Electronic Supplementary Information

Photoinduced charge separation in wide-band capturing, multi-modular bis(donor styryl)BODIPY-fullerene systems

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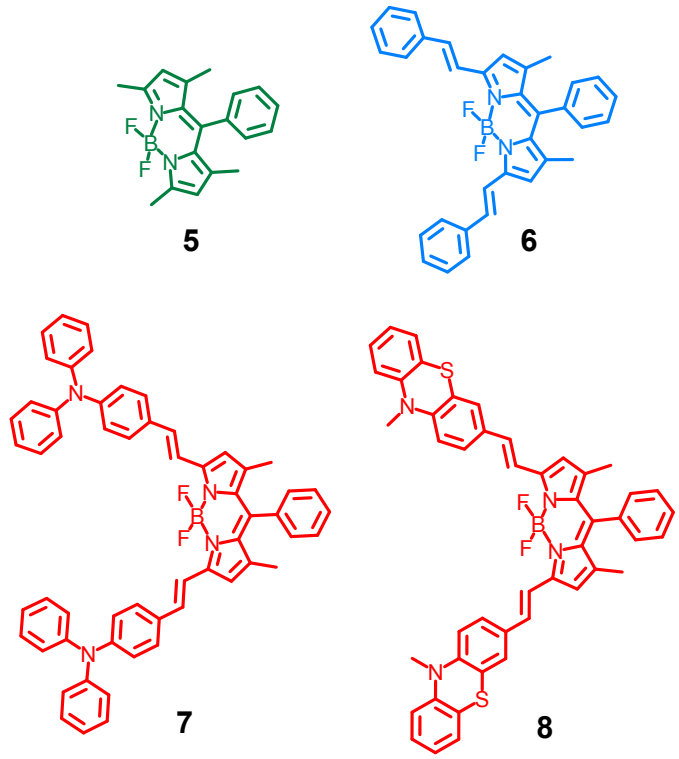


Fig. S1. Structure of the BODIPY (**5**), bis(phenyl styryl)BODIPY (**6**), bis(triphenylamine styryl)BODIPY (**7**), and bis(phenothiazine styryl)BODIPY-C_{60} (**8**) used as control compounds.

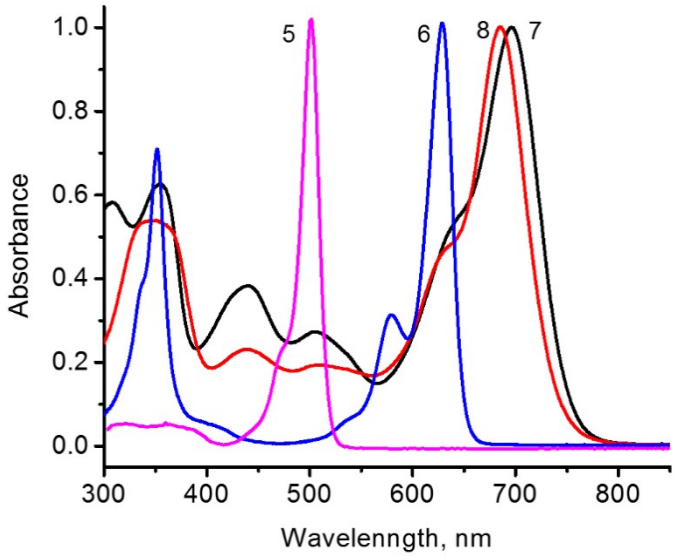


Fig. S2. Absorption spectra (normalized to the most intense peak maxima) of the indicated compounds in benzonitrile.

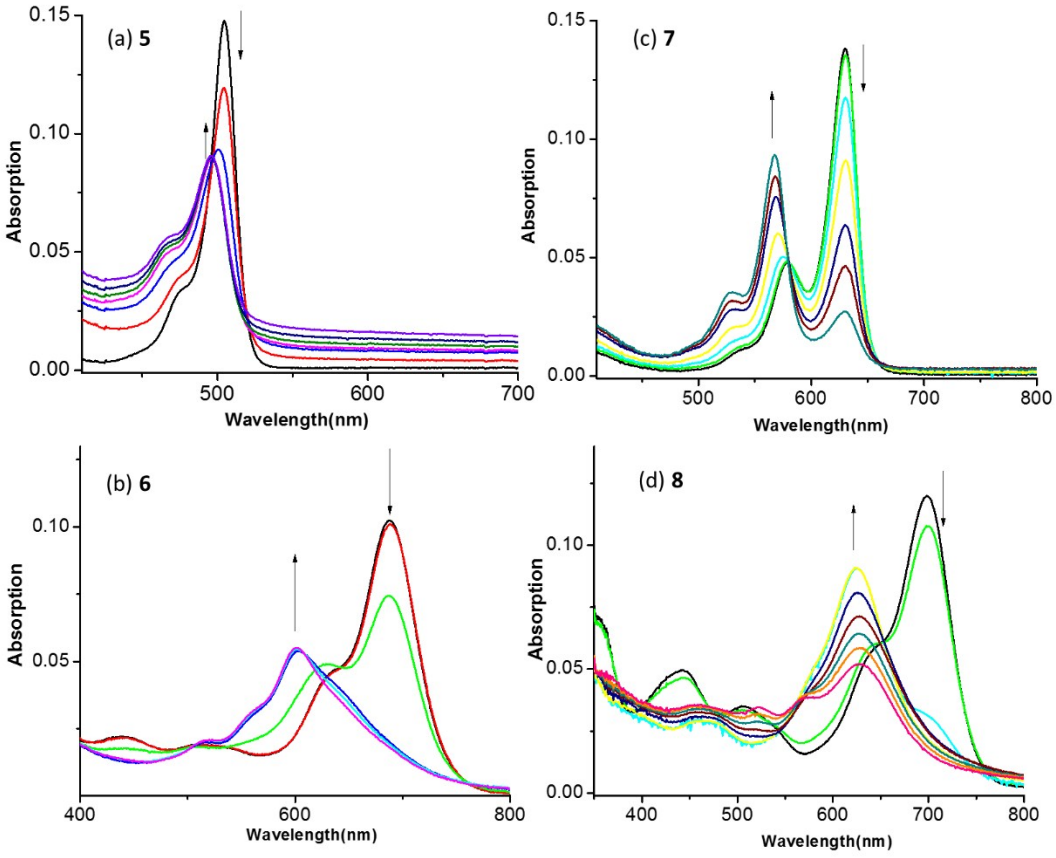
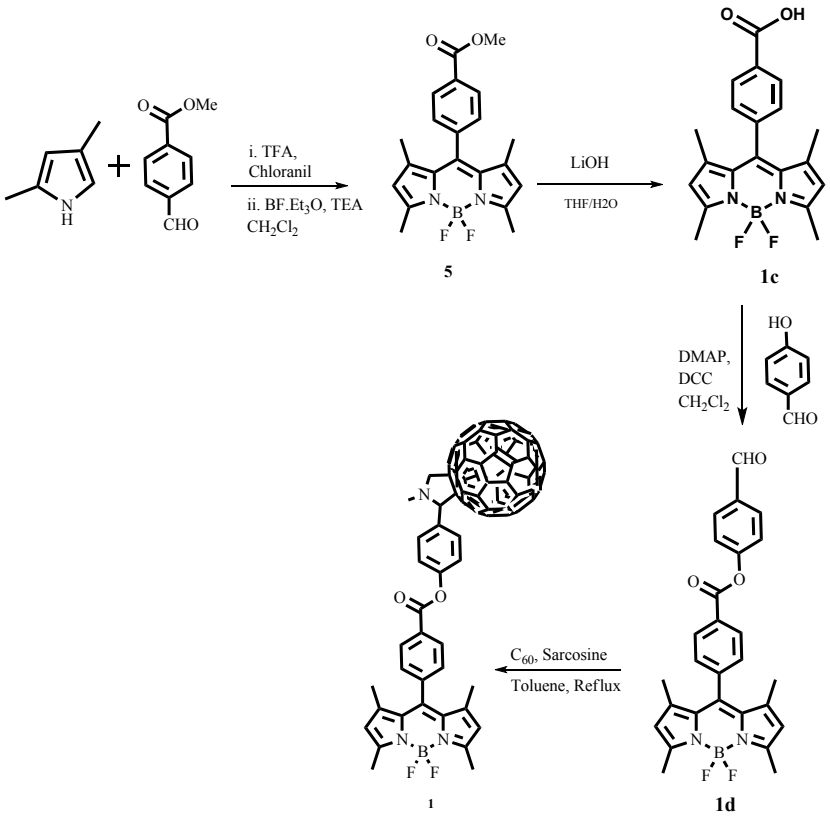


Fig. S3. Spectral changes observed during chemical oxidation of compound **5-8** in benzonitrile. Nitrosonium tetrafluroborate was used as an oxidizing agent.

