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Supporting Information

Fluoranthene Derivatives as Blue Fluorescent Materials for Non-doped Organic Light-Emitting Diodes

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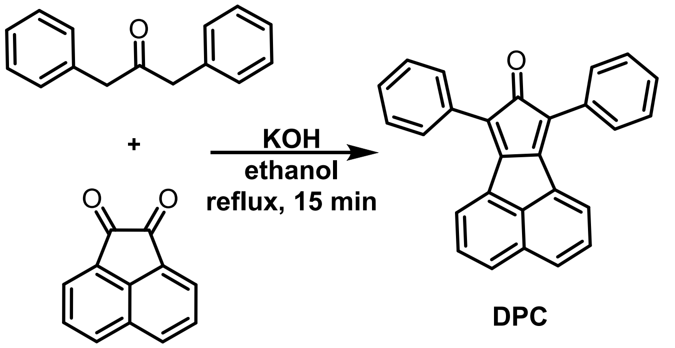
1. Synthesis of precursor materials

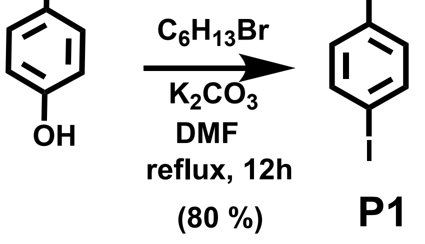
7,9-diphenyl-8H-cyclopenta[a]acenaphthylen-8-one (DPC)



Procedure

A two-necked 250 mL round bottom flask was equipped with a reflux condenser and rubber septum and charged with acenenapthenequinone (5.00 g, 27.5 mmol) and diphenylacetone (5.75 g, 27.5 mmol). Ethanol (70 mL) was added and the mixture brought to reflux, at which point ethanolic potassium hydroxide (2.5 mL) was added drop by drop. The reaction immediately became violent and a black precipitate formed. After 15 minutes the reaction vessel was capped and cooled to 0 °C. Pure DPC (9.10 g, 93% yield) was then collected by filtration as a deep purple crystalline solid. ^{1}H NMR (400 MHz, CDCl$_3$, ppm): δ 8.01 (d, J= 7 Hz, 2H), 7.9 (d, J= 8.2 Hz, 2H), 7.8 (d, J= 7.3 Hz, 4H), 7.6 (t, J=7.4, 2H), 7.5 (t, J= 7.6, 4H), 7.4 (t, J= 7.4, 2H).^{13}C NMR (101 MHz, CDCl$_3$): δ 204.51, 193.38, 128.96, 128.75, 128.52, 121.06, 89.97, 65.11, 52.96, 40.14, 39.93, 39.72, 39.51, 39.30, 39.09, 38.88, 0.39.

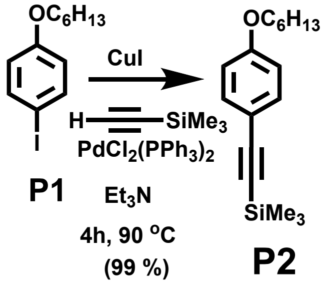
1-(Hexyloxy)-4-iodobenzene (P1)



Procedure

A mixture of 4-Iodophenol (5.0 g, 22.7 mmol) and anhydrous potassium carbonate (6.28 g, 45.5 mmol) was taken in *N,N*-dimethylforamide (20 mL). To the above reaction mixture 1-bromohexane (5.63 g, 34.1 mmol) was added. Reaction mixture was reflux for 16h. Reaction mixture was poured into 150 mL water and extracted with dichloromethane. The organic layer was washed with distilled water. The organic layer was dried over anhydrous sodium sulphate, filtered and subjected to rotary evaporation. Product was further purified using column chromatography with 2% ethyl acetate/hexane as eluent. Colourless liquid was obtained (90% yield). ^{1}H NMR (400 MHz, $CDCl_3$, ppm): δ 7.52 (d, 2H, *J*= 8.8 Hz), 6.66 (d, 2H, *J*= 9.2 Hz), 3.90 (t, 2H, *J*= 6.4 Hz), 1.79-1.75 (m, 2H), 1.47-1.43 (m, 2H), 1.35-1.31 (m, 4H), 0.90 (t, 3H, *J*= 4.32 Hz). ^{13}C NMR (100 MHz, $CDCl_3$, ppm): δ 159.01, 138.12, 116.93, 82.36, 77.32, 77.00, 76.68, 68.11, 31.53, 29.09, 25.65, 22.56, 13.99.

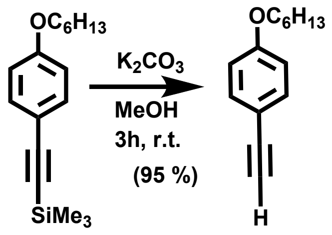
((4-(hexyloxy)phenyl)ethynyl)trimethylsilane (P2)



Procedure

A reaction mixture of compound P**1** (2.0 g, 6.5 mmol), trimethylsilyacetylene (0.7 g, 7.0 mmol), bis(triphenylphosphinepalladium(II))dichloride (4% mol) and copper iodide (10% mol) was taken in triethylamine (20 mL). In above reaction mixture was stirred at room temperature for 15 min and then refluxed for 4h under argon atmosphere. Reaction mixture was cooled to room temperature and subjected to solvent evaporation under reduced pressure. Residue was directly adsorbed over silica gel and purified using column chromatography with 2% ethylacetate/hexane as eluent. Colourless liquid was obtained. ^{1}H NMR (400 MHz, $CDCl_3$, ppm): δ 7.38 (d, 2H, *J*= 8.8 Hz), 6.79 (d, 2H, *J*= 8.8 Hz), 3.93 (t, 2H, *J*= 6.8 Hz), 1.78-1.72 (m, 2H), 1.46-1.42 (m, 2H), 1.34-1.31 (m, 4H), 0.90 (t, 3H, *J*= 4.32 Hz), 0.23 (s, 9H). ^{13}C NMR (100 MHz, $CDCl_3$, ppm): δ 159.36, 133.42, 115.01, 114.34, 105.34, 92.24, 77.32, 77.00, 76.68, 68.04, 31.56, 29.14, 25.67, 22.57, 13.99, 0.06.

Synthesis of 1-ethynyl-4-(hexyloxy)benzene (P3)

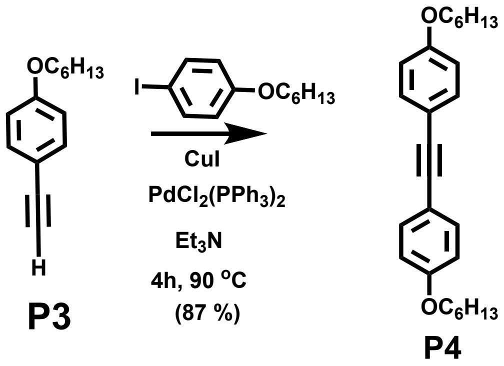


P2 **P3**

Procedure

Compound **P2** (1.7 g, 6.2 mmol) was treated with anhydrous potassium carbonate (85 mg, 0.6 mmol) in methanol (20 mL) at room temperature for 3 h under argon atmosphere. Solvent was evaporated and residue was extracted with dichloromethane/water mixture. Organic layer dried over anhydrous sodium sulphate, filtered and subjected to rotary evaporation. Product was further purified using column chromatography with 2% ethylacetate/hexane as eluent. Colourless liquid was obtained(95% yield).^{1}H NMR (400 MHz, $CDCl_3$, ppm): δ 7.4 (d, 2H, *J*= 8.8 Hz), 6.82 (d, 2H, *J*= 8.8 Hz), 3.94 (t, 2H, *J*= 6.8 Hz), 2.98 (s, 1H), 1.80-1.73 (m, 2H), 1.53-1.43 (m, 2H), 1.35-1.31 (m, 4H), 0.91 (t, 3H, *J*= 4.32 Hz). ^{13}C NMR (100 MHz, $CDCl_3$, ppm): δ 159.56, 133.55, 114.47, 113.89, 83.78, 77.32, 77.00, 76.68, 75.61, 68.08, 31.55, 29.12, 25.67, 22.57, 13.99.

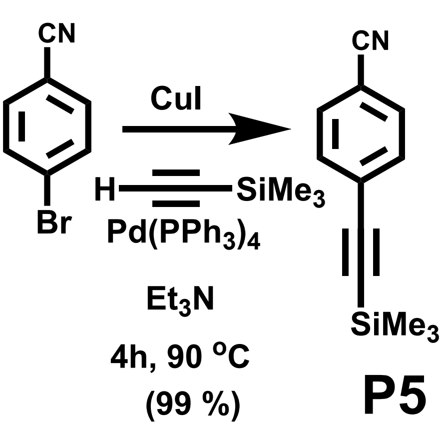
1,2-bis(4-(hexyloxy)phenyl)ethyne (P4)



Procedure

A mixture of compound **P1** (1.9 g, 6.2 mmol), **3** (1.2 g, 5.9 mmol), bis(triphenylphosphinepalladium(II))dichloride (4% mol) and copper iodide (10% mol) was taken in triethylamine (10 mL). In above reaction mixture was stirred at room temperature for 15 min, and then refluxed for 4 h under argon atmosphere. Reaction mixture was cooled to room temperature and solvent was evaporated and residue directly adsorbed over silica gel and purified using column chromatography with 2% ethylacetate/hexane as eluent. Crystalline white flakes were obtained(87% yield).^{1}H NMR (400 MHz, $CDCl_3$, ppm): δ 7.42 (d, 4H, *J*= 8.8 Hz), 6.82 (d, 4H, *J*= 8.8 Hz), 3.95 (t, 4H, *J*= 6.8 Hz), 1.80-1.73 (m, 4H), 1.53-1.43 (m, 4H), 1.35-1.31 (m, 8H), 0.91 (t, 6H, *J*= 4.32 Hz). ^{13}C NMR (100 MHz, $CDCl_3$, ppm): δ 138.17, 132.85, 115.55, 114.54, 87.98, 68.10, 31.60, 29.71, 29.20, 25.72, 22.61.Anal.Calcd for $C_{26}H_{34}O_2$: C, 82.49; H, 9.05; O, 8.45. Found: C, 82.31; H, 8.91.

