Supporting Information

Heptacyclic Aromatic Hydrocarbon Isomers with Two Azulene Units Fused

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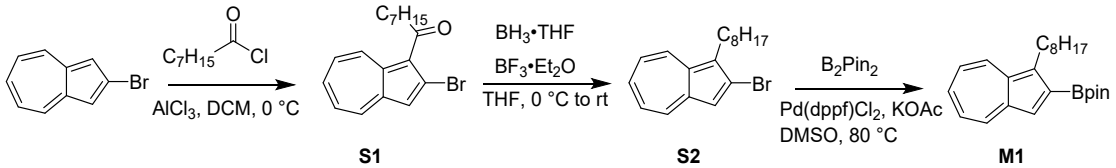
1. Experimental Section

1.1 General

All commercially available materials were purchased and used without further purification unless otherwise noted. All the anhydrous solvent was obtained from an MIKROUNA solvent purification system. All chemical shifts are referenced to residual protons in the NMR solvent ($CDCl_3$: δ 7.26 for protons and 77.16 for carbons). ^1H NMR and ^{13}C NMR spectra were measured on JEOL 400 MHz NMR and Bruker 600 MHz spectrometer. High-resolution mass spectrometry (HR-MS) was performed on a JEOL AccuTOF-DART mass spectrometer, the deviation of HRMS is less than 5 ppm. Absorption spectra were collected using PerkinElmer. Cyclic voltammetry (CV) was carried out on an Autolab using $^nBu_4NPF_6$ (0.1 M) in dichloromethane as supporting electrolyte and ferrocene as an internal reference at a scan rate of 50 mV/s. The CV cell consisted of a platinum button working electrode, a platinum wire counter electrode, and an $Ag/AgNO_3$ reference electrode. Detailed synthetic procedures are listed in the Supporting Information.

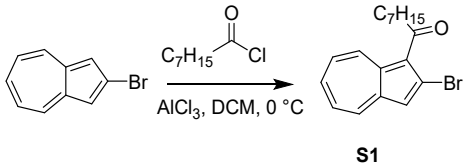
Theoretical calculations were performed with the Gaussian16 program. All calculations were carried out using the density functional theory (DFT) method with Becke's three-parameter hybrid exchange functionals and the Lee-Yang-Parr correlation functional (B3LYP) employing the 6-31G (d, p) basis set for all atoms. Time-dependent DFT (TD-DFT) calculations have been performed at the (R)B3LYP/6-31G (d, p) or (U)B3LYP/6-31G (d, p) level of theory. NICS values were calculated using the standard GIAO procedure. ACID plot was calculated by using the method devel-oped by Herges[5]. The single point energy, independent gradient mode based on Hirshfeld partition and the indexes of aromaticity were calculated at the B3LYP/6-31G* (d, p) level of theory.

1.2 Synthetic Procedures and Characterization Data



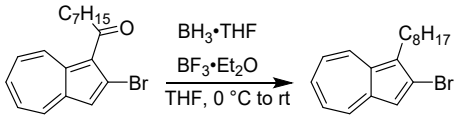
Scheme S1. Synthetic route of **M1**.

1-(2-bromoazulen-1-yl)octan-1-one **(S1)**



2-bromoazulene (1 g, 4.8 mmol, 1.0 eq) was dissolved in 30 mL of dry 1,2-dichloroethane in ice-water bath. Octanoyl chloride (864 mg, 5.3 mmol, 1.1 eq) and $AlCl_3$ (707 mg, 5.3 mmol, 1.1 eq) were added slowly and sequentially. The addition of $AlCl_3$ rapidly changed the color of the solution from purple to orange-red. The reaction was then stirred for 1h under ice bath conditions. The reaction mixture was poured into water and extracted three times with DCM, washed with water and dried over Na_2SO_4. The organic solvent was evaporated under reduced to give a crude product, which was purified by column chromatography on silica gel with PE/EA (50:1) to give compound **S1** as a violet oil in 57% yield (910 mg). **^{1}H NMR** (400 MHz, $CDCl_3$) δ (ppm): 9.44 (d, *J* = 10.0 Hz, 1 H), 8.32 (d, *J* = 10.0 Hz, 1 H), 7.79 (t, *J* = 10.0 Hz, 1 H), 7.54 (t, *J* = 9.6 Hz, 1 H), 7.45 (t, *J* = 9.6 Hz, 1 H), 7.33 (s, 1 H), 3.22 (t, *J* = 7.6 Hz, 2 H), 1.82-1.74 (m, 2 H), 1.43-1.25 (m, 8 H), 0.87 (t, *J* = 6.8 Hz, 3 H). **^{13}C NMR** (100 MHz, $CDCl_3$) δ (ppm): 200.0, 141.9, 140.5, 139.5, 138.0, 136.9, 129.5, 128.1, 128.0, 125.1, 121.4, 43.8, 31.9, 29.6, 29.4, 25.2, 22.8, 14.2.

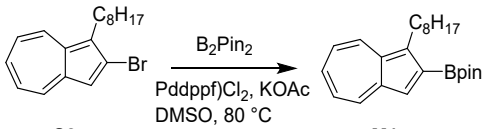
2-bromo-1-octylazulene **(S2)**



S1 **S2**

To a solution of **S1** (3.2 g, 9.6 mmol, 1.0 eq) in 100 mL dry THF in ice-water bath was added BH_3•THF (1.0 M in THF, 96 mL, 96 mmol, 10 eq) and stirred for 30 min, over which time the color of the mixture changed from violet to dark blue. Then BF_3•Et_2O (11 g, 48% BF_3) was added slowly. The solution was left to warm to room temperature and stirred overnight. The reaction mixture was quenched with MeOH and extracted three times with DCM, dried over Na_2SO_4. The organic solvent was evaporated under reduced to give a crude product, which was purified by column chromatography on silica gel with PE to give compound **S2** as a blue oil in 59% yield (1.8 g). **^{1}H NMR** (400 MHz, $CDCl_3$) δ (ppm): 8.25 (d, *J* = 9.6 Hz, 1 H), 8.18 (d, *J* = 9.6 Hz, 1 H), 7.58 (t, *J* = 9.6 Hz, 1 H), 7.37 (s, 1 H), 7.16 (t, *J* = 9.6 Hz, 1 H), 7.13 (t, *J* = 9.6 Hz, 1 H), 3.06(t, *J* = 8.0 Hz, 2 H), 1.70-1.63(m, 2 H), 1.46-1.29(m,10 H),0.90(t, *J* = 6.8 Hz, 3 H). **^{13}C NMR** (100 MHz, $CDCl_3$) δ (ppm): 139.1, 137.3, 135.3, 135.1, 133.0, 129.5, 129.4, 123.7, 123.1, 117.9, 32.1, 31.2, 29.8, 29.7, 29.4, 26.5, 22.8, 14.3.

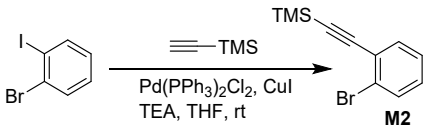
4,4,5,5-tetramethyl-2-(1-octylazulen-2-yl)-1,3,2-dioxaborolan **(M1)**



S2 **M1**

To a 100 ml Schlenk tube was added **S2** (1 g, 3.125 mmol, 1.0 eq), $Pd(dppf)Cl_2$ (115 mg, 0.16 mmol, 0.05 eq), Bis(pinacolato)diboron (1.59 g, 6.25 mmol, 2.0 eq), KOAC (920 mg, 9.38 mmol 3.0 eq). The flask was evacuated and backfilled with nitrogen for three times. Then 20 ml anhydrous DMSO was injected with syringe. The mixture was heated at 80 °C for 18 hours, after which it was cooled to room temperature. Then the mixture was poured into water and extracted three times with DCM, washed with water and dried over Na_2SO_4. The organic solvent was evaporated under reduced to give a crude product, which was purified by column chromatography on silica gel with PE/EA (20:1) to give compound **M1** as a dark blue oil in 78% yield (900 mg). **^{1}H NMR** (400 MHz, $CDCl_3$) δ (ppm): 8.28 (d, *J* = 9.6 Hz, 1 H), 8.21 (d, *J* = 9.2 Hz, 1 H), 7.70 (s, 1 H), 7.47 (t, *J* = 9.6Hz, 1 H), 6.99 (t, *J* = 9.6Hz, 1 H), 6.95 (t, *J* = 9.6Hz, 1 H), 3.26 (t, *J* = 7.6 Hz, 2 H), 1.67-1.60 (m, 2 H), 1.39(s, 12 H), 1.35-1.23(m, 10 H) 0.88 (t, *J* = 6.8 Hz, 3 H). **^{13}C NMR** (100 MHz, $CDCl_3$) δ (ppm):140.5, 139.6, 138.8, 137.8,136.9, 135.1, 125.0, 121.9, 121.2, 83.4, 33.6, 32.1, 30.1, 29.8, 29.5, 27.3, 25.1, 22.8, 14.3. **HR-MS** (m/z): $[M+H]^+$ calcd. for $C_{24}H_{36}BO_2$: 367.2803; Found: 367.2790; Error: 3.54ppm.

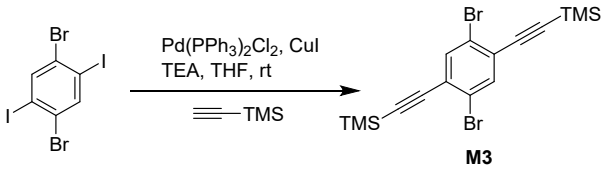
((2-bromophenyl)ethynyl)trimethylsilane **(M2)**[1]



M2

This compound was prepared according to the reported procedure. To a 200 ml Schlenk tube was added 1-bromo-2-iodobenzene (5 g, 17.7 mmol, 1.0 eq), $PdCl_2(PPh_3)_2$ (1.24 g, 1.77 mmol, 0.1 eq), CuI (673 mg, 3.53 mmol, 0.2 eq). The flask was evacuated and backfilled with nitrogen for three times. Then degassed dry THF (50 mL), triethylamine (30 mL), and ethynyltrimethylsilane (2.08 g, 21.2 mmol, 1.2 eq) was added with syringe. The mixture was stirred at room temperature for 24 hours. The reaction mixture was poured into water and extracted three times with EA, washed with water and dried over Na_2SO_4.The organic solvent was evaporated under reduced to give a crude product, which was purified by column chromatography on silica gel with n-hexane to give compound **M2** as a yellow oil in 94% yield (4.21 g). **^{1}H NMR** (400 MHz, $CDCl_3$) δ (ppm): 7.58 (d, *J* = 5.2 Hz, 1H), 7.49 (d, *J* = 4.8 Hz, 1H), 7.24 (t, *J* = 5.2 Hz, 1H), 7.15 (t, *J* = 5.2 Hz, 1H), 0.28 (s, 9H).

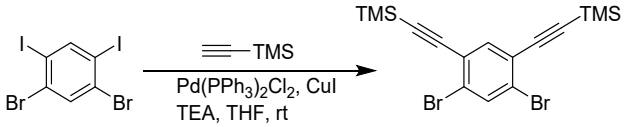
((2,5-dibromo-1,4-phenylene)bis(ethyne-2,1-diyl))bis(trimethylsilane) **(M3)**[2]



M3

This compound was prepared according to the reported procedure. Compound **M3** was obtained from 1,4-dibromo-2,5- diiodobenzene by a similar method with compound **M2** (eluting with n-hexane) in 85% yield (3.64 g), as a white solid. **^{1}H NMR** (400 MHz, $CDCl_3$) δ (ppm): 7.67 (s, 2 H), 0.27 (s, 18 H). **^{13}C NMR** (100 MHz, $CDCl_3$) δ (ppm): 136.6, 126.6, 123.9, 103.2, 101.5, -0.2.

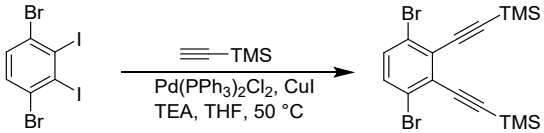
((4,6-dibromo-1,3-phenylene)bis(ethyne-2,1-diyl))bis(trimethylsilane) **(M4)**[3]



M4

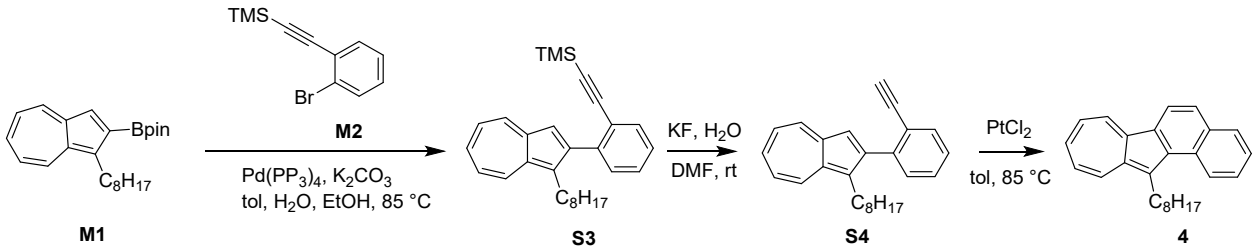
This compound was prepared according to the reported procedure. Compound **M4** was obtained from 1,5-dibromo-2,4-diiodobenzene by a similar method with compound **M2** (eluting with n-hexane) in 93% yield (0.82 g), as a yellow oil. **^{1}H NMR** (400 MHz, $CDCl_3$) δ (ppm): 7.80 (s, 1 H), 7.59 (s, 1 H), 0.26 (s, 18 H).

((3,6-dibromo-1,2-phenylene)bis(ethyne-2,1-diyl))bis(trimethylsilane) **(M5)**[4]



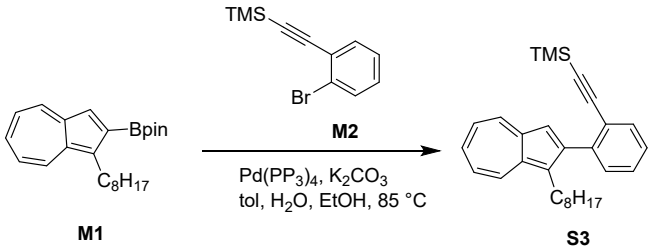
M5

1,4-dibromo-2,3-diiodobenzene was prepared according to the reported procedure. To a 100 ml Schlenk tube was added 1,4-dibromo -2,3-diiodobenzene (1 g, 2.05 mmol, 1.0eq), $PdCl_2(PPh_3)_2$ (144 mg, 0.2 mmol, 0.1 eq), CuI (78 mg, 0.41 mmol, 0.2 eq). The flask was evacuated and backfilled with nitrogen for three times. Then anhydrous THF (25 mL), triethylamine (20 mL), Trimethylsilylacetylene (443 mg, 4.5 mmol, 2.2 eq) was added with syringe. The mixture was stirred at 50°C for 24 hours. The reaction mixture was poured into water and extracted three times with EA, washed with water and dried over Na_2SO_4.The organic solvent was evaporated under reduced to give a crude product, which was purified by column chromatography on silica gel with n-hexane to give compound **M5** as a yellow oil in 15% yield (130 mg). **^{1}H NMR** (400 MHz, $CDCl_3$) δ (ppm): 7.35 (s,2H), 0.29 (s, 18 H). **^{13}C NMR** (100 MHz, $CDCl_3$) δ (ppm): 132.6, 129.2, 124.7, 105.7, 101.3, -.0.1. **HR-MS** (m/z): $[M+H]^+$ calcd. for $C_{16}H_{21}Br_2Si_2$: 428.9523; Found: 428.9503; Error: 4.7 ppm.



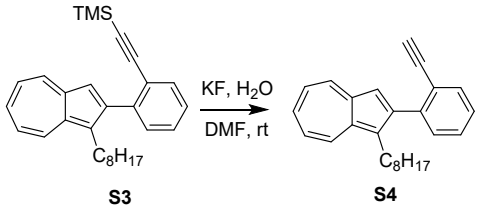
Scheme S2. Synthetic route of compound **4**.

trimethyl((2-(1-octylazulen-2-yl)phenyl)ethynyl)silane **(S3)**



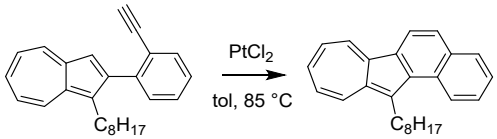
To a mixture of compound **M1** (500 mg, 1.36 mmol, 1 eq), **M2** (415 mg, 1.64 mmol, 1.2 eq), $Pd(PPh_3)_4$ (79 mg, 0.068 mmol, 0.05 eq), K_2CO_3 (566 mg, 4.09 mmol, 3 eq) under nitrogen atmosphere, 6 mL degassed toluene, 1.5 mL degassed water and 1.5 mL degassed EtOH were added and the mixture was heated at 85 °C for 24 h, after which it was cooled to room temperature. Then the mixture was poured into water and extracted three times with EA, washed with water and dried over Na_2SO_4. The organic solvent was evaporated under reduced to give a crude product, which was purified by column chromatography on silica gel with PE to give compound **S3** as a blue oil in 78% yield (210 mg). **^{1}H NMR** (400 MHz, $CDCl_3$) δ (ppm): 8.30 (d, *J* = 9.6 Hz, 1H), 8.22 (d, *J* = 9.2 Hz, 1H), 7.61 (d, *J* = 7.6 Hz, 1H), 7.51 (t, *J* = 7.6 Hz, 1H), 7.46 (s, 1H), 7.41-7.40 (m, 2H),7.34-7.31 (m, 1H), 7.10 (t, *J* = 9.6 Hz, 1H), 7.06 (t, *J* = 9.6 Hz, 1H), 3.05 (t, *J* = 7.6 Hz, 2H), 1.54-1.46 (m, 2H), 1.27-1.15 (m, 10H), 0.85 (t, *J* = 6.8 Hz, 3H), -0.05 (s, 9H). **^{13}C NMR** (100 MHz, $CDCl_3$) δ (ppm): 149.6, 141.8, 139.2, 136.8, 136.6, 135.8, 133.7, 132.6, 130.1, 129.9, 128.2, 127.1, 122.9, 122.3, 121.7, 118.8, 105.1, 97.3, 32.0, 32.0, 29.6, 29.4, 29.4, 25.9, 22.8, 14.3, -0.2. **HR-MS** (m/z): $[M+H]^+$ calcd. for $C_{29}H_{37}Si$: 413.2660; Found: 413.2654; Error: 1.5 ppm.

(2-ethynylphenyl)-1-octylazulene **(S4)**



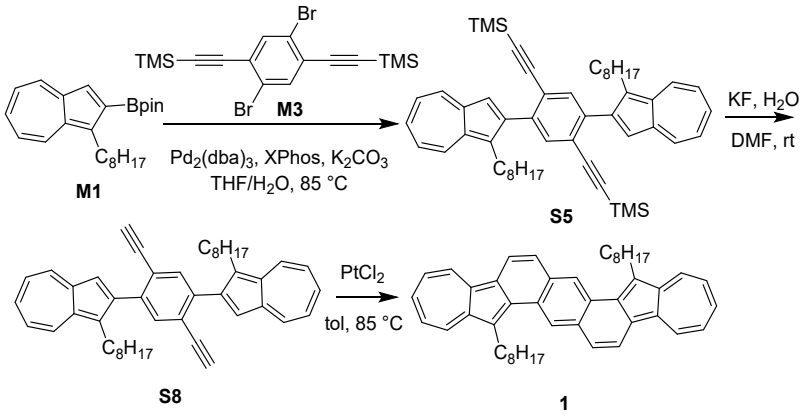
Compound **S3** (200 mg, 0.48mmol, 1.0 eq) was dissolved in DMF (20 mL) and aqueous KF (169 mg, 0.3 mmol, 6 eq) solution (5 mL) was added. The mixture was stirred at room temperature overnight and water (100 mL) was added. The reaction mixture was extracted three times with EA, washed with water and dried over Na_2SO_4.The organic solvent was evaporated under reduced to give a crude product, which was purified by column chromatography on silica gel with PE to give compound **S4** as a blue oil in 95% yield (157 mg).**^{1}H NMR** (400 MHz, $CDCl_3$) δ (ppm): 8.35 (d, *J* = 9.6 Hz, 1H), 8.28 (d, *J* = 9.2 Hz, 1H), 7.70 (d, *J* = 7.6 Hz, 1H), 7.54 (t, *J* = 9.6 Hz, 1H), 7.48 (s, 1H), 7.46-7.35 (m, 3H), 7.14 (d, *J* = 10.0 Hz, 1H), 7.10 (d, *J* = 9.6 Hz, 1H), 3.08 (t, *J* = 7.6 Hz, 2H), 2.91 (s, 1H), 1.55-1.50 (m, 2H), 1.29-1.18 (m, 10H), 0.88 (t, *J* = 6.8 Hz, 3H). **^{13}C NMR** (100 MHz, $CDCl_3$) δ (ppm): 149.4, 141.6, 139.3, 137.1, 136.6, 136.2, 134.0, 133.4, 130.3, 129.9, 128.5, 127.2, 122.5, 121.9, 121.8, 118.5, 83.3, 79.9, 32.0, 29.7, 29.4, 29.3, 25.8, 22.8,14.3. **HR-MS** (m/z): $[M+H]^+$ calcd. for $C_{26}H_{29}$: 341.2264; Found: 341.2259; Error: 1.5 ppm.

***12-octylnaphtho[2,1-a]azulene* (4)**



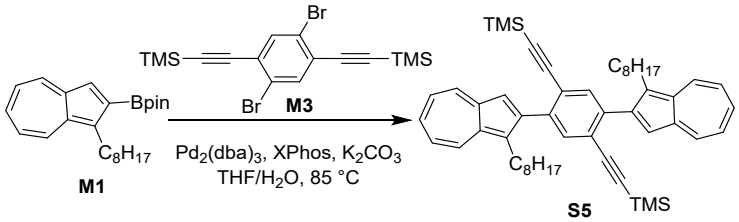
S4 **4**

Compound **S4** (50 mg, 0.146 mmol, 1 eq) and $PtCl_2$ (4 mg, 0.1 eq) was dissolved in 5 mL dry toluene under a nitrogen atmosphere. The mixture was heated at 85 ℃ for 12 h, after which it was cooled to room temperature. The crude mixture was filtered through celite and solvent was removed under reduced pressure, which was purified by column chromatography on silica gel with PE/DCM(20:1) to give compound **4** as a blue green solid in 66% yield (33 mg). **^{1}H NMR** (400 MHz, $CDCl_3$) δ (ppm): 8.84 (d, *J* = 8.28 Hz, 1H), 8.66 (dd, *J* = 8.68 Hz, 0.8 Hz, 1H), 8.45 (d, *J* = 8.64 Hz, 1H), 8.37 (d, *J* = 10.84 Hz, 1H), 8.10 (dd, *J* = 10.0 Hz, 1.6 Hz, 1H), 7.84 (d, *J* = 8.64 Hz, 1H), 7.74-7.64 (m, 2H), 7.48 (t, *J* =9.6 Hz, 1H), 7.22 (dd, *J* = 8.68 Hz, 10.64 Hz, 1H), 7.10 (dd, *J* = 8.92 Hz, 10.84 Hz, 1H), 3.63 (t, *J* = 8 Hz, 2H), 1.94-1.86 (m, 2H), 1.65-1.58 (m, 2H), 1.46-1.39 (m, 2H), 1.34-1.27 (m, 6H), 0.89 (t, *J* = 6.4 Hz, 3H) **^{13}C NMR** (100 MHz, $CDCl_3$) δ (ppm): 138.6, 138.0, 136.0, 134.9, 134.7, 133.5, 129.5, 129.1, 128.7, 128.5, 127.4, 126.2, 125.9, 125.8, 124.1, 123.2, 122.2, 119.4, 32.1, 30.3, 30.2, 29.8, 29.5, 27.8, 22.8, 14.3. **HR-MS** (m/z): $[M+H]^+$ calcd. for $C_{26}H_{29}$: 341.2264; Found: 341.2254; Error: 2.9 ppm.



