1,2,3-Triarylazulenes as Precursors of Azulene-Embedded Polycyclic Aromatic Hydrocarbons

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General

Synthesis: Sensitive reactions were conducted under N_2 using standard Schlenk techniques. Glassware was dried at 120 °C. Solvents for synthesis were treated as follows: 1,4-Dioxane (POCH): distilled over Na/benzophenone, $MeNO_2$ (POCH) dried over molecular sieves, THF (POCH) purified using mBraun solvent purification system, 1,2-dichloroethane (Acros, 99.8%, Extra Dry) and CH_2Cl_2 (ChemPur) were used without further purification.

1-Bromo-4-(*tert*-butyl)benzene (Sigma Aldrich, 97%), 1-iodo-4-methoxybenzene (Aldrich, 98%), 4-(*tert*-butyl)phenyl)boronic acid (Apollo Scientific, 98%), (4-methoxyphenyl)boronic acid (Apollo Scientific, 97%), *N*-iodosuccinimide (NIS, Alfa Aesar, 97%), $B_2(pin)_2$ (Alfa Aesar, 98%), $FeCl_3$ (POCH, pure for analysis), K_2CO_3 (Aldrich, pure for synthesis), Cs_2CO_3 (Sigma Aldrich, 99%) were used as received. Catalysts were purified by recrystallization under N_2: $Pd(dppf)Cl_2 \cdot CH_2Cl_2$ (Aldrich) from CH_2Cl_2/*n*-hexane (1/1) mixture, $[Ir(OMe)cod]_2$ (Aldrich, 98%) from CH_2Cl_2/MeOH (1/1) mixture.

Following compound were prepared according to the literature methods: 6-*tert*-butylazulene,[1] 2-bromo-7-(*tert*-butyl)pyrene,[2] 2-(7-(*tert*-butyl)pyren-2-yl)-4,4,5,5-tetramethyl-1,3,2-dioxaborolane.[2]

Chromatography: *Column chromatography*: standard glass columns and silica gel 60 (0.040-0.063 mm or 0.063-0.200 mm, Merck Millipore). Solvents for column chromatography were used without additional purification.
SEC (*Size exclusion chromatography*): Glass columns, BioBeads SX-1 stationary phase and CH_2Cl_2 as an eluent.
GPC (*Gel permeation chromatography*): JAI LaboACE LC-7080 recycling preparative system with JAIGEL-2HR (20ϕx600) and JAIGEL-2.5HR (20ϕx600) column using $CHCl_3$ stabilized with EtOH as an eluent.

NMR Spectroscopy: ^{1}H and ^{13}C NMR spectra were recorded with a Bruker Avance 500 MHz, Bruker Avance 600 MHz or JOEL 500 MHz spectrometers. For all the ^{1}H NMR spectra, the chemical shifts are given in ppm relative to the solvent residual peaks ($CDCl_3$, ^{1}H: 7.26 ppm, ^{13}C: 77.16 ppm; CD_2Cl_2, ^{1}H: 5.32 ppm, ^{13}C: 53.84 ppm). Coupling constants are given in Hz.

High Resolution Mass Spectrometry: HRMS spectra were recorded as follows: *ESI-HRMS*: Bruker qTOF compact or Shimadzu q-TOF LCMS 9030, *APCI-HRMS*: Bruker qTOF compact.

UV/Vis/NIR Spectroscopy: All measurements of CH_2Cl_2 solutions (c~10^{-5} M) were carried out in 10 mm quartz cuvettes using two-beam JASCO V-770 spectrophotometer.

Electrochemistry: Cyclic voltammetry (CV) and differential pulse voltammetry (DPV) measurements were carried out in CH_2Cl_2 (dried and degassed from mBraun solvent purification system) using a Metrohm Autolab/PGSTAT302N potentiostat / galvanostat in a glass cell under a N_2 atmosphere at room temperature. A platinum disk working electrode, a platinum wire auxiliary electrode and an Ag/AgCl reference electrode were used for all measurements. Tetrabutylammonium hexafluorophosphate (AmBeed) was used as a supporting electrolyte (0.1 M solution). CV: scan rate was 0.050 V s^{-1}. DPV: step size of 0.005

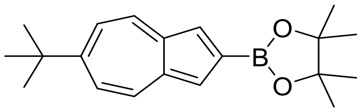
V, a modulation amplitude of 0.01 V, a modulation time of 0.05 s and an interval time of 0.5 s. All potentials were calibrated to the ferrocenium/ferrocene (Fc^{+}/Fc) redox couple.

X-ray single crystal diffraction: A suitable crystals were selected and measured using Rigaku XtaLAB Synergy-R diffractometer. The crystals were kept at 100 K during data collection. The structures were solved with the olex2.solve[3] or SHELXS[4] structure solution programs and refined with the SHELXL[5] refinement package using least squares minimization.[5]

Theoretical methods: Gaussian 16 software was used for density functional theory (DFT) and time-dependent density functional theory (TD-DFT) calculations.[6] B3LYP functional[7,8] and 6-31g(d) basis set were applied for neutral structure optimization, solvent model SCRF=(Solvent=Dichloromethane) was applied. Optimized ground-state geometries were examined by frequency analysis to possess no negative frequency. B3LYP functionals and 6-31g(d) basis sets were applied for TD-DFT calculations of UV/Vis/NIR spectra and NICS(0). UB3LYP/6-31G(d) level of theory was used for calculations of spin density of possible intermediates. Multiwfn software was used for analysis of the electronic transitions.[9]

Synthesis

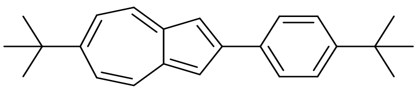
Compound 5, 2-(6-(*tert*-butyl)azulen-2-yl)-4,4,5,5-tetramethyl-1,3,2-dioxaborolane



6-*tert*-butylazulene (1.000 g, 5.43 mmol), 4,4'-dimethyl-2,2'bipirydyl (50 mg, 0.27 mmol), $B_2(pin)_2$ (758 mg, 2.98 mmol) and $[Ir(MeO)(COD)]_2$ (72 mg, 0.11 mmol) were placed in a Schlenk flask and purged with N_2. Next moisture- and oxygen-free THF was added, and the reaction mixture was stirred under N_2 for 24 h at 80 °C. After given time the solvent was removed under reduced pressure and the crude product was purified using silica gel chromatography (hexane/CH_2Cl_2; *v*/*v*; from 1/0 to 1/1) yielding 1.11 g (3.58 mmol) of product as a deep blue solid. Yield: 66%

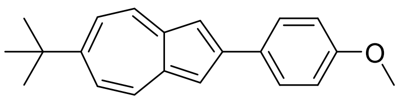
^1H NMR (500 MHz, $CDCl_3$) δ 8.29 (d, *J* = 10.8 Hz, 2H), 7.67 (s, 2H), 7.29 (d, *J* = 10.7 Hz, 2H), 1.45 (s, 9H), 1.40 (s, 12H).
^{13}C NMR (126 MHz, $CDCl_3$) δ 162.9, 139.6, 137.4, 124.7, 121.0, 83.7, 38.9, 32.0, 25.1 (C-B signal not visible).
ESI-HRMS (positive mode) *m*/*z* calcd for $C_{20}H_{27}BKO_2^+$ (M+K$^+$): 348.1772; found: 348.1793.

Compound 6a, 6-(*tert*-butyl)-2-(4-(*tert*-butyl)phenyl)azulene



2-(6-(*tert*-butyl)azulen-2-yl)-4,4,5,5-tetramethyl-1,3,2-dioxaborolane **5** (350 mg, 1.13 mmol), $Pd(dppf)Cl_2·CH_2Cl_2$ (20.6 mg, 0.028 mmol), 1-bromo-4-(*tert*-butyl)benzene (288 mg, 1.35 mmol), Cs_2CO_3 (735 mg, 2.26 mmol) were placed in a Schlenk flask and dissolved in 10 mL of 1,4-dioxane and 1 mL of H_2O. Rection mixture was degassed and stirred at 80 °C for 18 h. Solvents were evaporated under reduced pressure and crude mixture was purified using silica gel column (hexane to hexane/CH_2Cl_2, *v*/*v*, 1/1) yielding blue solid (235 mg, 0.742 mmol), yield: 66%
^1H NMR (500 MHz, $CDCl_3$) δ 8.22 (d, *J* = 10.8 Hz, 2H), 7.90 (d, *J* = 8.2 Hz, 2H), 7.59 (s, 2H), 7.49 (d, *J* = 8.2 Hz, 2H), 7.34 (d, *J* = 10.8 Hz, 2H), 1.46 (s, 9H), 1.38 (s, 9H).
^{13}C NMR (126 MHz, $CDCl_3$) δ 159.9, 151.2, 149.3, 140.2, 134.9, 134.1, 127.3, 126.0, 121.9, 113.9, 38.6, 34.8, 32.1, 31.5.
ESI-HRMS (positive mode) *m*/*z* calcd for $C_{24}H_{29}^+$ (M+H$^+$): 317.2264; found: 317.2279.

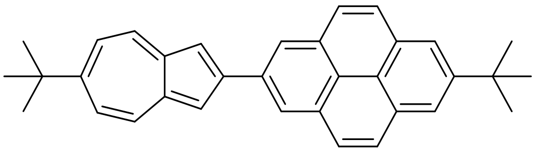
Compound 6b, 6-(*tert*-butyl)-2-(4-methoxyphenyl)azulene



2-(6-(*tert*-butyl)azulen-2-yl)-4,4,5,5-tetramethyl-1,3,2-dioxaborolane **5** (300 mg, 0.967 mmol), 1-iodo-4-methoxybenzene (339 mg, 1.45 mmol), $Pd(dppf)Cl_2·CH_2Cl_2$ (21.2 mg, 0.029 mmol), Cs_2CO_3 (630 mg, 1.93 mmol), 20 mL of 1,4-dioxane and 2 mL of water were used according to the procedure for **6a**. Reaction was carried out at 80 °C for 21 h, purification: silica gel column (hexane to CH_2Cl_2). Blue solid (70 mg, 0.241 mmol), yield: 25%.

^1H NMR (500 MHz, $CDCl_3$) δ 8.19 (d, *J* = 10.9 Hz, 2H), 7.92 – 7.88 (m, 2H), 7.53 (s, 2H), 7.33 (d, *J* = 10.9 Hz, 2H), 7.02 – 6.97 (m, 2H), 3.87 (s, 3H), 1.45 (s, 9H).
^{13}C NMR (126 MHz, $CDCl_3$) δ 159.9, 159.5, 149.1, 140.3, 134.5, 129.7, 128.8, 122.0, 114.5, 113.4, 55.5, 38.6, 32.1.
APCI-HRMS (positive mode) *m/z* calcd for $C_{21}H_{23}O^+$ (M+H$^+$): 291.1743; found: 291.1809.

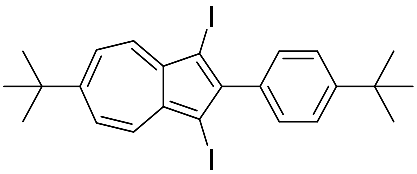
Compound 6c, 2-(*tert*-butyl)-7-(6-(*tert*-butyl)azulen-2-yl)pyrene



2-(6-(*tert*-butyl)azulen-2-yl)-4,4,5,5-tetramethyl-1,3,2-dioxaborolane **5** (227 mg, 0.732 mmol), 2-bromo-7-(*tert*-butyl)pyrene (271 mg, 0.804 mmol), Pd(dppf)Cl_2·CH_2Cl_2 (16.1 mg, 0.022 mmol), Cs_2CO_3 (477 mg, 1.46 mmol), 10 mL of 1,4-dioxane and 1 mL of water were used according to the procedure for **6a**. Reaction was carried out at 80 °C for 18 h, purification: silica gel column (hexane to CH_2Cl_2) and then solid was washed with hexane. Green solid (146 mg, 0.331 mmol), yield: 45%.
^1H NMR (500 MHz, $CDCl_3$) δ 8.72 (s, 2H), 8.32 (d, *J* = 10.8 Hz, 2H), 8.21 (s, 2H), 8.12 (d, *J* = 8.9 Hz, 2H), 8.06 (d, *J* = 8.9 Hz, 2H), 7.90 (s, 2H), 7.39 (d, *J* = 10.8 Hz, 2H), 1.60 (s, 9H), 1.49 (s, 9H).

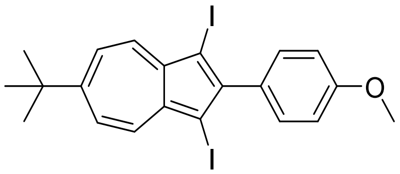
^{13}C NMR (126 MHz, $CDCl_3$) δ 160.5, 149.6, 149.3, 140.5, 135.4, 134.2, 131.6, 131.3, 128.1, 127.7, 124.6, 124.0, 123.1, 122.5, 122.2, 114.6, 38.7, 35.4, 32.1, 32.1.
APCI-HRMS (positive mode) *m/z* calcd for $C_{24}H_{33}^+$ (M+H$^+$): 441.2577; found: 441.2641.

Compound 7a, 6-(*tert*-butyl)-2-(4-(*tert*-butyl)phenyl)-1,3-diiodoazulene



Azulene **6a** (100 mg, 0.316 mmol) was dissolved in 50 mL of CH_2Cl_2 and the reaction mixture was cooled down to 0 °C. NIS (149 mg, 0.664 mmol) was added and the blue solution was stirred at room temperature for 3 h. Solvent was evaporated under reduced pressure and the crude product was purified using silica gel column (hexane/CH_2Cl_2, *v*/*v*, 1/1) yielding **7a** as a green solid (176 mg, 0.310 mmol), yield: 98%
^1H NMR (500 MHz, $CDCl_3$) δ 8.23 (d, *J* = 11.2 Hz, 2H), 7.57 (d, *J* = 11.2 Hz, 2H), 7.54 – 7.50 (m, 2H), 7.47 – 7.44 (m, 2H), 1.48 (s, 9H), 1.42 (s, 9H).
^{13}C NMR (126 MHz, $CDCl_3$) δ 162.8, 154.1, 151.2, 141.0, 138.4, 135.3, 130.4, 124.8, 123.8, 77.4, 39.0, 34.9, 31.9, 31.6.
ESI-HRMS (positive mode) *m/z* calcd for $C_{24}H_{26}I_2^+$ (M$^+$): 568.0118; found: 568.0133.

Compound 7b, 6-(*tert*-butyl)-1,3-diiodo-2-(4-methoxyphenyl)azulene



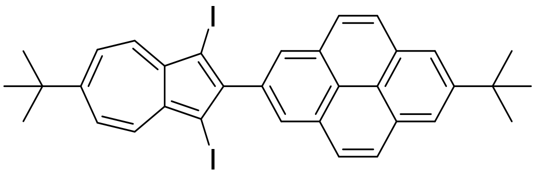
Azulene **6b** (70 mg, 0.241 mmol), NIS (136 mg, 0.602 mmol) and 50 mL of CH_2Cl_2 were used according to the procedure for **7a**. Reaction time: 1 h, purification: silica gel column (petroleum ether/CH_2Cl_2, *v*/*v*, 1/1), green solid, yield: 97% (127 mg, 0.234 mmol).

^{1}H NMR (500 MHz, $CDCl_3$) δ 8.19 (d, *J* = 10.9 Hz, 2H), 7.55 (d, *J* = 10.9 Hz, 2H), 7.46 – 7.42 (m, 2H), 7.05 – 7.02 (m, 2H), 3.89 (s, 3H), 1.46 (s, 9H).

^{13}C NMR (126 MHz, $CDCl_3$) δ 162.7, 159.7, 153.9, 141.0, 138.3, 132.1, 130.8, 123.8, 113.4, 77.5, 55.4, 39.0, 31.9.

APCI-HRMS (positive mode) *m*/*z* calcd for $C_{21}H_{21}I_2O^+$ (M^+): 542.9676; found: 542.9698.

Compound 7c, 2-(*tert*-butyl)-7-(6-(*tert*-butyl)-1,3-diiodoazulen-2-yl)pyrene



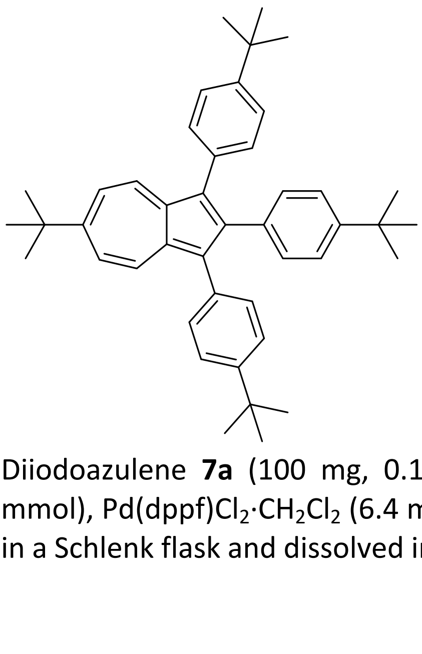
Azulene **6c** (110 mg, 0.250 mmol), NIS (124 mg, 0.602 mmol) and 50 mL of CH_2Cl_2 were used according to the procedure for **7a**. Reaction time: 1 h, purification: silica gel column (hexane/CH_2Cl_2, *v*/*v*, 1/1), green solid, yield: 84% (146 mg, 0.211 mmol).

^{1}H NMR (500 MHz, $CDCl_3$) δ 8.32 (d, *J* = 11.1 Hz, 2H), 8.26 (s, 2H), 8.25 (s, 2H), 8.14 (d, *J* = 8.9 Hz, 2H), 8.11 (d, *J* = 8.9 Hz, 2H), 7.64 (d, *J* = 11.1 Hz, 2H), 1.61 (s, 9H), 1.52 (s, 9H).

^{13}C NMR (126 MHz, $CDCl_3$) δ 163.2, 154.6, 149.5, 141.1, 138.6, 135.8, 131.3, 130.6, 128.0, 127.6, 127.1, 124.4, 124.0, 123.0, 122.5, 77.9, 39.1, 35.4, 32.1, 32.0.

APCI-HRMS (positive mode) *m*/*z* calcd for $C_{34}H_{31}I_2^+$ ($M+H^+$): 693.0510; found: 693.0499.

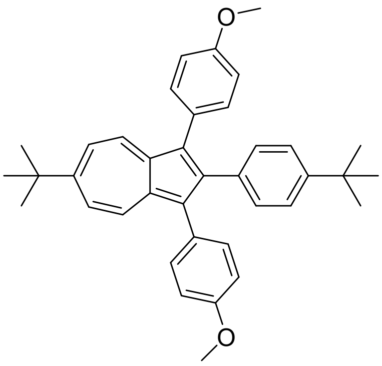
Compound 1a, 6-(*tert*-butyl)-1,2,3-tris(4-(*tert*-butyl)phenyl)azulene



Diiodoazulene **7a** (100 mg, 0.176 mmol (4-(*tert*-butyl)phenyl)boronic acid (94 mg, 0.528 mmol), $Pd(dppf)Cl_2{\cdot}CH_2Cl_2$ (6.4 mg, 0.0087 mmol), Cs_2CO_3 (172 mg, 0.528 mmol) were placed in a Schlenk flask and dissolved in 10 mL of 1,4-dioxane and 1 mL of H_2O. Rection mixture was

degassed and stirred at 80°C for 2 h. Solvents were evaporated under reduced pressure and crude mixture was purified using silica gel column (hexane to hexane/CH_2Cl_2, *v*/*v*, 1/1) yielding green solid (80 mg, 0.138 mmol), yield: 78%.
^{1}H NMR (500 MHz, $CDCl_3$) δ 8.26 (d, *J* = 11.0 Hz, 2H), 7.35 – 7.31 (m, 4H), 7.23 (d, *J* = 11.1 Hz, 2H), 7.21 – 7.18 (m, 4H), 7.10 – 7.06 (m, 2H), 6.97 – 6.94 (m, 2H), 1.41 (s, 9H), 1.35 (s, 18H), 1.25 (s, 9H).
^{13}C NMR (126 MHz, $CDCl_3$) δ 161.4, 149.1, 148.8, 147.3, 136.2, 134.8, 133.9, 133.7, 131.3, 131.1, 128.8, 124.8, 124.3, 121.6, 38.5, 34.6, 34.5, 32.0, 31.6, 31.5.
APCI-HRMS (positive mode) *m*/*z* calcd for $C_{44}H_{53}^{\cdot+}$ ($M^{\cdot+}$): 581.4142; found: 581.4092.

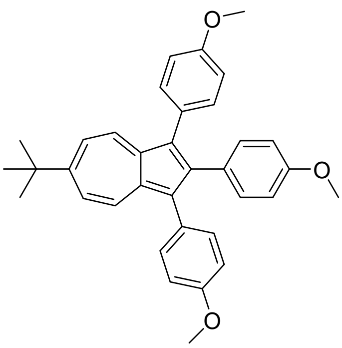
Compound 1b, 6-(*tert*-butyl)-2-(4-(*tert*-butyl)phenyl)-1,3-bis(4-methoxyphenyl)azulene



Diiodoazulene **7a** (100 mg, 0.176 mmol), (4-methoxyphenyl)boronic acid (80 mg, 0.528 mmol), Pd(dppf)Cl_2·CH_2Cl_2 (6.4 mg, 0.0087 mmol), Cs_2CO_3 (172 mg, 0.528 mmol), 20 mL of 1,4-dioxane and 2 mL of water were used according to the procedure for **1a**. Reaction carried out at 80 °C for 18 h, purification: silica gel column (hexane to hexane/CH_2Cl_2, *v*/*v*, 1/1). Green solid (67 mg, 0.127 mmol), yield: 72%.

^{1}H NMR (500 MHz, $CDCl_3$) δ 8.22 (d, *J* = 11.0 Hz, 2H), 7.23 (d, *J* = 11.0 Hz, 2H), 7.22 – 7.18 (m, 4H), 7.14 – 7.10 (m, 2H), 6.98 – 6.95 (m, 2H), 6.91 – 6.87 (m, 4H), 3.85 (s, 6H), 1.42 (s, 9H), 1.26 (s, 9H).
^{13}C NMR (126 MHz, $CDCl_3$) δ 161.5, 158.1, 149.2, 147.1, 136.2, 134.6, 133.8, 132.7, 131.0, 129.2, 128.3, 124.6, 121.5, 113.6, 55.4, 38.5, 34.6, 32.0, 31.5.
APCI-HRMS (positive mode) *m*/*z* calcd for $C_{38}H_{41}O_2^+$ ($M+H^+$): 529.3101; found: 529.3061.

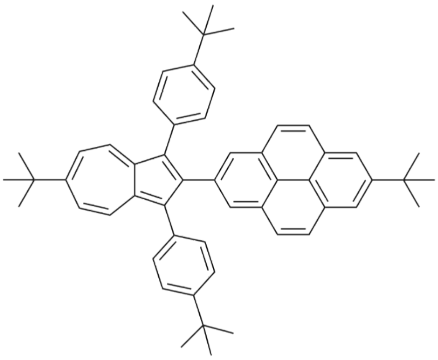
Compound 1c, 6-(*tert*-butyl)-1,2,3-tris(4-methoxyphenyl)azulene



Diiodoazulene **7b** (50 mg, 0.092 mmol, 1.0 equiv.), boronic acid (42 mg, 0.277 mmol), Pd(dppf)Cl_2·CH_2Cl_2 (2.0 mg, 0.0028 mmol), Cs_2CO_3 (90 mg, 0.277 mmol), 5 mL of 1,4-dioxane and 1 mL of water were used according to the procedure for **1a**. Reaction carried out at 80 °C for 18 h, purification: silica gel column (CH_2Cl_2). Green solid (43 mg, 085mmol), yield: 92%.

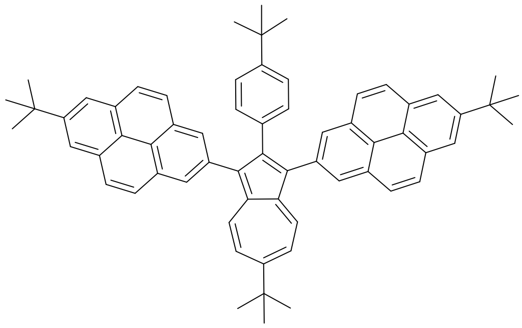
^{1}H NMR (500 MHz, $CDCl_3$) δ 8.21 (d, *J* = 11.0 Hz, 2H), 7.23 (d, *J* = 11.0 Hz, 2H), 7.22 – 7.19 (m, 4H), 6.99 – 6.95 (m, 2H), 6.92 – 6.89 (m, 4H), 6.69 – 6.65 (m, 2H), 3.85 (s, 6H), 3.75 (s, 3H), 1.42 (s, 9H).
^{13}C NMR (126 MHz, $CDCl_3$) δ 161.4, 158.3, 158.2, 146.7, 136.2, 134.4, 132.7, 132.6, 129.3, 129.2, 128.1, 121.6, 113.7, 113.3, 55.4, 55.2, 38.5, 32.0.
APCI-HRMS (positive mode) *m/z* calcd for $C_{35}H_{35}O_3^+$ (M+H$^+$): 503.2581; found: 503.2547.

Compound 1d, 2-(*tert*-butyl)-7-(6-(*tert*-butyl)-1,3-bis(4-(*tert*-butyl)phenyl)azulen-2-yl)pyrene



Diiodoazulene **7c** (90 mg, 0.130 mmol), 4-*tert*-butylphenylboronic acid (69 mg, 0.390 mmol), Pd(dppf)Cl_2·CH_2Cl_2 (2.9 mg, 0.0039 mmol), Cs_2CO_3 (85 mg, 0.260 mmol), 10 mL of 1,4-dioxane and 1 mL of water were used according to the procedure for **1a**. Reaction at 80 °C for 20 h, purification: silica gel column (hexane/CH_2Cl_2, *v*/*v*, 10/1), then GPC ($CHCl_3$). Green solid (44 mg, 0.062 mmol), yield: 48%.
^{1}H NMR (500 MHz, $CDCl_3$) δ 8.40 (d, *J* = 11.0 Hz, 2H), 8.13 (s, 2H), 7.90 (d, *J* = 9.0 Hz, 2H), 7.78 (s, 2H), 7.68 (d, *J* = 9.0 Hz, 2H), 7.31 (d, *J* = 11.0 Hz, 2H), 7.25 (d, J=8.6 Hz, 4H), 7.21 (d, *J* = 8.6 Hz, 4H), 1.55 (s, 9H), 1.46 (s, 9H), 1.29 (s, 18H).
^{13}C NMR (126 MHz, $CDCl_3$) δ 162.0, 149.1, 149.0, 147.3, 136.3, 135.2, 134.5, 133.5, 131.4, 131.2, 130.4, 129.3, 128.4, 127.7, 127.1, 125.0, 123.4, 122.9, 122.0, 121.8, 38.6, 35.3, 34.6, 32.1, 32.0, 31.5.
APCI-HRMS (positive mode) *m/z* calcd for $C_{54}H_{57}^+$ (M+H$^+$): 705.4455; found: 705.4449.

Compound 1e, 7,7'-(6-(*tert*-butyl)-2-(4-(*tert*-butyl)phenyl)azulene-1,3-diyl)bis(2-(*tert*-butyl)pyrene)



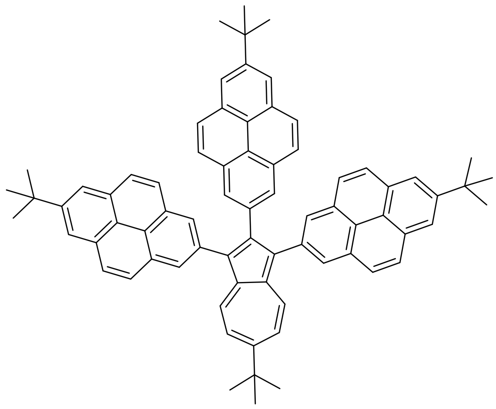
Diiodoazulene **7a** (100 mg, 0.176 mmol), 2-(7-(*tert*-butyl)pyren-2-yl)-4,4,5,5-tetramethyl-1,3,2-dioxaborolane (203 mg, 0.528 mmol), Pd(dppf)Cl_2·CH_2Cl_2 (3.9 mg, 0.0053 mmol), Cs_2CO_3 (115 mg, 0.352 mmol), 10 mL of 1,4-dioxane and 1 mL of water were used according to the procedure for **1a.** Reaction at 80°C for 24 h, purification: silica gel column (hexane/CH_2Cl_2, *v*/*v*, 10/1), then SEC (BioBeads SX-1, CH_2Cl_2). Blue solid (59 mg, 0.071 mmol), yield: 40%.

^{1}H NMR (500 MHz, $CDCl_3$) δ 8.46 (d, J = 11.1 Hz, 2H), 8.23 (s, 4H), 8.15 (s, 4H), 8.04 (d, J = 8.9 Hz, 4H), 7.97 (d, J = 8.9 Hz, 4H), 7.36 (d, J = 11.1 Hz, 2H), 6.96 (d, J = 8.5 Hz, 2H), 6.87 (d, J = 8.6 Hz, 2H), 1.61 (s, 18H), 1.46 (s, 9H), 1.09 (s, 9H).

^{13}C NMR (126 MHz, $CDCl_3$, 300 K) δ 162.0, 149.4, 149.0, 148.4, 137.0, 135.0, 134.4, 133.4, 131.3, 131.2, 131.0, 129.0, 128.3, 127.6, 127.6, 124.6, 123.4, 123.1, 122.5, 122.3, 38.7, 35.4, 34.5, 32.1, 32.0, 31.2.

APCI-HRMS (positive mode) *m*/*z* calcd for $C_{64}H_{60}^+$ (M+H$^+$): 828.4689; found: 828.4634.

Compound 1f, 7,7',7''-(6-(*tert*-butyl)azulene-1,2,3-triyl)tris(2-(*tert*-butyl)pyrene)



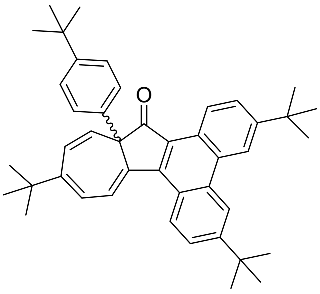
Diiodoazulene **7c** (100 mg, 0.144 mmol), 2-(7-(*tert*-butyl)pyren-2-yl)-4,4,5,5-tetramethyl-1,3,2-dioxaborolane (166 mg, 0.433 mmol), Pd(dppf)Cl_2·CH_2Cl_2 (3.2 mg, 0.0043 mmol), Cs_2CO_3 (141 mg, 0.433 mmol), 10 mL of 1,4-dioxane and 1 mL of water were used according to the procedure for **1a**. Reaction at 80 °C for 20 h, purification: silica gel column (hexane to hexane/CH_2Cl_2, *v*/*v*, 1/1), then SEC (BioBeads SX-1, CH_2Cl_2). Green solid (63 mg, 0.066 mmol), yield: 46%.

^{1}H NMR (500 MHz, $CDCl_3$) δ 8.56 (d, *J* = 11.0 Hz, 2H), 8.18 (s, 4H), 8.17 (s, 4H), 8.01 (s, 2H), 7.95 (d, *J* = 9.0 Hz, 4H), 7.88 (s, 2H), 7.84 (d, *J* = 9.0 Hz, 4H), 7.67 (d, *J* = 9.0 Hz, 2H), 7.41 (d, *J* = 11.0 Hz, 2H), 7.37 (d, *J* = 9.0 Hz, 2H), 1.58 (s, 18H), 1.49 (s, 9H), 1.48 (s, 9H).

^{13}C NMR (126 MHz, $CDCl_3$) δ 162.5, 149.0, 149.0, 147.9, 137.3, 135.4, 134.2, 133.9, 131.1, 131.0, 130.5, 129.5, 128.5, 128.3, 127.7, 127.6, 127.6, 127.1, 123.4, 123.4, 123.1, 122.7, 122.7,

122.3, 122.0, 38.8, 35.4, 35.3, 32.1, 32.0, 32.0. (one aromatic signal missing due to overlapping).
APCI-HRMS (positive mode) *m/z* calcd for $C_{73}H_{63}^+$ ($M+H^+$): 939.4924; found: 939.5025.

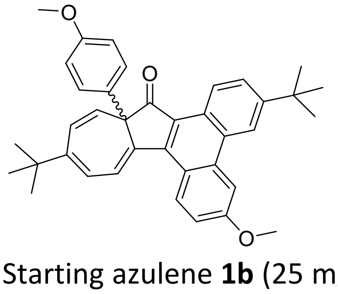
Compound 3a, 3,6,11-tri-*tert*-butyl-13*a*-(4-(*tert*-butyl)phenyl)azuleno[1,2-*l*]phenanthren-14(13*a*H)-one



Starting azulene **1a** (10 mg, 0.017 mmol) and 48 mg of K_2CO_3 (0.344 mmol) were placed in a screw-sealed vial and then 1 mL of dry 1,2-dichloroethane was added. The mixture was bubbled with N_2 and then 22 mg (0.138 mmol) of dry $FeCl_3$ in 0.4 mL of dry nitromethane was added to the reaction mixture. Vial was tightly closed and reaction mixture was stirred for 16 h at 80 °C. Solvent was removed under reduced pressure and mixture was passed through short silica column (hexane) yielding product as yellow solid (9.7 mg, 0.016 mmol). Yield: 93%

^{1}H NMR (500 MHz, $CDCl_3$) δ 9.16 (d, *J* = 8.7 Hz, 1H), 8.77 (d, *J* = 11.0 Hz, 1H), 8.77 (s, 1H), 8.63 (d, *J* = 1.7 Hz, 1H), 7.80 (dd, *J* = 8.7, 2.0 Hz, 1H), 7.72 (dd, *J* = 8.7, 1.8 Hz, 1H), 7.55 (d, *J* = 7.0 Hz, 1H), 7.15 – 7.11 (m, 2H), 7.09 – 7.06 (m, 2H), 6.63 (d, *J* = 10.1 Hz, 1H), 6.46 (d, *J* = 10.1 Hz, 1H), 6.40 (d, *J* = 6.9 Hz, 1H), 1.55 (s, 9H), 1.49 (s, 9H), 1.19 (s, 9H), 0.99 (s, 9H).
^{13}C NMR (126 MHz, $CDCl_3$) δ 204.8, 154.5, 152.7, 150.8, 149.4, 148.0, 137.4, 135.7, 132.0, 131.2, 128.7, 128.3, 127.1, 127.0, 126.7, 126.0, 125.9, 125.8, 125.7, 124.2, 123.8, 122.8, 119.7, 118.1, 60.7, 36.3, 35.6, 35.5, 34.4, 31.5, 31.4, 30.1, 29.8.
APCI-HRMS (positive mode) *m/z* calcd for $C_{44}H_{51}O^+$ ($M+H^+$): 595.3934; found: 595.3974.

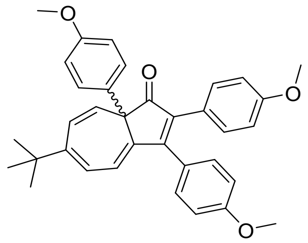
Compound 3b, 3,11-di-*tert*-butyl-6-methoxy-13*a*-(4-methoxyphenyl)azuleno[1,2-*l*]phenanthren-14(13*a*H)-one



Starting azulene **1b** (25 mg, 0.047 mmol) and 131 mg of K_2CO_3 (0.946 mmol) were placed in a Schlenk flask and then 5 mL of dry 1,2-dichloroethane was added. The mixture was bubbled with N_2 and then 123 mg (0.757 mmol) of dry $FeCl_3$ in 1.25 mL of dry nitromethane was added to the reaction mixture. Reaction mixture was stirred at 80 °C for 96 h. Solvent was removed under reduced pressure and mixture was purified using short silica gel column (eluent gradually changed from hexane to CH_2Cl_2) and washed with methanol yielding product as a yellow solid (15 mg, 0.028 mmol). Yield: 58%

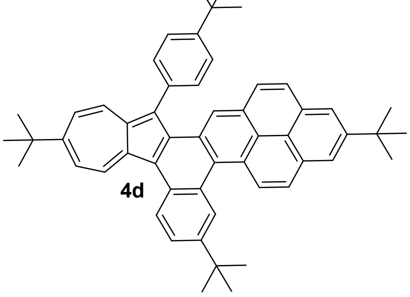
^{1}H NMR (500 MHz, $CDCl_3$) δ 9.16 (d, *J* = 8.7 Hz, 1H), 8.79 (d, *J* = 9.2 Hz, 1H), 8.51 (d, *J* = 1.7 Hz, 1H), 8.16 (d, *J* = 2.6 Hz, 1H), 7.73 (dd, *J* = 8.7, 1.8 Hz, 1H), 7.50 (d, *J* = 7.0 Hz, 1H), 7.34 (dd, *J* = 9.1, 2.6 Hz, 1H), 7.13 (d, *J* = 8.9 Hz, 2H), 6.63 (dd, *J* = 10.6, 8.7 Hz, 3H), 6.44 – 6.39 (m, 2H), 4.09 (s, 3H), 3.69 (s, 3H), 1.48 (s, 9H), 1.03 (s, 9H).
^{13}C NMR (126 MHz, $CDCl_3$) δ 204.5, 160.7, 158.4, 156.1, 154.6, 150.8, 148.1, 137.3, 137.2, 131.9, 131.1, 130.5, 129.0, 128.8, 128.4, 127.1, 127.0, 126.2, 125.9, 123.6, 122.8, 122.5, 118.3, 116.1, 112.9, 106.6, 55.7, 55.3, 36.4, 35.5, 31.5, 30.1.
APCI-HRMS (positive mode) *m/z* calcd for $C_{38}H_{39}O_3^+$ (M+H$^+$): 543.2894; found: 543.2931.

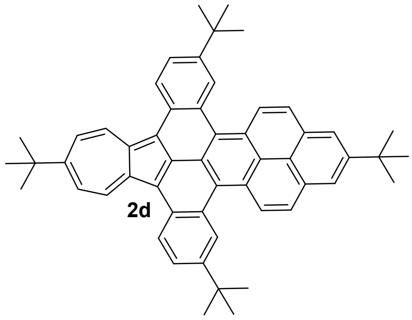
Compound 3c, 11-(*tert*-butyl)-3,6-dimethoxy-13*a*-(4-methoxyphenyl)azuleno[1,2-*l*]phenanthren-14(13*aH*)-one



Starting azulene **1c** (10 mg, 0.020 mmol) and 44 mg of K_2CO_3 (0.318 mmol) were placed in a Schlenk flask and then 2 mL of dry 1,2-dichloroethane was added. The mixture was bubbled with N_2 and then 65 mg (0.398 mmol) of dry $FeCl_3$ in 0.5 mL of dry nitromethane was added to the reaction mixture. Reaction mixture was stirred at 80 °C for 48 h. Solvent was removed under reduced pressure and mixture was passed through short silica column (CH_2Cl_2/hexane, *v*/*v*, 5/2) yielding product as a yellow solid (3 mg, 0.0058 mmol). Yield: 29%
^{1}H NMR (500 MHz, $CDCl_3$) δ 7.28 (d, J = 8.8 Hz, 2H), 7.20 (d, J = 8.9 Hz, 2H), 7.17 (d, J = 9.0 Hz, 2H), 6.95 (d, J = 8.8 Hz, 2H), 6.72 (d, J = 4.7 Hz, 2H), 6.70 (d, J = 4.6 Hz, 2H), 6.53 (d, J = 10.3 Hz, 1H), 6.38 (d, J = 10.4 Hz, 1H), 6.34 (d, J = 6.9 Hz, 1H), 6.20 (d, J = 6.9 Hz, 1H), 3.86 (s, 3H), 3.75 (s, 3H), 3.74 (s, 3H), 0.96 (s, 9H).
^{13}C NMR (126 MHz, $CDCl_3$) δ 204.9, 162.5, 160.2, 159.3, 158.5, 154.5, 141.7, 135.1, 132.4, 131.5, 131.3, 130.9, 130.5, 128.9, 128.1, 126.2, 123.9, 122.6, 122.0, 114.3, 113.6, 113.1, 55.5, 55.4, 55.3, 36.5, 30.0.
APCI-HRMS (positive mode) *m/z* calcd for $C_{35}H_{35}O_4^+$ (M+H$^+$): 519.2523; found: 519.2523.

