/ethyl acetate mixture as the eluent. Yield: 5 g, (90 %). mp: 217 ^{o}C. ^{1}H NMR (400 MHz, $CDCl_3$): δ = 8.04 (s, 1H), 7.89 – 7.87 (m, 2H), 7.68 – 7.51 (m, 9H), 6.84 (d, *J* = 8.1 Hz, 1H), 6.64 (s, 1H), 1.40 (s, 12H), 0.23 (s, 6H) ppm. ^{13}C NMR (100 MHz, $CDCl_3$): δ = 154.85, 148.68, 140.67, 140.31, 136.38, 132.04, 130.36, 129.64, 129.56, 129.03, 128.66, 128.42, 126.88, 111.16, 110.93, 83.64, 24.97, 9.28 ppm. ^{11}B NMR (128 MHz, $CDCl_3$): δ = 32.24 (s), -0.17 (s) ppm. HR-MS (ESI): calcd. for $C_{29}H_{32}B_2N_2O_2$ ($[M + H]^+$): 463.2733, found : 463.2733.

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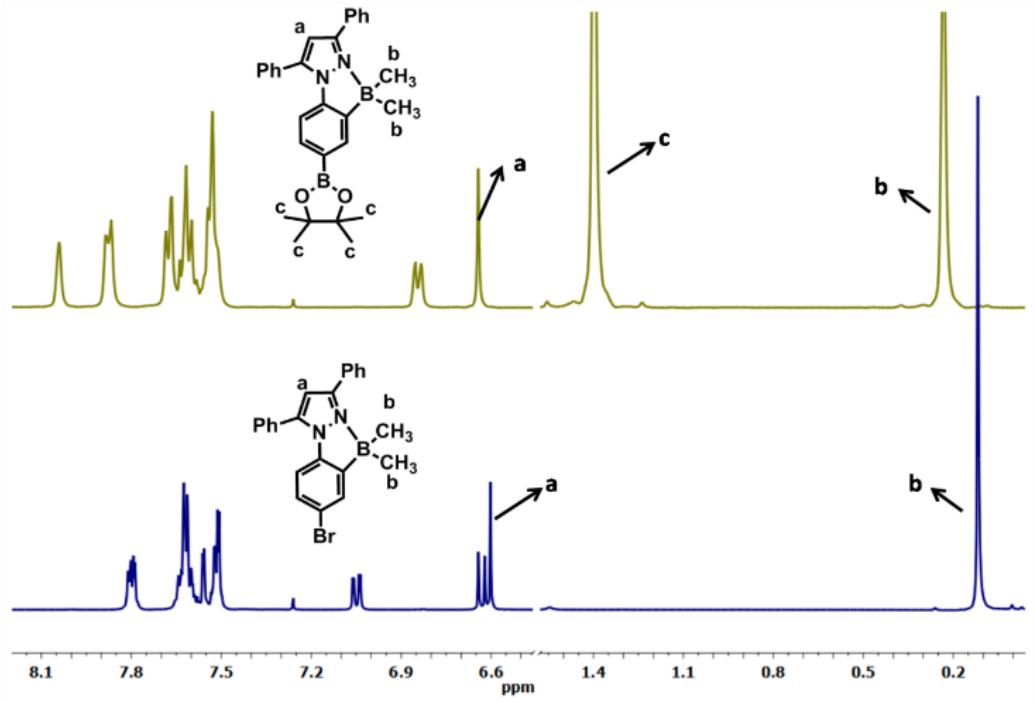


Figure S2: ^{1}H NMR spectrum of compound 5 and 6.

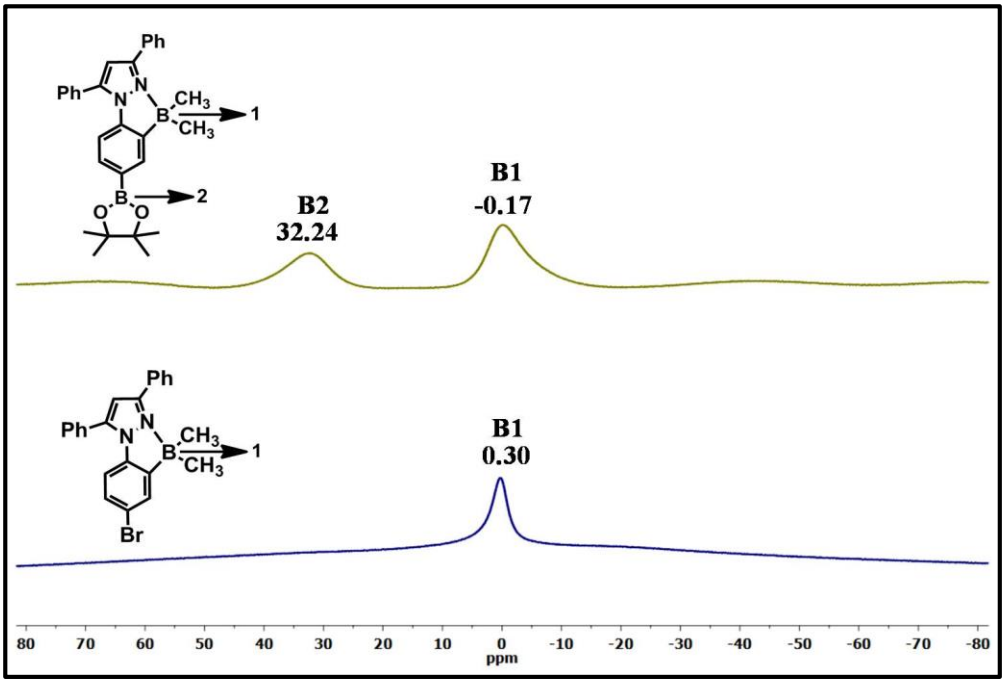


Figure S3: ^{11}B NMR spectrum of compound **5** and **6**.

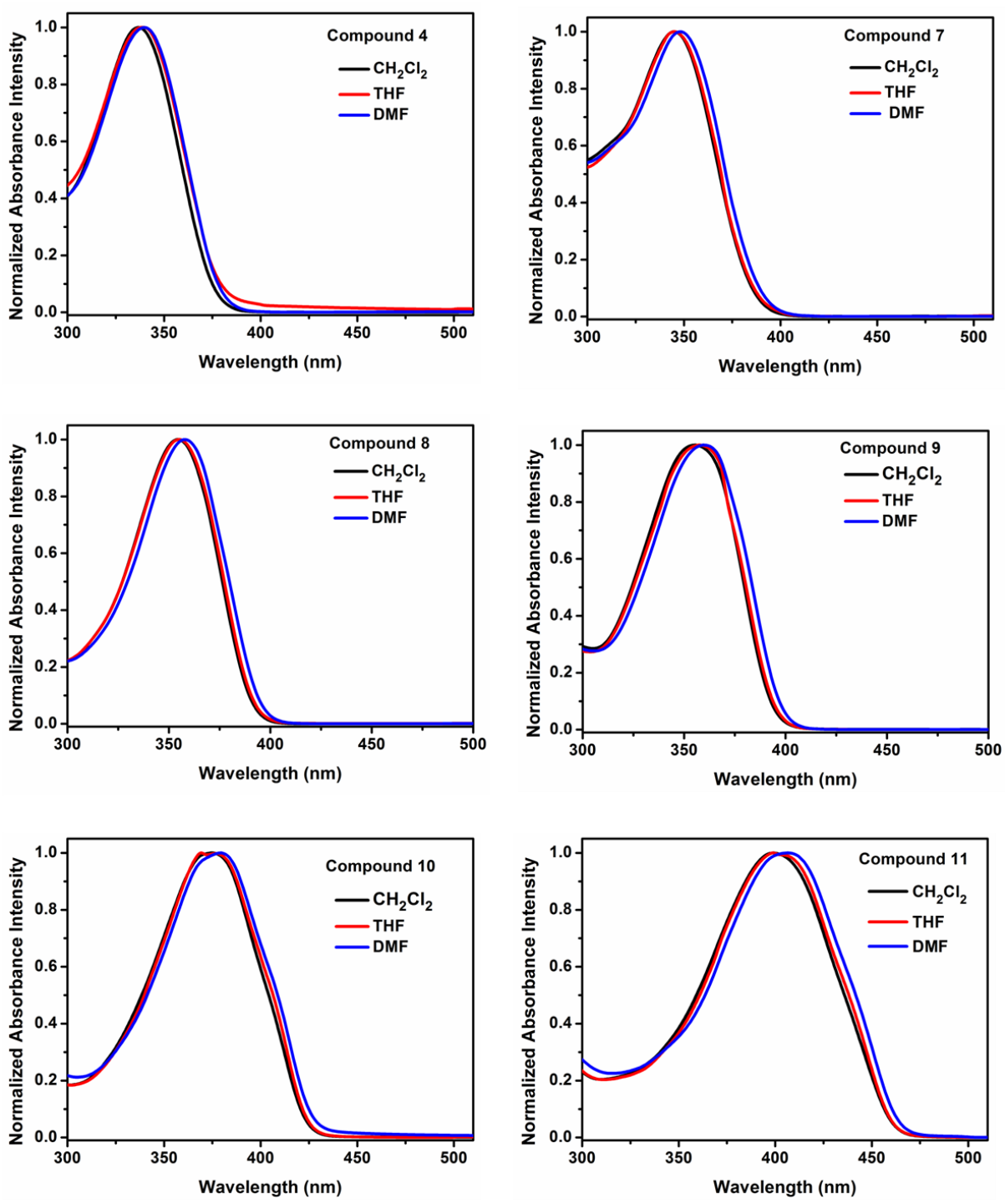


Figure S4: Comparison of normalized absorption spectra of **4** and **7-11** in different solvents.

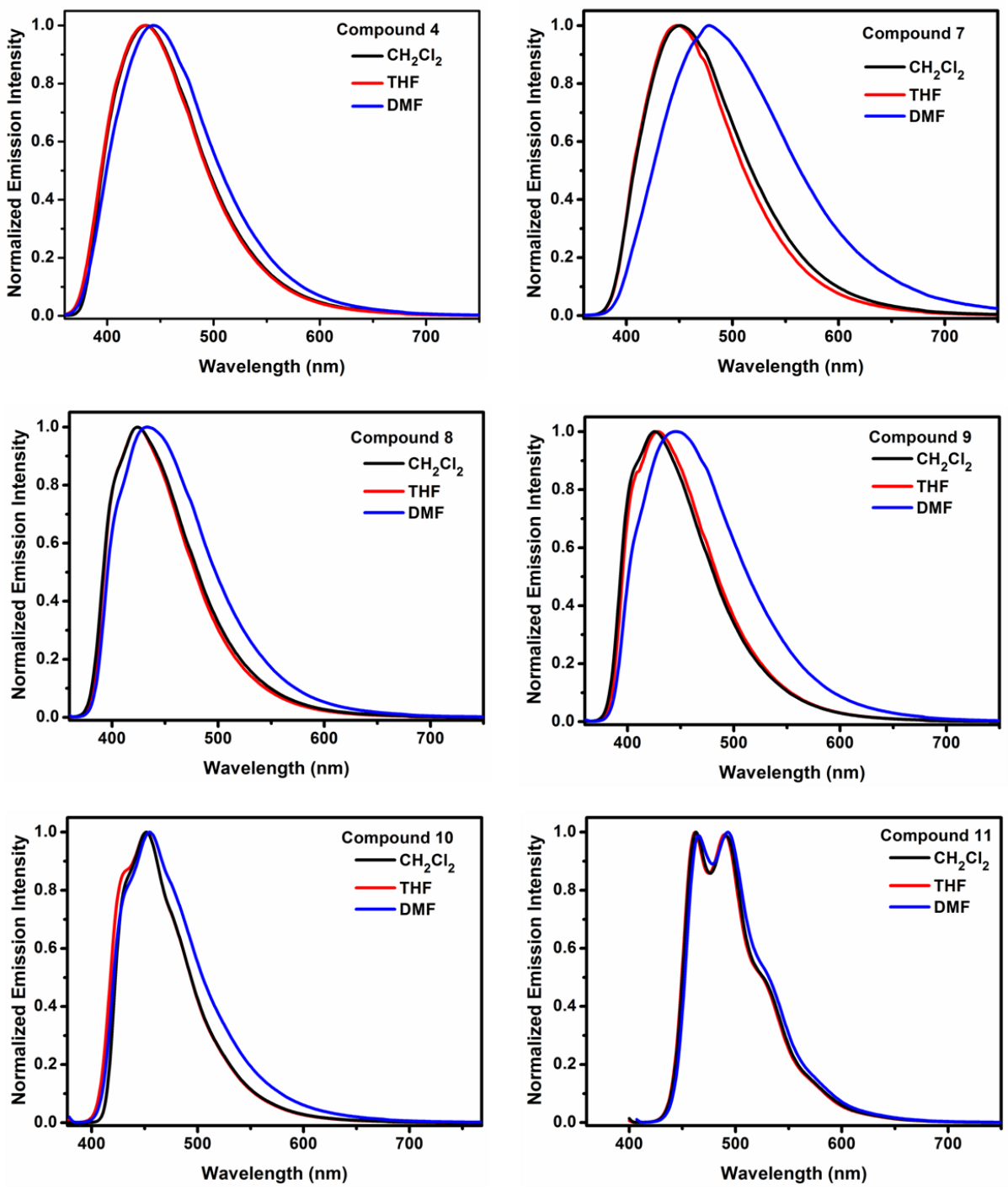


Figure S5: Comparison of normalized emission spectra of **4** and **7-11** in different solvents.

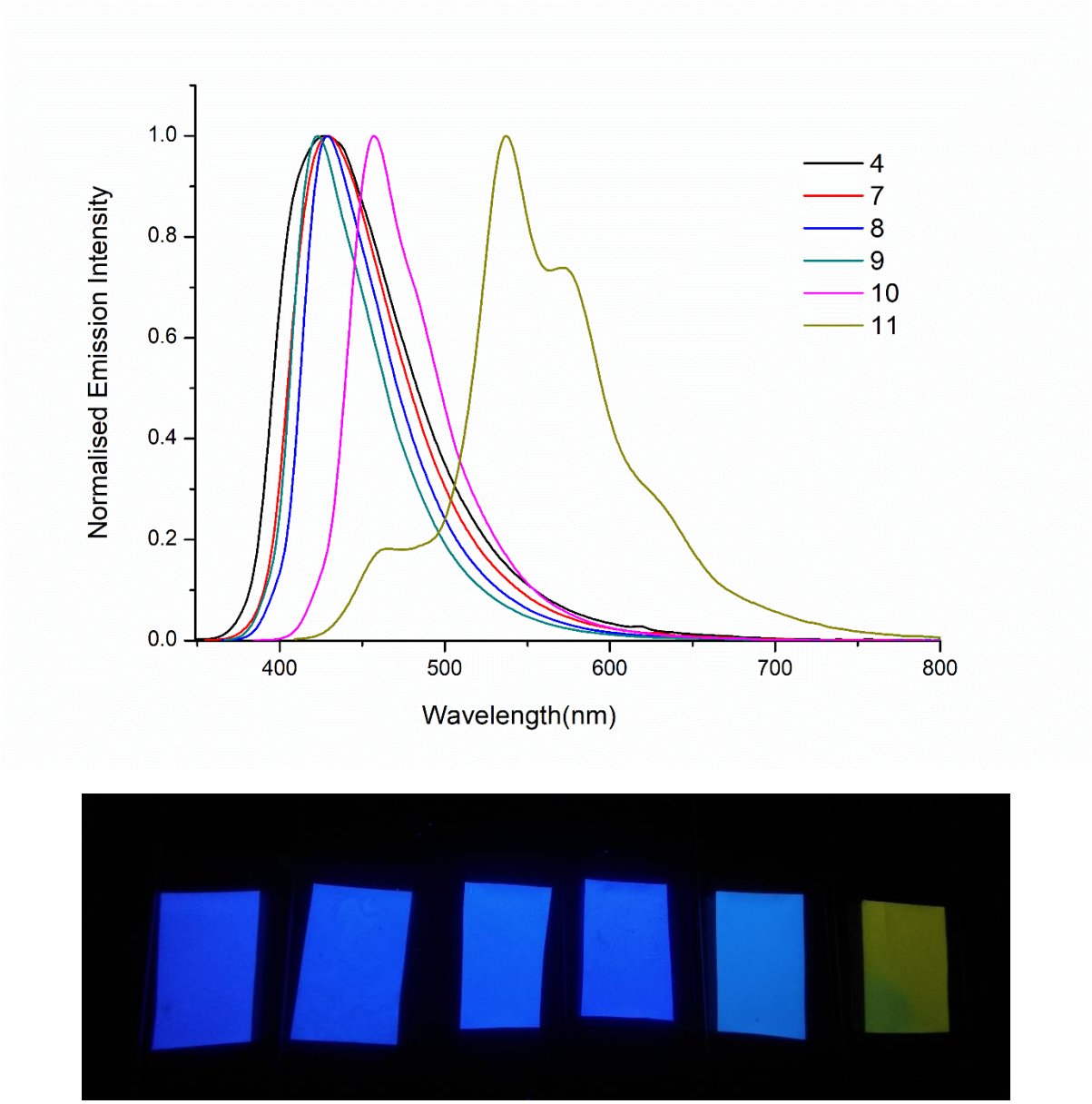


Figure S6: A comparison of normalized emission spectra of **4** and **7-11** in PMMA film (top). The fluorescence photograph of compounds **4** and **7-11** (left to right) in PMMA film (bottom). Irradiation was performed with a UV lamp with a wavelength of 365 nm.

