

Electronic Supplementary Information

Parent and Trisubstituted Triazacoronenes: Synthesis, Crystal Structure and Physicochemical Properties

Qitao Tan,^{*a} Huanhuan Chen,^a Huaida Xia,^a Bingxin Liu,^a Bin Xu^{*abc}

^a*Department of Chemistry, Innovative Drug Research Center, Shanghai University, Shanghai 200444, China*

^b*State Key Laboratory of Organometallic Chemistry, Shanghai Institute of Organic Chemistry, Chinese Academy of Sciences, Shanghai 200032, China*

^c*Shanghai Key Laboratory of Green Chemistry and Chemical Processes, Department of Chemistry, East China Normal University, Shanghai 200062, China*

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1. General Information

All reagents were obtained from commercial sources without further purification, and solvents were used as received except specifically mentioned. Silica gel plate GF254 were used for thin layer chromatography (TLC) and silica gel 300-400 mesh were used for flash column chromatography. All melting points were taken on a SGW X-4A digital melting point apparatus without correction. Infrared spectra were obtained using an AVATAR 370 FT-IR spectrometer. ^1H , ^{13}C , and ^{19}F NMR spectra were recorded with a Bruker AV-500 spectrometer operating at 500 MHz, 125 MHz and 470 MHz, respectively. Mass spectra and high resolution mass spectra were recorded with an Agilent 5975N using an electron impact (EI) or electrospray ionization (ESI) techniques. MALDI-TOF MS (solid-state analyte in TCNQ or DHB matrix) was carried out on a Thermo Fisher Scientific LTQ FT Ultra spectrometer. Ultraviolet spectra were measured on a PEGeneral spectrometer. Fluorescence spectra were recorded on a LS-55 spectrometer. The crystal structure was recorded on SMART APEXII X-ray diffraction spectrometer. The powder X-ray diffraction (XRD) was recorded on an 18KV D/MAX2500V+/PC X-ray diffraction measurement system, with Cu K α source ($\lambda = 1.54 \text{ \AA}$). Elemental analyses were carried out on an Elementar Vario EL elemental analyzer. Yields refer to chromatographically and spectroscopically pure compounds, unless otherwise indicated. TG analyses were performed on a TA Q500 V20.10 Build 36 thermal gravimetric analyzer with a heating rate of 10 $^{\circ}\text{C}/\text{min}$ under N_2 . Cyclic voltammetry (CV) and differential pulse voltammetry (DPV) were performed on a CHI660B electrochemical analyzer at room temperature in inert atmosphere with a three-electrode configuration in CH_2Cl_2 solution (distilled from CaH_2) containing the substrate (typically $\sim 1.00 \times 10^{-4} \text{ M}$) and 0.1 M tetrabutylammonium hexafluorophosphate ($n\text{-Bu}_4\text{NPF}_6$) as the supporting electrolyte. A glassy carbon disc served as the working electrode, a platinum wire and a commercial Ag/Ag^+ electrode (0.01 M AgNO_3 in CH_3CN) served as the counter and the reference electrodes, respectively. The scan rate was 0.1 V/s. The HOMO and LUMO energy values were estimated from the onset potentials of the first oxidation and reduction event, respectively. After calibration of the measurements against Fc/Fc^+ , the HOMO and LUMO energy levels were calculated according to the following equations:

$$E_{\text{HOMO}} (\text{eV}) = - [E^{\text{ox}}(\text{onset}) - E^{1/2}(\text{Fc}/\text{Fc}^+) + 4.8]$$

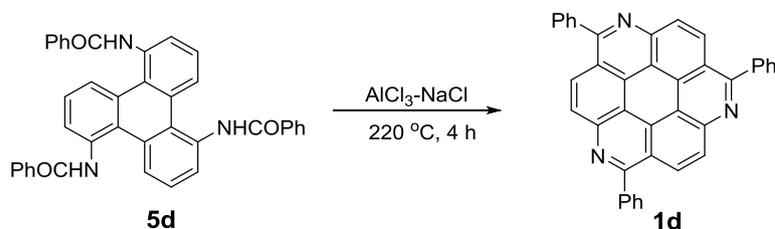
$$E_{\text{LUMO}} (\text{eV}) = - [E^{\text{red}}(\text{onset}) - E^{1/2}(\text{Fc}/\text{Fc}^+) + 4.8]$$

Where $E^{1/2}(\text{Fc}/\text{Fc}^+)$ is the half-wave potential of the Fc/Fc^+ couple (the oxidation potential of which is assumed at 4.8 eV) against the Ag/Ag^+ electrode. Theoretical calculations were carried out using the Gaussian 09 program, using density functional theory calculation at B3LYP/6-31G(d) level of theory.

2. Synthesis and Characterization

2.1

Table S1. The effect of molar ratios of AlCl₃-NaCl on the transformation of **5d** to **1d**.^a

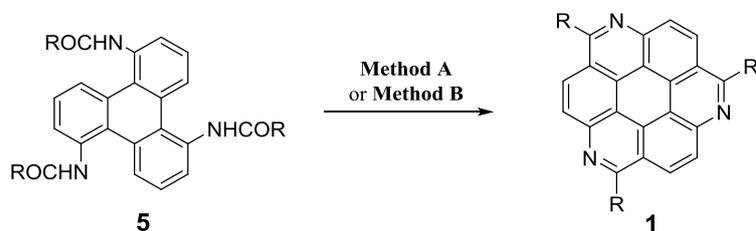


Entry	AlCl ₃ /NaCl (molar ratio)	Yield (%)
1	3 : 1	trace
2	1 : 1	61%
3	1 : 3	64%
4	1 : 5	42%

^aReaction conditions: **5d** (58.6 mg, 0.1 mmol), NaCl (292.2 mg, 5.0 mmol) and AlCl₃, N₂, sealed, 220 °C, 4 h.

2.2

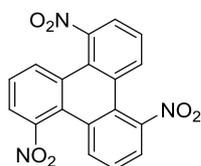
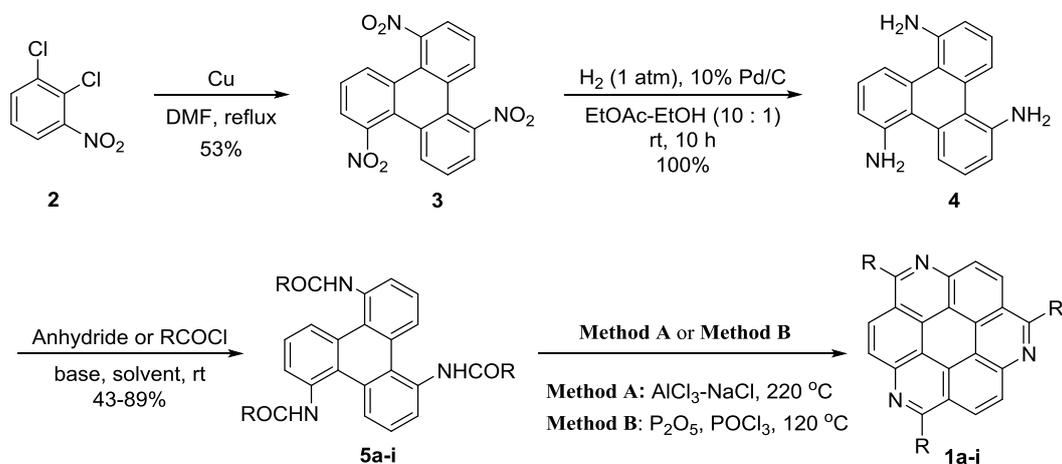
Table S2. Key cyclization methods for all TACs.



Compound	AlCl ₃ -NaCl ^a (Method A)	POCl ₃ -P ₂ O ₅ ^b (Method B)	Compound	AlCl ₃ -NaCl ^a (Method A)	POCl ₃ -P ₂ O ₅ ^b (Method B)
1a (R = H)	53%	trace	1f (R = 4-MeOC ₆ H ₄)	trace	67% ^c
1b (R = <i>n</i> -Bu)	79%	53%	1g (R = 4-ClC ₆ H ₄)	51%	74%
1c (R = CF ₃)	trace	15%	1h (R = 2-ClC ₆ H ₄)	56%	trace
1d (R = Ph)	74%	64%	1i (R = 2-FC ₆ H ₄)	50%	trace
1e (R = 4-MeC ₆ H ₄)	64%	63%			

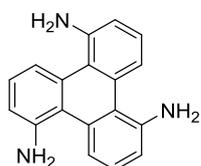
^aReaction condition: **5** (0.3 mmol), NaCl (876.6 mg, 15.0 mmol) and AlCl₃ (668.0 mg, 5.0 mmol), N₂, sealed, 220 °C, 4 h. ^bReaction conditions: **5** (0.3 mmol), P₂O₅ (0.94 g, 6.6 mmol), POCl₃ (3 mL), 120 °C, N₂, 12 h. ^cReaction conditions: **5f** (85.0 mg, 0.14 mmol), P₂O₅ (1.14 g, 8.0 mmol), POCl₃ (1.7 mL), 120 °C, N₂, 12 h.

2.3 Experimental Procedure



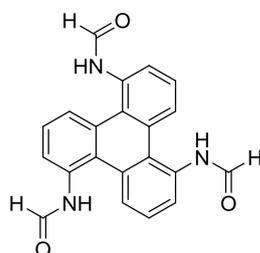
1,5,9-Trinitrotriphenylene (3)^[S1]

To a solution of 2,3-dichloronitrobenzene (30.0 g, 156.3 mmol) in DMF (240 mL) was added copper powder (60.0 g, 937.5 mmol). The mixture was stirred at reflux for 12 h under nitrogen atmosphere. After cooling to 120 °C, the hot solution was filtered through diatomite and washed by DMF (3 × 40 mL) to remove the excess copper powder. The filtrate was then slowly poured into a diluted ammonium solution 1.2 L (containing conc. NH₃·H₂O 300 mL) with vigorously stirring. A black solid precipitated and the aqueous layer was decanted. The solid was crushed into small pieces and washed with diluted ammonium solution and water successively. The resulted solid was then stirred with refluxing acetone (50 mL) for 30 min. The mixture was filtered and washed with acetone (2 × 5 mL) to give a brown yellow solid (10.0 g, 53%), the purity of which was determined by ¹H NMR to be > 90%. The solid can be directly used for the next step. Sample for spectra analysis was obtained as a yellow solid by chromatography packed with silica gel using hexane/dichloromethane (3 : 2, v/v) as eluent. M.p. 307-309 °C. IR (KBr, cm⁻¹): 3081, 1519, 1354, 873, 828, 770, 727, 672; ¹H NMR (500 MHz, CDCl₃): δ 8.15 (dd, *J* = 8.4, 1.1 Hz, 3H), 7.93 (dd, *J* = 7.8, 1.1 Hz, 3H), 7.68 (t, *J* = 8.1 Hz, 3H); ¹³C NMR (125 MHz, CDCl₃): δ 149.6, 129.5, 128.3, 128.2, 125.4, 122.4; HRMS (EI) *m/z* calcd for C₁₈H₉N₃O₆ [M]⁺ 363.0491, found 363.0493.



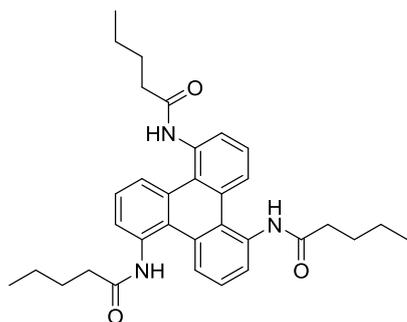
Triphenylene-1,5,9-triamine (**4**)

Activated palladium on carbon (10 % w/w, 0.60 g) was added to a solution of **3** (3.00 g, 8.26 mmol) in ethyl acetate (300 mL) and EtOH (30 mL) under a nitrogen atmosphere. The reaction flask was purged three times with H₂. Then the mixture was stirred at room temperature with a hydrogen balloon. After the reaction was complete, the catalyst was removed by filtration and washed with ethyl acetate. The filtrate was concentrated under reduced pressure to yield the amine **4** as a yellow solid in a quantitative yield, which could be directly used for the following reaction without further purification. Yield: 2.26 g (100%); M.p. 139-140 °C. IR (KBr, cm⁻¹): 3408, 3336, 2923, 1614, 1580, 1478, 1426, 1303, 1258, 762, 678, 589; ¹H NMR (500 MHz, DMSO-*d*₆): δ 8.21 (d, *J* = 7.9 Hz, 3H), 7.17 (t, *J* = 7.9 Hz, 3H), 6.88 (d, *J* = 7.7 Hz, 3H), 5.33 (br, 6H); ¹³C NMR (125 MHz, DMSO-*d*₆): δ 145.2, 132.3, 126.6, 118.3, 114.9, 114.0; HRMS (ESI) *m/z* calcd for C₁₈H₁₆N₃ [M+H]⁺ 274.1339, found 274.1326.



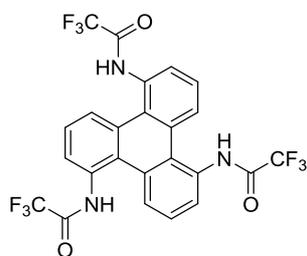
N,N',N''-(Triphenylene-1,5,9-triyl)triformamide (**5a**)

Formic acid (1.8 mL) was added to a solution of acetic anhydride (3.5 mL) at 0 °C. After stirred at 50 °C for 2 h, the mixture was cooled down to 0 °C. A solution of the amine **4** (2.40 g, 8.78 mmol) in THF (48 mL) was added dropwise over 15 min to the prepared mixture, which was then allowed to warm to ambient temperature after 40 min and stirred for 18 h. The resulting precipitate was filtered, rinsed with ethyl acetate, and dried to afford pure product **5a** as a pale yellow solid. Yield: 2.80 g (89%); M.p. 273-274 °C. IR (KBr, cm⁻¹): 3215, 2877, 1655, 1593, 1516, 1476, 1387, 1255, 1156, 809, 756; ¹H NMR (500 MHz, DMSO-*d*₆, 80 °C): δ 10.04 (s, 3H), 8.66 (d, *J* = 8.6 Hz, 3H), 8.40 (s, 3H), 7.73-7.50 (br, 3H), 7.53 (t, *J* = 8.0 Hz, 3H) (for variable-temperature ¹H NMR spectra of this compound, see Figure S2); ¹³C NMR (125 MHz, DMSO-*d*₆, 20 °C, as a mixture of rotamers^[S2]): δ 164.0, 160.3, 133.9, 132.9, 132.8, 132.7, 132.6, 130.7, 130.2, 127.0, 126.8, 126.6, 126.4, 126.0, 125.7, 125.4, 125.2, 125.0, 124.4, 124.1, 124.0, 123.8, 123.6; HRMS (ESI) *m/z* calcd for C₂₁H₁₅N₃NaO₃ [M+Na]⁺ 380.1006, found 380.1004.



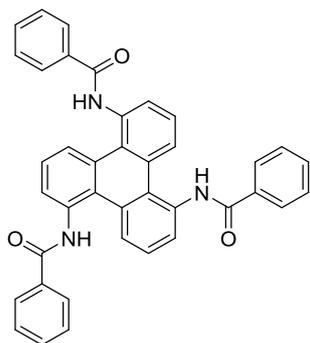
***N,N',N''*-(Triphenylene-1,5,9-triyl)tripentanamide (**5b**)**

To a solution of **4** (1.00 g, 3.66 mmol) in anhydrous THF (40 mL) with Et₃N (2.20 g, 22.00 mmol) was added dropwise valeroyl chloride (1.99 g, 16.50 mmol) dissolved in anhydrous THF (20 mL). The mixture was stirred at r.t. under N₂ for 22 h. To the reaction was added dichloromethane and saturated NaHCO₃ and the mixture was stirred for 5 min. The organic layer was separated and the aqueous phase was extracted with dichloromethane (3 × 20 mL). The combined organic phase was washed with brine and dried over Na₂SO₄. After filtration, the filtrate was evaporated in vacuum to give the crude product which was purified by washing with dichloromethane (150 mL) affording the pure product **5b** as a white solid. Yield: 0.97 g (50%); M.p. 293-294 °C. IR (KBr, cm⁻¹): 3250, 3023, 2955, 2866, 1649, 1518, 1470, 760; ¹H NMR (500 MHz, DMSO-*d*₆): δ 10.10 (s, 3H), 8.56 (dd, *J* = 6.7, 2 Hz, 3H), 7.37-7.49 (m, 6H), 2.39 (t, *J* = 7.3 Hz, 6H), 1.63 (m, 6H), 1.33-1.43 (m, 6H), 0.95 (t, *J* = 7.3 Hz, 9H); ¹³C NMR (125 MHz, CDCl₃: MeOD-*d*₄ = 0.7 mL : 0.3 mL): δ 173.8, 133.3, 130.6, 127.1, 126.5, 126.1, 123.9, 36.5, 27.6, 22.4, 13.6; HRMS (ESI) *m/z* calcd for C₃₃H₃₉N₃NaO₃ [M+Na]⁺ 548.2884, found 548.2883.



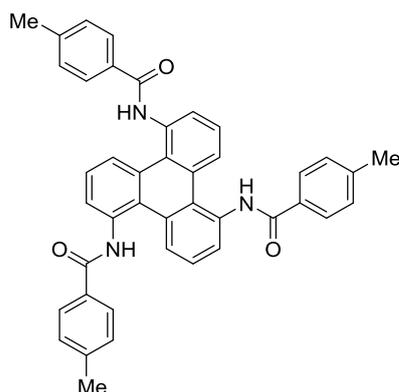
***N,N',N''*-(Triphenylene-1,5,9-triyl)tris(2,2,2-trifluoroacetamide) (**5c**)**

Following the procedure for **5a**, the reaction of **4** (1.00 g, 3.66 mmol), pyridine (3.47 g, 44.00 mmol), trifluoroacetic anhydride (3.84 g, 18.30 mmol) in dichloromethane (30 mL) afforded the desired product **5c** as a white solid after purification by column chromatography packed with silica gel using hexane/ethyl acetate (2 : 1, v/v) as eluent. Yield: 1.09 g (53%); M.p. 274-275 °C. IR (KBr, cm⁻¹): 3268, 3060, 2861, 1711, 1532, 1203, 1166, 720; ¹H NMR (500 MHz, DMSO-*d*₆): δ 11.87 (s, 3H), 8.50-8.60 (m, 3H), 7.55-7.68 (m, 6H); ¹⁹F NMR (470 MHz, DMSO-*d*₆): δ -74.3 (s, CF₃); ¹³C NMR (125 MHz, DMSO-*d*₆): δ 155.6 (q, ²*J*_{C-F} = 36.5 Hz), 131.7, 130.6, 129.0, 127.4, 127.3, 125.2, 116.6 (q, ¹*J*_{C-F} = 286.7 Hz); HRMS (MALDI/DHB) *m/z* calcd for C₂₄H₁₂F₉N₃NaO₃ [M+Na]⁺ 584.0627, found 584.0633.



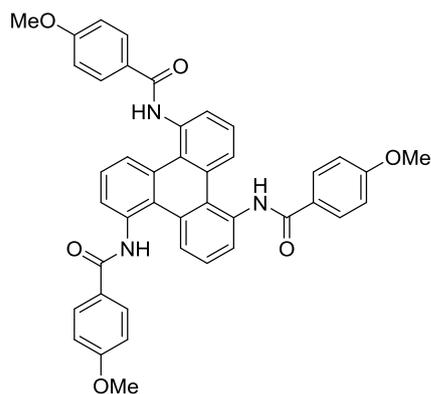
***N,N',N''*-(Triphenylene-1,5,9-triyl)tribenzamide (**5d**)**

Following the procedure described for **5b**, the reaction of **4** (1.53 g, 5.6 mmol), Et₃N (3.40 g, 33.6 mmol), benzoyl chloride (3.54 g, 25.2 mmol) in THF (58 mL) afforded the desired product **5d** as a white solid. Yield: 1.60 g (49%); M.p. 301-302 °C. IR (KBr, cm⁻¹): 3256, 3061, 3019, 1644, 1580, 1513, 1476, 1302, 702; ¹H NMR (500 MHz, DMSO-*d*₆): δ 10.73 (s, 3H), 8.73 (d, *J* = 8.2 Hz, 3H), 8.07 (d, *J* = 7.4 Hz, 6H), 7.50-7.67 (m, 12H), 7.43 (t, *J* = 8.0 Hz, 3H); ¹³C NMR (125 MHz, DMSO-*d*₆): δ 165.5, 134.5, 134.2, 131.7, 130.9, 128.6, 128.4, 127.7, 127.5, 126.1, 123.7; HRMS (ESI) *m/z* calcd for C₃₉H₂₇N₃NaO₃ [M+Na]⁺ 608.1945, found 608.1963.



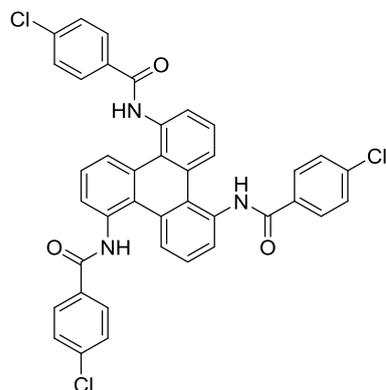
***N,N',N''*-(Triphenylene-1,5,9-triyl)tris(4-methylbenzamide) (**5e**)**

Following the procedure for **5b**, the reaction of **4** (0.88 g, 3.21 mmol), Et₃N (1.93 g, 19.10 mmol) and 4-methylbenzoyl chloride (2.24 g, 14.5 mmol) in THF (33 mL) afforded the desired product **5e** as a white solid. Yield: 1.11 g (55%); M.p. 298-299 °C. IR (KBr, cm⁻¹): 3448, 1648, 1523, 1498, 1472, 749; ¹H NMR (500 MHz, DMSO-*d*₆): δ 10.62 (s, 3H), 8.69 (d, *J* = 8.2 Hz, 3H), 7.98 (d, *J* = 7.8 Hz, 6H), 7.51 (d, *J* = 7.5 Hz, 3H), 7.30-7.44 (m, 9H), 2.42 (s, 9H); ¹³C NMR (125 MHz, DMSO-*d*₆): δ 165.3, 141.7, 134.2, 131.7, 130.8, 129.1, 128.4, 127.7, 127.4, 126.0, 123.6, 21.0; HRMS (ESI) *m/z* calcd for C₄₂H₃₃N₃NaO₃ [M+Na]⁺ 650.2420, found 650.2413.



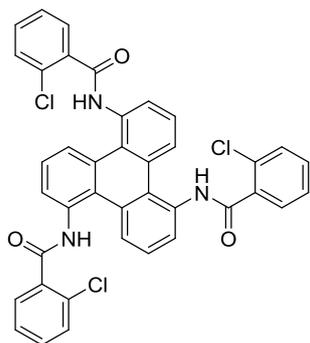
***N,N',N''*-(Triphenylene-1,5,9-triyl)tris(4-methoxybenzamide) (5f)**

Following the procedure for **5b**, the reaction of **4** (0.50 g, 1.83 mmol), Et₃N (1.11 g, 10.98 mmol), *p*-anisoyl chloride (1.40 g, 8.24 mmol) in THF (30 mL) afforded the desired product **5f** as a white solid. Yield: 0.59 g (48%); M.p. 226-227 °C. IR (KBr, cm⁻¹): 3249, 3066, 2936, 2837, 1654, 1604, 1498, 1467, 1251, 1174, 1023, 756; ¹H NMR (500 MHz, DMSO-*d*₆): δ 10.53 (s, 3H), 8.67 (d, *J* = 8.1 Hz, 3H), 8.04 (d, *J* = 8.7 Hz, 6H), 7.50 (d, *J* = 7.5 Hz, 3H), 7.38 (t, *J* = 8 Hz, 3H), 7.10 (d, *J* = 8.8 Hz, 6H), 3.86 (s, 9H); ¹³C NMR (125 MHz, DMSO-*d*₆): δ 165.4, 162.4, 134.8, 131.3, 130.1, 128.9, 127.9, 127.1, 126.4, 123.9, 114.2, 55.9; HRMS (MALDI/DHB) *m/z* calcd for C₄₂H₃₄N₃O₆ [M+H]⁺ 676.2442, found 676.2447.



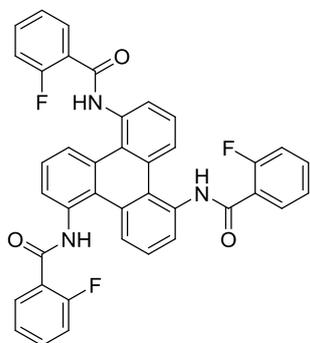
***N,N',N''*-(Triphenylene-1,5,9-triyl)tris(4-chlorobenzamide) (5g)**

Following the procedure for **5b**, the reaction of **4** (1.00 g, 3.66 mmol), Et₃N (2.22 g, 21.96 mmol), 4-chlorobenzoyl chloride (2.88 g, 16.47 mmol) in THF (38 mL) afforded the desired product **5g** as a white solid. Yield: 1.56 g (62 %); M.p. 295-296 °C. IR (KBr, cm⁻¹): 3266, 3065, 1648, 1594, 1517, 1482, 1273, 1092, 753; ¹H NMR (500 MHz, DMSO-*d*₆): δ 10.81 (s, 3H), 8.68 (d, *J* = 8.2 Hz, 3H), 8.08 (d, *J* = 8.5 Hz, 6H), 7.67 (d, *J* = 8.4 Hz, 6H), 7.54 (d, *J* = 7.5 Hz, 3H), 7.43 (t, *J* = 8.0 Hz, 3H); ¹³C NMR (125 MHz, DMSO-*d*₆): δ 164.9, 137.1, 134.4, 133.7, 131.2, 130.1, 129.1, 128.8, 127.8, 126.7, 124.2; HRMS (MALDI/DHB) *m/z* calcd for C₃₉H₂₄Cl₃N₃NaO₃ [M+Na]⁺ 710.0775, found 710.0780.



***N,N',N''*-(Triphenylene-1,5,9-triyl)tris(2-chlorobenzamide) (**5h**)**

To a solution of **4** (0.53 g, 1.94 mmol) in anhydrous dichloromethane (25 mL) with pyridine (844 mg, 10.67 mmol) and DMAP (23.7 mg, 0.19 mmol) was added dropwise 2-chlorobenzoyl chloride (1.36 g, 7.76 mmol) dissolved in anhydrous DCM (5 mL). The mixture was stirred at 40 °C under N₂ for 8 h. The reaction mixture was diluted with water, and neutralized with saturated NaHCO₃ solution. The resulting precipitate was recovered by filtration, washed with water, DCM and dried. The desired product **5h** was obtained as a white solid. Yield: 0.57 g (43%); M.p. > 300 °C. IR (KBr, cm⁻¹): 3229, 3063, 3023, 1655, 1510, 1470, 1302, 741; ¹H NMR (500 MHz, DMSO-*d*₆): δ 10.85 (s, 3H), 8.88 (d, *J* = 7.9 Hz, 3H), 7.75-7.68 (m, 3H), 7.66-7.58 (m, 9H), 7.57-7.49 (m, 6H); ¹³C NMR (125 MHz, DMSO-*d*₆): δ 165.8, 137.4, 134.0, 131.5, 131.1, 130.6, 130.3, 129.0, 128.5, 127.8, 127.4, 126.8, 125.0; HRMS (MALDI/DHB) *m/z* calcd for C₃₉H₂₅Cl₃N₃O₃ [M+H]⁺ 688.0956, found 688.0962.



***N,N',N''*-(Triphenylene-1,5,9-triyl)tris(2-fluorobenzamide) (**5i**)**

Following the procedure for **5h**, the reaction of **4** (1.50 g, 5.49 mmol), pyridine (2.39 g, 30.20 mmol), DMAP (67.10 mg, 0.55 mmol) 2-fluorobenzoyl chloride (3.48 g, 21.95 mmol) in DCM (65 mL) afforded the desired product **5i** as a white solid. Yield: 1.98g (57%); M.p. 293-294 °C. IR (KBr, cm⁻¹): 3254, 3072, 3031, 1647, 1519, 1480, 1304, 754; ¹H NMR (500 MHz, DMSO-*d*₆): δ 10.75 (s, 3H), 8.85 (d, *J* = 8.0 Hz, 3H), 7.76 (t, *J* = 7.0 Hz, 3H), 7.70-7.56 (m, 6H), 7.56-7.47 (m, 3H), 7.46-7.32 (m, 6H); ¹⁹F NMR (470 MHz, DMSO-*d*₆): δ -114.4 (m, Ar-F); ¹³C NMR (125 MHz, DMSO-*d*₆): δ 163.6, 159.7 (d, ¹*J*_{C-F} = 247.7 Hz), 134.0, 133.1 (³*J*_{C-F} = 8.4 Hz), 131.1, 130.4 (⁴*J*_{C-F} = 3.0 Hz), 128.5, 127.5, 126.7, 125.1, 125.0 (³*J*_{C-F} = 12.5 Hz), 124.6, 116.8 (²*J*_{C-F} = 21.8 Hz); HRMS (MALDI/DHB) *m/z* calcd for C₃₉H₂₅F₃N₃O₃ [M+H]⁺ 640.1843, found 640.1857.

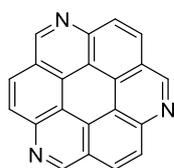
General procedures for the synthesis of TACs (1a-i)

Method A:

Compound **5** (0.3 mmol), sodium chloride (876.6 mg, 15.0 mmol), and anhydrous aluminum chloride (668.0 mg, 5.0 mmol) were charged into a sealed tube under N₂. The mixture was stirred at 220 °C for 4 h. After cooled to room temperature, the mixture was basified with 15% aqueous NaOH solution and filtered through diatomite, washed with water and dried. The product dispersed in the diatomite was dissolved in DCM/MeOH = 10 : 1, and filtered. The filtrate was evaporated in vacuum to give the crude product, which was further purified by column chromatography packed with silica gel or by washing with hot DCM or DCM/MeOH to afford the pure product **1**.

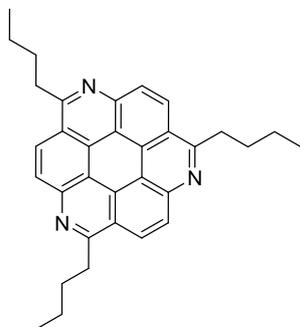
Method B:

A solution of amide compounds (0.3 mmol) and P₂O₅ (0.94 g, 6.6 mmol) in freshly distilled POCl₃ (3 mL) was stirred under reflux overnight. The mixture was concentrated under vacuum, and water was added slowly. The aqueous layer was adjusted to pH = 10 with 15 % aqueous NaOH solution and then filtered, washed with water, and dried. The resulting precipitate was dissolved in DCM/MeOH = 10 : 1, and filtered. The filtrate was evaporated in vacuum to give the crude product, which was purified by column chromatography or by washing with hot DCM or DCM/MeOH to afford pure product **1**.



1,5,9-Triazocoronene (1a)

Following **Method A**, Yield: 48.3 mg (53%), yellow solid, M.p. > 300 °C (hot washing with DCM/MeOH = 10 : 1). IR (KBr, cm⁻¹): 3049, 3029, 1630, 1595, 1448, 1358, 1307, 806, 775, 534; ¹H NMR (500 MHz, CDCl₃ : MeOD-*d*₄ = 0.5 mL : 0.2 mL): δ 10.24 (s, 3H), 9.03 (d, *J* = 8.7 Hz, 3H), 8.98 (d, *J* = 8.7 Hz, 3H); ¹³C NMR (125 MHz, TFA-*d*₁): δ 143.7, 129.7, 127.2, 118.5, 115.5, 113.8, 106.9; HRMS (ESI) *m/z* calcd for C₂₁H₁₀N₃ [M+H]⁺ 304.0869, found 304.0869.