Compound 4d: 4,9,14-tri-*tert*-butyl-17-(4-(*tert*-butyl)phenyl)azuleno[2,1-*k*]dibenzo[*m*,*pqr*]tetraphene and compound 2d: 2,7,12,17-tetra-*tert*-butylazuleno[1,2,3-*cd*]tribenzo[*a*,*f*,*lm*]perylene





Starting azulene **1d** (10 mg, 0.014 mmol) and 31 mg of K_2CO_3 (0.227 mmol) were placed in a Schlenk flask and then 2 mL of dry 1,2-dichloroethane was added. The mixture was bubbled with N_2 and then 18 mg (0.113 mmol) of dry $FeCl_3$ in 0.4 mL of dry nitromethane was added to the reaction mixture. Reaction mixture was stirred for 24 h at room temperature. Solvent was removed under reduced pressure and mixture was passed through short silica column (hexane/CH_2Cl_2, *v*/*v*, 7/3) and purified using GPC ($CHCl_3$) yielding product **4d** as a green solid (3.0 mg, 0.0043 mmol, yield: 30%) and traces of **2d**. Extension of the reaction time to 7 d followed by the same workup gave **4d** as a green solid (3.0 mg, 0.0043 mmol, yield: 30%) and **2d** as a red solid (3.5 mg, 0.0050 mmol, yield: 36%).

Compound 4d: 4,9,14-tri-tert-butyl-17-(4-(tert-butyl)phenyl)azuleno[2,1-k]dibenzo[m,pqr]tetraphene:

^{1}H NMR (500 MHz, $CDCl_3$) δ 9.38 (d, J = 10.2 Hz, 1H), 9.20 (d, J = 9.3 Hz, 1H), 9.02 (d, J = 2.0 Hz, 1H), 8.92 (d, J = 8.6 Hz, 1H), 8.53 (s, 1H), 8.24 (d, J = 1.7 Hz, 1H), 8.23 (d, J = 2.7 Hz, 1H), 8.21 (s, 1H), 8.16 (d, J = 1.7 Hz, 1H), 7.90 (d, J = 9.0 Hz, 1H), 7.83 (dd, J = 8.5, 2.0 Hz, 1H), 7.70 (d, J = 8.3 Hz, 2H), 7.60 – 7.51 (m, 4H), 7.38 (dd, J = 11.1, 1.9 Hz, 1H), 1.60 (s, 9H), 1.58 (s, 9H), 1.54 (s, 9H), 1.51 (s, 9H).

^{13}C NMR (126 MHz, $CDCl_3$) δ 160.8, 150.7, 149.4, 146.3, 139.7, 137.7, 135.9, 134.6, 134.5, 131.8, 131.3, 130.9, 130.6, 129.1, 129.0, 128.8, 128.5, 128.3, 127.9, 127.6, 127.3, 127.2, 127.0, 126.6, 126.0, 125.3, 125.3, 124.9, 123.9, 123.4, 122.8, 122.6, 122.5, 121.7, 121.3, 120.9, 38.6, 35.4, 35.2, 35.1, 32.1, 32.0, 31.8, 31.7.

APCI-HRMS (positive mode) *m*/*z* calcd for $C_{54}H_{55}^+$ ($M+H^+$): 703.4298; found: 703.4299.

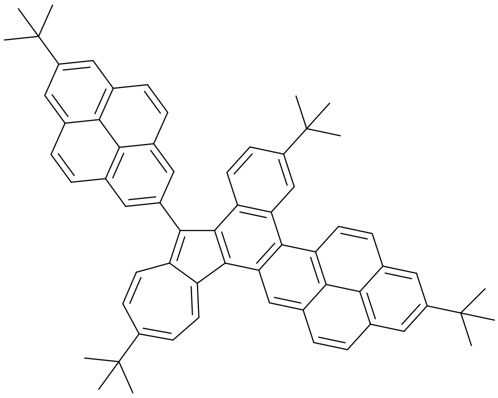
***Compound 2d: 2,7,12,17-tetra-tert-butylazuleno[1,2,3-cd]tribenzo[a,f,lm]perylene*:**

^{1}H NMR (500 MHz, CD_2Cl_2) δ 9.85 (d, *J* = 11.1 Hz, 2H), 9.24 (d, *J* = 10.6 Hz, 2H), 9.24 (s, 2H), 9.15 (d, *J* = 8.6 Hz, 2H), 8.40 (s, 2H), 8.33 (d, *J* = 9.2 Hz, 2H), 7.97 – 7.92 (m, 4H), 1.68 (s, 9H), 1.65 (s, 9H), 1.59 (s, 18H).

^{13}C NMR (151 MHz, CD_2Cl_2) δ 162.3, 150.0, 147.4, 138.3, 135.1, 134.9, 131.7, 130.3, 129.8, 128.8, 127.6, 126.9, 126.6, 126.0, 125.8, 125.4, 124.8, 123.9, 122.7, 122.6, 122.0, 118.3, 39.0, 35.6, 35.5, 32.4, 32.3, 32.1.

APCI-HRMS (positive mode) *m*/*z* calcd for $C_{54}H_{53}^+$ ($M+H^+$): 701.4142; found: 701.4146.

Compound 4e, 2,7,13-tri-*tert*-butyl-10-(7-(*tert*-butyl)pyren-2-yl)azuleno[1,2-*k*]dibenzo[*m*,*pqr*]tetraphene



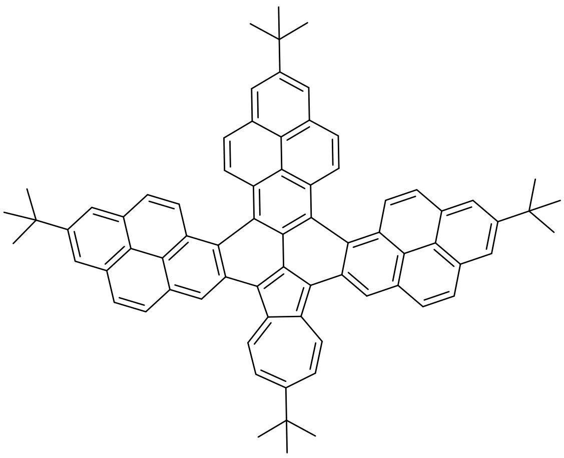
Starting azulene **1e** (35 mg, 0.042 mmol) and 117 mg of K_2CO_3 (0.844 mmol) were placed in a Schlenk flask and then 7 mL of dry 1,2-dichloroethane was added. The mixture was chilled in an ice bath and bubbled with N_2. Then 110 mg (0.675 mmol) of dry $FeCl_3$ in 1.75 mL of dry nitromethane was added to the reaction mixture. Reaction mixture was stirred for 18 h at room temperature. Solvent was removed under reduced pressure and mixture was passed through short silica column (hexane/CH_2Cl_2, *v*/*v*, 1/1) and purified using GPC ($CHCl_3$) yielding product as green solid (11 mg, 0.013 mmol). Yield: 32%

^{1}H NMR (500 MHz, $CDCl_3$) δ 9.72 – 9.68 (m, 2H), 9.20 (d, *J* = 9.3 Hz, 1H), 9.01 (d, *J* = 1.4 Hz, 1H), 8.46 (s, 2H), 8.35 – 8.25 (m, 7H), 8.18 – 8.13 (m, 5H), 7.74 (d, *J* = 8.6 Hz, 2H), 7.39 (dd, *J* = 11.1, 1.5 Hz, 1H), 7.15 (d, *J* = 8.7 Hz, 1H), 1.65 (s, 9H), 1.64 (s, 9H), 1.53 (s, 9H), 1.37 (s, 9H).

^{13}C NMR (126 MHz, $CDCl_3$) δ 160.9, 149.4, 149.1, 149.1, 140.3, 138.9, 136.3, 135.8, 134.8, 134.4, 131.8, 131.7, 131.5, 131.5, 131.3, 130.6, 130.3, 128.7, 128.2, 128.1, 128.0, 127.8, 127.8, 127.7, 127.7, 127.1, 126.9, 126.5, 125.3, 124.2, 124.1, 123.5, 123.4, 123.4, 123.2, 122.8, 122.7, 122.3, 122.0, 121.9, 120.5, 120.4, 38.6, 35.5, 35.4, 35.3, 32.2, 32.1, 32.0, 31.5.

APCI-HRMS (positive mode) *m*/*z* calcd for $C_{64}H_{59}^+$ (M+H$^+$): 827.4611; found: 827.4675.

Compound 2f, 2,9,16,23-tetra-*tert*-butylazuleno[1,2,3-*hi*]dinaphtho[8,1,2-*pqr*:2',1',8'-*yza*]pyreno[1,2,3-*uv*]hexacene



Starting azulene **1f** (12 mg, 0.013 mmol) and 35 mg of K_2CO_3 (0.252 mmol) were placed in a screw-sealed vial and then 2 mL of dry 1,2-dichloroethane was added. The mixture was bubbled with N_2 and the 33 mg (0.201 mmol) of dry $FeCl_3$ in 0.5 mL of dry nitromethane was added to the reaction mixture. Vial was tightly closed, and reaction mixture was stirred for 16 h at 80 °C. Solvent was removed under reduced pressure and mixture was passed through short silica column (hexane/CH_2Cl_2, *v*/*v*, 1/1) and purified using preparative TLC (hexane/CH_2Cl_2, *v*/*v*, 5/1) yielding product as a brown solid (5.7 mg, 0.006 mmol). Yield: 46%

^{1}H NMR (500 MHz, $CDCl_3$) δ 9.93 (d, *J* = 11.1 Hz, 2H), 9.69 (s, 2H), 8.72 (d, *J* = 9.5 Hz, 2H), 8.59 (d, *J* = 9.5 Hz, 2H), 8.39 (d, *J* = 8.9 Hz, 2H), 8.30 (dd, *J* = 9.1, 1.7 Hz, 4H), 8.26 (s, 2H), 8.22 (d, *J* = 8.9 Hz, 2H), 8.06 (d, *J* = 9.4 Hz, 2H), 8.02 – 7.98 (m, 4H), 1.69 (s, 9H), 1.66 (s, 18H), 1.62 (s, 9H).
^{13}C NMR (151 MHz, CD_2Cl_2) δ 162.4, 150.1, 149.6, 141.6, 135.5, 135.2, 131.9, 131.7, 131.4, 131.2, 130.8, 130.4, 129.1, 129.0, 128.7, 128.2, 128.1, 127.5, 127.3, 127.1, 125.1, 124.8, 123.9, 123.4, 123.3, 123.2, 123.1, 122.8, 122.7, 121.0, 117.2, 39.0, 35.6, 35.5, 32.2, 32.1, 32.0.
APCI-HRMS (positive mode) *m*/*z* calcd for $C_{74}H_{61}^+$ (M+H$^+$): 949.4768; found: 949.4730.

X-ray crystallography

Table S1. Detail of X-ray crystallography experiment of **1a**.

Crystal data CCDC 2371234	
Chemical formula	$C_{44}H_{52}$
M_r	580.85
Crystal system, space group	Monoclinic, $P2_1/c$
Temperature (K)	100
a, *b*, *c* (Å)	11.333 (2), 14.004 (3), 22.087 (5)
β (°)	96.66 (3)
V (Å^3)	3481.7 (13)
Z	4
Radiation type	Cu $K\alpha$
μ (mm^{-1})	0.46
Crystal size (mm)	0.15 × 0.14 × 0.08
Data collection	
Diffractometer	XtaLAB Synergy R, DW system, HyPix-Arc 150
Absorption correction	–
No. of measured, independent and observed [$I > 2\sigma(I)$] reflections	63206, 7210, 6176
R_{int}	0.024
$(\sin \theta/\lambda)_{max}$ (Å^{-1})	0.628
Refinement	
$R[F^2 > 2\sigma(F^2)]$, $wR(F^2)$, S	0.040, 0.107, 1.03
No. of reflections	7210
No. of parameters	409
H-atom treatment	H-atom parameters constrained
$\Delta\rho_{max}$, $\Delta\rho_{min}$ (e Å^{-3})	0.19, −0.21

Table S2. Detail of X-ray crystallography experiment of **3a**.

Crystal data CCDC 2371233	
Chemical formula	$C_{44}H_{50}O$
M_r	594.84
Crystal system, space group	Orthorhombic, $P2_12_12_1$
Temperature (K)	100
a, *b*, *c* (Å)	10.365 (2), 30.398 (6), 33.663 (6)
V (Å^3)	10606 (3)
Z	12
Radiation type	Mo *K*α
μ (mm^{-1})	0.06
Crystal size (mm)	0.33 × 0.25 × 0.12
Data collection	
Diffractometer	Xcalibur, Ruby, Gemini ultra
Absorption correction	–
No. of measured, independent and observed [$I > 2\sigma(I)$] reflections	37324, 21232, 10374
R_{int}	0.087
$(\sin \theta/\lambda)_{max}$ (Å^{-1})	0.679
Refinement	
$R[F^2 > 2\sigma(F^2)]$, $wR(F^2)$, S	0.091, 0.204, 1.00
No. of reflections	21232
No. of parameters	1252
H-atom treatment	H-atom parameters constrained
$\Delta\rho_{max}$, $\Delta\rho_{min}$ (e Å^{-3})	0.38, −0.33
Absolute structure	Flack x determined using 2308 quotients [(I+)-(I-)]/[(I+)+(I-)] (Parsons, Flack and Wagner, Acta Cryst. B69 (2013) 249-259).
Absolute structure parameter	−0.9 (10)

Table S3. Detail of X-ray crystallography experiment of **4e**.

Crystal data CCDC 2371235	
Chemical formula	$C_{64}H_{58}\cdot 1.5(C_6H_4Cl_2)$
M_r	1047.59
Crystal system, space group	Triclinic, *P*1
Temperature (K)	100
a, *b*, *c* (Å)	10.287 (2), 15.743 (3), 18.493 (4)
α, β, γ (°)	112.04 (3), 98.31 (3), 90.23 (3)
V ($Å^3$)	2741.4 (11)
Z	2
Radiation type	Cu *K*α
μ (mm^{-1})	1.85
Crystal size (mm)	0.27 × 0.20 × 0.12
Data collection	
Diffractometer	XtaLAB Synergy R, DW system, HyPix-Arc 150
Absorption correction	Multi-scan *CrysAlis PRO* 1.171.43.105a (Rigaku Oxford Diffraction, 2024) Empirical absorption correction using spherical harmonics, implemented in SCALE3 ABSPACK scaling algorithm.
T_{min}, T_{max}	0.846, 1.000
No. of measured, independent and observed [$I > 2\sigma(I)$] reflections	68595, 11179, 10382
R_{int}	0.021
$(\sin \theta/\lambda)_{max}$ ($Å^{-1}$)	0.629
Refinement	
$R[F^2 > 2\sigma(F^2)]$, $wR(F^2)$, S	0.042, 0.117, 1.03
No. of reflections	11179
No. of parameters	739
H-atom treatment	H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$, $\Delta\rho_{min}$ (e $Å^{-3}$)	0.68, −0.53

UV/Vis/NIR spectroscopy

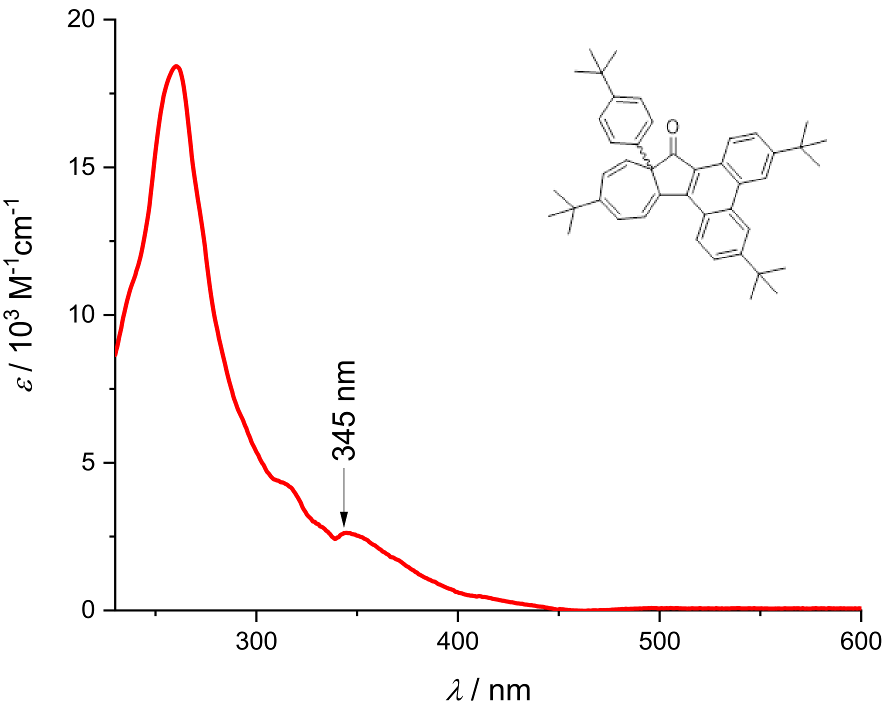


Figure S1. UV/Vis spectrum of compound **3a** (CH_2Cl_2, c~ 10^{-6} M).

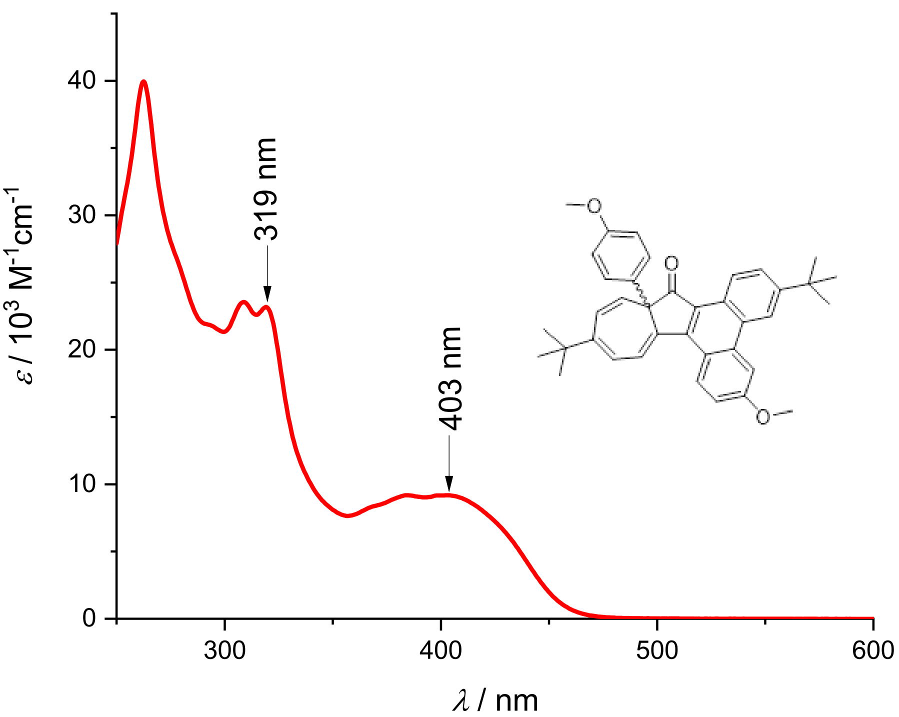


Figure S2. UV/Vis spectrum of compound **3b** (CH_2Cl_2, c~ 10^{-6} M).

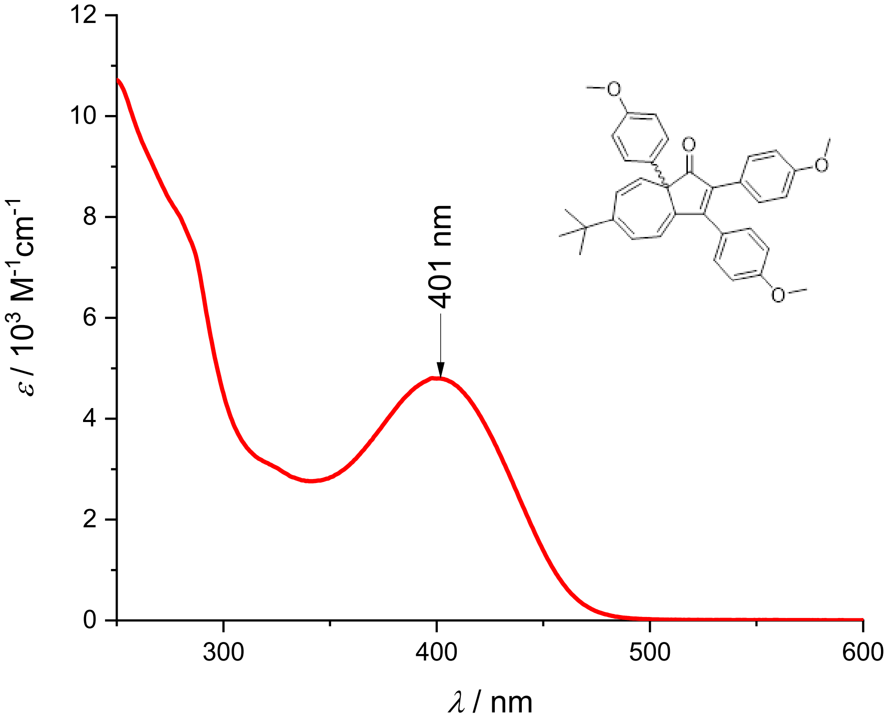


Figure S3. UV/Vis spectrum of compound **3c** (CH_2Cl_2, *c*~ 10^{-6} M).

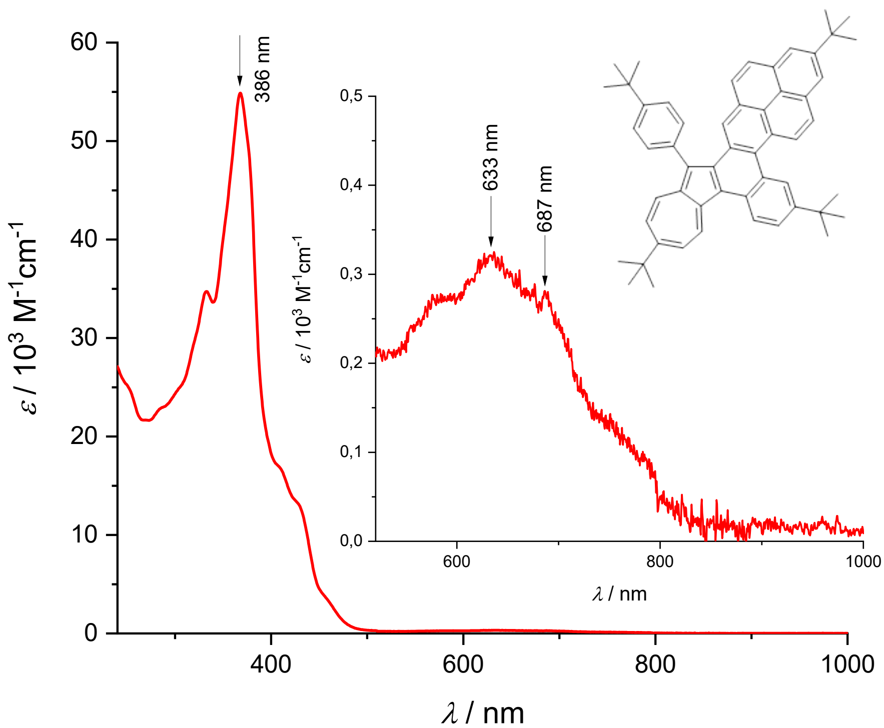


Figure S4. UV/Vis spectrum of compound **4d** (CH_2Cl_2, *c*~ 10^{-6} M).

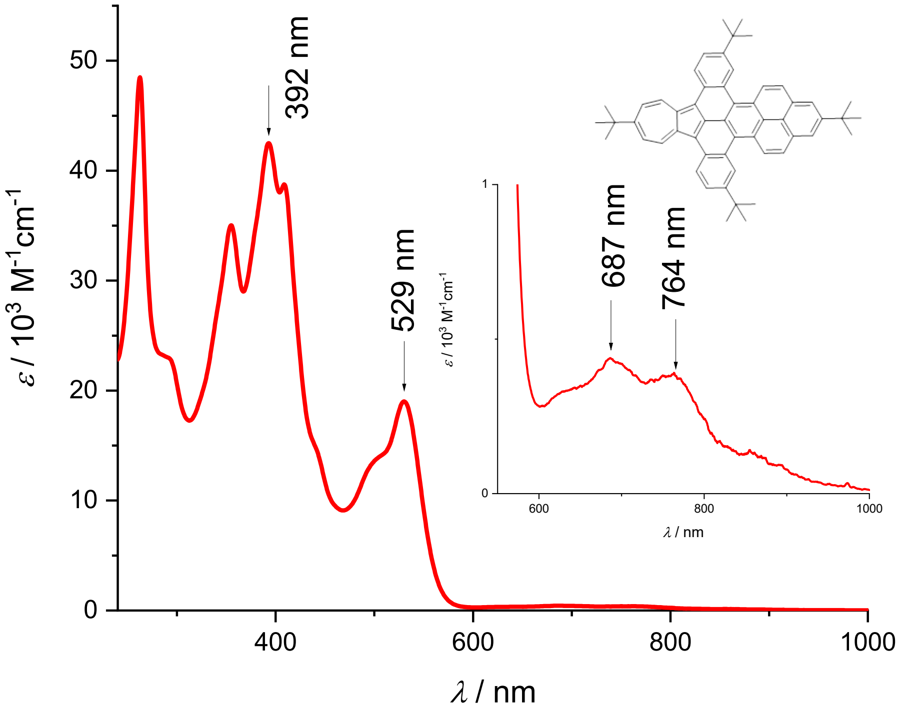


Figure S5. UV/Vis spectrum of compound **2d** (CH_2Cl_2, *c*~ 10^{-6} M).

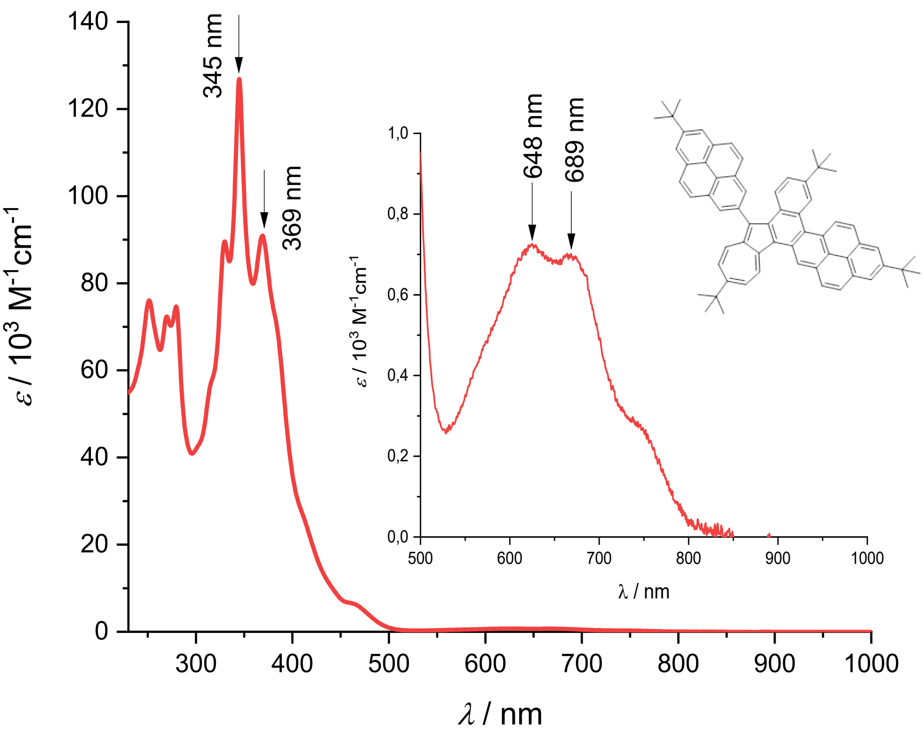


Figure S6. UV/Vis/NIR spectrum of compound **4e** (CH_2Cl_2, *c*~ 10^{-6} M).

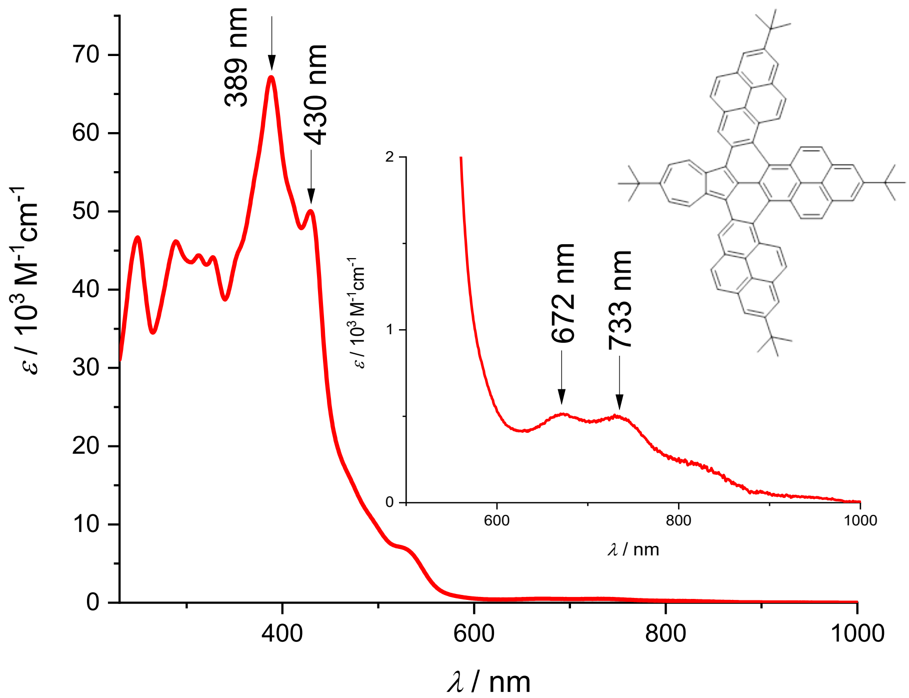


Figure S7. UV/Vis/NIR spectrum of compound **2f** (CH_2Cl_2, c~ 10^{-6} M).

Electrochemistry

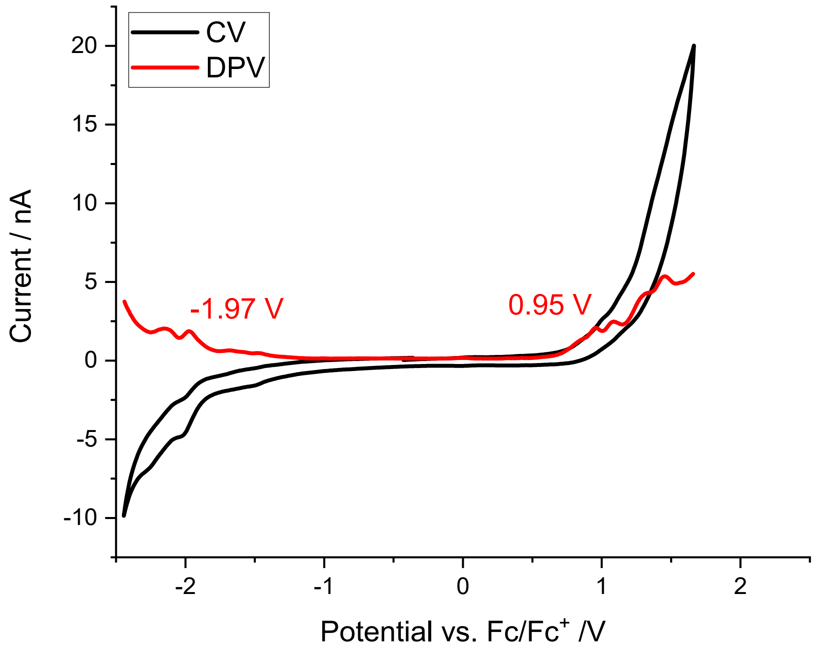


Figure S8. CV (black) and DPV (red) of compound **3a** ($[NBu_4][PF_6]$ in CH_2Cl_2 (0.1 M) as a supporting electrolyte, 50 mV/s scanning rate).

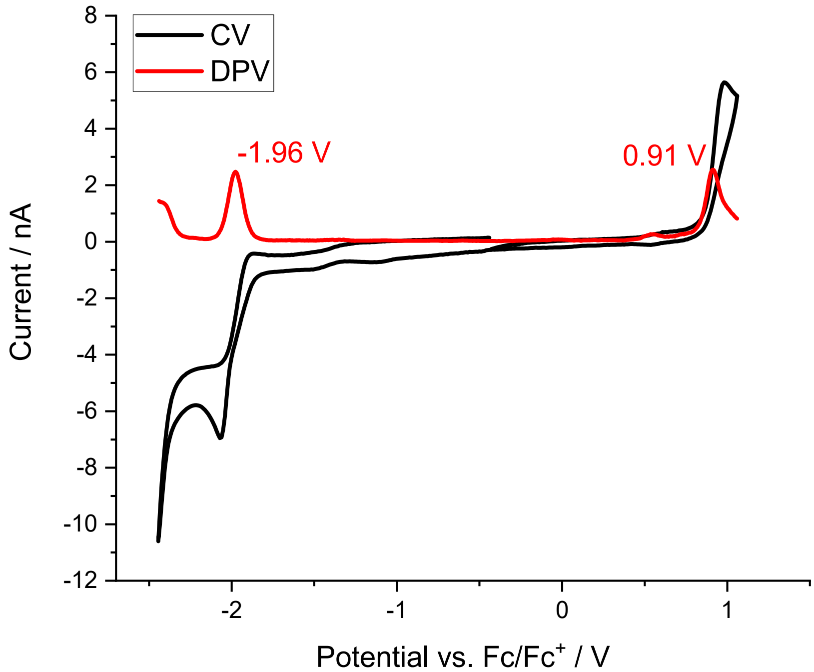


Figure S9. CV (black) and DPV (red) of compound **3b** ($[NBu_4][PF_6]$ in CH_2Cl_2 (0.1 M) as a supporting electrolyte, 50 mV/s scanning rate).

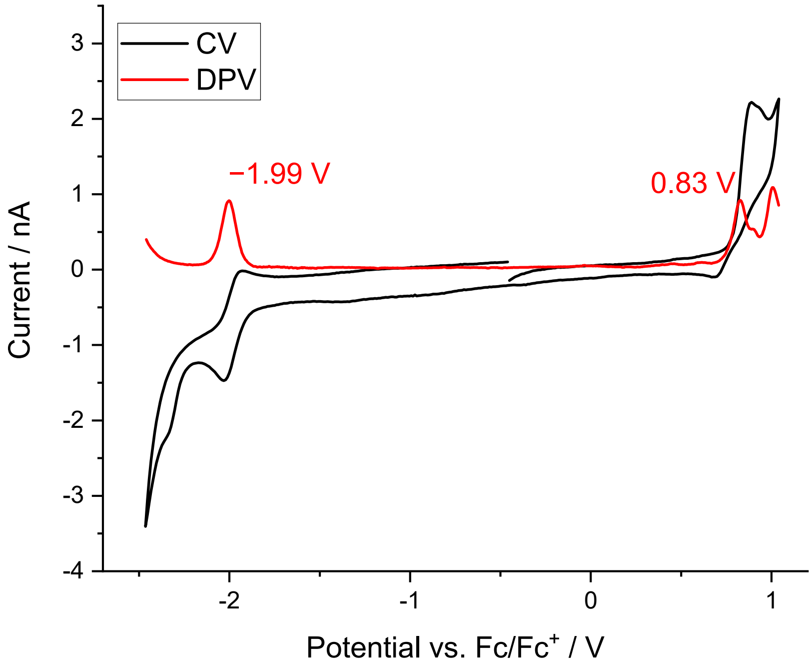


Figure S10. CV (black) and DPV (red) of compound **3c** ([NBu_4][PF_6] in CH_2Cl_2 (0.1 M) as a supporting electrolyte, 50 mV/s scanning rate).

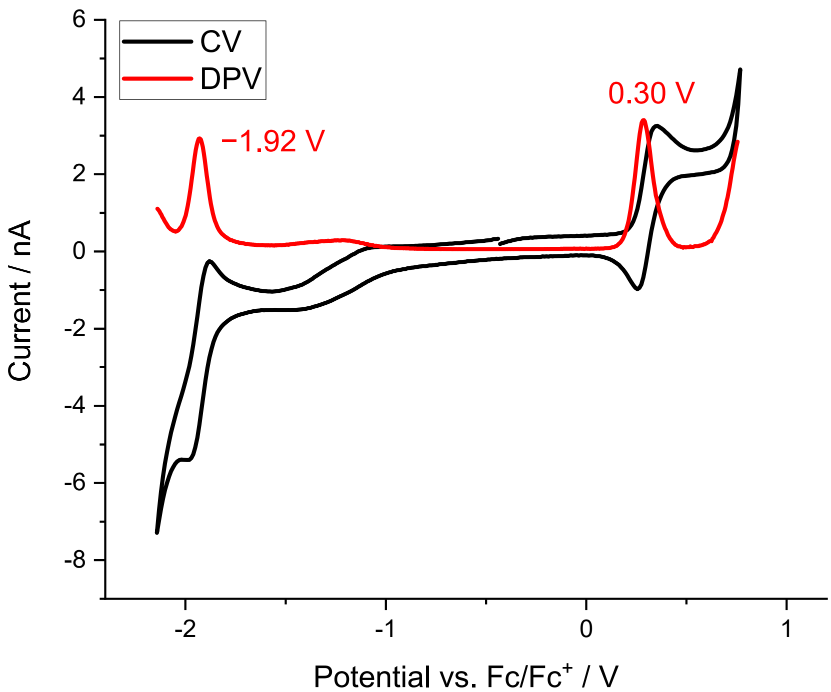


Figure S11. CV (black) and DPV (red) of compound **4d** ([NBu_4][PF_6] in CH_2Cl_2 (0.1 M) as a supporting electrolyte, 50 mV/s scanning rate).

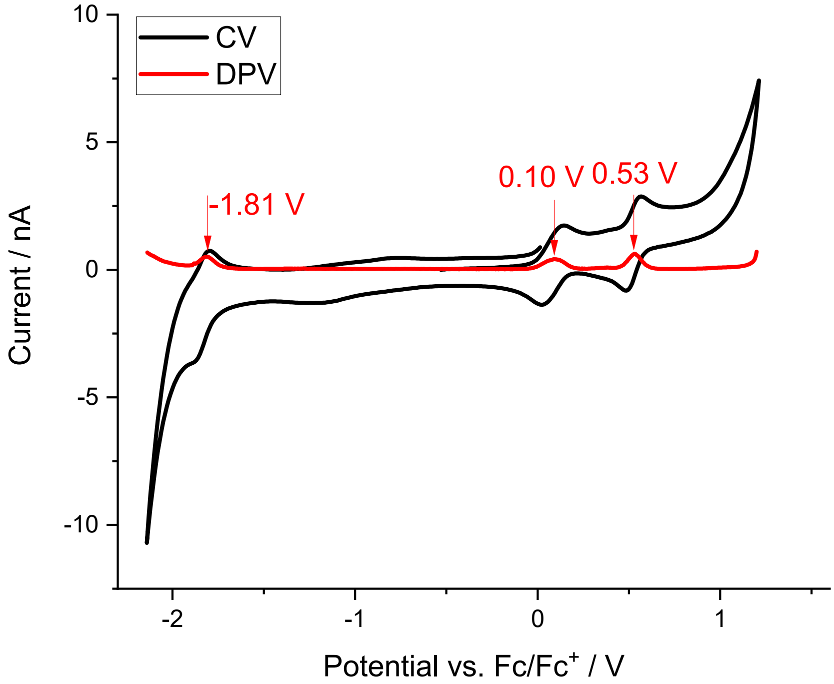


Figure S12. CV (black) and DPV (red) of compound **2d** ($[NBu_4][PF_6]$ in CH_2Cl_2 (0.1 M) as a supporting electrolyte, 50 mV/s scanning rate).