Table S1. Electrochemical data of **4** & **7-11**

Compound	$E_{pc}^{\#}$(V)	Compound	$E_{pc}^{\#}$(V)
4	-2.55, -2.82	**9**	-2.49, -2.76
7	-2.53, -2.76	**10**	-2.47, -2.74
8	-2.49, -2.74	**11**	-2.31, -2.49

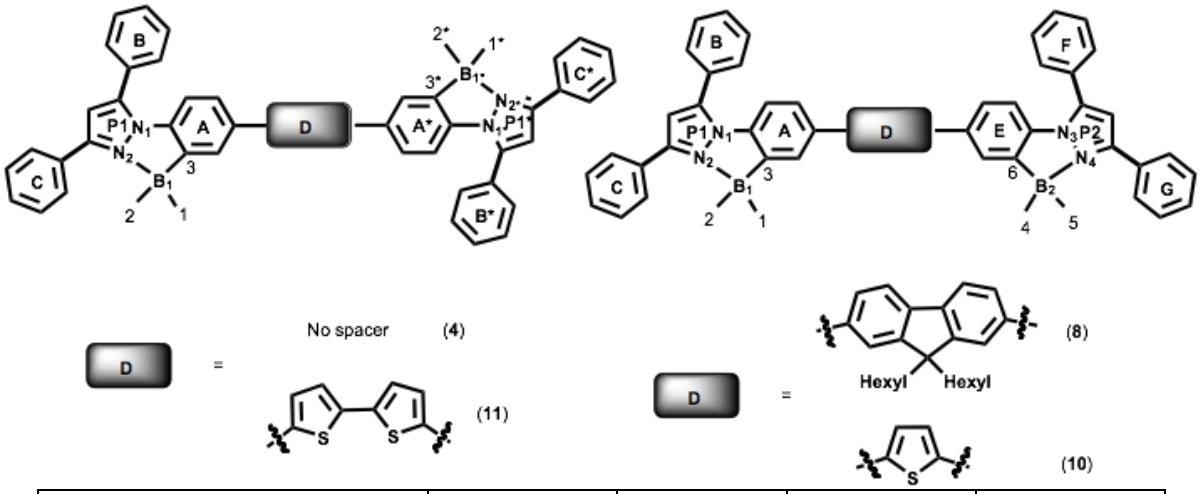
$^{\#}\mathbf{E_{pc}}$ = cathodic potential

Table S2: Crystal data and structure refinement parameters for compounds **4**, **8**, **10** and **11**.

Compound	4	8	10	11
Empirical formula	$C_{46}H_{40}N_4B_2$	$C_{71}H_{72}B_2N_4$	$C_{50}H_{42}B_2N_4S$	$C_{54}H_{44}B_2N_4S_2$
Formula weight	670.44	1002.94	752.55	834.67
Temperature/K	100.00	100.00	100.00	100.00
Crystal system	Monoclinic	Triclinic	Triclinic	Monoclinic
Space group	$P2_1/n$	P-1	P-1	$P2_1/c$
a/Å	12.284(4)	13.4091(6)	11.5795(5)	7.0486(17)
b/Å	7.108(2)	14.0249(7)	12.0816(5)	15.859(4)
c/Å	21.887(9)	19.5464(13)	16.8101(11)	19.155(5)
α/°	90	109.303(4)	97.113(4)	90
β/°	105.717(7)	95.233(4)	100.900(4)	95.549(6)
γ/°	90	112.832(3)	117.414(3)	90
Volume/Å^3	1839.7(11)	3094.0(3)	1989.06(19)	2131.2(9)
Z	2	2	2	2
ρ_{calcd}/g cm^{-3}	1.210	1.077	1.257	1.301
μ/mm^{-1}	0.070	0.062	0.123	0.169
F(000)	708.0	1072.0	792.0	876.0
2θ range for data collection/°	3.464 to 50.88	2.282 to 51.444	2.542 to 49.998	3.34 to 50.938

Index ranges	-14 ≤ h ≤ 14, -4 ≤ k ≤ 8, -26 ≤ l ≤ 26	-16 ≤ h ≤ 16, -16 ≤ k ≤ 17, -23 ≤ l ≤ 23	-13 ≤ h ≤ 13, -14 ≤ k ≤ 14, -19 ≤ l ≤ 19	-7 ≤ h ≤ 8, -19 ≤ k ≤ 19, -23 ≤ l ≤ 23
Reflns. collected	9945	38403	22351	27851
Independent reflns	3380 [R_{int} = 0.0800, R_{sigma} = 0.1002]	11760 [R_{int} = 0.0744, R_{sigma} = 0.0881]	6973 [R_{int} = 0.0530, R_{sigma} = 0.0576]	3937 [R_{int} = 0.1428, R_{sigma} = 0.1165]
Data/restraints/ parameters	3380/0/237	11760/27/713	6973/0/519	3937/0/283
GOF on F^2	1.029	0.940	1.086	0.978
Final R indices [$I > 2\sigma(I)$]	R_1 = 0.0770, wR_2 = 0.1886	R_1 = 0.0569, wR_2 = 0.1477	R_1 = 0.0633, wR_2 = 0.1632	R_1 = 0.0559, wR_2 = 0.1223
R indices (all data)	R_1 = 0.1389, wR_2 = 0.2299	R_1 = 0.1060, wR_2 = 0.1669	R_1 = 0.0821, wR_2 = 0.1740	R_1 = 0.1252, wR_2= 0.1524
Largest diff. peak and hole [e Å^{-3}]	0.39 and -0.31	0.28 and -0.28	0.40 and -0.27	0.30 and -0.24

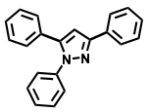
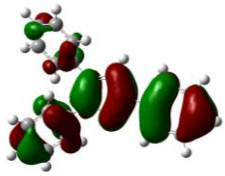
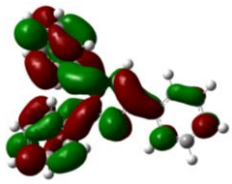
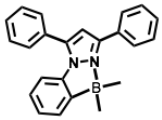
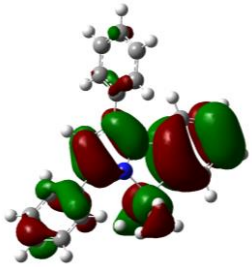
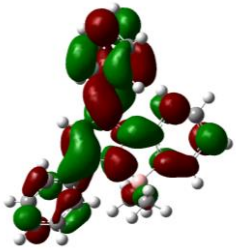
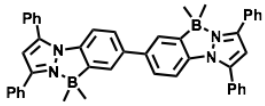
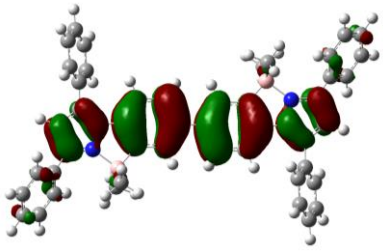
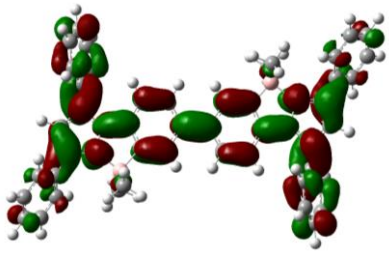
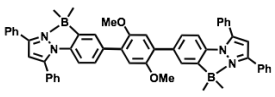
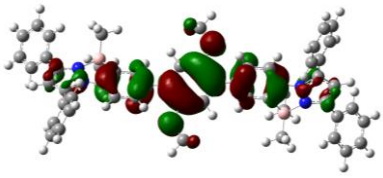
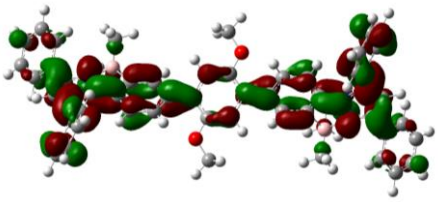
Table S3: Comparison of bond length [Å], angle [deg], deviation of boron atom from C_2N_2B plane [Å] and inter planar angle [deg] data for compounds **4**, **8**, **10** and **11**.



	4	**8**	**10**	**11**
B1-C1	1.612(6)	1.606(4)	1.613(5)	1.617(5)
B1-C2	1.625(5)	1.610(4)	1.615(6)	1.613(5)
B1-C3	1.604(6)	1.609(3)	1.606(5)	1.602(5)

B1-N2	1.654(5)	1.648(3)	1.672(5)	1.664(4)
C1-B1-C2	115.2(3)	113.7(2)	116.9(3)	113.6(3)
C1-B1-C3	114.6(3)	117.0(2)	110.2(3)	113.9(3)
C2-B1-C3	109.6(3)	110.3(2)	110.8(3)	111.9(3)
C1-B1-N2	109.7(3)	109.3 (2)	112.8(3)	108.6(3)
C2-B1-N2	110.8(3)	110.2(2)	109.0(3)	112.7(3)
C3-B1-N2	95.1(3)	94.6(2)	95.1(2)	94.7(2)
B2-C4		1.613(4)	1.621(6)	
B2-C5		1.616(3)	1.608(6)	
B2-C6		1.607(3)	1.604(5)	
B2-N4		1.649(3)	1.648(5)	
C4-B2-C5		113.0(2)	116.0(4)	
C4-B2-C6		115.2(2)	108.0(3)	
C5-B2-C6		111.6(2)	114.8(3)	
C4-B2-N4		109.2(2)	110.2(3)	
C5-B2-N4		112.1 (2)	114.8(3)	
C6-B2-N4		94.3 (2)	95.3(3)	
Deviation of B1 from C_2N_2B Plane (Å)	-0.076	-0.035	-0.069	-0.017
Pyrazole P1//Plane A	14.50(10)	6.35(9)	11.62(12)	10.17(9)
Pyrazole P1//Plane B	57.66(12)	84.21(9)	42.73(11)	62.86(10)
Pyrazole P1//Plane C	32.02(12)	60.99(9)	13.40(10)	29.87(11)
PlaneA//Plane D		34.11(6)	15.65(10)	9.46(9)
Deviation of B2 from C_2N_2B Plane (Å)		0.055	0.055	
Pyrazole P2//Plane E		19.32(7)	7.33(11)	
Pyrazole P2//Plane F		60.29(7)	37.79(12)	
Pyrazole P2//Plane G		40.79(9)	37.29(12)	
Plane E //Plane D		36.41(6)	4.17(9)	

Table S4. Computed orbitals from DFT (B3LYP:6-31G(d)) calculations for compounds **Pz, Pz-B, 4** & **7-11** (color red indicates negative and green indicates positive)

Compound	HOMO	LUMO
Pz 	 -5.6304	 -0.9248
Pz-B 	 -5.712	 -1.306
4 	 -5.195	 -1.469
7  Instead of hexyl, OMe was used to reduce the computation time	 -4.868	 -1.332

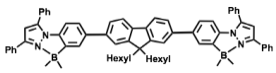
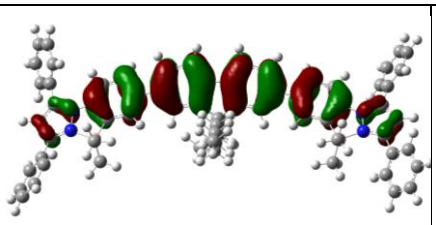
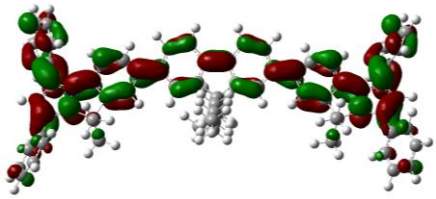
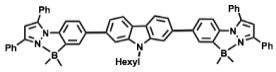
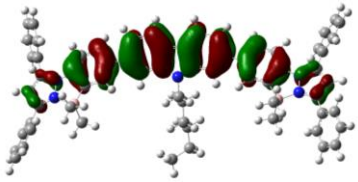
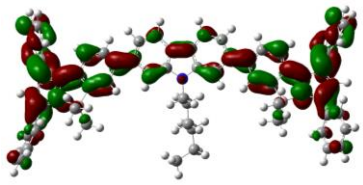
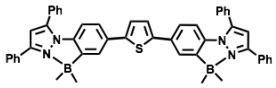
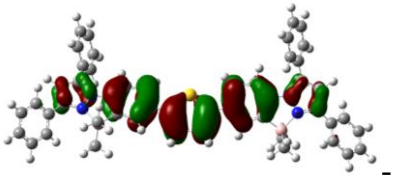
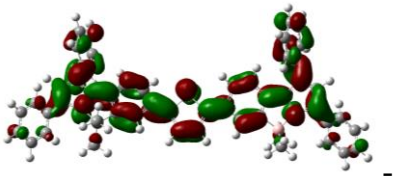
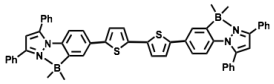
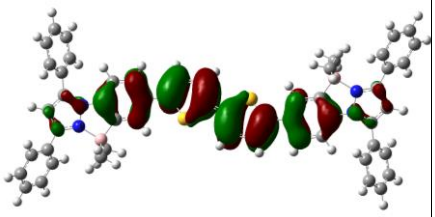
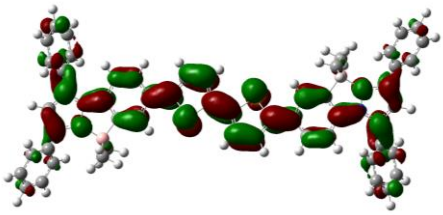
8 	 -5.059	 -1.442
9 	 -5.004	 -1.387
10 	 4.978	 1.550
11 	 -4.76	 -1.659

Table S5. Calculated electronic transitions for compound **Pz, Pz-B, 4, 7-11** from TD-DFT (B3LYP) calculations using 6-31G(d) as the basis set.