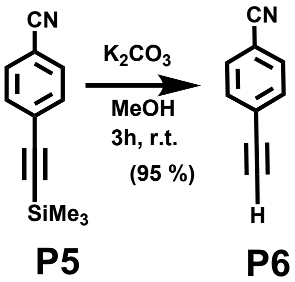
4-((trimethylsilyl)ethynyl)benzonitrile (P5)



Procedure

A reaction mixture of 4-bromobenzonitrile (1.82 g, 10mmol), trimethylsilyacetylene (0.98 g, 11.0 mmol), tetrakis(triphenylphosphinepalladium(0)) (4% mol) and copper iodide (10% mol) was taken in triethylamine (20 mL). In above reaction mixture was stirred at room temperature for 15 min and then refluxed for 4h under argon atmosphere. Reaction mixture was cooled to room temperature and subjected to solvent evaporation under reduced pressure. Residue was directly adsorbed over silica gel and purified using column chromatography with 2% ethylacetate/hexane as eluent.White solid powder was obtained (yield 85 %). ^{1}H NMR (400 MHz, $CDCl_3$, ppm): δ 7.59 (d, J = 8.3 Hz, 2H), 7.53 (d, J = 8.1 Hz, 2H), 0.26 (s, 9H). ^{13}C NMR (100 MHz, $CDCl_3$, ppm): δ 132.43, 131.90, 128.01, 118.39, 111.79, 102.97, 99.55, 29.68, -0.30.

4-ethynylbenzonitrile (P6)

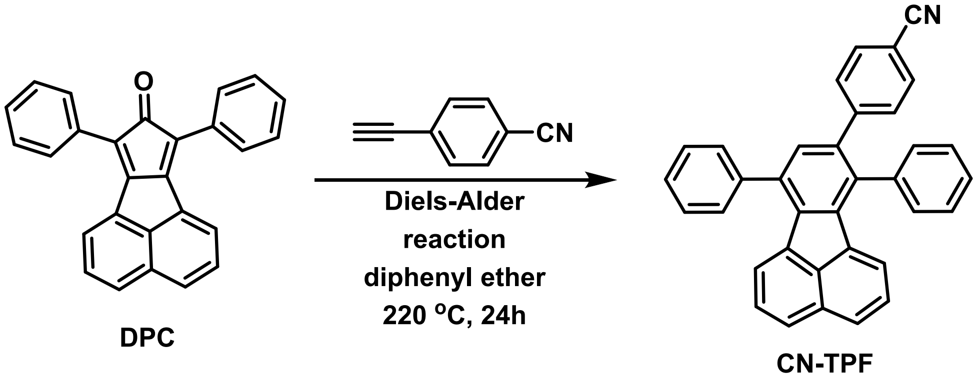


Procedure

Compound **P5** (1.7 g, 6.2 mmol) was treated with anhydrous potassium carbonate (85 mg, 0.6 mmol) in methanol (20 mL) at room temperature for 3 h under argon atmosphere. Solvent was evaporated and residue was extracted with dichloromethane/water mixture. Organic layer dried over anhydrous sodium sulphate, filtered and subjected to rotary evaporation. Product was further purified using column chromatography with 2% ethylacetate/hexane as eluent. Colourless liquid was obtained (95% yield). ^{1}H NMR (400 MHz, $CDCl_3$, ppm): δ 7.62 (d, *J* = 8.2 Hz, 2H), 7.57 (d, *J* = 8.3 Hz, 2H), 3.30 (s, 1H). ^{13}C NMR (100 MHz, $CDCl_3$, ppm): δ 132.65, 132.00, 126.98, 118.21, 112.33, 81.84, 81.51, 29.67.

Synthesis of fluoranthene derivatives

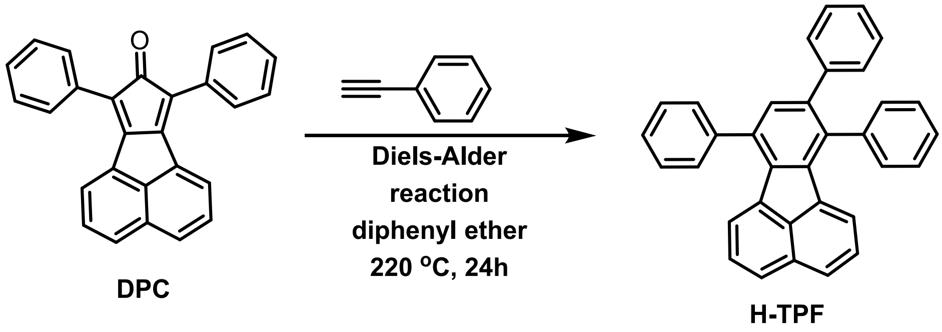
8-(4-cyanophenyl)-7,10-dipenylfluoranthene (CN-TPF)



Procedure

The compound DPC (1 mmol) and **P6** (1 mmol) were dissolved in diphenyl ether (5 mL) and kept in a sealed Teflon tube at 220 ^{o}C. After 24 h, reaction mixture was cooled down to room temperature; diphenyl ether was stripped under vacuum. Residue was diluted with hexane to precipitate the crude product. The resulting yellow solid was purified via column chromatography using 4:1 hexane/chloroform as eluent to afford green crystalline solid (yield 66%).^{1}H NMR (400 MHz, $CDCl_3$, ppm): δ 7.76 (t, *J* = 8.7 Hz, 2H), 7.69 (d, *J* = 7.3 Hz, 2H), 7.60 – 7.51 (m, 3H), 7.46 (d, *J* = 8.1 Hz, 2H), 7.39 (dd, *J* = 13.4, 5.5 Hz, 4H), 7.35 – 7.26 (m, 7H), 6.72 (d, *J* = 7.1 Hz, 1H).^{13}C NMR (100 MHz, $CDCl_3$, ppm): δ 146.03, 140.35, 138.69, 138.55, 138.42, 138.18, 136.71, 136.14, 135.89, 135.50, 133.12, 131.37, 130.61, 130.20, 129.73, 129.03, 128.74, 128.04, 127.76, 127.68, 127.62, 127.06, 126.97, 123.54, 123.33, 118.95, 110.11. ESI-MS: 455.27 (M^+). Elemental Analysis: ($C_{35}H_{21}N$) Calc. (%): C, 92.28; H, 4.65; N, 3.07; Found (%): C, 92.23; H, 4.67; N, 3.10.

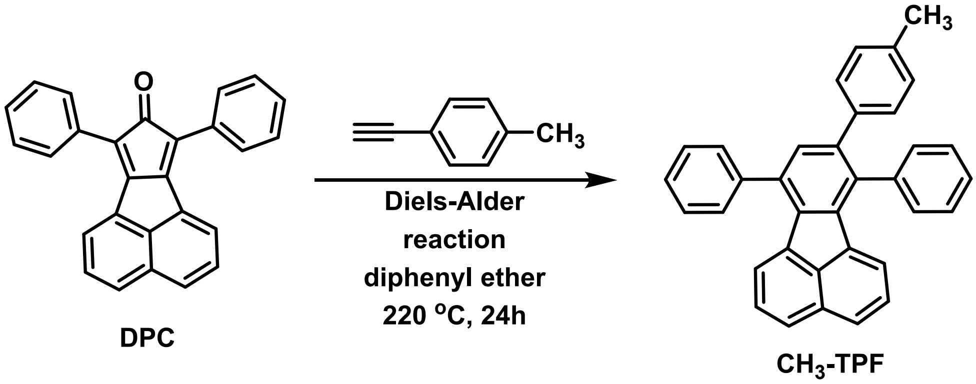
7,8,10-triphenylfluoranthene (TPF)



Procedure

Same as above. Green crystalline solid (yield 66%).^{1}H NMR (400 MHz, $CDCl_3$, ppm): δ 7.72 (dd, *J* = 10.1, 7.3 Hz, 4H), 7.53 (dt, *J* = 20.3, 7.0 Hz, 3H), 7.36 (d, *J* = 11.0 Hz, 6H), 7.30 (dd, *J* = 16.1, 9.0 Hz, 3H), 7.23 (d, *J* = 7.1 Hz, 2H), 7.17 (q, *J* = 6.4 Hz, 3H), 6.69 (d, *J* = 7.1 Hz, 1H).^{13}C NMR (100 MHz, $CDCl_3$, ppm): δ 141.01, 140.79, 139.33, 138.22, 137.92, 136.62, 136.18, 135.92, 135.71, 133.14, 131.14, 130.33, 129.96, 129.72, 129.13, 128.62, 128.45, 127.80, 127.62, 127.53, 127.27, 126.63, 126.33, 123.34, 122.91. ESI-MS: 431.73 (M^++H). Elemental Analysis: ($C_{34}H_{22}$) Calc. (%): C, 94.85; H, 5.15; Found (%): C, 94.18; H, 5.82

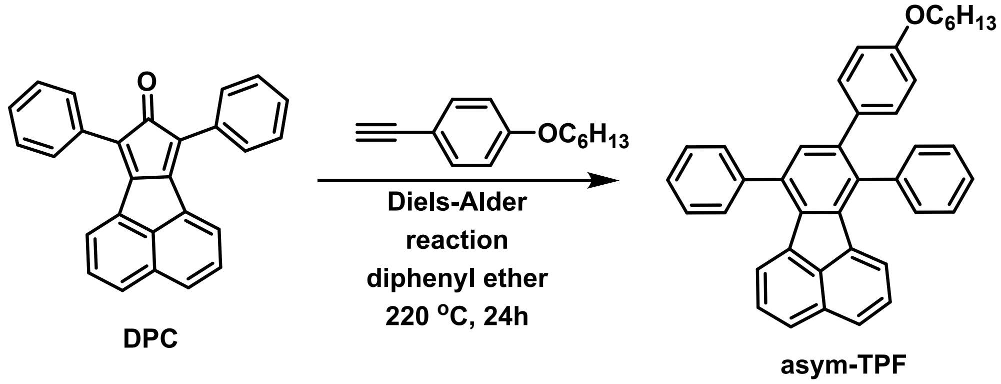
7,10-diphenyl-8-(p-tolyl)fluoranthene (CH_3-TPF)



Procedure

Same as above. Greenish-Yellow crystalline powder (yield 65 %). ^{1}H NMR (400 MHz, $CDCl_3$, ppm): δ 7.73 – 7.67 (m, 4H), 7.57 – 7.48 (m, 3H), 7.40 – 7.36 (m, 5H), 7.34 (d, *J* = 8.0 Hz, 2H), 7.32 (s, 1H), 7.28 (d, *J* = 7.1 Hz, 2H), 7.24 (d, *J* = 8.1 Hz, 1H), 7.13 – 7.09 (m, 2H), 6.97 (d, *J* = 7.9 Hz, 2H), 6.65 (d, *J* = 7.1 Hz, 1H), 2.26 (s, 3H).^{13}C NMR (101 MHz, $CDCl_3$, ppm): δ 140.85, 140.68, 139.51, 138.26, 138.02, 137.90, 136.68, 136.17, 135.97, 135.91, 135.51, 133.13, 131.22, 130.32, 129.80, 129.70, 129.13, 128.61, 128.47, 128.30, 127.76, 127.60, 127.51, 127.22, 126.56, 123.31, 122.83, 21.07. ESI-MS: 445.73 (M^++H). Elemental Analysis: ($C_{35}H_{24}$) Calc. (%): C, 94.56; H, 5.44; Found (%): C, 94.49; H, 5.51.