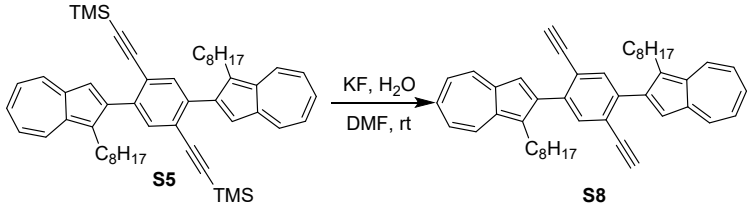
Scheme S3. Synthetic route of **1**.

***((2,5-bis(1-octylazulen-2-yl)-1,4-phenylene)bis(ethyne-2,1-diyl))bis(trimethylsilane)* (S5)**



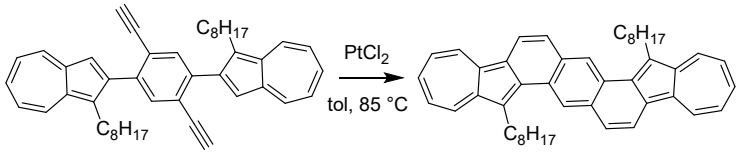
A mixture of **M1** (1.2 g, 3.28 mmol, 2.2 eq), **M3** (638 mg, 1.49 mmol, 1 eq), $Pd_2(dba)_3$ (136 mg, 0.149 mmol, 0.1 eq), XPhos (142 mg, 0.297 mmol, 0.2 eq) and K_2CO_3 (1.03 g, 7.4mmol, 5 eq) was dissolved in THF/H_2O (12 mL/ 3 mL) under nitrogen atmosphere. The reaction mixture was stirred at 85 ℃ for 12 h, after which it was cooled to room temperature. The reaction mixture was poured into water and extracted three times with EA, washed with water and dried over Na_2SO_4.The organic solvent was evaporated under reduced to give a crude product, which was purified by column chromatography on silica gel with PE/DCM(15:1) to give compound **S5** as a blue oil in 78% yield (870 mg). **^{1}H NMR** (400 MHz, $CDCl_3$) δ (ppm): 8.34 (d, *J* = 9.6 Hz, 2H), 8.24 (d, *J* = 9.6 Hz, 2H), 7.66 (s, 2H), 7.55-7.51 (m, 4H), 7.12 (t, *J* = 10.0 Hz, 2H), 7.08 (t, *J* = 9.6 Hz, 2H), 3.14 (t, *J* = 7.2 Hz, 4H),1.60-1.56 (m, 4H), 1.30-1.22 (m, 20H), 0.86 (t, *J* = 6.8 Hz, 6H), -0.03 (s, 18H). **^{13}C NMR** (100 MHz, $CDCl_3$) δ (ppm): 148.4, 140.2, 139.2, 136.9, 136.7, 136.0, 134.2, 133.8, 130.0, 122.6, 122.4, 121.7, 118.7, 104.7, 99.0, 32.1, 32.0, 29.7, 29.5, 29.4, 26.0, 22.8, 14.2, -0.3. **HR-MS** (m/z): $[M+H]^+$ calcd. for $C_{52}H_{67}Si_2$: 747.4776; Found: 747.4769; Error: 0.9 ppm.

***2,2'-(2,5-diethynyl-1,4-phenylene)bis(1-octylazulene)* (S8)**



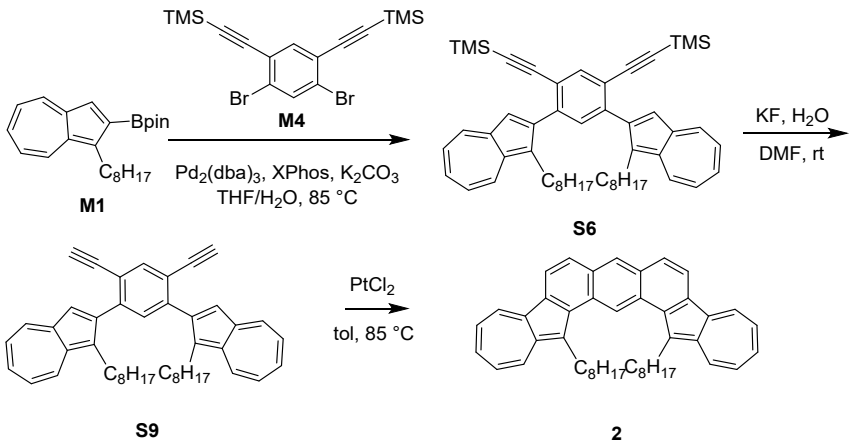
Compound **S5** (750 mg, 1 mmol, 1.0 eq) was dissolved in DMF (30 mL) and aqueous KF (700 mg, 12 mmol, 12 eq) solution (5 mL) was added. The mixture was stirred at room temperature overnight. The reaction mixture was poured into water and extracted three times with EA, washed with water and dried over Na_2SO_4.The organic solvent was evaporated under reduced to give a crude product, which was purified by column chromatography on silica gel with PE/DCM(10:1) to give compound **S8** as a blue oil in 86% yield (518 mg). **^{1}H NMR** (400 MHz, $CDCl_3$) δ (ppm): 8.36 (d, *J* = 9.6 Hz, 2H), 8.29 (d, *J* = 9.2 Hz, 2H), 7.69 (s, 2H), 7.57-7.53 (m, 4H), 7.14 (t, *J* = 9.6 Hz, 2H), 7.11 (t, *J* = 9.6 Hz, 2H), 3.13 (t, *J* =7.6 Hz, 4H), 2.98 (s, 2H), 1.62-1.52 (m, 4H), 1.29-1.21 (m, 20H), 0.85 (t, *J* = 6.8 Hz, 6H). **^{13}C NMR** (100 MHz, $CDCl_3$) δ (ppm): 147.9, 140.2, 139.3, 137.3, 136.7, 136.4, 135.1, 134.2, 130.0, 122.6, 122.0, 121.9, 118.4, 82.8, 81.3, 32.0, 32.0, 29.7, 29.5, 29.4, 25.9, 22.8, 14.2. **HR-MS** (m/z): $[M+H]^+$ calcd. for $C_{46}H_{51}$: 603.3986; Found: 603.4004; Error: 3.0 ppm.

8,17-dioctyldiazuleno[2,1-a:2',1'-h]anthracene **(1)**



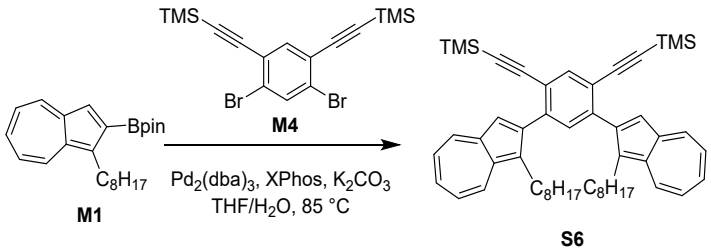
S8 **1**

The compound **1**was obtained from compound **S8** by a similar method with **4** (eluting with PE/DCM (3:1)) as a brownish black solid in 46% yield (175 mg). **^{1}H NMR** (400 MHz, $CDCl_3$) δ (ppm): 9.47 (s, 2H), 8.79 (d, *J* = 8.4 Hz, 2H), 8.51 (d, *J* = 10.4 Hz, 2H), 8.46 (d, *J* = 8.8 Hz, 2H), 8.04 (d, *J* = 8.8 Hz, 2H), 7.58 (t, *J* = 9.6 Hz, 2H), 7.29 (t, *J* = 9.2 Hz, 2H), 7.19 (t, *J* = 10.0 Hz, 2H), 3.81 (t, *J* = 8.0 Hz, 4H), 2.08-2.00 (m, 4H), 1.80-1.72 (m, 4H), 1.58-1.50 (m, 4H), 1.39-1.31 (m, 12H), 0.91 (t, *J* = 6.8 Hz, 6H). **^{13}C NMR** (100 MHz, $CDCl_3$) δ (ppm): 138.7, 137.0, 136.4, 135.2, 133.6, 132.9, 130.4, 128.7, 127.5, 126.8, 126.2, 124.1, 123.6, 122.1, 119.2, 32.1, 30.4, 30.4, 29.9, 29.6, 27.9, 22.9, 14.3. **HR-MS** (m/z): $[M+H]^+$ calcd. for $C_{46}H_{51}$: 603.3986; Found: 602.3903; Error: 1.7 ppm.



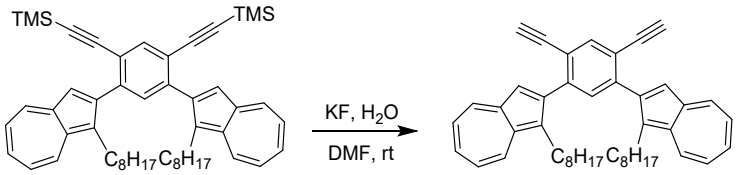
Scheme S4. Synthetic route of **2**.

((4,6-bis(1-octylazulen-2-yl)-1,3-phenylene)bis(ethyne-2,1-diyl))bis(trimethylsilane) **(S6)**



A mixture of **M1** (500 mg, 1.36 mmol, 2.2 eq), **M4** (266 mg, 0.62 mmol, 1 eq), $Pd_2(dba)_3$ (57 mg, 0.062 mmol, 0.1 eq), XPhos (59 mg, 0.12 mmol, 0.2 eq) and K_2CO_3 (429 mg, 3.1 mmol, 5 eq) was dissolved in THF/H_2O (8 mL/ 2 mL) under nitrogen atmosphere. The reaction mixture was stirred at 85 ℃ for 12 h, after which it was cooled to room temperature. The reaction mixture was poured into water and extracted three times with EA, washed with water and dried over Na_2SO_4. The organic solvent was evaporated under reduced to give a crude product, which was purified by column chromatography on silica gel with PE/DCM (15:1) to give compound **S6** as a blue oil in 61% yield (285mg). **^{1}H NMR** (400 MHz, $CDCl_3$) δ (ppm): 8.30 (d, *J* = 9.6 Hz, 2H), 8.21 (d, *J* = 9.2 Hz, 2H), 7.87 (s, 1H), 7.53-7.48 (m, 5H), 7.10 (t, *J* = 9.6 Hz, 2H), 7.06 (t, *J* = 9.6 Hz, 2H), 3.10 (t, *J* = 9.6 Hz, 4H), 1.52-1.47 (m, 4H), 1.19-1.12 (m, 20H), 0.83 (t, *J* = 6.8 Hz, 6H), 0.00 (s, 18H). **^{13}C NMR** (100 MHz, $CDCl_3$) δ (ppm): 148.7, 141.2, 139.2, 137.0, 136.7, 136.1, 133.8, 131.9, 129.9, 122.4, 121.8, 121.8, 118.8, 104.3, 98.1, 32.1, 32.1, 29.7, 29.6, 29.5, 26.1, 22.8, 14.3, -0.2. **HR-MS** (m/z): $[M+H]^+$ calcd. for $C_{52}H_{67}Si_2$: 747.4776; Found: 747.4761; Error: 2.0 ppm.

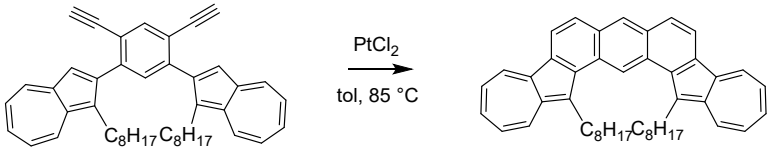
2,2'-(4,6-diethynyl-1,3-phenylene)bis(1-octylazulene) **(S9)**



S6 **S9**

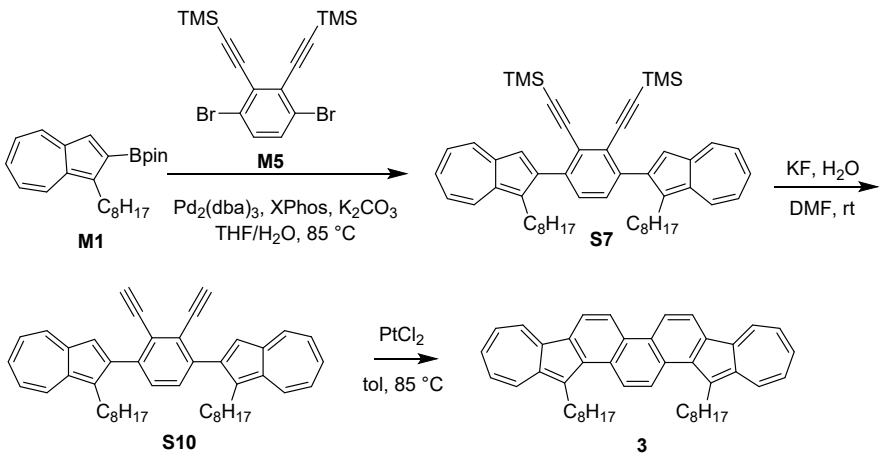
The compound **S9** was obtained from compound **S6** by a similar method with **S8** (eluting with PE/DCM (10:1)) as a blue oil in 92% yield. **^{1}H NMR** (400 MHz, $CDCl_3$) δ (ppm): 8.33 (d, *J* = 10.0 Hz, 2H), 8.26 (d, *J* = 9.6 Hz, 2H), 7.96(s, 1H), 7.55-7.45 (m, 5H), 7.12 (t, *J* = 10.0 Hz, 2H), 7.08 (t, *J* = 10.0 Hz, 2H), 3.11 (t, *J* = 7.6 Hz, 4H), 2.97 (s,2H), 1.54-1.50 (m, 4H), 1.23-1.15 (m, 20H), 0.84 (t, *J* = 6.8 Hz, 6H). **^{13}C NMR** (100 MHz, $CDCl_3$) δ (ppm): 148.3, 141.6, 139.3, 138.4, 137.4, 136.7, 136.5, 134.2, 132.3, 129.8, 122.7, 122.0, 120.9, 118.5, 82.4, 80.6, 32.2, 32.0, 29.8, 29.6, 29.4, 26.0, 22.8, 14.3. **HR-MS** (m/z): $[M+H]^+$ calcd. for $C_{46}H_{51}$: 603.3986; Found: 603.4004; Error: 3.0 ppm.

***16,18-dioctyldiazuleno[2,1-a:1',2'-j]anthracene* (2)**



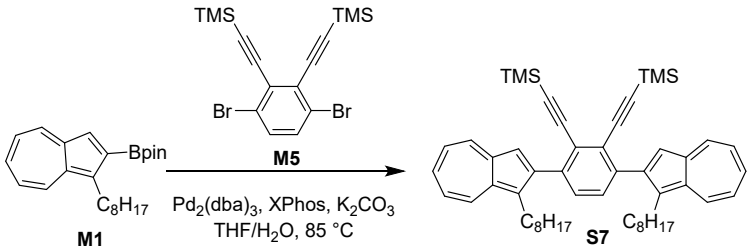
S9 **2**

The compound **2** was obtained from compound **S9** by a similar method with **4** (eluting with PE/DCM (3:1)) as a brownish black solid in 42% yield. **^{1}H NMR** (400 MHz, $CDCl_3$) δ (ppm): 10.43 (s,1H), 8.80 (d, *J* = 8.4 Hz, 2H), 8.72 (s,1H), 8.56 (d, *J* = 10.8 Hz, 2H), 8.49 (d, *J* = 8.8 Hz, 2H), 7.99 (d, *J* = 8.8 Hz, 2H), 7.60 (t, *J* = 10.0 Hz, 2H), 7.32 (t, *J* = 9.2 Hz, 2H), 7.23 (t, *J* = 10.0 Hz, 2H), 3.99 (t, *J* = 7.6 Hz, 4H), 2.08-2.04 (m, 4H), 1.30-1.16 (m, 20H), 0.80 (t, *J* = 6.8 Hz, 6H). **^{13}C NMR** (100 MHz, $CDCl_3$) δ (ppm): 139.3, 137.1, 136.4, 135.8, 133.7, 133.3, 130.2, 128.3, 128.2, 127.4, 126.7, 123.8, 123.5, 123.4, 122.3, 112.0, 32.0, 30.7, 30.0, 29.6, 29.5, 27.5, 22.4, 14.2. **HR-MS** (m/z): $[M]^+$ calcd. for $C_{46}H_{50}$: 602.3913; Found: 602.3893; Error: 3.3 ppm.



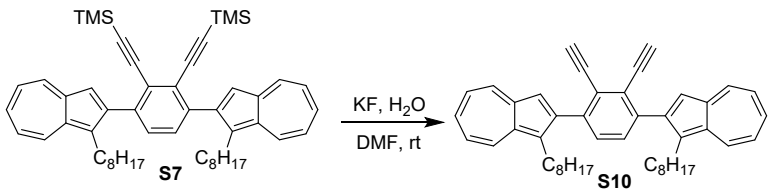
Scheme S5. Synthetic route of **3**.

***((3,6-bis(1-octylazulen-2-yl)-1,2-phenylene)bis(ethyne-2,1-diyl))bis(trimethylsilane)* (S7).**



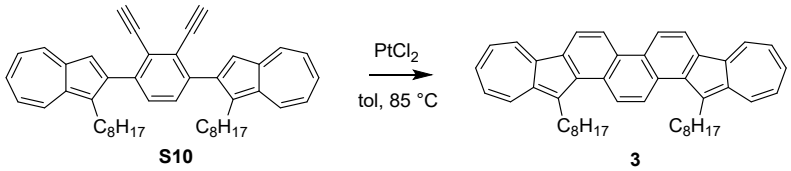
A mixture of **M1** (433 mg, 1.18 mmol, 2.2 eq), **M5**(230 mg, 0.54 mmol, 1 eq), $Pd_2(dba)_3$ (50 mg, 0.05 mmol, 0.1 eq), XPhos (51 mg, 0.1 mmol, 0.2 eq) and K_2CO_3 (370 mg, 2.68 mmol, 5 eq) was dissolved in THF/H_2O (8 mL/ 2 mL) under nitrogen atmosphere. The reaction mixture was stirred at 85 ℃ for 12 h, after which it was cooled to room temperature. The reaction mixture was poured into water and extracted three times with EA, washed with water and dried over Na_2SO_4. The organic solvent was evaporated under reduced to give a crude product, which was purified by column chromatography on silica gel with PE/DCM (15:1) to give compound **S7** as a blue oil in 68% yield (273 mg). **^{1}H NMR** (400 MHz, $CDCl_3$) δ (ppm): 8.33 (d, *J* = 9.6 Hz, 2H), 8.24 (d, *J* = 9.2 Hz, 2H), 7.55-7.50 (m,4H), 7.43 (s,2H), 7.12 (t, *J* = 9.6 Hz, 2H), 7.08 (t, *J* = 9.6 Hz, 2H), 3.10 (t, *J* = 7.6 Hz, 4H), 1.57-1.53 (m,4H), 1.26-1.19 (m,20H), 0.85(t, *J* = 6.8 Hz, 6H). **^{13}C NMR** (100 MHz, $CDCl_3$) δ (ppm): 149.2, 141.0, 139.2, 136.9, 136.7, 136.0, 133.8, 130.0, 129.4, 125.8, 122.4, 121.7, 118.9, 103.3, 102.2, 32.1, 32.0, 29.7, 29.6, 29.5, 26.0, 22.8, 14.3, -0.2. **HR-MS** (m/z): $[M+H]^+$ calcd. for $C_{52}H_{67}Si_2$: 747.4776; Found: 747.4798; Error: 2.9 ppm.

***2,2'-(2,3-diethynyl-1,4-phenylene)bis(1-octylazulene)* (S10)**



Compound **S10** was obtained from compound **S7** by a similar method with **S8** (eluting with PE/DCM (10:1)) as a blue oil in 90% yield. **^{1}H NMR** (400 MHz, $CDCl_3$) δ (ppm): 8.36 (d, *J* = 9.6 Hz, 2H), 8.29 (d, *J* = 9.6 Hz, 2H), 7.55 (t, *J* = 10.0 Hz, 2H), 7.53 (s, 2H), 7.45 (s, 2H), 7.14 (t, *J* = 9.6 Hz, 2H), 7.11 (t, *J* = 9.6 Hz, 2H), 3.18 (s, 2H), 3.11 (t, *J* = 7.6 Hz, 4H), 1.58-1.54 (m, 4H), 1.27-1.20 (m, 20H), 0.85(t, *J* = 6.8 Hz, 6H). **^{13}C NMR** (100 MHz, $CDCl_3$) δ (ppm): 148.8, 141.2, 139.3, 137.3, 136.6, 136.4, 134.2, 130.0, 123.0, 125.2, 122.6, 122.0, 118.5, 84.4, 81.8, 32.1, 32.0, 29.8, 29.5, 29.4, 26.0, 22.8, 14.3. **HR-MS** (m/z): $[M+H]^+$ calcd. for $C_{46}H_{51}$: 603.3986; Found: 603.4004; Error: 3.0 ppm.

***3,18-dioctyldiazuleno[2,1-a:1',2'-i]phenanthrene* (3)**



Compound **S10** (198 mg, 0.33 mmol, 1 eq) and $PtCl_2$ (18 mg, 0.066 mmol, 0.2 eq) was dissolved in 6 mL dry toluene under a nitrogen atmosphere. The mixture was heated at 85 ℃ for 12 h, after which it was cooled to room temperature. The crude mixture was filtered through celite and solvent was removed under reduced pressure, which was purified by column chromatography on silica gel with PE/DCM(10:1) to give crude product, which washed with a minimum amount of methanol to compound **3** as a brownish black solid in 28% yield (55 mg). **^{1}H NMR** (400 MHz, $CDCl_3$) δ (ppm): 9.05 (s, 2H), 8.97 (d, *J* = 9.2 Hz, 2H), 8.64 (t, *J* = 8.4 Hz, 2H), 8.34 (d, *J* = 8.4 Hz, 2H), 7.43 (t, *J* = 8.8 Hz, 2H), 7.20 (t, *J* = 8.8 Hz, 2H), 7.07 (t, *J* = 8.4 Hz, 2H), 3.73 (t, *J* = 7.6 Hz, 4H), 2.04-1.97 (m, 4H), 1.37-1.25 (m, 20H), 0.89 (t, *J* = 6.8 Hz, 6H). **^{13}C NMR** (100 MHz, $CDCl_3$) δ (ppm): 138.8, 138.7, 135.6, 134.9, 133.4, 132.0, 128.9, 128.8, 128.2, 126.4, 124.6, 123.5, 122.4, 119.4, 118.4, 32.0, 30.4, 30.2, 29.7, 29.5, 27.9, 22.8, 14.2. **HR-MS** (m/z): $[M+H]^+$ calcd. for $C_{46}H_{51}$: 603.3986; Found: 603.4004; Error: 3.0 ppm.