Compound	Transition	MO contributions	Energy gap eV (nm)	Oscillator strength/f
Pz	$S_0 \rightarrow S_1$	HOMO→LUMO	4.22 (293)	0.1696
		HOMO→LUMO+1		
	$S_0 \rightarrow S_2$	HOMO-4→LUMO	4.69 (264)	0.0657
		HOMO-1→LUMO		
		HOMO→LUMO+1		
		HOMO→LUMO+2		
		HOMO→LUMO+3		
	$S_0 \rightarrow S_3$	HOMO-1→LUMO	4.69 (263)	0.0926
		HOMO→LUMO+1		
		HOMO→LUMO+2		
		HOMO→LUMO+3		
Pz-B	$S_0 \rightarrow S_1$	HOMO→LUMO	3.89 (318)	0.2109
	$S_0 \rightarrow S_2$	HOMO-1→LUMO	4.34 (285)	0.0028
		HOMO→LUMO+1		
	$S_0 \rightarrow S_3$	HOMO-1→LUMO	4.38 (282)	0.1604
		HOMO→LUMO+1		
		HOMO→LUMO+2		

4	$S_0 \rightarrow S_1$	HOMO→LUMO	3.27 (378)	1.0616
	$S_0 \rightarrow S_2$	HOMO-1→LUMO	3.60 (343)	0.0000
		HOMO→LUMO+1		
	$S_0 \rightarrow S_3$	HOMO-1→LUMO		
		HOMO→LUMO+1	3.86 (320)	0.0000
		HOMO→LUMO+9		
7	$S_0 \rightarrow S_1$	HOMO→LUMO	3.11 (398)	0.7530
	$S_0 \rightarrow S_2$	HOMO→LUMO+1	3.28 (376)	0.0005
	$S_0 \rightarrow S_3$	HOMO-2→LUMO+1	3.76 (329)	0.4457
		HOMO-1→LUMO		
8	$S_0 \rightarrow S_1$	HOMO-1→LUMO+1	3.20 (387)	1.5103
		HOMO→LUMO		
	$S_0 \rightarrow S_2$	HOMO-1→LUMO	3.40 (363)	0.0187
		HOMO→LUMO+1		
	$S_0 \rightarrow S_3$	HOMO-2→LUMO+1	3.81 (325)	0.0051
		HOMO-1→LUMO		
		HOMO→LUMO+1		
9	$S_0 \rightarrow S_1$	HOMO-2→LUMO+1	3.20 (387)	1.3715
		HOMO→LUMO		
	$S_0 \rightarrow S_2$	HOMO-1→LUMO	3.34 (370)	0.0020
		HOMO→LUMO+1		
	$S_0 \rightarrow S_3$	HOMO-2→LUMO	3.38 (366)	0.0349
		HOMO-1→LUMO		

		HOMO→LUMO+1		
10	$S_0 \rightarrow S_1$	HOMO→LUMO	3.01 (410)	1.3367
	$S_0 \rightarrow S_2$	HOMO→LUMO+1	3.30 (374)	0.0082
	$S_0 \rightarrow S_3$	HOMO→LUMO+2	3.80 (325)	0.2755
11	S0→S1	HOMO→LUMO	2.72 (454)	1.7669
	S0→S2	HOMO→LUMO+1	3.05 (405)	0.0000
	S0→S3	HOMO→LUMO+2	3.41 (362)	0.2876

