Electronic Supplementary Material (ESI) for RSC Advances.

Experimental

All chemicals and starting materials were commercially available and were used without further purification. Solvents were distilled as per the standard methods and purged with nitrogen before use. All reactions were carried out under argon atmosphere unless otherwise indicated. Column chromatography was carried out on Merck silica gel. Thin layer chromatography (TLC) was performed on silica gel (Merck TLCSilicaGel60).

Measurements

NMR spectra were measured in deuterated chloroform by using Bruker Avance 400 MHz (^{1}H and ^{13}C NMR).

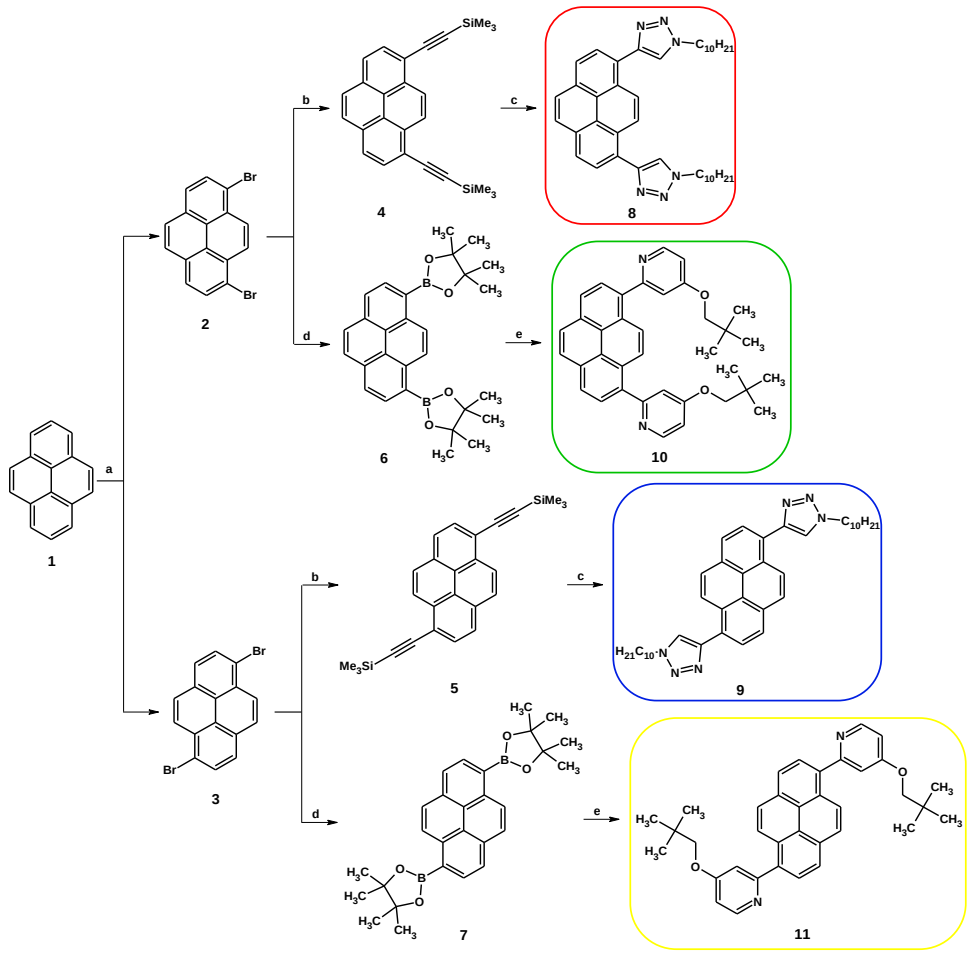
High-resolution mass spectrometry (HRMS) measurements were conducted by using Mass Spectrometer QTOF (Impact HD, Bruker).

Thermogravimetric analysis (TGA) was carried out by using Pyris 1 TGA Perkin-Elmer.

UV/Vis spectra were measured by using Perkin–Elmer Lambda Bio 40 UV/Vis spectrophotometer at room temperature with a conventional 1.0 cm quartz cell.

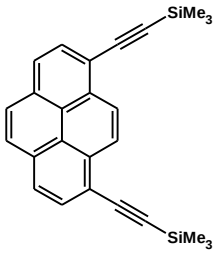
The emission and excitation spectra were measured by using spectrophotometer Hitachi F-7000. The quantum yields of fluorescence were determined by the absolute method at room temperature, using the integrating sphere with solvent as a blank (FLS-980 spectrophotometer). The time-resolved measurement has been prepared at optically diluted solutions at room temperature using the time-correlated single photon counting methods on the FLS-980 spectrophotometer. Excitation wavelengths were obtained using the picosecond pulsed diode EPLED–375 nm and nm with 50 ns pulse period as light sources. PMT (Hamamatsu, R928P) in cooled housing was used as a detector. The system was leveled at emission wavelengths. In addition, for the analysis of a fluorescence decay, an instrument response function was got. The IRF contains information about the time response of the overall optical and electronic system. The IRF was designated using LUDOX solution as a standard at 375 nm.

- **Synthesis route for disubstituted pyrene derivatives 1a-b and 2a-b**



Scheme S1. Synthesis of disubstituted pyrene derivatives **8-11**.

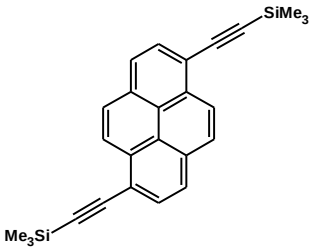
4



^{1}H NMR (400 MHz, $CDCl_3$) δ 8.66 (s, 2H), 8.19 – 8.06 (m, 4H), 8.03 (s, 2H), 0.40 (s, 18H).

^{13}C NMR (101 MHz, $CDCl_3$) δ 132.43, 131.51, 130.38, 128.29, 126.62, 125.14, 124.09, 118.46, 104.07, 100.89, 0.35.

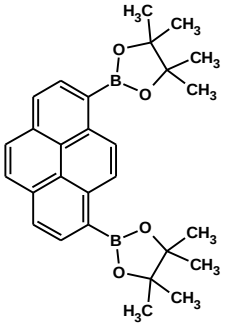
5



^{1}H NMR (400 MHz, $CDCl_3$) δ 8.57 (d, J = 9.1 Hz, 2H), 8.18 – 8.09 (m, 6H), 0.39 (s, 18H).

^{13}C NMR (101 MHz, $CDCl_3$) δ 132.40, 131.30, 130.32, 128.26, 126.42, 125.12, 124.05, 118.38, 104.07, 100.80, 0.34.

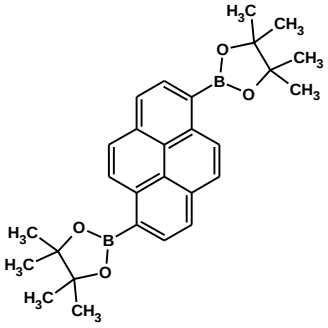
6



^{1}H NMR (400 MHz, $CDCl_3$) δ 9.12 (d, *J* = 9.2 Hz, 2H), 8.53 (d, *J* = 7.7 Hz, 2H), 8.19 (d, *J* = 7.7 Hz, 2H), 8.16 – 8.09 (m, 2H), 1.26 (s, 24H).

^{13}C NMR (101 MHz, $CDCl_3$) δ 136.53, 133.80, 133.17, 129.25, 127.99, 124.56, 124.50, 84.01, 83.60, 25.17, 25.14.

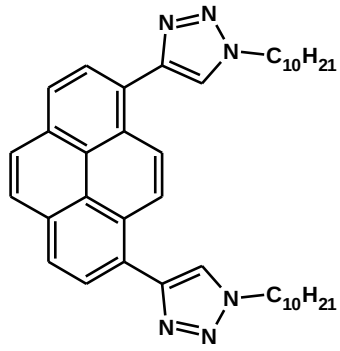
7



^{1}H NMR (400 MHz, $CDCl_3$) δ 9.12 (d, *J* = 9.2 Hz, 2H), 8.54 (d, *J* = 7.7 Hz, 2H), 8.19 (d, *J* = 7.7 Hz, 2H), 8.13 (d, *J* = 9.2 Hz, 2H), 1.50 (s, 24H).

^{13}C NMR (101 MHz, $CDCl_3$) δ 136.63, 133.85, 133.26, 129.32, 128.02, 124.59, 84.07, 25.23.

Procedure for synthesis 8 and 9: In a 150 mL round-bottom flask, bis((trimethylsilyl)ethynyl)pyrene **4**/**5** (0.438 g, 1.110 mmol), decyl azide (0.488 g, 2.660 mmol), ethanol (50 mL) and water (50 mL) were placed. The mixture was saturated with argon, and then KF (0.155 g, 2.660 mmol), $CuSO_4 \cdot 5H_2O$ (0.663 g, 2.660 mmol), sodium ascorbate (0.527 g, 2.660 mmol) and pyridine (2 mL) were added. The mixture was stirred at room temperature for 48 h. Then, dichloromethane (30 mL) and 5% solution of ammonia (20 mL) were added, and the mixture was stirred for 30 min. The mixture was extracted with water (50 mL) and dichloromethane (2 x 50 mL). The combined organic layers were dried with anhydrous $MgSO_4$, and the volatile fractions were evaporated. The crude product was purified by column chromatography (silica gel; CH_2Cl_2, ethyl acetate).

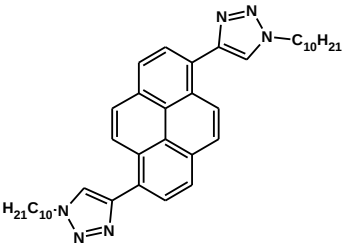


8 was obtained as yellow solid (0.630 g, 92%)

^{1}H NMR (400 MHz, $CDCl_3$) δ 8.69 (s, 2H), 8.29 (d, *J* = 7.9 Hz, 2H), 8.23 (d, *J* = 8.0 Hz, 2H), 8.09 (s, 2H), 7.96 (s, 2H), 4.52 (t, *J* = 7.2 Hz, 4H), 2.04 (dd, *J* = 14.1, 7.1 Hz, 4H), 1.75 (s, 4H), 1.51 – 1.35 (m, 10H), 1.27 (s, 12H), 0.87 (dd, *J* = 8.4, 5.1 Hz, 8H).

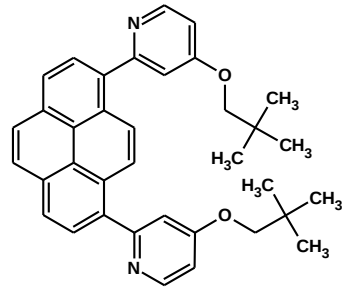
^{13}C NMR (101 MHz, $CDCl_3$) δ 147.46, 147.25, 131.55, 131.08,

128.93, 128.32, 128.13, 127.83, 127.48, 127.36, 125.82, 125.61, 125.56, 125.38, 125.29, 125.05, 122.95, 50.71, 31.98, 30.55, 29.61, 29.54, 29.39, 29.17, 26.74, 22.78, 14.21.
HRMS (ESI): *m/z* calcd. for $C_{40}H_{53}N_6$ [MH^+] 617.4326; found 617.4322.

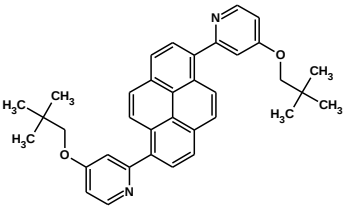


9 was obtained as yellow solid (0.603 g, 88%)
^{1}H NMR (400 MHz, $CDCl_3$) δ 8.73 (d, *J* = 9.2 Hz, 2H), 8.24 (q, *J* = 7.9 Hz, 4H), 8.12 (d, *J* = 9.3 Hz, 2H), 7.95 (s, 2H), 4.54 (t, *J* = 7.2 Hz, 4H), 2.12 – 2.01 (m, 6H), 1.51 – 1.37 (m, 10H), 1.28 (s, 14H), 0.88 (t, *J* = 6.6 Hz, 8H).
^{13}C NMR (101 MHz, $CDCl_3$) δ 147.62, 131.24, 129.12, 128.18, 127.55, 126.04, 125.44, 125.08, 122.88, 50.73, 32.01, 30.57, 29.63, 29.57, 29.40, 29.21, 26.82, 22.78, 14.16.
HRMS (ESI): *m/z* calcd. for $C_{40}H_{53}N_6$ [MH^+] 617.4326; found 617.4326.

Procedure for synthesis 10 and 11: In 100 mL round-bottom flask, bis(4,4,5,5-tetramethyl-1,3,2-dioxaborolan-2-yl)pyrene **6**/**7** (0.86 g, 1.89 mmol), 2-bromo-4-(2,2-dimethylpropyloxy)pyridine (1.030 g, 4.200 mmol), potassium phosphate trihydrate (0.173 g, 12.000 mmol), [$Pd(PPh_3)_4$] (0.173 g, 0.150 mmol) and 40 mL of DME/water mixture (3:1 v/v) were placed. The mixture was saturated with argon, heated to 105 ºC and stirred for 48 h. After cooling to room temperature, the mixture was extracted with chloroform (3 x 50 mL) and water (3 x 50 mL). The combined organic layers were dried, and the solvent was evaporated. The crude product was purified by column chromatography (silica gel; dichloromethane:ethyl acetate (2:1)).



10 was obtained as yellow solid (0.809 g, 81%)
^{1}H NMR (400 MHz, $CDCl_3$) δ 8.68 (d, *J* = 5.7 Hz, 2H), 8.43 (d, *J* = 9.2 Hz, 2H), 8.24 (d, *J* = 7.9 Hz, 2H), 8.15 (d, *J* = 7.8 Hz, 2H), 8.11 (d, *J* = 9.3 Hz, 2H), 7.27 (d, *J* = 2.4 Hz, 2H), 6.93 (dd, *J* = 5.8, 2.4 Hz, 2H), 3.76 (s, 4H), 1.08 (d, *J* = 4.6 Hz, 18H).
^{13}C NMR (101 MHz, $CDCl_3$) δ 165.98, 161.32, 150.92, 136.43, 131.25, 129.05, 128.06, 127.66, 125.54, 125.33, 124.88, 112.33, 108.96, 77.95, 32.01, 26.69.
HRMS (ESI): *m/z* calcd. for $C_{36}H_{37}N_2O_2$ [MH^+] 529.2850; found 529.2865.



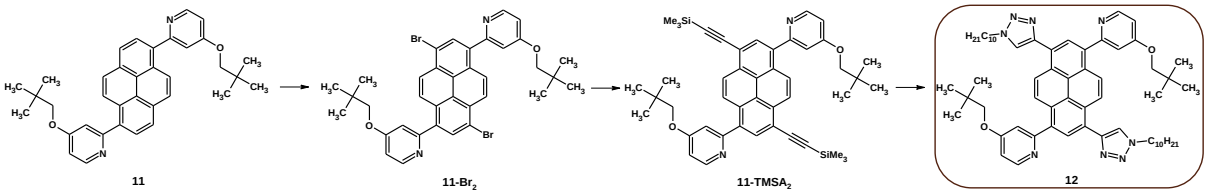
11 was obtained as yellow solid (0.729 g, 73%)

^{1}H NMR (400 MHz, $CDCl_3$) δ 8.67 (d, *J* = 5.8 Hz, 2H), 8.43 (d, *J* = 9.2 Hz, 2H), 8.24 (d, *J* = 7.9 Hz, 2H), 8.15 (d, *J* = 7.9 Hz, 2H), 8.11 (d, *J* = 9.3 Hz, 2H), 7.27 (s, 2H), 6.93 (dd, *J* = 5.8, 2.4 Hz, 2H), 3.76 (s, 4H), 1.09 (s, 18H).

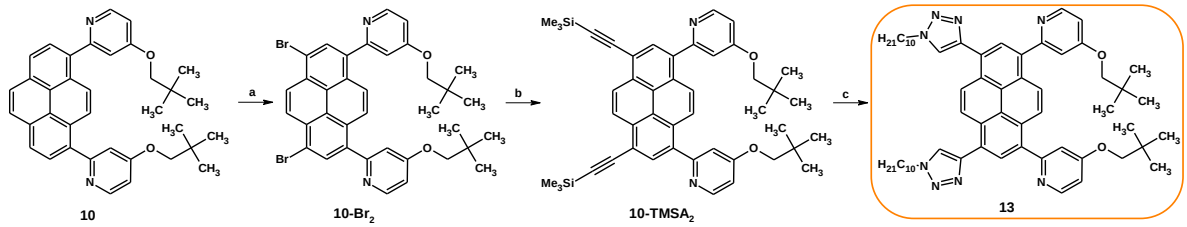
^{13}C NMR (101 MHz, $CDCl_3$) δ 165.95, 161.29, 150.90, 136.41, 131.23, 129.03, 128.04, 127.64, 125.53, 125.31, 124.87, 112.31, 108.93, 77.93, 31.99, 26.67.

HRMS (ESI): *m/z* calcd. for $C_{36}H_{37}N_2O_2$ [MH^+] 529.2850; found 529.2861.

- **Synthesis route for tetrasubstituted pyrene derivatives 12 and 13**

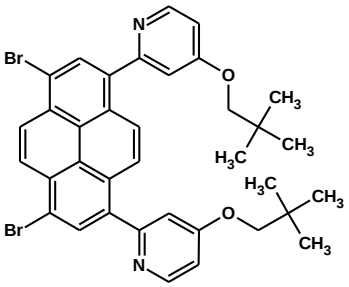


Scheme S2. Synthesis of tetrasubstituted pyrene derivative **12**.

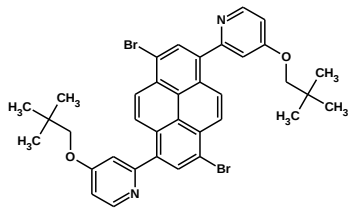


Scheme S3. Synthesis of tetrasubstituted pyrene derivative **13**.

Procedure for synthesis 10-Br_2 and 11-Br_2: In a 25 mL round-bottom flask, bis(4-(2,2-dimethylpropyloxy)pyrid-2-yl)pyrene (0.350 g, 0.660 mmol) was dissolved in dichloromethane (25 mL) and heated up to 40 °C. Over 15 min and under vigorous stirring, bromine (0.420 g, 2.640 mmol) was added to the solution. The obtained mixture was stirring at 40 °C for 2 hours. Then, the mixture was cooled down, and methanol (5 mL) was added, the obtained precipitate was collected by filtration, washed with water and dried in vacuum.