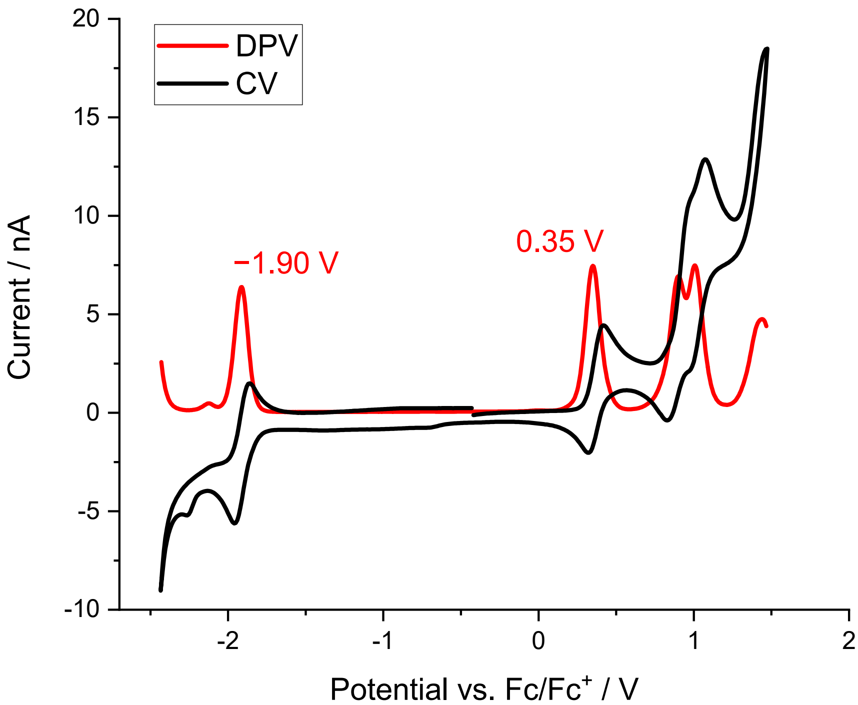


Figure S13. CV (black) and DPV (red) of compound **4e** ($[NBu_4][PF_6]$ in CH_2Cl_2 (0.1 M) as a supporting electrolyte, 50 mV/s scanning rate).

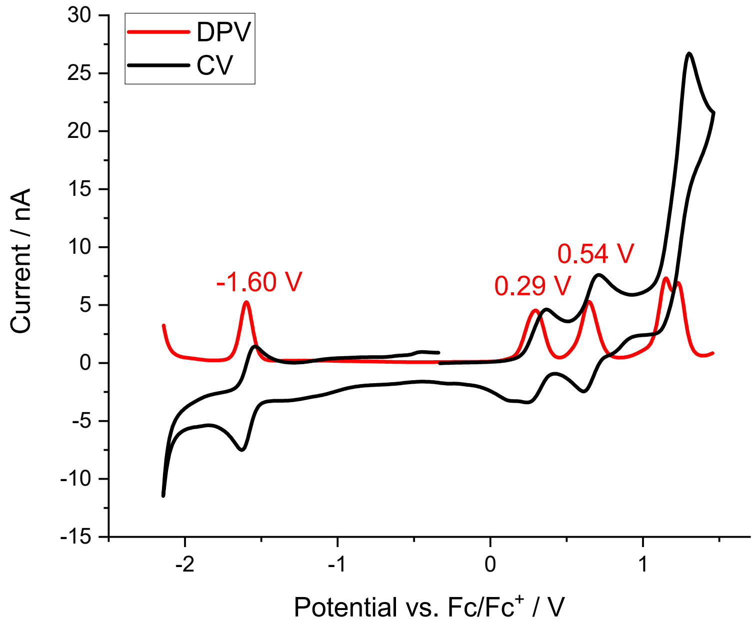


Figure S14. CV (black) and DPV (red) of compound **2f** ($[NEt_4][PF_6]$ in CH_2Cl_2 (0.1 M) as a supporting electrolyte, 50 mV/s scanning rate).

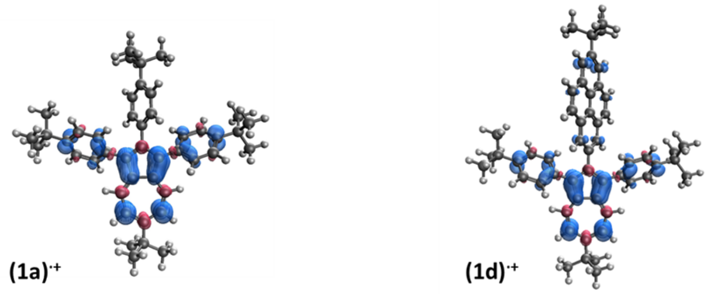
Table S4. Experimental and DFT-calculated HOMO and LUMO levels.

	3a	3b	3c	2d	4d	4e	2f
E_{HOMO} **(DFT)**[a]	−5.45 eV	−5.42 eV	−5.30 eV	−4.67 eV	−4.88 eV	−4.95 eV	−4.75 eV
E_{LUMO} **(DFT)**[a]	−2.28 eV	−2.23 eV	−2.20 eV	−2.18 eV	−2.12 eV	−2.14 eV	−2.25 eV
E_g **(DFT)**	3.17 eV	3.19 eV	3.10 eV	2.49 eV	2.76 eV	2.81 eV	2.50 eV
E_{HOMO} **(EXP)**[b]	−5.71 eV	−5.63 eV	−5.83 eV	−4.90 eV	−5.10 eV	−5.15 eV	−5.09 eV
E_{LUMO} **(EXP)**[b]	−2.84 eV	−2.81 eV	−2.82 eV	−2.99 eV	−2.88 eV	−2.90 eV	−3.20 eV
E_g **(EXP)**	2.92 eV	2.87 eV	2.82 eV	1.91 eV	2.22 eV	2.25 eV	1.89 eV
E_{ox}[c]	0.95 V	0.91 V	0.83 V	0.10 V	0.30 V	0.35 V	0.29 V
E_{red}[c]	−1.97 V	−1.96 V	−1.99 V	−1.81 V	−1.92 V	−1.90 V	−1.60 V

[a]B3LYP/6-31G(d) level of theory; [b]Calculated according to the known procedure using the experimentally determined redox potentials ($E_{LUMO} = -(E_{red} + 4.8$ eV) and $E_{HOMO} = -(E_{ox} + 4.8$ eV)) and the energy level of Fc^+/Fc with respect to the vacuum level (−4.8 eV);[10] [c]Potentials versus Fc/Fc^+ in CH_2Cl_2, 25°C, $[NBu_4][PF_6]$ (0.1 M) as a supporting electrolyte.

DFT calculations

Spin densities of radical cations



	(1a)·+	(1d)·+	(1e)·+	(1f)·+
C1	0.055	0.041	0.024	0.011
C2	0.052	0.053	0.080	0.083
C3	-0.006	0.019	-0.005	0.014
C4	-0.005	0.026	-0.005	0.022
C5	0.065	0.052	0.067	0.091
C6	0.052	0.049	0.039	0.013

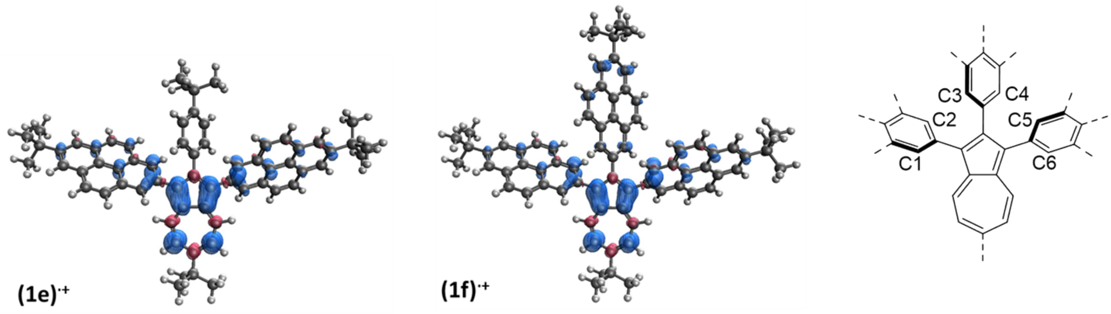


Figure S15. DFT-calculated spin densities of radical cations **(1a)**$^{\cdot+}$, **(1d)**$^{\cdot+}$, **(1e)**$^{\cdot+}$ and **(1f)**$^{\cdot+}$, UB3LYP/6-31G(d).

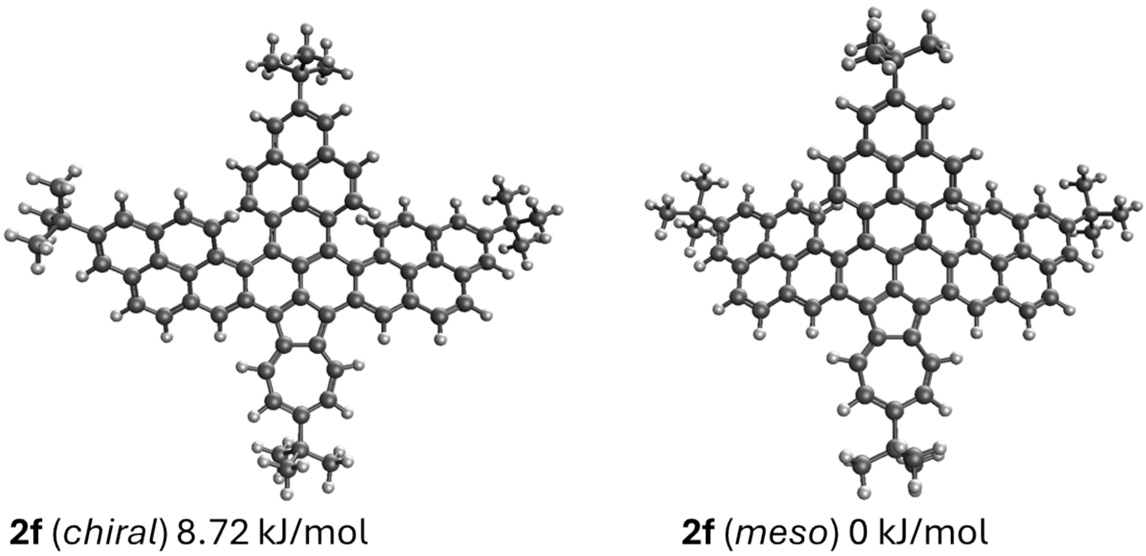


Figure S16. DFT-calculated energy difference between two possible isomers of **2f**: chiral (*P,P* or *M,M*) and *meso* (*P,M*) form, B3LYP/6-31G(d).

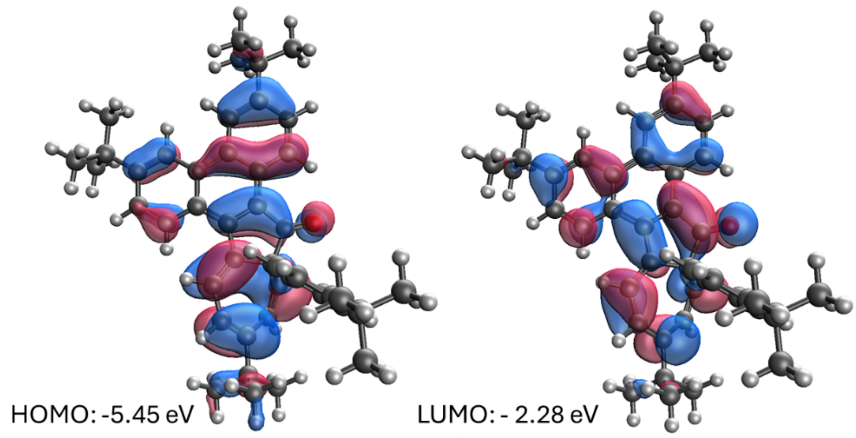


Figure S17. HOMO and LUMO plots of compound **3a**, B3LYP/6-31G(d).

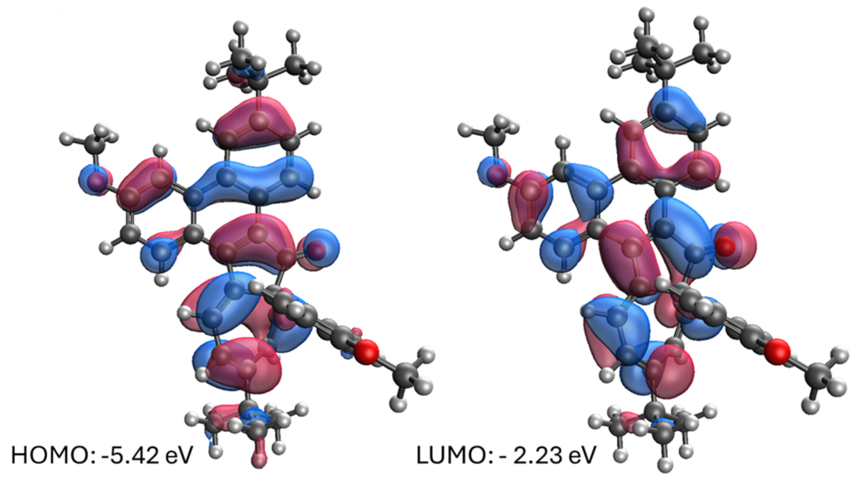


Figure S18. HOMO and LUMO plots of compound **3b**, B3LYP/6-31G(d).

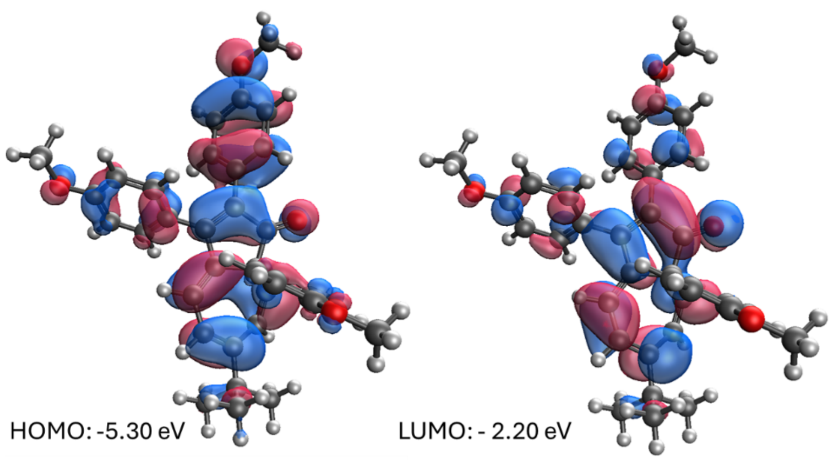


Figure S19. HOMO and LUMO plots of compound **3c**, B3LYP/6-31G(d).

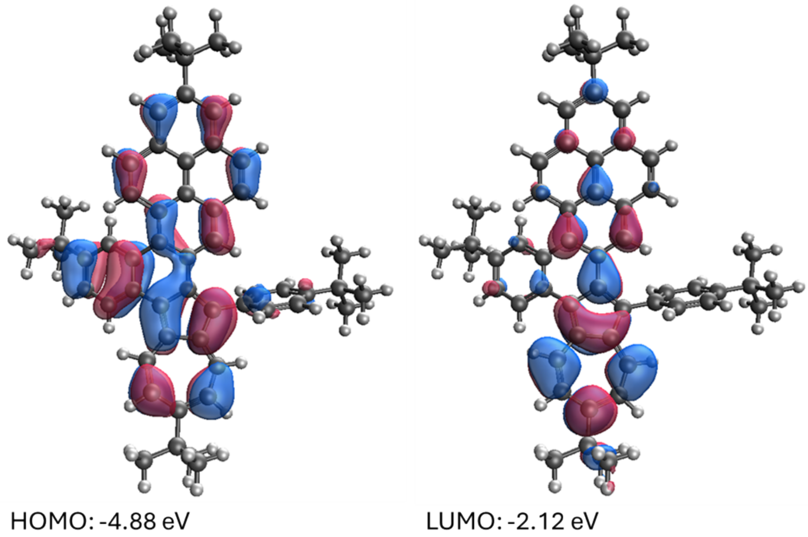


Figure S20. HOMO and LUMO plots of compound **4d**, B3LYP/6-31G(d).

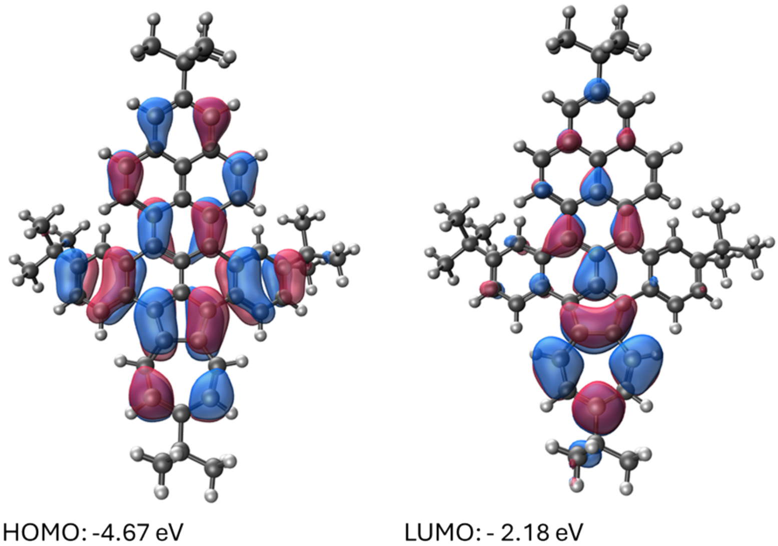


Figure S21. HOMO and LUMO plots of compound **2d**, B3LYP/6-31G(d).

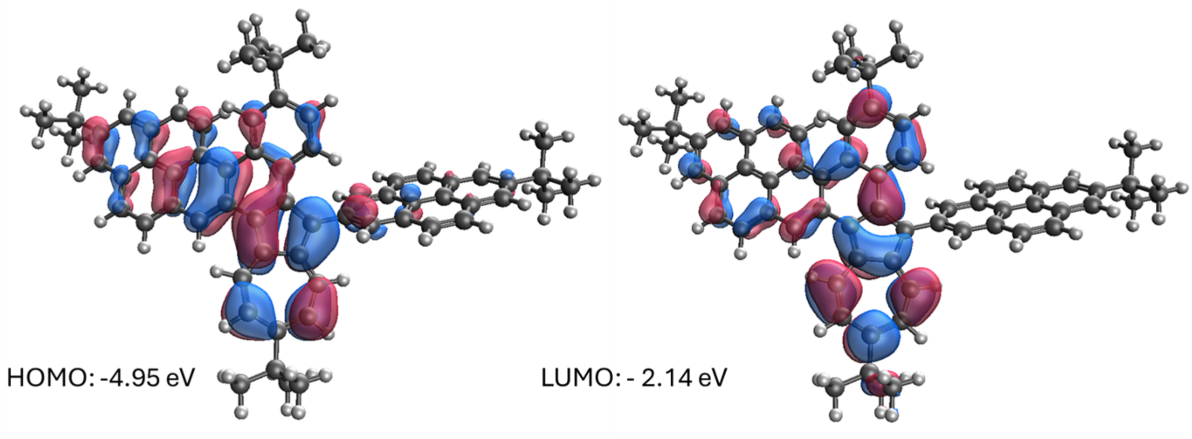


Figure S22. HOMO and LUMO plots of compound **4e**, B3LYP/6-31G(d).

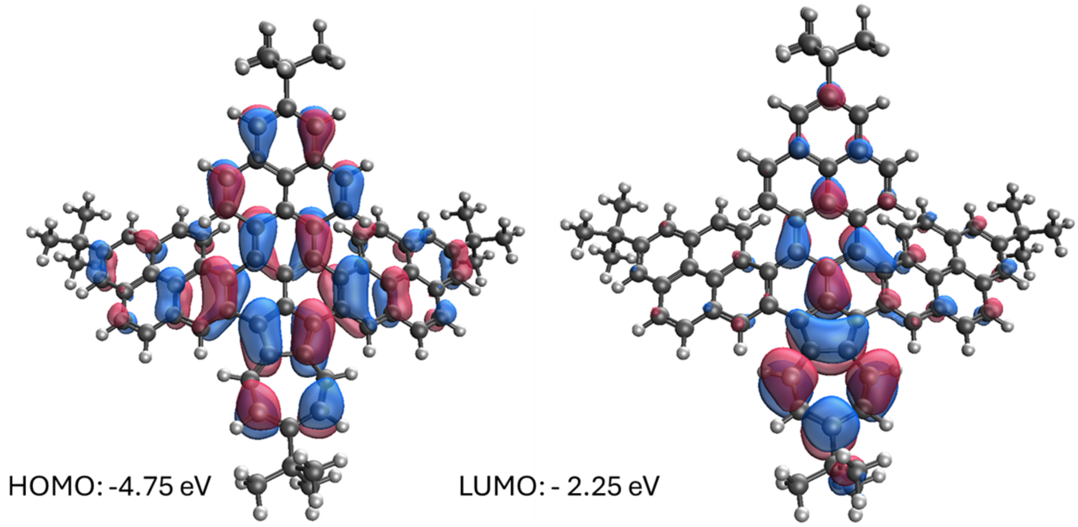


Figure S23. HOMO and LUMO plots of compound **2f**, B3LYP/6-31G(d).

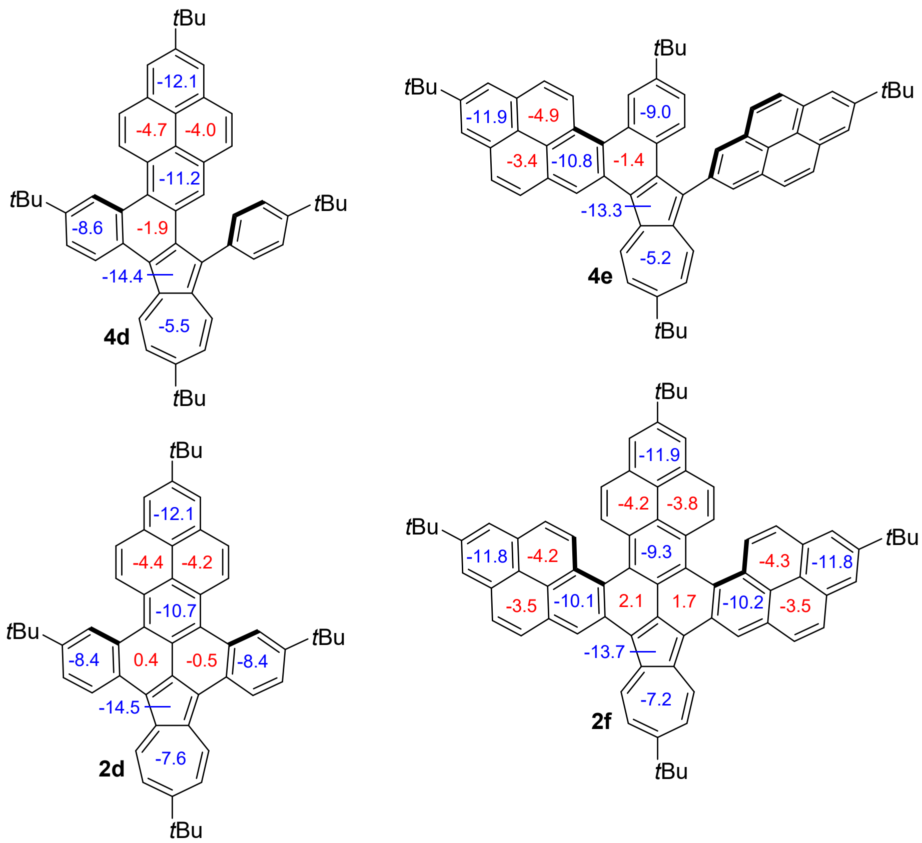


Figure S24. NICS(0) values of compounds **4d**, **2d**, **4e** and **2f**, B3LYP/6-31G(d).

Analysis of electronic transitions

Table S5. Electronic transition contributing to UV/Vis/NIR spectrum of compound **4d**, B3LYP/6-31G(d).

Transition	Energy	Wavelength	Oscillator strength	Contributions
$S_0 \rightarrow S_1$	2.01 eV	617 nm	f= 0.02360	H -> L 92.9%, H-1 -> L 5.2%
$S_0 \rightarrow S_2$	2.63 eV	471 nm	f= 0.30900	H -> L+1 90.4%
$S_0 \rightarrow S_3$	2.69 eV	460 nm	f= 0.01710	H-1 -> L 86.2%
$S_0 \rightarrow S_4$	2.90 eV	427 nm	f= 0.50590	H-2 -> L 68.7%, H -> L+2 26.0%
$S_0 \rightarrow S_5$	3.14 eV	395 nm	f= 1.29340	H-1 -> L+1 78.3%, H -> L+2 10.8%, H-2 -> L 6.1%
$S_0 \rightarrow S_6$	3.27 eV	379 nm	f= 0.11610	H-2 -> L+1 83.9%, H -> L+3 6.5%
$S_0 \rightarrow S_7$	3.31 eV	375 nm	f= 0.64400	H -> L+2 59.1%, H-2 -> L 18.2%, H-1 -> L+1 16.1%
$S_0 \rightarrow S_8$	3.59 eV	345 nm	f= 0.56990	H-1 -> L+2 95.1%
$S_0 \rightarrow S_9$	3.70 eV	335 nm	f= 0.35450	H -> L+3 88.0%, H-2 -> L+1 6.2%
$S_0 \rightarrow S_{10}$	3.72 eV	334 nm	f= 0.11760	H-2 -> L+2 77.5%, H-3 -> L 13.8%

Table S6. Electronic transition contributing to UV/Vis/NIR spectrum of compound **2d**, B3LYP/6-31G(d).

Transition	Energy	Wavelength	Oscillator strength	Contributions
$S_0 \rightarrow S_1$	1.79 eV	692 nm	f= 0.01780	H -> L 95.1%
$S_0 \rightarrow S_2$	2.30 eV	540 nm	f= 0.68030	H -> L+1 95.3%
$S_0 \rightarrow S_3$	2.66 eV	465 nm	f= 0.01810	H-1 -> L 89.8%
$S_0 \rightarrow S_4$	2.74 eV	453 nm	f= 0.06190	H -> L+2 64.1%, H-2 -> L 28.2%
$S_0 \rightarrow S_5$	2.97 eV	418 nm	f= 1.33470	H-1 -> L+1 60.5%, H-2 -> L 31.9%
$S_0 \rightarrow S_6$	3.06 eV	405 nm	f= 0.20060	H-2 -> L+1 73.2%, H -> L+3 9.6%
$S_0 \rightarrow S_7$	3.13 eV	396 nm	f= 0.55430	H-1 -> L+1 30.0%, H-2 -> L 29.6%, H -> L+2 23.7%, H-2 -> L+1 10.4%
$S_0 \rightarrow S_8$	3.43 eV	361 nm	f= 0.52820	H -> L+3 80.2%, H-2 -> L+1 10.5%
$S_0 \rightarrow S_9$	3.49 eV	355 nm	f= 0.50040	H-1 -> L+2 96.5%
$S_0 \rightarrow S_{10}$	3.59 eV	345 nm	f= 0.00920	H-2 -> L+2 85.3%

Table S7. Electronic transition contributing to UV/Vis/NIR spectrum of compound **4e**, B3LYP/6-31G(d).

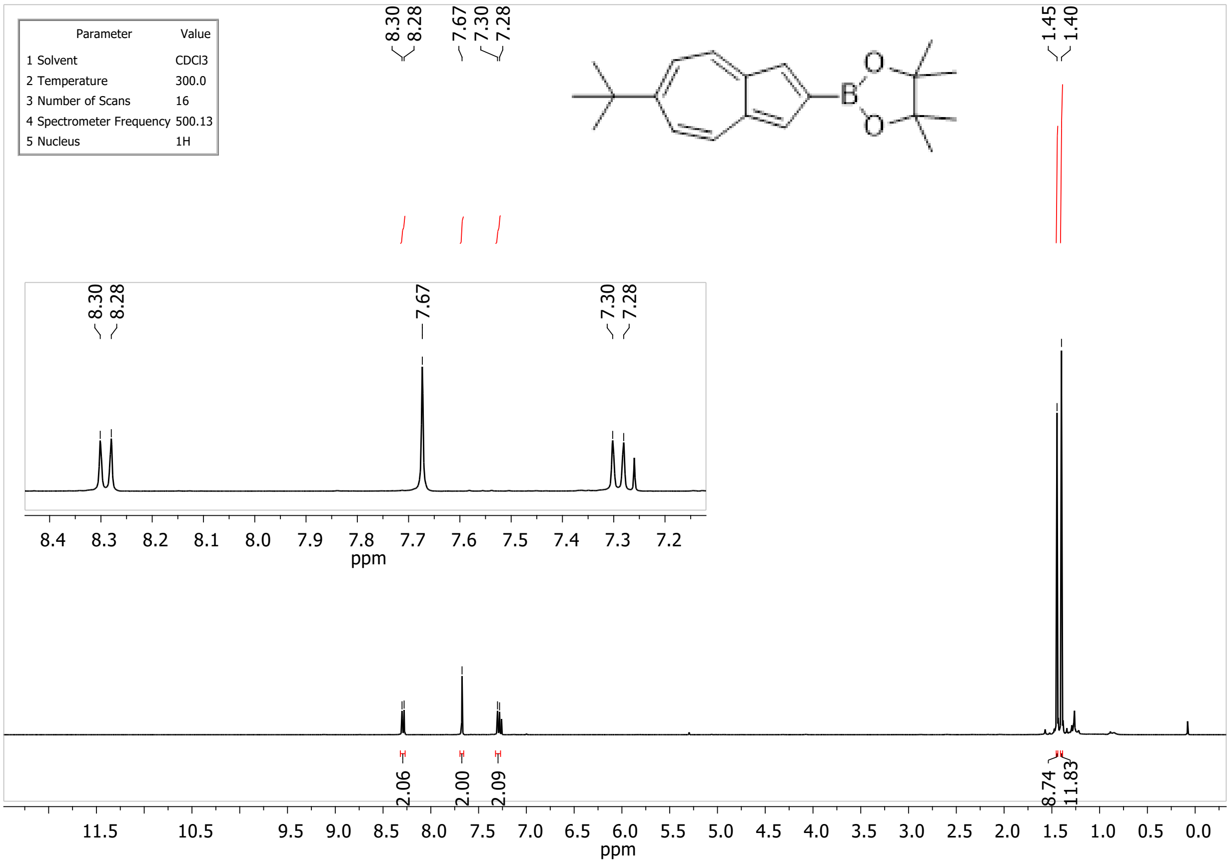
Transition	Energy	Wavelength	Oscillator strength	Contributions
$S_0 \rightarrow S_1$	2.05 eV	605 nm	f= 0.03730	H -> L 95.0%
$S_0 \rightarrow S_2$	2.58 eV	480 nm	f= 0.21780	H-1 -> L 92.3%
$S_0 \rightarrow S_3$	2.77 eV	448 nm	f= 0.04220	H -> L+1 87.7%
$S_0 \rightarrow S_4$	2.86 eV	434 nm	f= 0.00620	H-2 -> L 97.1%
$S_0 \rightarrow S_5$	2.89 eV	429 nm	f= 0.08580	H -> L+2 68.5%, H-3 -> L 22.4%
$S_0 \rightarrow S_6$	2.94 eV	422 nm	f= 0.00550	H -> L+3 40.5%, H-3 -> L 27.3%, H -> L+2 22.7%
$S_0 \rightarrow S_7$	3.11 eV	399 nm	f= 1.22720	H-1 -> L+1 65.4%, H -> L+3 17.9%, H-1 -> L+2 5.5%
$S_0 \rightarrow S_8$	3.24 eV	383 nm	f= 0.10450	H-1 -> L+2 54.7%, H-1 -> L+3 27.6%, H-1 -> L+1 9.5%
$S_0 \rightarrow S_9$	3.26 eV	381 nm	f= 1.10830	H-3 -> L 42.1%, H -> L+3 28.9%, H-1 -> L+1 15.0%
$S_0 \rightarrow S_{10}$	3.35 eV	371 nm	f= 0.00180	H-1 -> L+3 57.3%, H-1 -> L+2 35.4%

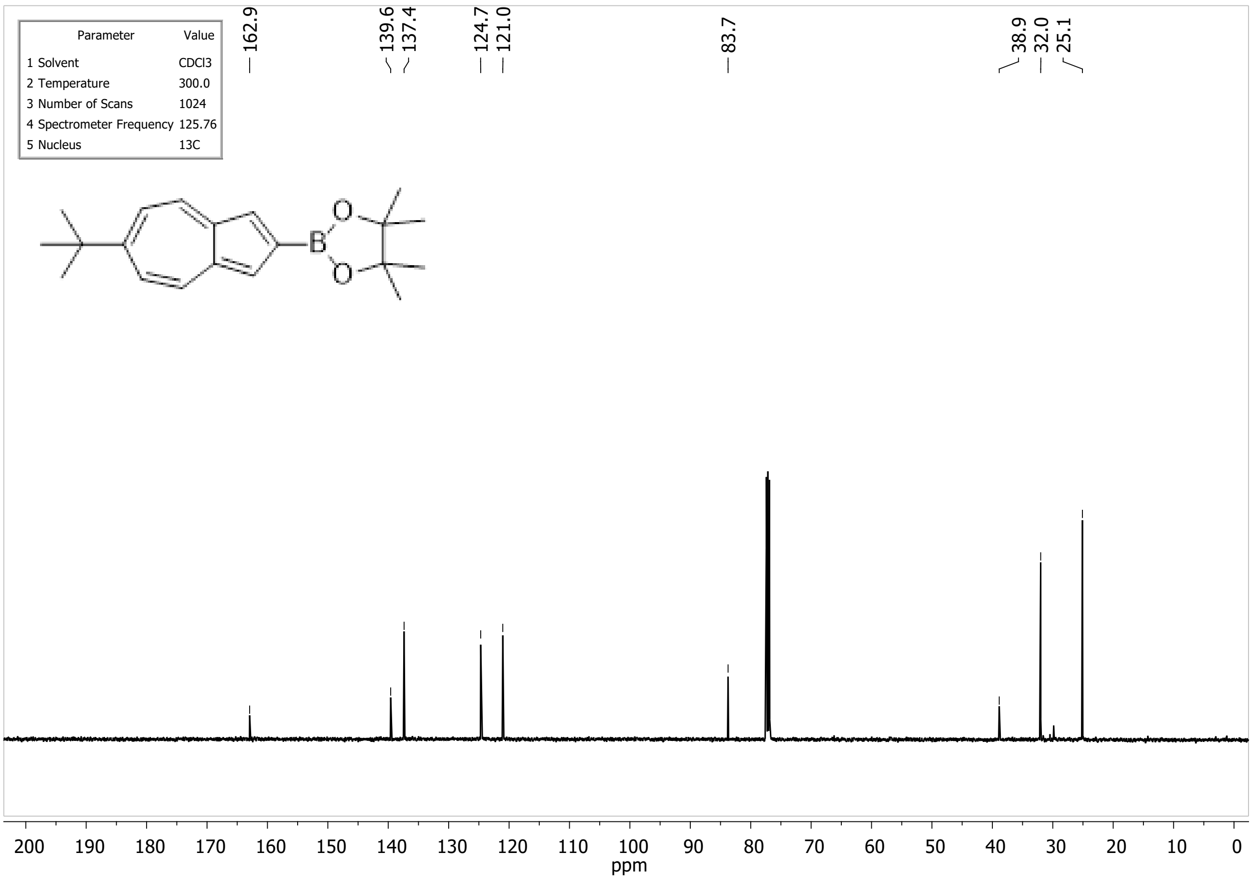
Table S8. Electronic transition contributing to UV/Vis/NIR spectrum of compound **2f**, B3LYP/6-31G(d).

