Electronic Supplementary Material (ESI) for Organic Chemistry Frontiers.

Supporting Information

Ring-expansion Approach toward Extended Asymmetric Benzopentafulvalene: Overcrowded Olefinic Structure and Chain-length Dependent Property

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Table of Contents

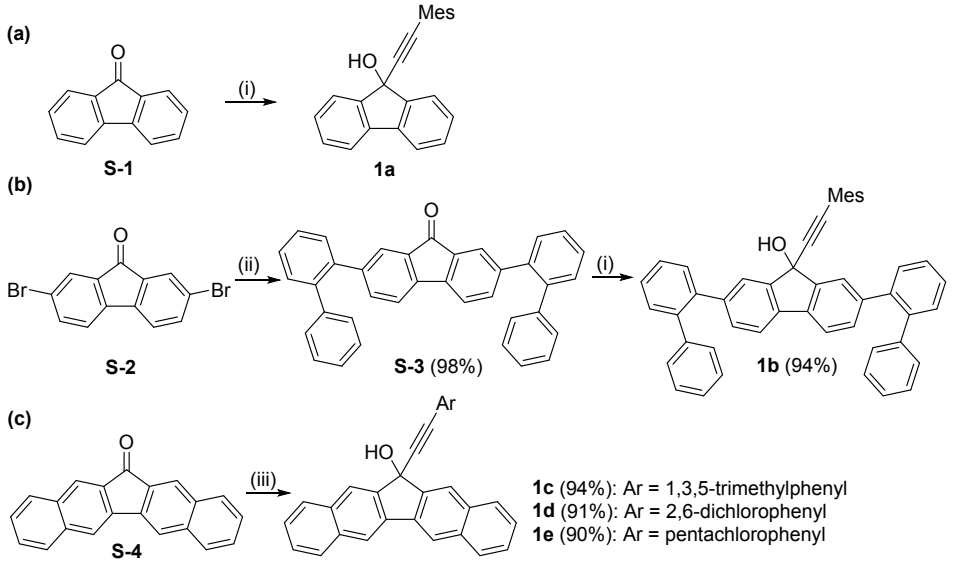
Experimental Procedures

General method

Solvents were purified and dried by standard methods prior to use. All commercially available reagents were used without further purification unless otherwise noted. Column chromatography was generally performed on silica gel (200 - 300 mesh) and reactions were monitored by thin layer chromatography (TLC) using silica gel GF254 plates with UV light to visualize the course of reaction. ^{1}H NMR and ^{13}C NMR data were recorded on a 400 MHz spectrometer at room temperature. All chemical shifts are quoted in ppm, relative to tetramethylsilane, using residual solvent peak as a reference standard. The following abbreviations were used to explain the multiplicities: s = singlet, d = doublet, t = triplet, q = quartet, m = multiplet. Cyclic voltammetry (CV) and differential pulse voltammetry (DPV) were performed on a Chenhua 650D electrochemical using a three-electrode cell with a glassy carbon working electrode, a platinum wire counter electrode, and an $Ag/AgNO_3$ or Ag/AgCl reference electrode in anhydrous solvents containing recrystallized tetrabutylammonium hexafluorophosphate ($TBAPF_6$, 0.10 M) as supporting electrolyte at 298 K. The potential was externally calibrated against the ferrocene/ferrocenium couple. Absorption spectra were recorded on a Shimadzu UV-3600 plus. High-resolution mass spectra (HRMS) were recorded on a Finnigan MAT TSQ 7000 or an Agilent 1200-6520 Q-TOF mass spectrometer system operating in a MALDI-TOF mode. Electron spin resonance (ESR) spectra were performed on a JES-FA200 spectrometer.

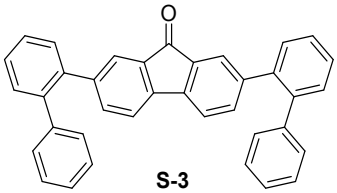
Synthetic procedures

Scheme S1. Preparation of starting materials 1a[a]-1e



Reagent and conditions: (i) trimethylphenylalkynyl lithium, dry THF, -78 ℃ to r.t.; [a]Compound **1a** was synthesized according to our previous procedure.[1] (ii) 2-biphenylboronic acid, $Pd(PPh_3)_4$, aqueous K_2CO_3 (2M), toluene, ethanol (1~2 mL), 80 ℃. (iii) lithiated 1,3,5-trimethylphenyl/2,6-dichlorophenyl/pentachlorophenyl alkyne reagents,[2] dry THF, -78 ℃ to r.t

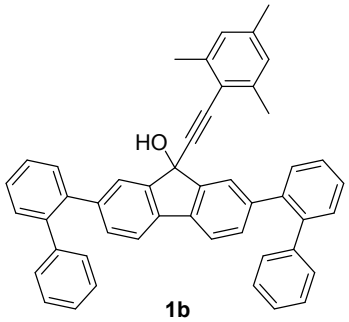
Synthesis of compound S-3



S-3

To a solution of 2,7-dibromo-9H-fluoren-9-one (compound **S-2** in Scheme S1, 500.0 mg, 1.48 mmol) in toluene (40 mL), 2-biphenylboronic acid (322.2 mg, 1.63 mmol), $Pd(PPh_3)_4$ (68.4 mg, 0.07 mmol), aqueous solution K_2CO_3 (2.0 M, 10 mL) and ethanol (1~2 mL) were added under argon atmosphere. The reaction mixture was stirred at 80 ℃, and monitored by TLC to confirm consumption of starting material. Upon completion, the solution was diluted with dichloromethane (50 mL) and water (15 mL), and washed with brine (20 mL). After removal of the solvent, the residue was purified by silica gel chromatography (petroleum ether/CH_2Cl_2 = 1:1) to afford compound **S-3** (703 mg, 98% yield) as a yellow solid. ^{1}H NMR (400 MHz, $CDCl_3$): δ 7.56 (s, 2H), 7.45 (s, 8H) 7.24 - 7.18 (m, 12H), 7.12 (d, *J* = 7.8 Hz, 2H). ^{13}C NMR (100 MHz, $CDCl_3$): δ 193.51, 142.58, 142.35, 141.04, 140.49, 139.22, 136.36, 134.48, 130.71, 130.11, 129.81, 128.10, 127.98, 127.63, 126.72, 125.44, 119.67. MS (APCI, *m/z*) calcd for $C_{37}H_{24}O$ $[M+Na]^+$, 507.1227; found: 507.1229, (error = 0.4 ppm).

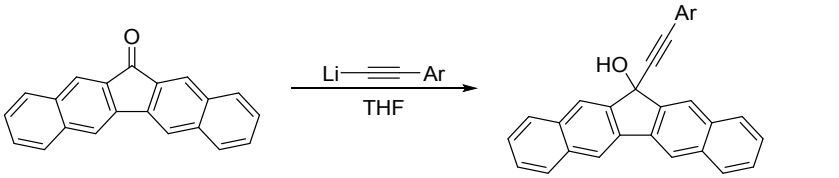
Synthesis of 1b



1b

A solution of 2-ethynyl-1,3,5-trimethylbenzene (143 mg, 0.99 mmol) in THF (30 mL) was cooled to -78 ℃, and *n*-BuLi (0.40 mL, 0.99 mmol, 2.5 M in hexane) was added dropwise under N_2 atmosphere. The freshly prepared lithium acetylide was kept stirring at -78 ℃ for 1 h, and was slowly added to a solution of compound **S-4** (400.0 mg, 0.83 mmol) in THF (20 mL) at -78 ℃. The mixture was then warmed up to the room temperature and stirred for another 1 h. Upon completion of reaction, the solution was diluted with water (20 mL) and dichloromethane (50 mL). The organic layer was dried by anhydrous $MgSO_4$. After filtration, the organic solvents were evaporated to dryness. The residue was purified by column chromatography on silica gel (petroleum ether/CH_2Cl_2 = 1:1) to afford compound **1b** (488 mg, 94% yield) as a white solid. ^{1}H NMR (400 MHz, $CDCl_3$): δ 7.61 (s, 2H), 7.51 - 7.49 (m, 10H), 7.40 - 7.38 (m, 2H), 7.20 - 7.18 (m, 8H), 7.10 (d, *J* = 8.2 Hz, 2H), 6.85 (s, 2H), 2.42 (s, 1H), 2.31 - 2.29 (m, 9H). ^{13}C NMR (100 MHz, $CDCl_3$): δ 147.61, 141.82, 141.34, 140.59, 140.46, 140.18, 137.92, 137.02, 131.47, 130.61, 130.40, 129.85, 127.92, 127.63, 127.55, 127.50, 127.42, 126.49, 125.56, 119.56, 119.18, 96.32, 81.04, 75.07, 21.33, 20.94. HRMS (MALDI-TOF, *m/z*) calcd for $C_{48}H_{36}O$ $[M]^+$, 628.2766; found: 628.2749 (error = -2.7 ppm).

General procedure for synthesis of 1c-1e



S-4

1c (94%): Ar = 1,3,5-trimethylphenyl
1d (91%): Ar = 2,6-dichlorophenyl
1e (90%): Ar = pentachlorophenyl

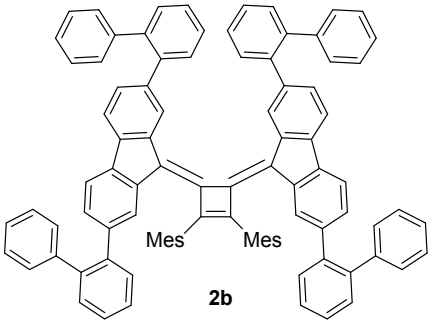
A solution of corresponding 1,3,5-trimethylphenyl/2,6-dichlorophenyl/pentachlorophenyl alkyne (1.71 mmol) in THF (20 mL) was cooled to -78 ℃, and *n*-BuLi (0.68 mL, 1.71 mmol, 2.5 M in hexane) was added dropwise under N_2 atmosphere. The freshly prepared lithium acetylide was kept stirring at -78 ℃ for 1 h, and slowly added to a solution of dibenzo[b,h]fluoren-12-one[3] (compound **S-4**, 400 mg, 1.43 mmol) in THF (80 mL) at -78 ℃. The mixture was then warmed up to the room temperature and stirred for another 1 h. Upon completion of reaction, the solution was diluted with water (20 mL) and dichloromethane (50 mL). The organic layer was dried by anhydrous $MgSO_4$. After filtration, the organic solvents were evaporated to dryness. The residue was purified by column chromatography on silica gel.

Compound **1c** (94 % yield) was obtained as a white solid. ^{1}H NMR (400 MHz, $CDCl_3$): δ 8.28 (s, 2H), 8.24 (s, 2H), 7.95 - 7.92 (m, 4H), 7.54 -7.48 (m, 4H), 6.82 (s, 2H), 2.94 (s, 1H), 2.37 (s, 6H), 2.25 (s, 3H). ^{13}C NMR (100 MHz, $CDCl_3$): δ 147.24, 146.09, 140.58, 137.43, 134.59, 134.33, 134.23, 133.99, 128.72, 128.51, 128.30, 127.51, 126.70, 126.31, 126.17, 126.00, 123.87, 122.69, 119.32, 118.90, 81.84, 22.86, 21.29, 20.94. HRMS (MALDI-TOF, *m/z*) calcd for $C_{32}H_{24}O$ $[M]^+$, 424.1827; found: 424.1830 (error = 0.7 ppm).

Compound **1d** (91 % yield) was obtained as a white solid. ^{1}H NMR (400 MHz, $CDCl_3$): δ 8.31 (s, 2H), 8.19 (s, 2H), 7.92 (d, *J* = 7.8 Hz, 4H), 7.54 - 7.47 (m, 4H), 7.28 (d, *J* = 8.1 Hz, 2H), 7.13 (t, *J* = 8.1 Hz, 1H), 3.09 (s, 1H). ^{13}C NMR (100 MHz, $CDCl_3$): δ 145.06, 137.70, 136.57, 137.69, 134.18, 129.36, 128.81, 128.36, 127.43, 126.83, 126.21, 124.36, 119.39, 100.12, 78.51, 74.63. HRMS (MALDI-TOF, *m/z*) calcd for $C_{29}H_{16}Cl_2O$ $[M]^+$, 450.0578; found: 450.0589 (error = 2.4 ppm).

Compound **1e** (90 % yield) was obtained as a white solid compound. ^{1}H NMR (400 MHz, $CDCl_3$): δ 8.30 (d, *J* = 7.5 Hz, 2H), 8.26 (s, 2H), 7.96 - 7.93 (m, 4H), 7.55 - 7.51 (m, 4H), 2.98 (s, 1H). ^{13}C NMR (100 MHz, $CDCl_3$): δ 144.67, 136.53, 135.01, 134.76, 134.16, 131.77, 131.70, 130.45, 128.81, 128.41, 127.05, 126.41, 124.41, 119.56, 119.53, 102.18, 78.10, 74.65. HRMS (MALDI-TOF, *m/z*) calcd for $C_{29}H_{13}Cl_5O$ $[M]^+$, 553.9380; found: 553.9377 (error = -0.5 ppm).

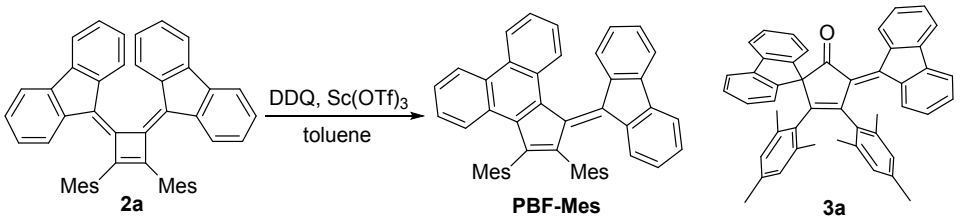
Synthesis of compound 2b



2b

To a solution of compound **1b** (400.0 mg, 0.64 mmol) in dry DCM (100 mL), anhydrous $SnCl_2$ (603 mg, 3.18 mmol) was added at room temperature. The resulting mixture was kept stirring for 6 h, and monitored by TLC to confirm consumption of starting material. Upon completion, the mixture was evaporated to dryness. The residue was purified by column chromatography on silica gel (petroleum ether/CH_2Cl_2= 4:1) to afford compound **2b** (249 mg, 64% yield) as a yellow solid. ^{1}H NMR (400 MHz, $CDCl_3$): δ 7.89 (s, 2H), 7.32 - 7.30 (m, 6H), 7.25 - 7.24 (m, 6H), 7.18 - 7.12 (m, 14H), 7.07 - 7.02 (m, 8H), 6.85 (d, *J* = 7.6 Hz, 2H), 6.81 - 6.79 (m, 4H), 6.72 - 6.66 (m, 6H), 6.58 - 6.56 (m, 2H), 5.91 (d, *J* = 7.7 Hz, 2H), 2.41 (s, 6H), 2.08 (s, 6H), 1.94 (s, 6H). ^{13}C NMR (100 MHz, $CDCl_3$): δ 160.39, 146.22, 141.81, 141.77, 140.49, 140.18, 140.07, 139.84, 139.68, 139.17, 138.93, 138.79, 138.43, 138.24, 137.70, 135.93, 135.85, 131.31, 130.72, 130.43, 130.30, 130.16, 130.11, 129.84, 129.81, 129.76, 129.61, 128.82, 128.79, 127.89, 127.80, 127.23, 126.95, 126.87, 126.76, 126.25, 126.07, 124.90, 118.08, 117.70, 21.14, 20.92, 20.46. HRMS (MALDI-TOF, *m/z*) calcd for $C_{96}H_{70}$ $[M]^+$, 1222.5478; found: 1222.5474 (error = -0.3 ppm).

Synthesis of target PBF-Mes and compound 3a



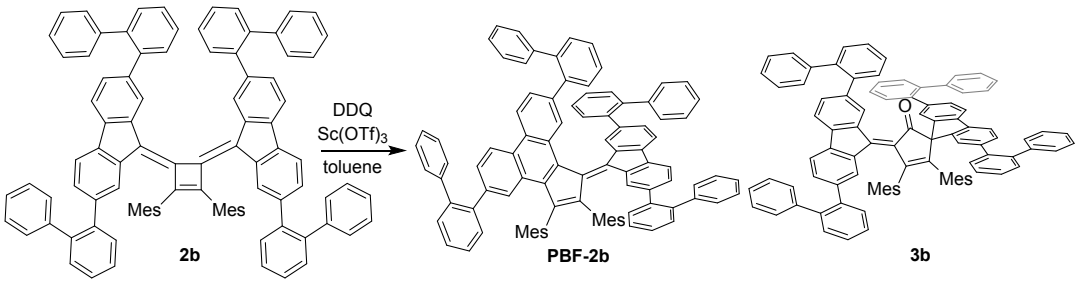
To a solution of compound **2a**[1] (150 mg, 0.24 mmol) in toluene (40 mL), DDQ (277 mg, 1.22 mmol) and $Sc(OTf)_3$ (600 mg, 1.22 mmol) were added under argon atmosphere. The reaction mixture was stirred at 120 ℃, and monitored by TLC to confirm consumption of starting material. Upon completion and filtration, the organic solvents were evaporated to dryness. The residue was purified by column chromatography on silica gel (petroleum ether/CH_2Cl_2 = 4:1) to afford compound **PBF-Mes** (129 mg, 86% yield) as a red solid. The same reaction could produce a yellowish **3a** (14 mg, 9% yield) when exposure to the air, while the major part is the ring-expansion compound **PBF-Mes**.

Compound **PBF-Mes**: ^{1}H NMR (400 MHz, $CDCl_3$): δ 8.66 (d, *J* = 8.3 Hz, 1H), 8.61 (d, *J* = 8.3 Hz, 1H), 8.13 (d, *J* = 8.2 Hz, 1H), 7.54 - 7.48 (m, 3H), 7.39 - 7.36 (m, 2H), 7.28 (s, 1H), 7.23 - 7.19 (m, 2H), 7.15 - 7.07 (m, 2H), 6.87 - 6.83 (m, 2H), 6.80 - 6.75 (m, 2H), 6.65 - 6.59 (m, 2H), 6.34 (s, 1H), 2.30 (s, 3H), 2.26 (s, 3H), 2.09 (s, 3H), 2.03 (s, 3H), 1.97 (s, 3H), 1.63 (s, 3H). ^{13}C NMR (100 MHz, $CDCl_3$): δ 147.04, 145.46, 145.16, 141.44, 141.24, 140.77, 139.57, 139.20, 137.79, 137.08, 136.93, 136.71, 136.59, 136.38, 135.76, 133.82, 133.59, 131.89, 130.53, 130.31, 130.24, 129.32, 129.17, 129.12, 128.78, 128.68, 128.44, 128.28, 128.18, 127.80, 127.70, 126.81, 126.75, 126.60, 126.36, 125.66, 124.08, 123.61, 123.56, 123.12, 119.23, 119.05, 21.90, 21.37, 21.29, 21.14, 20.98, 20.81. HRMS (MALDI-TOF, *m/z*) calcd for $C_{48}H_{38}$ $[M]^+$, 614.2974; found 614.2969 (error = -0.8 ppm).

Compound **3a**: ^{1}H NMR (400 MHz, $CDCl_3$): δ 8.71 (d, *J* = 8.0 Hz, 1H), 7.72 (d, *J* = 7.5 Hz, 2H), 7.54 (d, *J* = 11.9 Hz, 1H), 7.52 (d, *J* = 7.5 Hz, 1H), 7.33 - 7.28 (m, 4H), 7.24 - 7.22 (m, 1H), 7.17 - 7.09 (m, 4H), 7.02 (d, *J* = 7.9 Hz, 1H), 6.79 (t, *J* = 7.6 Hz, 1H), 6.66 (s, 2H), 6.48 (s, 2H), 2.14 (s, 3H), 2.09 (s, 6H), 2.04 (s, 3H), 1.69 (s, 6H). ^{13}C NMR (100 MHz, $CDCl_3$): δ 199.48, 152.14, 147.96, 143.88, 141.63, 141.15, 141.06, 138.65, 137.69, 137.34, 137.23, 136.96, 136.92, 136.74, 136.61,

132.84, 132.72, 129.57, 129.46, 129.28, 128.91, 128.85, 128.22, 127.55, 127.53, 126.57, 125.90, 124.20, 120.41, 119.19, 118.98, 22.86, 22.08, 20.88, 20.74. HRMS (MALDI-TOF, *m/z*) calcd for $C_{48}H_{38}O$ $[M]^+$, 630.2923; found: 630.2906 (error = -2.7 ppm).

Synthesis of compound PBF-2b and 3b

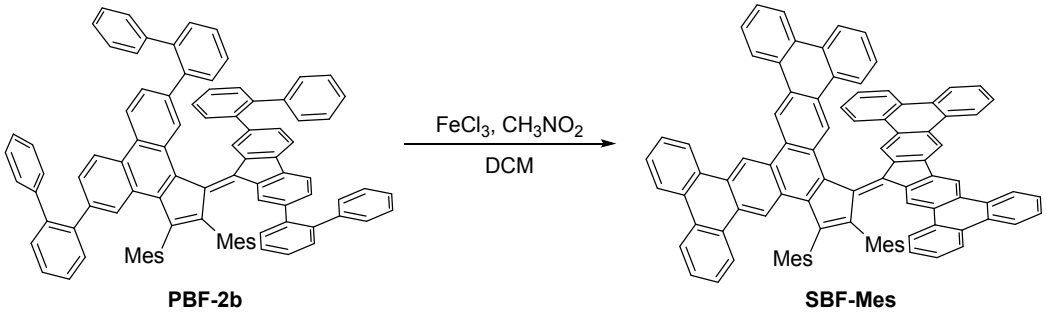


To a solution of compound **2b** (200 mg, 0.16 mmol) in toluene (40 mL), DDQ (185 mg, 0.82 mmol) and $Sc(OTf)_3$ (402 mg, 0.82 mmol) were added under argon atmosphere. The reaction mixture was stirred at 120 ℃. The reaction was monitored by TLC to confirm consumption of starting material. Upon completion and filtration, the red solvent was evaporated to dryness. The residue was purified by column chromatography on silica gel (petroleum ether/CH_2Cl_2 = 3:1) to afford compound **PBF-2b** (172 mg, 86% yield) as a red solid. The same reaction could produce a yellowish **3b** (8 mg, 4% yield) when exposure to the air, while the major part is the ring-expansion compound **PBF-2b**.

Compound **PBF-2b**: ^{1}H NMR (400 MHz, $CDCl_3$): δ 8.25 (s, 1H), 8.16 (d, *J* = 8.1 Hz, 1H), 8.10 (d, *J* = 8.7 Hz, 1H), 7.48 (s, 1H), 7.36 - 7.29 (m, 9H), 7.21 - 7.06 (m, 21H), 7.00 - 6.89 (m, 9H), 6.86 - 6.84(m, 2H), 6.75 (d, *J* = 8.7 Hz, 1H), 6.71 (s, 1H), 6.58 (d, *J* = 7.6 Hz, 1H), 6.54 - 6.52 (m, 2H), 6.34 (d, *J* = 7.7 Hz, 1H), 6.24 (s, 1H), 2.29 (s, 3H), 2.22 (s, 3H), 2.19 (s, 3H), 1.99 (s, 3H), 1.89 (s, 3H), 1.80 (s, 3H). ^{13}C NMR (100 MHz, $CDCl_3$): δ 146.68, 145.91, 145.50, 141.66, 141.52, 141.51, 141.43, 140.18, 140.14, 140.03, 139.85, 139.76, 139.71, 139.64, 139.58, 139.54, 139.36, 139.25, 137.15, 136.88, 136.80, 136.51, 135.85, 133.72, 132.63, 131.94, 131.18, 131.15, 130.90, 130.84, 130.53, 130.38, 130.35, 130.33, 130.26, 129.90, 129.86, 129.39, 128.79, 128.74, 128.33, 128.30, 128.25, 128.07, 127.94, 127.86, 127.79, 127.55, 127.52, 127.40, 127.28, 127.18, 127.07, 127.04, 126.49, 126.34, 126.31, 126.28, 124.20, 122.30, 122.00, 118.86, 118.45, 22.37, 21.59, 21.42, 21.03. HRMS (APCI, *m/z*) calcd for $C_{96}H_{70}$ $[M]^+$, 1222.5478; found: 1222.5471 (error = -0.6 ppm).

Compound **3b**: ^{1}H NMR (400 MHz, $CDCl_3$): δ 8.76 (s, 1H), 7.54 (s, 1H), 7.52 (s, 1H), 7.41 - 7.38 (m, 5H), 7.35 - 7.34 (m, 3H), 7.32 - 7.28 (m, 7H), 7.24 - 7.18 (m, 6H), 7.16 - 7.12 (m, 6H), 7.10 - 7.05 (m, 4H), 7.02 - 6.96 (m, 7H), 6.90 - 6.85 (m, 6H), 6.75 - 6.73 (m, 1H), 6.52 (s, 2H), 6.48 (s, 2H), 1.88 (s, 9H), 1.67 (s, 9H). ^{13}C NMR (100 MHz, $CDCl_3$): δ 198.28, 152.34, 148.46, 141.91, 141.18, 141.14, 140.91, 140.78, 140.56, 140.53, 140.47, 139.97, 129.94, 139.72, 139.46, 139.40, 139.36, 138.37, 137.91, 137.14, 137.10, 137.08, 136.99, 136.88, 132.75, 132.56, 131.72, 131.36, 131.06, 130.59, 130.54, 130.46, 130.43, 130.35, 130.15, 130.00, 129.76, 129.62, 129.38, 128.72, 128.07, 127.81, 127.77, 127.74, 127.51, 127.47, 127.32, 127.13, 127.01, 126.31, 126.23, 125.57, 119.76, 118.57, 118.32, 78.48, 23.09, 22.69, 21.98, 20.98, 20.76. HRMS (MALDI-TOF, *m/z*) calcd for $C_{96}H_{70}O$ $[M]^+$, 1238.5427; found: 1238.5430 (error = 0.2 ppm).

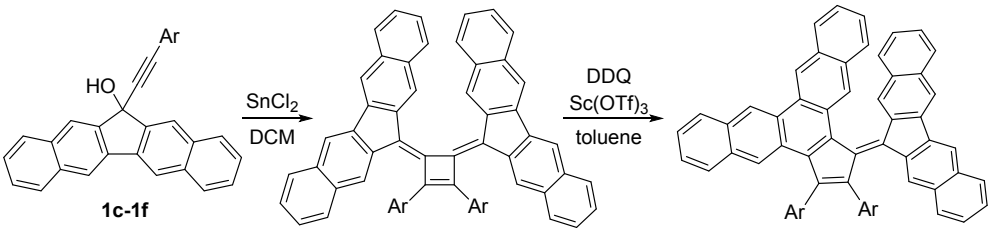
Synthesis of target SBF-Mes



PBF-2b **SBF-Mes**

Ferric chloride (311 mg, 1.92 mmol) was dissolved in anhydrous nitromethane (3 mL), and was then slowly added to the solution **PBF-2b** (150 mg, 0.12 mmol) in anhydrous DCM (50 mL) under an argon atmosphere at 0 ℃. The reaction mixture was stirred at room temperature, and monitored by TLC to confirm consumption of starting material. The reaction was quenched by water (5 mL). The organic layer was separated and evaporated to dryness. The residue was purified by column chromatography on silica gel (petroleum ether/CH_2Cl_2 = 3:1) to afford **SBF-Mes** (130 mg, 86% yield) as an purple solid. ^{1}H NMR (400 MHz, $CDCl_3$): δ 10.50 (s, 1H), 10.26 (s, 1H), 9.07 (d, *J* = 8.2 Hz, 1H), 9.04 (d, *J* = 8.0 Hz, 1H), 8.99 (s, 1H), 8.69 (d, *J* = 8.0 Hz, 1H), 8.64 (d, *J* = 8.1 Hz, 1H), 8.58 (d, *J* = 8.1 Hz, 1H), 8.52 (d, *J* = 7.7 Hz, 1H), 8.14 (s, 1H), 8.01 - 7.99 (m, 1H), 7.94 - 7.92 (m, 1H), 7.86 - 7.82 (m, 1H), 7.80 - 7.78 (m, 2H), 7.72 - 7.66 (m, 2H), 7.61 - 7.59 (m, 2H), 7.57 - 7.48 (m, 4H), 7.45 - 7.41 (m, 4H), 7.37 - 7.33 (m, 2H), 7.21 - 7.15 (m, 7H), 6.99 - 6.97 (m, 4H), 6.82 - 6.80 (m, 1H), 6.60 (s, 1H), 6.27 (s, 1H), 6.18 (s, 1H), 2.55 (s, 3H), 2.26 (s, 3H), 2.08 (s, 3H), 2.01 (s, 3H), 1.73 (s, 3H), 1.69 (s, 3H). ^{13}C NMR (100 MHz, $CDCl_3$): δ 163.29, 161.59, 161.04, 150.49, 149.84, 148.27, 140.17, 139.58, 139.55, 139.34, 138.73, 138.65, 138.52, 138.24, 138.17, 137.83, 137.54, 136.20, 136.06, 135.93, 135.79, 135.52, 134.16, 134.11, 133.59, 132.89, 132.63, 132.49, 132.04, 131.79, 130.92, 130.34, 130.23, 129.67, 129.34, 129.23, 128.82, 128.76, 128.54, 128.27, 128.24, 128.19, 127.85, 127.72, 127.23, 126.53, 126.50, 126.33, 126.06, 125.54, 124.87, 124.52, 124.47, 124.18, 124.15, 123.71, 123.39, 122.60, 119.17, 118.80, 117.87, 21.24, 21.09, 20.95, 20.73, 20.60, 20.17. HRMS (APCI, *m/z*) calcd for $C_{96}H_{62}$ $[M]^+$, 1214.4852; found: 1214.4832 (error = -1.6 ppm).

General procedure for synthesis of target NBF-Mes/ DCP/PCP



1c-1f

NBF-Mes (64%): Ar = 1,3,5-trimethylphenyl
NBF-DCP (32%): Ar = 2,6-dichlorophenyl
NBF-PCP (64%): Ar = pentachlorophenyl

To a solution of compound **1c-1f** (0.47 mmol) in dry DCM (50 mL), anhydrous $SnCl_2$ (447 mg, 2.36 mmol) was added at room temperature. The resulting mixture was kept stirring for 6 h. The

reaction was monitored by TLC to confirm consumption of starting material. Upon completion, the mixture was filtered and evaporated to dryness. The resulting cyclobutene derivative was used in next step without further purification. To a solution of crude cyclobutene derivative in toluene (40 mL), DDQ (267 mg, 1.18 mmol) and $Sc(OTf)_3$ (580 mg, 1.18 mmol) were added under argon atmosphere. The reaction mixture was stirred at 120 ℃, and monitored by TLC to confirm consumption of starting material. Upon completion, the mixture was evaporated to dryness. The residue was purified by column chromatography on silica gel (petroleum ether/CH_2Cl_2= 4:1) to afford the desired compounds.