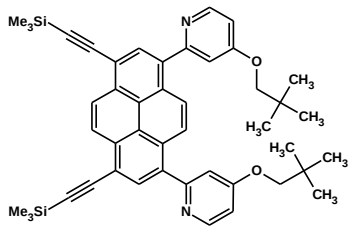


10-Br_2 ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.68 (d, *J* = 5.8 Hz, 2H), 8.57 – 8.39 (m, 6H), 7.26 (d, *J* = 2.4 Hz, 2H), 6.93 (dd, *J* = 5.8, 2.4 Hz, 2H), 3.76 (s, 4H), 1.08 (s, 18H).



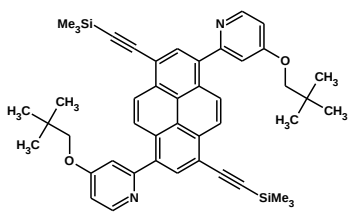
11-Br$_2$ ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.67 (d, *J* = 5.7 Hz, 2H), 8.55 – 8.35 (m, 6H), 7.25 (d, *J* = 2.3 Hz, 2H), 6.96 (dd, *J* = 5.7, 2.3 Hz, 2H), 3.77 (s, 4H), 1.09 (s, 18H).

Procedure for synthesis 10-TMSA$_2$ and 11-TMSA$_2$: In a 50mL three-necked round-bottom flask triethylamine (20 mL) was placed and saturated with argon for 15 minutes. Then **2a/2b-Br$_2$** (0.250 g, 0.360 mmol), [$Pd(PPh_3)_4$] (0.052 g, 0.045 mmol) and CuI (0.009 g, 0.045 mmol) were added and stirred for 30 seconds. Next, DBU (0.055 g, 0.360 mmol) was added, and the stirred during an additional 30 seconds. Trimethylsilylacetylene (TMSA) (0.088 g, 0.90 mmol) was added by syringe. The obtained mixture was stirred at 90 °C for 16 hours. After cooling the mixture to room temperature, the solvent was evaporated. The crude product was dissolved in dichloromethane and purified by column chromatography (silica gel; hexane).



10-TMSA$_2$ ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.65 (d, *J* = 5.7 Hz, 2H), 8.61 (s, 2H), 8.46 (d, *J* = 9.4 Hz, 2H), 8.31 (s, 2H), 7.25 (d, *J* = 2.2 Hz, 2H), 6.93 (dd, *J* = 5.8, 2.4 Hz, 2H), 3.76 (s, 4H), 1.09 (s, 18H), 0.35 (s, 18H).

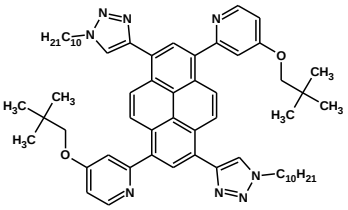
^{13}C NMR (101 MHz, $CDCl_3$) δ 165.95, 160.22, 150.84, 136.38, 132.08, 131.69, 129.10, 126.77, 126.25, 124.74, 118.12, 112.24, 109.01, 103.72, 100.91, 77.91, 31.89, 29.70, 26.56, 0.12.



11-TMSA$_2$ ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.67 (d, *J* = 5.8 Hz, 2H), 8.62 (d, *J* = 9.4 Hz, 2H), 8.47 (d, *J* = 9.4 Hz, 2H), 8.30 (s, 2H), 7.25 (d, *J* = 2.3 Hz, 2H), 6.94 (dd, *J* = 5.8, 2.4 Hz, 2H), 3.76 (s, 4H), 1.09 (s, 18H), 0.35 (s, 18H).

Procedure for synthesis 12 and 13: In a 100 mL round-bottom flask, **10**/**11-TMSA$_2$** (0.260 g, 0.360 mmol), decyl azide (0.163 g, 0.890 mmol), ethanol (50 mL) and water (50 mL) were placed. The mixture was saturated with argon and then KF (0.055 g, 0.890 mmol), $CuSO_4 \cdot 5H_2O$ (0.220 g, 0.890 mmol), sodium ascorbate (0.200 g, 0.890 mmol) and pyridine (0.7 mL) were added. The mixture was stirred at room temperature for 24 hours. Then, dichloromethane (20 mL) and 5% solution of ammonia (10 mL) were added, and the mixture

was stirred for 30 min. The mixture was extracted with water (25 mL) and dichloromethane (2 x 25 mL). The combined organic layers were dried with anhydrous $MgSO_4$, and the volatile fractions were evaporated. The crude product was purified by column chromatography (silica gel; CH_2Cl_2, ethyl acetate).

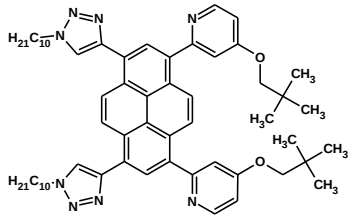


12 was obtained as yellow solid (0.221 g, 65%)

^{1}H NMR (400 MHz, $CDCl_3$) δ 8.74 (d, *J* = 9.6 Hz, 2H), 8.65 (d, *J* = 5.8 Hz, 2H), 8.47 (d, *J* = 9.6 Hz, 2H), 8.45 (s, 2H), 8.00 (s, 2H), 7.32 (d, *J* = 2.2 Hz, 2H), 6.93 (dd, *J* = 5.8, 2.3 Hz, 2H), 4.51 (t, *J* = 7.2 Hz, 4H), 3.76 (s, 4H), 2.09 – 1.99 (m, 4H), 1.41 (dd, *J* = 25.4, 13.1 Hz, 8H), 1.30 (d, *J* = 35.6 Hz, 18H), 1.09 (s, 18H), 0.86 (t, *J* = 6.8 Hz, 8H).

^{13}C NMR (101 MHz, $CDCl_3$) δ 166.02, 160.72, 150.81, 147.30, 136.29, 129.60, 129.14, 128.93, 128.87, 126.17, 126.11, 125.73, 123.21, 112.40, 109.26, 78.01, 50.63, 32.00, 31.96, 30.54, 29.60, 29.52, 29.37, 29.16, 26.72, 26.67, 22.76, 14.20.

HRMS (ESI): *m/z* calcd. for $C_{60}H_{79}N_8O_2$ [MH^+] 943.6321; found 943.6320.



13 was obtained as yellow solid (0.255 g, 75%)

^{1}H NMR (400 MHz, $CDCl_3$) δ 8.75 (d, *J* = 9.4 Hz, 2H), 8.66 (d, *J* = 5.0 Hz, 2H), 8.47 (s, 2H), 8.45 (s, 2H), 8.01 (s, 2H), 7.31 (d, *J* = 11.1 Hz, 2H), 6.94 (d, *J* = 3.1 Hz, 2H), 4.49 (t, *J* = 6.6 Hz, 4H), 3.76 (s, 4H), 2.02 (s, 4H), 1.39 (s, 8H), 1.25 (s, 18H), 1.08 (s, 18H), 0.86 (s, 8H).

^{13}C NMR (126 MHz, $CDCl_3$) δ 166.08, 160.37, 150.52, 147.15, 135.85, 129.10, 128.86, 128.75, 126.05, 125.99, 125.71, 123.27, 112.44, 109.25, 77.99, 50.60, 31.90, 30.45, 29.52, 29.44, 29.30, 29.08, 26.60, 22.70, 14.15.

HRMS (ESI): *m/z* calcd. for $C_{60}H_{79}N_8O_2$ [MH^+] 943.6321; found 943.6302.

Theoretical calculations

Table S1. Contours of selected orbitals with the contribution in their creation for compounds **8-11** (pyrene/heteroaryl), for molecules **12-13** (pyrene/pyridyl/triazolyl).

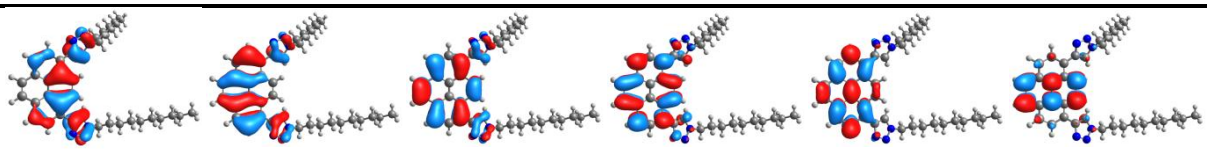
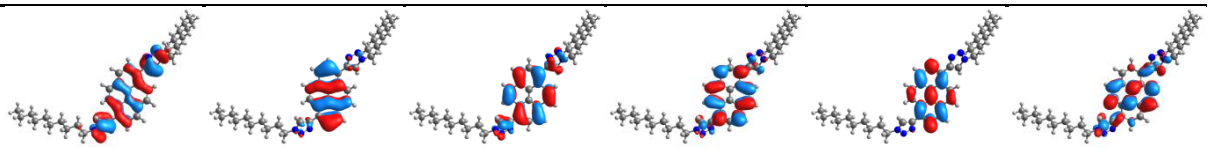
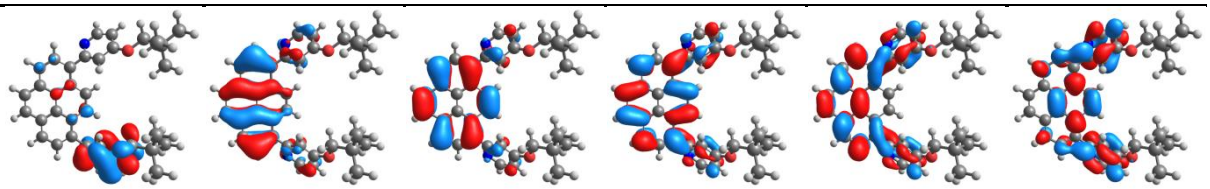
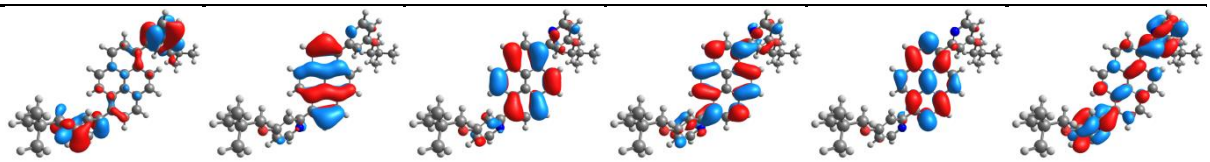
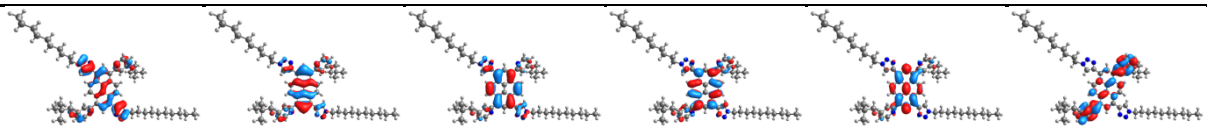
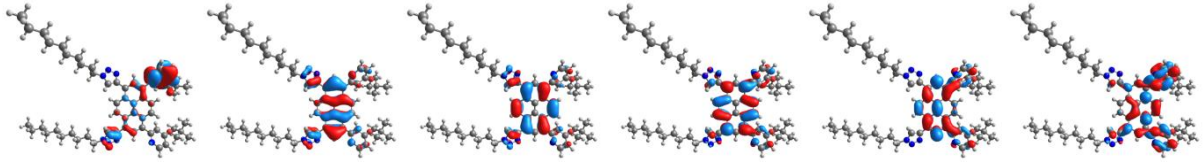
	HOMO-2	HOMO-1	HOMO	LUMO	LUMO+1	LUMO+2
8						
	55/45	78/22	80/20	84/16	93/7	86/14
9						
	38/62	92/8	81/19	85/15	95/5	76/24
10						
	8/92	85/15	86/14	79/21	71/29	52/48
11						
	12/88	91/9	87/13	80/20	89/11	36/64
12						
	28/22/50	73/14/13	75/9/16	74/14/12	81/13/6	39/59/2
13						
	14/75/11	72/11/17	75/10/15	74/15/11	75/21/4	48/44/8

Table S2. Contours of selected orbitals with the contribution in their creation for compounds **P1** and **P4** (pyrene/heteroaryl).

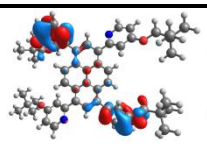
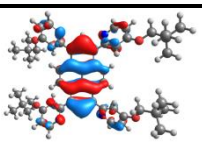
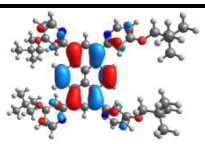
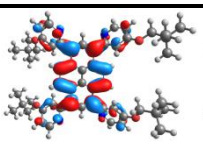
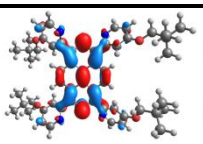
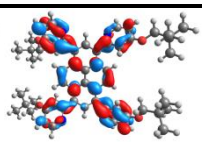
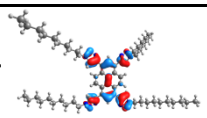
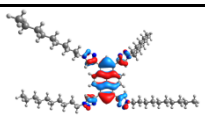
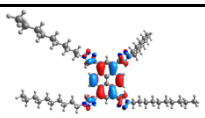
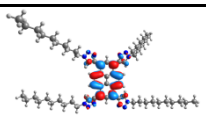
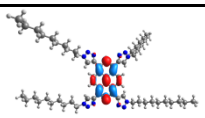
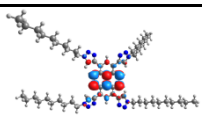
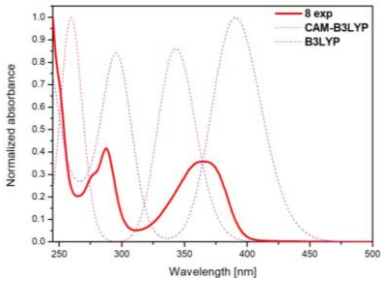
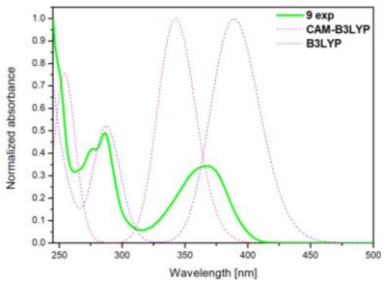
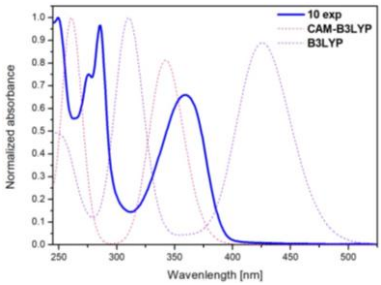
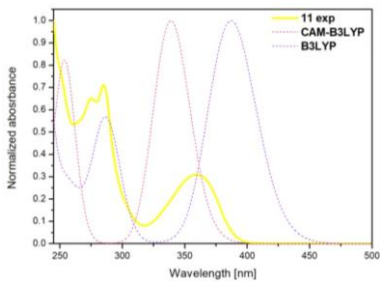
	HOMO-2	HOMO-1	HOMO	LUMO	LUMO+1	LUMO+2
P1						
	9/91	70/30	54/46	52/48	68/32	32/68
P4						
	30/70	69/31	72/28	76/24	88/12	77/23

Table S3. Experimental and theoretically calculated maxima of absorption with CAM-B3LYP or B3LYP hybrid potential and 6-31G(d,p) basis set in chloroform of **8-13**.

8		**experimental**	277, 287, 365
		CAM-B3LYP	260, 343
		B3LYP	295, 390
9		**experimental**	277, 286, 367
		CAM-B3LYP	254, 342
		B3LYP	288, 389
10		**experimental**	276, 286, 359
		CAM-B3LYP	261, 342
		B3LYP	247, 310, 425
11		**experimental**	275, 285, 359
		CAM-B3LYP	254, 339
		B3LYP	286, 387

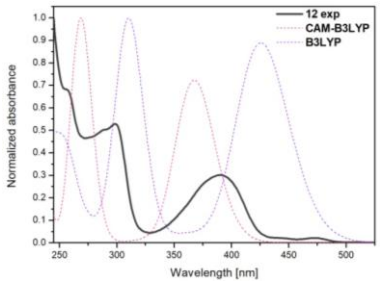
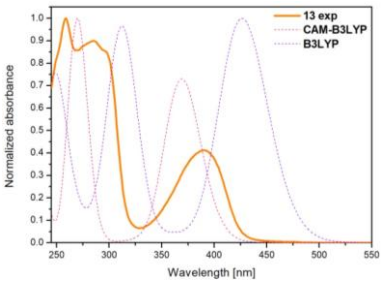
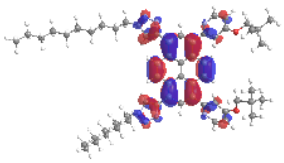
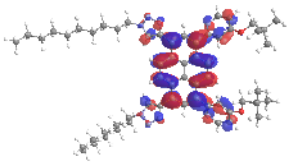
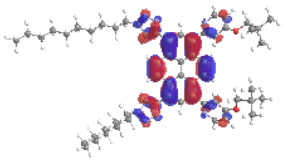
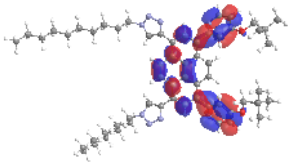
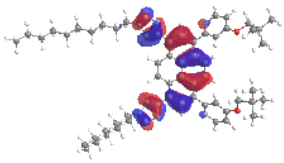
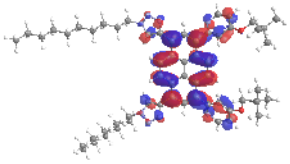
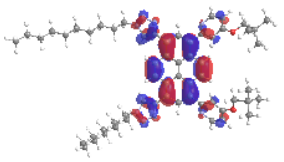
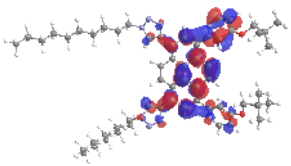
12		**experimental**	255, 298, 390
		CAM-B3LYP	269, 368
		B3LYP	246, 310, 425
13		**experimental**	259, 285, 297, 390
		CAM-B3LYP	270, 369
		B3LYP	249, 312, 426

Table S4. Natural transition orbitals (NTOs) with pairs occupied (holes) and unoccupied (electrons) with contribution higher than 25% for **13** presenting the nature of absorption spectra (6-31G(d,p)/B3LYP) with the contribution of (pyrene/pyridyl/triazolyl) substituents. For each state, the respective number of the state, transition energy, and the oscillator strength are listed.

experimental		**Hole**	**Electron**
390 nm	S_1 2.909 eV (0.870) 98%		
		0.79/0.08/0.13	0.78/0.13/0.09
297 nm	S_3 3.922 eV (0.598) 65%		
		0.79/0.08/0.13	0.52/0.47/0.01
	S_3 3.922 eV (0.598) 32%		
		0.61/0.02/0.37	0.78/0.13/0.09
	S_5 4.088 eV (0.273) 54%		
		0.79/0.08/0.13	0.69/0.23/0.08