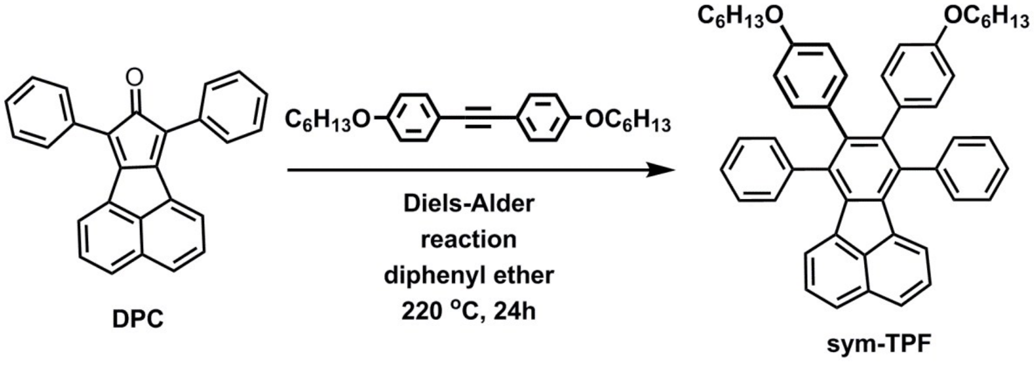
8-(4-(hexyloxy)phenyl)-7,10-diphenylfluoranthene (asym-TPF)



Procedure

Same as above. Green crystalline powder was obtained (yield 70 %). ^{1}H NMR (400 MHz, $CDCl_3$, ppm): δ 7.70 (t, *J* = 7.4 Hz, 12H), 7.52 (ddd, *J* = 14.4, 8.4, 4.5 Hz, 11H), 7.46 – 7.21 (m, 26H), 7.12 (d, *J* = 8.7 Hz, 6H), 6.68 (dd, *J* = 15.5, 7.9 Hz, 9H), 3.87 (t, *J* = 6.6 Hz, 6H), 1.79 – 1.67 (m, 6H), 1.41 (dd, *J* = 13.7, 6.2 Hz, 7H), 1.37 – 1.25 (m, 10H), 0.89 (t, *J* = 6.4 Hz, 7H).^{13}C NMR (101 MHz, $CDCl_3$, ppm): δ 157.74, 140.88, 140.42, 139.56, 138.26, 137.90, 136.71, 136.19, 136.00, 135.34, 133.17, 133.13, 131.16, 130.96, 130.33, 129.70, 129.13, 128.60, 128.51, 127.75, 127.60, 127.50, 127.21, 126.56, 126.51, 123.29, 122.77, 113.62, 67.86, 31.60, 29.26, 25.72, 22.58, 14.01. ESI-MS: 531.60 (M^++H). Elemental Analysis: ($C_{40}H_{34}O$) Calc. (%): C, 90.53; H, 6.46; O, 3.01; Found (%): C, 90.06; H, 6.52.

8,9-bis(4-(hexyloxy)phenyl)-7,10-diphenylfluoranthene (sym-TPF)



Procedure

Same as above. Greenish-yellow crystalline powder was obtained (yield 60 %). ^{1}H NMR (400 MHz, $CDCl_3$, ppm): δ 7.68 (d, *J* = 8.2 Hz, 2H), 7.35 – 7.23 (m, 12H), 6.77 (d, *J* = 8.5 Hz, 4H), 6.56 (d, *J* = 7.1 Hz, 2H), 6.43 (d, *J* = 8.5 Hz, 4H), 3.74 (t, *J* = 6.7 Hz, 4H), 1.71 – 1.59 (m, 4H), 1.32 (ddd, *J* = 15.9, 13.4, 7.7 Hz, 16H), 0.88 (t, *J* = 6.7 Hz, 6H).^{13}C NMR (100 MHz, $CDCl_3$, ppm): δ 156.60, 140.66, 140.17, 137.53, 136.64, 136.34, 133.26, 132.25, 130.09, 129.60, 128.16, 127.58, 126.74, 126.34, 123.04, 112.86, 67.68, 31.62, 29.68, 29.22, 25.67, 22.55, 14.00. ESI-MS = 707.93 (M^++H). Elemental Analysis: ($C_{52}H_{50}O_2$) Calc. (%): C, 88.34; H, 7.13; O, 4.53; Found (%): C, 88.19; H, 7.57.

CN-M-1

^{1}H NMR (400 MHz, CDCl$_3$) δ 7.76 (t, *J* = 8.7 Hz, 2H), 7.69 (d, *J* = 7.3 Hz, 2H), 7.60 – 7.51 (m, 3H), 7.46 (d, *J* = 8.1 Hz, 2H), 7.39 (dd, *J* = 13.4, 5.5 Hz, 4H), 7.35 – 7.26 (m, 7H), 6.72 (d, *J* = 7.1 Hz, 1H).

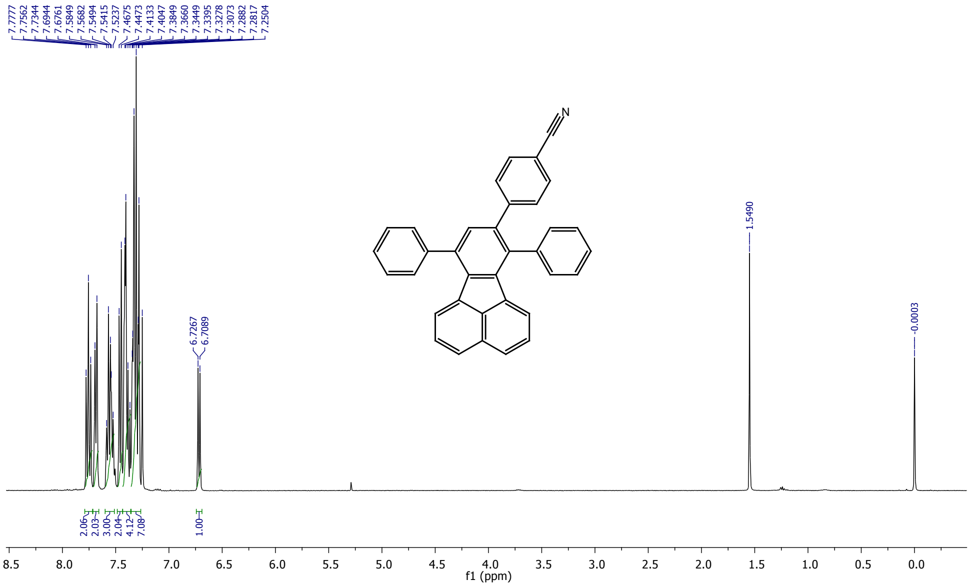


Figure S1 ^{1}H NMR spectra of CN-TPF

CN-M-1

^{13}C NMR (100 MHz, CDCl$_3$) δ 146.03, 140.35, 138.69, 138.55, 138.42, 138.18, 136.71, 136.14, 135.89, 135.50, 133.12, 131.37, 130.61, 130.20, 129.73, 129.03, 128.74, 128.04, 127.76, 127.68, 127.6
123.54, 123.33, 118.95, 110.11, 77.32, 77.00, 76.68.

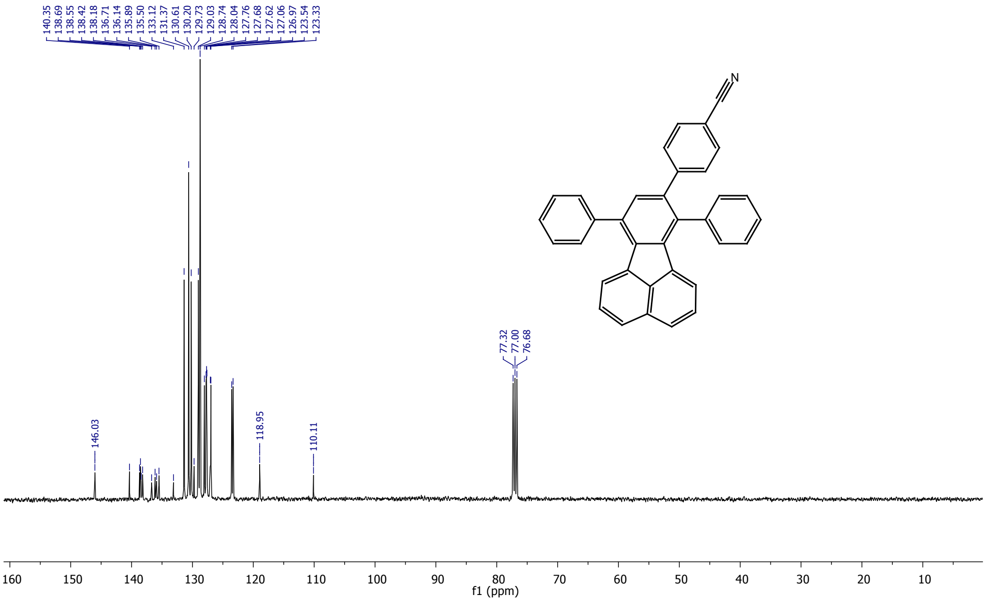


Figure S2 ^{13}C NMR spectra of CN-TPF.