Compound **NBF-Mes** (64% yield for two steps) was obtained as a purplish red solid. ^{1}H NMR (400 MHz, $CDCl_3$): δ 9.27 (s, 1H), 9.19 (s, 1H), 8.64 (s, 1H), 8.16 (s, 1H), 8.12 - 8.09 (m, 3H), 8.01 (d, *J* = 8.3 Hz, 1H), 7.77 (t, *J* = 8.9 Hz, 2H), 7.62 (s, 1H), 7.57 (s, 1H), 7.54 - 7.50 (m, 1H), 7.40 - 7.29 (m, 8H), 7.17 (t, *J* = 7.7 Hz, 1H), 7.07 - 7.06 (m, 2H), 6.90 (s, 1H), 6.86 (s, 1H), 6.73 (s, 1H), 6.20 (s, 1H), 2.51 (s, 3H), 2.38 (s, 3H), 2.17 (s, 3H), 2.06 (s, 3H), 1.85 (s, 3H), 1.68 (s, 3H). ^{13}C NMR (100 MHz, $CDCl_3$): δ 147.82, 142.01, 139.32, 139.25, 138.27, 137.39, 137.28, 137.11, 136.84, 136.52, 136.34, 135.73, 134.19, 134.06, 133.82, 133.41, 133.01, 132.38, 132.06, 131.73, 130.79, 130.16, 129.80, 129.74, 129.60, 128.85, 128.66, 128.49, 128.32, 128.27, 127.98, 127.84, 127.68, 127.40, 127.33, 127.21, 126.08, 125.71, 125.63, 125.55, 125.06, 123.16, 122.93, 122.33, 118.25, 118.00, 22.34, 21.85, 21.42, 21.25, 21.19, 20.51. HRMS (APCI, *m/z*) calcd for $C_{64}H_{47}^+$ $[M+H]^+$, 815.3672; found: 815.3677 (error = 0.6 ppm).

Compound **NBF-DCP** (32% yield for two steps) was obtained as a violet solid. ^{1}H NMR (400 MHz, $CDCl_3$): δ 9.30 (s, 1H), 9.23 (s, 1H), 8.80 (s, 1H), 8.31 (s, 1H), 8.14 - 8.12 (m, 2H), 8.09 (s, 1H), 8.06 - 8.02 (m, 2H), 7.80 - 7.76 (m, 2H), 7.64 (s, 1H), 7.57 - 7.51 (m, 2H), 7.45 - 7.41 (m, 5H), 7.38 - 7.30 (m, 5H), 7.21 - 7.18 (m, 1H), 7.15 - 7.09 (m, 3H), 6.73 - 6.65 (m, 2H). ^{13}C NMR (100 MHz, THF-d_8): δ 151.60, 139.55, 139.16, 139.01, 138.75, 138.22, 138.03, 137.41, 136.96, 136.58, 135.88, 135.30, 135.17, 133.49, 132.84, 132.74, 132.45, 132.30, 131.99, 131.16, 131.06, 130.53, 130.15, 129.82, 129.38, 128.92, 128.84, 128.69, 128.65, 128.56, 128.54, 128.50 , 128.43, 128.35, 128.29, 128.24, 127.91, 127.40, 127.04, 126.67, 126.58, 126.34, 126.23, 125.97, 125.31, 124.58, 124.33, 123.89, 123.24, 122.78, 122.69, 122.29, 119.67, 119.37, 119.33. MS (MALDI-TOF, *m/z*) calcd for $C_{54}H_{30}Cl_4$ $[M]^+$, 866.1102; found: 866.1085 (error = -2.0 ppm).

Compound **NBF-PCP** (64% yield for two steps) was obtained as a bluish violet solid. ^{1}H NMR (400 MHz, $CDCl_3$): δ 9.32 (s, 1H), 9.25 (s, 1H), 8.84 (s, 1H), 8.28 (s, 1H), 8.15 (d, *J* = 8.2 Hz, 1H), 8.10 - 8.06 (m, 3H), 7.81 - 7.80 (m, 2H), 7.77 (d, *J* = 8.2 Hz, 1H) 7.58 - 7.48 (m, 6H), 7.46 - 7.45 (m, 1H), 7.43 - 7.34 (m, 4H), 7.10 (d, *J* = 6.2 Hz, 2H). ^{13}C NMR (100 MHz, THF-d_8): δ 154.12, 153.77, 139.95, 139.57, 139.33, 139.26, 139.20, 138.19, 138.03, 137.92, 136.97, 136.87, 136.13, 136.01, 135.74, 135.40, 134.95, 134.70, 134.62, 134.38, 133.58, 133.44, 133.30, 133.25, 133.17, 133.04, 132.36, 132.20, 132.07, 131.90, 131.74, 131.24, 130.88, 130.60, 129.97, 129.68, 129.53, 129.44, 129.37, 129.12, 128.98, 128.85, 128.46, 128.19, 127.83, 127.46, 127.37, 127.09, 127.04, 126.88, 126.57, 126.53, 124.45, 124.07, 123.98, 122.37, 122.20, 120.20, 120.16. HRMS (MALDI-TOF, *m/z*) calcd for $C_{58}H_{24}Cl_{10}$ $[M]^+$, 1073.8704; found: 1073.8743 (error = 3.6 ppm).

Results and Discussion

X-ray crystallography of compound 3a

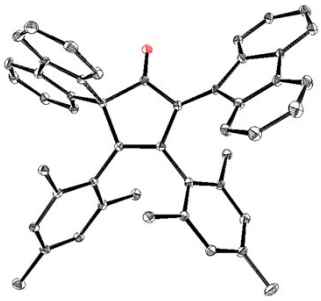


Figure S1. ORTEP plots of crystal structure **3a** (atoms: C, black; O, red). Thermal ellipsoids are shown at 30%, hydrogen atoms are omitted for clarify.

Theoretical calculations of reaction pathways

Density functional theory (DFT) calculations were performed with the Gaussian 09 program.[4] All geometry optimizations were carried out at the B3LYP level of density functional theory with the 6-31G(d,p) basis set (*vide infra*). The nature of the stationary points was assessed by means of vibrational frequency analysis. The transition states of the reaction paths were confirmed by intrinsic reaction coordinate (IRC) calculations. In the implicit solvent model by using B3LYP/6-31G(d,p) method, the CPCM polarizable conductor calculation model was used to the polarizable continuum model (PCM) in the self-consistent reaction field (SCRF) procedure.

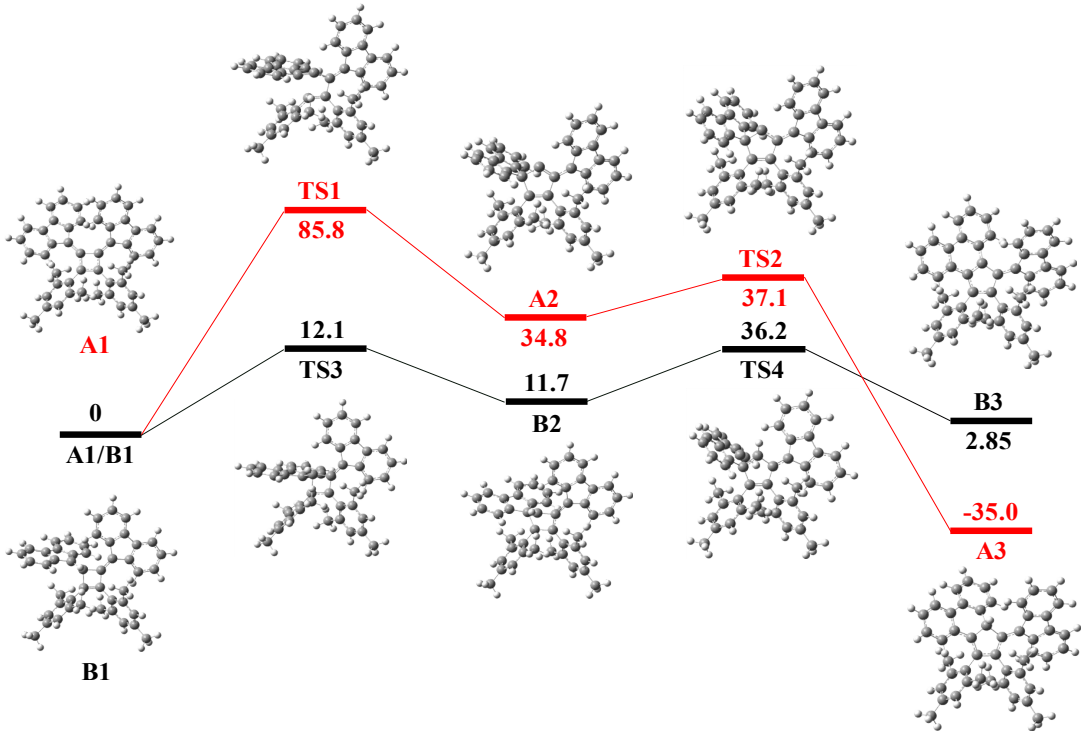


Figure S2. Optimized structures and relative energy (kcal/mol) associated with each transition state in the two possible reaction pathways (Path A: red; Path B: black).

Table S1. Summary of the control experiments.

Entry	Condition	Temperature	Reaction time	Yield by HPLC
1	DDQ (5 eq.)	120 ℃	3 days	1%
2	$Sc(OTf)_3$ (5 eq.)	20 ℃	3 days	-
3	$Sc(OTf)_3$ (5 eq.)	100 ℃	3 days	23%
4	$Sc(OTf)_3$ (5 eq.)	120 ℃	2 days	23%
5	$Sc(OTf)_3$ (5 eq.)/DDQ (1 eq.)	120 ℃	31 h	34%

The aromatic proton resonances of NBF-Mes/DCP/PCP

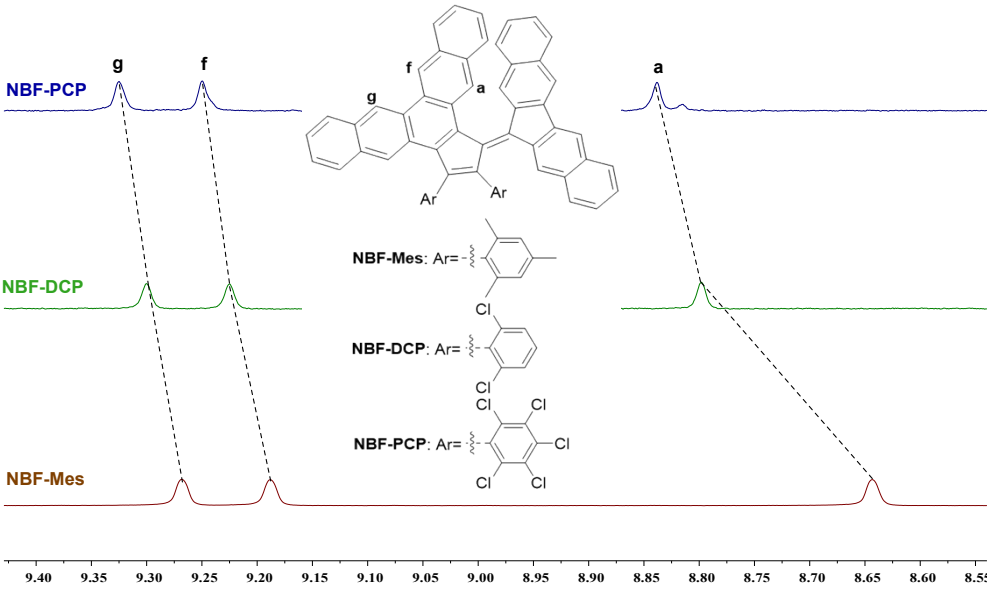


Figure S3. The downfield shifts for aromatic proton resonances from **NBF-Mes** to **NBF-DCP**, and to **NBF-PCP**.

The photophysical and electrochemical properties of new compounds.

Table S2. Summary of the photophysical and electrochemical properties of new compounds.

Cmpds	PBF-Mes	NBF-Mes	SBF-Mes	NBF-DCP	NBF-PCP
λ_{abs}^{max} (nm)	488	545	555	560	570
λ_{onset}^{max} (nm)	586	667	755	747	789
E_g^{opt} (eV)[a]	1.75	1.54	1.36	1.37	1.30
E_{red}^{1} (V)[b]	-1.37	-1.15	-1.09	-1.00	-0.89
E_{red}^{2} (V)[b]	-1.76	-1.59	-1.37	-1.57	-1.50
E_{ox} (V)[b]	0.49	0.47	0.51	0.57	0.65
E_g^{cv} (eV)[b]	1.86	1.62	1.60	1.57	1.54
LUMO (eV)[c]	-3.43	-3.65	-3.71	-3.80	-3.91
HOMO (eV)[c]	-5.29	-5.27	-5.31	-5.37	-5.45
Dipole Moment (D)[d]	1.09	2.10	2.22	3.08	5.19

[a]Calculated from the onset of UV absorption. [b]Onset potentials *vs* Fc/Fc^+, determined by cyclic voltammetric measurements in 0.10 M solution of *n*-$Bu_4N^+PF_6^-$ in CH_2Cl_2. [c]Estimated from onsets

of oxidative waves and reduction waves in CV measurements. [d]Obtained from DFT calculations at the B3LYP/6-31G(d,p) level on Gaussian 09 program.

Crystal packing of compound PBF-Mes and NBF-Mes

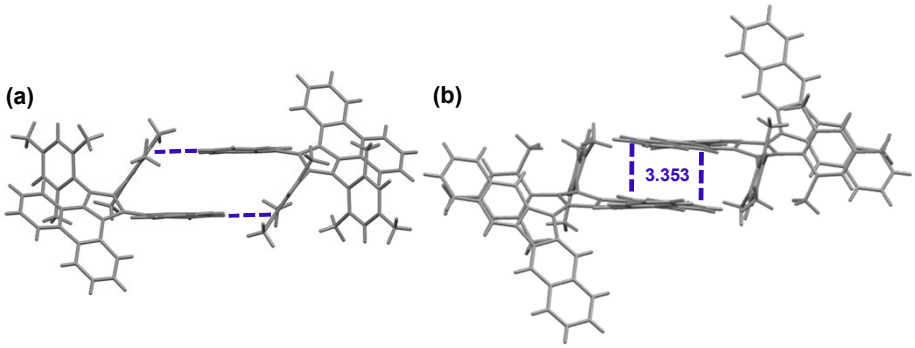


Figure S4. Crystal packing of small-sized **PBF-Mes** and larger-sized **NBF-Mes**.

DFT and TD-DFT calculations

DFT and time-dependent DFT (TD-DFT) were performed using the Gaussian 09 software package. All calculations were carried out using the DFT method with Becke's three-parameter hybrid exchange functionals and the Lee-Yang-Parr correlation functional (B3LYP) employing the 6-31G(d,p) basis set for all atoms.

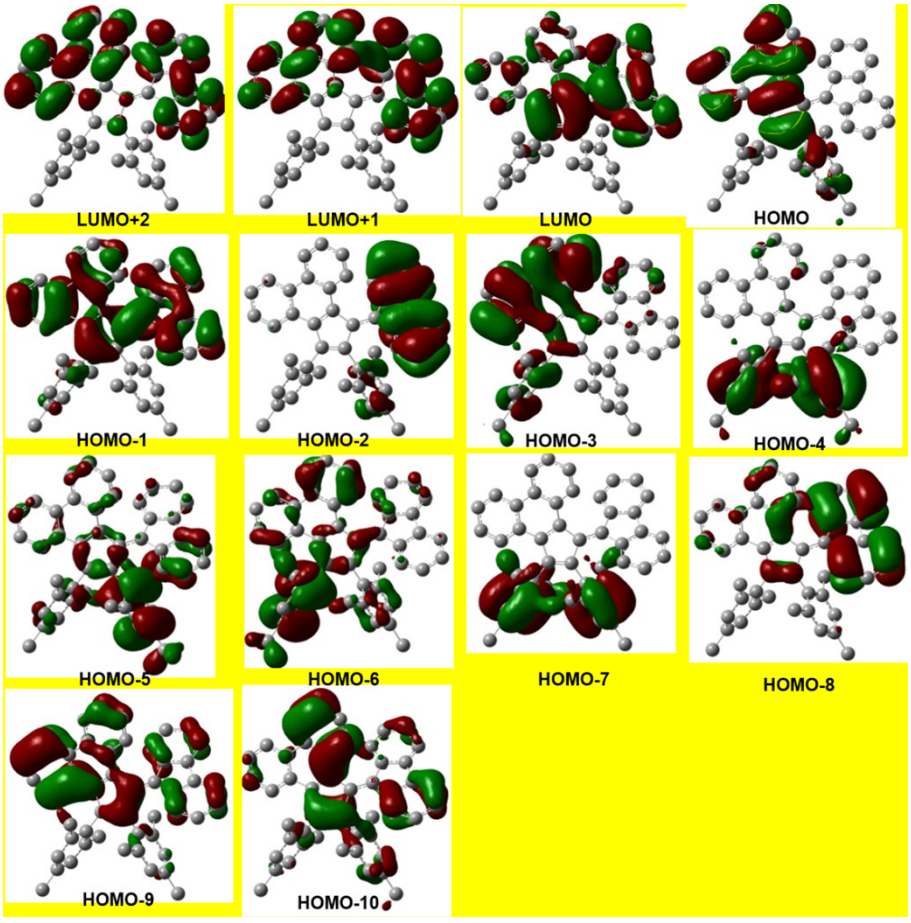


Figure S5. Calculated MOs profiles of **PBF-Mes** at the B3LYP/6-31G(d,p) level.

Table S3. Major electronic transitions of **PBF-Mes** calculated by TD-DFT.

excited state	Energy (cm^{-1})	Wavelength (nm)	Osc. Strength	Major contribs
1	14687.45760	680.85303	0.0044	H>L (99%)
2	20524.53232	487.22182	0.0539	H-2>L (79%) H-1>L (18%)
3	20987.49776	476.47414	0.2598	H-2>L (20%) H-1>L (65%)
4	22581.26032	442.84508	0.0623	H-4>L (53%) H-3>L (31%)
5	22882.91376	437.00728	0.0190	H-4>L (36%) H-3>L (55%)
6	23653.17856	422.77616	0.0058	H-6>L (46%) H-5>L (44%)
7	24225.02960	412.79619	0.1066	H-6>L (42%) H-5>L (47%)
8	25025.13712	399.59821	0.0282	H-7>L (95%)
9	28886.13984	346.18679	0.0488	H-8>L (92%)
10	30170.98992	331.44421	0.0642	H>L+1 (76%) H>L+2 (13%)
11	31096.92080	321.57525	0.0052	H-9>L (14%) H>L+1 (20%) H>L+2 (54%)
12	31300.98048	319.47881	0.0033	H-10>L (74%) H-9>L (19%)

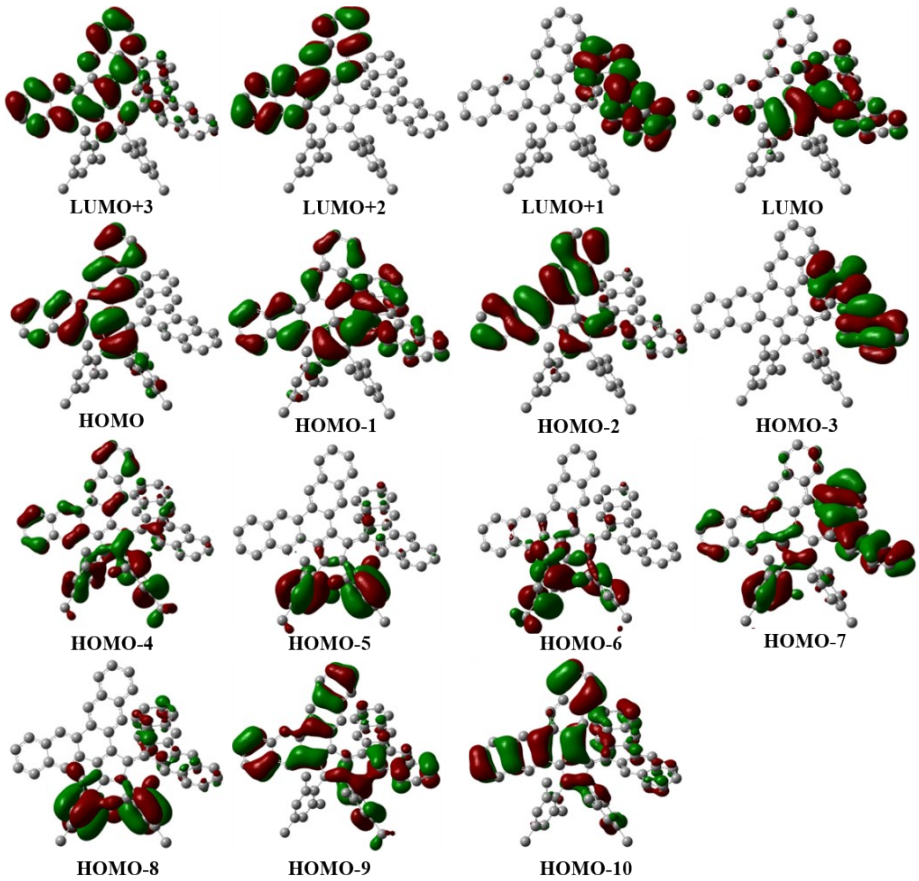


Figure S6. Calculated MOs profiles of **NBF-Mes** at the B3LYP/6-31G(d,p) level.

Table S4. Major electronic transitions of **NBF-Mes** calculated by TD-DFT method.

excited state	Energy (cm^{-1})	Wavelength (nm)	Osc. Strength	Major contribs
1	12429.89616	804.51195	0.0201	H>L (96%)
2	17428.95504	573.75786	0.0242	H-2>L (46%) H-1>L (52%)
3	18565.39808	538.63644	0.3641	H-2>L (46%) H-1>L (36%)
4	18725.90352	534.01962	0.0390	H-3>L (85%)
5	20620.51296	484.95398	0.1256	H-4>L (86%)
6	22461.08288	445.21450	0.0064	H-5>L (98%)
7	22874.0416	437.17678	0.0299	H-6>L (95%)
8	23057.13072	433.70530	0.0066	H>L+1 (98%)
9	24279.06912	411.87740	0.0104	H>L+2 (89%)
10	24498.45344	408.18903	0.0231	H-8>L (10%) H-7>L (80%)
11	24788.00848	403.42087	0.0161	H-8>L (76%) H-7>L (14%)
12	25940.58272	385.49635	0.0211	H-9>L (31%) H-2>L+1 (10%) H-1>L+1 (49%)
13	26126.09152	382.75912	0.0072	H-10>L (33%) H-9>L (38%) H-1>L+1 (18%)

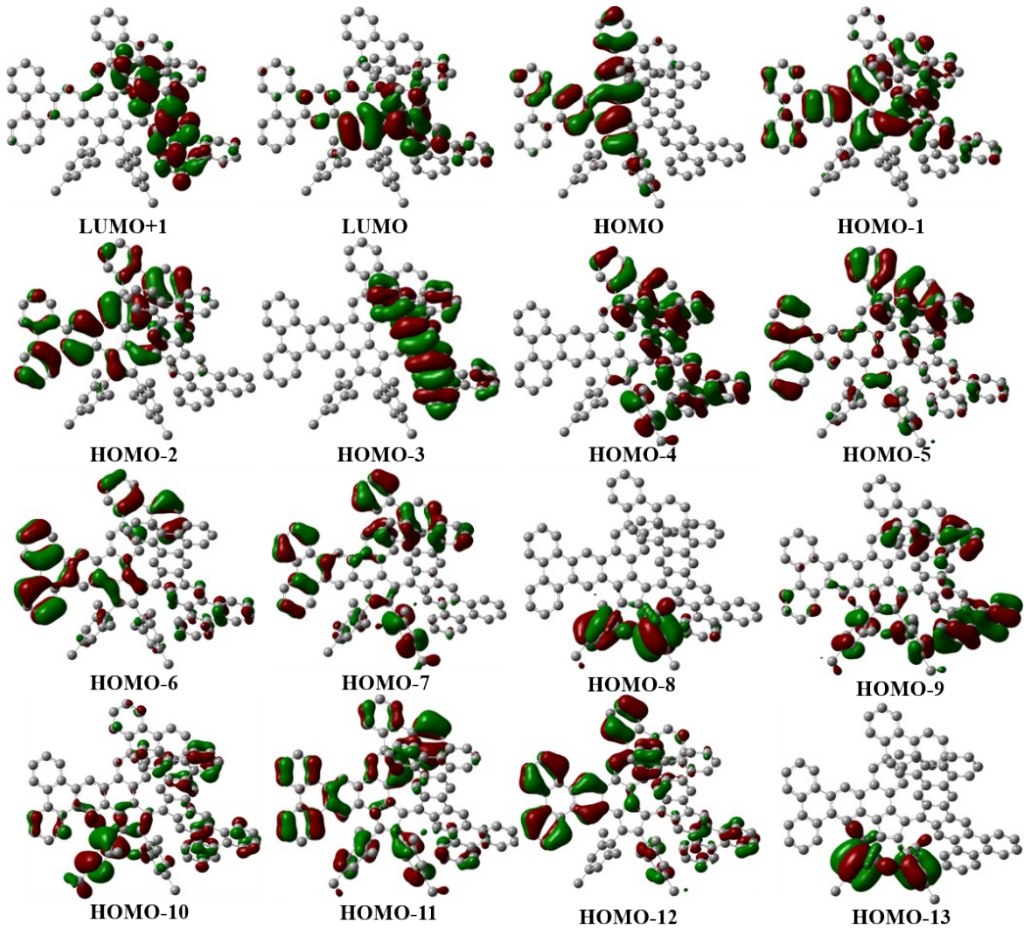


Figure S7. Calculated MOs profiles of **SBF-Mes** at the B3LYP/6-31G(d,p) level.

Table S5. Major electronic transitions of **SBF-Mes** calculated by TD-DFT method.

excited state	Energy (cm^{-1})	Wavelength (nm)	Osc. Strength	Major contribs
1	11734.64144	852.17772	0.0203	H>L (97%)
2	16097.32448	621.22125	0.2446	H-2>L (18%) H-1>L (80%)
3	16447.37152	607.99989	0.0006	H-3>L (98%)
4	17449.11904	573.09484	0.3539	H-2>L (79%) H-1>L (17%)
5	20066.40624	498.34534	0.0531	H-7>L (12%) H-4>L (72%)
6	20972.17312	476.82231	0.1068	H-5>L (74%)
7	21234.30512	470.93606	0.0117	H-8>L (88%)
8	21446.43040	466.27806	0.0286	H-10>L (10%) H-7>L (12%) H-6>L (50%)
9	22023.12080	454.06825	0.0213	H-7>L (55%) H-6>L (21%) H-5>L (16%)
10	22152.17040	451.42304	0.0172	H-10>L (27%) H-9>L (47%) H-6>L (12%)
11	22940.98608	435.90105	0.0354	H-11>L (23%) H-10>L (34%) H-9>L (31%)
12	23191.01968	431.20139	0.0081	H-11>L (61%) H-10>L (22%)
13	23926.60240	417.94484	0.0113	H-13>L (80%)

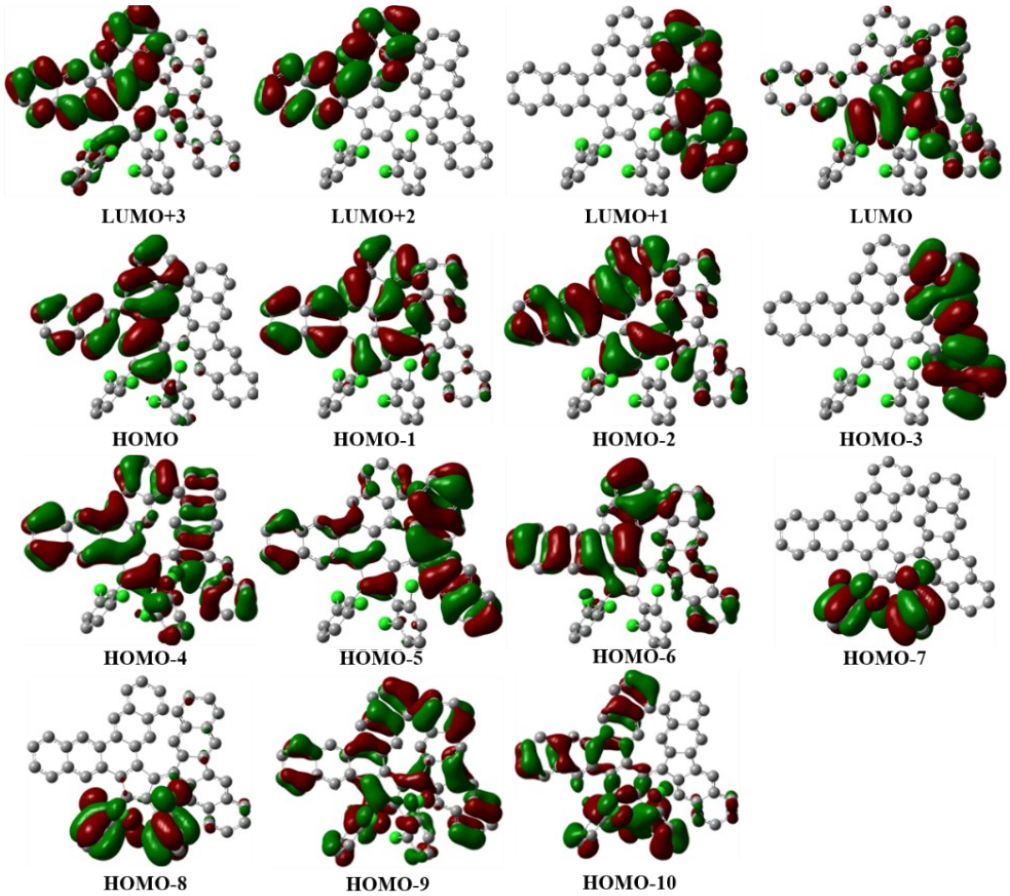


Figure S8. Calculated MOs profiles of **NBF-DCP** at the B3LYP/6-31G(d,p) level.