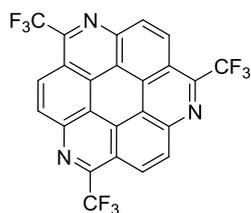


2,6,10-Tributyl-1,5,9-triazocoronene (1b)

Following **Method A**, Yield: 79 % (recrystallization with CH₃CN : THF = 4 : 1);

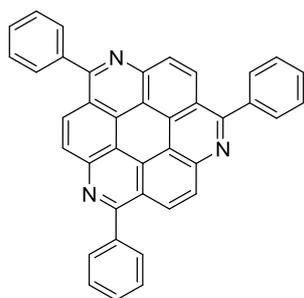
Following **Method B**, Yield: 53 % (hot washing with EtOH). Pale yellow solid, M.p. 158-159 °C; IR (KBr, cm^{-1}): 3061, 3025, 2954, 2922, 2857, 1910, 1626, 1448, 1261, 1097, 1025, 807, 696; ^1H NMR (500 MHz, CDCl_3): δ 9.10 (d, $J = 8.9$ Hz, 3H), 8.95 (d, $J = 8.9$ Hz, 3H), 3.93 (t, $J = 8.0$ Hz, 6H), 2.26-2.13 (m, 6H), 1.78-1.68 (m, 6H), 1.11 (t, $J = 7.4$ Hz, 9H); ^{13}C NMR (125 MHz, CDCl_3): δ 163.5, 142.9, 127.1, 125.4, 124.1, 119.8, 113.5, 36.7, 32.8, 23.4, 14.2; HRMS (MALDI/DHB) m/z calcd for $\text{C}_{33}\text{H}_{34}\text{N}_3$ $[\text{M}+\text{H}]^+$ 472.2747, found 472.2750.

Suitable single crystals for X-ray crystallography were obtained as brilliant yellow needles by slow diffusion of CH_3CN into a solution of compound **1b** in THF at room temperature.



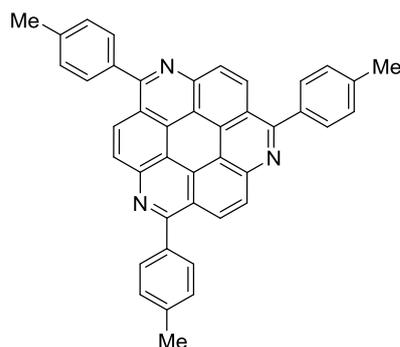
2,6,10-Tri(trifluoromethyl)-1,5,9-triazocoronene (**1c**)

Following **Method B**, Yield: 15% (purified by alkaline aluminum oxide column chromatography using petroleum ether/ethyl acetate = 5 : 1 as an eluent). Yellow solid, M.p. > 300 °C. IR (KBr, cm^{-1}): 3080, 2921, 2856, 1629, 1597, 1493, 1353, 1264, 1198, 1138, 1040, 904, 834, 737; ^1H NMR (500 MHz, CDCl_3): δ 9.62 (dq, $J = 9.2, 1.8$ Hz, 3H), 9.49 (d, $J = 9.2$ Hz, 3H); ^{19}F NMR (470 MHz, CDCl_3): δ -61.4 (s, CF_3); The poor solubility precluded solution ^{13}C NMR characterization. HRMS (MALDI/DHB) m/z calcd for $\text{C}_{24}\text{H}_7\text{F}_9\text{N}_3$ $[\text{M}+\text{H}]^+$ 508.0491, found 508.0503.



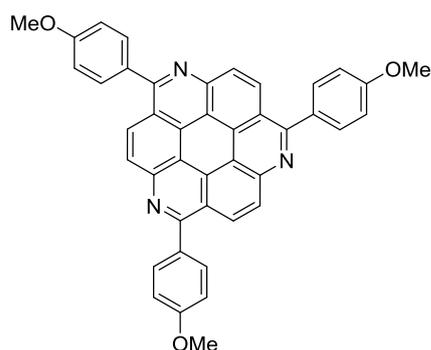
2,6,10-Triphenyl-1,5,9-triazocoronene (**1d**)

Following **Method A**, Yield: 74% (hot washing with DCM). Following **Method B**, Yield: 64%. Yellow solid, M.p. > 300 °C. IR (KBr, cm^{-1}): 3056, 1623, 1583, 1446, 1328, 1020, 829, 769, 707; ^1H NMR (500 MHz, CDCl_3 : TFA- $d_1 = 0.5$ mL : 15 μL): δ 9.69 (d, $J = 8.8$ Hz, 3H), 9.65 (d, $J = 9.0$ Hz, 3H), 8.19 (d, $J = 7.3$ Hz, 6H), 8.01-7.95 (m, 3H), 7.94-7.87 (m, 6H); ^{13}C NMR (125 MHz, CDCl_3 : TFA- $d_1 = 0.5$ mL : 15 μL): δ 163.9, 140.3, 134.5, 133.6, 131.7, 131.5, 130.2, 127.6, 125.7, 121.5, 115.3; HRMS (ESI) m/z calcd for $\text{C}_{39}\text{H}_{22}\text{N}_3$ $[\text{M}+\text{H}]^+$ 532.1808, found 532.1807.



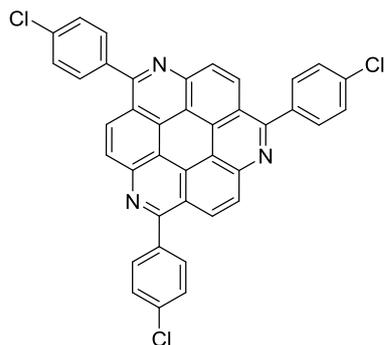
2,6,10-Tri(4-methylphenyl)-1,5,9-triazocoronene (1e)

Following **Method A**, Yield: 64 % (hot washing with DCM/MeOH = 20 : 1); Following **Method B**, Yield: 63 %. Yellow solid, M.p. > 300 °C. IR (KBr, cm^{-1}): 3028, 2860, 1623, 1583, 1478, 1440, 1377, 1324, 831, 731; ^1H NMR (500 MHz, CDCl_3 : TFA- d_1 = 0.5 mL : 10 μL): δ 9.62 (d, J = 9.1 Hz, 3H), 9.57 (d, J = 9.1 Hz, 3H), 8.12 (d, J = 7.7 Hz, 6H), 7.69 (d, J = 7.7 Hz, 6H), 2.66 (s, 9H); ^{13}C NMR (125 MHz, CDCl_3 : TFA- d_1 = 0.5 mL : 10 μL): δ 163.5, 144.0, 141.0, 133.4, 131.7, 130.7, 130.0, 127.3, 126.1, 121.1, 115.1, 21.9; HRMS (MALDI/DHB) m/z calcd for $\text{C}_{42}\text{H}_{28}\text{N}_3$ $[\text{M}+\text{H}]^+$ 574.2278, found 574.2281.



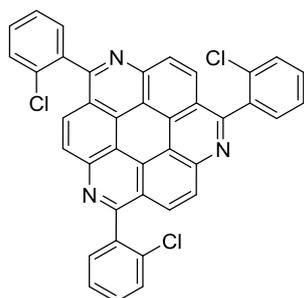
2,6,10-Tri(4-methoxyphenyl)-1,5,9-triazocoronene (1f)

Following **Method B**, Yield: 67% (hot washing with DCM/MeOH = 20 : 1). Yellow solid, M.p > 300 °C. IR (KBr, cm^{-1}): 3064, 3002, 2929, 2834, 1610, 1439, 1327, 1251, 1173, 1024, 836; ^1H NMR (500 MHz, TFA- d_1): δ 9.81 (d, J = 9.1 Hz, 3H), 9.57 (d, J = 9.1 Hz, 3H), 8.26 (d, J = 8.2 Hz, 6H), 7.48 (d, J = 8.3 Hz, 6H), 4.06 (s, 9H); ^{13}C NMR (125 MHz, CDCl_3 : TFA- d_1 = 0.5 mL : 0.1 mL): δ 166.5, 164.0, 138.6, 136.9, 134.9, 128.6, 123.8, 121.8, 121.0, 117.0, 115.4, 56.4; HRMS (MALDI/DHB) m/z calcd for $\text{C}_{42}\text{H}_{28}\text{N}_3\text{O}_3$ $[\text{M}+\text{H}]^+$ 622.2125, found 622.2128.



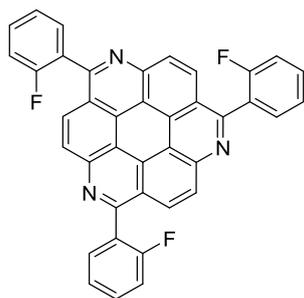
2,4,6-Tri(4-chlorophenyl)-1,5,9-triazocoronene (1g)

Following **Method A**, Yield: 51% (hot washing with DCM : MeOH = 20 : 1). Following **Method B**, Yield: 74%. Yellow solid, M.p. > 300 °C. IR (KBr, cm⁻¹): 2917, 1623, 1588, 1477, 1440, 1321, 1091, 1012, 836, 730; ¹H NMR (500 MHz, CDCl₃: TFA-*d*₁ = 0.45 mL : 30 μL): δ 9.72 (d, *J* = 8.8 Hz, 3H), 9.68 (d, *J* = 8.6 Hz, 3H), 8.17 (d, *J* = 7.5 Hz, 6H), 7.93 (d, *J* = 7.7 Hz, 6H); ¹³C NMR (125 MHz, CDCl₃: TFA-*d*₁ = 0.6 mL : 40 μL): δ 163.0, 141.7, 139.6, 134.8, 132.8, 130.7, 128.2, 127.6, 125.2, 121.5, 115.3; HRMS (MALDI/DHB) *m/z* calcd for C₃₉H₁₉Cl₃N₃ [M+H]⁺ 634.0639, found 634.0642.



2,6,10-Tri(2-chlorophenyl)-1,5,9-triazocoronene (1h)

Following **Method A**, Yield: 56% (purified by silica gel column chromatography using petroleum ether/dichloromethane = 1 : 5 as an eluent). Yellow solid, M.p. > 300 °C, IR (KBr, cm⁻¹): 3055, 1623, 1435, 1324, 829, 753, 733. This compound contains inseparable isomers, which are distinguishable from the ¹H NMR spectrum: Major isomer: ¹H NMR (500 MHz, CDCl₃): δ 9.23 (dd, *J* = 9.0, 1.8 Hz, 3H), 8.89 (d, *J* = 9.0 Hz, 3H), 7.90-7.84 (m, 3H), 7.79-7.73 (m, 3H), 7.69-7.62 (m, 6H); Minor isomer: ¹H NMR (500 MHz, CDCl₃): δ 9.16 (d, *J* = 9.0 Hz, 3H), 8.81 (d, *J* = 9.0 Hz, 3H), 8.03-8.01 (m, 3H), 7.79-7.73 (m, 3H), 7.69-7.62 (m, 6H). The ¹³C NMR of the two isomer was not assignable: ¹³C NMR (125 MHz, CDCl₃): δ 160.4, 160.2, 144.3, 144.1, 138.6, 138.5, 133.8, 133.7, 132.0, 131.9, 130.8, 130.3, 130.2, 129.2, 129.0, 128.7, 127.5, 127.4, 125.8, 125.5, 121.9, 121.7, 115.6, 115.3. Variable temperature ¹H NMR (500 MHz, DMSO-*d*₆, 80 °C): δ 9.22 (d, *J* = 9.0 Hz, 3H), 8.83 (d, *J* = 9.0 Hz, 3H), 7.96 (d, *J* = 7.0 Hz, 3H), 7.86 (d, *J* = 7.7 Hz, 3H), 7.83-7.73 (m, 6H) (see also Figure S1). HRMS (MALDI/DHB) *m/z* calcd for C₃₉H₁₉Cl₃N₃ [M+H]⁺ 634.0645, found 634.0641.



2,6,10-Tri(2-fluorophenyl)-1,5,9-triazocoronene (1i)

Following **Method A**, Yield: 50% (purified by silica gel column chromatography using petroleum ether/dichloromethane = 1 : 5 as an eluent). Yellow solid, M.p. > 300 °C. IR (KBr, cm^{-1}): 3058, 1619, 1449, 1328, 1214, 829, 755; ^1H NMR (500 MHz, CDCl_3): δ 9.20 (d, $J = 8.7$ Hz, 3H), 8.99 (d, $J = 7.5$ Hz, 3H), 8.09 (s, 3H), 7.77-7.68 (m, 3H), 7.59 (t, $J = 7.4$ Hz, 3H), 7.46 (t, $J = 9.2$ Hz, 3H); ^{19}F NMR (470 MHz, CDCl_3): δ -113.5 (s, Ar-F); ^{13}C NMR (125 MHz, CDCl_3): δ 160.4 (d, $^1J_{\text{C-F}} = 247.2$ Hz), 157.3, 144.1, 132.6 ($^4J_{\text{C-F}} = 3.2$ Hz), 131.5 ($^3J_{\text{C-F}} = 7.8$ Hz), 128.9, 128.5 ($^4J_{\text{C-F}} = 2.7$ Hz), 127.4 ($^3J_{\text{C-F}} = 15.4$ Hz), 125.4, 125.0 ($^4J_{\text{C-F}} = 3.3$ Hz), 121.6, 116.3 ($^2J_{\text{C-F}} = 21.3$ Hz), 114.9; HRMS (MALDI/DHB) m/z calcd for $\text{C}_{39}\text{H}_{19}\text{F}_3\text{N}_3$ $[\text{M}+\text{H}]^+$ 586.1526, found 586.1524.

3. Variable-temperature NMR Studies of **1h** and **5a**

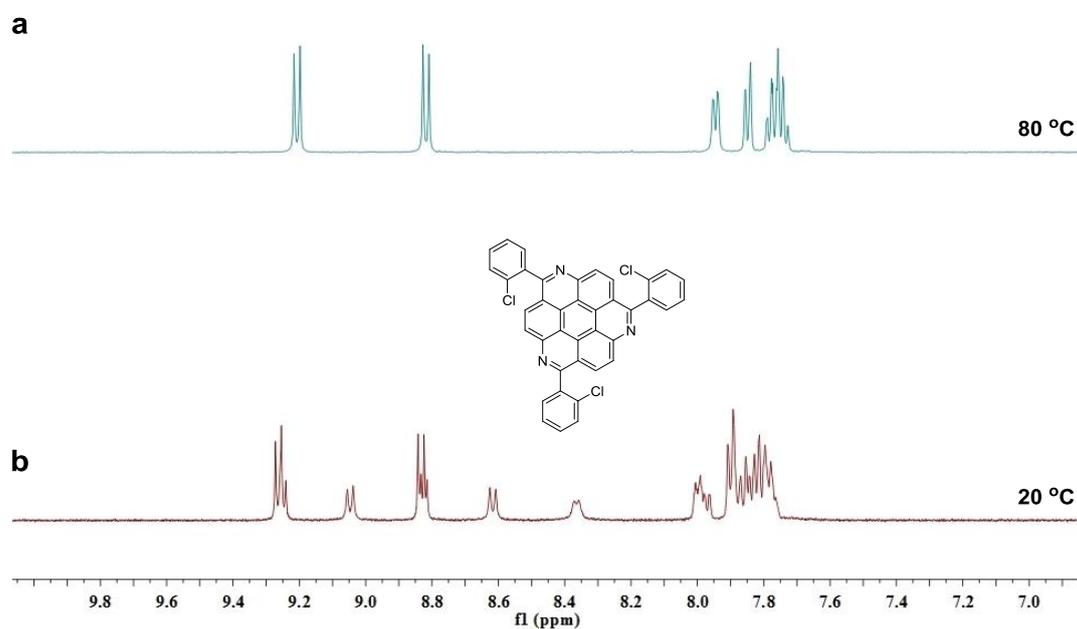


Figure S1. Variable-temperature ^1H NMR spectra of **1h** (DMSO- d_6 , 500 MHz).

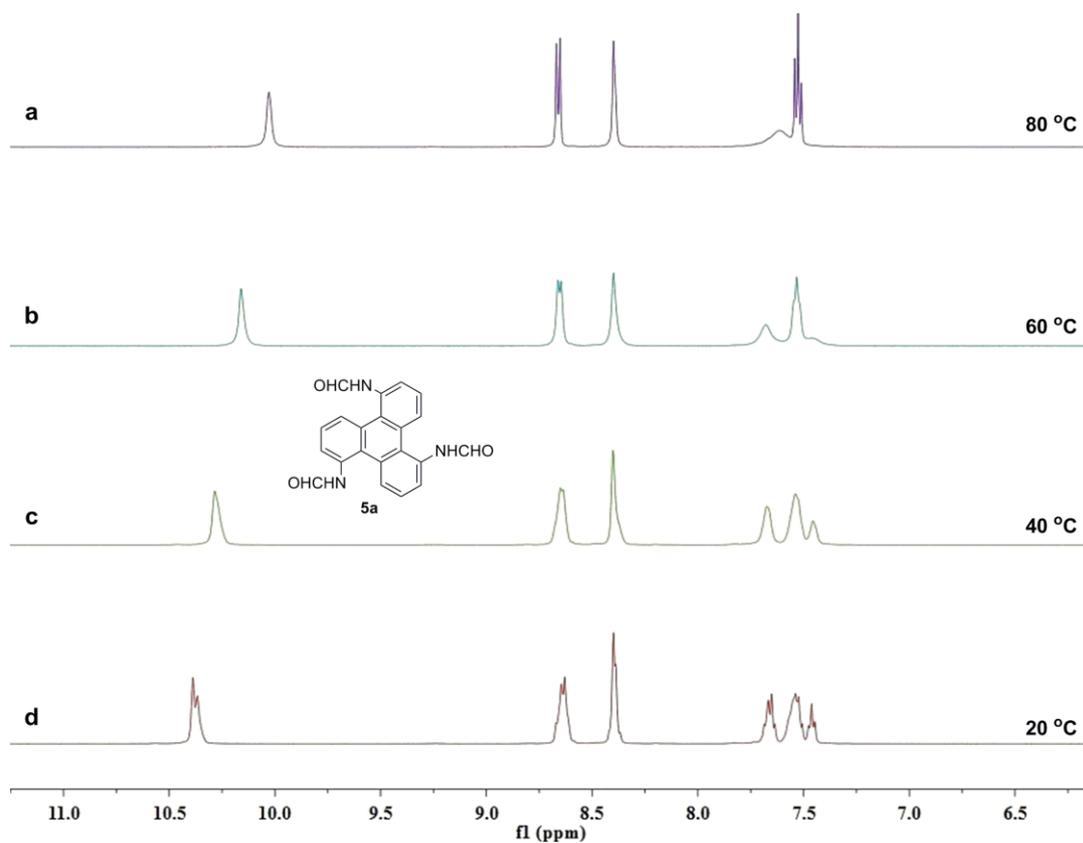


Figure S2. Variable-temperature ^1H NMR spectra of **5a** (DMSO- d_6 , 500 MHz).

4. X-ray Crystallography of **1b**

Suitable single crystals for X-ray crystallography were obtained as long brilliant yellow needles by slow diffusion of CH₃CN into a solution of compound **1b** in THF at room temperature.

The crystal structure was recorded on SMART APEXII X-ray diffraction spectrometer with a graphite-monochromatized MoK α ($\lambda = 0.71073 \text{ \AA}$) radiation at 293(2) K. The structure was solved and refined by SHELXL-97. The crystallographic details are given in the attached CIF file. The crystallographic data for the structure reported in this paper have been deposited with the Cambridge Crystallographic Data Centre as supplementary publication no. 1040955 for **1b**. These data can be obtained free of charge from The Cambridge Crystallographic Data Centre via http://www.ccdc.cam.ac.uk/data_request/cif. It should be noted that the last two carbon atoms of the *n*-butyl group are somewhat disordered but not affect the interpretation of the structure and solid stacking.

Table S3 X-ray crystallographic structure and data for **1b**

Formula	C ₃₃ H ₃₃ N ₃
Crystal dimensions	0.19 × 0.07 × 0.04 mm
Crystal color	Yellow
Temperature	293(2) K
Wavelength	0.71073 Å
Crystal system, space group	Triclinic, P-1
<i>a</i>	8.299(16) Å
<i>b</i>	12.11(2) Å
<i>c</i>	13.39(3) Å
α	76.13(2)°
β	87.13(3)°
γ	87.08(3)°
Volume	1304(4) Å ³
<i>Z</i>	2
Absorption coefficient	0.070 mm ⁻¹
F(000)	504
Theta range for data collection	2.86-25.00°
Limiting indices	-9 ≤ <i>h</i> ≤ 9, -14 ≤ <i>k</i> ≤ 14, -15 ≤ <i>l</i> ≤ 15
Absorption correction	None
Goodness-of-fit on F^2	1.186
Refinement method	Full-matrix least-squares on F^2
Final R indices [$I > 2\sigma(I)$]	R1 = 0.0814, wR2 = 0.2619
R indices (all data)	R1 = 0.1221, wR2 = 0.3043

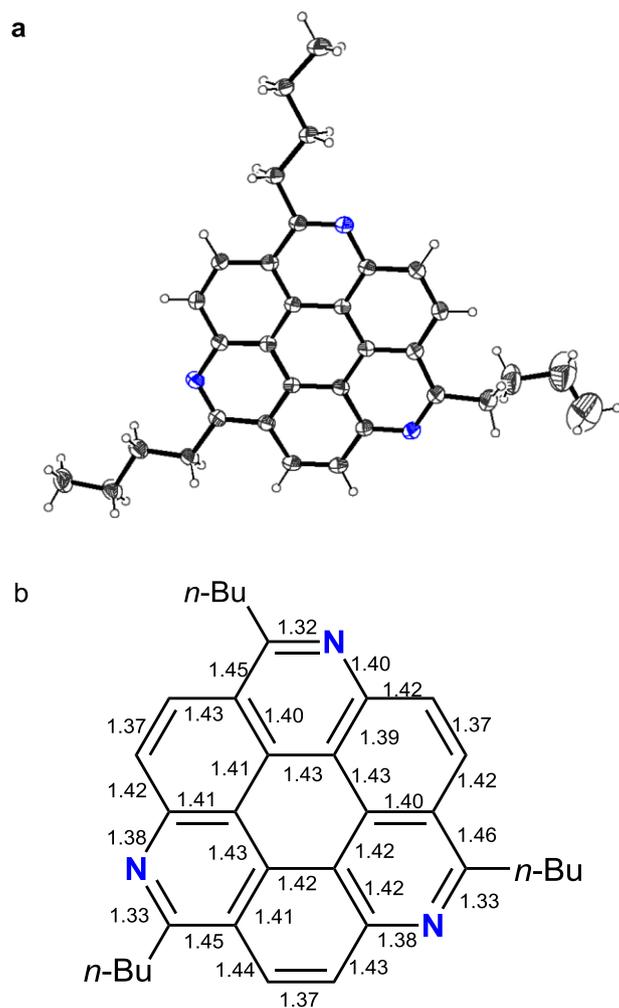


Figure S3. (a) Crystal structure of **1b**: Top view (thermal ellipsoids: 30% probability). (b) Bond lengths (Å). The terminal two carbon atoms of one *n*-butyl group are somewhat disordered.

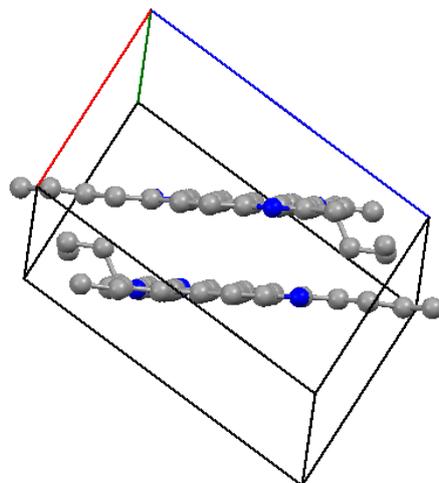


Figure S4. Two adjacent molecules in one unit cell.

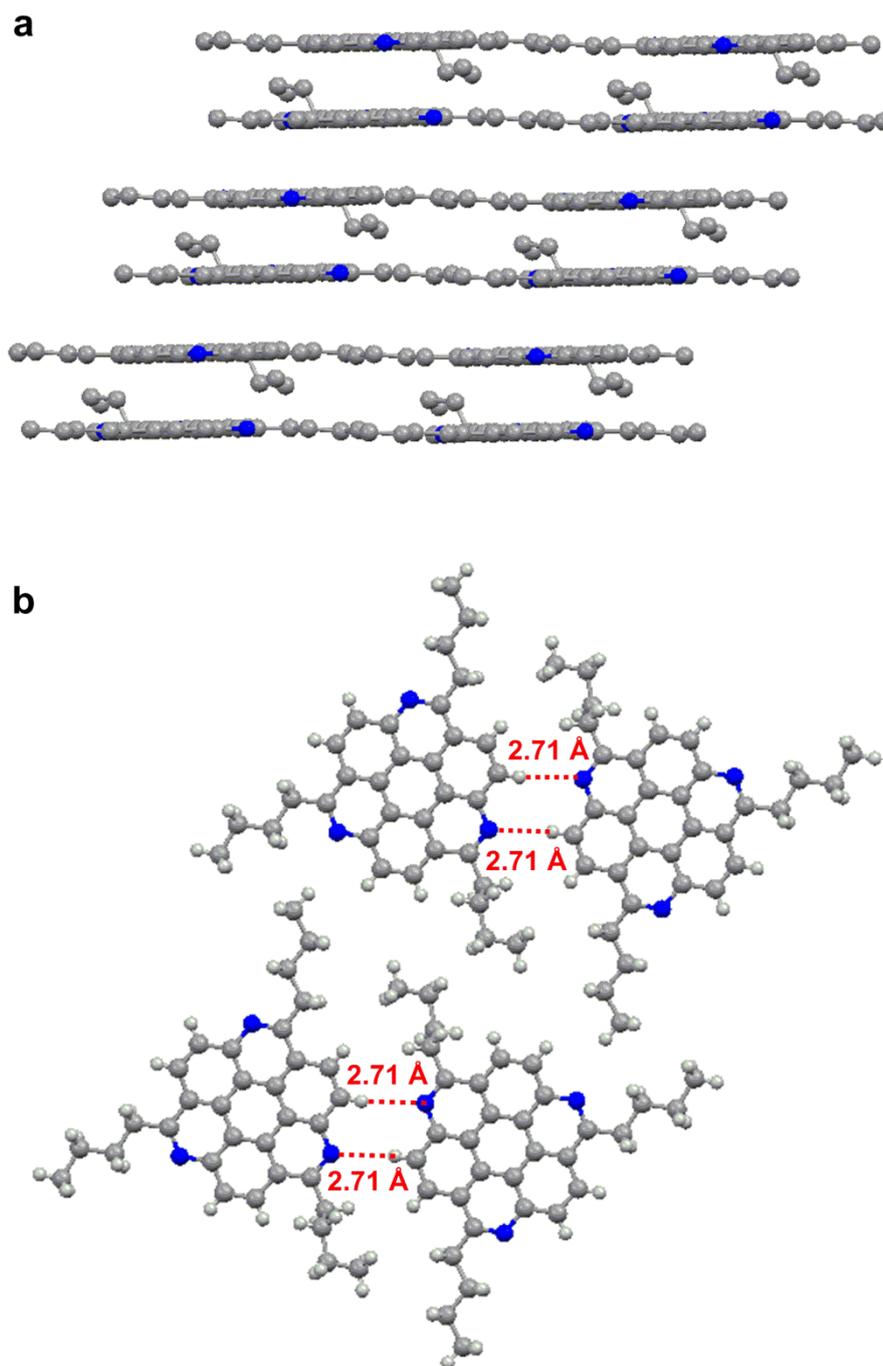
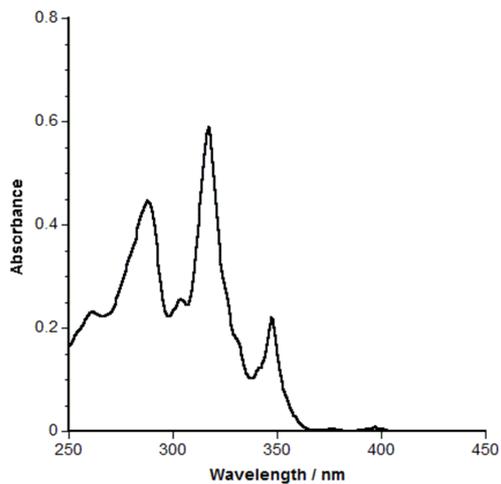


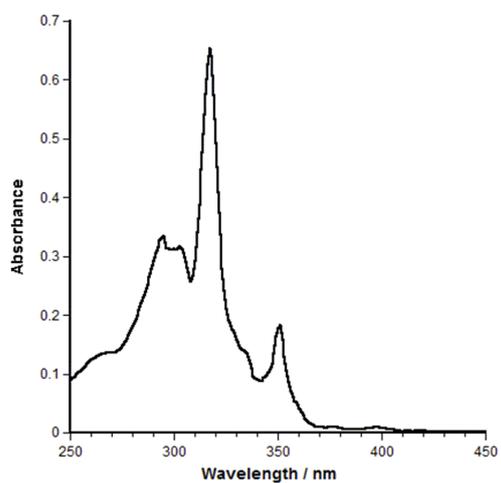
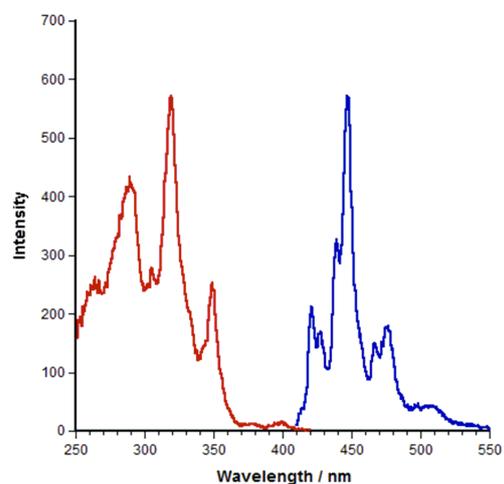
Figure S5. Packing diagram structure of **1b**: (a) Side view; (b) Top view, the dashed red lines indicate the CH- π interactions and the red numbers are the distances between the proton atoms to the nitrogen atoms.

