Electronic Supplementary Material (ESI) for Organic Chemistry Frontiers.

Donor- and acceptor-functionalized dibenzo[*a*,*e*]-pentalenes: Modulation of the electronic band gap

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Table of Contents

1 Materials and methods

Chemicals were purchased from Acros-Organics, Alfa Aesar, Fisher, Grüssing, KMF, Merck, Roth, Sigma-Aldrich, TCI-Europe or VWR and used directly without further purification unless otherwise noted. Experiments with moisture- or oxygen-sensitive substances were carried out under argon using standard Schlenk techniques. For reactions with $CeCl_3$, the argon was additionally dried over a silica gel column. Anhydrous solvents (THF, toluene, CH_2Cl_2) were obtained from a M. BRAUN solvent purification system (MB-SPS-800) and stored over 3 Å or 4 Å molecular sieves for a minimum duration of 48 h before use. CH_2Cl_2, ethyl acetate and cyclohexane were purchased in technical grade and purified by distillation. Other solvents were purchased and used in analytical or HPLC grade.

^1H and $^{13}C\{^1H\}$ **NMR spectra** were recorded at 300 K on the following spectrometers: Bruker *Avance dpx 300* [300 MHz (^1H resonance)], Bruker *Avance dpx 400 and Avance I 400* [400 MHz (^1H resonance), 101 MHz (^{13}C resonance)] and Bruker *AV III 500* [500 MHz (^1H resonance), 126 MHz (^{13}C resonance)]. ^1H-NMR spectra are referenced to the residual proton resonance of the respective solvent: $CDCl_3$: $\delta = 7.26$ ppm; CD_2Cl_2: $\delta = 5.32$ ppm; DMSO-d_6: $\delta = 2.50$ ppm.[1] ^{13}C-NMR spectra are referenced to the carbon resonance of the deuterated solvent: $CDCl_3$: $\delta = 77.16$ ppm; CH_2Cl_2: $\delta = 53.84$ ppm; DMSO-d_6: $\delta = 39.52$ ppm.[1] NMR spectra were analyzed using MestReNova software.[33] Analysis followed first order, and the following abbreviations for multiplicities were used: singlet (s), broad singlet (br), doublet (d), triplet (t), quartet (q), multiplet (m) and combinations thereof *i.e.* doublet of doublets (dd). Coupling constants (*J*) are given in Hertz [Hz]. Assignments of signals followed analysis of 2D NMR spectra.

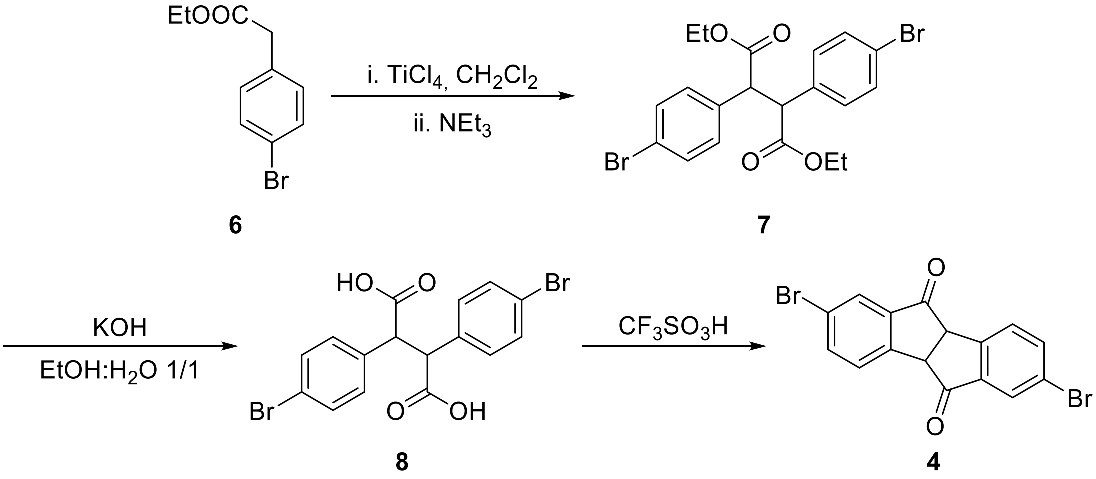
Electrospray ionization **mass spectra** (ESI-MS) were recorded with a *Bruker Daltonik micrOTOF-Q* time-of-flight spectrometer or a *Thermo Fisher Scientific Orbitrap XL* mass spectrometer. Electron-impact ionization **mass spectra** (EI-MS) were recorded with a *Thermo Finnigan MAT 90* or a *MAT 95 XL* sector-field device. Only the structurally significant and the strongest fragmentation peaks are reported.

IR spectra were recorded with a *Nicolet 380 FT-IR* spectrometer (*Smart Orbit, Thermo Electron Cooperation*) neat. Absorption bands are reported in ν (cm^{-1}) and the absorption strength is marked with s (strong), m (medium) and w (weak). Absorption spectra were recorded with a Lambda 18 UV/Vis spectrometer (PerkinElmer).

Melting points were recorded with a *Reichert Thermovar* and are not corrected.

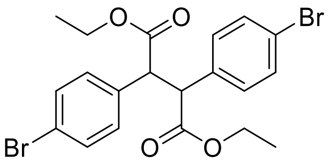
Silica gel layered alumina plates (Merck, Silica Gel 60 F254) were used for TLC, and compounds were detected using UV light (λ = 366 and 254 nm). For flash column chromatography, silica gel (Merck 60, 40–63 µm) was used as the stationary phase. Eluents are described in the respective synthetic procedures. Melting points were measured with a Reichert Thermovar and are uncorrected.

2 Synthetic manipulations



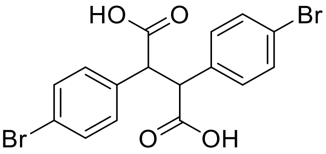
Scheme S1. Synthesis of diketone 4 from ester 6.

2.1 Diethyl 2,3-bis(4-bromophenyl)succinate (7)



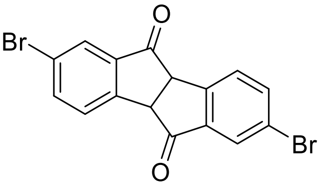
7 was prepared in analogy to a literature procedure.[2] $TiCl_4$ (32.8 g, 172 mmol) was added to a stirred solution of ethyl 2-(4-bromophenyl)acetate (**6**, 20.0 g, 82.0 mmol) in dry CH_2Cl_2 (280 mL) at -50 °C. After stirring for 30 min at -50 °C NEt_3 (17.1 g 169 mmol) was added dropwise. The resulting black solution was stirred at -50 °C for 90 min. The reaction was quenched with aq. sat. NH_4Cl (150 mL) and extracted with CH_2Cl_2 (3 × 100 mL). The combined organic extracts were dried (Na_2SO_4), and the solvent was removed under reduced pressure. Column chromatography (silica gel, cyclohexane/EtOAc 5:1 to 1:1) afforded **7** (19.8 g, 40.9 mmol, 99%) as a white solid. R_f = 0.45 (cyclohexane/EtOAc 5:1); ^{1}H NMR (400 MHz, $CDCl_3$): δ = 7.31–7.28 (m, 4H), 7.92–7.89 (m, 4H), 4.23–4.06 (m, 6H), 1.20 (t, *J* = 7.1 Hz, 6H) ppm; ^{13}C NMR (101 MHz, $CDCl_3$): δ = 172.5, 134.8, 131.9, 130.1, 121.8, 61.6, 54.3, 27.1, 14.1 ppm; MS (ESI$^+$): *m/z* = 561 $[M+Na]^+$, 485 $[M]^+$, 439 $[M\text{-}OEt]^+$; HRMS (ESI$^+$): calcd. for $C_{20}H_{20}Br_2O_4Na$ 506.9600 $[M+Na]^+$, found 506.9603.

2.2 2,3-Bis(4-bromophenyl)succinic acid (8)



7 (15.0 g, 31.0 mmol) and KOH (8.69 g, 155 mmol) were refluxed in EtOH/H2O (1:1, 300 mL) for 4 h. Aq. HCl (10% w/w, 100 mL) was added at 0 °C. The resulting solid was filtered off and washed with H_2O (3x 50 mL) and pentane (3x 50 mL), yielding 13.3 g (31.0 mmol, quant.) of **8** as a white solid. ^{1}H NMR (400 MHz, DMSO-d_6, mixture of stereoisomers): δ = 12.62 (br, 2H), 7.59–7.55 (m, 1H), 7.43–7.40 (m, 1H), 7.38–7.35 (m, 3H), 7.15–7.12 (m, 3H), 4.21 (s, 2H) ppm; ^{13}C NMR (75 MHz, DMSO-d_6, mixture of stereoisomers): δ = 173.5, 171.9, 136.6, 135.9, 131.4, 131.2, 130.7, 130.5, 120.9, 120.4, 53.6, 52.8 ppm; MS (ESI$^+$): *m/z* = 471 $[M-H+2Na]^+$; MS (ESI$^-$): *m/z* = 425 $[M-H]^-$, 337 $[M-H-2CO_2]^-$; HRMS (ESI$^+$): calcd. for $C_{16}H_{11}NaBr_2O_4Na$ 470.8814 $[M-H+2Na]^+$, found 470.8808.

2.3 2,7-Dibromo-4b,9b-dihydrodibenzo[*a*,*e*]pentalene-5,10-dione (4)

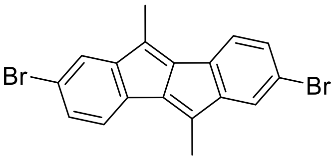


Trifluoromethanesulfonic acid (6 mL) was added to **8** (1.40 g, 3.27 mmol), and the mixture was stirred for 18 h at 75 °C. After cooling to rt, the mixture was poured onto ice. The aqueous phase was extracted with CH_2Cl_2 (5x 25 mL). The combined organic extracts were washed with sat. aq. $NaHCO_3$ (50 mL), dried ($Na_2SO_{4,}$), and the solvent was removed under reduced pressure. Recrystallization from *i*-PrOH afforded **4** (720 mg, 1.84 mmol, 53%) as a beige-colored solid. R_f = 0.30 (cyclohexane/CH_2Cl_2 1:2); ^{1}H NMR (400 MHz, $CDCl_3$): δ = 7.84–7.83 (m, 2H), 7.79–7.78 (m, 4H), 4.36 (s, 2H) ppm; ^{13}C NMR (101 MHz, $CDCl_3$): δ = 199.5, 148.0, 138.9, 136.6, 128.2, 127.9, 123.9, 52.5 ppm; MS (EI$^+$): *m/z* = 390 $[M]^+$, 311 $[M-Br]^+$, 283 $[M-Br-CO]^+$, 255 $[M-Br-2CO]^+$, 176 $[M-2Br-2CO]^+$; HRMS (EI$^+$): calcd. for $C_{16}H_8Br_2O_2$ 389.8891 [M], found 389.8891.

2.4 General procedure A for the Grignard-addition, one-pot reaction including elimination to dibenzopentalenes

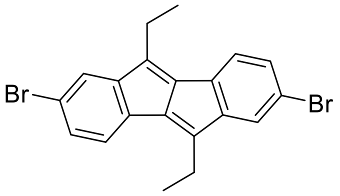
4 was suspended in anh. toluene at 50-60 °C. The Grignard-reagent (3 M in anh. Et_2O) was added, and the suspension was stirred at 110 °C for the specified time. After cooling to rt, conc. HCl was added, and the mixture was stirred at rt for the specified time. The suspension was extracted with CH_2Cl_2. The combined organic extracts were washed with brine, dried ($Na_2SO_{4,}$), and the solvent was removed under reduced pressure. Several runs of column chromatography (silica gel, cyclohexane/EE) afforded pure dibenzopentalenes. Yields are not optimized, mixtures were discarded and not further purified.

2.4.1 2,7-Dibromo-5,10-dimethyl-dibenzo[*a*,*e*]pentalene (3a)



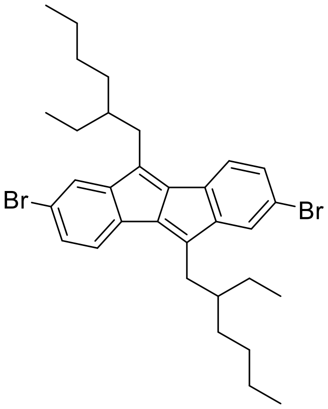
According to general procedure A, dione **4** (500 mg, 1.28 mmol) was reacted with methylmagnesium bromide (1.50 mL, 4.50 mmol) in anh. toluene (30 mL) for 70 min. After cooling to rt, reaction with conc. HCl (20 mL) over 30 min and purification afforded **3a** (90.0 mg, 232 µmol, 18%) as a red-orange crystalline solid. $R_f = 0.86$ (cyclohexane/CH_2Cl_2 1:2); ^1H NMR (400 MHz, CD_2Cl_2): $\delta = 7.09$ (dd, $J = 7.8, 1.8$ Hz, 2H), 7.05 (d, $J = 1.7$ Hz, 2H), 7.02 (d, $J = 7.8$ Hz, 2H), 2.15 (s, 6H) ppm; ^{13}C NMR was omitted due to poor solubility; MS (EI^+): $m/z = 386$ $[M]^+$, 371 $[M-Me]^+$, 307 $[M-Br]^+$, 228 $[M-2Br]^+$; HRMS (EI^+): calcd. for $C_{18}H_{12}Br_2$ 385.9306 [M], found 385.9302.

2.4.2 2,7-Dibromo-5,10-diethyl-dibenzo[*a*,*e*]pentalene (3b)



According to general procedure A, dione **4** (196 mg, 500 µmol) was reacted with ethylmagnesium bromide (600 µL, 1.80 mmol) in anh. toluene (12 mL) for 105 min. After cooling to rt, reaction with conc. HCl (8 mL) over night and purification afforded **3b** (10 mg, 24 µmol, 5%) as a red crystalline solid. R_f = 0.79 (cyclohexane/EE 6:1); ^{1}H NMR (300 MHz, $CDCl_3$): δ = 7.08–7.03 (m, 4H), 6.96 (dd, *J* = 7.6, 0.7 Hz, 2H), 2.55 (q, *J* = 7.6 Hz, 4H), 1.24 (t, *J* = 7.6 Hz, 6H) ppm; ^{13}C NMR (75 MHz, $CDCl_3$): δ = 152.0, 142.7, 142.6, 134.0, 129.7, 124.4, 123.1, 121.5, 19.9, 13.2 ppm; MS (EI$^+$): *m/z* = 414 [M]$^+$, 385 [M-Et]$^+$, 335 [M-Br]$^+$, 256 [M-2Br]$^+$; HRMS (EI$^+$): calcd. for $C_{20}H_{16}Br_2$ 413.9619 [M], found 413.9618.

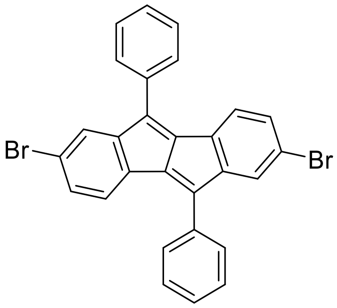
2.4.3 2,7-Dibromo-5,10-bis(2-ethylhexyl)-dibenzo[*a*,*e*]pentalene (3c)



This procedure is based on the $CeCl_3$-mediated addition of Grignard reagents to ketones.[3] Anh. $CeCl_3$ (189 mg, 765 µmol) was dried at 140 °C for 1 h *in vacuo*. Under Argon, it was cooled to 0 °C, at which temperature anh. THF (5 mL) was added. The white suspension was stirred at rt for 3.5 h, then 2-ethylhexylmagnesium bromide (1 M in Et_2O, 765 µL, 765 µmol) was added at 0 °C. After stirring at this temperature for 1.5 h, dione **4** (100 mg, 255 µmol) was added, and the stirring was continued at 0 °C for 65 min. The reaction was quenched by addition of conc. HCl (3 mL) and warmed to rt overnight. The solvent was removed under reduced pressure and the residue diluted with H_2O. The aqueous phase was extracted with CH_2Cl_2 (2x 10 ml). The combined org. extracts were washed with brine, dried (Na_2SO_4), and the solvent was removed under reduced pressure. Column chromatography (silica gel, cyclohexane) afforded **3c** (4 mg, 7 µmol, 3% over two steps) as a red-orange, slightly oily solid. R_f = 0.51 (pentane); ^{1}H NMR (500 MHz, $CDCl_3$): δ = 7.05 (dd, *J* = 7.8, 1.8 Hz, 2H), 7.00 (d, *J* = 1.8 Hz, 2H), 6.95 (d, *J* = 7.8 Hz, 2H), 2.49–2.42 (m, 4H), 1.71–1.63 (m, 2H), 1.47–1.26 (m, 16H), 0.92 (t, *J* = 7.4 Hz, 6H), 0.88 (t, *J* = 7.0 Hz, 6H) ppm; ^{13}C NMR (101 MHz, $CDCl_3$):

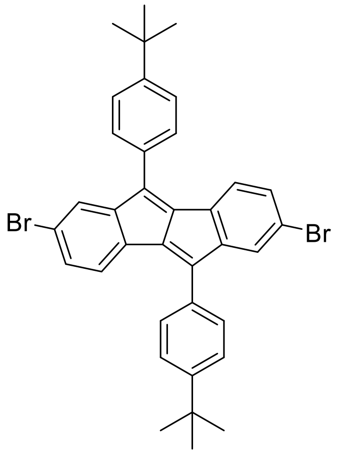
δ = 152.8, 143.9, 140.9, 134.2, 129.6, 124.6, 123.0, 121.3, 39.4, 33.3, 31.7, 29.0, 26.6, 23.2, 14.2, 11.2 ppm; HRMS (EI$^+$): calcd. for $C_{32}H_{40}Br_2$ 582.1497 [M], found 582.1473.

2.4.4 2,7-Dibromo-5,10-diphenyl-dibenzo[*a*,*e*]pentalene (3d)



According to general procedure A, dione **4** (196 mg, 500 µmol) was reacted with phenylmagnesium bromide (600 µL, 1.80 mmol) in anh. toluene (12 mL) for 110 min. After cooling to rt, reaction with conc. HCl (8 mL) over night and purification afforded **3d** (62 mg, 121 µmol, 24%) as an orange-colored crystalline solid. R_f = 0.81 (cyclohexane/CH_2Cl_2 1:2); ^{1}H NMR (500 MHz, CD_2Cl_2): δ = 7.64–7.61 (m, 4H), 7.57–7.54 (m, 4H), 7.51–7.48 (m, 2H), 7.17 (d, *J* = 1.8 Hz, 2H), 7.07 (d, *J* = 7.9 Hz, 2H), 7.02 (dd, *J* = 8.0, 1.8 Hz, 2H) ppm; ^{13}C NMR (126 MHz, CD_2Cl_2): δ = 151.8, 143.4, 140.9, 133.9, 133.3, 130.5, 129.7, 129.4, 128.7, 126.2, 123.5, 122.4 ppm; HRMS (EI$^+$): calcd. for $C_{20}H_{16}Br_2$ 509.9619 [M], found 509.9623.

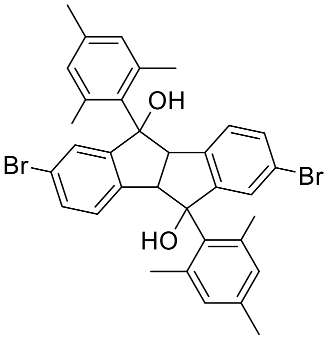
2.4.5 2,7-Dibromo-5,10-bis(4-*tert*-butylphenyl)-dibenzo[*a*,*e*]pentalene (3e)



4-*tert*-Butylphenylbromide (726 mg, 328 µmol) in anh. THF (4 mL) was cooled to -50 °C, at which temperature *n*-BuLi (1.6 M in *n*-hexane, 183 µL, 293 µmol) was added. After stirring at this temperature for 20 min, the solution was added to **4** (50 mg, 128 µmol) in anh. THF

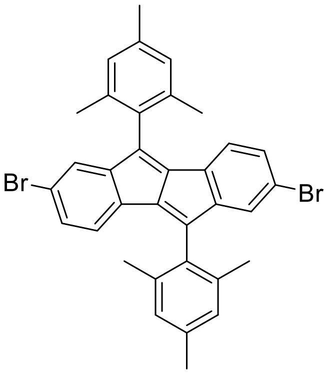
(11 mL) at -50 °C. Stirring of the red solution was continued at -50 °C for 1 h, and the solution was then warmed to rt. After 1 h at rt TFA (3 mL) was added and the resulting yellow solution was stirred for 2 d at rt. The solvent was removed under reduced pressure and the residue was dissolved in CH_2Cl_2 (10 mL). The organic phase was washed with H_2O (10 mL) and brine (2x 10 mL), dried (Na_2SO_4), and the solvent was removed under reduced pressure. Column chromatography (silica, cyclohexane) afforded **3e** (9.0 mg, 10% over two steps) as a red solid. $R_f = 0.94$ (cyclohexane/CH_2Cl_2 1:1); HRMS (EI^+): calcd. for $C_{36}H_{32}Br_2$ 622.0871 [M], found 622.0866.

2.5 2,7-Dibromo-4b,5,9b,10-tetrahydro-5,10-bis(2,4,6-trimethylphenyl)-indeno[2,1-*a*]indene-5,10-diol (9)



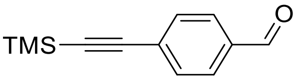
This procedure is based on the $CeCl_3$-mediated addition of Grignard reagents to ketones.[2] Anh. $CeCl_3$ (1.13 g, 4.59 mmol) was dried at 130-135 °C for 2 h *in vacuo*. Under Argon, it was cooled to 0 °C, at which temperature anh. THF (25 mL) was added. The white suspension was stirred at rt for 15 h, then mesitylmagnesium bromide (1 M in Et_2O, 4.59 mL, 4.59 mmol) was added at 0 °C. After stirring at this temperature for 2.5 h, dione **4** (600 mg, 1.53 mmol) was added, and stirring was continued at 0 °C for 8 h. The reaction was quenched by addition of HOAc (10%, w/w, 30 mL) and warmed to rt. After 20 min, the solution was diluted with Et_2O (60 mL) and the two phases were separated. The aqueous phase was extracted with Et_2O (2x 60 mL). The combined organic extracts were washed with brine (50 mL) and sat. aq. $NaHCO_3$ (2 x 50 mL), dried ($Na_2SO_{4,}$), and the solvent was removed under reduced pressure. Column chromatography (silica, cyclohexane/CH_2Cl_2 3:1 to 1:2) afforded **9** (599 mg, 947 µmol, 62%) as a colorless solid. R_f = 0.60 (cyclohexane/CH_2Cl_2 1:1); ^{1}H NMR (400 MHz, $CDCl_3$): δ = 7.40 (dd, *J* = 8.1, 1.9 Hz, 2H), 7.14 (d, *J* = 1.9 Hz, 2H), 7.09 (d, *J* = 8.1 Hz, 2H), 6.94–6.93 (m, 2H), 6.84 (br, 2H), 4.53 (s, 2H), 3.03 (s, 2H), 2.56 (s, 6H), 2.31 (s, 6H), 1.74 (s, 6H) ppm; ^{13}C NMR (101 MHz, $CDCl_3$): δ = 154.9, 138.3, 137.8, 136.7, 136.3, 135.6, 132.8, 132.0, 131.6, 127.9, 126.8, 122.6, 87.7, 61.7, 25.6, 23.9, 20.7 ppm; MS (EI$^+$): *m/z* = 613 $[M-OH]^+$, 493 $[M-H_2O-Mes]^+$; HRMS (ESI$^+$): calcd. for $C_{34}H_{32}Br_2O_2Na$ 653.0661 $[M+Na]^+$, found 653.0659.

2.6 2,7-Dibromo-5,10-bis(2,4,6-trimethylphenyl)-dibenzo[*a*,*e*]pentalene (3f)



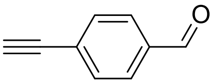
To a suspension of diol **9** (30 mg, 47 µmol) in toluene (1 mL), *p*-toluenesulfonic acid (4.0 mg, 17 µmol) was added. The solution was stirred at 110 °C for 3.5 h, cooled to rt and continued stirring overnight. The red suspension was diluted by CH_2Cl_2 (10 mL), washed with aq. NaOH (1 M, 5 mL) and brine, dried ($Na_2SO_{4,}$), and the solvent was removed under reduced pressure. Column chromatography (silica, cyclohexane/EE 10:1) afforded **3f** (25 mg, 42 µmol, 88%) as a red crystalline solid. $R_f = 0.61$ (cyclohexane); m.p. 342-344 °C; ^{1}H NMR (300 MHz, $CDCl_3$): δ = 6.99 (s, 4H), 6.90 (dd, *J* = 7.8, 1.8 Hz, 2H), 6.63 (d, *J* = 1.8 Hz, 2H), 6.41 (d, *J* = 7.8 Hz, 2H), 2.37 (s, 6H), 2.25 (s, 12H) ppm; ^{13}C NMR (101 MHz, $CDCl_3$): δ = 152.5, 144.6, 139.7, 138.1, 136.3, 133.4, 130.0, 128.8, 128.6, 125.5, 123.3, 122.3, 21.3, 20.3 ppm; HRMS (EI$^+$): calcd. for $C_{34}H_{28}Br_2$ 594.0558 [M], found 594.0555.

2.7 4-(Trimethylsilylethynyl)benzaldehyde (10)



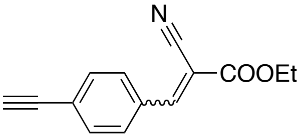
10 was prepared using a modified literature procedure.[4] Trimethylsilylacetylene (2.98 g, 29.7 mmol) was added to a mixture of CuI (93 mg, 486 mmol), 4-bromobenzaldehyde (5.05 g, 27.0 mmol), and $PdCl_2(PPh_3)_2$ (344 mg, 486 µmol) in degassed Et_3N (30 mL), and the mixture was heated to 80 °C for 3.5 h. After cooling to rt, sat. aq. NH_4Cl (30 mL) was added, and the mixture was extracted with CH_2Cl_2 (4x 30 mL). The combined organic extracts were washed with brine (2x 40 mL), dried ($Na_2SO_{4,}$), and the solvent was removed under reduced pressure. Column chromatography (silica gel, cyclohexane/EE 99:1 to 40:1) afforded **10** (4.63 g, 22.9 mmol, 85%) as a yellow solid. $R_f = 0.50$ (cyclohexane/EE 10:1); ^{1}H NMR (400 MHz, $CDCl_3$): δ = 10.00 (s, 1H), 7.81 (d, *J* = 8.3 Hz, 2H), 7.60 (d, *J* = 8.1 Hz, 2H), 0.27 (s, 9H) ppm; ^{13}C NMR (101 MHz, $CDCl_3$): δ = 191.6, 135.7, 132.6, 129.6, 104.0, 99.2, -0.1 ppm; HRMS (EI$^+$): calcd. for $C_{12}H_{14}OSi$ 202.0814 [M], found 202.0815.

2.8 4-Ethynylbenzaldehyde (11)



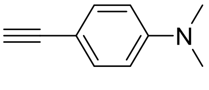
11 was prepared using a modified literature procedure.[5] K_2CO_3 (307 mg, 2.22 mmol) was added to a solution of **10** (4.50 g, 22.2 mmol) in MeOH/Et_2O (5:1, 24 mL). The suspension was stirred at rt for 25 h. After adding sat. aq. NH_4Cl (30 mL), the mixture was extracted with Et_2O (4x30 mL). The combined organic extracts were washed with brine, dried ($Na_2SO_{4,}$), and the solvent was removed under reduced pressure. Column chromatography (silica gel, cyclohexane/EE 1:0 to 9:1) afforded **11** (2.39 g, 18.4 mmol, 83%) as a yellowish solid. R_f = 0.40 (cyclohexane/EE 10:1); ^{1}H NMR (300 MHz, $CDCl_3$): δ = 10.01 (s, 1H), 7.85–7.81 (m, 2H), 7.65–7.61 (m, 2H), 3.29 (s, 0.2H) ppm; ^{13}C NMR (75 MHz, $CDCl_3$): δ = 191.5, 136.1, 132.8, 129.6, 128.4, 82.8, 81.2 ppm; HRMS (EI$^+$): calcd. for C_9H_6O 130.0340 [M-H]$^·$, found 130.0342.

2.9 Ethyl 2-cyano-3-(4-ethynylphenyl)-propenoate (12)



12 was prepared in analogy to a literature procedure.[5] R_f = 0.75 (CH_2Cl_2); ^{1}H NMR (300 MHz, $CDCl_3$): δ = 8.21 (s, 1H), 7.98–7.92 (m, 2H), 7.62–7.56 (m, 2H), 4.39 (q, J = 7.1 Hz, 2H), 3.30 (s, 1H), 1.40 (t, J = 7.1, 3H) ppm; ^{13}C NMR (75 MHz, $CDCl_3$): δ = 162.4, 153.8, 133.0, 131.7, 131.0, 127.2, 115.4, 103.9, 82.8, 81.4, 63.0, 14.3 ppm; HRMS (ESI$^+$): calcd. for $C_{14}H_{11}NO_2$ 248.0682 [M+Na]$^+$, found 248.0682.

2.10 1-(Dimethylamino)-4-ethynylbenzene (13)

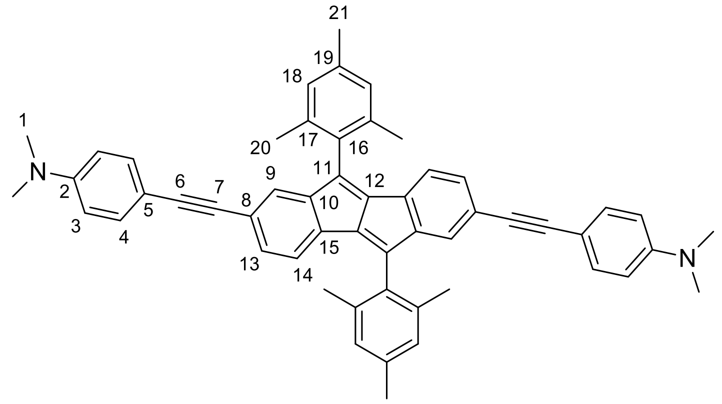


13 was prepared according to a literature procedure.[6] R_f = 0.42 (cyclohexane/EE 95:5); ^{1}H NMR (300 MHz, $CDCl_3$): δ = 7.37 (d, J = 8.8 Hz, 2H), 6.62 (d, J = 8.8 Hz, 2H), 2.98 (s, 6H) ppm; ^{13}C NMR (75 MHz, $CDCl_3$): δ = 150.5, 133.3, 111.8, 108.9, 85.0, 74.9, 40.3 ppm; HRMS (EI$^+$): calcd. for $C_{10}H_{10}N$ 144.0813 [M-H]$^·$, found 144.0812.

2.11 General procedure B for the Sonogashira reaction

A modified procedure from the literature was employed.[7] In a glovebox: A suspension of $Pd(PhCN)_2Cl_2$ (6 mol% or 12 mol%), CuI (6 mol% or 12 mol%) and **3f** in a mixture of abs. toluene and abs. $HN(i\text{-}Pr)_2$ was stirred for 2 min, then $P(t\text{-}Bu)_3$ (10% in hexane, 12 mol% or 24 mol%) was added, and the stirring was continued for 2 min. A solution of the respective alkyne in abs. toluene was added, and the suspension was stirred at rt for the time indicated. After that, the solvent was removed under reduced pressure and column chromatography afforded the product. Yields are not optimized; mixtures were discarded and not further purified.