Scheme S1: Synthetic methodology adopted for control compound **1**



Synthesis of **1c:** In a round-bottomed flask, compound **2a** (0.082 g, 0.215 mmoles) were dissolved in 2.5 mL of THF. To this solution, lithium hydroxide monohydrate (0.054 g, 1.07 mmoles) dissolved in 1.0 mL of water were rapidly added drop wise. The reaction mixture was stirred for 5 hours at room temperature. The mixture was then diluted with a 0.1 M solution of hydrochloric acid and extracted with dichloromethane and the organic phases were dried on sodium sulfate and evaporated under reduced pressure. The resulting mixture was purified by means of flash chromatography on silica gel using a methylene chloride/MeOH (99.05:1 drop % v/v) to afford compounds **1c**.

Yield (45.5 %) ^{1}H NMR ($CDCl_3$, 400 MHz, 25 °C), δ (ppm):), 8.12-8.16 (d, 2H, Ar-H), 7.66–7.70 (d, 2 H) 7.56–7.60 (d, 2H), 7.38–7.42 (d, 2 H), 7.32–7.37 (t, 4 H), 7.24–7.29 (m, 2 H), 6.60 (s, 2 H, 1.40 (s, 6 H).

Synthesis of **1d:** In a round-bottom flask, **1c**(0.021 g, 0.026 mmoles) and 4-hydoxy benzaldehyde (0.0157 g, 0.129 mmoles) were dissolved dry methylene chloride(25 mL), to this, 4-dimethylaminopyrdine, DMAP (0.016 g, 0.129) mmoles) was added The resulting solution was cooled to 0 °C, followed by addition of dicyclohexylcarbodiimide, DCC(0.027 g, 0.129 mmoles). The reaction mixture was stirred under nitrogen for 6 hours at room temperature. Excess solvent was removed under vacuum and the crude compound was washed with water several times and extracted with dichloromethane. Purification of the crude compound

was carried out on a silica gel column with hexane/ dichloromethane (1/9) as eluent giving the compound **1d.**

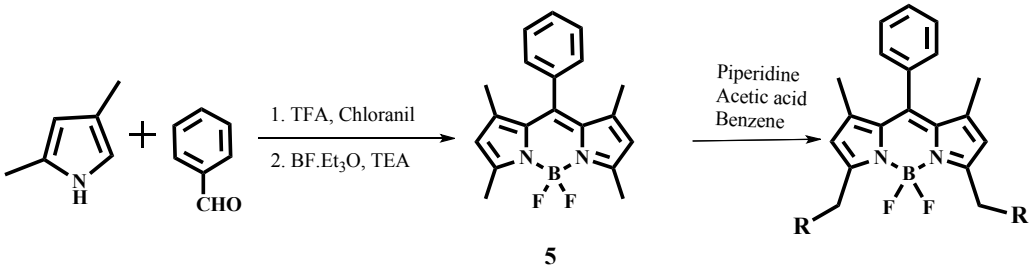
Yield (40%) ^{1}H NMR ($CDCl_3$, 400 MHz, 25 °C), δ (ppm): 10.14 (s, 1 H) 8.35- 8.39(d, 2H) 8.01-8.06(d, 2H), 7.35-7.40(m, 4 H), 6.01 (s, 2 H), 2.5(s, 2.53), 1.40 (s, 6 H)

Synthesis of **1:** Using Prato's[5] of synthesis, Compound **2** was synthesized as follows, to dry toluene (25 mL) in a round-bottomed flask, compound **2d** (0.0194 g, 0.0299 mmoles.), C_{60} (0.0645 g, 0.0896 mmoles), and sarcosine (0.0133 g, 0.149 mmoles) were refluxed for 12 hours. After cooling to room temperature, the solvent was evaporated and the crude was purified on silica by flash chromatography using toluene/hexane 9.5/0.5 v/v) solvent system affording the final compounds **1.**

Yield (83%) ^{1}H NMR ($CDCl_3$, 400 MHz, 25 °C), δ (ppm):8.18-8.22(d, 2H), 7.23-7.31(m, 4H), 7.04-7.15(m, 2H), 5.92(s, 1H), 4.90 (s, 2H), 4.26 (dd, 1H), 2.78(s, 3H) 2.49(s, 2.53), 1.39 (s, 6 H).

^{13}C NMR ($CDCl_3$) :164.4, 159.05, 155.7, 151.4, 146.0, 142.7, 140.2, 136.4, 132.6, 129.2, 122.6, 119.8, 116.2, 110.0, 107.3, 104.0, 101.1, 96.7, 91.9, 88.9, 86.1, 83.1, 77.2, 74.8, 70.1, 64.1, 60.9, 58.1, 52.3, 47.9, 42.9, 40.1, 37.3, 33.8, 30.8, 27.3, 23.0, 19.8 MS (MALDI): Calcd, : 1219.22 [M^+]; found 1219.7.

Scheme S2. Synthetic methodology adopted for control compounds **5-8**.



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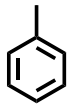
6



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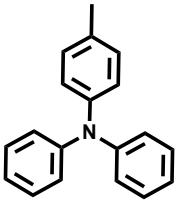

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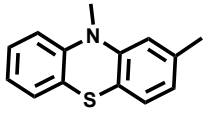


Synthesis of compounds 5-8

Synthesis of ***5*****:** The aryl-difluoroboron dipyrrin compounds was synthesized according to the procedure of Imahori and coworkers.[31]

To a mixture of aryl-aldehyde (12.4 mmol) and 2,4-dimethylpyrrole (2.16 mL, 21.1 mmol) in 800 mL of CH_2Cl_2, trifluoroacetic acid (0.19 mL, 2.47 mmol) was added. The reaction mixture was stirred for 2 hourd at room temperature under nitrogen. After which the solution mixture was washed with 0.1M NaOH (200 mL) followed by water (200 mL). The organic layer was dried over anhydrous Na_2SO_4 and evaporated under reduced pressure. The residue was dissolved in toluene (50 mL) and *p*-chloranil (2.73 g, 11.1 mmol) was added. After 10 minutes, Et_3N (8 mL) was added followed by $BF_3{\cdot}Et_2O$ (7 mL) and the mixture was stirred for 3 hours. To quench the reaction the mixture was poured into water. The organic layer was extracted and dried over anhydrous Na2SO4 and evaporated under reduced pressure. The crude product was purified using column chromatography using mixtures of CH_2Cl_2 and hexane as eluent.

Data for **5**: Yield: 8.71%. (^{1}H NMR in $CDCl_3$, 400 MHz, 25 °C), δ (ppm): 8.19 (d, 2 H), 7.41 (d, 2 H), 6.00 (s, 2H), 2.57 (s, 6 H), 1.37 (s, 6 H). ^{13}C NMR ($CDCl_3$): 155.43, 143.17, 141.74, 134.99, 131.43, 129.13, 129.04, 129.00, 128.94, 121.22, 121.2, 77.3, 77.05, 76.79, 14.61, 14.59, 14.57, 14.34, 14.33.

Synthesis of **6, 7** and **8***:* Synthesis of styrl compounds was accomplished according to the procedure of Rurack et. al.[32]**.** A mixture of a corresponding aldehyde (4 equiv), piperidine (10 equiv), and AcOH (10 equiv) and compound **5** (1 equiv) in toluene (20 mL) were refluxed and a reaction monitored using UV. The water formed during the reaction was removed azeotropically with a Dean–Stark apparatus. When all the starting material had been consumed, the mixture was cooled to room temperature and washed with water. The organic phase was dried over Na_2SO_4 and solvent was evaporated under reduced pressure. The residue was purified by silica gel column chromatography to afford the desired the control compounds **6, 7** and **8.**

Data for **6**: Yield (3.2 %). ^{1}H NMR in $CDCl_3$, 400 MHz, 25 °C), δ (ppm):), 7.64–7.77 (d, 2H), 7.54–7.58 (d,4 H, Ar-H,) 7.44–7.48 (4 H, Ar-H), 7.34–7.38 (t, 4 H, Ar-H), 7.28–7.3 (d, 2 H, CH-H), 7.20–7.24 (d,1 H, Ar-H), 6.81–6.85 (d, 2 H, Ar-H), 6.60 (s, 2 H, pyrrole-H), 1.50 (s, 6 H, CH_3-H). MS (MALDI): ^{13}C NMR ($CDCl_3$):152.62, 142.25, 139.15, 136.59, 136.22, 135.09, 133.39, 129.12, 129.02, 128.94, 128.80, 128.59, 128.39, 127.58, 119.29, 117.85, 77.45, 77.30, 77.20, 77.05, 76.95, 76.79, 14.65. Calcd, 500.22 [M+]; found 500.4.

