Supporting Information

Push-pull photochromic dyes for semi-transparent solar cells with light-adjustable optical properties and high color-rendering index.

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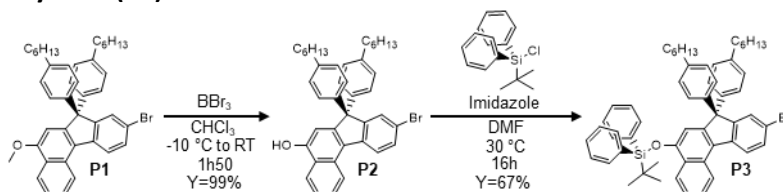[b] G-Lyte, Hub de l'énergie, 15 Rue Baudelocque, 80039 Amiens France
[c] LRCS, CNRS UMR7314, Université de Picardie Jules Verne, Hub de l'énergie, 15 Rue Baudelocque, 80039 Amiens France
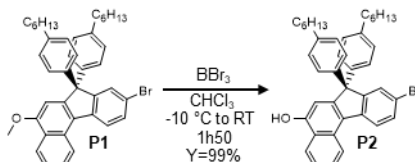[d] Solaronix SA, Rue de l'Ouriette 129, 1170 Aubonne, Switzerland

Synthesis:

Synthesis of the π-system (P3):

**P1** was synthesized according to the procedure described previously.[1]

Synthesis of P2:

P1 (3.310 g, 5.126 mmol, 1 eq.) was solubilized in anhydrous chloroform (30 mL) and the solution was stirred 5 minutes at -10 °C. 1M BBr_3 in DCM (24 mL, 24 mmol, 4.68 eq.) was added dropwise to the solution. The reaction mixture was allowed to warm up to RT and react for 2 hours. The reaction mixture was poured on saturated $NaHCO_3$ aqueous solution (30 mL), diluted with DCM (20 mL) and stirred in an ice bath for 10 minutes. The aqueous layer was then extracted with DCM and the organic layers are combined and washed with water and brine. The organic layer was dried over Na_2SO_4, filtered off and concentrated under vacuum. The resulting oil was purified by column chromatography (Hex/DCM: 8/2 to 6/4) to obtain **P2** (3.239 g, quantitative) as an expended white foam.

^{1}H NMR (400 MHz, Acetone) δ: 9.28 (s, 1H), 8.76 (d, J = 8.5 Hz, 1H), 8.39 (d, J = 8.2 Hz, 1H), 8.31 (d, J = 9.0 Hz, 1H), 7.74 (t, J = 7.1 Hz, 1H), 7.64 − 7.54 (m, 3H), 7.19 − 7.09 (m, 8H), 6.99 (s, 1H), 2.58 (t, 4H), 1.65 − 1.53 (m, 4H), 1.40 − 1.23 (m, 12H), 0.94 − 0.82 (m, 6H).

^{13}C NMR (100 MHz, Acetone) δ: 155.75, 155.03, 152.72, 143.02, 142.48, 141.75, 131.35, 131.18, 129.57, 129.25, 128.94, 128.67, 125.99, 125.64, 124.54, 124.39, 124.24, 119.34, 107.09, 65.90, 36.08, 32.41, 32.24, 23.24, 14.33.

Elem. Ana. (Calc., found for $C_{41}H_{43}OBr$): C (77.96, 77.87), H (6.86, 6.42).
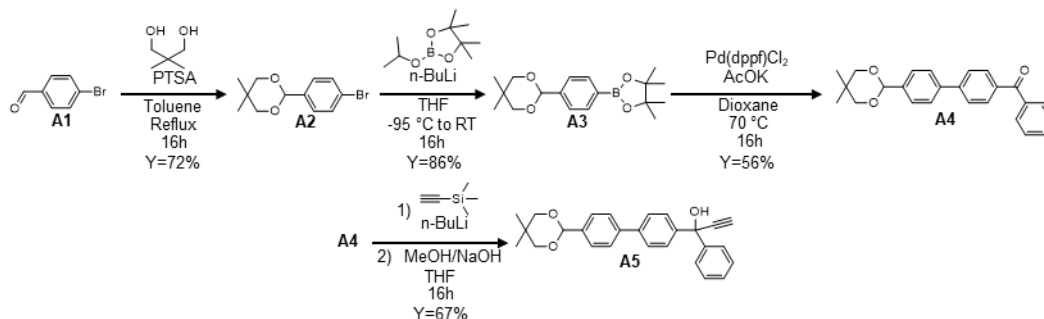
Synthesis of P3:
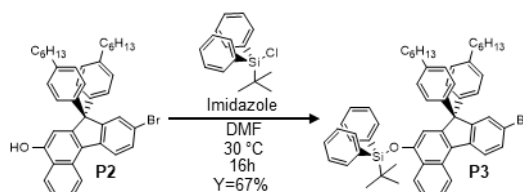
P2 (3.239 g, 5.127 mmol, 1 eq.) and imidazole (0.567 g, 1.62 eq.) are dried under vacuum and placed under argon. DMF (20 mL) was added and the solution was degassed for 5 minutes. TBDPSCl (1.374 g, 1.3 mL, 5 mmol, 0.97 eq.) was then added to the solution and the reaction mixture was heated to 30°C and allowed to react overnight. The reaction mixture was then poured on 1M HCl (30 mL) and diluted with DCM (20 mL). The aqueous layer was extracted with DCM and the organic layers are combined and washed with water and brine. The organic layer was dried over Na_2SO_4, filtered off and concentrated under vacuum. The resulting oil was purified by column chromatography (Hex/DCM: 8/2 to 6/4) to obtain **P3** (3.010 g, 3.459 mmol, 67% yield) as a white solid.

^{1}H NMR (400 MHz, Acetone) δ: 8.81 (d, J = 8.4 Hz, 1H), 8.69 (d, J = 7.7 Hz, 1H), 8.35 (d, J = 8.4 Hz, 1H), 7.81 (t, J = 7.0 Hz, 1H), 7.77 − 7.70 (m, 5H), 7.62 (dd, J = 8.3, 1.9 Hz, 1H), 7.58 − 7.48 (m, 3H), 7.39 (t, J = 7.5 Hz, 4H), 6.91 (d, J = 8.3 Hz, 4H), 6.72 (d, J = 7.9 Hz, 5H), 2.60 − 2.51 (m, 4H), 1.60 (dd, J = 14.0, 6.8 Hz, 4H), 1.43 − 1.26 (m, 12H), 1.21 (s, 9H), 0.92 (t, J = 6.7 Hz, 6H).

^{13}C NMR (100 MHz, Acetone) δ: 155.54, 152.77, 151.84, 142.55, 142.02, 141.38, 136.18, 132.82, 131.40, 131.24, 131.07, 129.68, 129.12, 128.95, 128.75, 128.46, 128.23, 126.96, 126.42, 124.85, 124.60, 124.42, 119.77, 112.45, 65.63, 36.04, 32.48, 32.20, 27.03, 23.28, 20.13, 14.37.
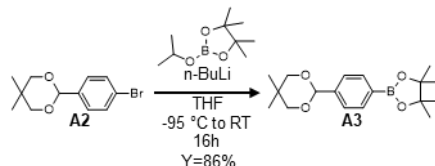
Elem. Ana. (Calc., found for $C_{57}H_{61}OBrSi$): C (78.68, 78.08), H (7.07, 6.91).

Synthesis of the acceptor (A5):

A2 was synthesized according to a well-known procedure described elsewhere.[2]

Synthesis of A3:

A2 (10.39 g, 38.46 mmol, 1 eq.) was solubilized in anhydrous THF (150 mL) and cooled at -96°C. *n*-BuLi (2.5 M, 20 mL, 1.30 eq.) was added dropwise and the solution was stirred for 30 minutes . iPrOB(pin) (10.734 g, 11.77 mL, 1.50 eq.) was then added to the reaction mixture which was allowed to reach RT and react overnight. EtOAc (50 mL) and water (50 mL) was added to the flask and the solution was stirred at RT for 10 minutes. The organic phase was separated and washed with water and brine before being concentrated under vacuum to obtain **A3** as a white powder (9.468 g, 29.75 mmol, 81% yield).

^{1}H NMR (400 MHz, CDCl$_3$) δ: 7.81 (d, *J* = 8.1 Hz, 2H), 7.50 (d, *J* = 7.9 Hz, 2H), 5.40 (s, 1H), 3.77 (d, *J* = 11.2 Hz, 2H), 3.64 (d, *J* = 10.6 Hz, 2H), 1.34 (s, 12H), 1.29 (s, 3H), 0.80 (s, 3H).

^{13}C NMR (100 MHz, CDCl$_3$) δ: 134.93, 125.54, 101.77, 83.93, 77.81, 30.42, 25.01, 23.21, 22.06.

HRMS: Calc. 318.20 g.mol^{-1}, found 318.10 g.mol^{-1}.

Synthesis of A4:
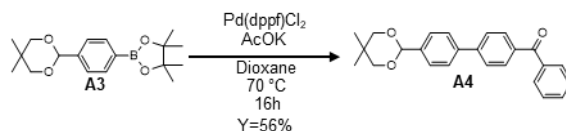
A3 (3 g, 9.43 mmol, 1.10 eq.) and bromo-benzophenone (2.28 g, 8.73 mmol, 1 eq.) are dried under vacuum and placed under argon in a round bottom flask. Dioxane (100 mL) and 1M AcOK (26 mL, 3 eq.) are added and the mixture was degassed for 10 minutes under stirring with argon. Pd(dppf)Cl$_2$ (125 mg, 2% eq.) was added to the mixture and degassed for 5 minutes with argon and the reaction mixture was left to react overnight at 70°C. Once the starting material was consumed, EtOAc (30 mL) and water (20 mL) were added to the mixture that was left under stirring for 10 minutes at RT. The organic layer was then collected, washed with water and brine, dried over Na$_2$SO$_4$, filtrated through a plug of aluminum oxide and concentrated under vacuum. The crude product obtained was purified by column chromatography (hexane/DCM: 8/2 to 6/4) to obtain **A4** (1.84 g, 4.94 mmol, 56% yield) as a white solid.

^{1}H NMR (400 MHz, CDCl$_3$) δ: 7.89 (d, *J* = 8.4 Hz, 2H), 7.84 (d, *J* = 7.0 Hz, 2H), 7.72 − 7.57 (m, 7H), 7.50 (t, *J* = 7.5 Hz, 2H), 5.47 (s, 1H), 3.81 (d, *J* = 11.1 Hz, 2H), 3.69 (d, *J* = 10.8 Hz, 2H), 1.32 (s, 3H), 0.83 (s, 3H).

^{13}C NMR (100 MHz, CDCl$_3$) δ: 145.09, 140.69, 138.65, 132.53, 130.86, 130.16, 128.46, 127.44, 127.18, 126.94, 101.51, 78.01, 30.44, 23.22, 22.06.

HRMS: Calc. 372.17 g.mol^{-1}, found 372.04 g.mol^{-1}.

Synthesis of A5:
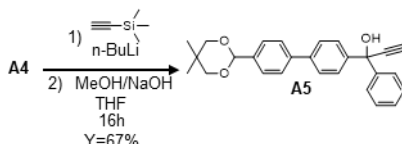
Trimethylsilylacetylene (2.11 mL, 2.5 eq.) was solubilized in anhydrous THF (100 mL) at -10°C. Then, *n*-BuLi (3.66 mL, 1.50 eq.) was added dropwise and the solution was stirred 30 minutes at -10°C. **A4** (2.27 g, 1 eq.) was then added to the mixture which was allowed to reach RT and react overnight. Water (20 mL), NaHCO$_3$ saturated (30 mL) and EtOAc (30 mL) are then added to stop the reaction and the organic phase was washed with water and brine, dried over Na$_2$SO$_4$ and concentrated under vacuum. The resulting intermediate was dissolved in MeOH (100 mL) and water (5 mL), and NaOH (3 g, excess) was added to the solution under stirring. After completion, the organic layer was extracted with EtOAc, washed with water and brine, dried with Na$_2$SO$_4$, filtered through a plug of aluminum oxide and concentrated under vacuum. The obtained powder was purified by column chromatography (Hex/DCM: 4/6 to 2/8) to give **A5** as a white powder (1.63 g, 4.09 mmol, 67% yield).

^{1}H NMR (400 MHz, Acetone) δ: 7.78 − 7.69 (m, 4H), 7.68 − 7.61 (m, 4H), 7.58 (d, *J* = 8.3 Hz, 2H), 7.35 (t, *J* = 7.6 Hz, 2H), 7.26 (t, *J* = 7.3 Hz, 1H), 5.76 (s, 1H), 5.47 (s, 1H), 3.74 (d, *J* = 10.9 Hz, 2H), 3.68 (d, *J* = 10.8 Hz, 2H), 3.38 (s, 1H), 1.27 (s, 3H), 0.79 (s, 3H).

^{13}C NMR (100 MHz, Acetone) δ: 146.83, 146.80, 146.24, 146.20, 141.56, 140.53, 139.41, 128.88, 128.16, 127.71, 127.42, 127.39, 127.31, 126.82, 102.05, 87.92, 87.89, 77.97, 76.40, 23.28, 21.93.

HRMS: Calc. 398.19 g.mol^{-1}, found 398.04 g.mol^{-1}.

Donor groups (C1-5):
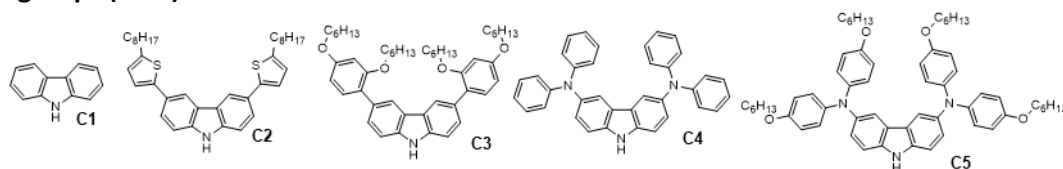
C1 and **C4** were purchased from Sigma Aldrich and Ikamba Organics, respectively.

C3 was synthesized according to a procedure described before.[3]

D5 was synthesized according to the literature.[4]

Synthesis of C2:
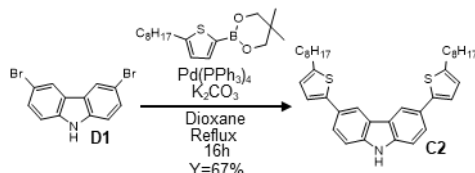
3,6-dibromocarbazole (**D1**, 0.490 g, 1.51 mmol, 1 eq.) and 5,5-dimethyl-2-(5-octylthiophen-2-yl)-1,3,2-dioxaborinane (1.592 g, 5.164 mmol, 3 eq.) are dried under vacuum and placed under argon. Dioxane (24 mL) and 2 mol.L^{-1} K$_2$CO$_3$ (16 mmol, 8.0 mL, 10 eq.) are added and the solution was degassed with argon for 10 minutes under stirring. Pd(PPh$_3$)$_4$ (0.181 g, 0.157 mmol, 10% eq.) was then added and the

mixture was immediately heated to 110 °C for 24 h. At the end of the reaction, EtOAc (50 mL) and water (50 mL) are added and the organic phase was then extracted with ethyl acetate, washed with brine, dried over MgSO$_4$, filtered and concentrated under vacuum. The resulting crude product was purified by precipitation in pentane to give **C2** as a white solid (0.729 g, 1.01 mmol, 67% yield).

^{1}H NMR (400 MHz, Acetone) δ: 10.45 (s, 1H), 8.45 (s, 2H), 7.68 (dd, J = 8.4, 1.6 Hz, 2H), 7.53 (d, J = 8.4 Hz, 2H), 7.26 (d, J = 3.4 Hz, 2H), 6.82 (d, J = 3.3 Hz, 2H), 2.85 (t, J = 7.5 Hz, 4H), 1.78 – 1.68 (m, 4H), 1.48 – 1.25 (m, 20H), 0.94 – 0.83 (m, 6H).

^{13}C NMR (100 MHz, Acetone) δ: 126.14, 124.87, 122.50, 117.96, 112.33, 32.61, 32.56, 30.74, 23.33, 14.36.

HRMS: Calc. 555.30 g.mol^{-1}, found 555.95 g.mol^{-1}.

Synthesis of C5:
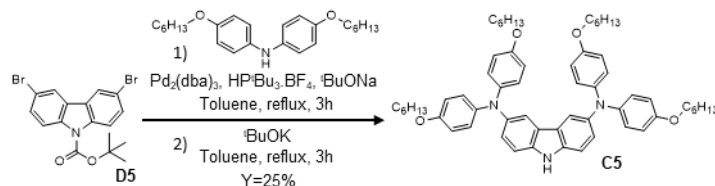
1. **D5** (1.283 g, 3.02 mmol, 1 eq.), di(4-hexyloylphenyl)amine (2.3396 g, 6.33 mmol, 2.1 eq.) and sodium *tert*-butoxide (0.879 g, 9.15 mmol, 3.03 eq.) are dried under vacuum and placed under argon. Dry toluene (12.75 mL) was added and the mixture was degassed for 10 minutes. Pd$_2$(dba)$_3$ (109 mg, 119 μmol, 4% eq.) and HP(^{t}Bu)$_3$·BF$_4$ (73 mg, 252 μmol, 8% eq.) are added and the solution was further degassed 5 minutes and the reaction mixture was heated at 125 °C (reflux) for 3 hours. Once the starting material was consumed, water (30 mL) was added and the mixture was allowed to cool down. The organic layer was extracted with toluene, washed with brine, dried over Na$_2$SO$_4$, filtered through a plug of celite and concentrated under vacuum. The resulting crude was purified by column chromatography (Hex/DCM: 7/3 to 5/5) to obtain the protected intermediate (1.679 g, 1.675 mmol, 55% yield).