1.3 Thermodynamic Stability

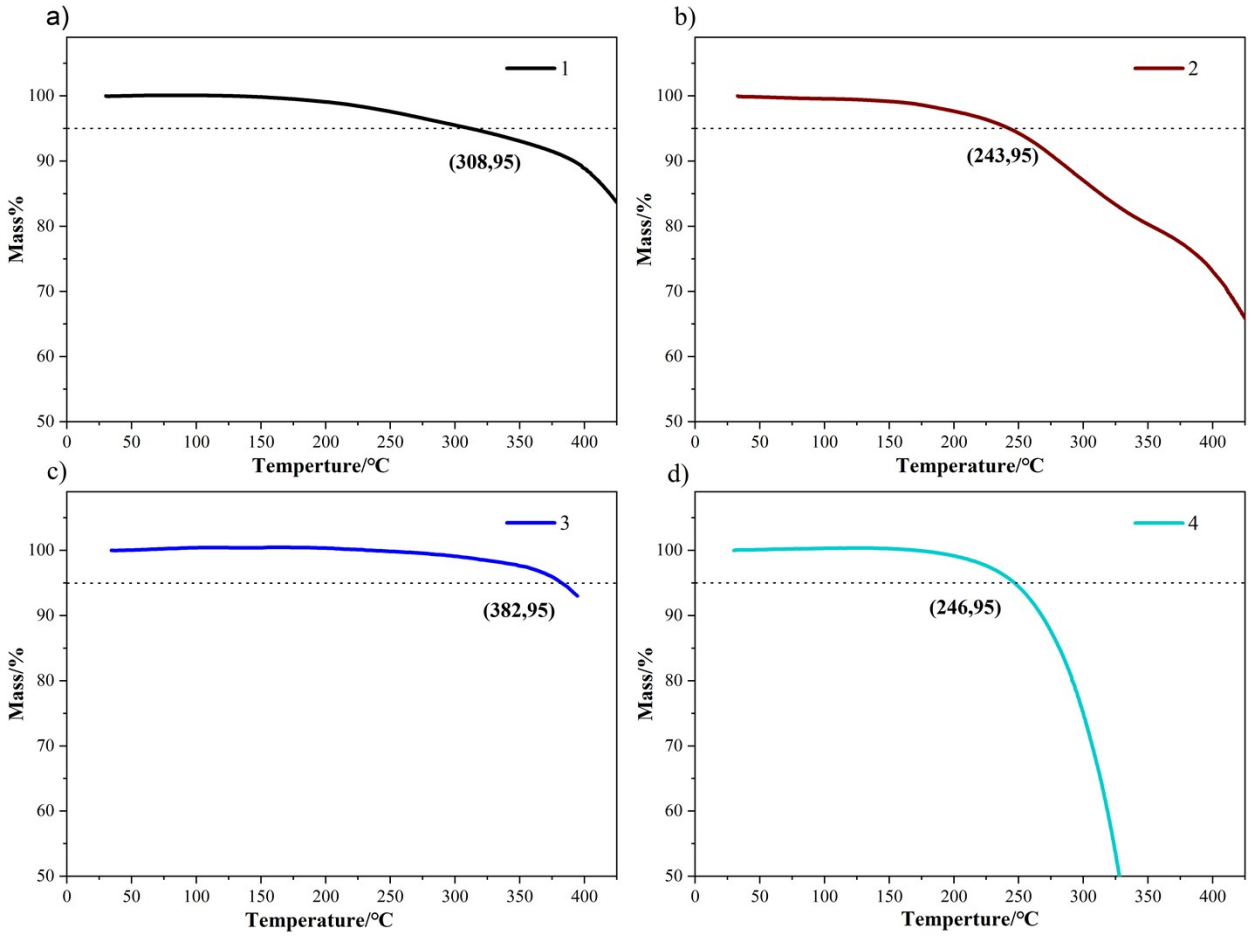
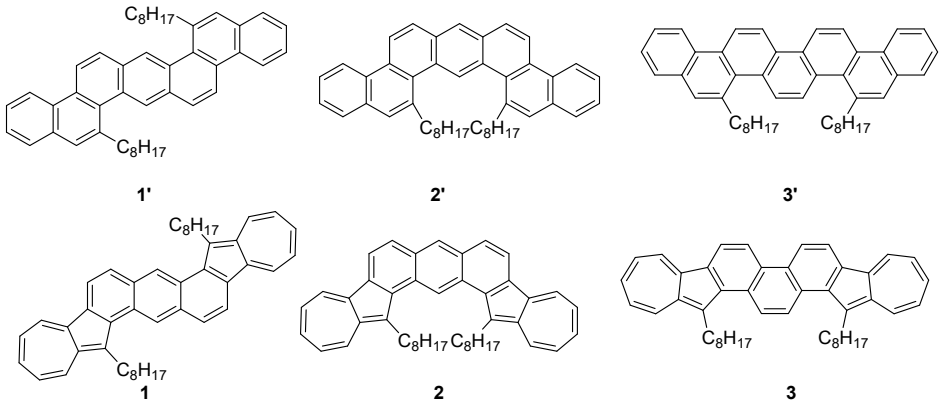


Figure S1. TGA curves of **1-4**

To gain insights into the origin of the stability features of compounds **1'-3'** and **1-3**, density functional theory calculations (DFT) are employed to study the energy and structural relationships between isomers **1**, **2**, and **3**. We performed calculations for the single point energy and independent gradient model (IGM) of these compounds using the B3LYP/6-31G*(d,p) level of theory. The single point energy calculations show that the values for isomer **3** (-1783.15145 au) and **3'** (-1783.22611 au) have the lowest energy values among both the naphthene-fusing and azulene-fusing polycyclic aromatic hydrocarbons (PHAs) (Table S1).

Table S1. The single point energy of compounds **1'-3'** and **1-3**.



Comp.	Single point energy (a.u.)
1'	-1783.22545
2'	-1783.22538
3'	-1783.22611
1	-1783.13583
2	-1783.14995
3	-1783.15145

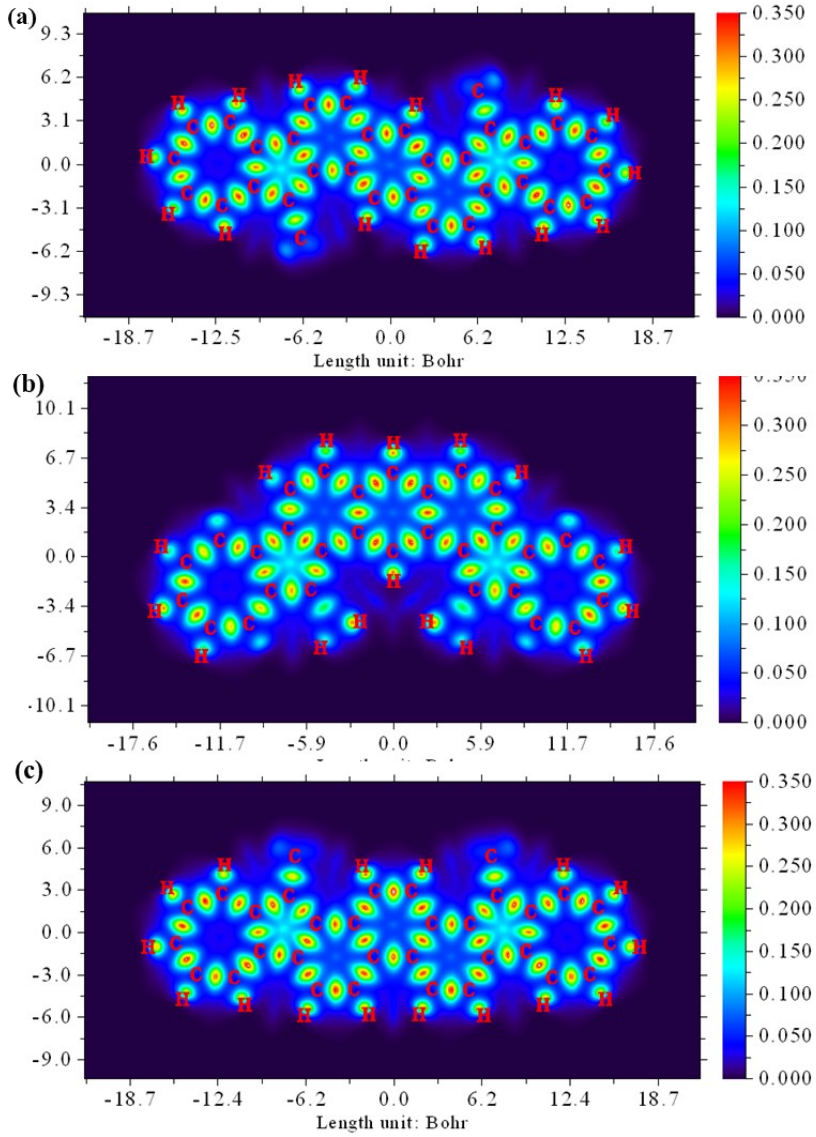


Figure S2. Independent Gradient Mode based on Hirshfeld partition[6, 7]. (a) Isomer **1**, (b) Isomer **2**, (c) Isomer **3**.

We employed IGM analysis via Multiwfn to visually study the intrafragment interaction, which can be individually revealed by δ_g^{intra} functions. Strong atomic interactions lead to an increase in the δ_g^{intra} of the interacting region. As shown in Figure S2, isomer **3** exhibits a high δ_g^{intra} value on a global scale compared to isomers **1** and **2**. Both the single-point energy calculation and IGM results align with our experimental findings.

2. Crystallographic Data

Table S2. Crystallographic data for **1** (CCDC: 2336236).

Empirical formula	$C_{46}H_{50}$
Formula weight	602.86
Temperature	193.00 K
Crystal system	triclinic
Space group	P-1
Unit cell dimensions	a=5.4401(2)Å α=101.504(3)°
	b=9.1230(3)Å β=95.881(2)°
	c=17.9486(6)Å γ=94.474(2)°
Volume	863.86(5) $Å^3$
Z	1
ρ_{calc}	1.159 g/cm^3
μ	0.483 mm^{-1}
F(000)	326.0
Crystal size	0.13 × 0.12 × 0.11 mm^3
Radiation	CuKα (λ = 1.54178)
2θ range for data collection	9.944 to 136.37°
Index ranges	-6≤h≤5, -10≤k≤10, -21≤l≤2
Reflections collected	8555
Independent reflections	3101 [R_{int}=0.0453, R_{sigma} = 0.0397]
Data/restraints/parameters	3101/0/209
Goodness-of-fit on F^2	1.051
Final R indexes [I>=2σ (I)]	R_1 = 0.0479, wR_2 = 0.1288
R_1 = 0.0479, wR_2 = 0.1288	R_1 = 0.0631, wR_2 = 0.1381
Largest diff. peak/hole	0.23/-0.19 e $Å^{-3}$

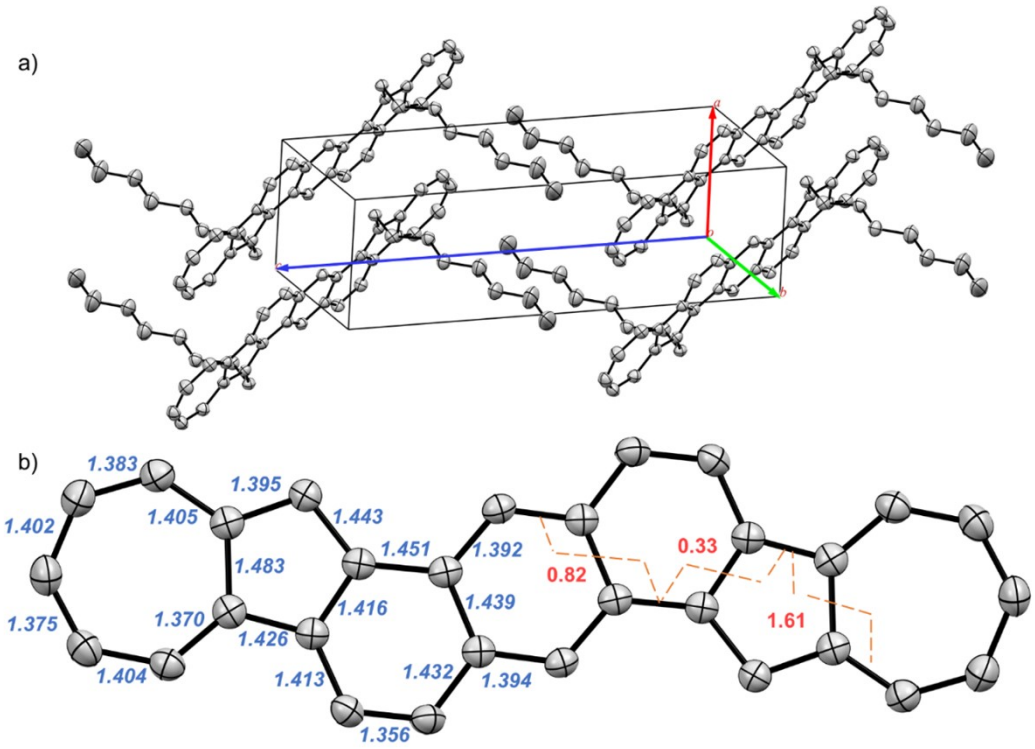


Figure S3. a) Single cell structure of compound **1**; b) Bond length (blue, Å) of **1**and dihedral angel (red, °) of skeleton plane of **1**.

3. Theoretical Calculations

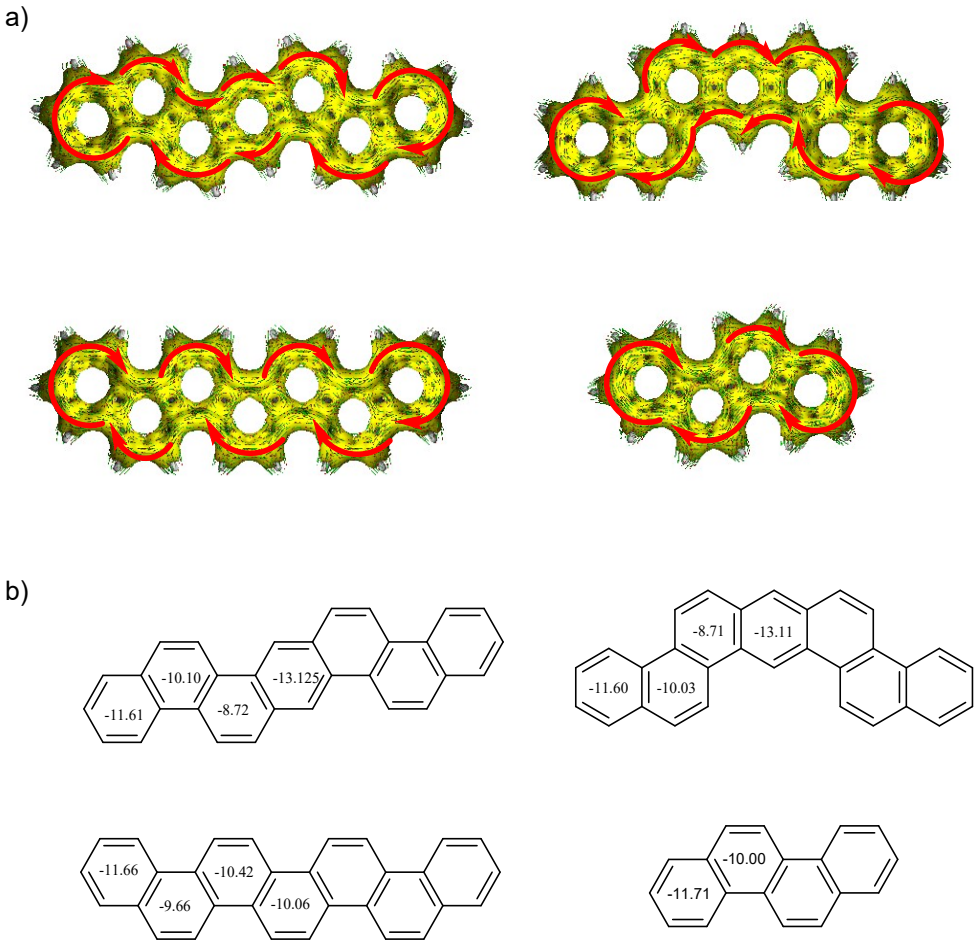
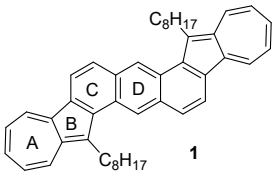
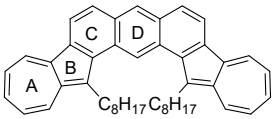


Figure S4. Calculated ACID and NICS(1)zz values (in ppm) of the isomer of **1-4**. Calculations were done at GIAO B3LYP/6-31G (d, p) level based on optimized geometry.

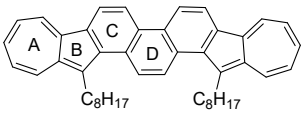
Table S3. The values of NICS(1)zz, MCI, FLU, HOMA, and NCBO for each ring of compounds **1-4.**



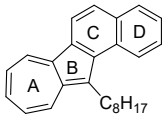
1



2



3



4

Comp.	Ring	NICS(1)zz	MCI	FLU	HOMA	NCBO
1	A	-10.65	0.02031	0.01403	0.4631	0.5731
	B	-18.31	0.02203	0.03278	-0.0489	0.4662
	C	-10.50	0.01069	0.02529	0.4147	0.4694
	D	-15.55	0.04071	0.01423	0.6368	0.5893
2	A	-10.87	0.02160	0.01358	0.5214	0.5782
	B	-18.11	0.02757	0.03259	0.0374	0.4876
	C	-10.96	0.00910	0.02573	0.3938	0.4569
	D	-15.59	0.03804	0.01430	0.6338	0.5799
3	A	-9.81	0.02171	0.01513	0.4860	0.5786
	B	-17.35	0.03183	0.03438	-0.0111	0.5018
	C	-13.13	0.02082	0.01894	0.5817	0.5245
	D	-13.00	0.03100	0.01928	0.4750	0.5605
4	A	-10.18	0.02179	0.00924	0.4235	0.5789
	B	-18.03	0.05233	0.02755	0.6200	0.5543
	C	-12.41	0.03208	0.02002	0.5474	0.5637
	D	-14.44	0.05490	0.00760	0.5138	0.6165

Table S4. Optical predictions for **1** via TD-DFT at the B3LYP /6-311g(d,p) level.[8]

Exited state	Excitation energy / eV (Wavelength / nm)	Excitation amplitudes	Oscillator strength f
S1	1.6638 (745.17)	0.17620 (HOMO-1–LUMO+1) 0.68025 (HOMO–LUMO)	0.0119
S2	1.9268 (643.48)	0.50649 (HOMO-1–LUMO) 0.48517 (HOMO–LUMO+1)	0.0000
S3	2.3765 (521.72)	-0.48571 (HOMO-1–LUMO) 0.50961 (HOMO–LUMO+1)	0.0000
S4	2.5283 (490.38)	0.44437 (HOMO-2–LUMO) 0.15656 (HOMO-1–LUMO+1) 0.51895 (HOMO–LUMO+2)	0.0077
S5	2.6592 (466.24)	0.65500 (HOMO-1–LUMO+1) -0.17522 (HOMO–LUMO) -0.14770 (HOMO–LUMO+2)	0.0168
S6	2.9335 (422.66)	0.11115 (HOMO-4–LUMO) 0.45395 (HOMO-2–LUMO+1) 0.22003 (HOMO-1–LUMO+2) 0.47726 (HOMO–LUMO+3)	0.0000
S7	3.0190 (410.68)	-0.11028 (HOMO-3–LUMO) 0.50556 (HOMO-2–LUMO) 0.17762 (HOMO-1–LUMO+3) -0.43709 (HOMO–LUMO+2)	1.5355
S8	3.0337 (408.69)	0.12572 (HOMO-2–LUMO+1) 0.56971 (HOMO-1–LUMO+2) -0.38534 (HOMO–LUMO+3)	0.0000
S9	3.3904 (365.69)	0.60534 (HOMO-2–LUMO+2) -0.32797 (HOMO–LUMO+4)	0.0700
S10	3.4630 (358.03 nm	0.55545 (HOMO-3–LUMO) 0.37802 (HOMO-1–LUMO+3) -0.13898 (HOMO–LUMO+4)	0.0003

Table S5. Optical predictions for **2** via TD-DFT at the B3LYP /6-311g (d, p) level.

Exited state	Excitation energy / eV (Wavelength / nm)	Excitation amplitudes	Oscillator strength f
S1	1.8564 (667.87)	-0.44289 (HOMO-1–LUMO+1) 0.54259 (HOMO–LUMO)	0.0094
S2	1.8973 (653.47)	-0.41994 (HOMO-1–LUMO) 0.54775 (HOMO–LUMO+1)	0.0114
S3	2.2009 (563.34)	0.54921 (HOMO-1–LUMO) 0.43065 (HOMO–LUMO+1)	0.0000
S4	2.4441 (507.28)	0.53716 (HOMO-1–LUMO+1) 0.43477 (HOMO–LUMO)	0.4141
S5	2.9147 (425.38)	0.52876 (HOMO-2–LUMO) -0.41350 (HOMO-1–LUMO+2) 0.18221 (HOMO–LUMO+3)	0.0085
S6	3.0006 (413.19)	-0.15190 (HOMO-3–LUMO) 0.37779 (HOMO-2–LUMO+1) -0.12848 (HOMO-1–LUMO) 0.55927 (HOMO–LUMO+2)	0.0245
S7	3.0610 (405.05)	-0.10099 (HOMO-3–LUMO+1) 0.35869 (HOMO-1–LUMO+2) 0.58460 (HOMO–LUMO+3)	0.0036
S8	3.1480 (393.85)	-0.37570 (HOMO-2–LUMO+1) 0.52021 (HOMO-1–LUMO+3) 0.27620 (HOMO–LUMO+2)	0.0221
S9	3.1573 (392.69)	0.39676 (HOMO-3–LUMO+1) 0.40131 (HOMO-2–LUMO) 0.35947 (HOMO-1–LUMO+2) -0.18688 (HOMO–LUMO+3)	0.2511
S10	3.2357 (383.18)	0.50628 (HOMO-3–LUMO) 0.35238 (HOMO-2–LUMO+1) 0.28019 (HOMO-1–LUMO+3) 0.10294 (HOMO–LUMO+1) -0.11412 (HOMO–LUMO+2)	0.0008

Table S6. Optical predictions for **3** via TD-DFT at the B3LYP /6-311g(d,p) level.