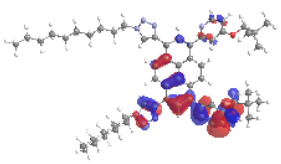
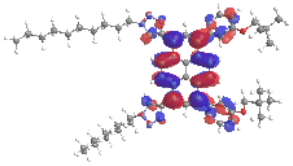
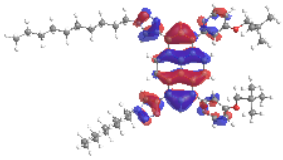
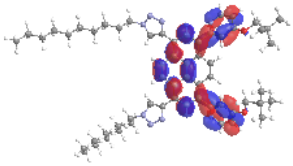
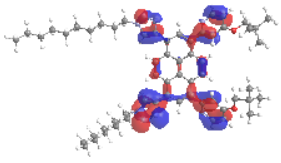
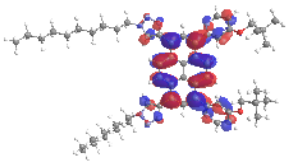
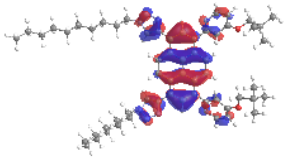
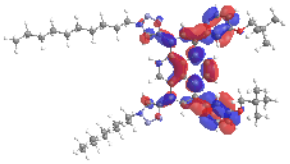
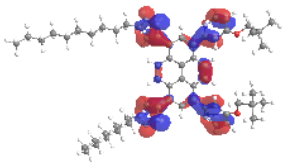
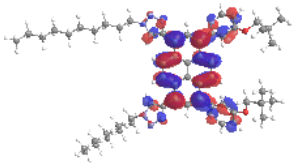
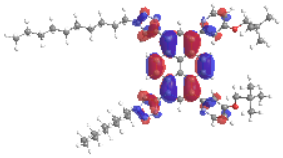
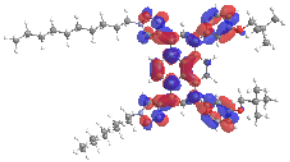
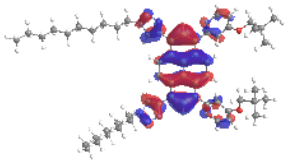
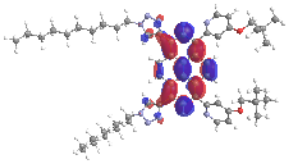
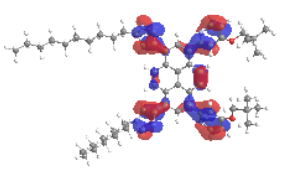
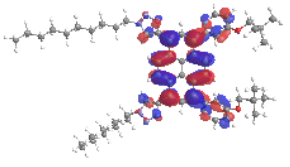
	S_5 4.088 eV (0.273) 40%		
		0.22/0.70/0.08	0.78/0.13/0.09
285 nm	S_{19} 4.785 eV (0.184) 48%		
		0.76/0.09/0.15	0.64/0.35/0.01
	S_{19} 4.785 eV (0.184) 45%		
		0.12/0.31/0.57	0.78/0.13/0.09
	S_{22} 4.926 eV (0.128) 62%		
		0.76/0.09/0.15	0.49/0.44/0.07
	S_{22} 4.926 eV (0.128) 28%		
		0.15/0.29/0.56	0.78/0.13/0.09
259 nm	S_{24} 4.998 eV (0.131) 85%		
		0.79/0.08/0.13	0.45/0.28/0.26
	S_{25} 5.068 eV (0.299) 41%		
		0.76/0.09/0.15	0.93/0.01/0.06
	S_{25} 5.068 eV (0.299) 40%		
		0.18/0.39/0.43	0.78/0.13/0.09

Table S5. Contours of selected orbitals with the contribution in their creation for compound **14** (pyrene/pyridyl/triazolyl).

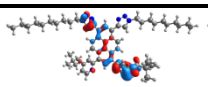
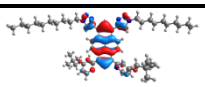
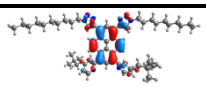
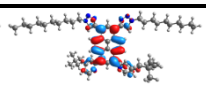
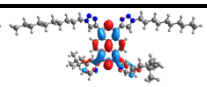
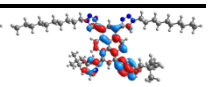
	HOMO-2	HOMO-1	HOMO	LUMO	LUMO+1	LUMO+2
14						
	17/68/15	72/10/18	75/10/15	74/15/11	77/19/4	44/46/10

Table S6. The angles between the pyrene and pyridyl/triazolyl substituent for molecule **14**.

	Angle [°]	
	ground state	
	pyridyl	triazolyl
14	44.81	34.72

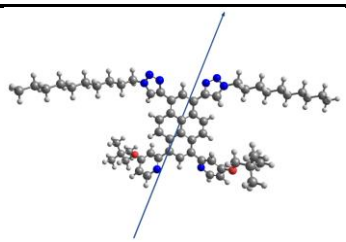
Table S7. Calculated absorption spectra by TD-DFT method (6-31G(d,p)/B3LYP) with oscillator strengths for **14**.

	Calculated wavelengths [nm] (oscillator strengths)	Transitions (contribution)
14	426.58 (0.8561)	HOMO→LUMO (98%)
	317.42 (0.3267)	H-1→LUMO (12%), HOMO→L+1 (27%), HOMO→L+3 (42%)
	308.09 (0.6451)	H-1→LUMO (25%), HOMO→L+1 (29%), HOMO→L+3 (24%)
	256.96 (0.2853)	H-12→LUMO (35%), H-1→L+1 (52%)
	248.97 (0.1995)	H-12→LUMO (24%), H-1→L+1 (18%), H-1→L+3 (20%), HOMO→L+9 (24%)

Table S8. TD-DFT calculated (6-31G(d,p)/CAM-B3LYP) wavelengths of emission with oscillator strengths for **14**.

	Calculated wavelengths [nm] (oscillator strengths)	Transitions (contribution)
14	471.30 (1.1978)	HOMO→LUMO (98%)
	352.24 (0.0607)	H-1→LUMO (58%), HOMO→L+1 (30%)

Table S9. Calculated dipole moment B3LYP/6-31G** for molecule **14**.

	ground state (μ_g) [D]
14	
	4.62

Optical properties

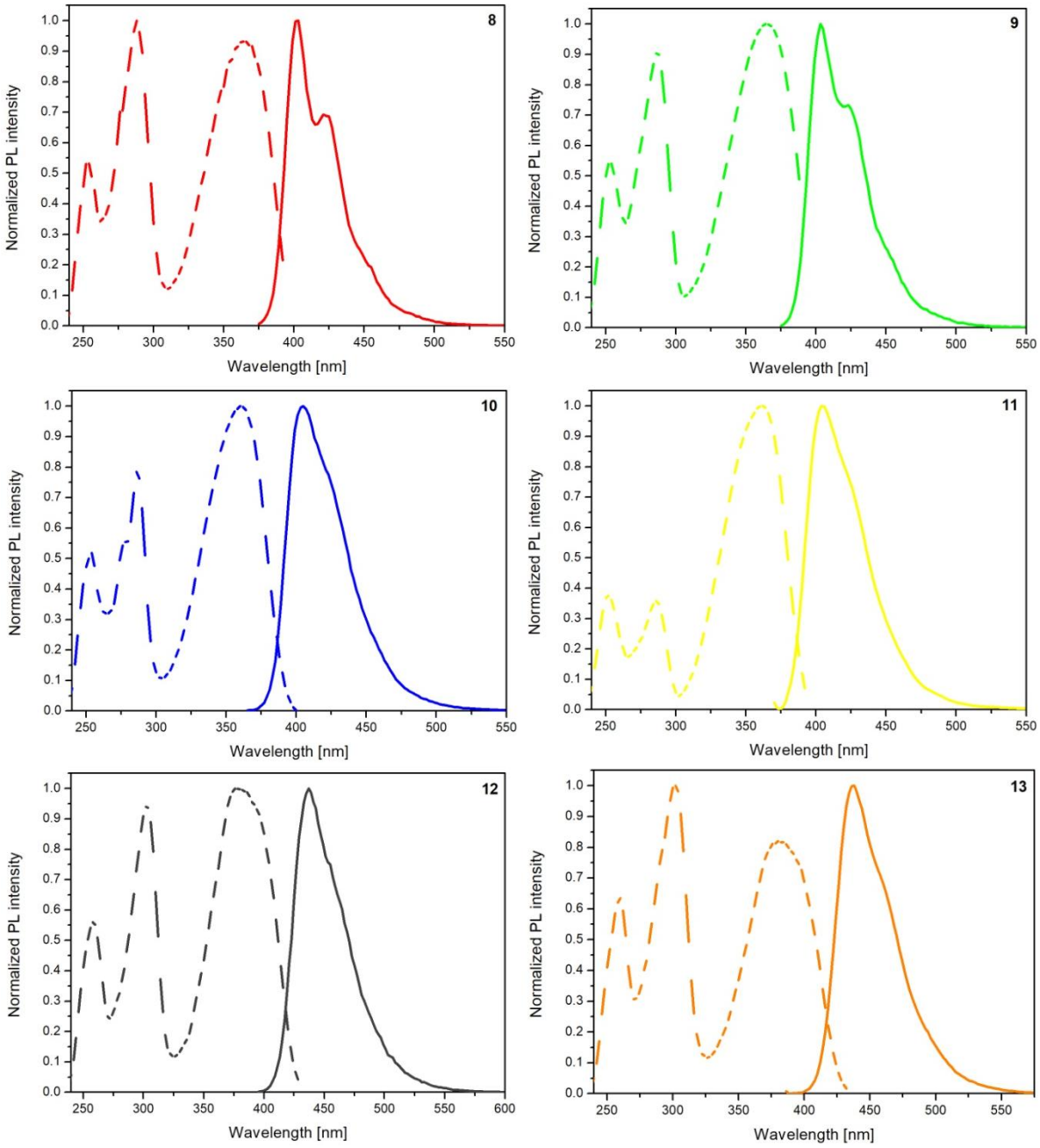


Figure S1. Excitation and emission spectra in CH_2Cl_2 solution of **8-13**.

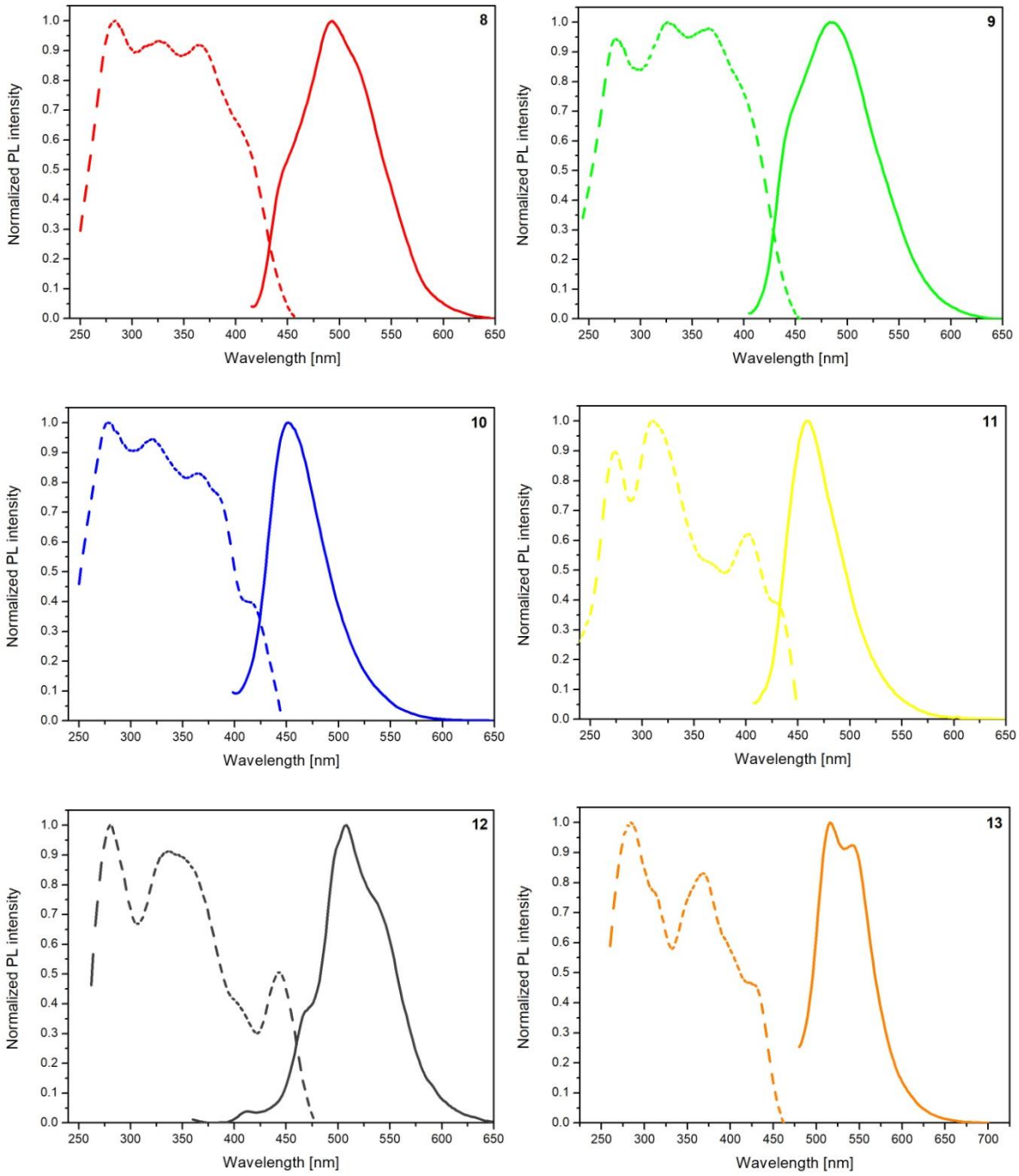
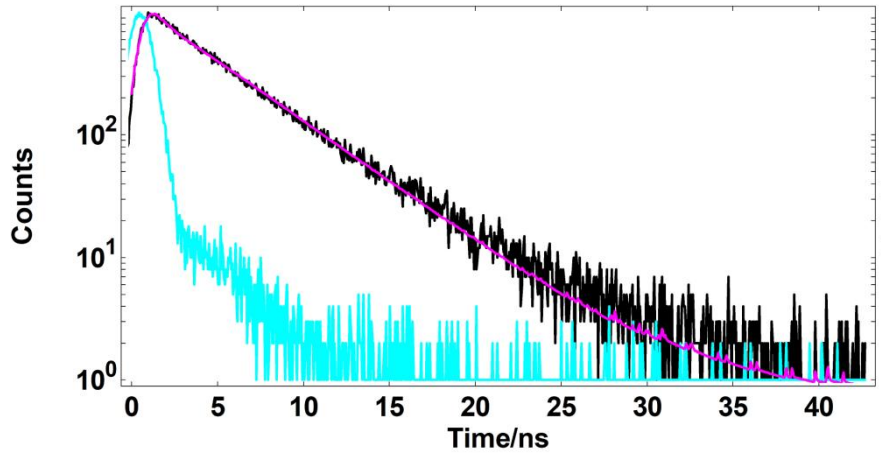
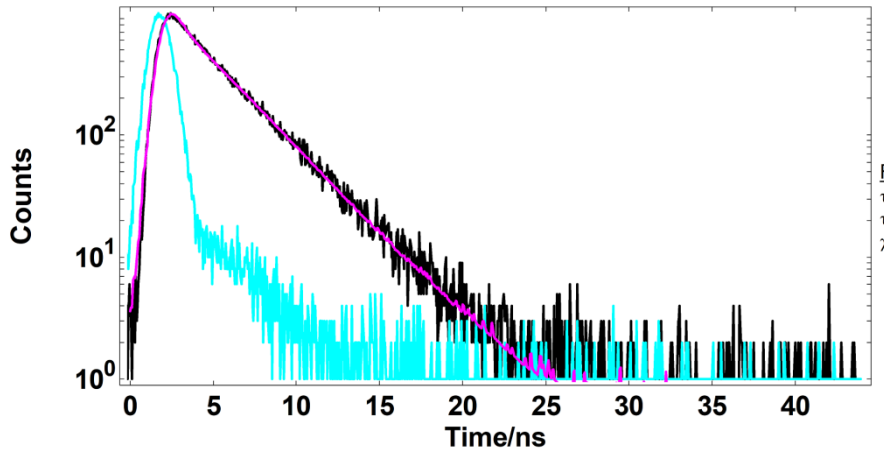


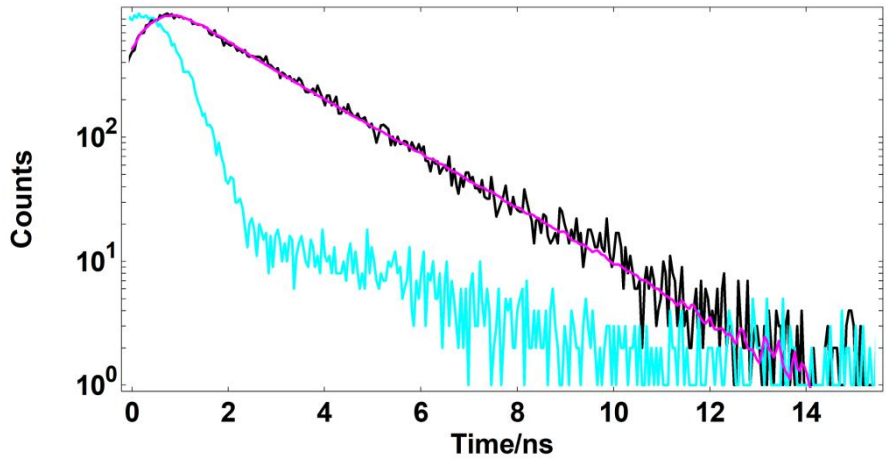
Figure S2. Excitation and emission spectra in the solid-state of **8**-**13**.