M-1

^{1}H NMR (400 MHz, CDCl$_3$) δ 7.72 (dd, J = 10.1, 7.3 Hz, 4H), 7.53 (dt, J = 20.3, 7.0 Hz, 3H), 7.36 (d, J = 11.0 Hz, 6H), 7.30 (dd, J = 16.1, 9.0 Hz, 3H), 7.23 (d, J = 7.1 Hz, 2H), 7.17 (q, J = 6.4 Hz, 3H), 6.69 (d, J = 7.1 Hz, 1H).

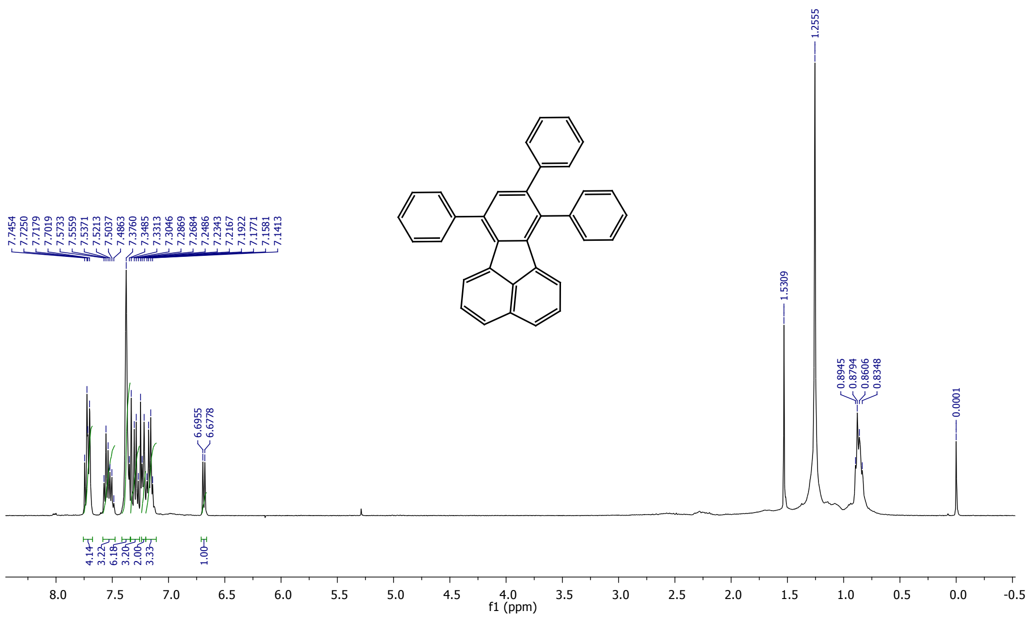


Figure S3 ^{1}H NMR spectra of TPF.

M-1

^{13}C NMR (100 MHz, CDCl$_3$) δ 141.01, 140.79, 139.33, 138.22, 137.92, 136.62, 136.18, 135.92, 135.71, 133.14, 131.14, 130.33, 129.96, 129.72, 129.13, 128.62, 128.45, 127.80, 127.62, 127.53, 127.2
123.34, 122.91, 77.32, 77.00, 76.68, 31.92, 30.03, 29.69, 29.35, 22.68, 14.10.

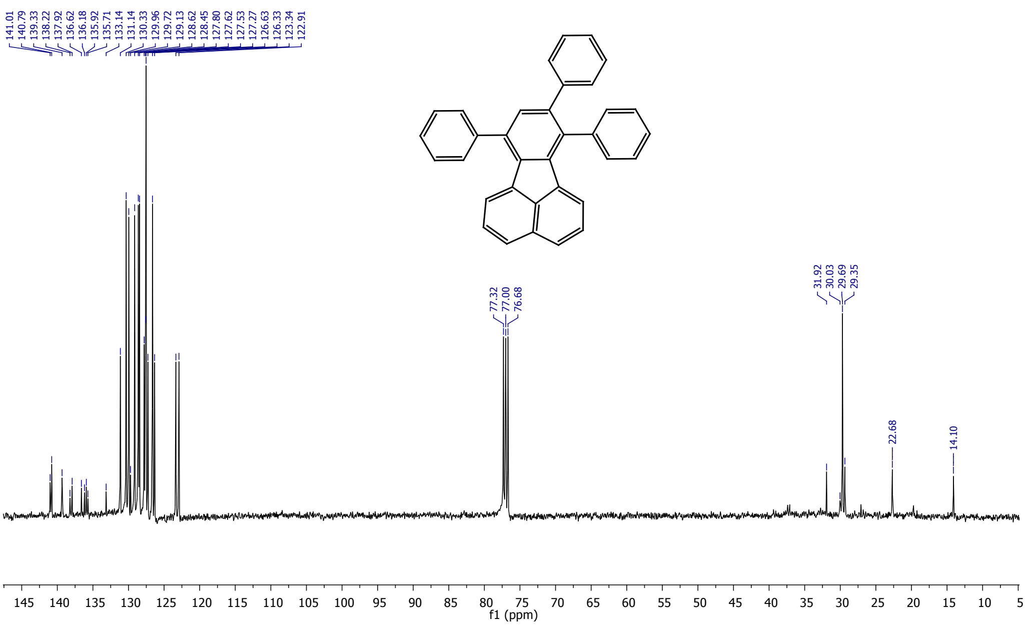


Figure S4 ^{13}C NMR spectra of TPF.

CH3-M-1

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.73 – 7.67 (m, 4H), 7.57 – 7.48 (m, 3H), 7.40 – 7.36 (m, 5H), 7.34 (d, J = 8.0 Hz, 2H), 7.32 (s, 1H), 7.28 (d, J = 7.1 Hz, 2H), 7.24 (d, J = 8.1 Hz, 1H), 7.13 – 7.09 (m, 2H), 6.97 (d, J = 7.9 Hz, 2H), 6.65 (d, J = 7.1 Hz, 1H), 2.26 (s, 3H).

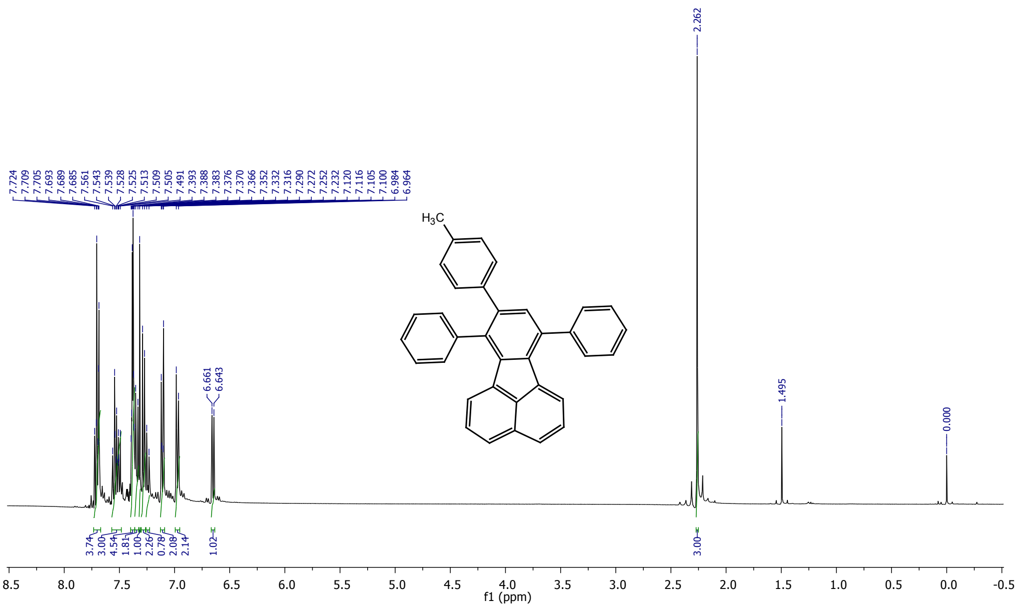


Figure S5 ^{1}H NMR spectra of CH_3-TPF.

CH3-M-1

^{13}C NMR (101 MHz, $CDCl_3$) δ 140.85, 140.68, 139.51, 138.26, 138.02, 137.90, 136.68, 136.17, 135.97, 135.91, 135.51, 133.13, 131.22, 130.32, 129.80, 129.70, 129.13, 128.61, 128.47, 128.30, 127.
127.22, 126.56, 123.31, 122.83, 77.32, 77.00, 76.68, 21.07.

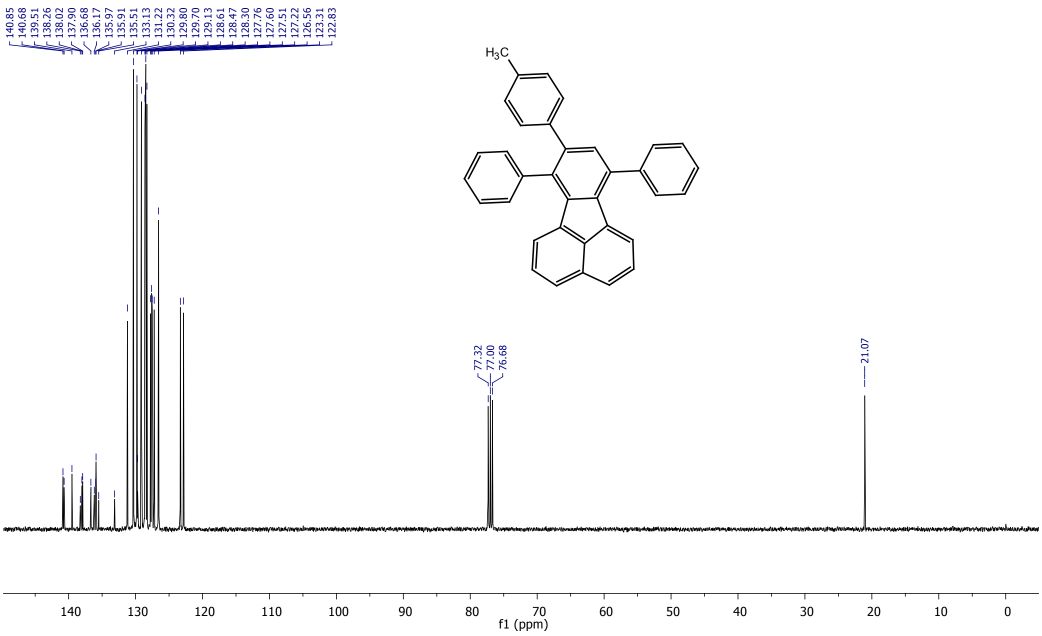


Figure S6 ^{13}C NMR spectra of CH_3-TPF.