2. The protected carbazole intermediate (0.9453 g, 0.943 mmol, 1 eq.) and ^{t}BuOK (0.524 g, 4.67 mmol, 4.95 eq.) are dried under vacuum and placed under argon. Dry toluene (20 mL) was added and the reaction mixture was heated at 130 °C (reflux) for 3 hours and then at 50 °C for 16 hours. Once the starting material was consumed, water (30 mL) was added and the mixture was allowed to cool down. The organic layer was extracted with EtOAc, washed with water and brine, dried over Na$_2$SO$_4$, filtered and concentrated under vacuum. The resulting crude product was purified by column chromatography (Hex/DCM: 7/3 to 5/5) to obtain **C5** (0.554 g, 0.614 mmol, 65% yield).

1H NMR (400 MHz, Acetone) δ: 10.23 (s, 1H), 7.68 (d, J = 1.9 Hz, 2H), 7.46 (d, J = 8.6 Hz, 2H), 7.16 (dd, J = 8.6, 2.1 Hz, 2H), 6.99 – 6.93 (m, 8H), 6.88 – 6.81 (m, 8H), 3.97 (t, J = 6.5 Hz, 8H), 1.83 – 1.74 (m, 8H), 1.57 – 1.46 (m, 8H), 1.46 – 1.26 (m, 16H), 1.00 – 0.87 (m, 12H).
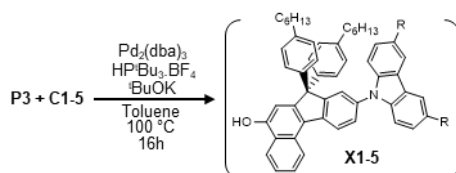
^{13}C NMR (100 MHz, Acetone) δ: 155.25, 143.52, 141.76, 138.16, 125.10, 124.69, 117.29, 115.93, 112.58, 68.74, 32.36, 26.51, 23.30, 14.31.

Elem. Ana. (Calc., found for C$_{60}$H$_{75}$N$_3$O$_4$): C (79.87, 79.55), H (8.38, 8.39), N (4.66, 4.66).

Final assembly of the dyes (SF1-5):
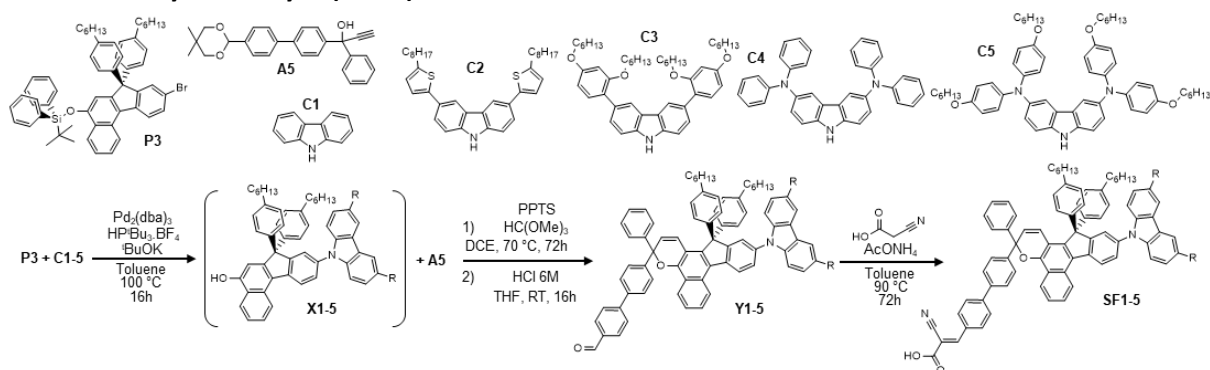
Synthesis of X1-5:

General procedure:

P3 (1.00 eq.), **C1-5** (1.00 eq.), ^{t}BuOK (3.00 eq.), Pd$_2$(dba)$_3$ (2% eq.) and HP^{t}Bu$_3$BF$_4$ (8% eq.) are dried under vacuum and placed under argon. Degassed toluene (20 mL, freeze-pump-thaw method) was added and the solution was left to react at 100 °C for 16 hours. With these reaction conditions, ^{t}BuOK deprotected partially or totally the TBDPS group *in-situ*. If the deprotection was not complete, TBAF (1M in THF, 1 eq.) was added to the mixture at 50 °C and the deprotection was carried to completion. Once the starting material was consumed, water (20 mL) and EtOAc (20 mL) were added to the mixture that was left under stirring for 10 minutes. The organic layer was extracted, washed with water, dried with Na$_2$SO$_4$, filtered off and concentrated under vacuum. The resulting crude product was purified by column chromatography (Hexane/DCM) to obtain **X1-5** as greyish foams. **X1-5** are highly unstable under air or irradiation and were used directly after their purification by column chromatography, based only on TLC plates without further purifications.

**P3 + C1** give **X1** with an 80% yield (column chromatography: hexane/DCM: 9/1 to 8/2).

P3 + C2 give **X2** with a 59% yield (column chromatography: hexane/DCM: 9/1 to 8/2).

P3 + C3 give **X3** with a 61% yield (column chromatography: hexane/DCM: 25/75 to 35/65).

P3 + C4 give **X4** with an 83% yield (column chromatography: hexane/DCM: 8/2 to 6/4).

P3 + C5 give **X5** with a 72% yield (column chromatography: hexane/DCM: 7/3 to 5/5).

Synthesis of Y1-5:
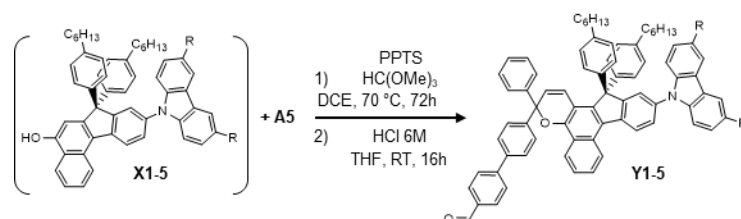
General procedure:

1) **X1-5** (1 eq.), **A5** (1.20 eq.) and pyridinium *p*-toluenesulfonate (0.10 eq.) are dried under vacuum and placed under argon. 1,2-dichloroethane (15 mL) and trimethylorthoformate (4.00 eq.) are then added and the mixture was heated at 70°C for 72 hours. At the end of the reaction, the organic layer was extracted with DCM and washed with water, dried over Na$_2$SO$_4$, filtered off and concentrated under

vacuum. The protected intermediate was then purified by column chromatography (Hex/DCM: 8/2 to 6/4).

2) The products are directly solubilized in THF (20 mL) and 6M HCl (5 mL) was added before leaving the mixture to react for 4 hours at RT. Once the starting material was consumed, water (15 mL) and EtOAc (20 mL) are added to the reaction mixture and the organic layer was washed with water and brine, dried over Na_2SO_4, filtered off and concentrated under vacuum. The resulting product was purified by column chromatography (Hex/DCM: 7/3 to 5/5) to obtain **Y1-5** as greyish solids.

Y1 obtained with a 50% yield.

^{1}H NMR (400 MHz, Acetone) δ: 10.10 (s, 1H), 8.96 (d, J = 8.5 Hz, 1H), 8.67 (d, J = 8.9 Hz, 2H), 8.22 (d, J = 7.7 Hz, 2H), 8.01 (d, J = 8.5 Hz, 2H), 7.87 (d, J = 8.3 Hz, 2H), 7.82 (ddd, J = 8.4, 6.9, 1.4 Hz, 1H), 7.77 − 7.67 (m, 5H), 7.63 − 7.58 (m, 2H), 7.56 (dd, J = 5.3, 3.3 Hz, 2H), 7.42 − 7.27 (m, 13H), 7.26 − 7.19 (m, 4H), 6.96 (d, J = 9.8 Hz, 1H), 6.21 (d, J = 9.8 Hz, 1H), 2.65 (dd, J = 15.2, 7.2 Hz, 4H), 1.72 − 1.57 (m, 4H), 1.45 − 1.22 (m, 12H), 0.96 − 0.80 (m, 6H).

^{13}C NMR (100 MHz, Acetone) δ: 192.59, 158.29, 149.69, 148.56, 146.93, 145.66, 145.09, 142.77, 142.70, 141.53, 140.67, 140.33, 140.23, 139.75, 136.77, 136.32, 131.00, 129.89, 129.84, 129.37, 129.31, 129.24, 129.05, 128.68, 128.64, 128.59, 128.50, 128.02, 127.79, 127.01, 126.90, 126.60, 126.57, 125.11, 124.45, 124.40, 124.34, 124.18, 123.84, 121.32, 121.07, 116.28, 110.69, 83.23, 65.97, 36.22, 32.58, 32.56, 32.40, 32.38, 29.93, 29.91, 23.40, 14.48.

Elem. Ana. (Calc., found for $C_{75}H_{65}NO_2$): C (88.98, 88.71), H (6.47, 6.44), N (1.38, 0.93).

Y2 obtained with a 62% yield.

^{1}H NMR (400 MHz, Acetone) δ: 10.10 (s, 1H), 8.95 (d, *J* = 8.6 Hz, 1H), 8.66 (d, *J* = 8.4 Hz, 2H), 8.54 (s, 2H), 8.01 (d, *J* = 8.3 Hz, 2H), 7.87 (d, *J* = 8.3 Hz, 2H), 7.81 (t, *J* = 7.1 Hz, 1H), 7.75 − 7.66 (m, 6H), 7.65 − 7.57 (m, 5H), 7.54 (d, *J* = 7.3 Hz, 2H), 7.40 − 7.32 (m, 7H), 7.32 − 7.26 (m, 6H), 7.25 − 7.18 (m, 5H), 6.96 (d, *J* = 9.9 Hz, 1H), 6.86 (d, *J* = 3.5 Hz, 2H), 6.20 (d, *J* = 9.8 Hz, 1H), 2.93 − 2.86 (m, 5H), 2.65 (dd, *J* = 14.4, 8.0 Hz, 5H), 1.81 − 1.71 (m, 5H), 1.71 − 1.58 (m, 5H), 1.52 − 1.23 (m, 40H), 0.96 − 0.80 (m, 14H).

^{13}C NMR (100 MHz, Acetone) δ: 192.49, 158.23, 149.62, 148.49, 146.82, 145.54, 145.26, 144.99, 143.25, 142.68, 142.61, 141.09, 140.70, 140.17, 140.07, 139.66, 136.66, 135.87, 130.89, 129.78, 129.73, 129.29, 129.23, 129.13, 128.96, 128.56, 128.49, 128.39, 127.91, 127.66, 126.79, 126.48, 126.28, 126.22, 125.11, 124.99, 124.79, 124.28, 124.17, 124.06, 123.71, 122.91, 118.13, 116.14, 111.17, 83.13, 65.88, 36.12, 32.62, 32.55, 32.48, 32.46, 32.32, 32.30, 30.75, 23.33, 23.29, 14.37.

HRMS: Calc. 1399.727 g.mol^{-1}, found 1399.731 g.mol^{-1} (3 ppm).

Y3 obtained with a 42% yield.

^{1}H NMR (400 MHz, Acetone) δ: 10.08 (s, 1H), 8.93 (d, J = 8.6 Hz, 1H), 8.64 (t, 2H), 8.36 (sd, J = 1.4 Hz, 2H), 7.98 (d, J = 8.4 Hz, 2H), 7.85 (t, J = 7.9 Hz, 2H), 7.79 (t, J = 7.0 Hz, 1H), 7.76 − 7.69 (m, 3H), 7.67 (d, J = 8.6 Hz, 2H), 7.58 (d, J = 8.6 Hz, 2H), 7.56 − 7.49 (m, 5H), 7.39 − 7.24 (m, 13H), 7.19 (dd, J = 8.3, 4.7 Hz, 5H), 6.95 (d, J = 9.9 Hz, 1H), 6.69 (sd, J = 2.3 Hz, 2H), 6.63 (dd, J = 8.4, 2.4 Hz, 2H), 6.17 (d, J = 9.9 Hz, 1H), 4.05 (dd, J = 14.4, 6.4 Hz, 9H), 2.63 (dd, J = 15.2, 7.6 Hz, 5H), 1.87 − 1.77 (m, 5H), 1.76 − 1.66 (m, 5H), 1.66 − 1.57 (m, 5H), 1.57 − 1.12 (m, 44H), 0.98 − 0.91 (m, 7H), 0.87 − 0.77 (m, 7H), 0.70 (t, J = 7.1 Hz, 7H).

^{13}C NMR (100 MHz, Acetone) δ: 192.46, 160.53, 158.13, 157.99, 149.50, 148.34, 146.80, 145.54, 144.98, 142.62, 142.55, 140.32, 140.25, 140.22, 140.16, 139.62, 136.63, 136.53, 132.03, 131.77, 130.87, 129.77, 129.73, 129.23, 129.17, 129.11, 128.89, 128.56, 128.47, 128.36, 127.89, 127.66, 126.74, 126.46, 126.11, 125.01, 124.66, 124.33, 124.18, 124.08, 124.03, 123.73, 121.93, 116.16, 109.87, 106.66, 101.14, 83.10, 70.83, 69.02, 68.63, 65.84, 42.52, 36.14, 32.45, 32.37, 32.35, 32.32, 30.08, 26.85, 26.53, 23.32, 23.27, 14.36, 14.33, 14.29.

Elem. Ana. (Calc., found for $C_{111}H_{121}NO_6$): C (85.18, 83.54), H (7.79, 7.60), N (0.89, 1.23).

Y4 obtained with a 31% yield.

^{1}H NMR (400 MHz, Acetone) δ: 10.10 (s, 1H), 8.94 (d, J = 8.5 Hz, 1H), 8.70 – 8.63 (m, 2H), 8.01 (d, J = 8.4 Hz, 2H), 7.92 – 7.85 (m, 4H), 7.81 (ddd, J = 8.4, 6.9, 1.4 Hz, 1H), 7.77 – 7.67 (m, 6H), 7.60 (d, J = 8.6 Hz, 2H), 7.55 (d, J = 7.2 Hz, 2H), 7.40 – 7.17 (m, 27H), 7.04 (d, J = 7.6 Hz, 9H), 7.00 – 6.93 (m, 6H), 6.22 (d, J = 9.8 Hz, 1H), 2.62 (dd, J = 14.5, 6.5 Hz, 5H), 1.66 – 1.54 (m, 5H), 1.39 – 1.21 (m, 15H), 0.94 – 0.78 (m, 7H).

^{13}C NMR (100 MHz, Acetone) δ: 192.60, 158.33, 149.72, 149.61, 148.56, 146.94, 145.64, 145.09, 142.79, 142.72, 141.80, 140.72, 140.31, 140.22, 139.79, 139.21, 136.77, 136.18, 131.00, 130.11, 129.87, 129.82, 129.40, 129.34, 129.24, 129.06, 128.67, 128.65, 128.61, 128.50, 128.03, 127.77, 126.90, 126.58, 126.44, 125.23, 125.08, 124.41, 124.22, 124.17, 123.84, 123.64, 122.75, 119.78, 116.25, 111.90, 83.24, 36.16, 32.48, 32.34, 23.36, 14.47.

Elem. Ana. (Calc., found for $C_{99}H_{83}N_3O_2$): C (88.29, 88.20), H (6.21, 6.01), N (3.12, 2.78).

Y5 obtained with a 25% yield.

^{1}H NMR (400 MHz, Acetone) δ: 10.06 (s, 1H), 8.90 (d, J = 8.6 Hz, 1H), 8.65 – 8.58 (m, 2H), 7.97 (d, J = 8.4 Hz, 2H), 7.84 (d, J = 8.3 Hz, 2H), 7.77 (t, J = 7.8 Hz, 1H), 7.72 – 7.61 (m, 8H), 7.57 (d, J = 8.6 Hz, 2H), 7.51 (d, J = 7.2 Hz, 2H), 7.36 – 7.22 (m, 8H), 7.21 – 7.13 (m, 7H), 7.05 (dd, J = 8.8, 2.2 Hz, 2H), 6.92 (d, J = 9.0 Hz, 11H), 6.80 (d, J = 9.1 Hz, 11H), 6.18 (d, J = 9.8 Hz, 1H), 3.92 (t, J = 6.5 Hz, 8H), 2.59 (dd, J = 14.9, 6.9 Hz, 4H), 1.79 – 1.69 (m, 8H), 1.56 (dd, J = 14.8, 7.4 Hz, 4H), 1.52 – 1.42 (m, 8H), 1.40 – 1.18 (m, 42H), 0.94 – 0.76 (m, 27H).

^{13}C NMR (100 MHz, Acetone) δ: 192.48, 160.68, 158.08, 155.45, 149.51, 148.34, 146.82, 145.52, 144.98, 143.17, 143.04, 142.62, 142.55, 140.23, 140.13, 139.66, 137.99, 136.65, 136.38, 130.88, 129.73, 129.67, 129.26, 129.20, 129.11, 128.89, 128.54, 128.48, 128.38, 127.90, 127.65, 126.74, 126.44, 126.13, 125.42, 125.10, 124.94, 124.79, 124.20, 124.04, 123.95, 123.74, 116.84, 116.12, 115.97, 111.34, 68.73, 36.02, 32.36, 32.20, 30.47, 30.28, 30.12, 30.09, 26.51, 23.31, 23.24, 14.36, 14.33.

HRMS: Calc. 1746.003 g.mol^{-1}, found 1746.006 g.mol^{-1} (2 ppm).