Counts
Time/ns
Fit Results
τ1 0.04ns
τ2 4.24ns
χ2 0.962

8


Counts
Time/ns
Fit Results
τ1 0.03ns
τ2 2.89ns
χ2 1.023

9


Counts
Time/ns
Fit Results
τ1 0.03ns
τ2 1.78ns
χ2 1.145

10

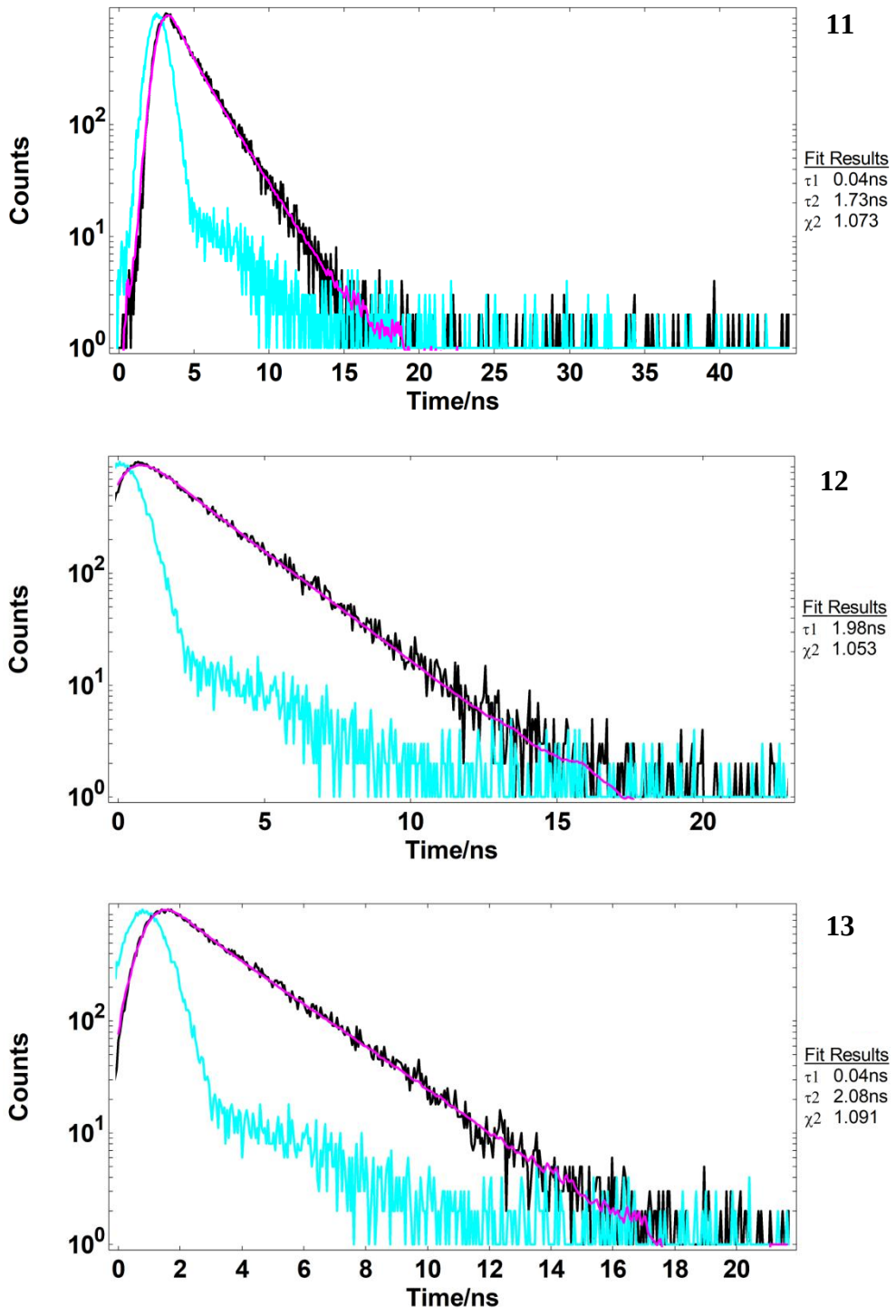


Figure S3. Decay curves of **8-13** in CH_2Cl_2 solution.

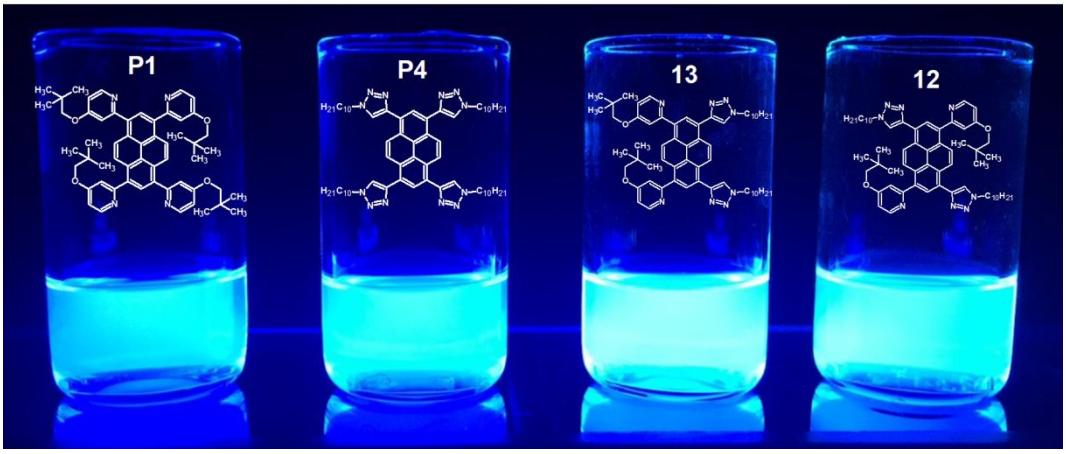


Figure S4. Dichloromethane solutions of **P1**, **P4**, **12** and **13** irradiated by wavelength 360 nm.

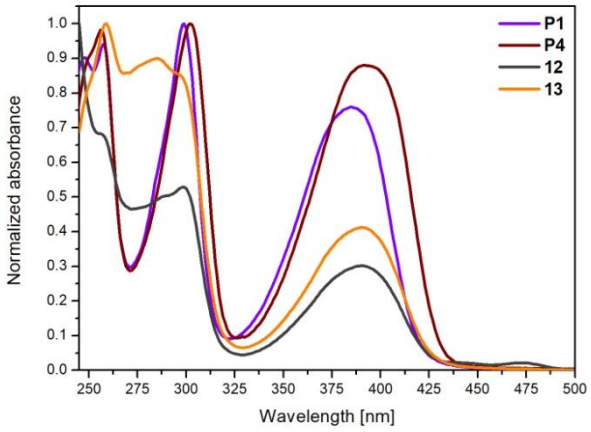


Figure S5. Comparison of absorption spectra recorded in CH_2Cl_2 solution (c = 10^{-5} mol/L) for **P1**, **P4**, **12**, and **13**.

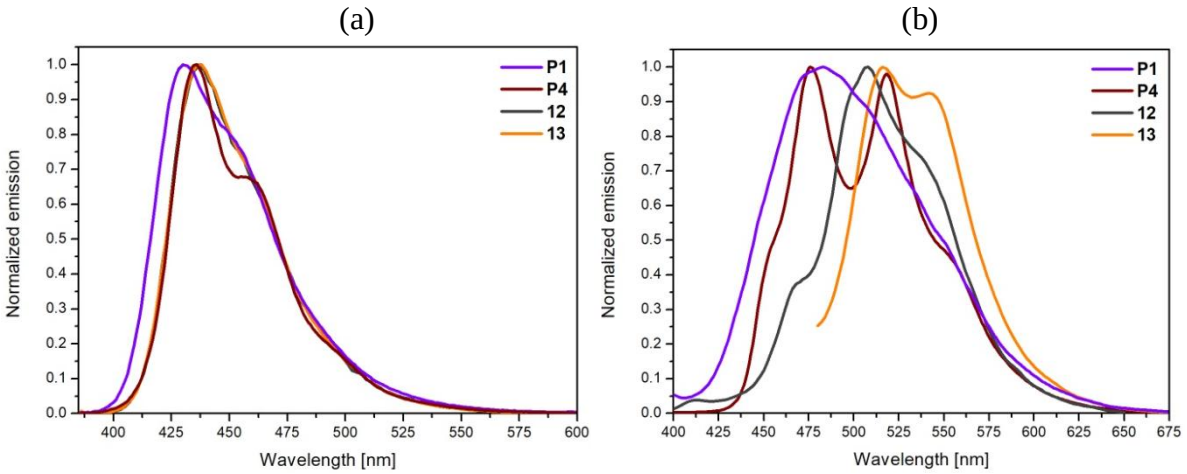


Figure S6. Comparison of emission spectra recorded in (a) CH_2Cl_2 solution (c = 10^{-5} mol/L), and (b) the solid state for **P1**, **P4**, **12**, and **13**.

^{1}H and ^{13}C NMR spectra of compounds 8-13

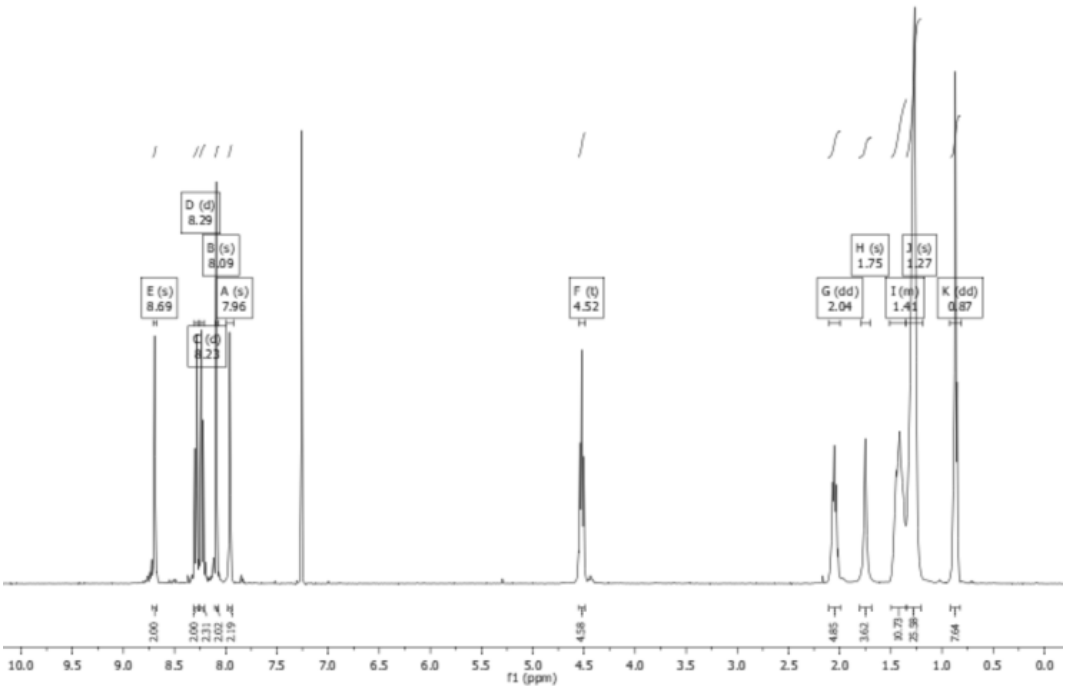


Figure S7. ^{1}H NMR plot of **8**.

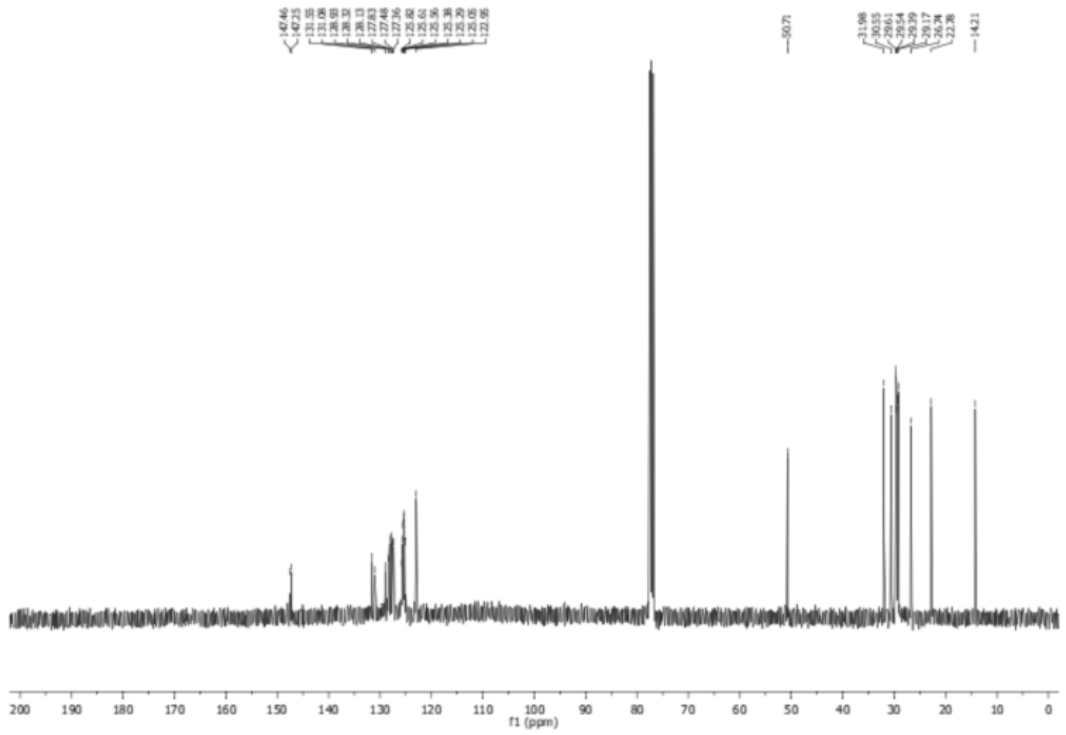


Figure S8. ^{13}C NMR plot of **8**.

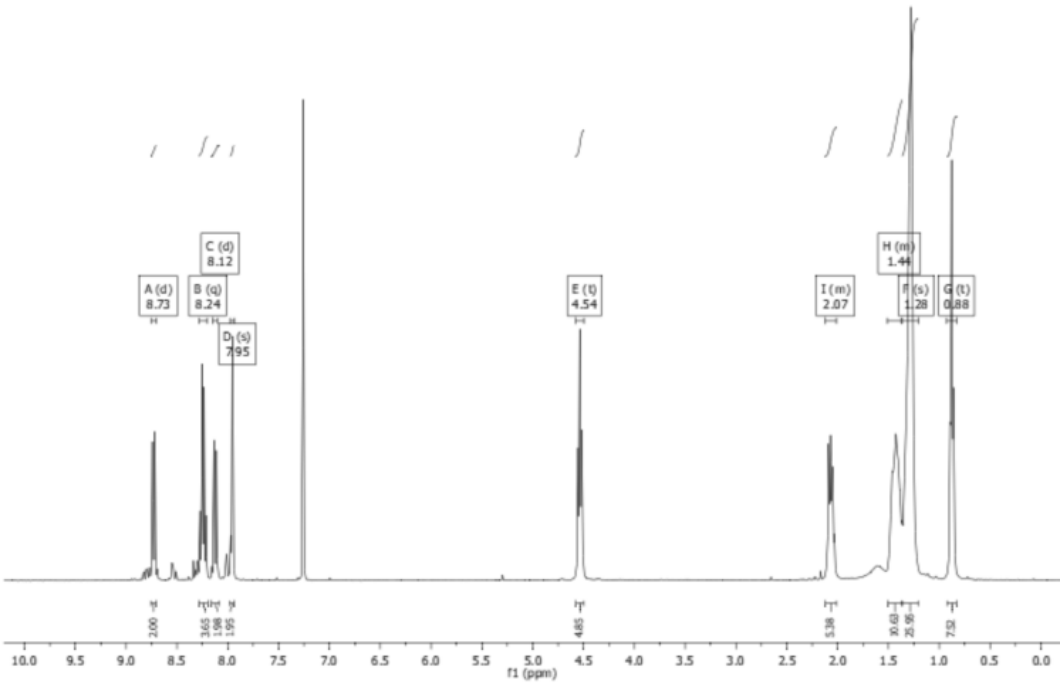


Figure S9. ^{1}H NMR plot of **9**.

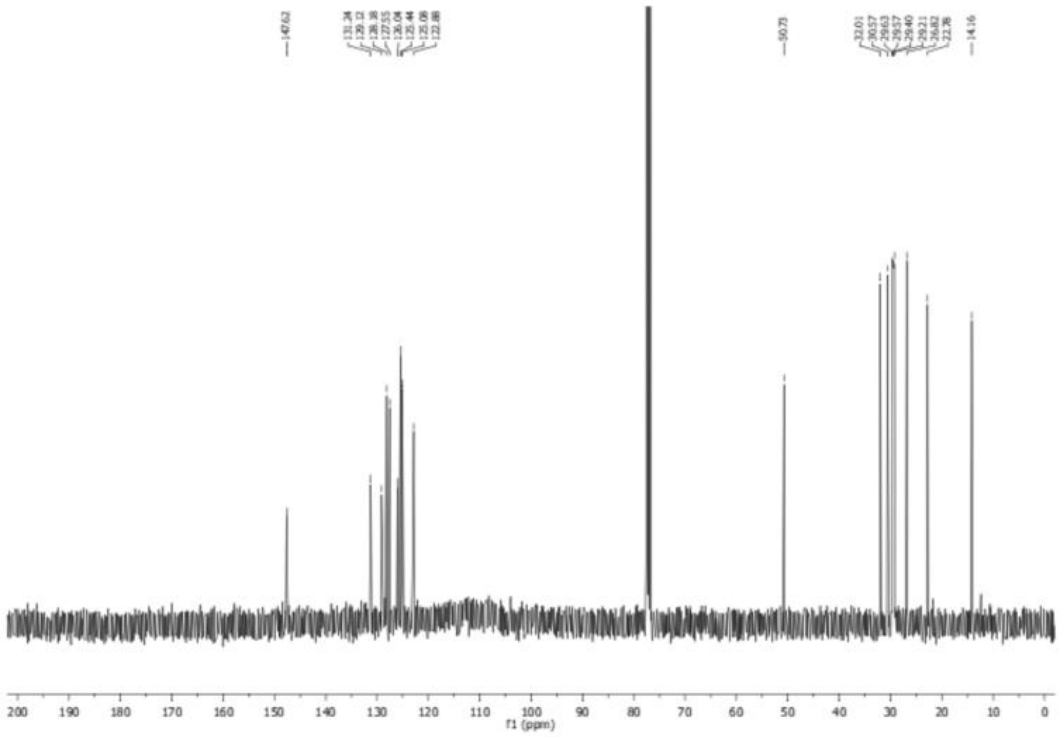


Figure S10. ^{13}C NMR plot of **9**.