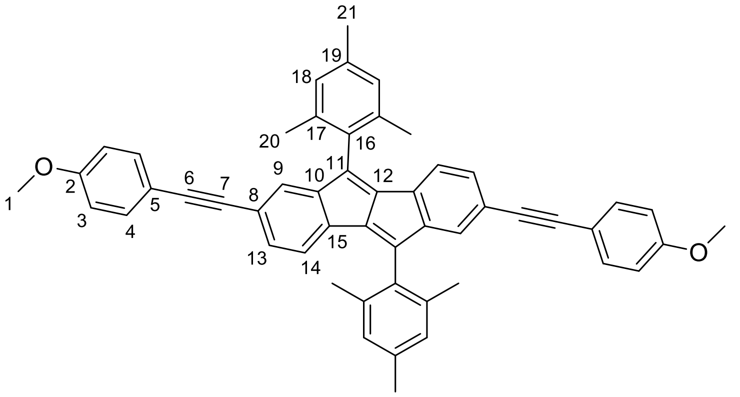
2.11.1 2,7-Bis[(4-ethynylphenyl)dimethylamine]-5,10-bis(2,4,6-trimethylphenyl)-dibenzo[*a*,*e*]pentalene (5a)



(Atom numbering for NMR assignment, does not correspond with the IUPAC numbering)

According to general procedure B: To a suspension of $Pd(PhCN)_2Cl_2$ (12 mol%, 6.4 mg, 17 µmol), CuI (12 mol%, 3.2 mg, 17 µmol) and **3f** (82 mg, 138 µmol) in a mixture of abs. toluene (5 mL) and abs. HN*i*Pr$_2$ (357 µL, 2.54 mmol) P(*t*-Bu)$_3$ (24 mol%, 99 µL, 33 µmol) was added followed by a solution of alkyne **13** (44 mg, 303 µmol) in abs. toluene (3 mL). The mixture was stirred at rt for 5 d. After washing with H_2O (10 mL), the solvent was removed under reduced pressure. Several purification steps afforded **7a** (20 mg, 28 µmol, 20%) as a brown solid, i.e. column chromatography (deactivated silica gel, cyclohexane/CH_2Cl_2/NEt_3 2:1:0.04 to 1:1:0.04), column chromatography (deactivated silica gel, cyclohexane/EE/NEt_3 1:0:0.02 to 1:1:0), extraction of the crystallized product from silica with CH_2Cl_2, then, the received solid was suspended in MeOH (2 mL), stirred at rt for 1.5 h, filtered and the residue was washed with cold MeOH. R_f = 0.43 (cyclohexane/EE 6:1); m.p. >350 °C; ^{1}H NMR (500 MHz, $CDCl_3$): δ = 7.31 (d, *J* = 8.9 Hz, 4H, H-4), 7.00 (s, 4H, H-18), 6.90 (dd, *J* = 7.6, 1.5 Hz, 2H, H-13), 6.64 (s, 2H, H-9), 6.61 (d, *J* = 9.0 Hz, 4H, H-3), 6.52 (d, *J* = 7.6 Hz, 2H, H-14), 2.97 (s, 12H, H-1), 2.38 (s, 6H, H-21), 2.29 (s, 12H, H-20) ppm; ^{13}C NMR (126 MHz, $CDCl_3$): δ = 150.7 (C-10 or* C-12), 150.1 (C-2), 144.9 (C-10 or* C-12), 139.7 (C-11), 137.7 (C-19), 136.5 (C-17), 133.9 (C-15), 132.8 (C-4), 130.3 (C-13), 129.6 (C-16), 128.5 (C-18), 124.9 (C-9), 123.6 (C-8), 122.0 (C-14), 111.9 (C-3), 110.2 (C-5), 91.3 (C-6), 88.1 (C-7), 40.4 (C-1), 21.4 (C-21), 20.4 (C-20) ppm; IR: $\tilde{\nu}$ = 2915 (m), 2361 (m), 2342 (m), 2186 (m), 2160 (w); 1607 (s), 1589 (m), 1521 (s), 1480 (w), 1441 (m), 1361 (s), 1225 (m), 1196 (m), 1140 (m), 1112 (m), 1069 (m), 944 (w), 883 (w), 854 (w), 835 (m), 814 (s), 669 (w), 528 (m), 513 (w), 488 (w), 472 (w), 447 (w), 427 (w) cm^{-1}; HRMS (ESI$^+$): calcd. for $C_{54}H_{48}N_2$ 724.3812 [M]$^+$, found 724.3811; UV/Vis (CH_2Cl_2): λ_{abs} (ε[rel]) = 241 (sh, 0.30), 366 (1), 446 (0.26) nm. *Carbon atoms 10 and 12 could not be unambiguously assigned.

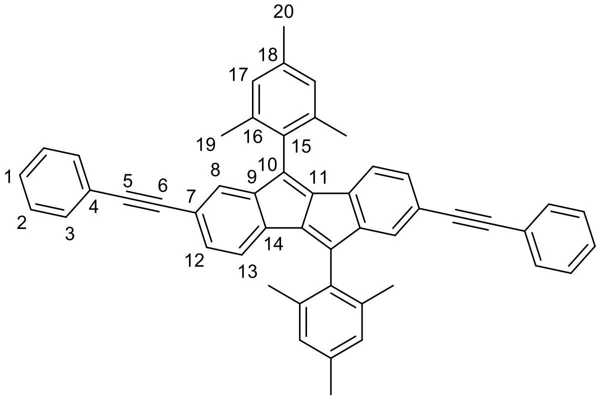
2.11.2 2,7-Bis[4-ethynylanisole]-5,10-bis(2,4,6-trimethylphenyl)-dibenzo[*a*,*e*]pentalene (5b)



(Atom numbering for NMR assignment, does not correspond with the IUPAC numbering)

According to general procedure B: To a suspension of Pd(PhCN)$_2$Cl$_2$ (12 mol%, 3.8 mg, 10 µmol), CuI (12 mol%, 1.9 mg, 10 µmol) and **3f** (50 mg, 84 µmol) in a mixture of abs. toluene (3 mL) and abs. HN*i*Pr$_2$ (216 µL, 1.54 mmol) P(*t*-Bu)$_3$ (24 mol%, 60 µL, 20 µmol) was added followed by a solution of 4-ethynylanisole (24 mg, 184 µmol) in abs. toluene (2 mL). The mixture was stirred at rt for 5 d. Several purification steps afforded **5b** (16 mg, 23 µmol, 27%) as a brown solid, i.e. column chromatography (silica gel, cyclohexane/EE 99:1 to 9:1), column chromatography (silica gel, cyclohexane/EE 99:1 to 96:4), prep. TLC (silica gel, cyclohexane/EE 10:1), prep. TLC (silica gel, cyclohexane/CH$_2$Cl$_2$ 3:2), fivefold prep. TLC (silica gel 60 RP-18, MeCN), prep. TLC (silica gel, cyclohexane/CH$_2$Cl$_2$ 6:1). R_f = 0.55 (cyclohexane/EE 6:1); m.p. 313-315 °C; ^{1}H NMR (500 MHz, CDCl$_3$): δ = 7.39–7.37 (m, 4H, H-4), 7.01 (s, 4H, H-18), 6.93 (dd, *J* = 7.6, 1.4 Hz, 2H, H-13), 6.84–6.82 (m, 4H, H-3), 6.66 (br, 2H, H-9), 6.55 (d, *J* = 7.6 Hz, 2H, H-14), 3.81 (s, 6H, H-1), 2.39 (s, 6H, H-21), 2.29 (s, 12H, H-20) ppm; ^{13}C NMR (126 MHz, CDCl$_3$): δ = 159.7 (C-2), 150.7 (C-10 or* C-12), 144.8 (C-10 or* C-12), 140.0 (C-11), 137.8 (C-19), 136.5 (C-17), 134.4 (C-15), 133.1 (C-4), 130.7 (C-13), 129.4 (C-16), 128.5 (C-18), 125.1 (C-9), 123.1 (C-8), 122.1 (C-14), 115.5 (C-5), 114.1 (C-3), 90.0 (C-6), 88.7 (C-7), 55.4 (C-1), 21.4 (C-21), 20.4 (C-20) ppm; IR: $\tilde{\upsilon}$ = 2916 (m), 2835 (m), 2358 (w), 2335 (w), 1604 (m), 1567 (w), 1508 (s), 1464 (m), 1440 (m), 1414 (m), 1380 (w), 1287 (m), 1247 (s), 1170 (s), 1116 (w), 1073 (w), 1031 (s), 971 (w), 954 (w), 893 (w), 851 (w), 832 (s), 805 (m), 790 (m), 771 (w), 733 (w), 707 (w), 688 (w), 672 (w), 627 (w), 581 (w), 564 (w), 532 (m), 521 (m), 467 (m) cm^{-1}; HRMS (APCI$^+$): calcd. for C$_{52}$H$_{42}$O$_2$H 699.3258 [M+H]$^+$, found 699.3251; UV/Vis (CH$_2$Cl$_2$): λ$_{abs}$ (ε[rel]) = 238 (sh, 0.34), 347 (1), 393 (0.12), 416 (0.17), 442 (0.19) nm. *Carbon atoms 10 and 12 could not be unambiguously assigned.

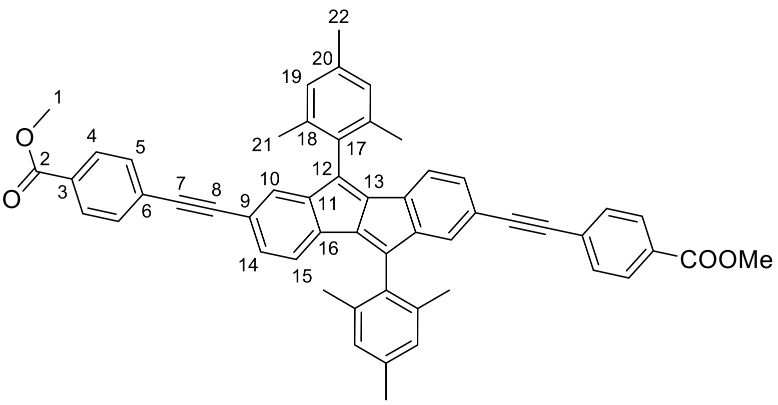
2.11.3 2,7-Bis[ethynyl-benzene]-5,10-bis(2,4,6-trimethylphenyl)-dibenzo[*a*,*e*]pentalene (5c)



(Atom numbering for NMR assignment, does not correspond with the IUPAC numbering)

According to general procedure B: To a suspension of $Pd(PhCN)_2Cl_2$ (6 mol%, 1.9 mg, 5 µmol), CuI (6 mol%, 1.0 mg, 5 µmol) and **3f** (50 mg, 84 µmol) in a mixture of abs. toluene (3 mL) and abs. HN*i*Pr_2 (216 µL, 1.54 mmol) P(*t*-Bu)$_3$ (12 mol%, 30 µL, 10 µmol) was added followed by a solution of phenylacetylene (20 µL, 184 µmol) in abs. toluene (1 mL). The mixture was stirred at rt for 5 d. Column chromatography (silica gel, cyclohexane/EE 1:0 to 50:1) afforded **5c** (19 mg, 30 µmol, 35%) as a red solid. $R_f = 0.82$ (cyclohexane/EE 6:1); m.p. 324-326 °C; ^{1}H NMR (400 MHz, $CDCl_3$): δ = 7.45–7.43 (m, 4H, H-3) 7.31–7.28 (m, 6H, H-1/H-2), 7.01 (s, 4H, H-17), 6.96 (dd, *J* = 7.6, 1.4 Hz, 2H, H-12), 6.68 (dd, *J* = 1.5, 0.6 Hz, 2H, H-8), 6.56 (dd, *J* = 7.5, 0.6 Hz, 2H, H-13), 2.39 (s, 6H, H-20), 2.30 (s, 12H, H-19) ppm; ^{13}C NMR (101 MHz, $CDCl_3$): δ = 150.7 (C-9 or* C-11), 144.8 (C-9 or* C-11), 140.2 (C-10), 137.9 (C-18), 136.5 (C-16), 134.7 (C-14), 131.7 (C-3), 131.0 (C-12), 129.3 (C-15), 128.6 (C-17), 128.4 (C-2), 128.3 (C-1), 125.2 (C-8), 123.4 (C-4), 122.8 (C-7), 122.1 (C-13), 90.0 (C-5 or* C-6), 90.0 (C-5 or* C-6), 21.4 (C-20), 20.4 (C-19) ppm; IR: $\tilde{\upsilon}$ = 2917 (m), 2235 (w), 2199 (w), 1894 (w), 1739 (w), 1621 (m), 1599 (m), 1567 (w), 1490 (m), 1438 (s), 1379 (m), 1327 (w), 1262 (m), 1182 (m), 1069 (m), 1024 (m), 972 (w), 949 (w), 913 (w), 891 (m), 854 (m), 832 (s), 752 (s), 737 (s), 686 (s), 637 (m), 580 (m), 565 (w), 526 (s), 510 (m), 481 (w), 466 (w), 430(w) cm^{-1}; HRMS (EI$^+$): calcd. for $C_{50}H_{38}$ 638.2974 [M], found 638.2972; UV/Vis (CH_2Cl_2): λ_{abs} (ε[rel]) = 237 (sh, 0.32), 342 (1), 393 (0.08), 414 (0.14), 440 (0.16) nm. *Carbon atoms 9 and 11, and 5 and 6, respectively, could not be unambiguously assigned.

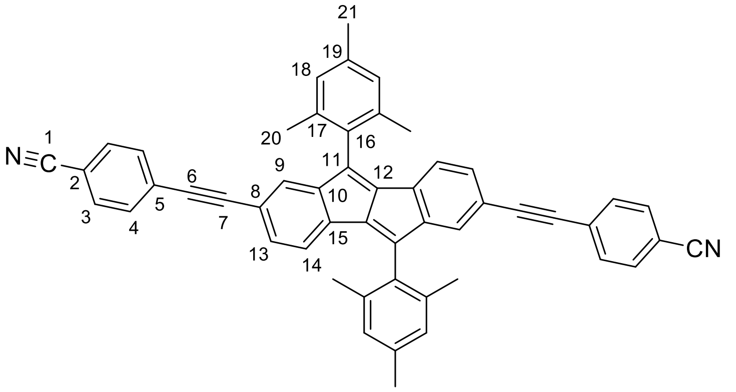
2.11.4 2,7-Bis[methyl 4-ethynylbenzoate]-5,10-bis(2,4,6-trimethylphenyl)-dibenzo[*a*,*e*]pentalene (5d)



(Atom numbering for NMR assignment, does not correspond with the IUPAC numbering)

According to general procedure B: To a suspension of Pd(PhCN)$_2$Cl$_2$ (6 mol%, 1.6 mg, 4 µmol), CuI (6 mol%, 0.8 mg, 4 µmol) and **3f** (41 mg, 69 µmol) in a mixture of abs. toluene (3 mL) and abs. HN*i*Pr$_2$ (181 µL, 1.28 mmol) was added P(*t*-Bu)$_3$ (12 mol%, 25 µL, 8 µmol) was added followed by a solution of methyl 4-ethynylbenzoate (24 mg, 151 µmol) in abs. toluene (1 mL). The mixture was stirred at rt for 25 h. Column chromatography (silica gel, cyclohexane/EE 1:0 to 5:1) afforded **5d** (17 mg, 23 µmol, 33%) as a brown solid. R_f = 0.46 (cyclohexane/EE 6:1); m.p. 333-335 °C; ^{1}H NMR (400 MHz, CDCl$_3$): δ = 7.99–7.96 (m, 4H, H-4), 7.52–7.48 (m, 4H, H-5), 7.02 (s, 4H, H-19), 6.99 (dd, J = 7.6, 1.5 Hz, 2H, H-14), 6.70 (d, J = 1.3 Hz, 2H, H-10), 6.59 (d, J = 7.6 Hz, 2H, H-15), 3.91 (s, 6H, H-1), 2.39 (s, 6H, H-22), 2.30 (s, 12H, H-21) ppm; ^{13}C NMR (101 MHz, CDCl$_3$): δ = 166.7 (C-2), 150.7 (C-11 or* C-13), 144.8 (C-11 or* C-13), 140.5 (C-12), 138.0 (C-20), 136.4 (C-18), 135.2 (C-16), 131.5 (C-5), 131.3 (C-14), 129.6 (C-4), 129.5 (C-3), 129.2 (C-17), 128.6 (C-19), 128.1 (C-6), 125.3 (C-10), 122.2 (C-9), 122.2 (C-15), 93.0 (C-8), 89.3 (C-7), 52.3 (C-1), 21.4 (C-22), 20.4 (C-21) ppm; IR: $\tilde{\nu}$ = 2918 (m), 2206 (w), 2184 (w), 2158 (w), 1717 (s), 1622 (w), 1604 (m), 1435 (m), 1404 (m), 1378 (w), 1307 (w), 1274 (s), 1174 (m), 1143 (w), 1106 (m), 1015 (m), 971 (w), 893 (w), 856 (m), 833 (m), 768 (s), 732 (m), 694 (m), 677 (w), 648 (w), 580 (w), 568 (w), 531 (w), 513 (w), 454 (w), 426 (w), 411 (w) cm^{-1}; HRMS (APCI$^+$): calcd. for C$_{54}$H$_{42}$O$_4$H 755.3156 [M+H]$^+$, found 755.3136; UV/Vis (CH$_2$Cl$_2$): λ_abs (ε[rel]) = 237 (sh, 0.31), 294 (sh, 0.20), 364 (1), 416 (0.14), 441 (0.15) nm. *Carbon atoms 11 and 13 could not be unambiguously assigned.

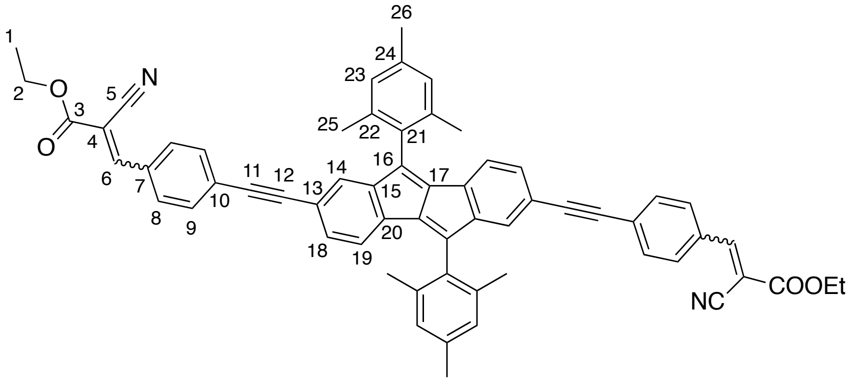
2.11.5 2,7-Bis[4-ethynylbenzonitrile]-5,10-bis(2,4,6-trimethylphenyl)-dibenzo[*a*,*e*]pentalene (5e)



(Atom numbering for NMR assignment, does not correspond with the IUPAC numbering)

According to general procedure B: To a suspension of $Pd(PhCN)_2Cl_2$ (12 mol%, 3.8 mg, 10 µmol), CuI (12 mol%, 1.9 mg, 10 µmol) and **3f** (50 mg, 84 µmol) in a mixture of abs. toluene (3 mL) and abs. HN*i*Pr_2 (216 µL, 1.54 mmol) was added P(*t*-Bu)$_3$ (24 mol%, 60 µL, 20 µmol) was added followed by a solution of 4-ethynylbenzonitrile (23 mg, 184 µmol) in abs. toluene (2 mL). The mixture was stirred at rt for 4 d. Column chromatography (silica gel, cyclohexane/EE 99:1 to 98:2) afforded **5e** (43 mg, 62 µmol, 74%) as a red solid. $R_f = 0.58$ (cyclohexane/EE 6:1); m.p. >350 °C; ^{1}H NMR (400 MHz, $CDCl_3$): δ = 7.60–7.57 (m, 4H, H-3), 7.52–7.49 (m, 4H, H-4), 7.03 (s, 4H, H-18), 6.99 (dd, *J* = 7.6, 1.4 Hz, 2H, H-13), 6.70 (dd, *J* = 1.3, 0.5 Hz, 2H, H-9), 6.60 (dd, *J* = 7.6, 0.4 Hz, 2H, H-14), 2.39 (s, 6H, H-21), 2.29 (s, 12H, H-20) ppm; ^{13}C NMR (101 MHz, $CDCl_3$): δ = 150.7 (C-10 or* C-12), 144.7 (C-10 or* C-12), 140.6 (C-11), 138.1 (C-19), 136.4 (C-17), 135.5 (C-15), 132.1 (C-3), 132.1 (C-4), 131.5 (C-13), 129.1 (C-16), 128.6 (C-18), 128.3 (C-5), 125.4 (C-9), 122.2 (C-14), 121.8 (C-8), 118.7 (C-1), 111.5 (C-2), 94.4 (C-7), 88.4 (C-6), 21.4 (C-21), 20.4 (C-20) ppm; IR: $\tilde{\upsilon}$ = 2917 (m), 2207 (w), 2193 (w), 1997 (w), 1972 (w), 1905 (w), 1603 (m), 1496 (w), 1436 (m), 1404 (m), 1377 (m), 1271 (w), 1173 (m), 1141 (w), 1115 (w), 1073 (m), 1016 (m), 973 (w), 892 (m), 827 (s), 732 (m), 703 (m), 677 (w), 666 (m), 612 (w), 581 (m), 549 (s), 513 (m), 481 (m), 455 (m), 426 (m), 408 (m) cm^{-1}; HRMS (APCI$^+$): calcd. for $C_{52}H_{36}N_2H$ 689.2951 $[M+H]^+$, found 689.2937; UV/Vis (CH_2Cl_2): λ_{abs} (ε[rel]) = 245 (0.30), 294 (sh, 0.20), 367 (1), 415 (0.13), 442 (0.14) nm. *Carbon atoms 10 and 12 could not be unambiguously assigned.

2.11.6 2,7-Bis[ethyl 2-cyano-3-(4-ethynylphenyl)-propanoate]-5,10-bis(2,4,6-trimethylphenyl)-dibenzo[*a*,*e*]pentalene (5f)



(Atom numbering for NMR assignment, does not correspond with the IUPAC numbering)

According to general procedure B: To a suspension of $Pd(PhCN)_2Cl_2$ (12 mol%, 3.8 mg, 10 µmol), CuI (12 mol%, 1.9 mg, 10 µmol) and **3f** (50 mg, 84 µmol) in a mixture of abs. toluene (3 mL) and abs. HN*i*Pr$_2$ (216 µL, 1.54 mmol) was added P(*t*-Bu)$_3$ (24 mol%, 60 µL, 20 µmol) was added followed by a solution of alkyne **12** (41 mg, 184 µmol) in abs. toluene (2 mL). The mixture was stirred at rt for 4 d. Column chromatography (silica gel, cyclohexane/EE 99:1 to 9:1) afforded **5f** (19 mg, 22 µmol, 26%) as a red-brown solid. R_f = 0.30 (cyclohexane/EE 6:1); m.p. 320-323 °C; ^{1}H NMR (400 MHz, $CDCl_3$): δ = 8.19 (s, 2H, H-6), 7.94 (d, *J* = 8.5 Hz, 4H, H-8), 7.54 (d, *J* = 8.4 Hz, 4H, H-9), 7.03 (s, 4H, H-23), 7.00 (dd, J = 7.6, 1.4 Hz, 2H, H-18), 6.71 (d, *J* = 1.4 Hz, 2H, H-14), 6.60 (d, *J* = 7.6 Hz, 2H, H-19), 4.39 (q, *J* = 7.1 Hz, 4H, H-2), 2.40 (s, 6H, H-26), 2.30 (s, 12H, H-25), 1.40 (t, *J* = 7.1 Hz, 6H, H-1) ppm; ^{13}C NMR (101 MHz, $CDCl_3$): δ = 162.6 (C-3), 153.9 (C-6), 150.7 (C-15 or* C-17), 144.8 (C-15 or* C-17), 140.6 (C-16), 138.1 (C-24), 136.4 (C-22), 135.4 (C-20), 132.2 (C-9), 131.6 (C-18), 131.1 (C-8), 130.9 (C-7), 129.1 (C-21), 128.6 (C-23), 128.6 (C-10), 125.4 (C-14), 122.2 (C-19), 122.0 (C-13), 115.6 (C-4), 103.1 (C-5), 94.6 (C-12), 89.4 (C-11), 62.9 (C-2), 21.4 (C-26), 20.4 (C-25), 14.3 (C-1) ppm; IR: $\tilde{\upsilon}$ = 2917 (m), 2224 (w), 2195 (m), 2171 (w), 1732 (s), 1594 (s), 1509 (m), 1442 (m), 1415 (w), 1380 (w), 1366 (w), 1315 (w), 1262 (s), 1204 (s), 1177 (s), 1145 (m), 1115 (w), 1086 (m), 1013 (m), 972 (w), 937 (w), 893 (m), 831 (s), 759 (m), 726 (m), 692 (m), 675 (w), 649 (w), 581 (m), 567 (w), 527 (m), 480 (w), 469 (w), 454 (w), 441 (w), 431 (w), 410 (w) cm^{-1}; HRMS (APCI$^+$): calcd. for $C_{62}H_{48}N_2O_4H$ 885.3687 [M+H]$^+$, found 885.3683; UV/Vis (CH_2Cl_2): λ_{abs} (ε[rel]) = 234 (sh, 0.38), 311 (0.48), 414 (1) nm. *Carbon atoms 15 and 17 could not be unambiguously assigned.

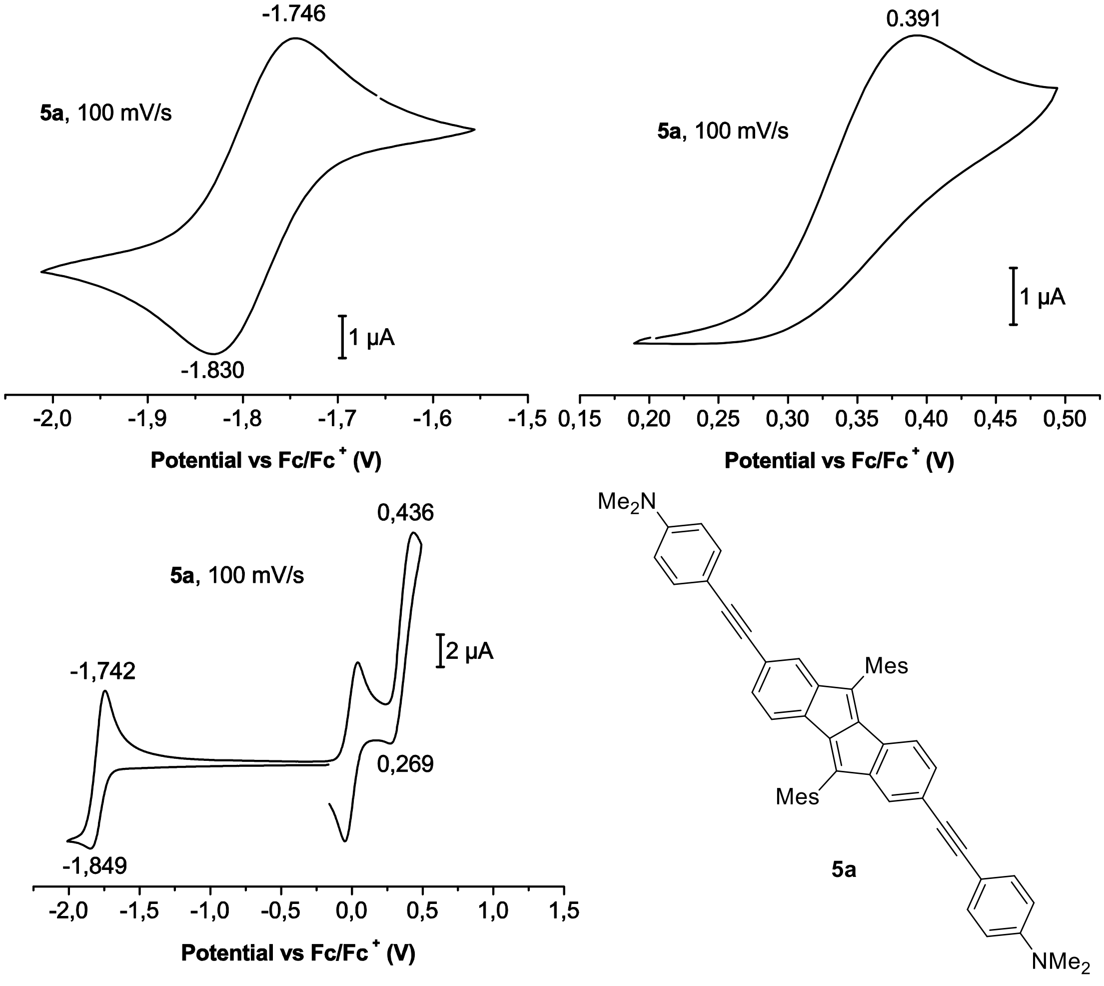
3 Cyclic voltammetry measurements

Cyclic voltammograms (CVs) were measured inside a glovebox using a PGSTAT128N by Metrohm Autolab. As working electrode a glassy carbon disc electrode (2 mm diameter) or a platinum disc electrode (2 mm diameter) was used, as counter electrode a platinum rod and as reference electrode a Ag/AgNO$_3$-electrode containing a silver wire immersed in an inner chamber filled with 1 M AgNO$_3$ and 0.1 M *n*-Bu$_4$NPF$_6$ in abs. acetonitrile. The analyte solution contained 10 mL of solvent (abs. CH$_2$Cl$_2$) with 0.1 M *n*-Bu$_4$NPF$_6$ and the specified analyte concentration. The ferrocene/ferrocenium redox couple was used as internal reference. LUMO levels were calculated using the following equation:

E_{LUMO} (eV) = - ($E_{i,Fc}$ + x)

$E_{i,Fc}$ = ionization energy of ferrocene = 4.8 eV[8]

x = onset of the first reduction peak Calibrated vs. Fc/Fc$^+$ with unit eV.



5a

Figure S1. Cyclic voltammograms of DBP 5a (GC-electrode).

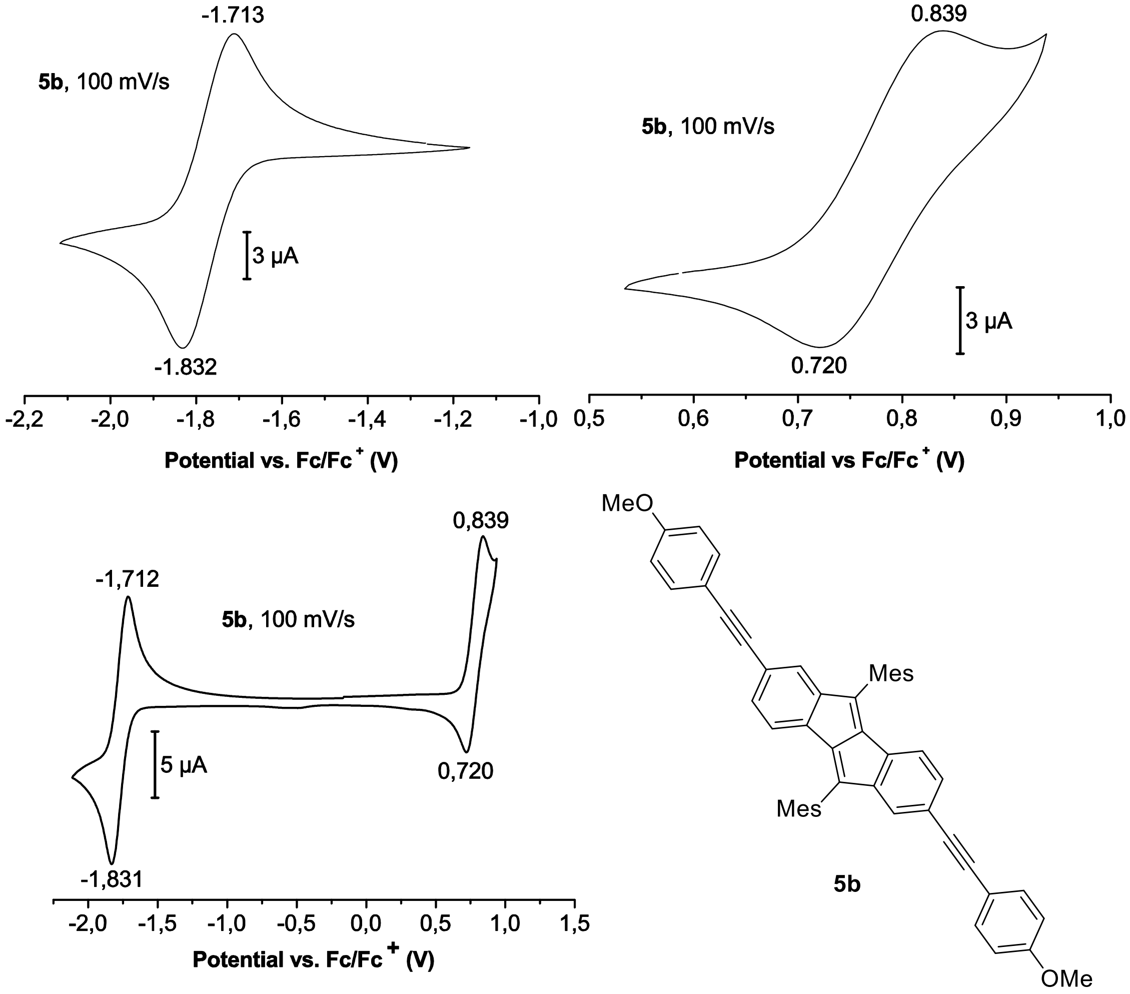


Figure S2. Cyclic voltammograms of DBP 5b (GC-electrode).