Synthesis of SF1-5:
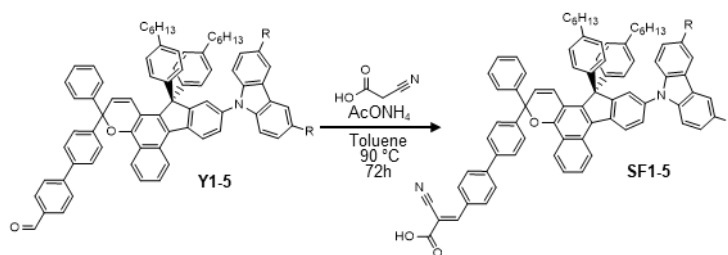
General procedure:

SF1-5 (1.00 eq.), cyanoacetic acid (8.00 eq.) and ammonium acetate (16 eq.) are dried under vacuum and placed under argon. Toluene (15 mL) was then added and the solution was stirred at 90 °C for 72 hours. Once the starting material was consumed, water (10 mL) and EtOAc (15 mL) are added to the reaction mixture and the organic layer was extracted, washed with water and brine, dried over Na$_2$SO$_4$, filtered off and concentrated under vacuum. The resulting crude product was purified by column chromatography (pure DCM to DCM/MeOH: 9/1) to obtain **SF1-5** as greyish solids.

SF1 (137 mg) was obtained with a 39% yield.

^{1}H NMR (400 MHz, THF) δ: 8.84 (d, J = 8.6 Hz, 1H), 8.54 (t, J = 8.4 Hz, 2H), 8.26 (s, 1H), 8.10 (d, J = 7.7 Hz, 4H), 7.76 (d, J = 8.4 Hz, 2H), 7.71 – 7.66 (m, 2H), 7.63 – 7.55 (m, 4H), 7.50 (d, J = 8.5 Hz, 2H), 7.44 (d, J = 7.0 Hz, 2H), 7.34 – 7.16 (m, 13H), 7.11 (d, J = 8.2 Hz, 4H), 6.89 (d, J = 9.8 Hz, 1H), 5.98 (d, J = 9.8 Hz, 1H), 2.65 – 2.57 (m, 4H), 1.68 – 1.57 (m, 4H), 1.41 – 1.24 (m, 13H), 0.86 (dt, J = 9.7, 7.1 Hz, 6H).

^{13}C NMR (100 MHz, THF) δ: 158.33, 149.66, 148.40, 145.61, 145.18, 142.46, 141.60, 140.74, 140.52, 140.47, 139.68, 136.35, 132.46, 132.14, 131.12, 129.99, 129.03, 128.91, 128.71, 128.66, 128.48, 128.37, 128.22, 127.90, 127.59, 126.68, 126.58, 126.32, 126.25, 124.97, 124.45, 124.06, 123.92, 123.77, 120.91, 120.66, 116.08, 110.66, 83.34, 65.97, 36.45, 32.75, 32.64, 30.15, 23.54, 14.47.

HRMS: Calc. 1078.507 g.mol^{-1}, found 1078.508 g.mol^{-1} (1 ppm).

SF2 (85 mg) was obtained with a 62% yield.

^{1}H NMR (400 MHz, THF) δ: 8.85 (d, J = 8.6 Hz, 1H), 8.59 – 8.52 (m, 2H), 8.40 (sd, J = 1.5 Hz, 2H), 8.26 (s, 1H), 8.11 (d, J = 8.2 Hz, 2H), 7.77 (d, J = 8.4 Hz, 2H), 7.74 – 7.66 (m, 2H), 7.66 – 7.54 (m, 6H), 7.51 (d, J = 8.4 Hz, 2H), 7.44 (d, J = 7.2 Hz, 2H), 7.32 (d, J = 8.3 Hz, 4H), 7.30 – 7.17 (m, 7H), 7.13 (d, J = 7.7 Hz, 4H), 6.90 (d, J = 9.9 Hz, 1H), 6.77 (d, J = 3.5 Hz, 2H), 5.99 (d, J = 9.8 Hz, 1H), 2.85 (t, J = 7.5 Hz, 4H), 2.63 (t, J = 7.6 Hz, 4H), 1.80 – 1.69 (m, 4H), 1.69 – 1.58 (m, 4H), 1.50 – 1.24 (m, 34H), 0.96 – 0.81 (m, 12H).

^{13}C NMR (100 MHz, THF) δ: 158.39, 153.16, 149.71, 148.47, 145.64, 145.36, 145.17, 145.03, 143.66, 142.51, 141.26, 140.91, 140.47, 140.42, 139.64, 136.05, 132.32, 132.22, 131.12, 129.98, 129.08, 128.92, 128.66, 128.54, 128.38, 128.25, 127.90, 127.61, 126.68, 126.35, 126.10, 125.93, 124.97, 124.90, 124.27, 124.07, 124.00, 123.76, 122.59, 117.92, 116.87, 116.07, 111.15, 83.36, 66.00, 36.47, 32.91, 32.78, 32.67, 31.04, 30.40, 30.28, 30.18, 30.10, 23.61, 23.56, 14.50.

HRMS: Calc. 1466.733 g.mol^{-1}, found 1466.730 g.mol^{-1} (2 ppm).

SF3 (117 mg) was obtained with a 50% yield.

^{1}H NMR (400 MHz, THF) δ: 8.86 (d, J = 8.6 Hz, 1H), 8.58 – 8.52 (m, 2H), 8.25 (d, J = 1.3 Hz, 3H), 8.09 (d, J = 8.2 Hz, 2H), 7.79 – 7.73 (m, 3H), 7.69 (t, J = 7.7 Hz, 2H), 7.64 – 7.54 (m, 3H), 7.50 (d, J = 8.5 Hz, 2H), 7.48 – 7.41 (m, 4H), 7.35 – 7.16 (m, 11H), 7.11 (d, J = 8.1 Hz, 4H), 6.90 (d, J = 9.8 Hz, 1H), 6.61 (d, J = 2.3 Hz, 2H), 6.56 (dd, J = 8.4, 2.3 Hz, 2H), 5.98 (d, J = 9.8 Hz, 1H), 3.98 (dt, J = 16.6, 6.4 Hz, 9H), 2.61 (t, J = 7.6 Hz, 4H), 1.84 – 1.56 (m, 24H), 1.56 – 1.13 (m, 40H), 0.93 (t, J = 7.1 Hz, 6H), 0.84 (dt, J = 9.4, 7.0 Hz, 6H), 0.73 (t, J = 7.0 Hz, 6H).

^{13}C NMR (100 MHz, THF) δ: 160.56, 158.30, 158.12, 152.86, 149.56, 148.32, 145.66, 145.25, 145.21, 142.44, 140.58, 140.55, 140.48, 140.39, 139.67, 136.80, 132.15, 131.99, 131.82, 131.13, 130.02, 129.03, 128.91, 128.86, 128.66, 128.41, 128.37, 128.23, 127.92, 127.60, 126.68, 126.30, 125.97, 125.24, 125.01, 124.51, 124.23, 124.05, 123.89, 123.80, 121.77, 116.10, 109.81, 106.34, 101.35, 83.33, 69.17, 68.64, 65.97, 36.49, 32.75, 32.68, 32.58, 30.39, 30.29, 30.18, 26.98, 26.81, 23.60, 23.55, 14.47, 14.45, 14.41.

HRMS: Calc. 1630.925 g.mol^{-1}, found 1630.925 g.mol^{-1} (0 ppm).

SF4 (125 mg) was obtained with a 61% yield.

^{1}H NMR (400 MHz, THF) δ: 8.81 (d, J = 8.6 Hz, 1H), 8.52 (dd, J = 8.4, 4.8 Hz, 2H), 8.23 (s, 1H), 8.03 (s, 2H), 7.83 (d, J = 2.0 Hz, 2H), 7.75 – 7.59 (m, 5H), 7.59 – 7.51 (m, 3H), 7.47 (d, J = 8.3 Hz, 2H), 7.41 (d, J = 7.3 Hz, 2H), 7.34 – 7.06 (m, 25H), 6.99 (d, J = 7.6 Hz, 8H), 6.91 – 6.81 (m, 5H), 5.95 (d, J = 9.8 Hz, 1H), 2.56 (dd, J = 15.0, 6.9 Hz, 4H), 1.63 – 1.49 (m, 4H), 1.37 – 1.18 (m, 12H), 0.83 (dt, J = 13.8, 6.8 Hz, 6H).

^{13}C NMR (100 MHz, THF) δ: 149.67, 145.16, 142.51, 141.62, 140.84, 140.49, 140.45, 139.32, 136.17, 131.09, 129.96, 129.77, 129.06, 128.89, 128.61, 128.48, 127.90, 127.56, 126.92, 125.40, 124.18, 123.74, 123.43, 122.33, 120.07, 116.05, 116.01, 111.79, 111.77, 36.40, 32.68, 32.66, 32.59, 30.69, 30.65, 30.36, 30.10, 23.52, 23.51, 14.47.

HRMS: Calc. 1412.654 g.mol^{-1}, found 1412.652 g.mol^{-1} (1 ppm).

SF5 (25 mg) was obtained with a 21% yield.

^{1}H NMR (400 MHz, THF) δ: 8.82 (d, J = 8.7 Hz, 1H), 8.52 (dd, J = 12.4, 8.1 Hz, 2H), 8.26 – 8.15 (m, 1H), 8.06 (d, J = 8.3 Hz, 2H), 7.73 (d, J = 8.4 Hz, 2H), 7.70 – 7.62 (m, 4H), 7.62 – 7.53 (m, 4H), 7.48 (d, J = 8.5 Hz, 2H), 7.42 (d, J = 7.1 Hz, 2H), 7.35 – 7.26 (m, 4H), 7.26 – 7.14 (m, 5H), 7.08 (dd, J = 8.4, 1.8 Hz, 4H),

7.02 (dd, J = 8.8, 2.1 Hz, 2H), 6.96 – 6.79 (m, 9H), 6.78 – 6.67 (m, 8H), 5.96 (d, J = 9.9 Hz, 1H), 3.88 (t, J = 6.4 Hz, 8H), 2.85 – 2.35 (m, 8H), 1.63 – 1.52 (m, 4H), 1.52 – 1.41 (m, 8H), 1.41 – 1.20 (m, 32H), 0.97 – 0.79 (m, 18H).

^{13}C NMR (100 MHz, THF) δ: 158.38, 155.56, 149.71, 148.47, 145.26, 143.57, 143.00, 142.59, 142.57, 140.63, 139.87, 138.46, 136.60, 135.63, 131.94, 131.19, 130.06, 129.16, 129.00, 128.80, 128.71, 128.24, 128.03, 127.66, 126.76, 126.41, 126.10, 125.40, 125.33, 125.18, 124.18, 117.73, 116.15, 115.87, 111.49, 83.43, 71.64, 71.49, 68.85, 66.10, 59.36, 36.50, 32.76, 32.69, 30.81, 30.54, 30.19, 26.92, 24.69, 23.70, 23.62, 20.66, 14.56, 14.06.

HRMS: Calc. 1813.010 g.mol^{-1}, found 1813.011 g.mol^{-1} (1 ppm).