Exited state	Excitation energy / eV (Wavelength / nm)	Excitation amplitudes	Oscillator strength f
S1	1.7737 (699.01)	-0.20253 (HOMO-1–LUMO+1) 0.67160 (HOMO–LUMO)	0.0110
S2	1.9543 (634.41)	0.54876 (HOMO-1–LUMO) -0.43413 (HOMO–LUMO+1)	0.0011
S3	2.4246 (511.37)	0.43528 (HOMO-1–LUMO) 0.55298 (HOMO–LUMO+1)	0.0176
S4	2.6092 (475.18)	0.66947 (HOMO-1–LUMO+1) 0.20781 (HOMO–LUMO)	0.0000
S5	2.6927 (460.45)	-0.45206 (HOMO-2–LUMO) 0.52633 (HOMO–LUMO+2)	0.0052
S6	2.9860 (415.22)	-0.12043 (HOMO-4–LUMO) -0.42610 (HOMO-2–LUMO+1) -0.23591 (HOMO-1–LUMO+2) 0.48663 (HOMO–LUMO+3)	0.0083
S7	3.1027 (399.60)	0.11085 (HOMO-2–LUMO+1) 0.57086 (HOMO-1–LUMO+2) 0.38637 (HOMO–LUMO+3)	0.0015
S8	3.1383 (395.07)	0.43497 (HOMO-2–LUMO) 0.33648 (HOMO-1–LUMO+3) 0.43692 (HOMO–LUMO+2)	1.0271
S9	3.3942 (365.28)	0.65001 (HOMO-3–LUMO) -0.18606 (HOMO-2–LUMO+1) 0.13284 (HOMO-2–LUMO+2)	0.0001
S10	3.5861 (345.74)	0.11773 (HOMO-3–LUMO+1) -0.30387 (HOMO-2–LUMO) 0.57842 (HOMO-1–LUMO+3) -0.13225 (HOMO–LUMO+2) -0.17430 (HOMO–LUMO+4)	1.6797

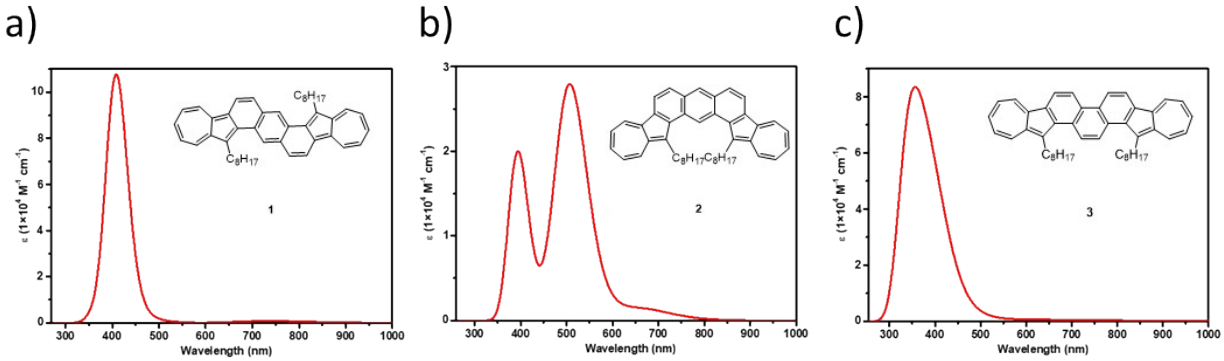


Figure S5. The UV-Vis spectra estimated from TD-DFT calculation.

4. Spectroscopic Measurement[9]

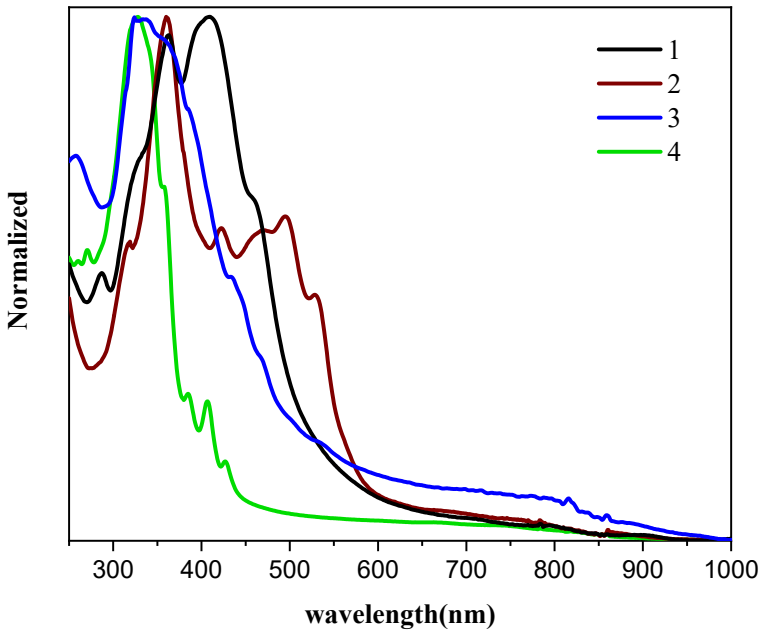


Figure S6. UV-vis spectra of **1-4** in thin film.

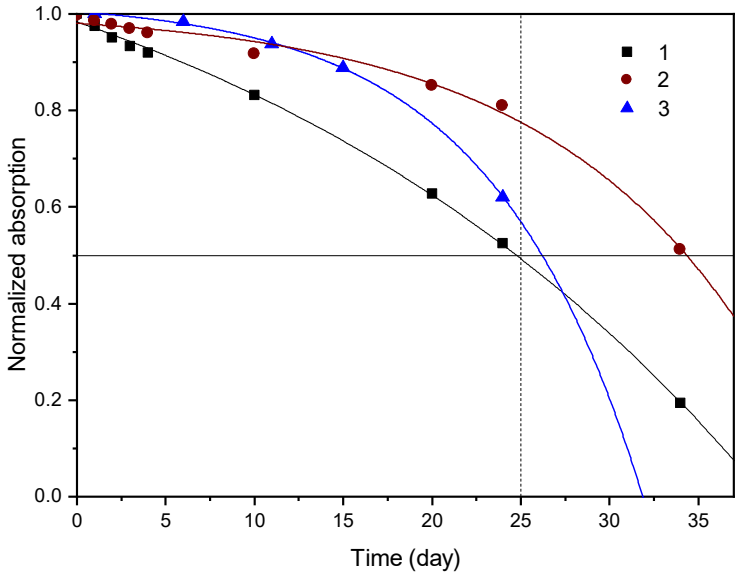


Figure S7. Absorption spectral changes of **1-3** under ambient air and light conditions.

5. Protonation Behavior

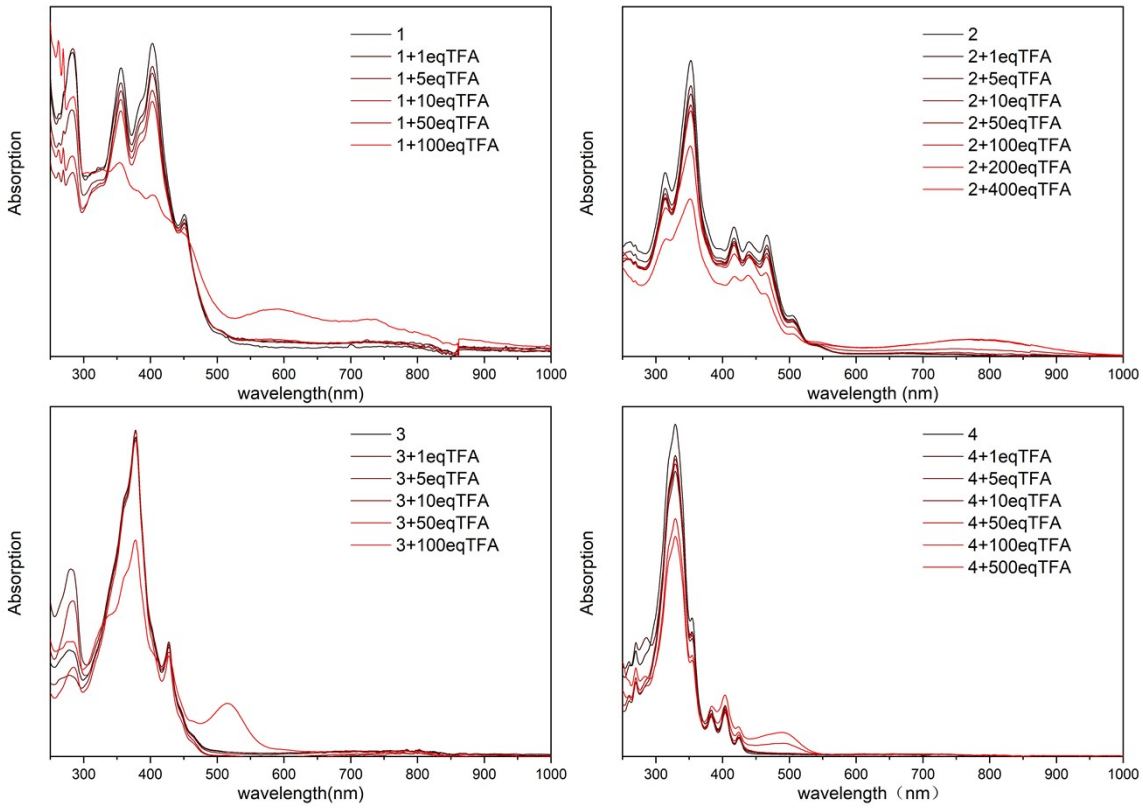


Figure S8. The change of UV-vis spectra during protonation behavior.

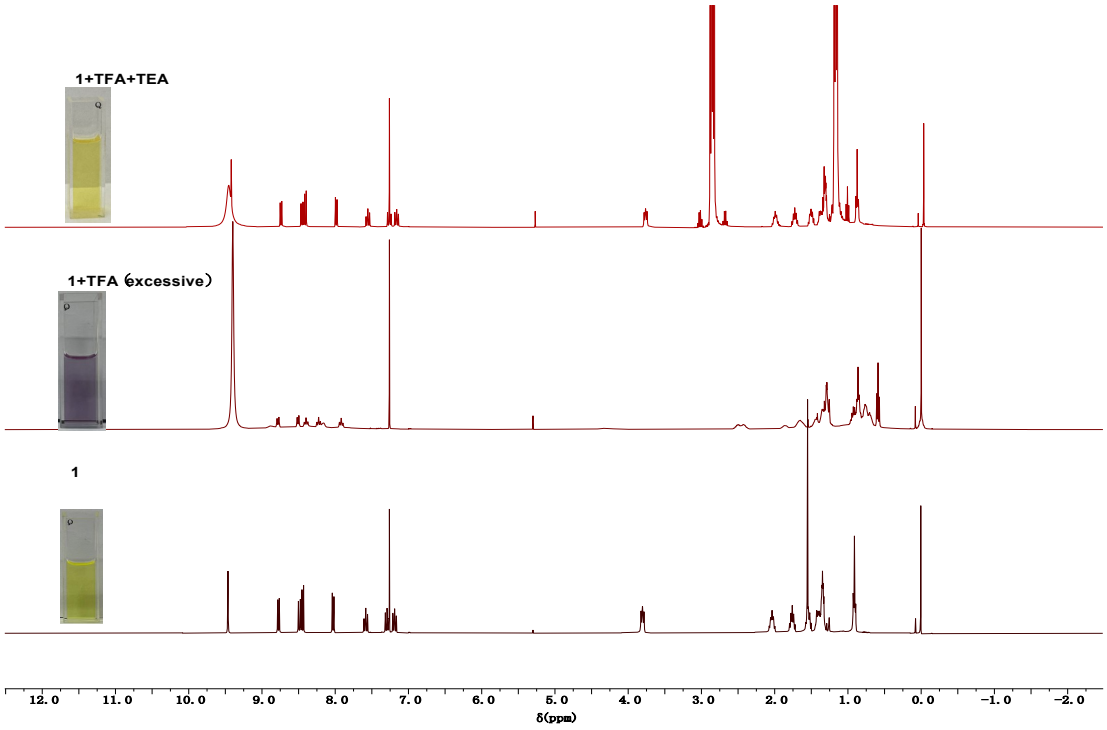


Figure S9. ^{1}H NMR change and reccover in protonation behavior.

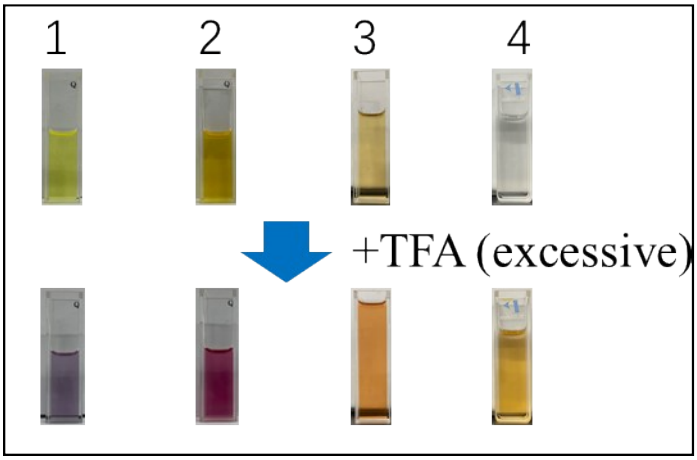


Figure S10. Color change in protonation behavior.

6. OFETs

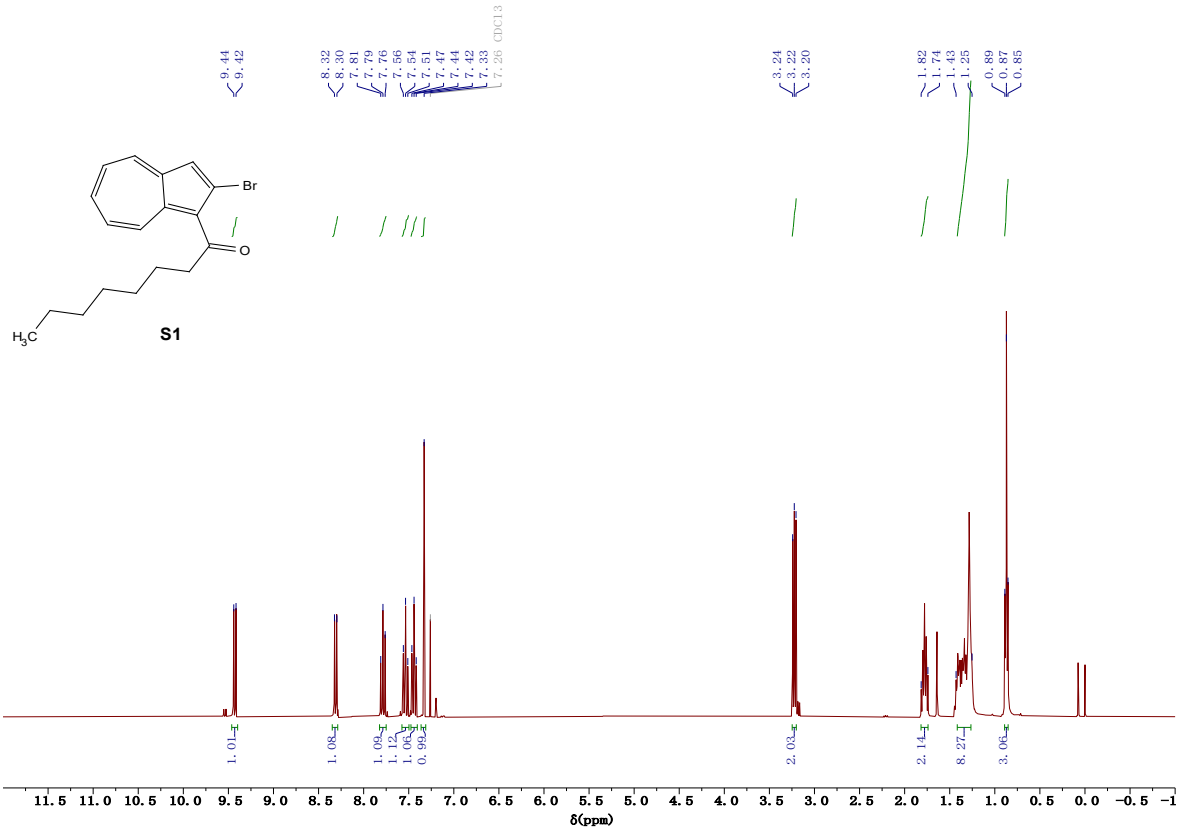
The charge transport properties of compound **1** were characterized by fabricating thin-film transistors with a bottom-gate/bottom-contact (BG/BC) device configuration. Source and drain electrodes (3 nm Cr and 30 nm Au) were patterned on the n^{++}-Si wafers with 300 nm silicon dioxide (SiO_2/Si) by using standard thermal evaporation procedures. The as-patterned SiO_2/Si substrates were then subjected to the cleaning procedures and octadecyltrichlorosilane (OTS) modified process. The substrates were rinsed with deionized water, hot piranha solution (H_2SO_4/H_2O_2 = 2:1), deionized water, ethanol, and finally were dried in an oven at 80 °C. The OTS modification procedures were carried out in a vacuum oven. Before modification process, a small drop of OTS surrounded by those cleaned SiO_2/Si substrates in a Petri dish was put into the vacuum oven. Then, the vacuum oven was heated up to 120 °C and kept for 3 h. After the temperature cooled down, the SiO_2/Si wafers were washed immediately by hexane, ethanol, and chloroform, followed by blown dry with high-purity nitrogen gas. The sample of compound **1** was dissolved in the chlorobenzene to obtain a solution (7 mg/mL). The small molecule thin films were deposited on the surface of OTS-modified SiO_2/Si substrates by spin-coating the polymer solution (900 rpm for **1** s and 1800 rpm for 60 s), followed by the thermal treatment at 150 °C for 20 min in a nitrogen-filled glovebox. To achieve the best-performed device performance, the channel length (L) and width (W) of the OFET devices were 20 μm and 1400 μm, respectively.

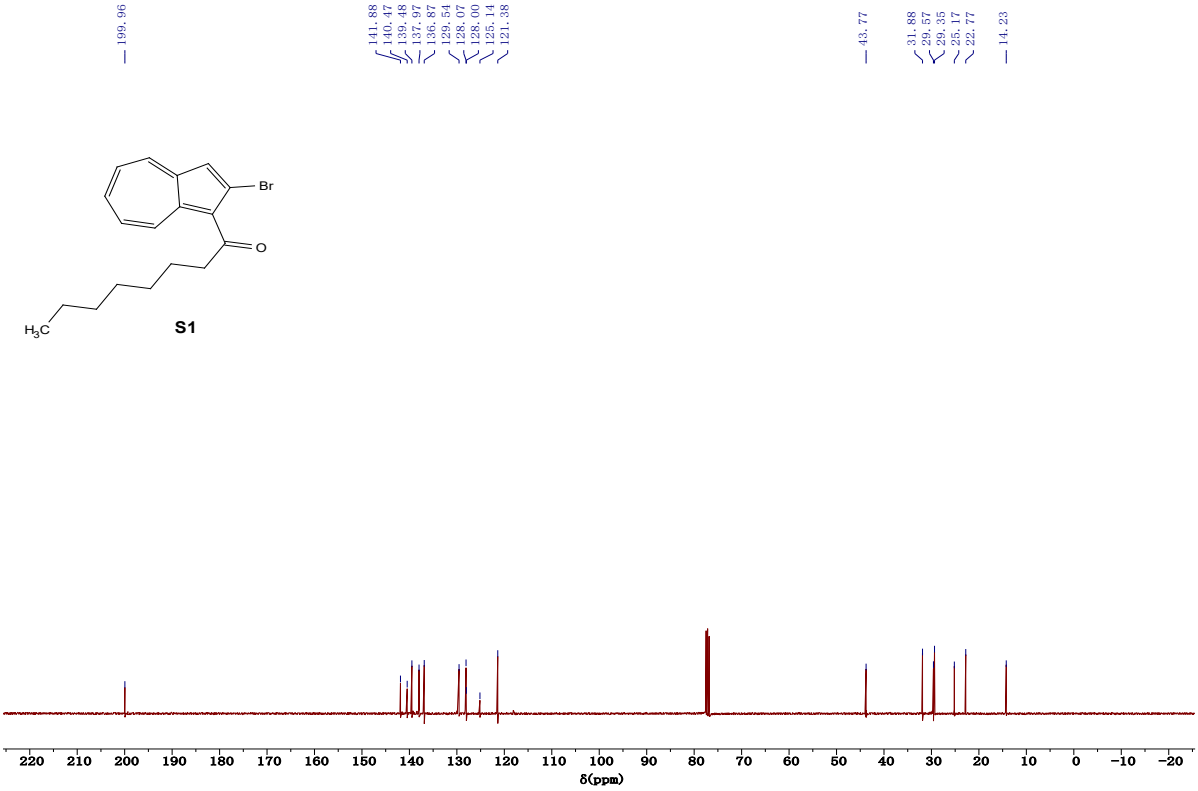
Characterization of OFET devices were performed at room temperature using a Keithley 4200 in a N_2-filled glove box. The mobilities were calculated in the saturation region according to the equation:

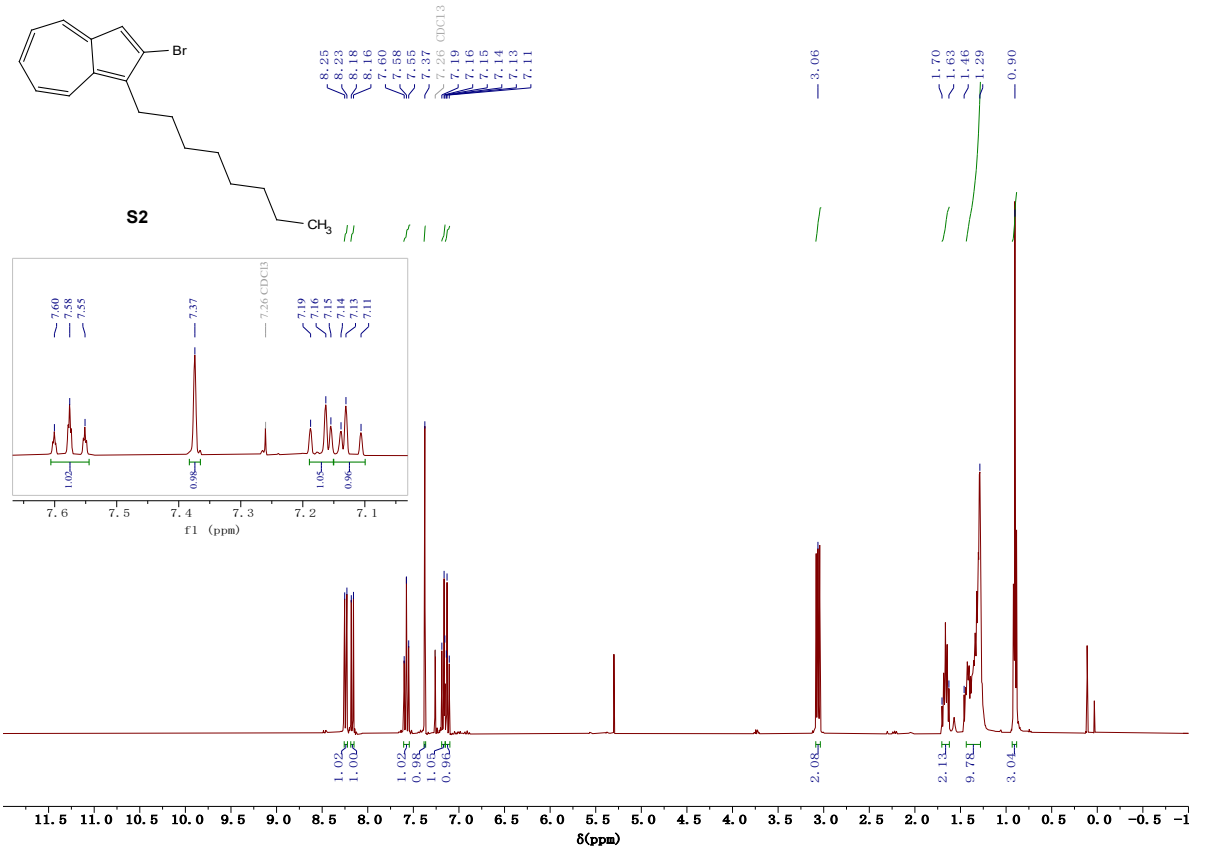
$$I_{DS} = \frac{W}{2L} C_i \mu (V_G - V_T)^2$$

where I_{DS} is the drain-source current, μ is the field-effect mobility, V_G is the gate voltage, V_T is the threshold voltage, W is the channel width, L is the channel width length, C_i is the capacitance of the insulating layer. In this work, the 300 nm SiO_2 surface layer with the capacitance value of 11.5 nF cm^{-2} was adopted as the dielectric layer.