Transition	Energy	Wavelength	Oscillator strength	Contributions
$S_0 \rightarrow S_1$	1.83 eV	677 nm	f= 0.04930	H -> L 91.4%, H-1 -> L 5.5%
$S_0 \rightarrow S_2$	2.21 eV	560 nm	f= 0.38040	H -> L+1 94.9%
$S_0 \rightarrow S_3$	2.40 eV	516 nm	f= 0.13420	H-1 -> L 90.2%, H -> L 6.1%
$S_0 \rightarrow S_4$	2.51 eV	494 nm	f= 0.07640	H-2 -> L 63.8%, H -> L+2 28.0%
$S_0 \rightarrow S_5$	2.63 eV	472 nm	f= 0.34180	H-1 -> L+1 76.2%, H-2 -> L 13.7%, H -> L+2 5.4%
$S_0 \rightarrow S_6$	2.65 eV	469 nm	f= 0.00850	H -> L+3 80.1%, H-2 -> L+1 11.0%
$S_0 \rightarrow S_7$	2.68 eV	462 nm	f= 0.81920	H-2 -> L+1 81.0%, H -> L+3 9.6
$S_0 \rightarrow S_8$	2.72 eV	456 nm	f= 0.58530	H -> L+2 52.2%, H-2 -> L 17.2%, H-1 -> L+1 14.5%, H-3 -> L 7.7%
$S_0 \rightarrow S_9$	2.98 eV	416 nm	f= 0.25920	H -> L+4 40.2%, H-3 -> L 37.8%, H-1 -> L+2 13.6%
$S_0 \rightarrow S_{10}$	3.04 eV	408 nm	f= 0.01830	H-3 -> L+1 38.1%, H-1 -> L+3 23.4%, H -> L+5 20.4%, H-2 -> L+2 7.5%

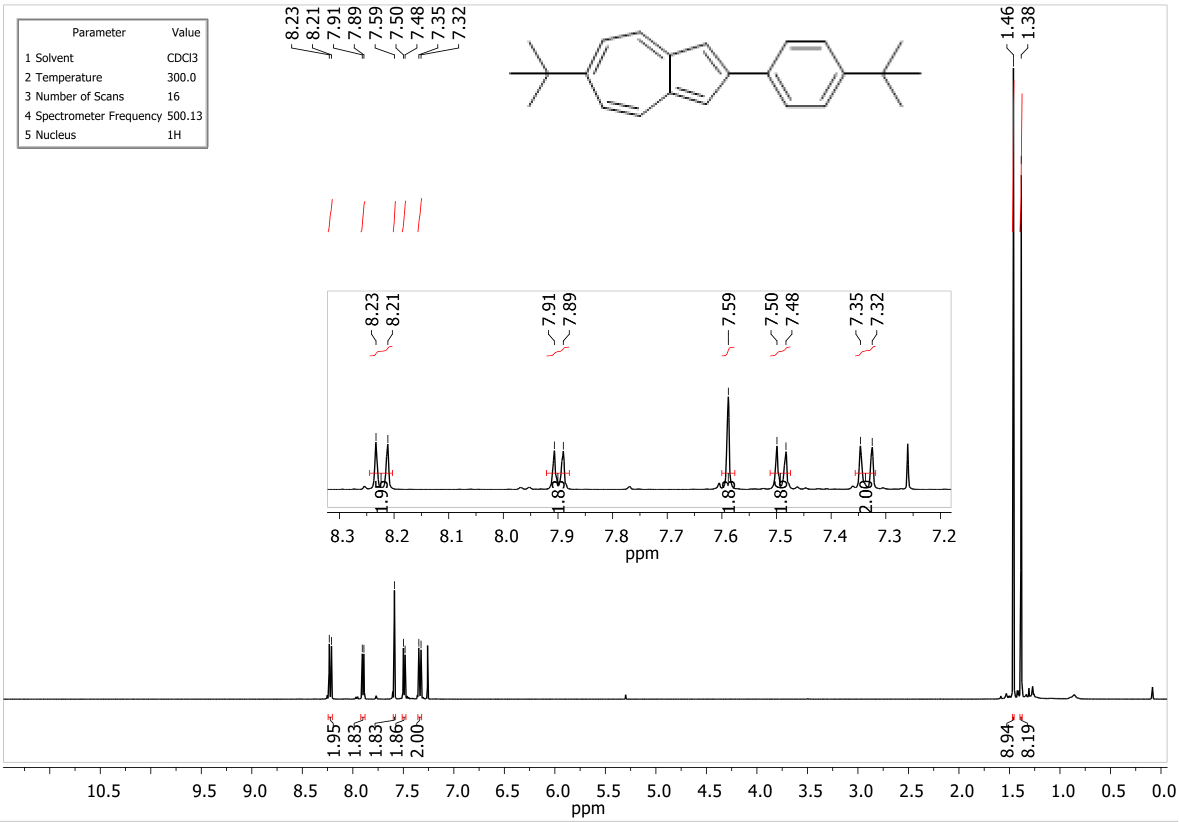
NMR Spectra

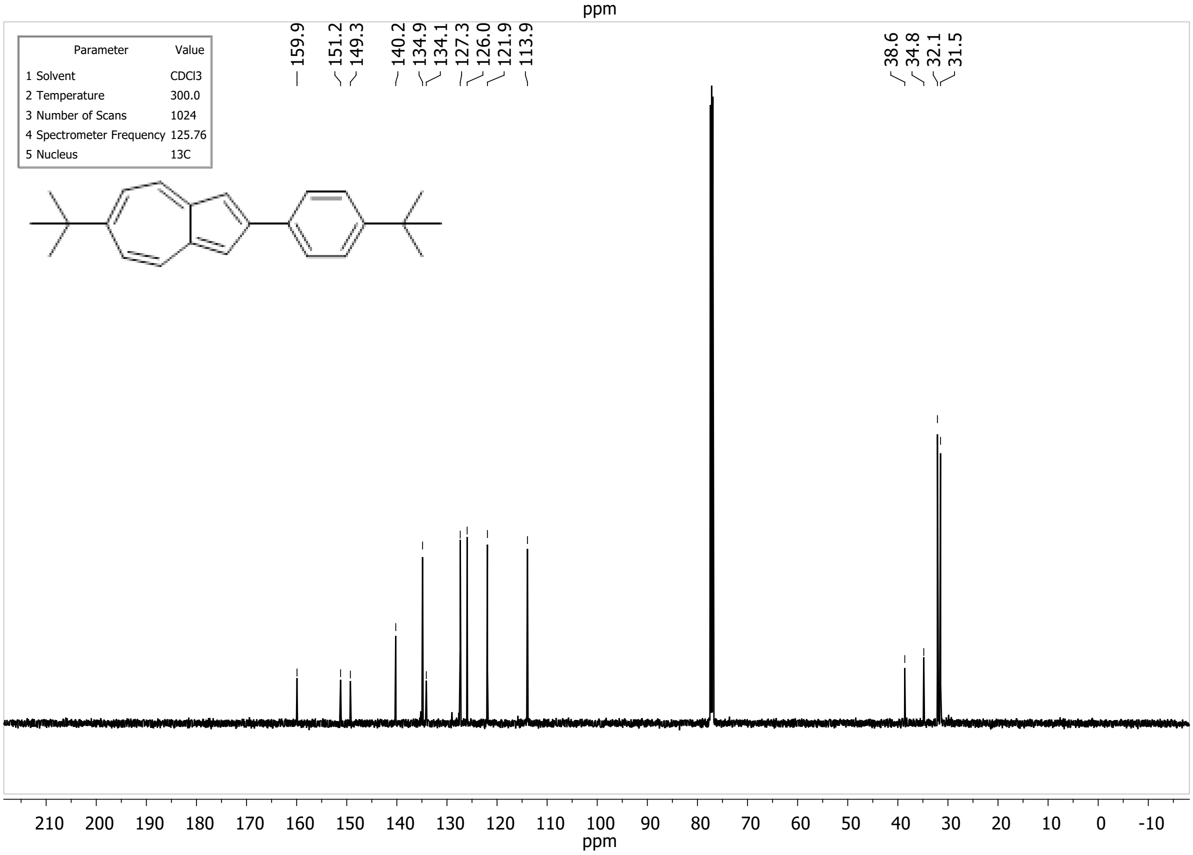
Compound 5, 2-(6-(*tert*-butyl)azulen-2-yl)-4,4,5,5-tetramethyl-1,3,2-dioxaborolane



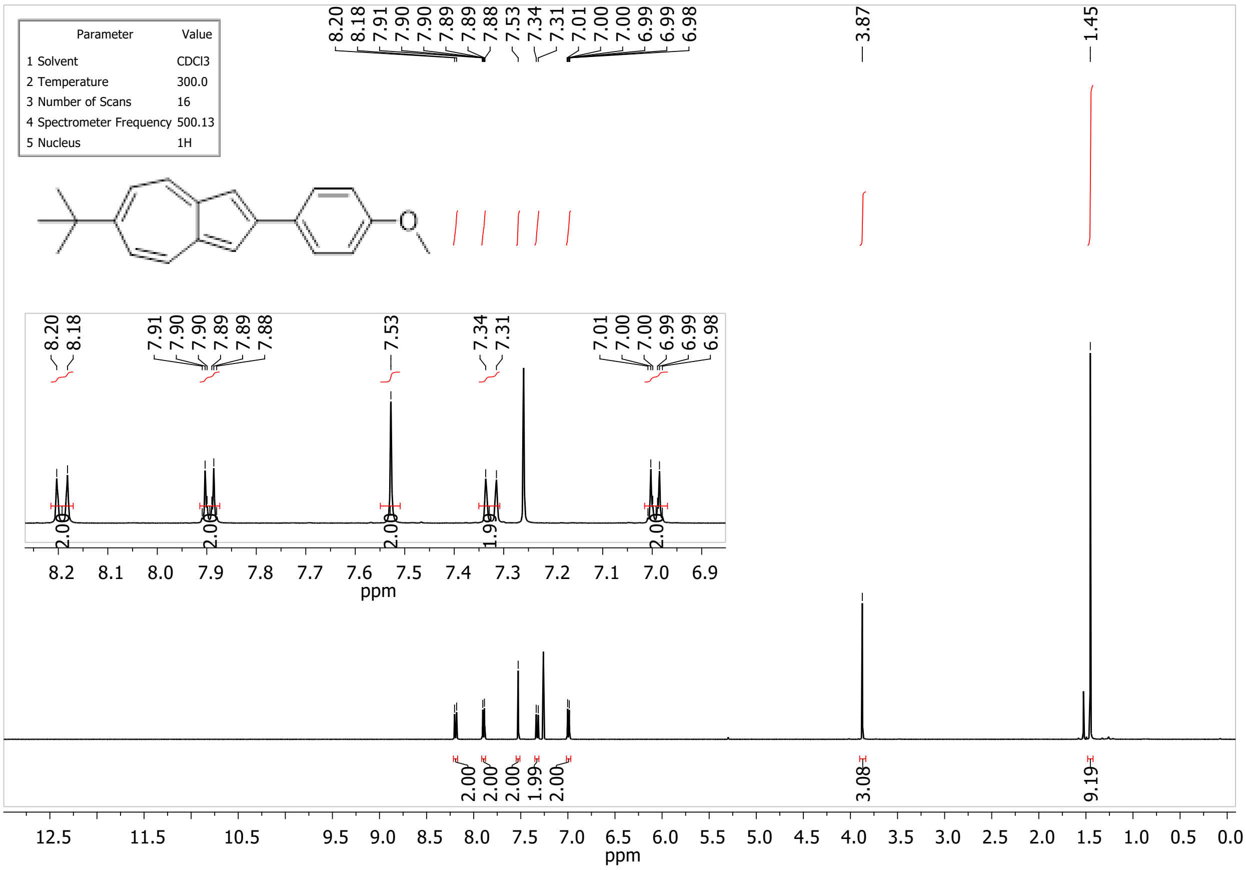


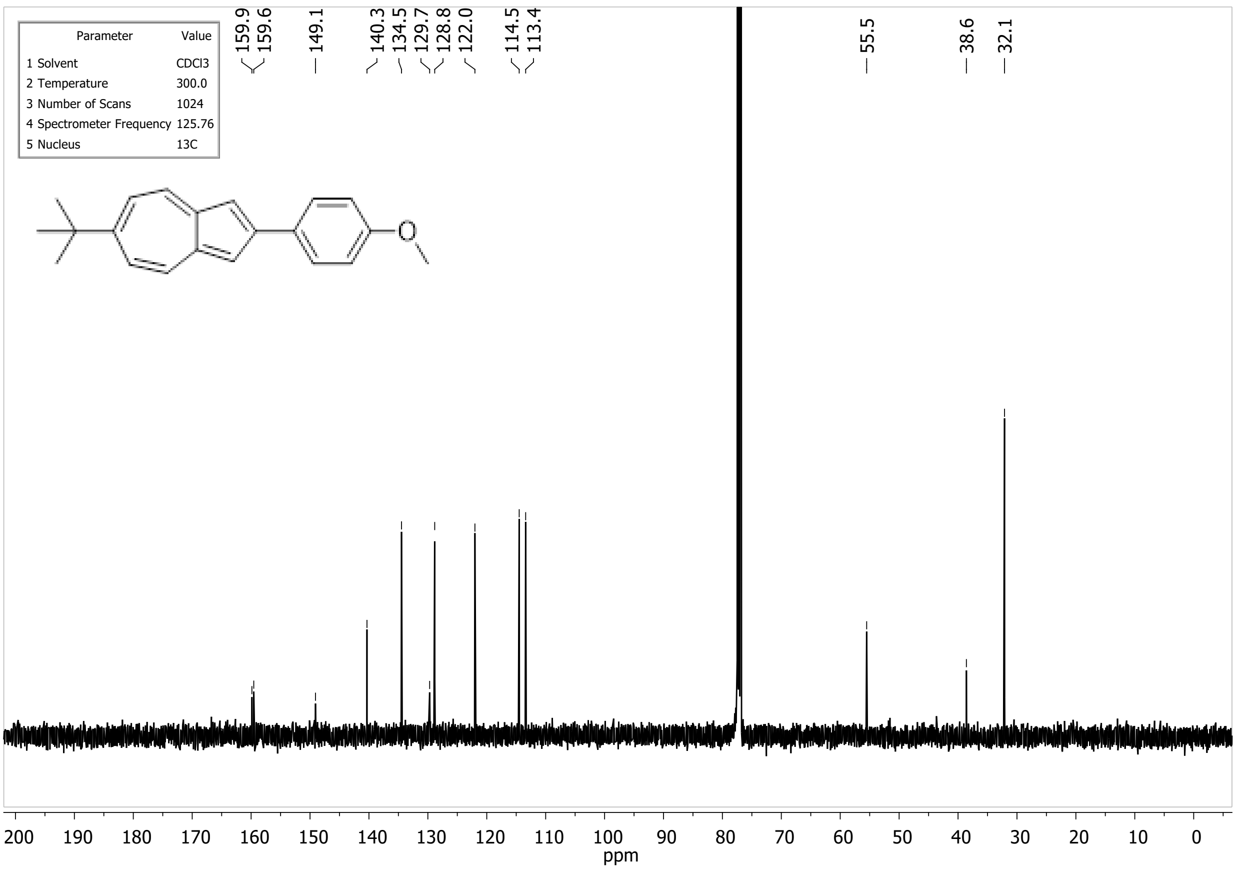
Compound 6a, 6-(*tert*-butyl)-2-(4-(*tert*-butyl)phenyl)azulene



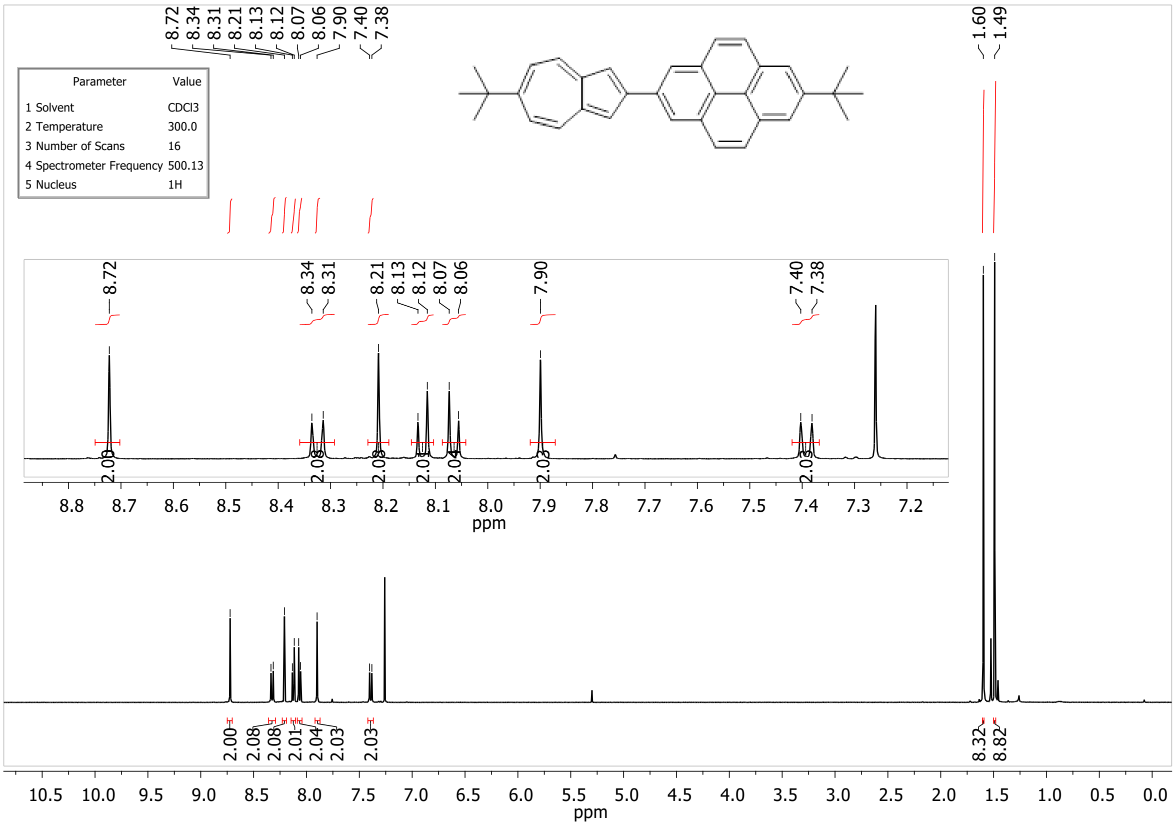


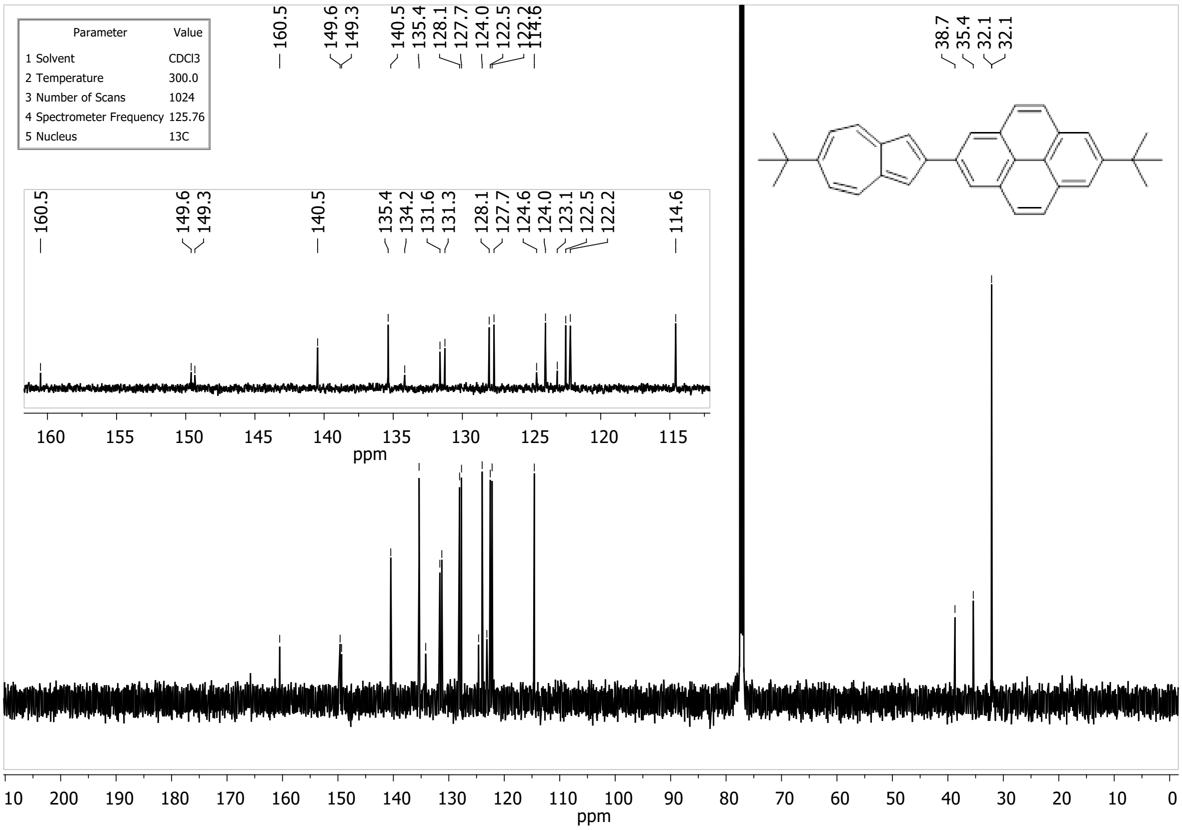
Compound 6b, 6-(*tert*-butyl)-2-(4-methoxyphenyl)azulene



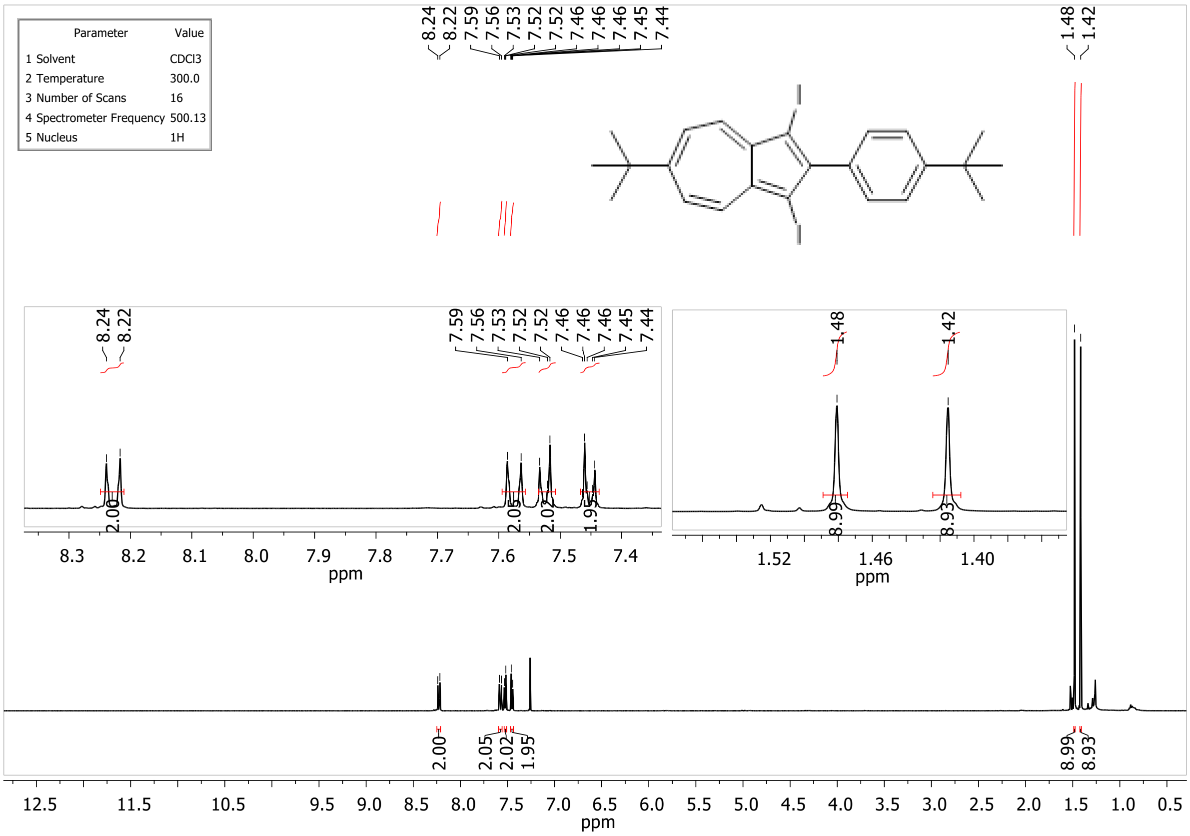


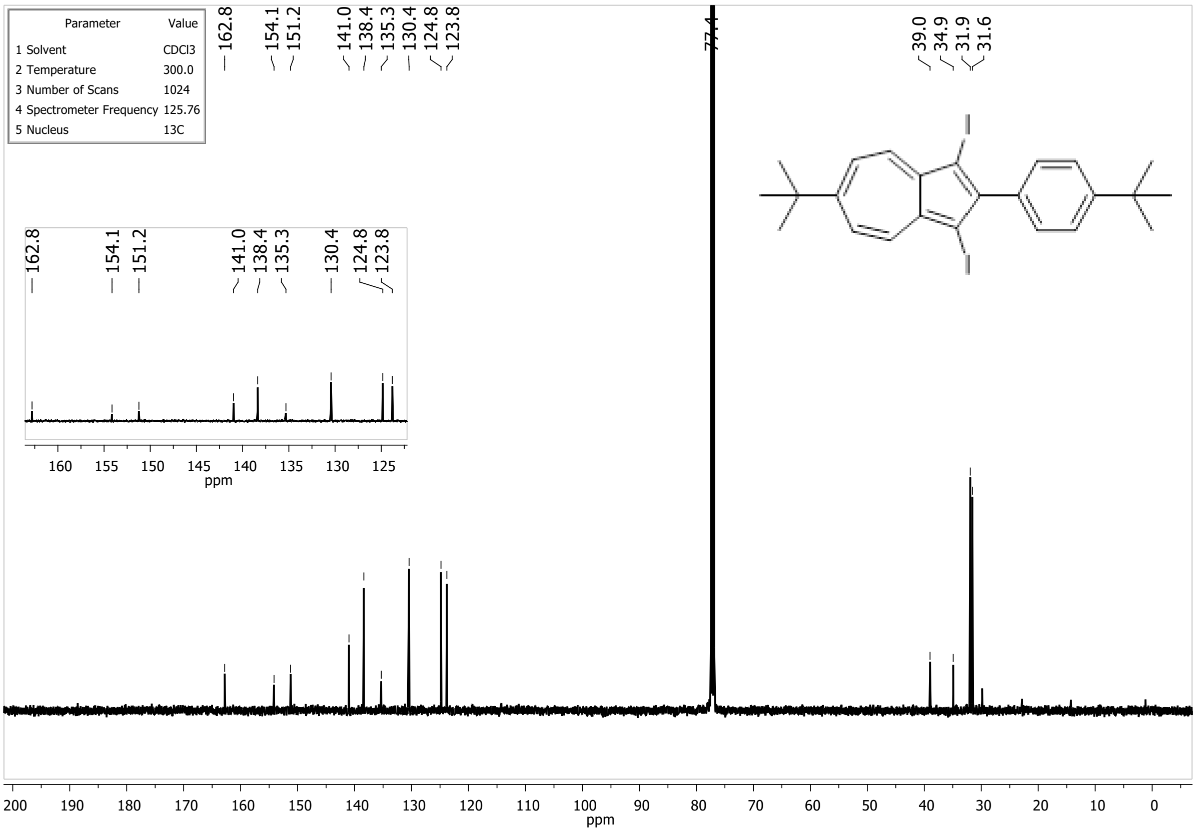
Compound 6c, 2-(*tert*-butyl)-7-(6-(*tert*-butyl)azulen-2-yl)pyrene



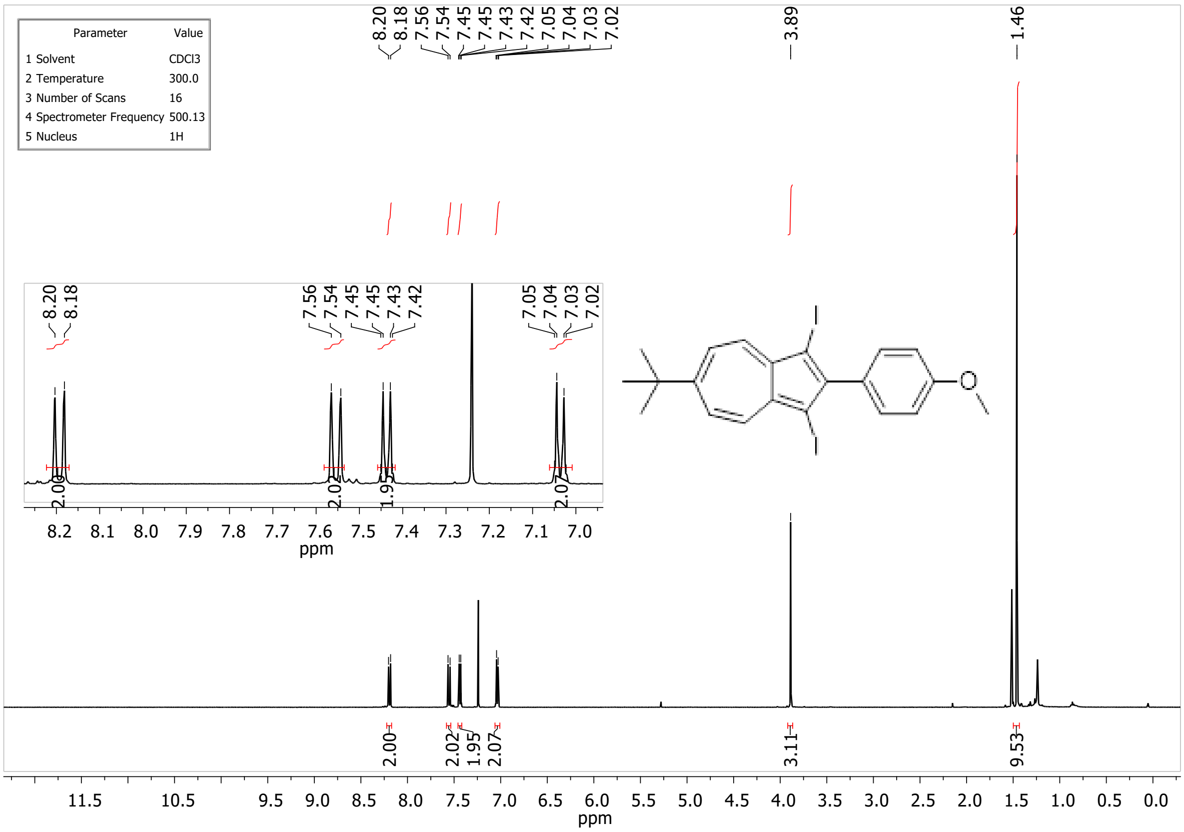


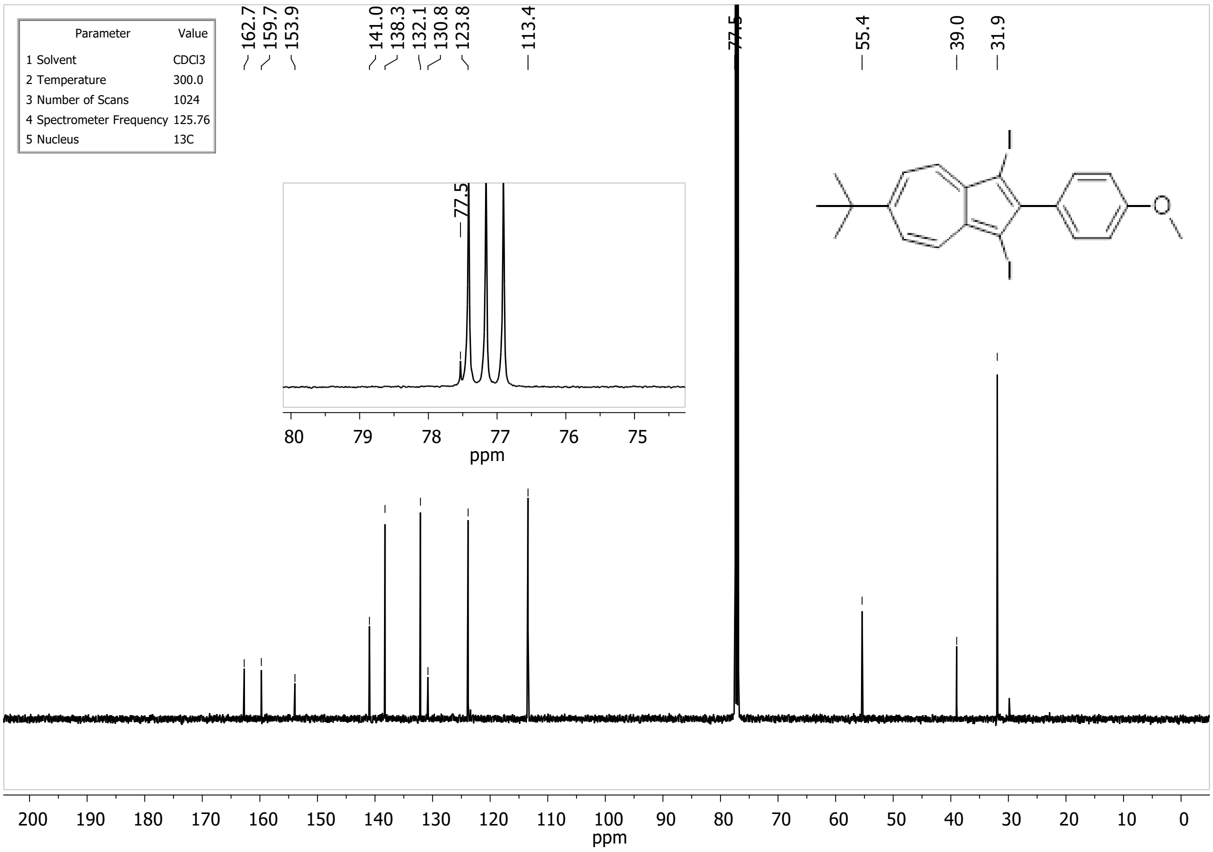
Compound 7a, 6-(*tert*-butyl)-2-(4-(*tert*-butyl)phenyl)-1,3-diiodoazulene



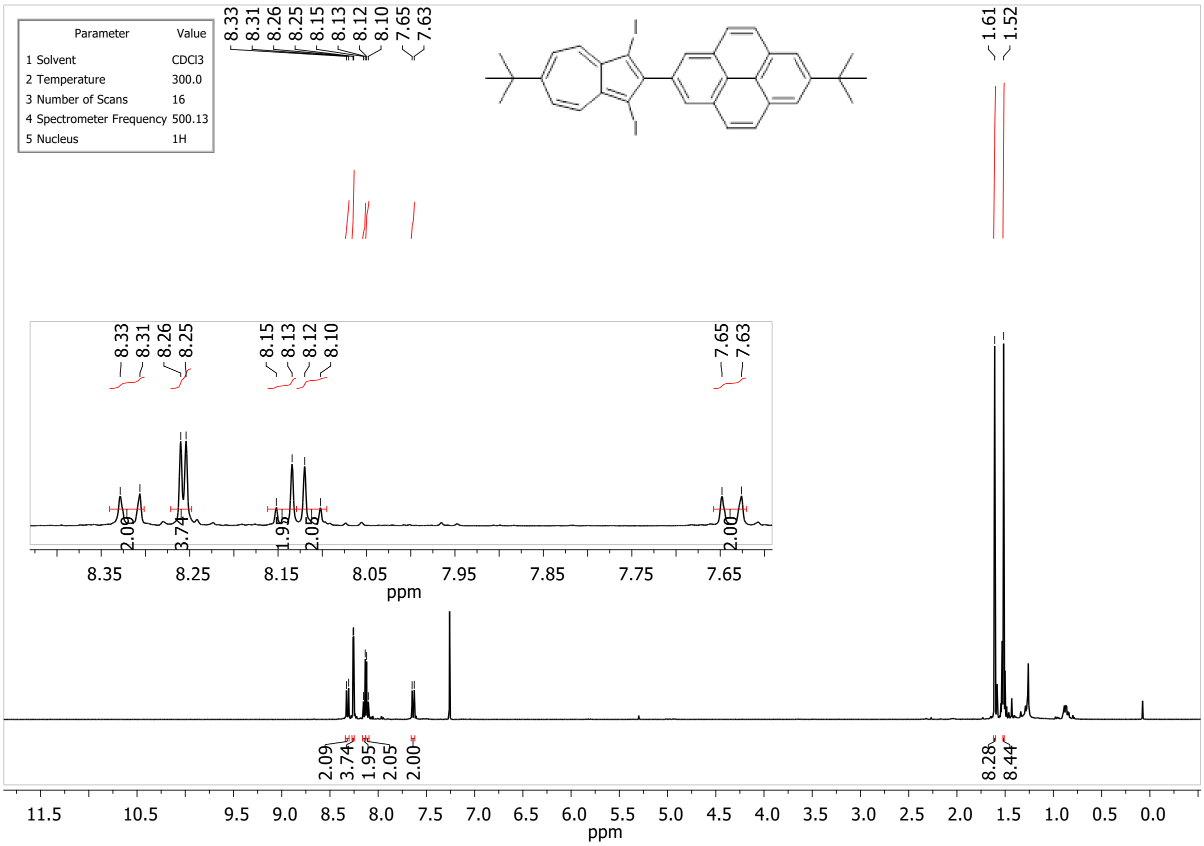


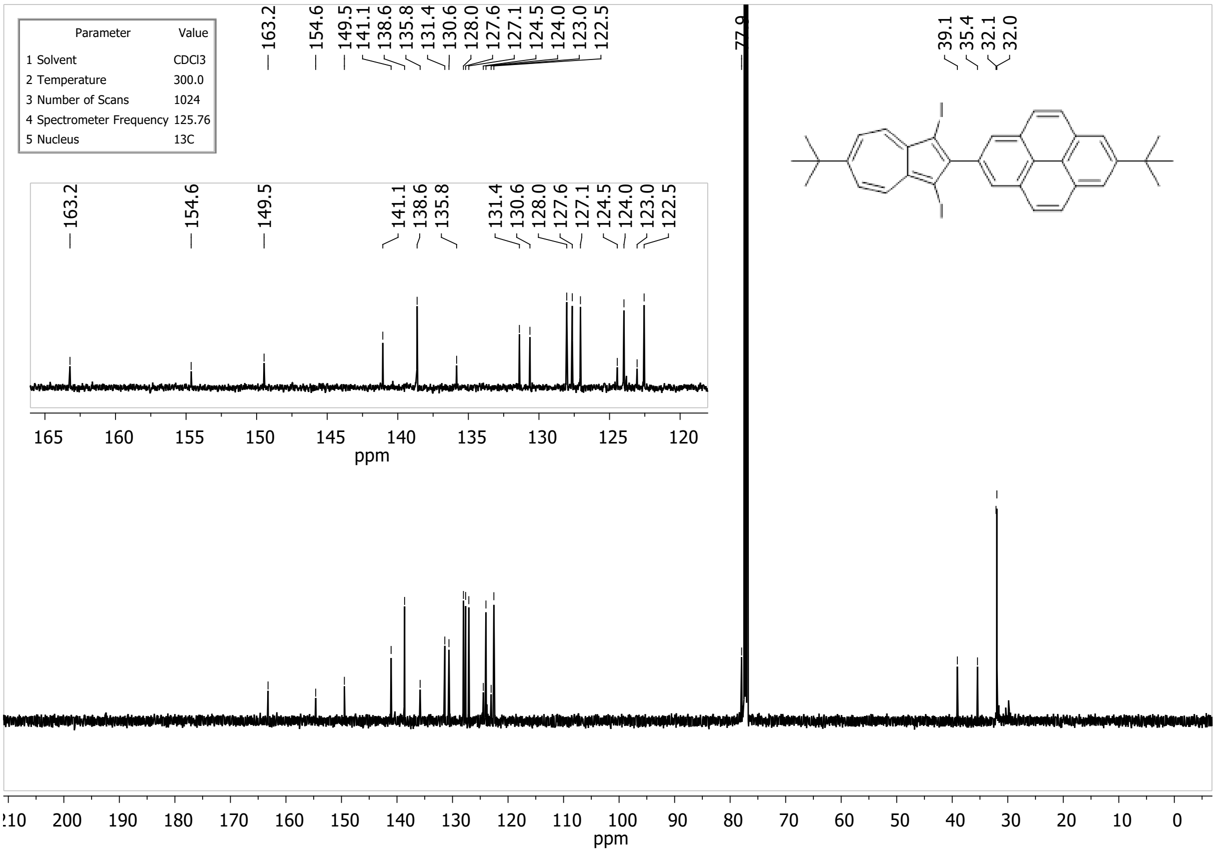
Compound 7b, 6-(*tert*-butyl)-1,3-diiodo-2-(4-methoxyphenyl)azulene



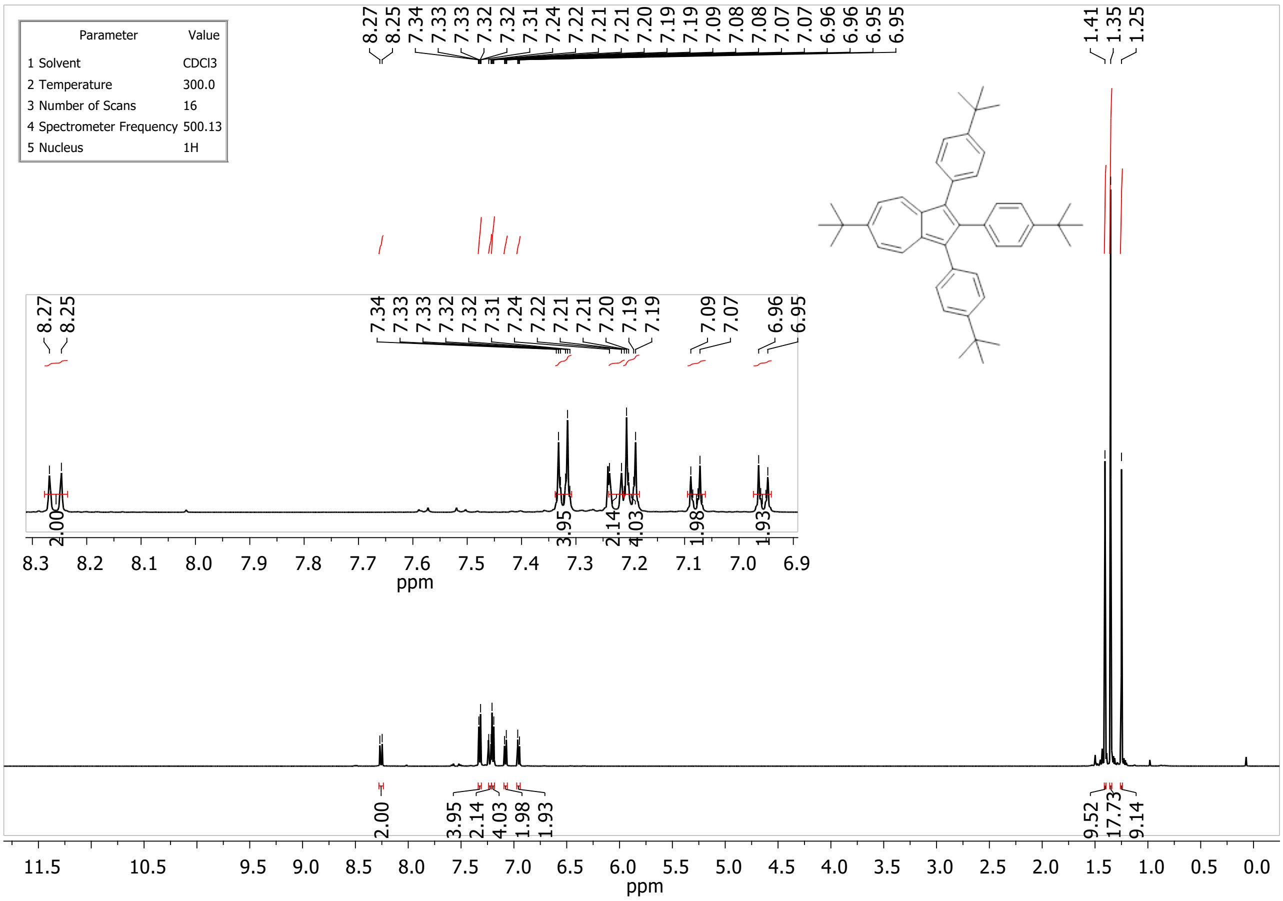


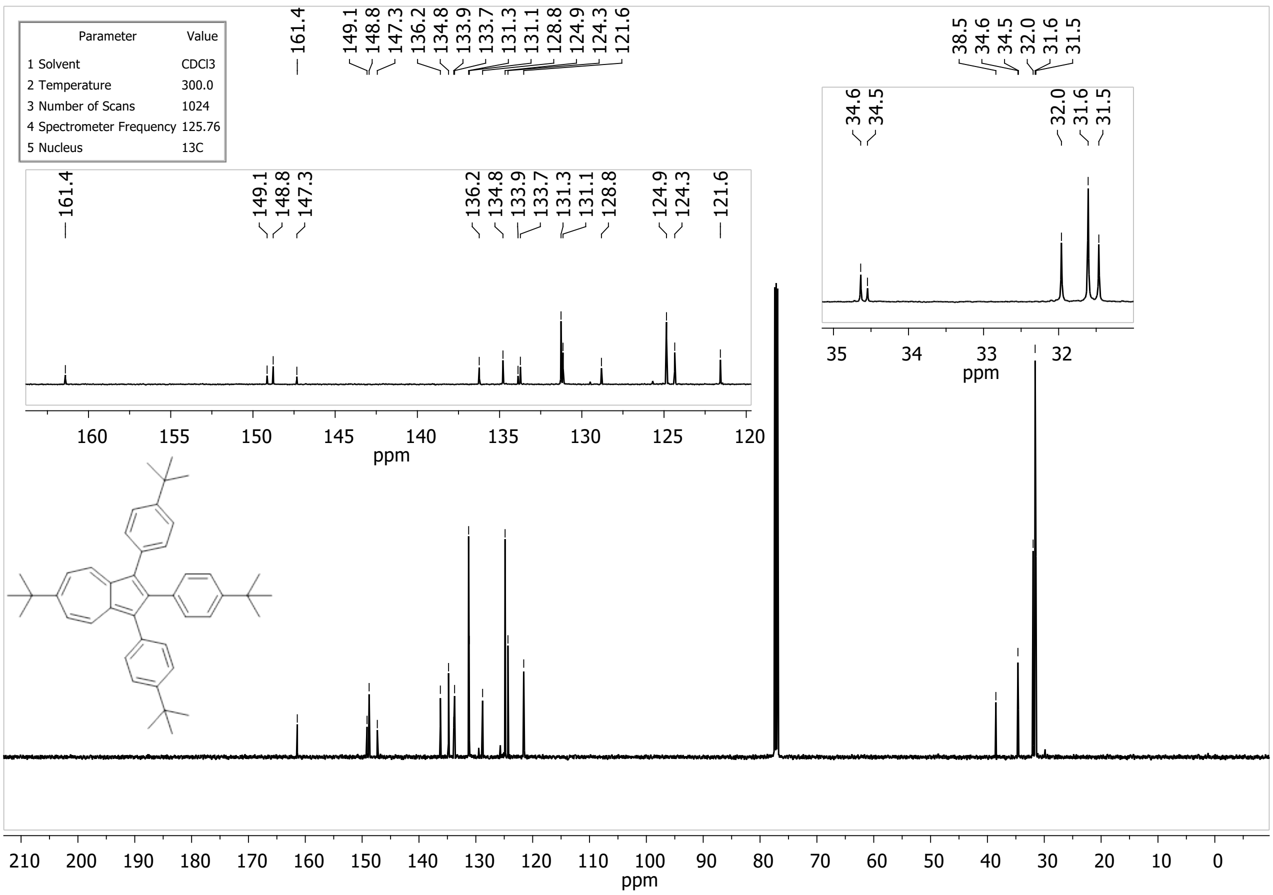
Compound 7c, 2-(*tert*-butyl)-7-(6-(*tert*-butyl)-1,3-diiodoazulen-2-yl)pyrene