NMR Spectra:
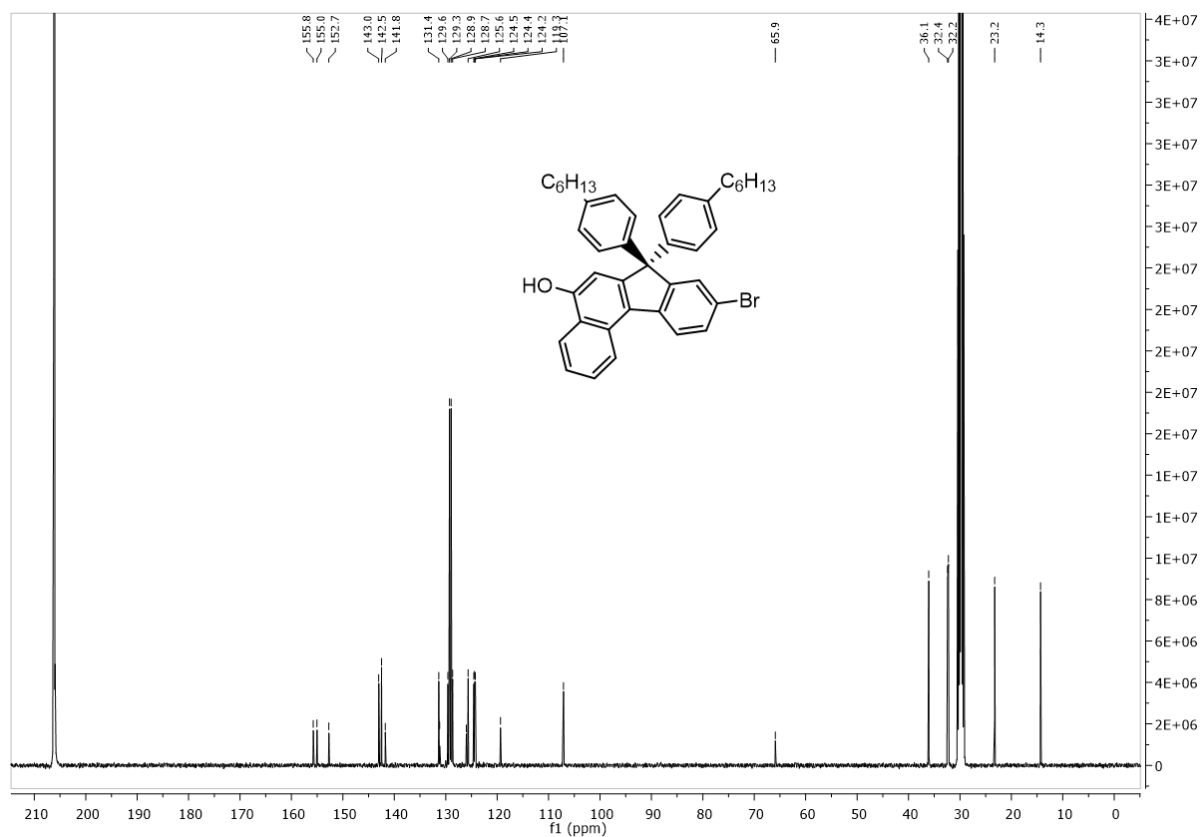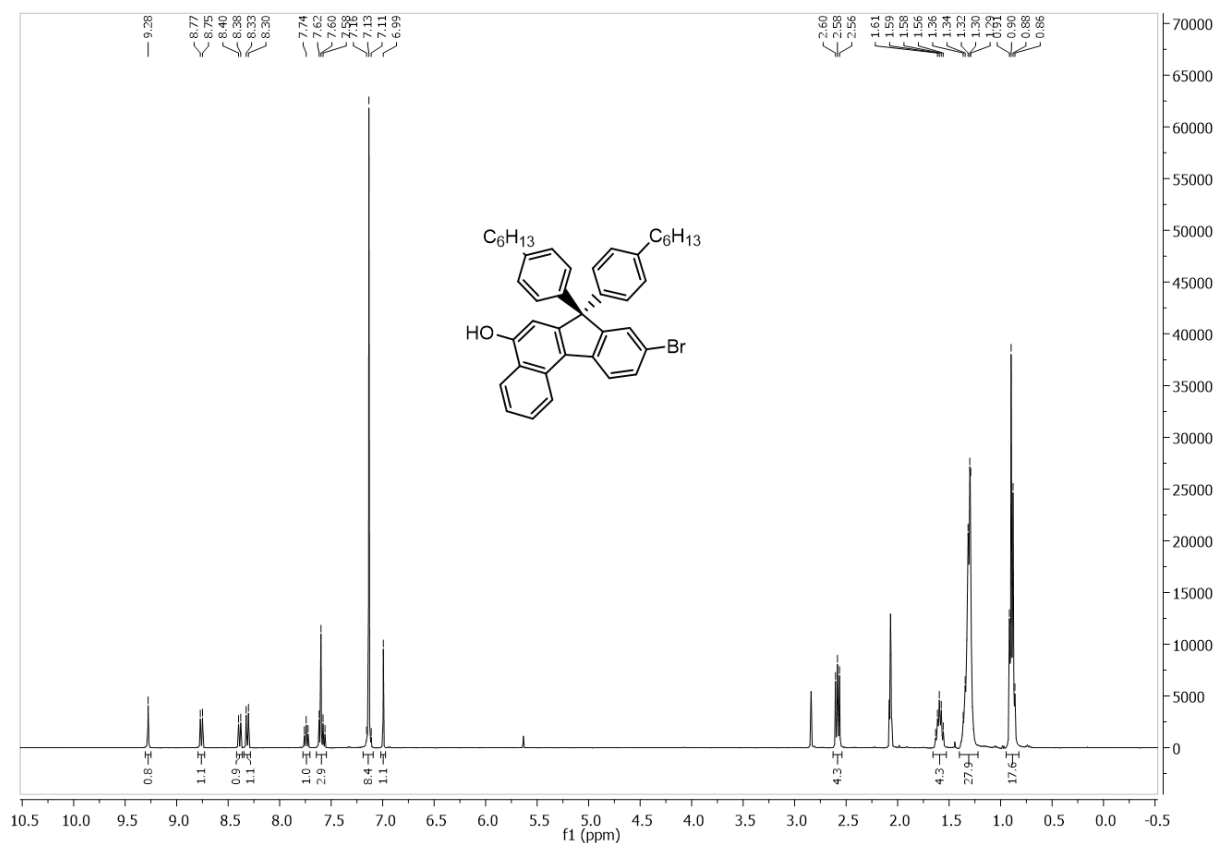
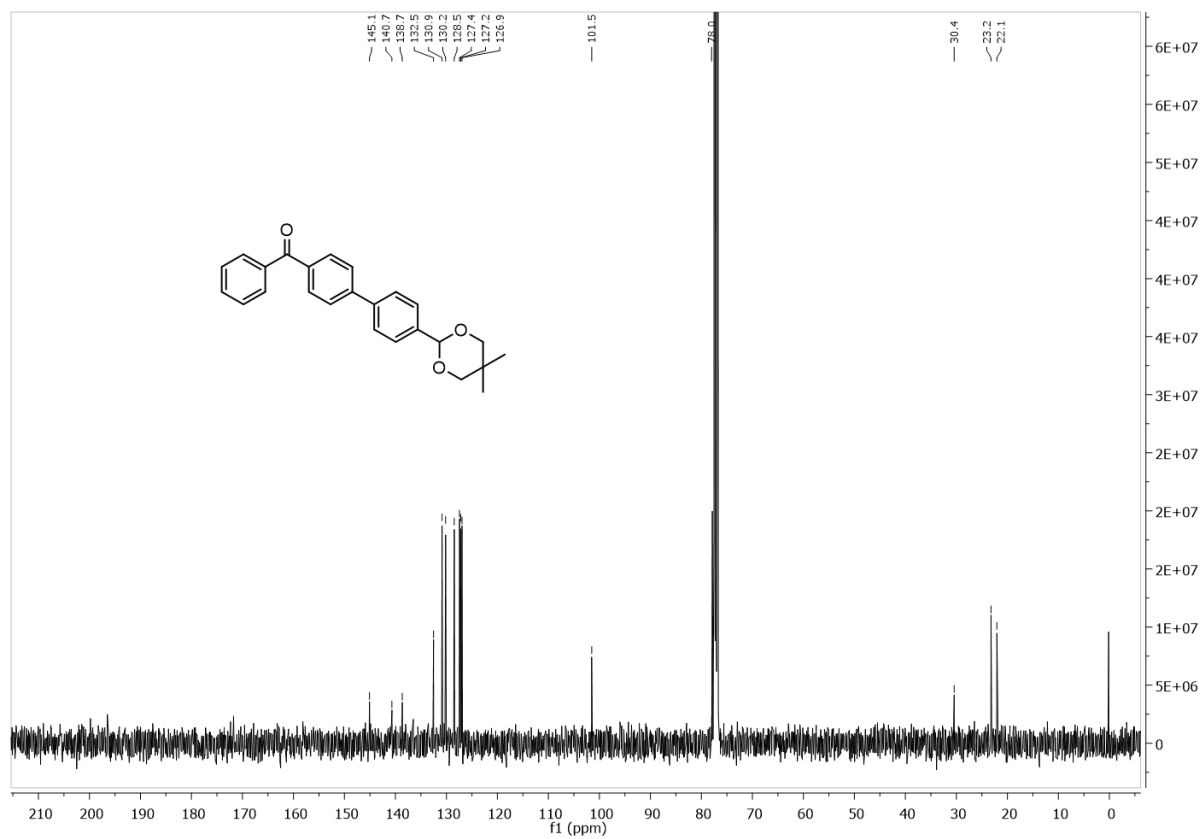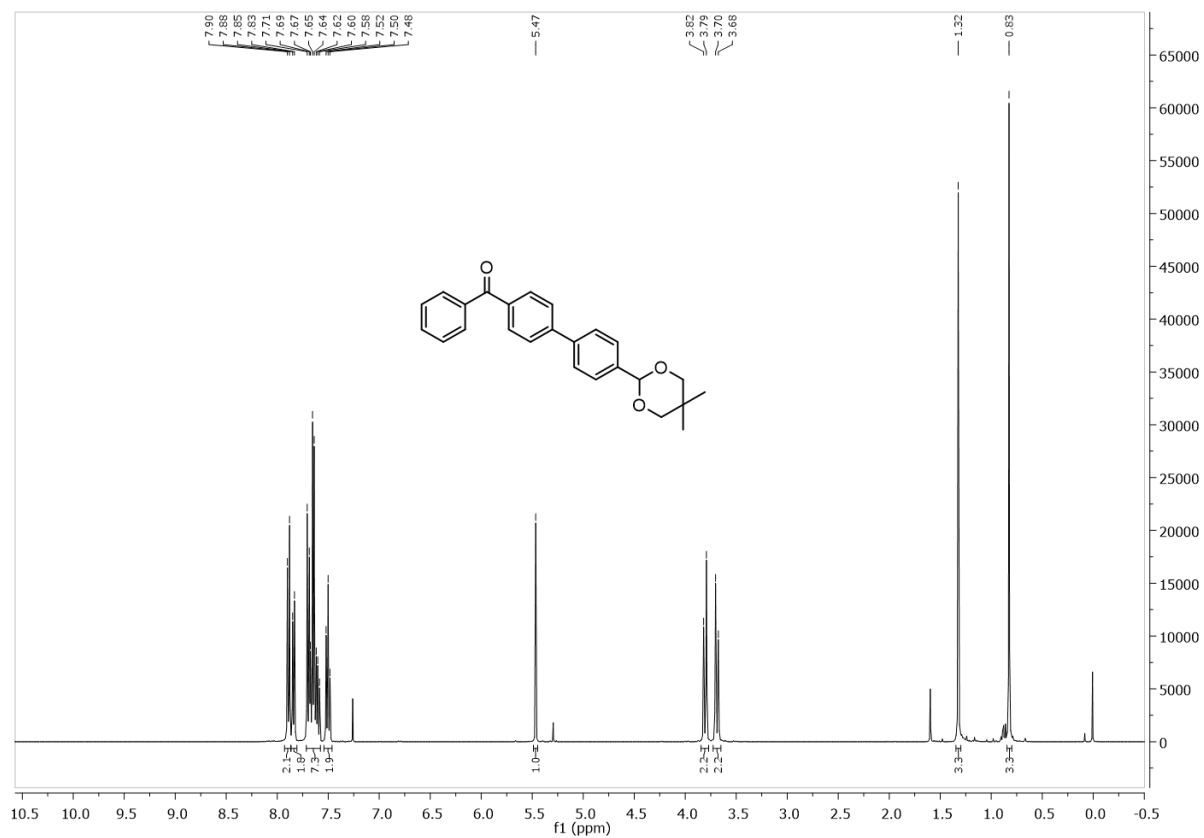^{1}H and ^{13}C spectra of **P2** in acetone (D6).
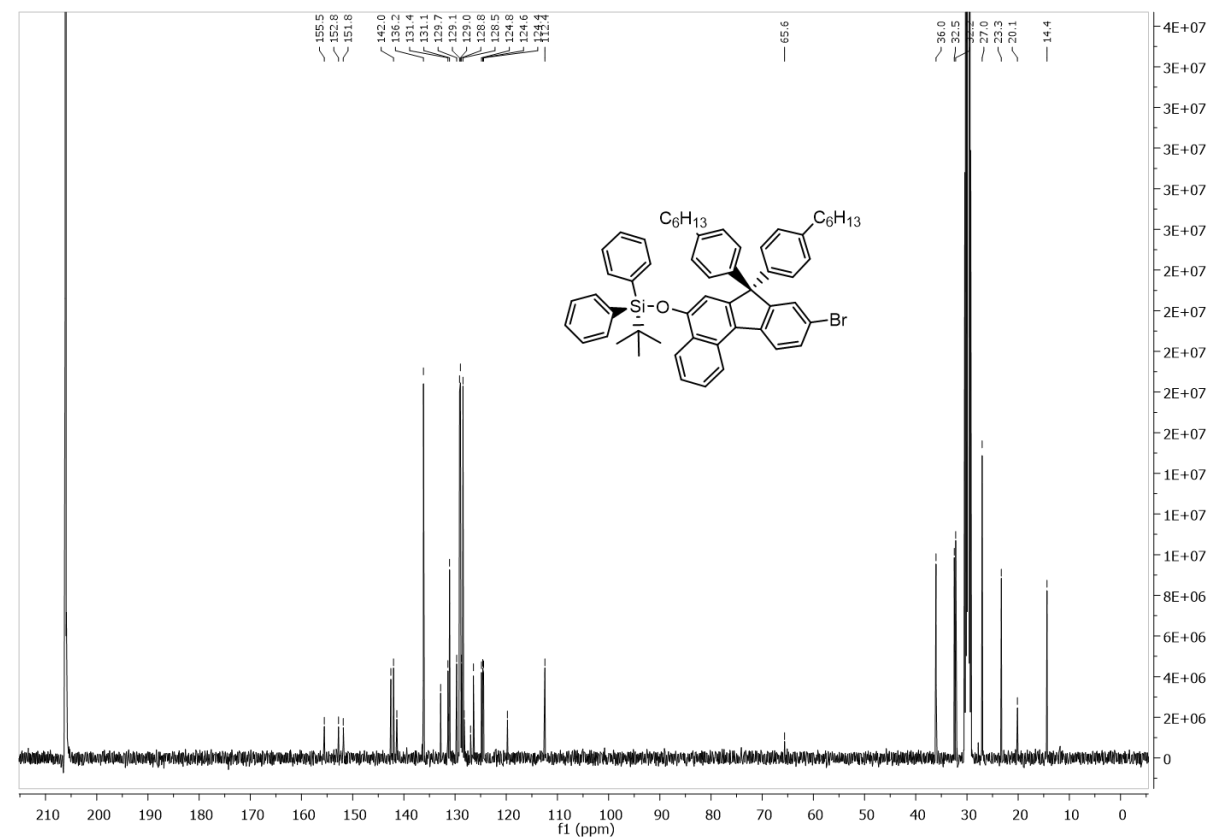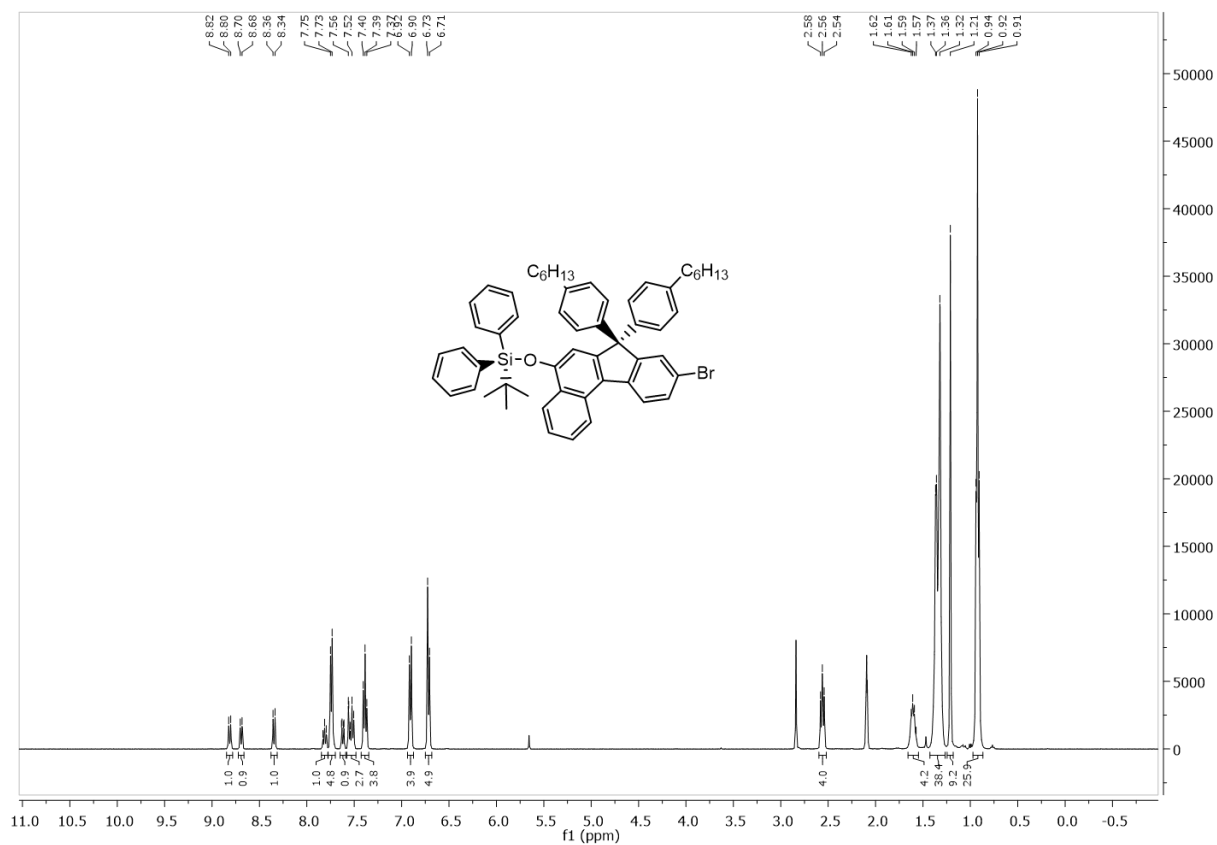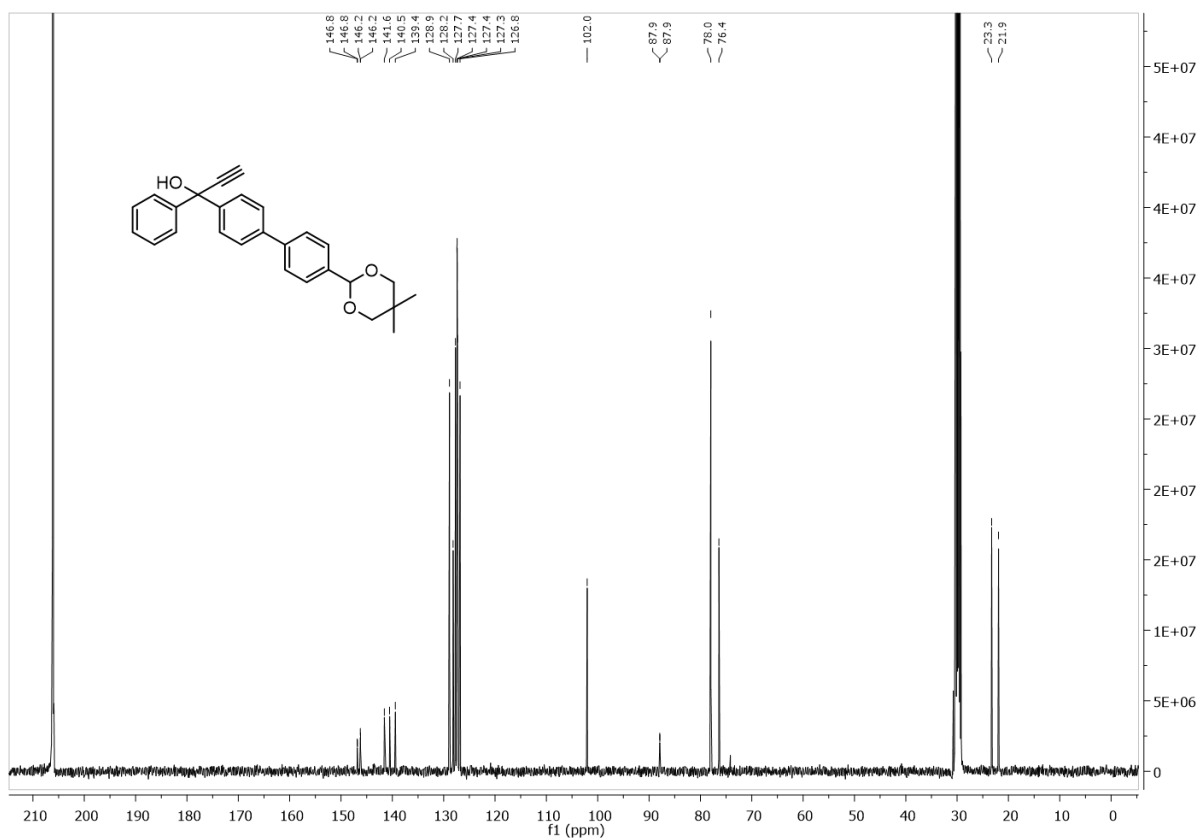
¹H and ¹³C spectra of **P3** in acetone (D6).
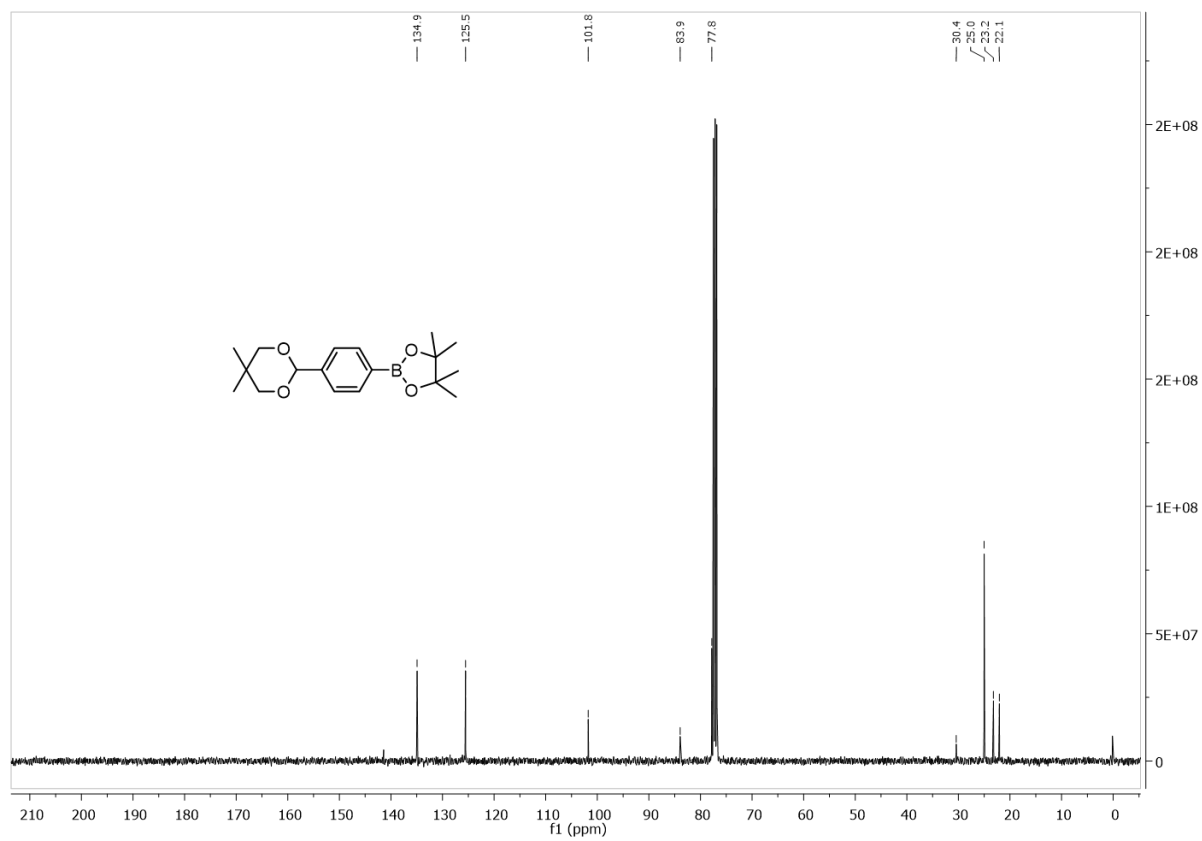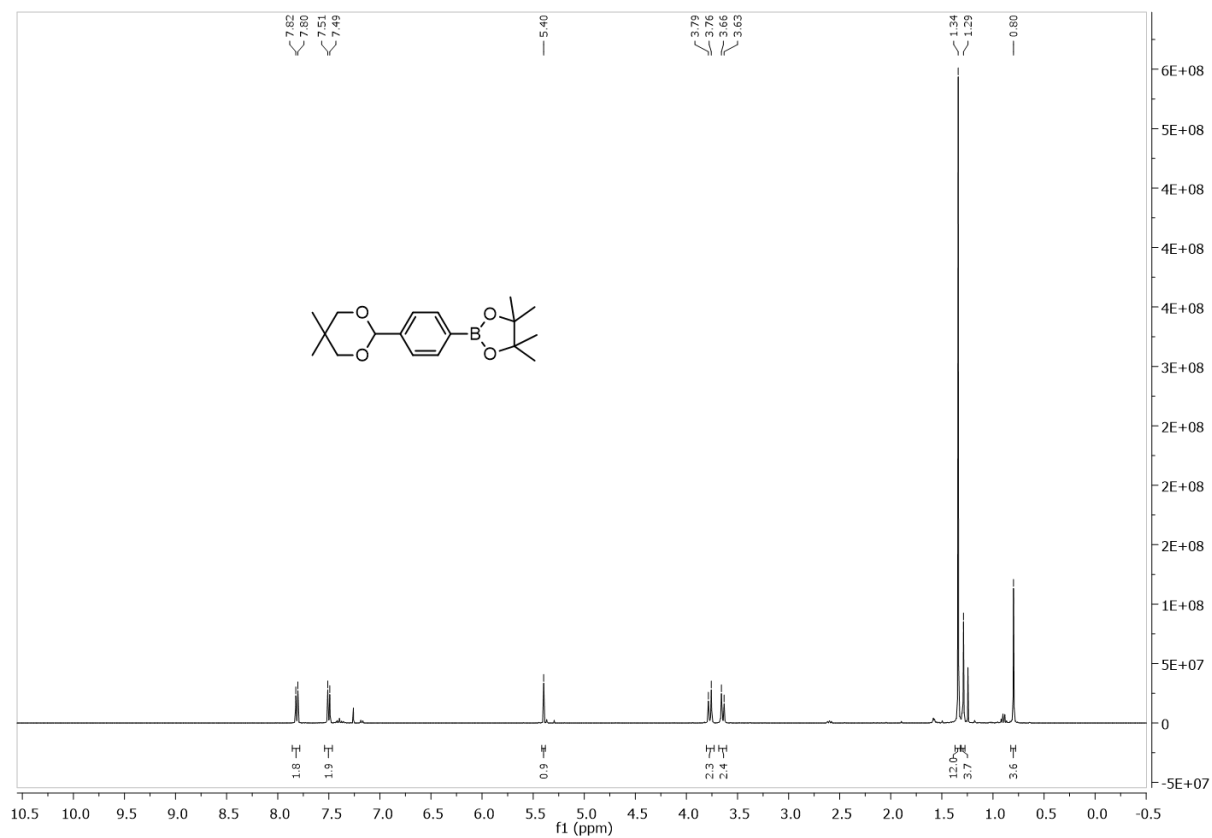
^{1}H and ^{13}C spectra of **A3** in chloroform (CDCl$_3$).