7.NMR Spectra of All New Compounds



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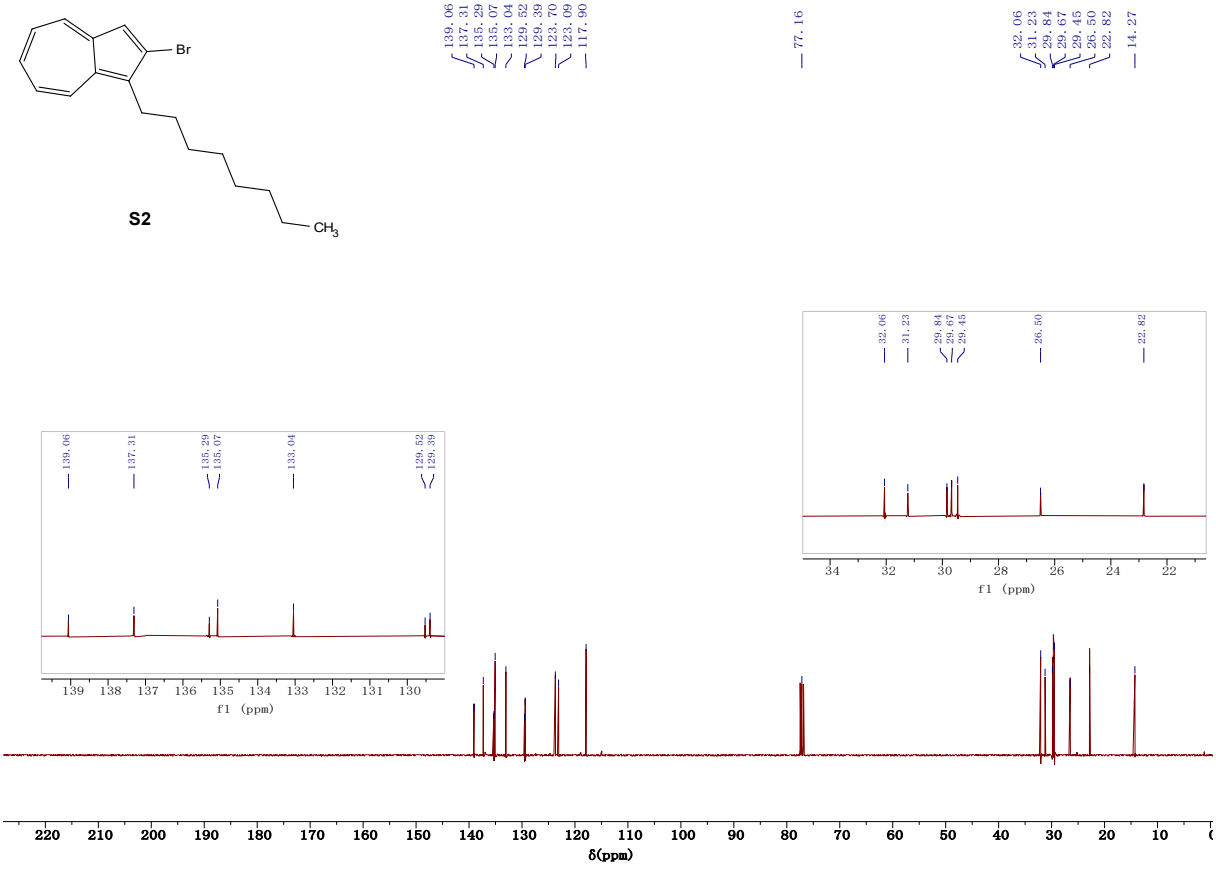
S2
CH3
8.25
8.23
8.18
8.16
7.60
7.58
7.55
7.37
7.26 CDCl3
7.19
7.16
7.15
7.14
7.13
7.11
3.06
1.70
1.63
1.46
1.29
0.90
1.02
1.00
1.02
0.98
1.05
0.96
2.08
2.13
9.78
3.04
δ(ppm)
f1 (ppm)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CH3
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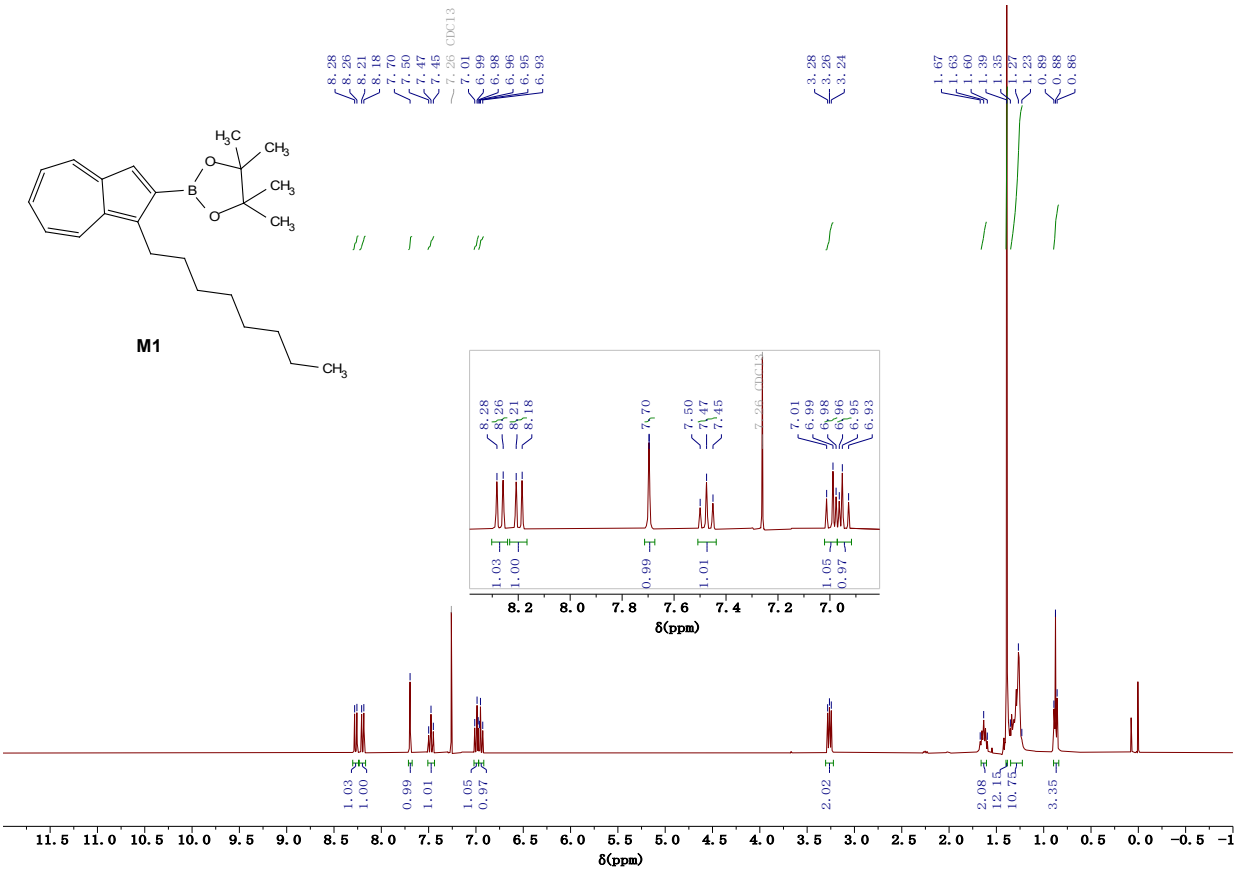
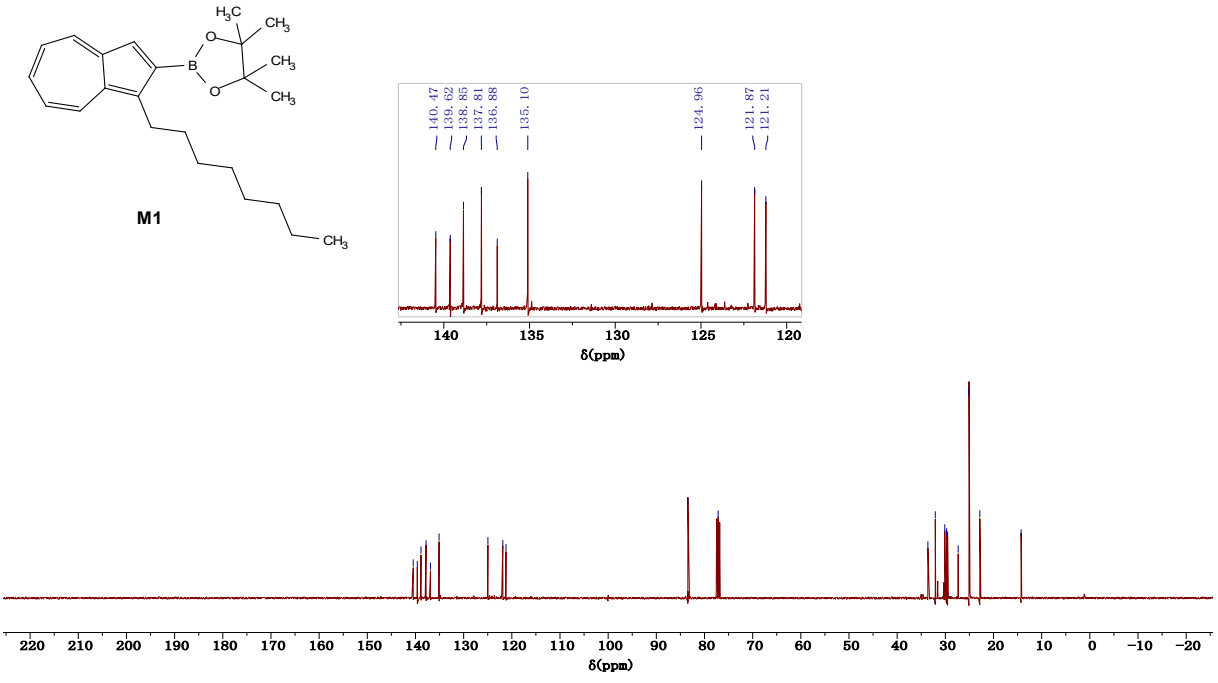
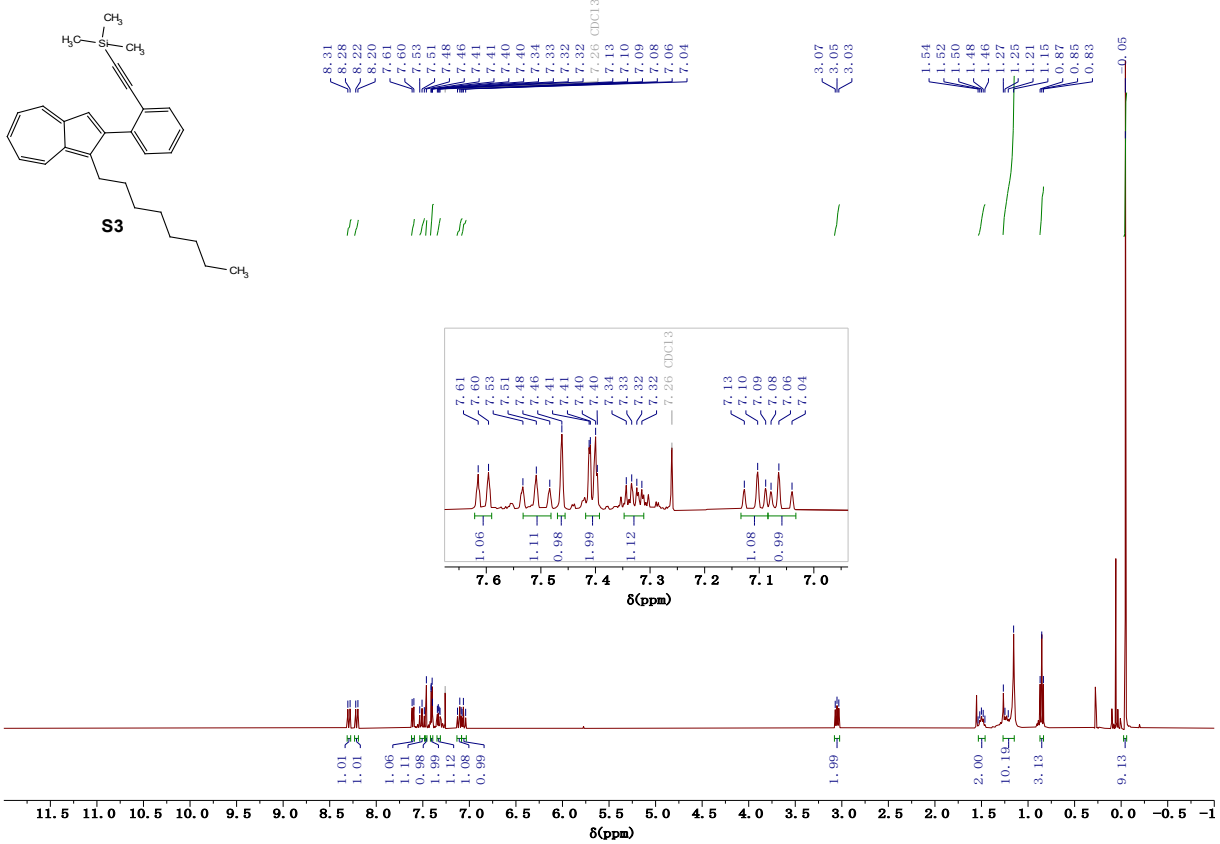
135.29
135.07
133.04
129.52
129.39
123.70
123.09
117.90
77.16
32.06
31.23
29.84
29.67
29.45
26.50
22.82
14.27
δ(ppm)
f1 (ppm)


M1
δ(ppm)


M1
δ(ppm)


S3
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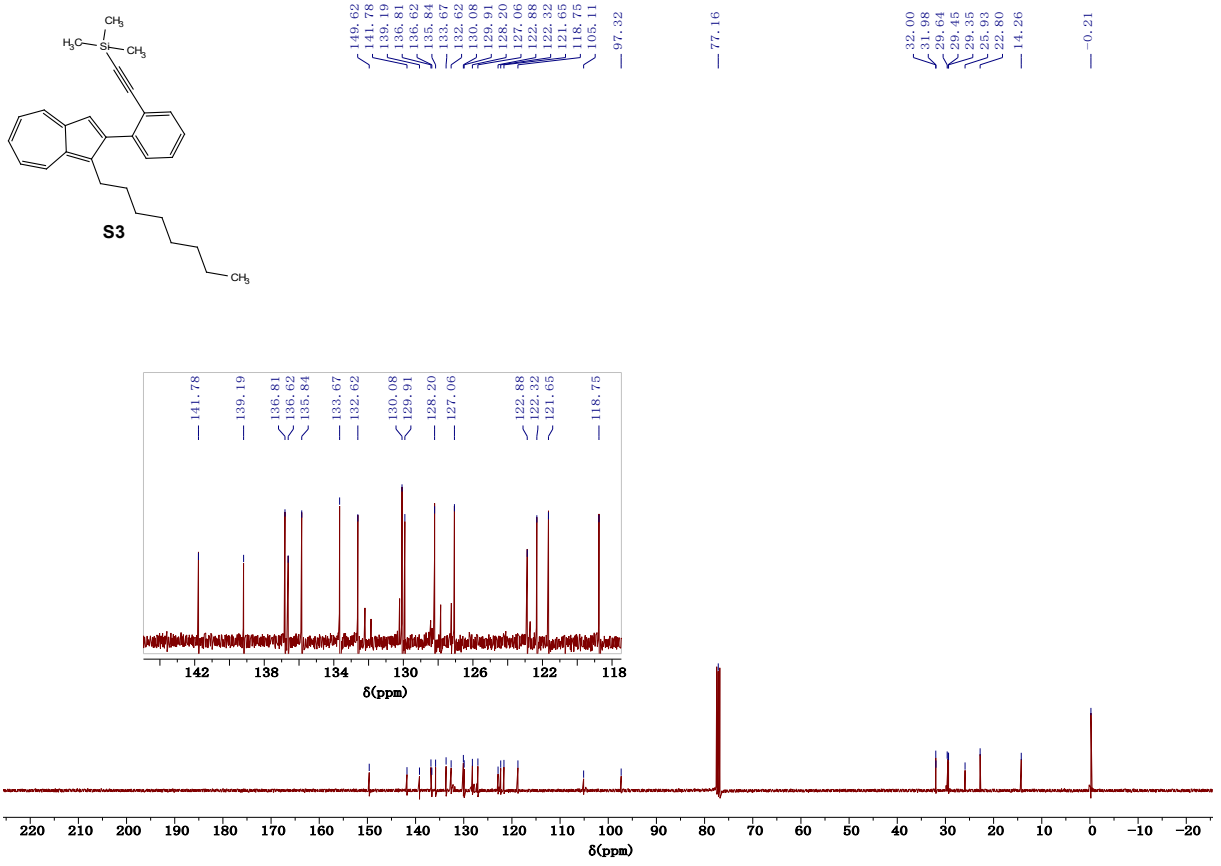
8.22
8.20
7.61
7.60
7.53
7.51
7.48
7.46
7.41
7.40
7.34
7.33
7.32
7.26 CDCl3
7.13
7.10
7.09
7.08
7.06
7.04
3.07
3.05
3.03
1.54
1.52
1.50
1.48
1.46
1.27
1.25
1.21
1.15
0.87
0.85
0.83
-0.05
1.06
1.11
0.98
1.99
1.12
1.08
0.99
δ(ppm)


S3
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139.19
136.81
136.62
135.84
133.67
132.62
130.08
129.91
128.20
127.06
122.88
122.32
121.65
118.75
105.11
97.32
77.16
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31.98
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29.45
29.35
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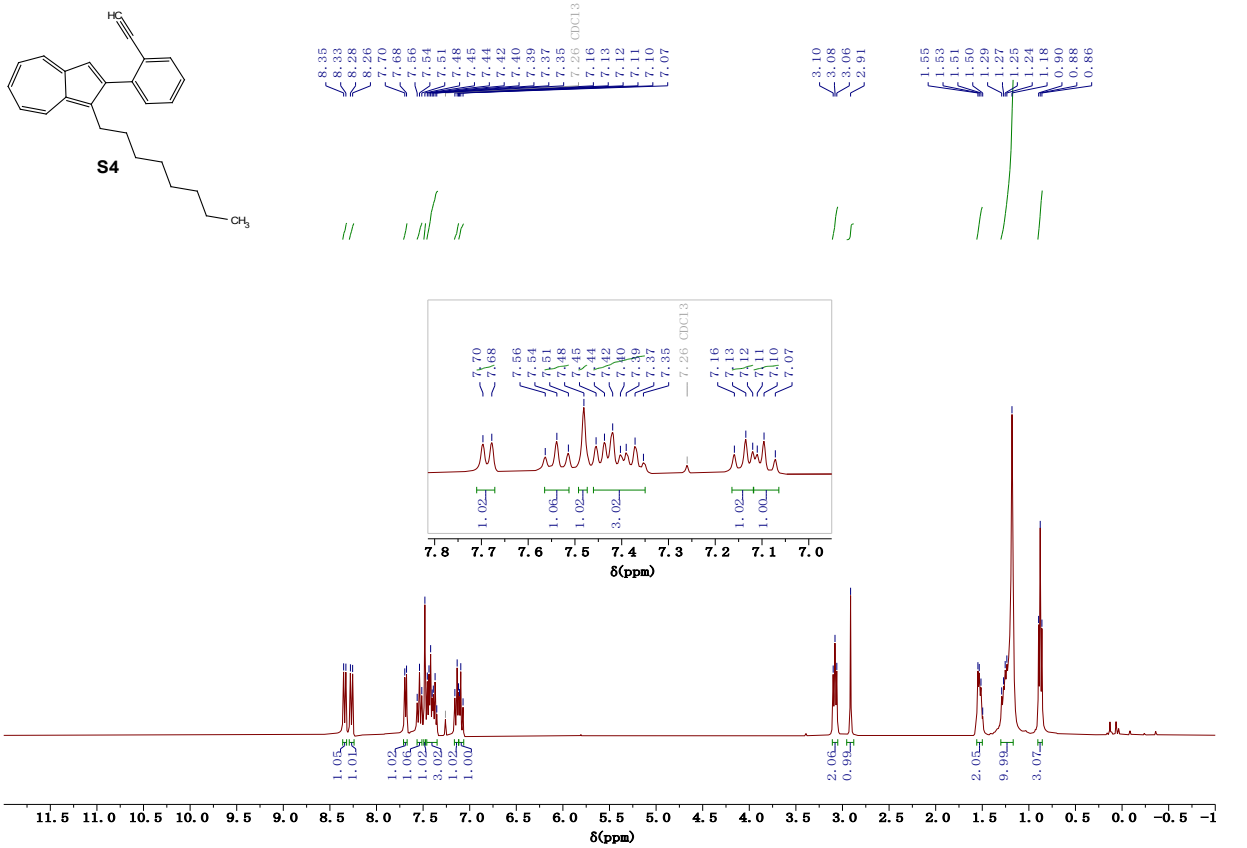
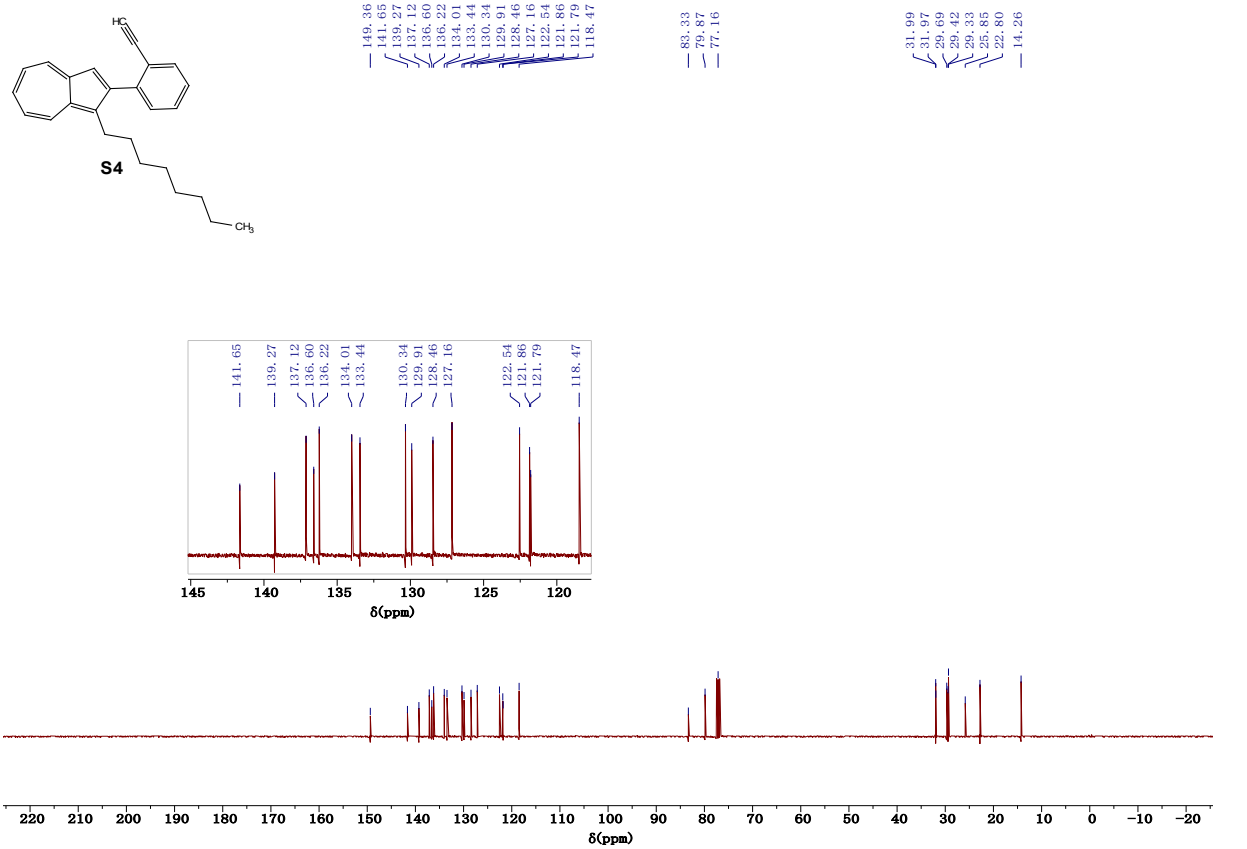
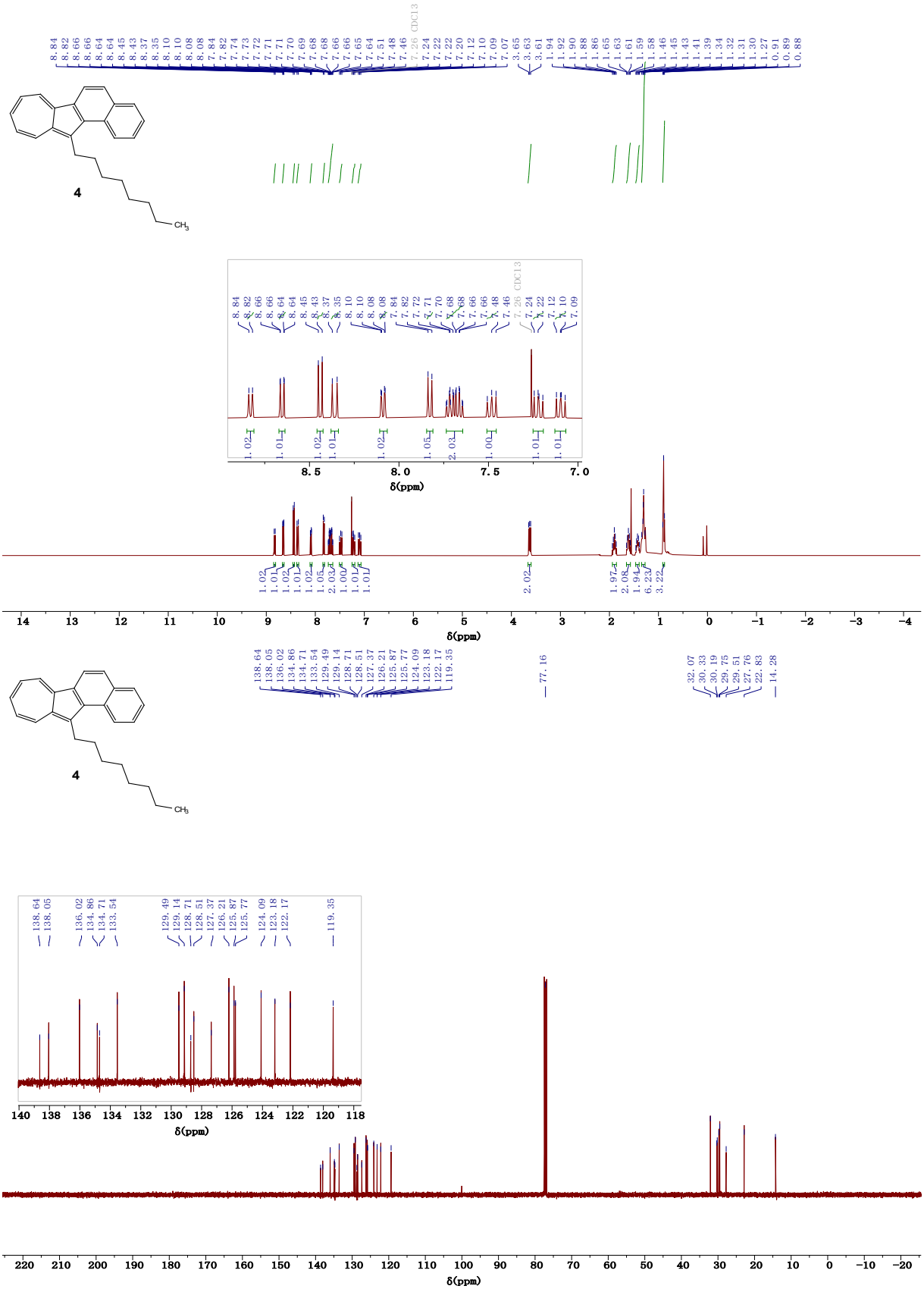
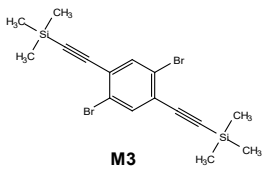
22.80
14.26
-0.21
δ(ppm)