Table S6. Major electronic transitions of **NBF-DCP** calculated by TD-DFT method.

excited state	Energy (cm^{-1})	Wavelength (nm)	Osc. Strength	Major contribs
1	11329.74832	882.63214	0.0207	H>L (95%)
2	15551.28336	643.03375	0.0178	H-2>L (28%) H-1>L (71%)
3	17381.36800	575.32871	0.4049	H-2>L (64%) H-1>L (24%)
4	17879.82208	559.28968	0.0888	H-3>L (87%)
5	22567.54880	443.11414	0.0381	H-4>L (88%)
6	22806.29056	438.47552	0.0850	H-5>L (87%)
7	23132.94736	432.28387	0.0076	H>L+1 (97%)
8	24463.77136	408.76772	0.0010	H>L+2 (87%)
9	25032.39616	399.48233	0.0151	H-6>L (77%)
10	25301.78720	395.22900	0.0042	H-8>L (27%) H-7>L (69%)
11	25755.07392	388.27301	0.0154	H-9>L (13%) H-2>L+1 (20%) H-1>L+1 (45%)
12	26153.51456	382.35779	0.0014	H-8>L (61%) H-7>L (27%) H-9>L (59%)
13	26834.25120	372.65806	0.0071	H-1>L+1 (13%) H>L+3 (12%)
14	27102.02912	368.97606	0.0236	H-2>L+1 (30%) H-1>L+1 (17%) H>L+3 (38%)
15	27277.85920	366.59768	0.0055	H-10>L (67%) H-2>L+1 (15%)

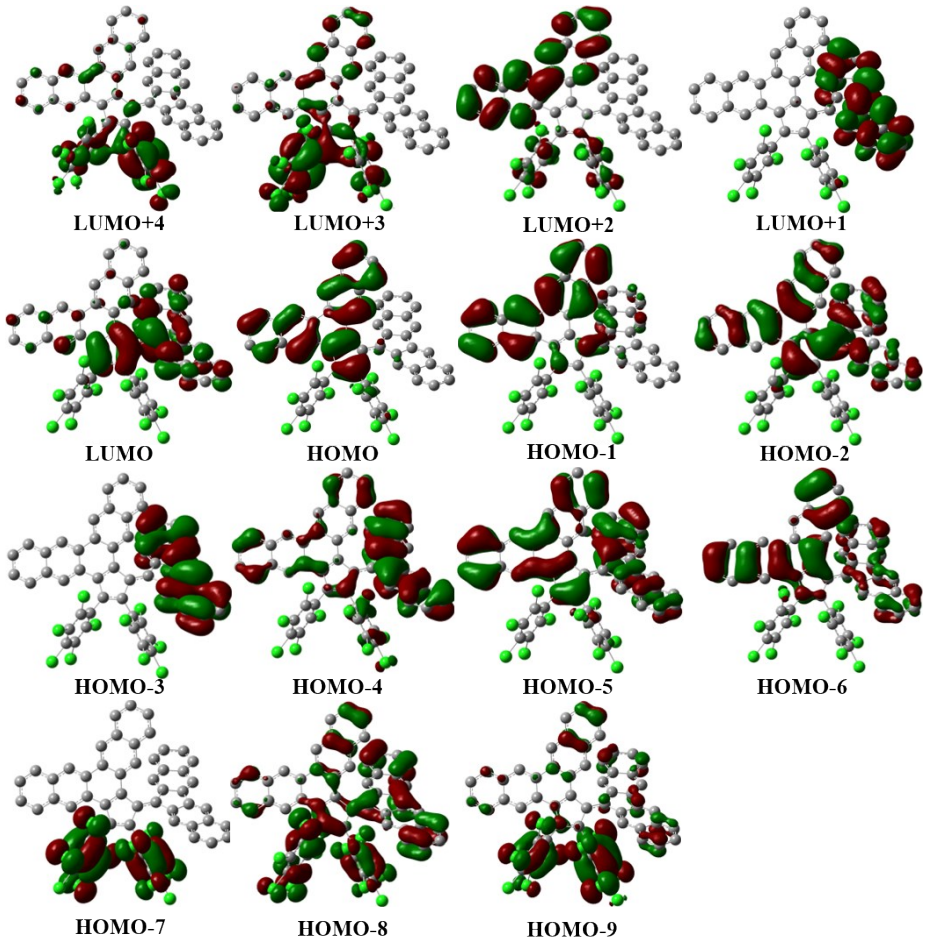


Figure S9. Calculated MOs profiles of **NBF-PCP** at the B3LYP/6-31G(d,p) level.

Table S7. Major electronic transitions of **NBF-PCP** calculated by TD-DFT method.

excited state	Energy (cm^{-1})	Wavelength (nm)	Osc. Strength	Major contribs
1	11091.81312	901.56586	0.0210	H>L (95%)
2	14749.56272	677.98620	0.0136	H-1>L (90%)
3	16937.76000	590.39684	0.2002	H-3>L (47%) H-2>L (46%)
4	17261.19056	579.33431	0.2878	H-3>L (49%) H-2>L (43%)
5	22182.01312	450.81571	0.0889	H-4>L (90%)
6	22349.77760	447.43175	0.0433	H-5>L (90%)
7	23528.16176	425.02258	0.0158	H>L+1 (98%)
8	24354.88576	410.59523	0.0189	H-6>L (84%)
9	24929.15648	401.13672	0.0020	H>L+2 (85%)
10	25384.86288	393.93555	0.0286	H>L+3 (92%)
11	25476.81072	392.51381	0.0014	H-9>L (26%) H-8>L (18%) H-7>L (54%) H-8>L (39%)
12	25818.79216	387.31479	0.0032	H-2>L+1 (22%) H-1>L+1 (18%)
13	26175.29168	382.03968	0.0012	H-9>L (45%) H-7>L (37%)
14	26330.15120	379.79273	0.0681	H>L+4 (91%)
15	26682.61792	374.77582	0.0419	H-9>L (15%) H-8>L (23%) H-1>L+1 (39%)

Differential pulse voltammograms

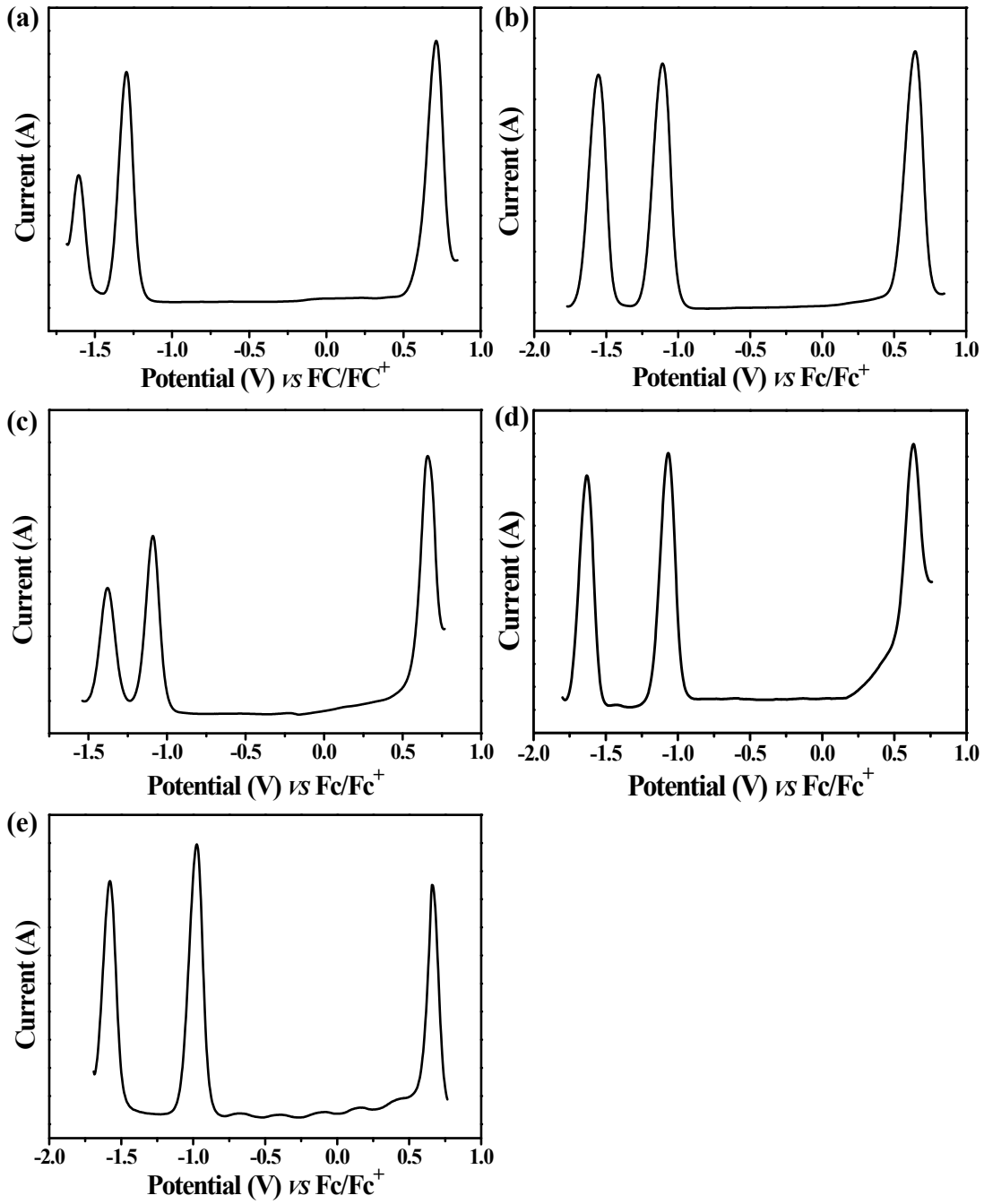


Figure S10. Differential pulse voltammograms of **PBF-Mes**, **NBF-Mes**, **SBF-Mes**, **NBF-DCP** and **NBF-PCP** in DCM (1.0 mM); redox potentials were determined by using 0.10 M *n*-$Bu_4N^+PF_6^-$ as a supporting electrolyte; the electrode potential was externally calibrated by the ferrocene/ferrocenium redox couple.

Characterization of NBF-PCP radical ions

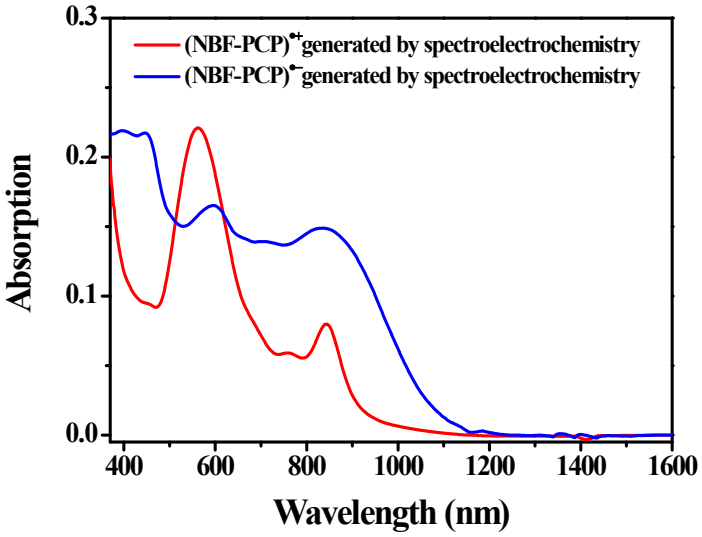


Figure S11. UV-*vis*-NIR spectra of **(NBF-PCP)**$^{\bullet+}$ and **(NBF-PCP)**$^{\bullet-}$ by in-situ measurement of one-electron oxidation and reduction of **NBF-PCP** through the electrochemistry (DCM solution containing 0.10 M *n*-$Bu_4^+NPF_6^-$).

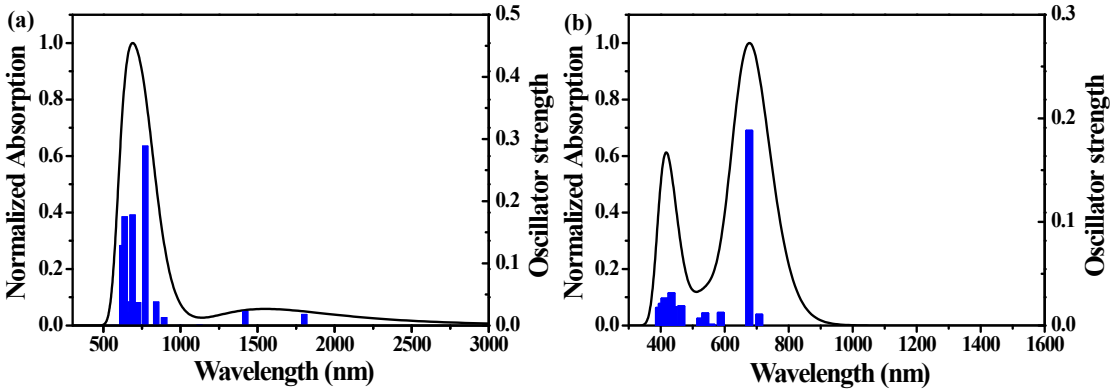


Figure S12. Calculated absorption spectra of **(NBF-PCP)**$^{\bullet+}$ at the UM06/6-31G(d,p) level (a) and **(NBF-PCP)**$^{\bullet-}$ at the CAM-B3LYP/6-31G(d,p) level (b).

Table S8. Major electronic transitions of **(NBF-PCP)**$^{\bullet+}$ calculated by TD-DFT method.

excited state	Energy (cm^{-1})	Wavelength (nm)	Osc. Strength	Major contribs
1	5546.71312	1802.86952	0.0179	H-2(B)>L(B) (19%) H(B)>L(B) (75%)
2	7044.49504	1419.54816	0.0227	H-2(B)>L(B) (77%) H(B)>L(B) (20%)
3	8899.58304	1123.64815	0.0010	H-2(A)>L(A) (29%) H-1(A)>L(A) (13%) H-2(B)>L+1(B) (20%) H(B)>L+1(B) (29%)
4	10000.53744	999.94626	0.0003	H-1(B)>L(B) (85%)

5	11188.60032	893.76684	0.0128	H-1(A)>L(A) (36%) H(A)>L(A) (31%) H-1(B)>L(B) (10%) H-1(B)>L+1(B) (14%)
6	11879.01568	841.82059	0.0379	H-3(A)>L(A) (19%) H-2(A)>L(A) (11%) H(A)>L(A) (45%)
7	12966.25856	771.2325	0.2887	H-2(A)>L(A) (14%) H-4(B)>L(B) (56%) H(B)>L+1(B) (16%)
8	13807.50064	724.24404	0.0372	H-4(A)>L(A) (20%) H-1(A)>L(A) (12%) H-1(B)>L+1(B) (48%)
9	14013.17344	713.61423	0.0055	H-4(A)>L(A) (16%) H-3(B)>L(B) (33%) H-3(B)>L+1(B) (21%) H-1(B)>L+1(B) (13%)
10	14514.85376	688.94941	0.1779	H-3(A)>L(A) (25%) H-1(A)>L(A) (18%) H(A)>L(A) (12%) H-4(B)>L(B) (12%) H(B)>L+1(B) (18%)
11	14767.30704	677.17154	0.0379	H-3(A)>L(A) (27%) H-2(A)>L(A) (21%) H-4(B)>L(B) (12%) H-3(B)>L(B) (10%) H(B)>L+1(B) (20%)
12	15347.22368	651.58365	0.0200	H-4(A)>L(A) (13%) H-3(A)>L(A) (11%) H-3(B)>L(B) (42%) H-3(B)>L+1(B) (11%)
13	15690.01168	637.34816	0.1751	H-2(A)>L(A) (12%) H-2(B)>L+1(B) (59%)
14	16073.12768	622.15645	0.1288	H-10(B)>L(B) (14%) H-8(B)>L(B) (17%) H-5(B)>L(B) (50%)
15	17703.18544	564.87009	0.0004	H-5(A)>L(A) (20%) H-6(B)>L(B) (26%) H-4(B)>L+1(B) (12%)

Table S9. Major electronic transitions of **(NBF-PCP)$^{\bullet-}$** calculated by TD-DFT method.

excited state	Energy (cm^{-1})	Wavelength (nm)	Osc. Strength	Major contribs
1	14,131.73776	707.62706	0.0105	H-1(B)>L(B) (15%) H(B)>L(B) (53%)
2	14,781.82512	676.50645	0.1880	H-1(B)>L(B) (75%) H(B)>L(B) (10%)
3	17,019.22256	587.57090	0.0121	H-3(A)>L+1(A) (16%) H-2(B)>L+2(B) (10%) H(B)>L(B) (28%)
4	17,897.56640	558.73518	0.0007	H-4(A)>L(A) (21%) H-4(B)>L(B) (16%) H-3(B)>L+1(B) (14%)
5	18,550.07344	539.08142	0.0116	H-1(A)>L+1(A) (15%) H(B)>L+2(B) (12%)
6	19,100.95392	523.53406	0.0066	H(A)>L(A) (69%)

7	21,549.67008	464.04423	0.0185	H-3(B)>L(B) (69%)
8	22,723.21488	440.07857	0.0177	H(A)>L+1(A) (24%) H(A)>L+2(A) (22%)
9	23,067.61600	433.50817	0.0310	H(A)>L+1(A) (16%) H(A)>L+2(A) (24%)
10	24,505.71248	408.06812	0.0120	H-4(A)>L(A) (15%) H-4(B)>L(B) (61%)
11	24,796.07408	403.28965	0.0208	H(A)>L+4(A) (30%)
12	25,346.14800	394.53727	0.0170	H(A)>L+1(A) (20%) H(B)>L+1(B) (11%) H(B)>L+2(B) (14%)

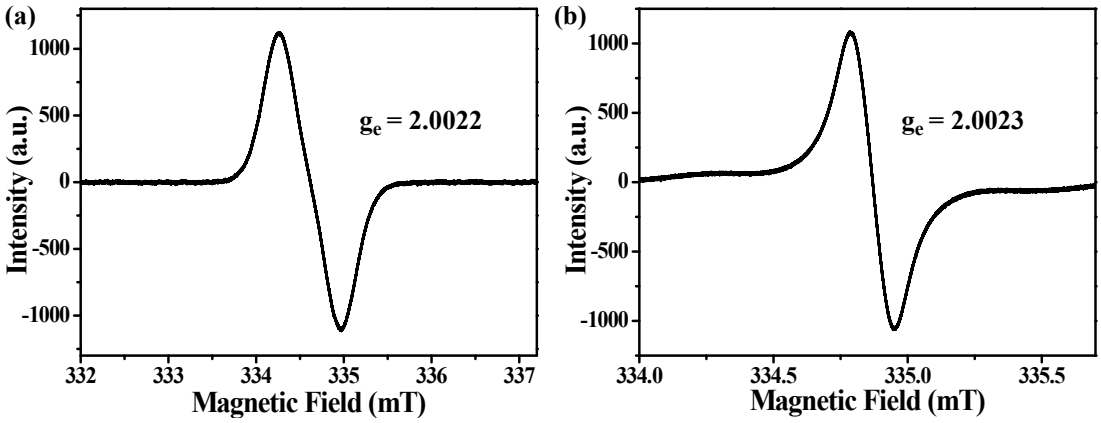


Figure S13. ESR spectra of **(NBF-PCP)**$^{\bullet+}$[SbF_6^-] (a) and **(NBF-PCP)**$^{\bullet-}$[$CoCp_2^+$] (b) recorded in air-degassed DCM solution at room temperature.

OFET devices

Thin film deposition and device fabrication

Heavily doped silicon substrates with a 300 nm SiO_2 dielectric modified with octadecyl trichlorosilane (OTS) through thermal vapor at 150 ℃ were used for the device fabrication. A homogeneous layer of **NBF-PCP** was spin-coated from chlorobenzene solution (5 mg mL^{-1}). Source and drain gold electrodes were thermal vapor deposited at a thickness of 50 nm. The channel length and width were estimated as 20 μm and 1000 μm, respectively.

The parameters of charge carrier mobilities

The charge carrier mobilities of OFETs were calculated in the saturation regime from a plot of the square root of the drain current vs. gate voltage using the following equation:

$$I_{DS} = \frac{WC_i}{2L}\mu(VG - VT)^2$$

where I_{DS} is the drain-source current, C_i is the capacitance per unit area of the gate dielectric (10 nF/cm^2), L is the channel length, W is the channel width, V_G and V_T are the gate-source voltage and threshold voltage, respectively.

Crystal data and Structural Refinement

Table S10. Crystal data and structure refinement for **PBF-Mes** (CCDC:1975936).

Identification code	**PBF-Mes**
Empirical formula	$C_{48}H_{38}$
Formula weight	614.78
Temperature	296.15 K
Wavelength	0.71073 Å
Crystal system	Monoclinic
Space group	P 1 2/n 1
a	17.963(3) Å
b	8.2911(13) Å
c	25.855(4) Å
α	90°
β	104.810(3)°
γ	90°
Volume	3722.7(10) $Å^3$
Z	4
Density (calculated)	1.097 Mg/m^3
Absorption coefficient	0.062 mm^{-1}
F(000)	1304
Crystal size	0.1 x 0.05 x 0.03 mm^3
Theta range for data collection	1.629 to 25.500°.
Index ranges	-14<=h<=21, -10<=k<=9, -31<=l<=31
Reflections collected	24085
Independent reflections	6895 [R(int) = 0.0910]
Completeness to theta = 25.242°	99.70%
Absorption correction	Semi-empirical from equivalents
Max. and min. transmission	0.7456 and 0.6133
Refinement method	Full-matrix least-squares on F2
Data / restraints / parameters	6895/1/440
Goodness-of-fit on F2	0.999
Final R indices [I>2sigma(I)]	R1 = 0.0652, wR2 = 0.1468
R indices (all data)	R1 = 0.1575, wR2 = 0.1906
Extinction coefficient	0.0041(7)
Largest diff. peak and hole	0.277 and -0.178 $e.Å^{-3}$

Table S11. Crystal data and structure refinement for compound **3a** (CCDC:1975939).

Identification code	**3a**
Empirical formula	$C_{48}H_{38}$ O
Formula weight	630.78
Temperature	293(2) K
Wavelength	0.71073 Å
Crystal system	Triclinic
Space group	P -1
a	11.2454(12) Å
b	17.5859(19) Å
c	19.671(2) Å
α	87.747(3)°
β	66.860(3)°
γ	61.993(2)°
Volume	3516.0(7) $Å^3$

Z	4
Density (calculated)	1.192 Mg/m^3
Absorption coefficient	0.069 mm^{-1}
F(000)	1336
Crystal size	0.200 x 0.150 x 0.100 mm^3
Theta range for data collection	1.863 to 24.999°.
Index ranges	-13<=h<=13, -20<=k<=13, -23<=l<=18
Reflections collected	19643
Independent reflections	12381 [R(int) = 0.0533]
Completeness to theta = 25.242°	97.30%
Absorption correction	Semi-empirical from equivalents
Max. and min. transmission	0.7456 and 0.6347
Refinement method	Full-matrix least-squares on F2
Data / restraints / parameters	12381/387/1157
Goodness-of-fit on F2	1.032
Final R indices [I>2sigma(I)]	R1 = 0.0950, wR2 = 0.2394
R indices (all data)	R1 = 0.2185, wR2 = 0.3045
Extinction coefficient	0.0015(8)
Largest diff. peak and hole	0.357 and -0.262 $e.Å^{-3}$

Table S12. Crystal data and structure refinement for **NBF-Mes** (CCDC:1975937)

Identification code	**NBF-Mes**
Empirical formula	$C_{64}H_{46}$
Formula weight	815.01
Temperature	173(2) K
Wavelength	0.71073 Å
Crystal system	Triclinic
Space group	P-1
a	17.0406(16) Å
b	17.1796(17) Å
c	21.2035(19) Å
α	87.747(3)°
β	66.860(3)°
γ	61.993(2)°
Volume	4958.2(8) Å3
Z	4
Density (calculated)	1.092 Mg/m^3
Absorption coefficient	0.062 mm^{-1}
F(000)	1720
Crystal size	0.18 x 0.16 x 0.10 mm^3
Theta range for data collection	1.542 to 25.000°.
Index ranges	-20<=h<=20, -20<=k<=20, -25<=l<=25
Reflections collected	74625
Independent reflections	17409 [R(int) = 0.1218]
Completeness to theta = 25.242°	96.90%
Absorption correction	Semi-empirical from equivalents
Max. and min. transmission	0.7456 and 0.4347
Refinement method	Full-matrix least-squares on F2
Data / restraints / parameters	17409/0/1162
Goodness-of-fit on F2	1.083
Final R indices [I>2sigma(I)]	R1 = 0.0716, wR2 = 0.1811
R indices (all data)	R1 = 0.1219, wR2 = 0.2134
Extinction coefficient	0.0048(6)

Largest diff. peak and hole	0.313 and -0.260 e.Å^{-3}

Table S13. Crystal data and structure refinement for **SBF-Mes** (CCDC:1975938)

Identification code	**SBF-Mes**
Empirical formula	$C_{96}H_{62}$
Formula weight	1215.45
Temperature	99.8(8) K
Wavelength	1.54184 Å
Crystal system	Orthorhombic
Space group	Pccn
a	14.9085(6) Å
b	32.282(2) Å
c	28.907(2) Å
α	90°
β	90°
γ	90°
Volume	13912.3(14) Å^3
Z	8
Density (calculated)	1.161 Mg/m^3
Absorption coefficient	0.499 mm^{-1}
F(000)	5104
Crystal size	0.3x0.3x0.1 mm^3
Theta range for data collection	3.606 to 66.598°.
Index ranges	-16<=h<=18, -39<=k<=39, -35<=l<=35
Reflections collected	12306
Independent reflections	12306 [R(int) = 0.2086]
Completeness to theta = 66.598°	100.00%
Absorption correction	Semi-empirical from equivalents
Max. and min. transmission	1.00000 and 0.50474
Refinement method	Full-matrix least-squares on F2
Data / restraints / parameters	12306/484/871
Goodness-of-fit on F2	0.982
Final R indices [I>2sigma(I)]	R1 = 0.0890, wR2 = 0.2353
R indices (all data)	R1 = 0.1568, wR2 = 0.2712
Extinction coefficient	n/a
Largest diff. peak and hole	1.006 and -0.281 e.Å^{-3}

Table S14. Crystal data and structure refinement for **NBF-PCP** (CCDC:1975940).

Empirical formula	**NBF-PCP**
Formula weight	1075.27
Temperature	293(2) K
Wavelength	1.54184 Å
Crystal system	Triclinic
Space group	P-1
a	8.4481(5) Å
b	17.6335(7) Å
c	19.2134(8) Å
α	103.740(4)
β	95.972(4)
γ	92.279(4)
Volume	2759.2(2) Å^3
Z	2
Density (calculated)	1.294 Mg/m^3

Absorption coefficient	4.902 mm^{-1}
F(000)	1084
Theta range for data collection	4.844 to 66.595°.
Reflections collected	9697
Completeness to theta = 66.595°	99.90%
Refinement method	Full-matrix least-squares on F2
Data / restraints / parameters	9697/0/613
Goodness-of-fit on F2	1.089
Final R indices [I>2sigma(I)]	R1 = 0.1002, wR2 = 0.2773
R indices (all data)	R1 = 0.1396, wR2 = 0.3293
Extinction coefficient	n/a
Largest diff. peak and hole	1.521 and -0.611 $Å^{-3}$

NMR/mass spectra for new compounds

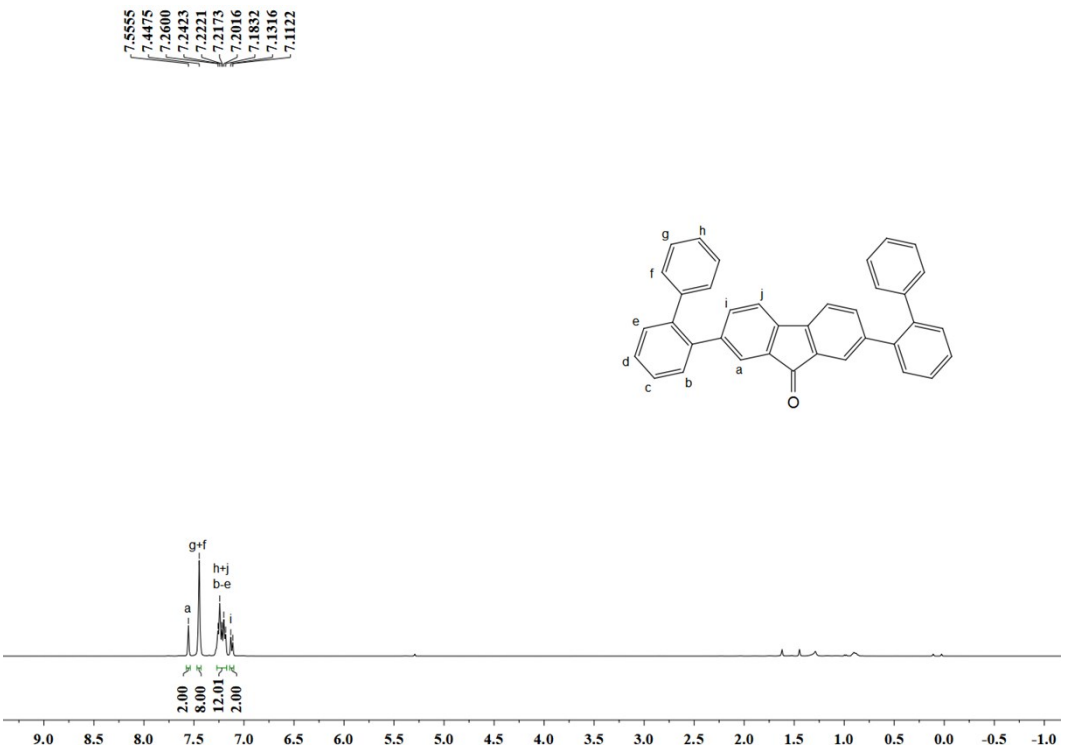


Figure S14. ^{1}H NMR spectrum (400 MHz) of compound **S-3** in $CDCl_3$ at 298 K.

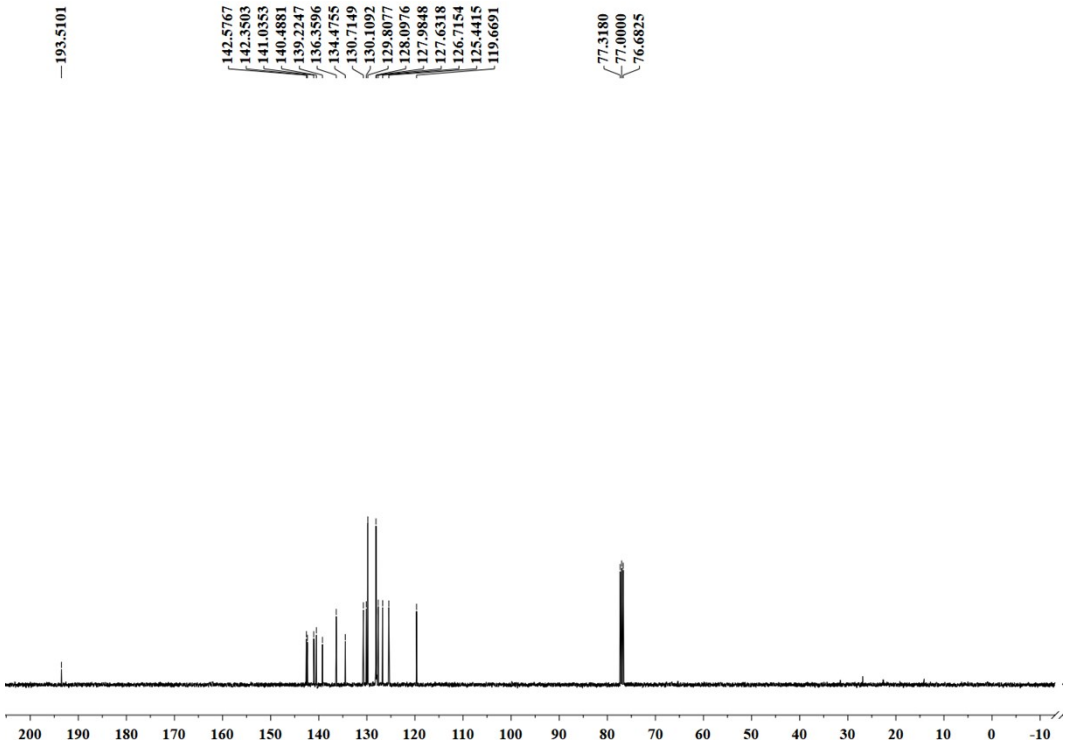


Figure S15. ^{13}C NMR spectrum (100 MHz) of compound **S-3** in $CDCl_3$ at 298 K.