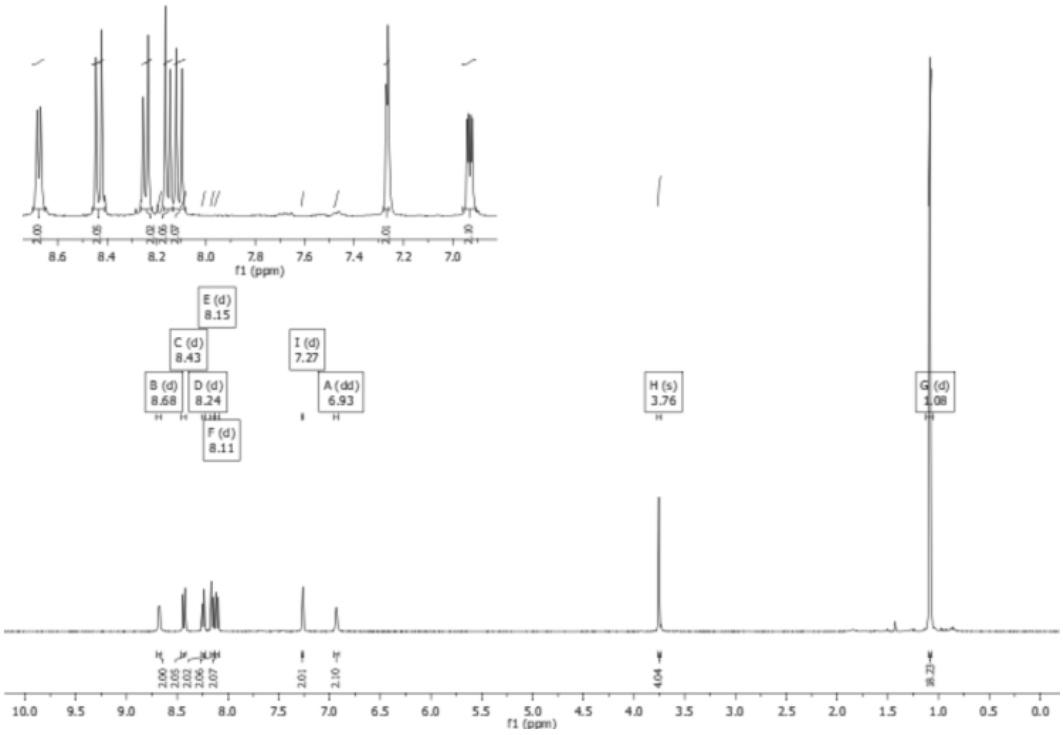


Figure S11. ^{1}H NMR plot of **10**.

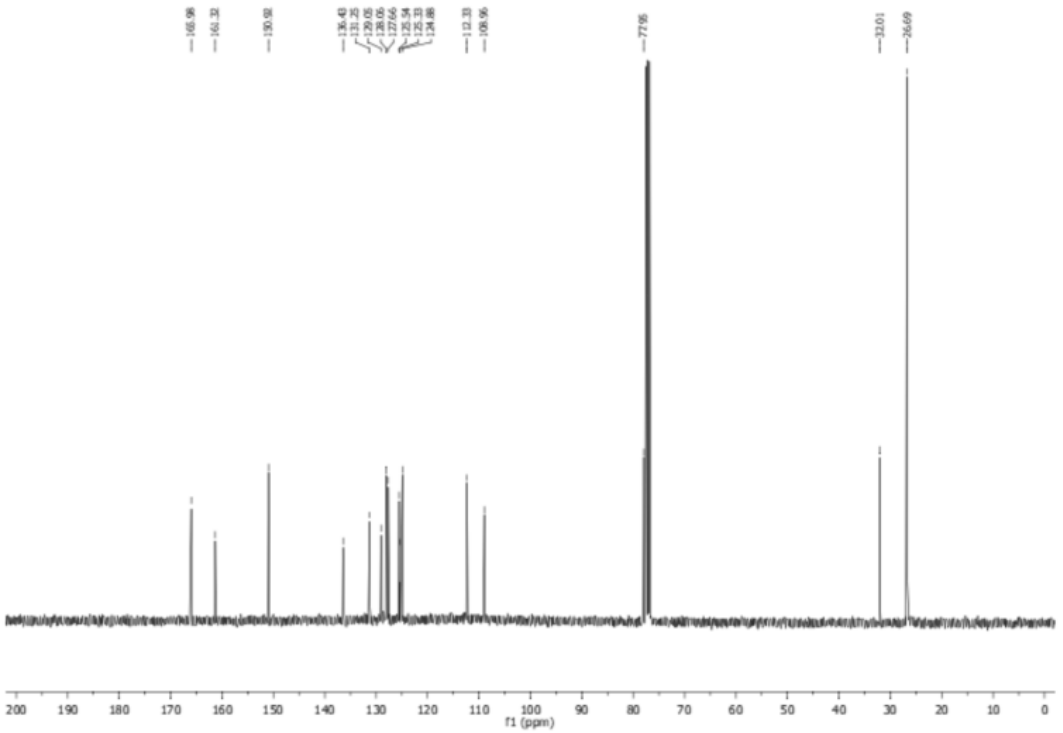


Figure S12. ^{13}C NMR plot of **10**.

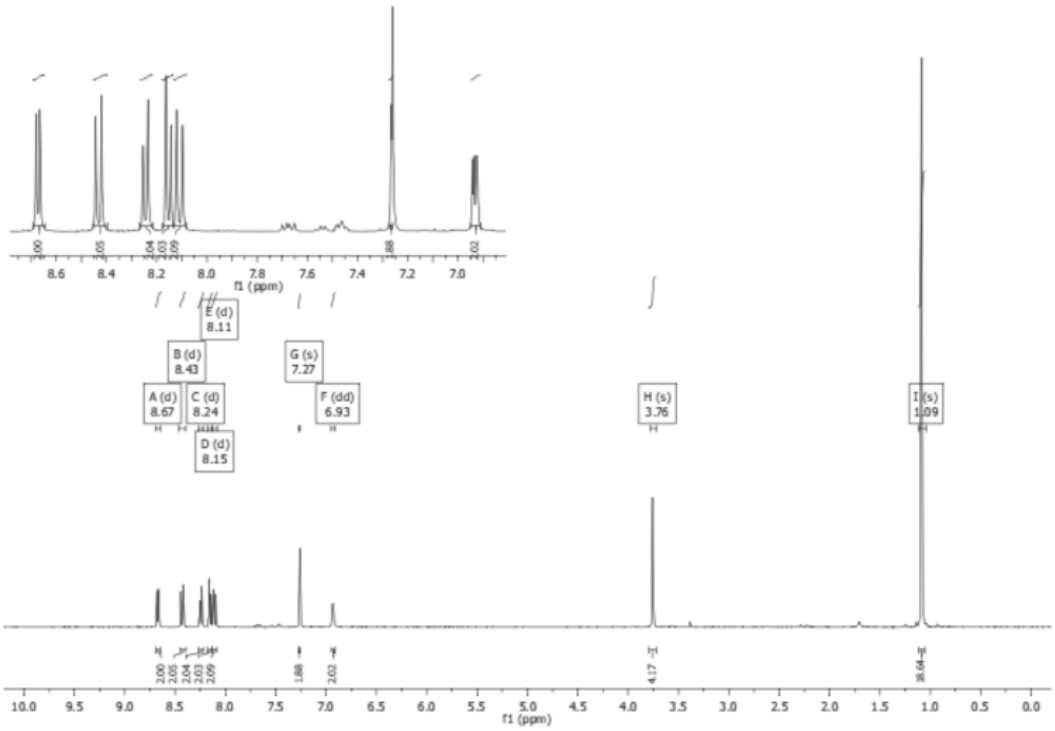


Figure S13. ^{1}H NMR plot of **11**.

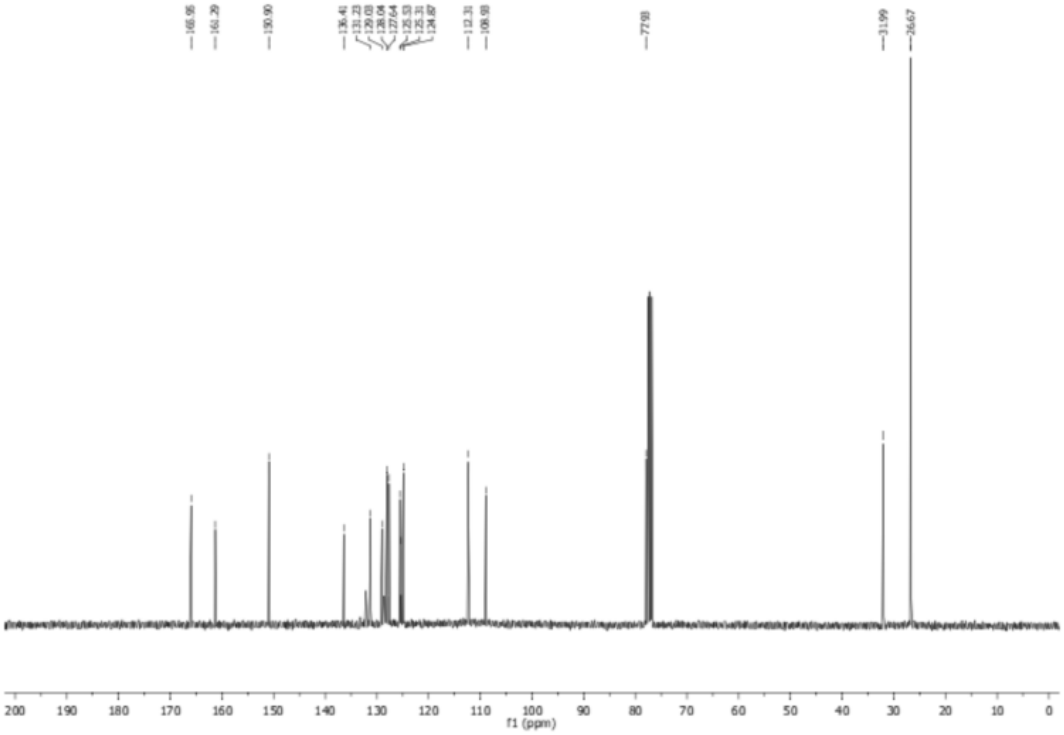


Figure S14. ^{13}C NMR plot of **11**.

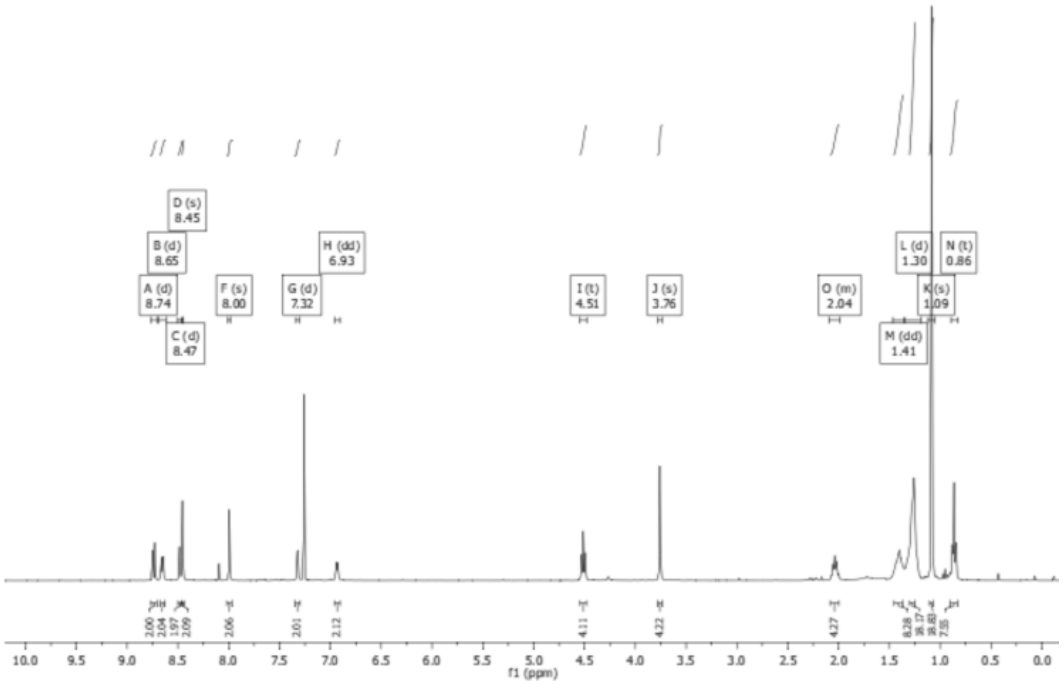


Figure S15. ^{1}H NMR plot of **12**.

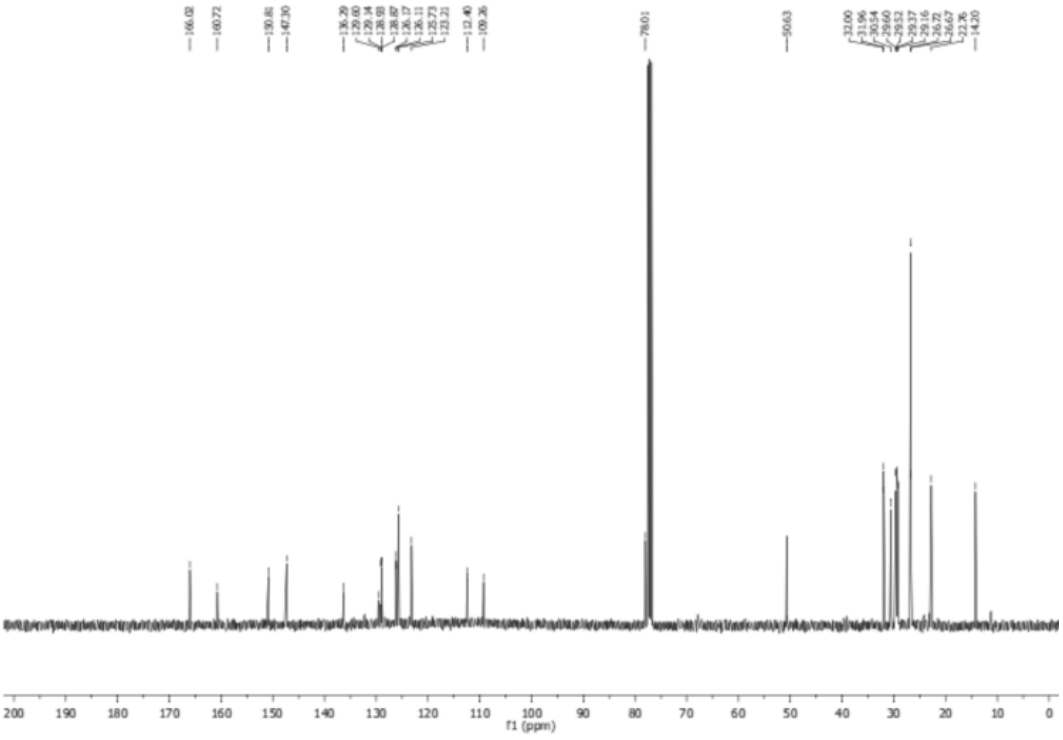


Figure S16. ^{13}C NMR plot of **12**.

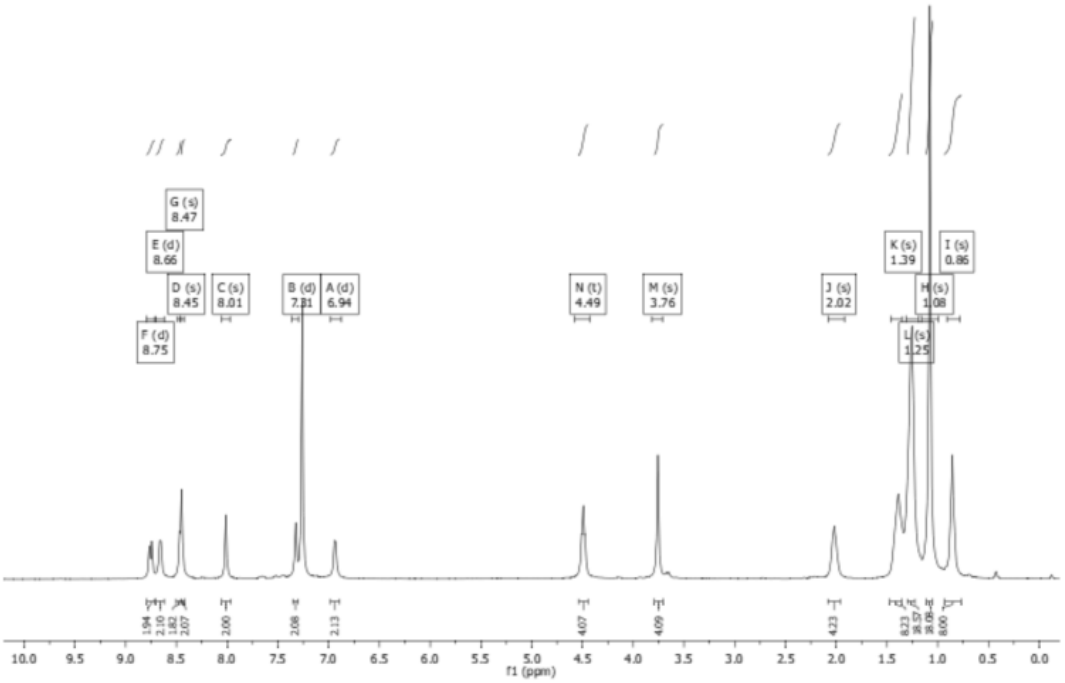


Figure S17. ^{1}H NMR plot of **13**.