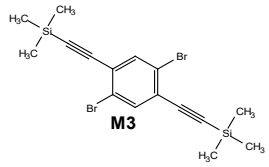

S4
CDCl3
δ(ppm)


S4
CDCl3
δ(ppm)


4
CH3
δ(ppm)
4
CH3
δ(ppm)
δ(ppm)


M3

7.67
7.26 CDCl3
0.27
2.01
17.93
δ(ppm)


M3

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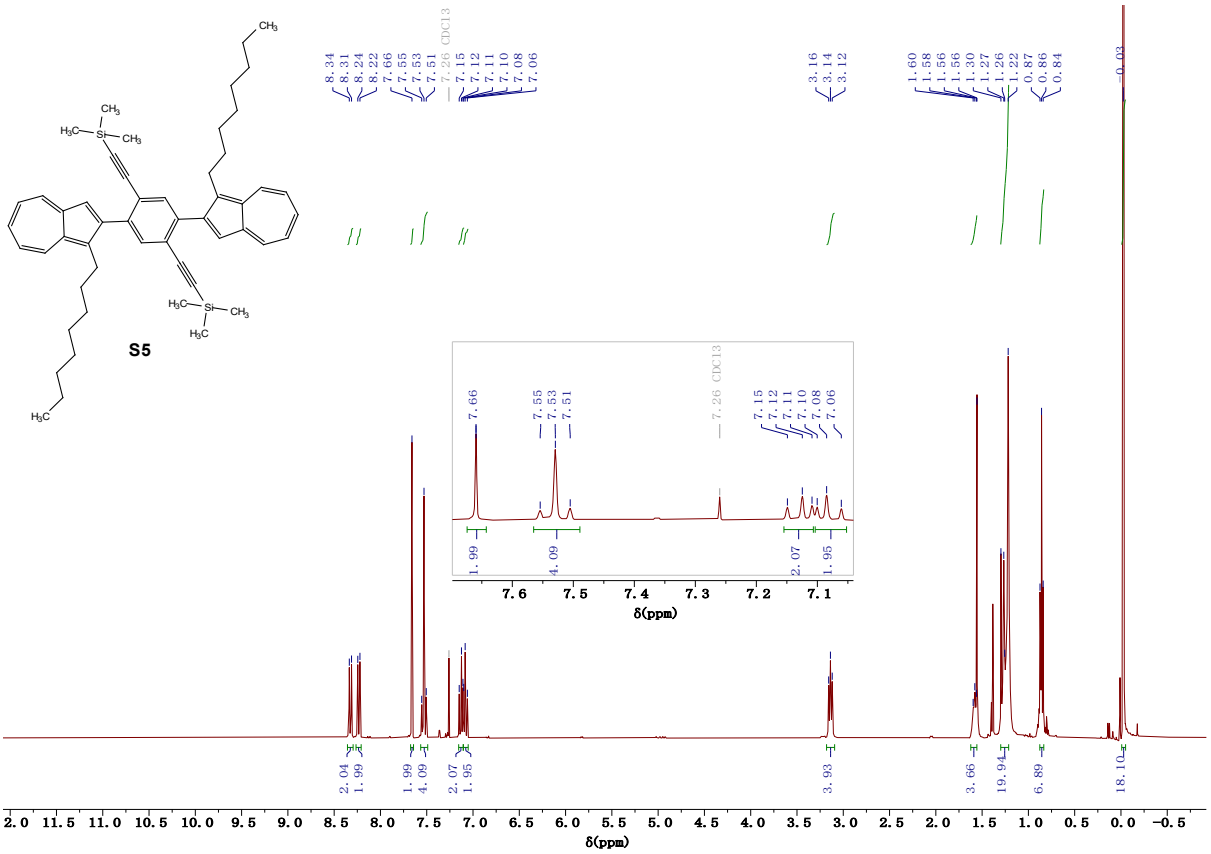
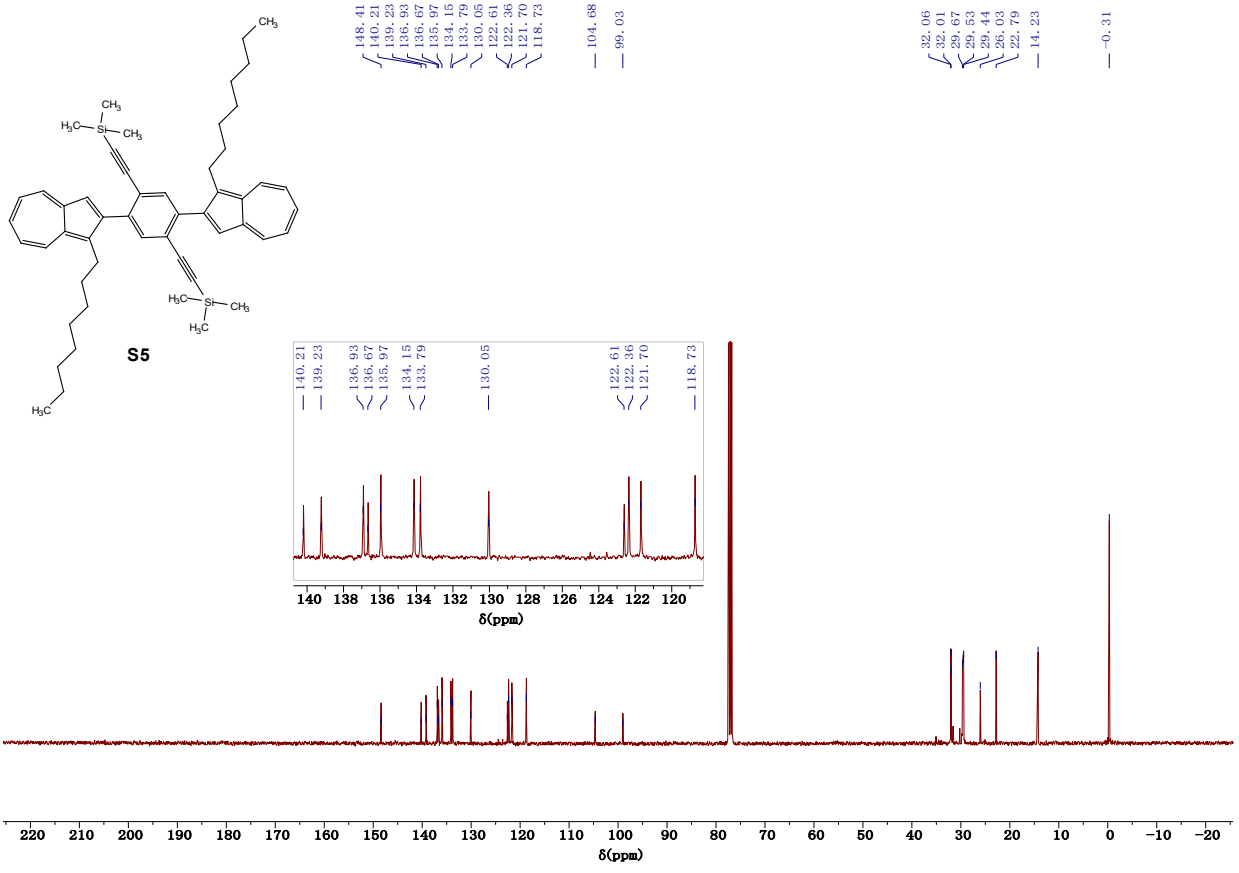
123.85
103.21
101.49
77.16
-0.18
δ(ppm)