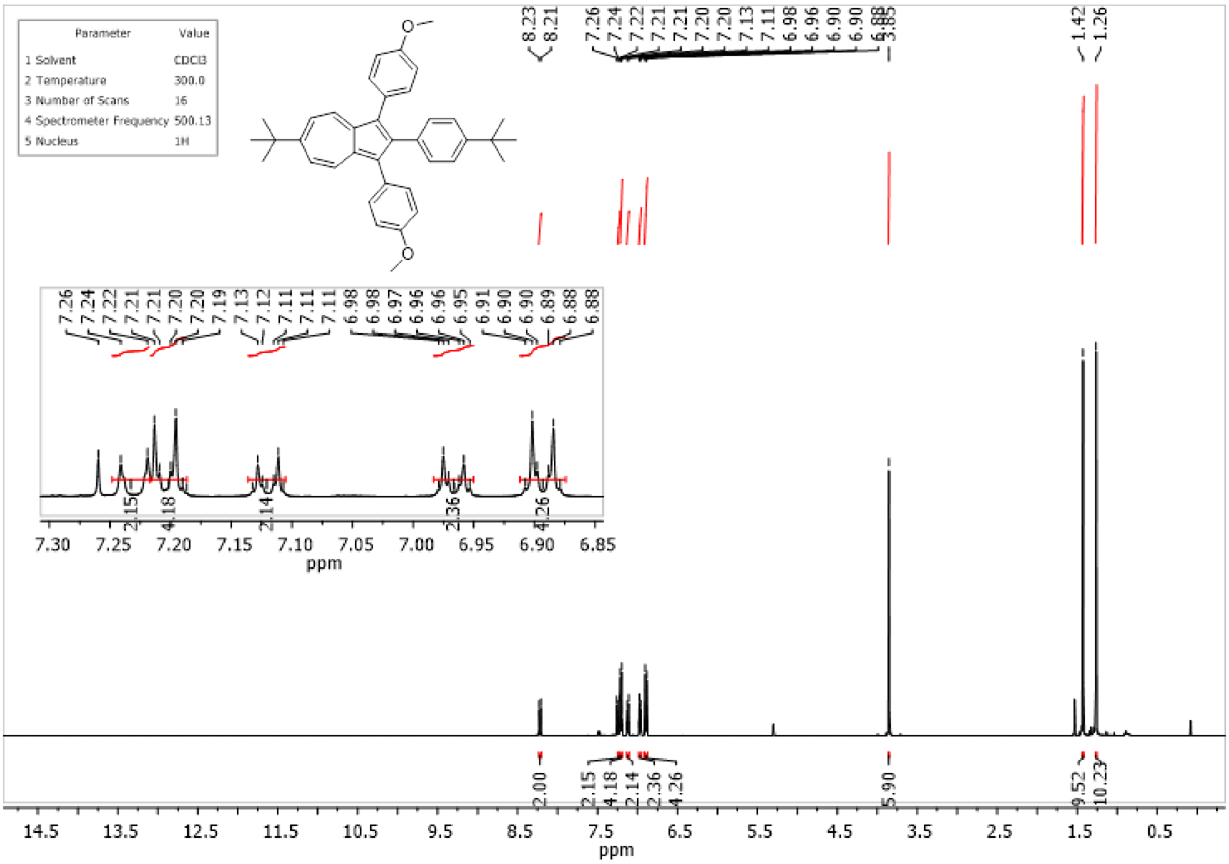


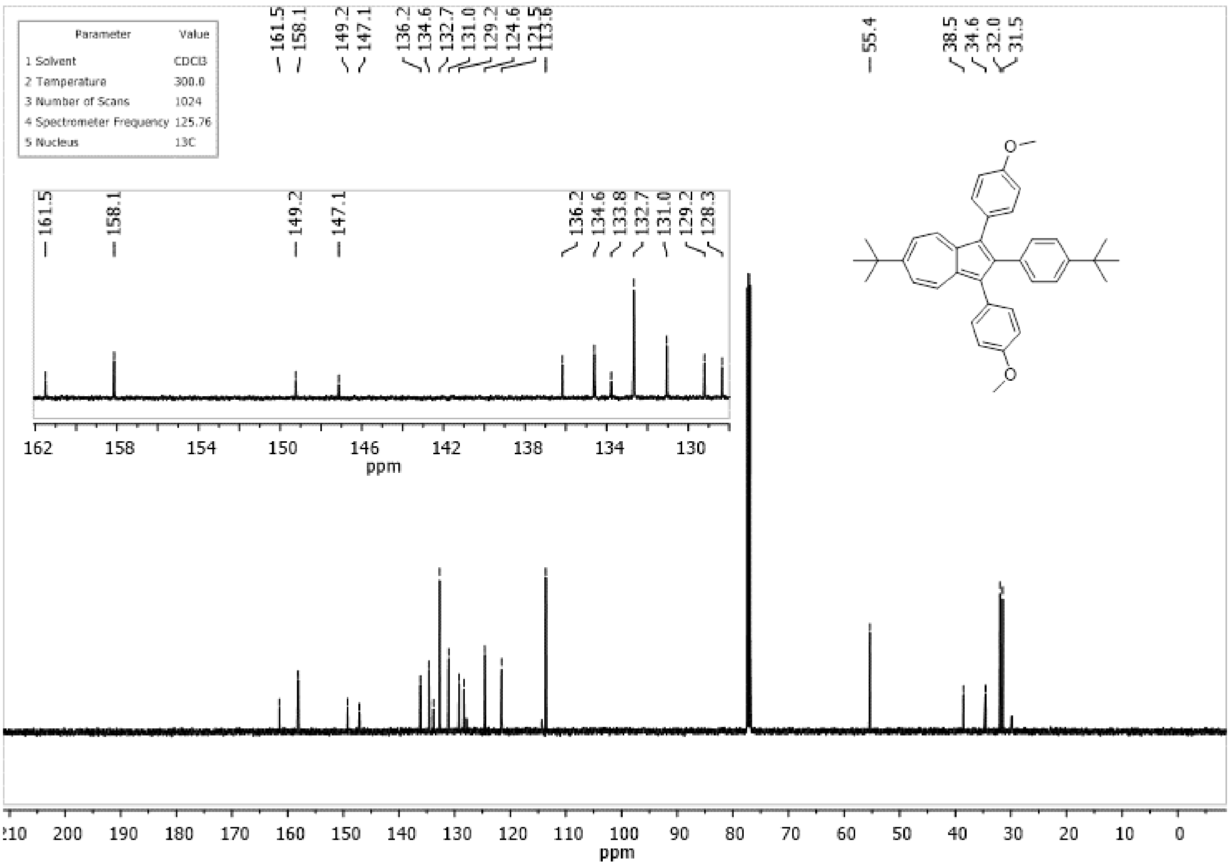
Compound 1a, 6-(*tert*-butyl)-1,2,3-tris(4-(*tert*-butyl)phenyl)azulene



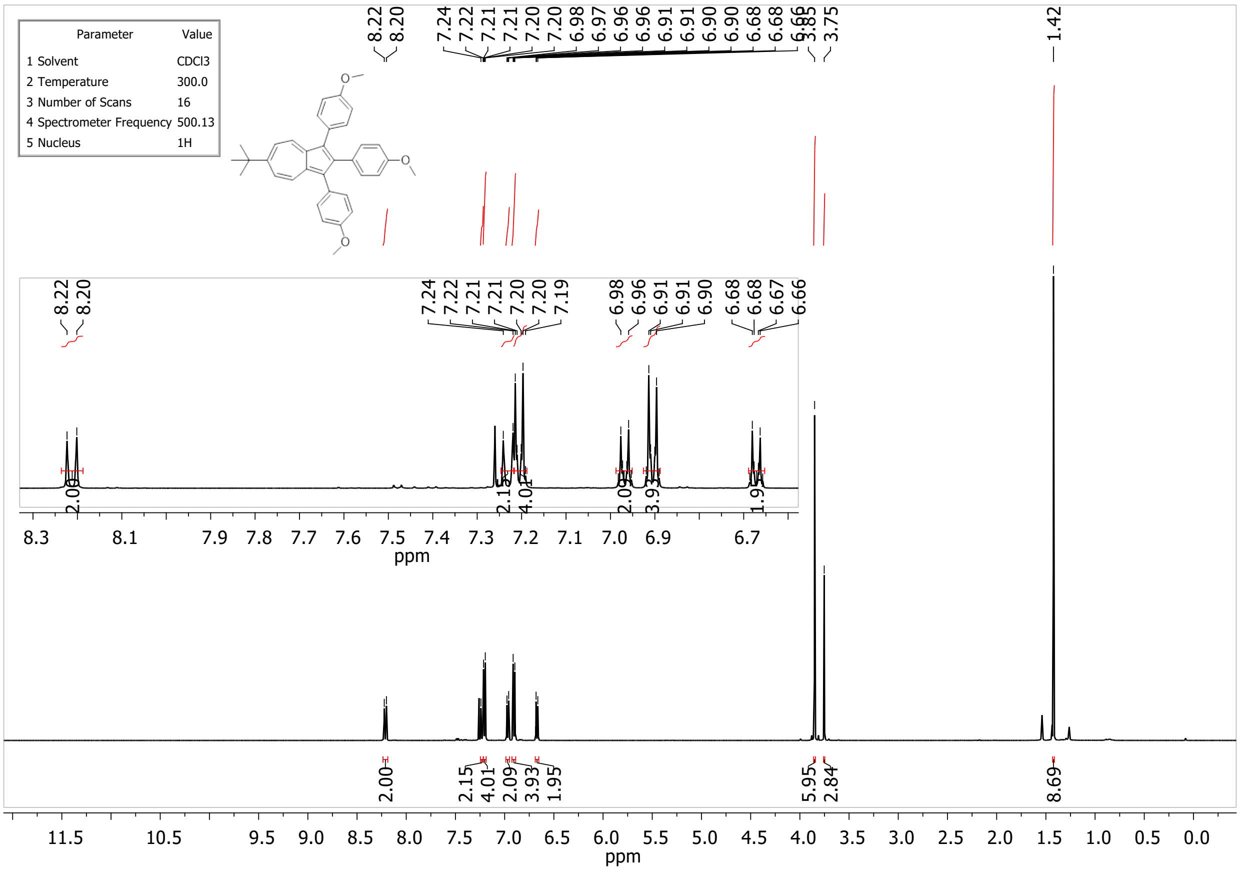


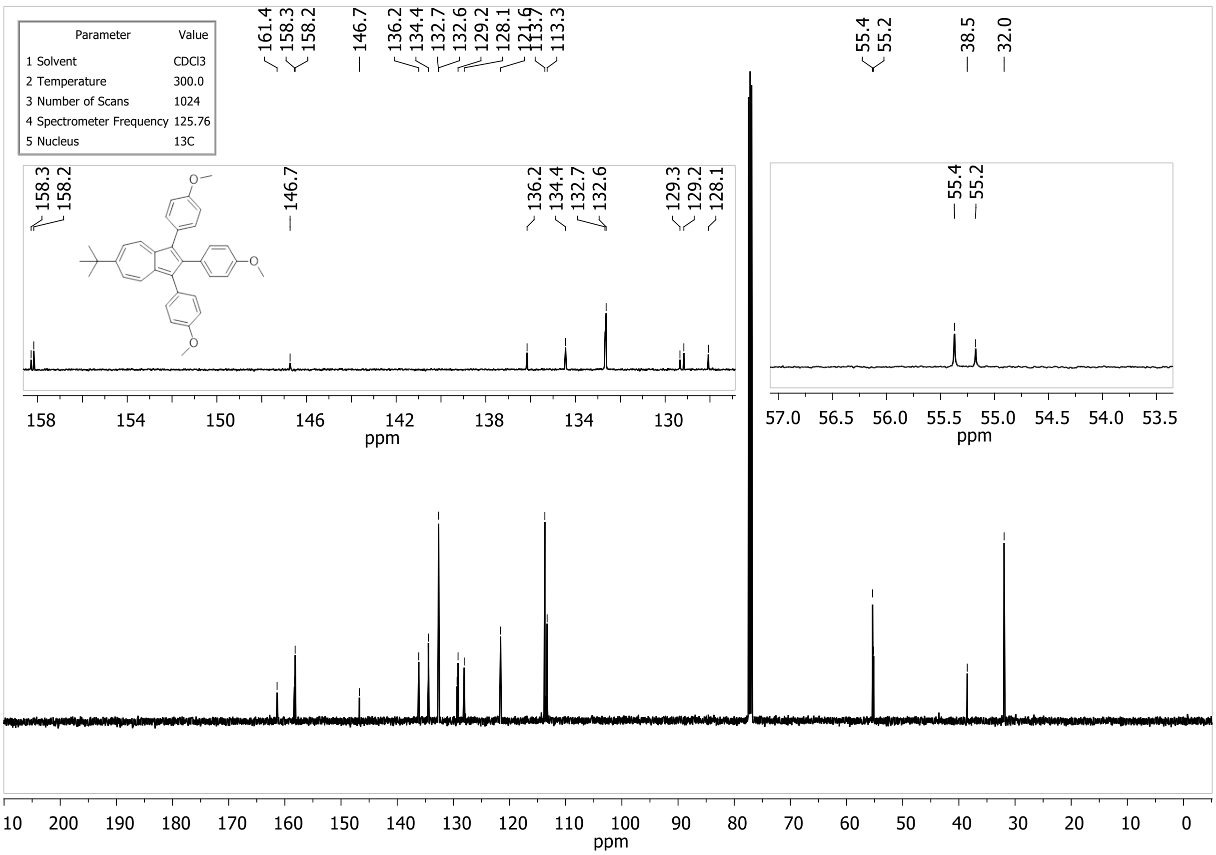
Compound 1b, 6-(*tert*-butyl)-2-(4-(*tert*-butyl)phenyl)-1,3-bis(4-methoxyphenyl)azulene



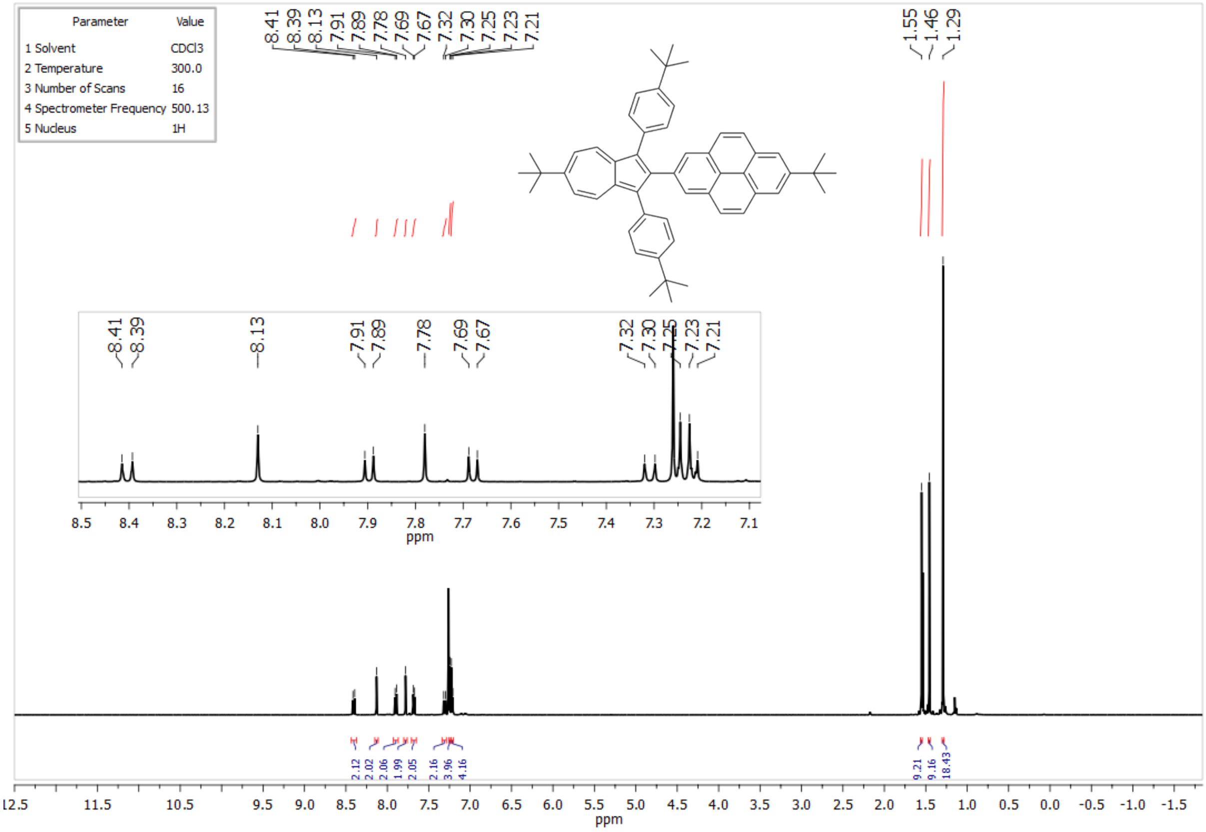


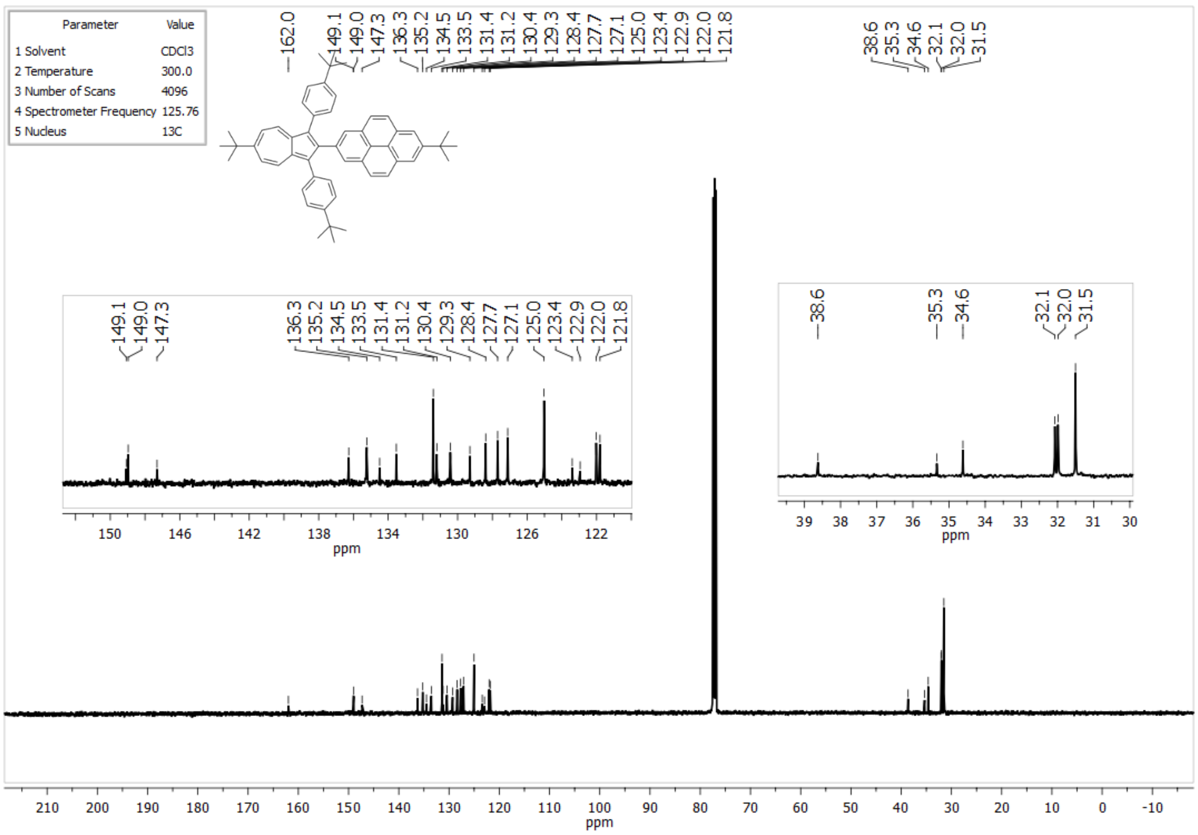
Compound 1c, 6-(*tert*-butyl)-1,2,3-tris(4-methoxyphenyl)azulene



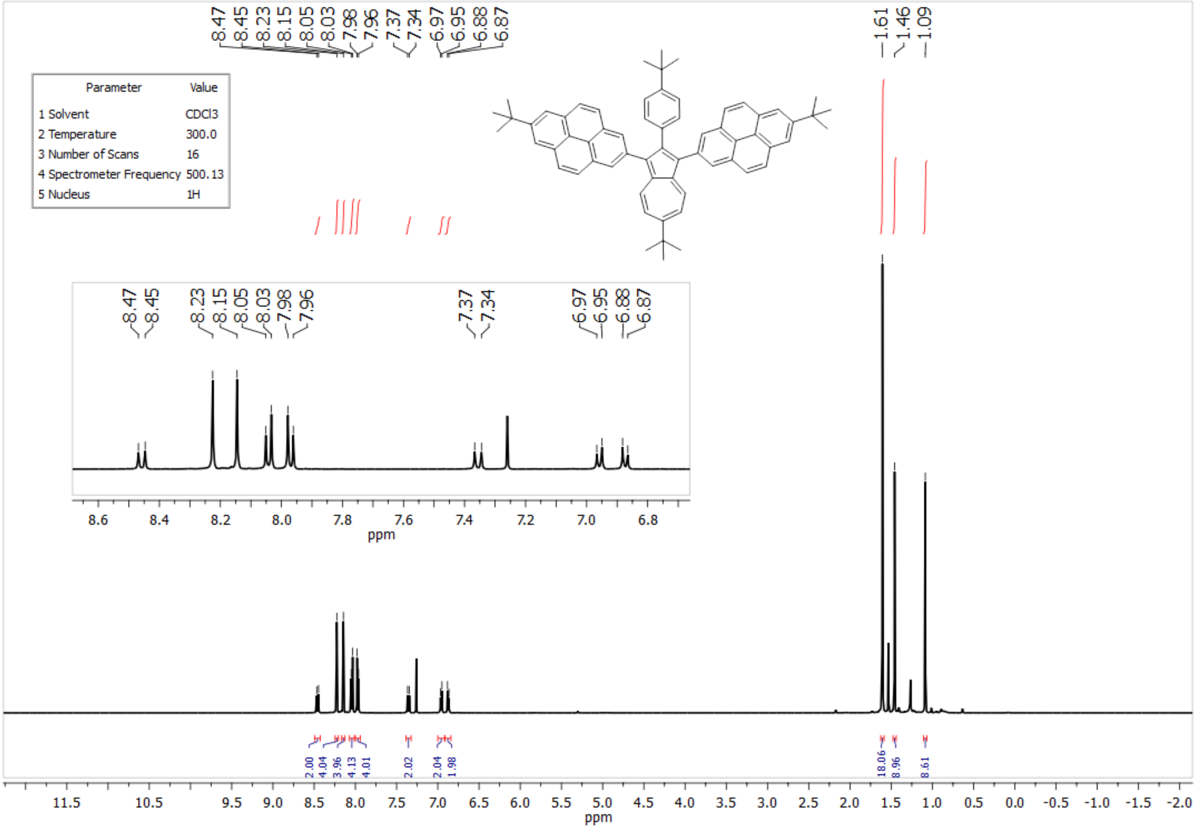


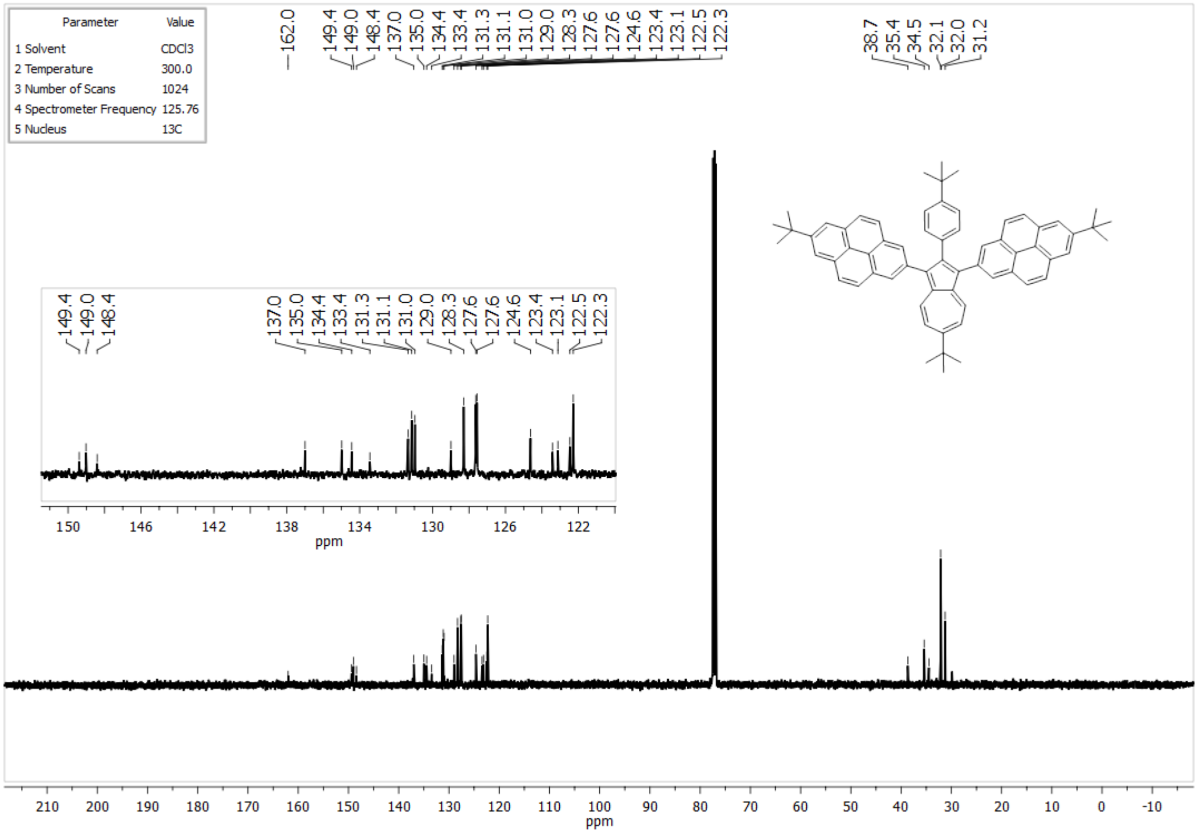
Compound 1d, 2-(*tert*-butyl)-7-(6-(*tert*-butyl)-1,3-bis(4-(*tert*-butyl)phenyl)azulen-2-yl)pyrene



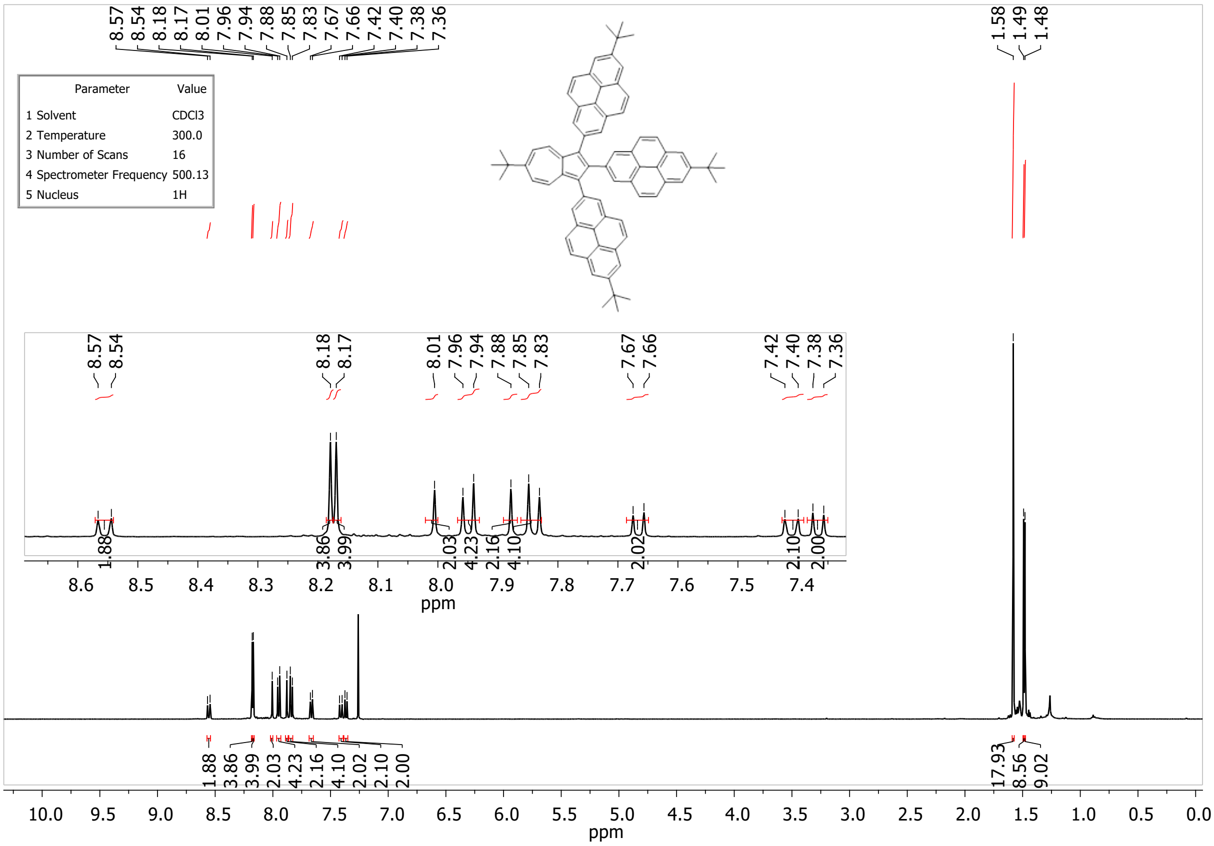


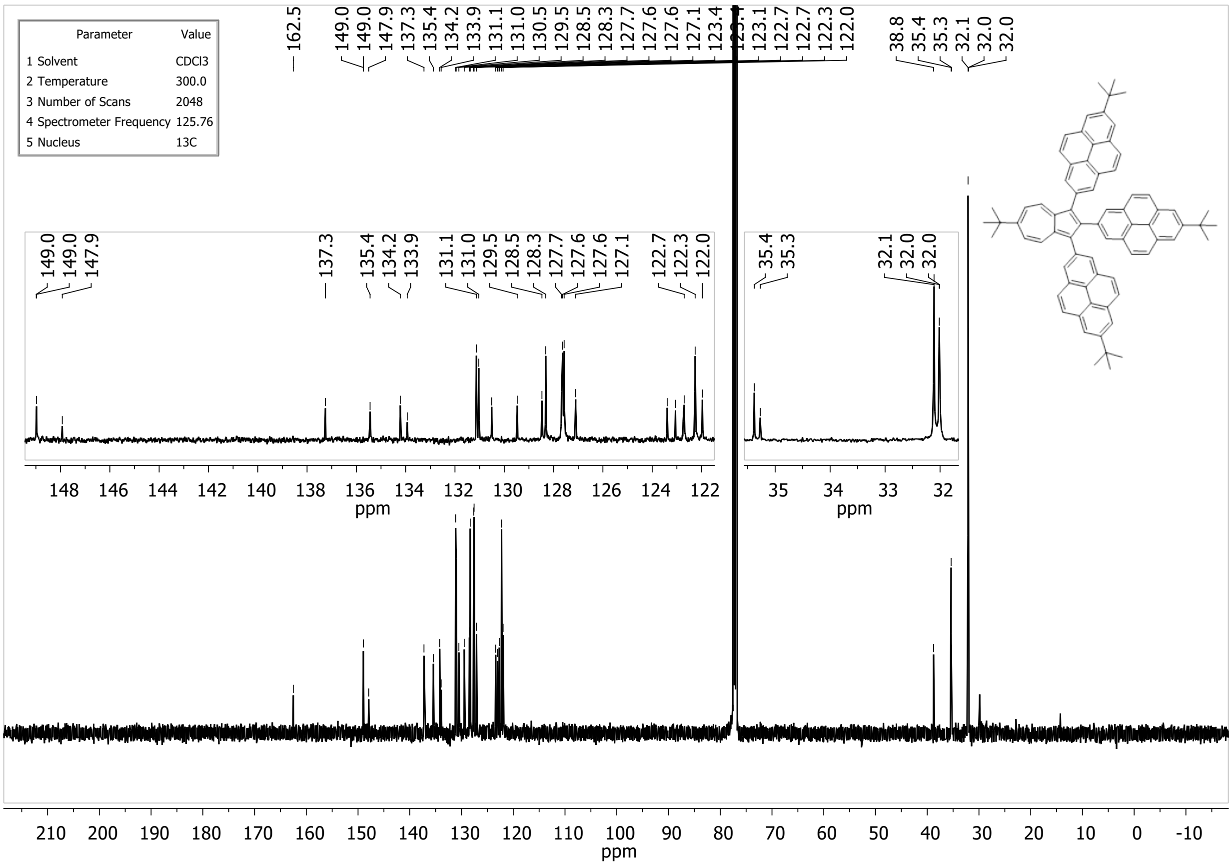
Compound 1e, 7,7'-(6-(*tert*-butyl)-2-(4-(*tert*-butyl)phenyl)azulene-1,3-diyl)bis(2-(*tert*-butyl)pyrene)



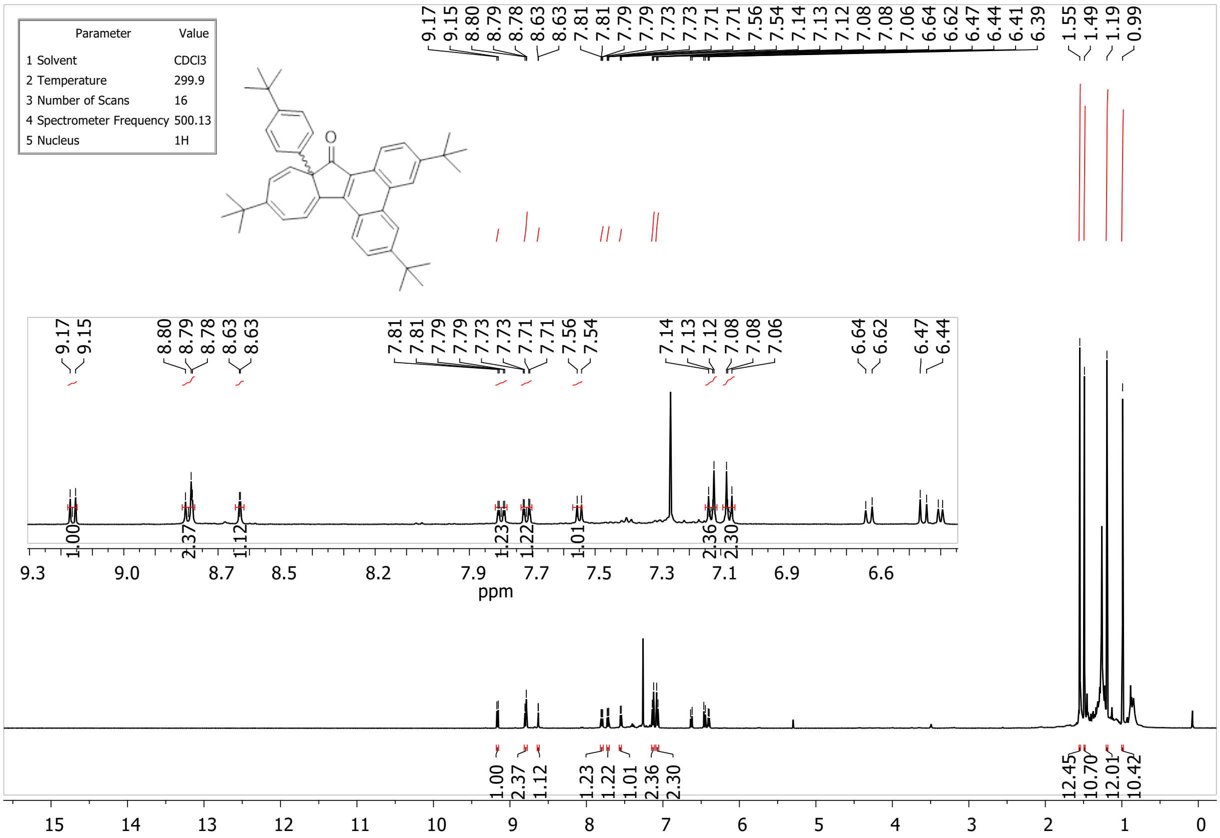


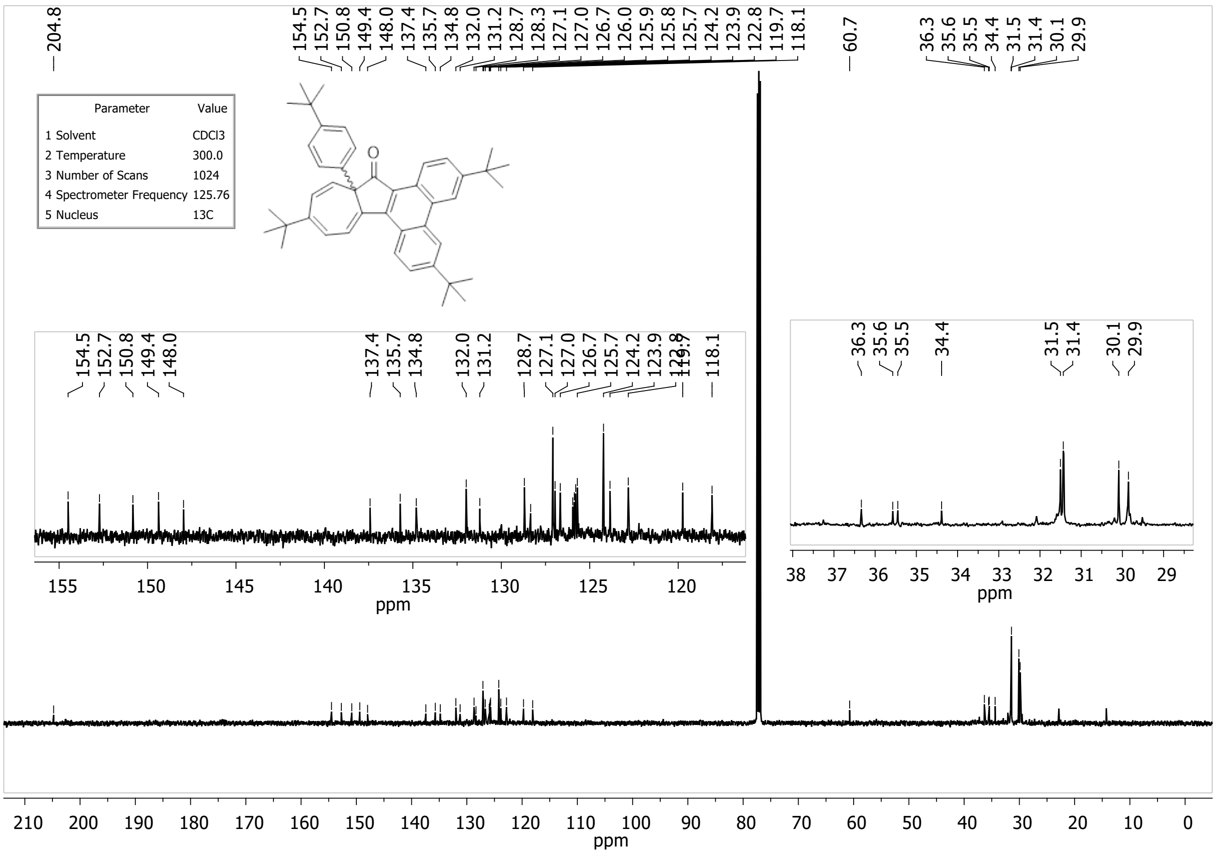
Compound 1f, 7,7',7''-(6-(*tert*-butyl)azulene-1,2,3-triyl)tris(2-(*tert*-butyl)pyrene)