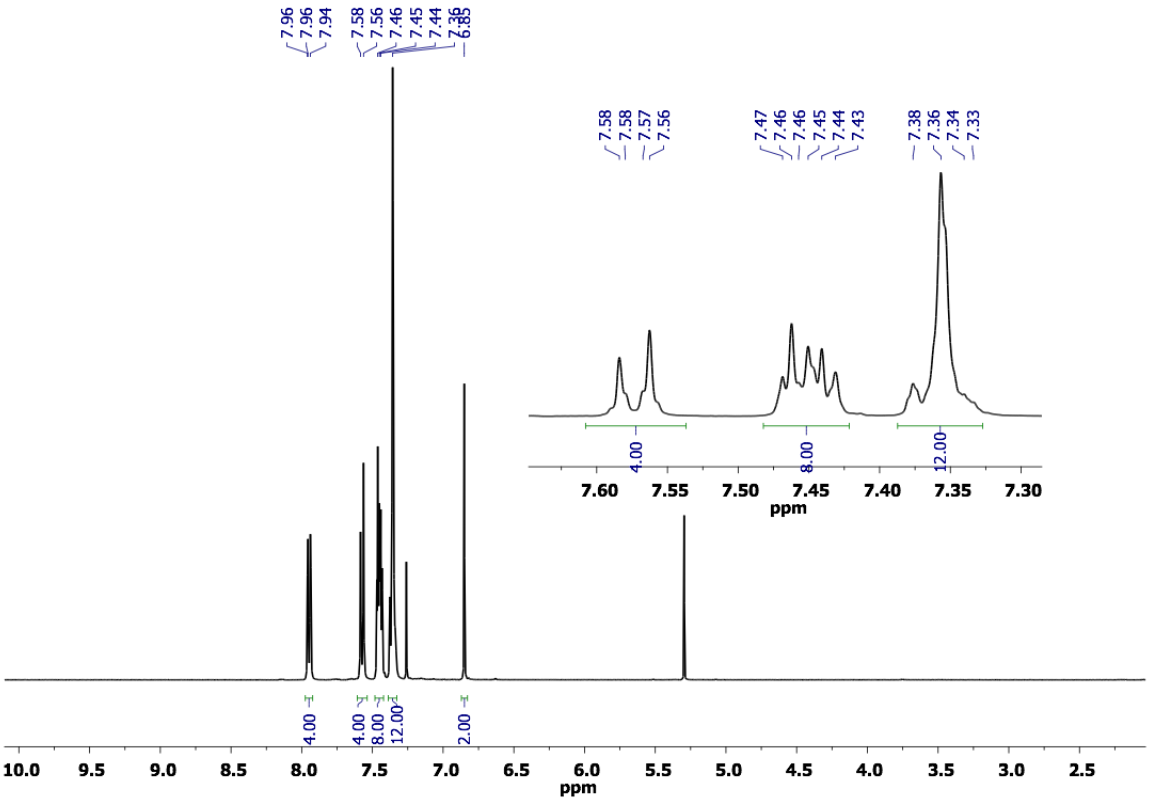


Figure S6. ^{1}H NMR spectrum of compound **3**

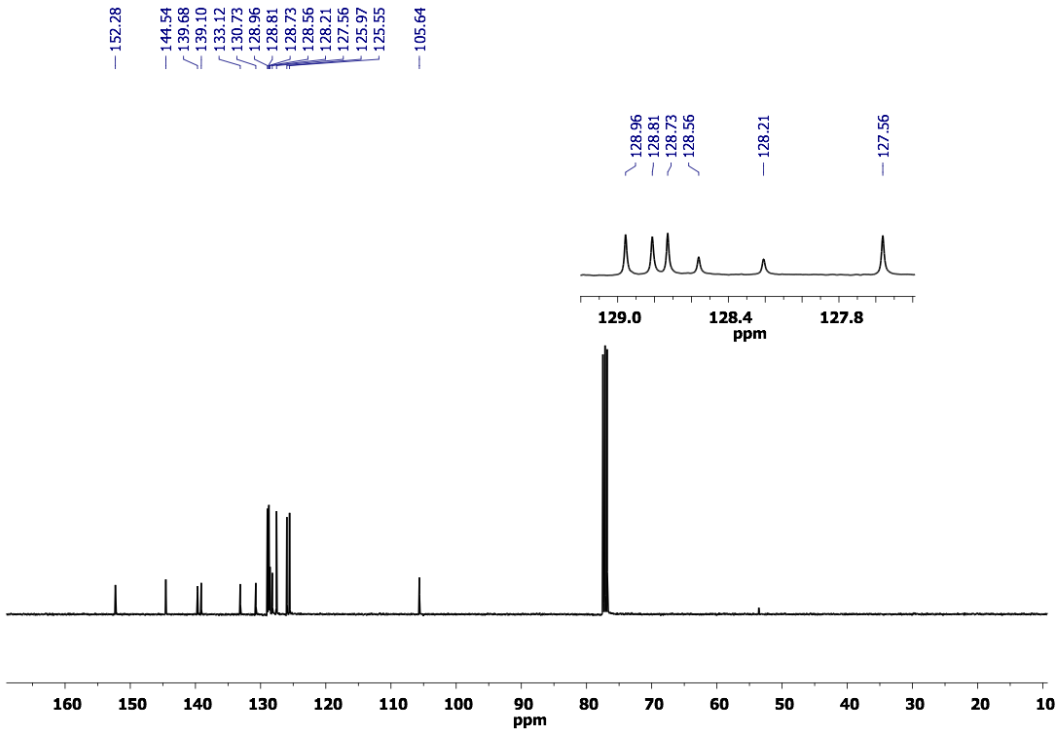


Figure S7. ^{13}C NMR spectrum of compound **3**

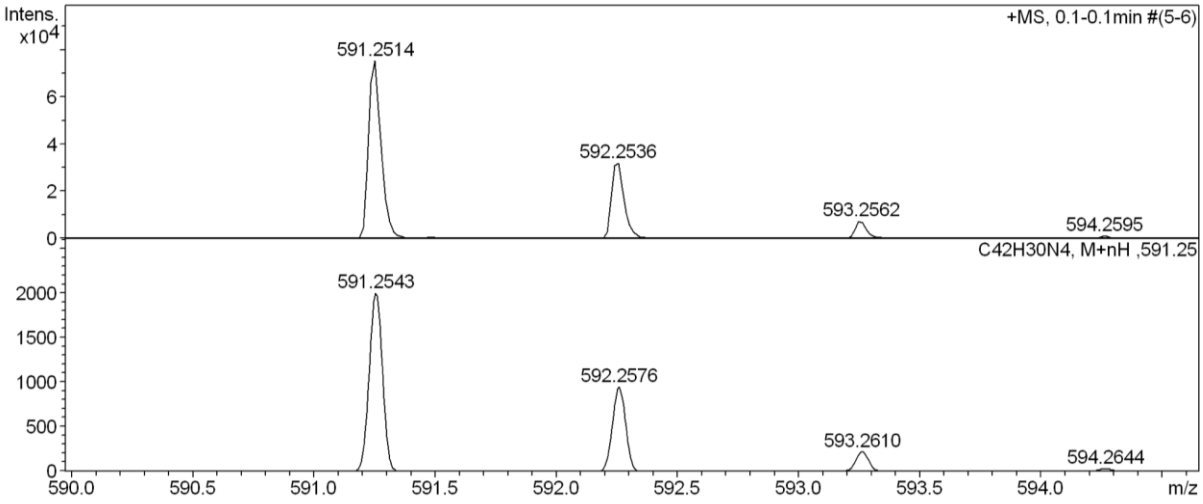


Figure S8. HRMS of compound **3**

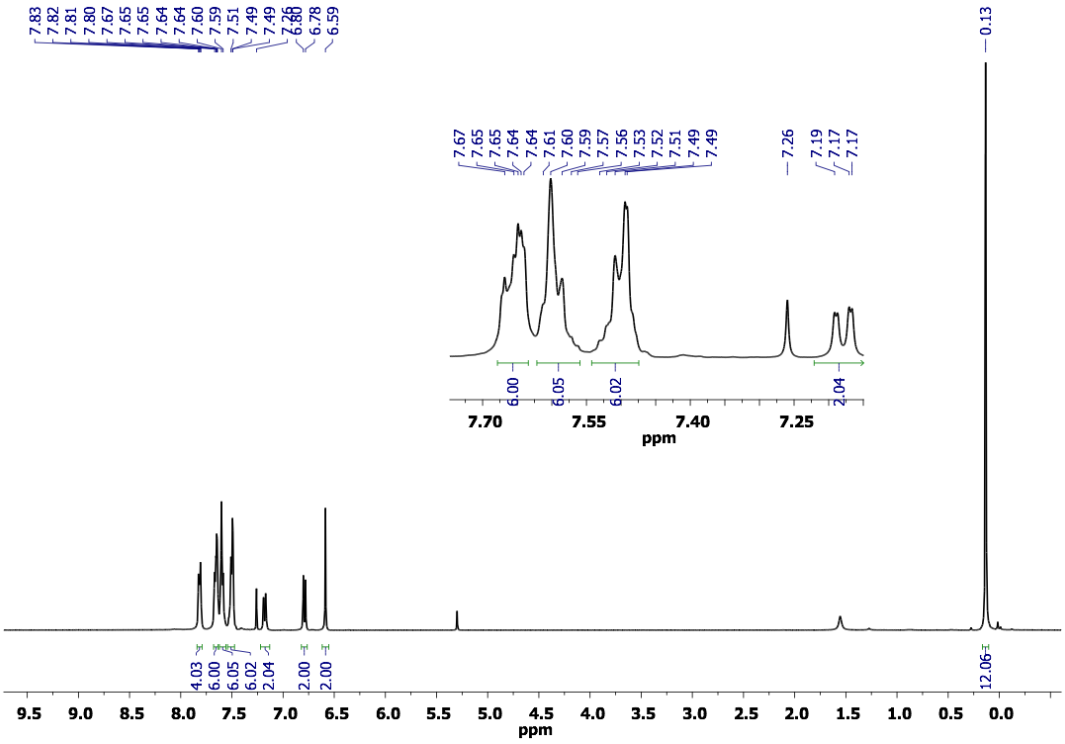


Figure S9. ^{1}H NMR spectrum of compound **4**

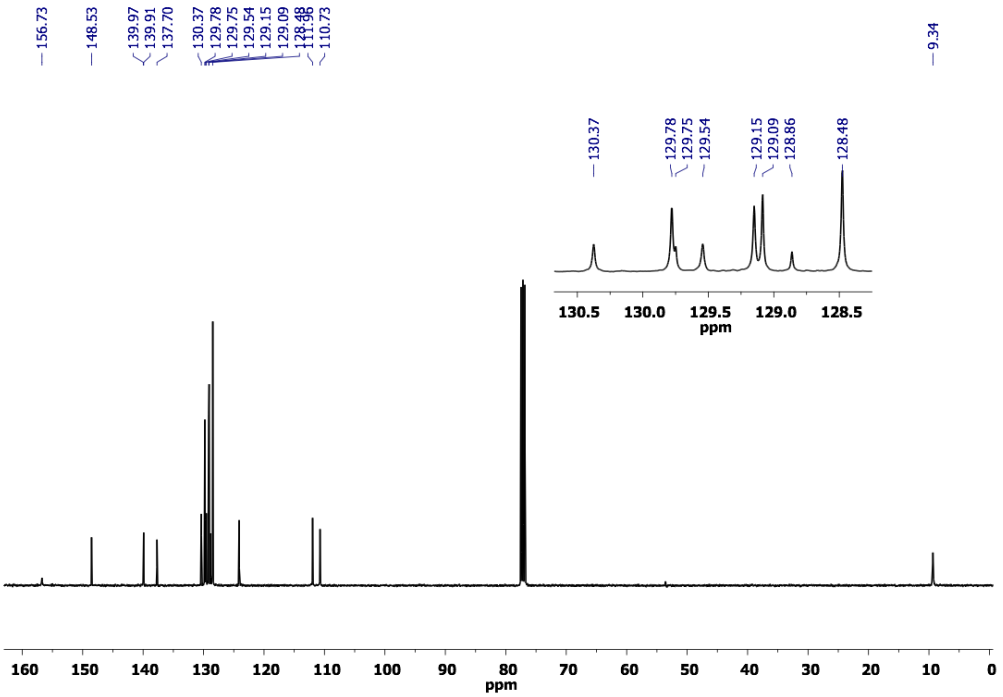


Figure S10. ^{13}C NMR spectrum of compound **4**

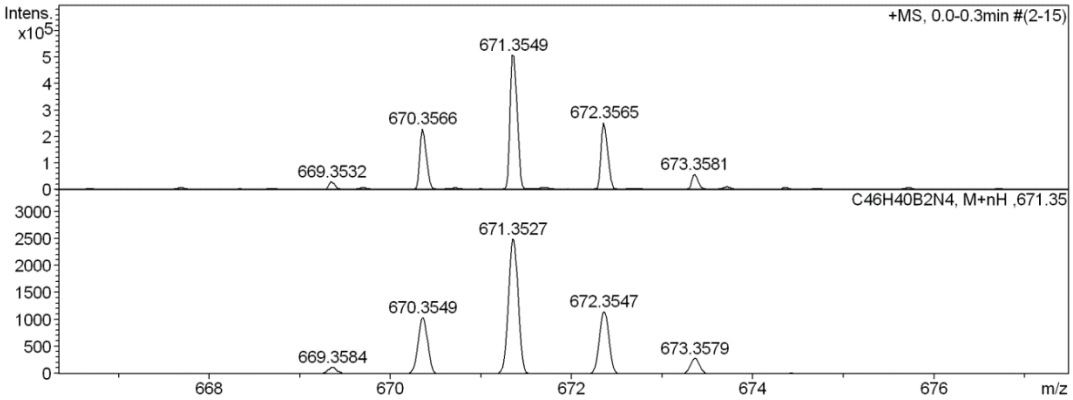


Figure S11. HRMS of compound **4**

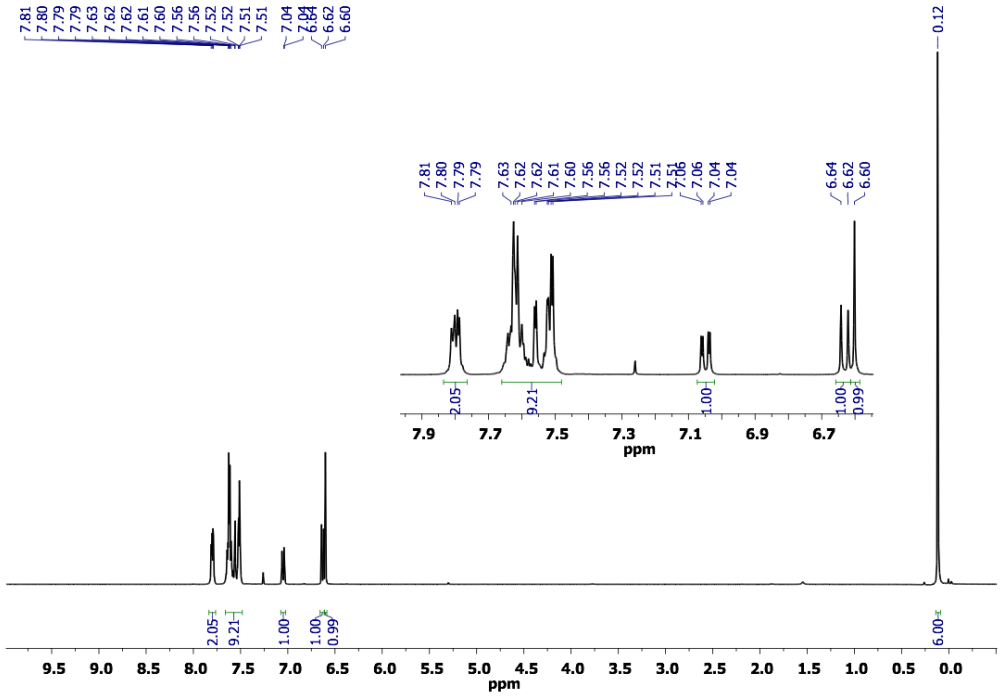


Figure S12. ^{1}H NMR spectrum of compound **5**

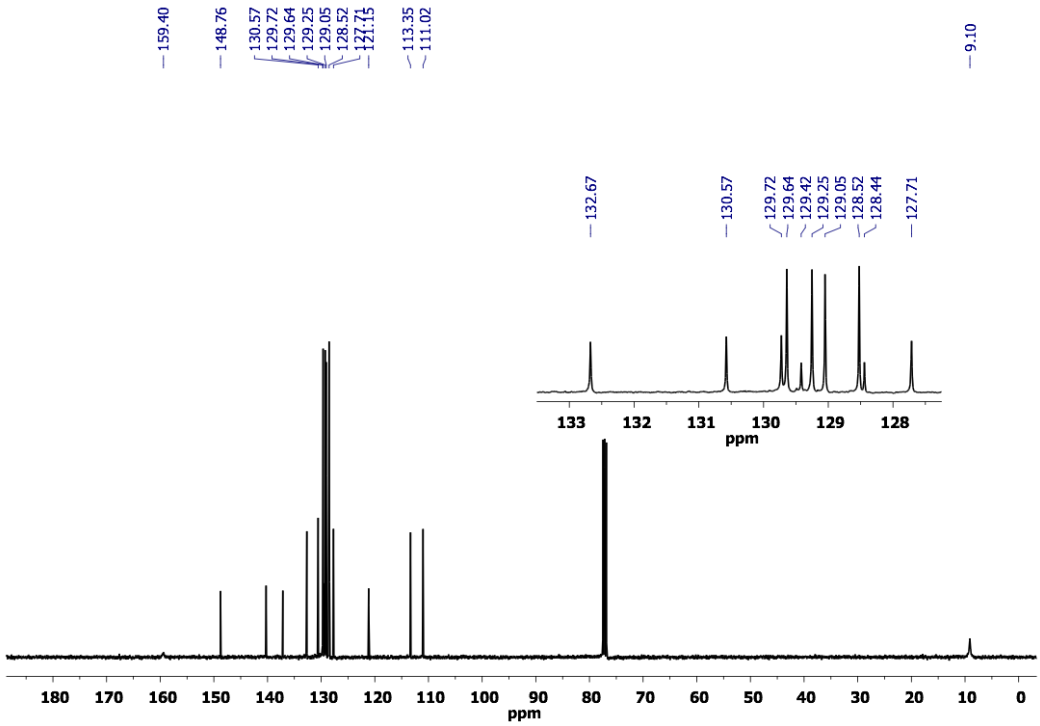


Figure S13. ^{13}C NMR spectrum of compound **5**

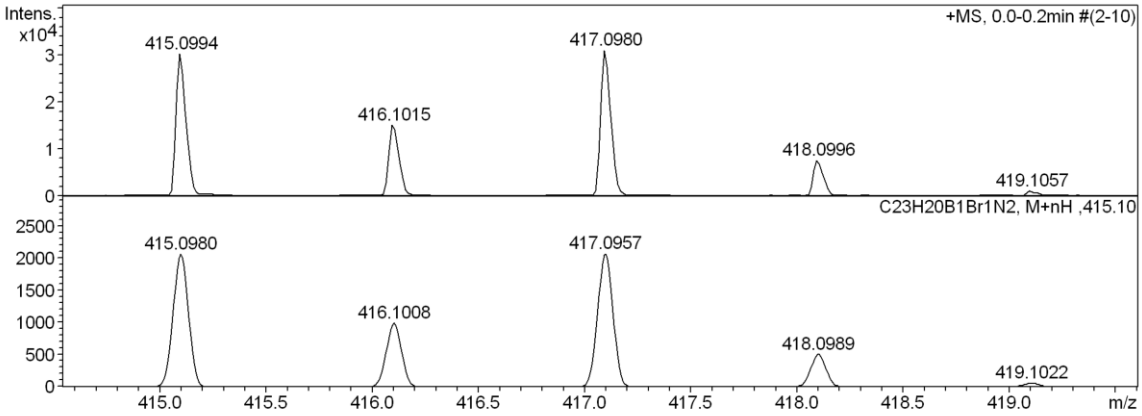


Figure S14. HRMS of compound **5**

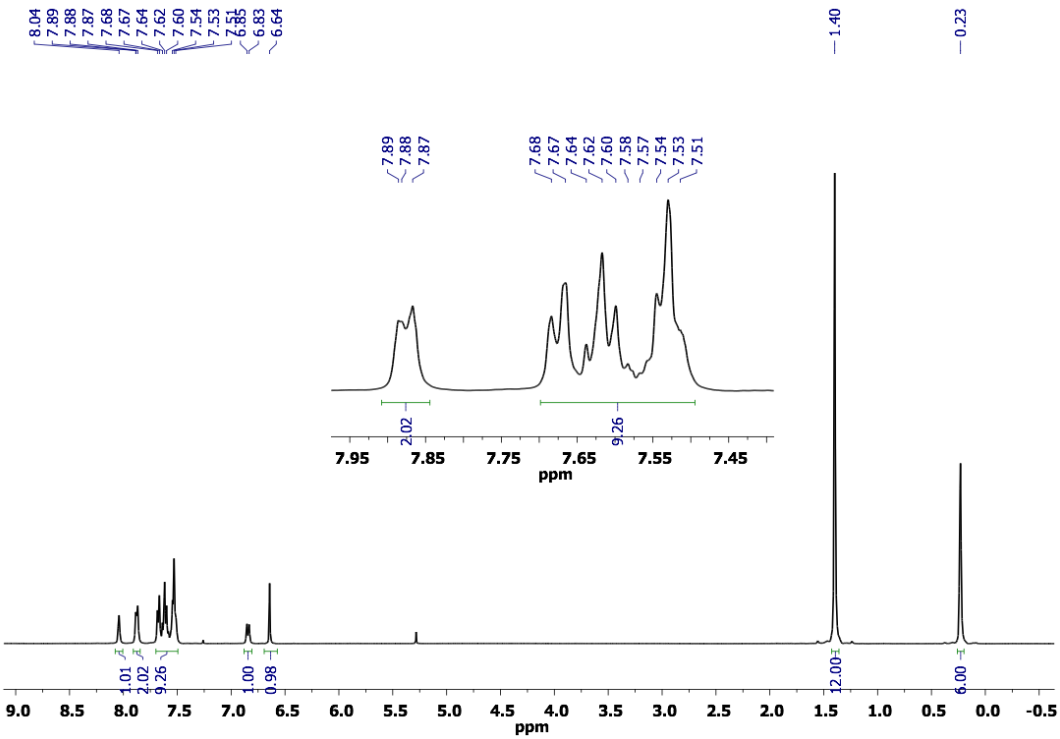


Figure S15. ^{1}H NMR spectrum of compound **6**

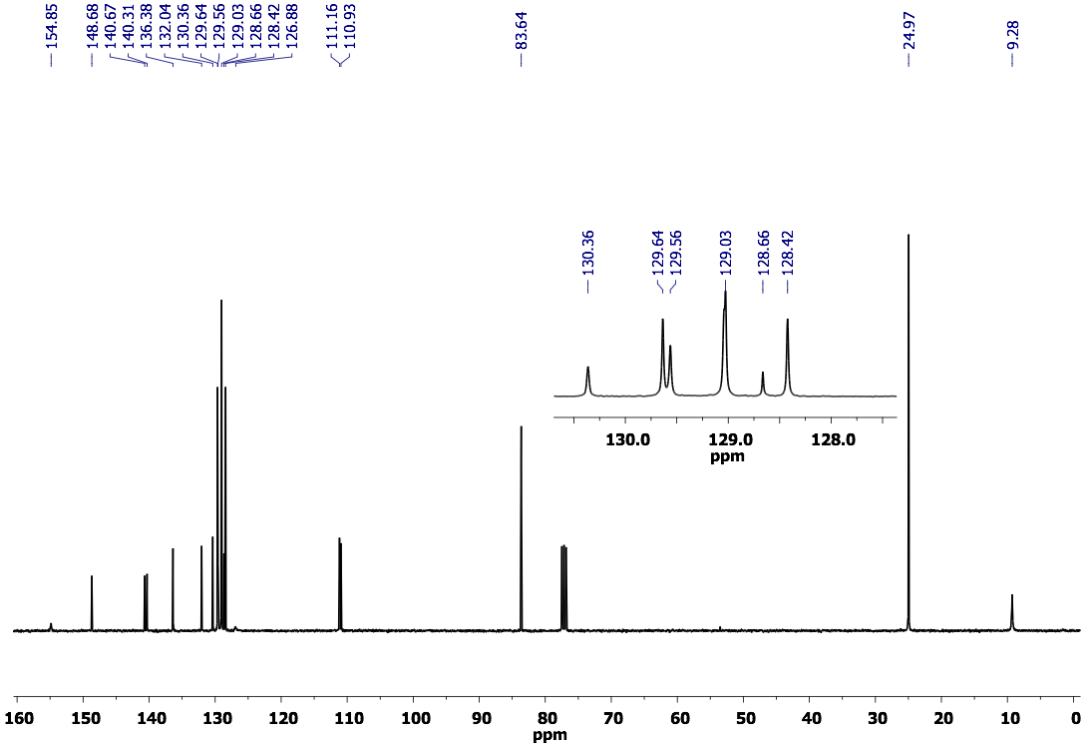


Figure S16. ^{13}C NMR spectrum of compound **6**

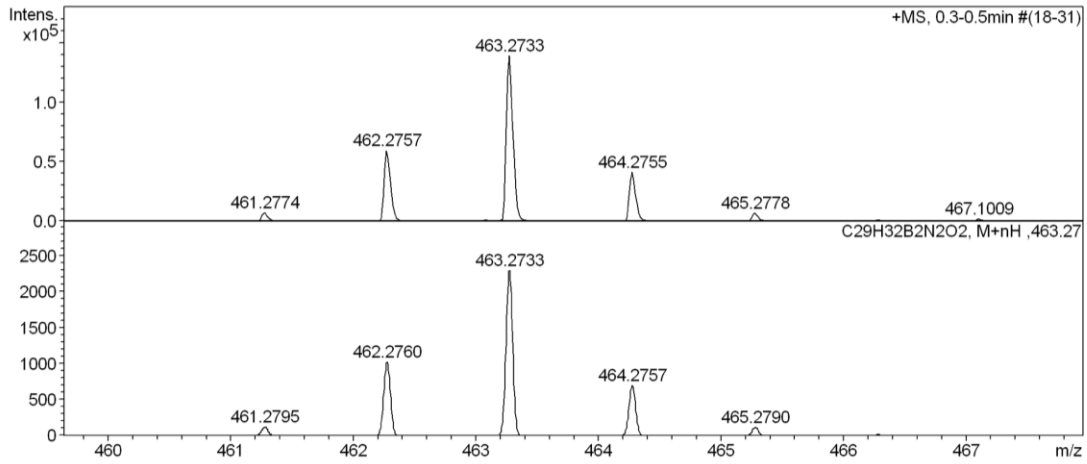


Figure S17. HRMS of compound **6**

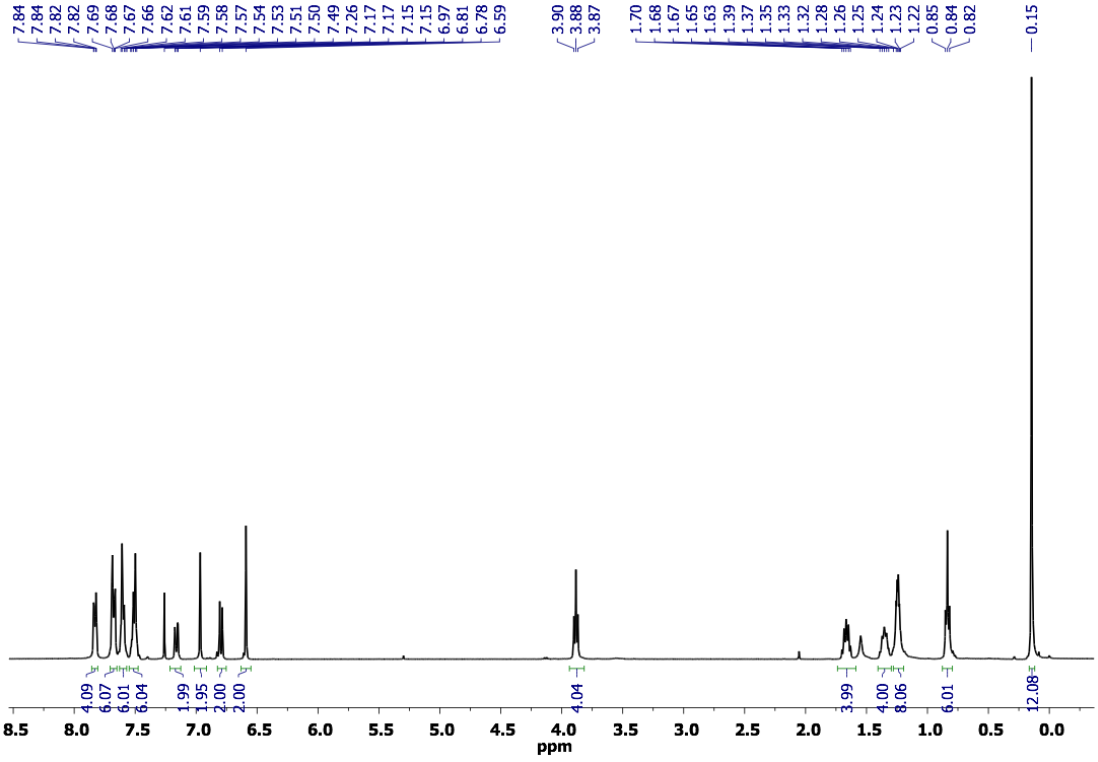


Figure S18. ^{1}H NMR spectrum of compound **7**

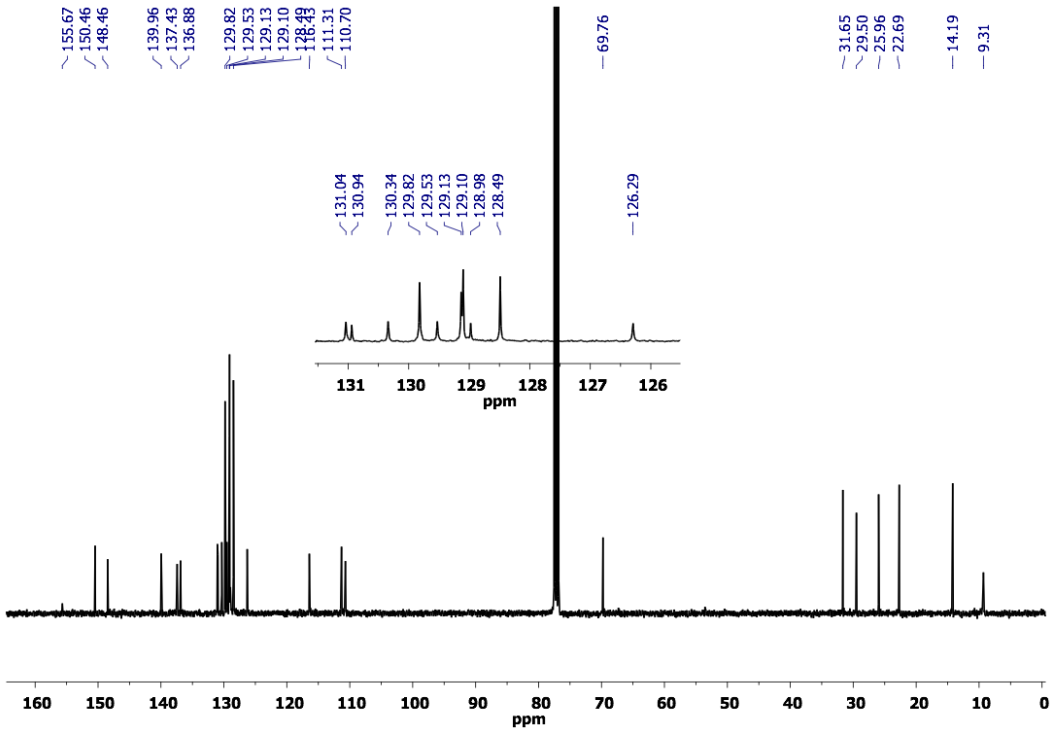


Figure S19. ^{13}C NMR spectrum of compound **7**

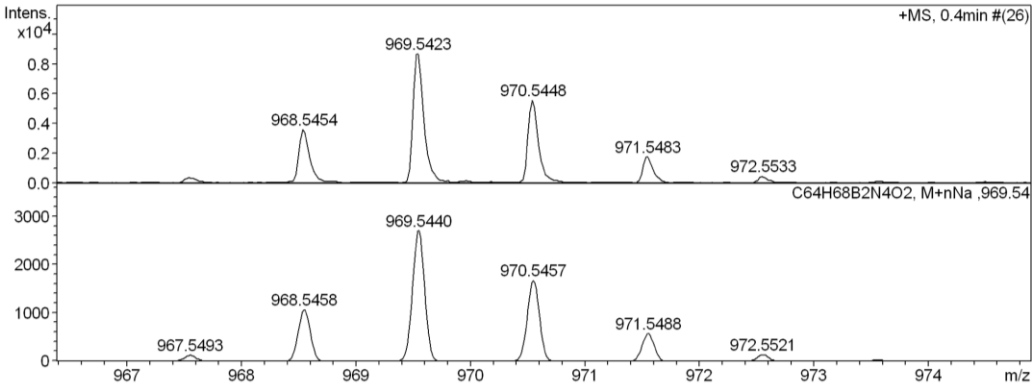


Figure S20. HRMS of compound **7**

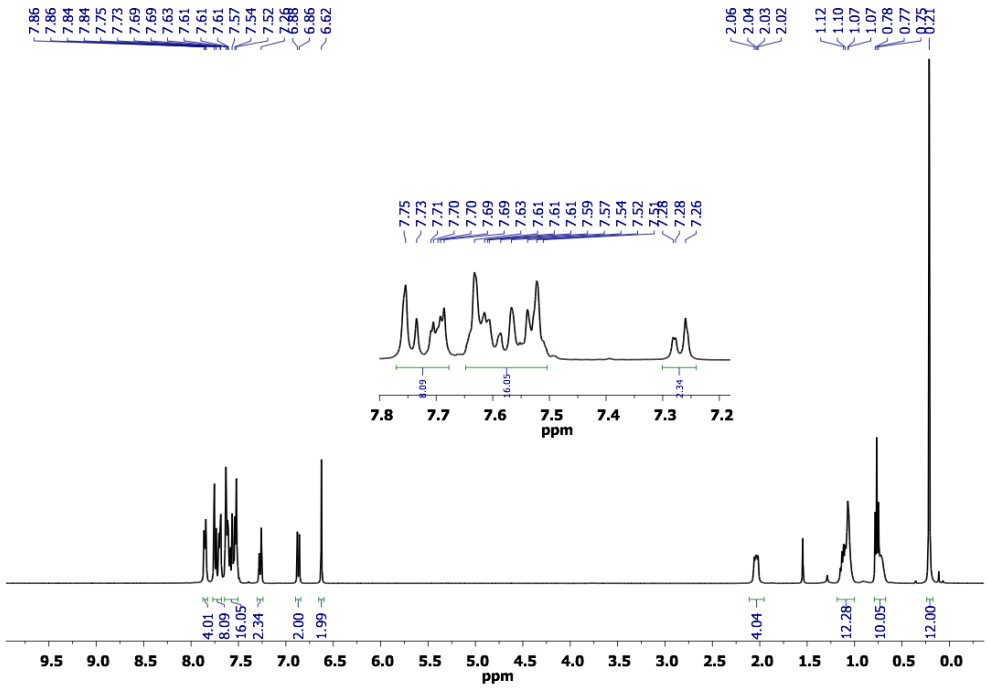


Figure S21. ^{1}H NMR spectrum of compound **8**

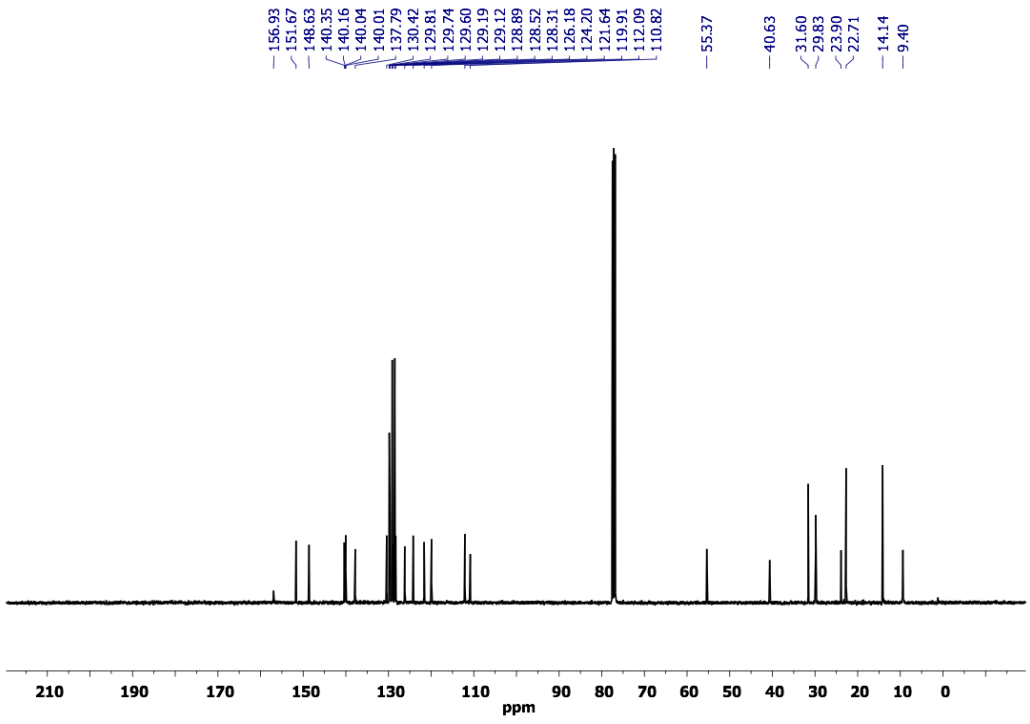


Figure S22. ^{13}C NMR spectrum of compound **8**

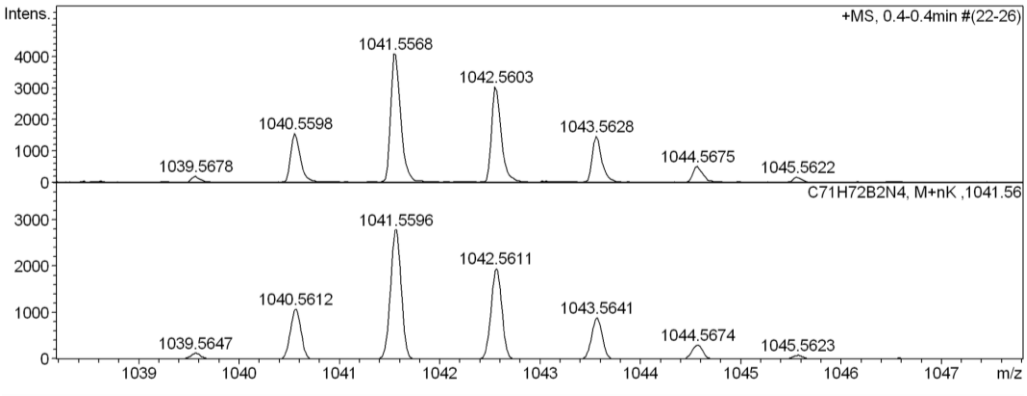


Figure S23. HRMS of compound **8**

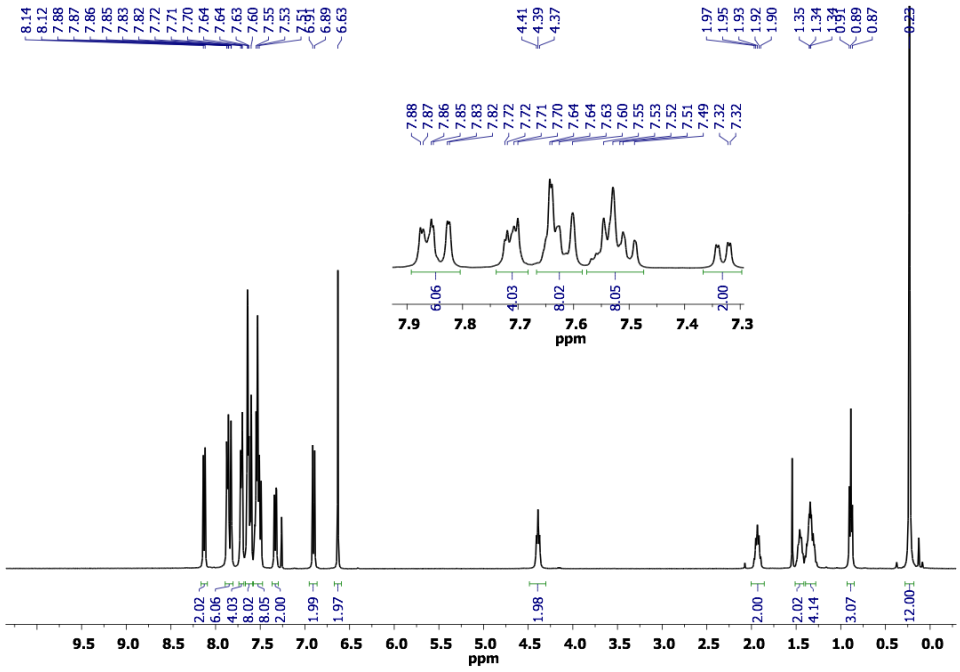


Figure S24. ^{1}H NMR spectrum of compound **9**

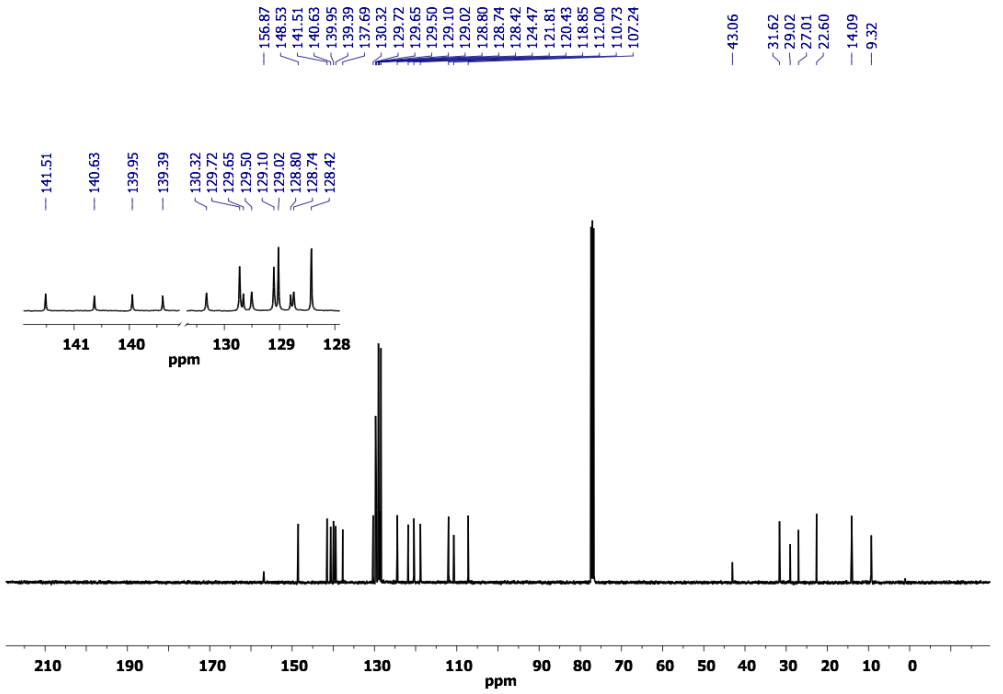


Figure S25. ^{13}C NMR spectrum of compound **9**