Data for **7**: Yield (3.8%). ^{1}H NMR (400 MHz, $CDCl_3$) δ = 7.6 (d, 2H), 7.42-7.8 (m, 10H), 7.24-7.29 (m, 6H), 7.16 (d, 2H), 7.08-7.15 (m, 9H), 7.00-7.08 (m, 8H), 6.60(s, 2H), 1.50(s, 6H). MS (MALDI): ^{13}C NMR

($CDCl_3$):147.84, 129.36, 129.13, 128.99, 128.84, 124.79, 123.81, 123.80, 123.56, 122.42, 77.40, 77.27, 77.15, 77.01, 76.90, 76.76, 59.52, 53.43, 50.91, 38.15, 37.10, 31.93, 31.24, 30.04, 29.66, 29.38, 27.01, 22.70, 19.73, 14.59, 14.13. Calcd.: 834.37 [M^+]; found : 834.8

Data for **8**: Yield (2.9%). ^{1}Hnmr ($CDCl_3$): δ= 7.50–7.56 (d, 2 H CH-H), 7.23–7.44 (m, 9H, Ar-H), 7.32 (d, 2 H, Ar-H), 7.06–7.16 (m, 7 H, Ar-H), 6.87–6.92 (t, 2 H, Ar-H), 6.75–6.79 (d, 4H), 6.54(s, 2H), 3.35(s, 3H), 1.39(s, 6H). MS (MALDI): ^{13}C NMR ($CDCl_3$):152.34, 146.28, 135.00, 129.01, 128.53, 127.53, 127.21, 125.96, 122.77, 114.26, 114.21, 77.31, 77.06, 76.81, 35.49, 30.95, 14.6. Calcd: 770.25 [M^+]; found: 770.1.

Table S1. Crystal data and structure refinement for str0958.

Identification code	p-1	
Empirical formula	C33 H27 B F2 N2	
Formula weight	500.38	
Temperature	220(2) K	
Wavelength	0.71073 Å	
Crystal system	Triclinic	
Space group	P - 1	
Unit cell dimensions	a = 8.2790(4) Å	α= 100.217(2)°.
	b = 8.3562(4) Å	β= 98.258(2)°.
	c = 19.2301(9) Å	γ = 96.502(2)°.
Volume	1282.48(11) $Å^3$	
Z	2	
Density (calculated)	1.296 Mg/m^3	
Absorption coefficient	0.085 mm^{-1}	
F(000)	524	
Crystal size	0.25 x 0.24 x 0.06 mm^3	
Theta range for data collection	1.09 to 27.10°.	
Index ranges	-10<=h<=10, -10<=k<=10, -24<=l<=24	
Reflections collected	37665	
Independent reflections	5440 [R(int) = 0.0359]	
Completeness to theta = 27.10°	96.0 %	
Absorption correction	Semi-empirical from equivalents	
Max. and min. transmission	0.9949 and 0.9789	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	5440 / 0 / 345	
Goodness-of-fit on F^2	1.003	
Final R indices [I>2sigma(I)]	R1 = 0.0769, wR2 = 0.2091	
R indices (all data)	R1 = 0.0979, wR2 = 0.2254	
Largest diff. peak and hole	0.327 and -0.325 $e.Å^{-3}$	

Table S2. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$x 10^3) for str0958. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
F(1)	1507(3)	1576(2)	2115(1)	58(1)
N(1)	840(3)	3650(3)	3032(1)	42(1)
C(1)	846(4)	3016(4)	3637(2)	45(1)
B(1)	1900(4)	3235(4)	2450(2)	44(1)
N(2)	1520(3)	4323(3)	1896(1)	41(1)
F(2)	3563(2)	3531(3)	2748(1)	58(1)
C(2)	-215(4)	3768(4)	4053(2)	49(1)
C(3)	-923(4)	4856(4)	3696(2)	47(1)
C(4)	-265(4)	4795(3)	3051(2)	43(1)
C(5)	-518(3)	5643(3)	2489(2)	42(1)
C(6)	341(3)	5395(3)	1913(2)	41(1)
C(7)	259(4)	6048(4)	1275(2)	47(1)
C(8)	1383(4)	5375(4)	894(2)	46(1)
C(9)	2170(4)	4328(3)	1288(2)	43(1)
C(10)	1781(4)	1707(4)	3769(2)	47(1)
C(11)	1704(4)	980(4)	4331(2)	50(1)
C(12)	2508(4)	-416(4)	4468(2)	51(1)
C(13)	2821(5)	-681(5)	5170(2)	65(1)
C(14)	3613(6)	-1981(7)	5316(3)	91(2)
C(15)	4031(6)	-3059(6)	4758(4)	97(2)
C(16)	3707(5)	-2838(5)	4064(3)	82(1)
C(17)	2959(5)	-1524(4)	3916(2)	64(1)
C(18)	3494(4)	3414(3)	1119(2)	45(1)
C(19)	4149(4)	3420(4)	525(2)	46(1)
C(20)	5497(4)	2534(4)	326(2)	46(1)
C(21)	5548(4)	1969(4)	-391(2)	53(1)
C(22)	6728(4)	1043(4)	-602(2)	59(1)
C(23)	7913(4)	702(4)	-95(2)	65(1)
C(24)	7946(4)	1296(5)	622(2)	66(1)
C(25)	6729(4)	2200(4)	837(2)	58(1)
C(26)	-1732(4)	6845(3)	2502(2)	42(1)
C(27)	-3423(4)	6310(4)	2339(2)	48(1)
C(28)	-4526(4)	7428(4)	2339(2)	54(1)
C(29)	-3979(4)	9093(4)	2515(2)	58(1)

C(30)	-2301(4)	9638(4)	2682(2)	61(1)
C(31)	-1189(4)	8522(4)	2675(2)	54(1)
C(32)	-2161(5)	5890(5)	3967(2)	64(1)
C(33)	-819(5)	7243(5)	1031(2)	59(1)

Table S3. Bond lengths [Å] and angles [°] for str0958.

F(1)-B(1)	1.401(4)
N(1)-C(1)	1.361(4)
N(1)-C(4)	1.396(4)
N(1)-B(1)	1.536(4)
C(1)-C(2)	1.398(4)
C(1)-C(10)	1.447(4)
B(1)-F(2)	1.389(4)
B(1)-N(2)	1.540(4)
N(2)-C(9)	1.357(4)
N(2)-C(6)	1.397(3)
C(2)-C(3)	1.367(4)
C(2)-H(2A)	0.9400
C(3)-C(4)	1.420(4)
C(3)-C(32)	1.505(4)
C(4)-C(5)	1.399(4)
C(5)-C(6)	1.397(4)
C(5)-C(26)	1.498(4)
C(6)-C(7)	1.425(4)
C(7)-C(8)	1.374(4)
C(7)-C(33)	1.504(4)
C(8)-C(9)	1.410(4)
C(8)-H(8A)	0.9400
C(9)-C(18)	1.447(4)
C(10)-C(11)	1.336(5)
C(10)-H(10A)	0.9400
C(11)-C(12)	1.452(4)
C(11)-H(11A)	0.9400
C(12)-C(13)	1.398(5)
C(12)-C(17)	1.403(5)
C(13)-C(14)	1.380(5)
C(13)-H(13A)	0.9400
C(14)-C(15)	1.384(8)
C(14)-H(14A)	0.9400
C(15)-C(16)	1.372(8)
C(15)-H(15A)	0.9400
C(16)-C(17)	1.373(5)
C(16)-H(16A)	0.9400