S5
δ(ppm)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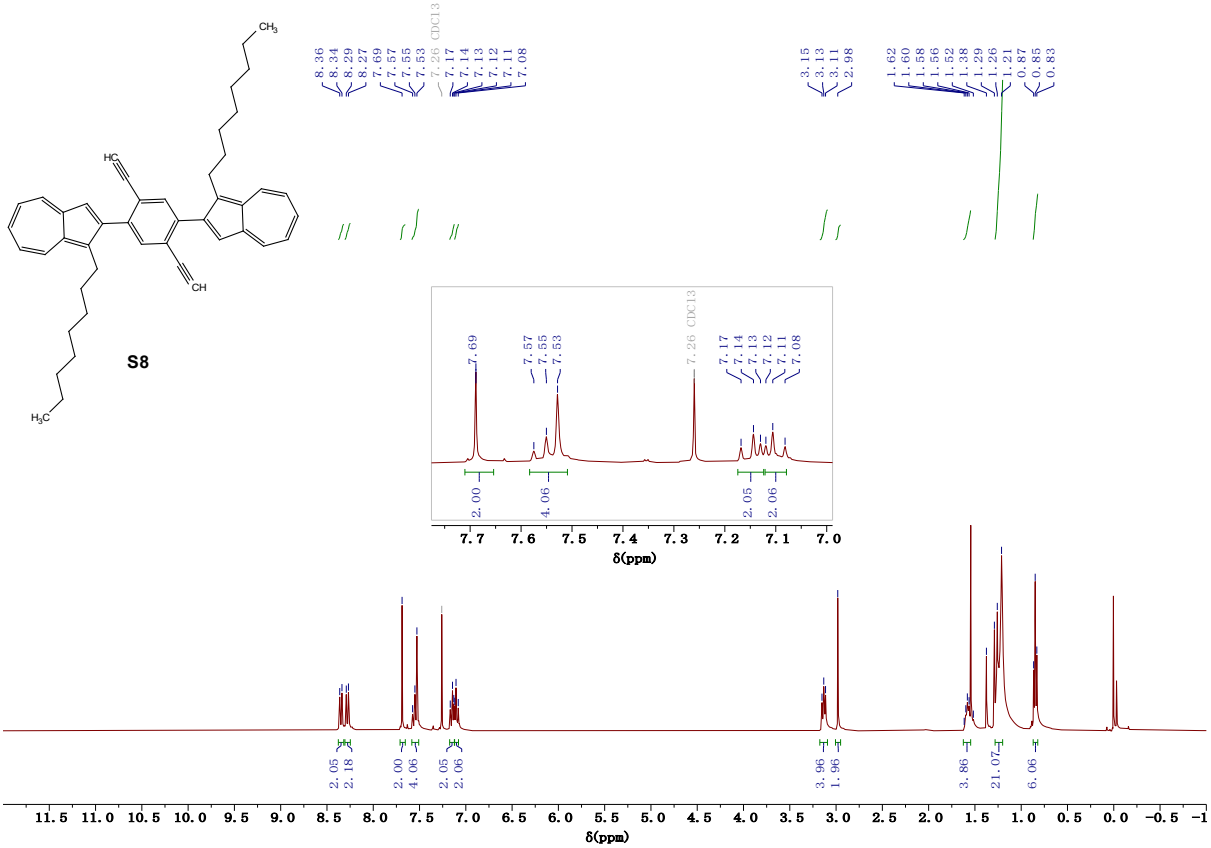
δ(ppm)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7.12
7.11
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3.15
3.13
3.11
2.98
1.62
1.60
1.58
1.56
1.52
1.38
1.29
1.26
1.21
0.87
0.85
0.83
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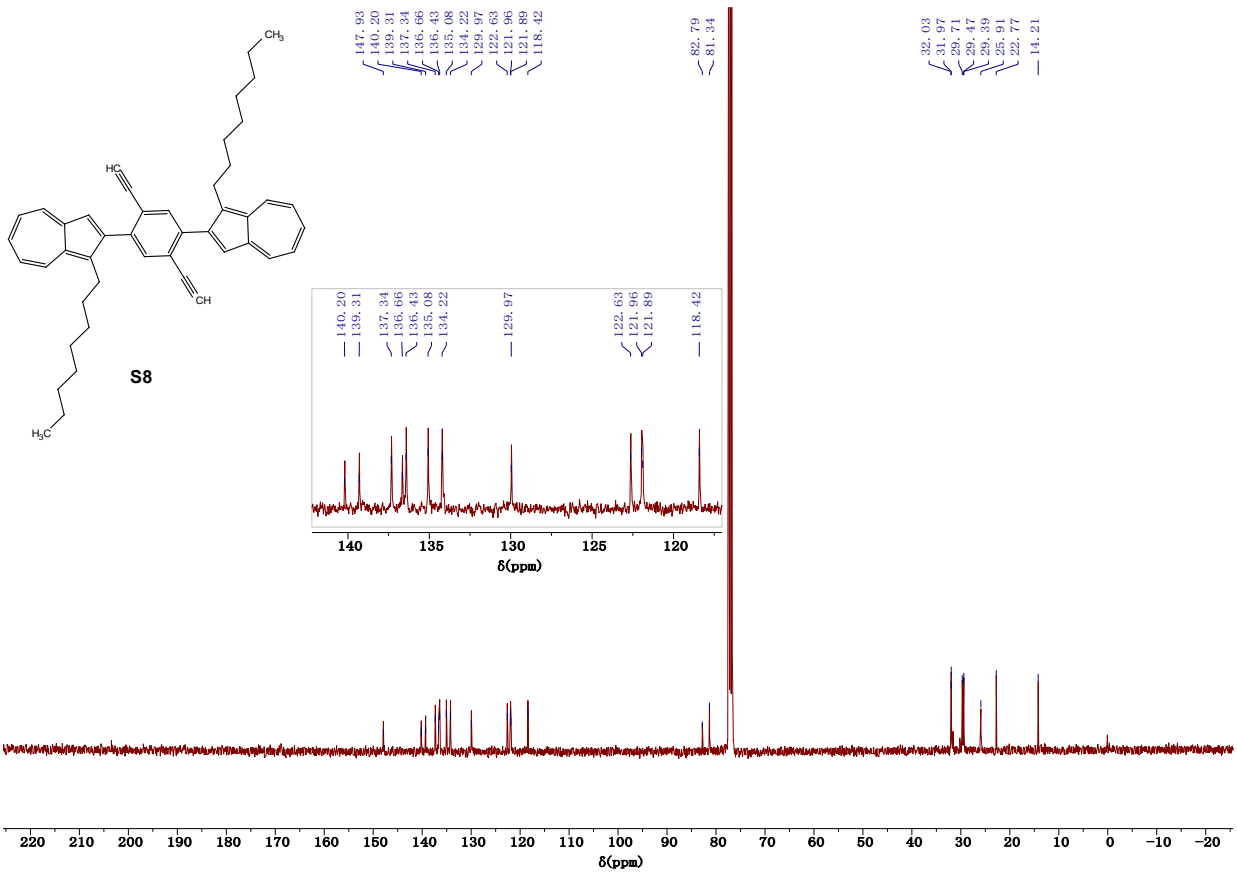
2.05
2.06
3.96
1.96
3.86
21.07
6.06
δ(ppm)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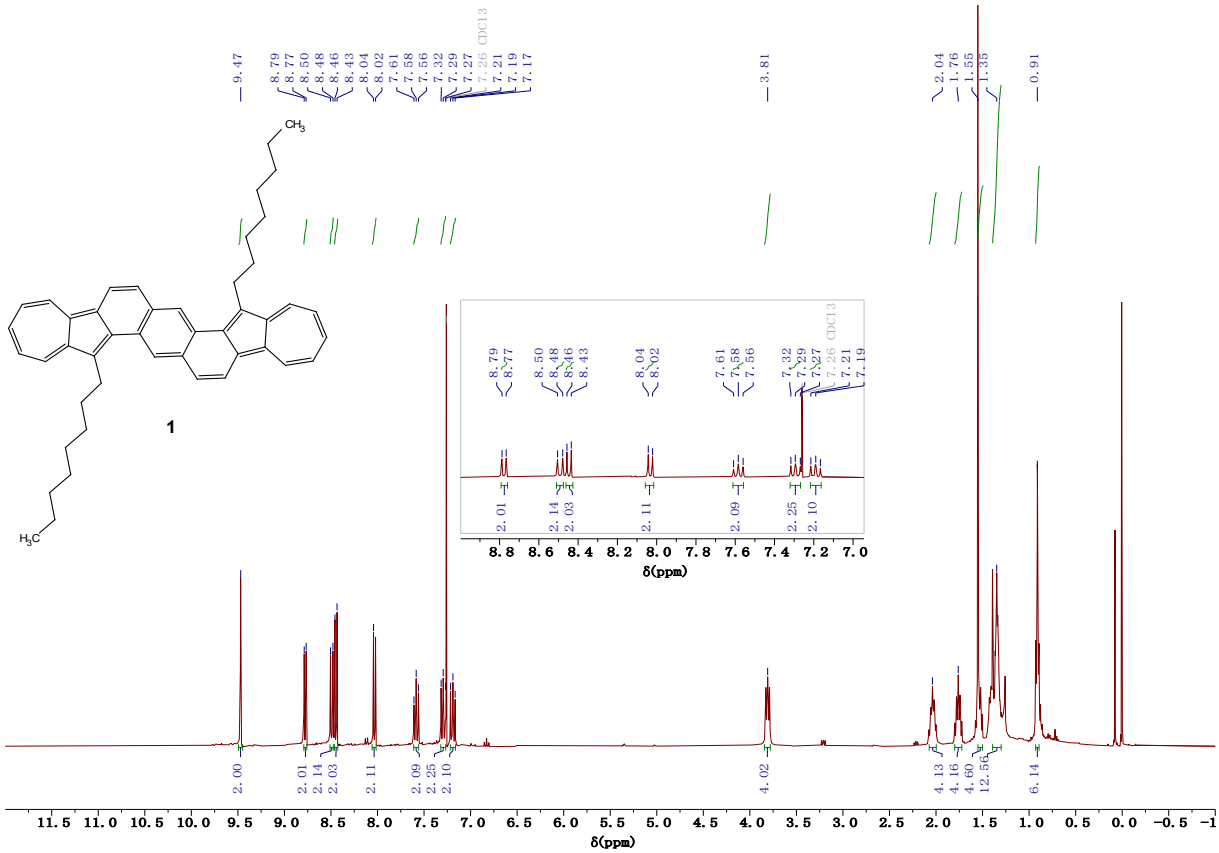
29.39
25.91
22.77
14.21
δ(ppm)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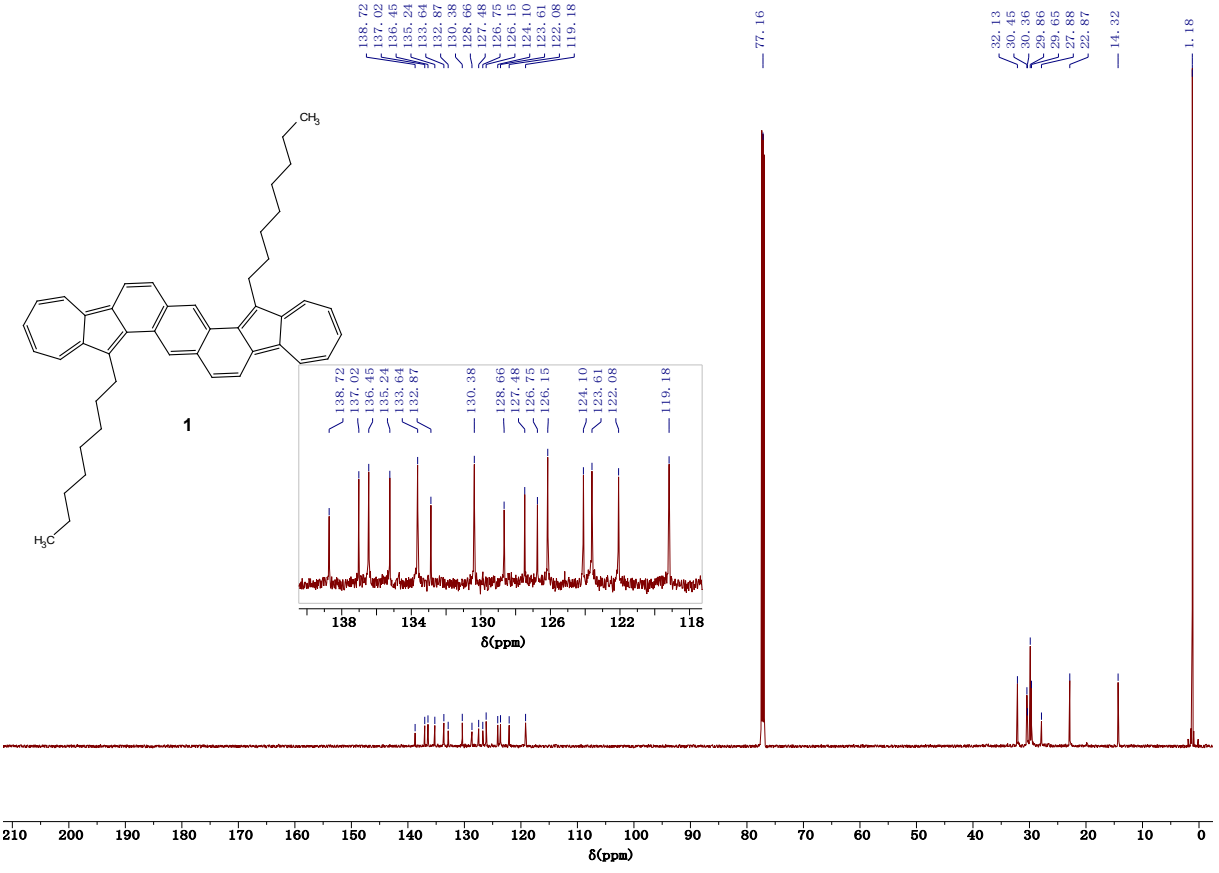
7.29
7.27
7.26
CDCl3
7.21
7.19
7.17
3.81
2.04
1.76
1.55
1.35
0.91
CH3
H3C
1
δ(ppm)
2.00
2.01
2.14
2.03
2.11
2.09
2.25
2.10
4.02
4.13
4.16
4.60
12.56
6.14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122.08
119.18
77.16
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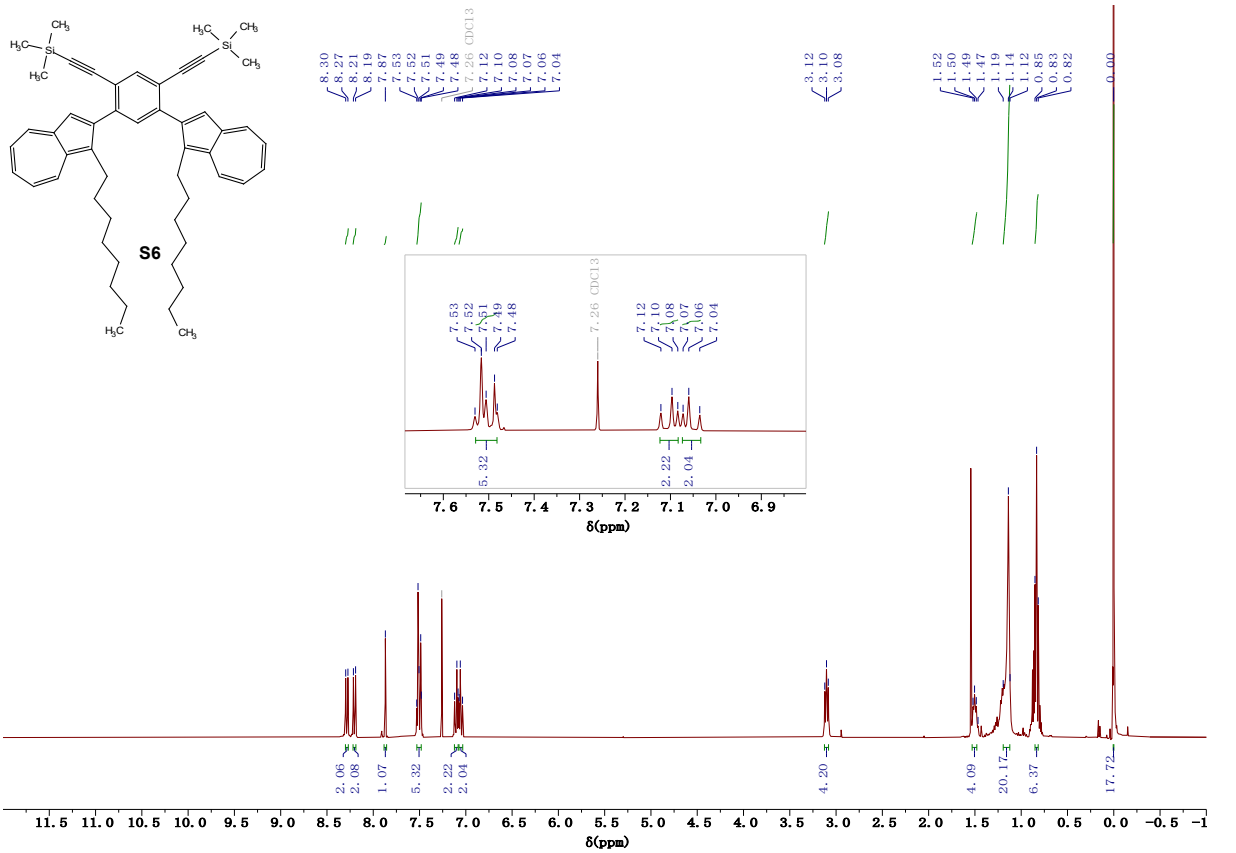
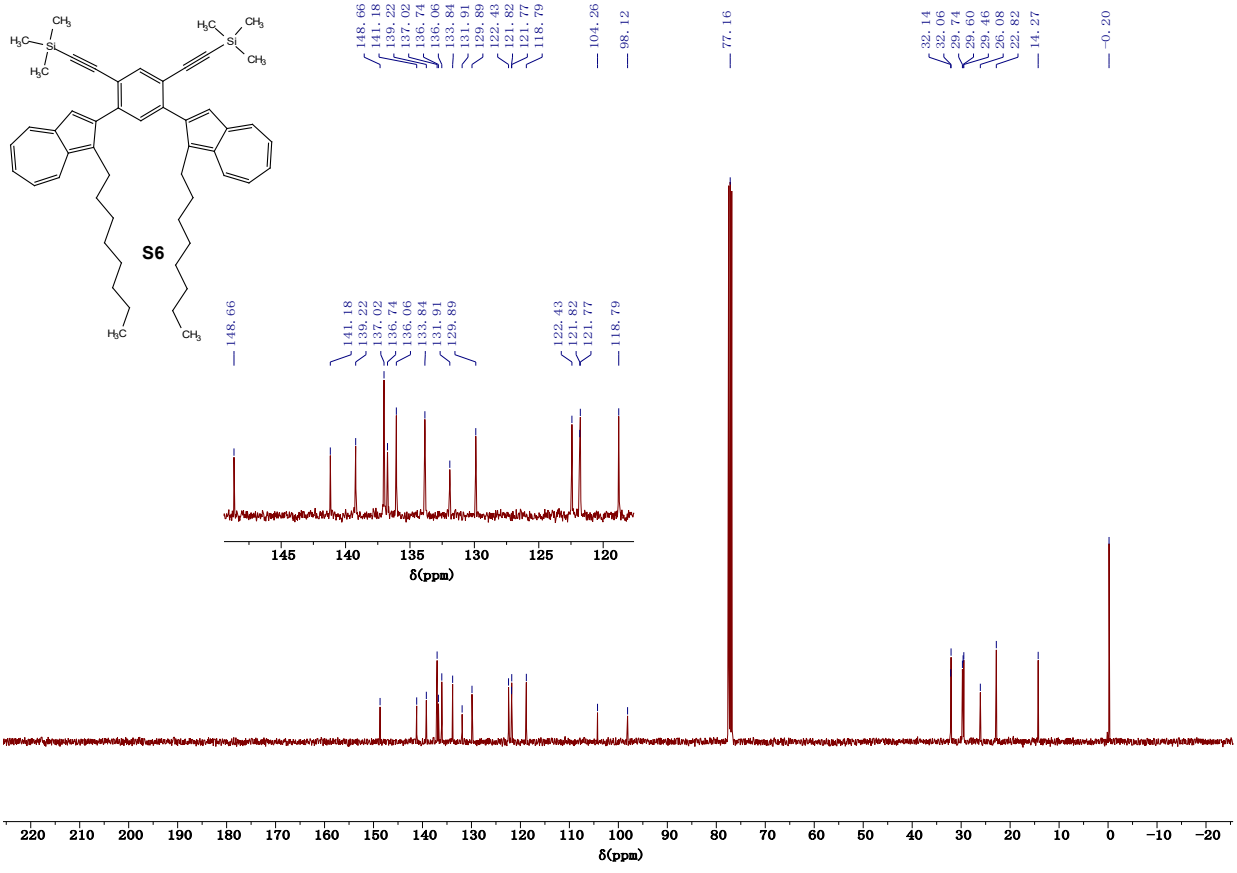
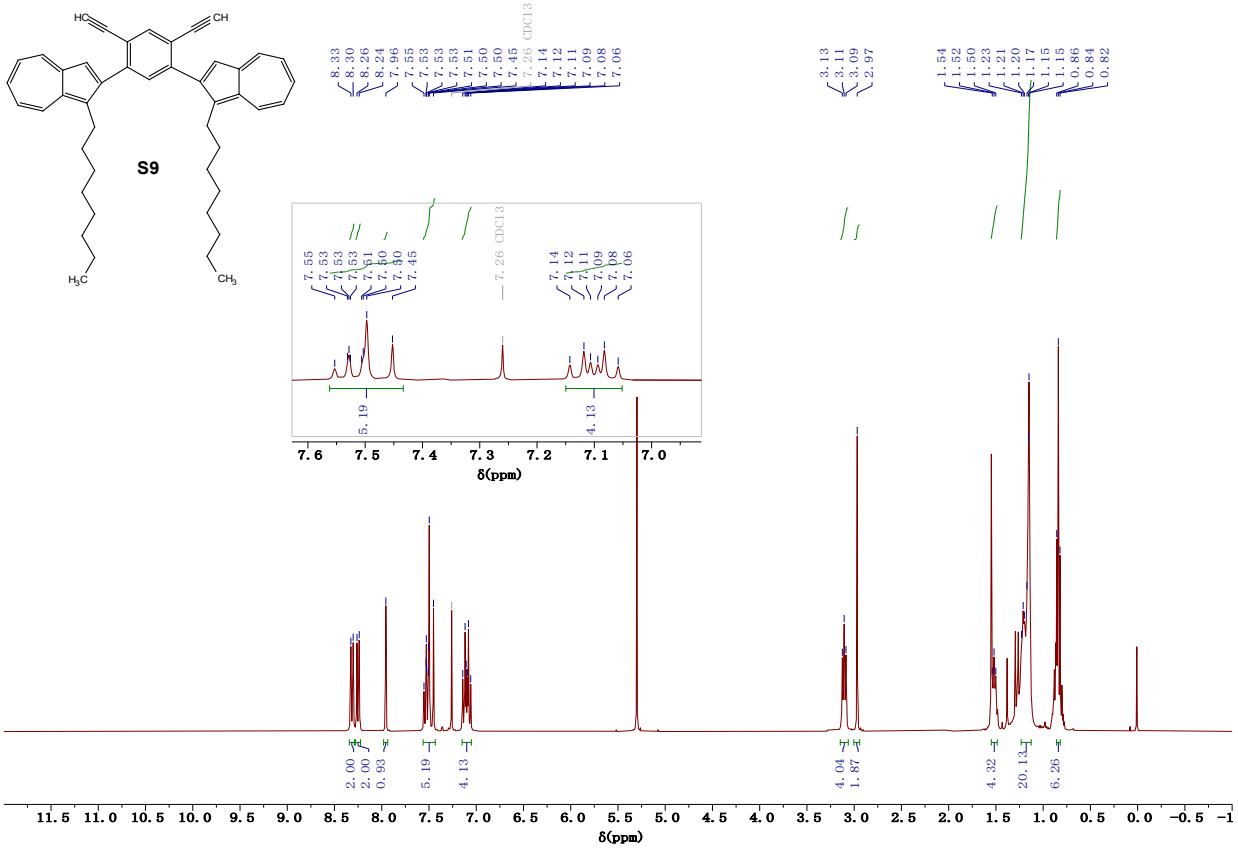
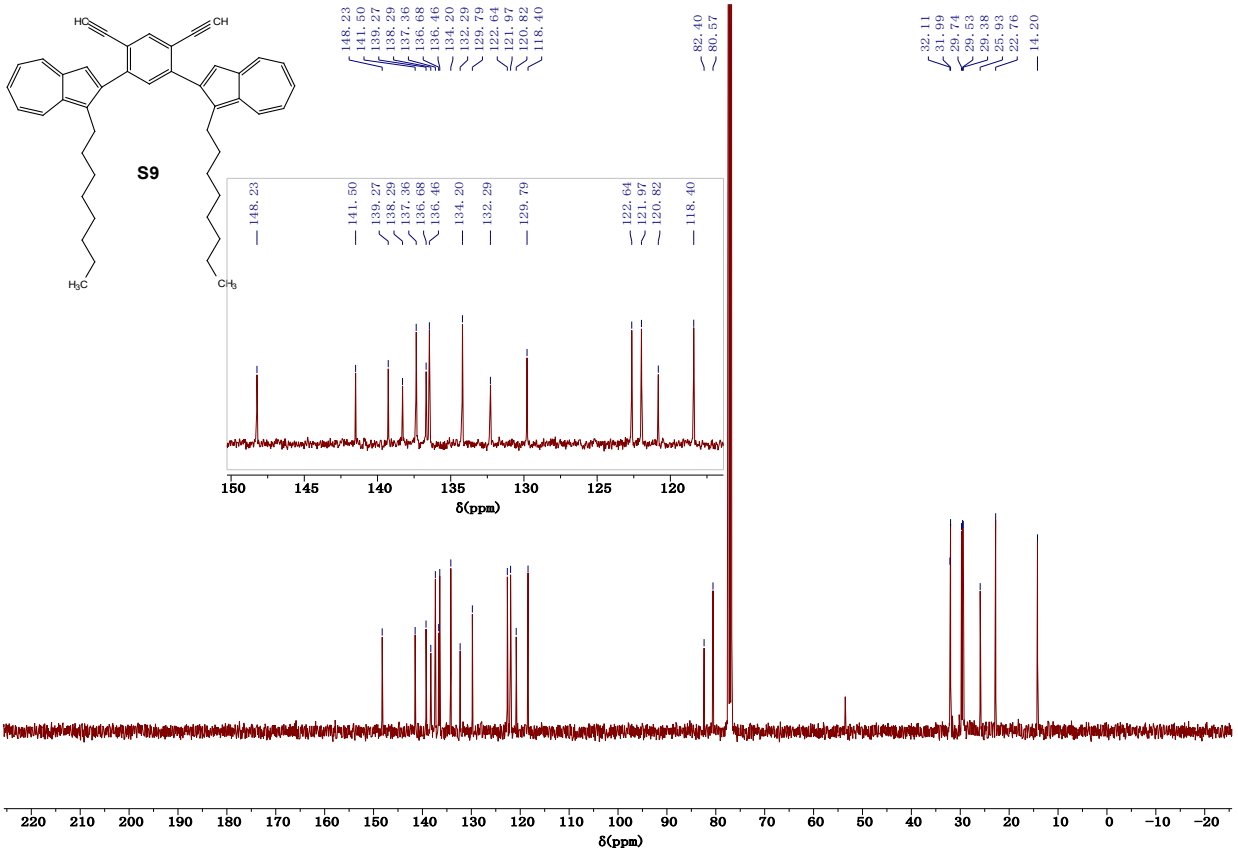
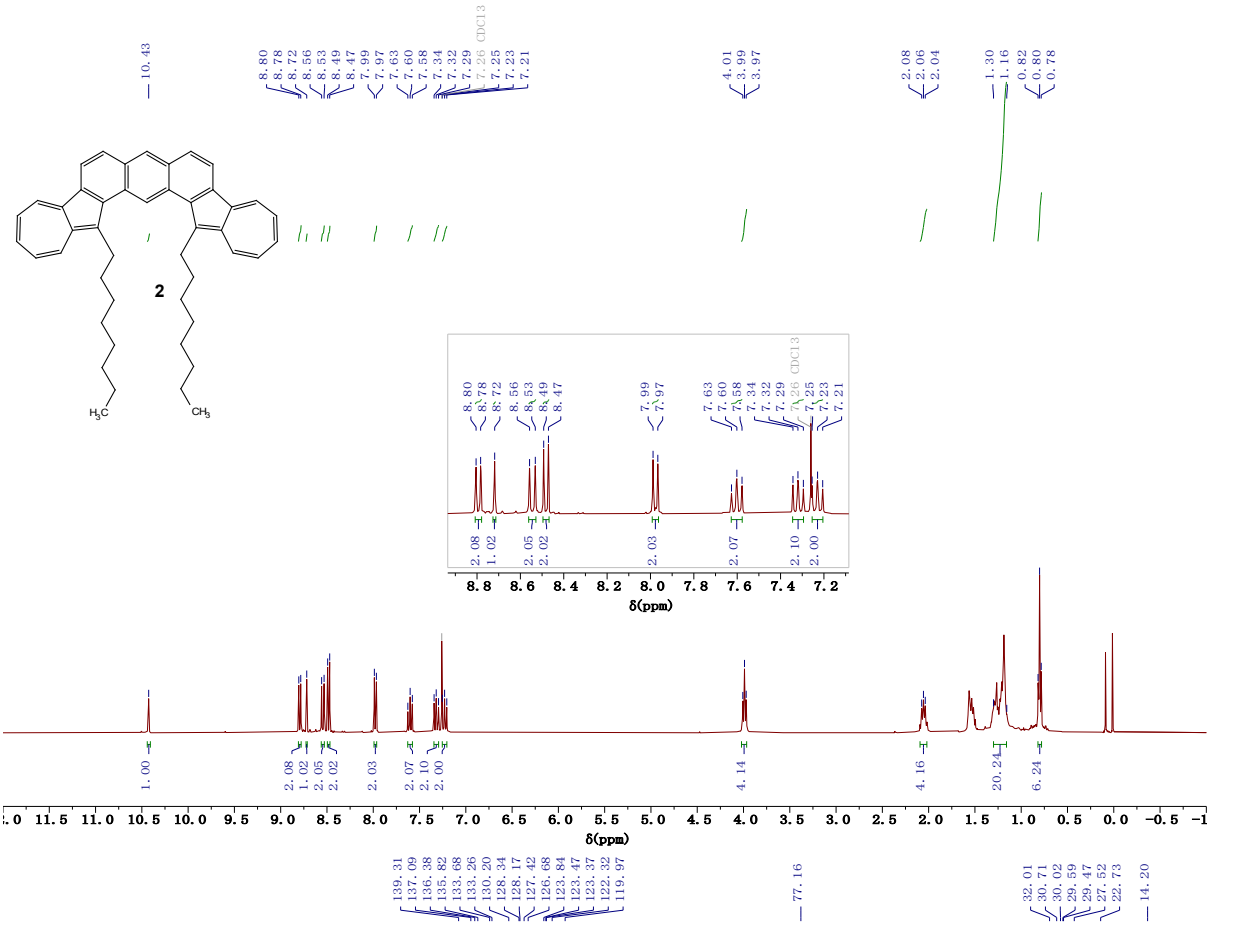
14.32
1.18
CH3
H3C
1
δ(ppm)

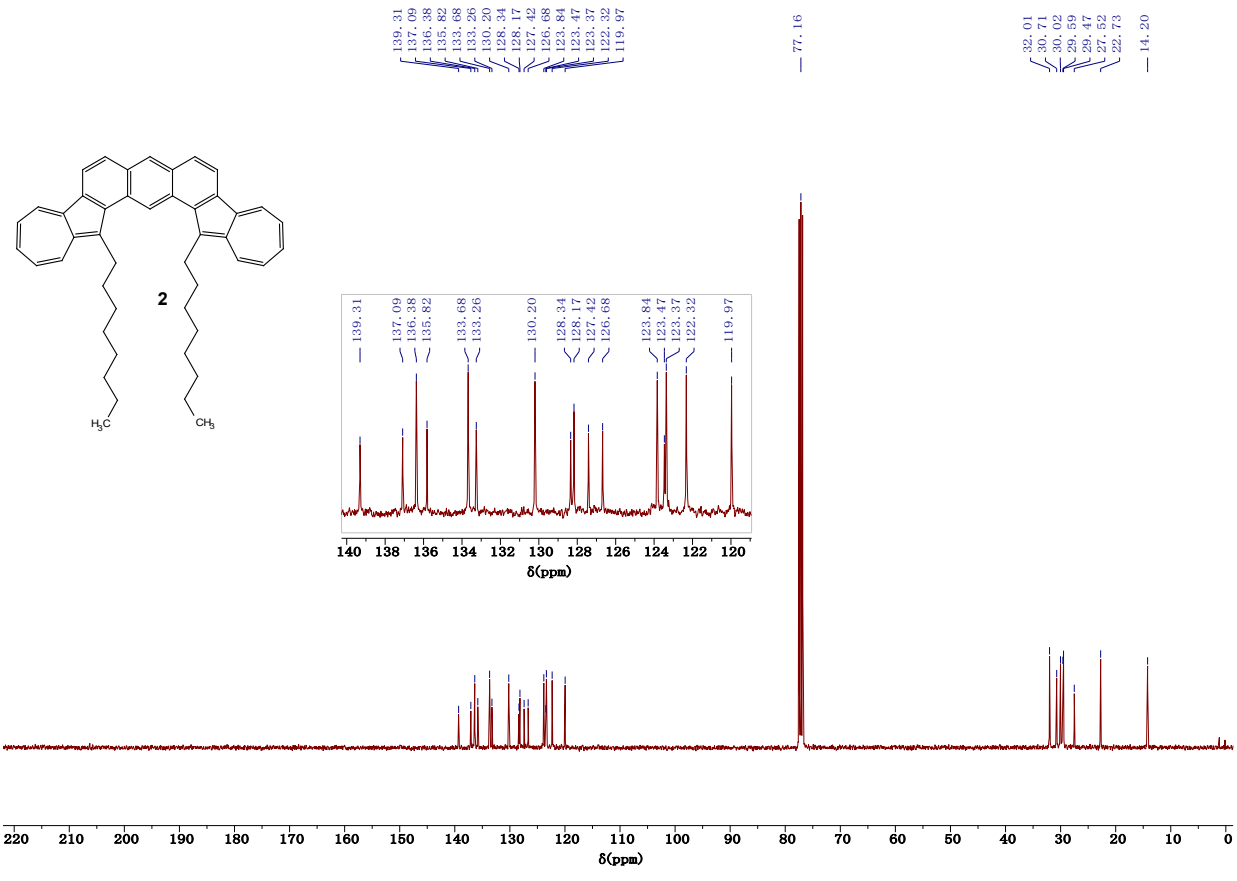

S6
δ(ppm)