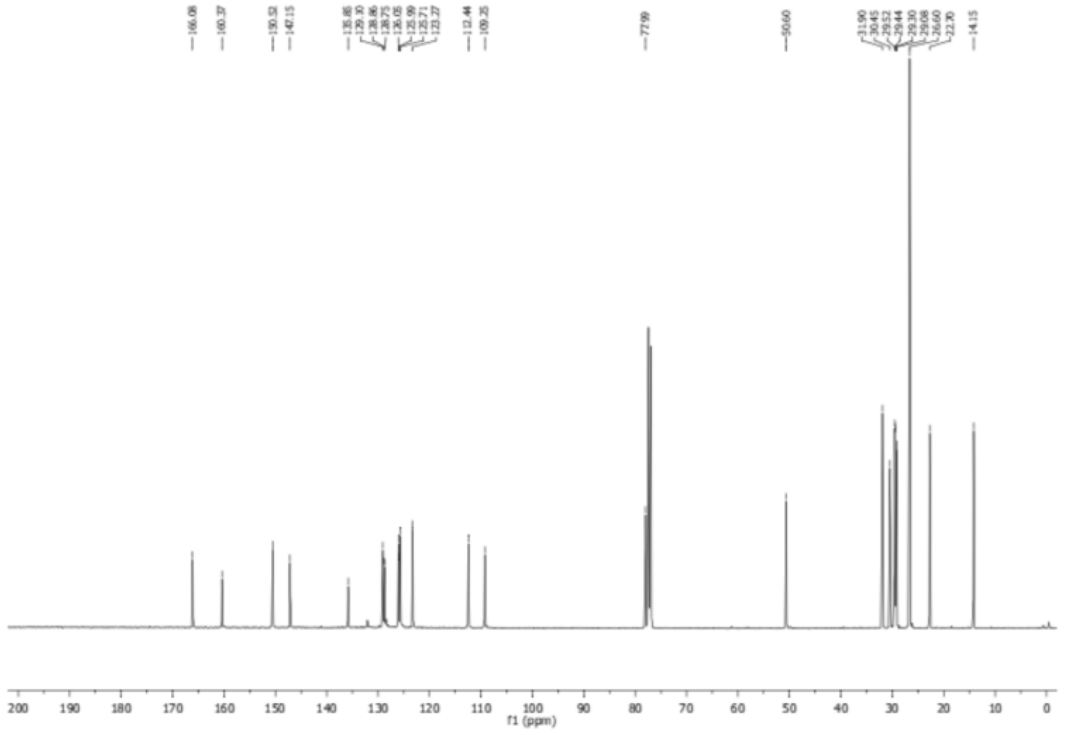
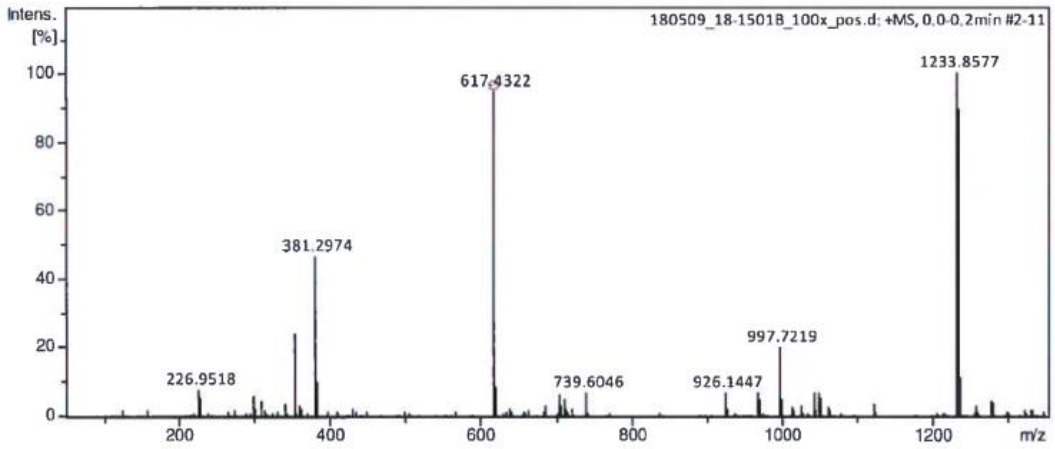


Figure S18. ^{13}C NMR plot of **13**.

MS spectra of compounds 8-13



The isotopic pattern of peak 617 m/z (experimental at the top, theoretical at the bottom)

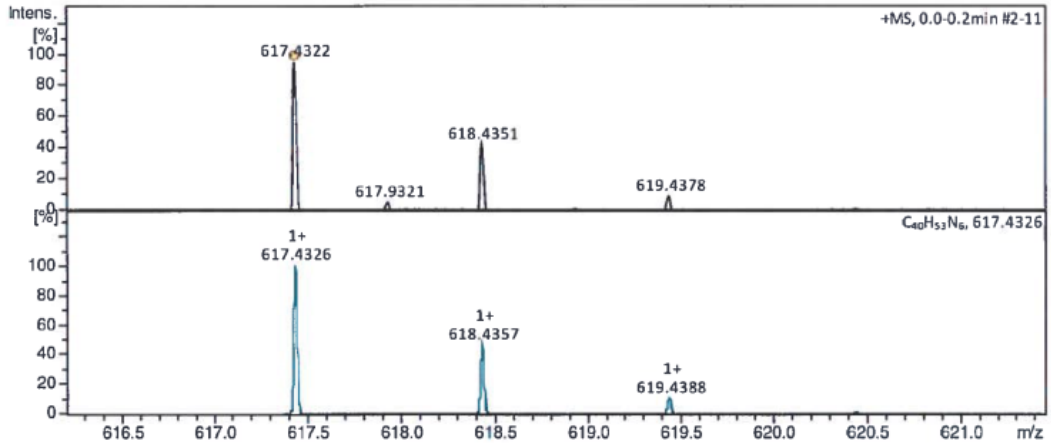
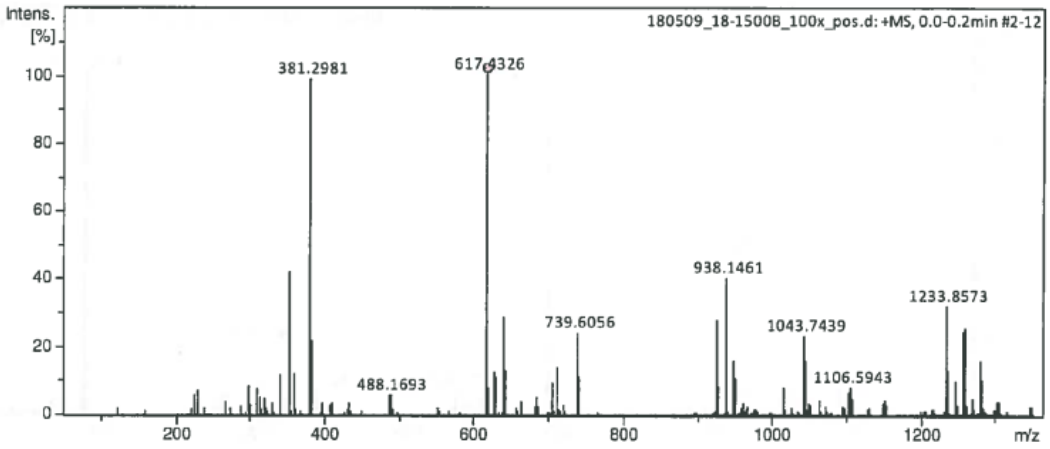


Figure S19. MS spectrum of **8**.



The isotopic pattern of peak 617 m/z (experimental at the top, theoretical at the bottom)

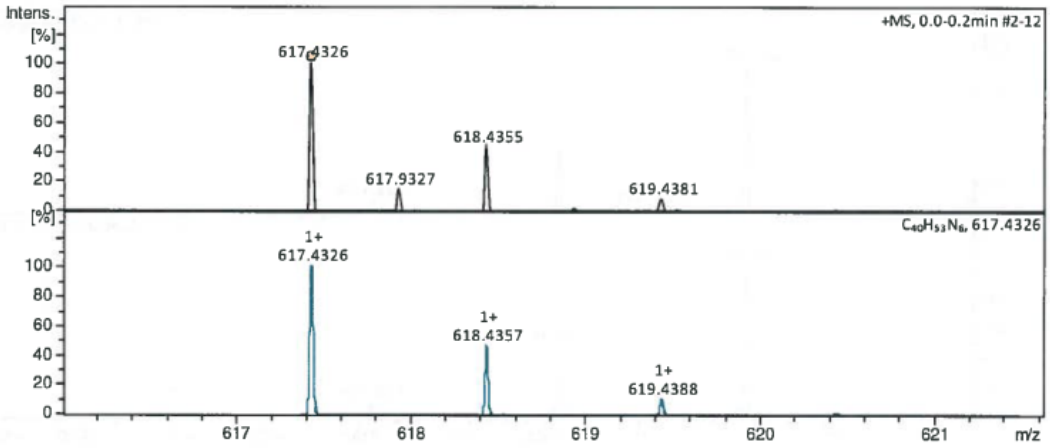
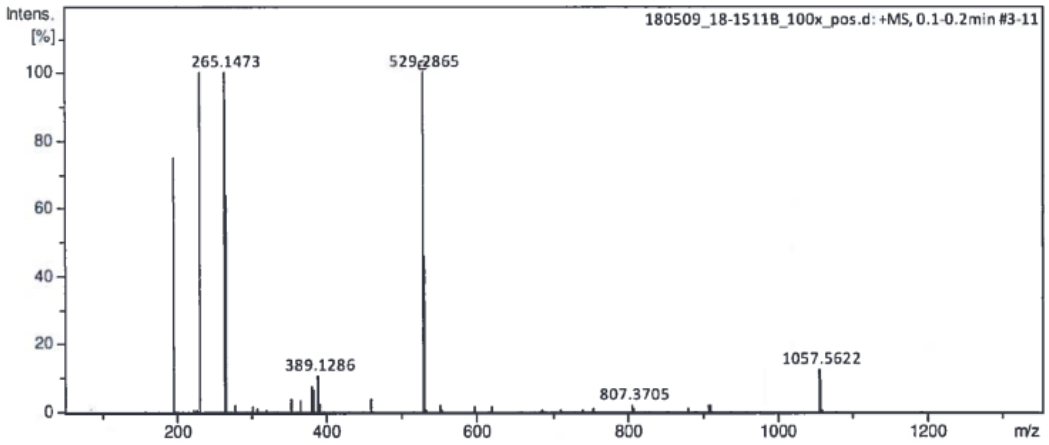


Figure S20. MS spectrum of **9**.



The isotopic pattern of peak 529 m/z (experimental at the top, theoretical at the bottom)

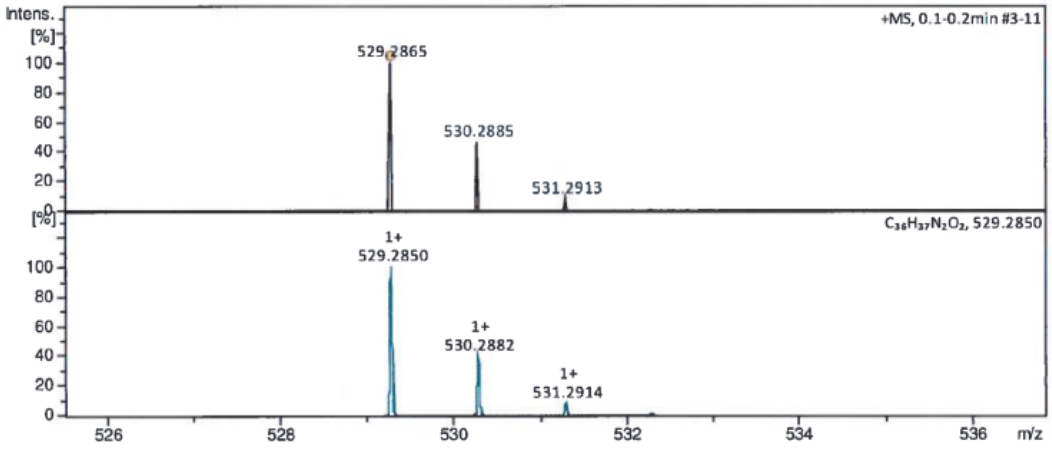
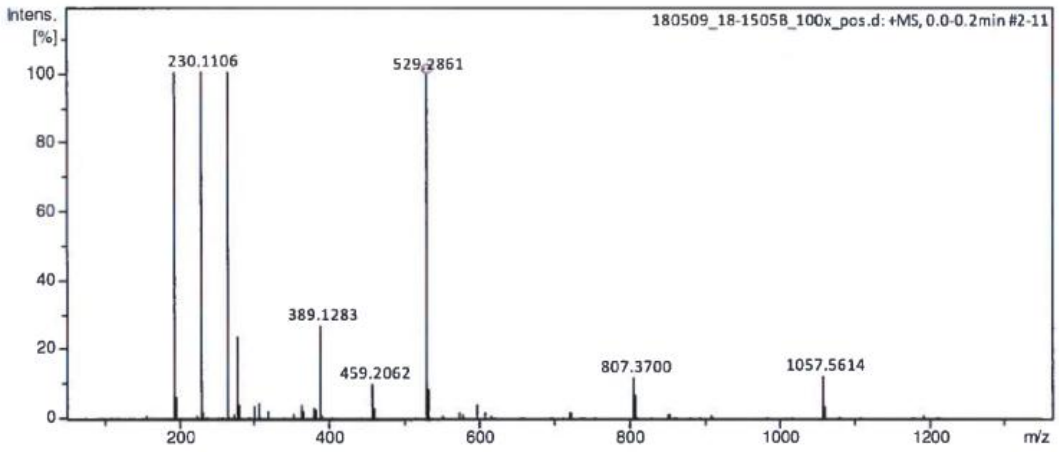


Figure S21. MS spectrum of **10**.



The isotopic pattern of peak 529 m/z (experimental at the top, theoretical at the bottom)

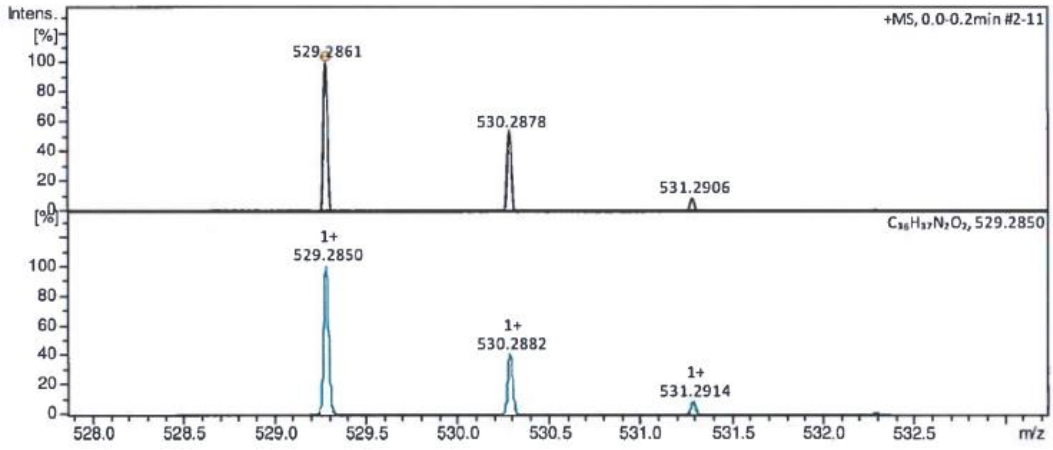
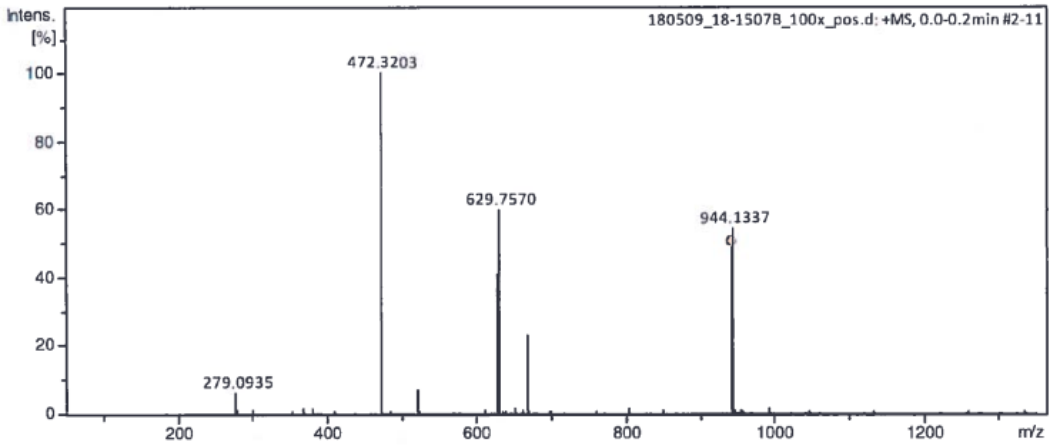


Figure S22. MS spectrum of **11**.



The isotopic pattern of peak 943 m/z (experimental at the top, theoretical at the bottom)

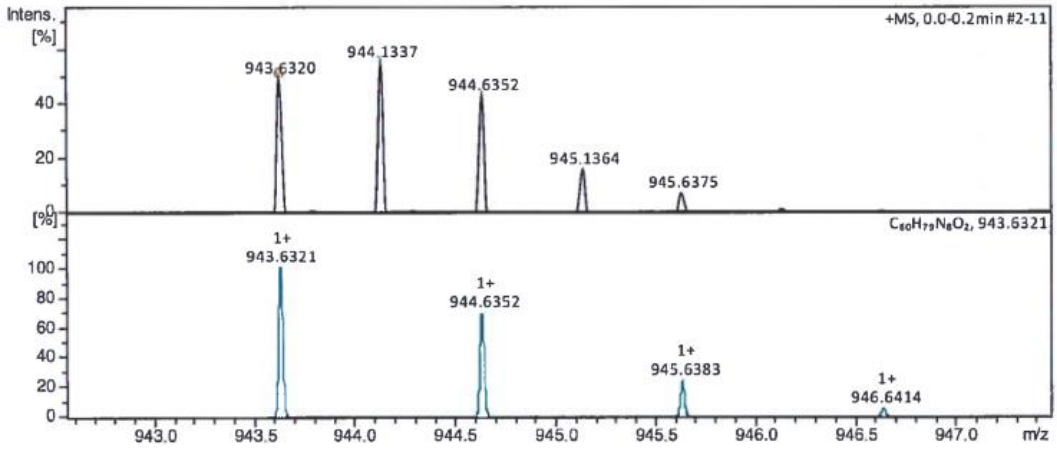
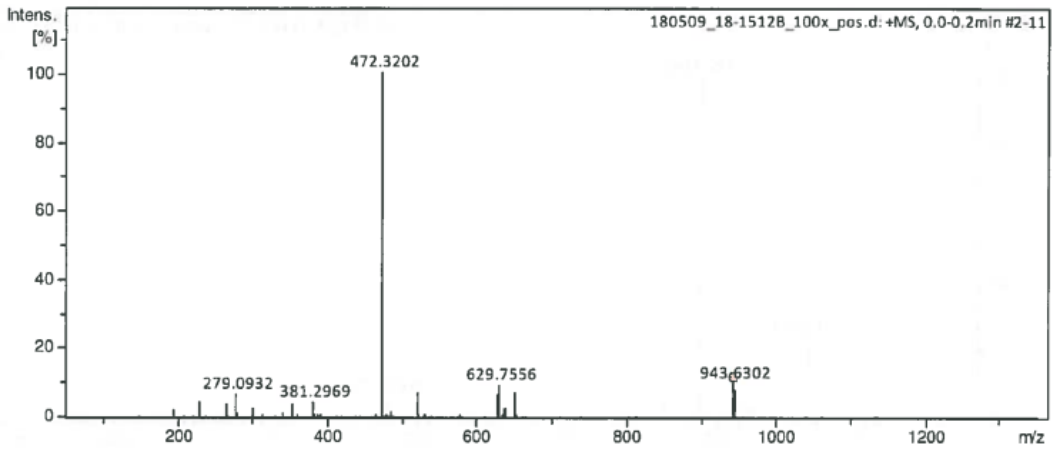


Figure S23. MS spectrum of **12**.