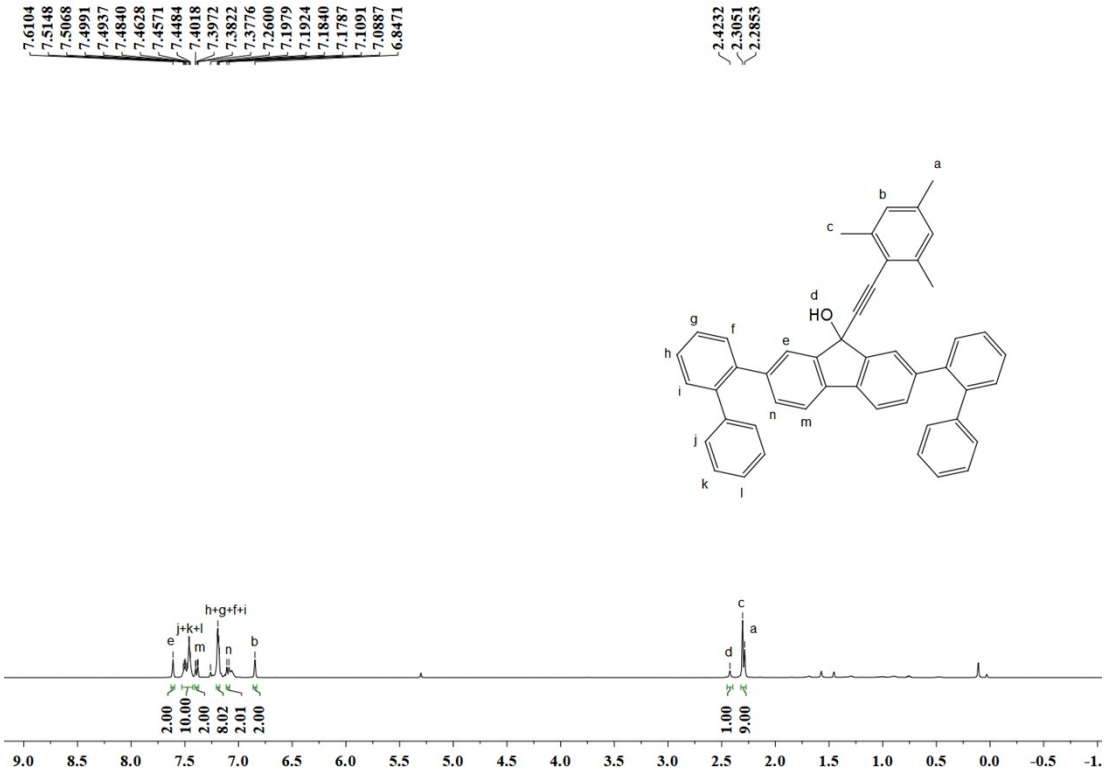


Figure S16. ^{1}H NMR spectrum (400 MHz) of compound **1b** in $CDCl_3$ at 298 K.

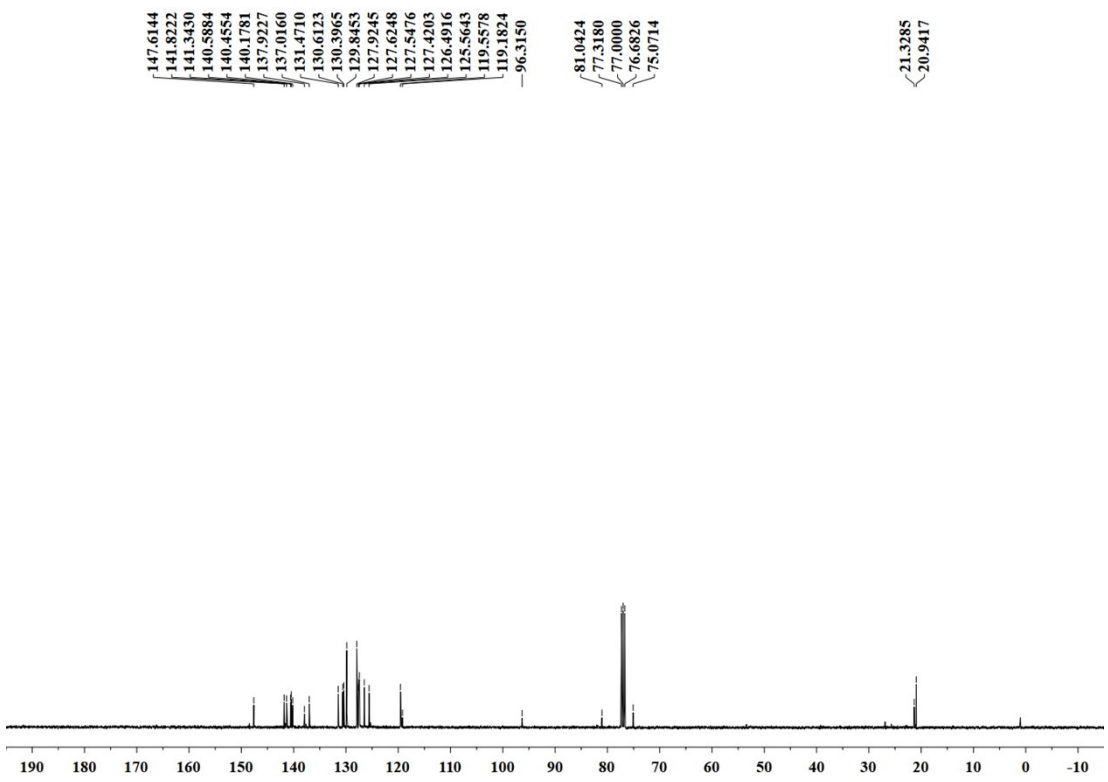


Figure S17. ^{13}C NMR spectrum (100 MHz) of compound **1b** in $CDCl_3$ at 298 K.

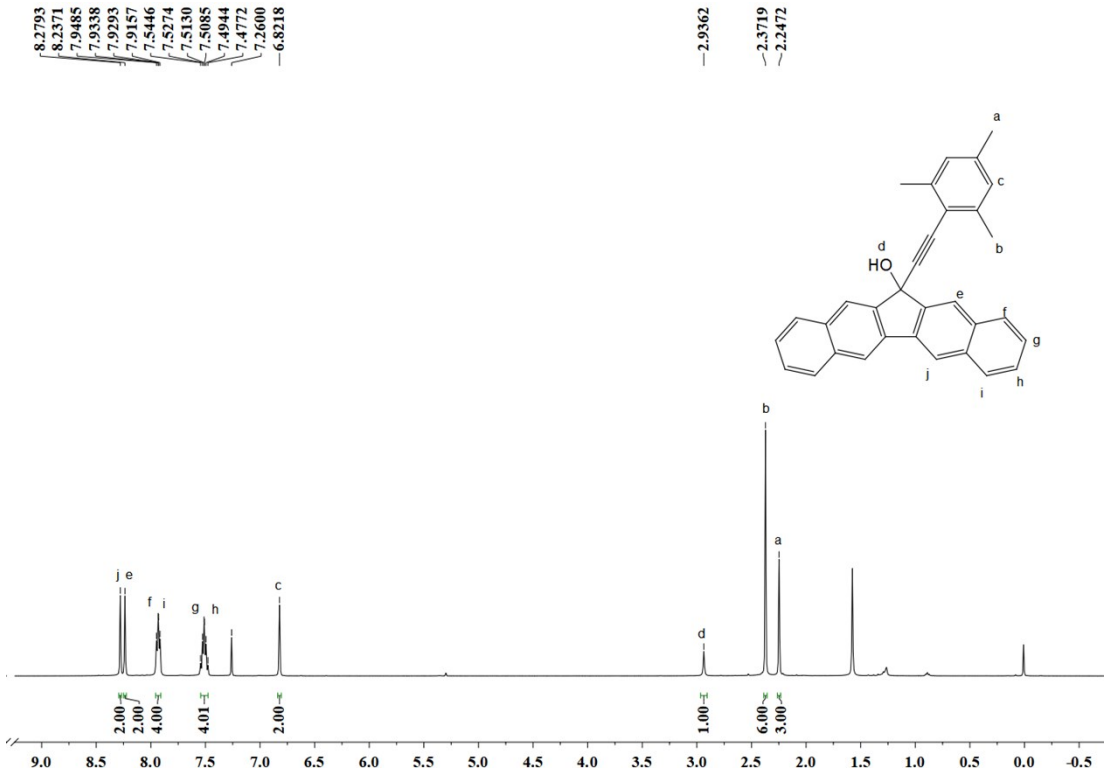


Figure S18. ^{1}H NMR spectrum (400 MHz) of compound **1c** in $CDCl_3$ at 298 K.

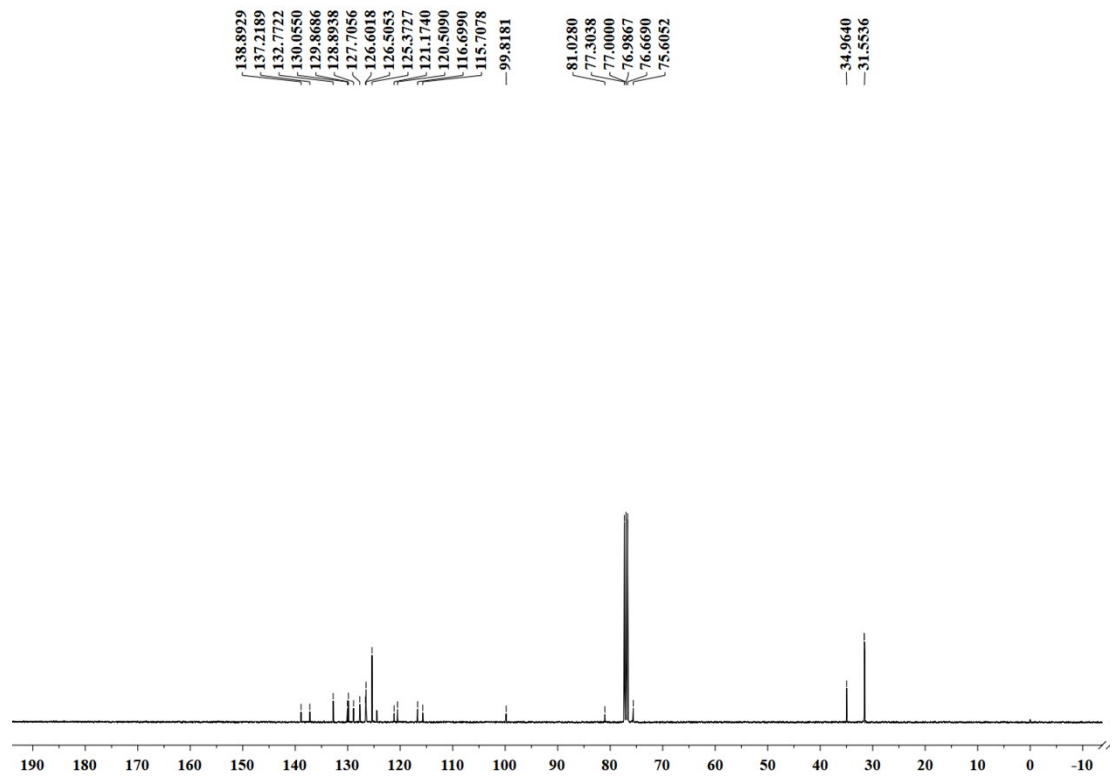


Figure S19. ^{13}C NMR spectrum (100 MHz) of compound **1c** in $CDCl_3$ at 298 K.

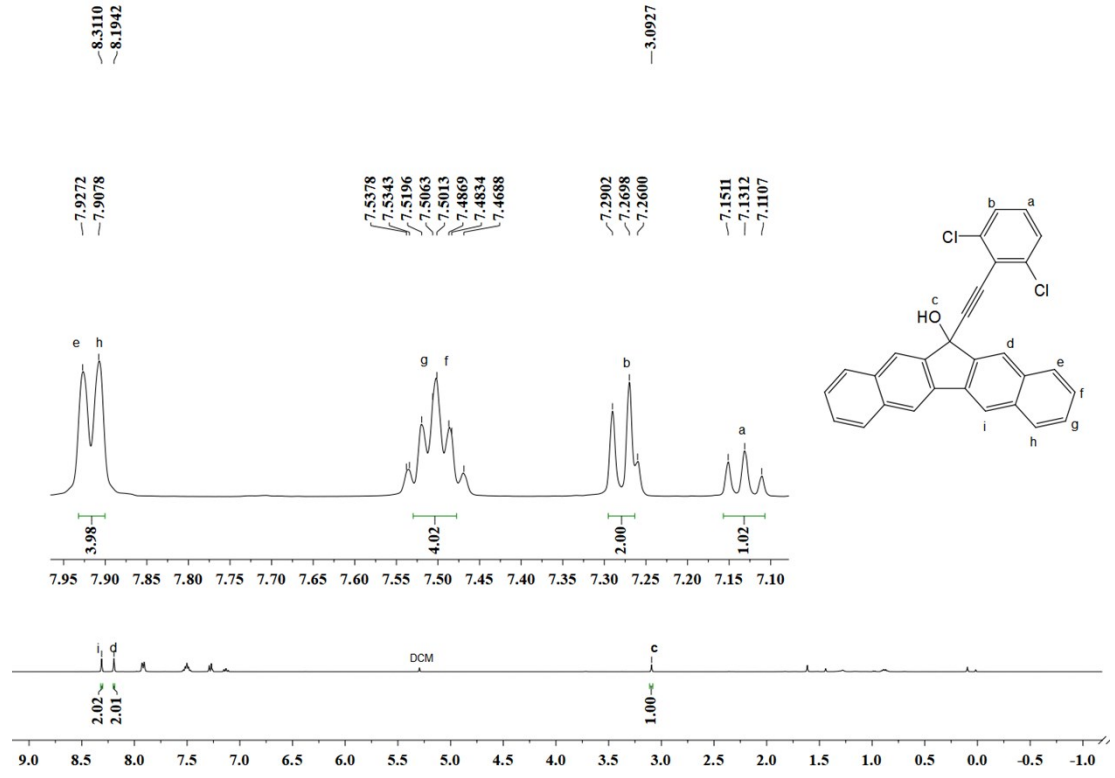


Figure S20. ^{1}H NMR spectrum (400 MHz) of compound **1d** in $CDCl_3$ at 298 K.

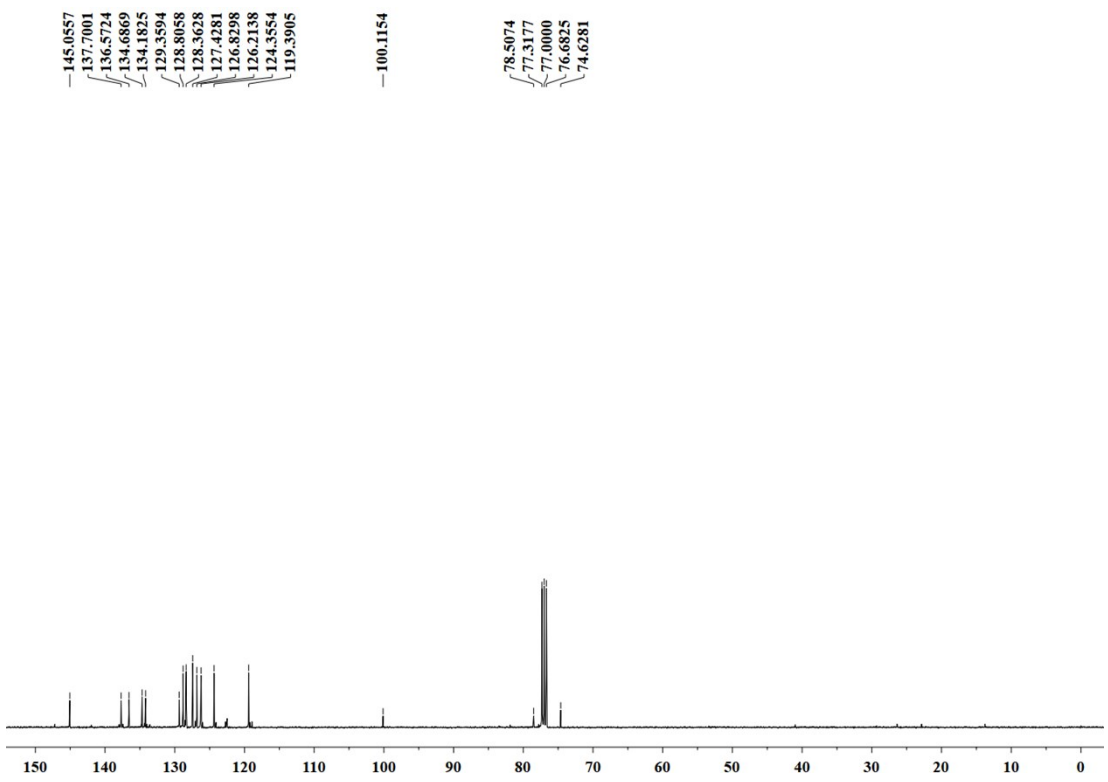


Figure S21. ^{13}C NMR spectrum (100 MHz) of compound **1d** in $CDCl_3$ at 298 K.

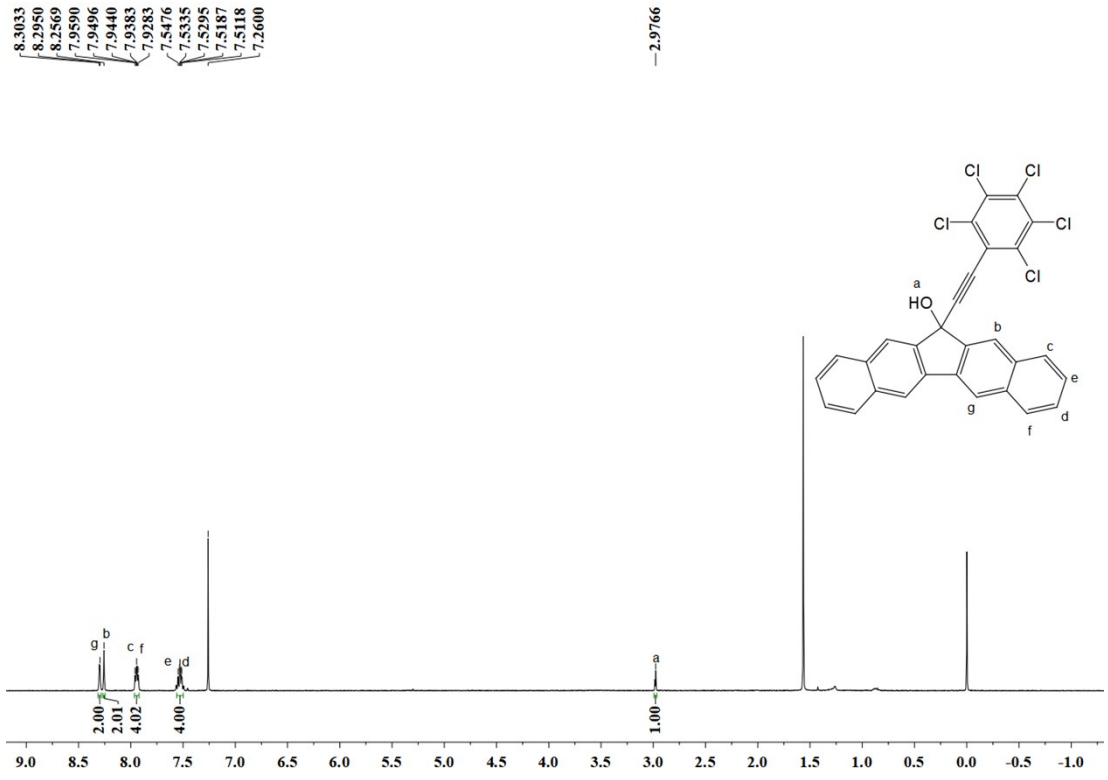


Figure S22. ^{1}H NMR spectrum (400 MHz) of compound **1e** in $CDCl_3$ at 298 K.

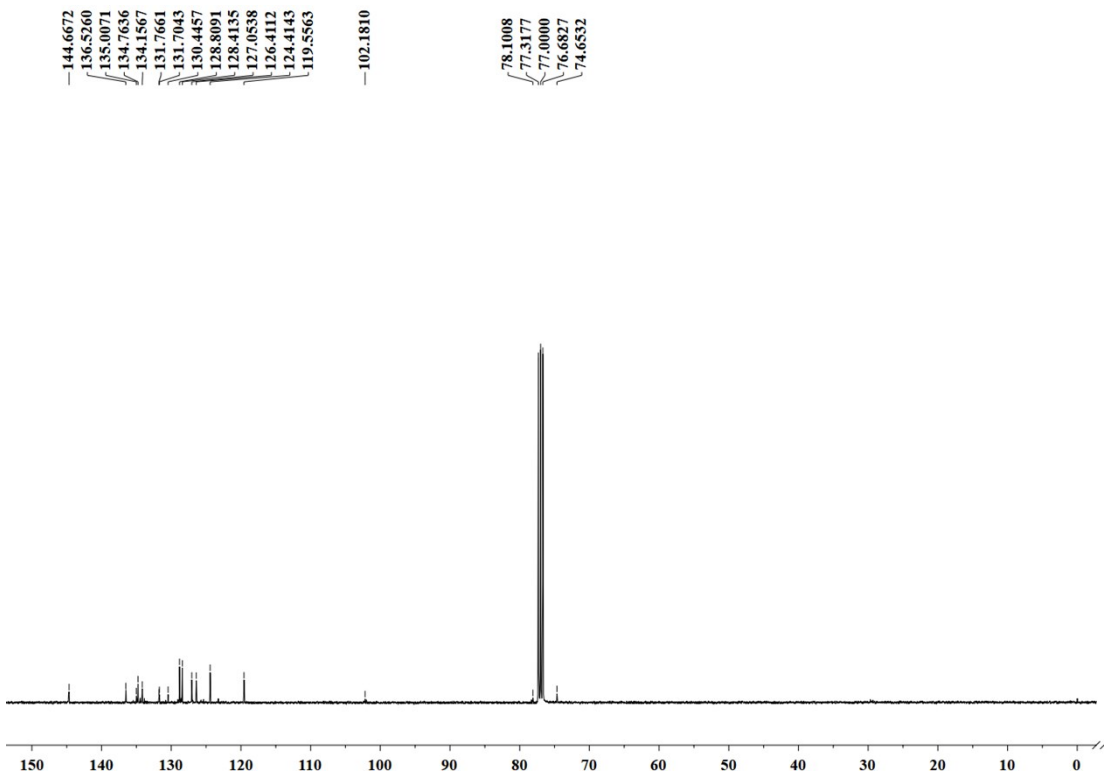


Figure S23. ^{13}C NMR spectrum (100 MHz) of compound **1e** in $CDCl_3$ at 298 K.

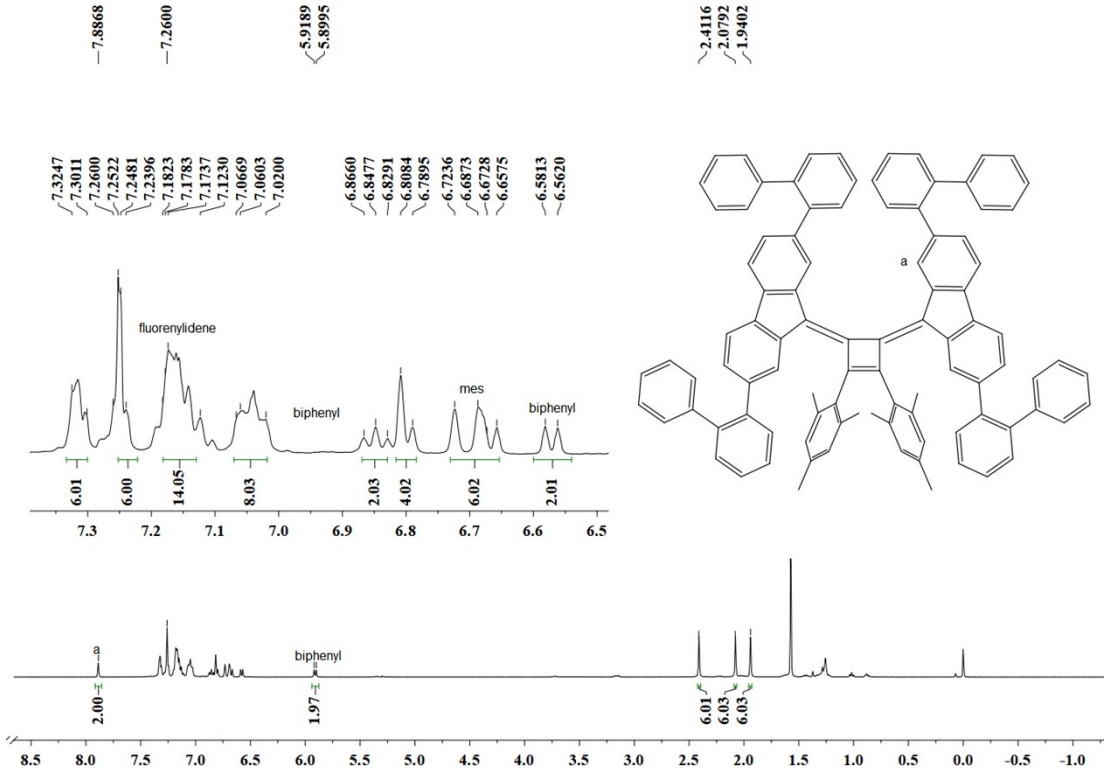


Figure S24. ^{1}H NMR spectrum (400 MHz) of compound **2b** in $CDCl_3$ at 298 K.

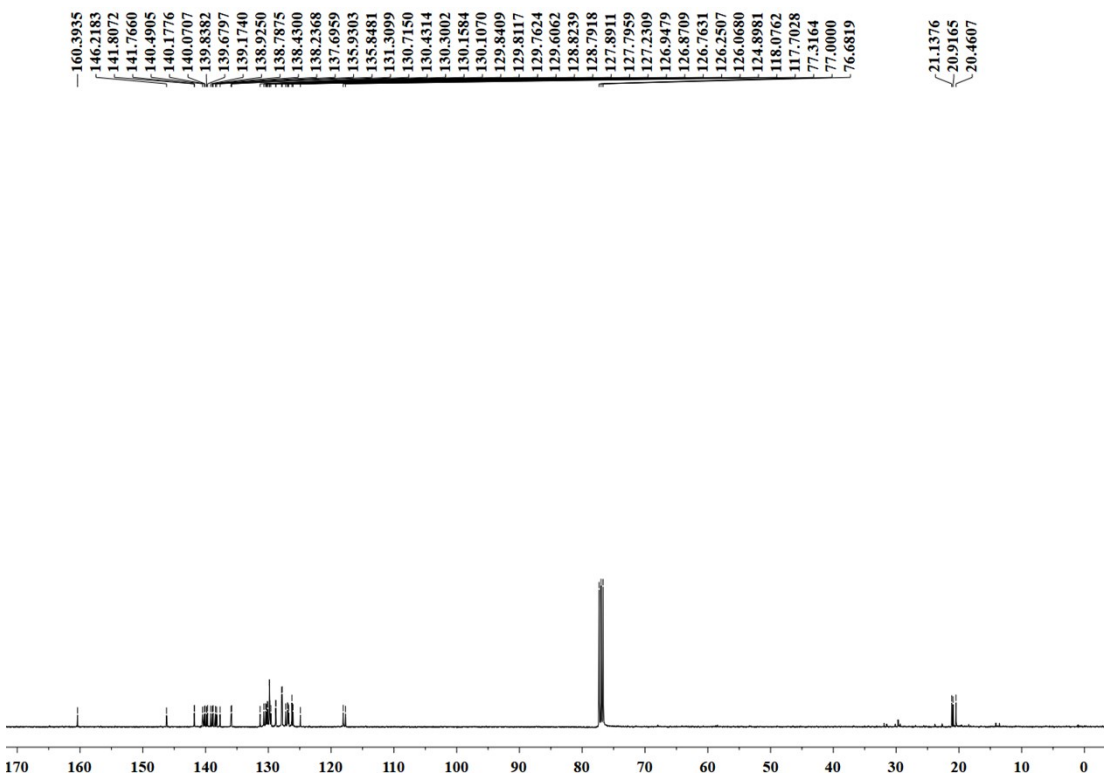


Figure S25. ^{13}C NMR spectrum (100 MHz) of compound **2b** in $CDCl_3$ at 298 K.

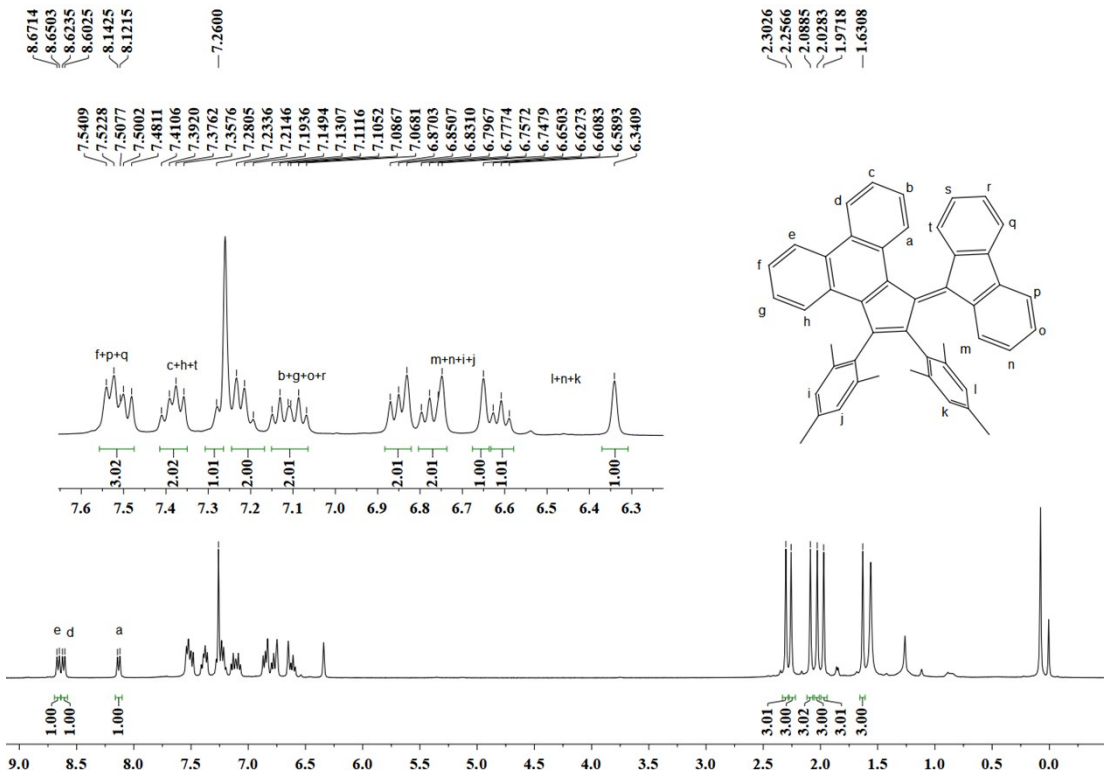


Figure S26. ^{1}H NMR spectrum (400 MHz) of compound **PBF-Mes** in $CDCl_3$ at 298 K.