^{1}H and ^{13}C spectra of **A4** in chloroform (CDCl$_3$).
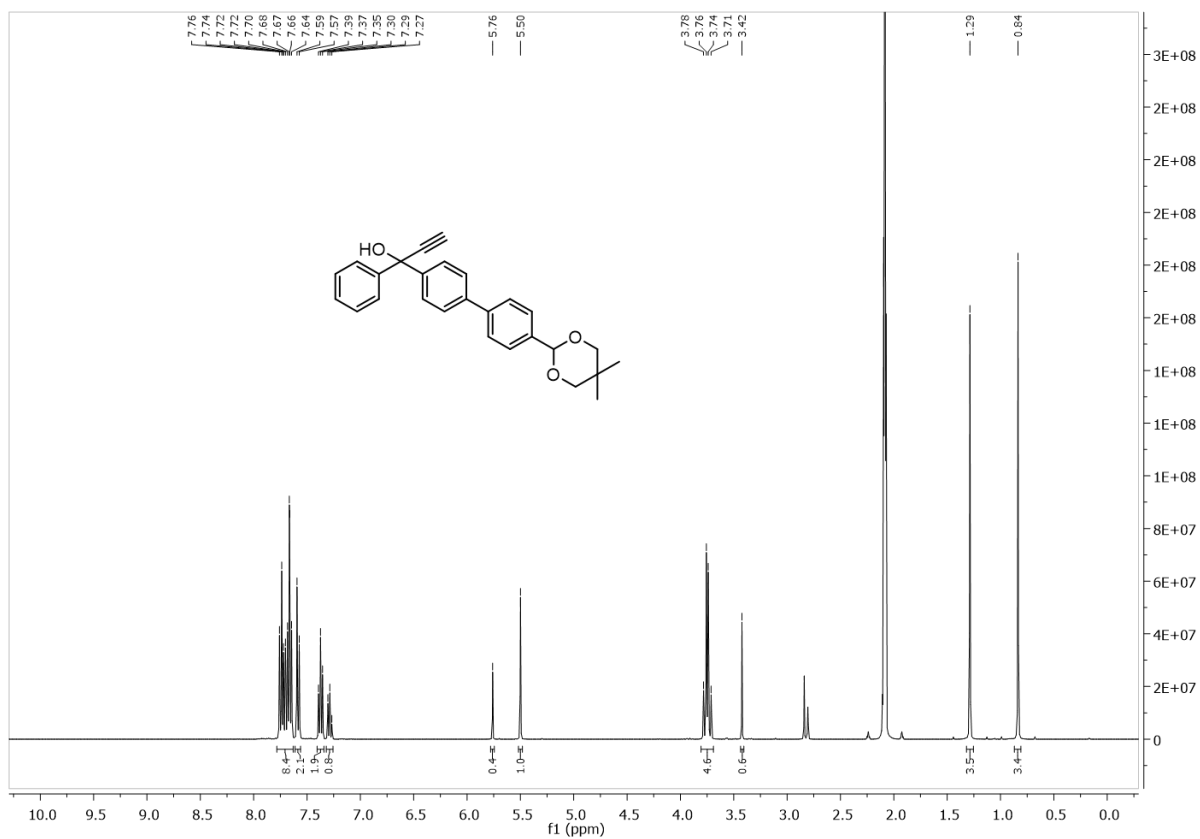
^{1}H and ^{13}C spectra of **A5** in acetone (D6).
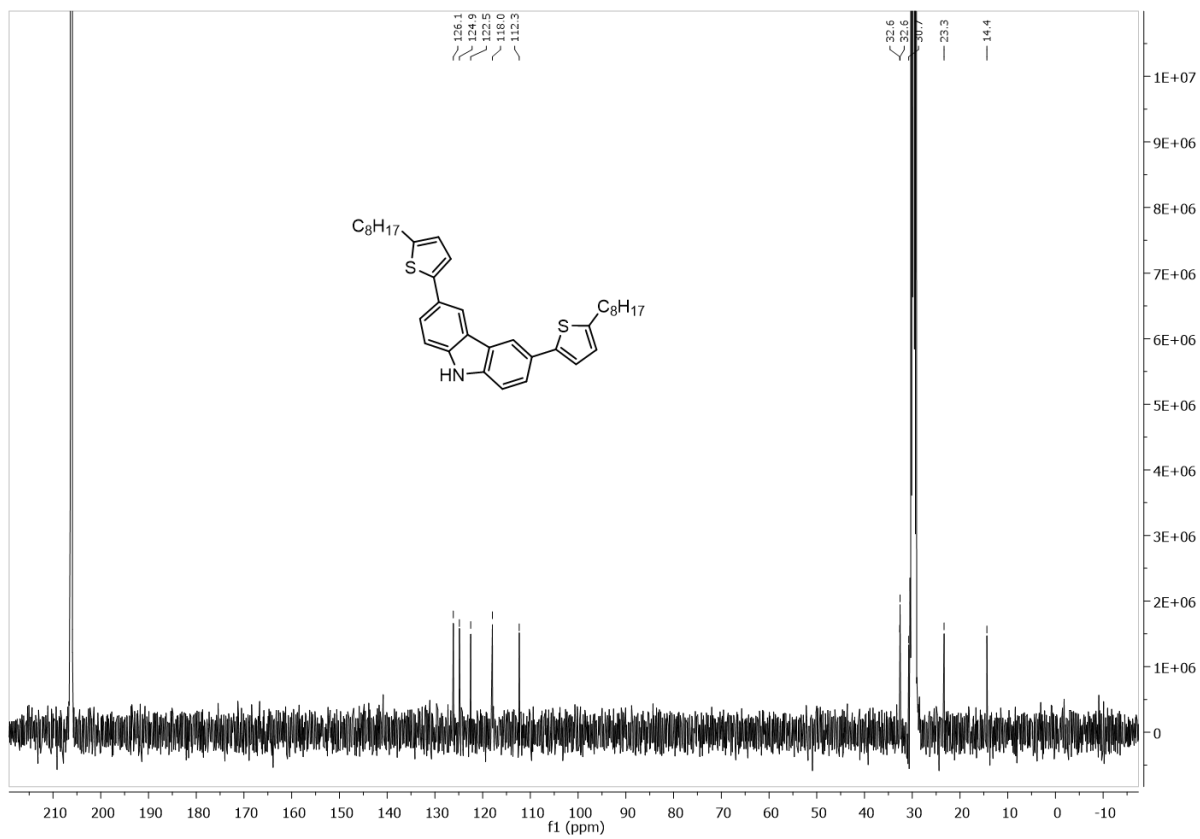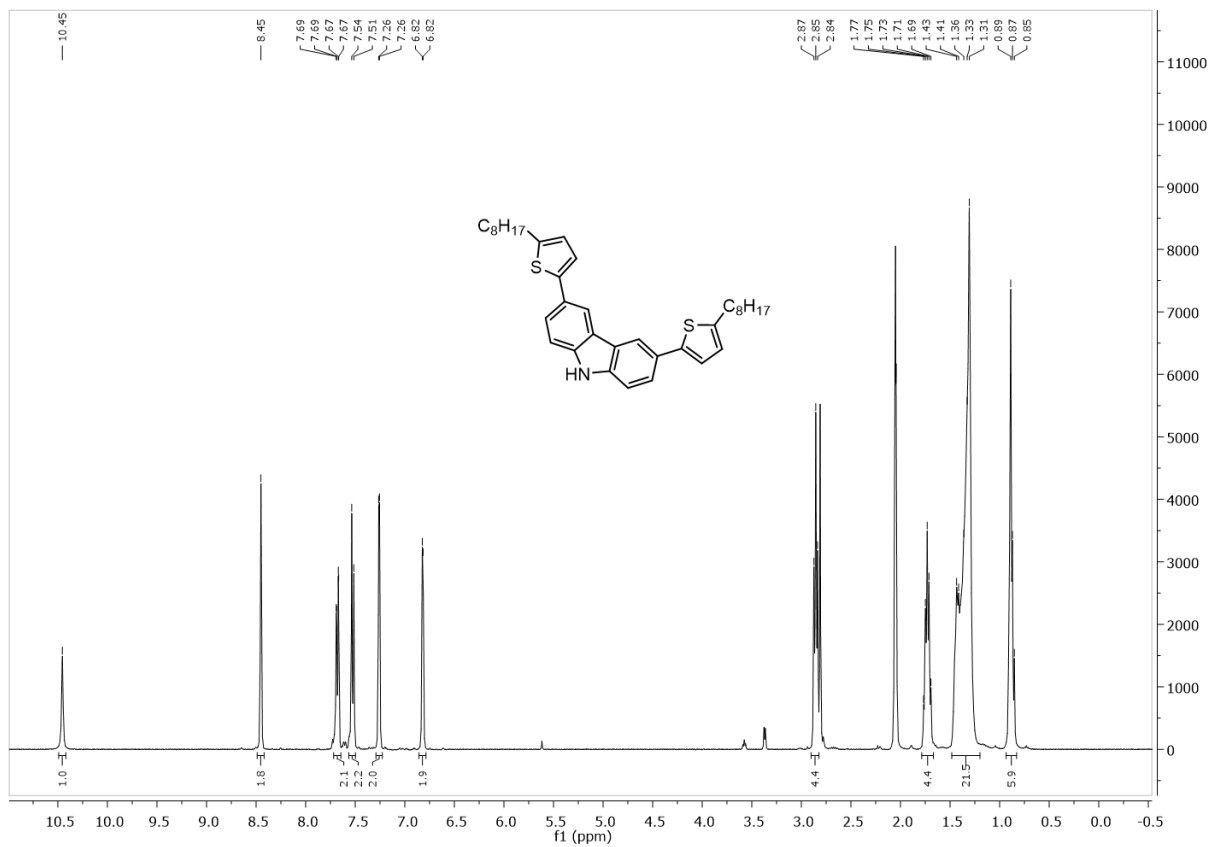
^{1}H and ^{13}C spectra of **C2** in acetone (D6).
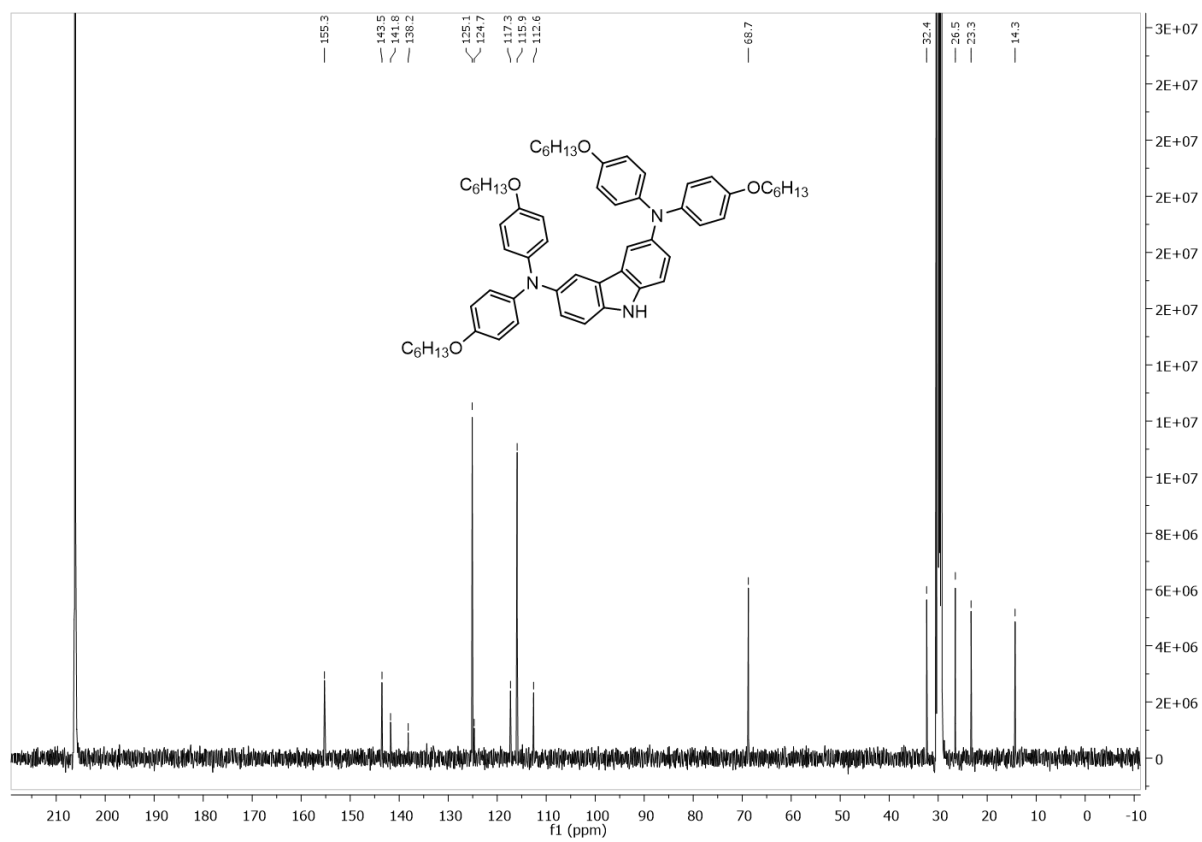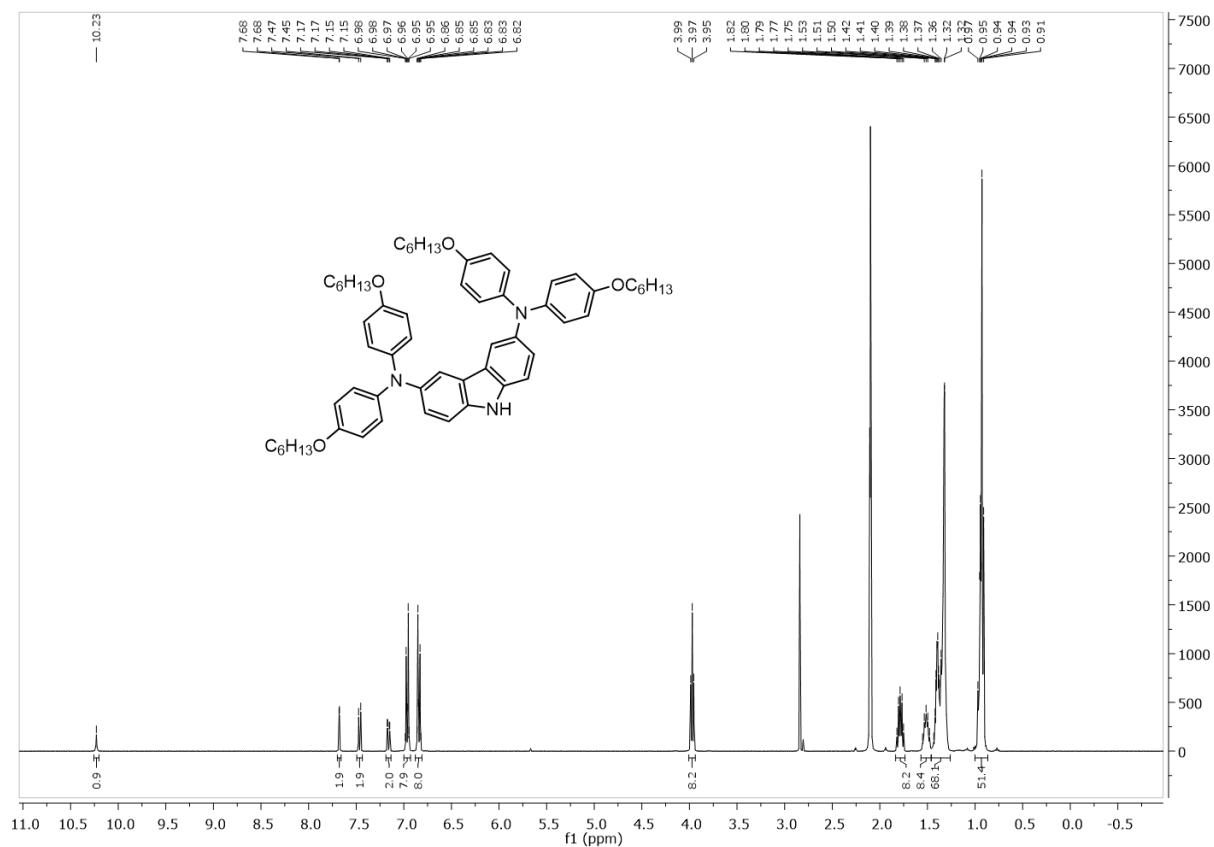
^{1}H and ^{13}C spectra of **C5** in acetone (D6).