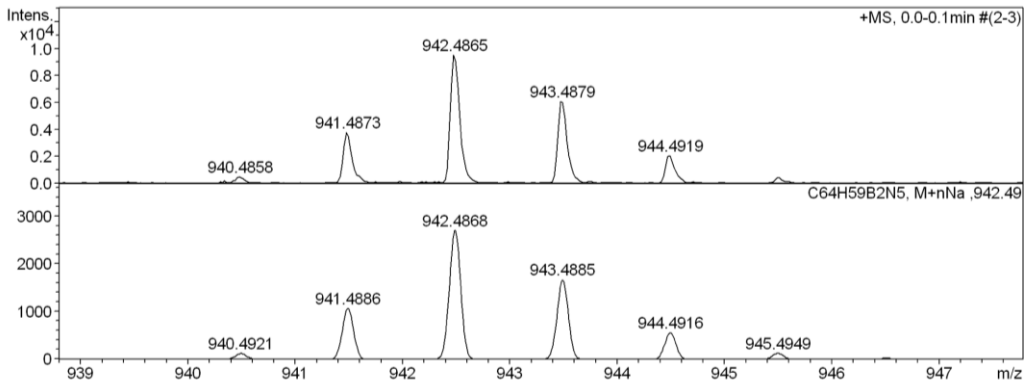


Figure S26. HRMS of compound **9**

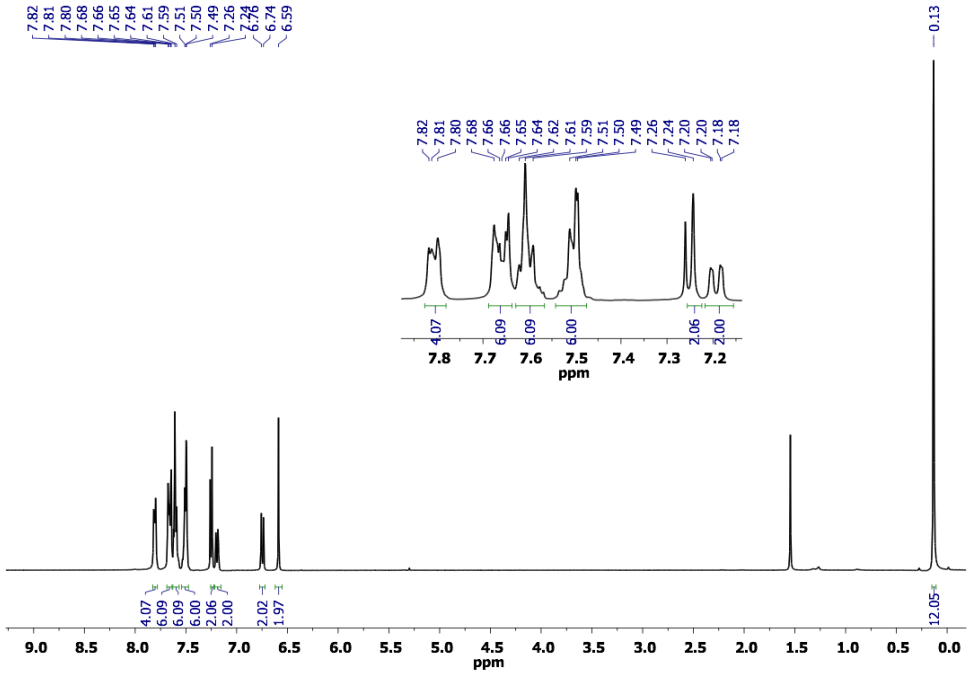


Figure S27. ^{1}H NMR spectrum of compound **10**

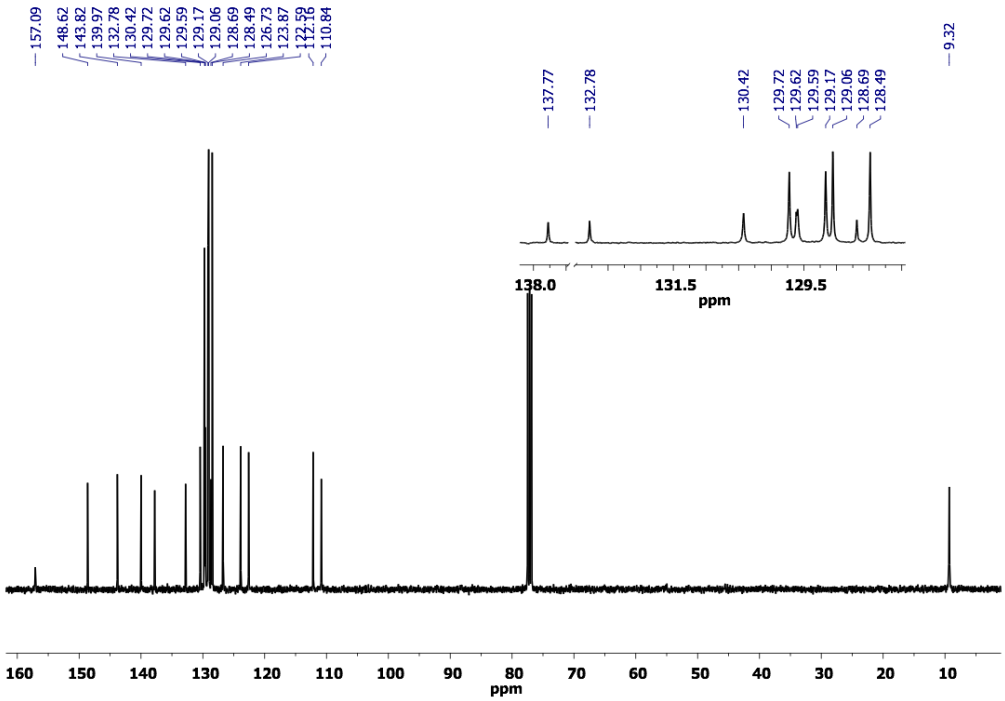


Figure S28. ^{13}C NMR spectrum of compound **10**

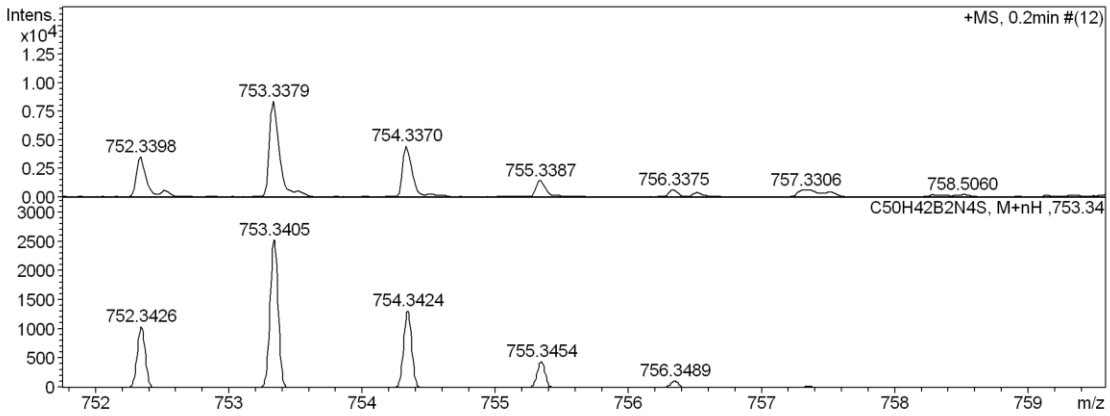


Figure S29. HRMS of compound **10**

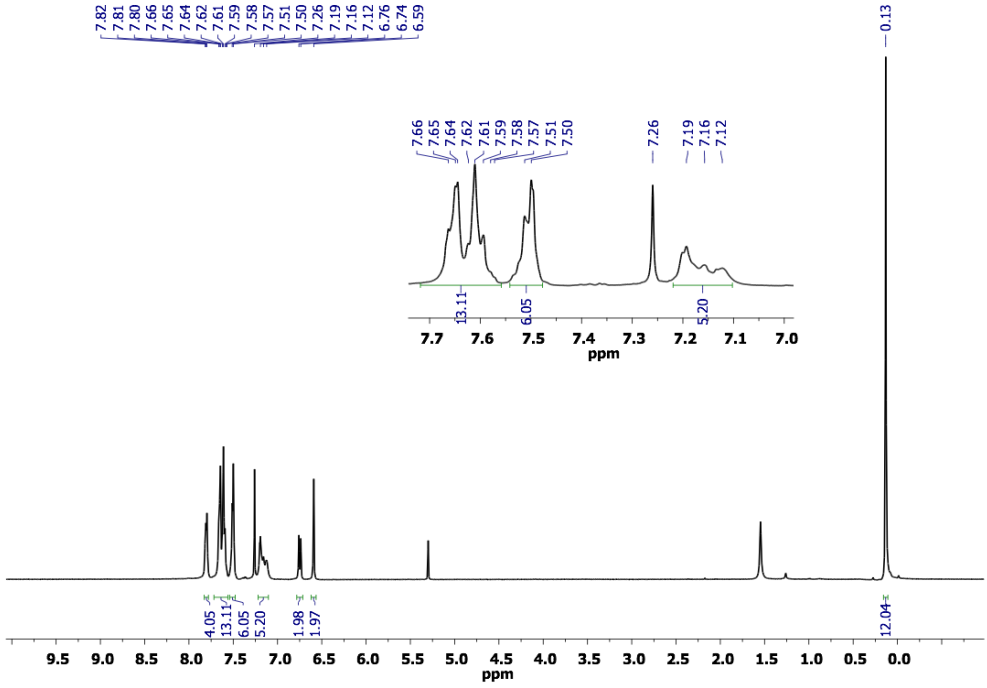


Figure S30. ^{1}H NMR spectrum of compound **11**

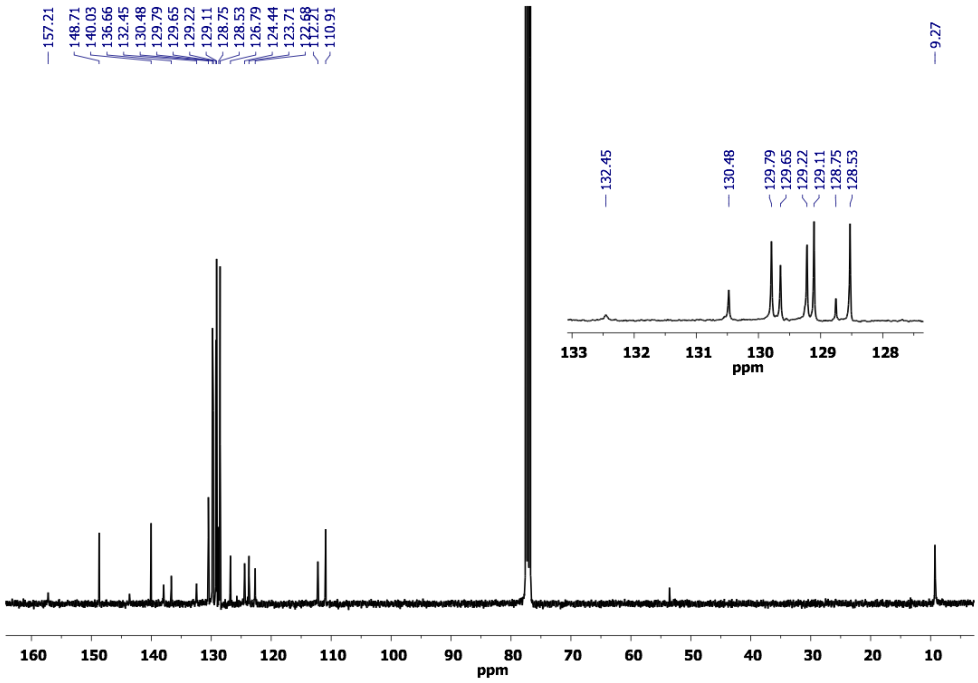


Figure S31. ^{13}C NMR spectrum of compound **11**

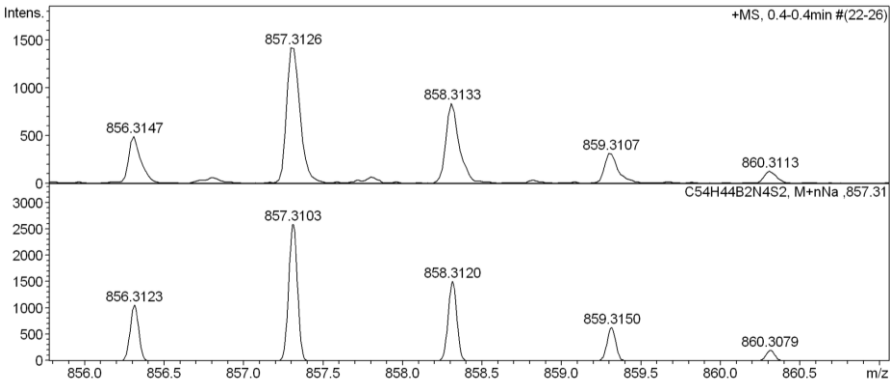


Figure S32. HRMS of compound **11**

Optimized x,y,z coordinates for compounds **4** and **7-11** calculated on Gaussian 03 at the B3LYP//6-31g(d) level

Compound **4**

N	-3.738925	-3.918374	0.916289
N	-3.111384	-3.850419	-0.297380
C	-7.451469	-6.045670	3.877468
H	-8.148893	-6.365493	4.646915
C	-7.913473	-5.738265	2.596251
H	-8.972434	-5.813217	2.364463
C	-7.018357	-5.326672	1.610795
H	-7.380923	-5.072837	0.618557
C	-5.647301	-5.211393	1.893823
C	-4.728965	-4.823770	0.807583
C	-2.139931	-2.108982	0.879976
C	-1.271165	-1.026051	0.994712
H	-1.239374	-0.510076	1.948769
C	-0.461609	-0.582363	-0.071974
C	-2.174212	-2.772286	-0.350510
C	-3.681964	-4.718937	-1.181422
C	-3.220116	-4.984405	-2.557266
C	-4.139095	-4.925791	-3.615871
H	-5.161202	-4.617000	-3.416342
C	-3.742560	-5.244716	-4.914409
H	-4.462441	-5.187944	-5.726158
C	-2.425406	-5.628512	-5.170600
H	-2.116210	-5.875146	-6.182509
C	-1.899473	-5.383253	-2.821627
H	-1.186329	-5.453070	-2.005321
C	-1.505913	-5.697718	-4.121129
H	-0.481618	-6.005071	-4.312615
C	-1.414864	-2.377415	-1.448978
H	-1.470389	-2.881429	-2.405301
C	-0.567091	-1.284156	-1.290771
H	0.018970	-0.981989	-2.150230
C	-2.390348	-3.398033	3.230088
H	-1.751743	-2.627859	3.686098