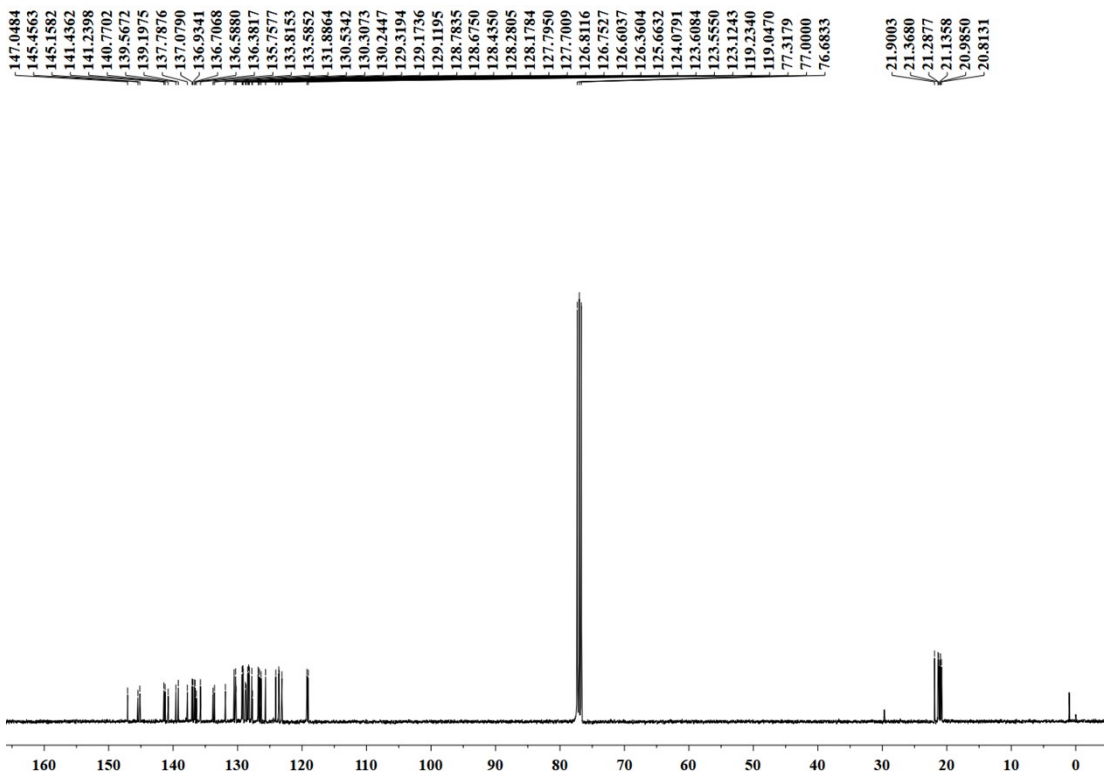


Figure S27. ^{13}C NMR spectrum (100 MHz) of compound **PBF-Mes** in $CDCl_3$ at 298 K.

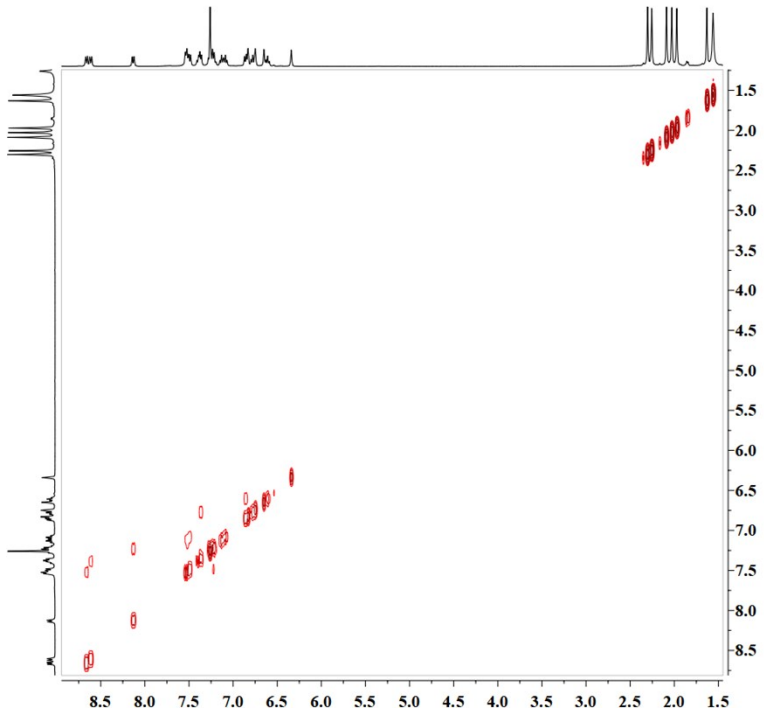


Figure S28. COSY spectrum (400 MHz) of compound **PBF-Mes** in $CDCl_3$ at 298 K.

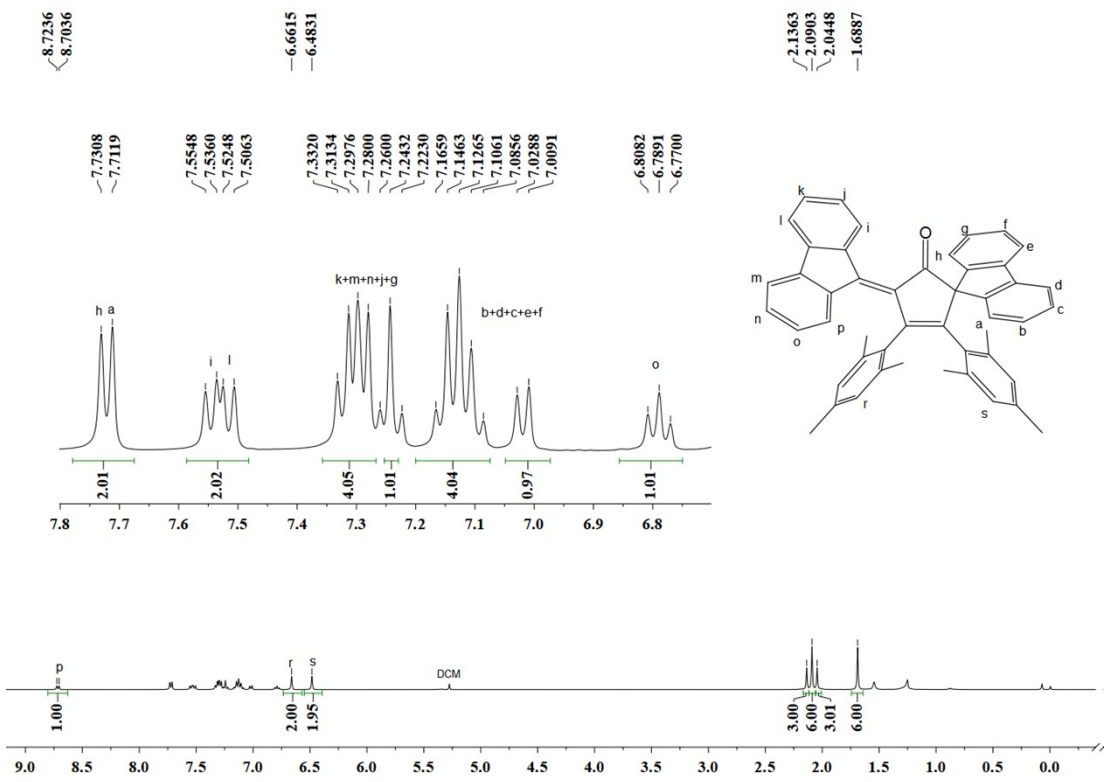


Figure S29. ^{1}H NMR spectrum (400 MHz) of compound **3a** in $CDCl_3$ at 298 K.

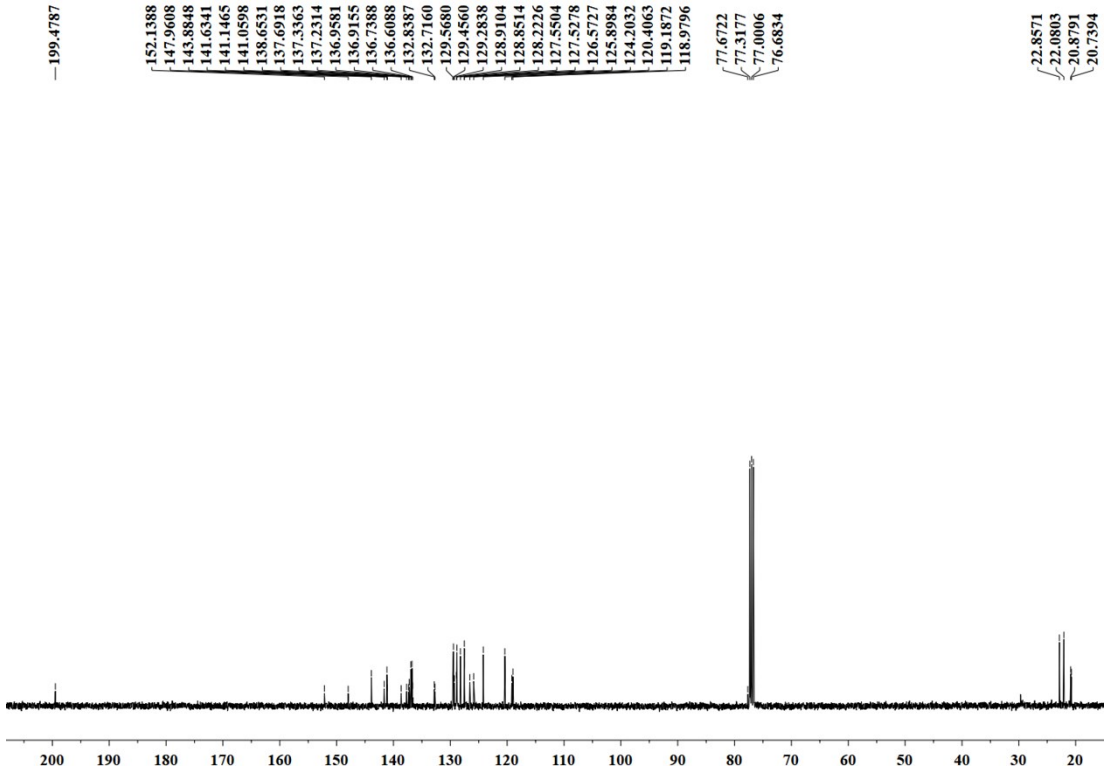


Figure S30. ^{13}C NMR spectrum (100 MHz) of compound **3a** in $CDCl_3$ at 298 K.

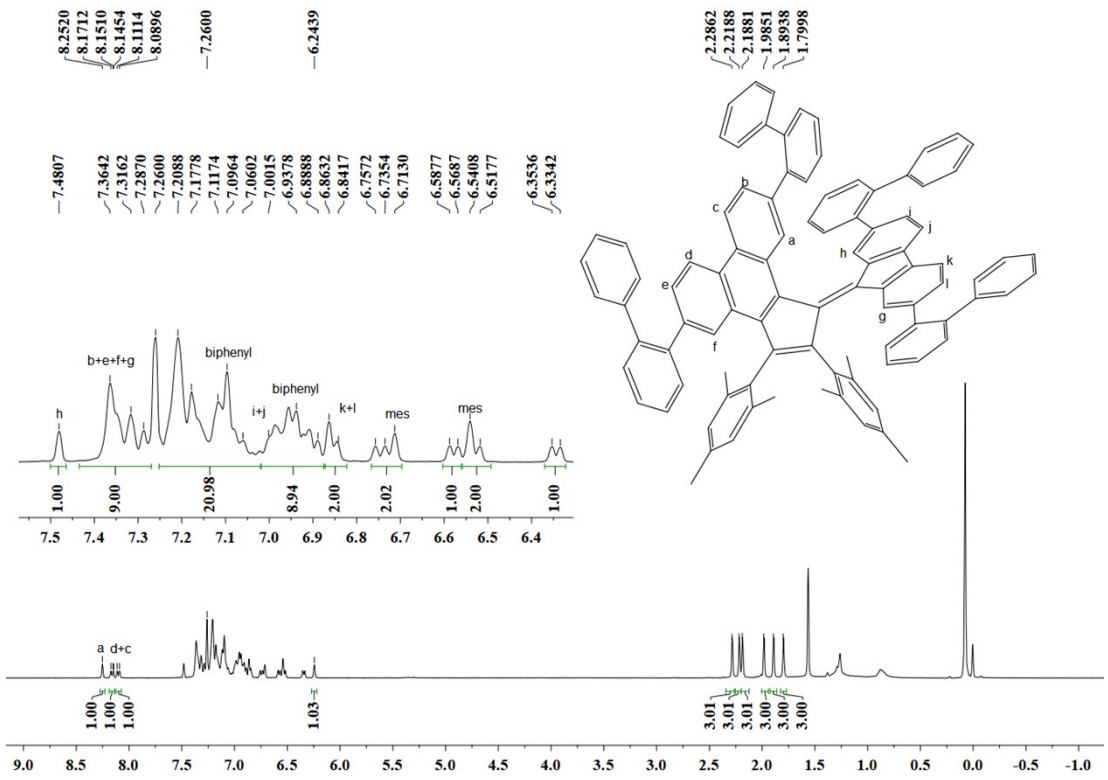


Figure S31. ^{1}H NMR spectrum (400 MHz) of compound **PBF-2b** in $CDCl_3$ at 298 K.

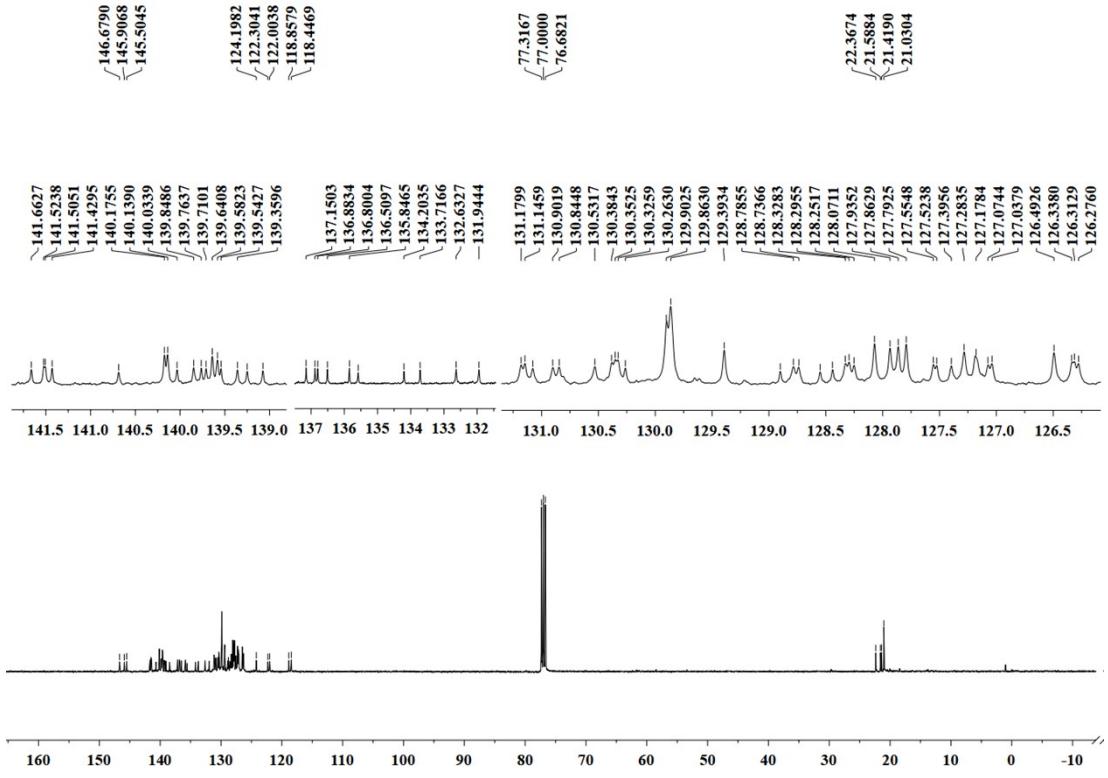


Figure S32. ^{13}C NMR spectrum (100 MHz) of compound **PBF-2b** in $CDCl_3$ at 298 K.

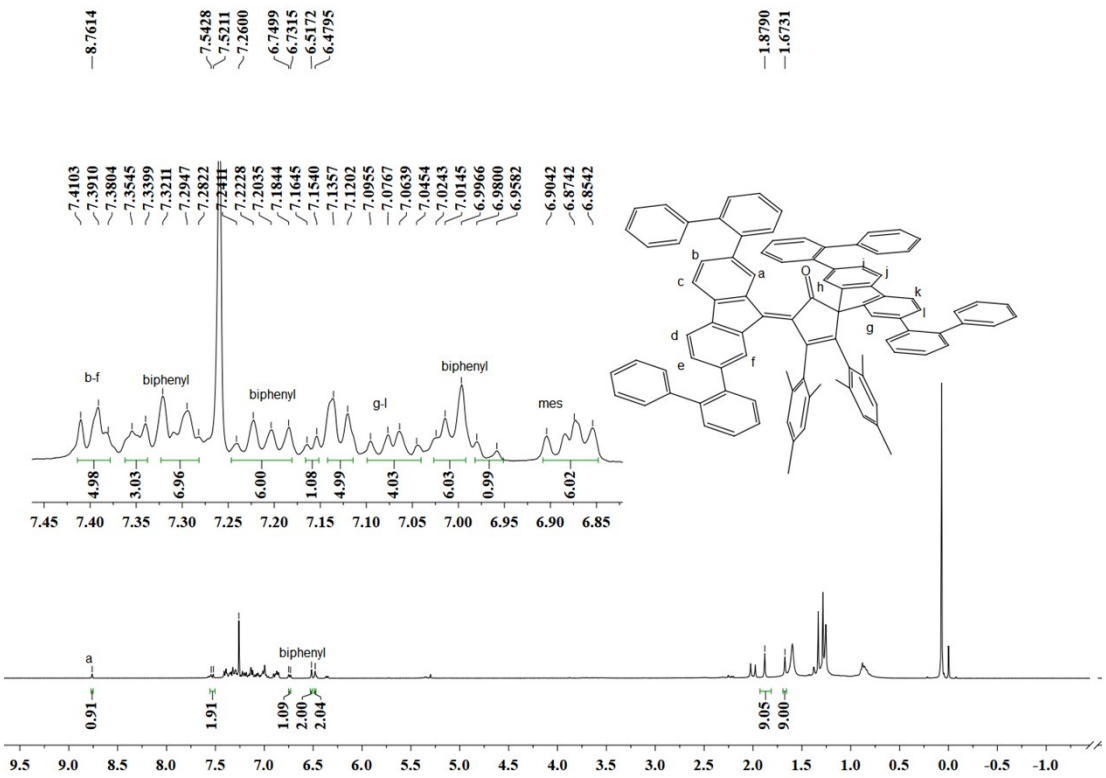


Figure S33. ^{1}H NMR spectrum (400 MHz) of compound **3b** in $CDCl_3$ at 298 K.

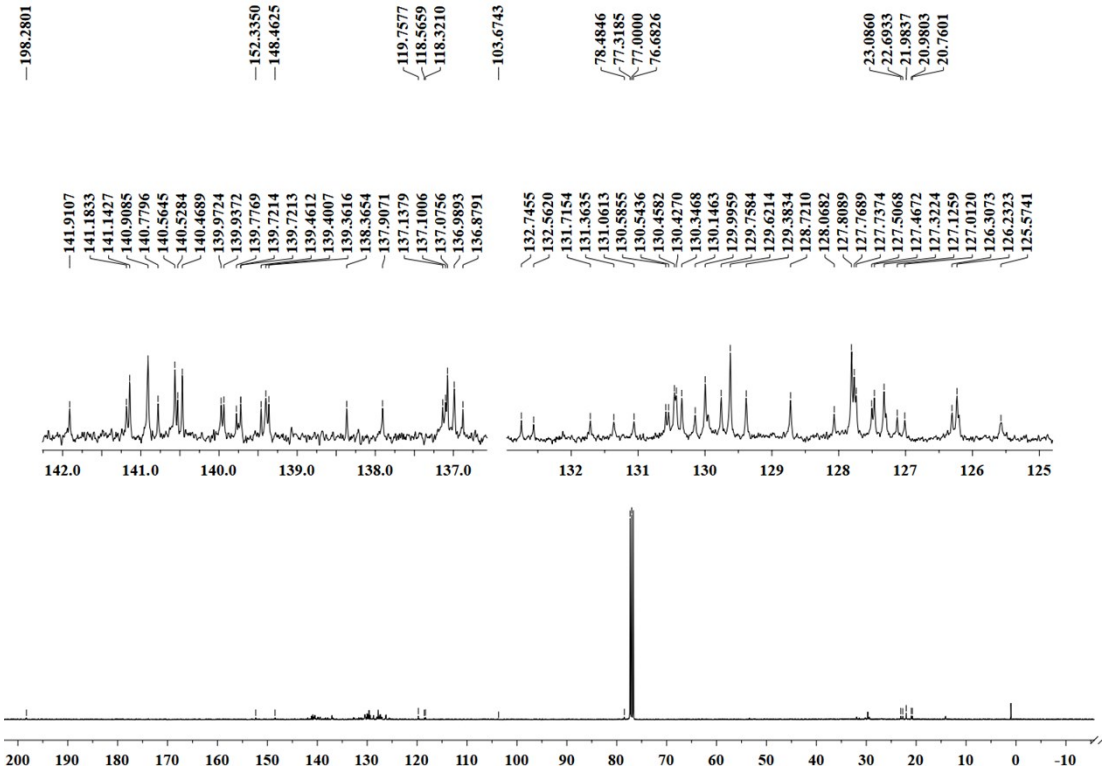


Figure S34. ^{13}C NMR spectrum (100 MHz) of **3b** in $CDCl_3$ at 298 K.

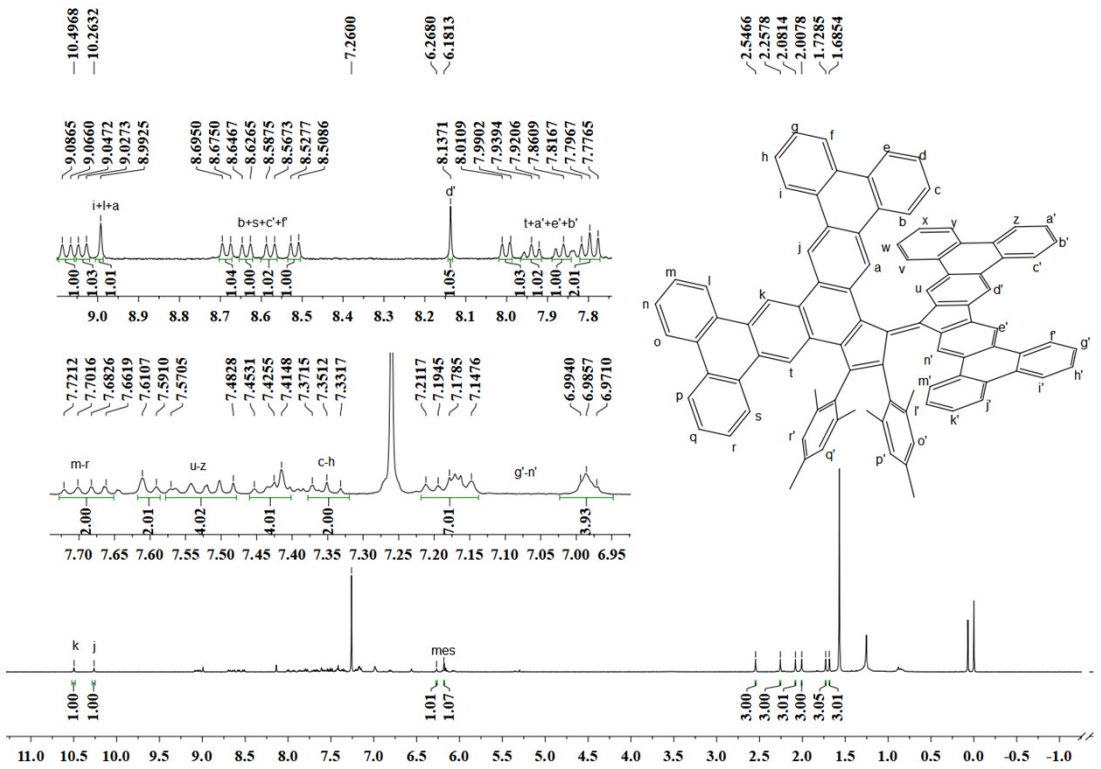


Figure S35. ^{1}H NMR spectrum (400 MHz) of compound **SBF-Mes** in $CDCl_3$ at 298 K.

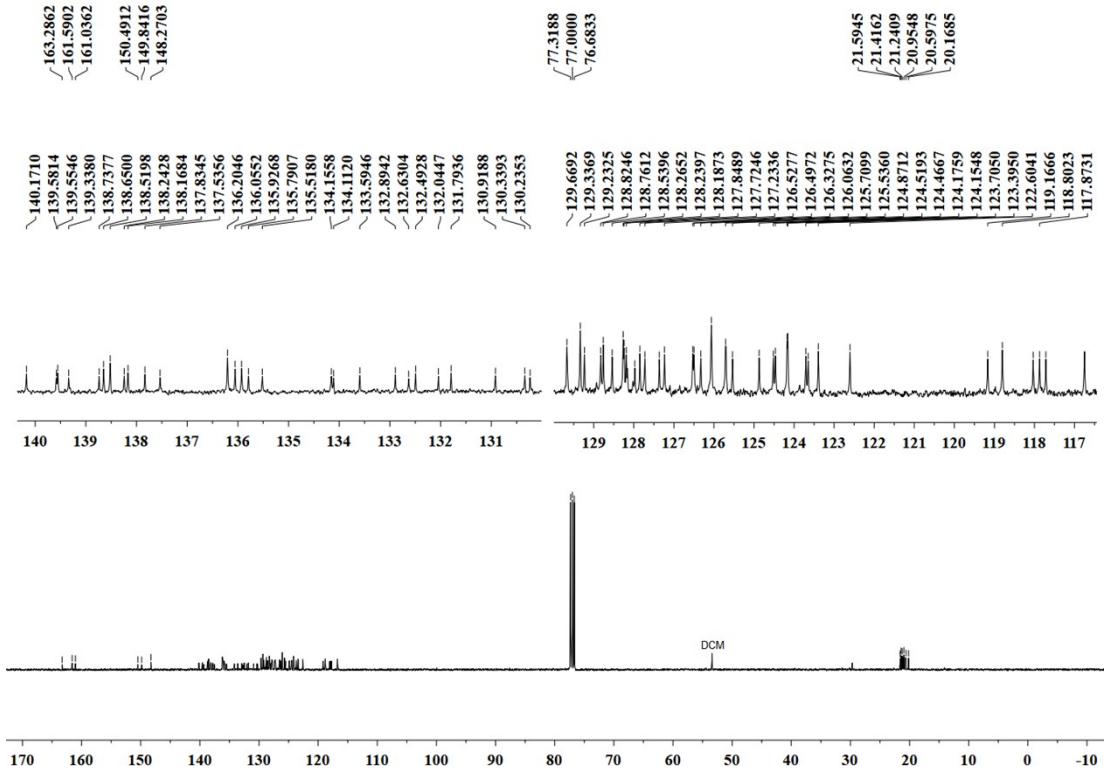


Figure S36. ^{13}C NMR spectrum (100 MHz) of **SBF-Mes** in $CDCl_3$ at 298 K.

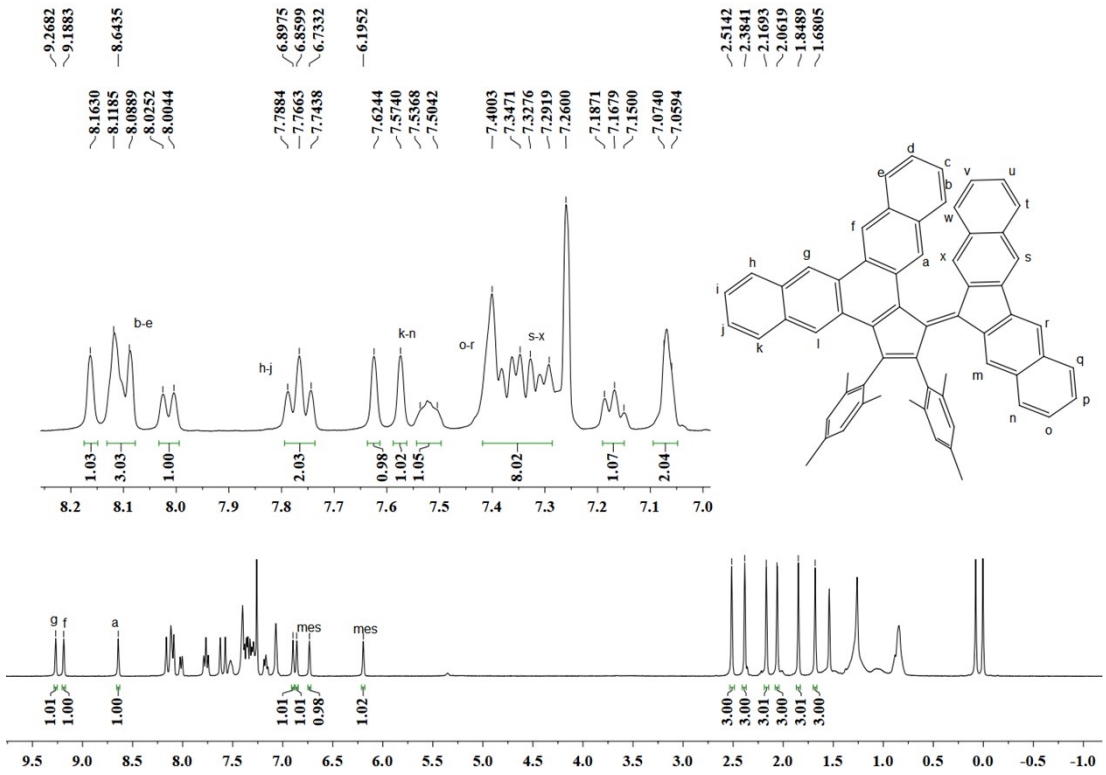


Figure S37. ^{1}H NMR spectrum (400 MHz) of compound **NBF-Mes** in $CDCl_3$ at 298 K.