^{1}H and ^{13}C spectra of **Y1** in acetone (D6).
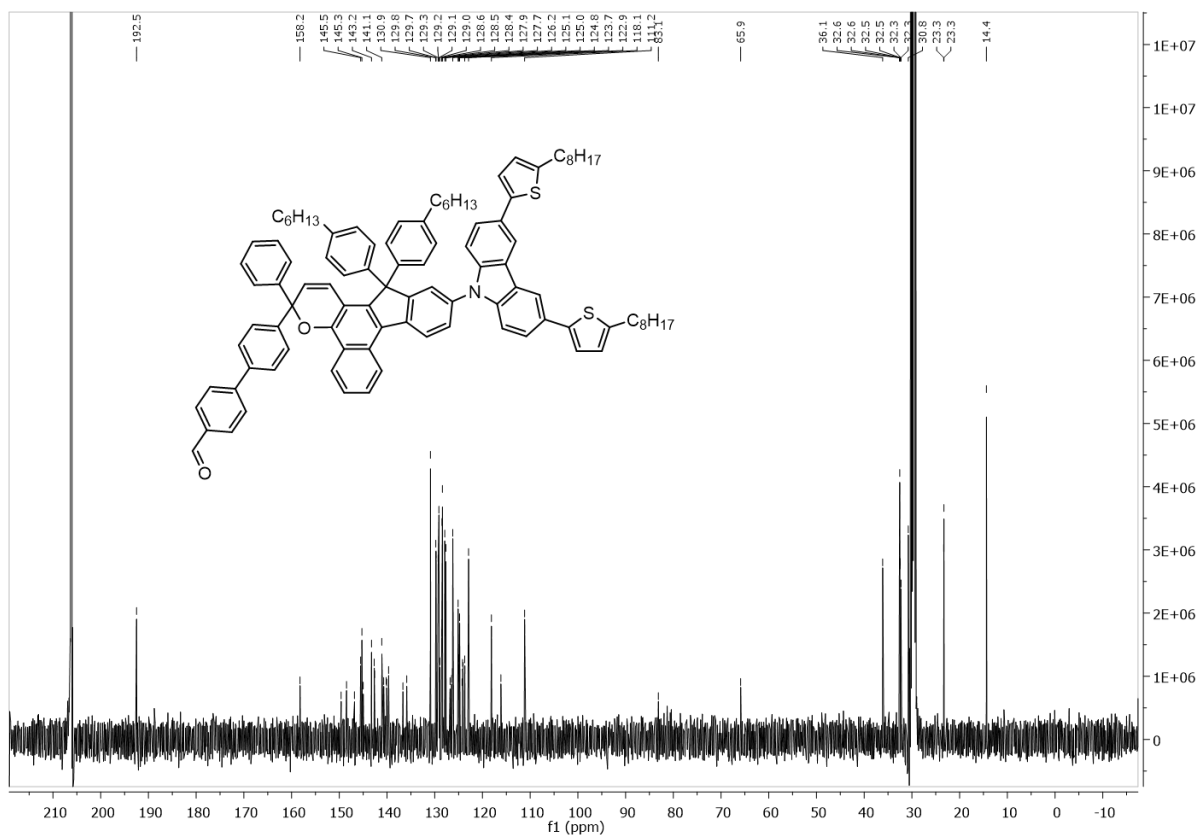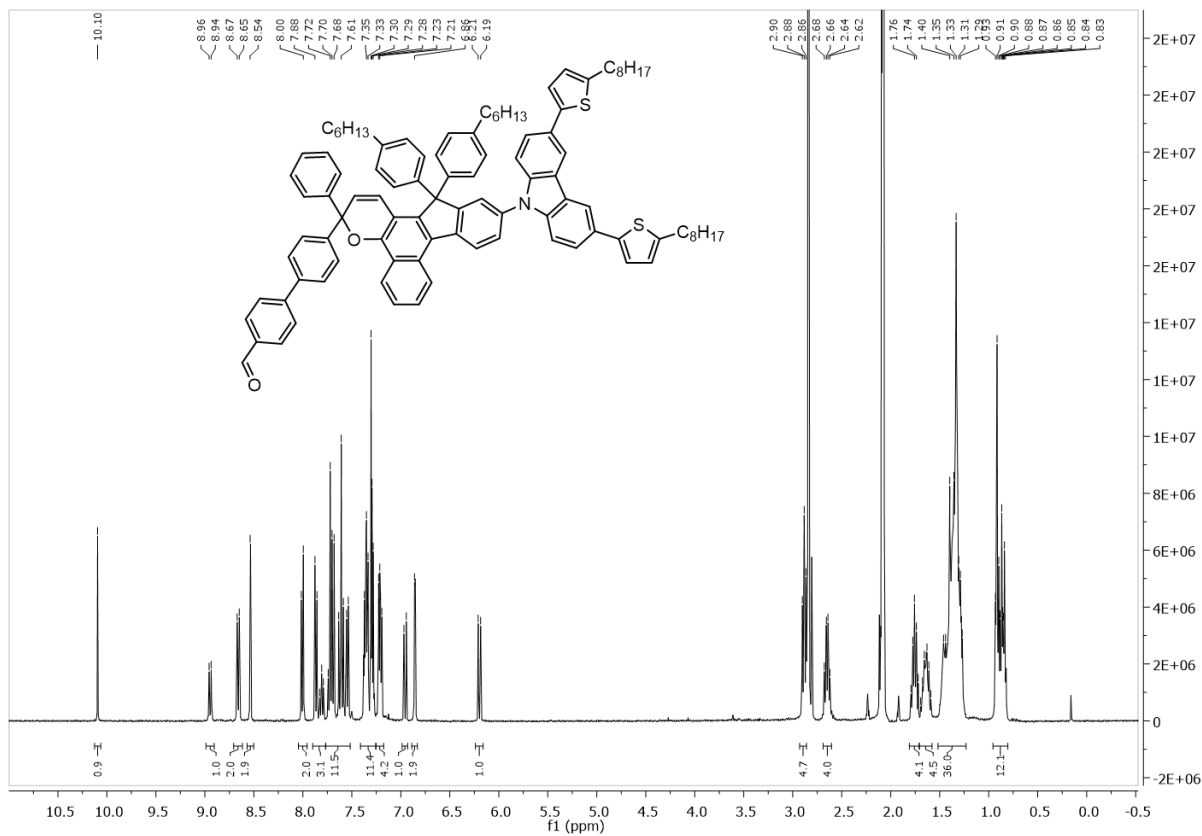
^{1}H and ^{13}C spectra of **Y2** in acetone (D6).
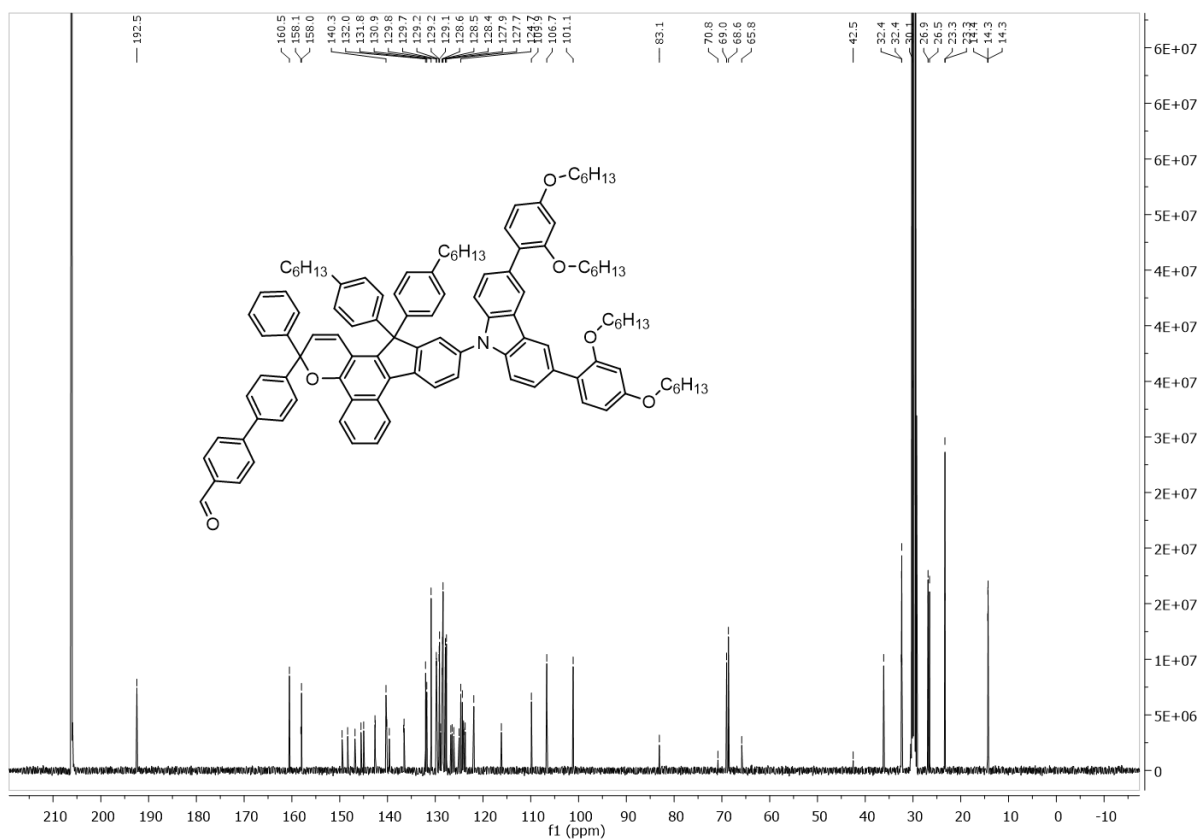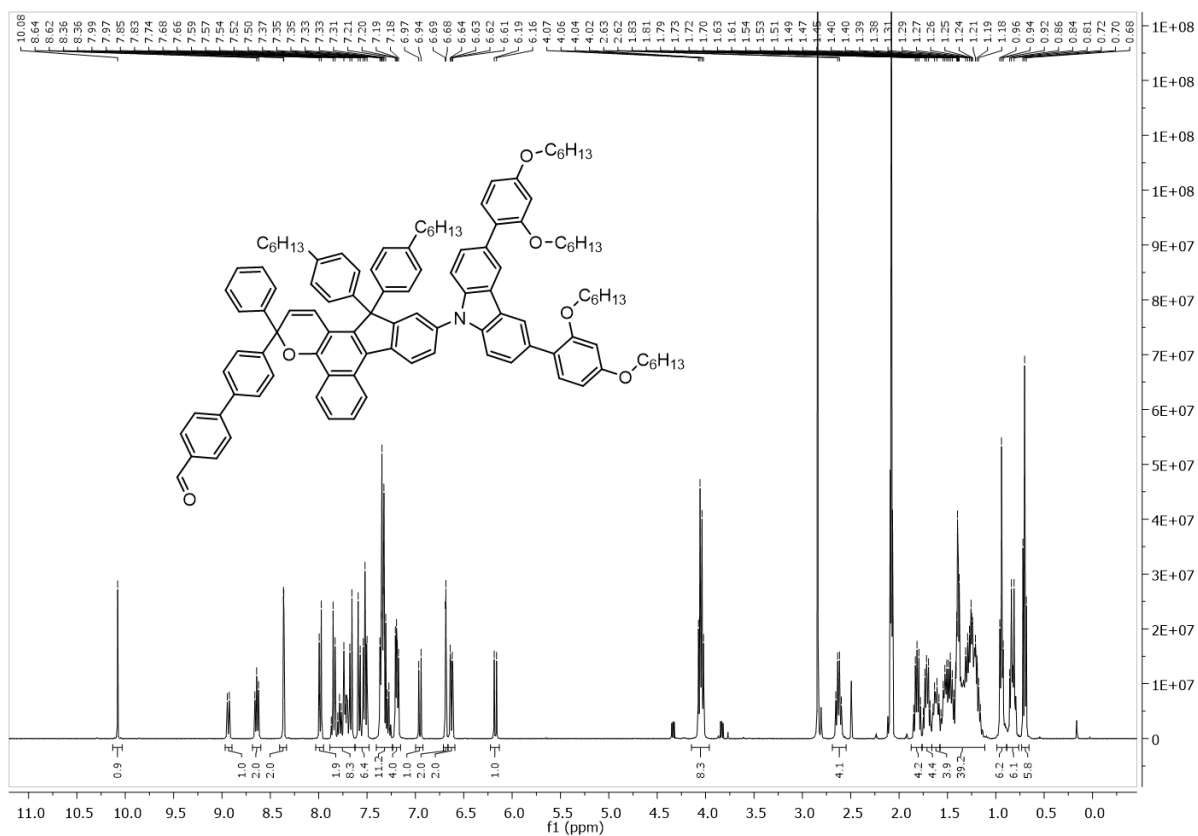
^{1}H and ^{13}C spectra of **Y3** in acetone (D6).