5. Photophysical Properties

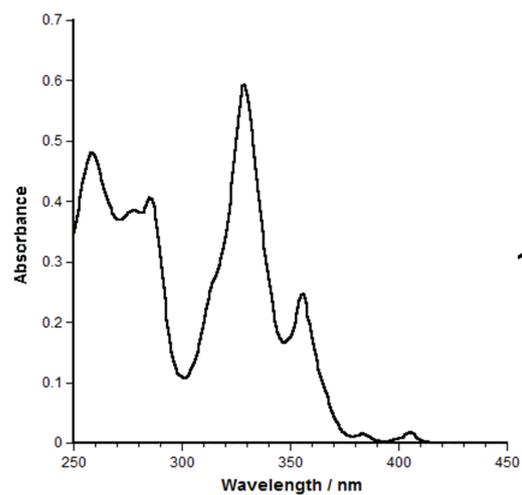
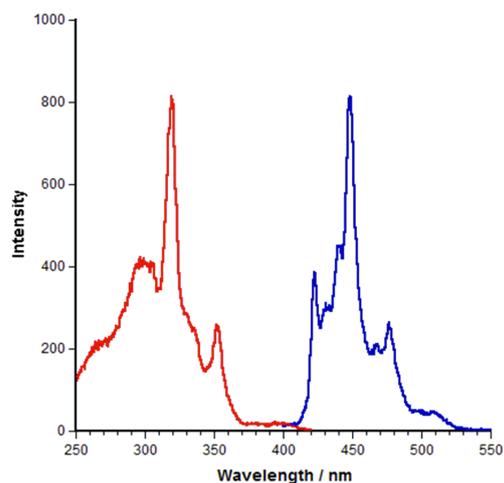
5.1 The electronic, emission and excitation spectra



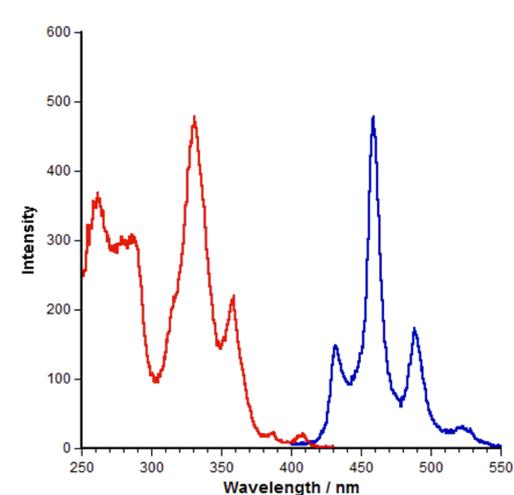
1a

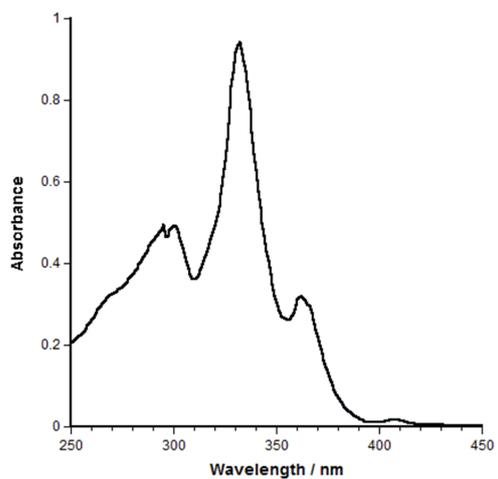


1b

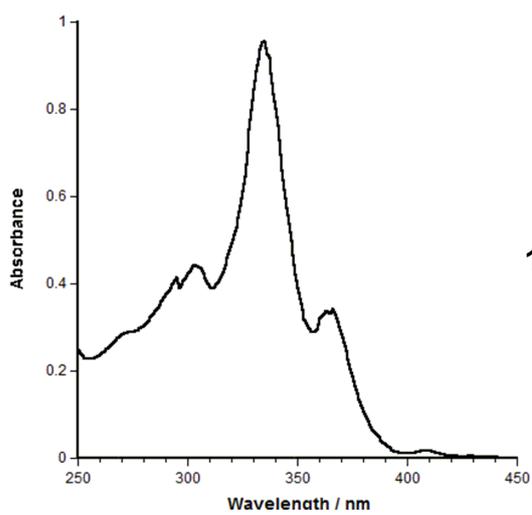
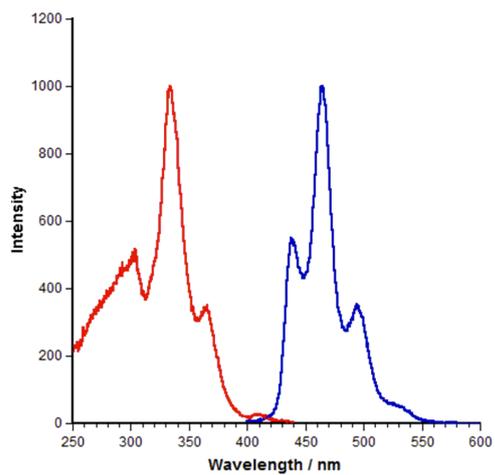


1c

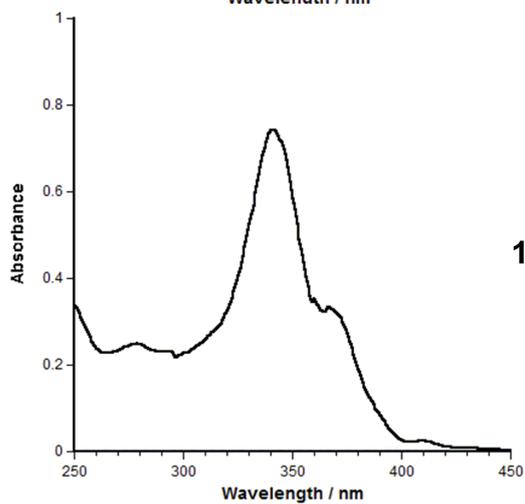
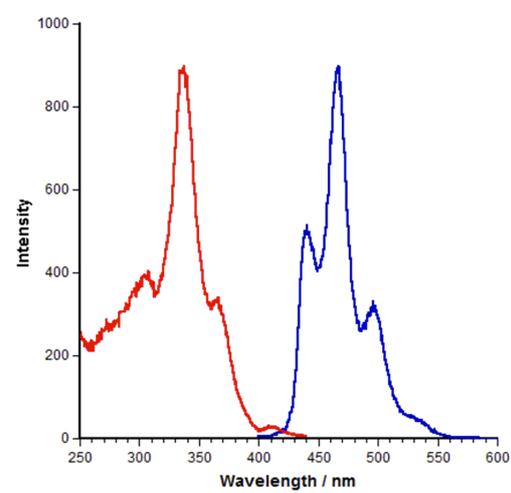




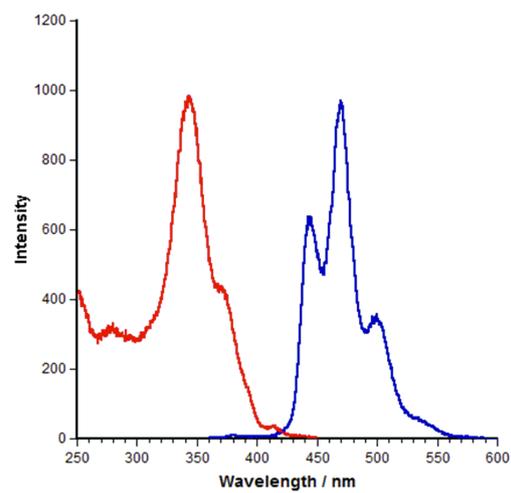
1d



1e



1f



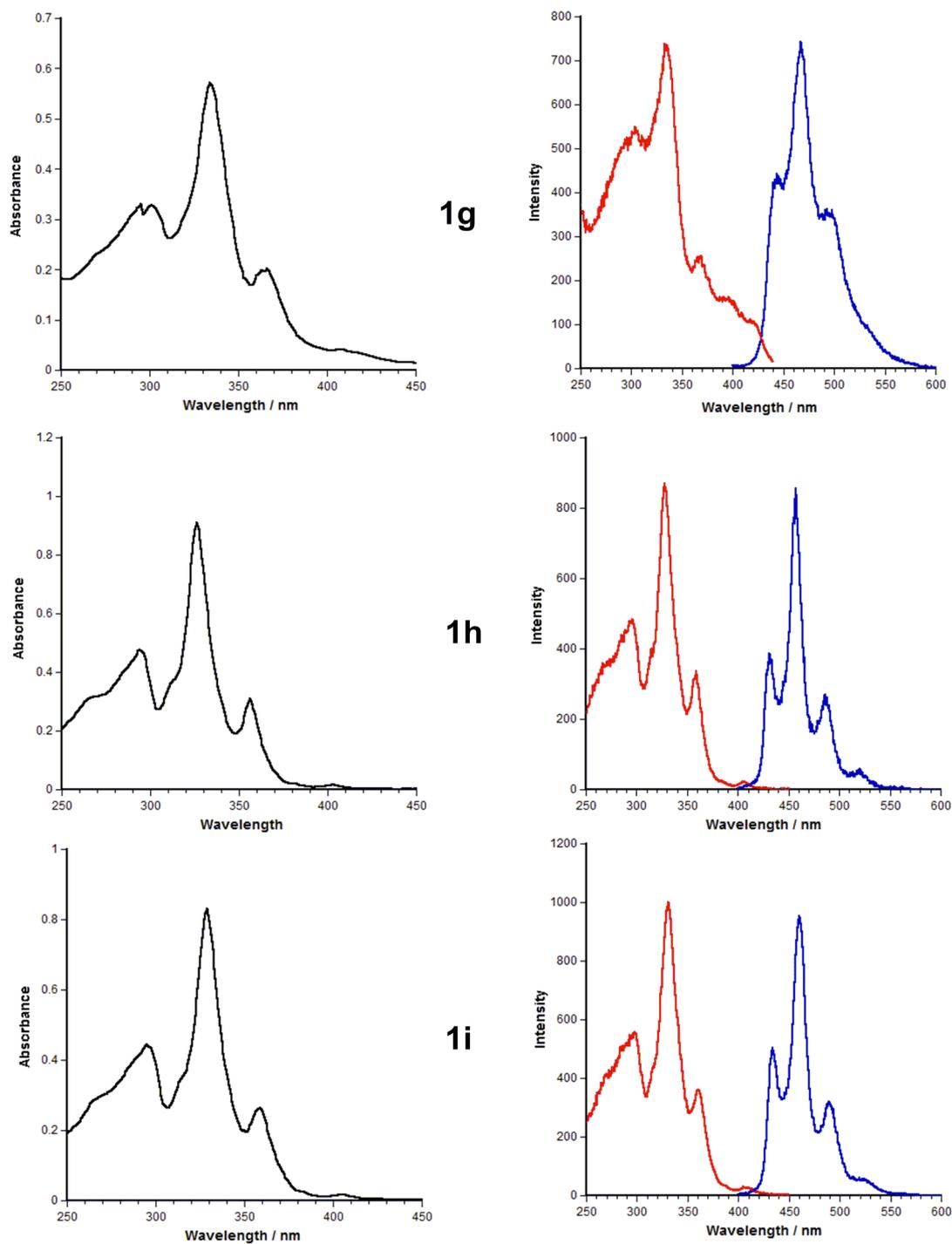
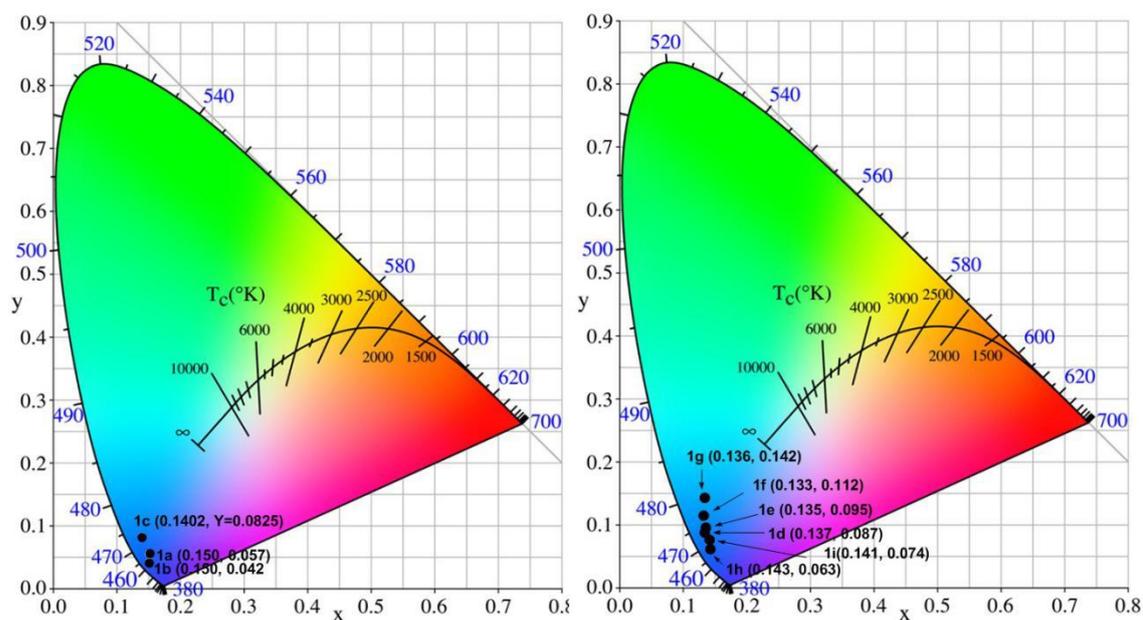


Figure S6. UV-Vis absorption (black) (1×10^{-5} M in CH_2Cl_2), emission (blue) and excitation spectra (red).

Table S4. Data of UV/vis absorption, Emission and Excitation spectra.

TACs	λ / nm	λ_{\max} / nm	ϵ / $M^{-1} \text{ cm}^{-1}$	E_g^a / eV	λ_{em}^b (nm)	λ_{exc} (nm)	Stock Shift (nm)
1a	397, 348, 317, 304, 289	317	58900	3.06	447	319	130
1b	398, 351, 317, 304	317	66200	3.08	448	319	131
1c	405, 356, 329, 286, 258	329	59300	3.00	458	331	129
1d	408, 362, 332, 301, 295	332	94100	2.99	465	334	133
1e	409, 366, 335, 304, 295	335	95500	2.94	467	337	132
1f	409, 369, 341	341	74300	2.92	470	344	129
1g	410, 366, 334, 302	334	57200	2.82	467	336	133
1h	403, 356, 326, 311, 295	326	91000	3.00	457	327	131
1i	405, 359, 329, 297	329	83100	2.95	460	331	131
Coronene ^c	340, 323, 301, 290	301	-	-	443	-	142

^aThe optical E_g was determined as the intersection of the x axis and a tangent line passing through the inflection point of the lowest-energy absorption. ^bExcited at the λ_{\max} of the absorption. ^cIn THF solution, see, Ref. [S3].

**Figure S7.** CIE chromaticity diagrams of **1a-1i** in solution.

6. Acid-induced Spectroscopic Changes for Selected TACs

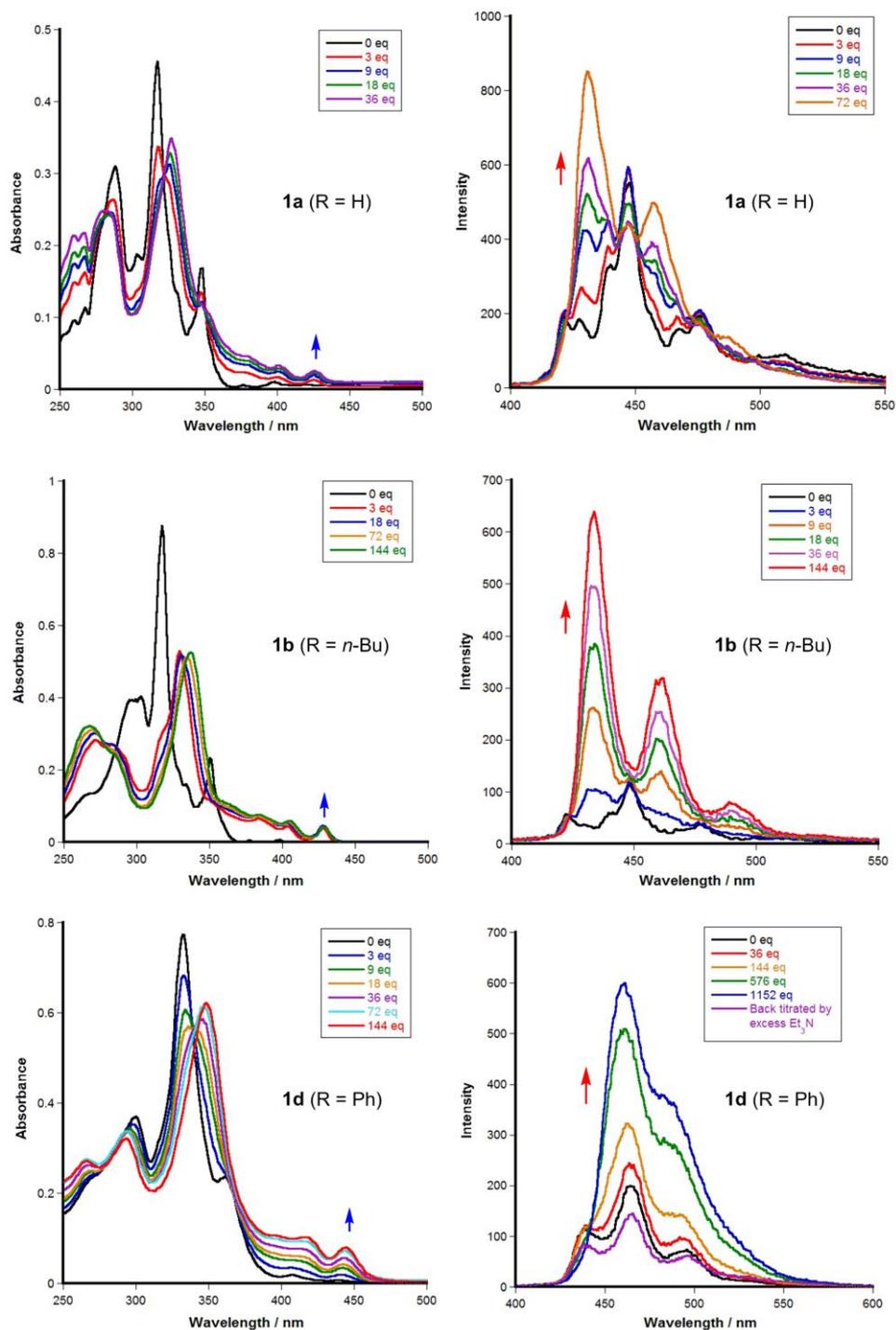


Figure S8. Acid-induced UV-vis absorption (left) and emission (right) changes of typical TACs in CH_2Cl_2 solution by adding trifluoroacetic acid. The wavelength where the absorbance is independent of the acid titration was selected as the excitation wavelength.

7. Electrochemical Properties (CV and DPV Measurement)

7.1 Cyclovoltammetry Measurements

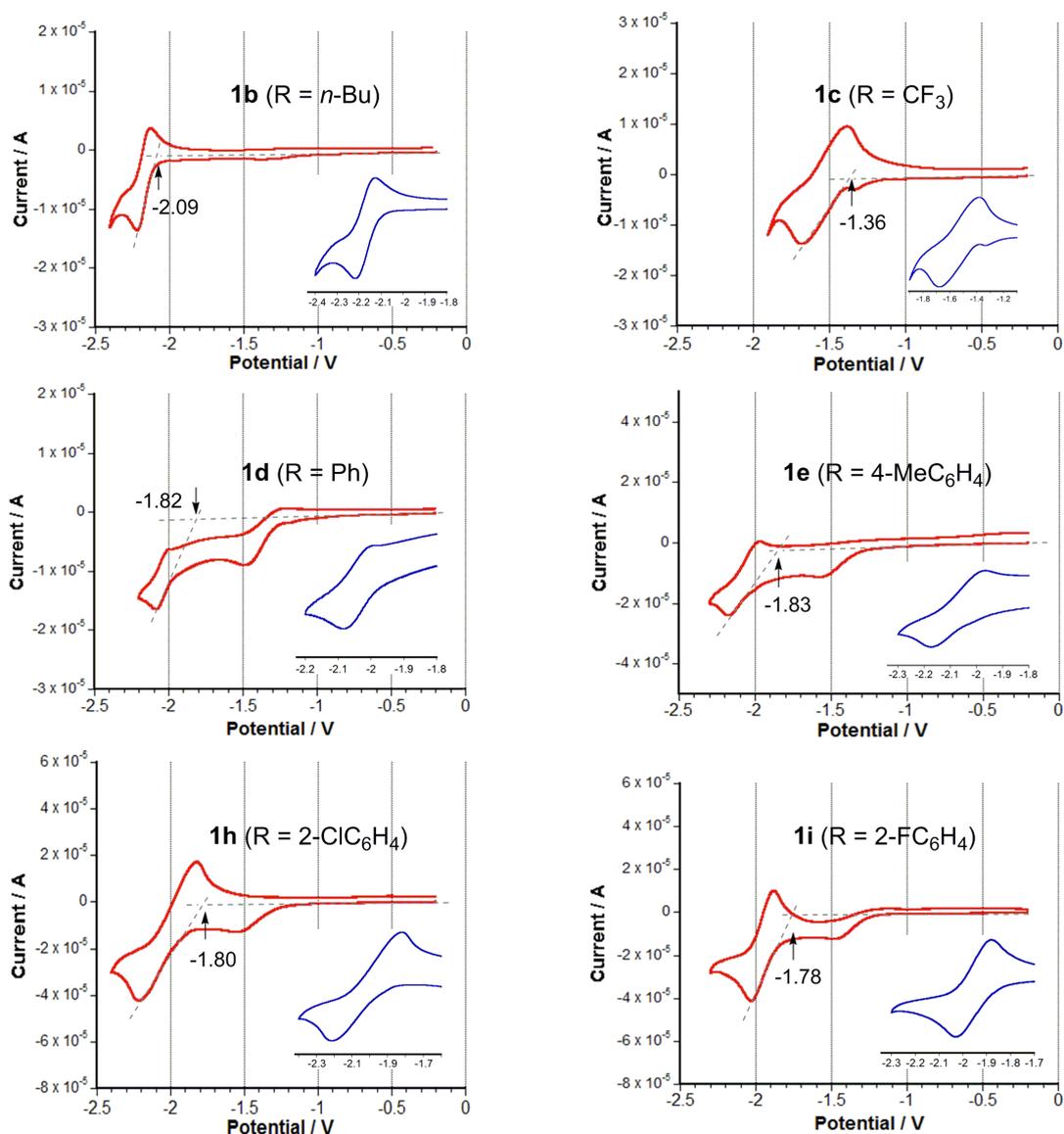


Figure S9. Cyclic voltammograms (red curves) of **1b-1e**, **1h** and **1i** in CH₂Cl₂ containing 0.10 M *n*-Bu₄NPF₆. Scan rate: 100 mV/s. The potentials were calibrated using the ferrocene/ferrocenium (Fc/Fc⁺) redox couple (0.20 V vs. Ag/Ag⁺) as an external standard which was measured under the same condition before and after measurement of the samples. The insets (blue curves) are the magnified reductive curves. The arrows indicate the onset of reductive potentials.

7.2 Differential Pulse Voltammetry (DPV) Measurements

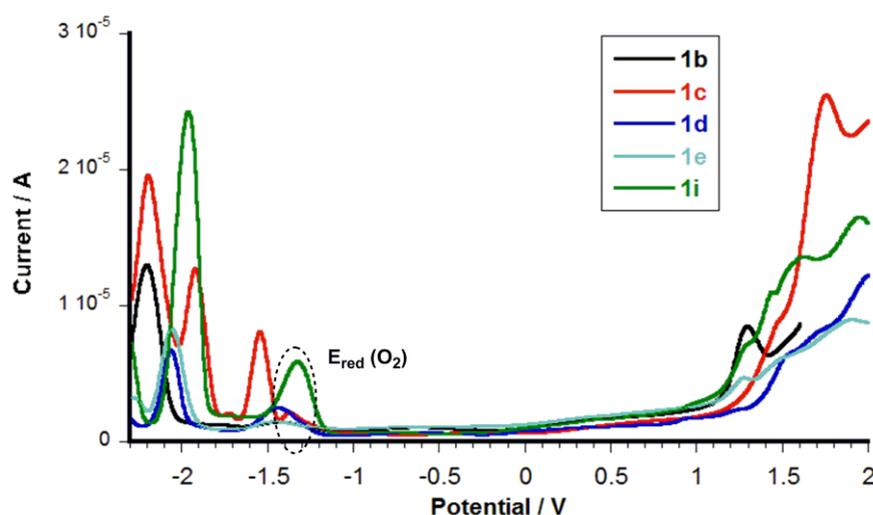


Figure S10. DPV Measurement of **1b-1e** and **1i** in CH_2Cl_2 using $n\text{-Bu}_4\text{NPF}_6$ (0.1 M) as electrolyte. The potentials were calibrated using the ferrocene/ferrocenium (Fc/Fc^+) redox couple (0.196 V vs. Ag/Ag^+) as an external standard. Conditions: $\text{Incr E (V)} = 0.004$; $\text{Amplitude (V)} = 0.05$; $\text{Pulse width (s)} = 0.05$; $\text{Sample width (s)} = 0.0167$; $\text{Pulse period (s)} = 0.2$; $\text{Quiet time (s)} = 2$; $\text{Sensitivity} = 1e^{-5}$. The peaks in the cycled (dash line) are corresponding to the reductive potential of oxygen which became weaker by bubbling nitrogen to the system, but it was difficult to be completely suppressed.

8. Theoretic Calculations

8.1 HOMO and LUMO Levels

Calculations were carried out using the density functional theory (DFT) with Becke's three-parameter hybrid exchange functional and the Lee-Yang-Parr correlation functional (B3LYP)^[S4] employing the 6-31G(d) basis set for all atoms using the Gaussian 09 program.^[S5] The computational data was shown in Table S5 together with the electrochemical and optical data for comparison. The results show that the HOMO and LUMO levels were uniformly overestimated in the DFT calculations, presumably because of the fact that the calculations were performed in vacuum. The calculated excitation energies E_g are systematically higher than the experimental E_g values.

Table S5. The calculated and experimental energy level for the HOMO and LUMO orbitals for representative TACs and all-carbon coronene.

Compound	Computational ^a			Experimental ^b			Optical ^c		
	E_{HOMO} [eV]	E_{LUMO} [eV]	E_{gap} [eV]	$E^{\text{red}}(\text{onset})$ [V]	E_{LUMO} [eV]	$E^{\text{ox}}(\text{onset})^{\text{d}}$ [V]	E_{HOMO} [eV]	E_{gap} [eV]	E_{gap} [eV]
1a	-6.22	-2.14	4.08	-	-	-	-	-	3.06
1b	-5.96	-1.89	4.07	-2.09	-2.71	1.14	-5.94	3.23	3.08
1c	-6.85	-2.88	3.97	-1.36	-3.44	1.54	-6.34	2.90	3.00
1d	-5.89	-2.08	3.81	-1.82	-2.98	1.20	-6.00	3.02	2.99
1e	-5.77	-1.99	3.78	-1.83	-2.97	-	-	-	2.94
1i	-5.97	-2.10	3.87	-1.78	-3.02	-	-	-	2.95
Coronene	-5.45	-1.41	4.04	-2.48 ^e	-1.92 ^f -1.90 ^g	-	-5.52 ^g	3.60	3.65 ^h

^aCalculations were performed at the B3LYP/6-31G(d) level of theory. ^b $E_{\text{HOMO}} = -E^{\text{ox}}(\text{onset}) - 4.80$; $E_{\text{LUMO}} = -E^{\text{red}}(\text{onset}) - 4.80$. E^{ox} and E^{red} were calibrated by the half-wave potential of Fc^+/Fc which was assumed to have an absolute energy level of -4.8 eV to vacuum. ^cThe optical E_{gap} was determined as the intersection of the x axis and a tangent line passing through the inflection point of the lowest-energy absorption. ^d $E^{\text{ox}}(\text{onset})$ was determined by DPV. ^e E^{red} vs SCE (see, Ref. [S6]). ^f $E_{\text{LUMO}} = -E^{\text{red}}(\text{vs SCE}) - 4.40$. ^gLUMO and HOMO were determined by inverse photoelectron spectroscopy (IPES) and ultraviolet photoelectron spectroscopy (UPS), respectively (see Ref. [S7]). ^hRef. [S3].

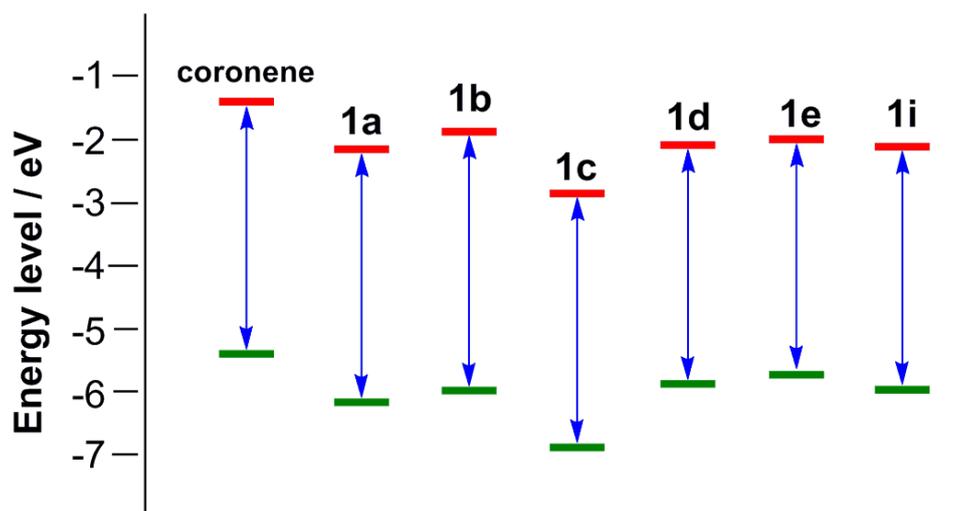


Figure S11. Schematic plot of HOMO-LUMO levels of compounds.

8.2 Molecular Orbitals

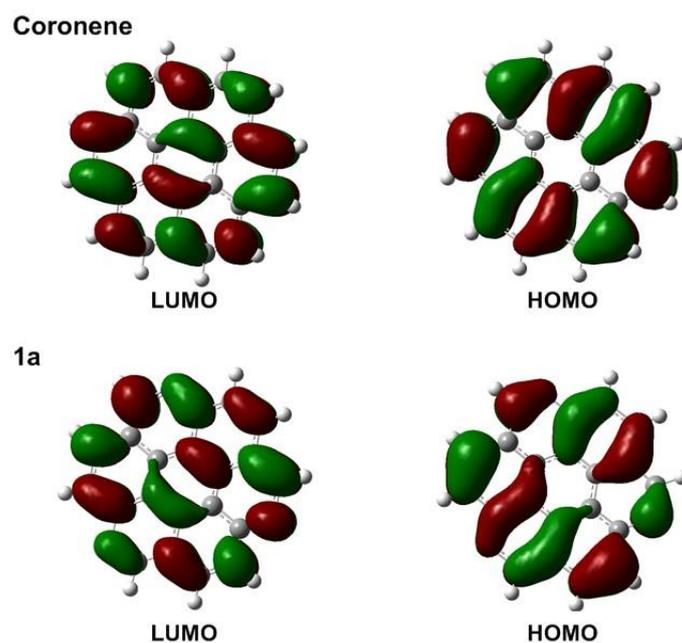


Figure S12. Calculated molecular orbitals of coronene and triazacoronene **1a**.

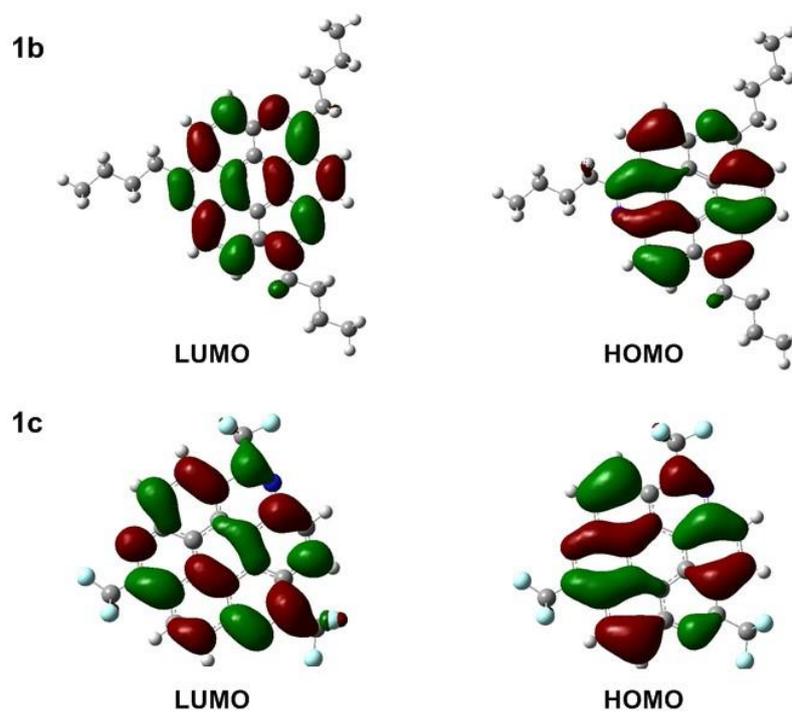


Figure S13. Calculated molecular orbitals of **1b** and **1c**.