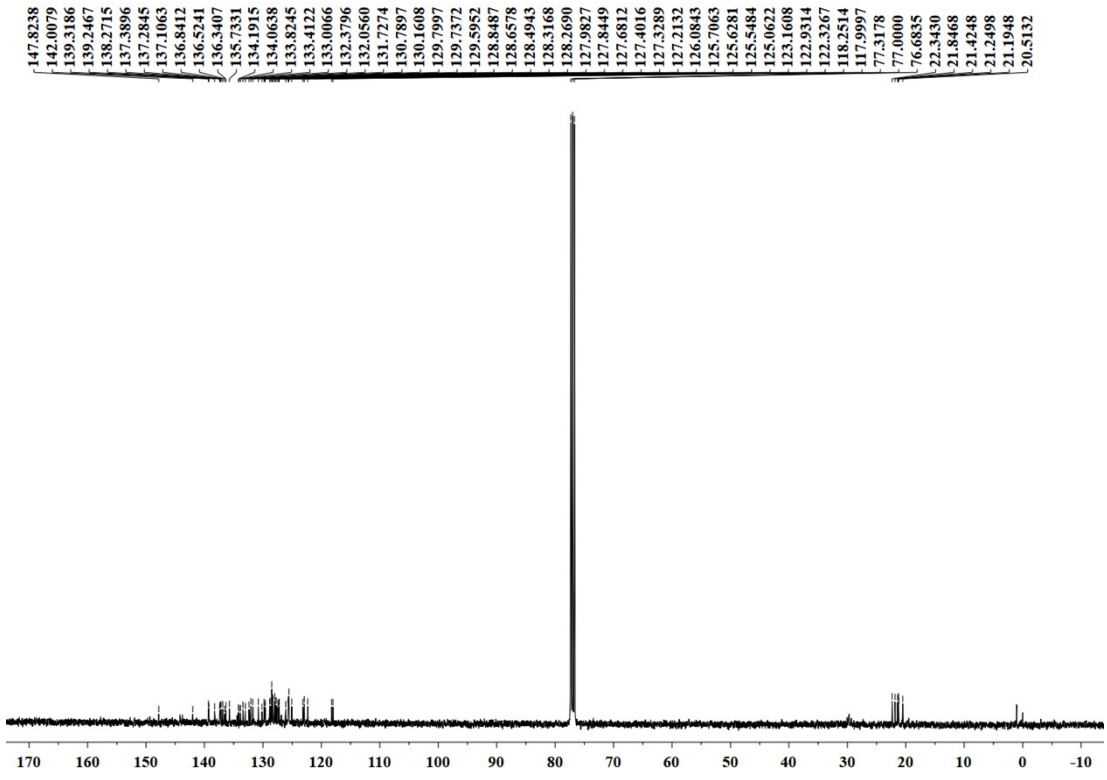


Figure S38. ^{13}C NMR spectrum (100 MHz) of compound **NBF-Mes** in $CDCl_3$ at 298 K.

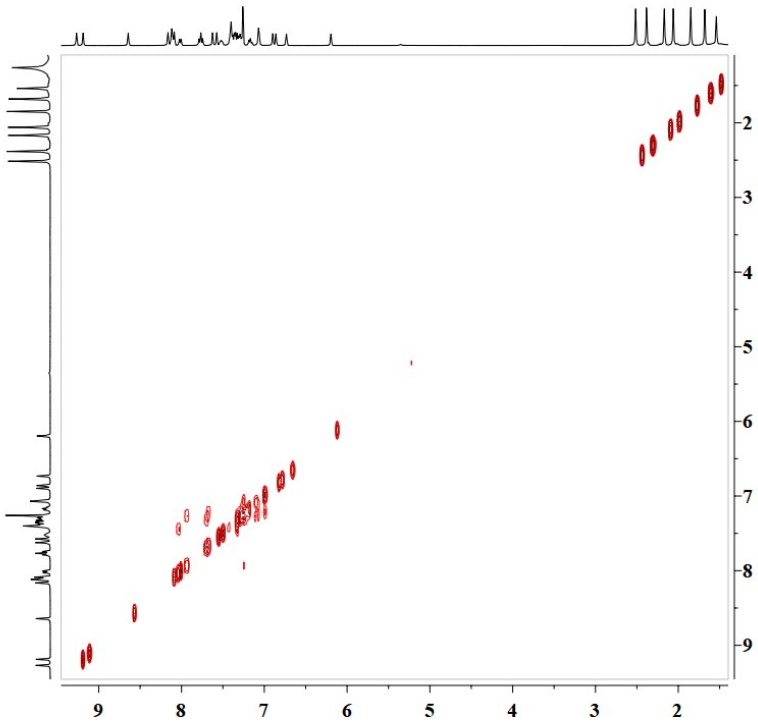


Figure S39. COSY spectrum (400 MHz) of **NBF-Mes** in $CDCl_3$ at 298 K

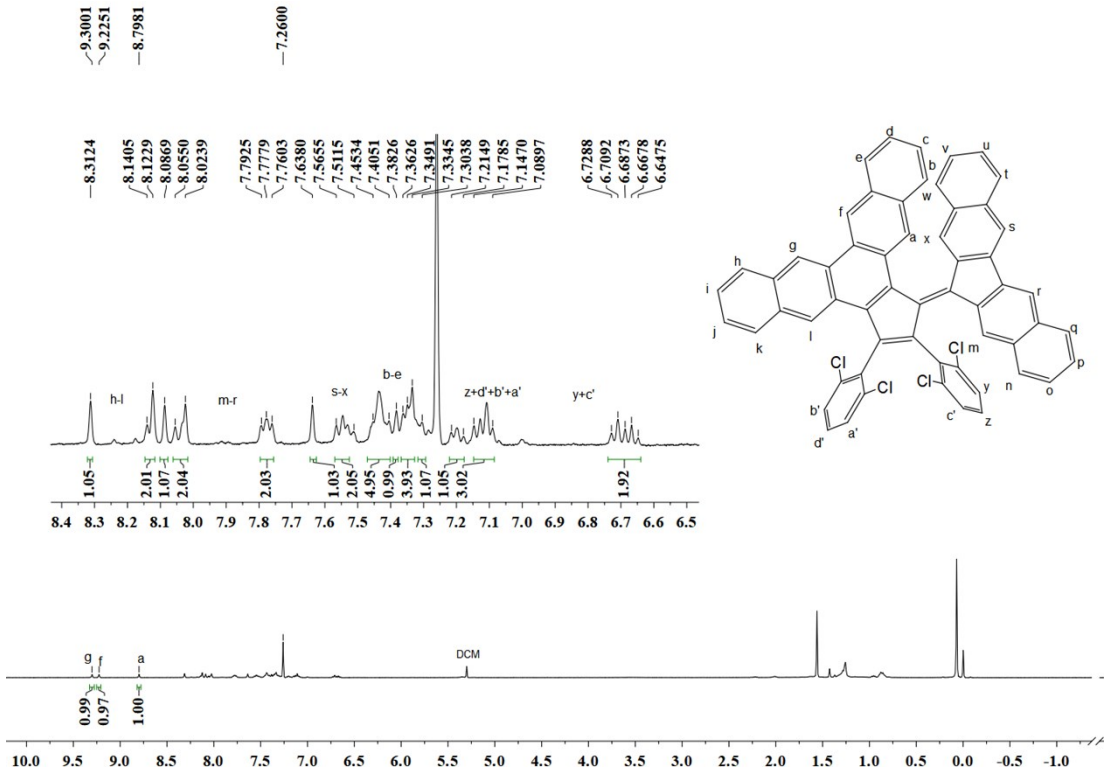


Figure S40. ^1H NMR spectrum (400 MHz) of compound **NBF-DCP** in $CDCl_3$ at 298 K.

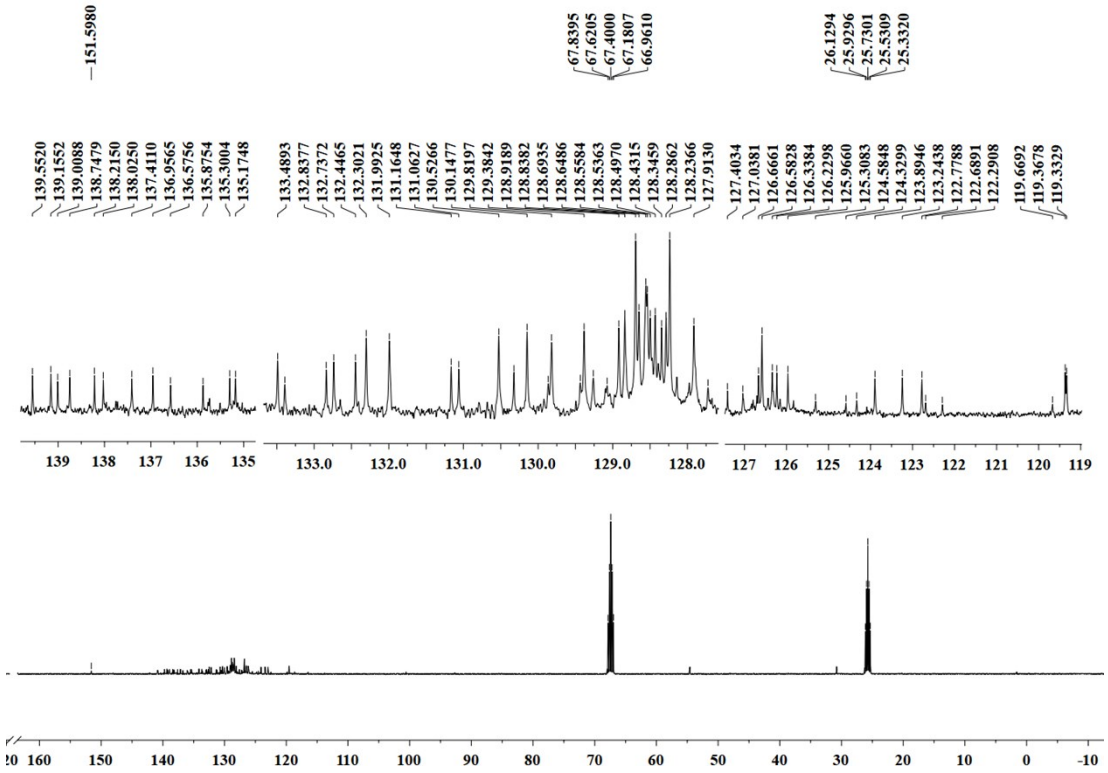


Figure S41. ^{13}C NMR spectrum (100 MHz) of compound **NBF-DCP** in THF-d_8 at 298 K

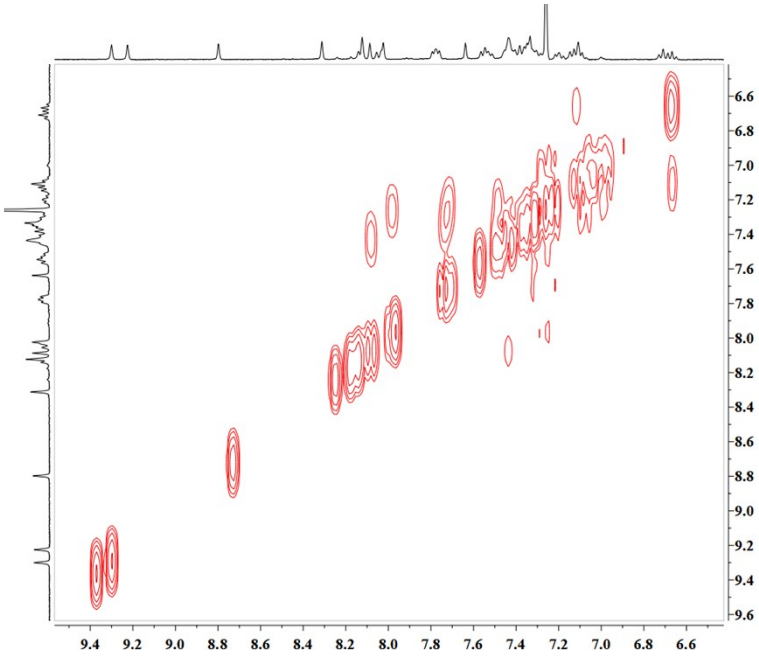


Figure S42. COSY spectrum (400 MHz) of compound **NBF-DCP** in $CDCl_3$ at 298 K.

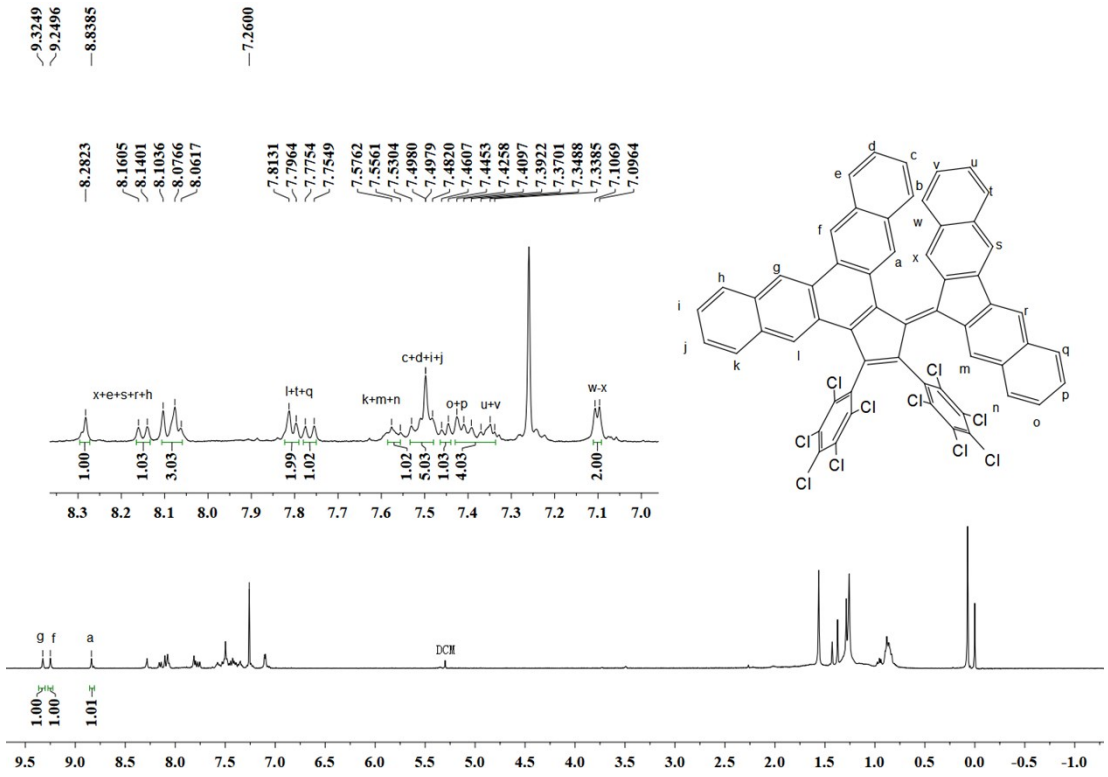


Figure S43. ^{1}H NMR spectrum (400 MHz) of **NBF-PCP** in $CDCl_3$ at 298 K.

Figure S44. ^{13}C NMR spectrum (100 MHz) of compound **NBF-PCP** in THF-d_8 at 298 K

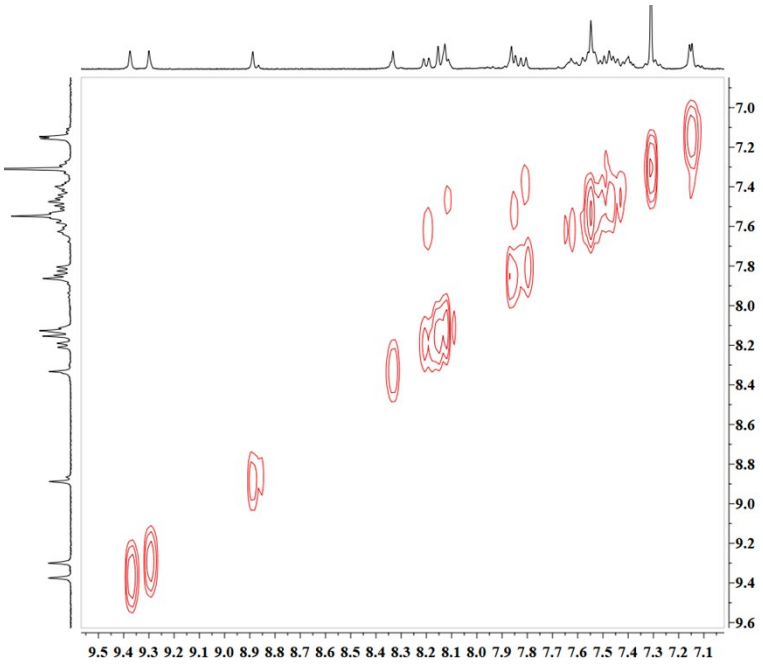


Figure S45. COSY spectrum (400 MHz) of compound **NBF-PCP** in $CDCl_3$ at 298 K.

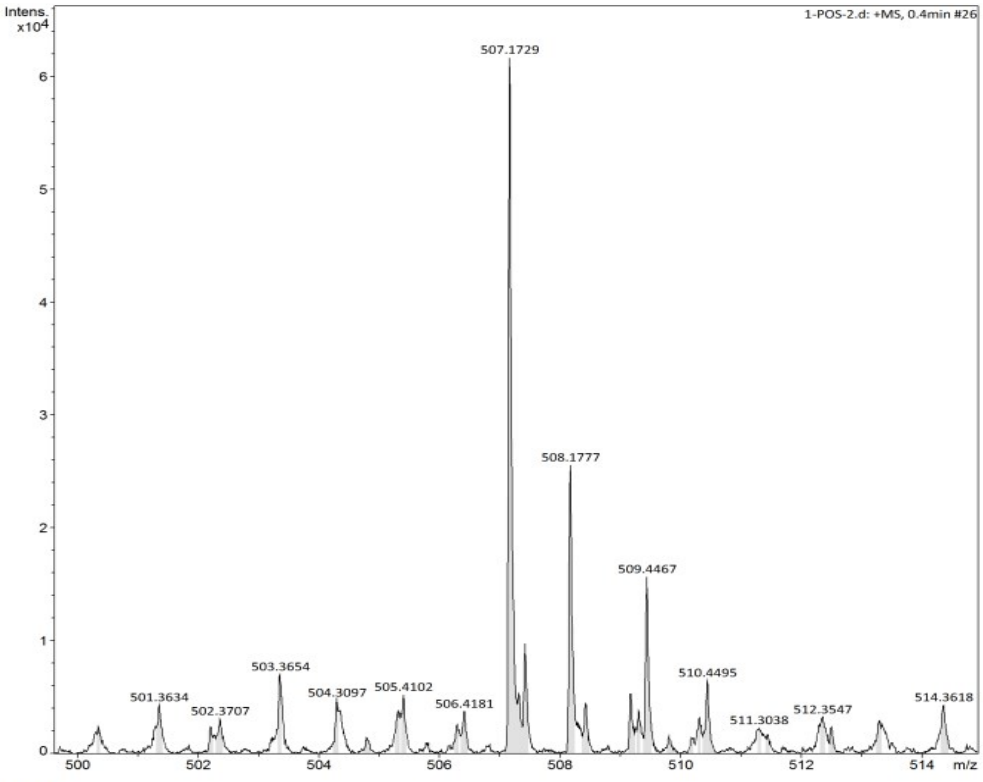


Figure S46. HR (APCI) mass spectrum of compound **S-3**.

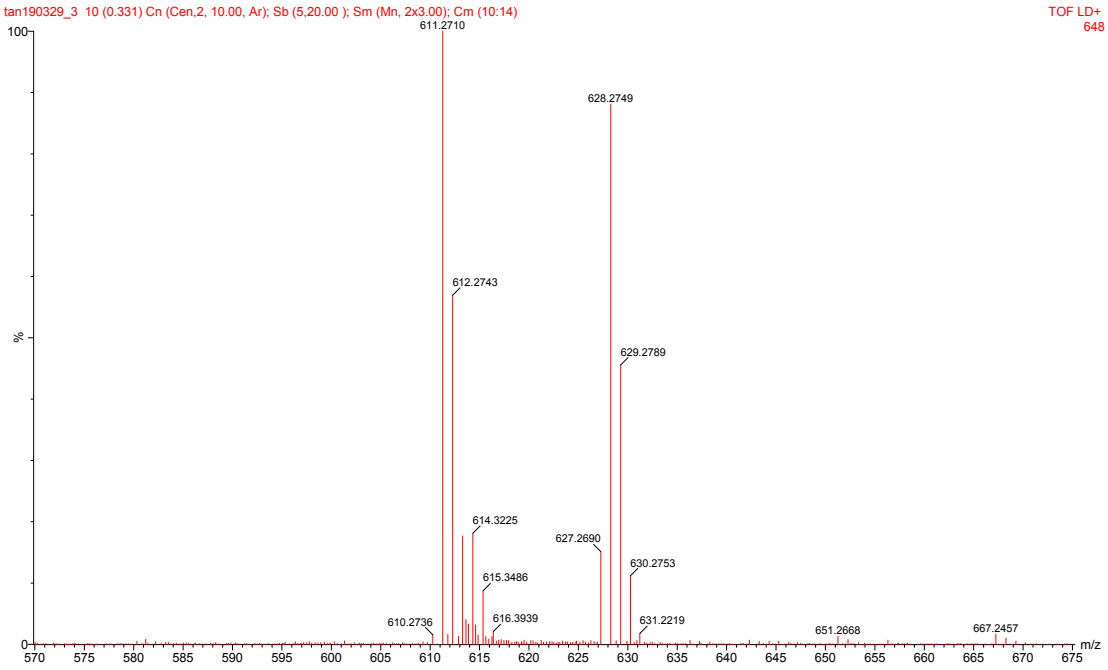


Figure S47. HR (MALDI-TOF) mass spectrum of compound **1b**.

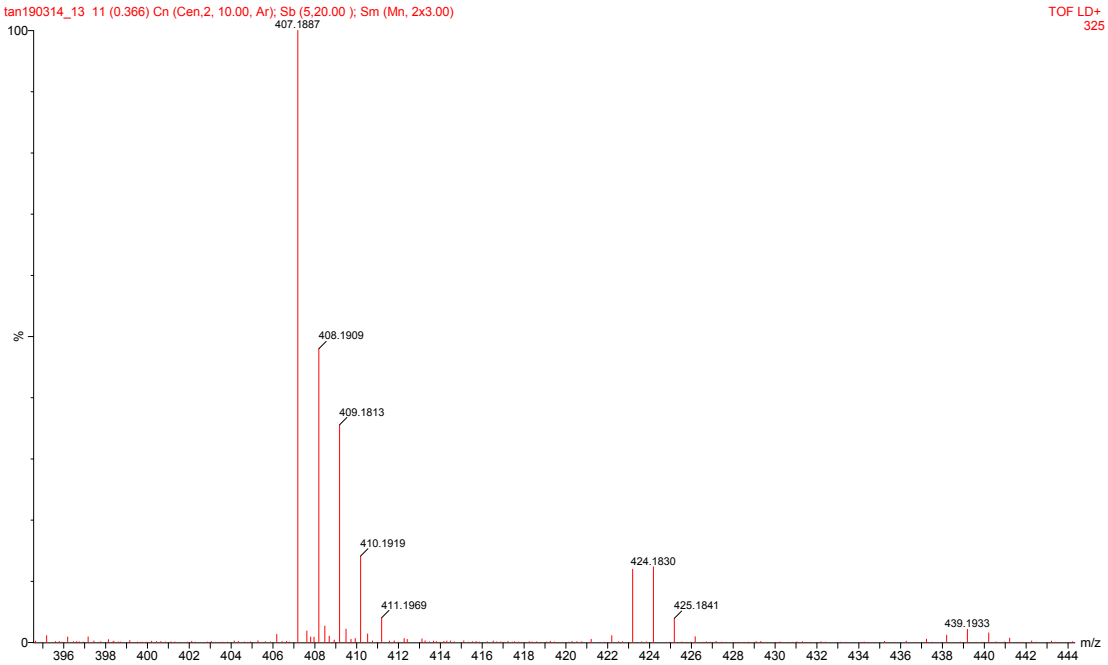


Figure S48. HR (MALDI-TOF) mass spectrum of compound **1c**.

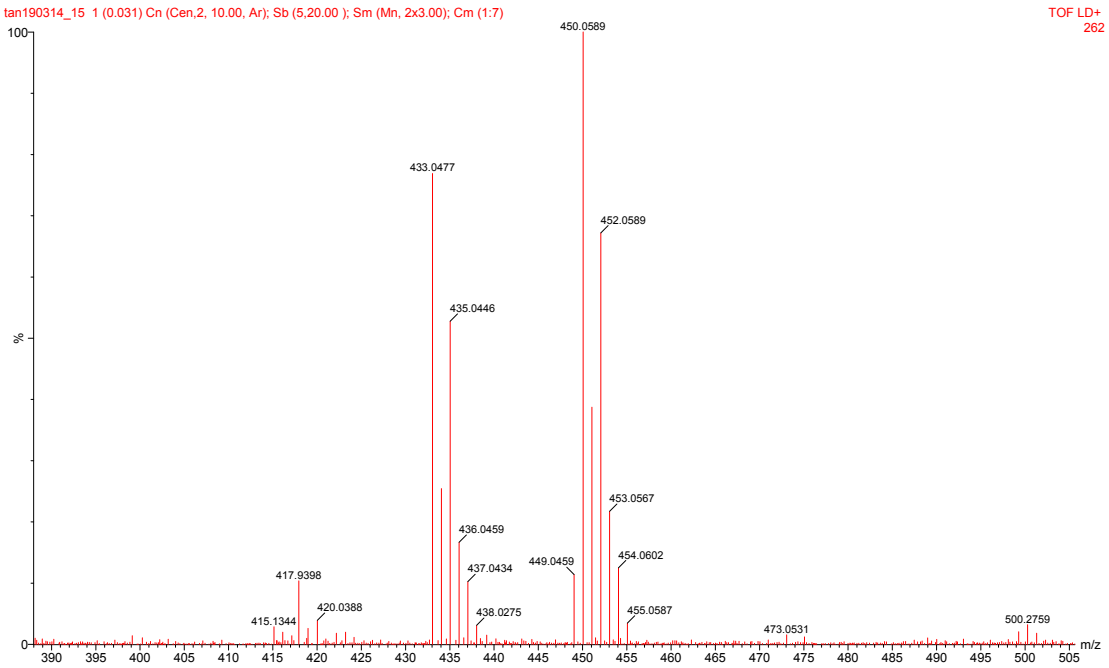


Figure S49. HR (MALDI-TOF) mass spectrum of compound **1d**.

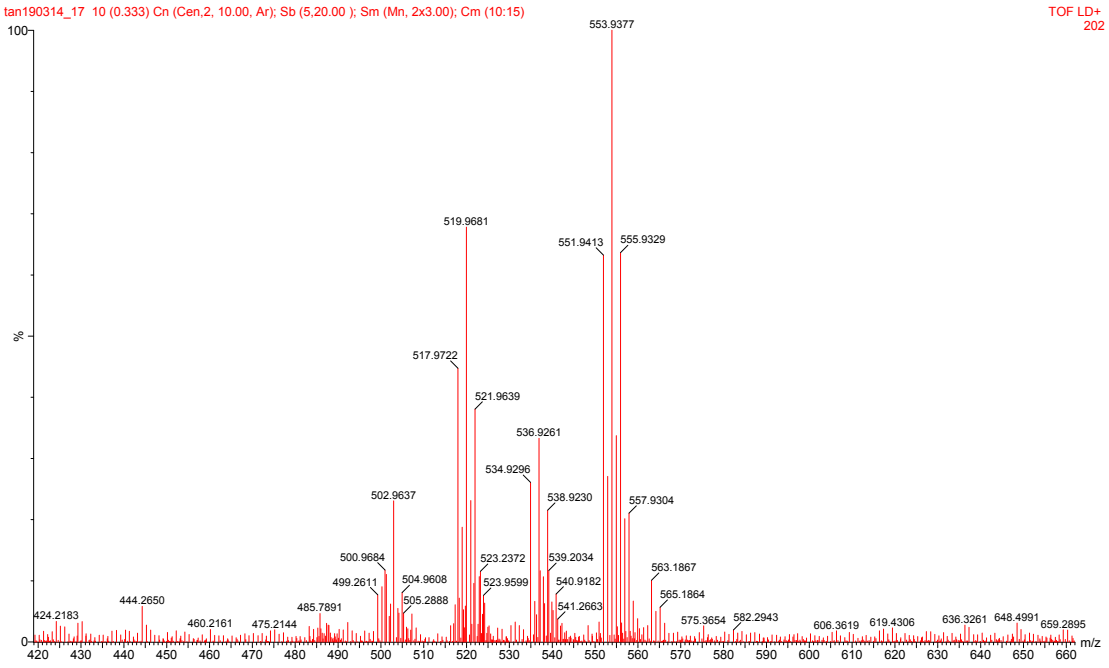


Figure S50. HR (MALDI-TOF) mass spectrum of compound **1e**.

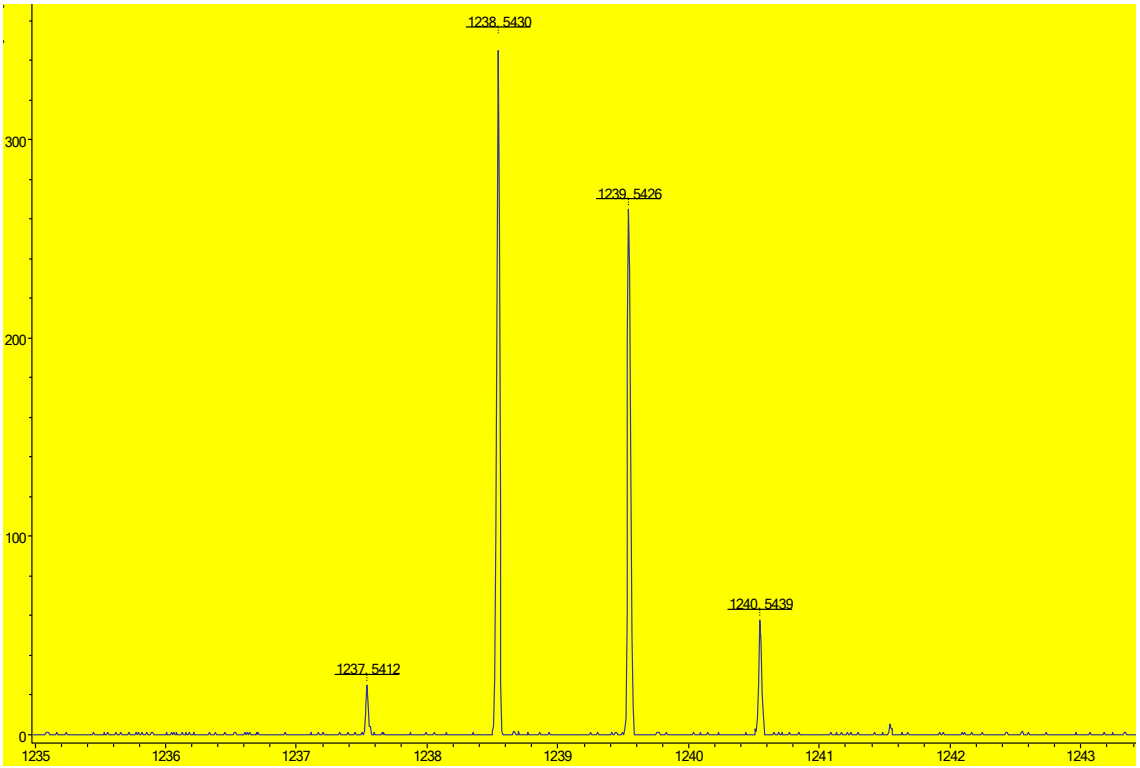


Figure S51. HR (MALDI-TOF) mass spectrum of compound **2b**.