M-7

^{1}H NMR (400 MHz, CDCl$_3$) δ 7.70 (t, J = 7.4 Hz, 12H), 7.52 (ddd, J = 14.4, 8.4, 4.5 Hz, 11H), 7.46 – 7.21 (m, 26H), 7.12 (d, J = 8.7 Hz, 6H), 6.68 (dd, J = 15.5, 7.9 Hz, 9H), 3.87 (t, J = 6.6 Hz, 6H), 1.79 – 1.67 (m, 6H), 1.41 (dd, J = 13.7, 6.2 Hz, 7H), 1.37 – 1.25 (m, 10H), 0.89 (t, J = 6.4 Hz, 7H).

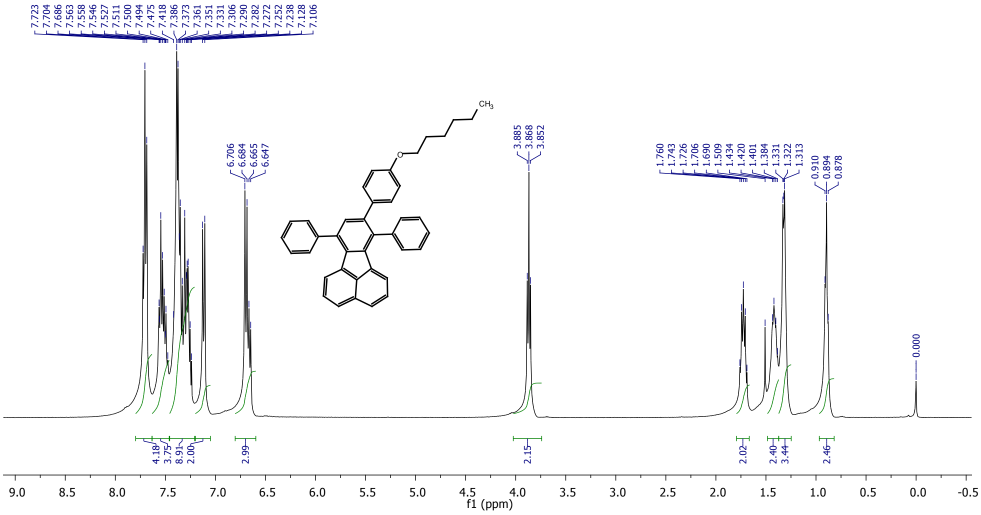


Figure S7 ^{1}H NMR spectra of asym-TPF.

M-7

^{13}C NMR (101 MHz, CDCl$_3$) δ 157.74, 140.88, 140.42, 139.56, 138.26, 137.90, 136.71, 136.19, 136.00, 135.34, 133.17, 133.13, 131.16, 130.96, 130.33, 129.70, 129.13, 128.60, 128.51, 127.75, 127.6
126.56, 126.51, 123.29, 122.77, 113.62, 77.32, 77.00, 76.68, 67.86, 31.60, 29.26, 25.72, 22.58, 14.01.

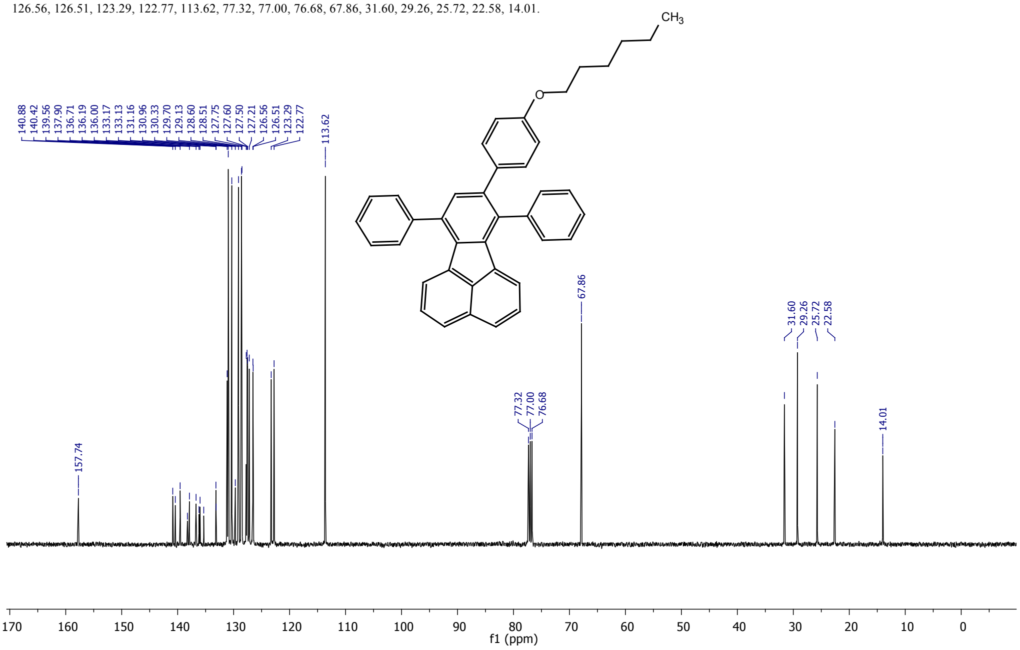


Figure S8 ^{13}C NMR spectra of asym-TPF.

M-3

^{1}H NMR (400 MHz, CDCl$_3$) δ 7.68 (d, *J* = 8.2 Hz, 2H), 7.35 – 7.23 (m, 12H), 6.77 (d, *J* = 8.5 Hz, 4H), 6.56 (d, *J* = 7.1 Hz, 2H), 6.43 (d, *J* = 8.5 Hz, 4H), 3.74 (t, *J* = 6.7 Hz, 4H), 1.71 – 1.59 (m, 4H), 1.32 (ddd, *J* = 15.9, 13.4, 7.7 Hz, 16H), 0.88 (t, *J* = 6.7 Hz, 6H).

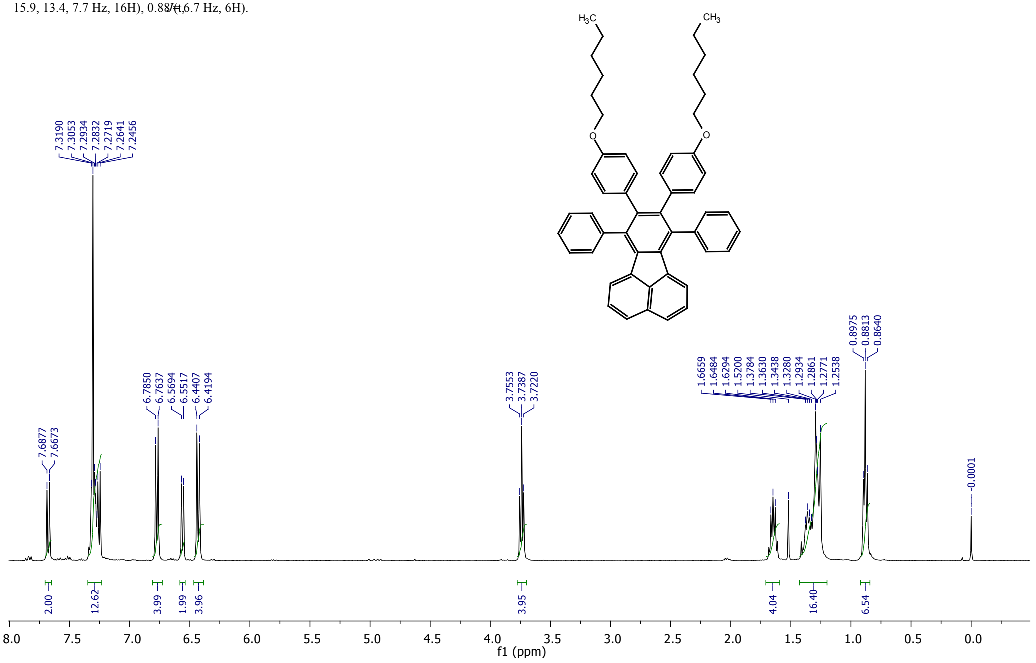


Figure S9 ^{1}H NMR spectra of sym-TPF.

M-3

^{13}C NMR (100 MHz, CDCl$_3$) δ 156.60, 140.66, 140.17, 137.53, 136.64, 136.34, 133.26, 132.25, 130.09, 129.60, 128.16, 127.58, 126.74, 126.34, 123.04, 112.86, 77.32, 77.00, 76.68, 67.68, 31.62, 29.
22.55, 14.00.