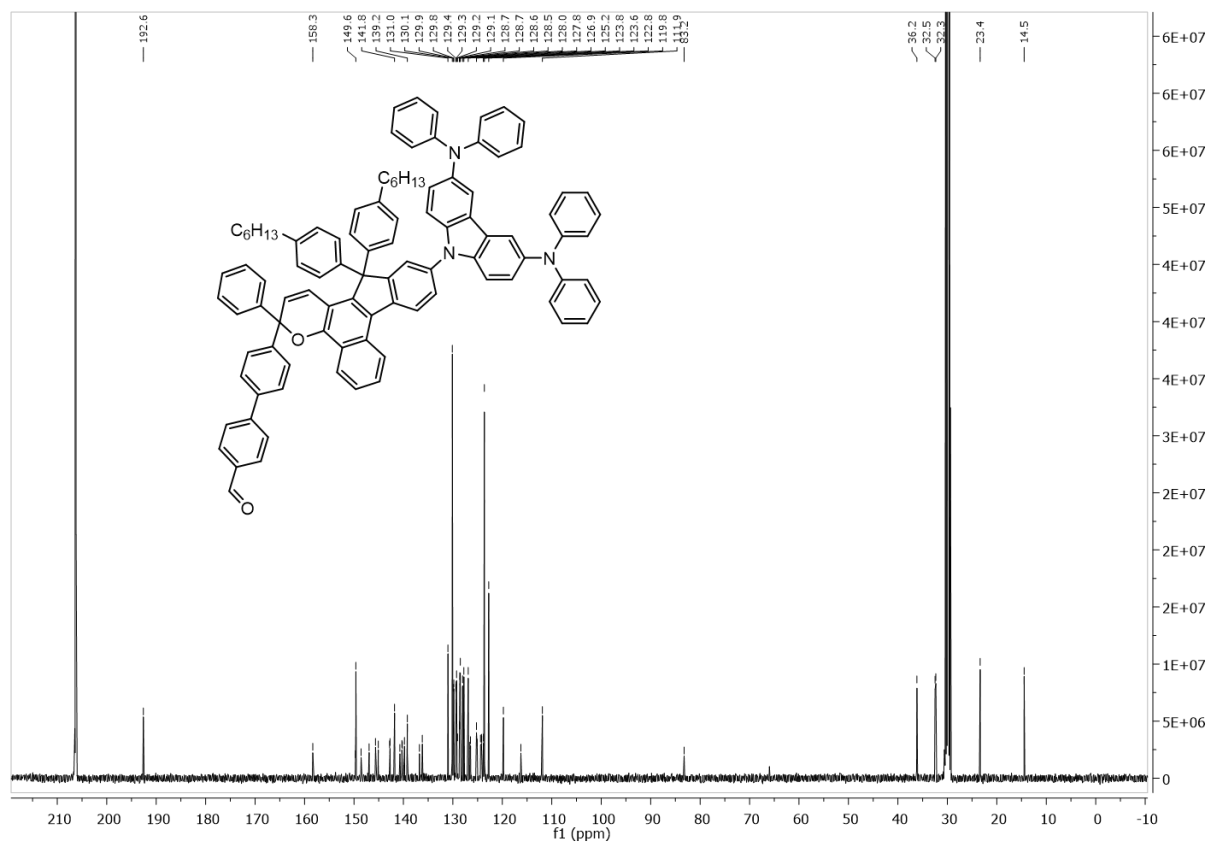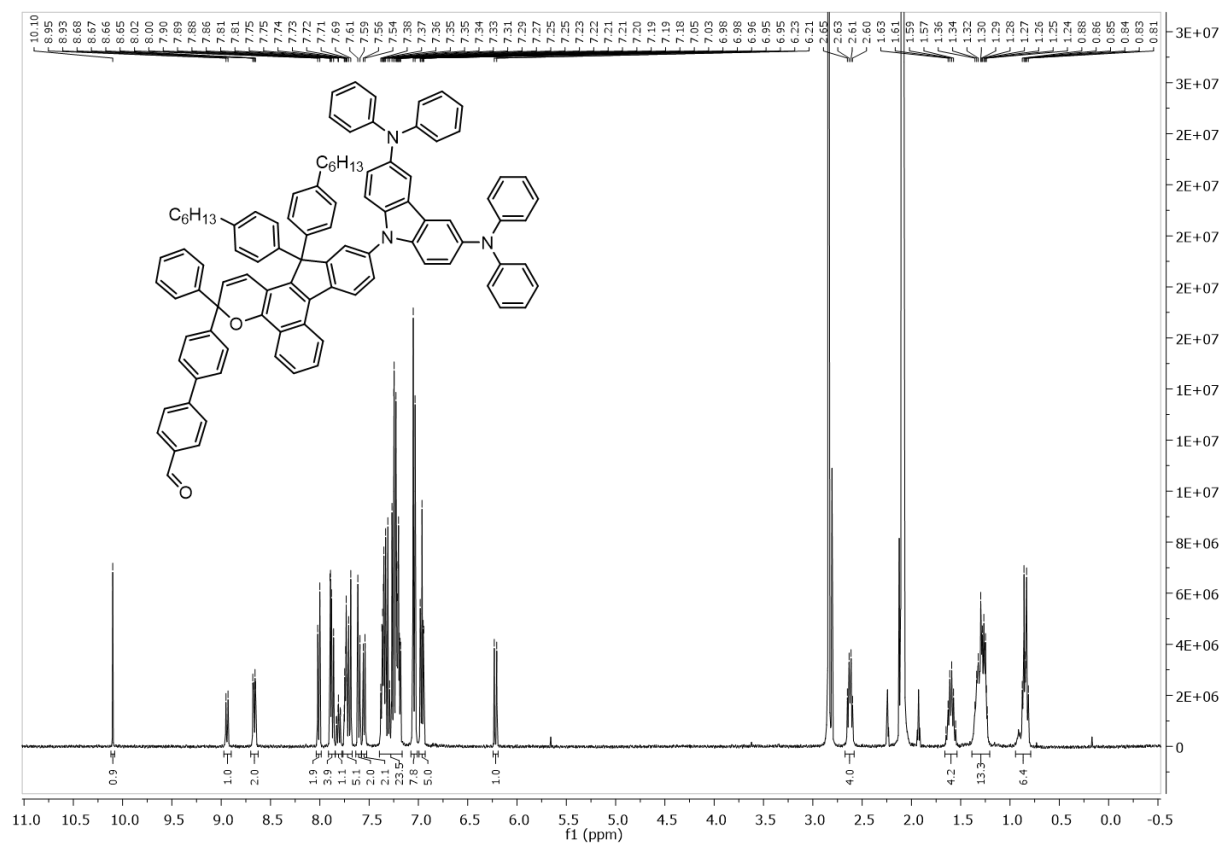
^{1}H and ^{13}C spectra of **Y4** in acetone (D6).
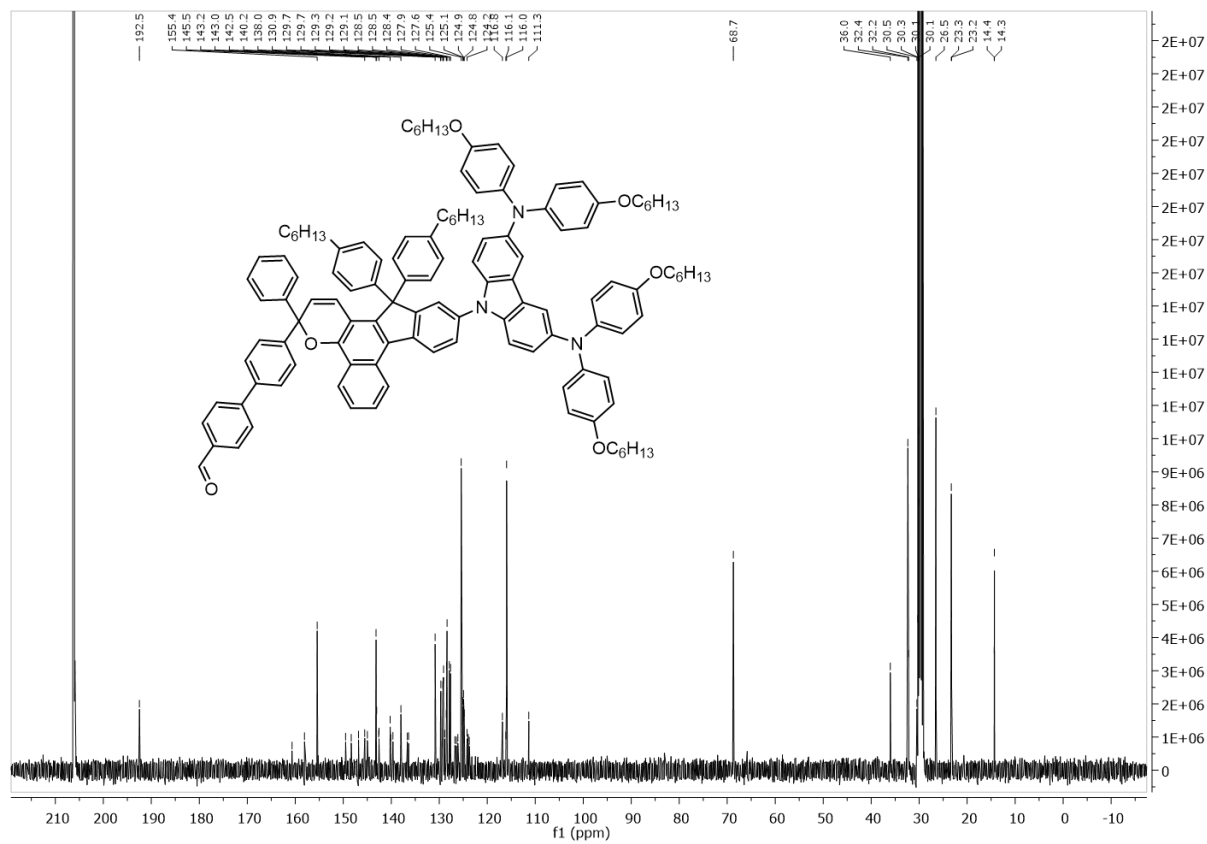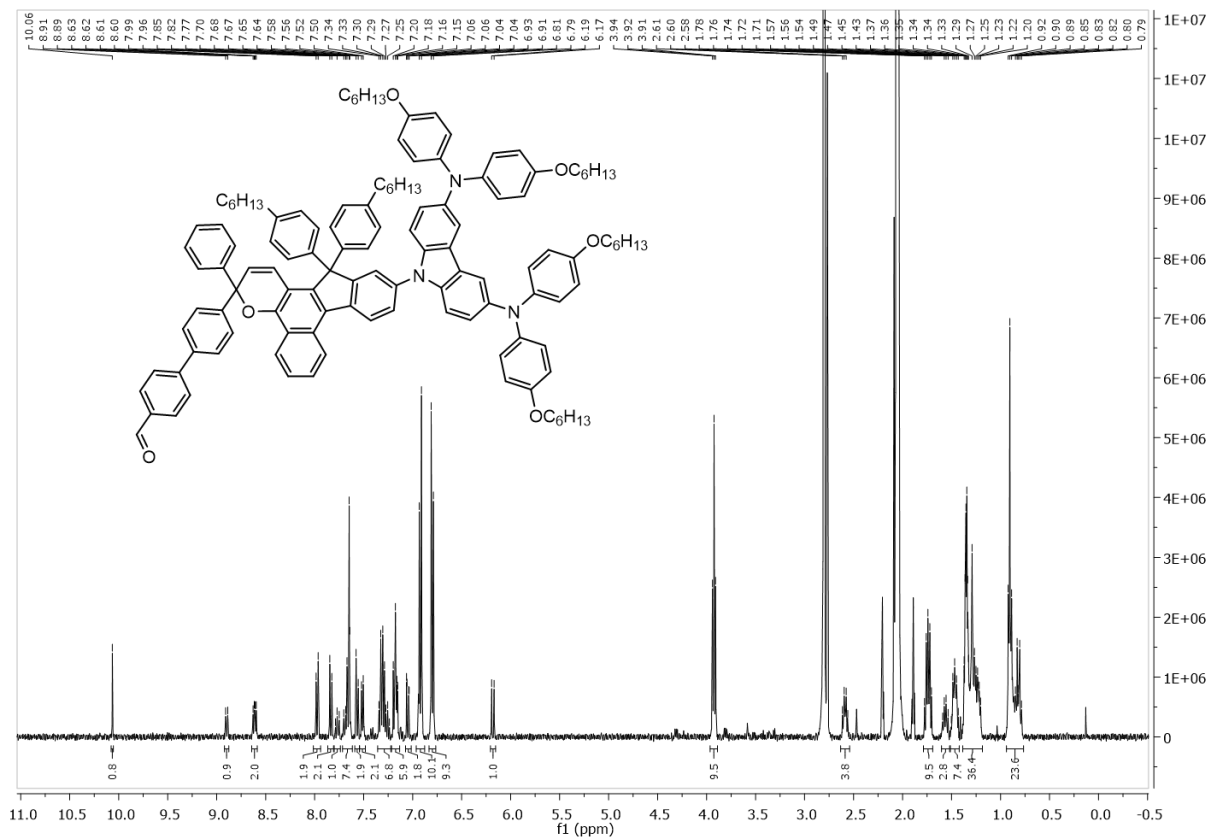
^{1}H and ^{13}C spectra of **Y5** in acetone (D6).
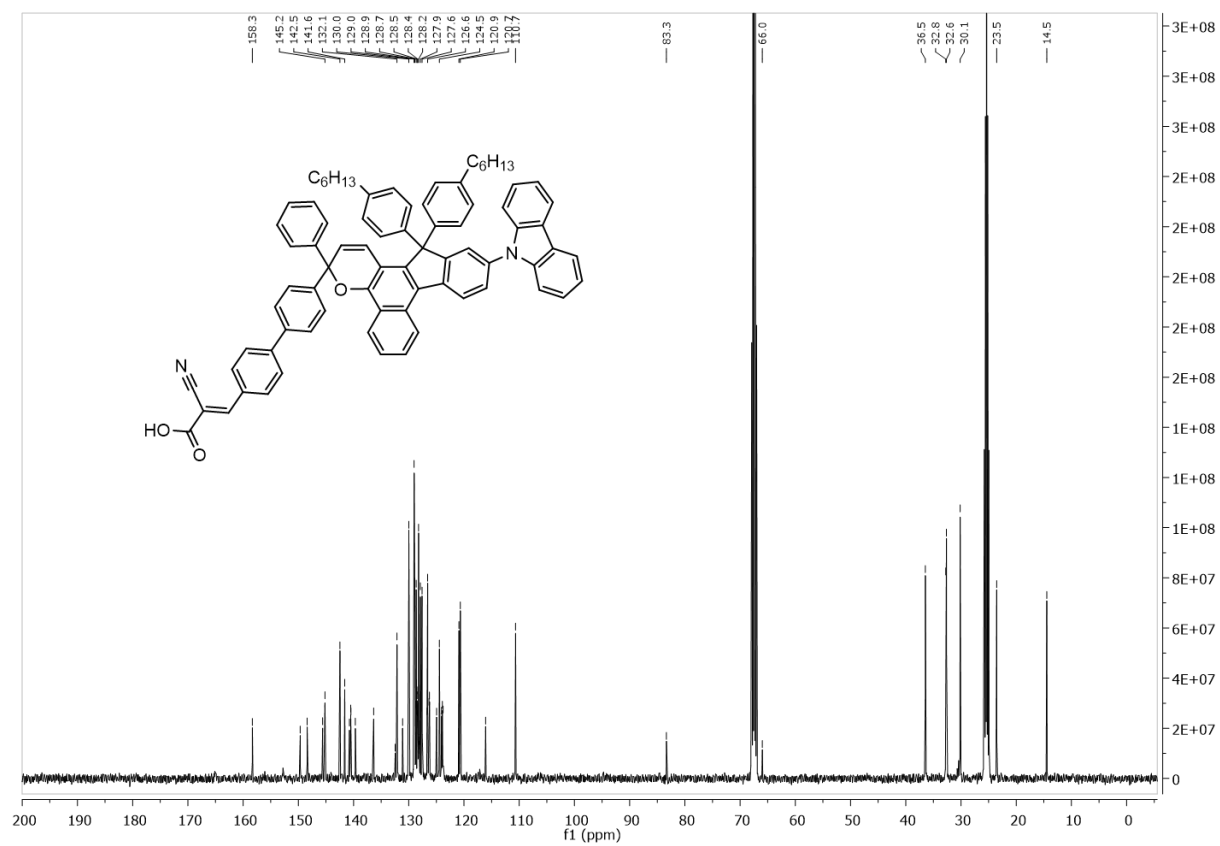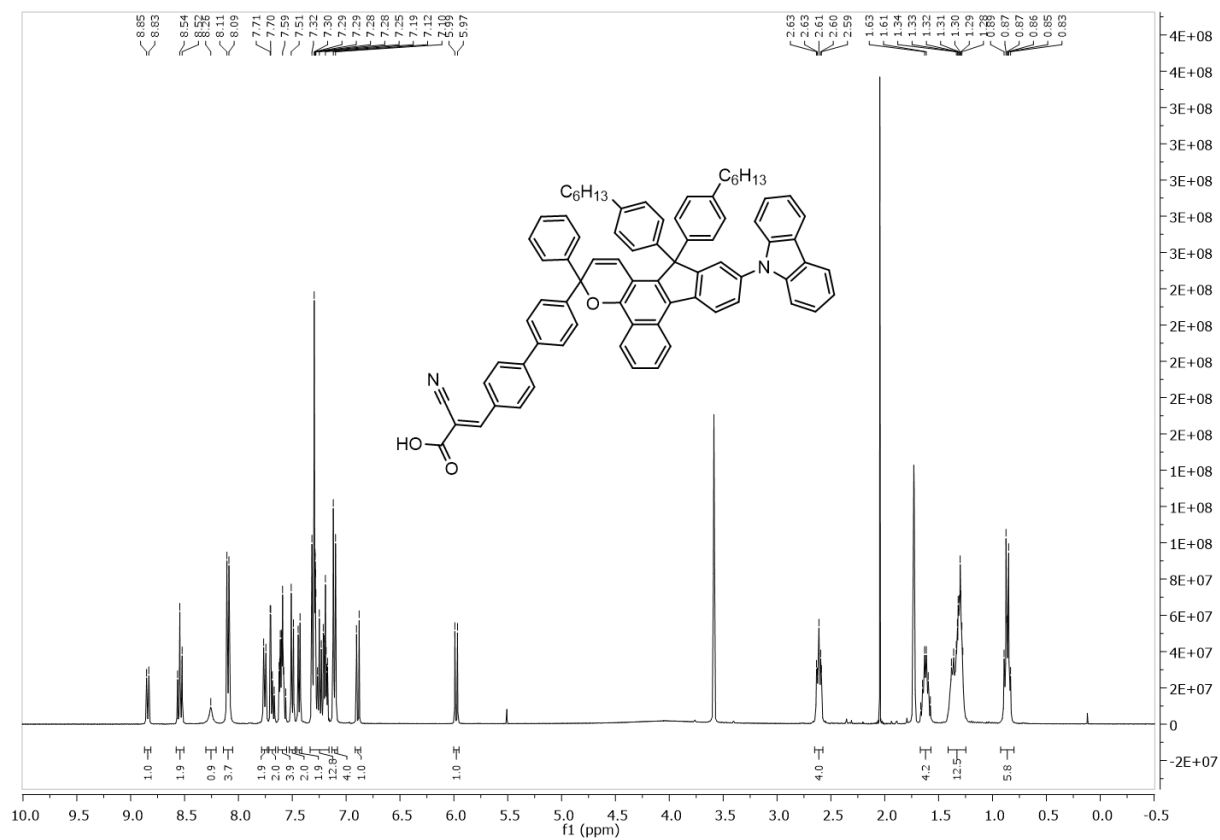