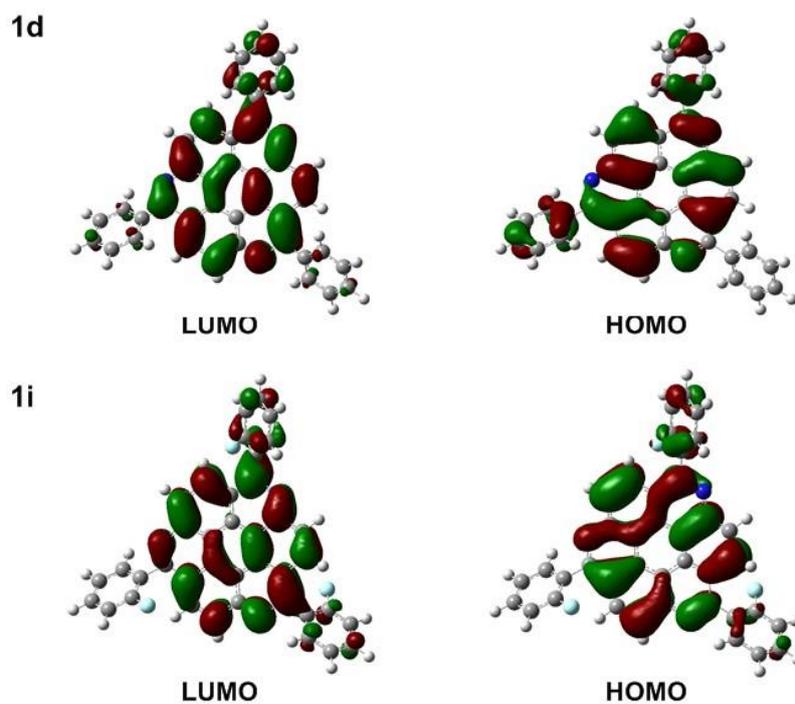


Figure S14. Calculated molecular orbitals of **1d** and **1i**.

8.3 Calculated Geometry of representative compounds (**1a-1d**, **1h** and **1i**)

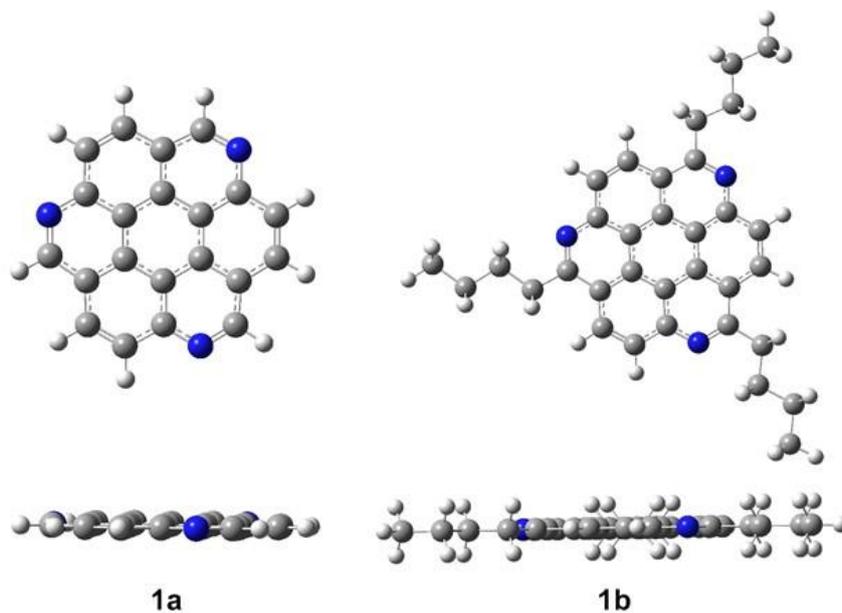


Figure S15. Calculated structure of **1a** (left) and **1b** (right).

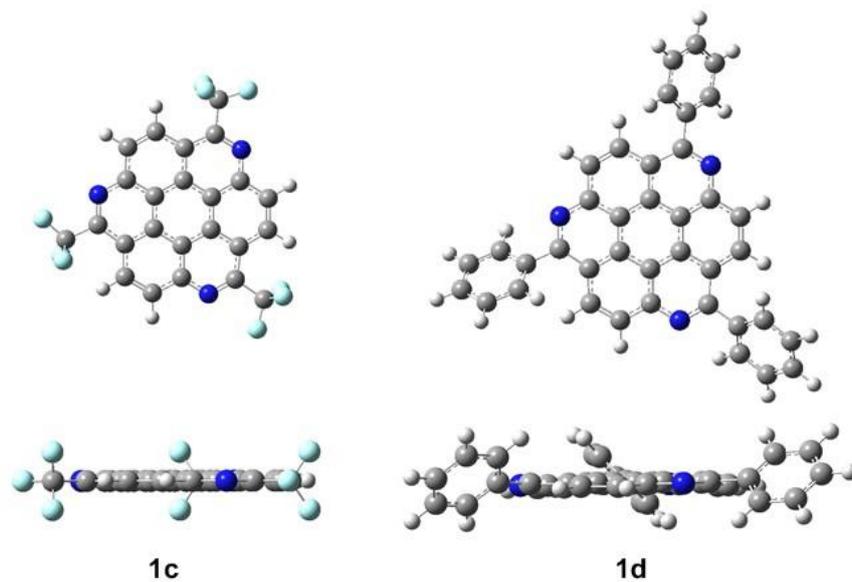


Figure S16. Calculated structure of **1c** (left) and **1d** (right).

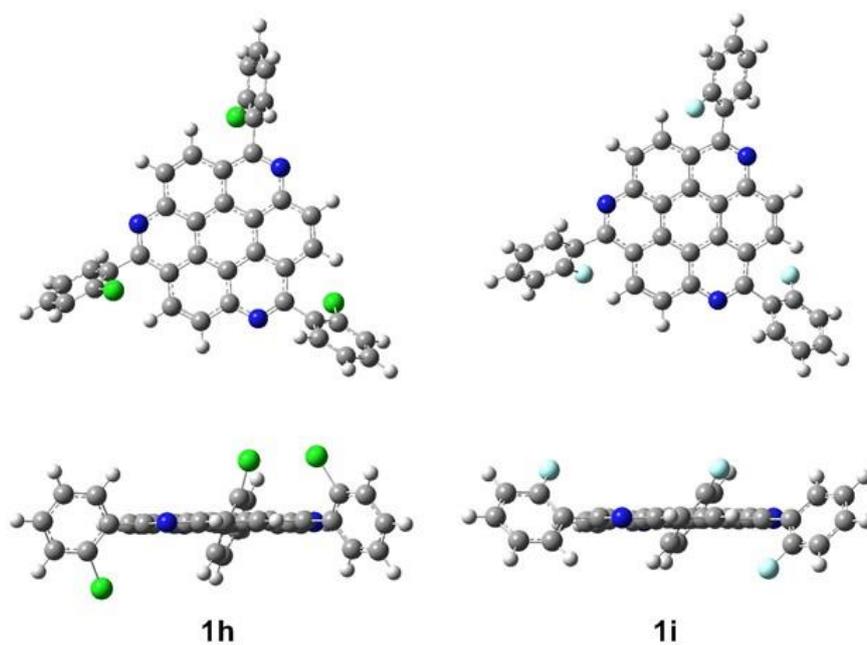


Figure S17. Calculated structure of **1i** (left) and **1j** (right).

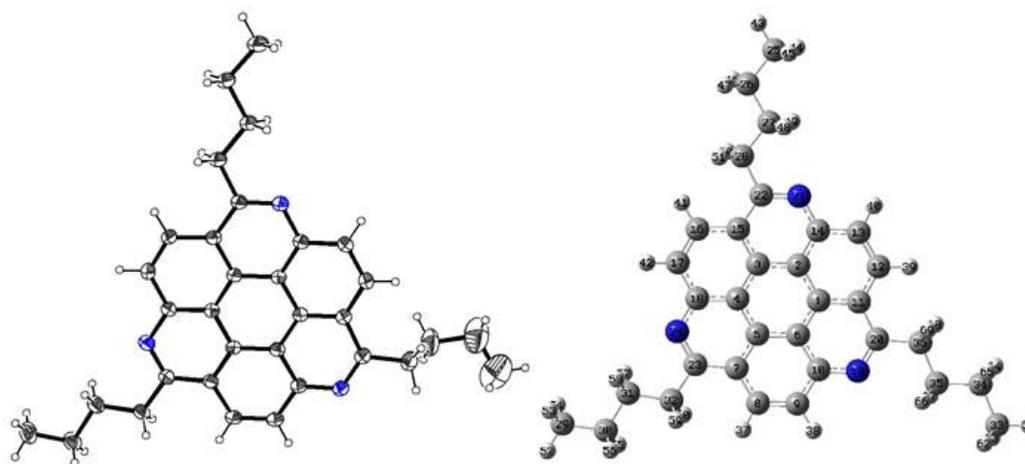


Figure S18. The comparison of the B3LYP/6-31G(d) calculated geometry (right) with the X-ray crystallographic structure (left) of **1b**.

Table S6. Selected Bond Distances (Å) of **1b** by DFT-B3LYP/6-31G(d).

Bond	Bond lengths	Bond	Bong lengths	Bond	Bond lengths
C1-C2	1.419	C14-N21	1.371	C28-H51	1.101
C1-C6	1.418	C15-C16	1.427	C29-C30	1.532
C1-C11	1.411	C15-C22	1.449	C29-H52	1.096
C2-C3	1.419	C16-C17	1.379	C29-H53	1.097
C2-C14	1.408	C16-H41	1.085	C29-H54	1.097
C3-C4	1.419	C17-C18	1.425	C30-C31	1.534
C3-C15	1.411	C17-H42	1.086	C30-H55	1.100
C4-C5	1.418	C18-N24	1.371	C30-H56	1.100
C4-C18	1.408	N19-C20	1.319	C31-C32	1.531
C5-C6	1.419	C20-C36	1.518	C31-H57	1.097
C5-C7	1.411	N21-C22	1.319	C31-H58	1.097
C6-C10	1.408	C22-C28	1.518	C32-H59	1.101
C7-C8	1.427	C23-N24	1.319	C32-H60	1.101
C7-C23	1.449	C23-C32	1.518	C33-C34	1.532
C8-C9	1.380	C25-C26	1.532	C33-H61	1.096
C8-H37	1.085	C25-H43	1.096	C33-H62	1.097
C9-C10	1.425	C25-H44	1.097	C33-H63	1.097
C9-H38	1.086	C25-H45	1.097	C34-C35	1.534
C10-N19	1.371	C26-C27	1.534	C34-H64	1.100
C11-C12	1.427	C26-H46	1.100	C34-H65	1.100
C11-C20	1.449	C26-H47	1.100	C35-C36	1.531
C12-C13	1.380	C27-C28	1.531	C35-H66	1.097
C12-H39	1.085	C27-H48	1.097	C35-H67	1.097
C13-C14	1.425	C27-H49	1.097	C36-H68	1.101
C13-H40	1.086	C28-H50	1.101	C36-H69	1.101

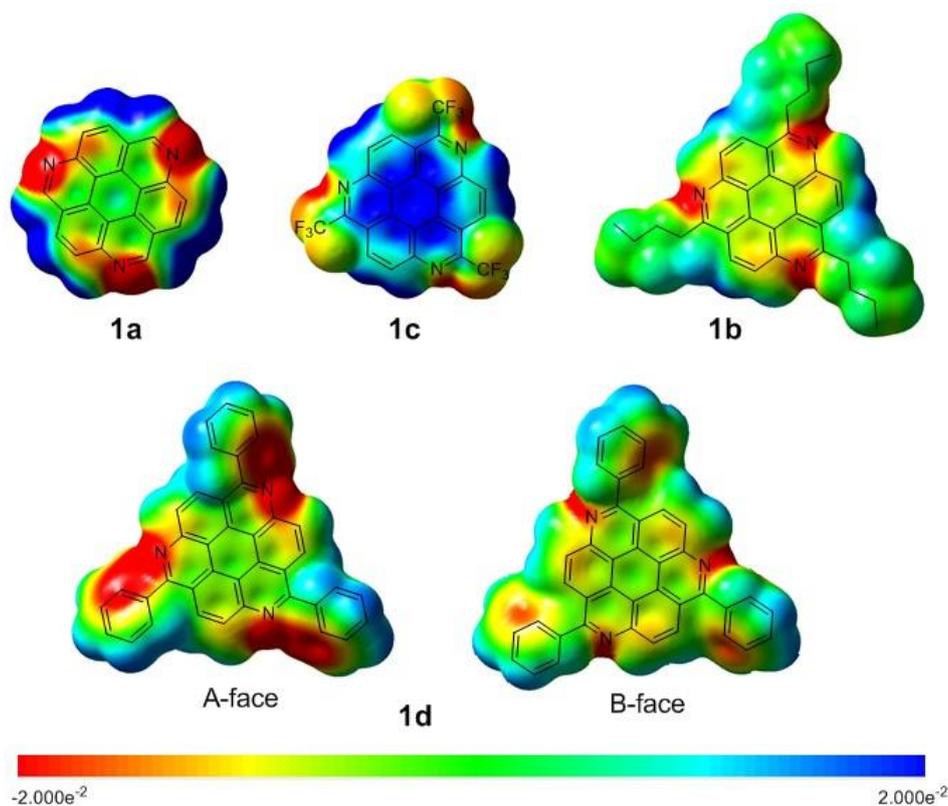


Figure S19. ESP (electrostatic potential) of **1a**, **1b**, **1c** and **1d**.

8.4 Nucleus Independent Chemical Shifts (NICS) calculation

To understand the aromatic nature, we calculate Nucleus Independent Chemical Shifts (NICS) to assess the magnetically-defined aromatic character of triazacoronene **1a** and **1c** as well as coronene, by the Gauge-Invariant Atomic Orbital (GIAO) method at B3LYP/6-31+g(d,p) level of theory.^[S8] NICS, as proposed by Schleyer *et. al.*, is the negative of the absolute shielding, computed at the ring center NICS(0) and NICS(1) is calculated 1 Å above or below the ring center.^[S9]

Table S7. NICS of **1a**, **1b** and coronene.

Calculation Method	1a			1b			Coronene ^[S10]	
	Central benzene ring	Outer benzene ring.	Out pyridine ring	Central benzene ring	Outer benzene ring.	Out pyridine ring	Central ring	Outer ring
NICS(0)	-0.178	-9.919	-8.203	-0.400	-10.211	-6.279	-0.514	-9.964
NICS(1)	-4.330	-11.732	-11.030	-4.274	-12.028	-9.739	-4.585	-11.975

9. Thermal Stability (TGA)

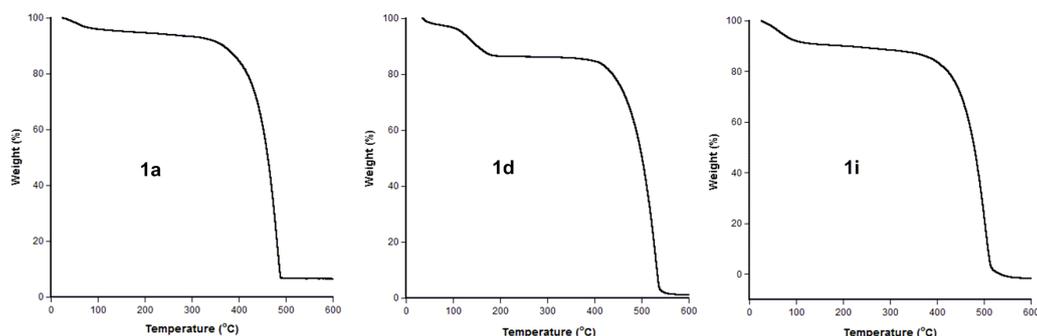
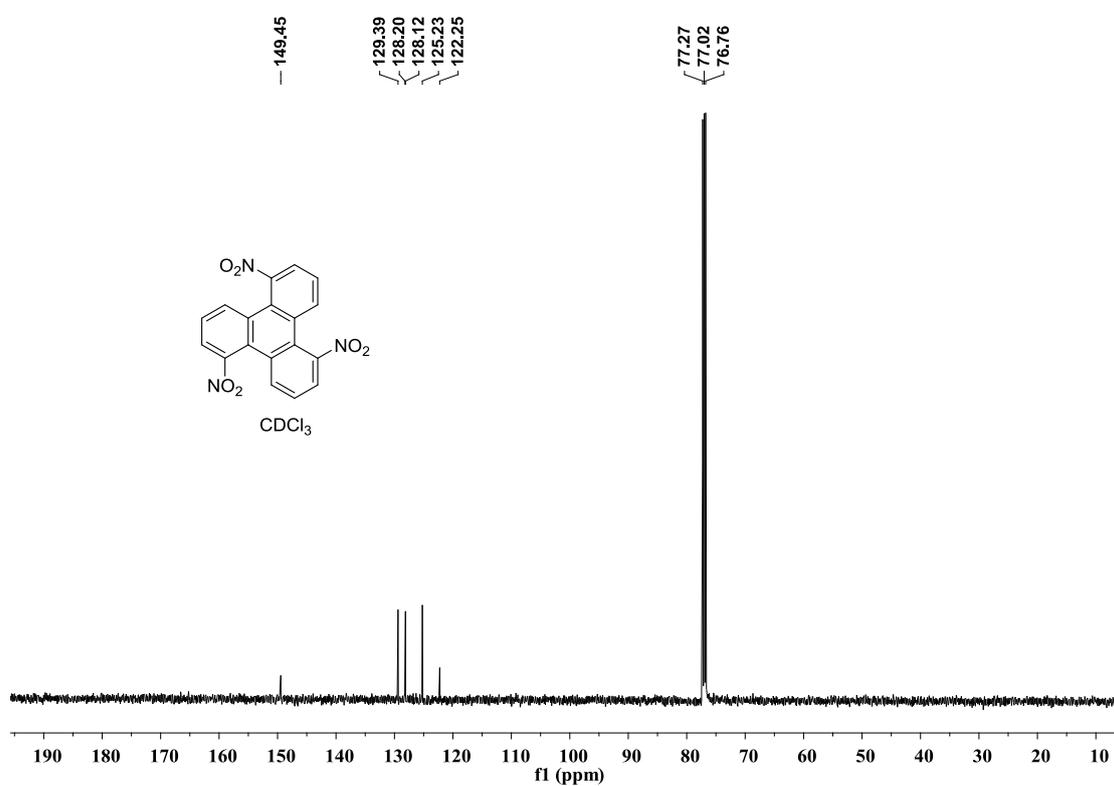
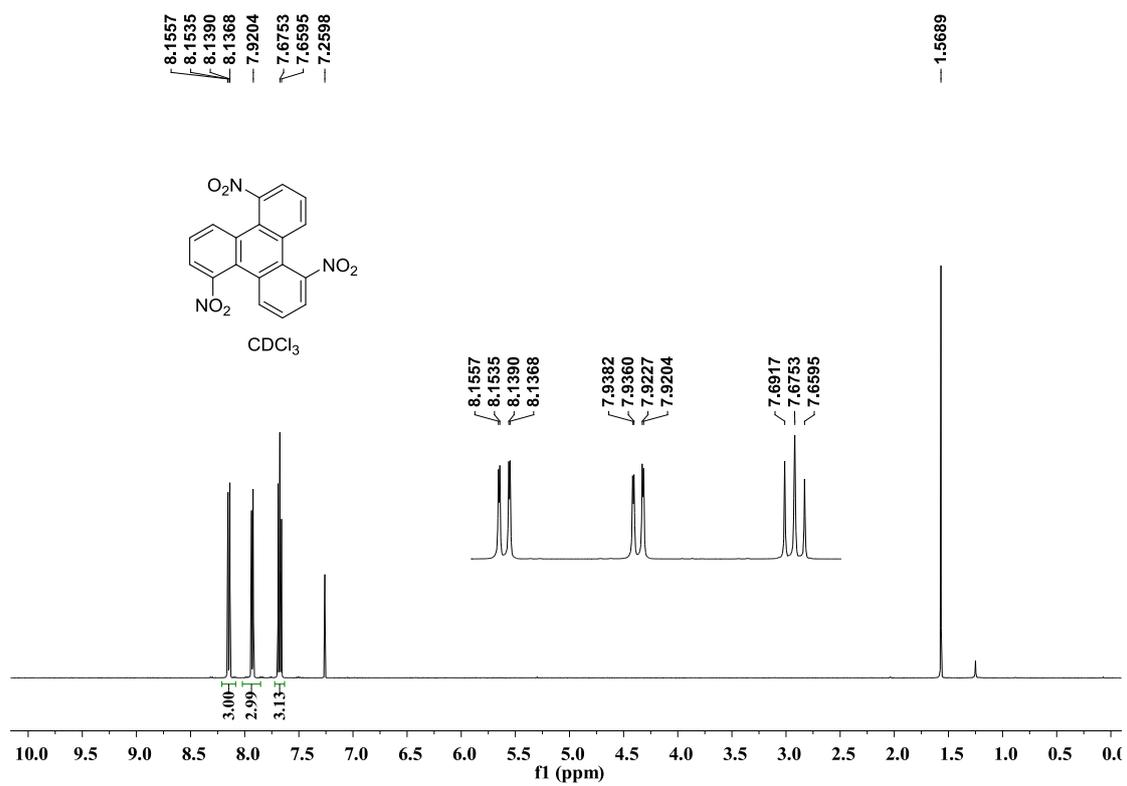


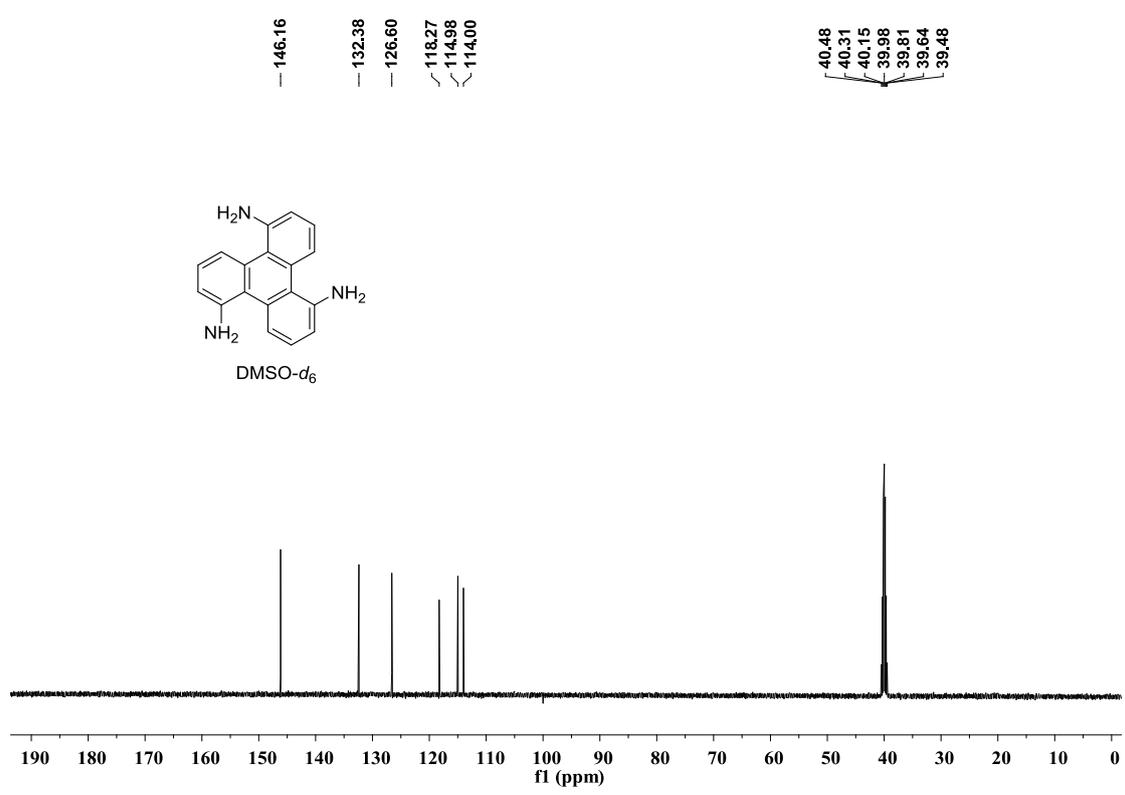
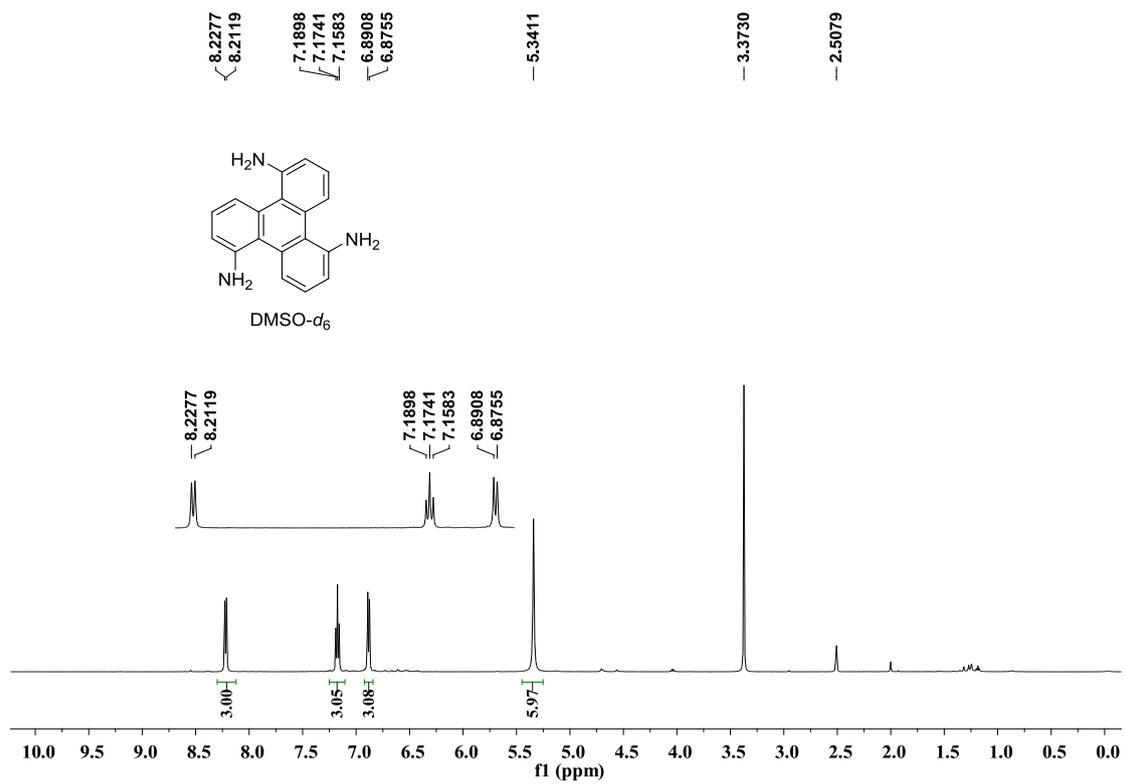
Figure 20. Thermal gravimetric analyses of selected TACs (heating rate 10 °C/min under nitrogen flow). The first slope is loss of volatiles (solvent residue or moisture).

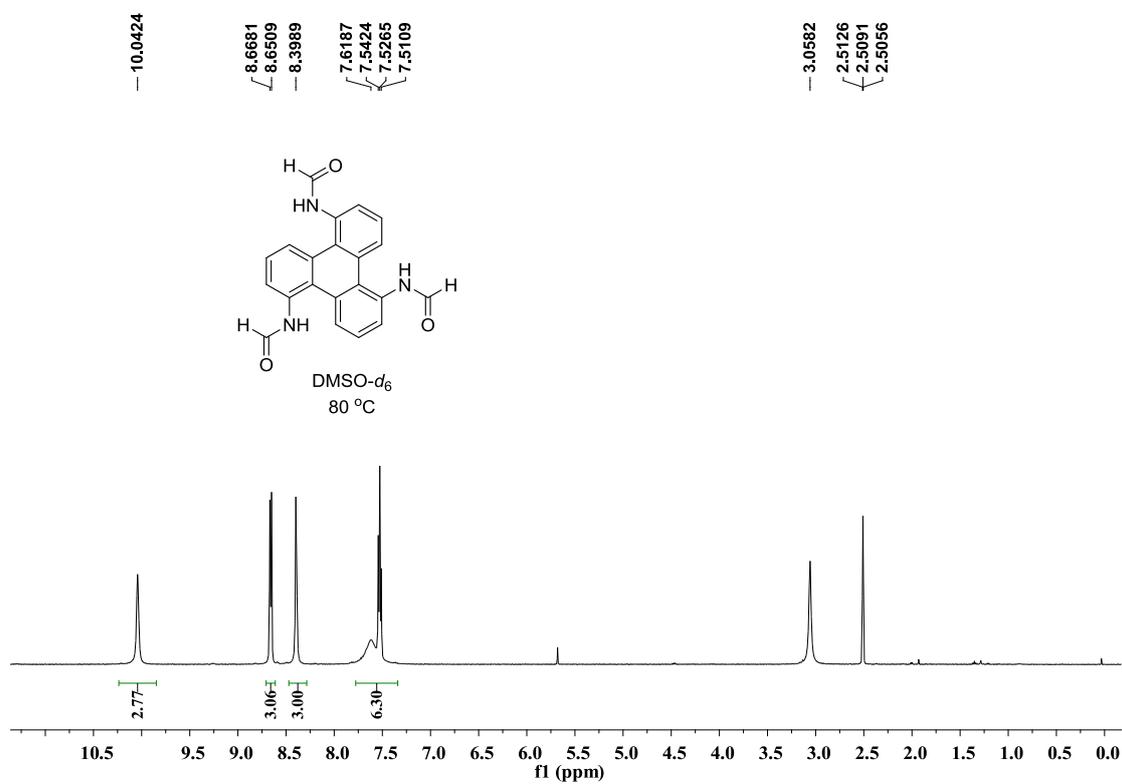
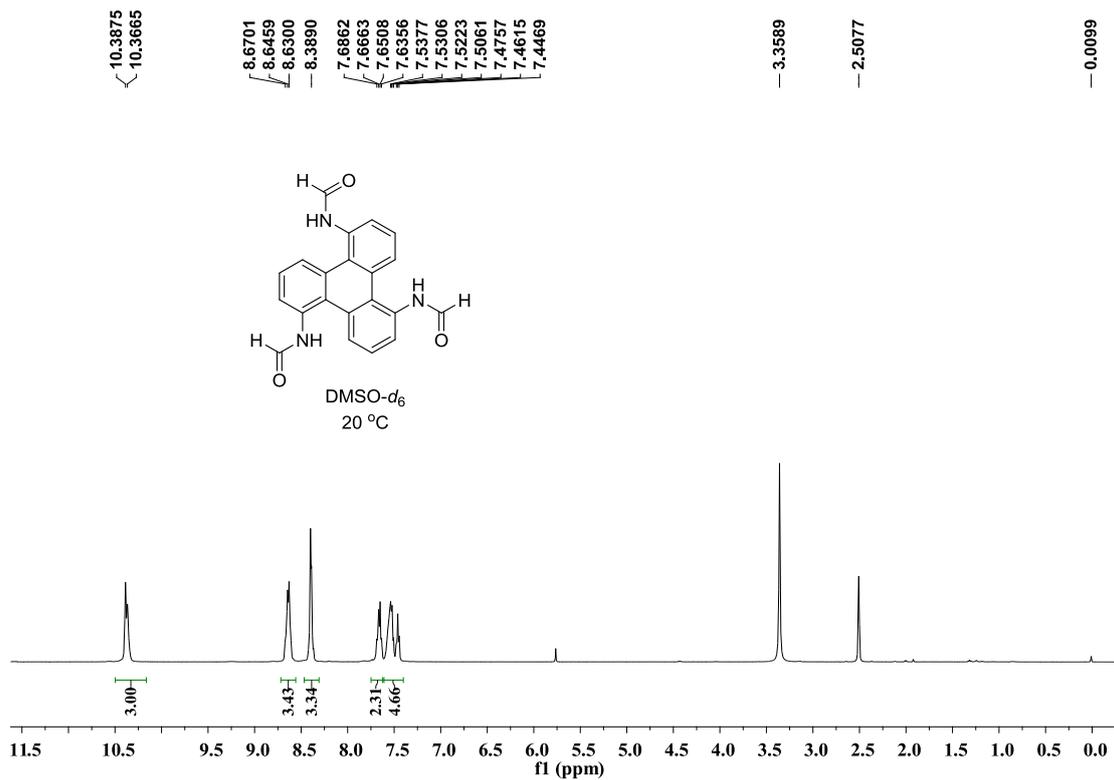
10. Reference