C(17)-H(17A)	0.9400
C(18)-C(19)	1.334(4)
C(18)-H(18A)	0.9400
C(19)-C(20)	1.466(4)
C(19)-H(19A)	0.9400
C(20)-C(21)	1.383(5)
C(20)-C(25)	1.400(5)
C(21)-C(22)	1.376(4)
C(21)-H(21A)	0.9400
C(22)-C(23)	1.372(6)
C(22)-H(22A)	0.9400
C(23)-C(24)	1.375(6)
C(23)-H(23A)	0.9400
C(24)-C(25)	1.392(5)
C(24)-H(24A)	0.9400
C(25)-H(25A)	0.9400
C(26)-C(31)	1.388(4)
C(26)-C(27)	1.394(4)
C(27)-C(28)	1.378(4)
C(27)-H(27A)	0.9400
C(28)-C(29)	1.379(5)
C(28)-H(28A)	0.9400
C(29)-C(30)	1.384(5)
C(29)-H(29A)	0.9400
C(30)-C(31)	1.383(4)
C(30)-H(30A)	0.9400
C(31)-H(31A)	0.9400
C(32)-H(32A)	0.9700
C(32)-H(32B)	0.9700
C(32)-H(32C)	0.9700
C(33)-H(33A)	0.9700
C(33)-H(33B)	0.9700
C(33)-H(33C)	0.9700
C(1)-N(1)-C(4)	107.4(2)
C(1)-N(1)-B(1)	126.4(3)
C(4)-N(1)-B(1)	126.2(3)
N(1)-C(1)-C(2)	109.4(3)
N(1)-C(1)-C(10)	122.1(3)
C(2)-C(1)-C(10)	128.4(3)

F(2)-B(1)-F(1)	108.3(3)
F(2)-B(1)-N(1)	110.4(3)
F(1)-B(1)-N(1)	110.6(3)
F(2)-B(1)-N(2)	110.8(3)
F(1)-B(1)-N(2)	109.6(3)
N(1)-B(1)-N(2)	107.1(2)
C(9)-N(2)-C(6)	108.3(2)
C(9)-N(2)-B(1)	126.5(2)
C(6)-N(2)-B(1)	125.0(2)
C(3)-C(2)-C(1)	108.2(3)
C(3)-C(2)-H(2A)	125.9
C(1)-C(2)-H(2A)	125.9
C(2)-C(3)-C(4)	107.1(3)
C(2)-C(3)-C(32)	124.2(3)
C(4)-C(3)-C(32)	128.7(3)
N(1)-C(4)-C(5)	119.6(3)
N(1)-C(4)-C(3)	107.9(3)
C(5)-C(4)-C(3)	132.4(3)
C(6)-C(5)-C(4)	121.3(3)
C(6)-C(5)-C(26)	119.2(3)
C(4)-C(5)-C(26)	119.5(3)
N(2)-C(6)-C(5)	120.6(3)
N(2)-C(6)-C(7)	107.6(2)
C(5)-C(6)-C(7)	131.8(3)
C(8)-C(7)-C(6)	107.0(3)
C(8)-C(7)-C(33)	124.1(3)
C(6)-C(7)-C(33)	128.9(3)
C(7)-C(8)-C(9)	108.2(3)
C(7)-C(8)-H(8A)	125.9
C(9)-C(8)-H(8A)	125.9
N(2)-C(9)-C(8)	108.8(3)
N(2)-C(9)-C(18)	122.8(3)
C(8)-C(9)-C(18)	128.3(3)
C(11)-C(10)-C(1)	123.1(3)
C(11)-C(10)-H(10A)	118.5
C(1)-C(10)-H(10A)	118.5
C(10)-C(11)-C(12)	126.0(3)
C(10)-C(11)-H(11A)	117.0
C(12)-C(11)-H(11A)	117.0

C(13)-C(12)-C(17)	118.9(3)
C(13)-C(12)-C(11)	119.1(3)
C(17)-C(12)-C(11)	121.9(3)
C(14)-C(13)-C(12)	120.2(4)
C(14)-C(13)-H(13A)	119.9
C(12)-C(13)-H(13A)	119.9
C(13)-C(14)-C(15)	119.4(5)
C(13)-C(14)-H(14A)	120.3
C(15)-C(14)-H(14A)	120.3
C(16)-C(15)-C(14)	121.2(4)
C(16)-C(15)-H(15A)	119.4
C(14)-C(15)-H(15A)	119.4
C(15)-C(16)-C(17)	119.8(5)
C(15)-C(16)-H(16A)	120.1
C(17)-C(16)-H(16A)	120.1
C(16)-C(17)-C(12)	120.4(4)
C(16)-C(17)-H(17A)	119.8
C(12)-C(17)-H(17A)	119.8
C(19)-C(18)-C(9)	123.2(3)
C(19)-C(18)-H(18A)	118.4
C(9)-C(18)-H(18A)	118.4
C(18)-C(19)-C(20)	125.9(3)
C(18)-C(19)-H(19A)	117.1
C(20)-C(19)-H(19A)	117.1
C(21)-C(20)-C(25)	118.2(3)
C(21)-C(20)-C(19)	119.5(3)
C(25)-C(20)-C(19)	122.3(3)
C(22)-C(21)-C(20)	121.5(3)
C(22)-C(21)-H(21A)	119.2
C(20)-C(21)-H(21A)	119.2
C(23)-C(22)-C(21)	119.7(4)
C(23)-C(22)-H(22A)	120.2
C(21)-C(22)-H(22A)	120.2
C(22)-C(23)-C(24)	120.6(3)
C(22)-C(23)-H(23A)	119.7
C(24)-C(23)-H(23A)	119.7
C(23)-C(24)-C(25)	119.7(4)
C(23)-C(24)-H(24A)	120.1
C(25)-C(24)-H(24A)	120.1

C(24)-C(25)-C(20)	120.2(4)
C(24)-C(25)-H(25A)	119.9
C(20)-C(25)-H(25A)	119.9
C(31)-C(26)-C(27)	118.5(3)
C(31)-C(26)-C(5)	120.4(3)
C(27)-C(26)-C(5)	121.1(3)
C(28)-C(27)-C(26)	120.5(3)
C(28)-C(27)-H(27A)	119.8
C(26)-C(27)-H(27A)	119.8
C(27)-C(28)-C(29)	120.7(3)
C(27)-C(28)-H(28A)	119.6
C(29)-C(28)-H(28A)	119.6
C(28)-C(29)-C(30)	119.3(3)
C(28)-C(29)-H(29A)	120.4
C(30)-C(29)-H(29A)	120.4
C(31)-C(30)-C(29)	120.2(3)
C(31)-C(30)-H(30A)	119.9
C(29)-C(30)-H(30A)	119.9
C(30)-C(31)-C(26)	120.7(3)
C(30)-C(31)-H(31A)	119.6
C(26)-C(31)-H(31A)	119.6
C(3)-C(32)-H(32A)	109.5
C(3)-C(32)-H(32B)	109.5
H(32A)-C(32)-H(32B)	109.5
C(3)-C(32)-H(32C)	109.5
H(32A)-C(32)-H(32C)	109.5
H(32B)-C(32)-H(32C)	109.5
C(7)-C(33)-H(33A)	109.5
C(7)-C(33)-H(33B)	109.5
H(33A)-C(33)-H(33B)	109.5
C(7)-C(33)-H(33C)	109.5
H(33A)-C(33)-H(33C)	109.5
H(33B)-C(33)-H(33C)	109.5

Symmetry transformations used to generate equivalent atoms:

Table S4. Anisotropic displacement parameters ($Å^2 x\ 10^3$) for str0958. The anisotropic displacement factor exponent takes the form: $-2\pi^2[\ h^2\ a^{*2}U^{11} + ...\ + 2\ h\ k\ a^*\ b^*\ U^{12}\ ]$