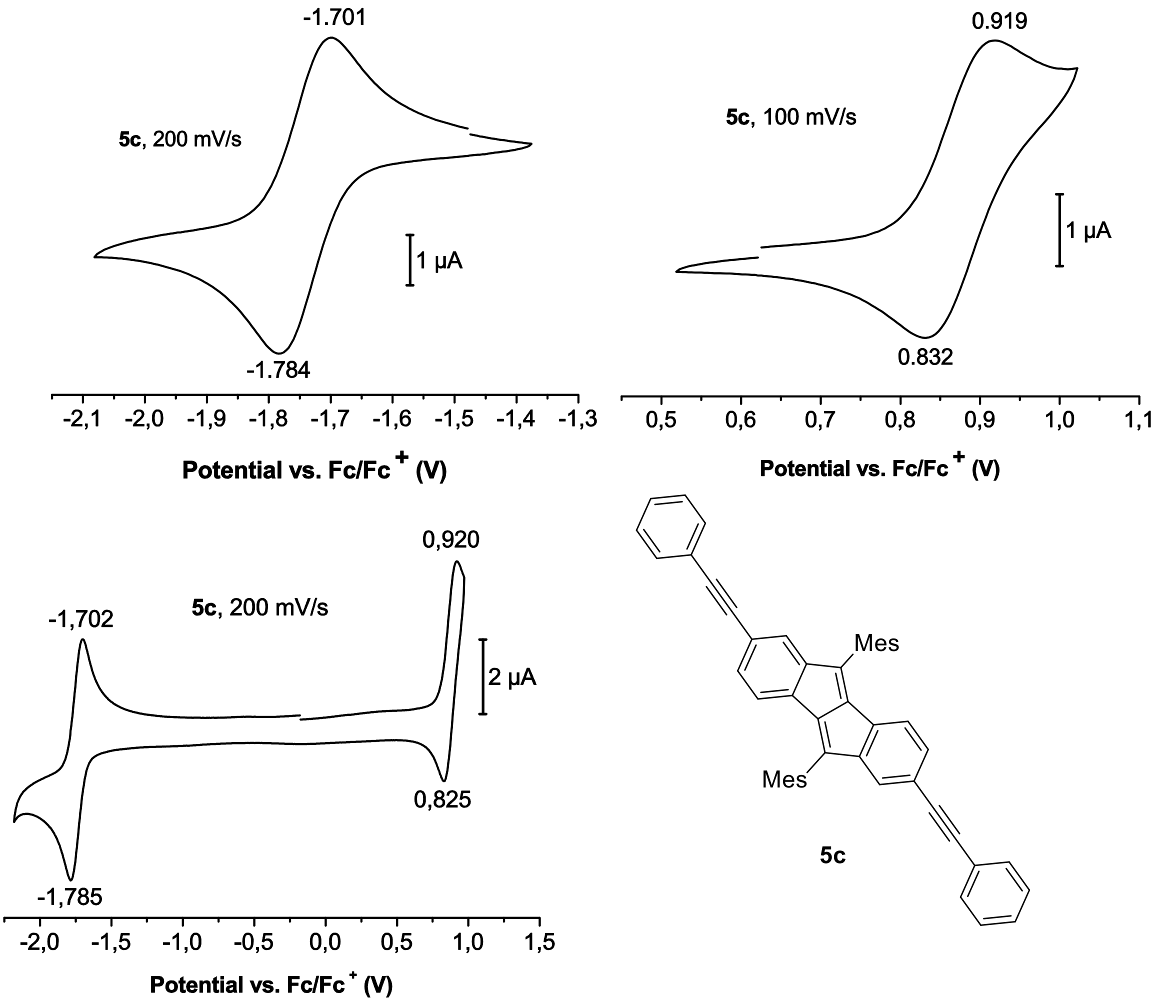


Figure S3. Cyclic voltammograms of DBP 5c (Pt-electrode).

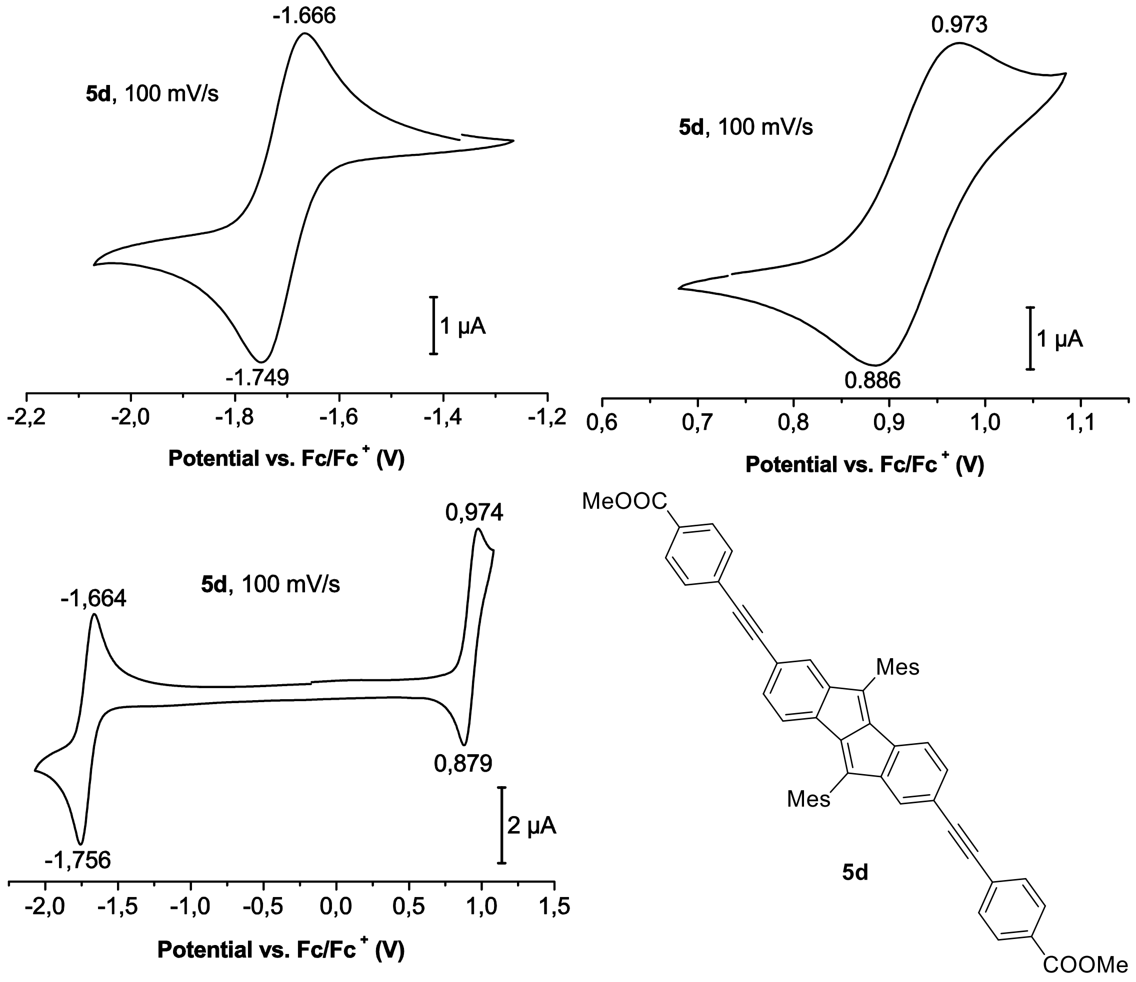


Figure S4. Cyclic voltammograms of DBP 5d (Pt-electrode).

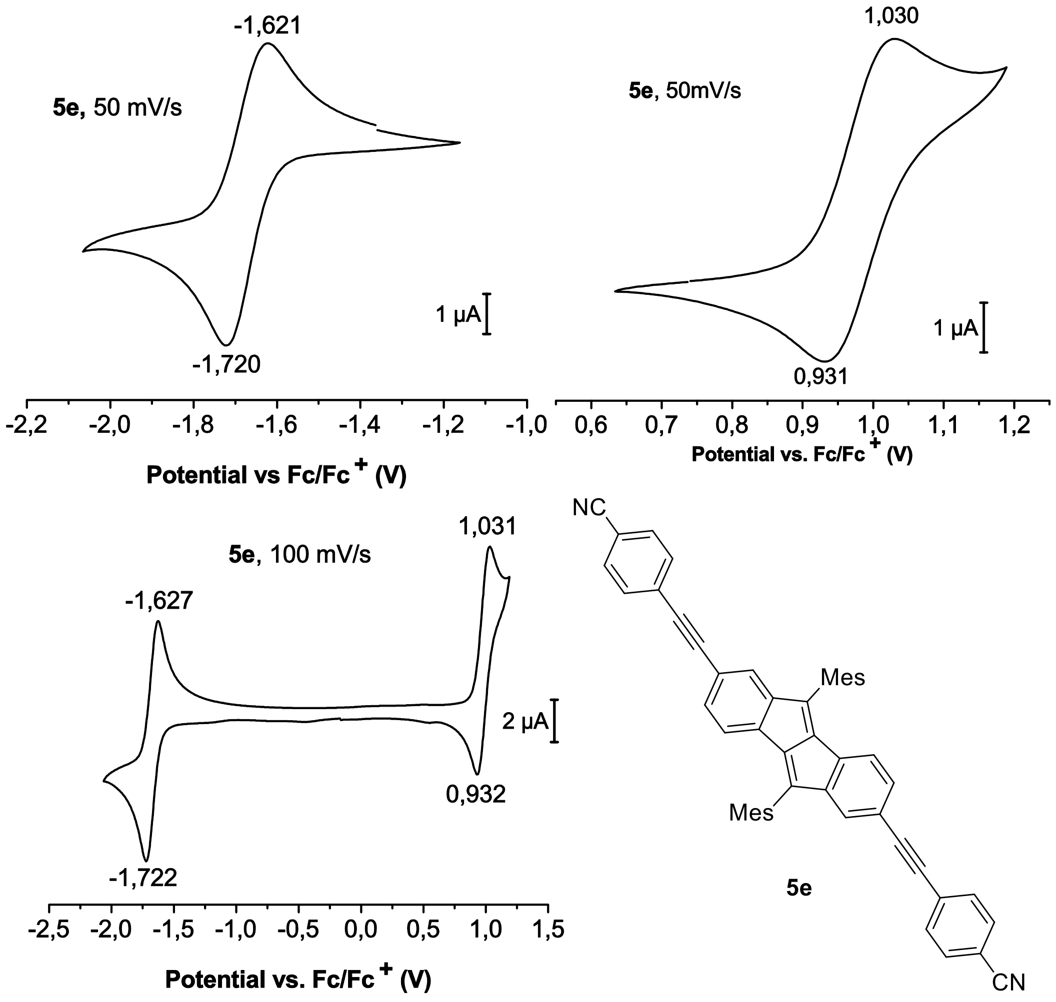
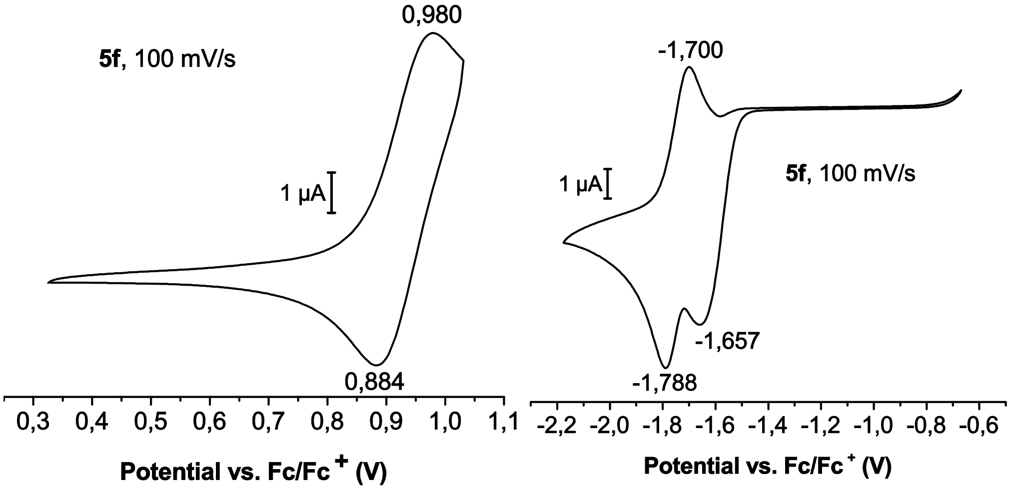
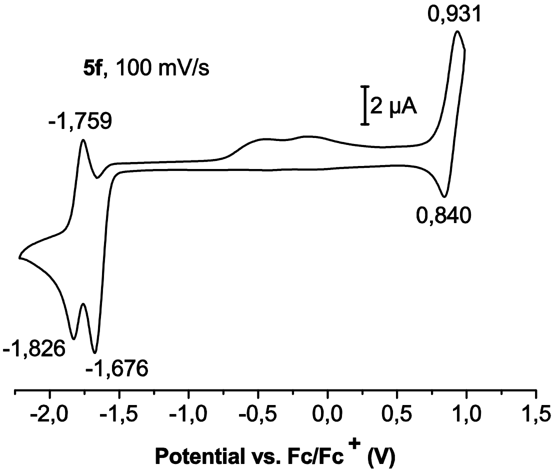
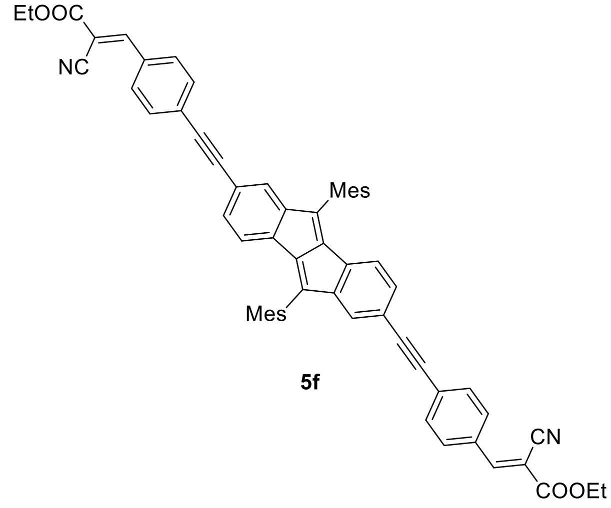


Figure S5. Cyclic voltammograms of DBP 5e (Pt-electrode).







5f

Figure S6. Cyclic voltammograms of DBP 5f (GC-electrode).

4 X-ray crystallography

Clear orange-red needles (**3a**), red blocks (**3b**), red needles (**3d**), clear yellowish-brown plates (**3e**), orange plates (**3f**) and reddish brown plates (**5c**) were grown at room temperature upon slow evaporation of diluted solutions in CH_2Cl_2 (**3a**, **3d** and **3e**), $CDCl_3$ (**3b**), EtOAc/cyclohexane (**3f**) and $CHCl_3$ (**5c**).

The data collections of **3a** and **3d** were performed on a STOE IPDS-2T diffractometer, those of **3b** and **3e** on a Bruker AXS X8-KappaApexII diffractometer, and those of **3f** and **5c** on a Bruker D8-Venture diffractometer using graphite monochromated Mo-Kα radiation (λ = 0.71073 Å) or Cu-Kα radiation (λ = 1.54178 Å). The diffractometers were equipped with a low–temperature device (Cryostream 700er or 800er series (STOE IPDS2T and Bruker D8Venture) or Kryoflex I (Bruker X8 KappaApexII)). Intensities were measured by fine-slicing ϕ- and ω-scans and corrected for background, polarization and Lorentz effects. A semi-empirical absorption correction was applied for the data sets following Blessing's method.[9] The structures were solved by direct methods and refined anisotropically by the least-squares procedure implemented in the ShelX program system.[10]

CCDC numbers 1496147 (**3a**), 1496148 (**3b**), 1496149 (**3d**), 1496150 (**3e**), 1496151 (**3f**), and 1496152 (**5c**) contain the supplementary crystallographic data for this paper, which can be obtained free of charge from the Cambridge Crystallographic Data Centre via www.ccdc.cam.ac.uk/data_request/cif.

5 NMR spectra

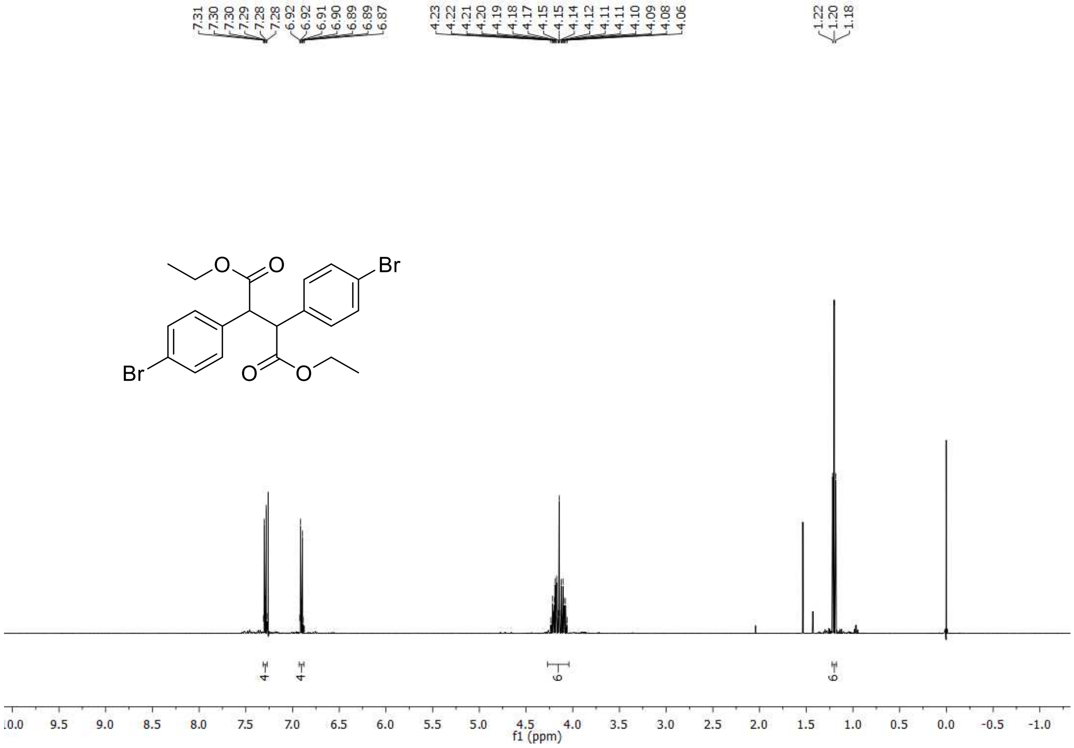


Figure S7 ^{1}H NMR spectrum of 7 in $CDCl_3$ (400 MHz).

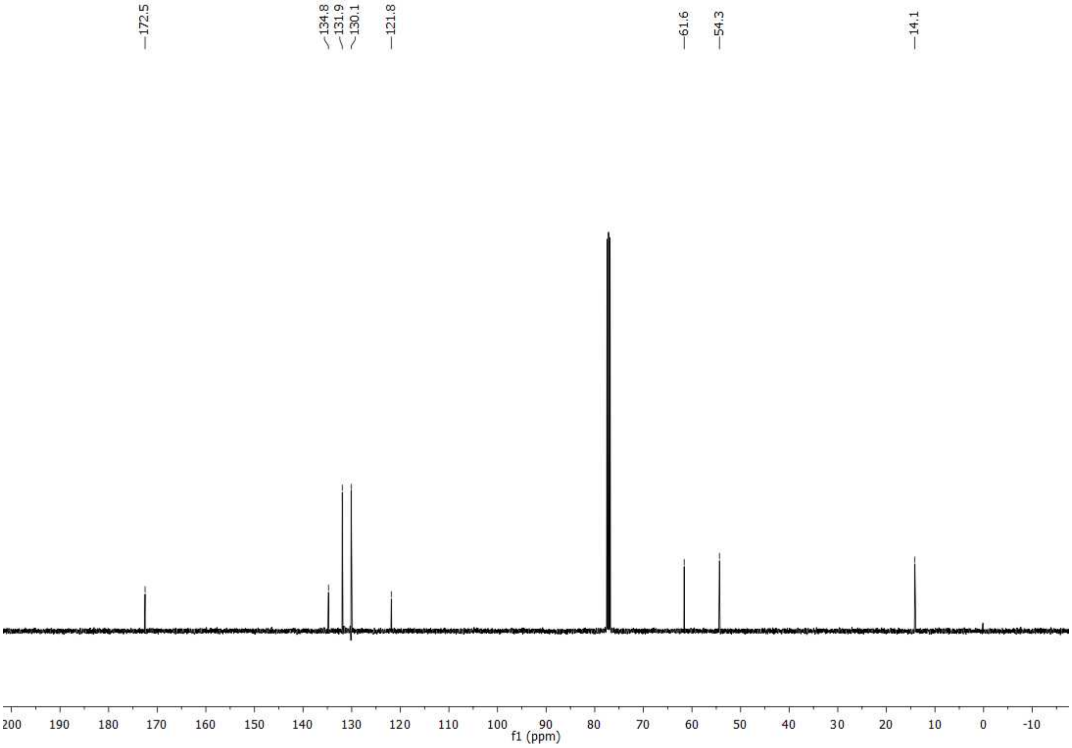


Figure S8 ^{13}C NMR spectrum of 7 in DMSO-d_6 (101 MHz).

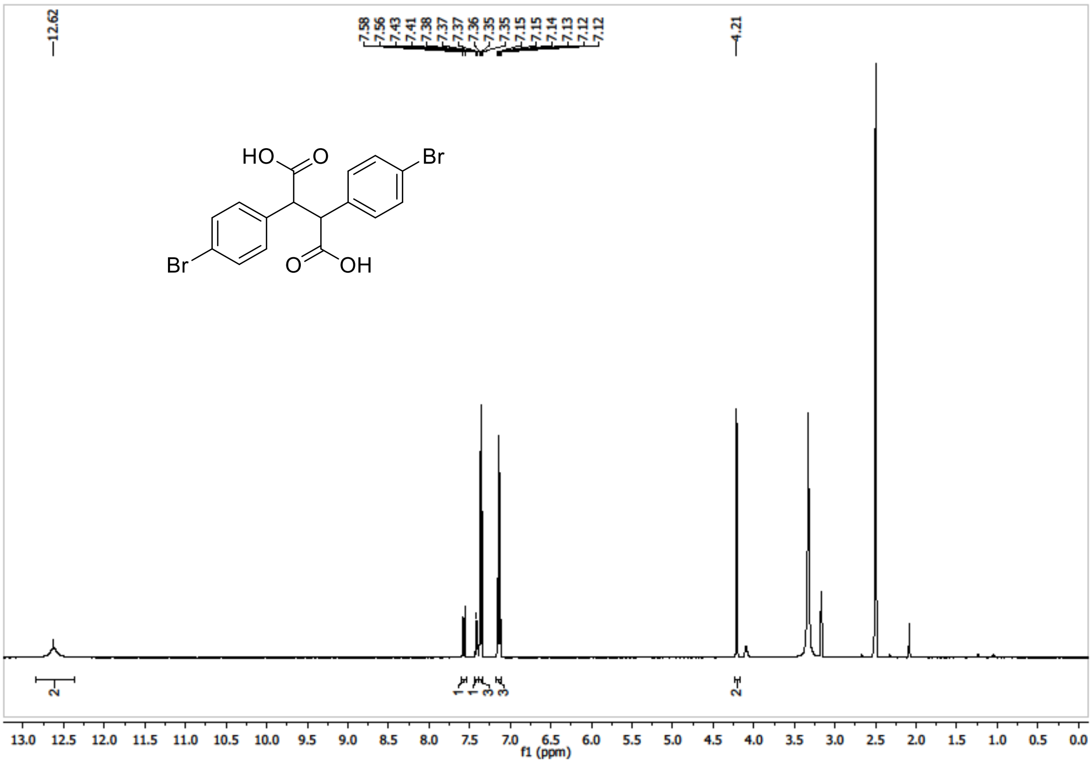


Figure S9 ^{1}H NMR spectrum of 8 in DMSO-d_6 (400 MHz).

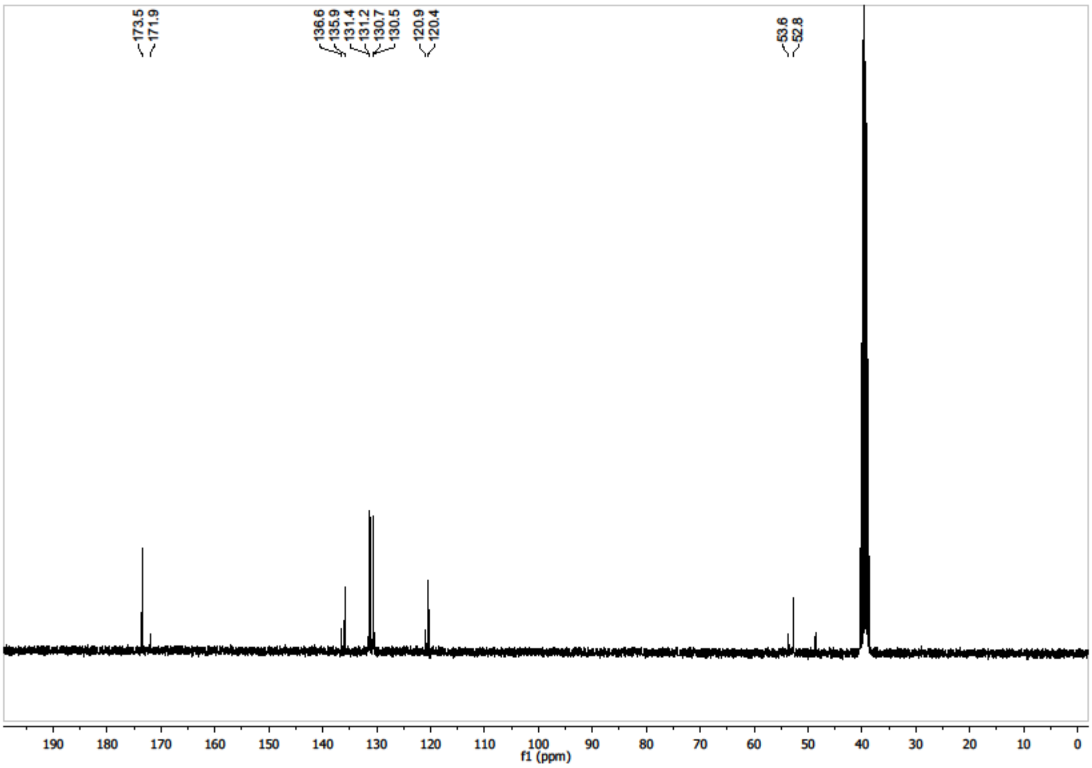


Figure S10 ^{13}C NMR spectrum of 8 in DMSO-d_6 (75 MHz).

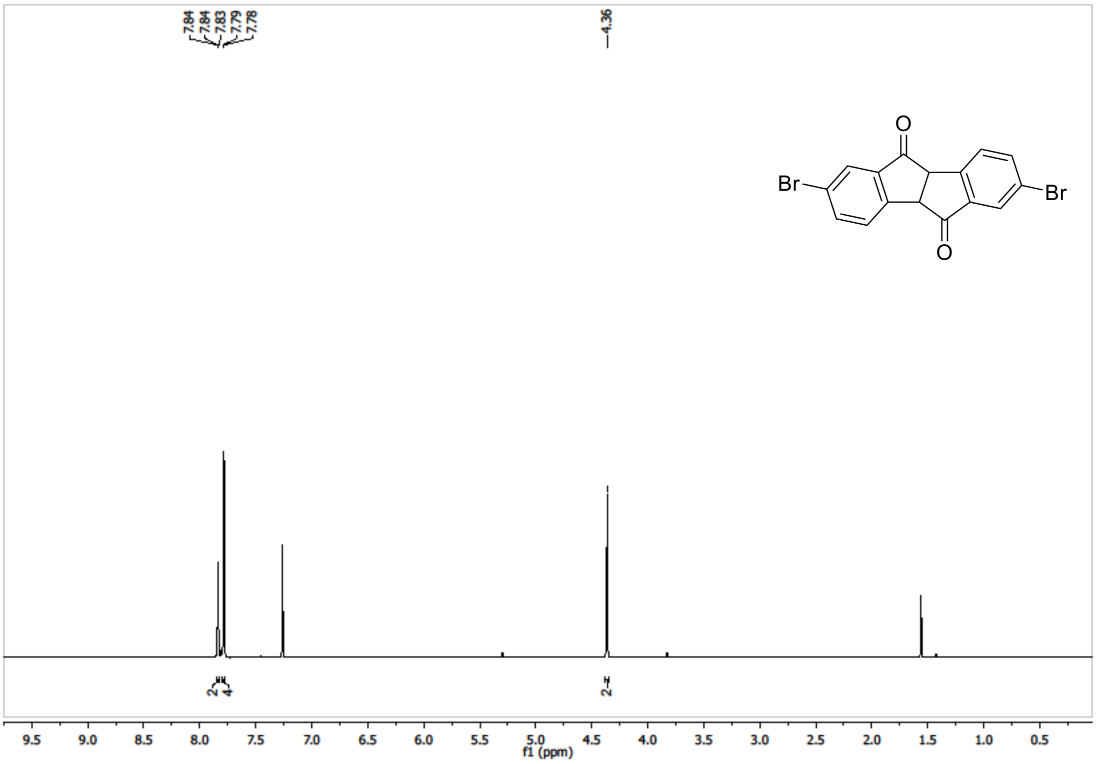


Figure S11 ^{1}H NMR spectrum of 4 in $CDCl_3$ (400 MHz).

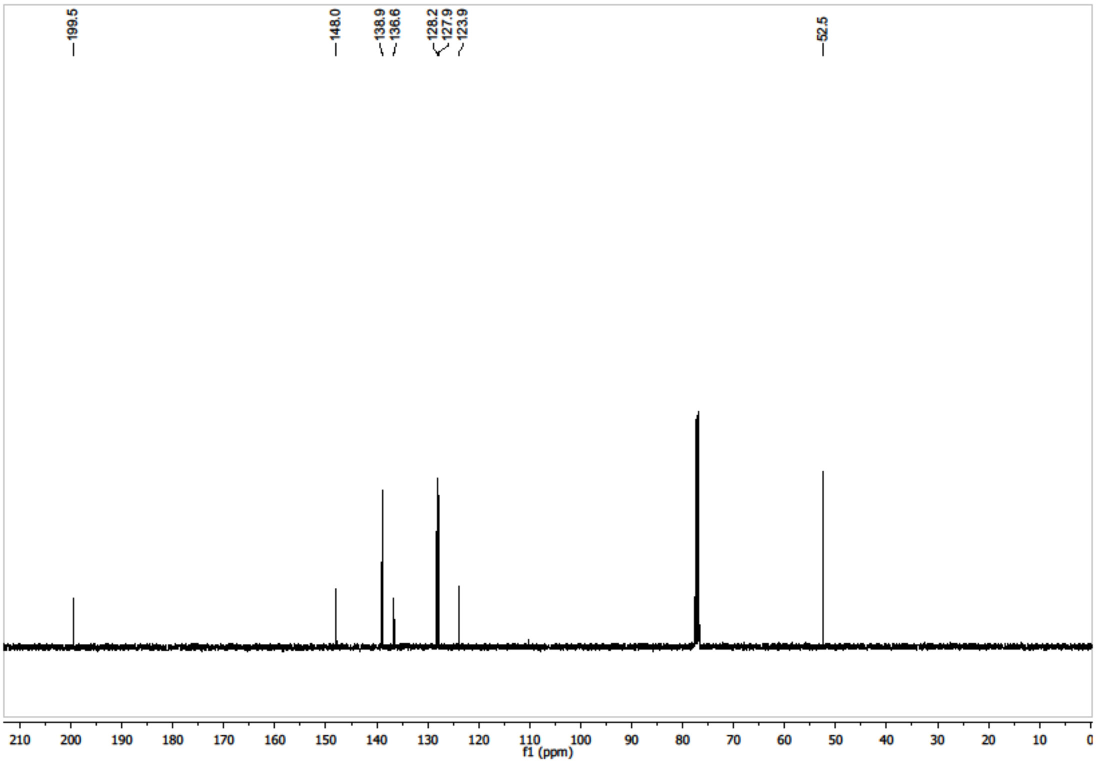


Figure S12 ^{13}C NMR spectrum of 4 in $CDCl_3$ (101 MHz).