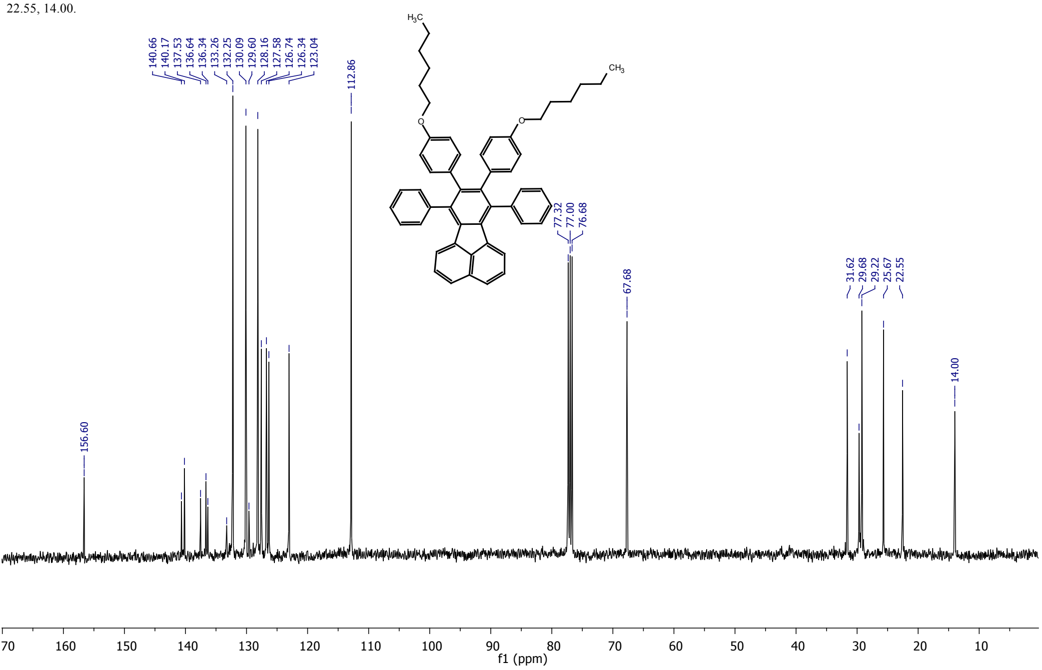


Figure S10 ^{13}C NMR spectra of sym-TPF.

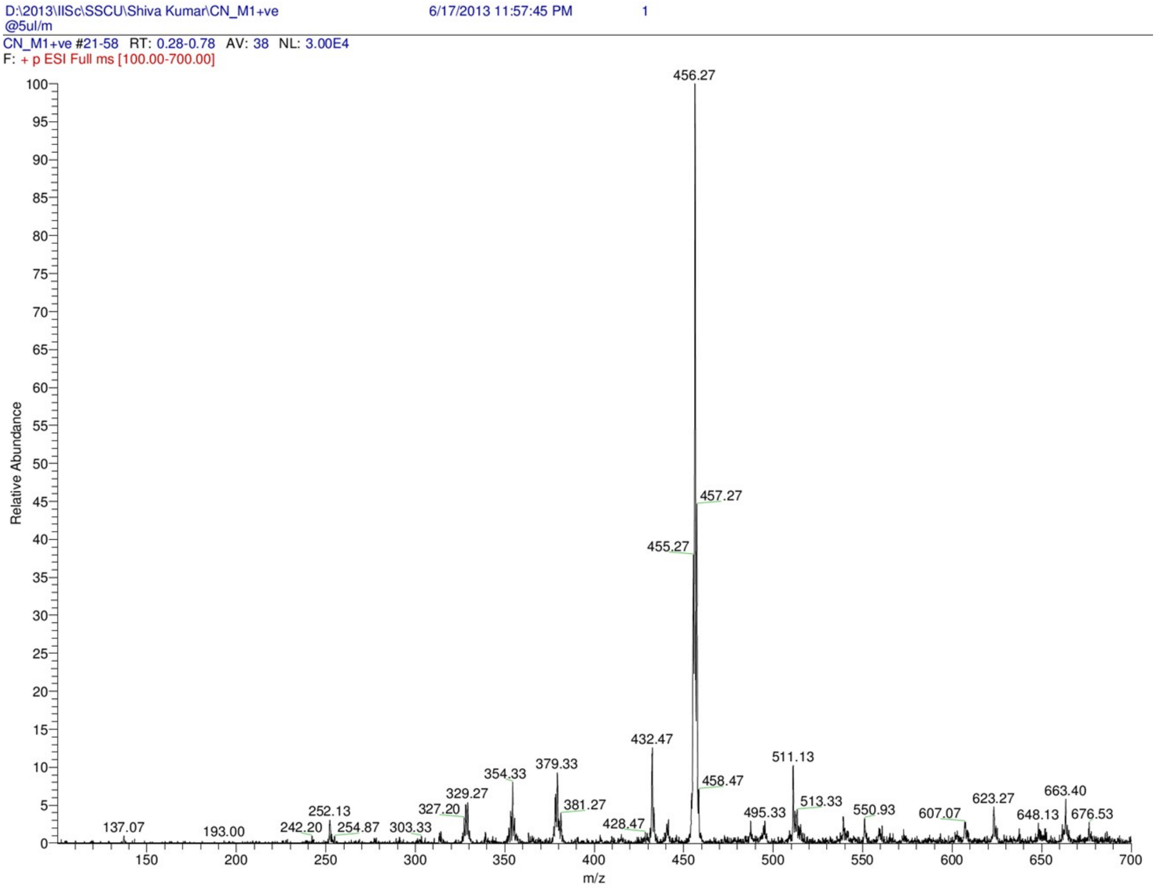


Figure S11 Mass spectra of CN-TPF.

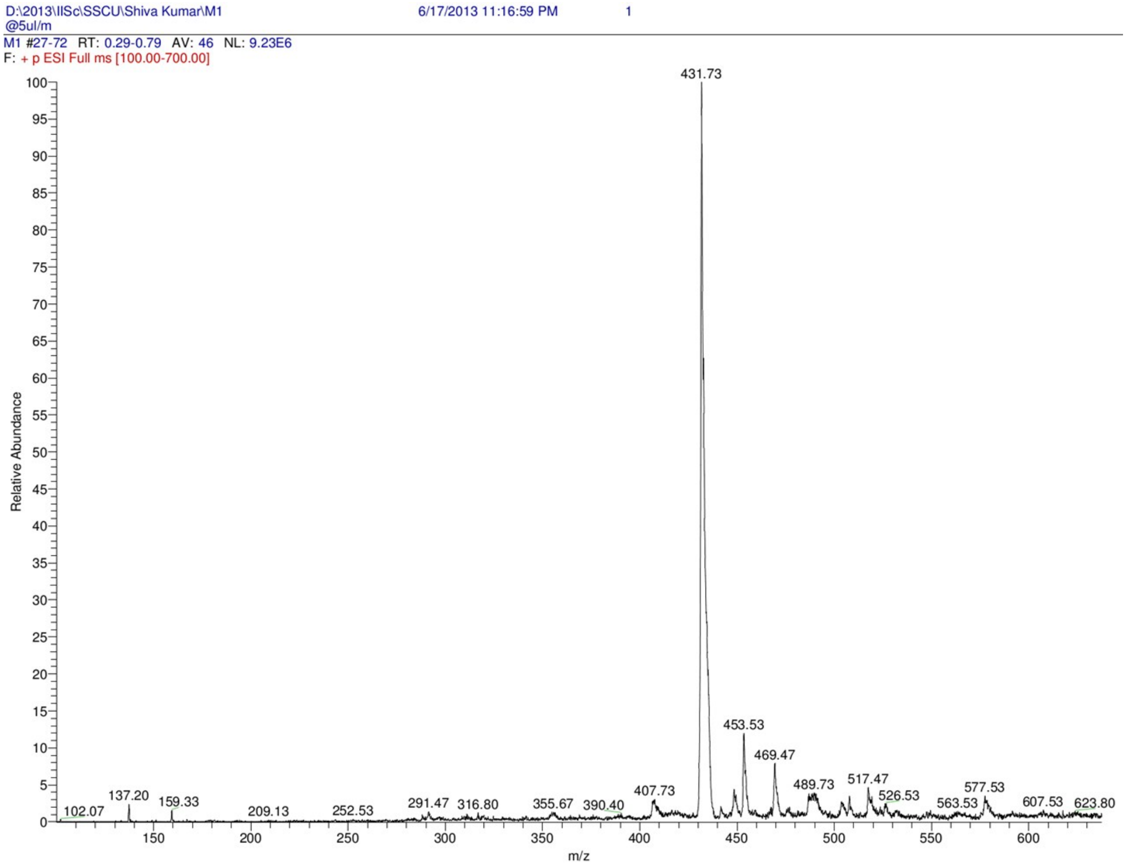


Figure S12 Mass spectra of TPF.

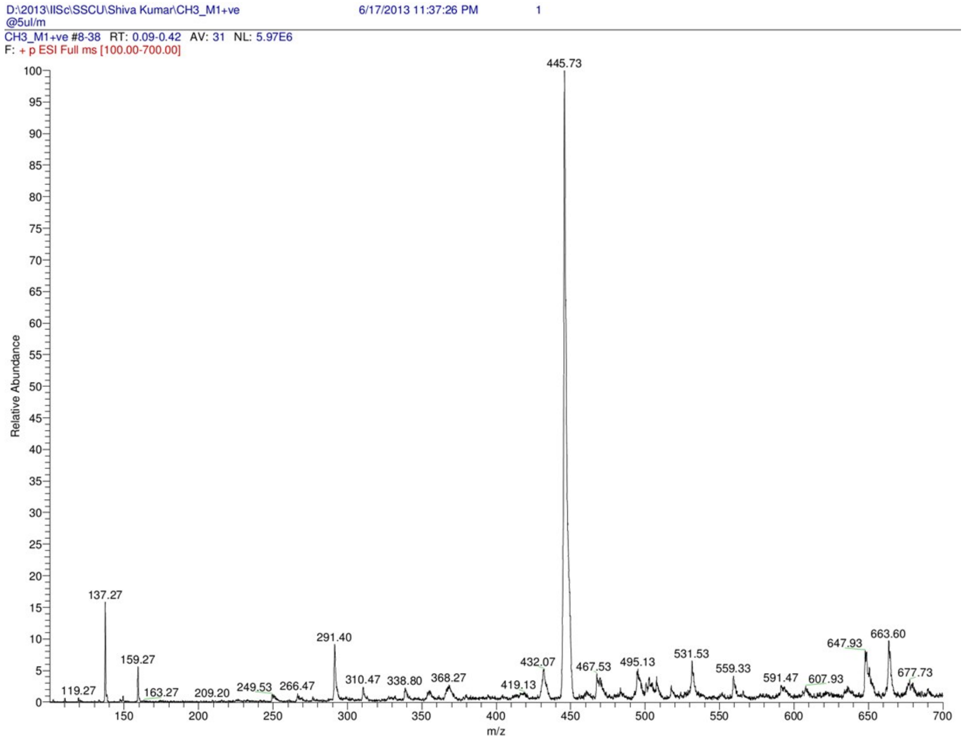


Figure S13 Mass spectra of CH_3-TPF.