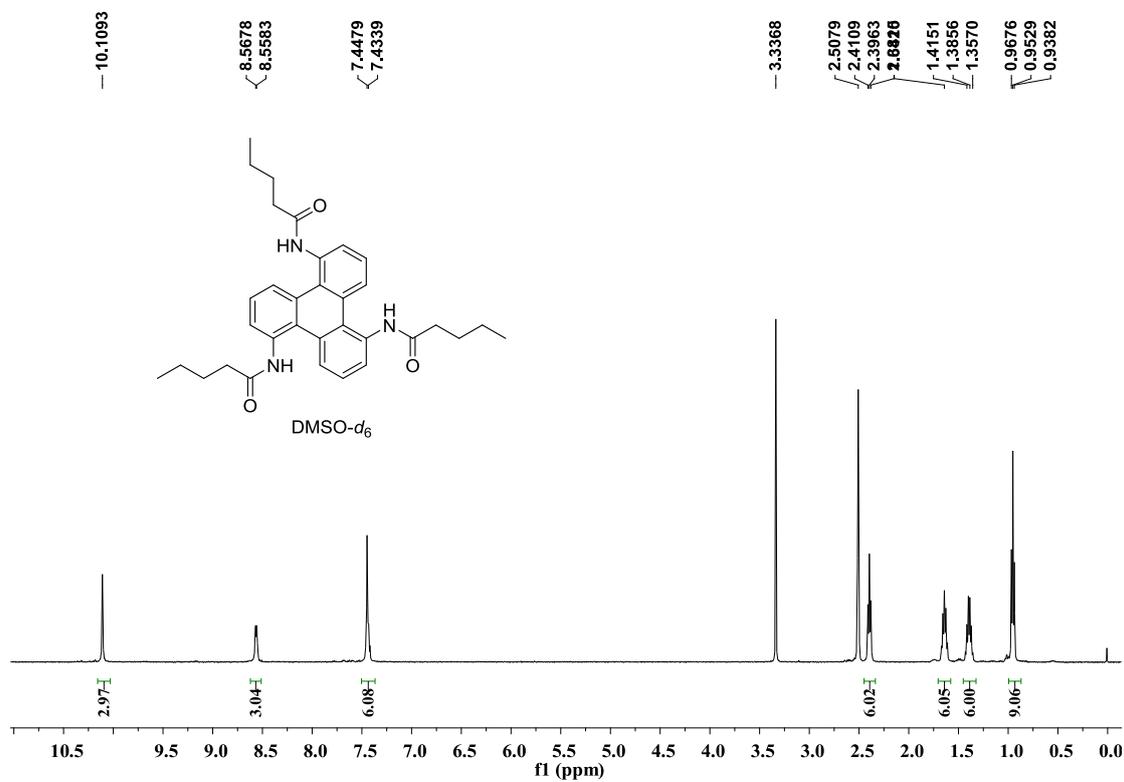
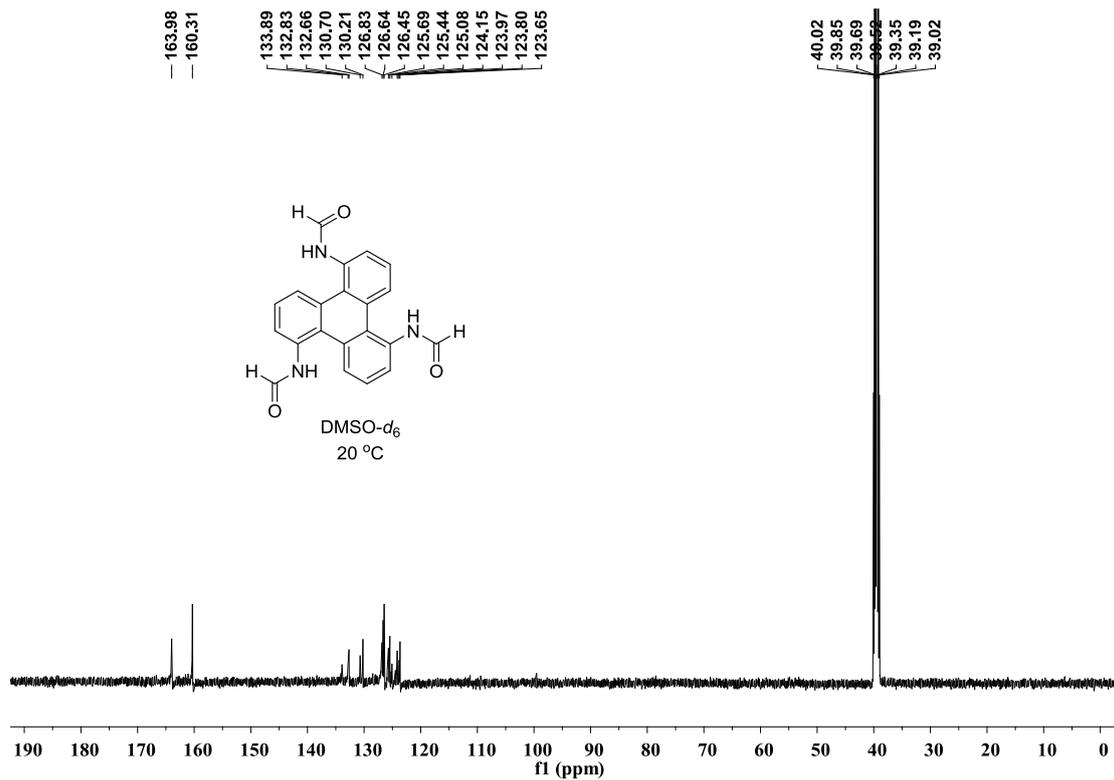
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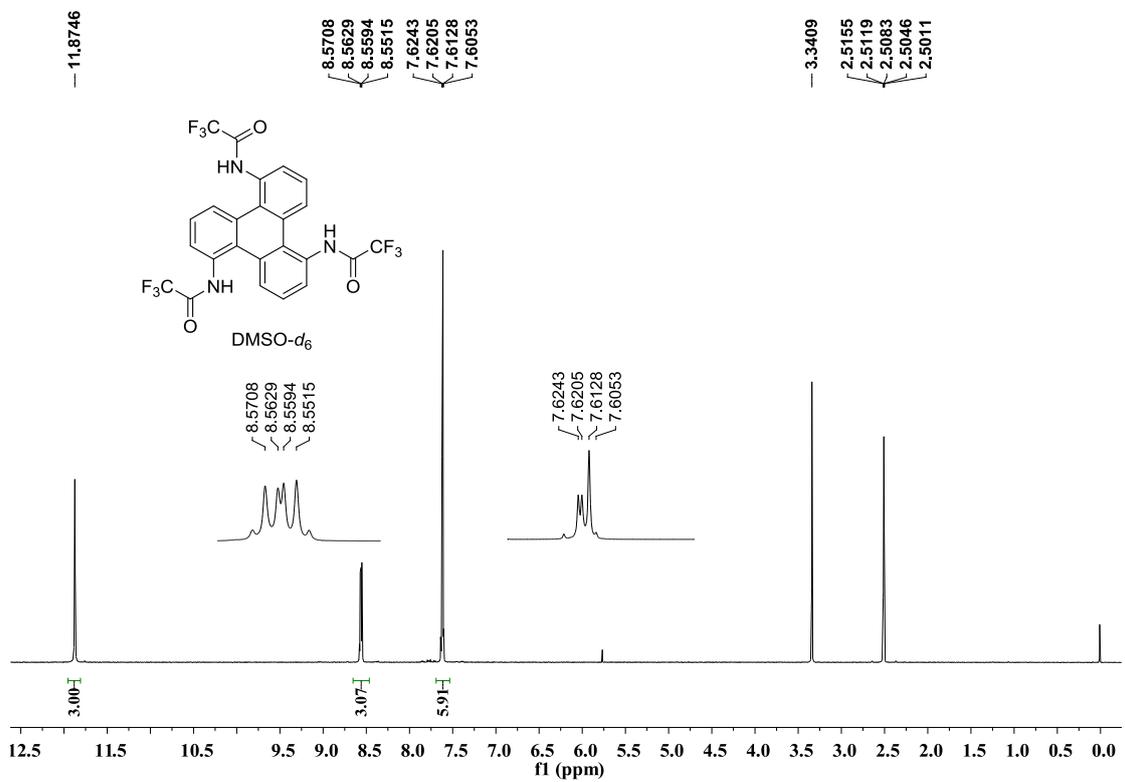
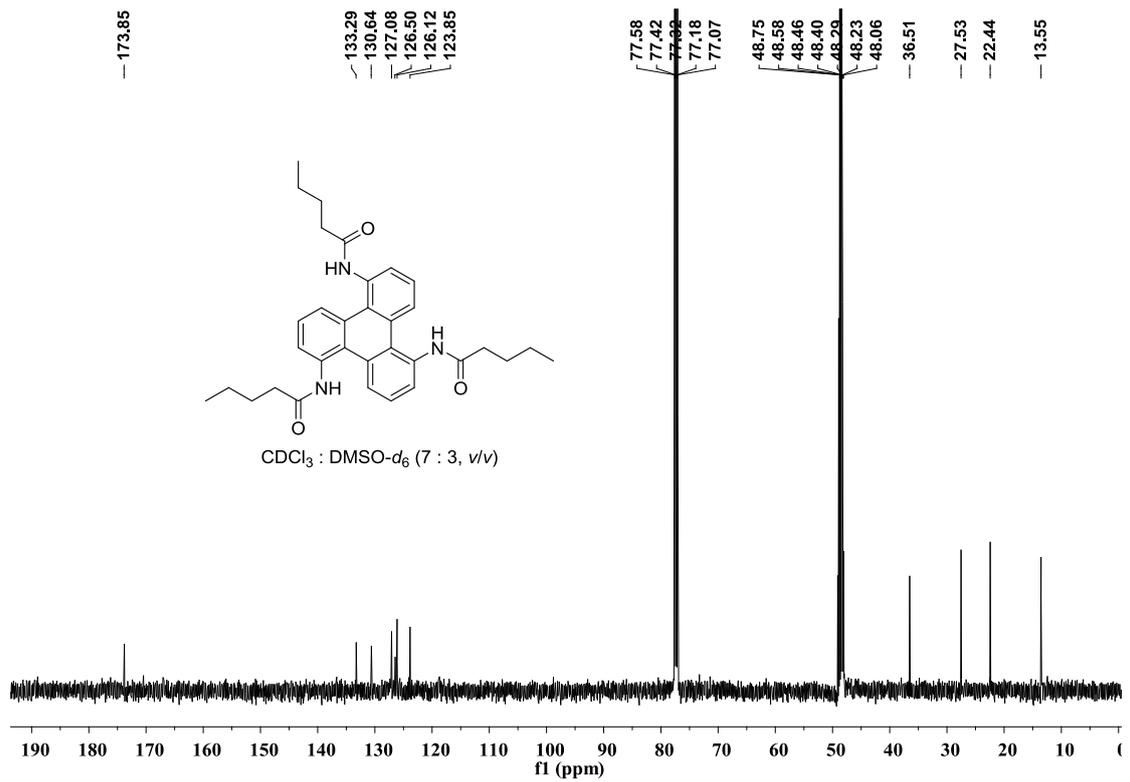
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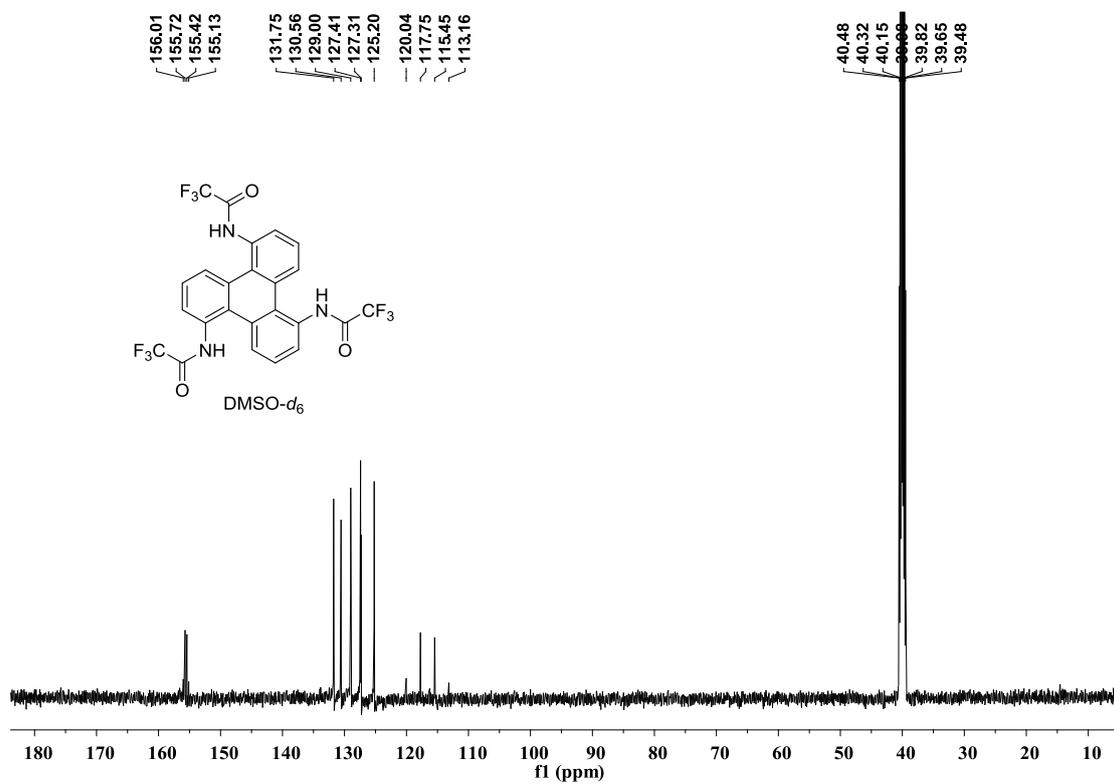
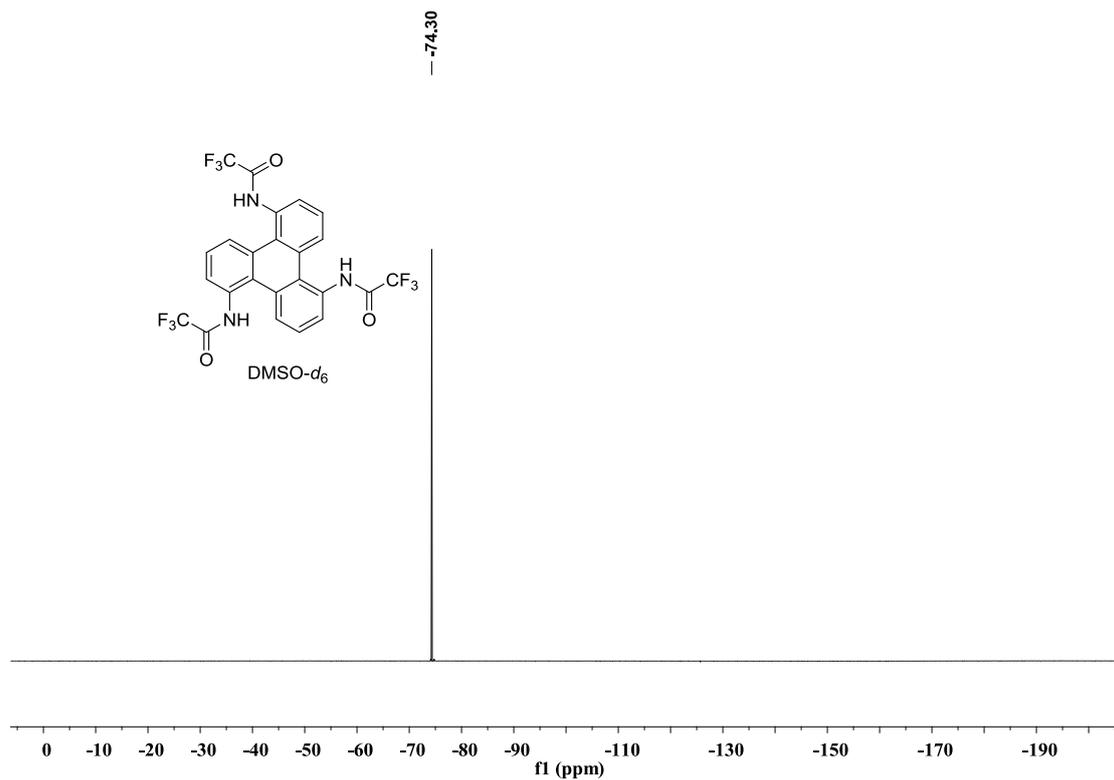


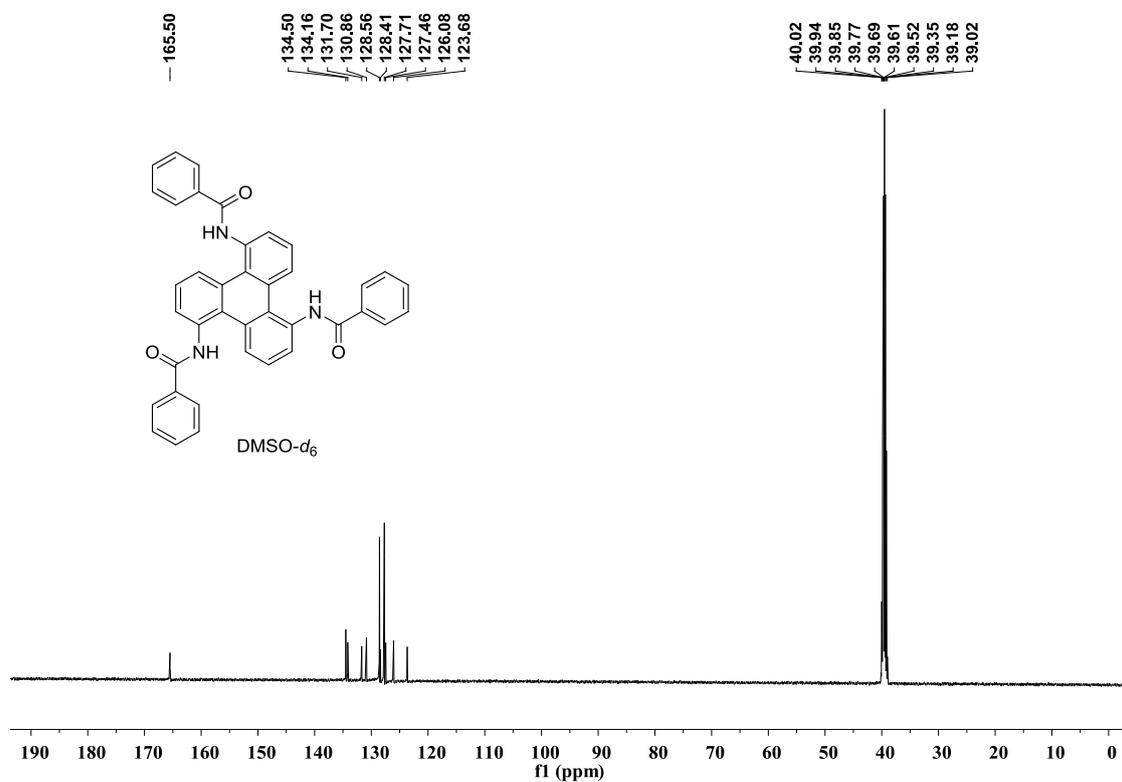
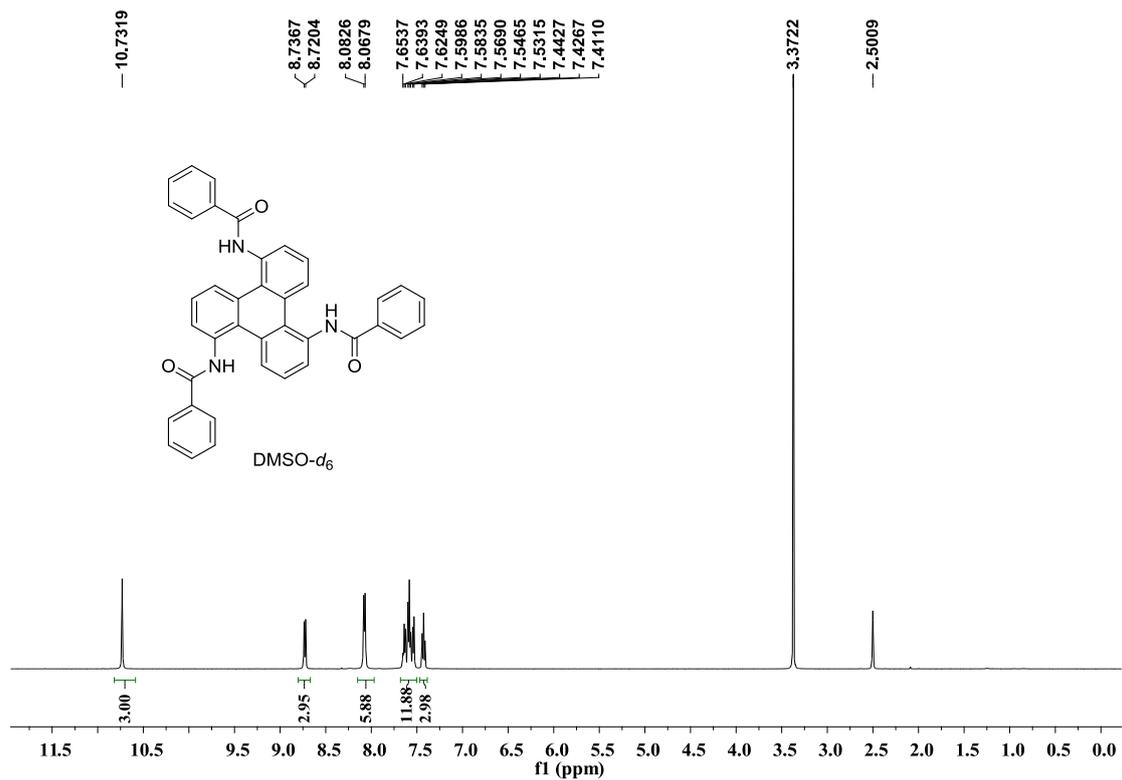


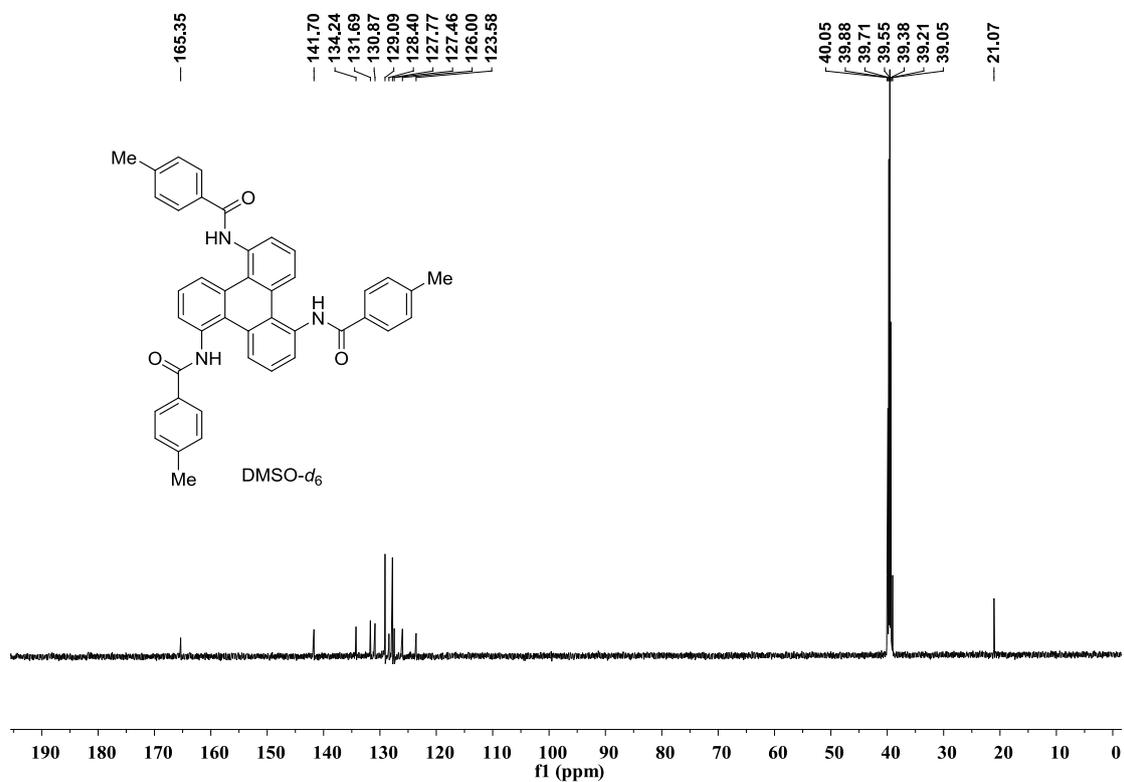
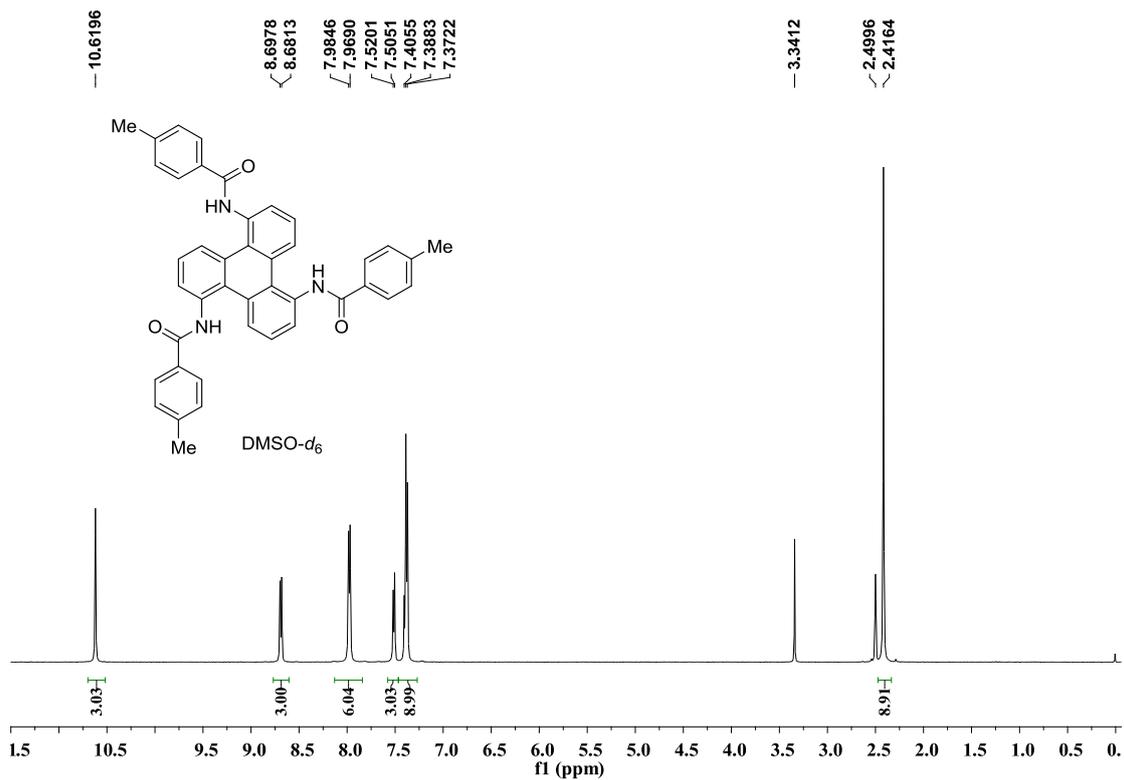


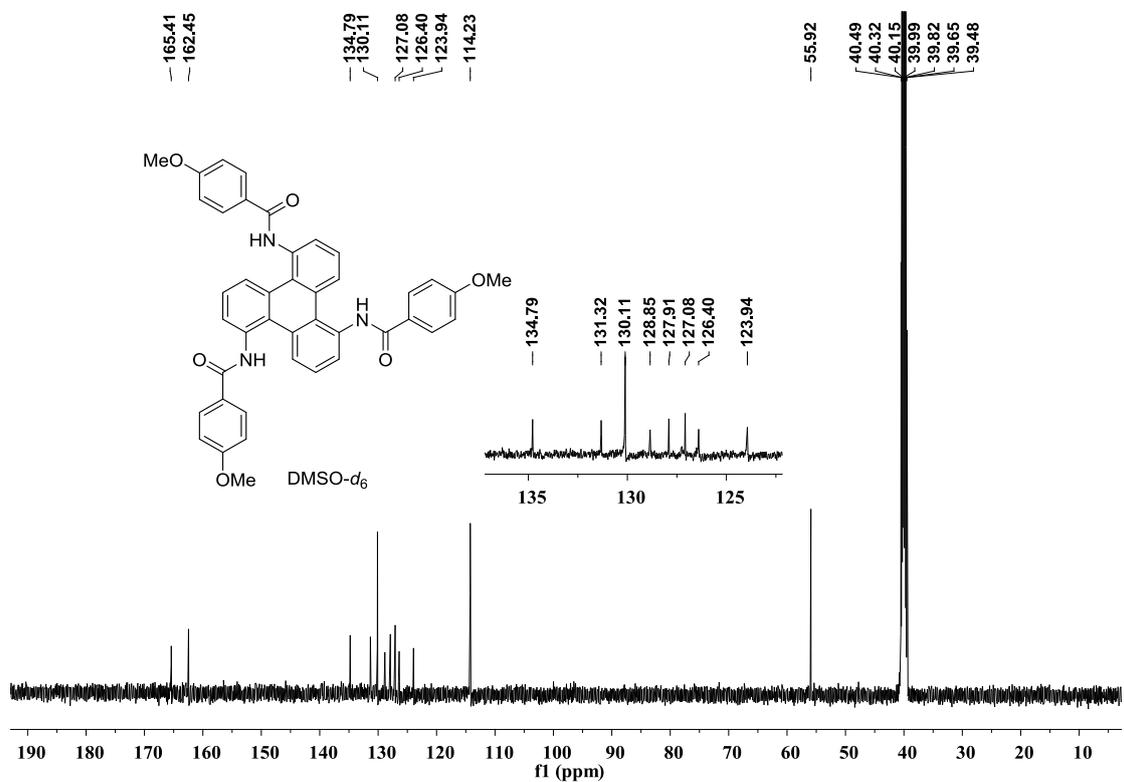
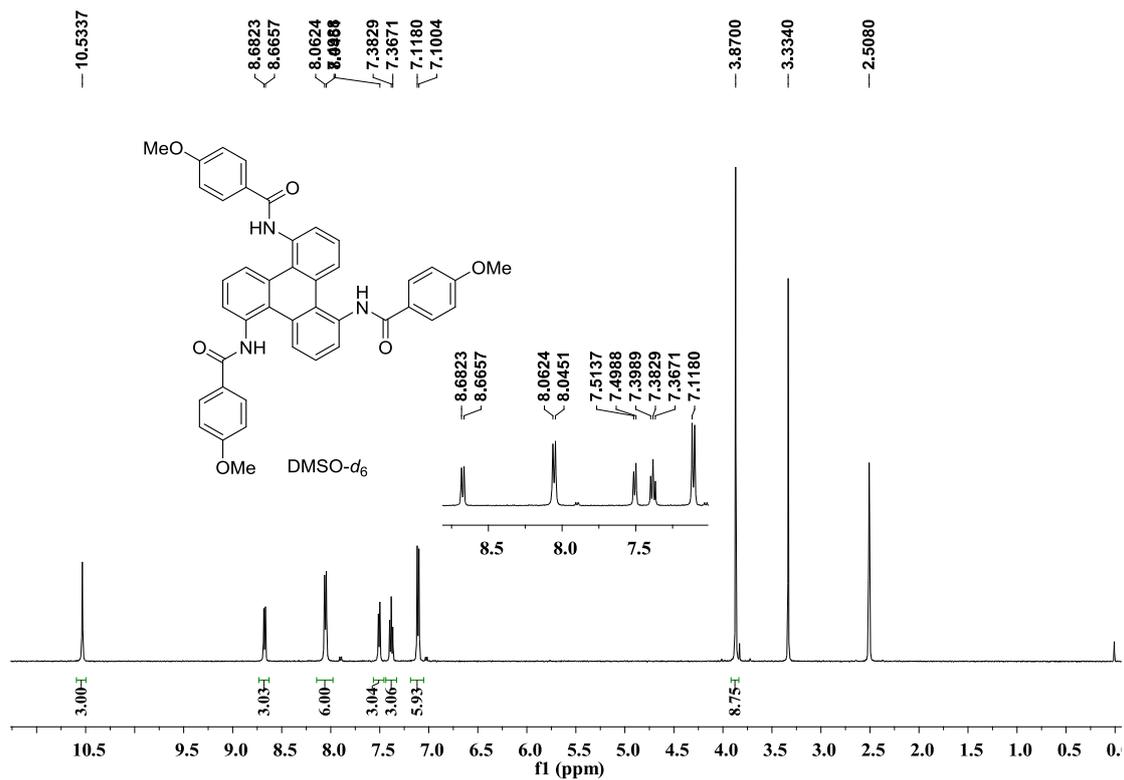