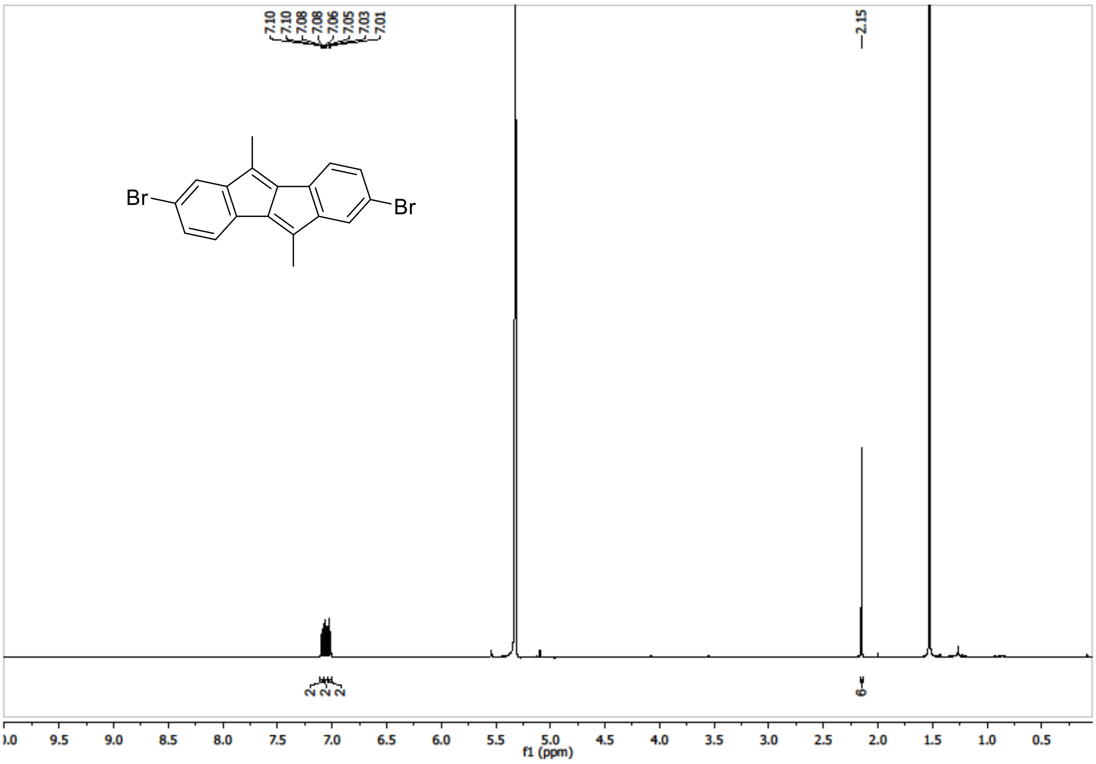


Figure S13 ^{1}**H NMR spectrum of 3a in** CD_2Cl_2 **(400 MHz).**

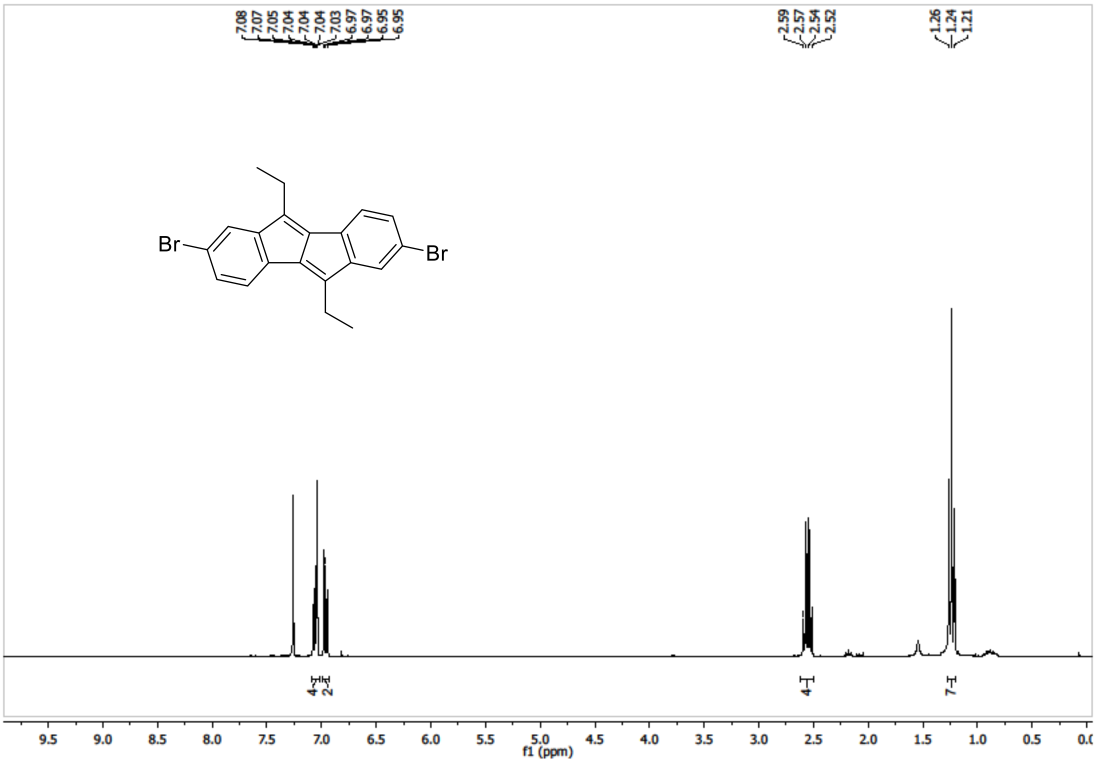


Figure S14 ^{1}H NMR spectrum of 3b in CDCl$_3$ (300 MHz).

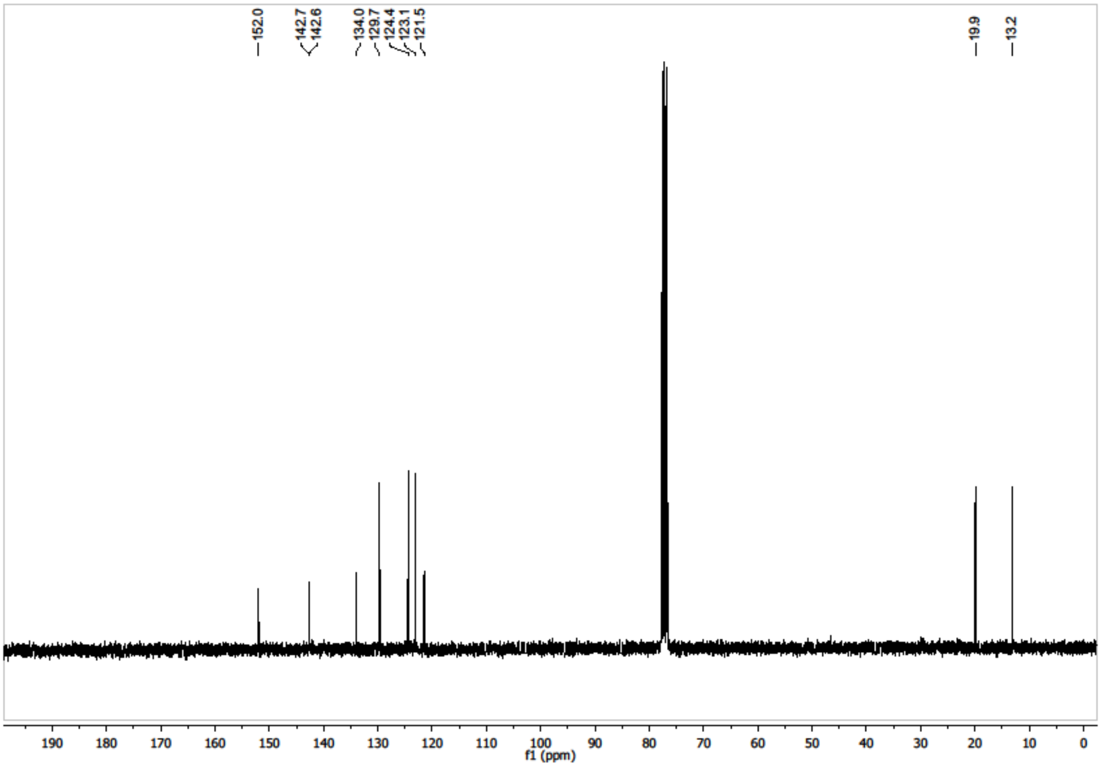


Figure S15 ^{13}C NMR spectrum of 3b in CDCl$_3$ (75 MHz).

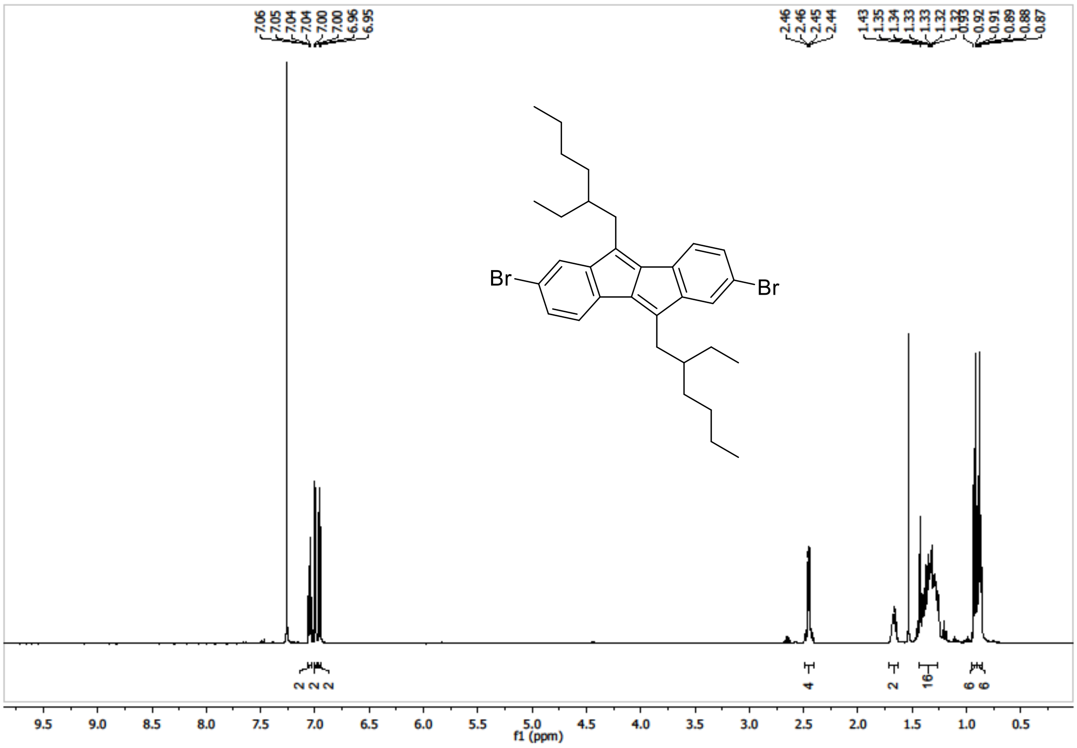


Figure S16 ^{1}H **NMR spectrum of 3c in** $CDCl_3$ **(500 MHz).**

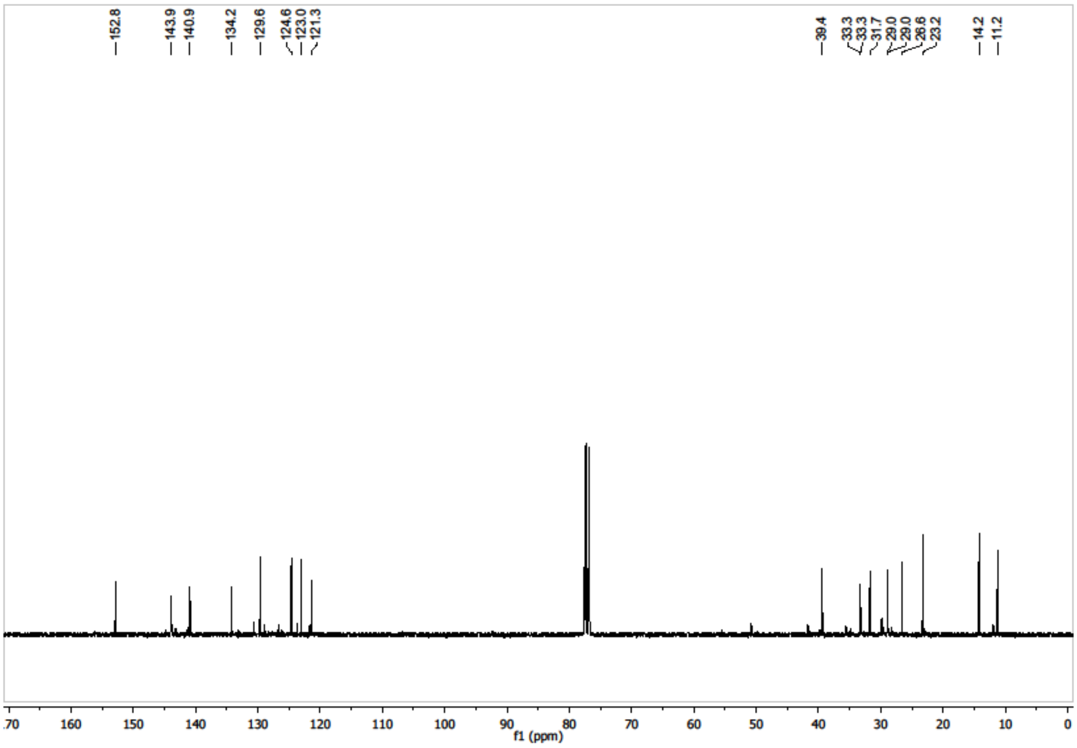


Figure S17 ^{13}C **NMR spectrum of 3c in** $CDCl_3$ **(101 MHz).**

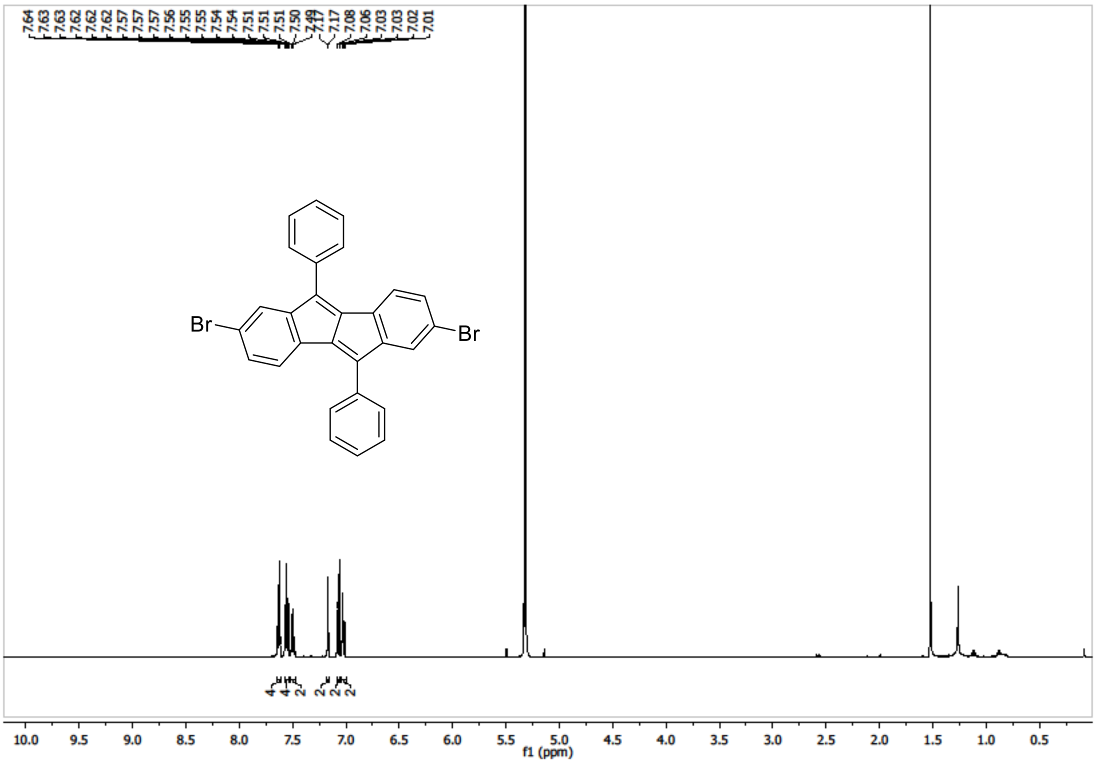


Figure S18 ^{1}H NMR spectrum of 3d in CD_2Cl_2 (500 MHz).

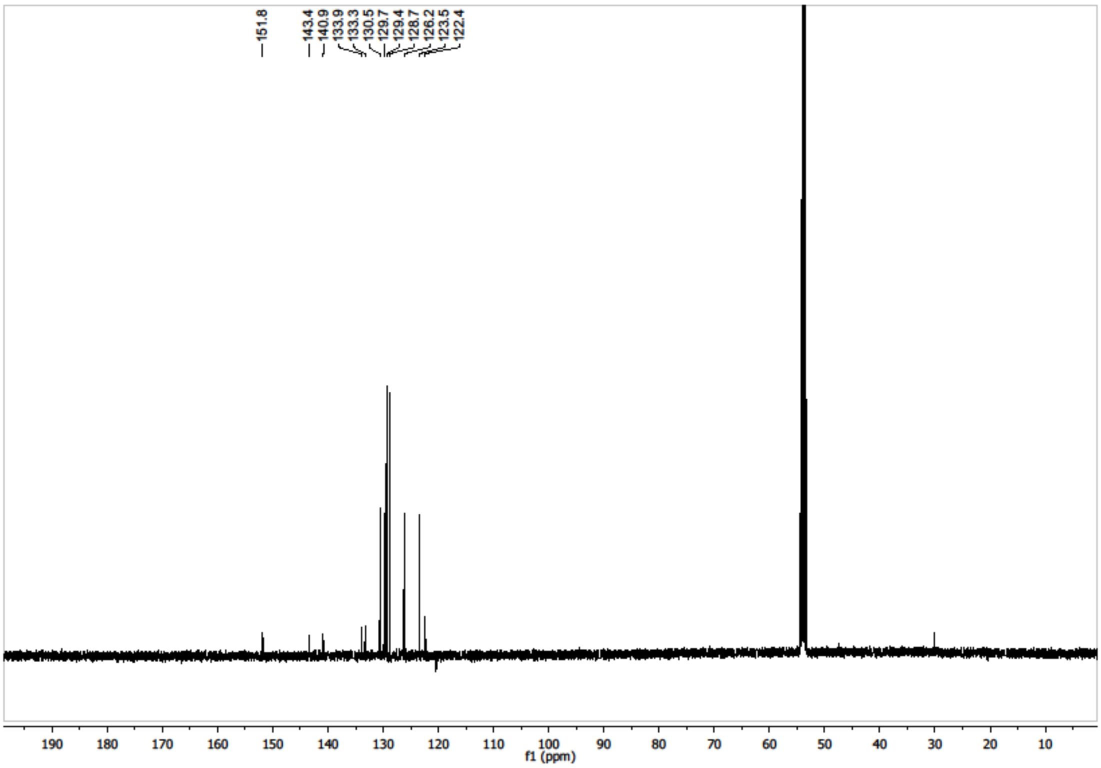


Figure S19 ^{13}C NMR spectrum of 3d in CD_2Cl_2 (126 MHz).

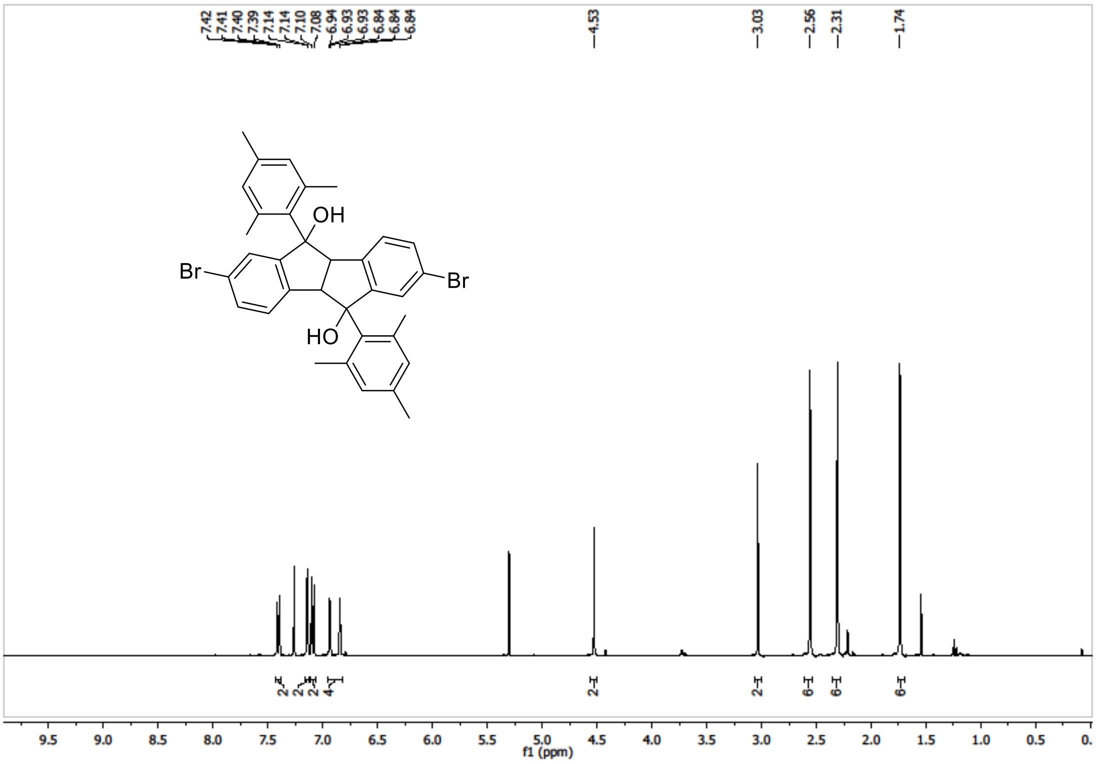


Figure S20 ^{1}H NMR spectrum of 9 in $CDCl_3$ (400 MHz).

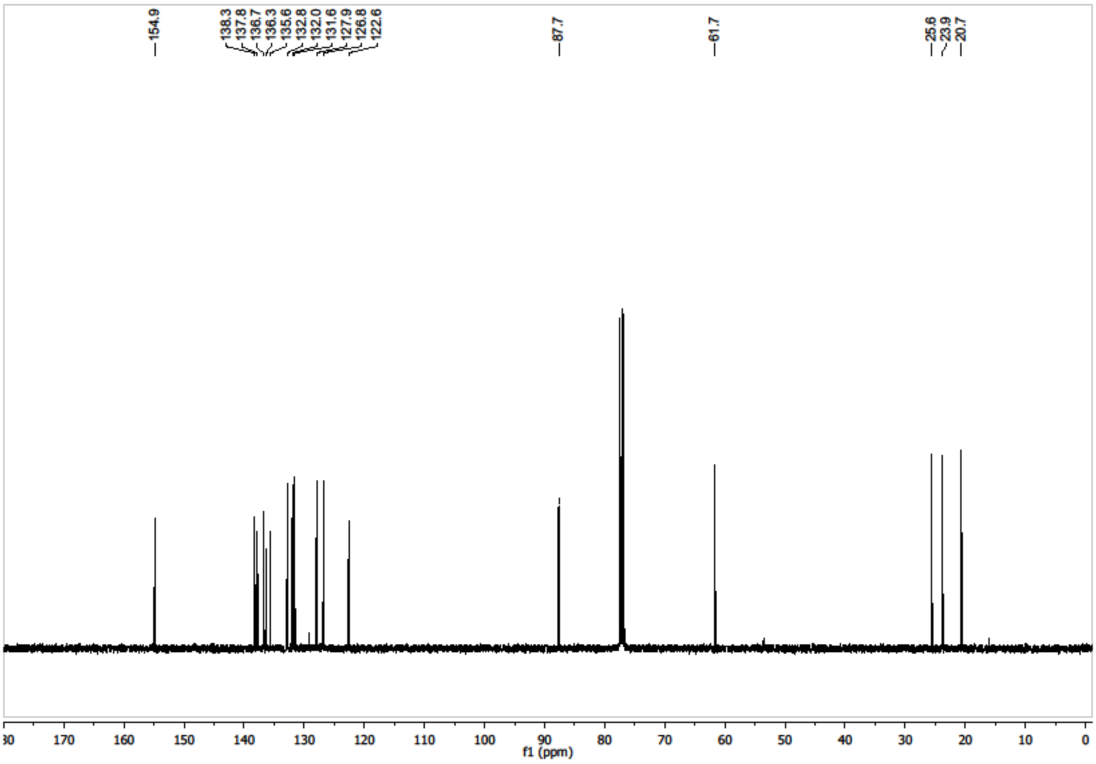


Figure S21 ^{13}C NMR spectrum of 9 in $CDCl_3$ (101 MHz).

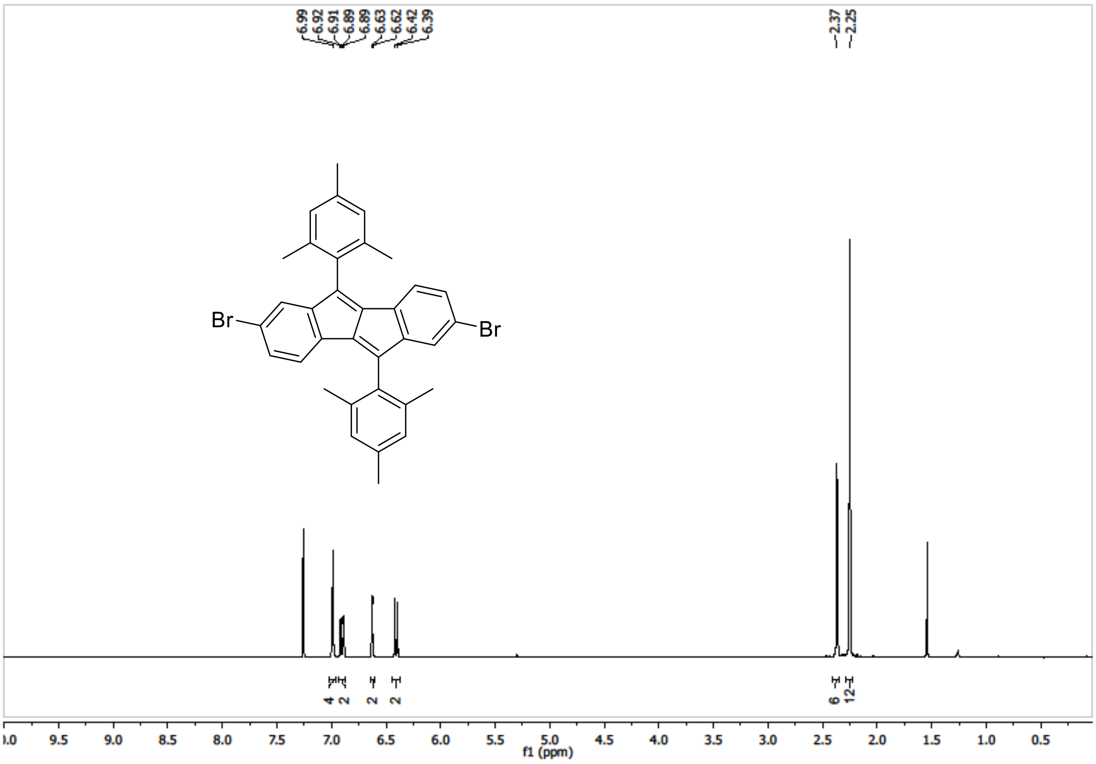


Figure S22 ^{1}H NMR spectrum of 3f in $CDCl_3$ (300 MHz).

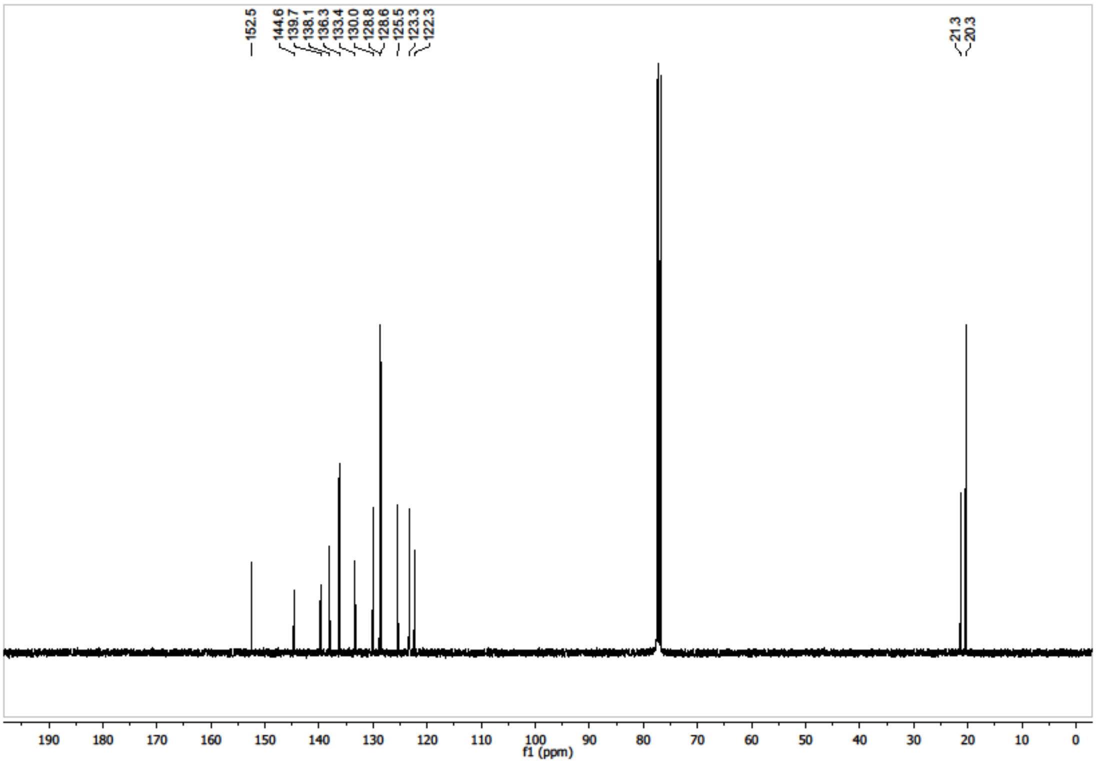


Figure S23 ^{13}C NMR spectrum of 3f in $CDCl_3$ (101 MHz).

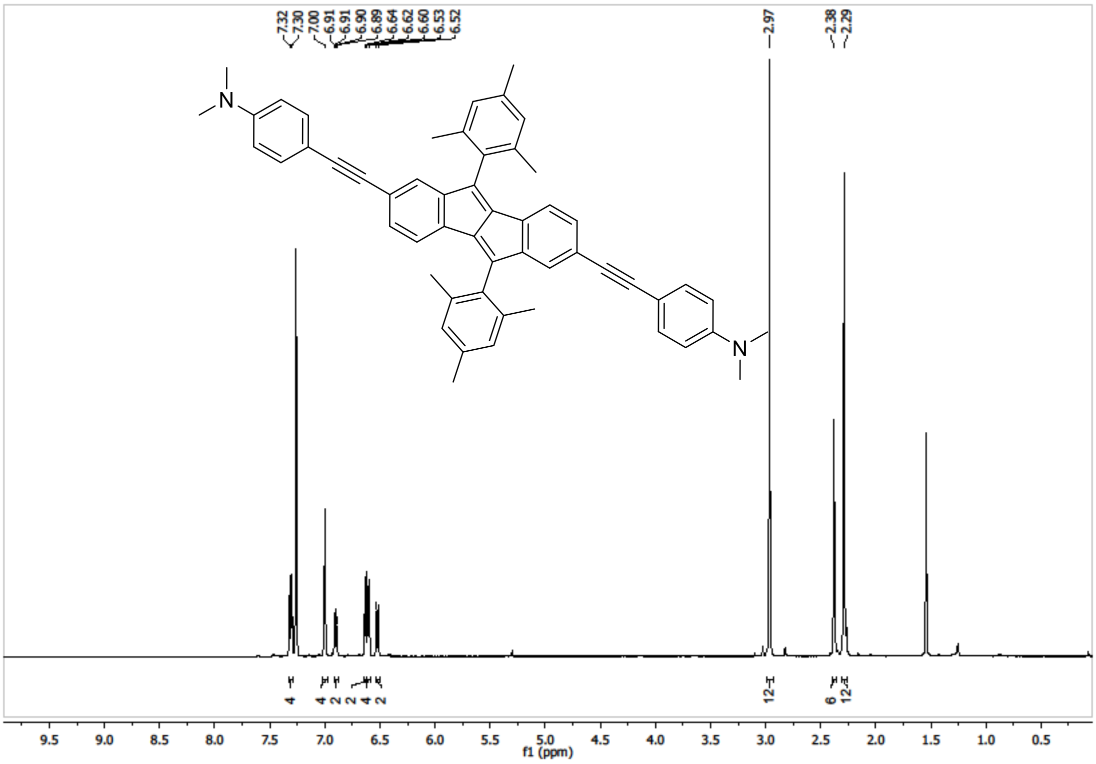


Figure S24 ^{1}H NMR spectrum of 5a in CDCl$_3$ (500 MHz).