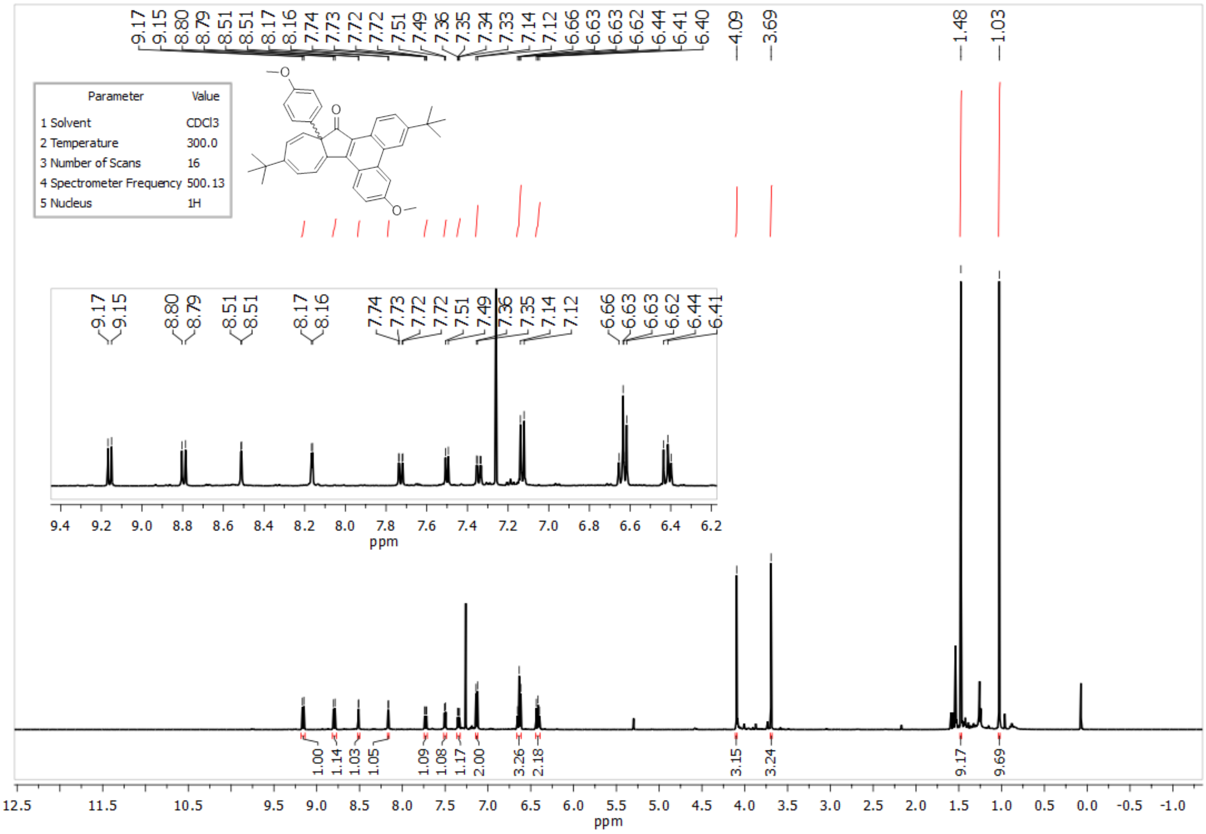


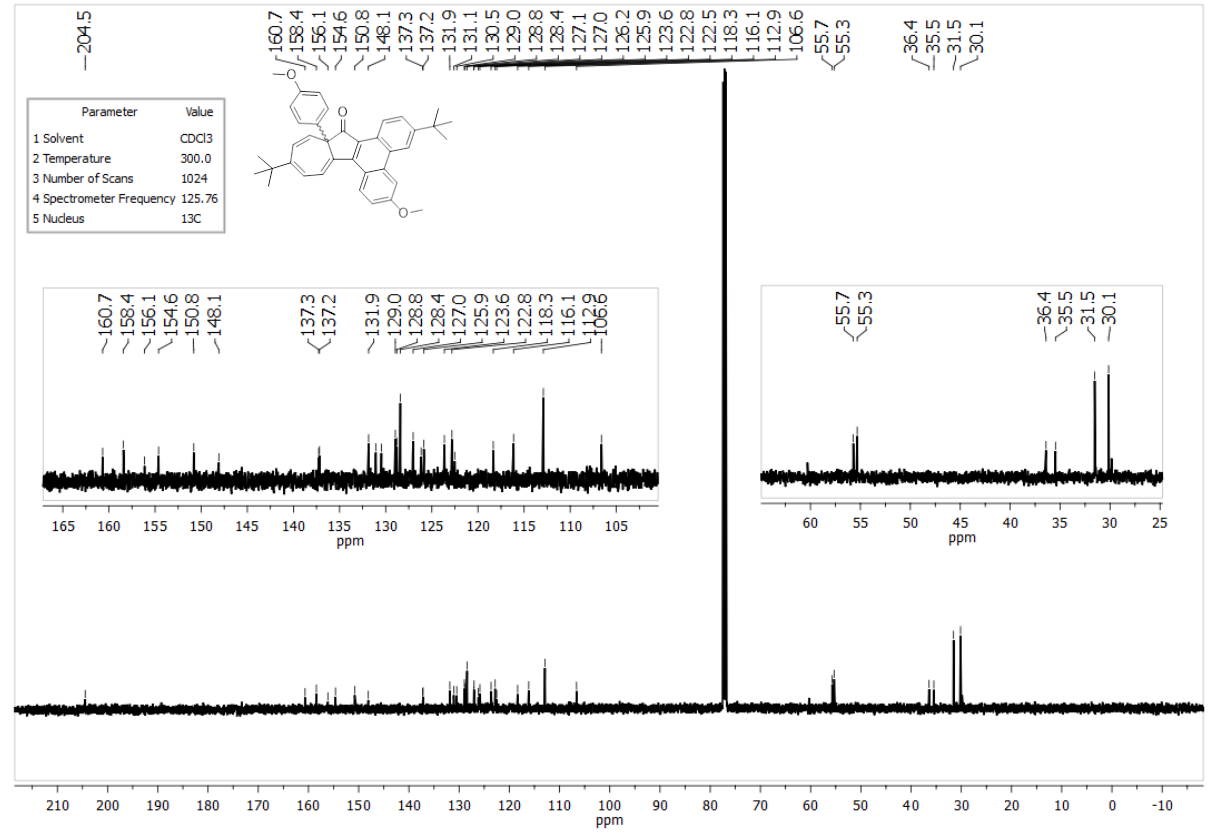
Compound 3a, 3,6,11-tri-*tert*-butyl-13*a*-(4-(*tert*-butyl)phenyl)azuleno[1,2-*l*]phenanthren-14(13*a*H)-one



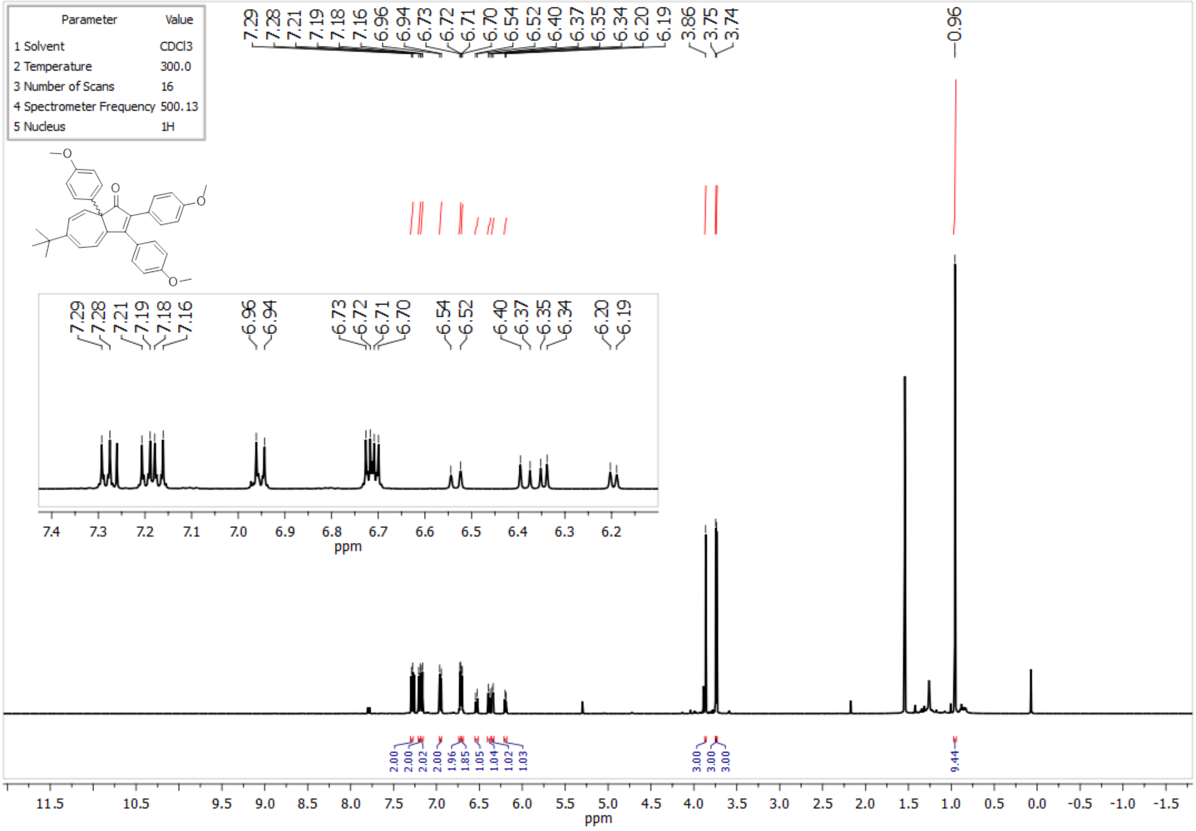


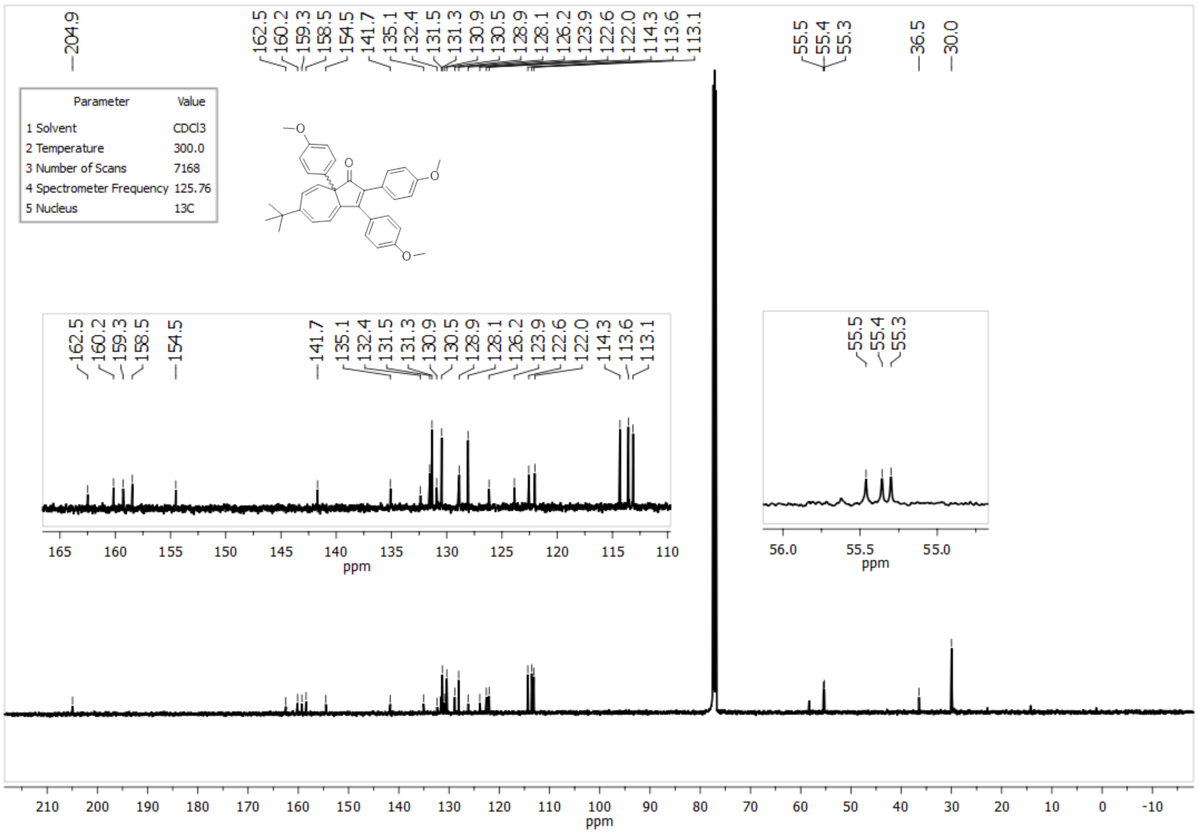
Compound 3b, 3,11-di-*tert*-butyl-6-methoxy-13*a*-(4-methoxyphenyl)azuleno[1,2-*l*]phenanthren-14(13*a*H)-one



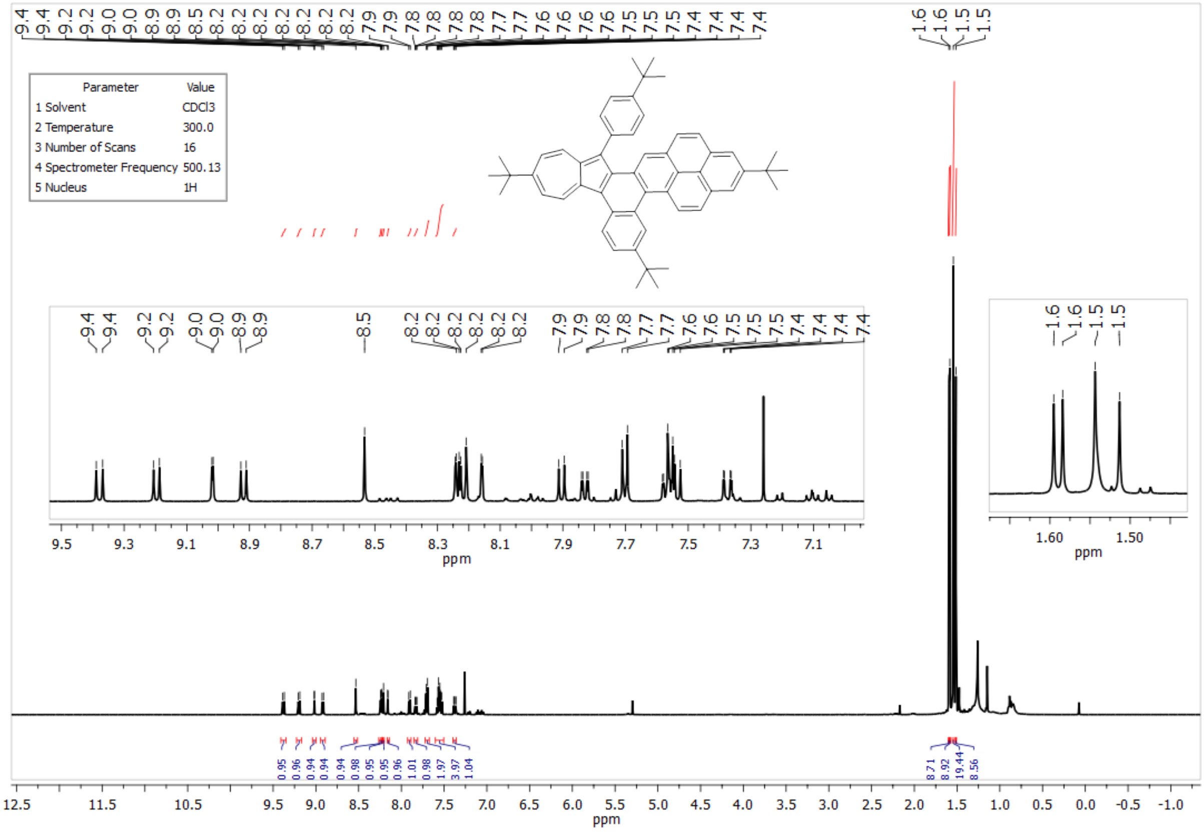


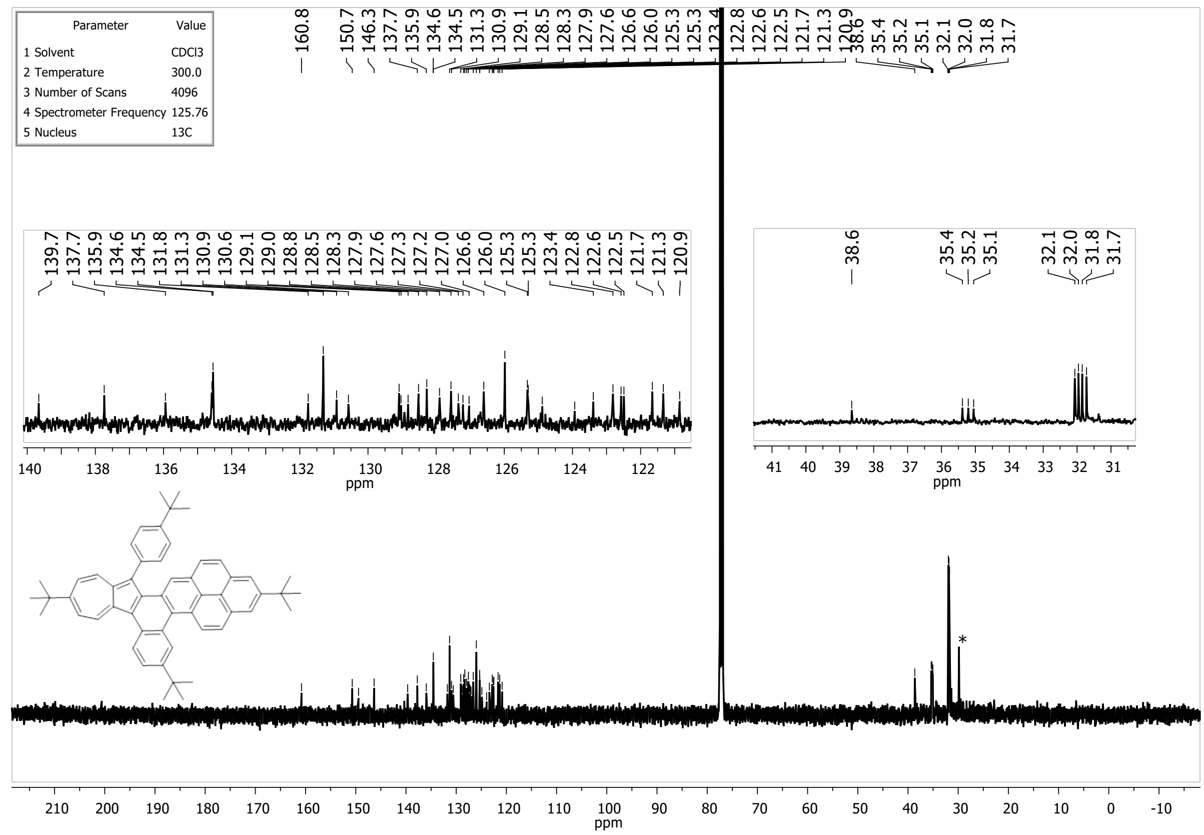
Compound 3c, 11-(*tert*-butyl)-3,6-dimethoxy-13*a*-(4-methoxyphenyl)azuleno[1,2-*l*]phenanthren-14(13*aH*)-one



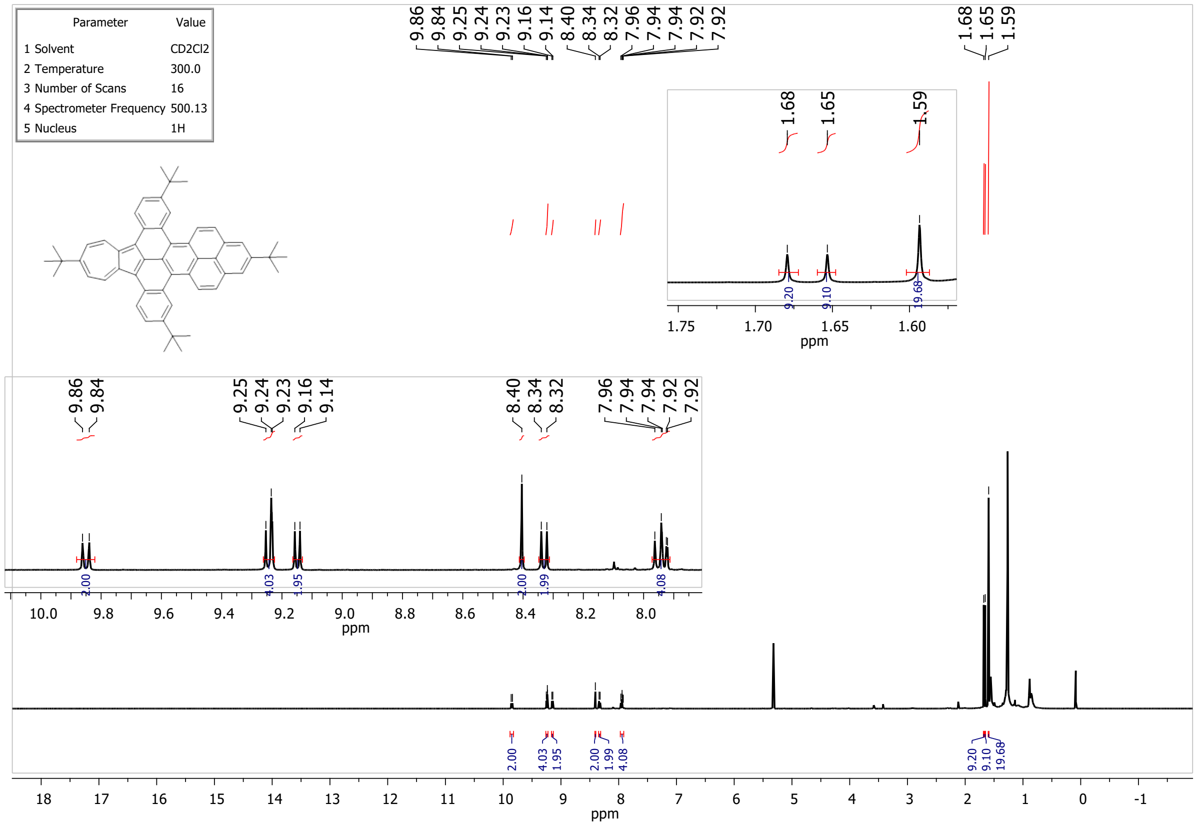


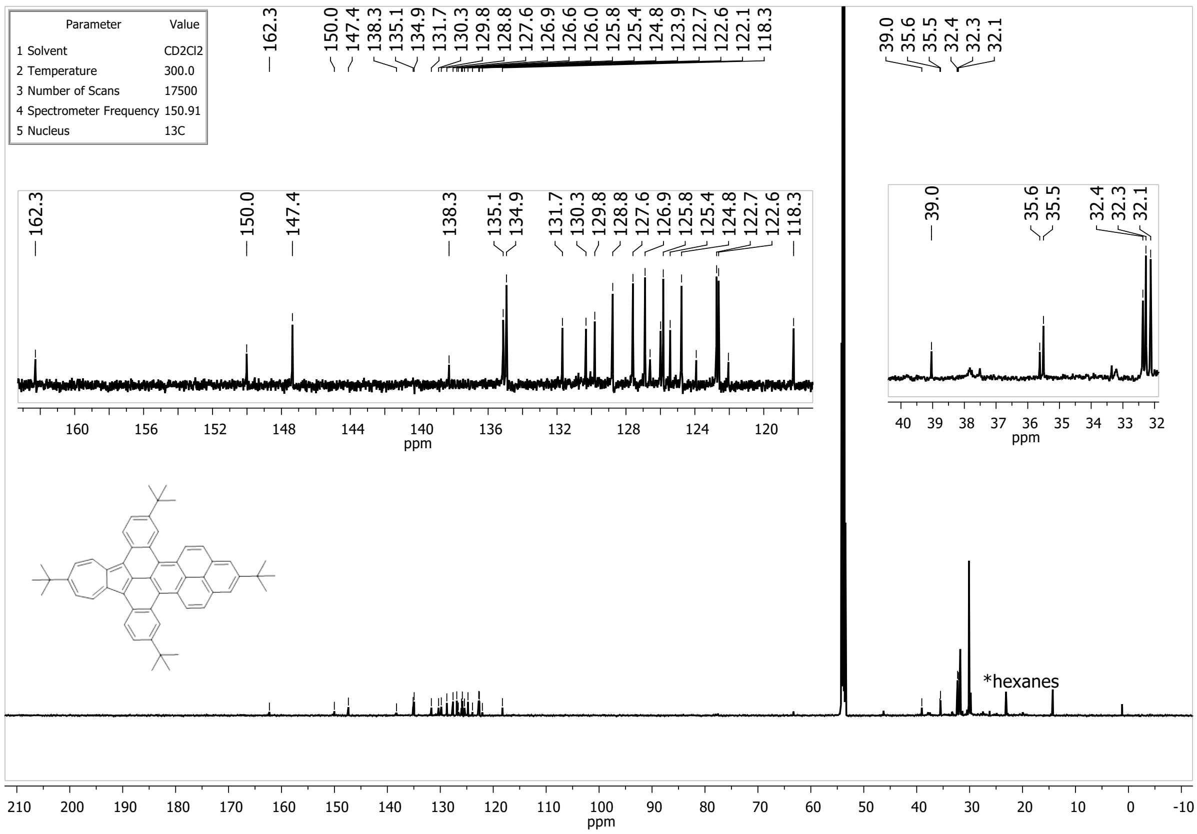
Compound 4d, 4,9,14-tri-*tert*-butyl-17-(4-(*tert*-butyl)phenyl)azuleno[2,1-*k*]dibenzo[*m*,*pqr*]tetraphene



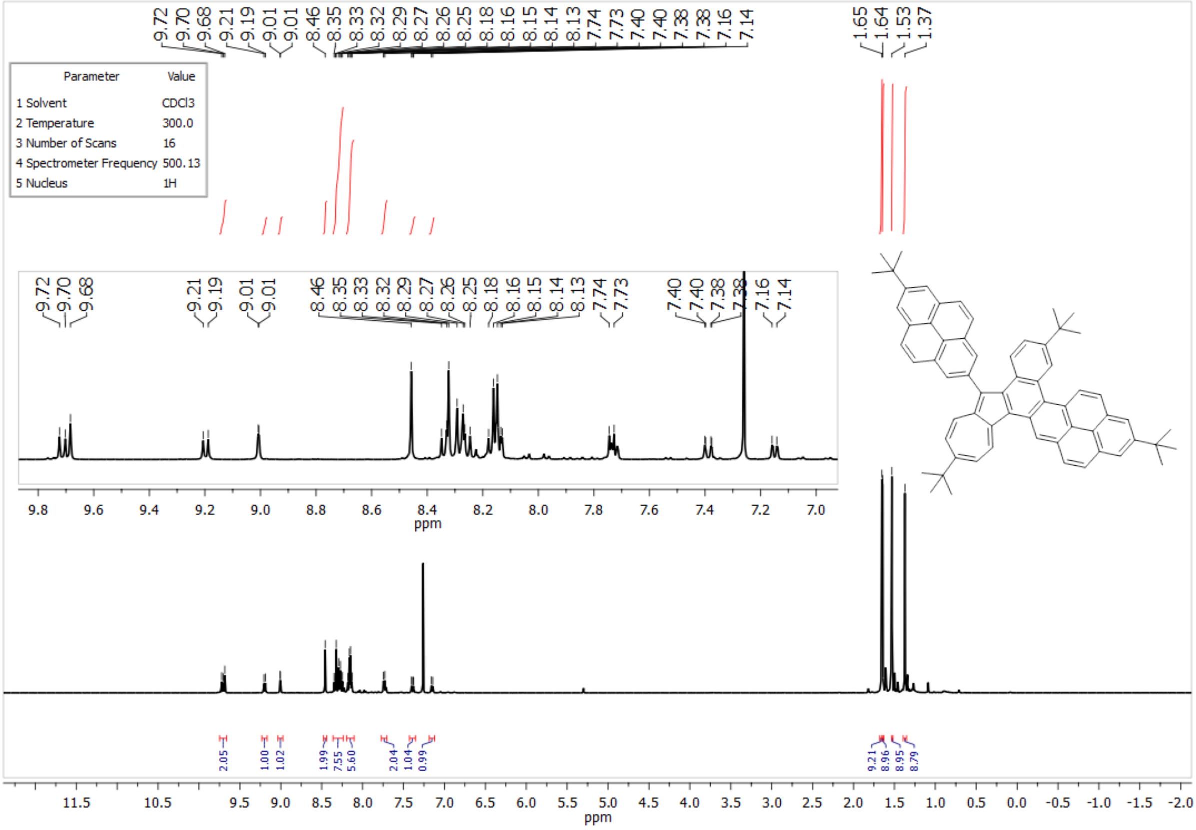


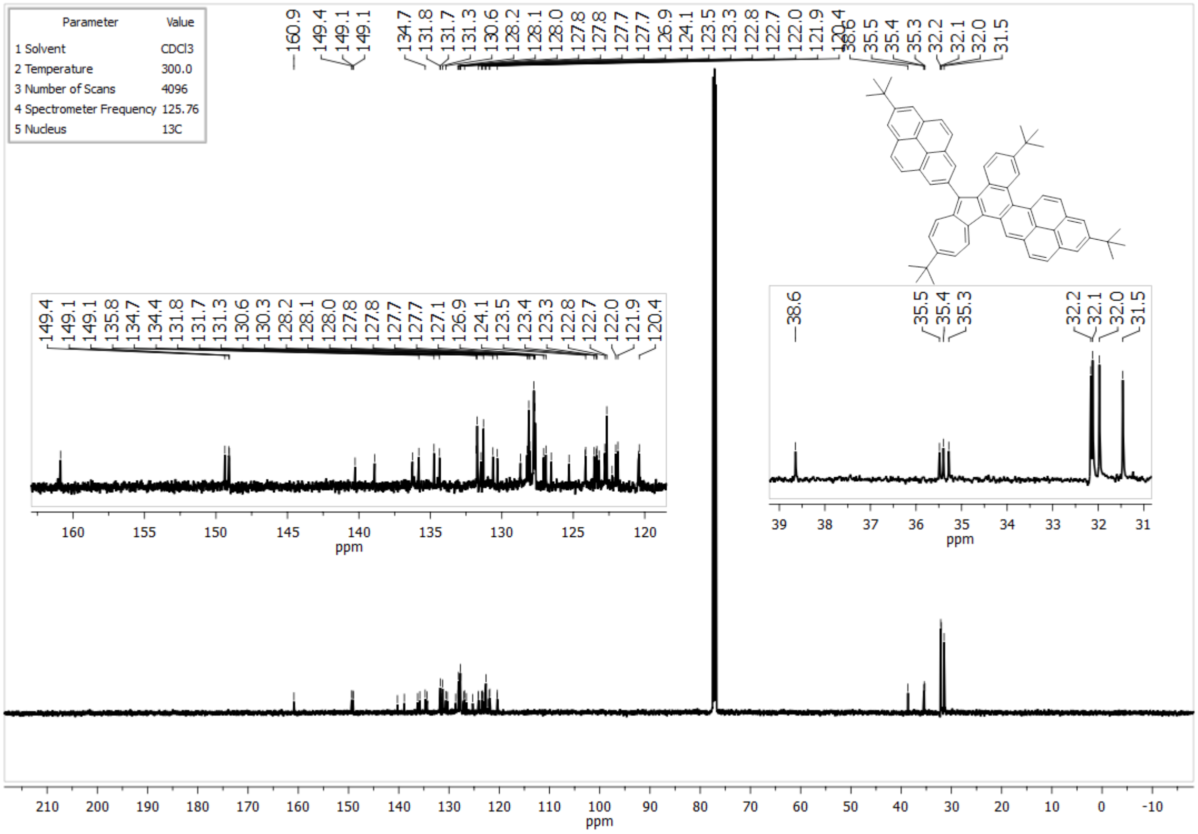
Compound 2d, 2,7,12,17-tetra-*tert*-butylazuleno[1,2,3-*cd*]tribenzo[*a*,*f*,*lm*]perylene



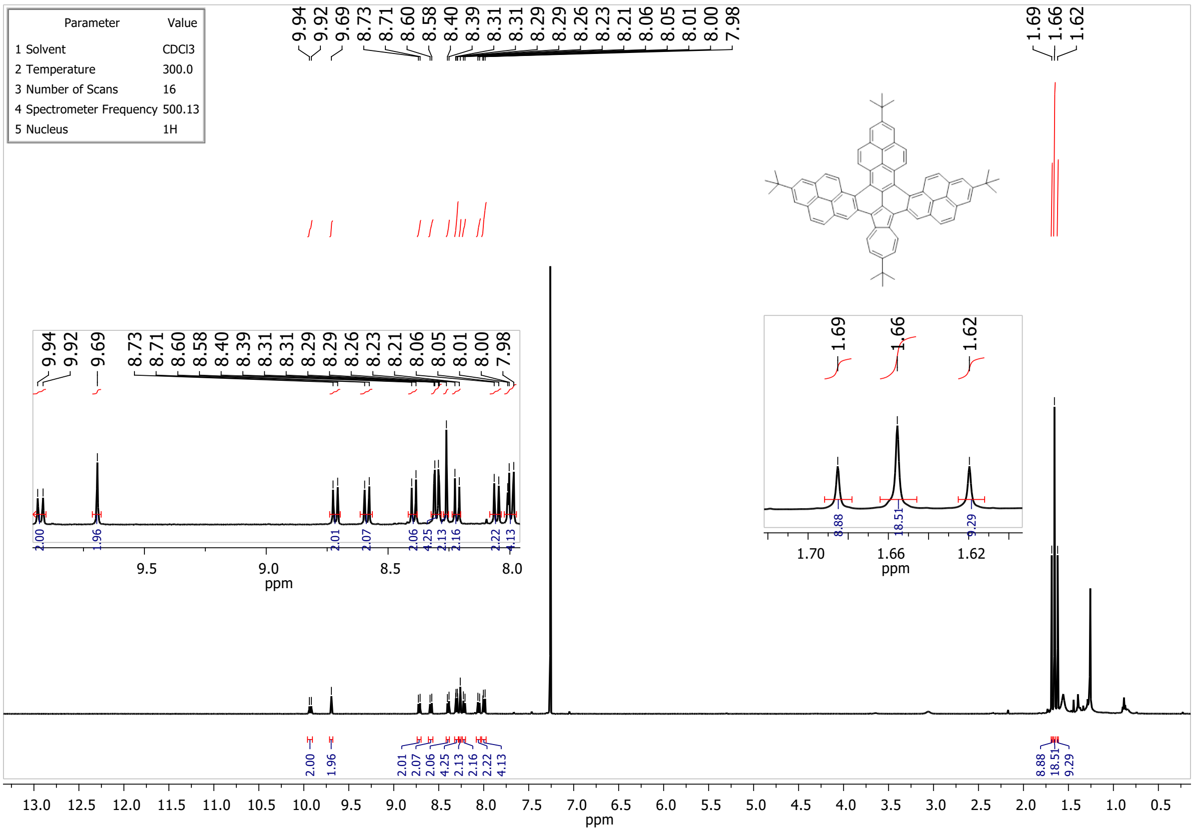


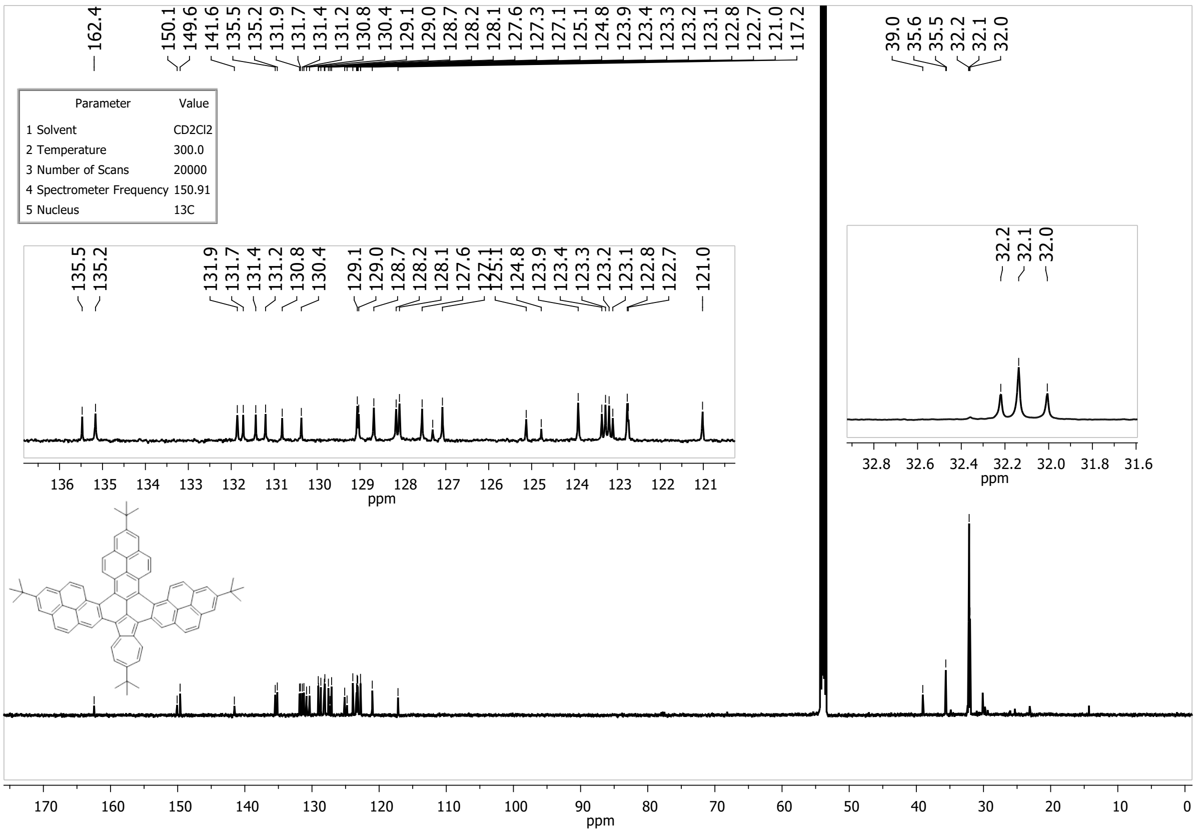
Compound 4e, 2,7,13-tri-*tert*-butyl-10-(7-(*tert*-butyl)pyren-2-yl)azuleno[1,2-*k*]dibenzo[*m*,*pqr*]tetraphene





Compound 2f, 2,9,16,23-tetra-*tert*-butylazuleno[1,2,3-*hi*]dinaphtho[8,1,2-*pqr*:2',1',8'-*yza*]pyreno[1,2,3-*uv*]hexacene