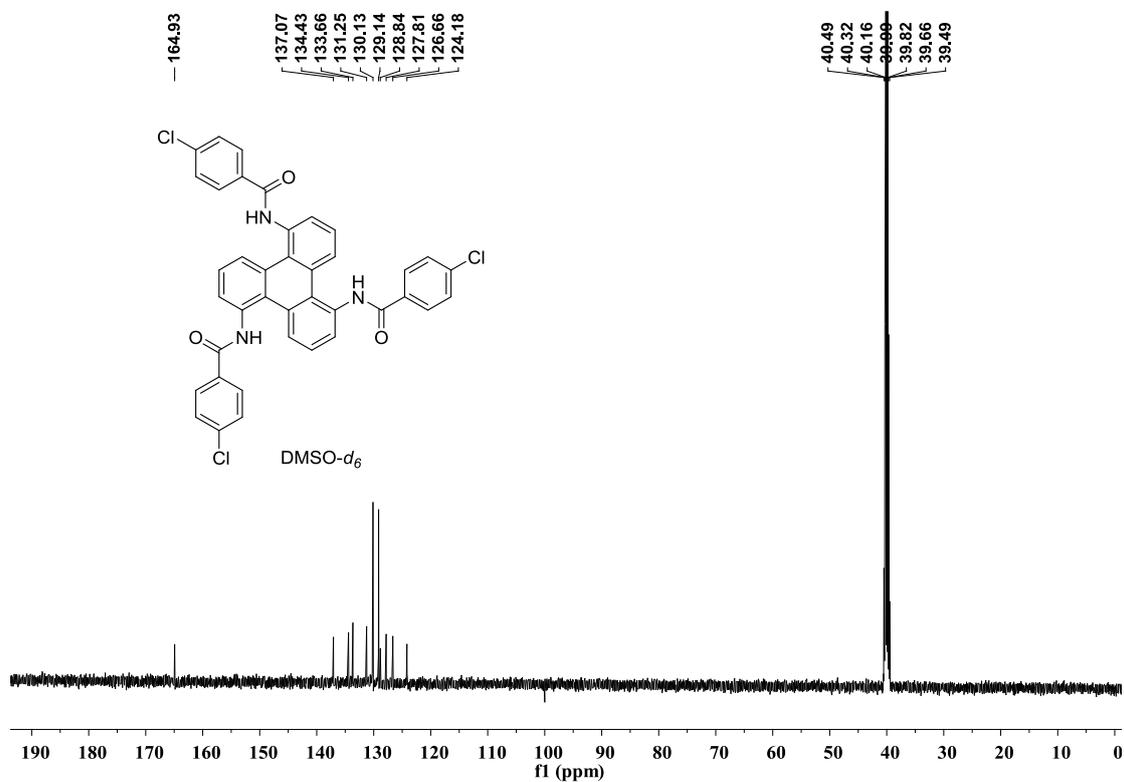
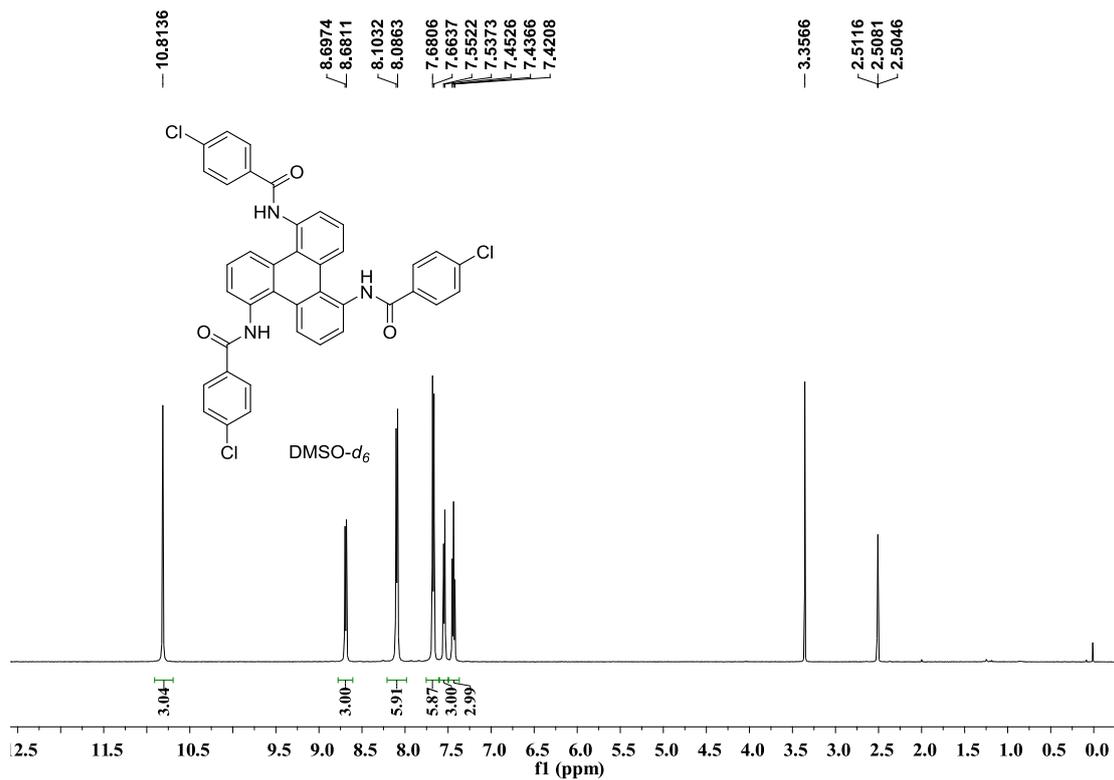


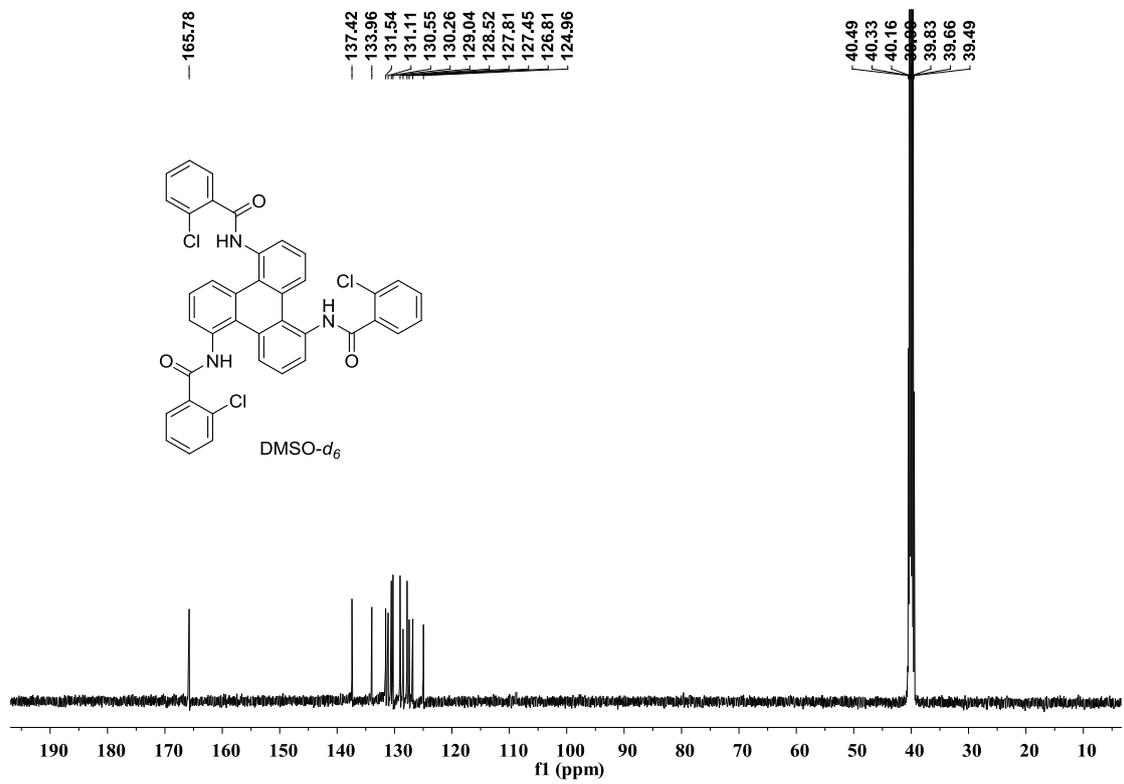
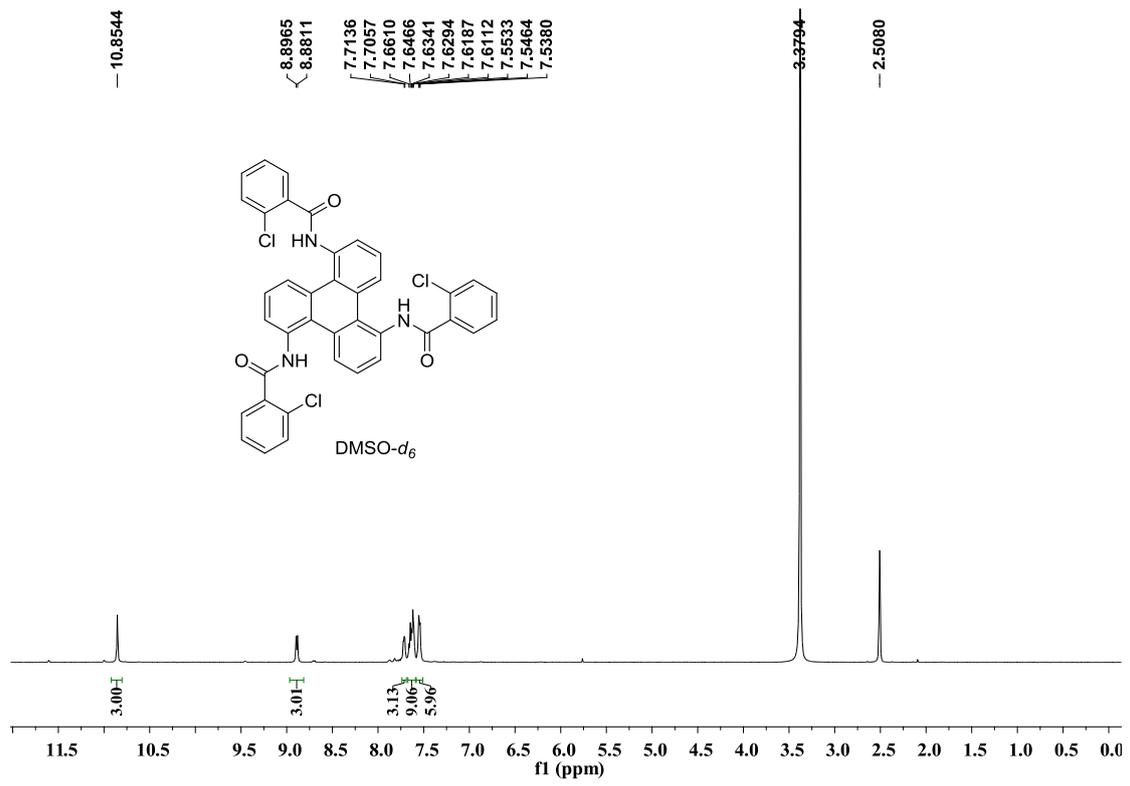


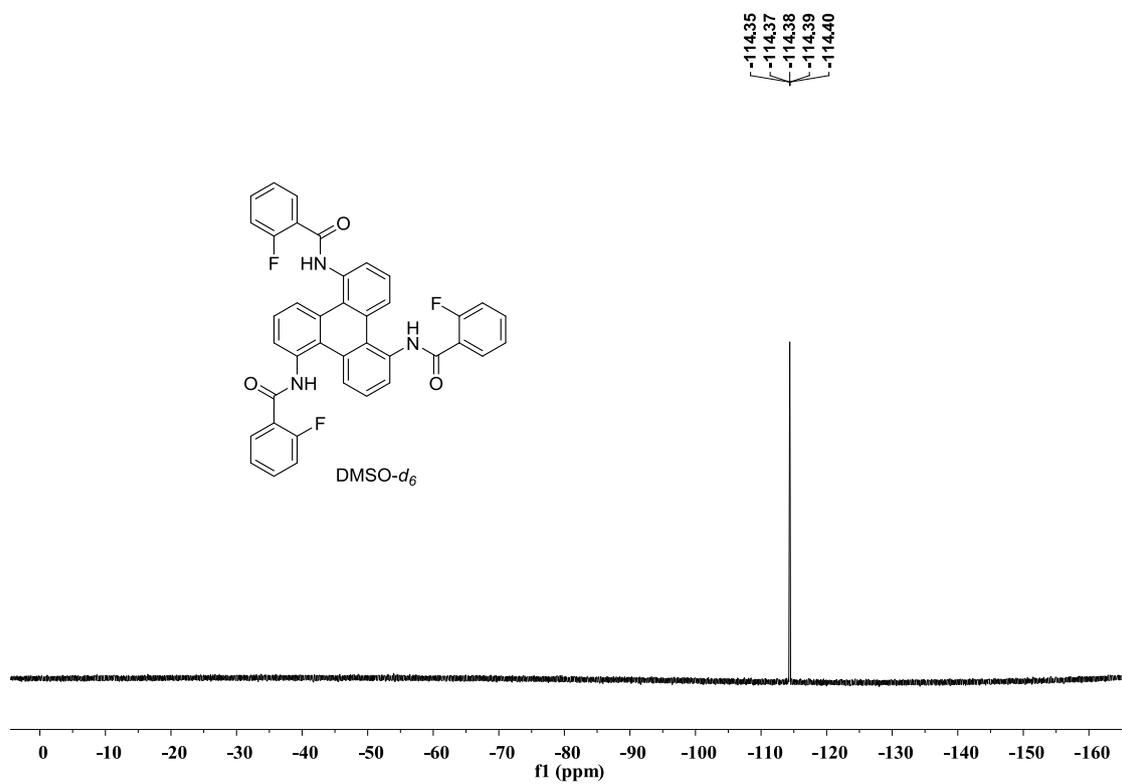
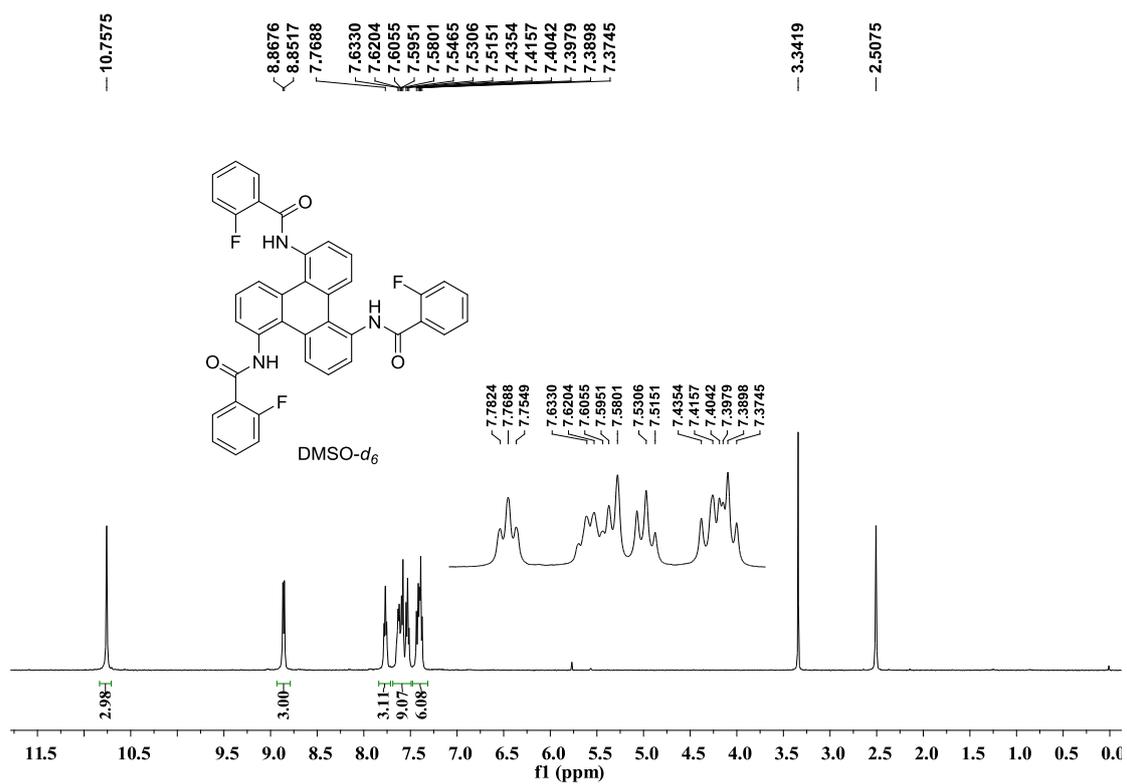


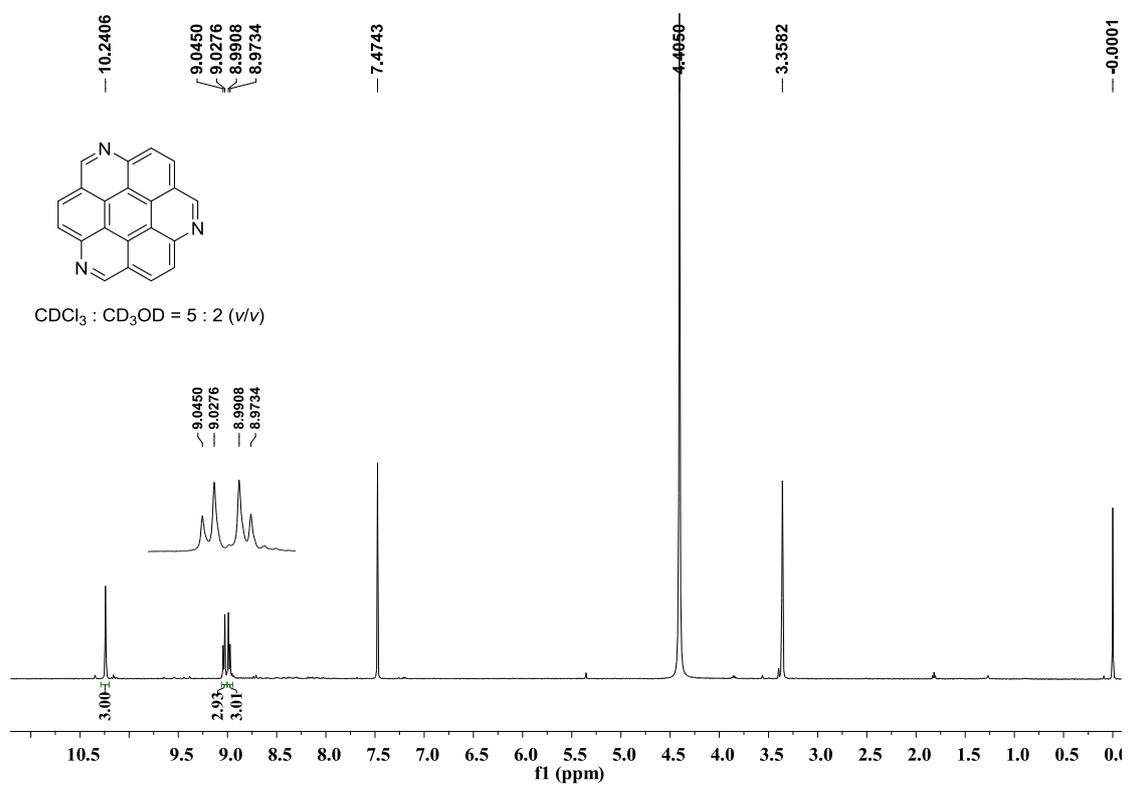
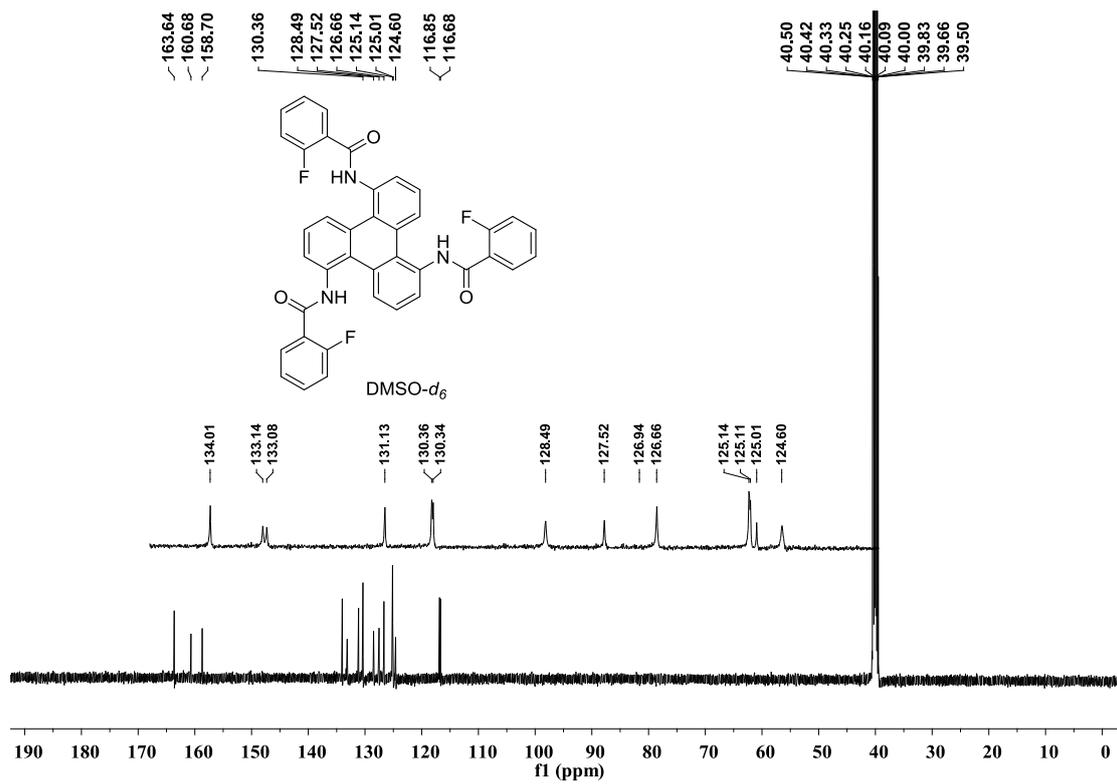


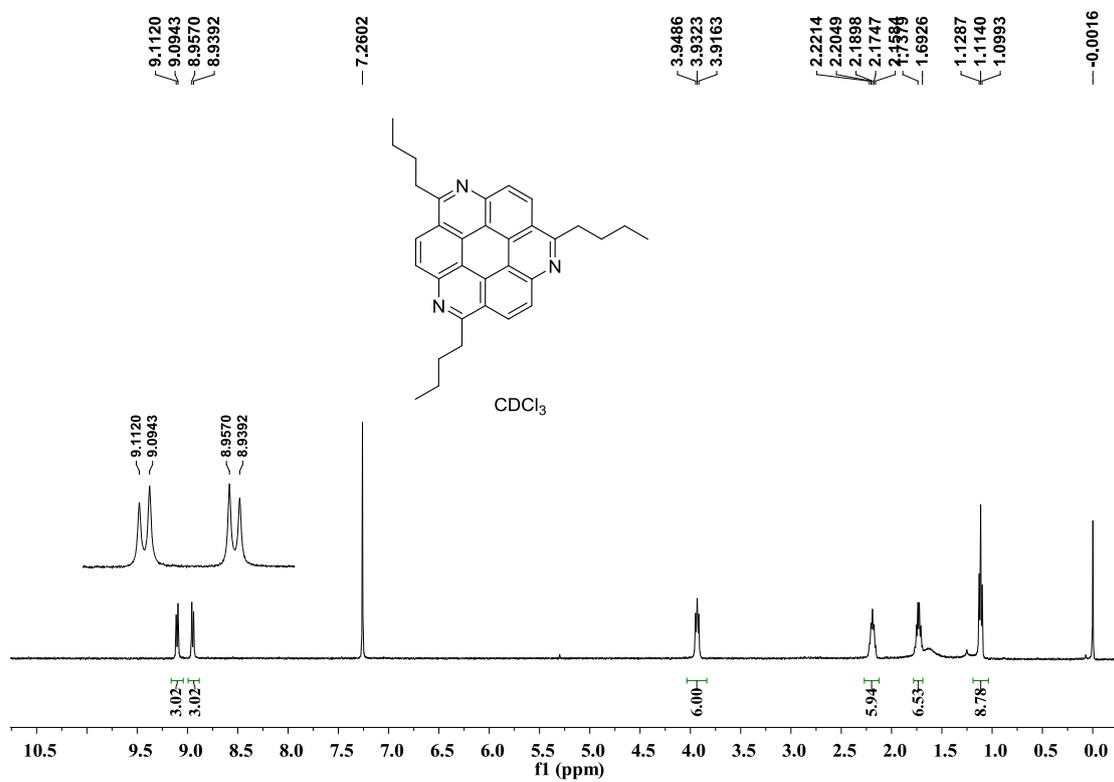
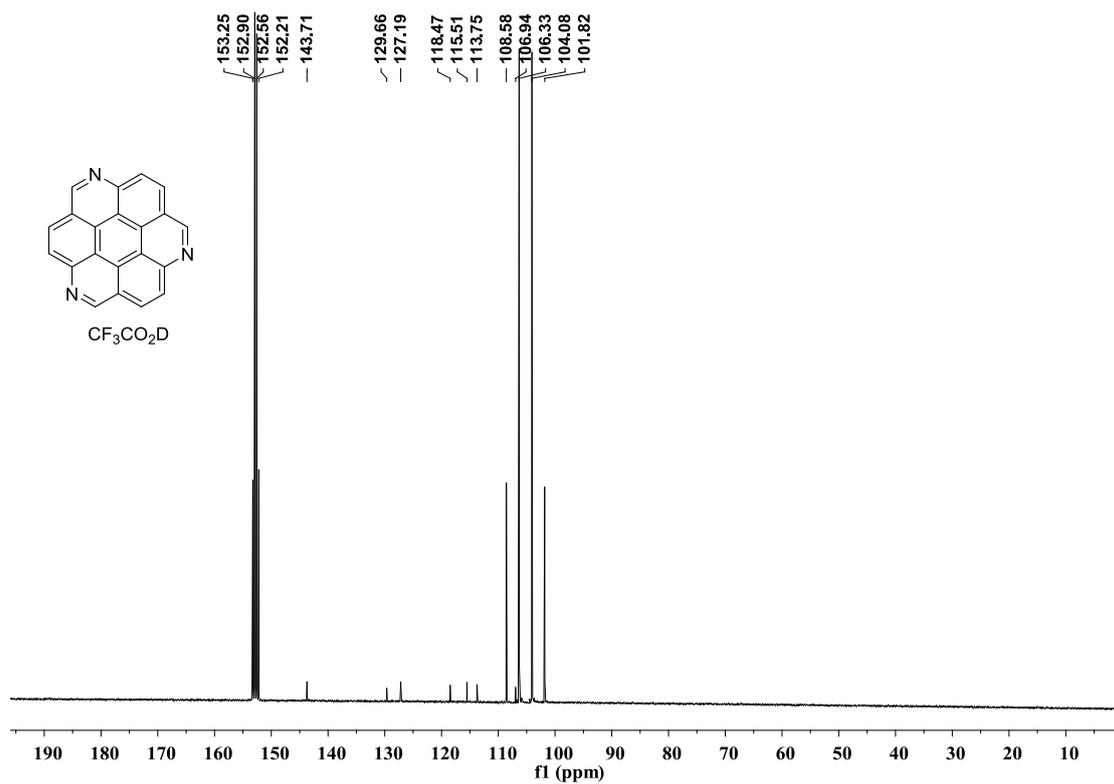


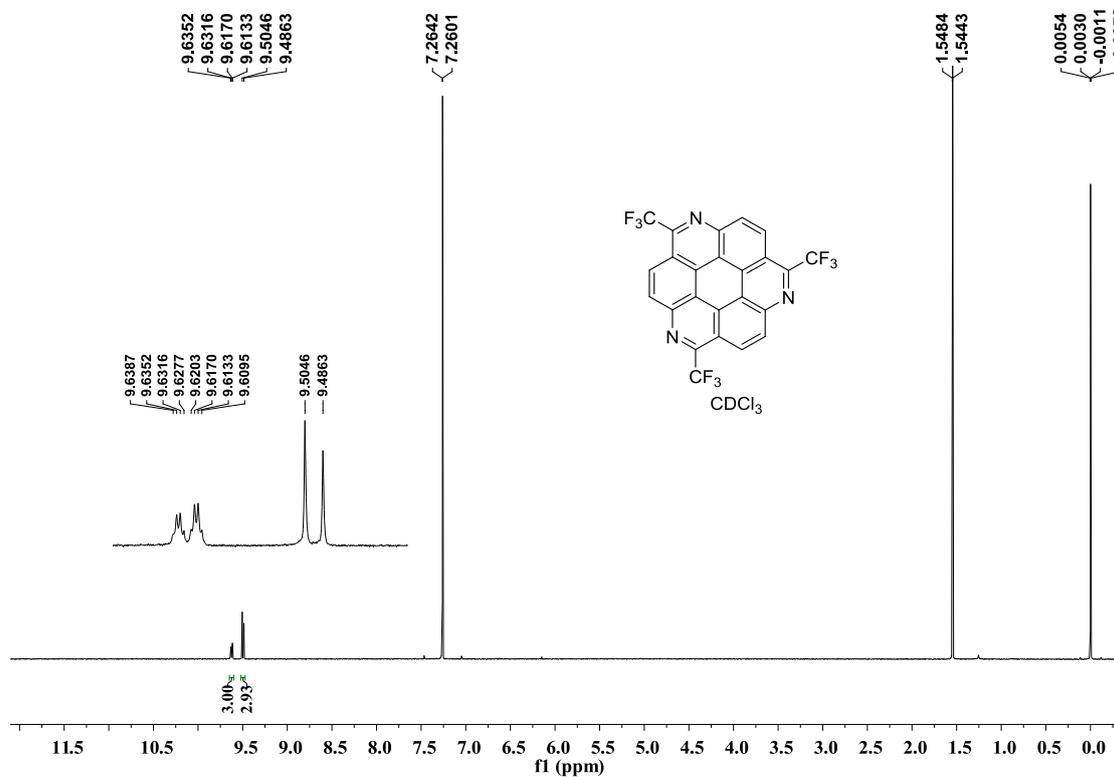
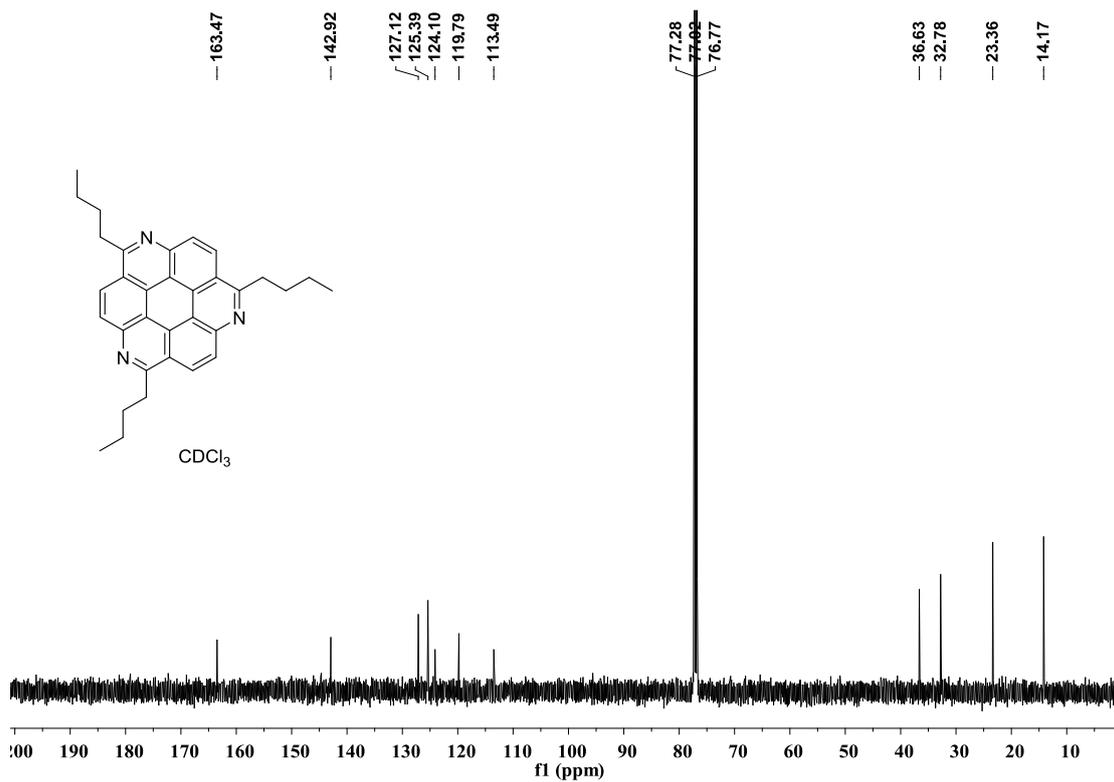