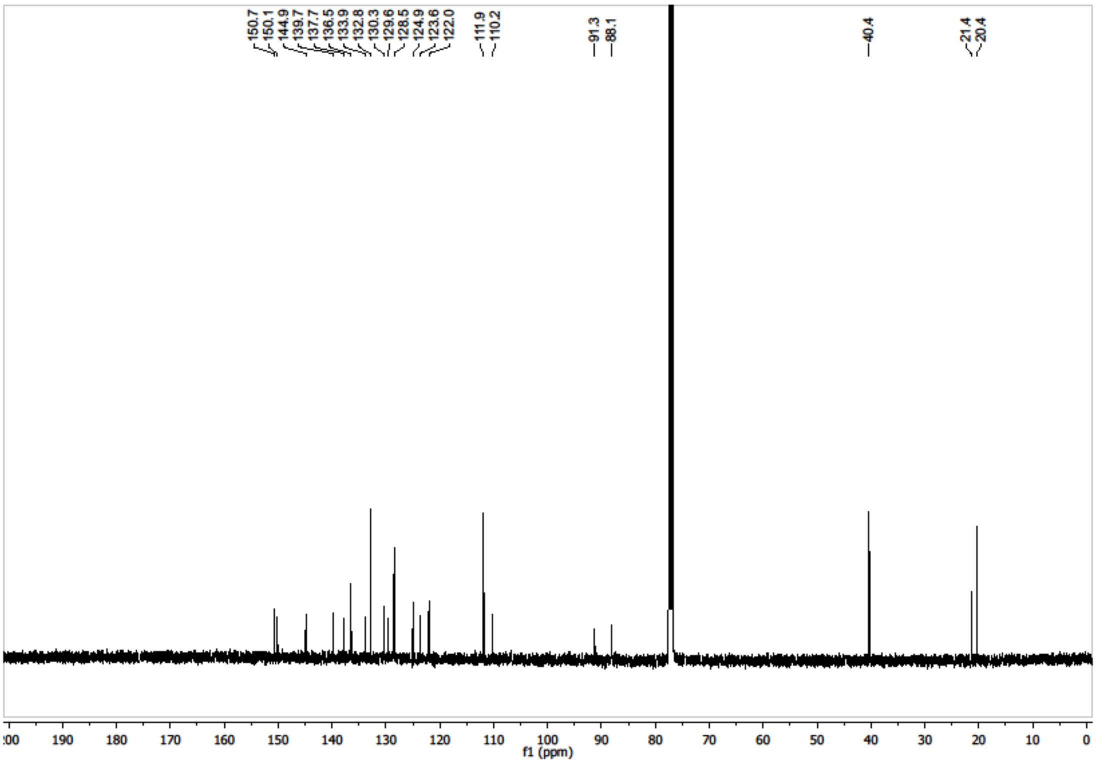


Figure S25 ^{13}C NMR spectrum of 5a in CDCl$_3$ (126 MHz).

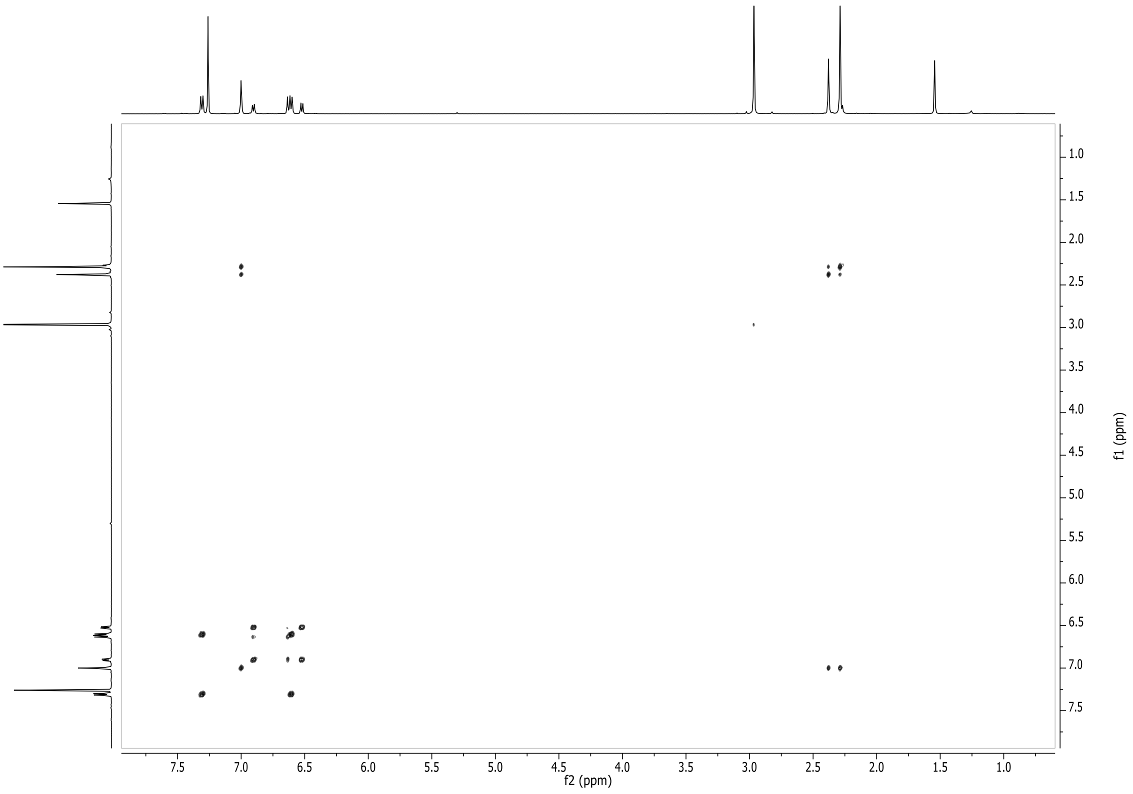


Figure S26 COSY NMR spectrum of 5a in $CDCl_3$ (500 MHz).

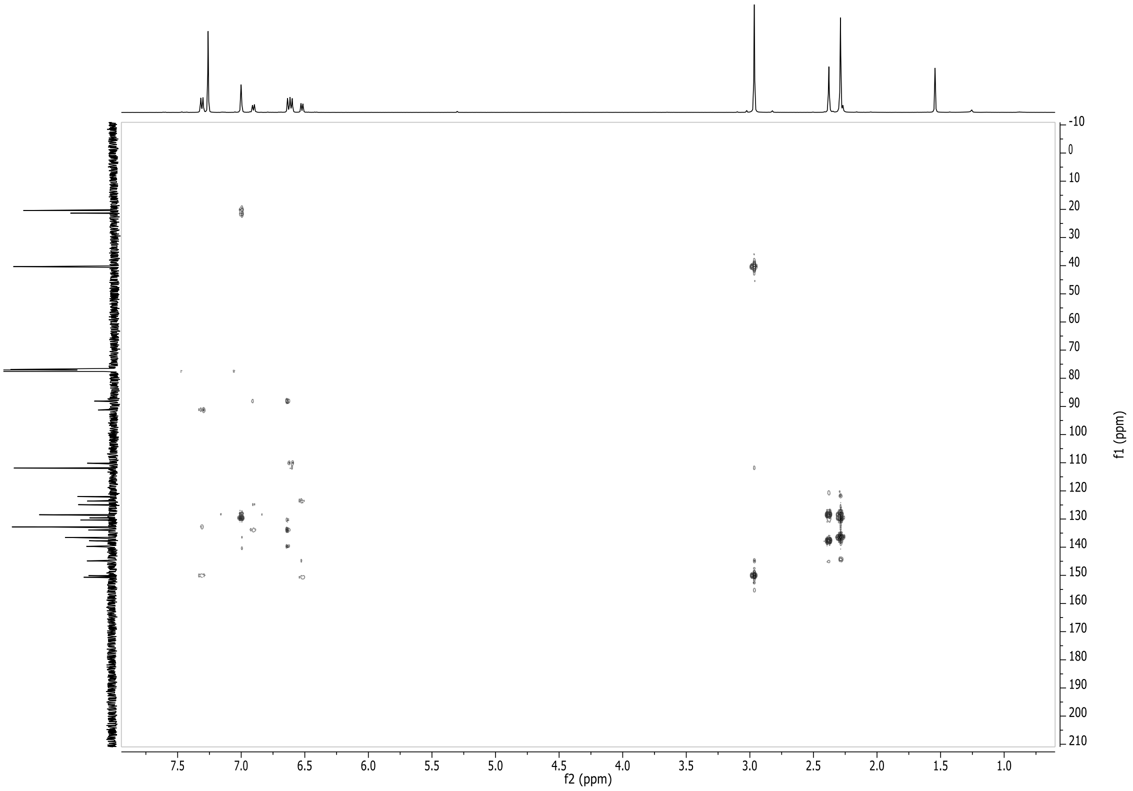


Figure S27 HMBC NMR spectrum of 5a in $CDCl_3$ (500 MHz).

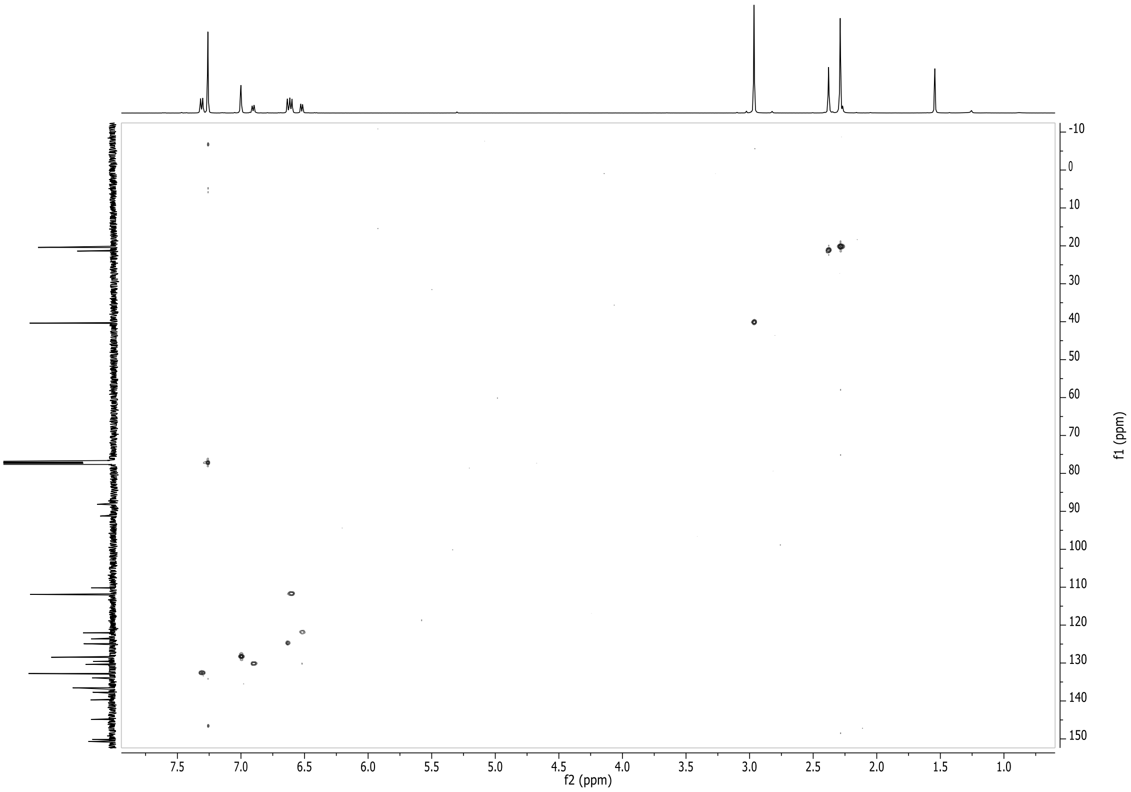


Figure S28 HSQC spectrum of 5a in $CDCl_3$ (500 MHz).

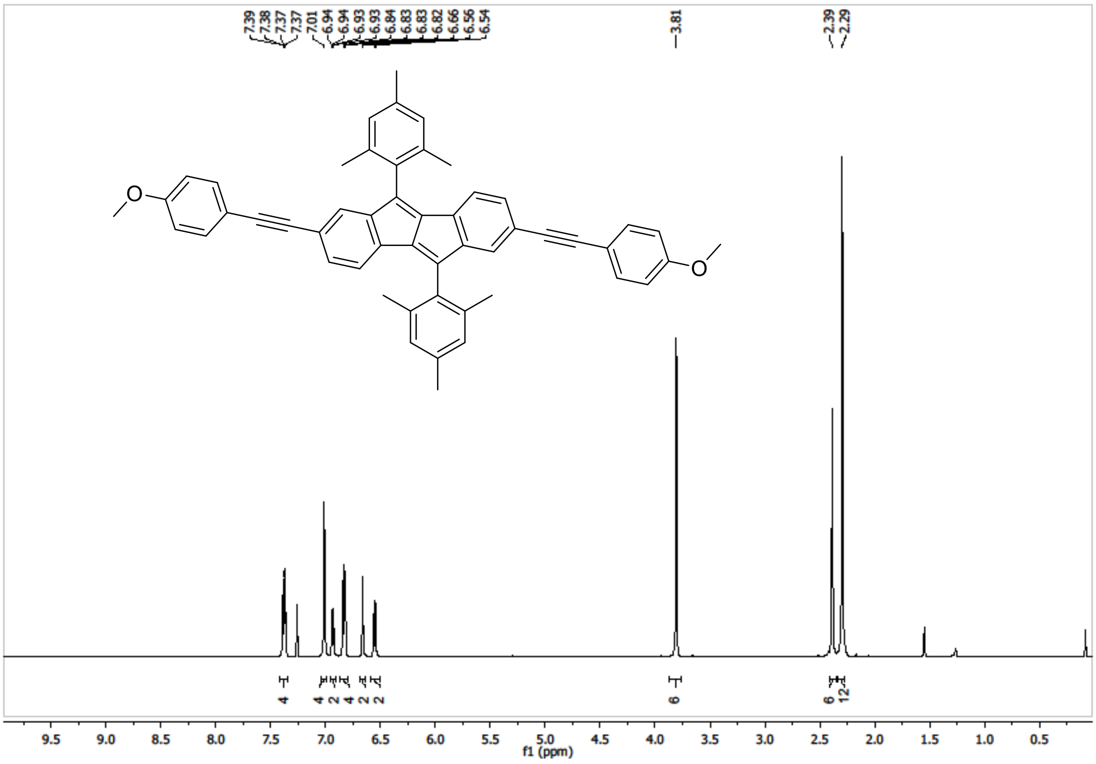


Figure S29 ^{1}H NMR spectrum of 5b in CDCl$_3$ (500 MHz).

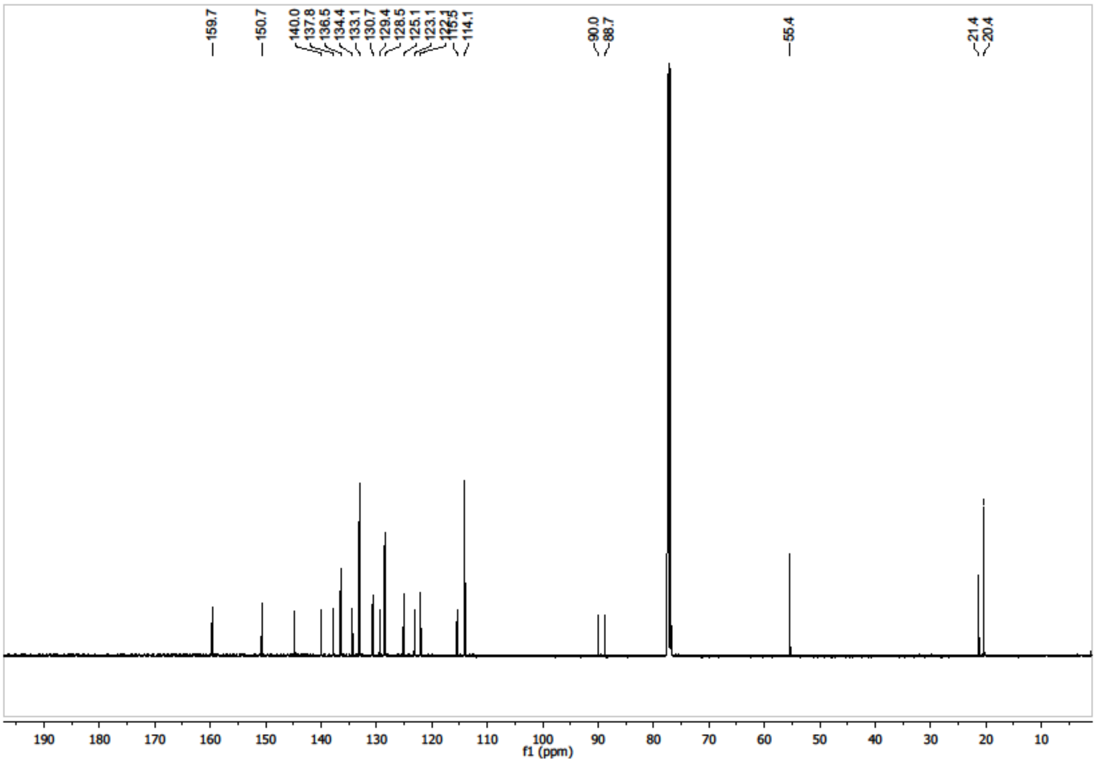


Figure S30 ^{13}C NMR spectrum of 5b in CDCl$_3$ (126 MHz).

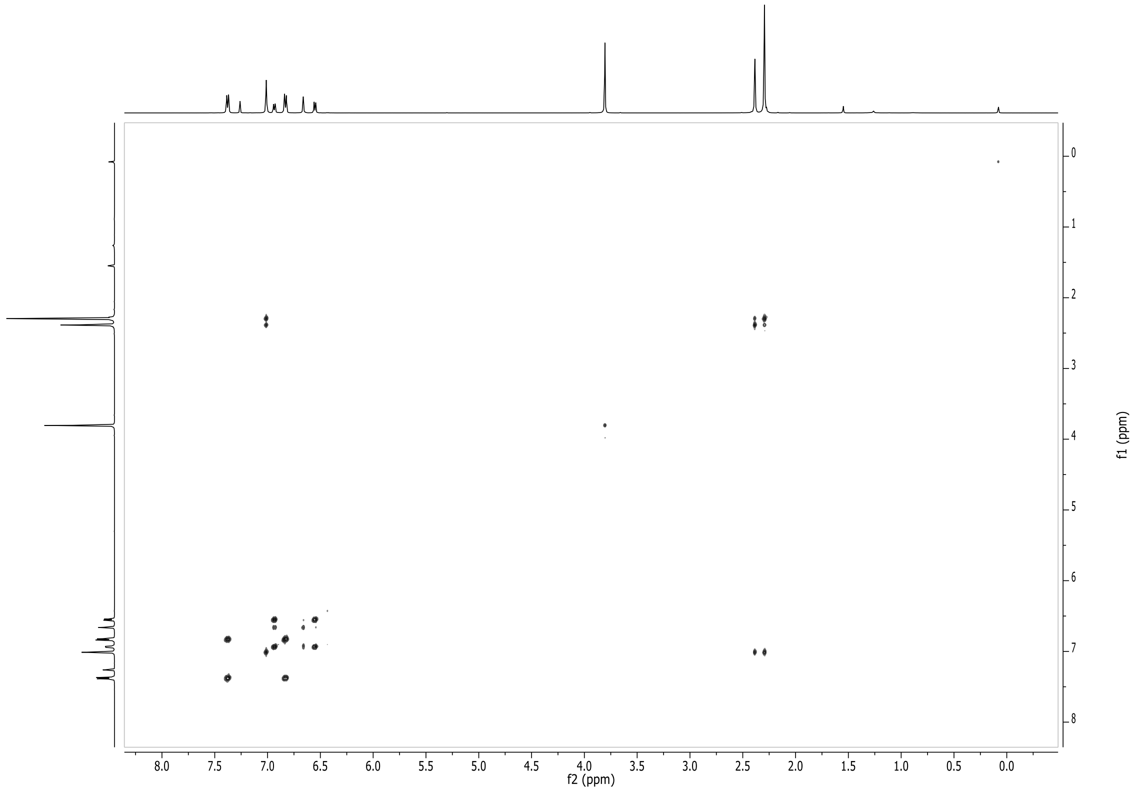


Figure S31 COSY NMR spectrum of 5b in CDCl$_3$ (500 MHz).

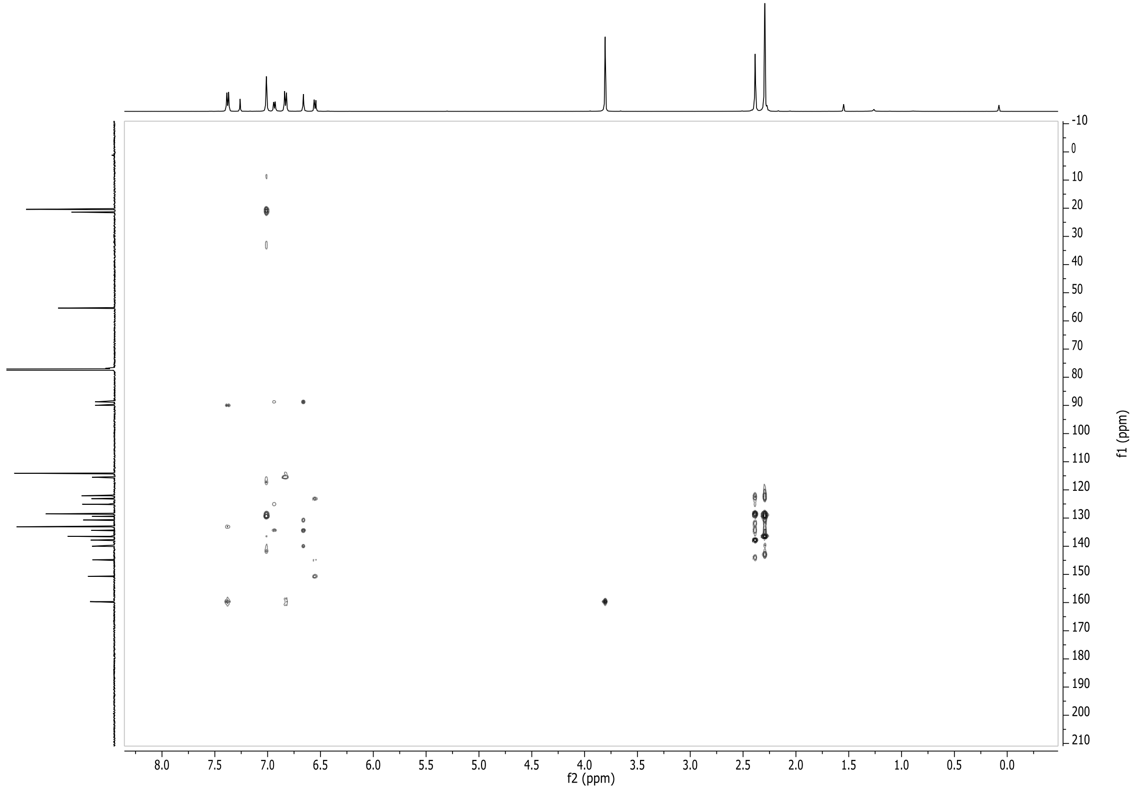


Figure S32 HMBC NMR spectrum of 5b in CDCl$_3$ (500 MHz).

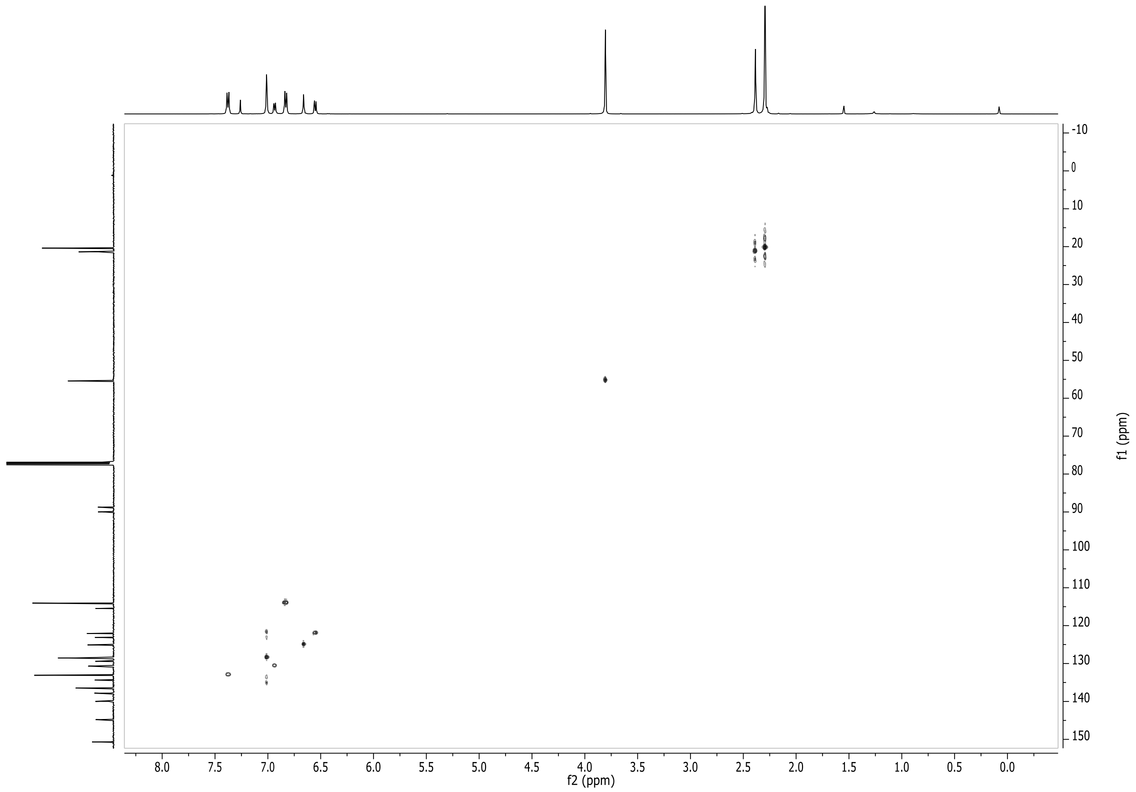


Figure S33 HSQC NMR spectrum of 5b in $CDCl_3$ (500 MHz).

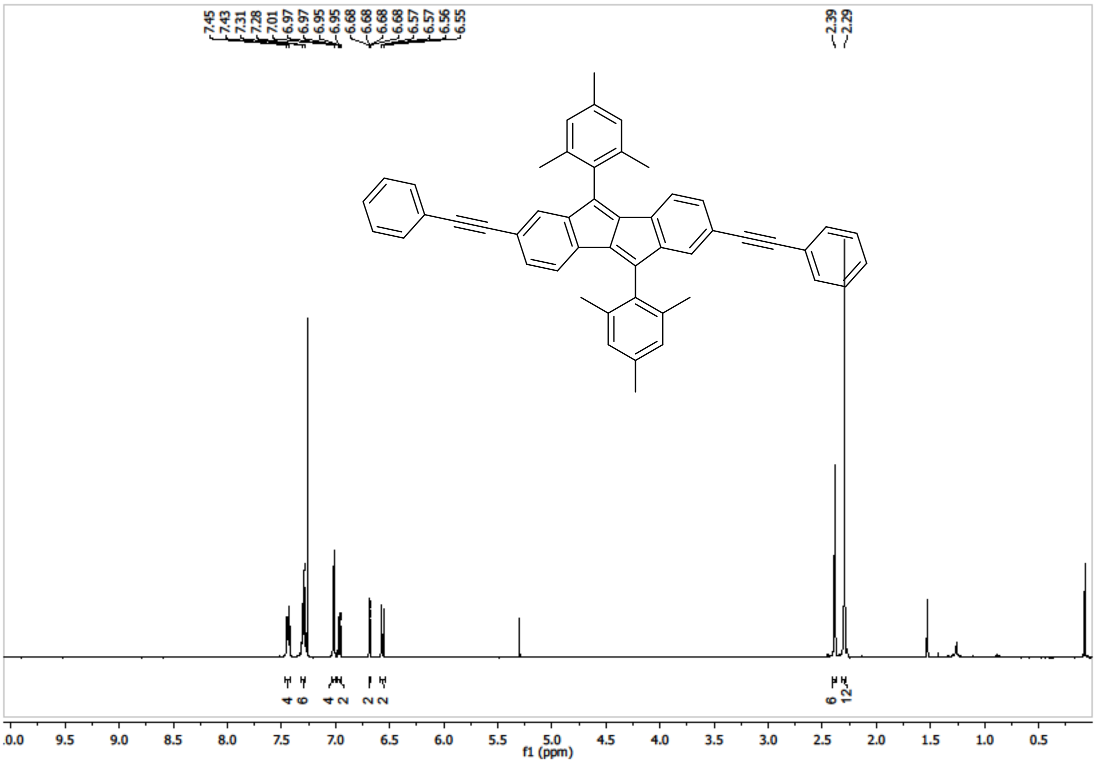


Figure S34 ^{1}H NMR spectrum of 5c in $CDCl_3$ (400 MHz).

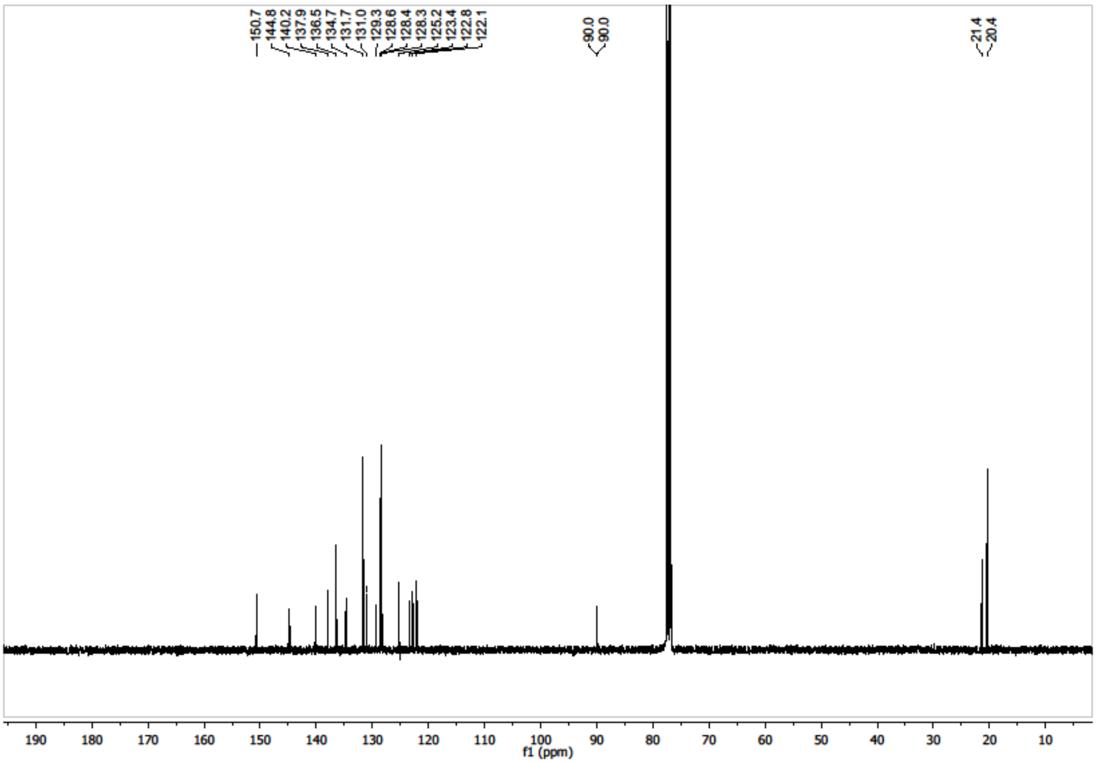


Figure S35 ^{13}C NMR spectrum of 5c in $CDCl_3$ (101 MHz).

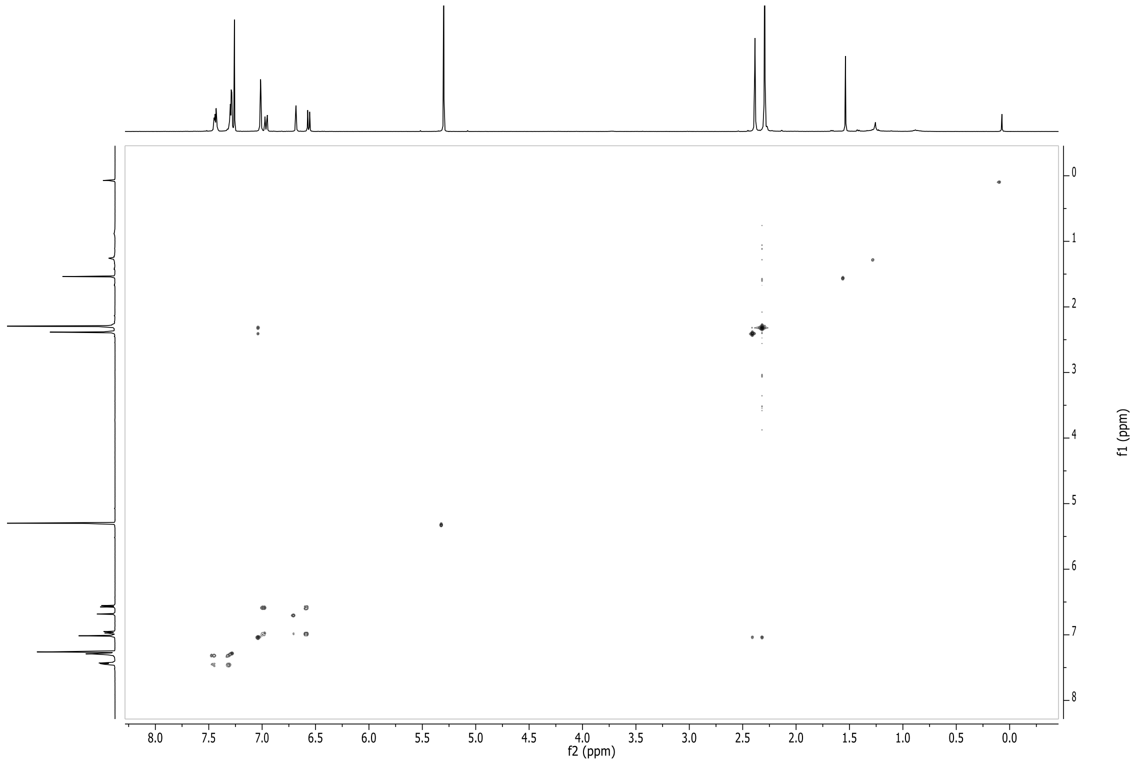


Figure S36 COSY NMR spectrum of 5c in CDCl$_3$ (400 MHz).