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
F(1)	75(1)	36(1)	64(1)	6(1)	21(1)	12(1)
N(1)	40(1)	38(1)	48(1)	5(1)	8(1)	5(1)
C(1)	41(2)	40(2)	50(2)	3(1)	4(1)	4(1)
B(1)	40(2)	38(2)	56(2)	7(1)	10(1)	9(1)
N(2)	38(1)	35(1)	52(1)	6(1)	11(1)	6(1)
F(2)	40(1)	72(1)	66(1)	20(1)	8(1)	16(1)
C(2)	50(2)	51(2)	47(2)	9(1)	10(1)	14(1)
C(3)	44(2)	44(2)	51(2)	3(1)	8(1)	9(1)
C(4)	40(2)	36(1)	50(2)	0(1)	10(1)	8(1)
C(5)	34(1)	35(1)	51(2)	-2(1)	5(1)	1(1)
C(6)	36(1)	36(1)	51(2)	5(1)	8(1)	5(1)
C(7)	42(2)	41(2)	57(2)	8(1)	9(1)	5(1)
C(8)	42(2)	41(2)	55(2)	11(1)	10(1)	8(1)
C(9)	39(2)	36(1)	51(2)	2(1)	8(1)	2(1)
C(10)	43(2)	43(2)	52(2)	3(1)	9(1)	7(1)
C(11)	47(2)	47(2)	54(2)	3(1)	7(1)	11(1)
C(12)	42(2)	43(2)	70(2)	14(1)	10(1)	5(1)
C(13)	53(2)	65(2)	86(3)	34(2)	20(2)	12(2)
C(14)	66(3)	99(4)	138(4)	78(3)	35(3)	27(2)
C(15)	61(3)	66(3)	190(6)	72(3)	42(3)	25(2)
C(16)	57(2)	47(2)	145(5)	17(2)	26(3)	15(2)
C(17)	54(2)	50(2)	86(3)	3(2)	9(2)	13(2)
C(18)	41(2)	36(1)	57(2)	6(1)	8(1)	6(1)
C(19)	40(2)	40(2)	57(2)	8(1)	9(1)	8(1)
C(20)	35(1)	36(1)	66(2)	9(1)	10(1)	2(1)
C(21)	46(2)	54(2)	64(2)	13(2)	19(2)	9(1)
C(22)	48(2)	55(2)	78(2)	9(2)	22(2)	8(2)
C(23)	44(2)	48(2)	106(3)	9(2)	23(2)	12(2)
C(24)	41(2)	55(2)	98(3)	10(2)	0(2)	10(2)
C(25)	49(2)	51(2)	70(2)	4(2)	3(2)	8(1)
C(26)	41(2)	39(1)	46(2)	4(1)	10(1)	7(1)
C(27)	40(2)	42(2)	58(2)	3(1)	8(1)	4(1)
C(28)	35(2)	56(2)	67(2)	2(2)	5(1)	9(1)
C(29)	48(2)	52(2)	71(2)	3(2)	6(2)	20(2)

C(30)	51(2)	40(2)	85(3)	2(2)	4(2)	9(1)
C(31)	40(2)	39(2)	77(2)	3(2)	3(2)	3(1)
C(32)	69(2)	76(2)	57(2)	15(2)	19(2)	38(2)
C(33)	58(2)	64(2)	65(2)	20(2)	16(2)	25(2)

Table S5. Hydrogen coordinates (x 10^4) and isotropic displacement parameters ($Å^2$x 10^3) for str0958.

	x	y	z	U(eq)
H(2A)	-408	3561	4501	58
H(8A)	1591	5578	447	55
H(10A)	2474	1352	3444	56
H(11A)	1072	1412	4669	60
H(13A)	2491	28	5543	78
H(14A)	3866	-2133	5790	110
H(15A)	4546	-3959	4856	116
H(16A)	3997	-3583	3691	99
H(17A)	2746	-1366	3441	77
H(18A)	3914	2784	1444	54
H(19A)	3705	4050	205	55
H(21A)	4757	2224	-741	64
H(22A)	6723	646	-1092	71
H(23A)	8710	56	-239	78
H(24A)	8786	1093	966	80
H(25A)	6734	2588	1327	70
H(27A)	-3815	5179	2228	57
H(28A)	-5663	7052	2218	65
H(29A)	-4738	9850	2521	69
H(30A)	-1917	10771	2800	73
H(31A)	-52	8904	2790	65
H(32A)	-2236	5792	4457	97
H(32B)	-3231	5516	3668	97
H(32C)	-1815	7030	3951	97
H(33A)	-751	7288	535	89
H(33B)	-448	8325	1327	89
H(33C)	-1951	6888	1072	89

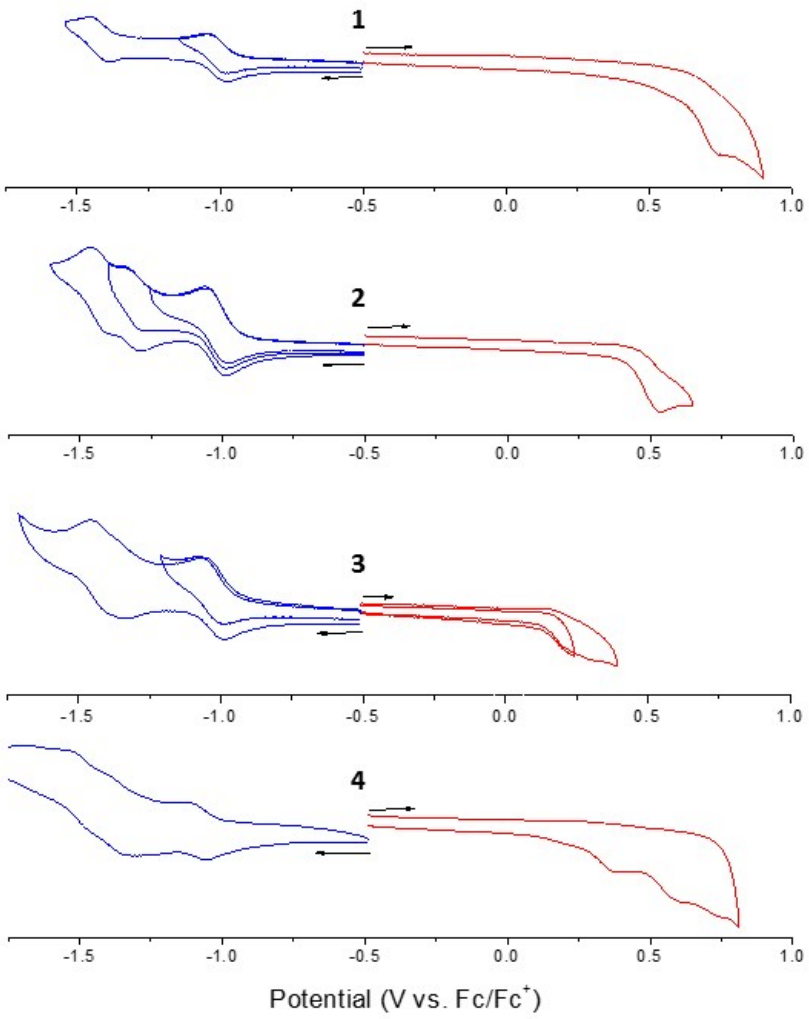


Fig. S4. Cyclic voltammograms (DPVs) corresponding to both oxidation and reduction processes of the indicated compounds in benzonitrile containing 0.1 M (*t*-Bu4N)ClO4. Scan rate = 5 mV/s, pulse width = 0.25 s, pulse height = 0.025 V.