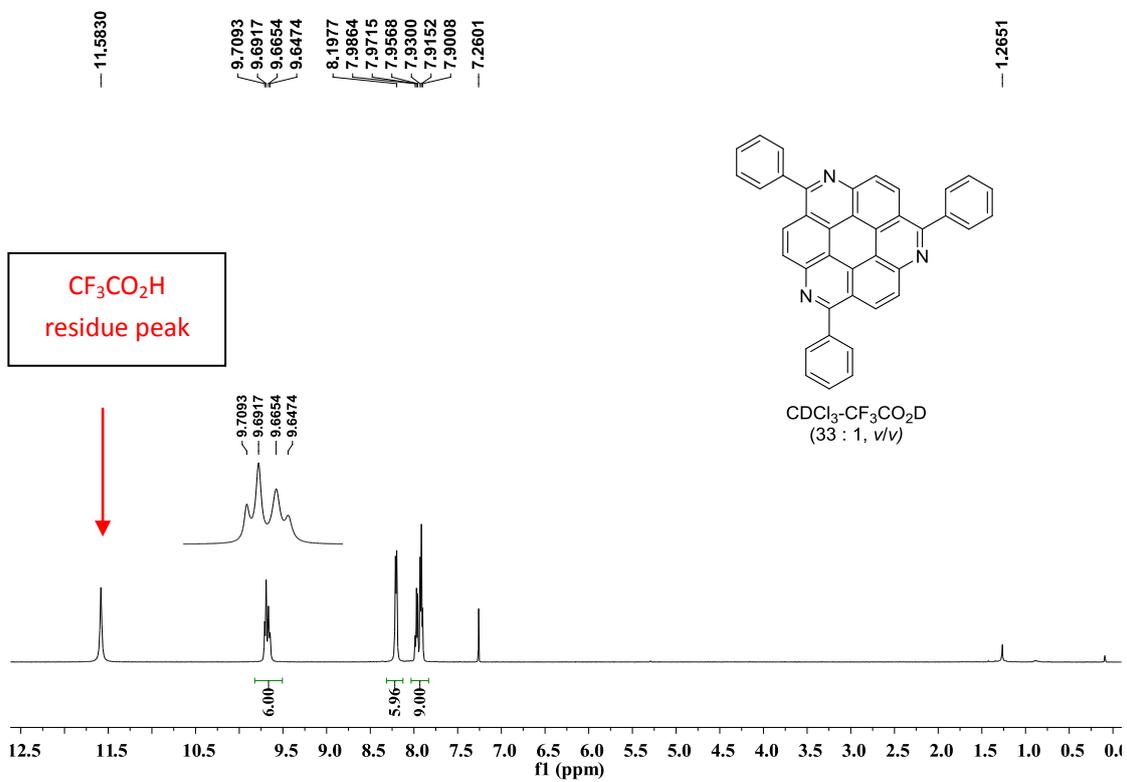
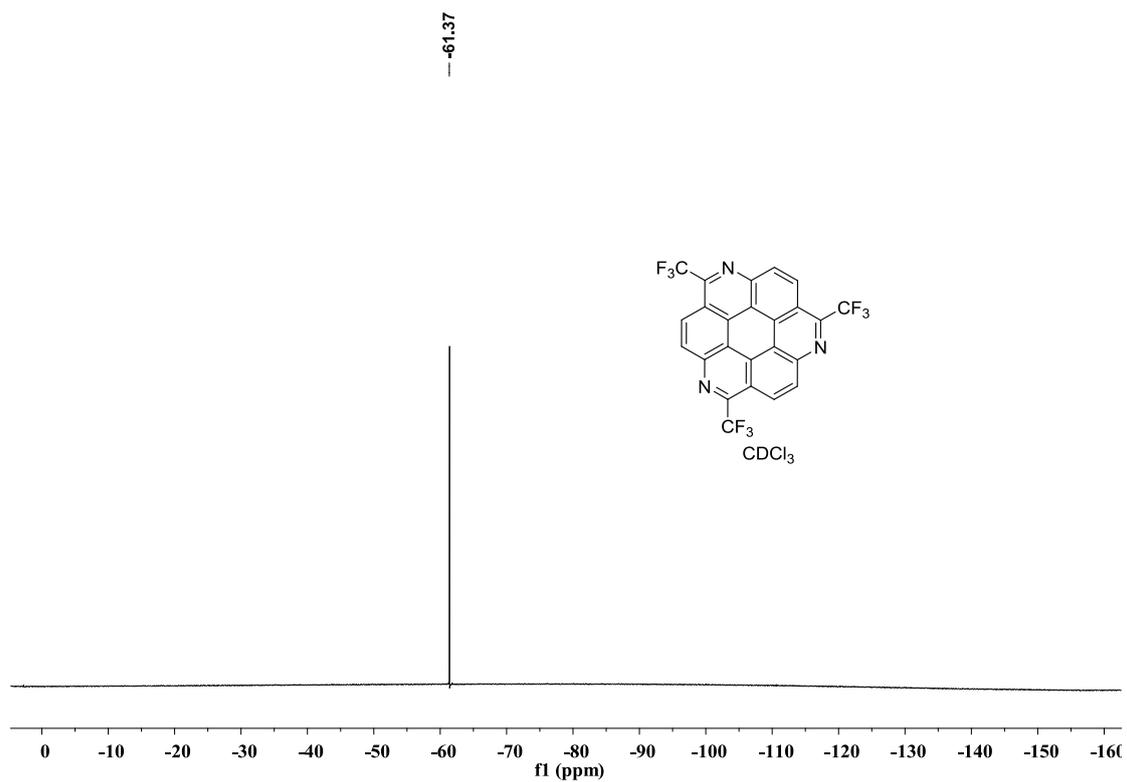


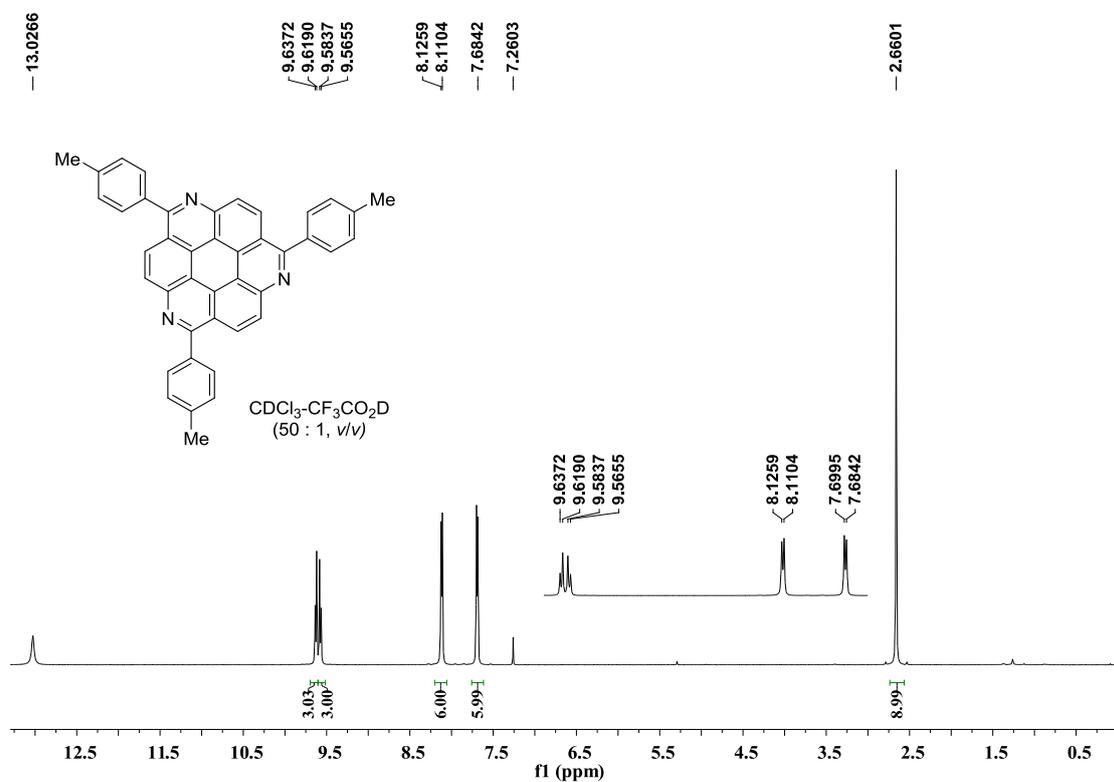
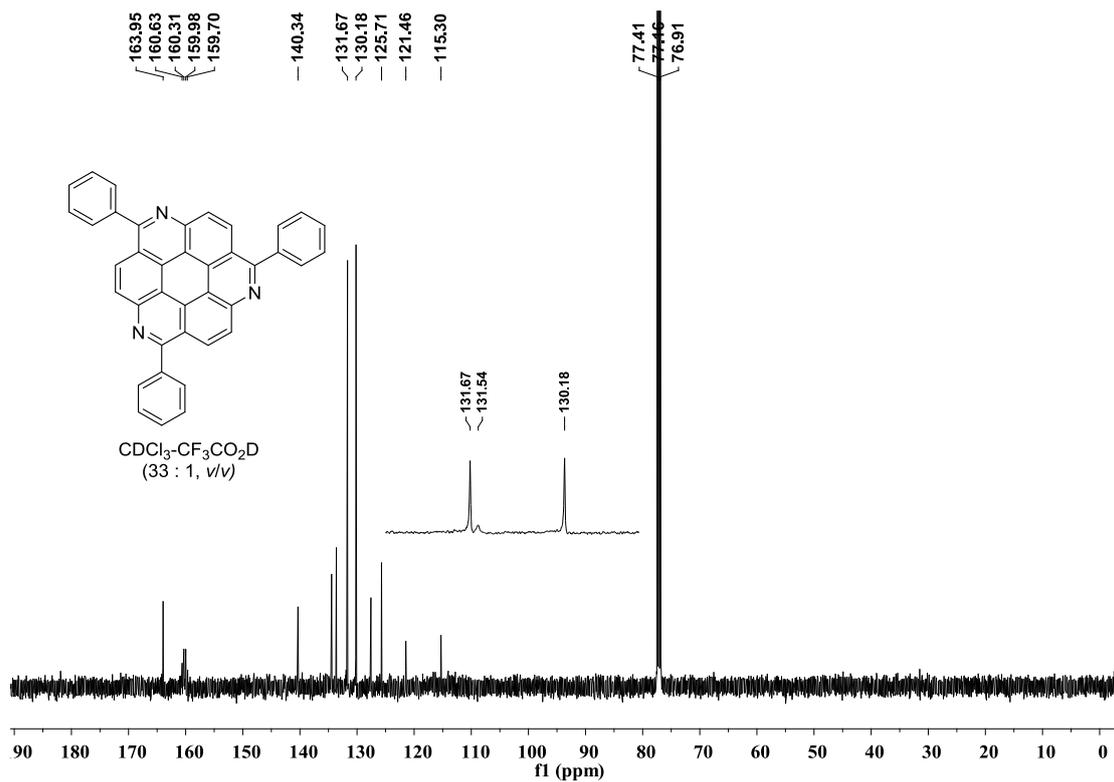


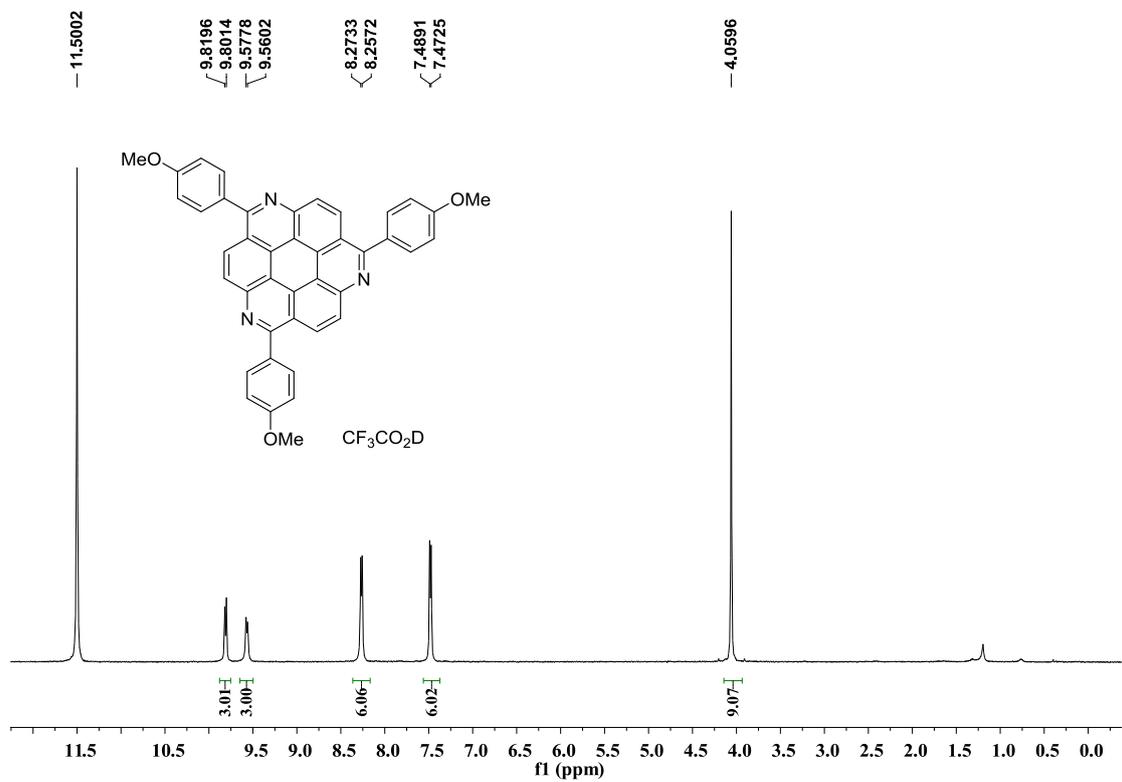
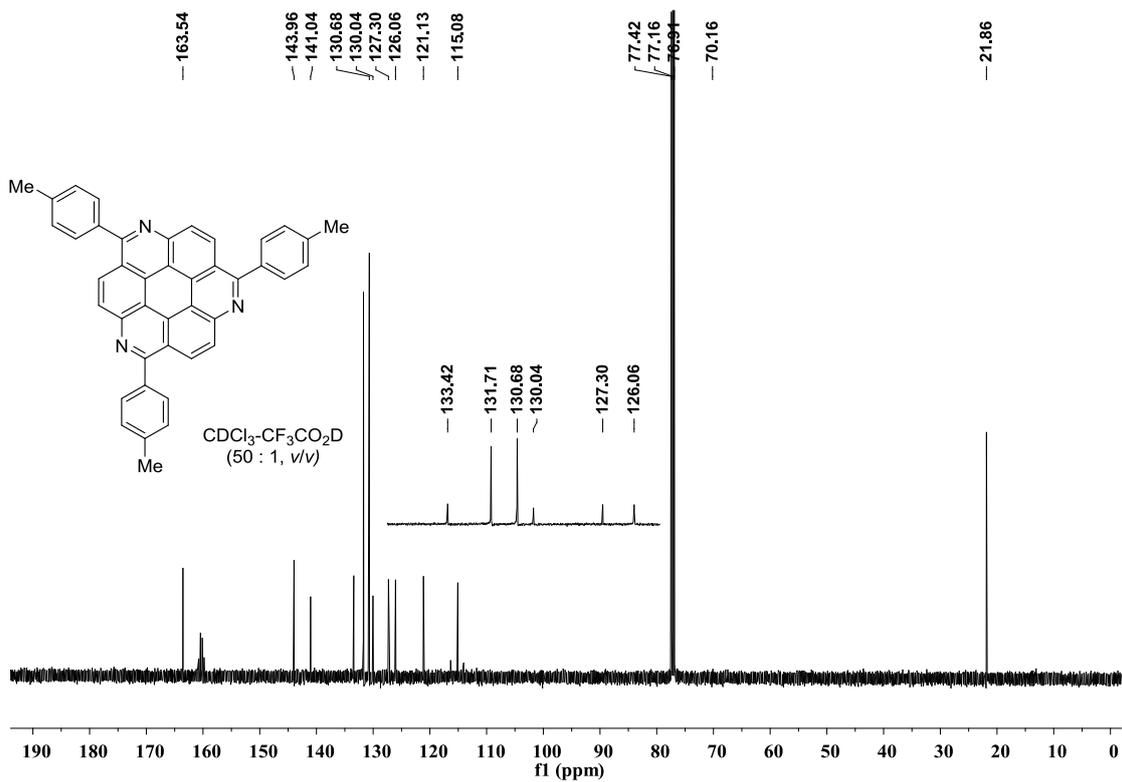


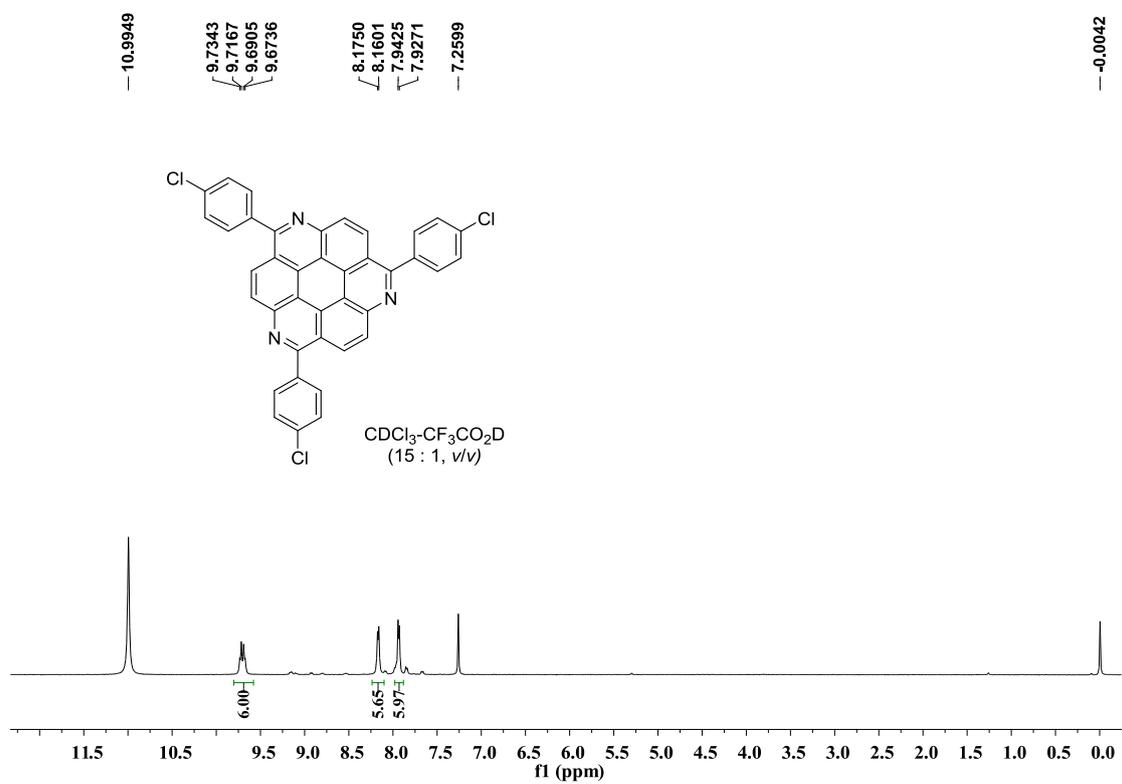
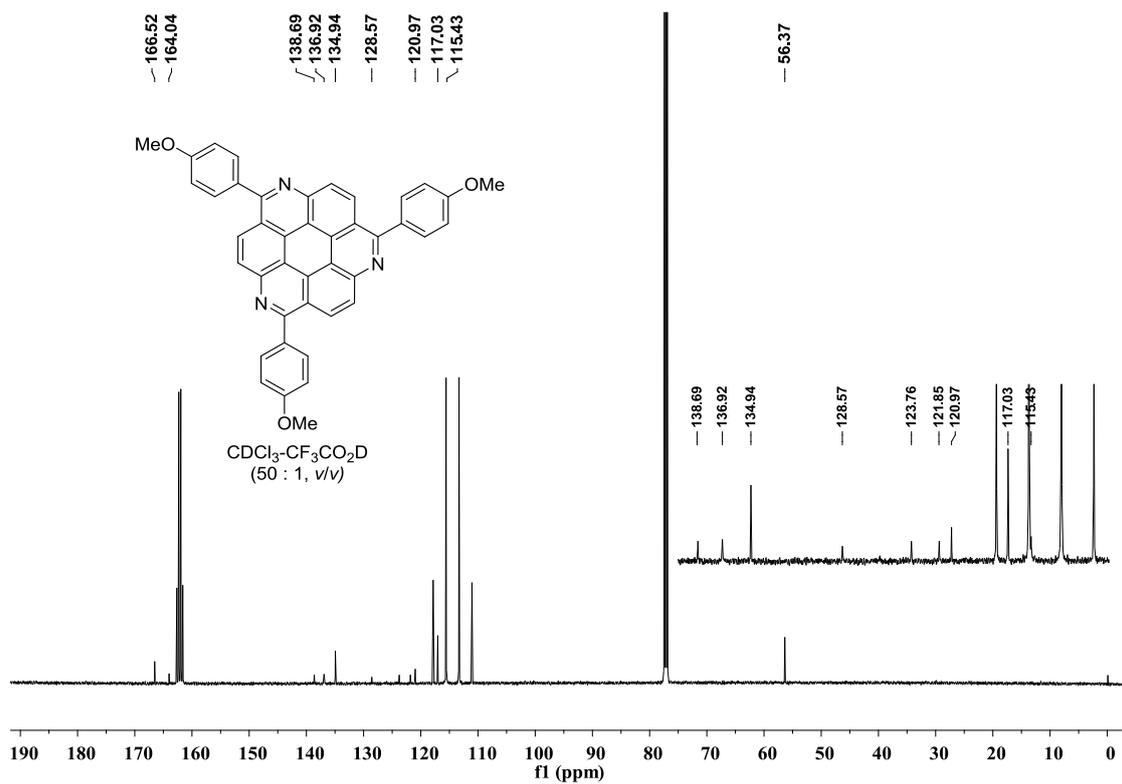


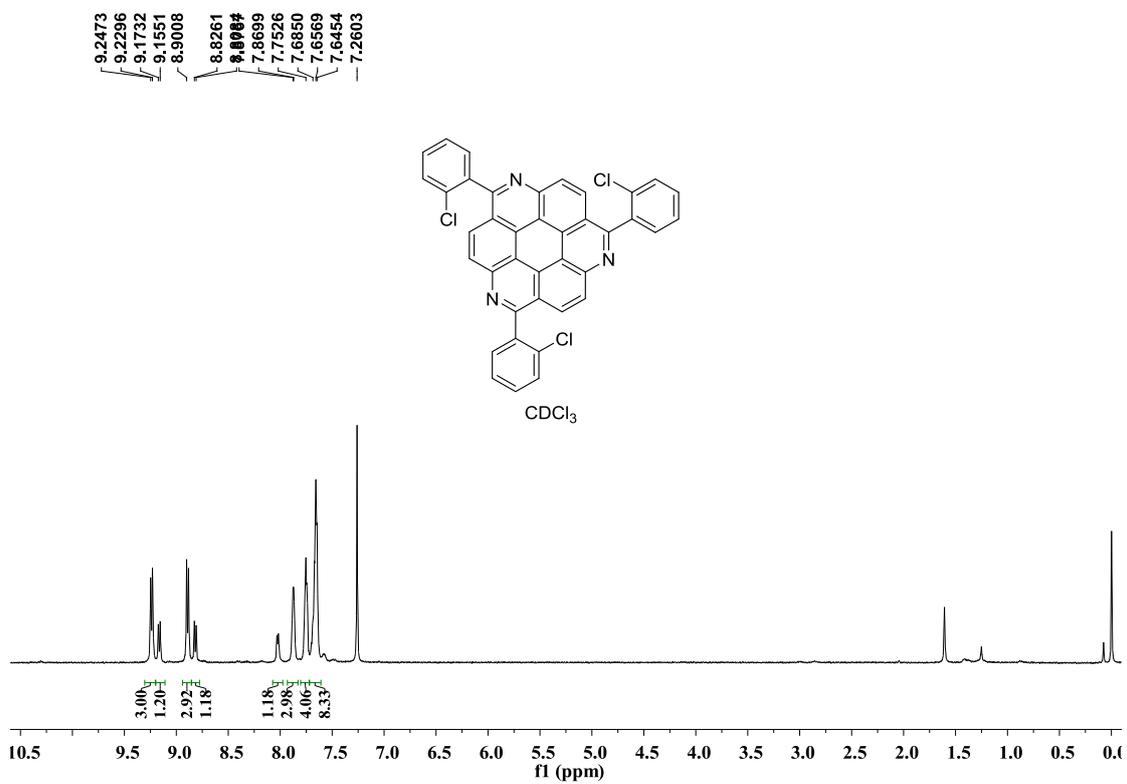
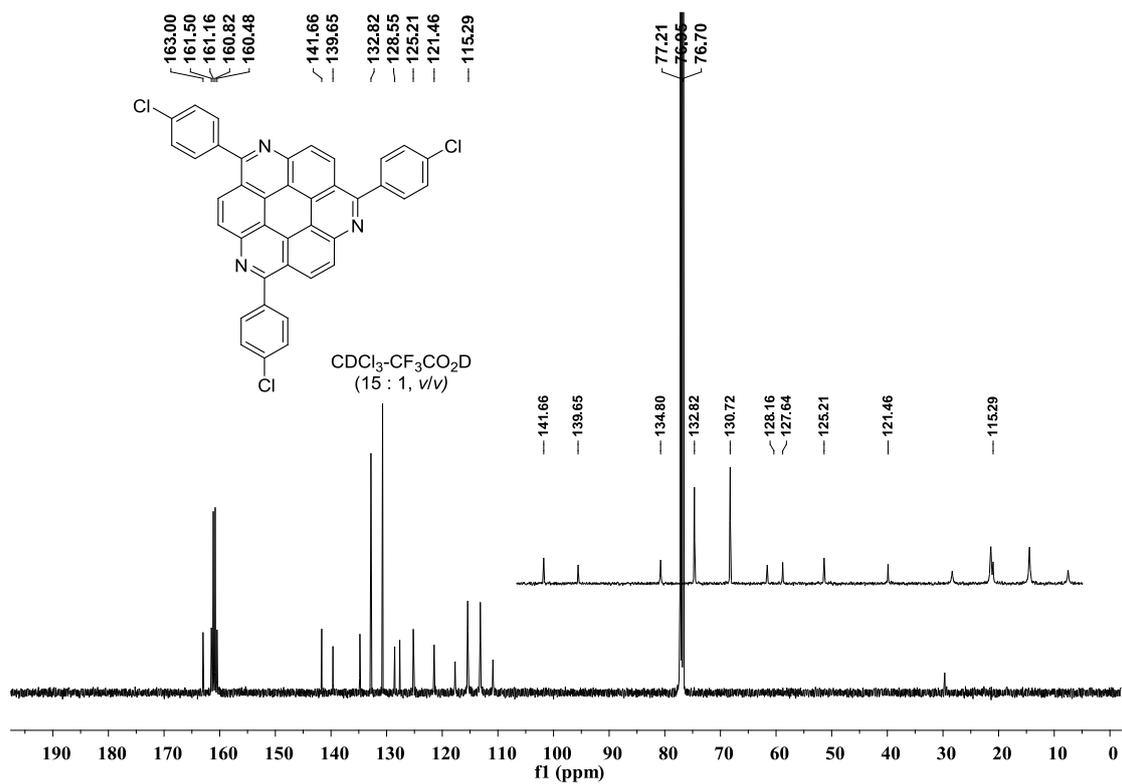