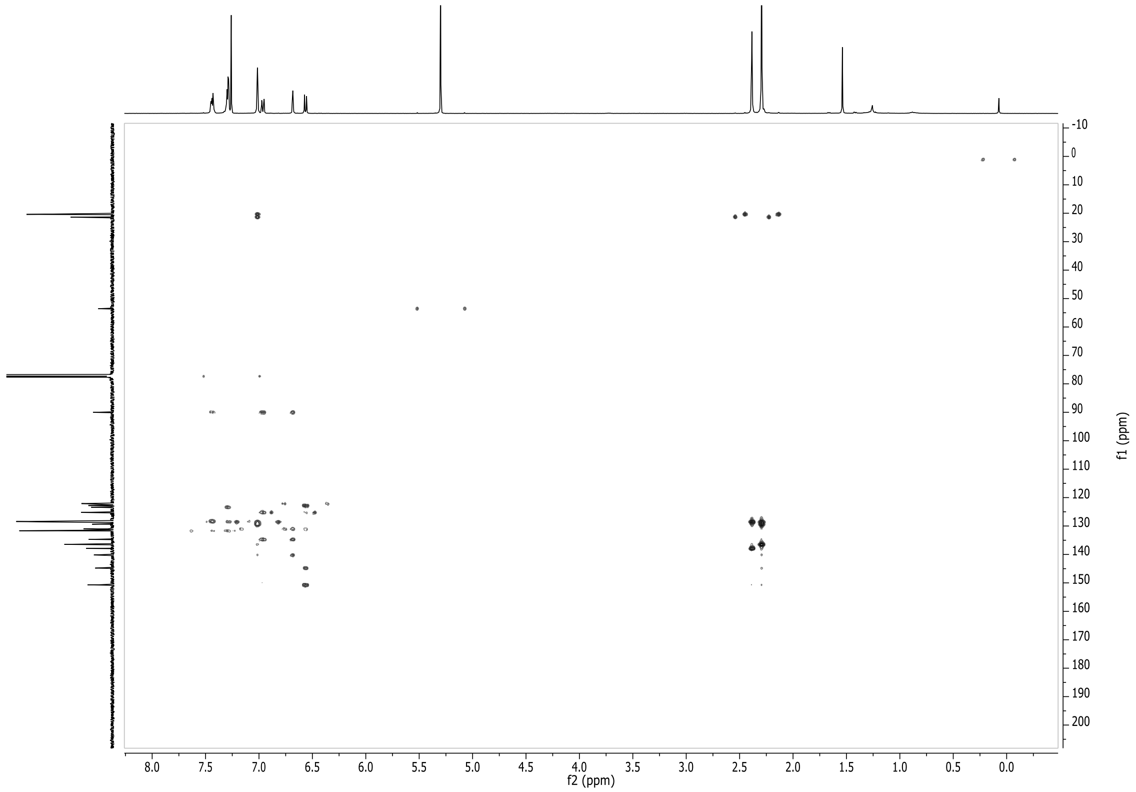


Figure S37 HMBC NMR spectrum of 5c in CDCl$_3$ (400 MHz).

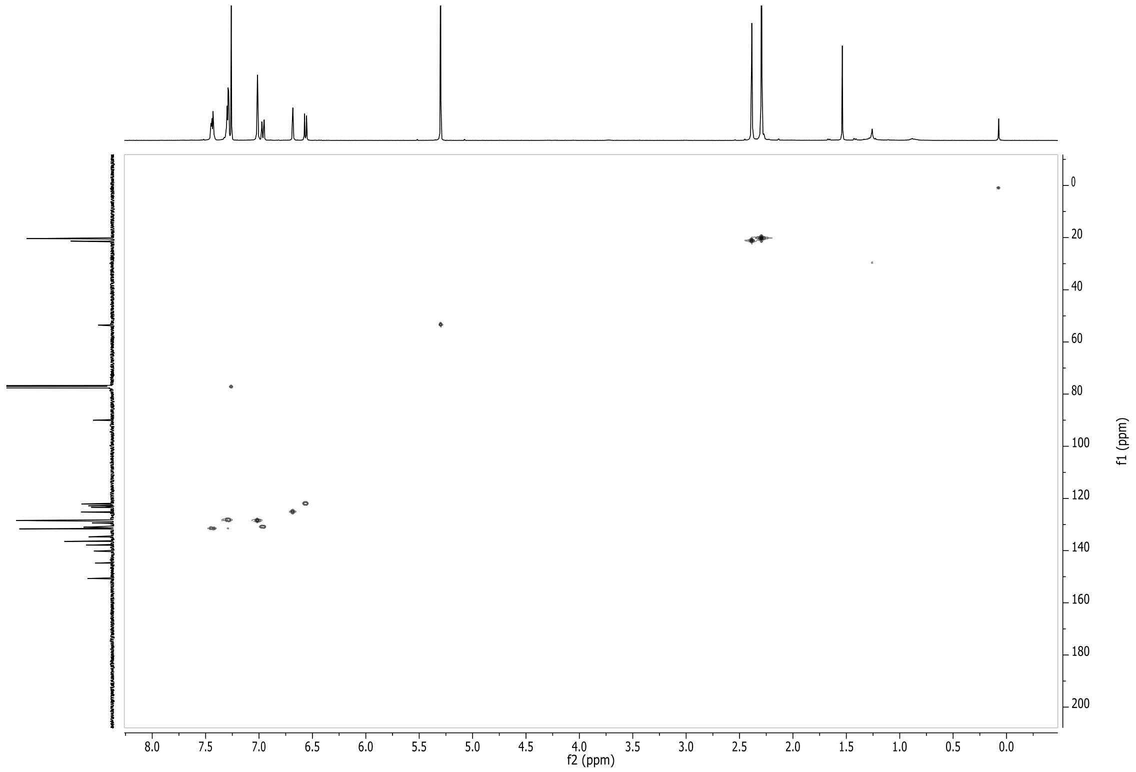


Figure S38 HMQC NMR spectrum of 5c in $CDCl_3$ (400 MHz).

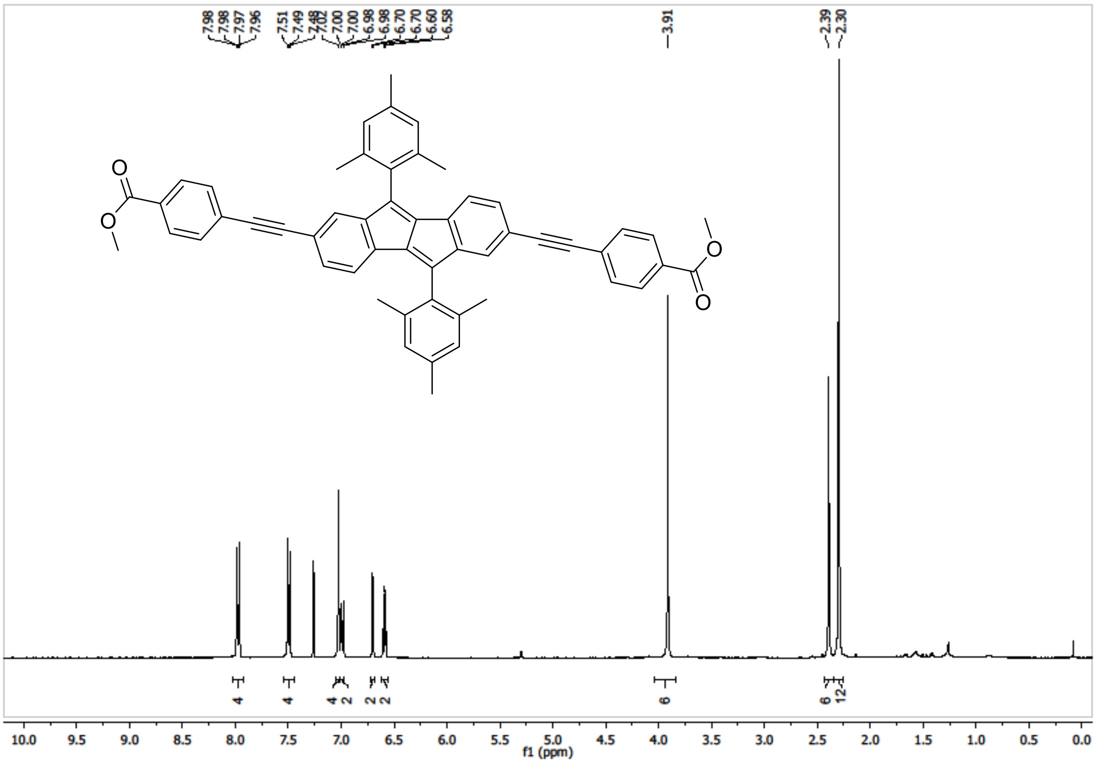


Figure S39 ^{1}H NMR spectrum of 5d in CDCl$_3$ (400 MHz).

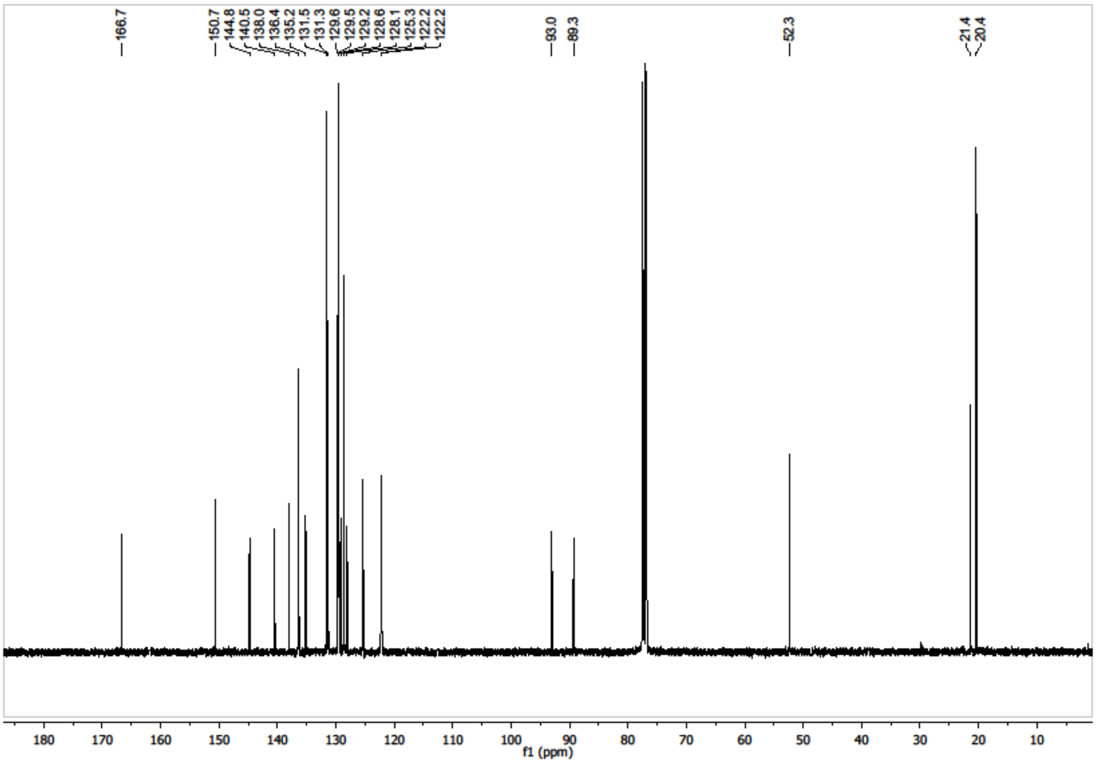


Figure S40 ^{13}C NMR spectrum of 5d in CDCl$_3$ (101 MHz).

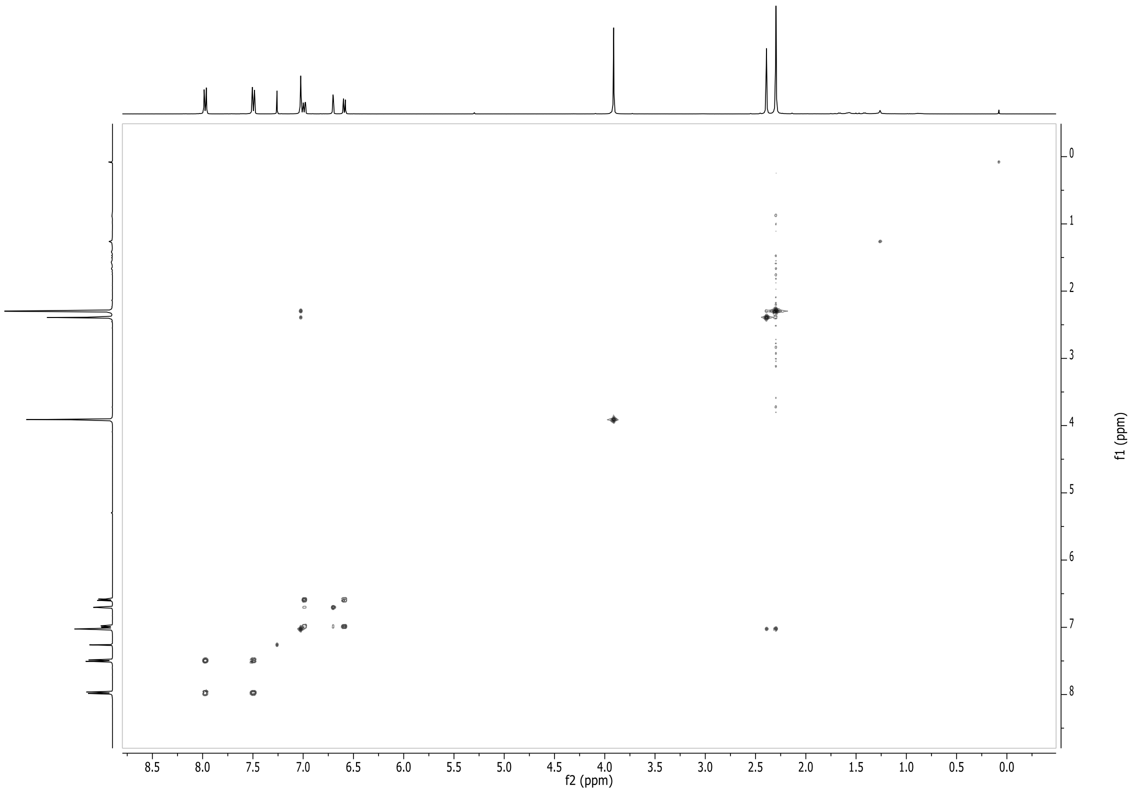


Figure S41 COSY NMR spectrum of 5d in $CDCl_3$ (400 MHz).

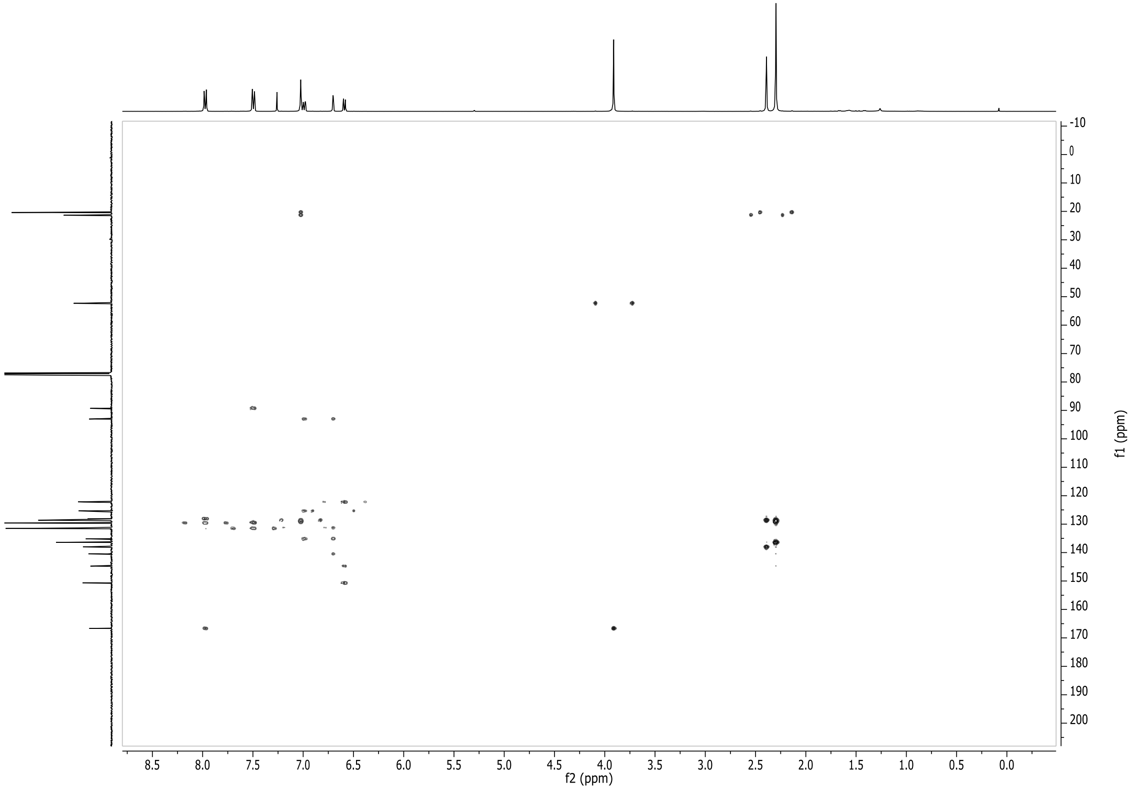


Figure S42 HMBC NMR spectrum of 5d in $CDCl_3$ (400 MHz).

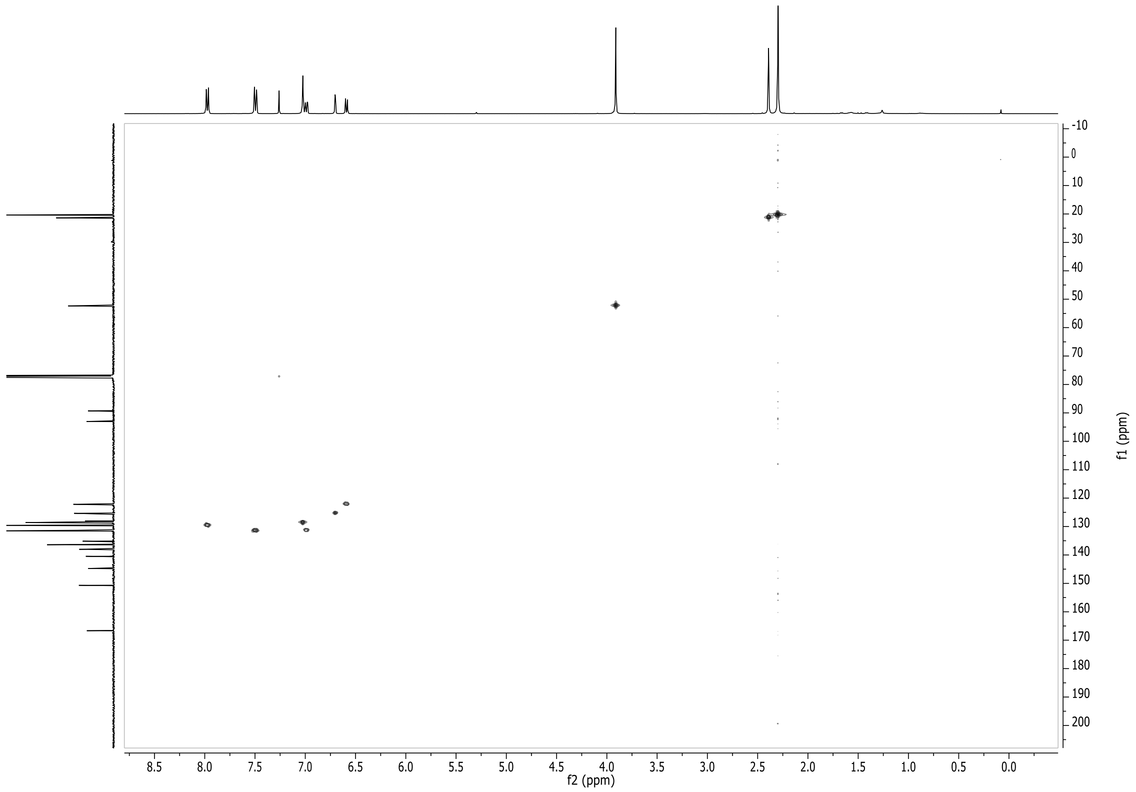


Figure S43 HMQC NMR spectrum of 5d in $CDCl_3$ (400 MHz).

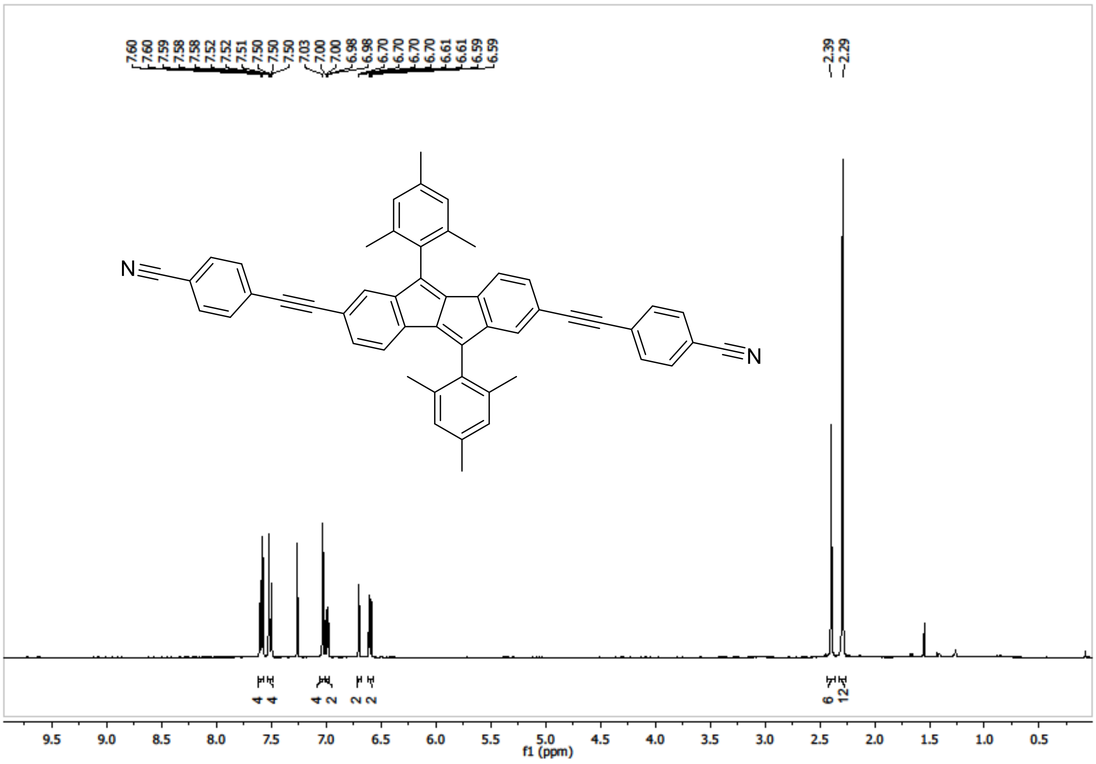


Figure S44 ^{1}H NMR spectrum of 5e in CDCl$_3$ (400 MHz).

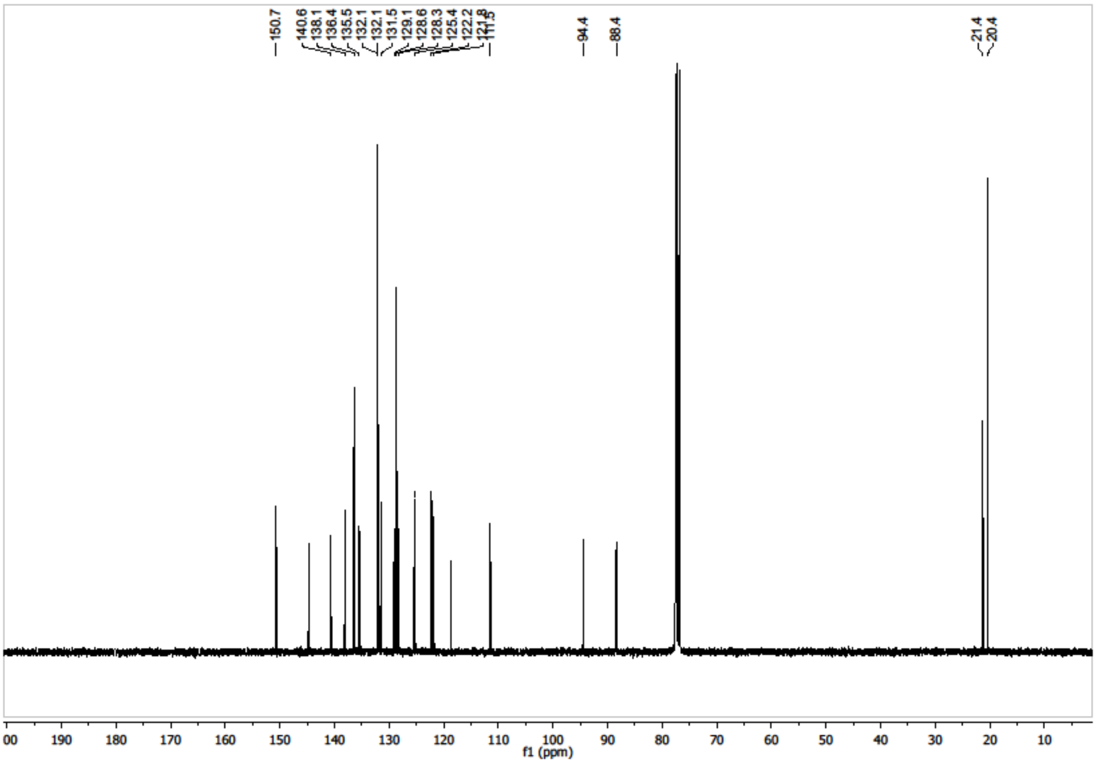


Figure S45 ^{13}C NMR spectrum of 5e in CDCl$_3$ (101 MHz).

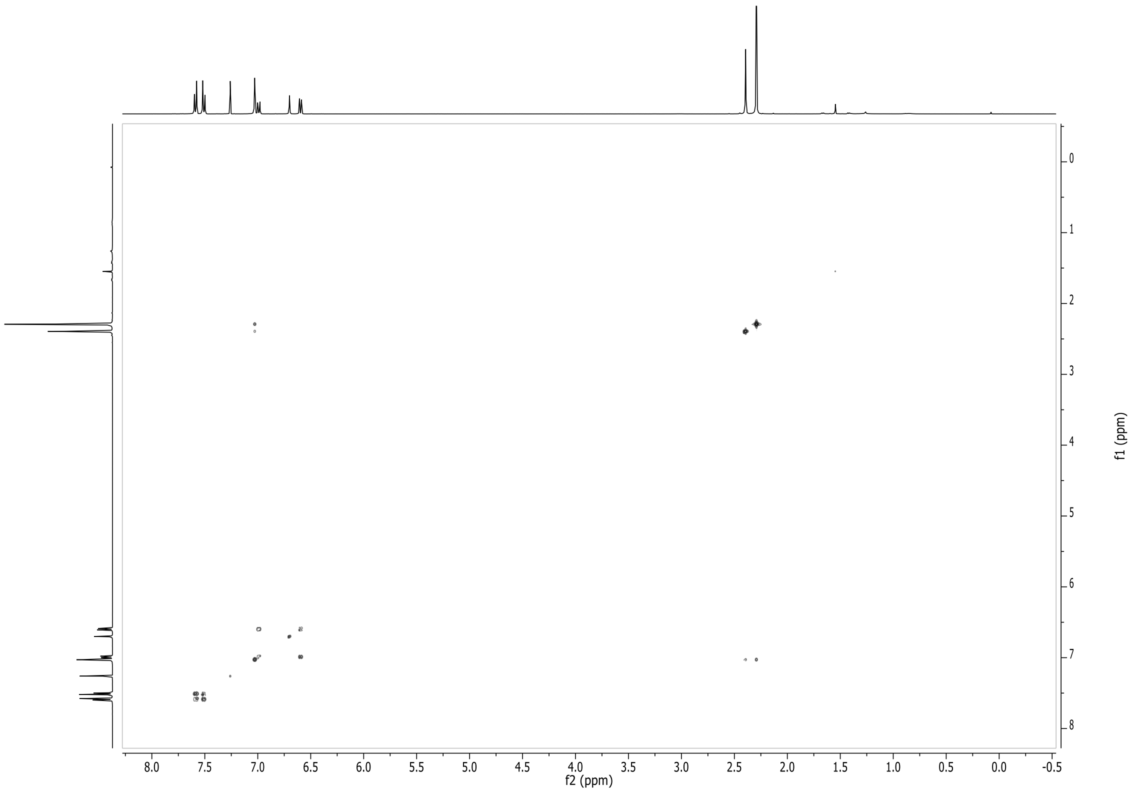


Figure S46 COSY NMR spectrum of 5e in $CDCl_3$ (400 MHz).

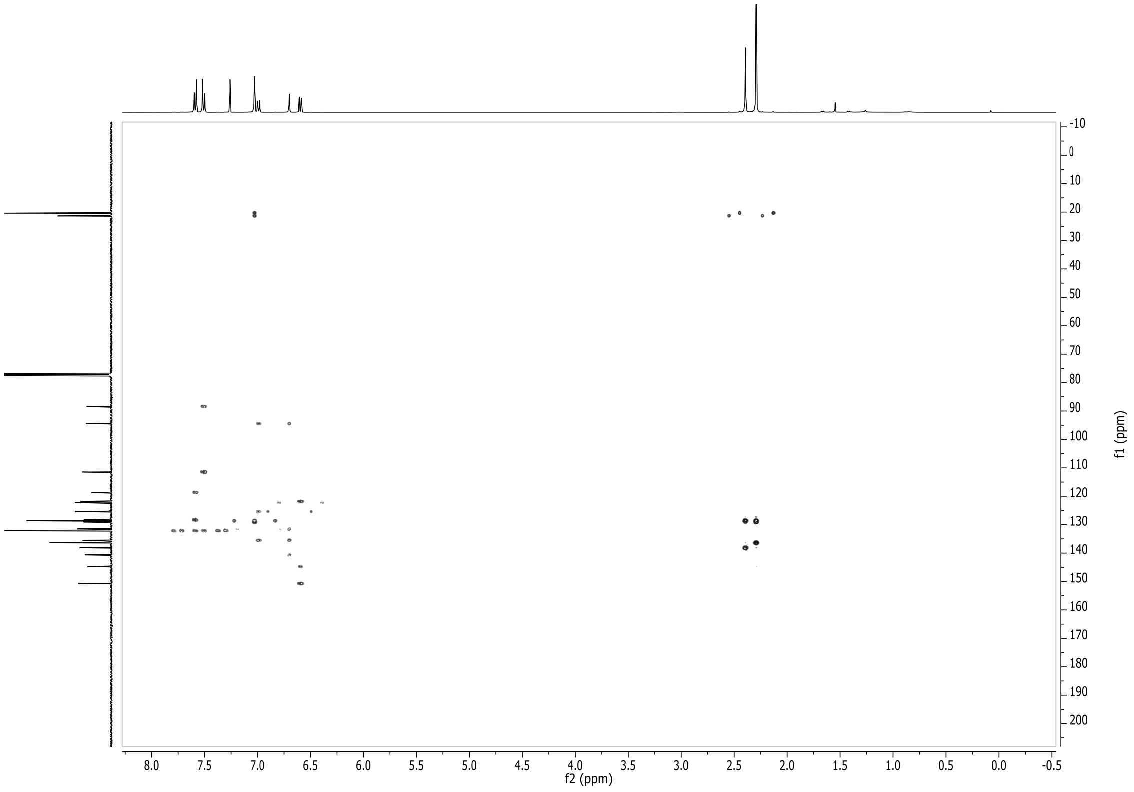


Figure S47 HMBC NMR spectrum of 5e in $CDCl_3$ (400 MHz).