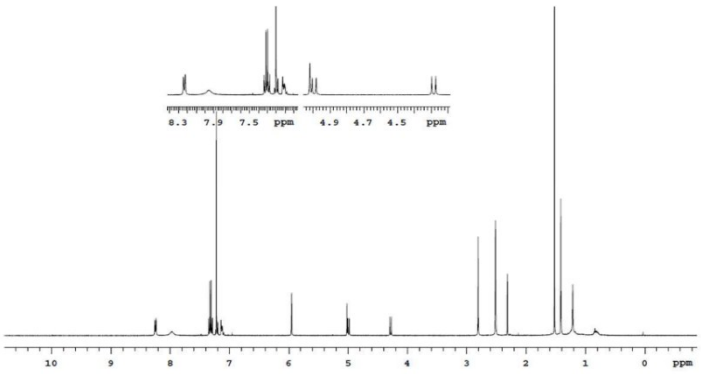


Fig. S5. ^{1}H NMR spectrum of **1** in $CDCl_3$

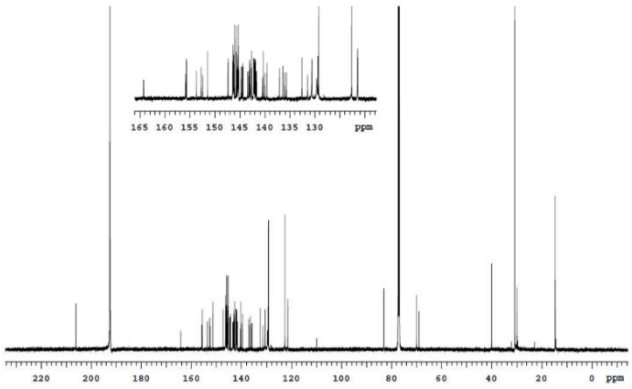


Fig. S6. ^{13}C NMR spectrum of **1** in $CDCl_3$

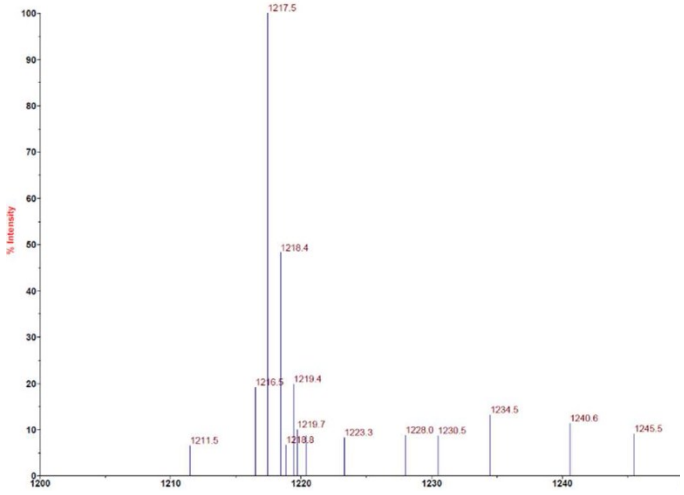


Fig. S7. MALDI spectrum of **1** in $CDCl_3$

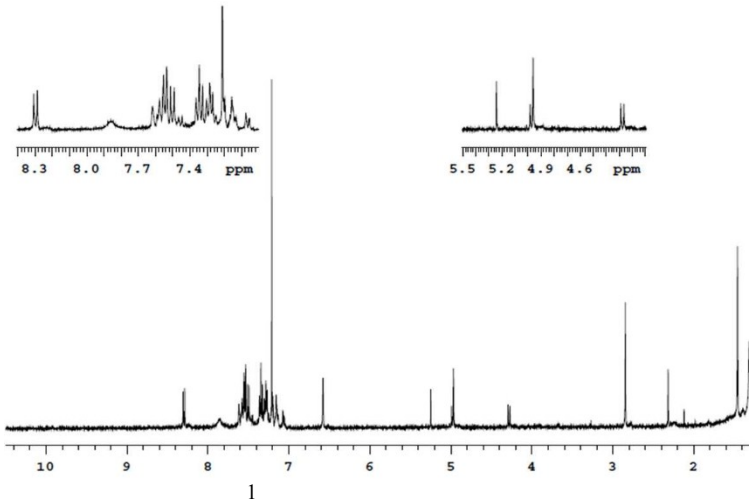


Fig. S8. ^{1}H NMR spectrum of **2** in $CDCl_3$.

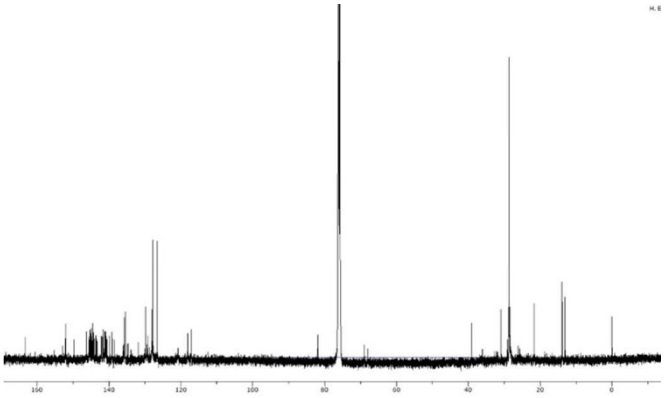


Fig. S9. ^{13}C NMR spectrum of **2** in $CDCl_3$.

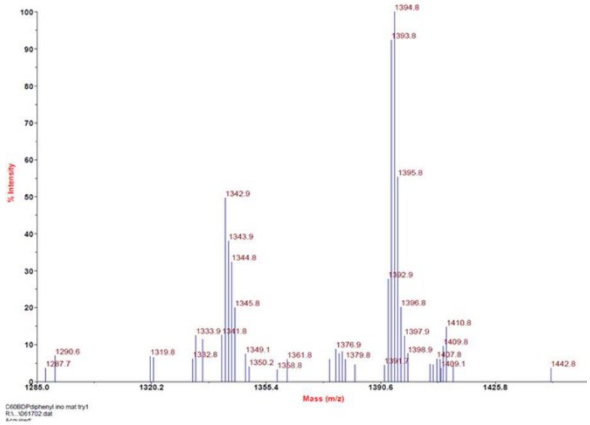


Fig. S10. MALDI mass spectrum of **2**

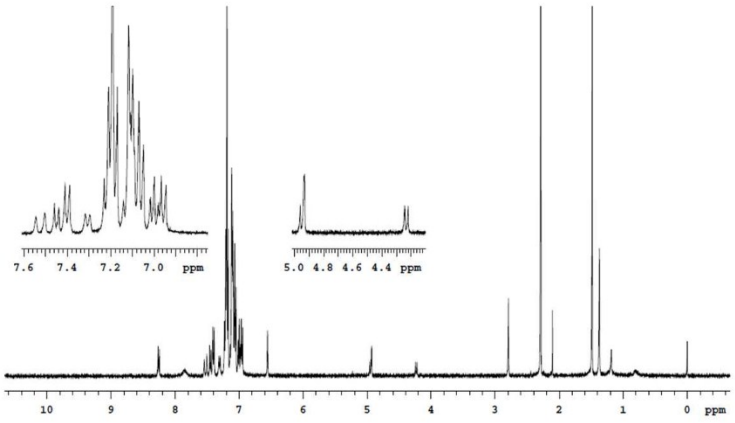


Fig. S11. ^{1}H NMR spectrum of **3** in $CDCl_3$.