H	-1.725293	-4.234049	2.970876
H	-3.068028	-3.738481	4.023475
C	-4.724448	-5.338815	-0.501053
H	-5.351799	-6.130026	-0.883643
C	-6.089118	-5.943216	4.164263
H	-5.720795	-6.190248	5.156187
C	-5.190230	-5.533442	3.180402
H	-4.131140	-5.477856	3.401406
C	-4.399501	-1.769729	2.358215
H	-4.019814	-0.925007	2.950523
H	-5.148779	-2.276176	2.981635
H	-4.923584	-1.340150	1.493665

B	-3.166303	-2.747868	1.953313
N	3.738925	3.918374	-0.916289
N	3.111384	3.850419	0.297380
C	7.451469	6.045670	-3.877468
H	8.148893	6.365493	-4.646915
C	7.913473	5.738265	-2.596251
H	8.972434	5.813217	-2.364463
C	7.018357	5.326672	-1.610795
H	7.380923	5.072837	-0.618557
C	5.647301	5.211393	-1.893823
C	4.728965	4.823770	-0.807583
C	2.139931	2.108982	-0.879976
C	1.271165	1.026051	-0.994712
H	1.239374	0.510076	-1.948769
C	0.461609	0.582363	0.071974
C	2.174212	2.772286	0.350510
C	3.681964	4.718937	1.181422
C	3.220116	4.984405	2.557266
C	4.139095	4.925791	3.615871
H	5.161202	4.617000	3.416342
C	3.742560	5.244716	4.914409
H	4.462441	5.187944	5.726158
C	2.425406	5.628512	5.170600
H	2.116210	5.875146	6.182509
C	1.899473	5.383253	2.821627
H	1.186329	5.453070	2.005321
C	1.505913	5.697718	4.121129
H	0.481618	6.005071	4.312615
C	1.414864	2.377415	1.448978
H	1.470389	2.881429	2.405301
C	0.567091	1.284156	1.290771
H	-0.018970	0.981989	2.150230
C	2.390348	3.398033	-3.230088
H	1.751743	2.627859	-3.686098
H	1.725293	4.234049	-2.970876
H	3.068028	3.738481	-4.023475
C	4.724448	5.338815	0.501053
H	5.351799	6.130026	0.883643
C	6.089118	5.943216	-4.164263
H	5.720795	6.190248	-5.156187
C	5.190230	5.533442	-3.180402
H	4.131140	5.477856	-3.401406
C	4.399501	1.769729	-2.358215
H	4.019814	0.925007	-2.950523
H	5.148779	2.276176	-2.981635
H	4.923584	1.340150	-1.493665
B	3.166303	2.747868	-1.953313