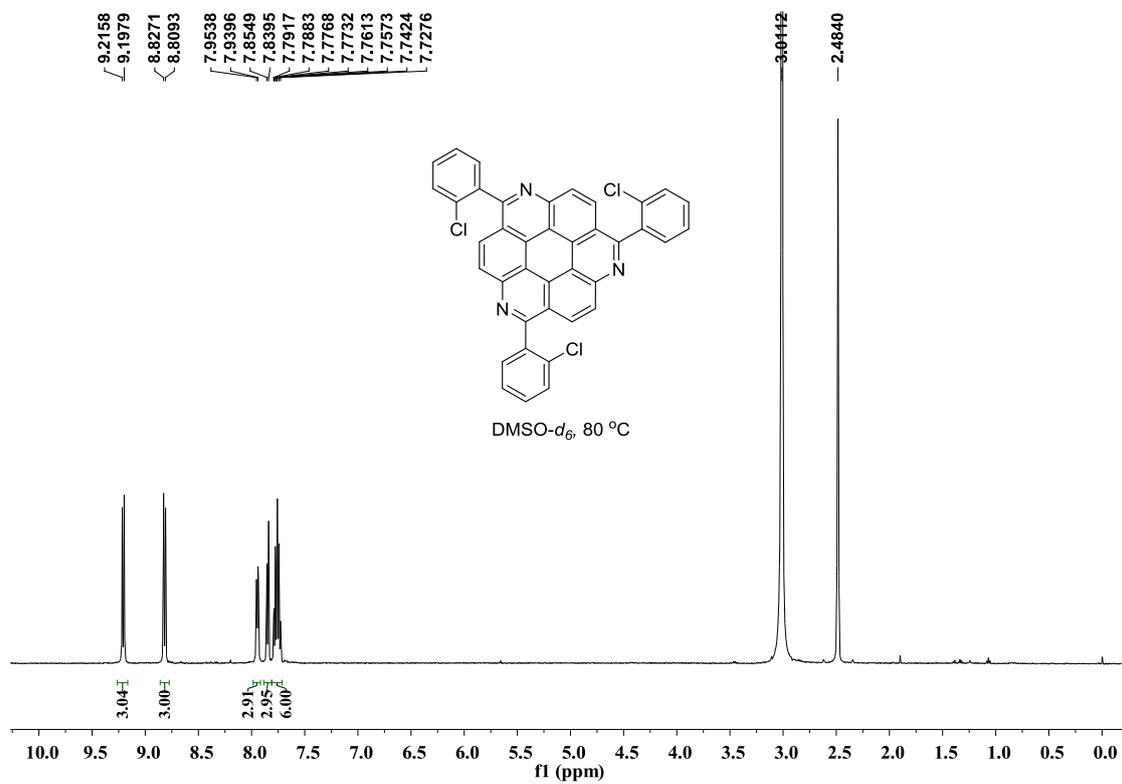
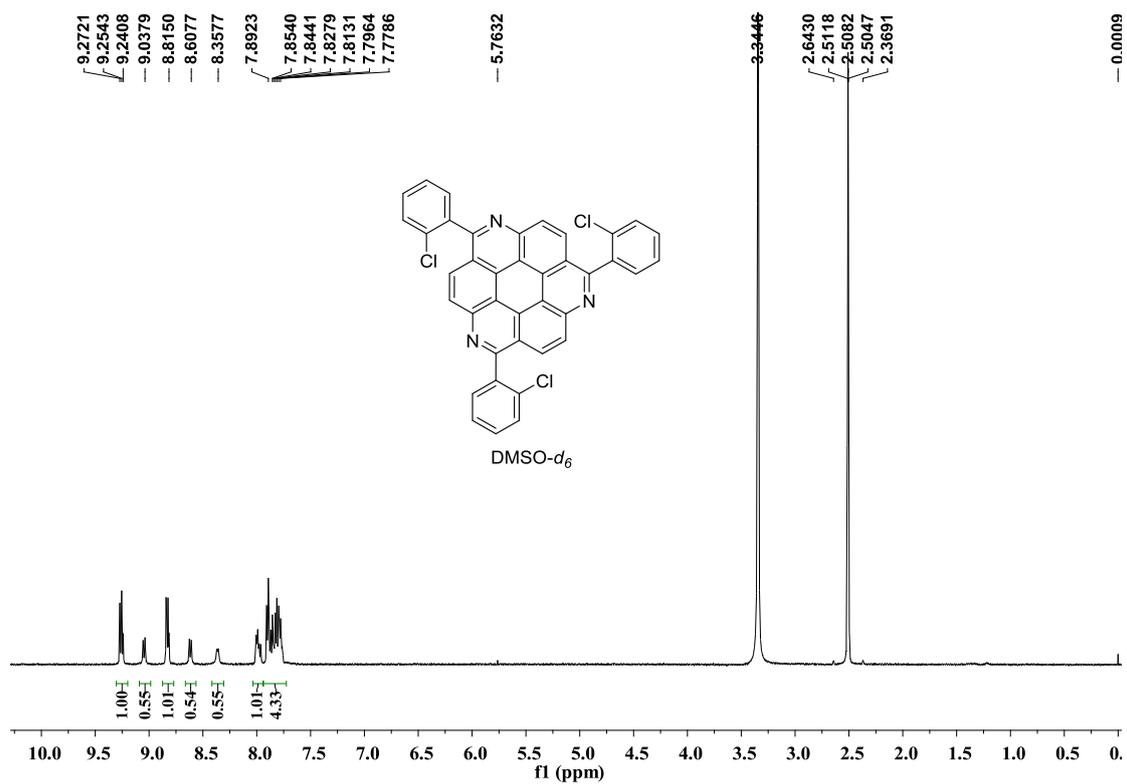


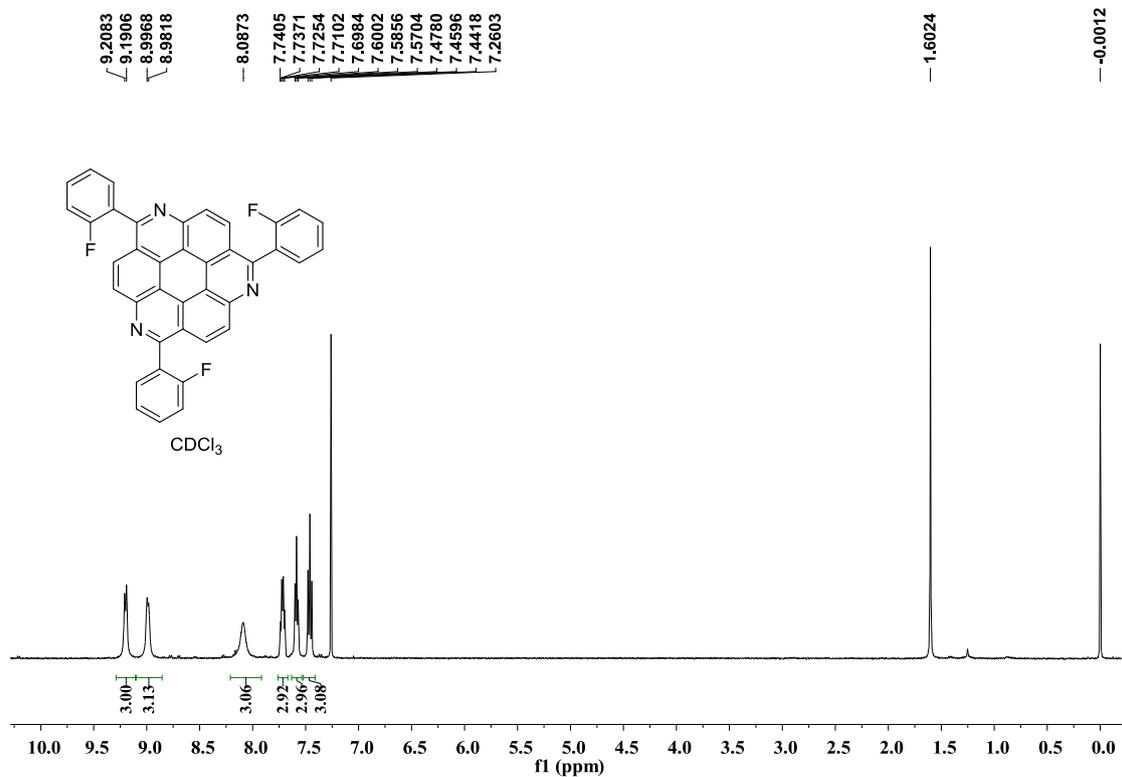
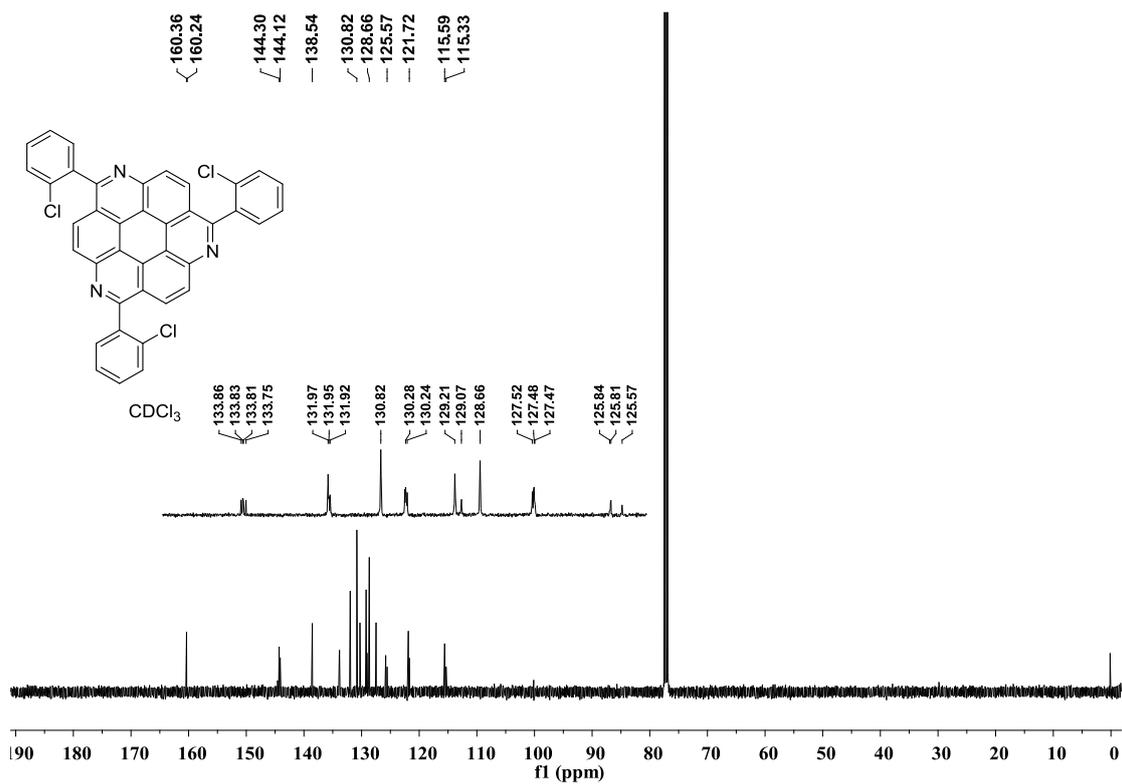


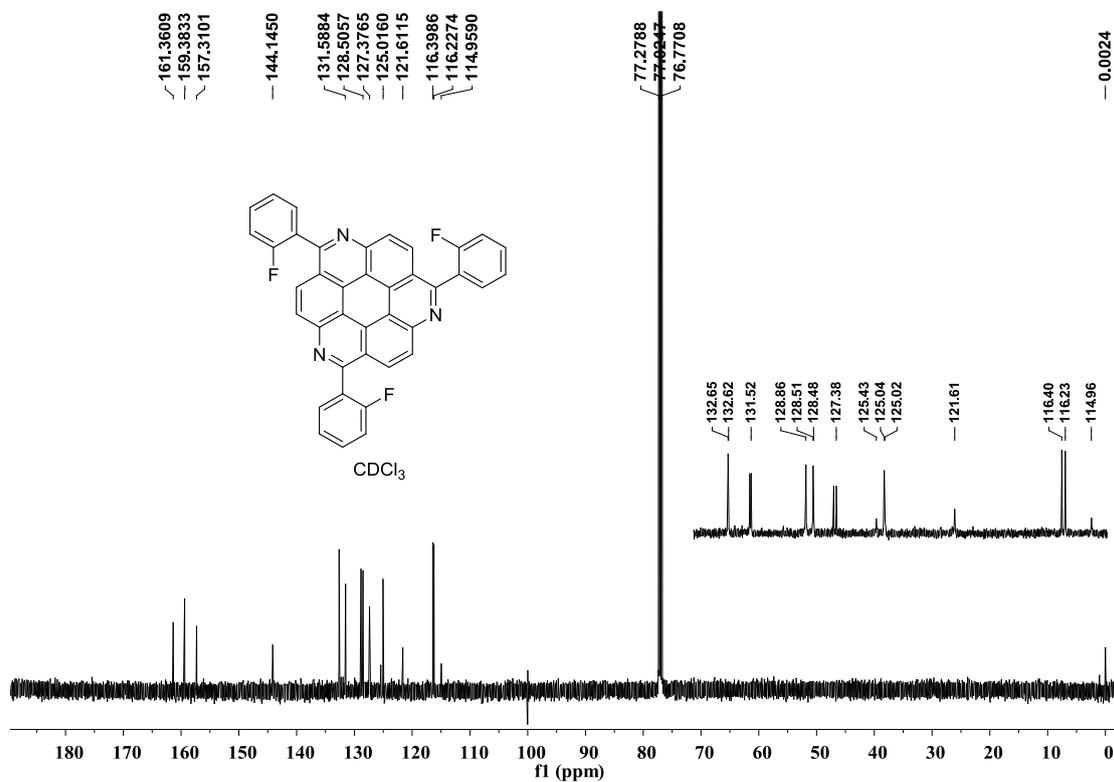
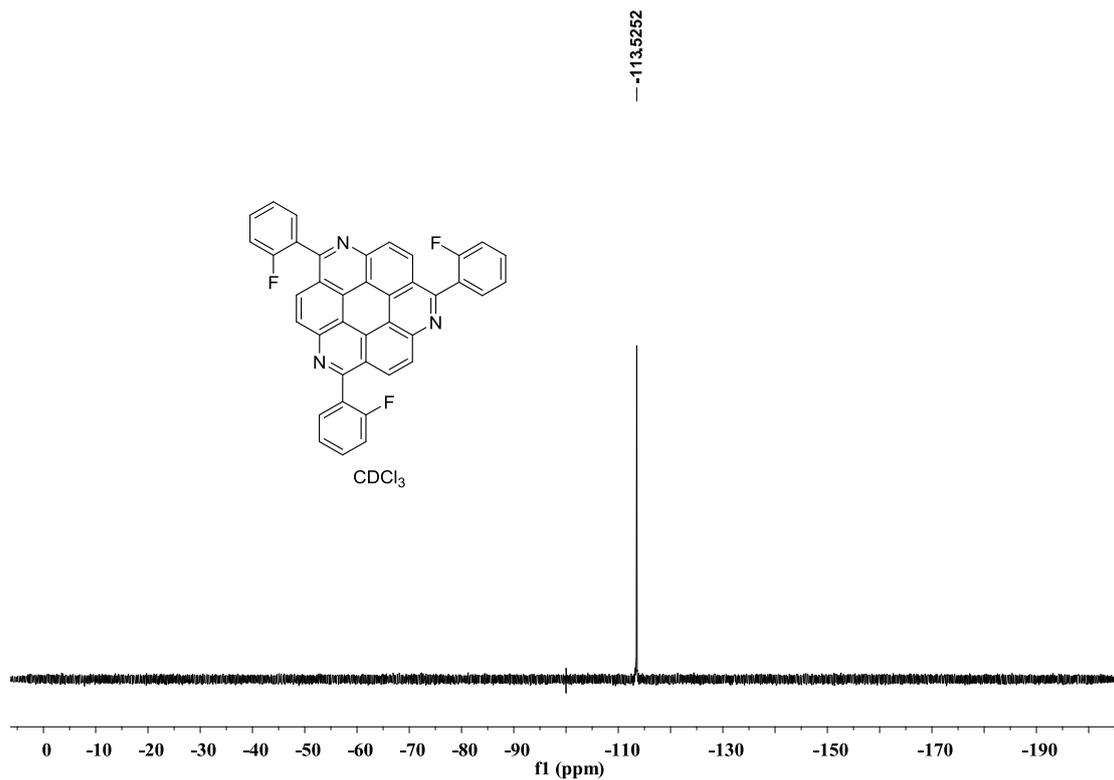




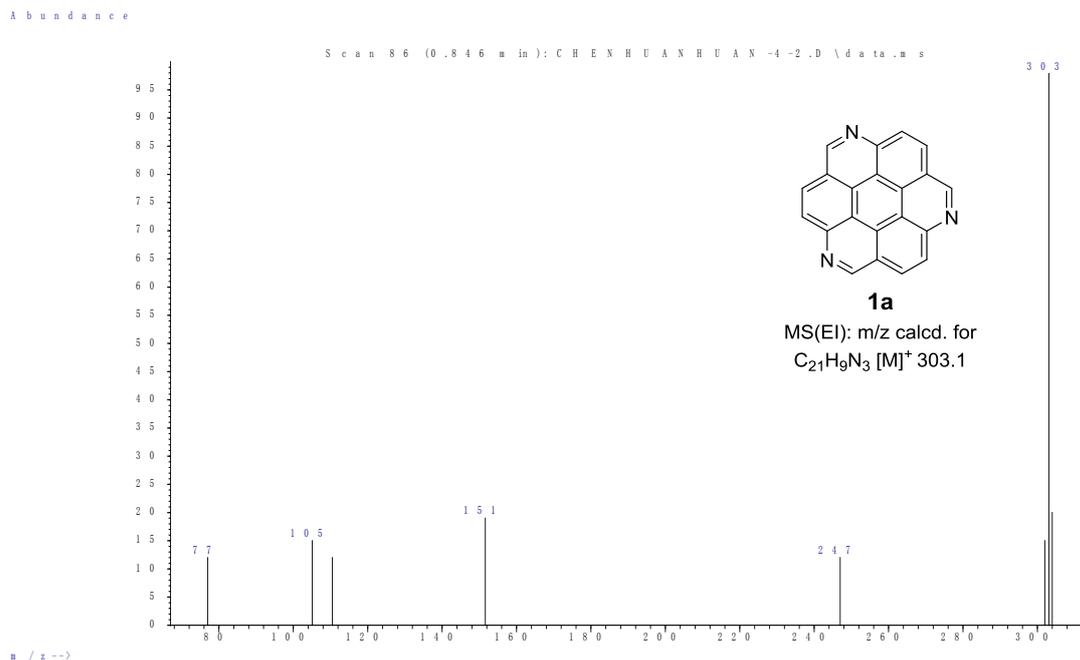




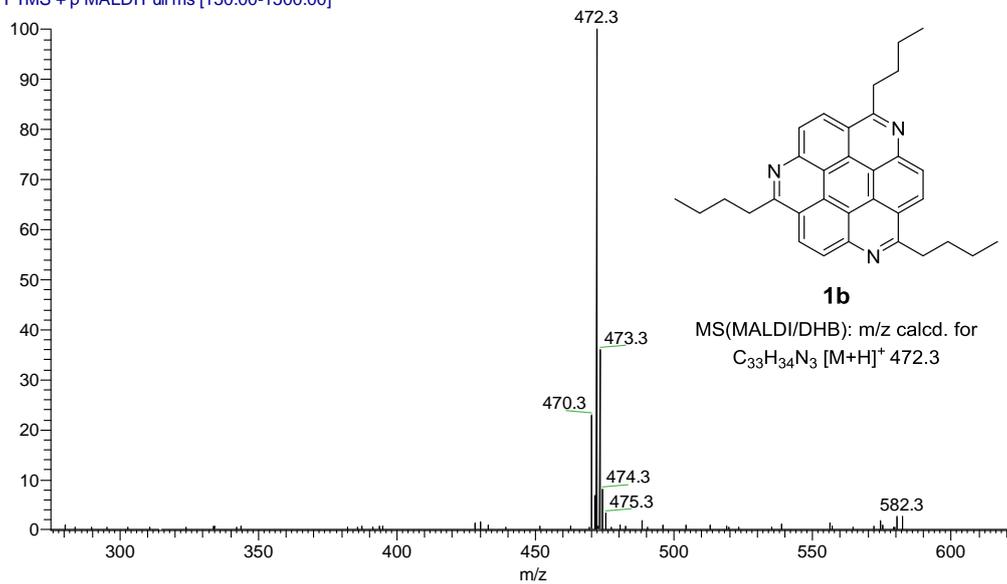




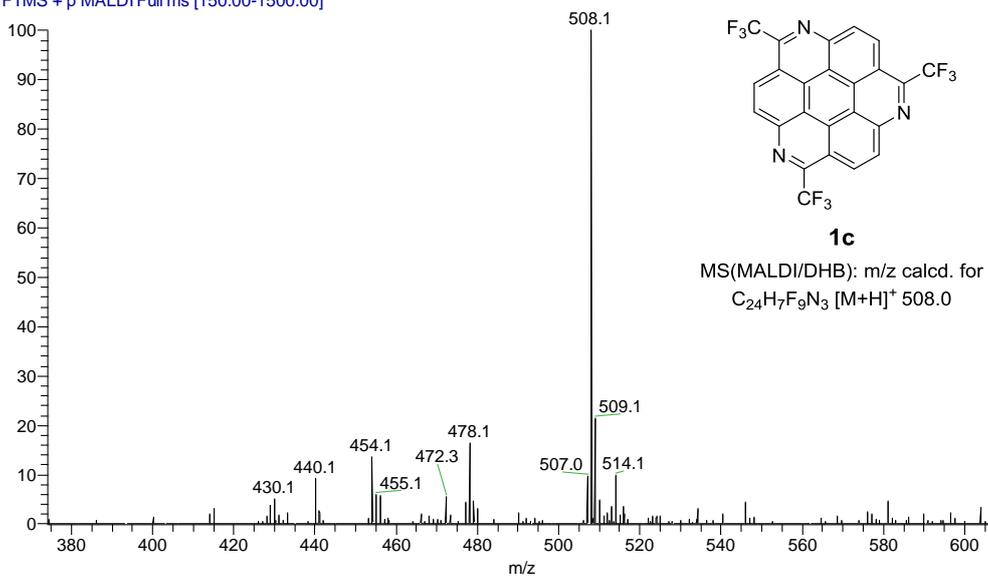
12. Copies of MS Spectra for Triazacoronenes



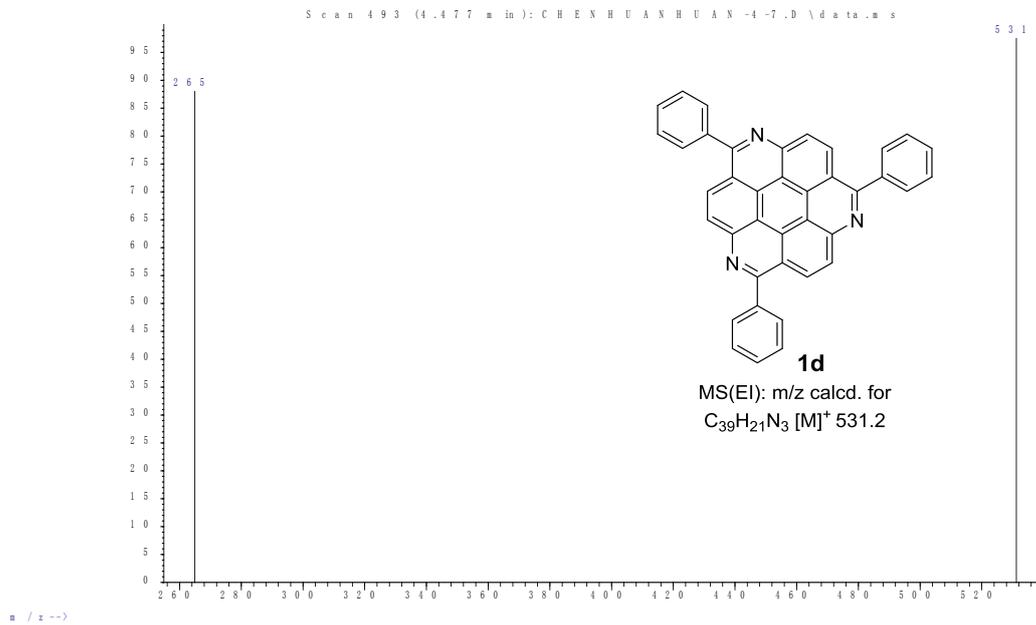
M150287 #13 RT: 0.8326 AV: 1 NL: 1.54E4
T: FTMS + p MALDI Full ms [150.00-1500.00]



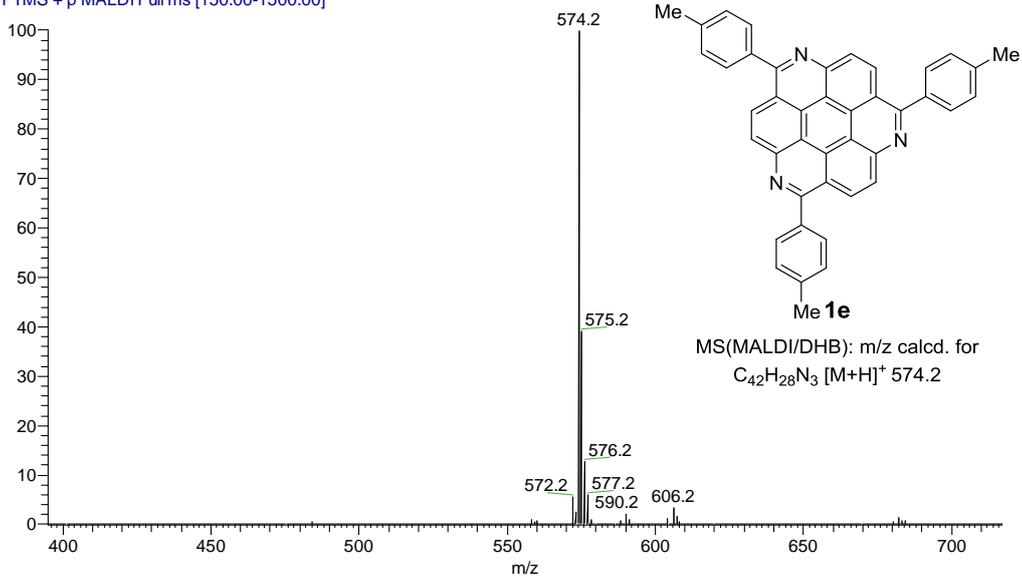
M150787 #5 RT: 0.2886 AV: 1 NL: 1.84E4
T: FTMS + p MALDI Full ms [150.00-1500.00]



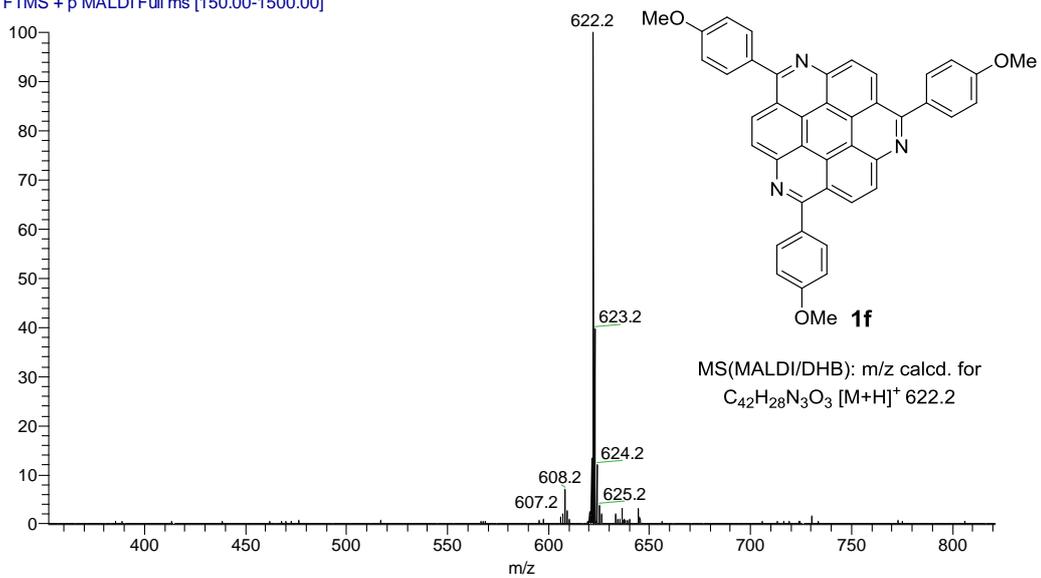
Abundance



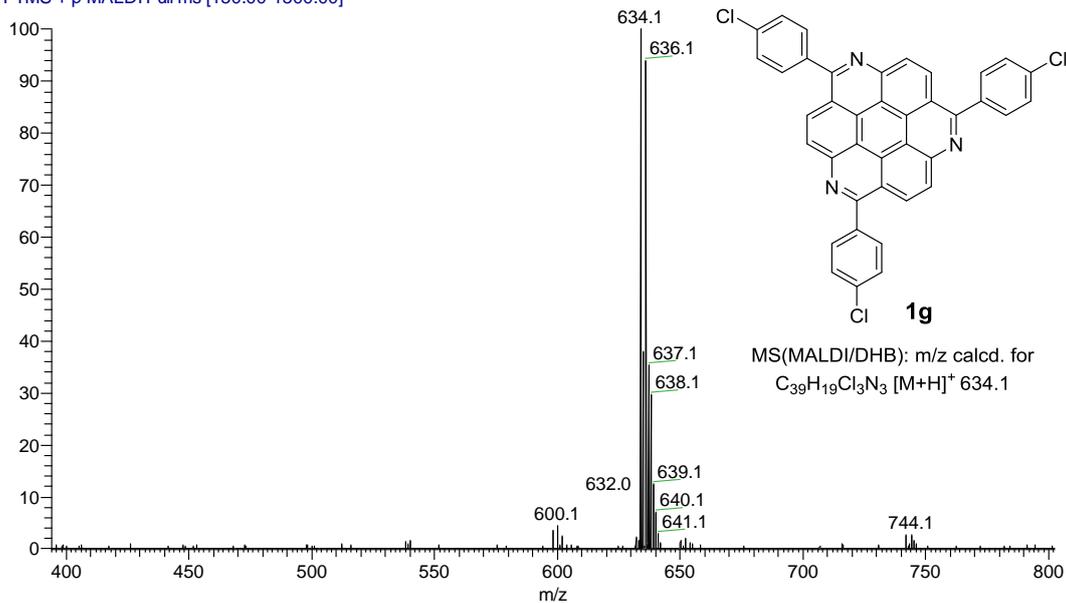
M150283 #10 RT: 0.6245 AV: 1 NL: 4.75E4
T: FTMS + p MALDI Full ms [150.00-1500.00]



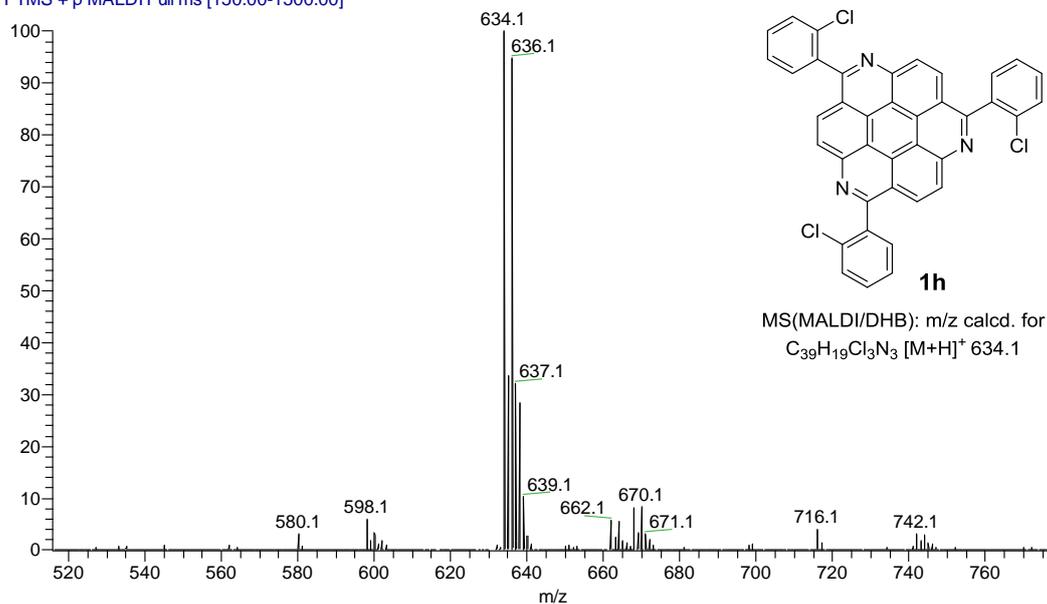
M150291 #24 RT: 1.5956 AV: 1 NL: 2.19E4
T: FTMS + p MALDI Full ms [150.00-1500.00]



M150285 #16 RT: 1.0407 AV: 1 NL: 1.69E4
T: FTMS + p MALDI Full ms [150.00-1500.00]



M150793 #5 RT: 0.2817 AV: 1 NL: 1.17E5
T: FTMS + p MALDI Full ms [150.00-1500.00]



M150795 #13 RT: 0.7188 AV: 1 NL: 5.33E5
T: FTMS + p MALDI Full ms [150.00-1500.00]