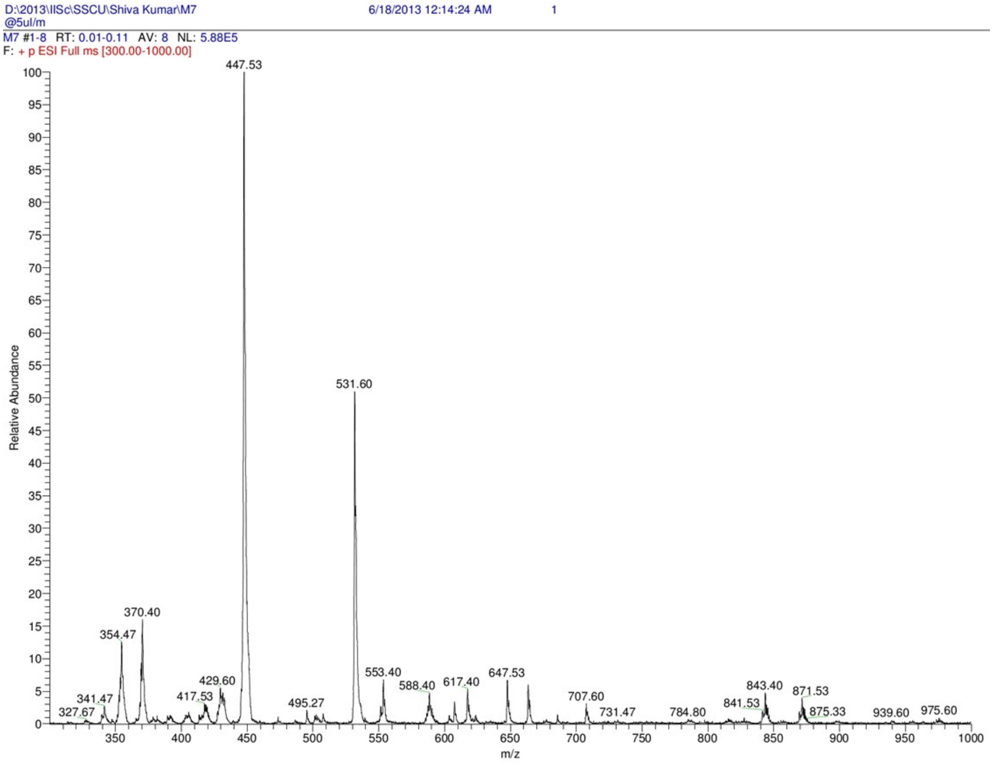


Figure S14 Mass spectra of asym-TPF.

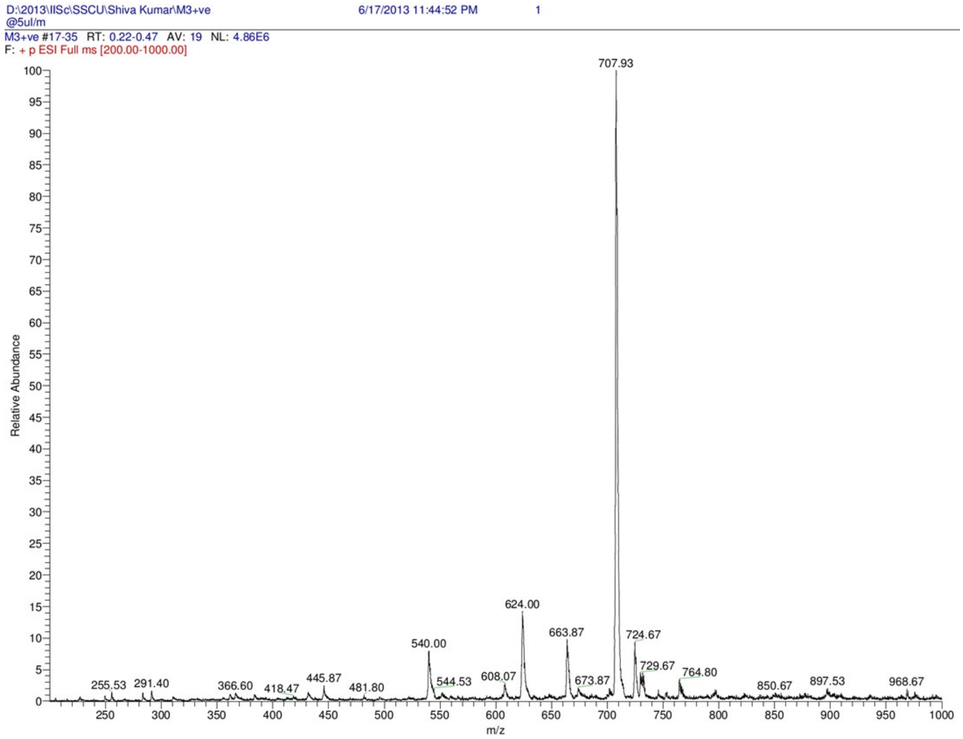


Figure S15 Mass spectra of sym-TPF.

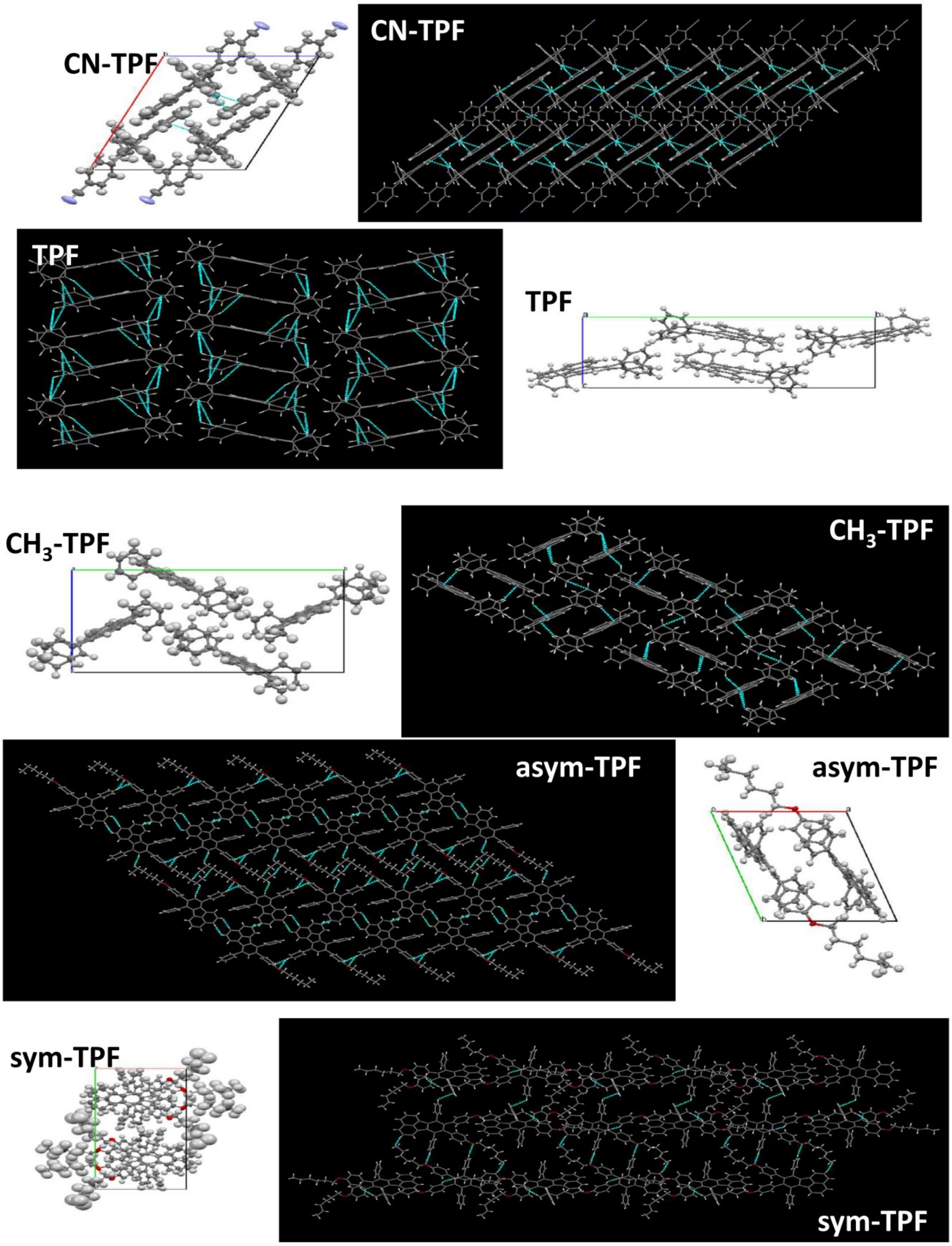


Figure S16 Supramolecular packing diagram of fluoranthene derivatives.

Table S1. Selective Crystallographic details of fluoranthene derivatives.

Molecule	**CN-TPF**	**TPF**	**CH$_3$-TPF**	**asym-TPF**	**sym-TPF**
Formula	$C_{35}H_{21}N$	$C_{34}H_{22}$	$C_{35}H_{24}$	$C_{40}H_{34}O$	$C_{56}H_{63}O_{4.5}$
Formula weight	455.53	430.52	444.54	530.67	808.06
Crystal system	Monoclinic	Monoclinic	Monoclinic	Triclinic	Monoclinic
Temperature	298K	110K	110K	110K	298K
Space group	$P2_1/c$	$P2_1/c$	$P2_1/c$	P-1	$P2_1/c$
a (Å)	13.735(2)	10.417(1)	10.717(5)	10.661(1)	12.522(2)
b (Å)	17.809(2)	24.645(1)	21.264(5)	12.346(1)	24.786(6)
c (Å)	10.840(1)	8.672(1)	11.420(5)	13.545(1)	15.897(2)
α(°)	90	90	90	65.98(1)	90
β(°)	112.05(1)	92.51(1)	113.40(1)	69.79(1)	108.86(1)
γ(°)	90	90	90	64.80(1)	90
Volume (Å^3)	2457.5(5)	2224.3(2)	2388.3(16)	1443.2(1)	4669.0(1)
Z	4	4	4	2	4
Density (g cm^{-3})	1.231	1.286	1.236	1.223	1.115
μ (mm^{-1})	0.071	0.073	0.070	0.071	0.071
F (000)	952	904	936	564	1740
Reflections collected	55107	18570	19714	23110	94880
Unique reflections	4315	4331	4596	5603	8196
L.S. parameters	325	307	318	422	489
R_{int}	0.0585	0.0422	0.0573	0.0399	0.1411
$R_1[I > 2\sigma(I)]$	0.0600	0.0406	0.0878	0.0435	0.1392
w$R_2[I > 2\sigma(I)]$	0.1688	0.0945	0.1669	0.1067	0.3497
$\Delta\rho_{min, max}$ (e Å^{-3})	-0.219/0.292	-0.211/0.193	-0.280/0.248	-0.193/0.247	-0.464/0.636
GOOF	1.100	1.009	1.116	1.070	1.226
CCDC No.	1402234	965009	965006	965010	1402235

Table S2 Summary of torsional angles.