Compound **7** (hexyl replaced by –Me)

C	-0.827145	1.101095	0.442785
C	-1.417464	-0.172133	0.444808
C	-0.556102	-1.289719	0.443441
C	0.827220	-1.101144	0.442789
C	1.417510	0.172064	0.444799
C	0.556154	1.289659	0.443397
C	-2.900205	-0.282214	0.432971
C	-3.581828	-1.192010	1.262503
C	-4.973627	-1.247039	1.290496
C	-5.673936	-0.368968	0.464393
C	-5.054464	0.535479	-0.404690
C	-3.660511	0.565454	-0.394905
N	-7.096038	-0.274254	0.329535
C	-8.186492	-0.968795	0.765184
C	-9.269217	-0.495950	0.031006
C	-8.782096	0.508032	-0.824204
N	-7.456226	0.632709	-0.628570
C	-8.204644	-1.961199	1.856478
C	-7.721531	-1.647761	3.137662
C	-7.815645	-2.576605	4.172376
C	-8.401682	-3.824454	3.946337
C	-8.895440	-4.139122	2.679438
C	-8.799713	-3.213392	1.640644
B	-6.119193	1.373155	-1.286535
C	-6.075686	1.041101	-2.876580
C	-9.577468	1.308705	-1.773192
C	-10.510146	0.653782	-2.594248
C	-11.313545	1.378859	-3.472151
C	-11.200722	2.768878	-3.538900
C	-10.283766	3.428497	-2.718666
C	-9.479305	2.706548	-1.837935
O	-1.144280	-2.529008	0.433892
C	-0.314900	-3.670943	0.312687
C	2.900228	0.282173	0.432921
C	3.660516	-0.565459	-0.394957
C	5.054487	-0.535455	-0.404770
C	5.673928	0.368987	0.464329
C	4.973605	1.247009	1.290505
C	3.581823	1.191930	1.262532
B	6.119248	-1.372866	-1.286823
C	6.080289	-2.964710	-0.939299
N	7.096028	0.274367	0.329424
N	7.456239	-0.632731	-0.628534
C	8.782142	-0.508156	-0.824066
C	9.269268	0.495782	0.031183
C	8.186497	0.968772	0.765204
C	9.577532	-1.308956	-1.772930
C	9.479451	-2.706822	-1.837385

C	10.283932	-3.428898	-2.717990
C	11.200826	-2.769388	-3.538386
C	11.313574	-1.379352	-3.471917
C	10.510153	-0.654146	-2.594137
C	8.204558	1.961291	1.856422
C	7.721844	1.647719	3.137725
C	7.815845	2.576641	4.172379
C	8.401372	3.824696	3.946146
C	8.894733	4.139494	2.679127
C	8.799123	3.213677	1.640392
O	1.144362	2.528942	0.433771
C	0.314923	3.670842	0.312595
C	-6.080335	2.964781	-0.937825
C	6.075904	-1.039823	-2.876720
H	-6.346958	3.199193	0.102660
H	-6.717576	3.570792	-1.594647
H	-5.055101	3.333778	-1.084510
H	11.825698	-3.335259	-4.224014
H	10.197394	-4.511292	-2.757119
H	8.784487	-3.224520	-1.187247
H	3.141172	-1.242965	-1.069061
H	-3.015456	-1.863908	1.896076
H	-5.472616	-1.957640	1.936949
H	-7.279262	-0.672697	3.320316
H	-7.438285	-2.321835	5.158835
H	-8.474854	-4.546288	4.755067
H	8.474467	4.546590	4.754829
H	7.438800	2.321782	5.158935
H	7.279960	0.672504	3.320500
H	5.472604	1.957585	1.936978
H	3.015415	1.863708	1.896219
H	-10.301255	-0.785672	0.161233
H	-9.351806	-5.107973	2.496416
H	-9.174829	-3.460295	0.651586
H	-10.587111	-0.429230	-2.554808
H	-12.023363	0.857136	-4.108336
H	-11.825586	3.334644	-4.224621
H	-10.197155	4.510877	-2.758017
H	-8.784301	3.224337	-1.187914
H	-3.141163	1.242937	-1.069016
H	-5.137061	1.417573	-3.307431
H	-6.890820	1.527174	-3.429717
H	-6.117789	-0.033205	-3.101866
H	1.489096	-1.958191	0.459702
H	5.137451	-1.416260	-3.307968
H	6.891270	-1.525417	-3.429945
H	6.117838	0.034622	-3.101357
H	12.023345	-0.857713	-4.108223
H	10.587068	0.428878	-2.554908
H	10.301310	0.785468	0.161467

H	9.173956	3.460658	0.651246
H	9.350697	5.108506	2.495964
H	5.055010	-3.333509	-1.086183
H	6.346961	-3.199980	0.100985
H	6.717445	-3.570234	-1.596645
H	-1.489017	1.958139	0.459713
H	0.289676	-3.636918	-0.603442
H	0.352811	-3.785525	1.177606
H	-0.991671	-4.526651	0.266741
H	-0.289684	3.636790	-0.603510
H	-0.352763	3.785380	1.177541
H	0.991654	4.526579	0.266622

Compound **8**

N	9.028654	-0.426901	0.036024
N	-9.097079	1.023026	0.143314
N	-9.001023	-0.237360	-0.378659
C	0.178001	5.820969	-2.381235
H	1.050402	6.140894	-1.793588
H	-0.705329	6.173233	-1.829444
C	11.208775	-5.089785	-0.912974
H	11.467212	-6.126698	-1.109030
C	10.354896	-4.769116	0.145232
H	9.953145	-5.554587	0.779251
C	10.022680	-3.439815	0.400514
H	9.371327	-3.191858	1.233615
C	10.534841	-2.412519	-0.409028
C	10.261173	-0.992990	-0.114179
C	7.673905	-0.778157	-0.262608
C	6.841704	0.330232	-0.064125
C	5.483070	0.155470	-0.321859
H	4.810068	1.001628	-0.205043
C	4.961524	-1.071126	-0.775067
C	3.511418	-1.229905	-1.047869
C	2.552559	-0.593477	-0.232570
H	2.885588	-0.006196	0.619501
C	1.198871	-0.739984	-0.500276
C	0.006055	-0.142076	0.247193
C	-1.162096	-0.701041	-0.566625
C	-2.523061	-0.516882	-0.368575
H	-2.881473	0.075167	0.469663
C	-3.456476	-1.124422	-1.234175
C	-4.914512	-0.937392	-1.029713
C	-5.432306	0.282121	-0.553443
H	-4.747958	1.104356	-0.358474
C	-6.796666	0.472839	-0.340157
B	-7.603591	1.750453	0.235481

C	-10.368402	1.195414	0.549337
C	-10.901258	2.424336	1.166223
C	-11.700786	2.311993	2.315489
H	-11.863492	1.333057	2.757801
C	-12.261546	3.444978	2.901873
H	-12.869550	3.343298	3.796701
C	-12.036422	4.705496	2.345332
H	-12.472071	5.589569	2.802862
C	-11.256287	-4.695490	-1.937490
H	-11.541685	-5.660773	-2.346350
C	-11.519455	-4.395629	-0.600073
H	-12.007470	-5.127391	0.037692
C	-11.152198	-3.156995	-0.074530
H	-11.348280	-2.925426	0.968429
C	-10.513130	-2.203637	-0.881488
C	-10.208494	-0.870673	-0.327260
C	-11.251775	4.824555	1.196896
H	-11.080321	5.801165	0.752631
C	-10.690004	3.693185	0.606586
H	-10.100047	3.788263	-0.297238
C	-11.090370	0.020107	0.275126
H	-12.149231	-0.133548	0.420844
C	-7.643398	-0.598303	-0.649391
C	-7.189230	-1.831586	-1.113364
H	-7.858559	-2.659143	-1.310519
C	-5.816424	-1.985016	-1.296099
H	-5.437190	-2.948156	-1.624177
C	-2.971638	-1.914207	-2.295032
H	-3.679642	-2.360864	-2.987207
C	-1.606540	-2.108990	-2.497192
H	-1.262791	-2.719316	-3.328778
C	-0.696763	-1.501770	-1.629421
C	0.767626	-1.526998	-1.587562
C	1.703312	-2.166081	-2.403419
H	1.385683	-2.768114	-3.251261
C	3.061084	-2.012110	-2.129062
H	3.791794	-2.481794	-2.781316
C	0.032933	1.415732	0.226139
H	-0.853892	1.775878	0.766944
H	0.900666	1.745999	0.814935
C	0.081973	2.077742	-1.156714
H	0.969371	1.729124	-1.700934
H	-0.787183	1.760830	-1.747793
C	0.107267	3.610559	-1.077108
H	0.978349	3.932324	-0.486689
H	-0.778493	3.963275	-0.527586
C	0.151187	4.288685	-2.452327
H	1.035989	3.935978	-3.002959
H	-0.720386	3.968483	-3.042624
C	-0.045812	-0.601066	1.733892

H	0.823322	-0.170844	2.251742
H	-0.930592	-0.140625	2.196344
C	-0.081026	-2.114401	1.982678
H	0.814846	-2.580832	1.552377
H	-0.940465	-2.552862	1.459021
C	-0.167821	-2.459860	3.475810
H	0.692928	-2.021266	4.003485
H	-1.061184	-1.982205	3.901545
C	-0.204467	-3.971052	3.745129
H	-1.076657	-4.408815	3.236570
H	0.679386	-4.432531	3.281963
C	-0.241338	-4.357344	5.233197
H	-0.121563	-5.446242	5.316208
H	0.628482	-3.917101	5.741922
C	-1.523740	-3.943173	5.965162
H	-1.652519	-2.855155	5.981394
H	-1.512876	-4.288162	7.005627
H	-2.409466	-4.373739	5.481019
C	11.186334	0.014768	0.135816
H	12.259752	-0.099423	0.162813
C	10.458492	1.174271	0.457299
N	9.145162	0.888358	0.392835
B	7.660872	1.639316	0.414216
C	7.678037	2.846491	-0.673205
H	7.975279	2.526138	-1.681064
H	8.344706	3.667497	-0.376747
H	6.670897	3.277761	-0.762287
C	11.022119	2.488010	0.819308
C	12.066132	3.013637	0.040495
H	12.398327	2.472222	-0.840930
C	12.656204	4.230738	0.375567
H	13.456022	4.629750	-0.242326
C	12.215934	4.937104	1.496543
H	12.674550	5.886953	1.757627
C	11.186222	4.416183	2.282168
H	10.844974	4.955567	3.161451
C	10.593966	3.198281	1.950666
H	9.809182	2.787463	2.574444
C	11.731478	-4.073941	-1.714661
H	12.395813	-4.316509	-2.539411
C	11.398807	-2.742840	-1.464059
H	11.797386	-1.951653	-2.092550
C	7.217777	-2.012246	-0.722604
H	7.880860	-2.852461	-0.883961
C	5.852774	-2.142465	-0.972032
H	5.470484	-3.103803	-1.302174
C	-7.500651	3.041890	-0.751238
H	-7.934846	2.877222	-1.747592
H	-6.440164	3.282008	-0.913132
H	-7.956207	3.946891	-0.329239

C	-7.288279	2.080558	1.795358
H	-7.943854	2.864606	2.197739
H	-6.258703	2.453019	1.892976
H	-7.373783	1.206951	2.455918
C	-10.261831	-2.509137	-2.229351
H	-9.787307	-1.769398	-2.867622
C	-10.627558	-3.748989	-2.750247
H	-10.429179	-3.972455	-3.794802
C	7.244591	2.104212	1.919166
H	6.158960	2.274119	1.951321
H	7.709505	3.050162	2.225042
H	7.462483	1.354286	2.692892
C	0.218558	6.489423	-3.759140
H	0.237704	7.582203	-3.674660
H	-0.659606	6.216923	-4.357675
H	1.109049	6.183221	-4.322058

Compound **9**

N	8.929480	-0.348859	0.018223
N	-8.973521	0.893161	-0.597056
N	-8.912147	-0.447714	-0.335829
C	11.239711	-4.749191	1.659179
H	11.526644	-5.728963	2.030837
C	10.340012	-3.962132	2.382181
H	9.930667	-4.324278	3.321152
C	9.970915	-2.704189	1.909060
H	9.282889	-2.088042	2.480754
C	10.492138	-2.220865	0.697539
C	10.178198	-0.862454	0.214258
C	7.596870	-0.857628	-0.094916
C	6.734108	0.161099	-0.516839
C	5.391742	-0.175736	-0.682840
H	4.696308	0.582349	-1.035679
C	4.914919	-1.479868	-0.450349
C	3.478416	-1.812239	-0.624612
C	2.492920	-0.880239	-0.266870
H	2.781750	0.071393	0.167379
C	1.150314	-1.218001	-0.441221
C	-1.107585	-1.227679	-0.484489
C	-2.458745	-0.901321	-0.361667
H	-2.772045	0.047629	0.061300
C	-3.421475	-1.842343	-0.755588
C	-4.867155	-1.525457	-0.637612
C	-5.350819	-0.227714	-0.890013
H	-4.649539	0.542743	-1.202227
C	-6.702000	0.093811	-0.770388
B	-7.471352	1.501102	-0.974296
C	-10.223063	1.303291	-0.310934
C	-10.718100	2.683776	-0.463426

C	-11.479986	3.247783	0.573094
H	-11.639754	2.681064	1.486212
C	-12.007316	4.531570	0.447238
H	-12.586466	4.958078	1.261731
C	-11.785629	5.268298	-0.717849
H	-12.195158	6.269963	-0.816264
C	-11.272807	-4.944961	0.927196
H	-11.583953	-5.964977	1.134941
C	-11.468487	-3.944865	1.880816
H	-11.929435	-4.183279	2.835320
C	-11.068012	-2.635546	1.614983
H	-11.211260	-1.857751	2.359557
C	-10.462524	-2.311931	0.391384
C	-10.120851	-0.906469	0.100402
C	-11.038085	4.711076	-1.756842
H	-10.869818	5.274697	-2.670399
C	-10.509992	3.426457	-1.635189
H	-9.949255	2.989954	-2.452919
C	-10.966282	0.197188	0.137889
H	-12.018285	0.184754	0.381051
C	-7.571508	-0.942643	-0.409813
C	-7.150640	-2.243254	-0.138056
H	-7.835528	-3.021114	0.174282
C	-5.789638	-2.517862	-0.256643
H	-5.433563	-3.515960	-0.020115
C	-3.000111	-3.095561	-1.261619
H	-3.750056	-3.807388	-1.592904
C	-1.653998	-3.419712	-1.377509
H	-1.358526	-4.386743	-1.776723
C	-0.685618	-2.488370	-0.986212
C	0.758875	-2.482073	-0.958710
C	1.749674	-3.404402	-1.313697
H	1.478136	-4.373601	-1.724475
C	3.087616	-3.068501	-1.147269
H	3.855343	-3.773254	-1.451695
C	-0.003558	0.871813	0.401158
H	0.876314	1.407633	0.026744
H	-0.878332	1.397431	0.001465
C	-0.025505	0.893269	1.937189
H	0.852109	0.351083	2.313495
H	-0.906597	0.340005	2.288467
C	-0.042909	2.319242	2.502566
H	0.838198	2.868397	2.137212
H	-0.919691	2.851706	2.108784
C	-0.055308	2.353866	4.037520
H	-0.951879	1.831990	4.403789
H	0.804556	1.778363	4.408604
C	-0.006195	3.765014	4.646340
H	0.119169	3.670922	5.733427
H	0.891718	4.284196	4.281563