Cartesian coordinates of DFT-optimized structures

Compound 3a

Energy: −4681847.344 kJ/mol

C	0.86938	-1.16403	-0.46896
C	1.68630	-0.09963	-1.18210
C	0.61401	0.93592	-1.60320
C	-0.66447	0.53062	-0.99994
C	-0.53549	-0.73623	-0.44285
C	1.47230	-2.23743	0.12155
C	2.83764	-2.64733	-0.04427
C	3.66373	-2.46156	-1.12765
C	3.21937	-1.75989	-2.31741
C	2.30865	-0.76271	-2.38700
C	-1.71279	-1.42481	0.04055
C	-1.89828	1.26421	-0.99400
C	2.68455	0.65763	-0.28527
C	-2.94907	-0.70962	0.11130
C	-4.08477	-1.38270	0.62003
C	-4.06848	-2.71228	1.02213
C	-2.85057	-3.41577	0.87912
C	-1.71591	-2.79260	0.40350
C	-2.00917	2.56649	-1.52684
C	-3.19255	3.27685	-1.43216
C	-4.32860	2.72870	-0.79865
C	-4.21838	1.43660	-0.28722
C	-3.03684	0.67120	-0.37345
C	3.80908	1.28475	-0.83752
C	4.66893	2.04189	-0.04515
C	4.44540	2.22034	1.33146
C	3.30875	1.60260	1.86985
C	2.44341	0.84214	1.07870
O	0.83710	1.88567	-2.34256
C	5.06310	-3.12890	-1.11600
C	5.85288	-2.60684	0.10911
C	5.88820	-2.79733	-2.37698
C	4.92625	-4.66717	-1.02437
C	-5.30713	-3.43519	1.57715
C	-5.65720	-4.63152	0.65930
C	-4.99347	-3.95639	3.00065
C	-6.54031	-2.51647	1.66194
C	-5.65632	3.49839	-0.65939
C	-6.78720	2.71142	-1.36437
C	-6.00299	3.66027	0.84022
C	-5.58647	4.90303	-1.28902
C	5.42431	3.06013	2.17150
C	5.47952	4.50129	1.61053
C	5.00809	3.13708	3.65270
C	6.83607	2.43057	2.09934
H	0.90025	-2.84362	0.81641
H	3.20384	-3.29543	0.74911
H	3.65546	-2.07913	-3.26033
H	2.01187	-0.39003	-3.36540
H	-5.01775	-0.84086	0.67919
H	-2.79681	-4.46977	1.13381
H	-0.82208	-3.38451	0.26427
H	-1.14378	3.00472	-2.00874
H	-3.22988	4.27566	-1.85173
H	-5.08490	1.00880	0.20195
H	4.02163	1.17274	-1.89611
H	5.53246	2.50265	-0.51749
H	3.07841	1.70501	2.92472
H	1.57753	0.37960	1.54324
H	6.85292	-3.05685	0.13221
H	5.35497	-2.85174	1.05260
H	5.96894	-1.51801	0.06437
H	6.89817	-3.20805	-2.26764
H	5.98131	-1.71642	-2.53075
H	5.45714	-3.23654	-3.28354
H	5.91744	-5.13702	-1.02297
H	4.36613	-5.06250	-1.87988
H	4.40833	-4.97729	-0.11100
H	-6.53374	-5.16176	1.05025
H	-4.83516	-5.35175	0.59279
H	-5.89064	-4.29129	-0.35611
H	-5.86275	-4.48651	3.40760
H	-4.75299	-3.12829	3.67729
H	-4.14732	-4.65145	3.00487
H	-7.38632	-3.07785	2.07338
H	-6.84106	-2.14301	0.67645
H	-6.36438	-1.65595	2.31743
H	-7.73820	3.24942	-1.26995
H	-6.92382	1.71506	-0.93104
H	-6.57173	2.58723	-2.43190
H	-6.94821	4.20481	0.95344
H	-5.22189	4.22286	1.36446
H	-6.11382	2.69277	1.34115
H	-6.55080	5.40804	-1.16455
H	-5.37243	4.85959	-2.36294
H	-4.82255	5.52739	-0.81200
H	6.18033	5.11015	2.19480
H	4.49360	4.97803	1.65823
H	5.81114	4.51998	0.56703
H	5.73346	3.74292	4.20739
H	4.97820	2.14617	4.12009
H	4.02407	3.60352	3.77630
H	7.54736	3.02283	2.68800
H	7.20982	2.38597	1.07096
H	6.83060	1.41003	2.49966

Compound 3b

Energy: −4457175.222 kJ/mol

C	-1.10195	-1.00235	0.20012
C	-1.70041	0.22819	0.86171
C	-0.44925	1.04234	1.27549
C	0.73061	0.36752	0.71986
C	0.36148	-0.86824	0.19828
C	-1.89906	-1.95029	-0.37508
C	-3.32084	-2.07457	-0.22548
C	-4.10759	-1.69508	0.83652
C	-3.54874	-1.05781	2.01399
C	-2.45913	-0.25869	2.07236
C	1.38153	-1.79620	-0.23069
C	2.08816	0.83314	0.72727
C	-2.51511	1.13373	-0.08091
C	2.74137	-1.35048	-0.28752
C	3.73256	-2.24874	-0.74392
C	3.41808	-3.55355	-1.10143
C	2.08983	-4.01343	-0.97858
C	1.10743	-3.15068	-0.55202
C	2.45152	2.10341	1.22419
C	3.75745	2.55312	1.14609
C	4.77279	1.76256	0.56593
C	4.41173	0.50351	0.08932
C	3.09626	-0.00026	0.16029
C	-3.51745	1.96995	0.41698
C	-4.20686	2.86399	-0.40816
C	-3.88482	2.94061	-1.76801
C	-2.86944	2.11871	-2.27918
C	-2.19534	1.23584	-1.44406

O	-0.49140	2.04605	1.97658
C	-5.61109	-2.07401	0.81745
C	-6.26759	-1.44501	-0.43581
C	-6.37072	-1.54803	2.05323
C	-5.77875	-3.61127	0.77097
O	4.31193	-4.47269	-1.54897
C	5.67957	-4.08913	-1.68322
C	6.23367	2.23852	0.44858
C	7.15813	1.26508	1.21849
C	6.64874	2.26774	-1.04203
C	6.43647	3.65117	1.02962
O	-4.49162	3.77029	-2.66789
C	-5.52259	4.63213	-2.19738
H	-1.45061	-2.67949	-1.04202
H	-3.79813	-2.66183	-1.00708
H	-4.05201	-1.25403	2.95709
H	-2.10739	0.07889	3.04532
H	4.76214	-1.92538	-0.79342
H	1.86909	-5.05037	-1.21026
H	0.10809	-3.53921	-0.41662
H	1.68249	2.72571	1.66527
H	3.98848	3.53752	1.53684
H	5.18427	-0.10927	-0.35928
H	-3.78047	1.92406	1.46896
H	-4.98315	3.48814	0.01952
H	-2.62371	2.18688	-3.33483
H	-1.41547	0.60855	-1.86525
H	-7.33559	-1.69313	-0.46622
H	-5.81392	-1.80901	-1.36304
H	-6.17061	-0.35347	-0.42145
H	-7.44035	-1.75545	1.93672
H	-6.25115	-0.46564	2.17511
H	-6.04622	-2.03494	2.97959
H	-6.84293	-3.87722	0.76573
H	-5.31691	-4.08261	1.64644
H	-5.32175	-4.04485	-0.12449
H	6.19765	-4.96910	-2.06611
H	6.10935	-3.80443	-0.71560
H	5.79187	-3.26059	-2.39235
H	8.20198	1.59208	1.13950
H	7.09754	0.24549	0.82355
H	6.89253	1.23027	2.28137
H	7.68829	2.60354	-1.13880
H	6.01472	2.95657	-1.61206
H	6.57355	1.27911	-1.50709
H	7.48705	3.94320	0.92265
H	6.18876	3.69401	2.09628
H	5.83043	4.39941	0.50636
H	-5.85926	5.19846	-3.06721
H	-5.14860	5.32596	-1.43434
H	-6.36526	4.06247	-1.78619

Compound 3c

Energy: −4348167.184 kJ/mol

C	0.56973	-0.82746	-0.38637
C	1.21697	0.46467	-0.83264
C	-0.01635	1.36655	-1.09848
C	-1.23107	0.65121	-0.65091
C	-0.87405	-0.62678	-0.27002
C	1.27112	-1.95201	-0.06798
C	2.67391	-2.17027	-0.27841
C	3.49225	-1.61215	-1.23046
C	2.99220	-0.68241	-2.23016
C	1.96827	0.19167	-2.11348
C	-1.78181	-1.67646	0.24204
C	-2.56915	1.25194	-0.77295
C	2.05822	1.15960	0.25511
C	-2.62787	-1.41928	1.33074
C	-3.47811	-2.39901	1.84266
C	-3.50638	-3.67041	1.25250
C	-2.67067	-3.94228	0.15762
C	-1.81702	-2.96247	-0.33170
C	-2.76447	2.61242	-0.48296
C	-4.01669	3.21708	-0.60198
C	-5.11344	2.46202	-1.03534
C	-4.93467	1.10395	-1.34696
C	-3.68667	0.51372	-1.21658
C	3.07767	2.05034	-0.09111
C	3.80005	2.75352	0.87766
C	3.49671	2.57627	2.23236
C	2.46734	1.69476	2.59452
C	1.75925	1.00456	1.61791
O	0.04358	2.46544	-1.63209
C	4.96238	-2.09837	-1.32028
C	5.65005	-1.87338	0.04840
C	5.77852	-1.32837	-2.37991
C	5.00724	-3.60266	-1.67925
O	-4.29980	-4.69749	1.66262
C	-5.17688	-4.47885	2.76560
O	-6.37803	2.94595	-1.19165
H	-3.57002	-0.53330	-1.47540
C	-6.61581	4.32064	-0.90061
O	4.13616	3.20398	3.26358
C	5.18398	4.11518	2.94888
H	0.73046	-2.77327	0.39791
H	3.09699	-2.96527	0.33211
H	3.49322	-0.70250	-3.19454
H	1.66860	0.76446	-2.98907
H	-4.10770	-2.16288	2.69243
H	-2.70674	-4.92862	-0.29448
H	-1.18360	-3.18797	-1.18427
H	-1.92335	3.21336	-0.15588
H	-4.12236	4.26791	-0.35848
H	-5.78906	0.53237	-1.69693
H	3.32834	2.19847	-1.13669
H	4.58852	3.42799	0.56393
H	2.23814	1.56348	3.64795
H	0.96978	0.32535	1.92528
H	6.69525	-2.20270	0.00285
H	5.16008	-2.43158	0.85223
H	5.63813	-0.81212	0.32160
H	6.82910	-1.63411	-2.32060
H	5.73531	-0.24525	-2.21926
H	5.43931	-1.53709	-3.40054
H	6.04672	-3.94552	-1.75177
H	4.52163	-3.79018	-2.64411
H	4.50408	-4.21611	-0.92470
H	-5.70914	-5.41956	2.91254
H	-5.89812	-3.68153	2.55003
H	-4.61906	-4.22973	3.67623
H	-7.67656	4.48695	-1.09391
H	-6.02024	4.97524	-1.54831
H	-6.39631	4.55101	0.14899
H	5.54561	4.49678	3.90506
H	4.81943	4.95063	2.33843
H	6.00649	3.61482	2.42280
H	-2.61685	-0.43741	1.79427

Compound 2d

Energy: −5488784.837 kJ/mol

C	2.51166	-3.58953	0.67258
C	0.20689	0.00148	0.23855
C	-0.17850	-5.92802	2.15623
C	1.90074	-4.72194	1.19555
C	0.52663	-4.73591	1.48216
C	-0.22688	3.62185	1.02077
C	2.39207	1.17218	-0.06520
C	0.49195	4.78484	1.29025
C	-0.19932	-3.58458	1.16130
C	1.86975	4.76659	0.99741
C	-0.45570	-1.25459	0.23522
C	1.78679	-2.42690	0.35216
C	0.36379	-2.44611	0.55116
C	3.69564	0.74554	-0.45543
C	3.69916	-0.75156	-0.42465
C	0.34702	2.45933	0.45558
C	-0.46484	1.25272	0.18907
C	8.14744	-0.06182	-1.96627
C	6.04483	-1.25202	-1.26872
C	-2.53524	-0.01737	-0.24944
C	1.62600	0.00414	0.12144
C	1.76725	2.43929	0.25565
C	-1.84342	-1.26750	-0.07913
C	-1.85395	1.24287	-0.12355
C	2.40394	-1.16825	-0.02008
C	4.75991	-1.56680	-0.82763
C	6.04275	1.23156	-1.31875
C	6.67353	-0.00824	-1.48412
C	2.48785	3.62247	0.52333
C	-0.14648	6.04142	1.90850
C	4.74533	1.54883	-0.88957
C	8.21975	-0.80583	-3.32344
H	7.85437	-1.83501	-3.25517
H	9.25877	-0.84465	-3.67101
H	7.62653	-0.28699	-4.08509
C	8.77976	1.33011	-2.16473
H	8.26764	1.91140	-2.93944
H	9.82042	1.20724	-2.48346
H	8.78664	1.91622	-1.23907
C	9.00095	-0.81465	-0.91475
H	8.97336	-0.29931	0.05219
H	10.04502	-0.85827	-1.24610
H	8.65952	-1.84236	-0.75830
H	6.64742	-2.12671	-1.49280
H	4.55406	-2.63268	-0.81697
H	6.63065	2.10549	-1.57034
H	4.53160	2.61268	-0.92163
H	3.59071	-3.59077	0.57530
H	3.56631	3.62672	0.42067
C	-2.57330	-2.47610	-0.36414
C	-3.93527	-0.02946	-0.56855
C	-3.90406	-2.47587	-0.65205
C	-4.64616	-1.25490	-0.72407
C	-2.59457	2.43504	-0.45061
C	-3.92511	2.41478	-0.73640
C	-4.65806	1.18564	-0.76590
C	-6.02543	-1.24322	-0.99950
C	-6.03306	1.14830	-1.03930
C	-6.74636	-0.05444	-1.14969
C	-8.25798	-0.02575	-1.44235
C	-8.50865	0.69222	-2.79002
C	-8.86577	-1.43848	-1.53060
C	-8.98330	0.74173	-0.31118
H	-2.03650	-3.41393	-0.40103
H	-4.41444	-3.41096	-0.86951
H	-6.52137	-2.20240	-1.10319
H	-6.54453	2.09737	-1.17690
H	-4.44295	3.33770	-0.98578
H	-2.06583	3.37552	-0.52008
H	-9.93999	-1.36313	-1.73301
H	-8.74340	-1.99468	-0.59425
H	-8.41758	-2.02622	-2.33975
H	-8.01231	0.16501	-3.61297
H	-9.58320	0.72591	-3.00688
H	-8.13849	1.72272	-2.77921
H	-8.62491	1.77270	-0.22283
H	-10.06142	0.77829	-0.50906
H	-8.83197	0.24897	0.65622
C	-1.65111	5.86448	2.18655
C	0.02792	7.23094	0.93375
C	0.55407	6.37335	3.24807
H	0.44061	5.55047	3.96329
H	1.62528	6.55704	3.11433
H	-2.21519	5.65425	1.27065
H	-2.05490	6.78716	2.61823
H	-1.84270	5.05518	2.90033
C	0.77985	-7.11045	2.39578
C	-1.33675	-6.42432	1.25828
C	-0.74854	-5.48378	3.52468
H	-0.96338	-6.74917	0.28011
H	-2.08682	-5.64411	1.09052
H	-1.84363	-7.27594	1.72821
H	0.05211	-5.13788	4.18858
H	-1.25801	-6.32275	4.01435
H	-1.47328	-4.66946	3.41975
H	1.20975	-7.48297	1.45885
H	0.23265	-7.93780	2.86131
H	1.60304	-6.84034	3.06684
H	2.52148	-5.58015	1.42738
H	-1.26821	3.58147	1.30550
H	-1.24377	-3.54479	1.44304
H	2.48130	5.64275	1.19360
H	-0.47327	7.03197	-0.02067
H	1.08335	7.43375	0.72300
H	-0.40755	8.14134	1.36339
H	0.11449	7.27409	3.69356

Compound 4d

Energy: −5491837.596 kJ/mol

C	-2.59742	3.13779	-0.67734
C	0.05841	-0.04048	0.22351
C	-2.30919	6.53456	1.15976
C	-2.57633	4.51403	-0.43186
C	-2.34669	5.02687	0.85168
C	1.07575	-3.61429	0.77387
C	-1.92790	-1.51986	-0.03347
C	0.54548	-4.87612	1.02808
C	-2.14471	4.09133	1.88362
C	-0.84371	-5.03302	0.84651
C	0.64610	1.23392	0.30215
C	-2.38788	2.21059	0.35253
C	-2.16830	2.72035	1.64521
C	-3.31491	-1.37875	-0.34652
C	-3.62827	0.06369	-0.21082
C	0.30219	-2.51983	0.31742
C	0.89762	-1.19546	0.09475
C	-7.93570	-1.45216	-1.49719
C	-6.11828	0.09491	-0.69389
C	2.85194	0.30604	-0.11492
C	-1.38555	-0.22138	0.16204
C	-1.11015	-2.68886	0.20485
C	2.02238	1.42528	0.20243
C	2.28173	-0.99941	-0.21797
C	-2.44288	0.74769	0.10279
C	-4.90008	0.64907	-0.33458
C	-5.54563	-2.27835	-1.17664
C	-6.45301	-1.22181	-1.10356

C	-1.64519	-3.96791	0.47613
C	1.39471	-6.05950	1.52492
C	-4.18095	-2.34731	-0.82858
C	-8.30764	-0.51884	-2.67679
H	-8.18706	0.53939	-2.42613
H	-9.35521	-0.67602	-2.95934
H	-7.68460	-0.73079	-3.55328
C	-8.23771	-2.89830	-1.93728
H	-7.66617	-3.18813	-2.82596
H	-9.30021	-2.98024	-2.19059
H	-8.03301	-3.62345	-1.14191
C	-8.84209	-1.13758	-0.28025
H	-8.60419	-1.79515	0.56373
H	-9.89296	-1.29710	-0.54882
H	-8.74095	-0.10266	0.06034
H	-6.93946	0.80487	-0.68413
H	-4.93096	1.71427	-0.11375
H	-5.93409	-3.22085	-1.54235
H	-3.74478	-3.32721	-0.99679
H	-2.76906	2.77904	-1.68887
H	-2.71808	-4.11354	0.46313
C	2.62335	2.72478	0.34889
C	4.24623	0.51658	-0.34179
C	3.96133	2.90811	0.18008
C	4.82136	1.81180	-0.18129
C	3.14229	-2.04079	-0.72427
C	4.46824	-1.83568	-0.97116
C	5.08556	-0.56169	-0.74484
C	6.19967	1.98521	-0.38849
C	6.45517	-0.33376	-0.94986
C	7.03844	0.92859	-0.76956
C	8.55102	1.11119	-0.99973
C	8.89760	0.74006	-2.46152
C	9.01352	2.55936	-0.75018
C	9.33192	0.18419	-0.03768
H	1.97798	3.56286	0.60033
H	4.40273	3.89438	0.30110
H	6.60644	2.98089	-0.24775
H	7.06798	-1.17569	-1.26130
H	5.07520	-2.64388	-1.37217
H	-2.01197	2.02930	2.46966
H	2.71176	-3.00415	-0.96609
H	10.09309	2.63374	-0.92218
H	8.82005	2.87795	0.28043
H	8.52170	3.26793	-1.42630
H	8.36388	1.38733	-3.16704
H	9.97350	0.85964	-2.63767
H	8.63517	-0.29758	-2.69277
H	9.08054	-0.87018	-0.19298
H	10.41136	0.29713	-0.19557
H	9.11383	0.43146	1.00775
C	2.88282	-5.69416	1.68126
C	1.28705	-7.22280	0.50981
C	0.86875	-6.53441	2.90088
H	0.93809	-5.73197	3.64443
H	-0.17683	-6.85585	2.84968
H	3.32607	-5.36842	0.73331
H	3.44196	-6.57228	2.02341
H	3.03325	-4.89910	2.42042
C	-2.55771	7.39488	-0.09368
C	-0.92097	6.90679	1.73350
C	-3.40045	6.87521	2.20281
H	-0.12667	6.68551	1.01102
H	-0.70025	6.35737	2.65468
H	-0.88045	7.97802	1.96543
H	-4.39816	6.63091	1.81997
H	-3.37959	7.94635	2.43761
H	-3.25594	6.32605	3.13916
H	-1.79703	7.22365	-0.86386
H	-2.52184	8.45622	0.17643
H	-3.54167	7.19878	-0.53474
H	-2.73966	5.18553	-1.26764
H	2.12141	-3.44024	0.98238
H	-1.96996	4.43592	2.89927
H	-1.31589	-5.98975	1.05121
H	1.66776	-6.92162	-0.47308
H	0.25194	-7.55688	0.38135
H	1.87490	-8.08268	0.85345
H	1.46132	-7.38410	3.26141
H	0.01685	2.10268	0.43942

Compound 4e

Energy: -6497620.397 kJ/mol

C	-3.69843	1.26140	0.94037
H	-3.57005	1.90851	1.62392
C	0.19491	-0.74607	0.85399
C	-6.47066	-0.73871	-0.58652
C	-4.98394	0.73717	0.71914
C	-5.17790	-0.19300	-0.33406
C	3.89406	-0.89398	-0.01562
C	1.06641	1.53458	0.52966
C	4.98353	-0.00621	-0.23392
C	-4.07209	-0.60791	-1.12356
C	4.78485	1.40175	-0.13411
C	-0.83122	-1.59567	1.30713
H	-1.73464	-1.31155	1.23145
C	-2.60587	0.84786	0.17327
C	-2.80382	-0.09862	-0.83712
H	-2.05762	-0.40245	-1.34059
C	0.54752	2.87144	0.52701
C	-0.91502	2.74792	0.33455
C	2.63415	-0.37273	0.42060
C	1.53402	-1.22539	0.89297
C	8.63960	-0.12905	-1.01451
H	9.37635	0.46772	-1.07488
C	-4.30384	-1.52550	-2.20813
H	-3.57113	-1.80475	-2.74451
C	7.77009	-2.35220	-1.13368
H	7.89342	-3.27904	-1.30159
C	-0.56585	7.45099	0.27597
C	-1.55781	5.16046	-0.04718
H	-2.26444	5.67316	-0.42173
C	5.90929	2.28836	-0.31860
H	5.77727	3.22730	-0.25930
C	4.12322	-2.28263	-0.34072
H	3.39689	-2.89295	-0.29052
C	-7.93124	-2.18715	-1.88435
H	-8.06383	-2.75967	-2.63085
C	0.76525	-3.26884	2.02965
C	-0.02916	0.65123	0.53359
C	2.42415	1.03735	0.39493
C	-0.55879	-2.83212	1.85926
H	-1.27612	-3.39454	2.12712
C	1.77648	-2.45879	1.52546
H	2.67578	-2.75247	1.61229
C	-1.24729	1.39224	0.38508
C	-9.00655	-1.91559	-1.03684
C	7.37930	0.39228	-0.72220
C	-1.78499	3.80343	-0.00498
H	-2.66556	3.53671	-0.24174
C	8.86374	-1.49488	-1.22243
C	0.74466	5.37087	0.86886
H	1.34028	5.99479	1.26683
C	-0.42874	5.91736	0.38295
C	-7.56595	-0.40379	0.24657
C	3.50893	1.88846	0.11219
H	3.36280	2.82681	0.08931
C	-5.53822	-1.99804	-2.48039
H	-5.66342	-2.57657	-3.22352
C	-8.80748	-1.02007	0.01307
H	-9.53524	-0.81967	0.59001
C	-6.66770	-1.64044	-1.66444
C	6.48577	-1.87966	-0.80120
C	7.14577	1.80752	-0.57390
H	7.87375	2.41216	-0.65716
C	6.27863	-0.49938	-0.58015
C	-7.34326	0.53619	1.31075
H	-8.06863	0.77881	1.87412
C	10.29127	-1.98959	-1.50712
C	5.34669	-2.74406	-0.71660
H	5.44828	-3.66456	-0.92867

C	1.20023	4.03361	0.86838
H	2.10063	3.91853	1.14847
C	-1.74368	7.92177	1.14354
H	-2.56482	7.47464	0.85003
H	-1.84943	8.89180	1.05234
H	-1.56787	7.69916	2.08159
C	0.68424	8.21451	0.73879
H	0.86946	7.99988	1.67689
H	0.53062	9.17824	0.64842
H	1.45017	7.95266	0.18638
C	-6.11821	1.08683	1.53110
H	-6.01030	1.71519	2.23546
C	-10.35329	-2.60422	-1.30270
C	10.31946	-3.47069	-1.89546
H	9.76588	-3.61022	-2.69200
H	9.96869	-4.00916	-1.15552
H	11.24180	-3.74073	-2.08727
C	1.12719	-4.55035	2.79124
C	1.89407	-5.49720	1.85604
H	1.34110	-5.70186	1.07318
H	2.10525	-6.32698	2.33269
H	2.72520	-5.06690	1.56528
C	2.01359	-4.18664	3.99169
H	2.83110	-3.74974	3.67372
H	2.24851	-5.00144	4.48298
H	1.52660	-3.57680	4.58446
C	-0.81179	7.82100	-1.19693
H	-0.06038	7.50757	-1.74236
H	-0.89244	8.79415	-1.28029
H	-1.63936	7.39699	-1.50645
C	-0.11404	-5.28707	3.30823
H	-0.60172	-4.70835	3.93087
H	0.16118	-6.10601	3.77078
H	-0.69505	-5.51772	2.55344
C	10.90485	-1.17514	-2.66529
H	11.78030	-1.54819	-2.89912
H	11.01121	-0.24138	-2.38745
H	10.31243	-1.21853	-3.44478
C	11.13963	-1.80157	-0.24362
H	10.77060	-2.34721	0.48189
H	11.12875	-0.85755	0.01962
H	12.06178	-2.07941	-0.42485
C	-11.32407	-2.43662	-0.14030
H	-11.56287	-1.49068	-0.04799
H	-10.90065	-2.74891	0.68647
H	-12.13298	-2.96254	-0.31190
C	-10.97196	-1.98838	-2.57382
H	-11.82799	-2.42529	-2.76525
H	-10.36232	-2.11872	-3.33002
H	-11.11865	-1.02948	-2.43414
C	-10.13489	-4.11377	-1.51593
H	-9.70441	-4.49672	-0.72315
H	-9.56174	-4.25358	-2.29846
H	-10.99942	-4.55154	-1.66177

Compound 2f (*chiral*)

Energy: -7503962.382 kJ/mol

C	3.57994	2.65426	-0.92695
C	0.00096	0.46080	-0.00124
C	6.24870	0.18445	-0.13110
C	4.83401	2.04445	-0.91180
C	4.95099	0.74391	-0.33191
C	-3.78109	0.06047	-0.04492
C	-1.12449	2.66733	0.28597
C	-4.94538	0.79281	0.33618
C	3.77798	0.02297	0.04524
C	-4.81335	2.09085	0.91915
C	1.24122	-0.21319	-0.19590
C	2.41639	1.99027	-0.49891
C	2.48057	0.57595	-0.22912
C	-0.71118	4.02815	0.14999
C	0.75367	4.01951	-0.14289
C	-2.47688	0.59870	0.22894
C	-1.24648	-0.20251	0.19068
C	-8.67191	0.37822	0.39992
C	3.97751	-1.19349	0.78994
C	-7.71357	-1.51291	-0.72449
C	0.08627	8.72746	-0.00820
C	1.27019	6.50801	-0.03551
C	-5.99183	2.76814	1.39183
C	-3.99496	-1.15115	-0.79325
C	7.69212	-1.59420	0.72766
C	-0.01278	-2.31295	-0.00763
C	0.00743	1.87793	0.00145
C	-2.39697	2.01188	0.50197
C	1.16048	-1.61818	-0.44401
C	-1.17903	-1.60924	0.43168
C	1.15035	2.65975	-0.28135
C	8.84022	-0.94310	0.26633
C	-7.40690	0.94535	0.59823
C	1.57513	5.15066	-0.12993
C	-8.85358	-0.85099	-0.25899
C	-1.20884	6.52544	0.03755
C	0.03044	7.17738	-0.00237
C	7.41442	0.87062	-0.58921
C	-3.55325	2.68716	0.93376
C	5.22055	-1.70212	1.03189
C	8.67304	0.28946	-0.38981
C	6.40337	-1.05989	0.53938
C	-6.41870	-0.99273	-0.53752
C	-7.22870	2.21775	1.24894
C	-6.24943	0.24800	0.13607
C	7.25108	2.14639	-1.23688
C	-10.27631	-1.41179	-0.44540
C	-5.24387	-1.64591	-1.03434
C	-1.51983	5.16212	0.13803
C	0.81479	9.21164	-1.28700
H	1.84143	8.83816	-1.34871
H	0.85828	10.30695	-1.29755
H	0.28227	8.88474	-2.18744
C	-1.30483	9.39139	0.01379
H	-1.90371	9.12563	-0.86438
H	-1.18114	10.47962	0.00824
H	-1.87345	9.13085	0.91330
C	6.02030	2.71033	-1.38060
C	10.25648	-1.51942	0.45469
C	-10.28299	-2.76030	-1.19006
H	-9.72173	-3.52934	-0.64725
H	-9.85911	-2.67287	-2.19691
H	-11.31411	-3.11567	-1.29518
C	0.85650	9.21507	1.24487
H	0.35313	8.89200	2.16322
H	0.90105	10.31041	1.24976
H	1.88468	8.84175	1.27496
C	-10.93020	-1.62384	0.94103
H	-11.94784	-2.01578	0.82412
H	-10.99586	-0.68979	1.50880
H	-10.35647	-2.34137	1.53903
C	-11.12353	-0.40677	-1.26205
H	-10.68780	-0.24285	-2.25444
H	-11.19837	0.56513	-0.76313
H	-12.14163	-0.79161	-1.39717
C	10.91104	-1.73610	-0.93070
H	10.98849	-0.80174	-1.49648
H	10.33068	-2.44601	-1.53138
H	11.92396	-2.13965	-0.81226
C	11.11271	-0.52501	1.27490
H	12.12628	-0.92107	1.41155
H	10.67664	-0.35809	2.26664
H	11.19915	0.44688	0.77783
C	10.24713	-2.86922	1.19702
H	9.67905	-3.63135	0.65158
H	9.82185	-2.77903	2.20304
H	11.27419	-3.23567	1.30393
H	2.14900	7.14512	-0.02476
H	2.64006	4.95046	-0.18114
H	-2.08606	7.16025	0.02706

H	-2.58608	4.97121	0.19626
H	3.50909	3.66730	-1.30438
H	8.13865	2.66325	-1.59361
H	5.91288	3.68794	-1.84428
H	3.11397	-1.69773	1.20430
H	5.32765	-2.60961	1.62128
H	7.77155	-2.54163	1.25002
H	9.54289	0.82747	-0.75759
H	-3.47103	3.69817	1.31429
H	-5.87312	3.74338	1.85777
H	-8.11009	2.74309	1.60859
H	-3.13765	-1.66316	-1.21104
H	-5.36168	-2.55037	-1.62637
H	-9.53526	0.92448	0.77088
H	-7.80409	-2.45809	-1.24914
C	2.16604	-2.37624	-1.13520
C	-0.01950	-3.74522	-0.01126
C	2.10026	-3.73453	-1.23989
C	1.03909	-4.47515	-0.62227
C	-2.19187	-2.36081	1.12118
C	-2.14081	-3.71950	1.21946
C	-1.08735	-4.46887	0.59677
C	1.00317	-5.88162	-0.62694
C	-1.06206	-5.87116	0.59173
C	-0.03169	-6.60247	-0.02051
C	-0.07359	-8.14234	-0.00222
C	-1.36590	-8.63076	-0.69929
C	1.13018	-8.77152	-0.72896
C	-0.06464	-8.63811	1.46371
H	2.98754	-1.84454	-1.59994
H	2.86635	-4.27733	-1.78797
H	1.81833	-6.40191	-1.11840
H	-1.88099	-6.39312	1.07975
H	-2.91164	-4.25685	1.76622
H	-3.00666	-1.82240	1.59001
H	1.05242	-9.86370	-0.68853
H	2.08137	-8.49033	-0.26292
H	1.16672	-8.48136	-1.78517
H	-1.39648	-8.30025	-1.74400
H	-1.41111	-9.72650	-0.68803
H	-2.26587	-8.25505	-0.20135
H	-0.92302	-8.25908	2.02817
H	-0.10285	-9.73380	1.49320
H	0.84669	-8.31588	1.98066

Compound 2f (*meso*)

Energy: −7503971.074 kJ/mol

C	-3.63059	2.68370	0.00481
C	-0.00171	0.42156	0.33359
C	-5.89635	0.11359	-1.46127
C	-4.79621	2.08088	-0.46936
C	-4.75396	0.70330	-0.83956
C	3.56567	-0.02555	-0.62470
C	1.15943	2.61005	0.56266
C	4.74751	0.74758	-0.84132
C	-3.56416	-0.05797	-0.62314
C	4.77514	2.12623	-0.47302
C	-1.25085	-0.24074	0.44115
C	-2.45179	1.96055	0.24594
C	-2.44848	0.53418	0.04747
C	0.72874	3.90418	0.97889
C	-0.76940	3.89521	0.98046
C	2.44320	0.55590	0.04455
C	1.25405	-0.22999	0.43935
C	8.20723	0.33062	-2.23106
C	-3.52948	-1.38207	-1.19346
C	7.01124	-1.72725	-2.53261
C	-0.08307	8.33058	2.56983
C	-1.26897	6.22401	1.87598
C	5.98542	2.88005	-0.67081
C	3.54477	-1.35033	-1.19391
C	-6.99083	-1.79269	-2.53528
C	0.01093	-2.17048	1.31911
C	-0.00781	1.84385	0.38036
C	2.43147	1.98296	0.24105
C	-1.24671	-1.54266	1.01770
C	1.26212	-1.53152	1.01614
C	-1.18540	2.60134	0.56707
C	-8.18303	-1.07732	-2.68718
C	7.09016	0.93256	-1.63746
C	-1.58188	4.94244	1.42458
C	8.19604	-0.99989	-2.68447
C	1.21257	6.24283	1.87132
C	-0.02785	6.86316	2.06964
C	-7.09795	0.86499	-1.63666
C	3.60342	2.71774	-0.00043
C	-4.61174	-1.93656	-1.81017
C	-8.20835	0.25228	-2.23195
C	-5.85159	-1.22678	-1.93410
C	5.86568	-1.17232	-1.93299
C	7.09584	2.30748	-1.21060
C	5.89627	0.16901	-1.46179
C	-7.11820	2.23908	-1.20788
C	9.46185	-1.59588	-3.32925
C	4.63310	-1.89454	-1.80923
C	1.53032	4.95479	1.41855
C	-0.79227	8.38039	3.94648
H	-1.81943	8.00587	3.90043
H	-0.83193	9.41507	4.30658
H	-0.24838	7.78384	4.68775
C	1.30776	8.97381	2.73865
H	1.91310	8.46056	3.49393
H	1.18375	10.01047	3.06963
H	1.87004	8.99395	1.79848
C	-6.01402	2.82238	-0.66660
C	-9.44196	-1.68539	-3.33416
C	9.26563	-3.06075	-3.76373
H	8.47247	-3.16185	-4.51321
H	9.02012	-3.70902	-2.91486
H	10.19241	-3.43752	-4.21063
C	-0.87134	9.18792	1.54778
H	-0.38099	9.17661	0.56764
H	-0.91683	10.22762	1.89226
H	-1.89932	8.83774	1.41401
C	9.84069	-0.76898	-4.58122
H	10.74547	-1.17889	-5.04617
H	10.03858	0.27935	-4.33442
H	9.03570	-0.79334	-5.32483
C	10.62711	-1.54732	-2.31213
H	10.39098	-2.13523	-1.41759
H	10.84818	-0.52353	-1.99264
H	11.53851	-1.96140	-2.76017
C	-10.60898	-1.64980	-2.31852
H	-10.84095	-0.62866	-1.99827
H	-10.36807	-2.23622	-1.42428
H	-11.51549	-2.07269	-2.76824
C	-9.82752	-0.86093	-4.58567
H	-10.72749	-1.27945	-5.05230
H	-9.02135	-0.87626	-5.32824
H	-10.03635	0.18505	-4.33790
C	-9.23038	-3.14771	-3.77002
H	-8.97916	-3.79437	-2.92161
H	-8.43547	-3.23991	-4.51879
H	-10.15282	-3.53338	-4.21831
H	-2.14428	6.81342	2.13078
H	-2.64521	4.72714	1.44338
H	2.08728	6.83289	2.11522
H	2.59557	4.74889	1.43343
H	-3.63693	3.75925	0.13299
H	-8.03331	2.81050	-1.34284
H	-6.03280	3.86814	-0.36956
H	-2.60511	-1.94405	-1.14926
H	-4.53881	-2.93403	-2.23702
H	-6.91695	-2.81611	-2.88736
H	-9.11280	0.84450	-2.34458

H	3.59882	3.79350	0.12598
H	5.99316	3.92637	-0.37528
H	8.00505	2.88816	-1.34587
H	2.62601	-1.92151	-1.14999
H	4.57055	-2.89311	-2.23516
H	9.10562	0.93198	-2.34382
H	6.94818	-2.75184	-2.88339
C	-2.44923	-2.19996	1.45695
C	0.01682	-3.45316	1.96242
C	-2.43189	-3.42219	2.05590
C	-1.20052	-4.10932	2.30511
C	2.47190	-2.17755	1.45520
C	2.46769	-3.39916	2.05406
C	1.24260	-4.09915	2.30445
C	-1.17133	-5.37713	2.91348
C	1.22158	-5.36299	2.91121
C	0.02663	-6.03126	3.21826
C	0.07379	-7.42173	3.87862
C	0.81293	-7.32274	5.23452
C	-1.33182	-7.99593	4.13844
C	0.83217	-8.40291	2.95297
H	-3.39452	-1.68939	1.33045
H	-3.36148	-3.88243	2.38171
H	-2.12369	-5.83869	3.15154
H	2.17690	-5.82174	3.15229
H	3.40195	-3.84977	2.37993
H	3.41178	-1.65718	1.32841
H	-1.24360	-8.98496	4.60165
H	-1.90212	-8.11477	3.21014
H	-1.91240	-7.36292	4.81907
H	0.29241	-6.63934	5.91536
H	0.86010	-8.30857	5.71278
H	1.83949	-6.96091	5.11489
H	1.85869	-8.07304	2.76177
H	0.88103	-9.39690	3.41384
H	0.32473	-8.50125	1.98630