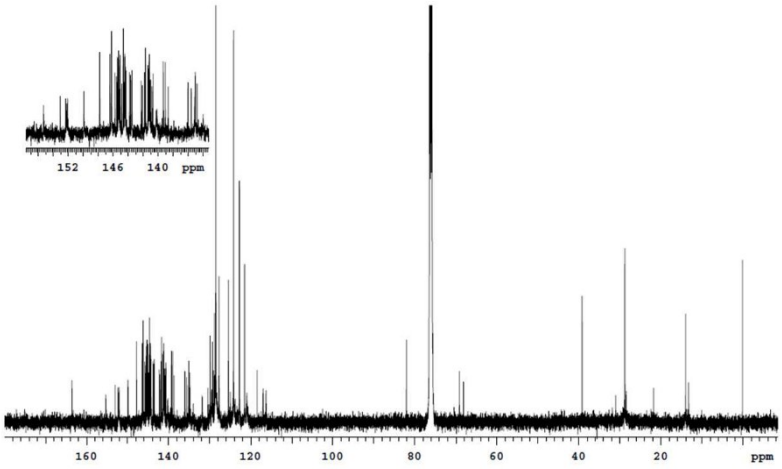


Fig. S12. ^{13}C- NMR spectrum of **3** in $CDCl_3$

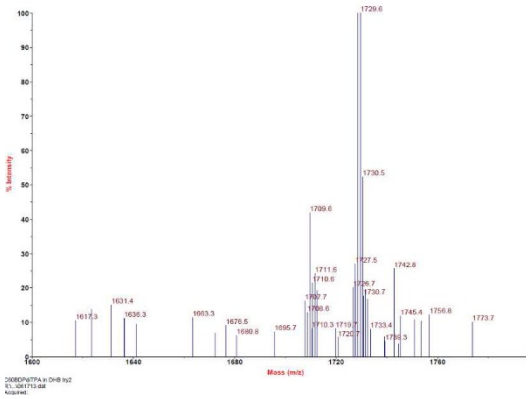


Fig. S12. MALDI-mass spectrum of **3**

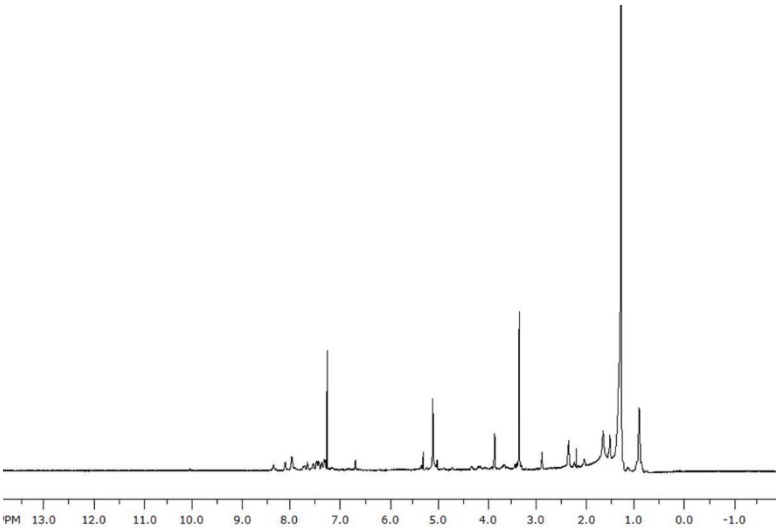


Fig. S13. ^{1}H NMR spectrum of **4** in $CDCl_3$

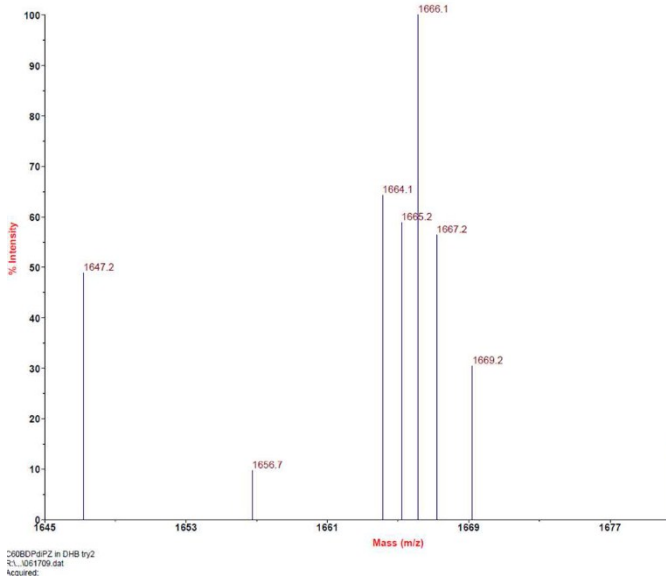


Fig. S14. MALDI-mass spectrum of **4**

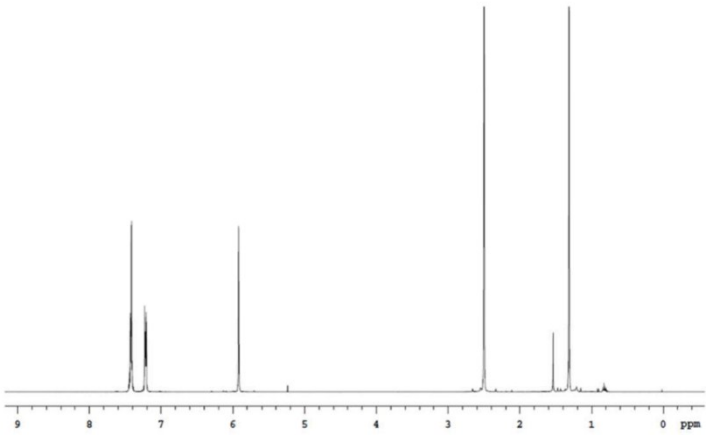


Fig. S15. ^{1}H NMR spectrum of **5** in $CDCl_3$

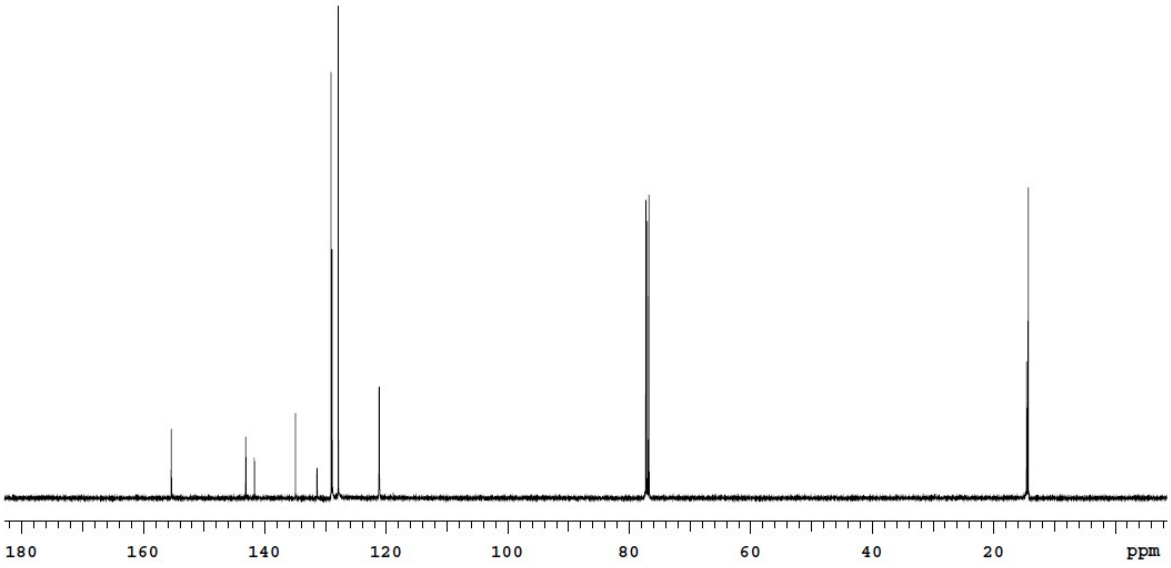


Fig. S16. ^{13}C NMR spectrum of **5** in $CDCl_3$

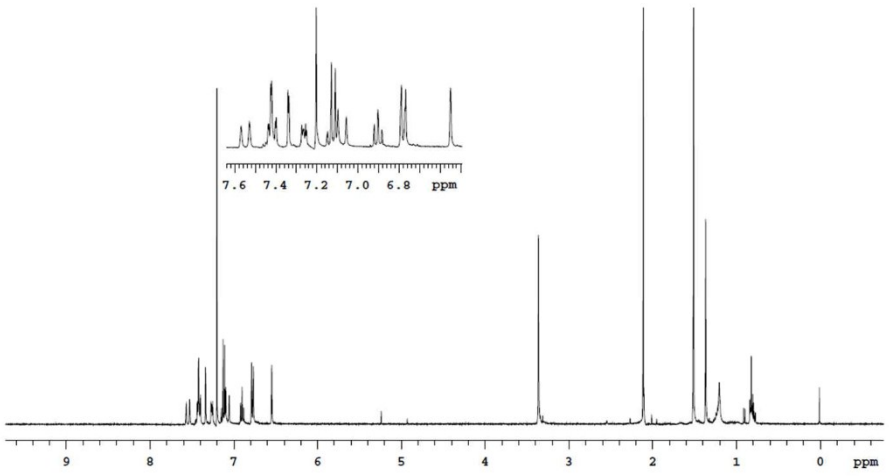


Fig. S17. ^{1}H NMR spectrum of **6** in $CDCl_3$

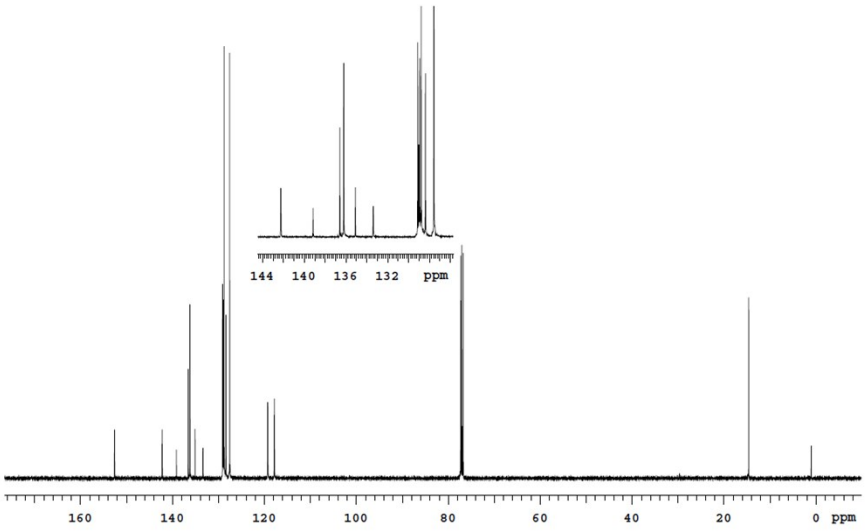
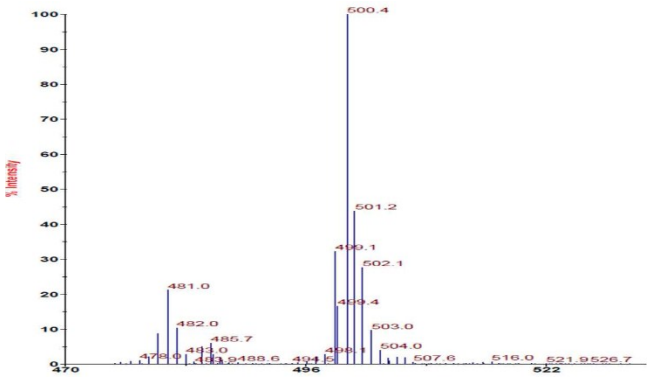