The isotopic pattern of peak 943 m/z (experimental at the top, theoretical at the bottom)

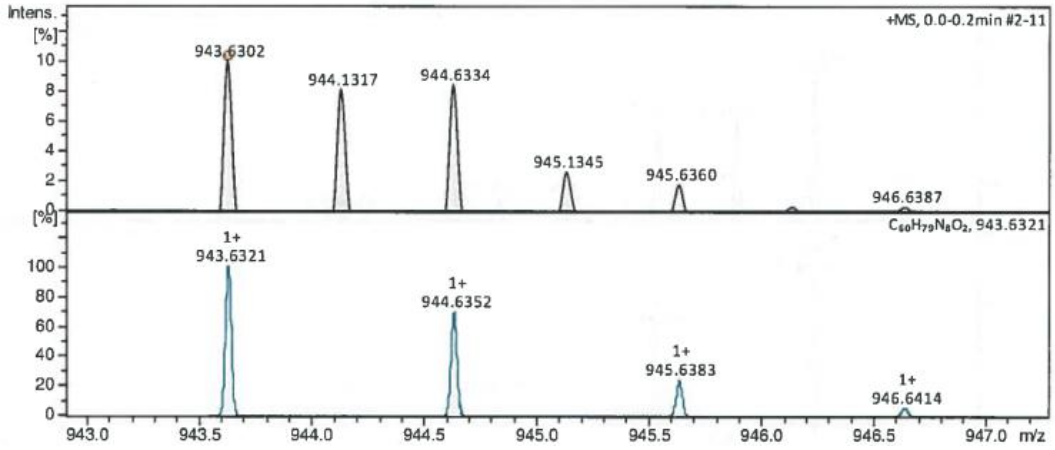


Figure S24. MS spectrum of **13**.

Cartesian coordinates of DFT-optimized structure of **8** by B3LYP /6-31G**/CH_2Cl_2:
Charge = 0; multiplicity=1

C	5.970938000	-0.952166000	-1.254463000
C	6.217747000	-2.313490000	-1.161697000
C	5.236153000	-3.193998000	-0.679041000
C	3.980694000	-2.660904000	-0.250884000
C	3.742214000	-1.250212000	-0.318082000
C	4.741559000	-0.399226000	-0.860644000
C	5.463329000	-4.608541000	-0.603442000
C	4.503926000	-5.449564000	-0.129525000
C	3.233112000	-4.949993000	0.310665000
C	2.970800000	-3.546118000	0.248236000
C	2.505946000	-0.765366000	0.228090000
C	1.546013000	-1.607000000	0.703630000
C	1.707691000	-3.033701000	0.688528000
C	2.235493000	-5.804852000	0.806307000
C	1.003150000	-5.307897000	1.202476000
C	0.707062000	-3.936610000	1.136449000
C	-0.644607000	-3.515414000	1.538933000
C	-1.486678000	-2.529010000	1.046905000
N	-2.626768000	-2.651296000	1.766803000
N	-2.521036000	-3.661310000	2.655508000
N	-1.332093000	-4.184084000	2.521545000
C	-3.876780000	-1.900309000	1.649757000
C	-4.789194000	-2.428464000	0.537497000
C	-6.103785000	-1.642663000	0.459880000
C	-7.044107000	-2.143779000	-0.643364000
C	-8.363733000	-1.365565000	-0.711972000
C	-9.311596000	-1.859061000	-1.812022000
C	-10.633353000	-1.083649000	-1.872019000
C	-11.585032000	-1.573886000	-2.970029000
H	6.731632000	-0.288284000	-1.650065000
H	6.423936000	-4.994812000	-0.932734000
H	4.684715000	-6.519419000	-0.073688000
H	2.351453000	0.304046000	0.305606000
H	0.652582000	-1.185551000	1.148031000
H	0.235991000	-5.984027000	1.563290000
H	-1.379401000	-1.802452000	0.258063000
H	-3.619777000	-0.850428000	1.482073000
H	-4.366606000	-1.977010000	2.623065000
H	-4.994190000	-3.489108000	0.725209000
H	-4.261490000	-2.371642000	-0.422850000
H	-5.884240000	-0.578643000	0.293563000
H	-6.618227000	-1.700836000	1.428983000
H	-7.257576000	-3.209323000	-0.480596000
H	-6.532241000	-2.080074000	-1.613855000
H	-8.148116000	-0.299329000	-0.871006000
H	-8.872361000	-1.430283000	0.260362000
H	-9.523619000	-2.926321000	-1.655698000

H	-8.805536000	-1.789893000	-2.785529000
H	-10.420670000	-0.016173000	-2.027318000
H	-11.138057000	-1.153047000	-0.897778000
C	4.558372000	1.049508000	-1.044461000
N	5.616252000	1.919035000	-0.943748000
N	5.213946000	3.130209000	-1.220027000
N	3.898475000	3.067038000	-1.514531000
C	3.448526000	1.793955000	-1.415495000
C	3.147680000	4.287498000	-1.809361000
C	2.458404000	4.870453000	-0.570948000
C	1.674087000	6.147191000	-0.895781000
C	0.971968000	6.746920000	0.328892000
C	0.169215000	8.014084000	0.010951000
C	-0.536402000	8.612822000	1.233841000
C	-1.351498000	9.872234000	0.915971000
C	-2.059967000	10.469106000	2.137884000
H	2.431375000	1.523092000	-1.647479000
H	2.419097000	4.048125000	-2.589286000
H	3.868248000	4.995196000	-2.225397000
H	3.220166000	5.077961000	0.189944000
H	1.783063000	4.116629000	-0.146666000
H	0.927294000	5.928480000	-1.672013000
H	2.354712000	6.893863000	-1.327465000
H	1.720565000	6.973652000	1.100722000
H	0.302026000	5.993494000	0.766745000
H	-0.577687000	7.784591000	-0.762503000
H	0.838491000	8.767721000	-0.427690000
H	0.211037000	8.849025000	2.004586000
H	-1.198767000	7.855135000	1.676513000
H	-2.098032000	9.634822000	0.144403000
H	-0.689872000	10.630772000	0.473733000
H	7.176097000	-2.713045000	-1.481349000
H	2.432538000	-6.871747000	0.862505000
C	-12.907684000	-0.799659000	-3.026666000
C	-13.853029000	-1.296038000	-4.124900000
C	-2.880662000	11.724975000	1.820234000
C	-3.586148000	12.313209000	3.045859000
H	-11.797431000	-2.641707000	-2.816425000
H	-11.082521000	-1.502634000	-3.945446000
H	-1.314166000	10.710259000	2.909064000
H	-2.719457000	9.709615000	2.582139000
H	-12.695481000	0.267139000	-3.181008000
H	-13.409618000	-0.870713000	-2.052093000
H	-13.391158000	-1.206616000	-5.114887000
H	-14.786054000	-0.723152000	-4.140493000
H	-14.112557000	-2.350537000	-3.976648000
H	-3.625916000	11.484068000	1.049795000
H	-2.222066000	12.484596000	1.377474000
H	-4.277214000	11.588166000	3.491041000
H	-4.163772000	13.206306000	2.785743000

H	-2.864294000	12.598044000	3.819951000

Cartesian coordinates of DFT-optimized structure of **9** by B3LYP /6-31G**/CH_2Cl_2:
Charge = 0; multiplicity=1

C	-2.312325000	-3.655974000	-1.175824000
C	-2.884272000	-2.487612000	-0.646219000
C	-2.042896000	-1.506880000	-0.055863000
C	-0.634106000	-1.761564000	0.041244000
C	-0.091660000	-2.976104000	-0.476699000
C	-0.949552000	-3.898110000	-1.096765000
C	-2.532452000	-0.245235000	0.430106000
C	-1.706311000	0.661180000	1.021335000
C	-0.304732000	0.408513000	1.176092000
C	0.237512000	-0.805837000	0.657465000
C	1.311089000	-3.226134000	-0.327469000
C	2.137139000	-2.320367000	0.264980000
C	1.645764000	-1.062059000	0.757643000
C	0.551595000	1.327162000	1.803056000
C	1.913065000	1.080361000	1.891017000
C	2.484982000	-0.087019000	1.359707000
C	-4.348647000	-2.355257000	-0.731725000
C	3.948049000	-0.225581000	1.461476000
N	-5.046193000	-2.860407000	-1.800855000
N	-6.326330000	-2.684989000	-1.609254000
N	-6.481323000	-2.078664000	-0.413784000
C	-5.278796000	-1.852216000	0.165430000
C	4.891302000	-0.697204000	0.561111000
N	6.083361000	-0.511946000	1.175553000
N	5.910736000	0.050992000	2.388844000
N	4.627841000	0.227222000	2.564419000
C	7.432849000	-0.771241000	0.671369000
C	8.092947000	0.481883000	0.086347000
C	9.517140000	0.203628000	-0.409032000
C	10.218198000	1.454828000	-0.952406000
C	11.645930000	1.186914000	-1.443916000
C	12.360240000	2.441290000	-1.961563000
C	13.789551000	2.174849000	-2.449550000
C	14.510619000	3.430481000	-2.954144000
C	-7.813442000	-1.690931000	0.051063000
C	-8.147564000	-0.230846000	-0.273091000
C	-9.556217000	0.158616000	0.191670000
C	-9.903344000	1.619066000	-0.121941000
C	-11.311672000	2.024057000	0.330796000
C	-11.653853000	3.485695000	0.018036000
C	-13.062255000	3.896731000	0.465347000
C	-13.401072000	5.359156000	0.153241000
H	-2.967409000	-4.385527000	-1.639004000
H	-3.579084000	-0.001482000	0.297670000
H	-2.101186000	1.609068000	1.376773000

H	1.706751000	-4.172030000	-0.687313000
H	3.185154000	-2.561310000	0.392871000
H	2.566744000	1.805450000	2.363331000
H	-5.185595000	-1.409322000	1.143639000
H	4.813357000	-1.105850000	-0.433278000
H	7.353057000	-1.563492000	-0.077558000
H	8.014336000	-1.158662000	1.511802000
H	8.108981000	1.259643000	0.858749000
H	7.475970000	0.863344000	-0.736819000
H	9.489392000	-0.568096000	-1.191003000
H	10.112508000	-0.215693000	0.413949000
H	10.242411000	2.223222000	-0.167153000
H	9.623064000	1.877728000	-1.773918000
H	11.620228000	0.428628000	-2.239488000
H	12.233709000	0.747793000	-0.625240000
H	12.384563000	3.198045000	-1.164500000
H	11.773363000	2.882237000	-2.779962000
H	13.764959000	1.423616000	-3.251999000
H	14.372937000	1.726107000	-1.632771000
H	-7.857814000	-1.875543000	1.128387000
H	-8.514332000	-2.370816000	-0.438381000
H	-8.054470000	-0.081932000	-1.355442000
H	-7.405396000	0.422881000	0.202335000
H	-9.645771000	-0.012964000	1.273479000
H	-10.292942000	-0.502017000	-0.285790000
H	-9.806563000	1.788950000	-1.203300000
H	-9.164757000	2.277385000	0.356755000
H	-11.409598000	1.851332000	1.412043000
H	-12.050080000	1.366808000	-0.149946000
H	-11.552362000	3.657811000	-1.062968000
H	-10.914916000	4.141886000	0.499765000
H	-13.164714000	3.723497000	1.546221000
H	-13.801440000	3.241810000	-0.017783000
H	-0.537415000	-4.819134000	-1.499378000
H	0.139193000	2.247847000	2.206159000
C	-14.809615000	5.772748000	0.597863000
C	-15.138276000	7.235139000	0.282879000
C	15.940722000	3.164313000	-3.440079000
C	16.655530000	4.423949000	-3.938240000
H	14.535610000	4.181792000	-2.151632000
H	13.928912000	3.880543000	-3.771545000
H	-13.297660000	5.533263000	-0.927494000
H	-12.662557000	6.014549000	0.637121000
H	-14.913167000	5.598584000	1.677555000
H	-15.547597000	5.118984000	0.113275000
H	-14.440048000	7.914827000	0.784772000
H	-16.150100000	7.498070000	0.608506000
H	-15.073151000	7.432178000	-0.793395000
H	15.915972000	2.415754000	-4.243832000
H	16.521108000	2.712998000	-2.623775000

H	16.117248000	4.878997000	-4.777644000
H	17.672318000	4.200359000	-4.277560000
H	16.727531000	5.177809000	-3.145831000

Cartesian coordinates of DFT-optimized structure of **10** by B3LYP /6-31G**/CH_2Cl_2:
Charge = 0; multiplicity=1

C	-1.411992000	-3.391545000	-1.110544000
C	-2.474644000	-2.485933000	-1.248427000
C	-2.255079000	-1.112970000	-0.962120000
C	0.074806000	-1.648616000	-0.309156000
C	-0.167406000	-2.989011000	-0.649606000
C	-3.233087000	-0.088041000	-1.206458000
C	-3.006960000	1.217588000	-0.891865000
C	-1.774734000	1.657195000	-0.295787000
C	-0.737681000	0.680684000	-0.140571000
C	1.350486000	-1.216008000	0.185525000
C	1.577357000	0.089080000	0.496846000
C	0.548326000	1.077012000	0.341793000
C	-1.523020000	3.004837000	0.072438000
C	-0.239814000	3.366467000	0.508884000
C	0.773552000	2.429318000	0.644834000
C	-2.561121000	4.075844000	0.042606000
N	-2.174952000	5.264057000	-0.458611000
C	-3.075693000	6.258803000	-0.445666000
C	-4.366141000	6.145234000	0.050509000
C	-4.759866000	4.912539000	0.591882000
C	-3.837773000	3.860452000	0.589594000
O	-6.014879000	4.842226000	1.090964000
C	-6.473470000	3.606774000	1.662774000
C	-7.918576000	3.782620000	2.152307000
C	-8.363659000	2.434575000	2.750615000
C	-7.978266000	4.877642000	3.233668000
C	-8.833432000	4.154922000	0.970729000
H	-1.588805000	-4.431496000	-1.362050000
H	-4.166054000	-0.358649000	-1.685780000
H	-3.765424000	1.954137000	-1.128480000
H	2.136318000	-1.957220000	0.302085000
H	2.547629000	0.408994000	0.866630000
H	-0.056886000	4.406230000	0.756743000
H	-2.742556000	7.208286000	-0.860661000
H	-5.057592000	6.980077000	0.037686000
H	-4.079393000	2.899285000	1.021743000
H	-5.819327000	3.329099000	2.499719000
H	-6.421389000	2.814488000	0.904177000
H	-7.726172000	2.137951000	3.590959000
H	-8.333226000	1.634274000	2.002647000
H	-9.391347000	2.505705000	3.120991000
H	-7.342829000	4.622397000	4.089373000
H	-9.002899000	4.997477000	3.600999000

H	-7.643590000	5.840899000	2.839069000
H	-8.813826000	3.378995000	0.196966000
H	-8.523368000	5.098083000	0.512543000
H	-9.869230000	4.265088000	1.308682000
C	-3.789744000	-3.038622000	-1.682486000
N	-3.749762000	-3.950061000	-2.682465000
C	-4.907416000	-4.498485000	-3.057744000
C	-6.151476000	-4.205854000	-2.497343000
C	-6.185349000	-3.277994000	-1.449899000
C	-4.979641000	-2.693209000	-1.037391000
O	-7.297023000	-2.896272000	-0.780426000
C	-8.560939000	-3.473299000	-1.144998000
C	-9.659847000	-2.897935000	-0.239165000
C	-9.368430000	-3.250473000	1.231346000
C	-9.738581000	-1.369479000	-0.411777000
C	-10.990374000	-3.540854000	-0.674857000
H	-4.850715000	-5.225465000	-3.866377000
H	-7.041479000	-4.697200000	-2.867970000
H	-4.990635000	-1.998419000	-0.206201000
H	-8.507557000	-4.564289000	-1.032849000
H	-8.775159000	-3.243086000	-2.197191000
H	-9.326847000	-4.336031000	1.376023000
H	-10.155591000	-2.855905000	1.882353000
H	-8.413509000	-2.828843000	1.556626000
H	-8.798776000	-0.890948000	-0.122250000
H	-10.538506000	-0.954962000	0.210607000
H	-9.949806000	-1.099472000	-1.452750000
H	-10.962646000	-4.631067000	-0.567847000
H	-11.225392000	-3.308240000	-1.719523000
H	-11.812351000	-3.166188000	-0.056690000
C	-0.976236000	-0.693256000	-0.469919000
H	0.631809000	-3.716509000	-0.537939000
H	1.752866000	2.736073000	1.001601000

Cartesian coordinates of DFT-optimized structure of **11** by B3LYP /6-31G**/CH_2Cl_2:
Charge = 0; multiplicity=1

C	-1.187401000	-3.720254000	0.776580000
C	-2.038510000	-2.691623000	0.400532000
C	-1.581875000	-1.365180000	0.355136000
C	-0.235575000	-1.079453000	0.733045000
C	0.642446000	-2.148189000	1.116941000
C	0.155217000	-3.481419000	1.105100000
C	-2.423891000	-0.286992000	-0.072027000
C	-1.981821000	1.000375000	-0.086452000
C	-0.651408000	1.345471000	0.341250000
C	0.226613000	0.276733000	0.725144000
C	1.972865000	-1.803102000	1.544622000
C	2.414939000	-0.515736000	1.530192000
C	1.572918000	0.562455000	1.103041000