Compound (1a)$^{\cdot+}$

Energy: –4486762.026 kJ/mol

C	0.34709	2.25004	-0.06412
C	1.03968	0.95782	-0.03796
C	0.07353	0.00692	0.00080
C	-1.25077	0.66823	-0.03812
C	-1.09025	2.01404	-0.09646
C	-2.14244	2.97884	-0.29173
C	-2.04791	4.31398	-0.26543
C	-0.90543	5.18821	0.00793
C	0.37089	4.76019	0.09544
C	0.95416	3.44179	-0.00544
C	0.30793	-1.44433	0.05210
C	-1.27046	6.70313	0.18418
C	-0.06956	7.60798	0.56825
C	-1.83753	7.27492	-1.13586
C	-2.31369	6.88114	1.31361
C	0.93333	-2.11135	-1.00249
C	1.14339	-3.49332	-0.94330
C	0.73024	-4.25547	0.16639
C	0.09609	-3.56955	1.21456
C	-0.11200	-2.18558	1.15861
C	0.97757	-5.77346	0.19552
C	0.46724	-6.46510	1.47992
C	0.25881	-6.43935	-0.99770
C	2.49271	-6.05413	0.09741
C	-2.54305	-0.03381	-0.06503
C	2.48683	0.71354	-0.03255
C	-3.40963	0.03004	1.02880
C	-4.63343	-0.65055	1.01067
C	-5.02519	-1.41817	-0.09831
C	-4.13605	-1.47369	-1.18950
C	-2.91394	-0.79325	-1.17475
C	3.12456	0.20423	1.09986
C	4.50528	-0.03058	1.09641
C	5.28984	0.24010	-0.03666
C	4.62974	0.75859	-1.16771
C	3.25056	0.99255	-1.16722
C	-6.35803	-2.18515	-0.14995
C	-7.22607	-2.01524	1.11736
C	6.80722	-0.01159	-0.07616
C	7.38126	-0.57829	1.24209
C	-7.19768	-1.68922	-1.34711
C	-6.08037	-3.69501	-0.31457
C	7.13496	-1.02835	-1.19096
C	7.54636	1.31323	-0.36323
H	-3.12406	2.56732	-0.52268
H	-2.98381	4.82845	-0.47701
H	1.15504	5.48907	0.28902
H	2.04320	3.45958	0.03724
H	0.69915	7.61479	-0.21318
H	0.39112	7.28791	1.51009
H	-0.38727	8.64892	0.70594
H	-1.12992	7.13401	-1.96126
H	-2.03343	8.35022	-1.04765
H	-2.78388	6.80652	-1.42437
H	-1.95191	6.44953	2.25422
H	-3.27367	6.41101	1.07692
H	-2.52249	7.94231	1.49473
H	1.26594	-1.56209	-1.87989
H	1.64017	-3.96773	-1.78664
H	-0.25591	-4.08793	2.10178
H	-0.60969	-1.69206	1.99038
H	-0.61511	-6.34119	1.60219
H	0.96002	-6.06805	2.37508
H	0.66678	-7.54315	1.45405
H	-0.81782	-6.23273	-0.97482
H	0.39009	-7.52764	-0.98092
H	0.64091	-6.08585	-1.96165
H	3.03770	-5.56776	0.91518
H	2.92133	-5.69278	-0.84378
H	2.69985	-7.12934	0.15152
H	-3.13678	0.60930	1.90844
H	-5.26334	-0.56283	1.89132
H	-4.38077	-2.05777	-2.07401
H	-2.25238	-0.86769	-2.03474
H	2.55027	-0.02189	1.99568
H	4.94095	-0.43444	2.00592
H	5.18416	0.98687	-2.07537
H	2.77722	1.38945	-2.06253
H	-7.49273	-0.96532	1.28581
H	-6.71133	-2.38493	2.01187
H	-8.16447	-2.57624	1.03160
H	6.93009	-1.54449	1.49641
H	7.21673	0.10735	2.08150
H	8.46337	-0.73896	1.16496
H	-7.38567	-0.61123	-1.27731
H	-8.16934	-2.19552	-1.38517
H	-6.70267	-1.87522	-2.30650
H	-5.45955	-4.07369	0.50611
H	-5.55971	-3.92092	-1.25162
H	-7.01361	-4.27026	-0.31981
H	6.60041	-1.97265	-1.03316
H	8.20770	-1.25279	-1.21838
H	6.86020	-0.65721	-2.18441
H	7.30984	2.06911	0.39507
H	7.28115	1.73299	-1.33973
H	8.63301	1.16796	-0.36185

Compound (1d)$^{\cdot+}$

Energy: −5494388.608 kJ/mol

C	3.66992	0.39030	0.08958
C	2.41775	0.92722	0.07291
C	1.40478	-0.15590	0.01449
C	2.05192	-1.35051	-0.05526
C	3.49031	-1.05212	-0.01665
C	4.46081	-1.96999	-0.10124
C	5.89671	-1.79644	-0.10103
C	6.67460	-0.70083	0.02820
C	6.15481	0.65704	0.20829
C	4.90044	1.12742	0.22905
C	-0.06590	0.01406	0.05003
C	8.23938	-0.80411	0.00510
C	8.78124	-2.24436	-0.19561
C	8.81791	0.03688	-1.15718
C	8.83180	-0.30813	1.34575
C	-0.85096	-0.72317	0.94929
C	-2.25072	-0.63599	0.94559
C	-2.88408	0.26373	0.06381
C	-2.10741	1.05348	-0.81164
C	-0.70900	0.90421	-0.82003
C	1.41909	-2.67492	-0.13222
C	2.13750	2.37102	0.10269
C	1.51190	-3.56322	0.94273
C	0.85593	-4.79962	0.90663
C	0.08884	-5.18588	-0.20433
C	0.03277	-4.29109	-1.29082
C	0.68621	-3.05463	-1.25706
C	1.55888	2.97037	1.22108
C	1.30666	4.34901	1.23812
C	1.62434	5.16641	0.13966
C	2.19725	4.54092	-0.98364
C	2.44559	3.16574	-1.00524
C	-4.29805	0.36706	0.05448
C	-4.93540	1.27930	-0.81011
C	-4.14868	2.07606	-1.65532
C	-2.75507	1.96081	-1.66057
C	-3.03279	-1.43410	1.79062
C	-4.42628	-1.34831	1.76333
C	-5.07242	-0.44986	0.90319
C	-6.47389	-0.35090	0.86476
C	-7.13923	0.56031	0.02172
C	-6.34129	1.36586	-0.81002
C	-8.67788	0.61911	0.00428
C	-9.24283	0.70069	1.44113
C	-9.24466	1.83486	-0.76368
C	-9.21351	-0.65762	-0.67581
H	4.16846	-3.01515	-0.20290
H	6.37669	-2.76443	-0.22935
H	6.91323	1.42533	0.35025
H	4.79457	2.19872	0.39384
H	8.44949	-2.67175	-1.14894
H	8.46683	-2.91113	0.61576
H	9.87815	-2.25572	-0.20733
H	8.39162	-0.27498	-2.11783
H	9.90625	-0.07917	-1.22436
H	8.62454	1.10779	-1.03784
H	8.40721	-0.86149	2.19158
H	8.64904	0.75728	1.51832
H	9.91928	-0.44652	1.37192
H	-0.11759	1.48867	-1.52164
H	2.07955	-3.28988	1.82994
H	1.29991	2.37104	2.09121
H	2.89007	2.71972	-1.89264
H	-4.61648	2.79233	-2.32714
H	-2.17788	2.58982	-2.33486
H	-2.56225	-2.14358	2.46786
H	-5.00378	-1.99129	2.42363
H	-7.05333	-1.01184	1.50623
H	-6.80246	2.07720	-1.49025
H	-8.82297	1.55663	1.98228
H	-9.02987	-0.19975	2.02686
H	-10.33341	0.81426	1.43111
H	-8.87222	2.77881	-0.34884
H	-10.33963	1.86221	-0.70780
H	-8.98521	1.80262	-1.82795
H	-8.91414	-1.56415	-0.13745
H	-8.83721	-0.74703	-1.70194
H	-10.30869	-0.65201	-0.72199
C	1.38202	6.68598	0.13273
C	0.70415	7.21622	1.41578
C	0.47119	7.06828	-1.05447
C	2.73361	7.41934	-0.00896
C	-0.67347	-6.52111	-0.26369
C	-0.08573	-7.39606	-1.39007
C	-2.16991	-6.26164	-0.54862
C	-0.60051	-7.33941	1.04550
H	0.43011	-7.62097	1.29048
H	-1.17496	-8.26989	0.96253
H	-1.01255	-6.77926	1.89319
H	-0.18624	-6.92423	-2.37381
H	-0.59417	-8.36581	-1.44334
H	0.98125	-7.58740	-1.22503
H	-2.33314	-5.79671	-1.52687
H	-2.60658	-5.59924	0.20834
H	-2.74147	-7.19722	-0.54299
H	-0.27748	6.75426	1.57279
H	0.54630	8.30006	1.35983
H	1.31729	7.02715	2.30456
H	3.41525	7.15192	0.80729
H	2.59786	8.50696	0.01261
H	3.23892	7.17754	-0.95063
H	-0.48452	6.53312	-1.00677
H	0.93007	6.83702	-2.02194
H	0.25284	8.14269	-1.05491
H	0.85698	4.75899	2.13830
H	2.46617	5.12047	-1.86403
H	-0.53694	-4.53897	-2.18389
H	0.95579	-5.44072	1.77787
H	-0.36892	-1.39982	1.65154
H	0.59848	-2.38324	-2.10835

Compound (1e)$^{\cdot+}$

Energy: −6501990.421 kJ/mol

C	0.77480	2.85916	-0.12605
C	1.20203	1.45316	-0.16484
C	0.06764	0.71238	-0.10128
C	-1.10053	1.62293	-0.02928
C	-0.67764	2.91125	-0.00749
C	-1.52324	4.06995	0.12478
C	-1.16295	5.35908	0.14805
C	0.15175	5.99476	0.04391
C	1.30777	5.32171	-0.12714
C	1.60066	3.90984	-0.20667
C	-0.00263	-0.75638	-0.02385
C	0.13299	7.55938	0.16266

C	-0.44068	7.98271	1.53647
C	1.53141	8.22542	0.06139
C	-0.72043	8.18109	-0.96709
C	-0.65556	-1.48873	-1.01759
C	-0.80146	-2.87703	-0.90370
C	-0.29697	-3.57579	0.20477
C	0.37511	-2.82430	1.18754
C	0.51608	-1.43723	1.07929
C	-2.50154	1.16838	0.01773
C	2.57400	0.91924	-0.18195
C	-3.35333	1.38863	-1.07239
C	-4.65873	0.87423	-1.08212
C	-5.11165	0.11329	0.01912
C	-4.26031	-0.10515	1.12521
C	-2.96582	0.43385	1.11493
C	3.00006	0.05357	-1.19725
C	4.29787	-0.48238	-1.19483
C	5.19345	-0.12537	-0.16240
C	4.77772	0.75807	0.85781
C	3.46832	1.26032	0.84147
C	-6.41515	-0.44362	0.00853
C	-6.86284	-1.22022	1.09723
C	-6.00523	-1.42271	2.18786
C	-4.72141	-0.87211	2.20243
C	-5.51920	1.08312	-2.16783
C	-6.80675	0.54021	-2.17230
C	-7.26587	-0.23056	-1.09462
C	-8.55090	-0.80100	-1.09257
C	-9.02029	-1.59192	-0.02486
C	-8.15336	-1.78083	1.06469
C	-0.47006	-5.09413	0.38044
C	-1.26123	-5.37631	1.67671
C	-1.23548	-5.77400	-0.77709
C	6.50841	-0.65499	-0.14768
C	7.40617	-0.29218	0.87674
C	6.98038	0.59715	1.87345
C	5.68214	1.11254	1.86686
C	4.72654	-1.36767	-2.19253
C	6.02239	-1.89114	-2.17432
C	6.92512	-1.54362	-1.15880
C	8.23350	-2.06086	-1.12631
C	9.14515	-1.73320	-0.10442
C	8.70686	-0.82832	0.87906
C	10.57597	-2.30411	-0.10195
C	11.44185	-1.44084	-1.03961
C	11.22725	-2.29965	1.30122
C	10.61616	-3.76983	-0.59449
C	-10.42974	-2.20835	-0.08210
C	-10.56452	-3.09293	-1.34141
C	-10.77422	-3.09887	1.13347
C	-11.48215	-1.08086	-0.13785
C	0.91492	-5.76923	0.47273
H	-2.58751	3.86852	0.23761
H	-1.99898	6.04640	0.26792
H	2.23461	5.88681	-0.20143
H	2.66552	3.71557	-0.33301
H	0.12634	7.52611	2.35636
H	-1.49097	7.69933	1.65895
H	-0.39257	9.07043	1.66663
H	2.20128	7.88256	0.85865
H	1.45772	9.31575	0.15757
H	2.00589	8.02393	-0.90598
H	-1.77677	7.90265	-0.89829
H	-0.35516	7.86908	-1.95239
H	-0.68320	9.27651	-0.93146
H	-1.08022	-0.98301	-1.88192
H	-1.33580	-3.38634	-1.70072
H	0.79136	-3.30980	2.06747
H	1.02325	-0.89391	1.87314
H	-2.98536	1.94821	-1.93067
H	-2.29799	0.25212	1.95509
H	2.30813	-0.21729	-1.99278
H	3.13738	1.92407	1.63862
H	-6.32769	-2.01944	3.03825
H	-4.07926	-1.05746	3.06074
H	-5.19283	1.66751	-3.02535
H	-7.44758	0.71848	-3.03304
H	-9.19576	-0.62460	-1.95173
H	-8.46540	-2.37792	1.91771
H	-2.23995	-4.88200	1.65710
H	-0.73347	-5.02396	2.56979
H	-1.43285	-6.45089	1.80950
H	-2.25011	-5.37193	-0.88105
H	-1.33333	-6.85282	-0.60593
H	-0.71700	-5.64525	-1.73426
H	7.65758	0.89456	2.67110
H	5.38462	1.79623	2.65890
H	4.05153	-1.66289	-2.99300
H	6.31991	-2.57883	-2.96291
H	8.53658	-2.72872	-1.92917
H	9.37989	-0.51694	1.67369
H	11.46653	-0.39553	-0.70925
H	11.05709	-1.45033	-2.06611
H	12.47553	-1.80411	-1.07043
H	11.40211	-1.28384	1.67241
H	12.20597	-2.79418	1.28549
H	10.60221	-2.82691	2.03143
H	10.34893	-3.86245	-1.65240
H	9.93080	-4.40061	-0.01648
H	11.62273	-4.19349	-0.49447
H	-9.80228	-3.88108	-1.35299
H	-10.45751	-2.51792	-2.26754
H	-11.54679	-3.57839	-1.38024
H	-10.07721	-3.93994	1.22693
H	-11.78113	-3.52323	1.03971
H	-10.75242	-2.53056	2.07056
H	-11.37473	-0.45853	-1.03306
H	-11.39905	-0.42044	0.73349
H	-12.49921	-1.48986	-0.15062
H	1.48789	-5.42341	1.34004
H	1.51466	-5.56258	-0.42155
H	0.81853	-6.85729	0.56611

Compound (1f)$^{\cdot+}$

Energy: –7509594.912 kJ/mol

C	0.58603	3.92141	-0.20988
C	1.07931	2.54071	-0.30406
C	-0.01396	1.74216	-0.20027
C	-1.22227	2.59017	-0.06936
C	-0.86049	3.89706	-0.02413
C	-1.75422	5.01228	0.16238
C	-1.45030	6.31414	0.23347
C	-0.16542	7.01056	0.14581
C	1.00955	6.40213	-0.11262
C	1.35705	5.01224	-0.29192
C	0.01276	0.26996	-0.12271
C	-0.23913	8.55773	0.39690
C	-0.78993	8.83763	1.81616
C	1.13078	9.28406	0.32124
C	-1.14520	9.24095	-0.65298
C	-0.63650	-0.50869	-1.08784
C	-0.61361	-1.91114	-1.01729
C	0.08229	-2.54163	0.03881
C	0.73256	-1.76242	1.01992
C	0.67813	-0.36538	0.93447
C	-2.59946	2.06936	-0.00095
C	2.47576	2.06920	-0.35414
C	-3.49709	2.31011	-1.04994
C	-4.78435	1.75212	-1.04129
C	-5.17133	0.92146	0.03380
C	-4.27247	0.67602	1.09601
C	-2.99814	1.26198	1.07034
C	2.90244	1.16714	-1.33780
C	4.20156	0.63501	-1.31900
C	5.10481	1.04693	-0.31461
C	4.69691	1.98402	0.65941
C	3.38227	2.47103	0.63666

C	-6.45667	0.32326	0.04068
C	-6.83877	-0.52274	1.10211
C	-5.93402	-0.75370	2.14804
C	-4.66839	-0.16163	2.14599
C	-5.69111	1.98836	-2.08296
C	-6.96080	1.40503	-2.06956
C	-7.35492	0.56531	-1.01807
C	-8.62114	-0.04556	-0.99952
C	-9.02579	-0.90447	0.04176
C	-8.11224	-1.12220	1.08693
C	0.13087	-3.95603	0.11550
C	0.83358	-4.58510	1.16437
C	1.47487	-3.79354	2.12717
C	1.42397	-2.40008	2.05717
C	-1.26278	-2.70403	-1.97272
C	-1.21740	-4.09892	-1.89331
C	-0.52083	-4.73906	-0.85765
C	-0.45592	-6.14112	-0.76738
C	0.24427	-6.79661	0.26557
C	0.88062	-5.98980	1.22339
C	6.41683	0.51209	-0.27572
C	7.32237	0.93178	0.71933
C	6.90828	1.88275	1.66257
C	5.61010	2.39702	1.63771
C	4.61966	-0.30975	-2.26525
C	5.91066	-0.84361	-2.21895
C	6.82047	-0.44366	-1.22935
C	8.12120	-0.97779	-1.16387
C	9.03938	-0.59421	-0.16879
C	8.61767	0.38547	0.74921
C	10.46312	-1.17963	-0.11092
C	11.39899	-0.25061	-0.90735
C	10.99202	-1.29171	1.33887
C	10.55237	-2.60067	-0.71510
C	0.29326	-8.33442	0.31230
C	0.94566	-8.87181	-0.97995
C	1.10488	-8.90032	1.50018
C	-1.13963	-8.89624	0.43134
C	-10.41661	-1.56340	0.00247
C	-10.55926	-2.40452	-1.28532
C	-10.69663	-2.50834	1.19318
C	-11.50686	-0.47086	0.01921
H	-2.80735	4.76085	0.27851
H	-2.31373	6.95941	0.38842
H	1.91040	7.00947	-0.17169
H	2.42178	4.87478	-0.47939
H	-0.18181	8.33701	2.57906
H	-1.82397	8.49974	1.93936
H	-0.78165	9.91120	2.03897
H	1.83509	8.89812	1.06759
H	1.02020	10.35785	0.51681
H	1.58483	9.18782	-0.67174
H	-2.18928	8.92080	-0.58023

H	-0.79858	9.02625	-1.67040
H	-1.14345	10.33016	-0.52509
H	-1.16624	-0.01816	-1.90219
H	1.17287	0.23768	1.69359
H	-3.18095	2.92636	-1.89002
H	-2.29701	1.06428	1.87928
H	2.20407	0.84702	-2.10910
H	3.05353	3.15973	1.41322
H	-6.20436	-1.40562	2.97582
H	-3.98895	-0.37139	2.96938
H	-5.41608	2.62745	-2.91921
H	-7.63930	1.60705	-2.89546
H	-9.30277	0.15263	-1.82487
H	-8.37266	-1.77327	1.91757
H	2.02569	-4.25630	2.94298
H	1.93812	-1.81619	2.81750
H	-1.81328	-2.24184	-2.78931
H	-1.73277	-4.68335	-2.65221
H	-0.96449	-6.73147	-1.52766
H	1.43380	-6.44154	2.04278
H	7.59232	2.22438	2.43615
H	5.31870	3.12382	2.39277
H	3.93745	-0.65112	-3.04092
H	6.19705	-1.58379	-2.96290
H	8.40661	-1.70711	-1.91765
H	9.30231	0.74388	1.51391
H	11.40901	0.76315	-0.49010
H	11.08509	-0.17022	-1.95483
H	12.42962	-0.62335	-0.89696
H	11.14920	-0.31189	1.80228
H	11.96157	-1.80305	1.36866
H	10.29808	-1.85790	1.97117
H	10.36614	-2.60463	-1.79448
H	9.83230	-3.27901	-0.24264
H	11.55220	-3.02878	-0.57435
H	1.95529	-8.46450	-1.11064
H	0.36868	-8.61347	-1.87468
H	1.02740	-9.96482	-0.95651
H	2.15054	-8.57287	1.46714
H	1.11099	-9.99690	1.48787
H	0.68004	-8.59222	2.46263
H	-1.76032	-8.63649	-0.43314
H	-1.64201	-8.50852	1.32562
H	-1.13059	-9.99022	0.50192
H	-9.77439	-3.16777	-1.34666
H	-10.49420	-1.79227	-2.19133
H	-11.52724	-2.91836	-1.31675
H	-9.97457	-3.33236	1.23225
H	-11.69407	-2.95767	1.11494
H	-10.65944	-1.97488	2.15008
H	-11.44915	0.18548	-0.85601
H	-11.41816	0.16110	0.91080
H	-12.50980	-0.91358	0.02265

Compound (4a)$^{\cdot+}$

Energy: −4483663.045 kJ/mol

C	0.25974	2.25085	-0.22222
C	-0.61735	1.23607	0.01393
C	0.13035	-0.04648	0.13070
C	1.46372	0.21862	0.07177
C	1.58903	1.67340	-0.07367
C	2.74064	2.35738	-0.00980
C	2.92245	3.79213	0.08129
C	2.09345	4.81269	-0.22606
C	0.76949	4.61782	-0.81990
C	-0.03370	3.54521	-0.78783
C	-0.61504	-1.33431	0.14028
C	2.50198	6.30467	-0.00038
C	1.40575	7.05502	0.79429
C	3.81300	6.48373	0.80883
C	2.72143	7.00796	-1.35842
C	-2.02573	-1.30249	-0.02837
C	-2.69912	-2.54860	-0.15552

C	-2.05839	-3.79778	-0.06536
C	-0.68245	-3.78089	0.16625
C	0.02077	-2.57844	0.26458
C	-2.80481	-5.13700	-0.19787
C	-2.22165	-5.93936	-1.38163
C	-2.63722	-5.95526	1.10112
C	-4.32269	-4.99162	-0.45101
C	2.59093	-0.71687	0.08047
C	-2.09694	1.23785	0.05306
C	3.07203	-1.25601	-1.11312
C	4.15951	-2.13523	-1.10007
C	4.80430	-2.49405	0.10059
C	4.31244	-1.92904	1.28933
C	3.22316	-1.04949	1.28062
C	-2.78075	0.00250	-0.01900
C	-4.19910	0.05180	0.01223
C	-4.94680	1.24355	0.14234

C	-4.22574	2.42599	0.28779
C	-2.82978	2.41852	0.26085
C	5.99558	-3.46807	0.07446
C	7.12409	-2.88773	-0.80519
C	-6.48506	1.19772	0.16614
C	-7.01075	0.52210	-1.11977
C	6.60266	-3.75029	1.46740
C	5.54193	-4.82348	-0.50933
C	-6.95876	0.39193	1.39452
C	-7.14865	2.59170	0.24658
H	3.67038	1.80201	0.10879
H	3.90557	4.01627	0.48955
H	0.37374	5.47334	-1.36448
H	-0.97196	3.62203	-1.33307
H	1.19935	6.55530	1.74804
H	0.46307	7.12598	0.24147
H	1.71391	8.08318	1.01871
H	3.74950	5.99716	1.78911
H	4.02436	7.54493	0.98912
H	4.67973	6.07891	0.27376
H	1.80420	7.06326	-1.95348
H	3.47577	6.48325	-1.95632
H	3.06922	8.03816	-1.21680
H	-3.76659	-2.54814	-0.33432
H	-0.12050	-4.70744	0.26243
H	1.08593	-2.66182	0.43788
H	-1.16522	-6.18867	-1.23340
H	-2.29788	-5.37289	-2.31739
H	-2.75742	-6.88577	-1.52002
H	-1.58985	-6.20673	1.30089
H	-3.18838	-6.90139	1.04632
H	-3.01349	-5.39966	1.96831
H	-4.52669	-4.44913	-1.38154
H	-4.82019	-4.46252	0.37020
H	-4.80427	-5.97300	-0.53907
H	2.60055	-0.99999	-2.05950
H	4.49773	-2.53876	-2.05217
H	4.75997	-2.15517	2.25318
H	2.86853	-0.62895	2.21943
H	-4.76736	-0.87078	-0.03404
H	-4.71792	3.38206	0.44059
H	-2.32671	3.36461	0.43907
H	7.44686	-1.90692	-0.43628
H	6.81384	-2.76099	-1.84813
H	8.00000	-3.54705	-0.81021
H	-6.68820	-0.52126	-1.20433
H	-6.65841	1.04939	-2.01424
H	-8.10683	0.51878	-1.14461
H	6.97927	-2.83379	1.93644
H	7.44716	-4.44636	1.39665
H	5.86844	-4.20355	2.14360
H	5.19489	-4.73345	-1.54455
H	4.71957	-5.25017	0.07720
H	6.36371	-5.54911	-0.50870
H	-6.61858	-0.64900	1.36350
H	-8.05316	0.37061	1.45500
H	-6.58177	0.83292	2.32495
H	-6.86308	3.22304	-0.60298
H	-6.87643	3.11700	1.16942
H	-8.24223	2.50995	0.23650

Compound (4d)$^{\cdot+}$

Energy: –5491253.190 kJ/mol

C	3.66338	0.14264	0.21096
C	2.45365	0.74680	0.07692
C	1.40596	-0.32323	-0.01364
C	2.01162	-1.57315	0.20298
C	3.46446	-1.30045	0.14383
C	4.43296	-2.18150	-0.14677
C	5.83475	-1.93615	-0.42701
C	6.61700	-0.86032	-0.19677
C	6.13687	0.35555	0.46103
C	4.88503	0.81193	0.60097
C	0.01094	-0.20730	-0.18396
C	8.12657	-0.83435	-0.60601
C	8.57580	-2.05881	-1.44557
C	8.43412	0.41165	-1.47100
C	9.02014	-0.81628	0.65500
C	-0.81713	-1.33877	0.04242
C	-2.25752	-1.08583	0.14344
C	-2.80844	0.15537	-0.27230
C	-1.95694	1.18553	-0.69070
C	-0.57903	1.00078	-0.60422
C	1.24769	-2.73804	0.35375
C	2.27963	2.20262	0.20736
C	1.81061	-3.99159	0.68396
C	1.06890	-5.17308	0.67456
C	-0.26973	-5.15535	0.30942
C	-0.83733	-3.88657	0.06290
C	-0.15469	-2.64125	0.17634
C	1.65692	2.74577	1.33329
C	1.46993	4.12907	1.44561
C	1.90343	5.00923	0.44018
C	2.53920	4.44331	-0.68225
C	2.72658	3.06232	-0.79837
C	-4.21425	0.40339	-0.26068
C	-4.74049	1.63000	-0.72356
C	-3.86070	2.61782	-1.17378
C	-2.48457	2.40305	-1.14413
C	-3.19343	-1.98321	0.71506
C	-4.57351	-1.75059	0.74121
C	-5.10029	-0.56815	0.23133
C	-6.48514	-0.32228	0.23547
C	-7.03265	0.88325	-0.24051
C	-6.13141	1.84888	-0.71484
C	-8.55526	1.10417	-0.21521
C	-9.06720	1.02172	1.23925
C	-8.99932	2.47345	-0.77799
C	-9.25233	0.01699	-1.06173
H	4.17010	-3.21816	-0.33076
H	6.27311	-2.80706	-0.90993
H	6.90913	1.00414	0.87036
H	4.76523	1.76978	1.10488
H	7.98898	-2.15187	-2.36679
H	8.48819	-2.99341	-0.87954
H	9.62798	-1.96961	-1.74274
H	7.78747	0.44572	-2.35563
H	9.47353	0.40339	-1.82030
H	8.29795	1.34792	-0.91964
H	8.80346	-1.67339	1.30331
H	8.88703	0.09320	1.24957
H	10.08210	-0.86468	0.38621
H	0.05092	1.83091	-0.91048
H	2.85126	-4.07212	0.98200
H	1.30189	2.09505	2.13001
H	3.21697	2.66241	-1.68345
H	-4.23558	3.57387	-1.53143
H	-1.82248	3.20308	-1.47045
H	-2.85640	-2.88374	1.22140
H	-5.22325	-2.50139	1.18528
H	-7.14676	-1.09397	0.62531
H	-6.49525	2.80427	-1.08431
H	-8.56834	1.76244	1.87550
H	-8.89406	0.03604	1.68483
H	-10.14588	1.21084	1.29000
H	-8.57660	3.30373	-0.20030
H	-10.09023	2.58021	-0.74242
H	-8.69779	2.59642	-1.82476
H	-9.08429	-0.98992	-0.66431
H	-8.88718	0.02789	-2.09556
H	-10.33719	0.17272	-1.08944
C	1.70370	6.53261	0.52648
C	1.00111	6.99841	1.82168
C	0.83653	7.00754	-0.65956
C	3.07401	7.24184	0.47049
C	-1.11874	-6.43015	0.17326
C	-0.35846	-7.72559	0.53858

C	-1.59758	-6.57763	-1.28706
C	-2.34734	-6.34665	1.10513
H	-2.04228	-6.19844	2.14778
H	-2.94160	-7.26680	1.05884
H	-3.01690	-5.52222	0.83747
H	0.50874	-7.88275	-0.11339
H	-1.00373	-8.60593	0.43214
H	-0.00643	-7.70694	1.57662
H	-0.74790	-6.61382	-1.97920
H	-2.23964	-5.74660	-1.59895
H	-2.17705	-7.49845	-1.42187
H	-0.00189	6.56586	1.91487
H	0.88369	8.08868	1.83716
H	1.57616	6.72369	2.71363
H	3.72773	6.90135	1.28226
H	2.96103	8.32811	0.56640
H	3.59852	7.05740	-0.47341
H	-0.13506	6.49920	-0.66632
H	1.31487	6.81460	-1.62610
H	0.64841	8.08619	-0.60482
H	0.97160	4.49036	2.34099
H	2.89799	5.07475	-1.49229
H	-1.86366	-3.87503	-0.29641
H	1.58531	-6.09447	0.92650

Compound (4e)$^{\cdot+}$

Energy: −6498847.177 kJ/mol

C	-0.89485	2.58075	0.11295
C	-1.21310	1.27588	-0.09529
C	0.06072	0.49733	-0.22307
C	1.14353	1.35042	0.05096
C	0.55611	2.70761	0.07586
C	1.21437	3.85651	-0.13742
C	0.67812	5.18683	-0.34870
C	-0.54857	5.70244	-0.12107
C	-1.64912	4.93356	0.46250
C	-1.82515	3.60688	0.52940
C	0.27447	-0.87336	-0.44509
C	-0.89171	7.19213	-0.45508
C	0.23101	7.94573	-1.21553
C	-2.14543	7.27041	-1.35925
C	-1.14720	7.98568	0.84647
C	1.60004	-1.37249	-0.34114
C	1.71943	-2.79240	-0.34452
C	0.67217	-3.70186	-0.60607
C	-0.57701	-3.15147	-0.85140
C	-0.77026	-1.77286	-0.75847
C	2.45373	0.86885	0.21065
C	-2.59783	0.78570	-0.02267
C	3.47275	1.67419	0.75566
C	4.80275	1.26377	0.82466
C	5.16257	0.03076	0.26328
C	4.15730	-0.82060	-0.26674
C	2.74166	-0.47282	-0.14109
C	-3.03863	0.08217	1.10500
C	-4.35303	-0.40141	1.17976
C	-5.24161	-0.16472	0.10603
C	-4.80476	0.55588	-1.02871
C	-3.48447	1.02557	-1.07954
C	6.54430	-0.32465	0.23430
C	6.95924	-1.51205	-0.39200
C	5.99813	-2.30643	-1.01076
C	4.64454	-1.95392	-0.96222
C	5.77742	2.08969	1.40320
C	7.11883	1.71259	1.41133
C	7.51952	0.51227	0.81847
C	8.87386	0.13512	0.78820
C	9.30685	-1.05633	0.17682
C	8.32288	-1.86320	-0.41464
C	0.93245	-5.21724	-0.59723
C	2.04953	-5.56613	-1.60517
C	1.36825	-5.65672	0.81696
C	-6.57137	-0.65221	0.16615
C	-7.46099	-0.41880	-0.90291
C	-7.01059	0.30121	-2.01877
C	-5.70030	0.78220	-2.08144
C	-4.80425	-1.11888	2.29486
C	-6.11508	-1.59917	2.35098
C	-7.00917	-1.37432	1.29454
C	-8.33019	-1.85359	1.33481
C	-9.24072	-1.63681	0.28145
C	-8.77730	-0.91217	-0.82977
C	-10.67518	-2.18782	0.37616
C	-11.38123	-1.59194	1.61354
C	-11.55495	-1.85972	-0.85162
C	-10.63170	-3.72586	0.50702
C	10.80182	-1.42098	0.16524
C	11.32341	-1.52647	1.61488
C	11.11338	-2.76647	-0.52878
C	11.59553	-0.32774	-0.58232
C	-0.30377	-6.06283	-0.98011
H	2.28797	3.82793	-0.30410
H	1.44520	5.83097	-0.77363
H	-2.46441	5.52365	0.87726
H	-2.75013	3.25851	0.98634
H	0.48008	7.44931	-2.16063
H	1.14343	8.02942	-0.61381
H	-0.07702	8.96927	-1.46231
H	-2.00665	6.68473	-2.27559
H	-2.35493	8.30511	-1.65583
H	-3.04644	6.90094	-0.85846
H	-0.28569	7.92249	1.52152
H	-2.02497	7.62456	1.39185
H	-1.32334	9.04673	0.63306
H	2.67466	-3.22681	-0.06048
H	-1.44311	-3.76449	-1.08331
H	-1.77838	-1.41832	-0.94501
H	3.21942	2.64045	1.18581
H	-2.34517	-0.09720	1.92498
H	-3.13634	1.57862	-1.95045
H	6.28613	-3.20331	-1.55471
H	3.96908	-2.57448	-1.54604
H	5.50060	3.04363	1.84742
H	7.84956	2.37643	1.86742
H	9.60586	0.79605	1.24934
H	8.59834	-2.78935	-0.91267
H	3.00761	-5.10609	-1.34035
H	1.78924	-5.22764	-2.61505
H	2.21816	-6.64853	-1.64911
H	2.30432	-5.18060	1.12883
H	1.52861	-6.74026	0.86222
H	0.60571	-5.40091	1.56223
H	-7.67891	0.49419	-2.85519
H	-5.38531	1.33521	-2.96382
H	-4.13704	-1.31364	3.13184
H	-6.43224	-2.15400	3.23130
H	-8.65096	-2.41122	2.21309
H	-9.43714	-0.71562	-1.67096
H	-11.39994	-0.49660	1.56743
H	-10.88661	-1.87315	2.54963
H	-12.41835	-1.94059	1.68305
H	-11.66254	-0.77800	-0.99338
H	-12.56493	-2.27105	-0.73538
H	-11.13879	-2.28575	-1.77200
H	-10.11821	-4.05045	1.41865
H	-10.10939	-4.17938	-0.34376
H	-11.64271	-4.14853	0.54134
H	10.75715	-2.27312	2.18422
H	11.24818	-0.57565	2.15363
H	12.37897	-1.82205	1.63464
H	10.60511	-3.60254	-0.03434
H	12.18812	-2.98355	-0.50544
H	10.81091	-2.75708	-1.58243
H	11.52119	0.64827	-0.09040
H	11.22971	-0.20723	-1.60896
H	12.66123	-0.57942	-0.63538
H	-0.66379	-5.81702	-1.98600

H	-1.13023	-5.91310	-0.27559
H	-0.06755	-7.13373	-0.97359

Compound (4f)$^{\cdot+}$
Energy: −7506432.872 kJ/mol

C	1.24139	-3.41144	0.78143
C	1.46928	-2.02745	0.50636
C	0.21051	-1.39259	0.42747
C	-0.82558	-2.35630	0.65231
C	-0.20202	-3.64112	0.83240
C	-0.80130	-4.89870	0.89026
C	-0.24108	-6.16677	1.07407
C	1.08956	-6.58867	1.25579
C	2.19687	-5.72737	1.18549
C	2.25746	-4.35316	0.94200
C	-0.12228	0.01594	0.27479
C	1.30442	-8.10246	1.50951
C	0.78293	-8.90480	0.29018
C	2.78342	-8.48152	1.72252
C	0.52512	-8.52028	2.78253
C	-1.51460	0.39033	0.23632
C	-1.84674	1.78594	0.43098
C	-0.81946	2.77054	0.33584
C	0.53769	2.37321	0.14409
C	0.85438	1.00564	0.18044
C	-2.20359	-1.97989	0.56891
C	2.82828	-1.45950	0.32377
C	-3.28487	-2.81475	0.91512
C	-4.59981	-2.50873	0.57249
C	-4.85102	-1.35346	-0.24612
C	-3.80337	-0.43598	-0.51697
C	-2.50746	-0.64417	0.08686
C	3.66808	-1.26182	1.42914
C	4.96631	-0.74784	1.27553
C	5.43649	-0.43547	-0.03574
C	4.58826	-0.64522	-1.16627
C	3.29752	-1.15404	-0.96407
C	-6.15169	-1.14241	-0.77982
C	-6.39883	-0.05918	-1.66656
C	-5.30289	0.78600	-2.01283
C	-4.06317	0.61263	-1.45602
C	-5.70318	-3.35718	0.92563
C	-6.95734	-3.11868	0.44899
C	-7.22587	-2.01652	-0.43792
C	-8.49393	-1.77852	-0.97119
C	-8.75976	-0.70893	-1.85565
C	-7.69884	0.12859	-2.18993
C	-1.12285	4.15576	0.46927
C	-0.10419	5.13878	0.31601
C	1.23645	4.70419	0.06348
C	1.54769	3.37314	-0.00138
C	-3.14420	2.23976	0.83668
C	-3.42995	3.56874	0.99833
C	-2.44436	4.57871	0.77770
C	-2.72068	5.95211	0.89869
C	-1.73711	6.93587	0.72036
C	-0.43653	6.50185	0.43257
C	6.75049	0.08177	-0.21681
C	7.22950	0.39098	-1.52361
C	6.35394	0.16681	-2.64372
C	5.09632	-0.32692	-2.47511
C	5.84405	-0.52308	2.39184
C	7.10025	-0.02586	2.21310
C	7.60118	0.29408	0.90428
C	8.89427	0.80500	0.69889
C	9.38020	1.11373	-0.57678
C	8.52669	0.89714	-1.67151
C	10.79607	1.67196	-0.81402
C	11.58364	0.70011	-1.72519
C	10.69352	3.05378	-1.50322
C	11.58557	1.84722	0.49704
C	-2.10825	8.42427	0.85466
C	-2.65573	8.68833	2.27795
C	-0.90039	9.35166	0.62262
C	-3.19565	8.77482	-0.18929
C	-10.18313	-0.51774	-2.40785
C	-11.16439	-0.30477	-1.22987
C	-10.28698	0.69788	-3.34783
C	-10.59647	-1.78106	-3.20118
H	-1.87580	-4.92025	0.75571
H	-0.98217	-6.95989	1.08461
H	3.16953	-6.18772	1.30743
H	3.26413	-3.94632	0.87843
H	1.32116	-8.62791	-0.62310
H	-0.28579	-8.75081	0.11129
H	0.93648	-9.97596	0.46113
H	3.39842	-8.27254	0.84017
H	2.85157	-9.55677	1.91558
H	3.22345	-7.96823	2.58481
H	-0.55186	-8.34848	2.69132
H	0.88115	-7.97042	3.66087
H	0.67272	-9.58931	2.97087
H	1.89732	0.72360	0.13848
H	-3.10514	-3.71864	1.48199
H	3.30431	-1.49443	2.42696
H	2.64990	-1.31781	-1.82181
H	-5.46165	1.57756	-2.74053
H	-3.25022	1.26352	-1.75451
H	-5.51367	-4.21076	1.57100
H	-7.77946	-3.77582	0.72060
H	-9.29881	-2.45184	-0.68998
H	-7.85111	0.95876	-2.87087
H	2.01432	5.45410	-0.05397
H	2.57426	3.05433	-0.15912
H	-3.91607	1.51184	1.04792
H	-4.42468	3.86921	1.31730
H	-3.73805	6.24472	1.14326
H	0.35955	7.22583	0.29768
H	6.72068	0.40091	-3.64011
H	4.45037	-0.49112	-3.33396
H	5.48329	-0.75935	3.38978
H	7.75049	0.13735	3.06902
H	9.52073	0.95646	1.57125
H	8.87199	1.12475	-2.67642
H	11.09921	0.56606	-2.69805
H	11.67780	-0.28705	-1.25876
H	12.59308	1.08697	-1.90756
H	10.18150	2.99378	-2.46935
H	11.69502	3.46164	-1.68348
H	10.14505	3.76613	-0.87642
H	11.72334	0.89550	1.02273
H	11.09512	2.55044	1.17980
H	12.58113	2.24607	0.27482
H	-1.90425	8.45263	3.03983
H	-3.54943	8.09267	2.49211
H	-2.92846	9.74429	2.38615
H	-0.10312	9.17851	1.35448
H	-1.21604	10.39518	0.72448
H	-0.47941	9.23357	-0.38243
H	-4.10503	8.18034	-0.05105
H	-2.83346	8.60318	-1.20923
H	-3.47454	9.83112	-0.10204
H	-10.89968	0.58824	-0.65251
H	-11.17611	-1.15765	-0.54305
H	-12.18394	-0.17292	-1.60963
H	-10.03199	1.63361	-2.83725
H	-11.31561	0.79273	-3.71097
H	-9.63834	0.59446	-4.22517
H	-10.58905	-2.68062	-2.57662
H	-9.92181	-1.95359	-4.04723
H	-11.61181	-1.66132	-3.59603

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