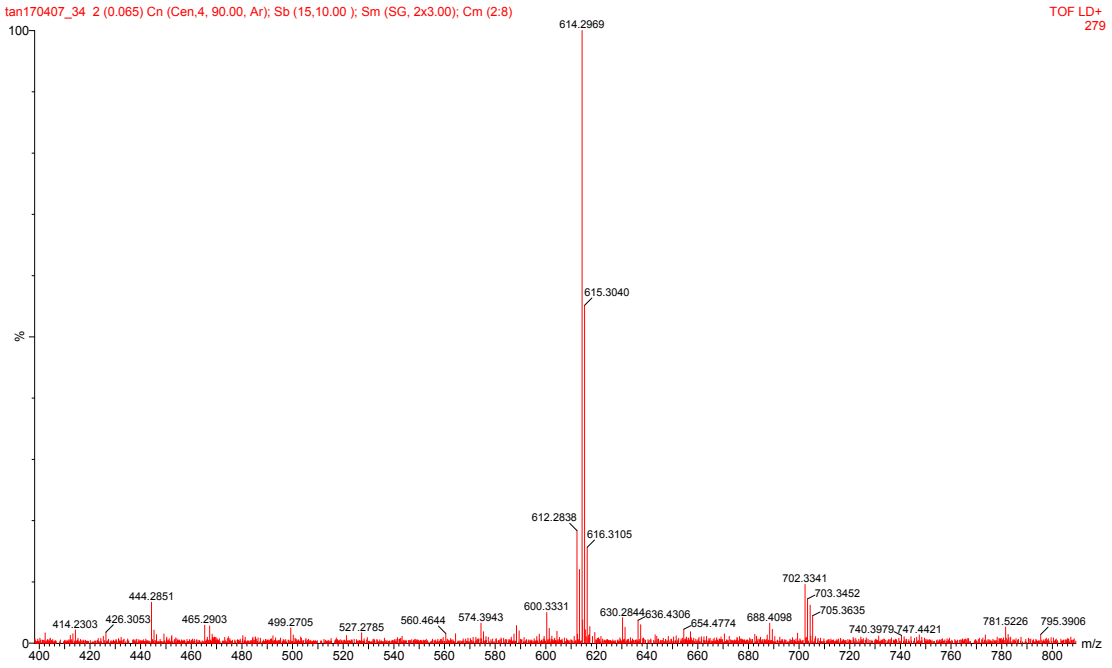


Figure S52. HR (MALDI-TOF) mass spectrum of compound **PBF-Mes**.

Figure S53. HR (MALDI-TOF) mass spectrum of compound **3a**.

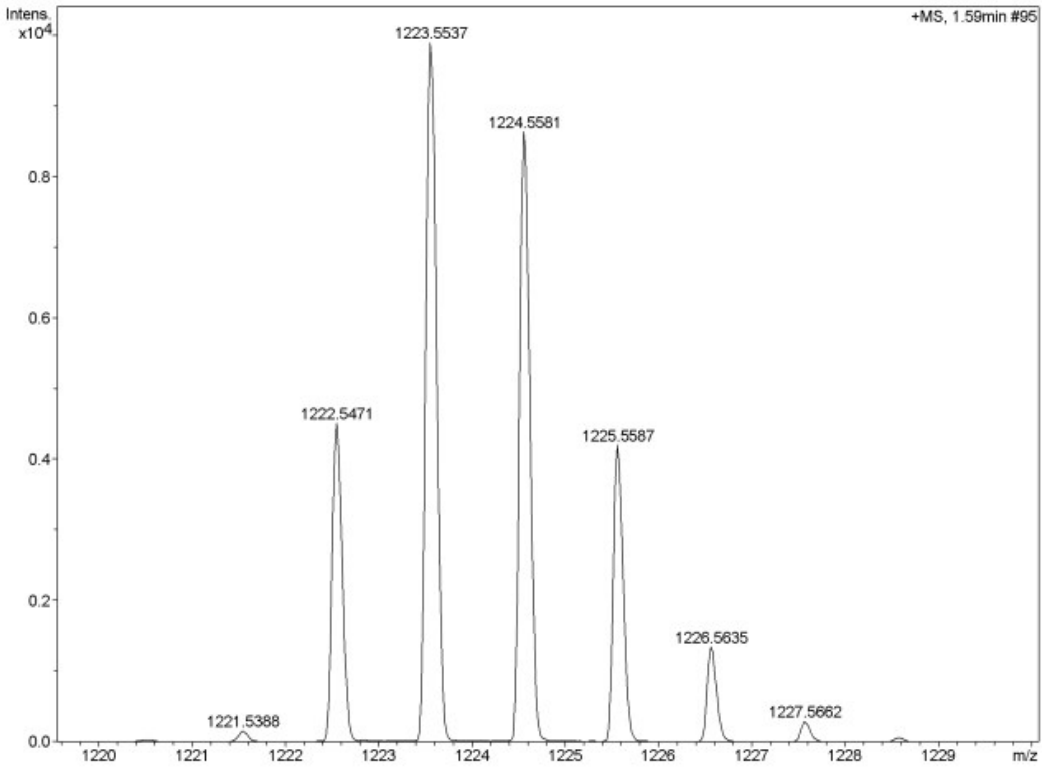


Figure S54. HR (ACPI) mass spectrum of compound **PBF-2b**.

Figure S55. HR (MALDI-TOF) mass spectrum of compound **3b**.

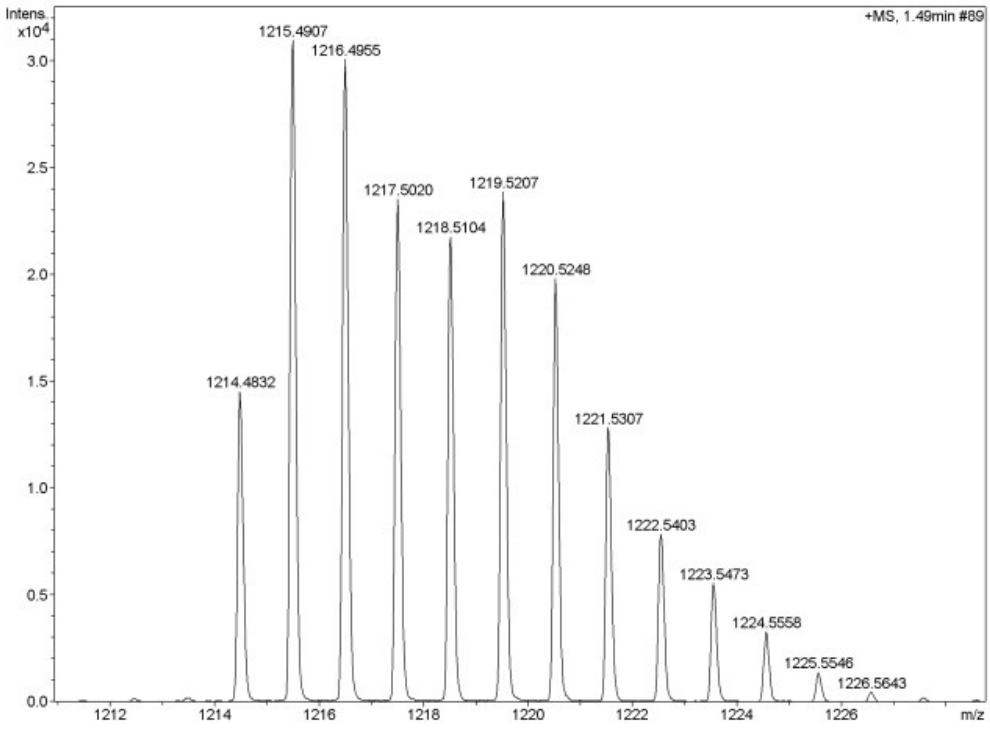


Figure S56. HR (APCI) mass spectrum of compound **SBF-Mes**.

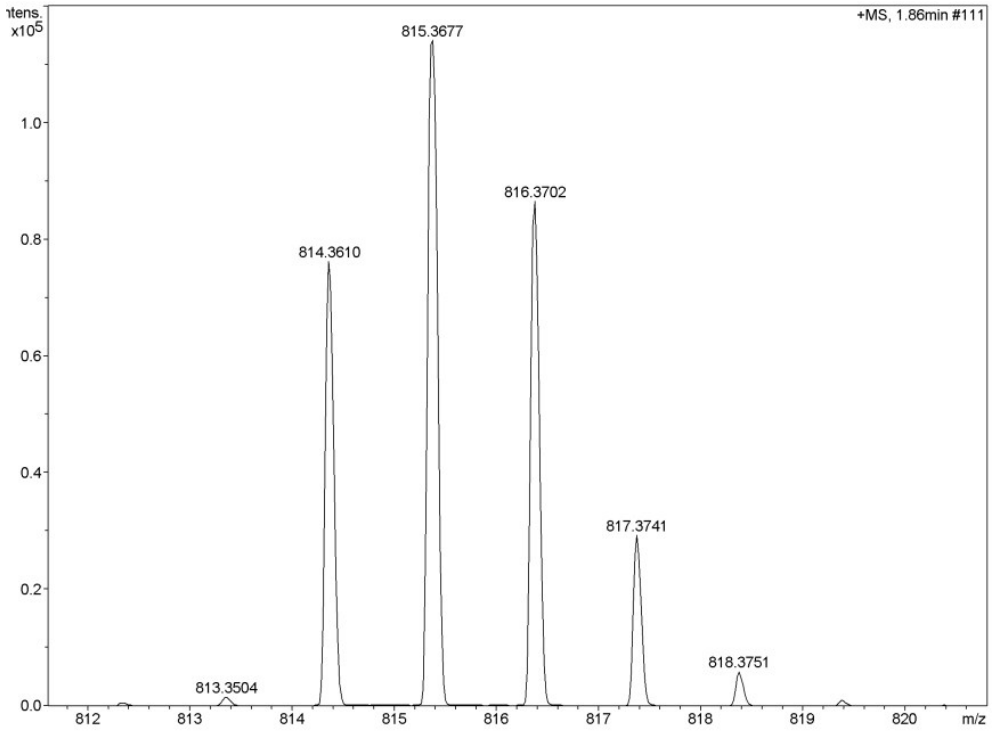


Figure S57. HR (APCI) mass spectrum of compound **NBF-Mes**.

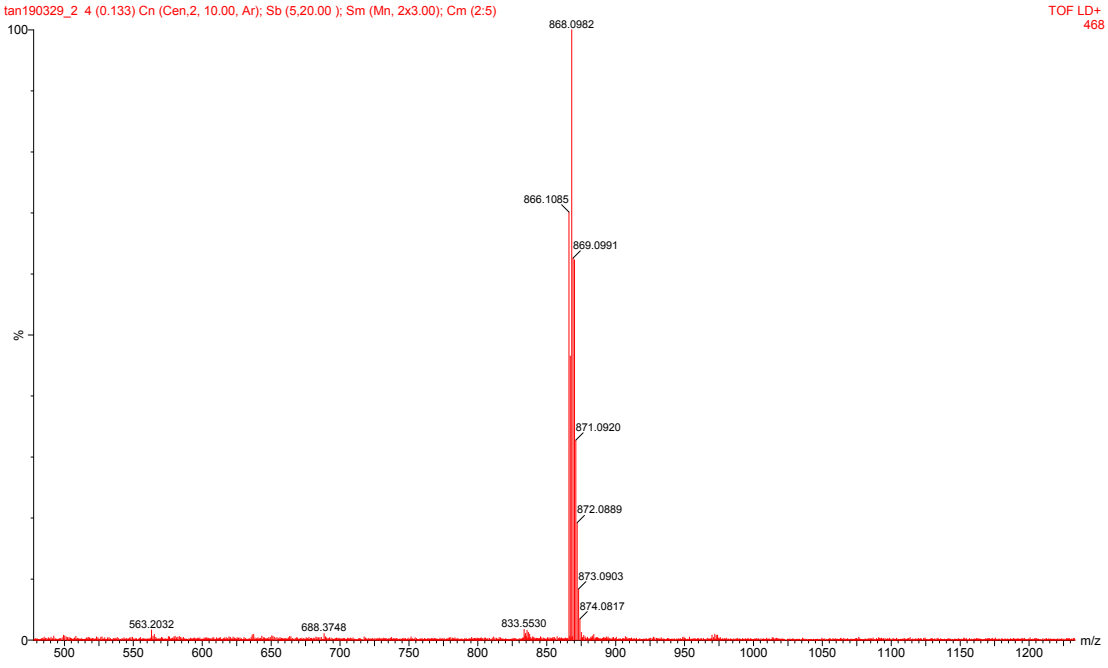


Figure S58. HR (MALDI-TOF) mass spectrum of compound **NBF-DCP**.

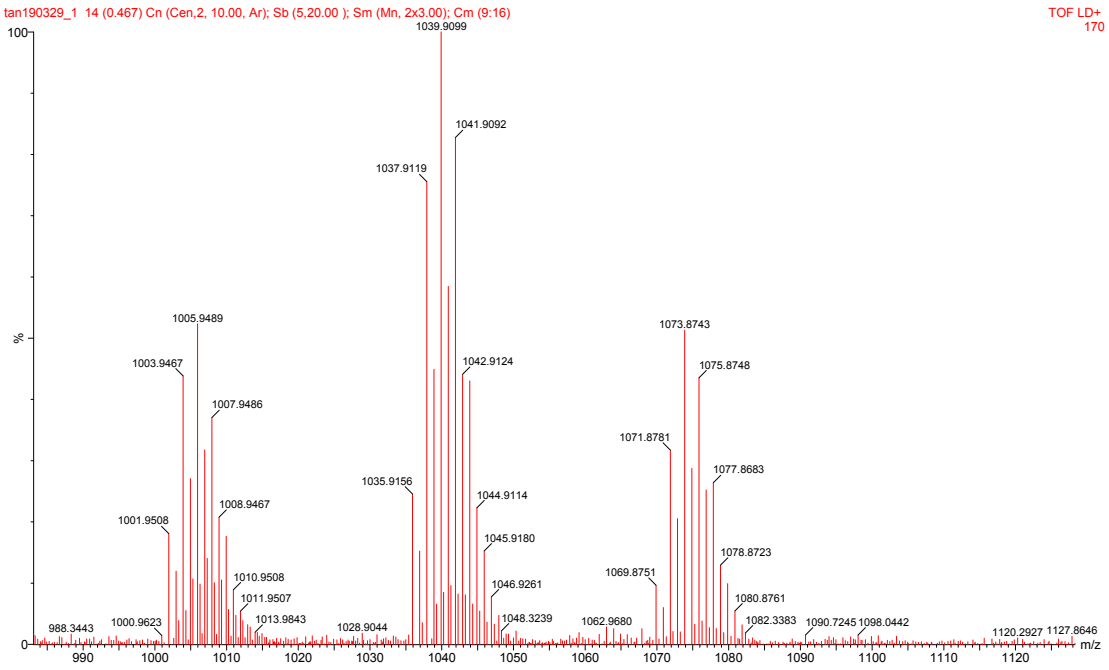


Figure S59. HR (MALDI-TOF) mass spectrum of compound **NBF-PCP**.

Computational results

Cartesian coordinates for optimized geometry A1 in the proposed radical cation mechanism (path A).

C	-0.02228600	0.13821300	-1.75512300
C	-0.65555300	-0.78396900	-0.83790200
C	0.10631100	-0.26837500	0.27350900
C	0.75666100	0.70897900	-0.57057300
C	-0.02650600	0.28770300	-3.13135100
C	1.58500000	1.79211500	-0.32794200
C	-1.13038300	-0.03441000	-4.05660200
C	-0.70449400	0.24696800	-5.38155700
C	0.68900900	0.70656700	-5.32818100

C	1.08761300	0.75961900	-3.96477000
C	2.56253100	1.93283300	0.76834900
C	3.17132100	3.21163400	0.66809300
C	2.56126800	3.92292400	-0.46248200
C	1.62531900	3.05127200	-1.08312300
C	3.02150700	1.01707600	1.72026000
C	4.04138900	1.40208200	2.59566000
C	4.61414800	2.67348300	2.51054900
C	4.18822500	3.58631200	1.53537000
C	2.73453600	5.22024300	-0.92115000
C	1.95879500	5.66500300	-2.00323500
C	1.01122200	4.82746800	-2.59597000
C	0.83178700	3.51922900	-2.13833600
C	-2.45435900	-0.41598400	-3.81863800
C	-3.32336800	-0.56492300	-4.90364300
C	-2.88808500	-0.31553900	-6.20749300
C	-1.57341900	0.10369800	-6.45467200
C	1.58358700	1.01750800	-6.34147200
C	2.89743000	1.37306500	-5.99897100
C	3.30823200	1.39222900	-4.66414000
C	2.41148400	1.08030500	-3.63861500
C	-1.60604800	-1.88993100	-0.95362000
C	-1.31829000	-2.99255500	-1.80581100

C	-2.22986400	-4.04628500	-1.86235800
C	-3.42917100	-4.04117700	-1.14067100
C	-3.69572300	-2.94046100	-0.32084500
C	-2.80762600	-1.87129900	-0.19578800
C	-3.18863500	-0.71118600	0.69653300
C	-0.04625400	-3.09556300	-2.61645800
C	-4.41030500	-5.17863300	-1.26315600
C	0.09620300	-0.57769300	1.70355100
C	-0.26751000	0.42036700	2.64841000
C	-0.29988600	0.07797000	4.00071700
C	0.03988500	-1.19861500	4.46007500
C	0.41440300	-2.15797700	3.51279900
C	0.43390000	-1.88612600	2.14515800
C	0.87535600	-2.97342100	1.19135100
C	-0.65975800	1.82593500	2.25326200
C	-0.02077100	-1.53835000	5.92708100
H	2.60190200	0.02136200	1.79064100
H	4.39570500	0.70072400	3.34395400
H	5.40812000	2.95301300	3.19585300
H	4.65828100	4.56179200	1.45729100
H	3.44429800	5.89090500	-0.44680800
H	2.08686200	6.67778400	-2.37222000
H	0.40624400	5.19446300	-3.41839100

H	0.08038400	2.88921900	-2.59628600
H	-2.81492900	-0.59782800	-2.81407400
H	-4.34951900	-0.87063100	-4.72763300
H	-3.57827700	-0.43233800	-7.03705700
H	-1.25110500	0.32278200	-7.46794900
H	1.28464500	0.97372900	-7.38416800
H	3.60617700	1.62011200	-6.78314200
H	4.33322800	1.64974200	-4.41884100
H	2.75055000	1.08162500	-2.61075400
H	-1.99338400	-4.90281100	-2.48862100
H	-4.62615900	-2.91136700	0.24007700
H	-2.67725800	-0.76128700	1.66282600
H	-2.94482000	0.25563300	0.24581400
H	-4.26305300	-0.72076100	0.89397200
H	0.81455700	-2.65471900	-2.10786600
H	0.18738300	-4.14293600	-2.82167800
H	-0.14952300	-2.58975200	-3.58231000
H	-3.89740100	-6.14287500	-1.32381800
H	-5.09934400	-5.20816900	-0.41552100
H	-5.01241200	-5.07595500	-2.17418800
H	-0.60289200	0.83510500	4.71948500
H	0.70371900	-3.14999800	3.84973300
H	1.37339600	-3.77847900	1.73628600

H	0.02534200	-3.41290600	0.66061900
H	1.57710400	-2.60186200	0.43786400
H	0.21783700	2.47808700	2.18923300
H	-1.16768500	1.86701500	1.28687500
H	-1.32982800	2.25595700	3.00157900
H	0.16340000	-0.65960400	6.55084200
H	-1.01183000	-1.92556800	6.19391800
H	0.70965900	-2.30792900	6.19078200

Cartesian coordinates for optimized structural geometry relative to transition state TS1 in the proposed radical cation mechanism (Path A).

C	1.57933900	0.42393600	-1.39684500
C	0.46730700	-0.01771100	-2.10762400
C	-0.35676800	-0.49829200	-0.95592500
C	0.18193900	0.00440300	0.19022900
C	1.58780800	1.35154400	-0.36787800
C	0.98292000	2.73078300	-0.51037800
C	1.67029600	3.60391200	0.35961300
C	2.71438900	2.84911900	1.07105800
C	2.68257600	1.50850400	0.63259300
C	-0.03431500	3.19142300	-1.33688500
C	-0.38770200	4.54452800	-1.27058700
C	0.28017800	5.41239400	-0.40128700
C	1.31707300	4.95022300	0.41608400

C	3.66313700	3.25828000	2.00451400
C	4.57760100	2.31717400	2.48993900
C	4.55146600	0.99183800	2.04377100
C	3.60038200	0.57688600	1.10557300
C	0.33128400	-0.02918400	-3.49958000
C	1.45279500	0.20673900	-4.41705600
C	0.96339400	0.17517300	-5.74830400
C	-0.48458100	-0.06462700	-5.69265700
C	-0.86803500	-0.19248900	-4.32614600
C	-1.42717700	-0.14559400	-6.70616700
C	-2.77362400	-0.34500700	-6.36543700
C	-3.16257100	-0.44758100	-5.02776600
C	-2.21882600	-0.36537800	-3.99947300
C	2.81533600	0.40216300	-4.17328700
C	3.67629200	0.59722100	-5.25786200
C	3.18545700	0.57748000	-6.56637500
C	1.82242000	0.36112900	-6.82149000
C	-1.44776000	-1.51276000	-0.99363700
C	-1.22287500	-2.77339600	-1.60980600
C	-2.25613800	-3.71286100	-1.61199500
C	-3.50932500	-3.45399900	-1.04931900
C	-3.71446900	-2.19875100	-0.47415200
C	-2.71381900	-1.22348100	-0.42568000

C	-3.05177400	0.10708300	0.20746100
C	0.07342100	-3.15592900	-2.29434500
C	-4.59486400	-4.50162000	-1.05275900
C	0.22746900	-0.29894200	1.59103500
C	0.77722200	-1.55239600	2.02114400
C	0.81581200	-1.83993200	3.37925200
C	0.32929800	-0.94818800	4.34656500
C	-0.19603300	0.27197100	3.91392700
C	-0.24298600	0.63085000	2.56750500
C	-0.81756100	1.98403700	2.22485300
C	1.30066100	-2.57672900	1.04787100
C	0.36022400	-1.31071300	5.80795600
H	-0.54863600	2.52736500	-2.02522400
H	-1.18183900	4.92284200	-1.90694900
H	-0.00262900	6.46033700	-0.36694900
H	1.84034800	5.63545000	1.07697600
H	3.70537200	4.28887200	2.34506700
H	5.32433900	2.62292900	3.21693000
H	5.27798200	0.28045100	2.42455800
H	3.59066400	-0.44947900	0.75103400
H	-1.13619400	-0.04919500	-7.74821800
H	-3.52098700	-0.40920600	-7.15082200
H	-4.20991100	-0.58932400	-4.77952500

H	-2.54452300	-0.44058300	-2.97025200
H	3.21199700	0.39011800	-3.16111300
H	4.73553500	0.75559600	-5.08090700
H	3.86823500	0.72390000	-7.39811900
H	1.45551100	0.34066100	-7.84368500
H	-2.07460100	-4.67938400	-2.07689100
H	-4.68722000	-1.96399900	-0.04816200
H	-4.13283900	0.27259200	0.18687500
H	-2.73889800	0.14213000	1.25704000
H	-2.57433000	0.94818000	-0.30413700
H	0.95736200	-2.71584800	-1.82814100
H	0.19931900	-4.24262700	-2.28218200
H	0.06975900	-2.84470600	-3.34597400
H	-4.45641800	-5.21042600	-0.22595300
H	-5.58614300	-4.05325000	-0.93635200
H	-4.58845800	-5.08306900	-1.98058200
H	1.23688300	-2.78944700	3.70081000
H	-0.57825500	0.97339700	4.65183800
H	-1.73966800	2.15782700	2.79006100
H	-0.11773500	2.77943900	2.50406700
H	-1.03925300	2.09999800	1.16481400
H	1.92724800	-2.13162700	0.26794900
H	1.89528600	-3.33231500	1.56813700

H	0.47498500	-3.09375700	0.54597300
H	-0.42799200	-2.03838000	6.04168800
H	1.31426300	-1.77304900	6.08326100
H	0.20335000	-0.43604300	6.44521400

Cartesian coordinates for optimized geometry A2 in the proposed cation mechanism (Path A).

C	-0.94207200	0.48404900	1.46620800
C	-0.96654400	-0.86071100	1.15410700
C	-0.82705100	-0.92846800	-0.34061900
C	-0.55556900	0.33662700	-0.81989000
C	-0.41396800	1.32386400	0.37527000
C	0.99450600	1.62413700	0.95870200
C	1.11317600	3.00928800	1.19998400
C	-0.11293800	3.68103100	0.76862400
C	-1.01534600	2.71988500	0.26835900
C	2.01894600	0.74100500	1.28561900
C	3.19859000	1.25945800	1.82449200
C	3.33152400	2.63484200	2.05281900
C	2.29353100	3.51674200	1.74665500
C	-0.46541400	5.03192200	0.79729600
C	-1.72280300	5.40753100	0.32519900
C	-2.61954700	4.44944000	-0.16233300
C	-2.27443100	3.09528300	-0.18696500
C	-1.00228200	-1.83214100	2.18570400

C	-1.59595700	-1.58361800	3.50091300
C	-1.36578600	-2.71586500	4.32627900
C	-0.62245800	-3.70774500	3.52945500
C	-0.42217400	-3.16783300	2.22470100
C	-0.12953200	-4.95478300	3.86211000
C	0.58052600	-5.68138600	2.88705600
C	0.79792100	-5.15502100	1.61380500
C	0.30706200	-3.89022700	1.27214900
C	-2.33609800	-0.49812000	3.97965000
C	-2.78682300	-0.52236100	5.30462600
C	-2.53657700	-1.62909800	6.11650200
C	-1.82786300	-2.74422600	5.62908700
C	-1.08596900	-2.16027200	-1.13478500
C	-2.30241500	-2.87613000	-0.96742000
C	-2.53264500	-4.02065800	-1.73546700
C	-1.59999600	-4.50498200	-2.65541300
C	-0.39649100	-3.80879300	-2.78201700
C	-0.11685300	-2.65105000	-2.04927800
C	1.23429900	-2.00439500	-2.24989800
C	-3.38147800	-2.46376800	0.01016000
C	-1.88943600	-5.72558100	-3.49286900
C	-0.60510200	0.80729400	-2.22732900
C	-1.80932000	0.69928700	-2.97710500

C	-1.84005000	1.15844700	-4.29715600
C	-0.72736400	1.71923900	-4.92225900
C	0.44387100	1.83652500	-4.16848100
C	0.52777000	1.41515400	-2.84148600
C	1.84769300	1.61817200	-2.13448600
C	-3.09880800	0.13841400	-2.42438800
C	-0.77677600	2.17262300	-6.35904500
H	1.91388800	-0.32698700	1.12027300
H	4.01647000	0.59048000	2.07161300
H	4.25351400	3.01975700	2.47696000
H	2.40548000	4.58042900	1.93221900
H	0.22289700	5.77857000	1.18107300
H	-2.01039500	6.45408700	0.33667400
H	-3.59287900	4.76089100	-0.52769500
H	-2.97776900	2.36237800	-0.56591500
H	-0.27494600	-5.37157600	4.85358000
H	0.97185900	-6.66286600	3.13600300
H	1.35431400	-5.72835700	0.88023600
H	0.48247900	-3.49384500	0.28177400
H	-2.56716300	0.34546500	3.33835400
H	-3.35210100	0.31692200	5.69506000
H	-2.90759000	-1.63993000	7.13652300
H	-1.65733600	-3.60324300	6.27020500

H	-3.47405200	-4.54963900	-1.60864600
H	0.35689500	-4.17750800	-3.47384800
H	1.95412100	-2.73767900	-2.62222500
H	1.18365100	-1.19251900	-2.98167700
H	1.63345100	-1.57894500	-1.32532200
H	-3.47737300	-1.38099900	0.11054500
H	-4.35058800	-2.85523100	-0.30876500
H	-3.19178000	-2.86732600	1.01256900
H	-2.55918400	-6.41799700	-2.97552900
H	-2.37569100	-5.44481700	-4.43502100
H	-0.97213100	-6.26262900	-3.74954400
H	-2.77285100	1.07954700	-4.85001700
H	1.32516800	2.27719000	-4.62786000
H	2.65055700	1.74505100	-2.86479900
H	1.83426800	2.51789200	-1.51136500
H	2.11421400	0.78152800	-1.48709300
H	-3.19488100	0.28061200	-1.34669000
H	-3.95496600	0.62106700	-2.90316600
H	-3.18030000	-0.93593600	-2.61715800
H	-1.80163400	2.37388300	-6.68137900
H	-0.18414400	3.07917800	-6.51264700
H	-0.36814800	1.40267700	-7.02494400

Cartesian coordinates for optimized structural geometry relative to TS2 in the proposed radical cation mechanism (Path A).