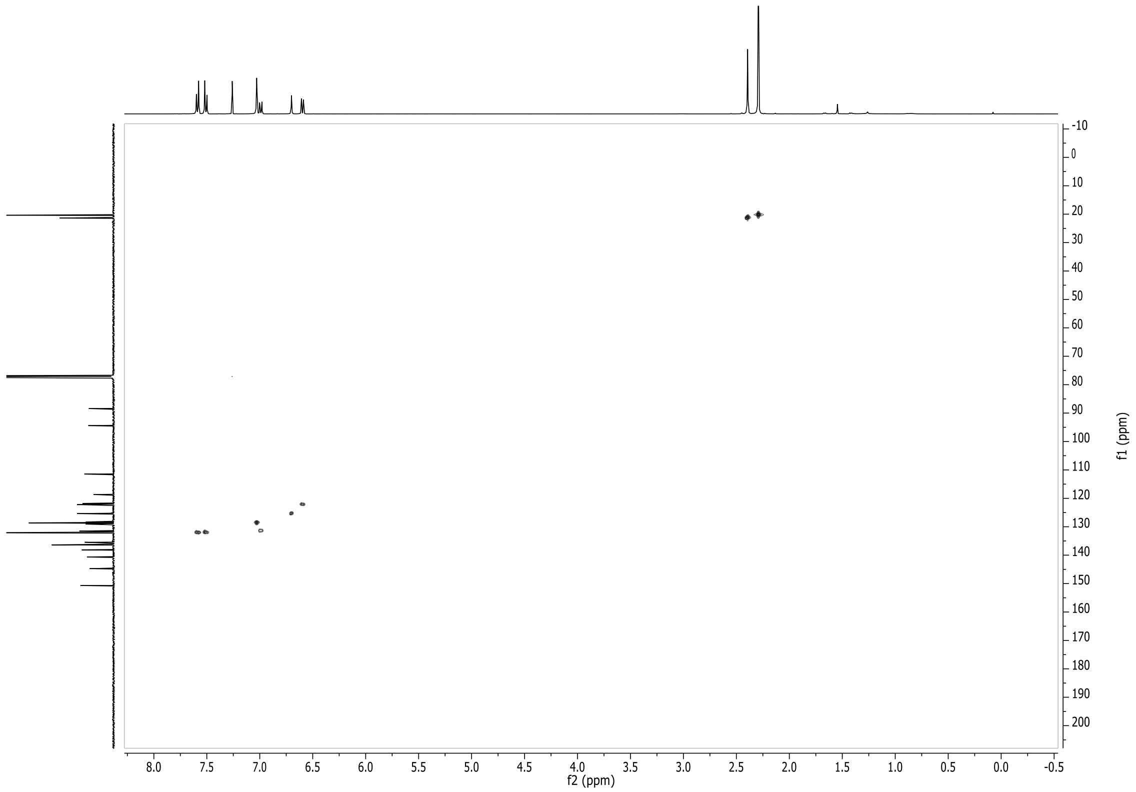


Figure S48 HMQC NMR spectrum of 5e in $CDCl_3$ (400 MHz).

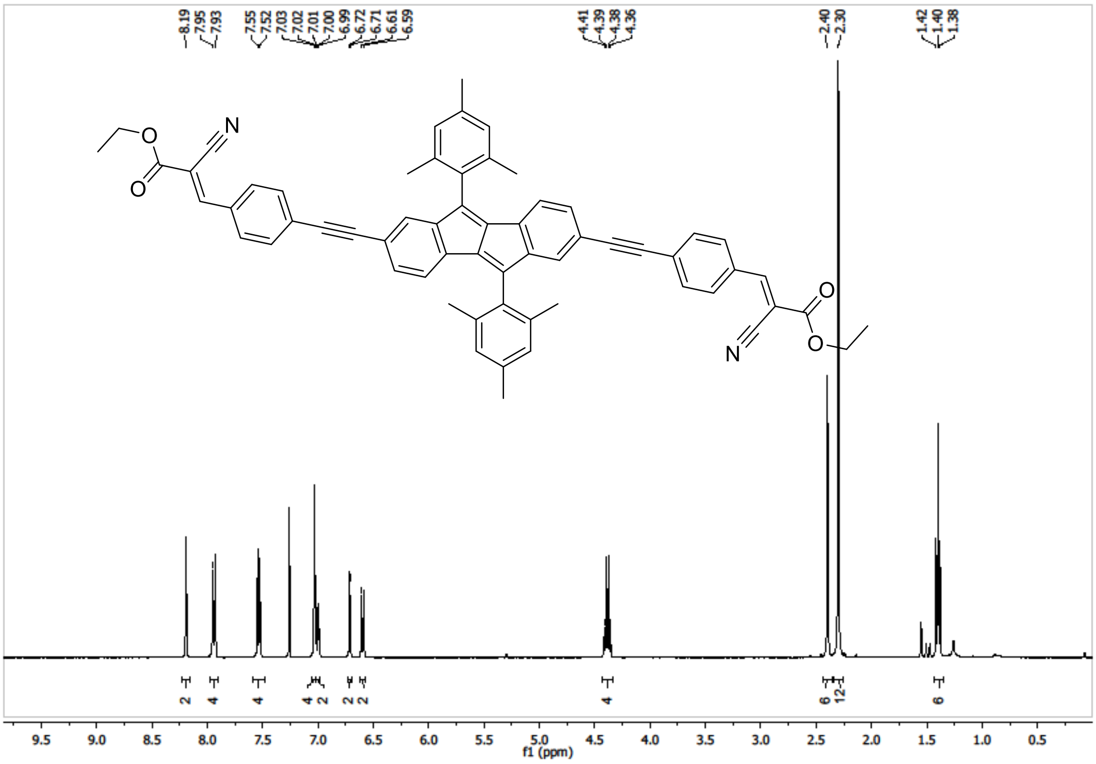


Figure S49 ^{1}H NMR spectrum of 5f in CDCl$_3$ (400 MHz).

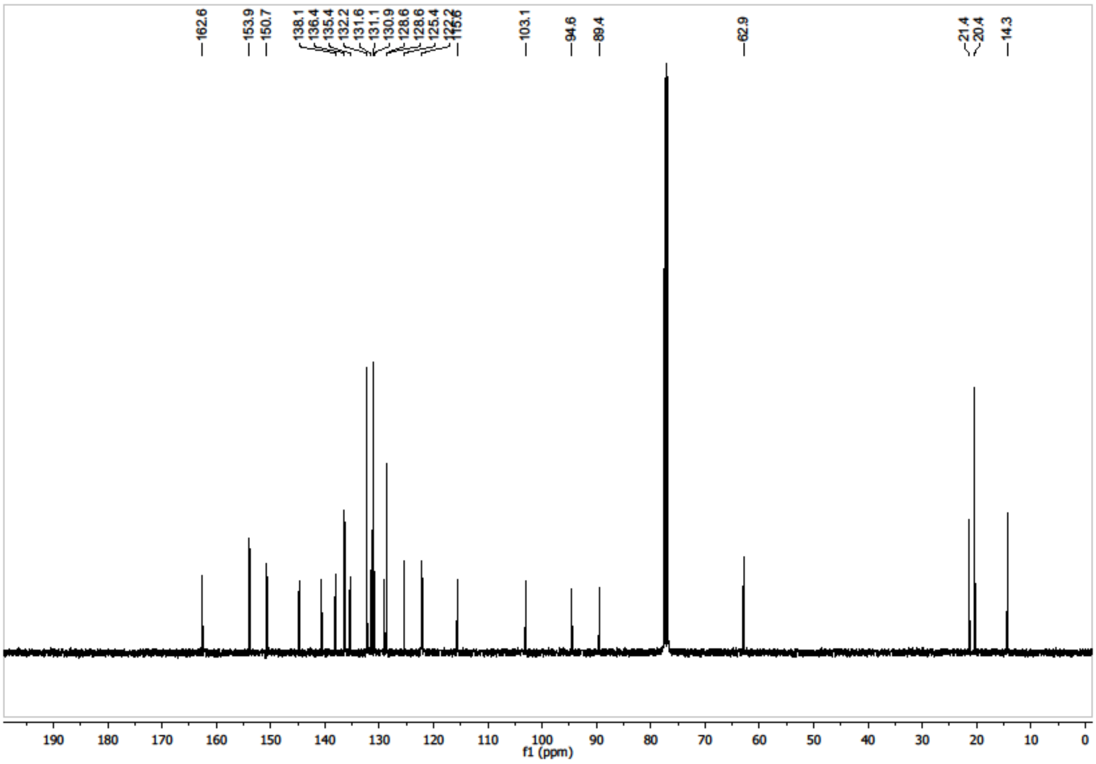


Figure S50 ^{13}C NMR spectrum of 5f in CDCl$_3$ (101 MHz).

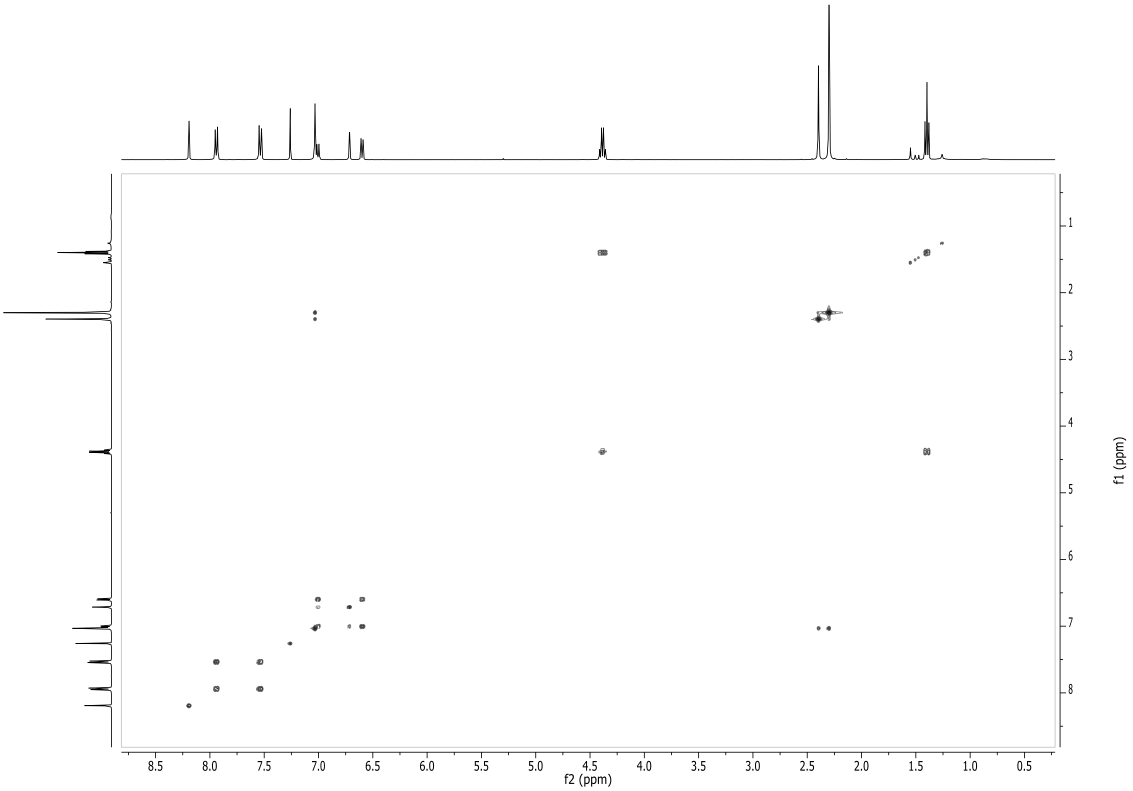


Figure S51 COSY NMR spectrum 5f in CDCl$_3$ (400 MHz).

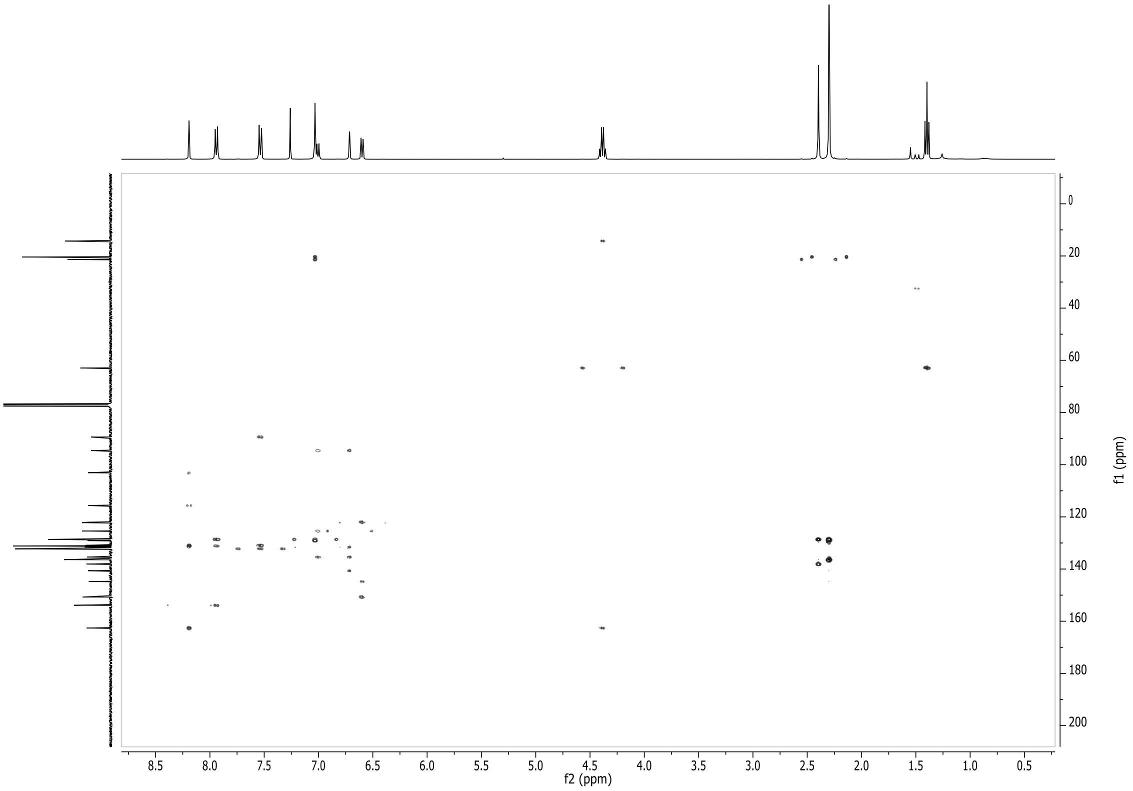


Figure S52 HMBC NMR spectrum of 5f in CDCl$_3$ (400 MHz).

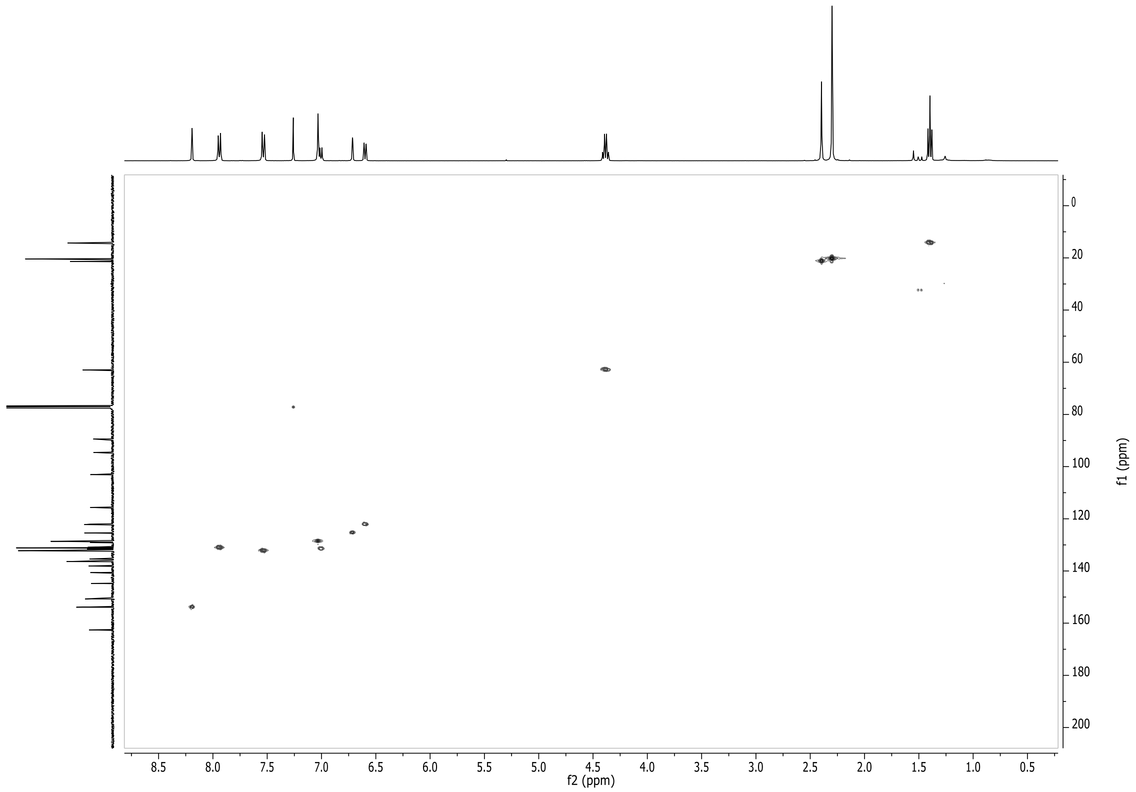


Figure S53 HMQC NMR spectrum of 5f in $CDCl_3$ (400 MHz).

6 DFT calculations

6.1 Computational details and results

For DFT calculations on **5a**-**f** all mesityl groups as well as the ethyl group in **5f** were replaced with methyl groups to increase computational speed. This will be indicated by an asterix, i.e. **5a***.

DFT calculations were performed with either the ORCA 3.0.2 program package[11] or the TURBOMOLE 6.6 program package.[12] The resolution-of-identity (RI, RIJDX for SP)[13,14] approximation for the Coulomb integrals was used in all DFT calculations employing matching auxiliary basis set def2-XVP/J.[15] Further, the D3 dispersion correction scheme[16,17] with the Becke-Johnson damping function[18,19,20] was applied. Using ORCA, the geometries of **5a***-**f*** were optimized without symmetry restrictions at the PBE[21]-D3/def2-SVP[22] level followed by harmonic vibrational frequency analyses to confirm minima as stationary points. The structures were then re-optimized using TPSS[23]-D3/def2-TZVP.[24] All further calculations were done using TURBOMOLE. Vertical excitation energies were calculated using TDDFT.

For **5c*** (R=H) different density functionals were tested in order to evaluate which one would furnish the best match of orbital energies and predicted vertical excitation energies (TDDFT) with experimental values from CV measurements and UV/Vis absorption spectra. Four different density functionals with varying amounts of HF exchange from 0% to 50% were chosen (see Table 1), since this has been shown to have a pronounced effect.[25] Geometries were optimized without symmetry restrictions at the *functional*-D3/def2-TZVP level of theory. The vertical excitation energies were then calculated using TDDFT at the same level of theory.

Table 1. Electronic energies (E_0), HOMO/LUMO energies and first singlet excitation energies from TDDFT calculations on 5c* calculated using different density functionals (*functional*-D3/def2-TZVP).

Density functional	**BHLYP[26]**	**B3LYP[27,28]**	**TPSSH[24,29]**	**BP86[30,31,32]**
HF exchange	50%	20%	10%	0%
E_0 [hartrees]	-1308.52517	-1308.53881	-1309.42005	-1309.40336
E_0 [kcal/mol]	-821112.6	-821121.2	-821674.2	-821663.7
E (LUMO) [eV]	-1.49	-2.51	-2.81	-3.31
E (HOMO) [eV]	-6.24	-5.32	-5.08	-4.90
E (gap) [eV] [a]	4.75	2.81	2.27	1.59
1st singlet excitation energy [eV] [b]	2.72	2.19	2.05	1.78

[a] The experimentally determined band gap (onset of the longest wavelength absorption) of **5c** amounts to 2.08 eV; [b] from TDDFT calculations.

The electronic as well as HOMO/LUMO energies can be found in Table 1. The best match to the experimentally determined band gap of 2.08 eV is found for the TPSSH functional, followed by B3LYP. The calculated vertical excitation energies of **5c*** are plotted in Figure S54 and listed in Table 2 together with experimental values from UV/Vis absorption spectra of **5c**. Here, the best match between theory and experiment is found for the B3LYP functional, followed by TPSSH.

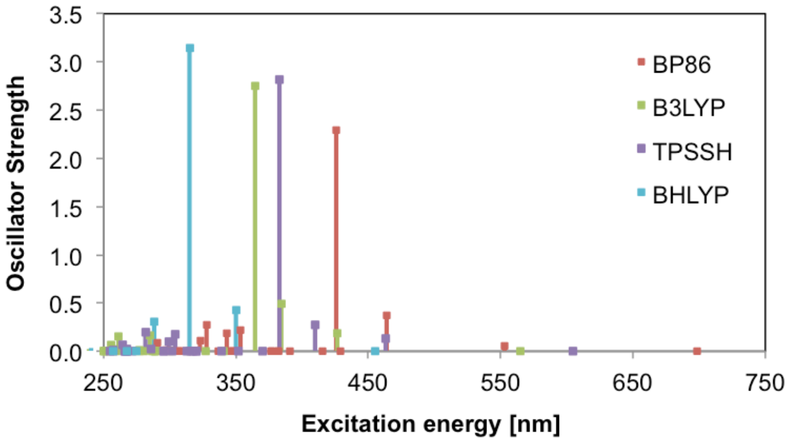


Figure S54. Vertical excitation energies of 5c* (R=H) calculated using TDDFT with different density functionals (*functional*-D3/def2-TZVP).

Table 2. Excitations energies of 5c* (R=H) in nm (with oscillator strengths) calculated using TDDFT, assigned to transitions (main contributions) and optical transitions of 5c (with extinction coefficients ε_{max} in M^{-1} cm^{-1}) from absorption spectra in CH_2Cl_2 solution.

Functional	HOMO → LUMO	HOMO-1 → LUMO	HOMO-2 → LUMO	HOMO → LUMO+1
BHLYP	455 (0.00)	350 (0.43)	288 (0.31)	315 (3.15)
B3LYP	565 (0.00)	427 (0.18)	384 (0.50)	364 (2.75)
TPSSH	605 (0.00)	463 (0.13)	410 (0.28)	383 (2.82)
BP86	698 (0.00)	553 (0.06)	464 (0.38)	426 (2.29)
Experiment	511 (-)	440 (14200); 414 (12400); 393 (7100)		342 (88700)

Based on these results, the TPSSH and B3LYP functional were used to assess orbital energies and vertical excitation energies of **5a***-**f***.

In order to increase computational speed, the geometries of **5a***-**f*** were optimized within the C_{2h} point group using TPSSH-D3/def2-TZVP and B3LYP-D3/def2-TZVP, followed by TDDFT calculations of the vertical excitation energies. The Cartesian coordinates can be found in Table 7-Table 18, electronic and orbital energies in Table 3 and Table 4.

Table 3. Electronic energies (E_0) and HOMO/LUMO energies of 5a*-f* calculated with B3LYP-D3/def2-TZVP in C_{2h} symmetry.

Compound	**5a***	**5b***	**5c***	**5d***	**5e***	**5f***
R	NMe_2	OMe	H	CO_2Me	CN	CPM [a]
E_0 [hartrees]	-1576.43008	-1537.57468	-1308.53883	-1764.28553	-1493.01267	-2103.53180
E_0 [kcal/mol]	-989225.6	-964843.5	-821121.2	-1107106.8	-936880.4	-1319987.2
E (LUMO) [eV]	-2.18	-2.37	-2.51	-2.71	-2.94	-3.04
E (HOMO) [eV]	-4.73	-5.09	-5.32	-5.52	-5.77	-5.69
E (gap) [eV]	2.55	2.72	2.81	2.81	2.83	2.65

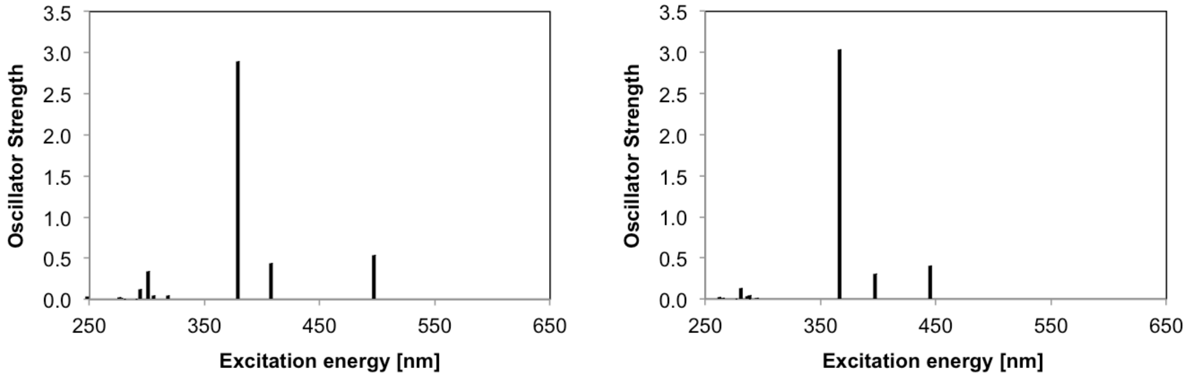
[a] CPM = CHC(CN)(CO_2Me).

Table 4. Electronic energies (E_0) and HOMO/LUMO energies of 5a*-f* calculated with TPSSH-D3/def2-TZVP in C_{2h} symmetry.

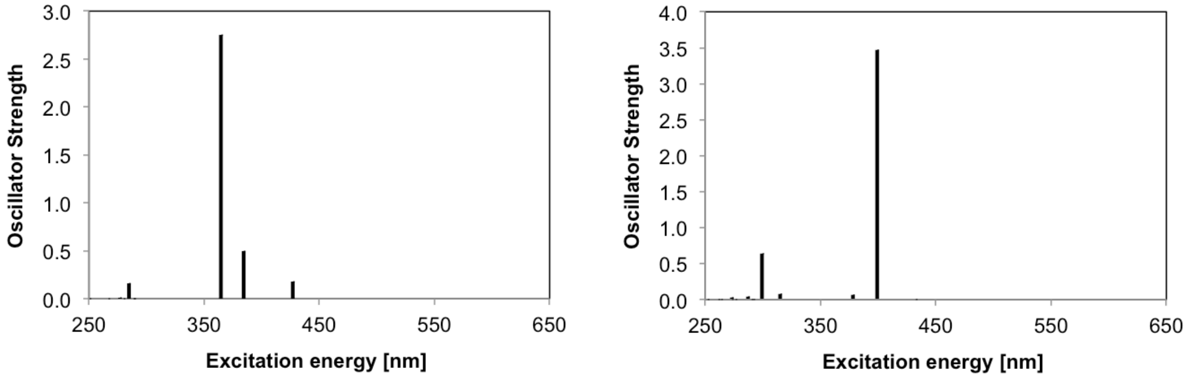
Compound	**5a***	**5b***	**5c***	**5d***	**5e***	**5f***
R	NMe_2	OMe	H	CO_2Me	CN	CPM [a]
E_0 [hartrees]	-1577.49434	-1538.57715	-1309.42011	-1765.39176	-1493.98580	-2104.83697
E_0 [kcal/mol]	-989893.5	-965472.5	-821674.2	-1107801.0	-937491.0	-1320806.2
E (LUMO) [eV]	-2.46	-2.66	-2.81	-3.02	-3.25	-3.34
E (HOMO) [eV]	-4.47	-4.84	-5.08	-5.30	-5.54	-5.48
E (gap) [eV]	2.01	2.18	2.27	2.27	2.29	2.14

[a] CPM = CHC(CN)(CO_2Me).

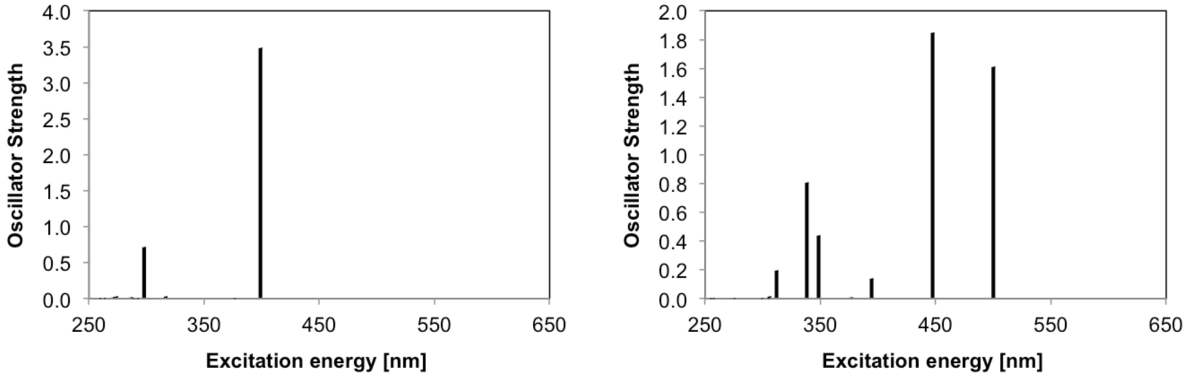
The vertical excitation energies of **5a*-f*** within the C_{2h} point group were calculated using TDDFT at the B3LYP-D3/def2-TZVP level of theory. The results are plotted in Figure S55 and listed in Table 5. For comparison, the optical transitions of **5a-f** from UV/Vis absorption spectra in solution are listed in Table 6. For all compounds apart from **5f**, the absorption maximum corresponds to the HOMO → LUMO+1 transition (Band 3 in Table 6). In the case of **5f**, Band 2 is the absorption maximum, which, according to the TDDFT calculations, corresponds to the HOMO-1 → LUMO transition. For **5f*** another long wavelength excitation was calculated (see Figure S55), which is assigned to the HOMO-3 → LUMO+1 transition.


a) **5a*** (R = NMe$_2$)

b) **5b*** (R = OMe)


c) **5c*** (R = H)

d) **5d*** (R = CO$_2$Me)


e) **5e*** (R = CN)

f) **5f*** (R = CPM)

Figure S55. Vertical excitation energies of 5a*-f* calculated within the C_{2h} point group using TDDFT at the B3LYP-D3/def2-TZVP level of theory (CPM = CHC(CN)(CO$_2$Me)).

Table 5. Excitations energies of 5a*-f* in nm (with oscillator strengths) calculated within the C_{2h} point group using TDDFT at the B3LYP-D3/def2-TZVP level of theory and assigned to transitions (main contributions).

	R	HOMO → LUMO a_g	HOMO-1 → LUMO b_u	HOMO-2 → LUMO b_u	HOMO → LUMO+1 b_u
5a	NMe_2	604 (0.00)	497 (0.53)	408 (0.44) [a]	379 (2.89)
5b	OMe	578 (0.00)	445 (0.40)	397 (0.31)	366 (3.04)
5c	H	565 (0.00)	427 (0.18)	384 (0.50)	365 (2.75)
5d	CO_2Me	562 (0.00)	433 (0.01)	378 (0.06)	399 (3.47)
5e	CN	558 (0.00)	434 (0.01)	376 (0.00)	399 (3.48)
5f	CPM [b]	570 (0.00)	447 (1.85)	395 (0.14)	500 (1.61)

[a] 49% HOMO→LUMO+1 and 45% HOMO-3→LUMO transition; [b] CPM = CHC(CN)(CO_2Me).

Table 6. Optical transitions (with extinction coefficients ε_{max} in M^{-1} cm^{-1}) of 5a-f from absorption spectra in CH_2Cl_2 solution.

	R	Band 1	Band 2	Band 3
5a	NMe_2	567 (-)	446 (24900)	366 (95900)
5b	OMe	532 (-)	442 (21400); 416 (19200); 393 (13500)	347 (112800)
5c	H	511 (-)	440 (14200); 414 (12400); 393 (7100)	342 (88700)
5d	CO_2Me	530 (-)	441 (14800); 416 (13800)	364 (98900)
5e	CN	530 (-)	442 (14100); 415 (13100)	367 (100800)
5f [a]	CPE [a]	534 (-)	414 (90600)	311 (43500)

[a] CPE = CHC(CN)(CO_2Et).

6.2 Cartesian coordinates of calculated structures

Cartesian coordinates are from optimizations in the C_{2h} point group and are listed in angstrom for two different methods: B3LYP or TPSSH with D3 and the def2-TZVP basis set.