Fig. S18. ^{13}C NMR spectrum of **6** in $CDCl_3$



Mass (m/z)

Fig. S19. MALDI-mass spectrum of **6**

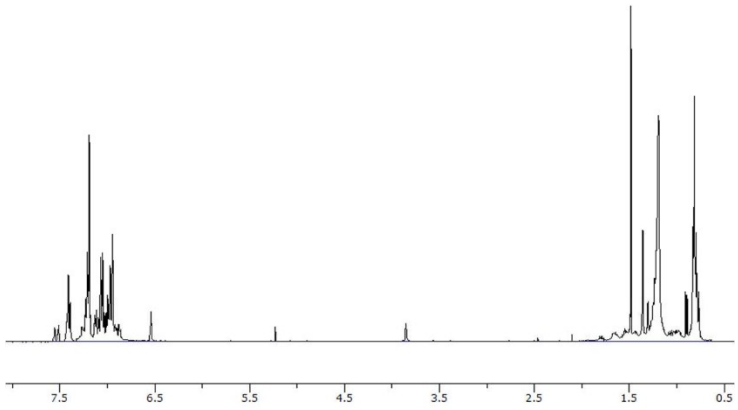


Fig. S20. ^{1}H NMR spectrum of **7** in $CDCl_3$

Fig. S21. ^{13}C NMR spectrum of **7** in $CDCl_3$

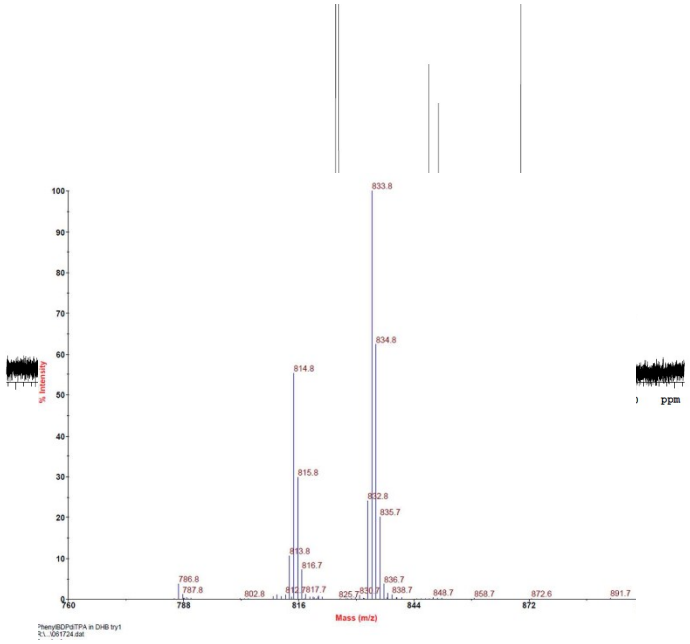


Fig. S22. MALDI mass spectrum of **7**

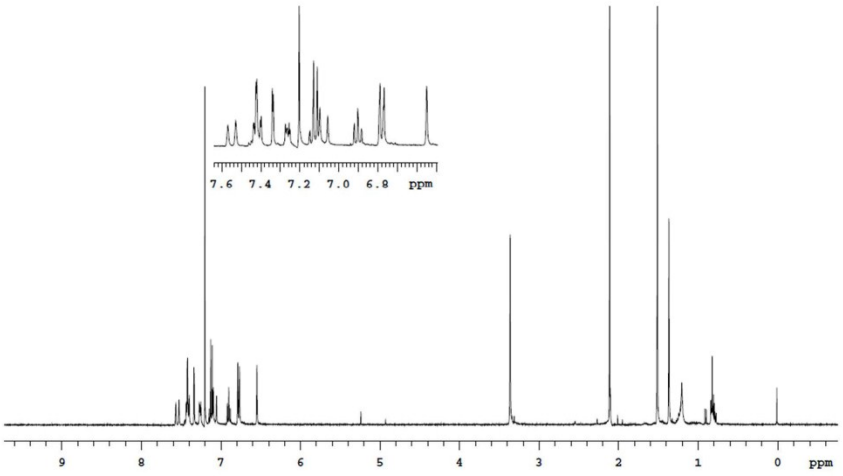


Fig. S23. ^{1}H NMR of **8** in $CDCl_3$

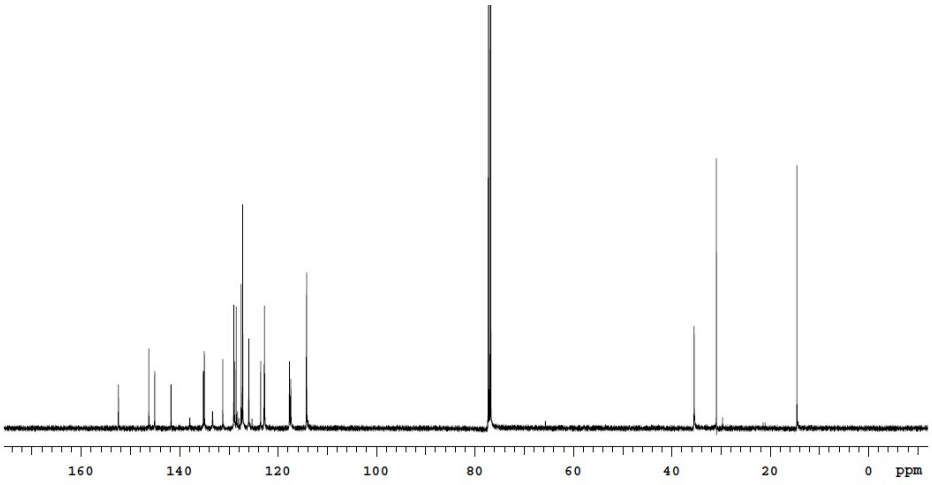


Fig. S24. ^{13}C NMR of **8** in $CDCl_3$

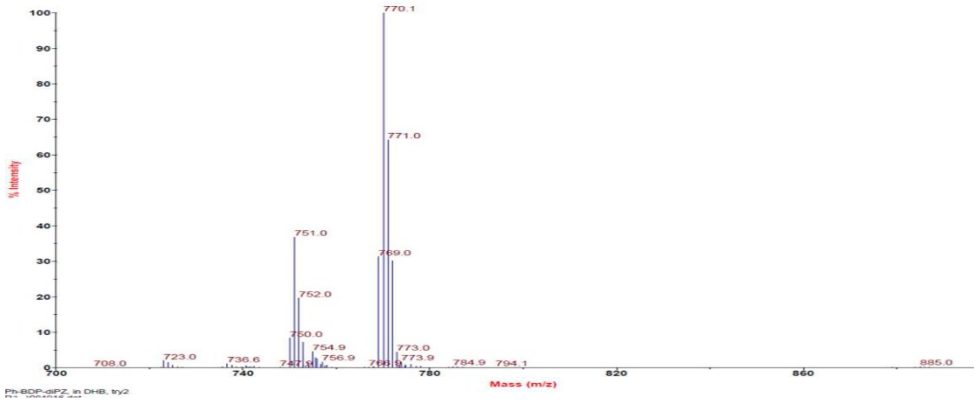


Fig. S25. MALDI-mass spectrum of **8=**