C	-1.243943	4.624552	4.362268
H	-1.369362	4.822528	3.291890
H	-1.173336	5.594400	4.867947
H	-2.157426	4.130643	4.716902
C	11.071083	0.168008	-0.059701
H	12.144234	0.126631	0.052852
C	10.306668	1.299166	-0.396682
N	9.003205	0.967883	-0.343619
B	7.503938	1.563063	-0.752572
C	7.547007	2.049549	-2.302157
H	7.896483	1.273824	-2.996962
H	8.183068	2.933516	-2.445877
H	6.536655	2.334682	-2.627954
C	10.827776	2.635655	-0.737272
C	11.904642	2.734501	-1.633539
H	12.293131	1.834100	-2.101225
C	12.456723	3.975876	-1.943525
H	13.283129	4.037290	-2.646378
C	11.944612	5.135661	-1.358665
H	12.373674	6.104118	-1.600950
C	10.881027	5.045026	-0.458977
H	10.483546	5.942300	0.007378
C	10.326870	3.804708	-0.145447
H	9.515345	3.736587	0.569028
C	11.771140	-4.271399	0.460363
H	12.470973	-4.878592	-0.107031
C	11.401721	-3.014280	-0.017658
H	11.807545	-2.644614	-0.954926
C	7.187099	-2.170024	0.133249
H	7.874259	-2.946457	0.444215
C	5.836799	-2.464004	-0.047391
H	5.488648	-3.472419	0.154643
C	-7.402376	2.020452	-2.516932
H	-7.888289	1.345759	-3.235993
H	-6.348736	2.088673	-2.822954
H	-7.824841	3.023809	-2.656931
C	-7.083853	2.633876	0.124937
H	-7.718270	3.527057	0.046642
H	-6.049948	2.969371	-0.039445
H	-7.140490	2.277880	1.162718
C	-10.280104	-3.321904	-0.567639
H	-9.832736	-3.076502	-1.526506
C	-10.678871	-4.629702	-0.297368
H	-10.533428	-5.401644	-1.047918
C	7.006533	2.711562	0.291157
H	5.917252	2.827529	0.197306
H	7.435508	3.700927	0.086565
H	7.200948	2.469932	1.345875
N	0.012464	-0.466028	-0.167474

Compound **10**

S	0.000075	0.363555	0.000493
N	-7.427406	-0.739623	0.083495
N	6.786344	0.330208	0.478328
N	-6.786198	0.330454	-0.478156
C	6.507733	-3.279976	0.290280
H	6.658573	-3.119100	1.367228
H	7.319549	-3.923624	-0.072235
H	5.585743	-3.870725	0.193415
C	-11.862462	-2.878501	1.758429
H	-12.667162	-3.493191	2.152521
C	-10.944565	-3.418792	0.856018
H	-11.036196	-4.454003	0.539075
C	-9.910176	-2.633982	0.348179
H	-9.213224	-3.050891	-0.368724
C	-9.776638	-1.295340	0.745603
C	-8.728591	-0.415085	0.197736
C	-5.035244	-1.066303	0.111999
C	-3.681783	-1.373424	0.219804
H	-3.386266	-2.313124	0.679325
C	-2.679681	-0.481759	-0.215440
C	-1.264867	-0.848837	-0.102361
C	1.264966	-0.848911	0.102883
C	2.679801	-0.481916	0.215947
C	3.075006	0.756935	0.757055
H	2.321998	1.456538	1.108338
C	4.418635	1.102457	0.877956
H	4.694280	2.063556	1.292352
C	5.365763	0.171994	0.453924
C	7.671414	1.335021	0.741833
C	7.362963	2.604041	1.428254
C	6.770339	2.620020	2.701732
H	6.487655	1.683636	3.174108
C	6.554481	3.827968	3.362544
H	6.096150	3.826958	4.347561
C	6.935504	5.033044	2.767336
H	6.767305	5.973175	3.285258
C	-6.936319	5.033092	-2.767746
H	-6.768374	5.973200	-3.285792
C	-6.553868	3.828129	-3.362254
H	-6.094683	3.827163	-4.346873
C	-6.769399	2.620209	-2.701280
H	-6.485644	1.683910	-3.173180
C	-7.363123	2.604145	-1.428315
C	-7.671355	1.335159	-0.741788
C	-5.365605	0.172254	-0.453567
C	-4.418408	1.102897	-0.877039
H	-4.693981	2.064189	-1.291047

C	-3.074799	0.757320	-0.756088
H	-2.321725	1.457089	-1.106912
N	7.427573	-0.739788	-0.083454
C	8.728729	-0.415100	-0.197833
C	8.912458	0.885668	0.304802
H	9.851974	1.406361	0.415005
C	7.536138	5.024863	1.507575
H	7.834725	5.958450	1.038933
C	7.750669	3.818181	0.841736
H	8.209536	3.810662	-0.142787
C	9.776870	-1.295103	-0.745824
C	10.711451	-0.755609	-1.645019
H	10.611010	0.278749	-1.961883
C	11.744923	-1.542535	-2.149384
H	12.454513	-1.113873	-2.851853
C	11.862846	-2.877895	-1.759040
H	12.667597	-3.492428	-2.153274
C	10.944047	-3.418898	-0.857969
H	11.035005	-4.454528	-0.542210
C	9.909598	-2.634295	-0.349948
H	9.211993	-3.051802	0.365951
B	6.341315	-1.904338	-0.566852
C	5.035318	-1.066359	-0.112016
C	3.681833	-1.373425	-0.219758
H	3.386259	-2.312940	-0.679615
C	6.477981	-2.102056	-2.173655
H	5.689722	-2.779645	-2.531096
H	7.435385	-2.558583	-2.458975
H	6.374554	-1.167727	-2.742043
C	0.706943	-2.108016	0.057387
H	1.299007	-3.014187	0.124052
C	-0.706888	-2.107971	-0.057167
H	-1.299008	-3.014092	-0.124043
C	-6.477943	-2.102009	2.173503
H	-5.689836	-2.779812	2.530883
H	-7.435453	-2.558295	2.458857
H	-6.374241	-1.167720	2.741904
C	-11.743723	-1.543667	2.150328
H	-12.452635	-1.115598	2.853844
C	-10.710318	-0.756535	1.646141
H	-10.609215	0.277427	1.964089
C	-8.912422	0.885646	-0.304901
H	-9.852019	1.406167	-0.415262
C	-7.752261	3.818183	-0.842504
H	-8.211973	3.810609	0.141625
C	-7.538055	5.024824	-1.508505
H	-7.837754	5.958324	-1.040402
B	-6.341379	-1.904232	0.566661
C	-6.508084	-3.279787	-0.290496
H	-5.586388	-3.870947	-0.193284

H	-6.658459	-3.118866	-1.367507
H	-7.320347	-3.923028	0.071722

Compound **11**

S	-2.144334	0.511043	0.228356
N	-8.757054	-0.593211	-0.173673
N	-9.067362	0.739028	-0.203345
C	-9.875157	-1.340665	0.059518
C	-10.922555	-0.438585	0.207627
H	-11.963836	-0.689937	0.343887
C	-10.387977	0.850454	0.030402
C	-11.137914	2.118670	0.076014
C	-12.074939	2.313433	1.104269
H	-12.186891	1.555298	1.874418
C	-12.838354	3.477993	1.156028
H	-13.551859	3.618495	1.963413
C	-12.681190	4.462376	0.178363
H	-13.275298	5.371266	0.218726
C	-11.759010	4.272275	-0.852246
H	-11.637545	5.029699	-1.621725
C	-10.994130	3.107999	-0.907987
H	-10.295786	2.955501	-1.721914
C	-9.947195	-2.814148	0.067953
C	-10.550182	-3.469071	1.152424
H	-10.891653	-2.886017	2.002865
C	-10.696714	-4.856073	1.147457
H	-11.158844	-5.351378	1.996833
C	-10.246370	-5.604554	0.058952
H	-10.359596	-6.685076	0.055886
C	-9.652698	-4.959733	-1.028899
H	-9.309798	-5.535791	-1.883841
C	-9.507358	-3.573607	-1.028867
H	-9.059772	-3.073428	-1.882903
C	-7.344440	-0.809986	-0.197411
C	-6.690643	-2.038716	-0.107930
H	-7.225736	-2.973870	-0.004167
C	-5.299178	-2.032676	-0.126827
H	-4.768586	-2.973846	-0.022686
C	-4.570364	-0.831426	-0.243781
C	-5.284719	0.380987	-0.319377
H	-4.734849	1.314598	-0.417522
C	-6.676485	0.417663	-0.284653
C	-3.106501	-0.867953	-0.277973
C	-2.278113	-1.898057	-0.669980
H	-2.654474	-2.842896	-1.046582
C	-0.897363	-1.596451	-0.576595
H	-0.113923	-2.293551	-0.855365
C	-0.636643	-0.323753	-0.109158

C	-7.609744	2.651933	0.960924
H	-7.662665	2.120644	1.920887
H	-8.400504	3.414081	0.960656
H	-6.653424	3.193696	0.950515
C	-7.628527	2.448408	-1.763194
H	-6.589751	2.754186	-1.952456
H	-8.224388	3.369989	-1.788442
H	-7.927715	1.828977	-2.620589
B	-7.695719	1.672183	-0.331862
S	2.144335	-0.511090	-0.228243
N	8.757054	0.593211	0.173669
N	9.067379	-0.739024	0.203307
C	9.875138	1.340686	-0.059541
C	10.922545	0.438624	-0.207691
H	11.963818	0.689994	-0.343977
C	10.387991	-0.850427	-0.030476
C	11.137949	-2.118629	-0.076137
C	12.074933	-2.313360	-1.104435
H	12.186835	-1.555213	-1.874580
C	12.838371	-3.477903	-1.156241
H	13.551843	-3.618381	-1.963660
C	12.681273	-4.462300	-0.178579
H	13.275399	-5.371176	-0.218979
C	11.759136	-4.272229	0.852074
H	11.637725	-5.029663	1.621552
C	10.994234	-3.107970	0.907862
H	10.295928	-2.955493	1.721825
C	9.947148	2.814170	-0.067959
C	10.550091	3.469120	-1.152439
H	10.891552	2.886084	-2.002896
C	10.696593	4.856125	-1.147458
H	11.158689	5.351451	-1.996840
C	10.246261	5.604583	-0.058932
H	10.359462	6.685107	-0.055856
C	9.652631	4.959735	1.028926
H	9.309740	5.535775	1.883884
C	9.507321	3.573606	1.028881
H	9.059767	3.073406	1.882922
C	7.344439	0.809971	0.197451
C	6.690629	2.038697	0.108022
H	7.225712	2.973859	0.004274
C	5.299165	2.032645	0.126951
H	4.768562	2.973812	0.022849
C	4.570365	0.831383	0.243886
C	5.284733	-0.381025	0.319431
H	4.734874	-1.314644	0.417563
C	6.676498	-0.417687	0.284674
C	3.106502	0.867898	0.278109
C	2.278114	1.897983	0.670164
H	2.654475	2.842814	1.046788

C	0.897364	1.596370	0.576796
H	0.113925	2.293454	0.855605
C	0.636645	0.323685	0.109324
C	7.609752	-2.651914	-0.960983
H	7.662647	-2.120598	-1.920933
H	8.400520	-3.414053	-0.960752
H	6.653438	-3.193687	-0.950567
C	7.628585	-2.448462	1.763141
H	6.589809	-2.754230	1.952423
H	8.224431	-3.370054	1.788344
H	7.927807	-1.829061	2.620545
B	7.695747	-1.672197	0.331828

Compound **Pz**

N	-0.265820	0.556302	-0.010346
N	1.042183	0.917598	-0.008005
C	-3.115537	3.653012	-0.270160
C	-2.010655	3.774685	0.575655
H	-1.875976	4.673225	1.171510
C	-1.076052	2.745231	0.668150
C	-1.245530	1.587909	-0.099007
C	-0.422545	-0.814696	-0.006761
C	-1.702140	-1.540578	0.083045
C	-1.902188	-2.682047	-0.710884
H	-1.133437	-2.975054	-1.420359
C	-3.076950	-3.425715	-0.604972
H	-3.215552	-4.304202	-1.229479
C	-4.073053	-3.039131	0.293099
H	-4.989943	-3.616510	0.374494
C	-3.274051	2.497439	-1.036889
H	-4.122203	2.399418	-1.708745
C	-2.337909	1.466176	-0.963384
H	-2.447651	0.579209	-1.576996
C	1.735781	-0.224489	-0.007296
C	0.858166	-1.337622	-0.014147
H	1.105982	-2.387856	0.029364
C	-2.708321	-1.164755	0.989417
H	-2.562462	-0.296539	1.624329
C	-3.883327	-1.907081	1.089008
H	-4.649879	-1.604474	1.797324
C	3.208168	-0.208506	-0.001188
C	3.945142	-1.402766	-0.021512
H	3.427926	-2.357854	-0.043617
C	5.339171	-1.380885	-0.015493
H	5.891063	-2.317172	-0.031389
C	6.022973	-0.164597	0.010057

H	7.109566	-0.147249	0.014397
C	5.298732	1.030389	0.029323
H	5.821817	1.983119	0.048407
C	3.906728	1.010710	0.024148
H	3.341412	1.936658	0.037850
H	-3.844287	4.456014	-0.335834
H	-0.210538	2.825869	1.315949

Compound **Pz-B**

N	0.763033	0.439613	-0.085698
N	-0.591977	0.261059	-0.072305
C	4.984471	-0.788494	-1.050218
H	5.618130	-0.364937	-1.825108
C	3.620561	-0.491386	-1.037740
H	3.197139	0.148423	-1.803964
C	2.786947	-1.029107	-0.044969
C	1.331859	-0.778494	-0.030843
C	0.312715	-1.748280	0.019313
H	0.441446	-2.821017	0.007792
C	-0.900010	-1.066449	-0.021714
C	-2.262037	-1.638019	-0.075375
C	-2.709727	-2.471081	0.961822
H	-2.071935	-2.637726	1.825799
C	-3.969698	-3.070715	0.893247
H	-4.307277	-3.708377	1.706038
C	-4.793514	-2.847893	-0.212922
H	-5.773793	-3.314221	-0.265839
C	3.343219	-1.882306	0.923154
H	2.706127	-2.297659	1.699721
C	4.707062	-2.177963	0.908062
H	5.125158	-2.831105	1.669709
C	-3.092696	-1.426025	-1.188653
H	-2.747318	-0.795778	-2.003907
C	-4.350964	-2.025513	-1.254312
H	-4.983425	-1.854931	-2.121564
C	-1.292109	1.503935	0.062806
C	-0.372112	2.559511	0.121275
C	-0.901085	3.847443	0.255561
H	-0.228636	4.701870	0.302912
C	-2.282997	4.052672	0.342513
H	-2.677541	5.060145	0.451890
C	-3.162845	2.965081	0.297921
H	-4.235040	3.125494	0.374493
C	-2.675016	1.662400	0.156421
H	-3.357768	0.822258	0.127908
B	1.159471	2.048627	0.040201
C	1.927747	2.587830	-1.291749
H	1.473392	2.250276	-2.235415

H	2.992372	2.319203	-1.313059
H	1.888052	3.687129	-1.304824
C	2.001080	2.262263	1.416387
H	2.988555	1.780288	1.380795
H	1.482201	1.888885	2.311288
H	2.180722	3.335397	1.578019
C	5.532443	-1.629852	-0.077968
H	6.594934	-1.858793	-0.089765