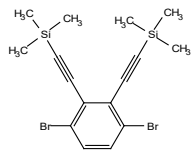

S6
δ(ppm)


S9
HC
CH
H3C
CH3
δ(ppm)


S9
HC
CH
H3C
CH3
δ(ppm)

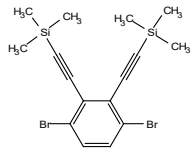

10.43
8.80
8.78
8.72
8.56
8.53
8.49
8.47
7.99
7.97
7.63
7.60
7.58
7.34
7.32
7.29
7.26 CDCl3
7.25
7.23
7.21
4.01
3.99
3.97
2.08
2.06
2.04
1.30
1.16
0.82
0.80
0.78
2
H3C
CH3
δ(ppm)
1.00
2.08
1.02
2.05
2.02
2.03
2.07
2.10
2.00
4.14
4.16
20.24
6.24


139.31
137.09
136.38
135.82
133.68
133.26
130.20
128.34
128.17
127.42
126.68
123.84
123.47
123.37
122.32
119.97
77.16
32.01
30.71
30.02
29.59
29.47
27.52
22.73
14.20
2
H3C
CH3
δ(ppm)



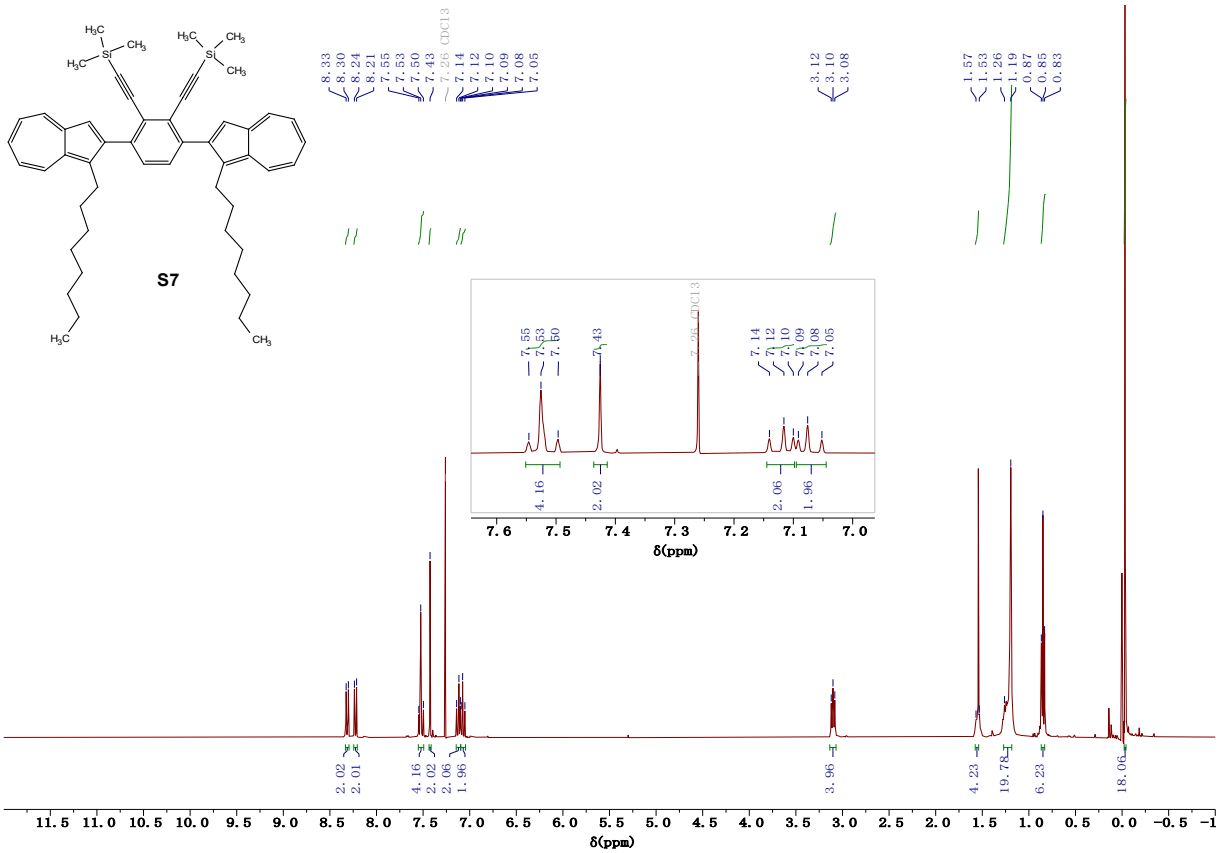
M5

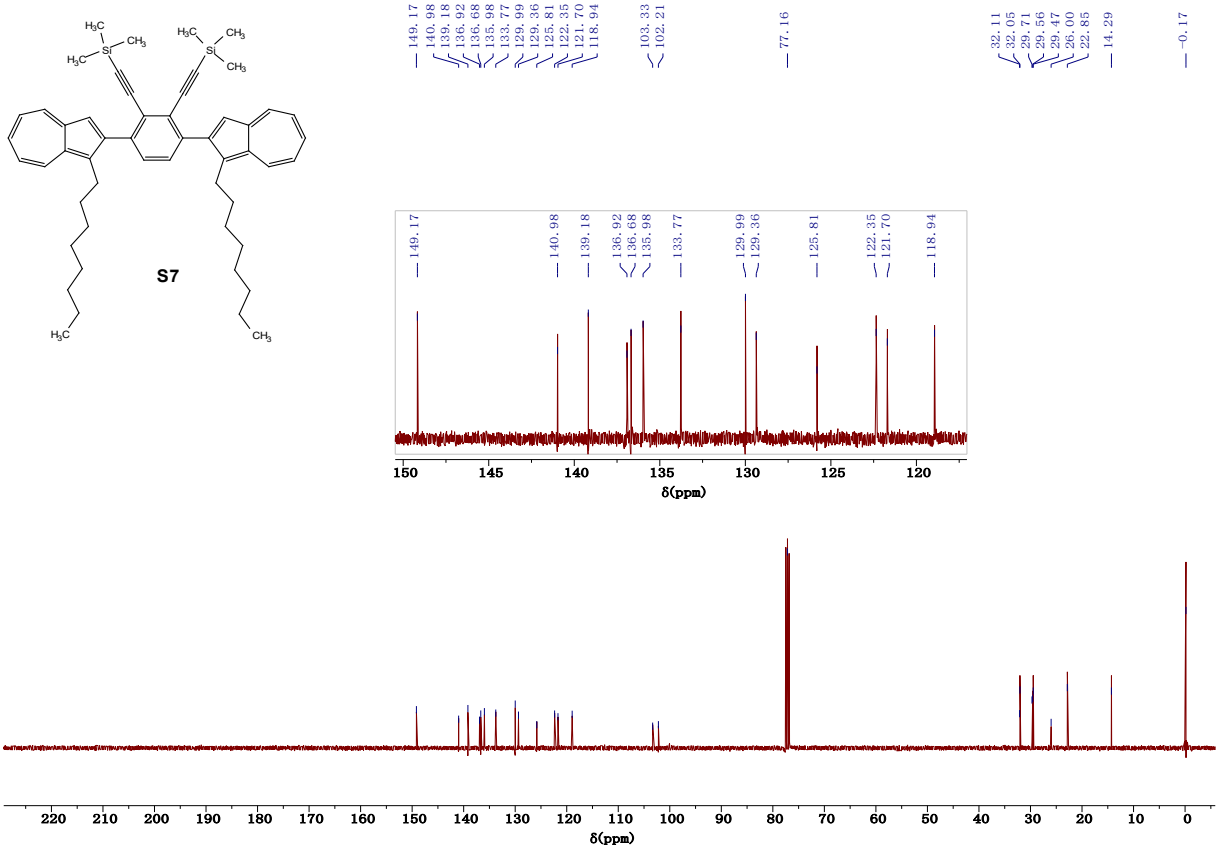
7.35
7.26 CDCl3
0.29
2.00
17.97
11.5 11.0 10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 −0.5 −1
δ(ppm)

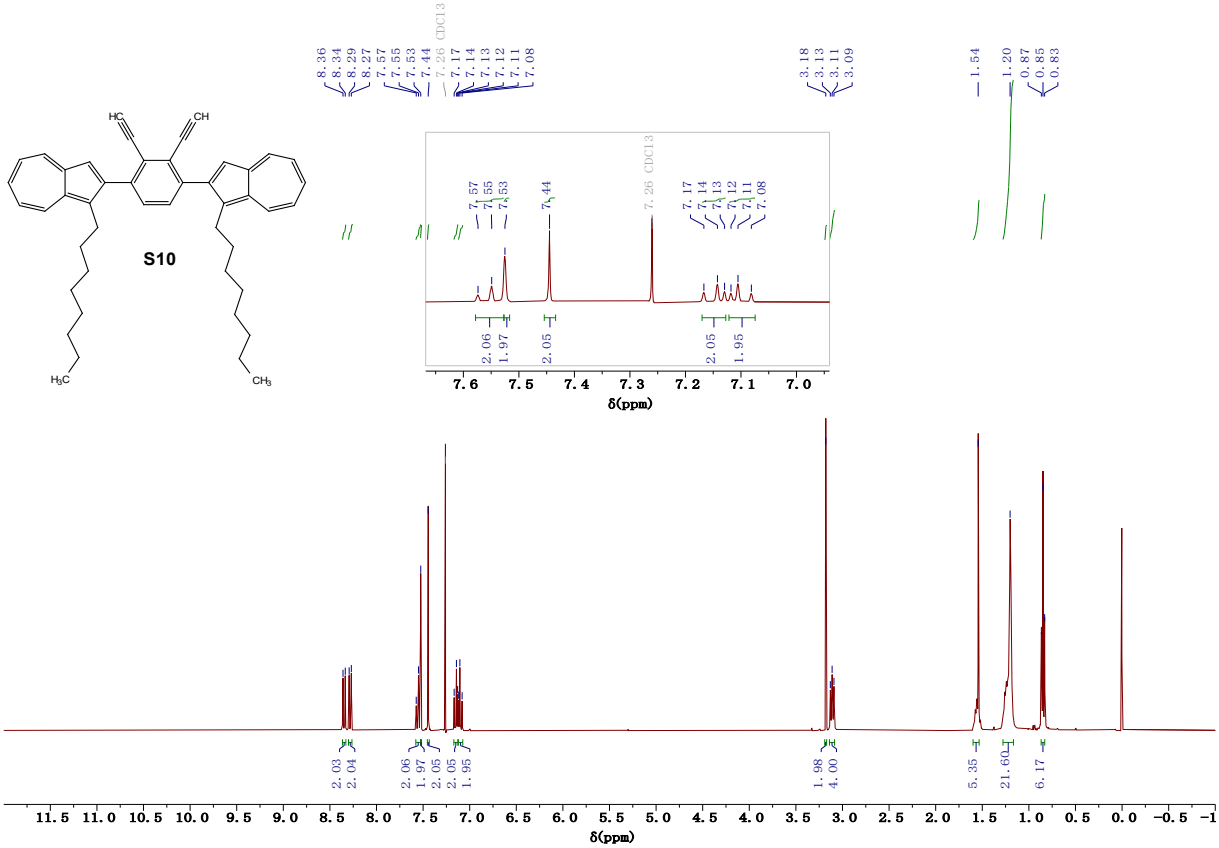


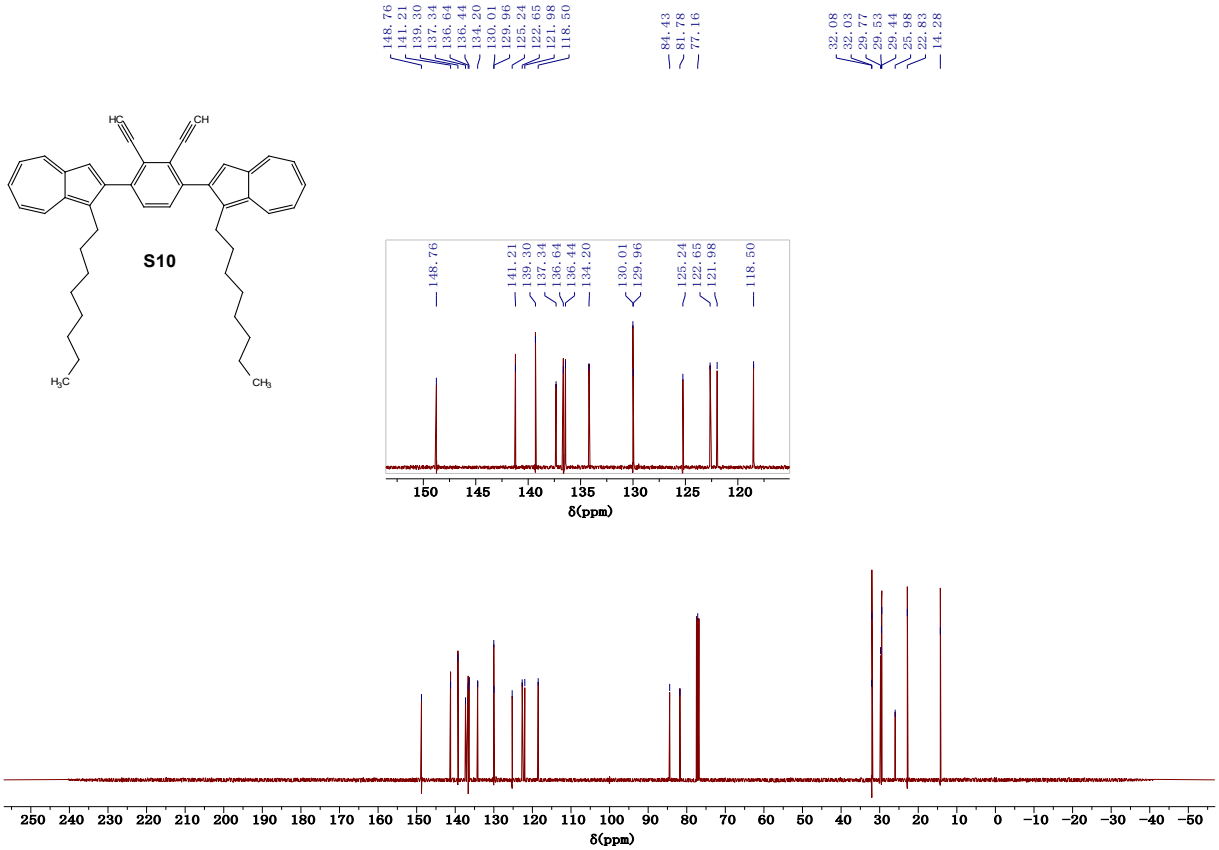
M5

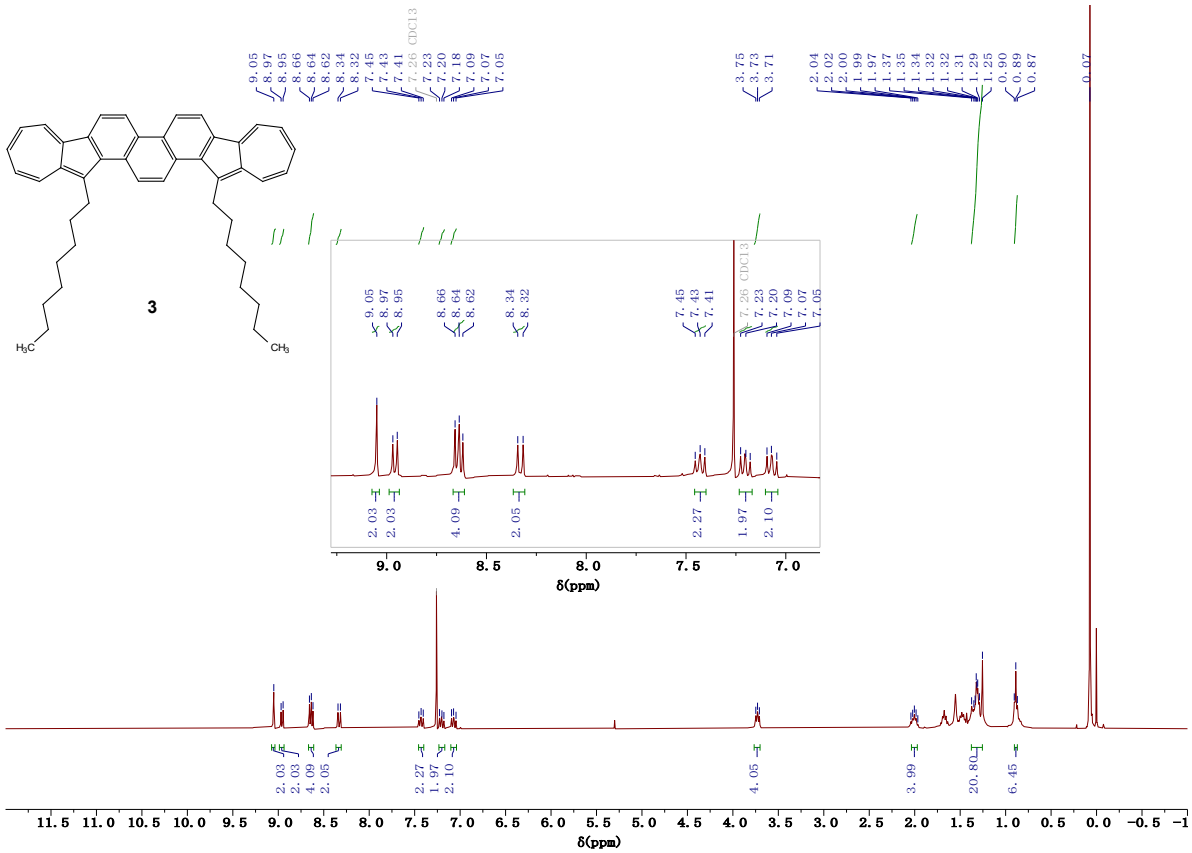
132.65
129.24
124.68
105.69
101.33
77.16
−0.05
220 210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 −10 −20
δ(ppm)

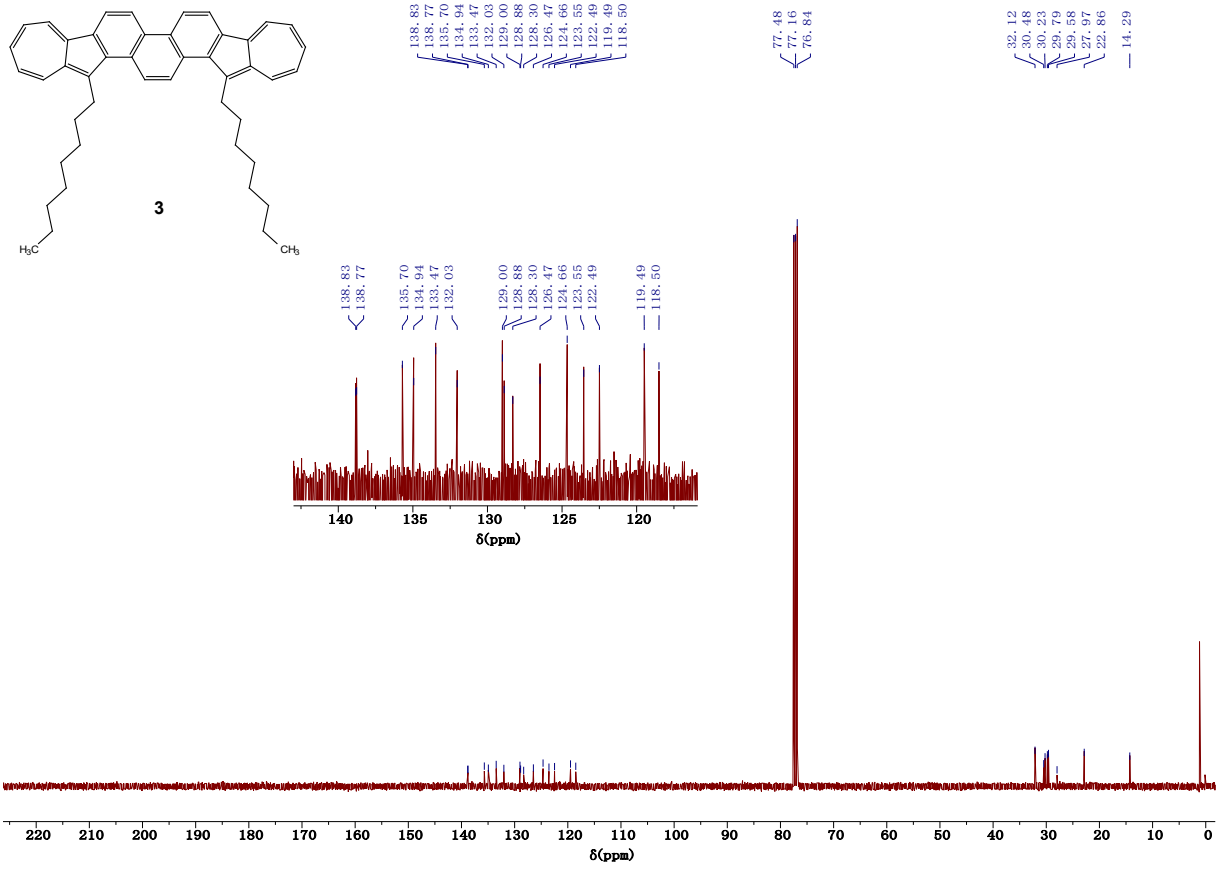

S7
δ(ppm)


S7
δ(ppm)


S10
HC
CH
H3C
CH3
8.36
8.34
8.29
8.27
7.57
7.55
7.53
7.44
7.26 CDCl3
7.17
7.14
7.13
7.12
7.11
7.08
3.18
3.13
3.11
3.09
1.54
1.20
0.87
0.85
0.83
2.03
2.04
2.06
1.97
2.05
2.05
1.95
1.98
4.00
5.35
21.60
6.17
δ(ppm)


S10
HC
CH
H3C
CH3
148.76
141.21
139.30
137.34
136.64
136.44
134.20
130.01
129.96
125.24
122.65
121.98
118.50
84.43
81.78
77.16
32.08
32.03
29.77
29.53
29.44
25.98
22.83
14.28
δ(ppm)


3
H3C
CH3
δ(ppm)


3
H3C
CH3
δ(ppm)

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