C	-0.164172000	2.678702000	0.353090000
C	1.178453000	2.917527000	0.681587000
C	2.029561000	1.888894000	1.057631000
C	1.001492000	-4.672050000	1.413569000
C	-1.010428000	3.869351000	0.044630000
N	0.466074000	-5.576939000	2.253619000
C	1.186140000	-6.681081000	2.507525000
C	2.432236000	-6.949994000	1.961084000
C	2.977803000	-6.016471000	1.067297000
C	2.245866000	-4.857217000	0.787456000
N	-0.475031000	4.774177000	-0.795501000
C	-1.195057000	5.878347000	-1.049395000
C	-2.441086000	6.147359000	-0.502851000
C	-2.986620000	5.213916000	0.391039000
C	-2.254727000	4.054629000	0.670863000
O	-4.189526000	5.519843000	0.927240000
C	-4.789358000	4.615015000	1.868286000
C	-6.135418000	5.190454000	2.332448000
C	-6.734825000	4.190702000	3.339808000
O	4.180777000	-6.322303000	0.531193000
C	4.780757000	-5.417272000	-0.409566000
C	6.127021000	-5.992476000	-0.873427000
C	6.726575000	-4.992519000	-1.880497000
C	5.909909000	-7.354378000	-1.559060000
C	7.074942000	-6.150166000	0.330097000
C	-5.917937000	6.552414000	3.017849000
C	-7.083652000	5.348116000	1.129165000
H	-1.548195000	-4.742745000	0.802793000
H	-3.432757000	-0.521164000	-0.400914000
H	-2.637839000	1.785248000	-0.442395000
H	2.628888000	-2.587983000	1.900543000
H	3.423811000	-0.281567000	1.859061000
H	1.539253000	3.940016000	0.655368000
H	0.735690000	-7.395923000	3.193664000
H	2.975206000	-7.857850000	2.198252000
H	2.606988000	-4.119225000	0.084159000
H	-0.744629000	6.593131000	-1.735609000
H	-2.984023000	7.055237000	-0.740008000
H	-2.615823000	3.316699000	1.374236000
H	-4.115398000	4.483617000	2.724992000
H	-4.936649000	3.637625000	1.389796000
H	-6.082349000	4.057639000	4.209987000
H	-6.895334000	3.207768000	2.882773000
H	-7.702837000	4.551609000	3.701911000
H	4.927784000	-4.439926000	0.069095000
H	4.107021000	-5.285850000	-1.266444000
H	6.886822000	-4.009619000	-1.423297000
H	6.074325000	-4.859438000	-2.750842000
H	7.694737000	-5.353249000	-2.242373000
H	5.243767000	-7.258943000	-2.424133000

H	5.467473000	-8.078304000	-0.869412000
H	6.863160000	-7.760143000	-1.913781000
H	7.254425000	-5.186125000	0.819709000
H	8.042848000	-6.546421000	0.005645000
H	6.658775000	-6.835251000	1.073760000
H	-5.251580000	6.456998000	3.882758000
H	-6.871038000	6.958358000	3.372767000
H	-5.475581000	7.276189000	2.327990000
H	-7.263383000	4.384039000	0.639717000
H	-6.667609000	6.033063000	0.385307000
H	-8.051421000	5.744525000	1.453838000
H	-3.066783000	-2.908933000	0.125093000
H	3.057838000	2.106199000	1.333058000

Cartesian coordinates of DFT-optimized structure of **12** by B3LYP /6-31G**/CH_2Cl_2:
Charge = 0; multiplicity=1

C	-1.236245000	-3.640209000	0.858663000
C	-2.106032000	-2.596645000	0.531677000
C	-1.598488000	-1.274015000	0.443683000
C	-0.229855000	-1.024466000	0.787457000
C	0.628933000	-2.113754000	1.149280000
C	0.116120000	-3.436175000	1.131198000
C	-2.389608000	-0.171273000	-0.016204000
C	-1.906779000	1.101134000	-0.032628000
C	-0.577674000	1.409429000	0.408971000
C	0.281136000	0.319951000	0.770259000
C	1.959652000	-1.806053000	1.586390000
C	2.442242000	-0.533531000	1.570949000
C	1.649046000	0.569829000	1.116431000
C	-0.066903000	2.732444000	0.432691000
C	1.283869000	2.937639000	0.712809000
C	2.153783000	1.893974000	1.038231000
C	0.947931000	-4.646180000	1.401248000
C	-3.516717000	-2.943076000	0.290638000
C	-0.899423000	3.942075000	0.163328000
C	3.561603000	2.243570000	1.292588000
N	0.419772000	-5.554505000	2.241389000
C	1.125672000	-6.675672000	2.456646000
C	2.351353000	-6.956878000	1.871282000
C	2.890507000	-6.016784000	0.980718000
C	2.172877000	-4.839846000	0.740828000
N	-3.868240000	-4.150229000	-0.260203000
N	-5.169845000	-4.251353000	-0.295634000
N	-5.682167000	-3.123141000	0.238320000
C	-4.691480000	-2.280160000	0.613006000
C	4.742225000	1.598118000	0.957405000
N	5.725339000	2.427110000	1.380378000
N	5.202042000	3.536433000	1.943244000
N	3.901424000	3.430633000	1.892022000

N	-0.369241000	4.853830000	-0.671836000
C	-1.075831000	5.974754000	-0.886162000
C	-2.304052000	6.252480000	-0.304478000
C	-2.845273000	5.308867000	0.581102000
C	-2.127130000	4.131980000	0.819713000
C	7.174429000	2.294967000	1.226156000
C	7.673618000	2.823158000	-0.123203000
C	9.198924000	2.731433000	-0.249955000
C	9.720478000	3.265893000	-1.589708000
C	11.246999000	3.199597000	-1.719863000
C	11.769253000	3.741042000	-3.056295000
C	13.296940000	3.688928000	-3.184792000
C	13.810027000	4.237413000	-4.523229000
C	-7.130728000	-2.923005000	0.288062000
C	-7.687337000	-2.306284000	-0.999660000
C	-9.205458000	-2.102601000	-0.929323000
C	-9.794512000	-1.522646000	-2.221211000
C	-11.310067000	-1.299135000	-2.151272000
C	-11.906239000	-0.737777000	-3.447898000
C	-13.419920000	-0.502366000	-3.374507000
C	-14.019179000	0.049944000	-4.673416000
O	-4.031805000	5.622014000	1.149086000
C	-4.629863000	4.705091000	2.078738000
C	-5.955747000	5.294412000	2.582492000
C	-6.561777000	4.277531000	3.568380000
O	4.074645000	-6.333123000	0.409527000
C	4.671264000	-5.419052000	-0.523831000
C	5.995625000	-6.010621000	-1.028944000
C	6.600149000	-4.996751000	-2.018851000
C	5.733537000	-7.346533000	-1.749048000
C	6.961185000	-6.225354000	0.151389000
C	-5.696132000	6.628596000	3.306690000
C	-6.918869000	5.511667000	1.400634000
H	-1.626748000	-4.649725000	0.900956000
H	-3.385915000	-0.364007000	-0.394783000
H	-2.529387000	1.900713000	-0.415553000
H	2.583654000	-2.606111000	1.965967000
H	3.440087000	-0.340912000	1.945618000
H	1.672405000	3.948308000	0.678283000
H	0.680974000	-7.394043000	3.142702000
H	2.883509000	-7.878670000	2.077105000
H	2.527902000	-4.094846000	0.041831000
H	-4.889823000	-1.337037000	1.095668000
H	4.949312000	0.670205000	0.449320000
H	-0.629504000	6.695945000	-1.568191000
H	-2.836563000	7.174314000	-0.509200000
H	-2.483745000	3.384276000	1.514996000
H	7.427413000	1.239051000	1.356348000
H	7.620570000	2.854343000	2.051692000
H	7.349745000	3.865172000	-0.230899000

H	7.196068000	2.256816000	-0.932644000
H	9.515831000	1.686338000	-0.126344000
H	9.665781000	3.292326000	0.571463000
H	9.390243000	4.306396000	-1.715694000
H	9.259630000	2.698895000	-2.410728000
H	11.578244000	2.158748000	-1.595071000
H	11.705120000	3.764773000	-0.895776000
H	11.430719000	4.779362000	-3.182411000
H	11.315454000	3.172653000	-3.880753000
H	13.636517000	2.649533000	-3.066950000
H	13.742792000	4.250451000	-2.353360000
H	-7.343462000	-2.289496000	1.153520000
H	-7.573166000	-3.904953000	0.471848000
H	-7.433176000	-2.962853000	-1.840064000
H	-7.188725000	-1.346358000	-1.184107000
H	-9.446063000	-1.437061000	-0.088419000
H	-9.691828000	-3.062818000	-0.708339000
H	-9.563864000	-2.197067000	-3.057526000
H	-9.296844000	-0.570238000	-2.452147000
H	-11.537592000	-0.615305000	-1.321056000
H	-11.805700000	-2.249215000	-1.906040000
H	-11.685792000	-1.426736000	-4.275656000
H	-11.404134000	0.207524000	-3.698928000
H	-13.639037000	0.191592000	-2.550320000
H	-13.921469000	-1.446185000	-3.116741000
H	-3.942588000	4.539121000	2.918664000
H	-4.804338000	3.742767000	1.578744000
H	-5.895815000	4.098245000	4.419838000
H	-6.757990000	3.315215000	3.082244000
H	-7.512233000	4.651721000	3.962007000
H	4.847526000	-4.455562000	-0.026748000
H	3.982215000	-5.254802000	-1.362660000
H	6.798023000	-4.033297000	-1.535656000
H	5.932401000	-4.819332000	-2.869312000
H	7.549500000	-5.372600000	-2.413568000
H	5.061072000	-7.208711000	-2.603408000
H	5.278136000	-8.076407000	-1.074339000
H	6.671224000	-7.768342000	-2.125658000
H	7.170985000	-5.281291000	0.667151000
H	7.913987000	-6.632098000	-0.203261000
H	6.543621000	-6.923969000	0.881458000
H	-5.025346000	6.489009000	4.162077000
H	-6.634901000	7.048732000	3.682461000
H	-5.239845000	7.360572000	2.634856000
H	-7.126942000	4.568833000	0.881914000
H	-6.500158000	6.212487000	0.673338000
H	-7.872704000	5.916850000	1.754282000
C	15.333076000	4.151435000	-4.714281000
C	16.144666000	5.031137000	-3.756100000
C	-15.531851000	0.291517000	-4.598416000

C	-16.122549000	0.840469000	-5.900606000
H	13.492050000	5.284603000	-4.630781000
H	13.320807000	3.687590000	-5.338948000
H	-13.804638000	-0.646053000	-5.497137000
H	-13.515426000	0.991817000	-4.934624000
H	15.572923000	4.436719000	-5.746597000
H	15.651532000	3.105077000	-4.608013000
H	15.850981000	6.083779000	-3.844507000
H	17.215909000	4.966223000	-3.973742000
H	16.004256000	4.735687000	-2.711348000
H	-15.745831000	0.988826000	-3.776884000
H	-16.035319000	-0.649004000	-4.336098000
H	-15.662673000	1.797910000	-6.171190000
H	-17.201996000	1.002823000	-5.814372000
H	-15.955837000	0.148030000	-6.733724000

Cartesian coordinates of DFT-optimized structure of **13** by B3LYP /6-31G**/CH_2Cl_2:
Charge = 0; multiplicity=1

C	-1.472602000	-3.414674000	-1.248273000
C	-2.517970000	-2.495503000	-1.341633000
C	-2.274441000	-1.133150000	-1.029551000
C	-0.989225000	-0.749890000	-0.522629000
C	0.044744000	-1.730791000	-0.374940000
C	-0.199271000	-3.065311000	-0.792753000
C	-3.241794000	-0.100084000	-1.261091000
C	-3.003474000	1.195367000	-0.919338000
C	-1.771816000	1.601241000	-0.306938000
C	-0.737573000	0.619354000	-0.160577000
C	1.274817000	-1.325961000	0.238127000
C	1.512937000	-0.030329000	0.580601000
C	0.546565000	1.001507000	0.347559000
C	-1.519521000	2.938639000	0.093079000
C	-0.240809000	3.292935000	0.523454000
C	0.798231000	2.366936000	0.642667000
C	-2.556086000	4.012827000	0.074542000
C	2.109385000	2.873802000	1.080930000
C	3.396790000	2.541434000	0.687675000
N	4.200780000	3.388383000	1.372332000
N	3.468878000	4.215664000	2.147810000
N	2.210871000	3.910273000	1.975074000
N	-2.175943000	5.196867000	-0.439161000
C	-3.075163000	6.193062000	-0.417096000
C	-4.358593000	6.082289000	0.097437000
C	-4.746579000	4.851780000	0.647752000
C	-3.824765000	3.799332000	0.639414000
C	5.654539000	3.536766000	1.300523000
C	6.099810000	4.450897000	0.153792000
C	7.625203000	4.594601000	0.093837000
C	8.097638000	5.524052000	-1.031078000

C	9.623198000	5.660870000	-1.105521000
C	10.100043000	6.597673000	-2.222215000
C	11.625968000	6.728477000	-2.301736000
C	12.105016000	7.668045000	-3.414936000
O	-5.996650000	4.782583000	1.158846000
C	-6.453767000	3.544795000	1.727105000
C	-7.900607000	3.716794000	2.212781000
C	-8.344237000	2.367075000	2.808402000
C	-7.965583000	4.810373000	3.295330000
C	-8.813032000	4.088513000	1.028993000
H	-1.659152000	-4.441242000	-1.539567000
H	-4.175355000	-0.356841000	-1.746518000
H	-3.751306000	1.947609000	-1.138748000
H	2.017899000	-2.079778000	0.468054000
H	2.441221000	0.223890000	1.077623000
H	-0.047962000	4.328443000	0.776795000
H	3.783464000	1.820271000	-0.013959000
H	-2.746823000	7.140301000	-0.840777000
H	-5.049857000	6.917373000	0.090243000
H	-4.061406000	2.839728000	1.078289000
H	6.084606000	2.536490000	1.196614000
H	5.968252000	3.940943000	2.265655000
H	5.632716000	5.433797000	0.287644000
H	5.724675000	4.047732000	-0.795315000
H	8.080030000	3.602799000	-0.038540000
H	7.993658000	4.974263000	1.056853000
H	7.649177000	6.517393000	-0.891184000
H	7.718343000	5.151493000	-1.992978000
H	10.069449000	4.666647000	-1.250676000
H	10.002142000	6.025458000	-0.140178000
H	9.657779000	7.593009000	-2.073485000
H	9.716119000	6.236721000	-3.187070000
H	12.067423000	5.732906000	-2.452888000
H	12.009933000	7.086300000	-1.335662000
H	-5.801220000	3.266723000	2.565084000
H	-6.397880000	2.754118000	0.966971000
H	-7.708725000	2.071812000	3.650751000
H	-8.309182000	1.567032000	2.060286000
H	-9.373424000	2.434770000	3.175275000
H	-7.332701000	4.554896000	4.152827000
H	-8.991606000	4.927893000	3.659469000
H	-7.630752000	5.774504000	2.903152000
H	-8.787563000	3.315193000	0.252655000
H	-8.505148000	5.034237000	0.574824000
H	-9.850361000	4.192778000	1.363979000
C	0.824691000	-4.123086000	-0.762237000
N	0.494675000	-5.426779000	-0.487451000
N	1.558223000	-6.177241000	-0.591665000
N	2.588222000	-5.380161000	-0.945812000
C	2.178797000	-4.094766000	-1.059930000

C	3.936565000	-5.931112000	-1.079901000
C	4.783190000	-5.729494000	0.181581000
C	6.191038000	-6.318165000	0.031971000
C	7.055439000	-6.126232000	1.284340000
C	8.466068000	-6.711908000	1.147401000
C	9.330138000	-6.519364000	2.399737000
C	10.741982000	-7.103290000	2.267022000
C	11.604935000	-6.910810000	3.519969000
C	-3.846423000	-3.016316000	-1.777785000
N	-3.835012000	-3.883800000	-2.815974000
C	-5.005965000	-4.404353000	-3.190298000
C	-6.235166000	-4.122666000	-2.592809000
C	-6.238862000	-3.237451000	-1.508543000
C	-5.018840000	-2.682980000	-1.096212000
O	-7.333076000	-2.868886000	-0.804455000
C	-8.610853000	-3.418865000	-1.162943000
C	-9.684901000	-2.854003000	-0.221518000
C	-9.365122000	-3.240556000	1.234588000
C	-9.753612000	-1.321592000	-0.359811000
C	-11.030354000	-3.475660000	-0.641920000
H	2.842810000	-3.303478000	-1.368694000
H	4.405549000	-5.459465000	-1.948412000
H	3.808383000	-6.993229000	-1.299687000
H	4.267370000	-6.196952000	1.028812000
H	4.848830000	-4.656646000	0.403382000
H	6.691505000	-5.855599000	-0.830259000
H	6.114580000	-7.389981000	-0.197038000
H	6.551895000	-6.587659000	2.145159000
H	7.128039000	-5.053654000	1.513395000
H	8.968640000	-6.251118000	0.285018000
H	8.392469000	-7.784449000	0.918282000
H	8.826520000	-6.980211000	3.261375000
H	9.401867000	-5.446556000	2.629259000
H	11.245841000	-6.642260000	1.405380000
H	10.670281000	-8.176034000	2.037355000
H	-4.973267000	-5.097453000	-4.029322000
H	-7.137674000	-4.590078000	-2.964451000
H	-5.005174000	-2.020676000	-0.238877000
H	-8.570167000	-4.513260000	-1.082432000
H	-8.840014000	-3.156035000	-2.204152000
H	-9.324403000	-4.329160000	1.354278000
H	-10.137316000	-2.858001000	1.910256000
H	-8.402317000	-2.829908000	1.550687000
H	-8.798751000	-0.858446000	-0.095537000
H	-10.525727000	-0.911981000	0.299864000
H	-10.000049000	-1.027824000	-1.386598000
H	-11.012343000	-4.567578000	-0.552448000
H	-11.281950000	-3.223794000	-1.678226000
H	-11.836721000	-3.102153000	-0.002795000
C	13.017637000	-7.493107000	3.388945000

C	13.871955000	-7.296678000	4.645001000
H	11.101941000	-7.372538000	4.381786000
H	11.676490000	-5.838097000	3.750778000
H	13.520322000	-7.031037000	2.528296000
H	12.946684000	-8.564920000	3.158547000
H	13.991778000	-6.232852000	4.880090000
H	14.872327000	-7.724147000	4.520462000
H	13.411067000	-7.776538000	5.516014000
C	13.631116000	7.795864000	-3.496718000
C	14.101238000	8.736859000	-4.610079000
H	11.666500000	8.664801000	-3.262876000
H	11.719796000	7.312483000	-4.381494000
H	14.069227000	6.800092000	-3.649896000
H	14.016203000	8.150795000	-2.530979000
H	13.760442000	8.389555000	-5.592211000
H	15.193592000	8.805633000	-4.642513000
H	13.708392000	9.749664000	-4.464468000