C	-0.86599300	0.60019600	1.35955500
C	-0.90893900	-0.79257100	1.07247200
C	-0.88588500	-0.90160100	-0.41311600
C	-0.65019500	0.34965500	-0.95716900
C	-0.50823600	1.35450900	0.17312000
C	0.77173900	1.45978700	1.09483400
C	0.85916500	2.81546500	1.55042700
C	-0.21668100	3.60262800	0.97206000
C	-0.99183900	2.78371300	0.12292100
C	1.81607600	0.54704000	1.35252300
C	2.88978800	0.96145500	2.12503300
C	2.94066200	2.27420800	2.63015600
C	1.93916100	3.20209900	2.34459400
C	-0.53520500	4.95515300	1.14084900
C	-1.62537500	5.47612400	0.44831500
C	-2.39213100	4.65828800	-0.39257700
C	-2.09079600	3.30180100	-0.55221700
C	-0.87223700	-1.72843000	2.12075300
C	-1.28871400	-1.40028500	3.49502900
C	-1.04650100	-2.52282900	4.32787900
C	-0.46942700	-3.58744200	3.49486300

C	-0.38256900	-3.11177800	2.15497800
C	-0.02414200	-4.85325500	3.83479400
C	0.52746600	-5.66758400	2.83164100
C	0.64076000	-5.20432500	1.52049600
C	0.19657500	-3.92402200	1.17279700
C	-1.90249600	-0.25980600	4.02425400
C	-2.20345200	-0.22221100	5.39054400
C	-1.93544700	-1.32229000	6.20686700
C	-1.36103800	-2.49014900	5.67619300
C	-1.16009600	-2.15388700	-1.17137300
C	-2.37555500	-2.85550700	-0.96026800
C	-2.62307100	-4.02308700	-1.68778800
C	-1.70980700	-4.53715200	-2.61163000
C	-0.50904800	-3.84618000	-2.78723300
C	-0.21290000	-2.66803300	-2.09358000
C	1.13643400	-2.02871800	-2.33511300
C	-3.43298500	-2.40142900	0.02366200
C	-2.01799800	-5.78455600	-3.40340100
C	-0.68999200	0.78146000	-2.37355100
C	-1.85001400	0.60680400	-3.17395500
C	-1.82590500	1.02518900	-4.50856000
C	-0.70284400	1.61289500	-5.09076500
C	0.41824100	1.81488700	-4.27781500

C	0.44342600	1.43422900	-2.93720700
C	1.69306700	1.72458900	-2.13727700
C	-3.14649100	0.03562100	-2.64777100
C	-0.69120000	2.01709400	-6.54378500
H	1.75684000	-0.47179800	0.98486200
H	3.69522400	0.26821200	2.34512600
H	3.78793200	2.57593800	3.23896700
H	2.01952200	4.22190000	2.70845600
H	0.05703000	5.59016500	1.79333800
H	-1.88231700	6.52529800	0.55754300
H	-3.23236900	5.08411000	-0.93289200
H	-2.69264200	2.68123500	-1.20669400
H	-0.08895000	-5.21412000	4.85710900
H	0.87861900	-6.66381400	3.08432600
H	1.07850100	-5.84063000	0.75777200
H	0.29594400	-3.58650200	0.15113900
H	-2.15504000	0.58242800	3.38910500
H	-2.67032400	0.66243200	5.81204000
H	-2.19100200	-1.28464000	7.26176500
H	-1.17717300	-3.34733800	6.31730900
H	-3.56297100	-4.54646100	-1.52591800
H	0.22827100	-4.23626100	-3.48557600
H	1.83853700	-2.76392100	-2.73926900

H	1.07143600	-1.20590400	-3.05504300
H	1.57192400	-1.61982800	-1.41731700
H	-3.51812400	-1.31314200	0.08325000
H	-4.41169700	-2.79830100	-0.26153800
H	-3.22329100	-2.76576900	1.03739300
H	-2.65114600	-6.47442800	-2.83628600
H	-2.55399100	-5.53830300	-4.32937500
H	-1.10412000	-6.31490400	-3.68932000
H	-2.72408500	0.89461600	-5.10810100
H	1.29981200	2.29106200	-4.70115400
H	2.51415600	2.00840100	-2.80146500
H	1.53994300	2.55765000	-1.44078600
H	2.02349200	0.86318500	-1.54843900
H	-3.31006300	0.27441900	-1.59300800
H	-3.99255300	0.43345400	-3.21648900
H	-3.17437400	-1.05515300	-2.73988200
H	-0.19702600	1.25273500	-7.15790400
H	-1.70545400	2.14464600	-6.93397100
H	-0.14502100	2.95416300	-6.69533400

Cartesian coordinates for optimized geometry A3 in the proposed radical cation mechanism (Path A).

C	0.56477600	1.15035200	0.99640100
C	0.33823600	-0.27957700	0.79707500

C	0.04024100	-0.43761600	-0.62248600
C	-0.01379100	0.85816600	-1.22828400
C	0.23638800	1.83410700	-0.22194900
C	1.25710000	1.84400800	2.03348600
C	1.29398500	3.28012600	1.98362700
C	0.63991900	3.99812300	0.88392900
C	0.17507700	3.27689000	-0.25864700
C	1.97313400	1.17068600	3.06143300
C	2.65719500	1.86929600	4.03437600
C	2.65372900	3.27314900	4.00967100
C	1.99427100	3.95725700	2.99569900
C	0.48074000	5.39482200	0.90382100
C	-0.09414300	6.07457300	-0.16278500
C	-0.53300500	5.36932800	-1.28859300
C	-0.40040000	3.99035600	-1.33495700
C	0.26985600	-1.26877200	1.78779700
C	-0.31347100	-1.09499400	3.13384400
C	-0.28483000	-2.34305700	3.80832900
C	0.37591200	-3.32041200	2.93104000
C	0.68124700	-2.67605900	1.70151500
C	0.74551500	-4.63679700	3.15728000
C	1.44359800	-5.32258800	2.15115500
C	1.78960400	-4.68402300	0.95825000

C	1.42633300	-3.35378800	0.73117100
C	-0.98497300	-0.01052500	3.70777900
C	-1.56153600	-0.15995000	4.97229000
C	-1.49422400	-1.38233300	5.64550600
C	-0.86545100	-2.49074700	5.05937400
C	-0.38375000	-1.68235500	-1.30272200
C	-1.58819500	-2.33177400	-0.91192500
C	-1.99386600	-3.47492700	-1.60311800
C	-1.24895600	-4.02283400	-2.65099600
C	-0.05442400	-3.38617100	-3.00095800
C	0.38824300	-2.22764600	-2.36280900
C	1.71950100	-1.64806600	-2.78503600
C	-2.48405200	-1.83172100	0.20096300
C	-1.72764300	-5.24581100	-3.39038500
C	-0.25054200	1.13539500	-2.67318900
C	-1.52419300	0.97358400	-3.26302900
C	-1.68001800	1.24450700	-4.62752800
C	-0.62036300	1.66783300	-5.43003300
C	0.62512900	1.85340500	-4.81911400
C	0.83165600	1.61266300	-3.45989600
C	2.19507100	1.90699400	-2.87269600
C	-2.74547400	0.57018900	-2.46886300
C	-0.80422300	1.91445200	-6.90688100

H	2.00921400	0.09010100	3.05821600
H	3.21089900	1.33680300	4.80025700
H	3.19381300	3.83129600	4.76786000
H	2.05930300	5.03795600	2.97917000
H	0.79312200	5.96516100	1.76995400
H	-0.20617800	7.15295700	-0.11494700
H	-0.98989900	5.89560400	-2.12020900
H	-0.76617800	3.44945000	-2.19660800
H	0.51953600	-5.12852700	4.09825500
H	1.73846700	-6.35462100	2.31339400
H	2.35428500	-5.22095300	0.20339500
H	1.72726500	-2.86377300	-0.18440800
H	-1.06649300	0.93717500	3.18911600
H	-2.07302400	0.68013700	5.43031800
H	-1.95135300	-1.48221800	6.62494700
H	-0.85320400	-3.44703100	5.57289200
H	-2.92724900	-3.95124500	-1.31302900
H	0.55925300	-3.80983700	-3.79211000
H	2.36647300	-2.43269300	-3.18641900
H	1.59429500	-0.89570400	-3.56903900
H	2.24941900	-1.17169500	-1.95557800
H	-2.41899100	-0.75284100	0.35005200
H	-3.52700800	-2.07657000	-0.01627900

H	-2.23636400	-2.30995800	1.15492600
H	-2.30443500	-5.90856600	-2.73929100
H	-2.37971300	-4.96325200	-4.22605600
H	-0.89267800	-5.81444400	-3.80852800
H	-2.66646500	1.12748500	-5.06958500
H	1.46197000	2.20514900	-5.41781100
H	2.95541900	1.92549000	-3.65720500
H	2.20884300	2.88793200	-2.38366700
H	2.50158600	1.17161000	-2.12525200
H	-2.67944500	0.88390900	-1.42395400
H	-3.64369600	1.02404900	-2.89613400
H	-2.89123200	-0.51456500	-2.48062600
H	-0.45767500	1.05444800	-7.49259800
H	-1.85507000	2.07979200	-7.15812200
H	-0.23135800	2.78420500	-7.24200800

Cartesian coordinates for optimized geometry B1 in the proposed cation mechanism (Path B).

C	-0.90292900	0.29498600	0.68823300
C	-0.89868200	-1.22945000	0.85805400
C	-0.88581200	-1.39585900	-0.60333000
C	-0.78503100	-0.05266400	-0.86715900
C	0.18763700	1.15832300	1.13837900
C	1.51236900	0.82891400	1.62763300
C	2.21861000	2.04601300	1.87354200

C	1.32262600	3.16779200	1.52433100
C	0.09506600	2.60335000	1.07815600
C	2.12599100	-0.40446700	1.88818400
C	3.44200800	-0.41586600	2.36416300
C	4.12074600	0.77899800	2.60040400
C	3.50917300	2.02784800	2.35899900
C	1.48995700	4.53675500	1.56111200
C	0.41955400	5.35556100	1.13870600
C	-0.78317800	4.80967100	0.69005500
C	-0.95892100	3.42097600	0.65629600
C	-0.91326500	-1.99796300	1.98281700
C	-0.75663500	-3.46898200	2.09805900
C	-0.86043400	-3.82895700	3.46556900
C	-1.08461100	-2.61242000	4.25339000
C	-1.09293500	-1.50261700	3.37254500
C	-1.27344900	-2.44489100	5.62190300
C	-1.47486200	-1.15632900	6.12391300
C	-1.49175600	-0.05515800	5.26267800
C	-1.30369500	-0.22125200	3.88808700
C	-0.47175400	-4.45135100	1.14573700
C	-0.33037500	-5.77996100	1.55858700
C	-0.45878300	-6.12977600	2.90513900
C	-0.71798800	-5.15147500	3.87088200

H	-1.87607500	0.75271900	0.89372900
C	-1.15394000	-2.52846700	-1.52040300
C	-0.19942000	-2.92604200	-2.48640400
C	-0.50545300	-3.98333600	-3.34721300
C	-1.73351100	-4.64777300	-3.30240800
C	-2.66345400	-4.23825200	-2.34114600
C	-2.40208900	-3.20104300	-1.44427600
C	-3.45067800	-2.86063500	-0.40868500
C	1.14966100	-2.25835400	-2.60575800
C	-2.05714900	-5.75684100	-4.27181500
C	-0.81679400	0.83467800	-2.03895200
C	-2.07401400	1.11433300	-2.64447800
C	-2.11882700	1.94653100	-3.76153100
C	-0.96566700	2.51949900	-4.31104600
C	0.25664200	2.24648900	-3.69416800
C	0.35754700	1.42524200	-2.56738500
C	1.72307300	1.22890600	-1.94882400
C	-3.35701600	0.50568100	-2.13078900
C	-1.04405600	3.38436400	-5.54363700
H	1.59545100	-1.33497500	1.73323400
H	3.93055800	-1.36292700	2.56548600
H	5.13585900	0.75182100	2.98403600
H	4.05302200	2.94604200	2.55670700

H	2.41606800	4.98819600	1.90227100
H	0.53865800	6.43424800	1.16405900
H	-1.58601600	5.46368700	0.36808200
H	-1.89370900	2.99879800	0.30337000
H	-1.27020700	-3.29919500	6.29195700
H	-1.62299300	-1.00947100	7.18917400
H	-1.65437500	0.94008500	5.66420900
H	-1.33017100	0.65400500	3.24930400
H	-0.35962900	-4.20393700	0.09816700
H	-0.11625200	-6.54647300	0.82062800
H	-0.34706500	-7.16673200	3.20633200
H	-0.79718400	-5.42436500	4.91885100
H	0.23931200	-4.29463000	-4.07530100
H	-3.62268400	-4.74660300	-2.28266100
H	-3.20356500	-3.30345700	0.56225300
H	-3.55737400	-1.78429300	-0.25539500
H	-4.42471200	-3.25422000	-0.70896500
H	1.60843400	-2.08302400	-1.62808000
H	1.83460800	-2.87679600	-3.19068600
H	1.06946400	-1.28964500	-3.10986700
H	-1.15055800	-6.23454700	-4.65262100
H	-2.68100800	-6.52586500	-3.80727200
H	-2.61062100	-5.36956300	-5.13600600

H	-3.08241100	2.14973400	-4.22214400
H	1.16433900	2.68649000	-4.10018200
H	2.49159300	1.16476400	-2.72441200
H	1.98774400	2.07954900	-1.31040900
H	1.78293800	0.32604300	-1.34047100
H	-3.47081200	0.62307800	-1.04730600
H	-4.22313400	0.97089700	-2.60678500
H	-3.39709800	-0.56751300	-2.34365300
H	-1.93366400	4.02102300	-5.52997500
H	-0.16428700	4.02533600	-5.64223200
H	-1.10401300	2.76658500	-6.44782600

Cartesian coordinates for optimized structural geometry relative to transition state TS3 in the proposed cation mechanism (Path B).

C	-1.11043400	0.32637200	0.90580500
C	-1.07798900	-1.17495200	1.01968500
C	-0.78944400	-1.26298400	-0.39626400
C	-0.58623200	0.14224800	-0.62570600
C	0.17787500	0.96119800	0.81347400
C	1.51951100	0.50636500	1.31253700
C	2.30590100	1.66039900	1.54511400
C	1.52614800	2.85574600	1.19506100
C	0.26138800	2.44709300	0.72227800
C	2.05646200	-0.75813600	1.55637400

C	3.36382100	-0.86029200	2.04340100
C	4.13015500	0.28275300	2.28528200
C	3.60371200	1.55294000	2.03664300
C	1.84065100	4.20816400	1.28539000
C	0.88240600	5.14986500	0.89262400
C	-0.37234600	4.74489900	0.42792100
C	-0.69556700	3.38620600	0.34441600
C	-1.14944500	-1.98356800	2.12017900
C	-0.85523300	-3.42728200	2.24524600
C	-1.04073600	-3.80679400	3.60014900
C	-1.45627900	-2.62141700	4.36407600
C	-1.50883500	-1.51865900	3.47607600
C	-1.75666800	-2.46712100	5.71034500
C	-2.11158200	-1.19514700	6.18049000
C	-2.16628100	-0.10238900	5.31203100
C	-1.87389700	-0.25764700	3.95298100
C	-0.38658400	-4.36411100	1.32015800
C	-0.13967600	-5.67456400	1.74359500
C	-0.34934100	-6.04550800	3.07371800
C	-0.79612500	-5.10862100	4.01531800
H	-2.01187800	0.91132700	1.06128800
C	-0.97923100	-2.33310500	-1.37847400
C	0.01011000	-2.56927700	-2.37562300

C	-0.19810500	-3.58456900	-3.30911800
C	-1.36490500	-4.35207600	-3.33154600
C	-2.32963900	-4.10214500	-2.34847700
C	-2.16557700	-3.13188500	-1.36158100
C	-3.27782200	-2.99199200	-0.34352500
C	1.31454000	-1.81203300	-2.43990100
C	-1.58939900	-5.40410900	-4.38658000
C	-0.79701300	0.95136800	-1.85704900
C	-2.11617200	1.07575400	-2.38192400
C	-2.32691000	1.83879400	-3.53015500
C	-1.28233200	2.47464300	-4.20885200
C	0.00195300	2.33639200	-3.68704500
C	0.27033200	1.60087300	-2.52645800
C	1.71302500	1.57145200	-2.06979200
C	-3.31995700	0.40030400	-1.76460600
C	-1.54093700	3.26241600	-5.46912700
H	1.48892900	-1.66276000	1.37832400
H	3.78333200	-1.84296300	2.23631500
H	5.14239200	0.18391400	2.66593100
H	4.20093400	2.44060400	2.22418500
H	2.80685300	4.53377500	1.65972800
H	1.11546300	6.20876900	0.95495800
H	-1.10341300	5.48931800	0.12815300

H	-1.66902600	3.08653000	-0.03123900
H	-1.71858800	-3.31103400	6.39305200
H	-2.34974700	-1.05939200	7.23130100
H	-2.44515700	0.87562900	5.69177800
H	-1.93726900	0.60460800	3.29874600
H	-0.21394700	-4.09617500	0.28486200
H	0.21933200	-6.40818100	1.02830000
H	-0.15491500	-7.06760400	3.38527600
H	-0.93665800	-5.40036000	5.05208600
H	0.57972500	-3.78130800	-4.04300700
H	-3.24443900	-4.68996200	-2.34835300
H	-3.06354800	-3.58116000	0.55531000
H	-3.44946000	-1.96281300	-0.02434800
H	-4.21395200	-3.37176500	-0.76238900
H	2.08491300	-2.42618800	-2.91527600
H	1.20623300	-0.90349100	-3.04125300
H	1.68487800	-1.51763700	-1.45492600
H	-2.19154700	-5.00083500	-5.21149400
H	-0.64499200	-5.75546200	-4.81238700
H	-2.13034300	-6.26685900	-3.98458100
H	-3.34126900	1.93544100	-3.91072300
H	0.83348700	2.82348700	-4.19201100
H	2.37428600	1.36254600	-2.91795400

H	2.00787300	2.54841600	-1.67110000
H	1.91214600	0.82570000	-1.30197100
H	-3.33732400	-0.66953200	-1.99906600
H	-3.35944100	0.49663800	-0.67458900
H	-4.24298600	0.83226700	-2.16074200
H	-0.71189800	3.93856800	-5.69785900
H	-1.66816900	2.59318800	-6.32986700
H	-2.45617600	3.85849800	-5.38728600

Cartesian coordinates for optimized geometry B2 in the proposed cation mechanism (Path B).

C	-1.41516500	0.58439500	0.56139000
C	-1.23762900	-0.87617500	0.83716400
C	-0.86011500	-1.06083700	-0.53914900
C	-0.68568900	0.34855700	-0.91856300
C	-0.13896000	1.25667000	0.29185100
C	1.17809000	0.99356800	0.99732800
C	1.76637300	2.23880800	1.30912500
C	0.91009300	3.32097700	0.80857500
C	-0.20379400	2.76093600	0.15348300
C	1.83919300	-0.18905800	1.31910200
C	3.07203200	-0.12189300	1.97820400
C	3.64072400	1.11106700	2.30677400
C	2.99281100	2.30032500	1.96995300
C	1.05256400	4.70537600	0.89799100

C	0.07324400	5.52257700	0.32886300
C	-1.03547100	4.96423700	-0.31416300
C	-1.18534700	3.57591400	-0.40183300
C	-1.27782200	-1.58173900	2.00814700
C	-0.82675000	-2.96013500	2.28986000
C	-1.03522900	-3.22474800	3.66868000
C	-1.62400000	-2.02838500	4.28931200
C	-1.76201800	-1.03451400	3.28851900
C	-2.00584400	-1.77553000	5.59890300
C	-2.52802100	-0.51350300	5.91683000
C	-2.66659000	0.47150000	4.93658900
C	-2.29434800	0.21544400	3.61282700
C	-0.21554500	-3.92249900	1.48192300
C	0.15763200	-5.14668000	2.04665300
C	-0.06960400	-5.40653800	3.39988800
C	-0.66458100	-4.44176600	4.22381000
H	-2.35673300	1.11992500	0.59232200
C	-0.97189600	-2.21647700	-1.42003600
C	0.04938300	-2.46490600	-2.38855200
C	-0.05813700	-3.58488800	-3.21083900
C	-1.15399800	-4.44996300	-3.15928800
C	-2.15064700	-4.18788900	-2.21108200
C	-2.08465400	-3.11532100	-1.32546800

C	-3.22685300	-2.97015700	-0.34366600
C	1.29318100	-1.62118200	-2.52182000
C	-1.27184500	-5.61686600	-4.10248400
C	-0.94105600	0.94000400	-2.26685300
C	-2.22369800	0.83890900	-2.87583600
C	-2.43064900	1.41424700	-4.13069000
C	-1.41569800	2.07089700	-4.83187000
C	-0.16450500	2.15701300	-4.22336300
C	0.09575800	1.62063400	-2.95803500
C	1.49432400	1.82405900	-2.41492700
C	-3.40492300	0.14098700	-2.24015300
C	-1.66511000	2.64698500	-6.20286800
H	1.42574500	-1.16006900	1.07513700
H	3.58933700	-1.04087300	2.23445500
H	4.59746100	1.14439600	2.81830600
H	3.44354700	3.25802100	2.21139400
H	1.90658800	5.14454600	1.40427500
H	0.17255100	6.60180400	0.38870200
H	-1.78743800	5.61205400	-0.75299300
H	-2.04447000	3.15918300	-0.91707100
H	-1.90373400	-2.53382400	6.36885700
H	-2.83157400	-0.30150900	6.93714000
H	-3.07506900	1.44130700	5.20059000

H	-2.42768200	0.99045300	2.86697300
H	-0.02900900	-3.74018300	0.43077400
H	0.62953300	-5.90037100	1.42481900
H	0.22513700	-6.36261800	3.82092900
H	-0.82117000	-4.64537900	5.27848900
H	0.74409300	-3.78803700	-3.91498200
H	-3.01110600	-4.84938800	-2.15796300
H	-2.98507400	-3.44826200	0.61086900
H	-3.48933700	-1.93372700	-0.13173000
H	-4.11639100	-3.46675600	-0.73795600
H	1.63115400	-1.20520100	-1.57139200
H	2.11000300	-2.22076900	-2.93051600
H	1.12282700	-0.78824800	-3.20995100
H	-0.29325200	-5.94321100	-4.46286700
H	-1.76996700	-6.46706300	-3.62850500
H	-1.86888000	-5.33961700	-4.98014400
H	-3.42043300	1.34617700	-4.57518600
H	0.64246200	2.66771900	-4.74304400
H	2.23064100	1.68113900	-3.21134100
H	1.61575900	2.84778700	-2.04683200
H	1.75276100	1.15020100	-1.60025600
H	-3.47838100	0.30823800	-1.16289300
H	-4.33684500	0.49558300	-2.68631700

H	-3.36243300	-0.94077400	-2.40170700
H	-2.66011000	3.09635400	-6.27191500
H	-0.92584200	3.41034600	-6.45803900
H	-1.60987600	1.86540700	-6.97023500

Cartesian coordinates for optimized structural geometry relative to transition state TS4 in the proposed cation mechanism (Path B).

C	-0.79877200	-0.81375600	1.12934700
C	-0.80369100	-0.92148900	-0.35383200
C	-0.72967100	0.34226600	-0.91510900
C	-0.76391100	1.34477900	0.17406100
C	0.58513700	1.53433900	1.20206900
C	0.58040400	2.93072200	1.51814400
C	-0.58951200	3.61297800	0.97309900
C	-1.30636400	2.74144400	0.12926000
C	1.75714700	0.76917100	1.39690900
C	2.87480600	1.36496200	1.95833400
C	2.84057900	2.71876500	2.33648000
C	1.70678300	3.50023200	2.11411700
C	-1.00563700	4.93560900	1.14516900
C	-2.13906800	5.37843700	0.46159900
C	-2.84300100	4.51167600	-0.37953900
C	-2.43864100	3.18021000	-0.54507800
C	-0.71726200	-1.74093900	2.16852700

C	-0.79417400	-1.37291600	3.61234600
C	-1.09937900	-2.54306700	4.35475900
C	-1.02294900	-3.69358800	3.44985600
C	-0.69310500	-3.22474600	2.14914700
C	-1.11849000	-5.04773200	3.73143400
C	-0.82960600	-5.97022600	2.71632200
C	-0.42525100	-5.52604800	1.45784000
C	-0.35230700	-4.15931600	1.16505700
C	-0.59172200	-0.17377500	4.30818000
C	-0.79367900	-0.13300300	5.69341700
C	-1.17754900	-1.27599600	6.39347800
C	-1.31480300	-2.49934300	5.72431000
C	-0.96473800	-2.16629600	-1.15639900
C	-2.19103500	-2.87498600	-1.08417500
C	-2.36196100	-4.01484800	-1.87425800
C	-1.35937400	-4.49348000	-2.72310300
C	-0.15048100	-3.79482400	-2.75850900
C	0.06597500	-2.63759900	-2.00247200
C	1.41682500	-1.96557700	-2.09672800
C	-3.31951800	-2.47545400	-0.15781900
C	-1.58339800	-5.71255200	-3.58447800
C	-0.70633600	0.75056500	-2.35105800
C	-1.82972300	0.55358800	-3.19057500

C	-1.76326800	0.96193800	-4.52810800
C	-0.62928100	1.56143200	-5.07377900
C	0.45616000	1.78392700	-4.22123700
C	0.43708300	1.40873000	-2.87713600
C	1.64785400	1.73454300	-2.03108600
C	-3.13263200	-0.04418100	-2.71116800
C	-0.56962700	1.95375700	-6.52974300
H	1.75855300	-0.29056400	1.16561500
H	3.77223000	0.77807600	2.12517700
H	3.71944400	3.16959800	2.78797600
H	1.72055700	4.55920100	2.35325000
H	-0.45781200	5.61334800	1.79351400
H	-2.47102800	6.40542100	0.57795300
H	-3.71253800	4.87434200	-0.91927800
H	-2.99162800	2.51794100	-1.20155900
H	-1.38623500	-5.39315700	4.72573400
H	-0.89273600	-7.03478900	2.92198300
H	-0.15790800	-6.24458600	0.68935400
H	-0.00857900	-3.85259500	0.18957200
H	-0.22146400	0.71925100	3.82288500
H	-0.63214300	0.79908300	6.22623100
H	-1.33770000	-1.22674800	7.46638900
H	-1.56489200	-3.40018100	6.27705700

H	-3.30820200	-4.54886700	-1.81886600
H	0.65295300	-4.15801900	-3.39565700
H	2.17506800	-2.67497400	-2.44144000
H	1.39879600	-1.13236500	-2.80784400
H	1.74840700	-1.56585800	-1.13285200
H	-3.41502200	-1.39258000	-0.04637900
H	-4.27408000	-2.85924900	-0.52974900
H	-3.17086000	-2.89365400	0.84513200
H	-2.26489300	-6.42344400	-3.10614700
H	-2.02960600	-5.43375500	-4.54807000
H	-0.64365200	-6.23071600	-3.80027200
H	-2.63681600	0.81055400	-5.15864600
H	1.34596800	2.27231200	-4.61261800
H	2.49408800	2.01190800	-2.66607800
H	1.45604900	2.58274900	-1.36239600
H	1.96197000	0.89253900	-1.40758800
H	-3.33342500	0.17871900	-1.65938700
H	-3.96812400	0.34454900	-3.30173100
H	-3.13795500	-1.13406400	-2.81531600
H	-1.57048600	2.09866900	-6.94803600
H	-0.00182200	2.87907600	-6.67325200
H	-0.07551500	1.17527600	-7.12572200
C	-0.88293600	0.62388500	1.41597500

H	-1.40165700	1.02553600	2.27574500

Cartesian coordinates for optimized geometry B3 in the proposed cation mechanism (Path B).

C	0.12091800	-0.25765000	0.88582100
C	-0.07527600	-0.41823800	-0.52195500
C	-0.13933800	0.86928300	-1.16608300
C	-0.02510700	1.85791200	-0.19102600
C	1.21799300	1.90882300	1.96614000
C	1.37315100	3.30616300	1.79706200
C	0.55958700	4.02694000	0.79477600
C	-0.05334500	3.29677100	-0.27152300
C	2.04561300	1.22655500	2.85770700
C	3.01996400	1.90404800	3.59343400
C	3.16907900	3.28147100	3.44481400
C	2.35815600	3.97008500	2.54777800
C	0.43143600	5.42208500	0.79894500
C	-0.24535100	6.08782000	-0.22037500
C	-0.81008600	5.37390400	-1.28381200
C	-0.71021500	3.99111300	-1.31193000
C	0.13428200	-1.24888300	1.87660100
C	-0.39830300	-1.11555100	3.25326200
C	-0.37274300	-2.39721200	3.86843200
C	0.28935600	-3.33599300	2.95322900
C	0.61337200	-2.63613200	1.76257200

C	0.66834600	-4.65637600	3.13383100
C	1.41389300	-5.28634400	2.12443800
C	1.79630100	-4.58631800	0.97848800
C	1.41139100	-3.25480300	0.79581600
C	-0.96602500	-0.03979300	3.94806400
C	-1.48828200	-0.24492200	5.22898500
C	-1.46360000	-1.51140700	5.81483700
C	-0.90423300	-2.60135900	5.13194200
C	-0.40745700	-1.68438600	-1.23340300
C	-1.61929900	-2.35820400	-0.92609900
C	-1.94958400	-3.50961500	-1.64448500
C	-1.12527000	-4.03346100	-2.64425800
C	0.07109000	-3.36576700	-2.91240200
C	0.44340600	-2.19942900	-2.23911500
C	1.78523400	-1.58607500	-2.57569000
C	-2.59336500	-1.88772400	0.13488500
C	-1.52629300	-5.26597100	-3.41660200
C	-0.27028900	1.12480200	-2.63325300
C	-1.50125000	0.94445100	-3.30532200
C	-1.57166200	1.21394400	-4.67572000
C	-0.46612300	1.65372600	-5.40758600
C	0.73092600	1.85814500	-4.71664800
C	0.85114700	1.61947000	-3.34413200

C	2.16917900	1.94915100	-2.67493200
C	-2.76228500	0.50965400	-2.59256900
C	-0.56097500	1.89457900	-6.89475100
H	1.94781300	0.15497300	2.97923900
H	3.66582700	1.35051900	4.26844000
H	3.92823100	3.81633800	4.00735900
H	2.52032900	5.03275500	2.40370600
H	0.85431800	6.00111600	1.61244900
H	-0.33307100	7.16982300	-0.18550400
H	-1.33884500	5.89613000	-2.07492300
H	-1.17364800	3.43172100	-2.11486500
H	0.41816200	-5.19304600	4.04426900
H	1.72037300	-6.32042500	2.25175400
H	2.40638600	-5.07454200	0.22516500
H	1.74713400	-2.71698200	-0.07930300
H	-0.99054400	0.96136800	3.53859600
H	-1.91548700	0.59337000	5.77013700
H	-1.87966500	-1.65545200	6.80750900
H	-0.89189200	-3.58588500	5.59024700
H	-2.88634400	-4.01255000	-1.41399200
H	0.74507900	-3.76635100	-3.66670500
H	2.50508100	-2.36687500	-2.84244500
H	1.71030800	-0.90810200	-3.43215700

H	2.20992800	-1.01597500	-1.74374100
H	-2.62893700	-0.79903700	0.22865000
H	-3.60418100	-2.23158100	-0.10315900
H	-2.34220900	-2.29376400	1.12211500
H	-2.05157200	-5.98571600	-2.78015600
H	-2.20436500	-5.00753000	-4.24038900
H	-0.65721100	-5.76631500	-3.85449100
H	-2.52463900	1.08084000	-5.18331400
H	1.59918600	2.22724300	-5.25835700
H	2.99193900	1.88777300	-3.39344900
H	2.16263600	2.97261200	-2.27893900
H	2.40346800	1.28449300	-1.83957400
H	-2.82133400	0.90972200	-1.57482500
H	-3.64680400	0.85634600	-3.13532600
H	-2.82929100	-0.58137600	-2.52156800
H	-1.56300300	2.22743700	-7.18404700
H	0.15892400	2.64937900	-7.22655000
H	-0.35032400	0.97444800	-7.45537800
C	0.10452400	1.23604300	1.16662400
H	-0.85177700	1.45981400	1.67038700

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