Table 7. Coordinates of the calculated structure of 5c* (R = H, B3LYP-D3/def2-TZVP).

	x	y	z
C	-5.071361	2.75047	0
C	-3.7229533	2.3128463	0
C	-2.6742835	3.2426977	0
C	-3.4257906	0.9312922	0
H	-2.91452	4.2971162	0
C	-1.3419696	2.8312321	0
C	-2.1098222	0.5241939	0
H	-4.2384739	0.2167166	0
H	-0.5545147	3.5733081	0
C	-1.0499352	1.4787849	0
C	-1.5388781	-0.8420498	0
C	-0.1869437	-0.7096414	0
C	-2.3672546	-2.0767426	0
C	1.0499352	-1.4787849	0
C	2.1098222	-0.5241939	0
C	2.3672546	2.0767426	0
C	1.3419696	-2.8312321	0
C	3.4257906	-0.9312922	0
C	2.6742835	-3.2426977	0
H	0.5545147	-3.5733081	0
C	3.7229533	-2.3128463	0
H	4.2384739	-0.2167166	0
H	2.91452	-4.2971162	0
C	5.071361	-2.75047	0
H	3.0198082	2.106353	0.8778991
H	1.7534345	2.9751883	0
H	3.0198082	2.106353	-0.8778991
H	-1.7534345	-2.9751883	0
H	-3.0198082	-2.106353	-0.8778991
H	-3.0198082	-2.106353	0.8778991
C	6.2226904	-3.1189253	0
C	-6.2226904	3.1189253	0
C	7.5732838	-3.55446	0
C	-7.5732838	3.55446	0
C	7.8826708	-4.9235655	0
C	9.2032525	-5.3448061	0
C	10.2377711	-4.4143083	0
C	9.9422852	-3.0546113	0
C	8.6245736	-2.6245015	0
H	7.0763073	-5.6446208	0
H	9.4271426	-6.4039793	0
H	10.7431245	-2.326152	0
H	8.3919138	-1.5680786	0
C	-8.6245736	2.6245015	0
C	-9.9422852	3.0546113	0
C	-10.2377711	4.4143083	0
C	-9.2032525	5.3448061	0
C	-7.8826708	4.9235655	0
H	-8.3919138	1.5680786	0
H	-10.7431245	2.326152	0
H	-9.4271426	6.4039793	0
H	-7.0763073	5.6446208	0
C	1.5388781	0.8420498	0
C	0.1869437	0.7096414	0
H	-11.2678027	4.7466733	0
H	11.2678027	-4.7466733	0

Table 8. Coordinates of the calculated structure of 5c* (R = H, TPSSH-D3/def2-TZVP).

	x	y	z
C	-5.062136	2.76738	0
C	-3.716799	2.325362	0
C	-2.663225	3.253463	0
C	-3.424508	0.941755	0
H	-2.901321	4.309673	0
C	-1.331995	2.837798	0
C	-2.107232	0.53074	0
H	-4.241042	0.229592	0
H	-0.542255	3.579323	0
C	-1.04369	1.481744	0
C	-1.544749	-0.835818	0
C	-0.188014	-0.7076	0
C	-2.380785	-2.067121	0
C	1.04369	-1.481744	0
C	2.107232	-0.53074	0
C	2.380785	2.067121	0
C	1.331995	-2.837798	0
C	3.424508	-0.941755	0
C	2.663225	-3.253463	0
H	0.542255	-3.579323	0
C	3.716799	-2.325362	0
H	4.241042	-0.229592	0
H	2.901321	-4.309673	0
C	5.062136	-2.76738	0
H	3.033694	2.090712	0.879081
H	1.771499	2.969619	0
H	3.033694	2.090712	-0.879081
H	-1.771499	-2.969619	0
H	-3.033694	-2.090712	-0.879081
H	-3.033694	-2.090712	0.879081
C	6.216634	-3.140243	0
C	-6.216634	3.140243	0
C	7.564962	-3.57837	0
C	-7.564962	3.57837	0
C	7.871538	-4.950069	0
C	9.192436	-5.373779	0
C	10.229914	-4.444406	0
C	9.937012	-3.082678	0
C	8.619365	-2.648994	0
H	7.062303	-5.669775	0
H	9.414407	-6.434658	0
H	10.740293	-2.354986	0
H	8.387949	-1.591029	0
C	-8.619365	2.648994	0
C	-9.937012	3.082678	0
C	-10.229914	4.444406	0
C	-9.192436	5.373779	0
C	-7.871538	4.950069	0
H	-8.387949	1.591029	0
H	-10.740293	2.354986	0
H	-9.414407	6.434658	0
H	-7.062303	5.669775	0
C	1.544749	0.835818	0
C	0.188014	0.7076	0
H	-11.260473	4.779309	0
H	11.260473	-4.779309	0

Table 9. Coordinates of the calculated structure of 5b* (R = OMe, B3LYP-D3/def2-TZVP).

	x	y	z
C	0.1809641	0.7113968	0
C	-1.0624744	1.4700794	0
C	-2.1142643	0.5067446	0
C	-1.5316644	-0.8547146	0
C	-0.1809641	-0.7113968	0
C	-1.3670395	2.8196767	0
C	-2.7029869	3.2197591	0
C	-3.7441947	2.2813235	0
C	-3.4337408	0.9022937	0
C	1.5316644	0.8547146	0
C	2.1142643	-0.5067446	0
C	1.0624744	-1.4700794	0
C	3.4337408	-0.9022937	0
C	3.7441947	-2.2813235	0
C	2.7029869	-3.2197591	0
C	1.3670395	-2.8196767	0
C	-5.0964328	2.7063018	0
C	-6.2515182	3.0643188	0
C	-7.6055385	3.4846908	0
C	-8.6542822	2.5470427	0
C	-9.9715966	2.955148	0
C	-10.2888324	4.3170043	0
C	-9.2629553	5.2623962	0
C	-7.9394841	4.8436407	0
C	-2.3495697	-2.0965454	0
C	5.0964328	-2.7063018	0
C	6.2515182	-3.0643188	0
C	7.6055385	-3.4846908	0
C	7.9394841	-4.8436407	0
C	9.2629553	-5.2623962	0
C	10.2888324	-4.3170043	0
C	9.9715966	-2.955148	0
C	8.6542822	-2.5470427	0
O	11.6132816	-4.6192536	0
C	11.9938402	-5.9854398	0
O	-11.6132816	4.6192536	0
C	-11.9938402	5.9854398	0
C	2.3495697	2.0965454	0
H	-2.9519087	4.2721988	0
H	-4.2398581	0.1802518	0
H	-0.5861899	3.5688358	0
H	0.5861899	-3.5688358	0
H	4.2398581	-0.1802518	0
H	2.9519087	-4.2721988	0
H	3.0019101	2.1319551	0.8778895
H	1.7278559	2.989615	0
H	3.0019101	2.1319551	-0.8778895
H	-1.7278559	-2.989615	0
H	-3.0019101	-2.1319551	-0.8778895
H	-3.0019101	-2.1319551	0.8778895
H	7.1468977	-5.5798818	0
H	9.4808972	-6.3199591	0
H	10.7793805	-2.2354809	0
H	8.4164453	-1.4917943	0
H	-8.4164453	1.4917943	0
H	-10.7793805	2.2354809	0
H	-9.4808972	6.3199591	0
H	-7.1468977	5.5798818	0
H	-11.6266912	6.500849	-0.8923822
H	-11.6266912	6.500849	0.8923822
H	-13.0811057	5.9934039	0
H	13.0811057	-5.9934039	0
H	11.6266912	-6.500849	-0.8923822
H	11.6266912	-6.500849	0.8923822

Table 10. Coordinates of the calculated structure of 5b* (R = OMe, TPSSH-D3/def2-TZVP).

	x	y	z
C	0.1801251	0.7098896	0
C	-1.0602349	1.4702331	0
C	-2.113131	0.5075938	0
C	-1.5352635	-0.8527116	0
C	-0.1801251	-0.7098896	0
C	-1.3648573	2.8226614	0
C	-2.7008242	3.2233509	0
C	-3.7444501	2.2838129	0
C	-3.4350091	0.9034512	0
C	1.5352635	0.8527116	0
C	2.113131	-0.5075938	0
C	1.0602349	-1.4702331	0
C	3.4350091	-0.9034512	0
C	3.7444501	-2.2838129	0
C	2.7008242	-3.2233509	0
C	1.3648573	-2.8226614	0
C	-5.094863	2.7090275	0
C	-6.25456	3.067051	0
C	-7.6078454	3.4842794	0
C	-8.6558141	2.5429045	0
C	-9.9752011	2.9482584	0
C	-10.2934741	4.310928	0
C	-9.2697913	5.2607643	0
C	-7.9447304	4.8448818	0
C	-2.3574838	-2.0935055	0
C	5.094863	-2.7090275	0
C	6.25456	-3.067051	0
C	7.6078454	-3.4842794	0
C	7.9447304	-4.8448818	0
C	9.2697913	-5.2607643	0
C	10.2934741	-4.310928	0
C	9.9752011	-2.9482584	0
C	8.6558141	-2.5429045	0
O	11.6203828	-4.6120243	0
C	11.983079	-5.987402	0
O	-11.6203828	4.6120243	0
C	-11.983079	5.987402	0
C	2.3574838	2.0935055	0
H	-2.950436	4.2769473	0
H	-4.2430638	0.1815952	0
H	-0.5837242	3.5734058	0
H	0.5837242	-3.5734058	0
H	4.2430638	-0.1815952	0
H	2.950436	-4.2769473	0
H	3.0100384	2.1248263	0.879128
H	1.7376912	2.9889232	0
H	3.0100384	2.1248263	-0.879128
H	-1.7376912	-2.9889232	0
H	-3.0100384	-2.1248263	-0.879128
H	-3.0100384	-2.1248263	0.879128
H	7.1525415	-5.5833821	0
H	9.4922881	-6.3191388	0
H	10.7822774	-2.2259941	0
H	8.414983	-1.4870871	0
H	-8.414983	1.4870871	0
H	-10.7822774	2.2259941	0
H	-9.4922881	6.3191388	0
H	-7.1525415	5.5833821	0
H	-11.6060833	6.4935816	-0.8944154
H	-11.6060833	6.4935816	0.8944154
H	-13.0707773	6.0046019	0
H	13.0707773	-6.0046019	0
H	11.6060833	-6.4935816	-0.8944154
H	11.6060833	-6.4935816	0.8944154

Table 11. Coordinates of the calculated structure of 5a* (R = NMe$_2$, B3LYP-D3/def2-TZVP).

	x	y	z
C	-5.0728777	2.7523308	0
C	-3.7249468	2.3161296	0
C	-2.6743034	3.2445785	0
C	-3.4254768	0.9340685	0
H	-2.913495	4.2993042	0
C	-1.3420425	2.8321889	0
C	-2.1096902	0.5266348	0
H	-4.2379492	0.219118	0
H	-0.5544743	3.5744522	0
C	-1.0489254	1.4800358	0
C	-1.5394569	-0.8401978	0
C	-0.1875056	-0.7099584	0
C	-2.3686519	-2.0747147	0
C	1.0489254	-1.4800358	0
C	2.1096902	-0.5266348	0
C	2.3686519	2.0747147	0
C	1.3420425	-2.8321889	0
C	3.4254768	-0.9340685	0
C	2.6743034	-3.2445785	0
H	0.5544743	-3.5744522	0
C	3.7249468	-2.3161296	0
H	4.2379492	-0.219118	0
H	2.913495	-4.2993042	0
C	5.0728777	-2.7523308	0
H	3.0213984	2.1045187	0.8778672
H	1.7546873	2.9732166	0
H	3.0213984	2.1045187	-0.8778672
H	-1.7546873	-2.9732166	0
H	-3.0213984	-2.1045187	-0.8778672
H	-3.0213984	-2.1045187	0.8778672
C	6.2258793	-3.1196634	0
C	-6.2258793	3.1196634	0
C	7.5739724	-3.552316	0
C	-7.5739724	3.552316	0
C	7.9024379	-4.9163899	0
C	9.2151409	-5.3446637	0
C	10.2824179	-4.4221173	0
C	9.951834	-3.0506261	0
C	8.6351744	-2.6345888	0
H	7.1049269	-5.6478023	0
H	9.4124808	-6.4058781	0
H	10.7301685	-2.3027976	0
H	8.4127612	-1.5755612	0
N	11.591044	-4.8423863	0
C	-8.6351744	2.6345888	0
C	-9.951834	3.0506261	0
C	-10.2824179	4.4221173	0
C	-9.2151409	5.3446637	0
C	-7.9024379	4.9163899	0
H	-8.4127612	1.5755612	0
H	-10.7301685	2.3027976	0
N	-11.591044	4.8423863	0
H	-9.4124808	6.4058781	0
H	-7.1049269	5.6478023	0
C	1.5394569	0.8401978	0
C	0.1875056	0.7099584	0
C	-11.9004222	6.2559603	0
H	-11.4993219	6.7611251	-0.8856587
H	-11.4993219	6.7611251	0.8856587
H	-12.9797155	6.385131	0
C	12.6655728	-3.8732541	0
H	13.6182789	-4.3966498	0
H	12.6336175	-3.2290019	0.8856317
H	12.6336175	-3.2290019	-0.8856317
C	-12.6655728	3.8732541	0
H	-12.6336175	3.2290019	0.8856317
H	-12.6336175	3.2290019	-0.8856317
H	-13.6182789	4.3966498	0
C	11.9004222	-6.2559603	0
H	12.9797155	-6.385131	0
H	11.4993219	-6.7611251	-0.8856587
H	11.4993219	-6.7611251	0.8856587

Table 12. Coordinates of the calculated structure of 5a* (R = NMe$_2$, TPSSH-D3/def2-TZVP).

	x	y	z
C	-5.0698545	2.758024	0
C	-3.7240132	2.3210067	0
C	-2.6702473	3.2498602	0
C	-3.4260815	0.9374312	0
H	-2.9093492	4.3059384	0
C	-1.338244	2.836055	0
C	-2.1081534	0.5289279	0
H	-4.2407919	0.2229963	0
H	-0.5500237	3.5795406	0
C	-1.0456476	1.4809193	0
C	-1.5436063	-0.8370664	0
C	-0.1871271	-0.7083895	0
C	-2.3781365	-2.0698211	0
C	1.0456476	-1.4809193	0
C	2.1081534	-0.5289279	0
C	2.3781365	2.0698211	0
C	1.338244	-2.836055	0
C	3.4260815	-0.9374312	0
C	2.6702473	-3.2498602	0
H	0.5500237	-3.5795406	0
C	3.7240132	-2.3210067	0
H	4.2407919	-0.2229963	0
H	2.9093492	-4.3059384	0
C	5.0698545	-2.758024	0
H	3.0310914	2.0950365	0.8791118
H	1.7669498	2.9712378	0
H	3.0310914	2.0950365	-0.8791118
H	-1.7669498	-2.9712378	0
H	-3.0310914	-2.0950365	-0.8791118
H	-3.0310914	-2.0950365	0.8791118
C	6.2274554	-3.1257774	0
C	-6.2274554	3.1257774	0
C	7.5744279	-3.5562051	0
C	-7.5744279	3.5562051	0
C	7.9049324	-4.9222946	0
C	9.2191797	-5.3485496	0
C	10.2836279	-4.4218411	0
C	9.9537801	-3.0495918	0
C	8.6358193	-2.6349089	0
H	7.1072921	-5.655365	0
H	9.4223957	-6.4107378	0
H	10.7353363	-2.3021645	0
H	8.4111401	-1.575132	0
N	11.5924862	-4.8400699	0
C	-8.6358193	2.6349089	0
C	-9.9537801	3.0495918	0
C	-10.2836279	4.4218411	0
C	-9.2191797	5.3485496	0
C	-7.9049324	4.9222946	0
H	-8.4111401	1.575132	0
H	-10.7353363	2.3021645	0
N	-11.5924862	4.8400699	0
H	-9.4223957	6.4107378	0
H	-7.1072921	5.655365	0
C	1.5436063	0.8370664	0
C	0.1871271	0.7083895	0
C	-11.9023745	6.2549681	0
H	-11.4996139	6.7568145	-0.8878667
H	-11.4996139	6.7568145	0.8878667
H	-12.9837359	6.3777411	0
C	12.6655416	-3.8671875	0
H	13.6176227	-4.3944419	0
H	12.6285837	-3.2247606	0.8878497
H	12.6285837	-3.2247606	-0.8878497
C	-12.6655416	3.8671875	0
H	-12.6285837	3.2247606	0.8878497
H	-12.6285837	3.2247606	-0.8878497
H	-13.6176227	4.3944419	0
C	11.9023745	-6.2549681	0
H	12.9837359	-6.3777411	0
H	11.4996139	-6.7568145	-0.8878667
H	11.4996139	-6.7568145	0.8878667

Table 13. Coordinates of the calculated structure of 5d* (R = CO_2Me, B3LYP-D3/def2-TZVP).

	x	y	z
C	-0.0282246	-0.7331644	0
C	1.345945	-1.2149364	0
C	2.1729929	-0.0524394	0
C	1.319054	1.1569482	0
C	0.0282246	0.7331644	0
C	1.9241927	-2.4721467	0
C	3.3136657	-2.5843275	0
C	4.1348196	-1.4482156	0
C	3.5457577	-0.1638241	0
C	-1.319054	-1.1569482	0
C	-2.1729929	0.0524394	0
C	-1.345945	1.2149364	0
C	-3.5457577	0.1638241	0
C	-4.1348196	1.4482156	0
C	-3.3136657	2.5843275	0
C	-1.9241927	2.4721467	0
C	5.5452629	-1.5824776	0
C	6.7495457	-1.6906975	0
C	8.1605016	-1.8172132	0
C	8.9812014	-0.6766029	0
C	10.3567202	-0.8040426	0
C	10.951564	-2.0675922	0
C	10.1428586	-3.2065105	0
C	8.7653021	-3.0847314	0
C	1.8594205	2.5419044	0
C	-5.5452629	1.5824776	0
C	-6.7495457	1.6906975	0
C	-8.1605016	1.8172132	0
C	-8.7653021	3.0847314	0
C	-10.1428586	3.2065105	0
C	-10.951564	2.0675922	0
C	-10.3567202	0.8040426	0
C	-8.9812014	0.6766029	0
C	-12.4342214	2.1425655	0
O	-13.1681587	1.1825813	0
C	12.4342214	-2.1425655	0
O	12.8869096	-3.4133363	0
C	14.3133017	-3.5627385	0
C	-1.8594205	-2.5419044	0
O	-12.8869096	3.4133363	0
O	13.1681587	-1.1825813	0
H	3.7774746	-3.5612218	0
H	4.1840484	0.7099603	0
H	1.3164871	-3.3672506	0
H	-1.3164871	3.3672506	0
H	-4.1840484	-0.7099603	0
H	-3.7774746	3.5612218	0
H	-2.4899405	-2.7123486	0.8778915
H	-1.0655105	-3.285899	0
H	-2.4899405	-2.7123486	-0.8778915
H	1.0655105	3.285899	0
H	2.4899405	2.7123486	-0.8778915
H	2.4899405	2.7123486	0.8778915
H	-8.1391467	3.9664876	0
H	-10.6002572	4.1850863	0
H	-10.9944972	-0.0691306	0
H	-8.5220997	-0.3025352	0
H	8.5220997	0.3025352	0
H	10.9944972	0.0691306	0
H	10.6002572	-4.1850863	0
H	8.1391467	-3.9664876	0
H	14.4948257	-4.6340439	0
H	14.745025	-3.0997443	0.8868624
H	14.745025	-3.0997443	-0.8868624
C	-14.3133017	3.5627385	0
H	-14.4948257	4.6340439	0
H	-14.745025	3.0997443	-0.8868624
H	-14.745025	3.0997443	0.8868624

Table 14. Coordinates of the calculated structure of 5d* (R = CO_2Me, TPSSH-D3/def2-TZVP).

	x	y	z
C	-0.0262889	-0.7315028	0
C	1.3461367	-1.2128118	0
C	2.1721981	-0.0491531	0
C	1.3207452	1.1583741	0
C	0.0262889	0.7315028	0
C	1.9270817	-2.471792	0
C	3.3168603	-2.5819351	0
C	4.1380711	-1.4426819	0
C	3.5476423	-0.157801	0
C	-1.3207452	-1.1583741	0
C	-2.1721981	0.0491531	0
C	-1.3461367	1.2128118	0
C	-3.5476423	0.157801	0
C	-4.1380711	1.4426819	0
C	-3.3168603	2.5819351	0
C	-1.9270817	2.471792	0
C	5.5469582	-1.5766928	0
C	6.7555638	-1.6864677	0
C	8.1647739	-1.8161091	0
C	8.9892568	-0.6754798	0
C	10.3653437	-0.8074904	0
C	10.9557175	-2.0747077	0
C	10.1441638	-3.2135556	0
C	8.7660676	-3.0878371	0
C	1.8627884	2.5442718	0
C	-5.5469582	1.5766928	0
C	-6.7555638	1.6864677	0
C	-8.1647739	1.8161091	0
C	-8.7660676	3.0878371	0
C	-10.1441638	3.2135556	0
C	-10.9557175	2.0747077	0
C	-10.3653437	0.8074904	0
C	-8.9892568	0.6754798	0
C	-12.4358278	2.1518605	0
O	-13.1767317	1.1921643	0
C	12.4358278	-2.1518605	0
O	12.884861	-3.4271521	0
C	14.3171304	-3.5583302	0
C	-1.8627884	-2.5442718	0
O	-12.884861	3.4271521	0
O	13.1767317	-1.1921643	0
H	3.7835346	-3.5588615	0
H	4.18638	0.7172718	0
H	1.3210291	-3.3695322	0
H	-1.3210291	3.3695322	0
H	-4.18638	-0.7172718	0
H	-3.7835346	3.5588615	0
H	-2.4940633	-2.7118476	0.8791472
H	-1.0688856	-3.2894725	0
H	-2.4940633	-2.7118476	-0.8791472
H	1.0688856	3.2894725	0
H	2.4940633	2.7118476	-0.8791472
H	2.4940633	2.7118476	0.8791472
H	-8.1354466	3.9679593	0
H	-10.6012292	4.193952	0
H	-11.0090828	-0.0631957	0
H	-8.5312548	-0.3055378	0
H	8.5312548	0.3055378	0
H	11.0090828	0.0631957	0
H	10.6012292	-4.193952	0
H	8.1354466	-3.9679593	0
H	14.5073731	-4.6288502	0
H	14.7377264	-3.0872553	0.8887321
H	14.7377264	-3.0872553	-0.8887321
C	-14.3171304	3.5583302	0
H	-14.5073731	4.6288502	0
H	-14.7377264	3.0872553	-0.8887321
H	-14.7377264	3.0872553	0.8887321

Table 15. Coordinates of the calculated structure of 5e* (R = CN, B3LYP-D3/def2-TZVP).

	x	y	z
C	-5.1105627	2.6684151	0
C	-3.7568346	2.2512687	0
C	-2.7239297	3.1990399	0
C	-3.4398828	0.8743154	0
H	-2.9811564	4.2493736	0
C	-1.3858256	2.8090544	0
C	-2.11777	0.48849	0
H	-4.2412147	0.147153	0
H	-0.610159	3.5631572	0
C	-1.0734789	1.4608214	0
C	-1.5250587	-0.8680394	0
C	-0.1752609	-0.7123145	0
C	-2.3330587	-2.115781	0
C	1.0734789	-1.4608214	0
C	2.11777	-0.48849	0
C	2.3330587	2.115781	0
C	1.3858256	-2.8090544	0
C	3.4398828	-0.8743154	0
C	2.7239297	-3.1990399	0
H	0.610159	-3.5631572	0
C	3.7568346	-2.2512687	0
H	4.2412147	-0.147153	0
H	2.9811564	-4.2493736	0
C	5.1105627	-2.6684151	0
H	2.9847904	2.1556929	0.8780026
H	1.7053957	3.0044551	0
H	2.9847904	2.1556929	-0.8780026
H	-1.7053957	-3.0044551	0
H	-2.9847904	-2.1556929	-0.8780026
H	-2.9847904	-2.1556929	0.8780026
C	6.2673601	-3.0201883	0
C	-6.2673601	3.0201883	0
C	7.6206527	-3.4358171	0
C	-7.6206527	3.4358171	0
C	7.9493054	-4.8018776	0
C	9.2692089	-5.2090434	0
C	10.2971083	-4.2587378	0
C	9.9805988	-2.8950817	0
C	8.6599436	-2.4903956	0
H	7.1547236	-5.5350649	0
H	9.516506	-6.2617104	0
H	10.7766498	-2.1632347	0
H	8.4146644	-1.4374176	0
C	11.6611375	-4.6779515	0
C	-8.6599436	2.4903956	0
C	-9.9805988	2.8950817	0
C	-10.2971083	4.2587378	0
C	-9.2692089	5.2090434	0
C	-7.9493054	4.8018776	0
H	-8.4146644	1.4374176	0
H	-10.7766498	2.1632347	0
C	-11.6611375	4.6779515	0
H	-9.516506	6.2617104	0
H	-7.1547236	5.5350649	0
C	1.5250587	0.8680394	0
C	0.1752609	0.7123145	0
N	-12.7632679	5.0165535	0
N	12.7632679	-5.0165535	0

Table 16. Coordinates of the calculated structure of 5e* (R = CN, TPSSH-D3/def2-TZVP).

	x	y	z
C	-5.1080598	2.6724834	0
C	-3.7563219	2.2543983	0
C	-2.7208487	3.203158	0
C	-3.4409603	0.8760366	0
H	-2.9786826	4.2546436	0
C	-1.3828296	2.8122987	0
C	-2.1165234	0.4896087	0
H	-4.2445282	0.1494208	0
H	-0.6066898	3.5677341	0
C	-1.0709643	1.4611235	0
C	-1.5288436	-0.8658872	0
C	-0.174553	-0.7107384	0
C	-2.3414159	-2.1124077	0
C	1.0709643	-1.4611235	0
C	2.1165234	-0.4896087	0
C	2.3414159	2.1124077	0
C	1.3828296	-2.8122987	0
C	3.4409603	-0.8760366	0
C	2.7208487	-3.203158	0
H	0.6066898	-3.5677341	0
C	3.7563219	-2.2543983	0
H	4.2445282	-0.1494208	0
H	2.9786826	-4.2546436	0
C	5.1080598	-2.6724834	0
H	2.993448	2.1478693	0.8791986
H	1.7159761	3.0036294	0
H	2.993448	2.1478693	-0.8791986
H	-1.7159761	-3.0036294	0
H	-2.993448	-2.1478693	-0.8791986
H	-2.993448	-2.1478693	0.8791986
C	6.2692362	-3.0250405	0
C	-6.2692362	3.0250405	0
C	7.621626	-3.4383101	0
C	-7.621626	3.4383101	0
C	7.9527009	-4.8059297	0
C	9.2741639	-5.2110393	0
C	10.3015519	-4.2571639	0
C	9.9827817	-2.8919357	0
C	8.6605787	-2.4893457	0
H	7.1580978	-5.5409112	0
H	9.5242392	-6.2642474	0
H	10.7788998	-2.1584154	0
H	8.4125986	-1.435749	0
C	11.6655595	-4.6736955	0
C	-8.6605787	2.4893457	0
C	-9.9827817	2.8919357	0
C	-10.3015519	4.2571639	0
C	-9.2741639	5.2110393	0
C	-7.9527009	4.8059297	0
H	-8.4125986	1.435749	0
H	-10.7788998	2.1584154	0
C	-11.6655595	4.6736955	0
H	-9.5242392	6.2642474	0
H	-7.1580978	5.5409112	0
C	1.5288436	0.8658872	0
C	0.174553	0.7107384	0
N	-12.7728808	5.0115368	0
N	12.7728808	-5.0115368	0

Table 17. Coordinates of the calculated structure of 5f* (R = CPM, B3LYP-D3/def2-TZVP).

	x	y	z
C	-5.0683042	2.745109	0
C	-3.7220129	2.3079175	0
C	-2.6743401	3.2400365	0
C	-3.4261046	0.9259854	0
H	-2.9158326	4.2940991	0
C	-1.3426263	2.8298023	0
C	-2.1101475	0.5202062	0
H	-4.2386879	0.2114549	0
H	-0.5553627	3.571773	0
C	-1.0509935	1.4767147	0
C	-1.5381299	-0.8450393	0
C	-0.1859866	-0.7096056	0
C	-2.3648542	-2.0803718	0
C	1.0509935	-1.4767147	0
C	2.1101475	-0.5202062	0
C	2.3648542	2.0803718	0
C	1.3426263	-2.8298023	0
C	3.4261046	-0.9259854	0
C	2.6743401	-3.2400365	0
H	0.5553627	-3.571773	0
C	3.7220129	-2.3079175	0
H	4.2386879	-0.2114549	0
H	2.9158326	-4.2940991	0
C	5.0683042	-2.745109	0
H	3.0172503	2.1103445	0.8778893
H	1.7506978	2.9784133	0
H	3.0172503	2.1103445	-0.8778893
H	-1.7506978	-2.9784133	0
H	-3.0172503	-2.1103445	-0.8778893
H	-3.0172503	-2.1103445	0.8778893
C	6.2207691	-3.1131692	0
C	-6.2207691	3.1131692	0
C	7.5669106	-3.5431987	0
C	-7.5669106	3.5431987	0
C	7.8851295	-4.9117304	0
C	9.2025001	-5.3181952	0
C	10.2606798	-4.3899146	0
C	9.9353478	-3.0202977	0
C	8.6194104	-2.6093629	0
H	7.0864198	-5.6405777	0
H	9.43424	-6.3760964	0
H	10.7142352	-2.2741091	0
H	8.3837592	-1.5539673	0
C	11.6010512	-4.9249302	0
C	-8.6194104	2.6093629	0
C	-9.9353478	3.0202977	0
C	-10.2606798	4.3899146	0
C	-9.2025001	5.3181952	0
C	-7.8851295	4.9117304	0
H	-8.3837592	1.5539673	0
H	-10.7142352	2.2741091	0
C	-11.6010512	4.9249302	0
H	-9.43424	6.3760964	0
H	-7.0864198	5.6405777	0
C	1.5381299	0.8450393	0
C	0.1859866	0.7096056	0
C	-12.8153183	4.3224954	0
H	-11.6635156	6.0082823	0
C	-13.0202634	2.915818	0
C	-14.0199866	5.2043255	0
N	-13.1780501	1.7731243	0
O	-13.9819499	6.4107834	0
O	-15.1512858	4.4868619	0
C	-16.3739071	5.2403426	0
C	12.8153183	-4.3224954	0
C	13.0202634	-2.915818	0
C	14.0199866	-5.2043255	0
O	13.9819499	-6.4107834	0
O	15.1512858	-4.4868619	0
C	16.3739071	-5.2403426	0
H	-17.1689522	4.5006586	0
H	-16.4305358	5.8689362	-0.8879414
H	-16.4305358	5.8689362	0.8879414
H	17.1689522	-4.5006586	0
H	16.4305358	-5.8689362	-0.8879414
H	16.4305358	-5.8689362	0.8879414
N	13.1780501	-1.7731243	0
H	11.6635156	-6.0082823	0

Table 18. Coordinates of the calculated structure of 5f* (R = CPM, TPSSH-D3/def2-TZVP).

	x	y	z
C	-5.0639894	2.7519091	0
C	-3.7200518	2.3132277	0
C	-2.6691355	3.2457117	0
C	-3.4265516	0.9296908	0
H	-2.9106112	4.3010713	0
C	-1.3378191	2.8338437	0
C	-2.1085433	0.5225182	0
H	-4.2417536	0.2161967	0
H	-0.5496145	3.5766442	0
C	-1.0474967	1.4775781	0
C	-1.5424566	-0.841918	0
C	-0.1856948	-0.7079417	0
C	-2.3746287	-2.0753492	0
C	1.0474967	-1.4775781	0
C	2.1085433	-0.5225182	0
C	2.3746287	2.0753492	0
C	1.3378191	-2.8338437	0
C	3.4265516	-0.9296908	0
C	2.6691355	-3.2457117	0
H	0.5496145	-3.5766442	0
C	3.7200518	-2.3132277	0
H	4.2417536	-0.2161967	0
H	2.9106112	-4.3010713	0
C	5.0639894	-2.7519091	0
H	3.0272235	2.1003499	0.8791141
H	1.7634623	2.9763957	0
H	3.0272235	2.1003499	-0.8791141
H	-1.7634623	-2.9763957	0
H	-3.0272235	-2.1003499	-0.8791141
H	-3.0272235	-2.1003499	0.8791141
C	6.2209695	-3.1207729	0
C	-6.2209695	3.1207729	0
C	7.565969	-3.548548	0
C	-7.565969	3.548548	0
C	7.886259	-4.9190885	0
C	9.2053838	-5.3226176	0
C	10.2621768	-4.3902443	0
C	9.9354135	-3.0192537	0
C	8.6181326	-2.6104347	0
H	7.0872597	-5.6494369	0
H	9.4422665	-6.3809077	0
H	10.7168816	-2.2727076	0
H	8.3790205	-1.5545772	0
C	11.6017417	-4.9223737	0
C	-8.6181326	2.6104347	0
C	-9.9354135	3.0192537	0
C	-10.2621768	4.3902443	0
C	-9.2053838	5.3226176	0
C	-7.886259	4.9190885	0
H	-8.3790205	1.5545772	0
H	-10.7168816	2.2727076	0
C	-11.6017417	4.9223737	0
H	-9.4422665	6.3809077	0
H	-7.0872597	5.6494369	0
C	1.5424566	0.841918	0
C	0.1856948	0.7079417	0
C	-12.816083	4.311021	0
H	-11.6719018	6.0070874	0
C	-13.0175654	2.9051249	0
C	-14.0190021	5.1907715	0
N	-13.1793292	1.7578567	0
O	-13.9838183	6.4012309	0
O	-15.1512289	4.4692329	0
C	-16.3663377	5.2425488	0
C	12.816083	-4.311021	0
C	13.0175654	-2.9051249	0
C	14.0190021	-5.1907715	0
O	13.9838183	-6.4012309	0
O	15.1512289	-4.4692329	0
C	16.3663377	-5.2425488	0
H	-17.1688426	4.5099201	0
H	-16.4084694	5.8707153	-0.8898264
H	-16.4084694	5.8707153	0.8898264
H	17.1688426	-4.5099201	0
H	16.4084694	-5.8707153	-0.8898264
H	16.4084694	-5.8707153	0.8898264
N	13.1793292	-1.7578567	0
H	11.6719018	-6.0070874	0

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