Compounds	Torsion angle about C13-C23(°)	Torsion angle about C16-C17(°)	Torsion angle about C15-C29(°)	Torsion angle about C14-C35(°)
CN-TPF	54.3(4)	-75.2(3)	-49.4(4)	-
TPF	128.4(1)	-61.6(2)	-51.4(2)	-
CH_3-TPF	83.4(5)	-67.5(5)	-53.9(5)	-
asym-TPF	-56.1(2)	65.2(2)	62.6(2)	-
sym-TPF	68.2(7)	-101.2(6)	-118.4(5)	62.5(7)

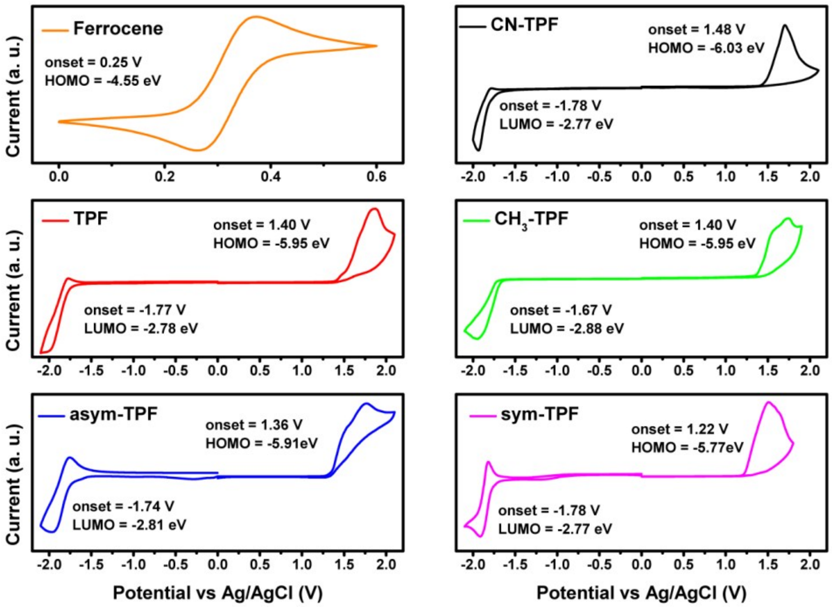


Figure S17 Cyclic voltammograms of fluoranthene derivatives in acetonitrile. Fc/Fc$^+$ couple was used as an internal reference and Bu4NF6 was used as supporting electrolyte with scan rate of 50 mV s^{-1}.

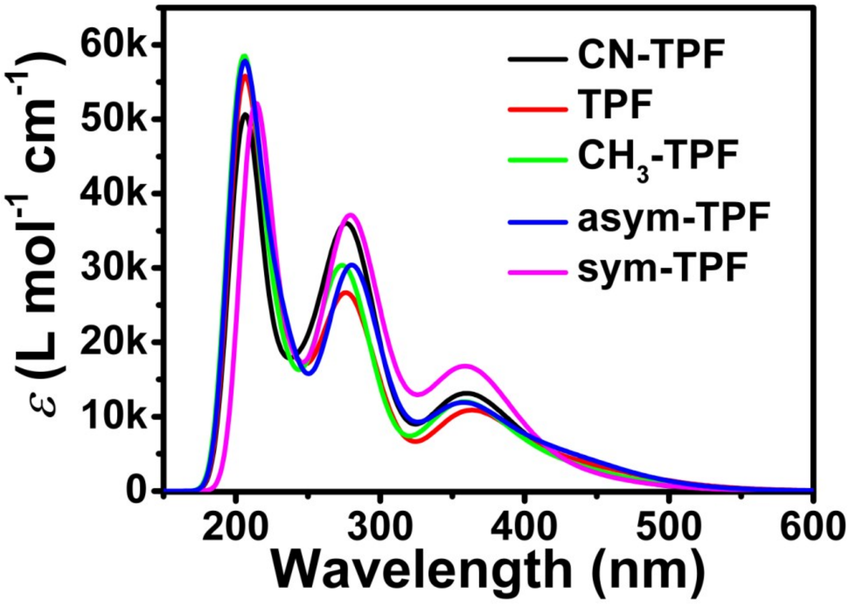


Figure S18 Simulated UV-visible absorption spectra of fluoranthene derivatives at TD-DFT/M062X/3-21G level of theory.

Table S3. Selected UV-visible key transitions of fluoranthene derivatives at the TD-DFT/M062X/3-21G level of theory in gaseous phase.

Compound	Expt. (nm)	TD-DFT/M062X/3-21G			Key transitions
		λ (nm)	λ (eV)	*f*	
CN-TPF	376	358	3.46	0.31	H-1→L, H→L
	329	285	4.33	0.10	H-4→L, H-2→L
	302	279	4.43	0.63	H-2→L+1, H→L+1
	243	241	5.13	0.18	H-1→L+1, H→L+2
TPF	375 329 295 243	362 287 279	3.42 4.30 4.43	0.25 0.12 0.38	H-1→L, H→L, H→L+1 H-5→L, H-4→L, H-2→L H-5→L, H-3→L, H-1→L, H→L+1
CH_3-TPF		498	2.48	0.07	H-1→L, H→L
	375	415	2.98	0.17	H-1→L, H→L, H→L+1
	329	325	3.81	0.32	H-5→L, H-4→L, H-3→L, H-1→L, H→L+1
	298	312	3.96	0.13	H-5→L, H-4→L, H-3→L, H-1→L+1, H→L+1
	243	279	4.43	0.07	H→L+2, H→L+4
		259	4.78	0.05	H-2→L+1, H-1→L+2, H→L+4, H→L+6, H→L+7
asym -TPF	377	427	2.90	0.10	H-1→L, H→L
	329	356	3.48	0.28	H-1→L, H→L, H→L+1
	300	280	4.42	0.62	H-3→L, H→L+1
	243	227	5.44	0.22	H-4→L, H→L+2, H→L+5, H→L+6
sym-TPF	376	360	3.44	0.40	H-1→L, H→L+2
	329	309	4.01	0.08	H-6→L, H-2→L, H→L
	300	283	4.37	0.57	H-3→L, H→L+1
	243	211	5.85	0.46	H-1→L+3, H-1→L+6

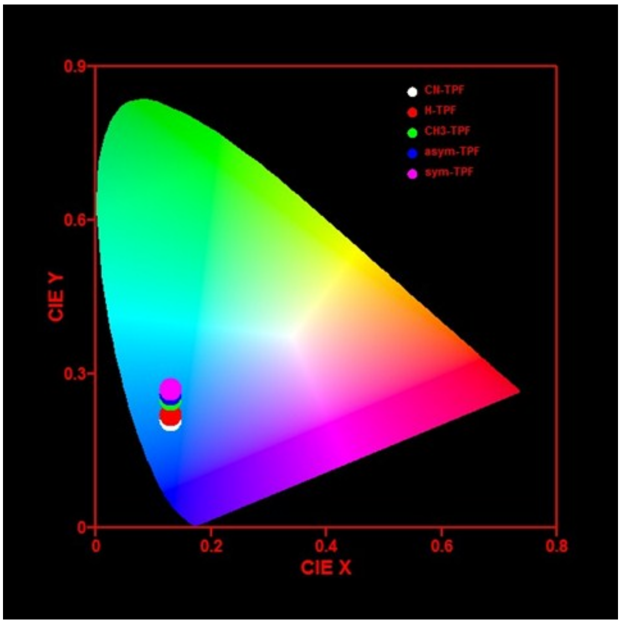


Figure S19 CIE 1931 chromaticity plot.

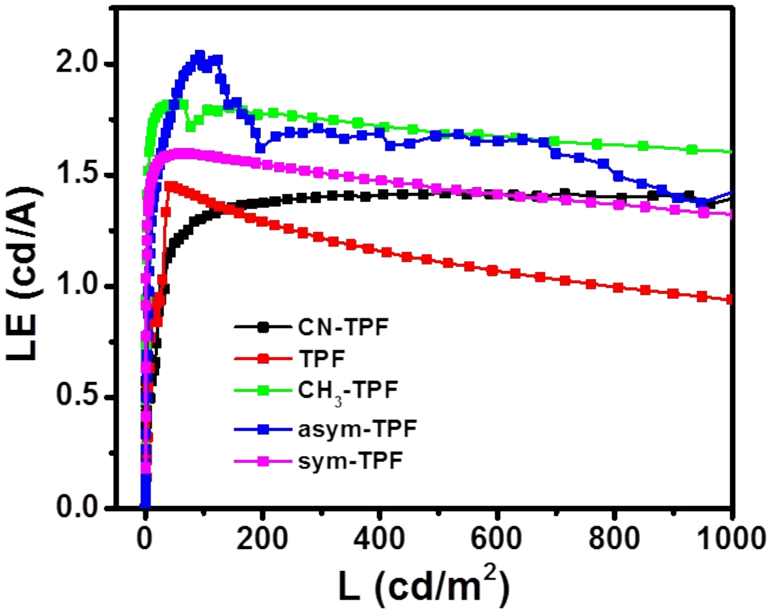


Figure S20 Luminescence efficiency-luminance (LE-L) characteristic plot.