^{1}H and ^{13}C spectra of **SF1** in THF (D8).
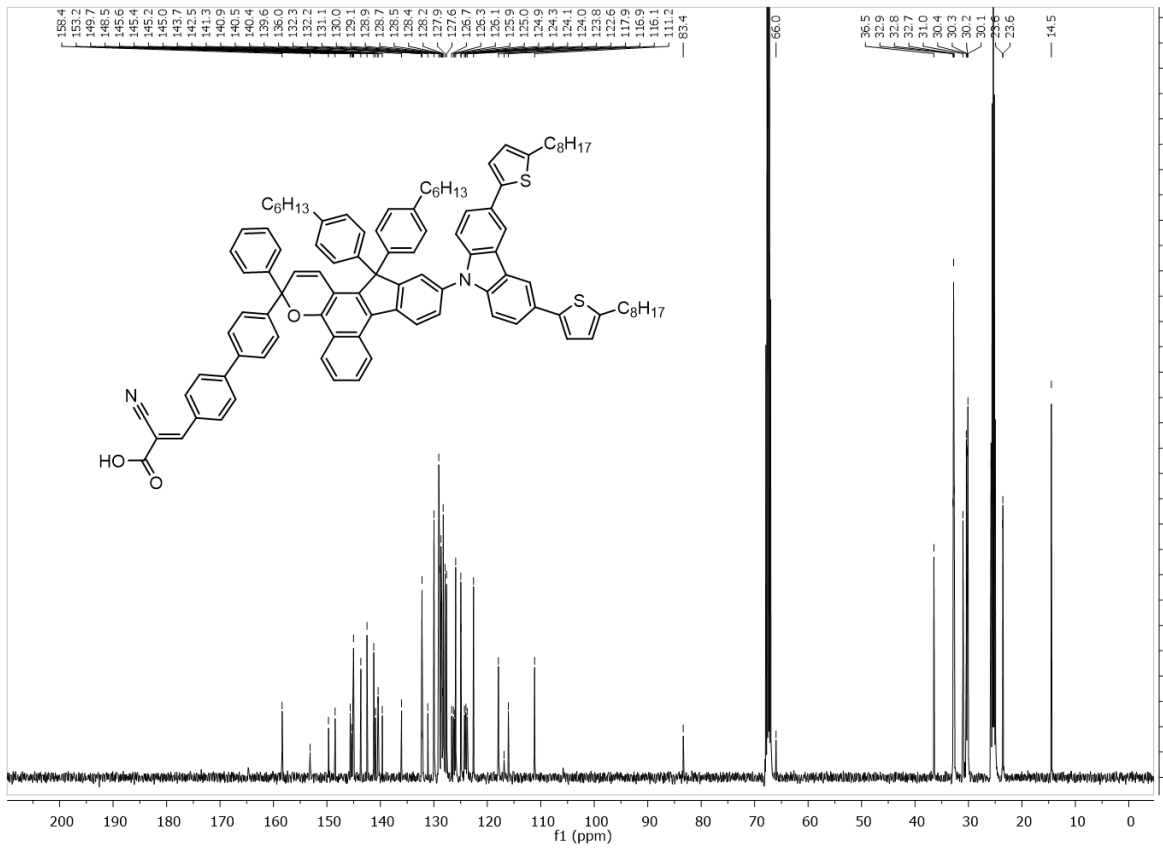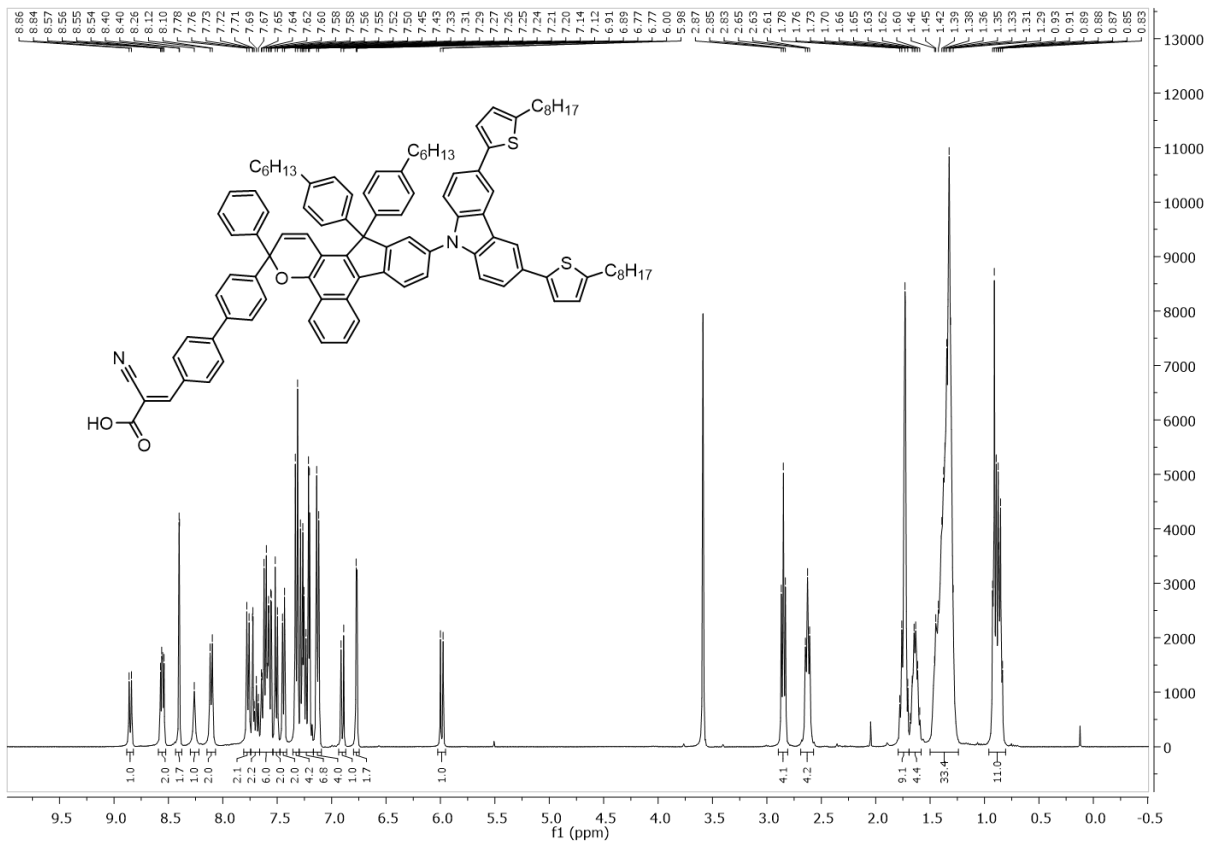
^{1}H and ^{13}C spectra of **SF2** in THF (D8).
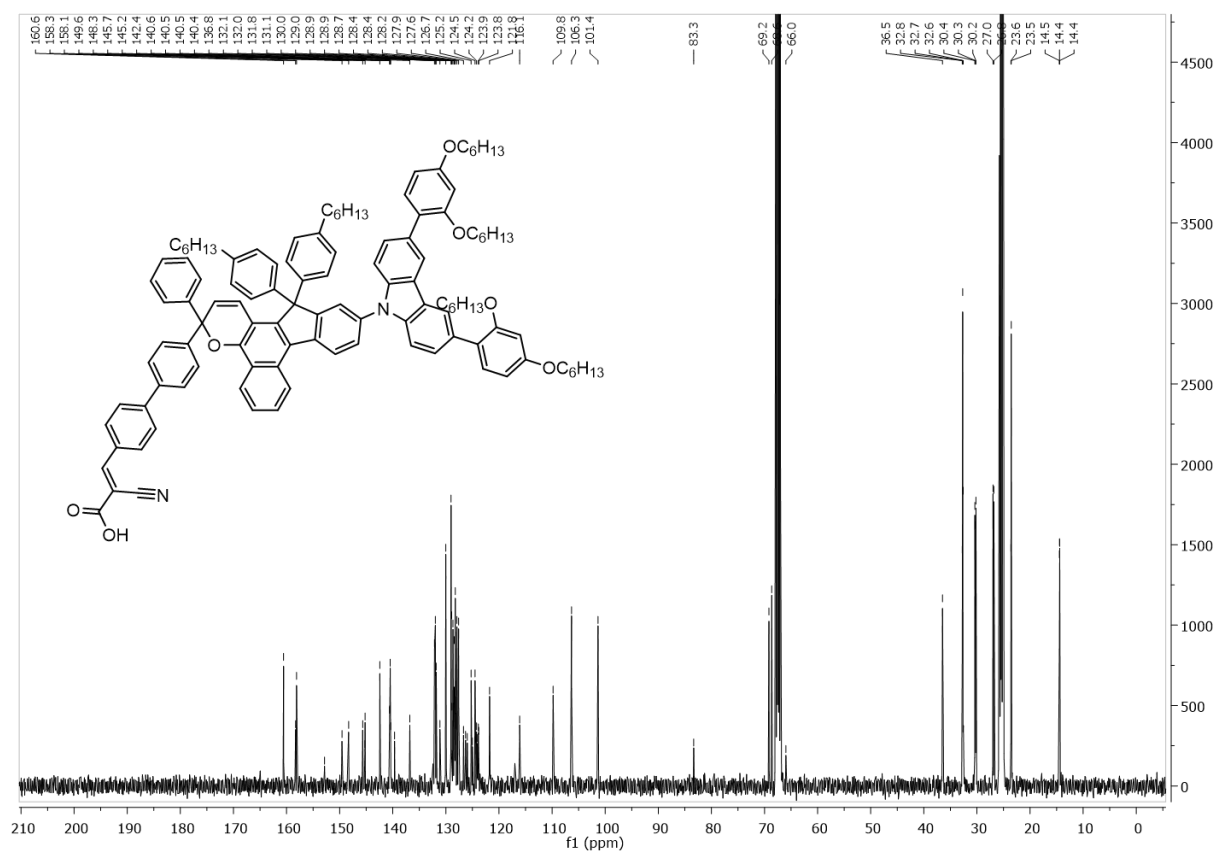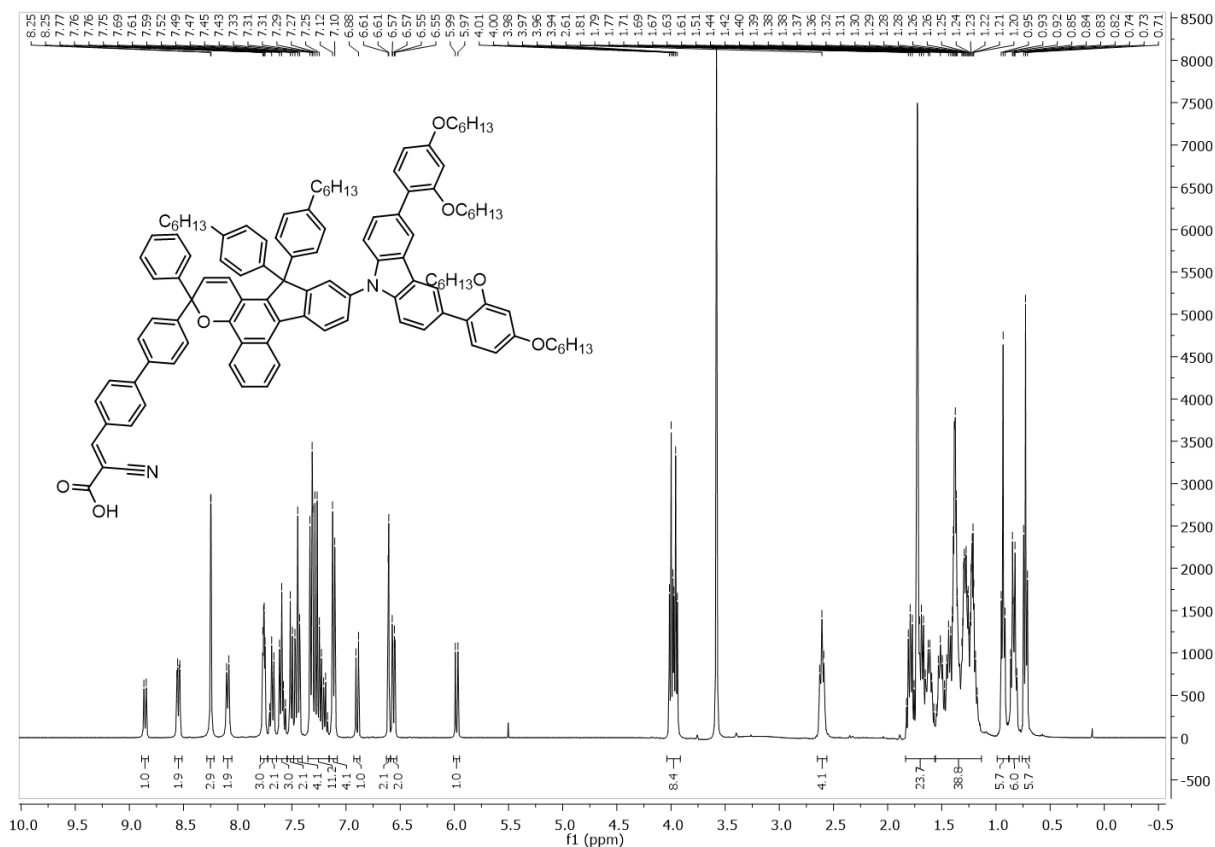
^{1}H and ^{13}C spectra of **SF3** in THF (D8).
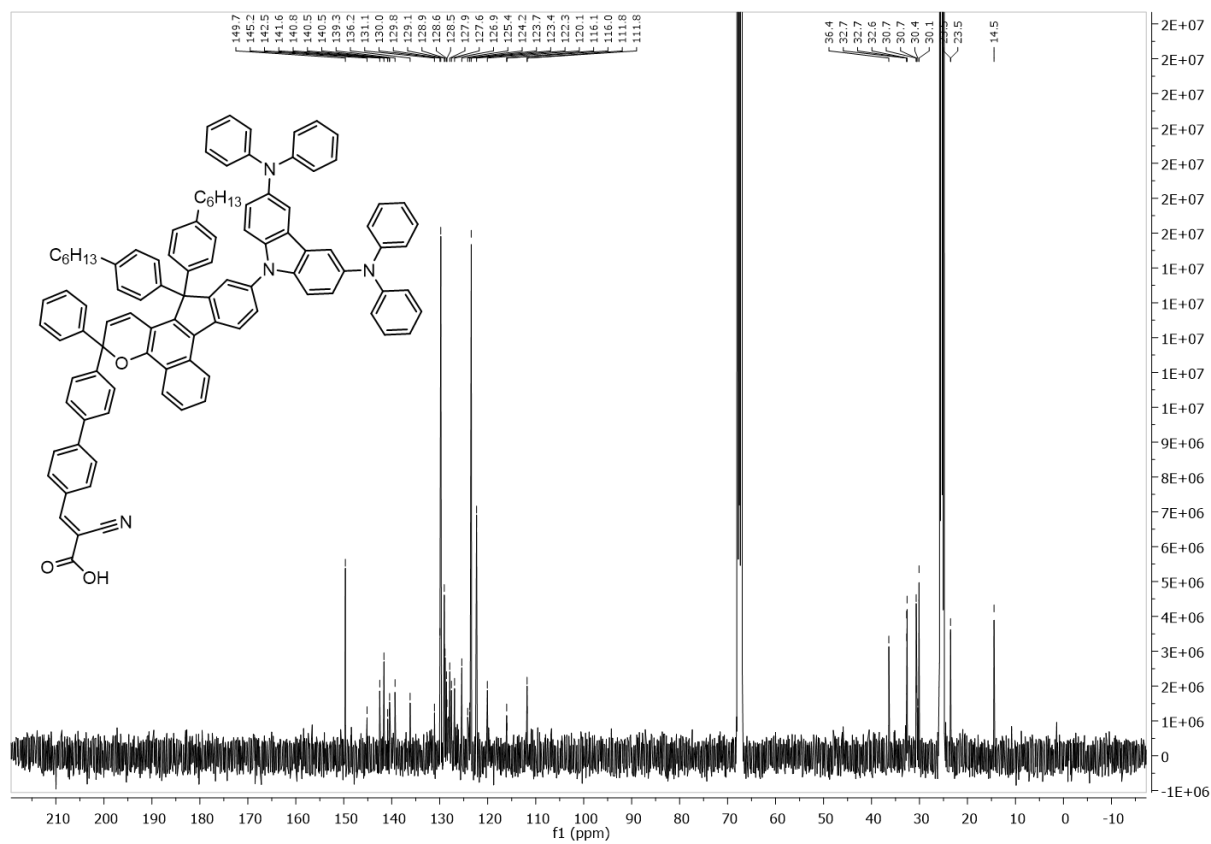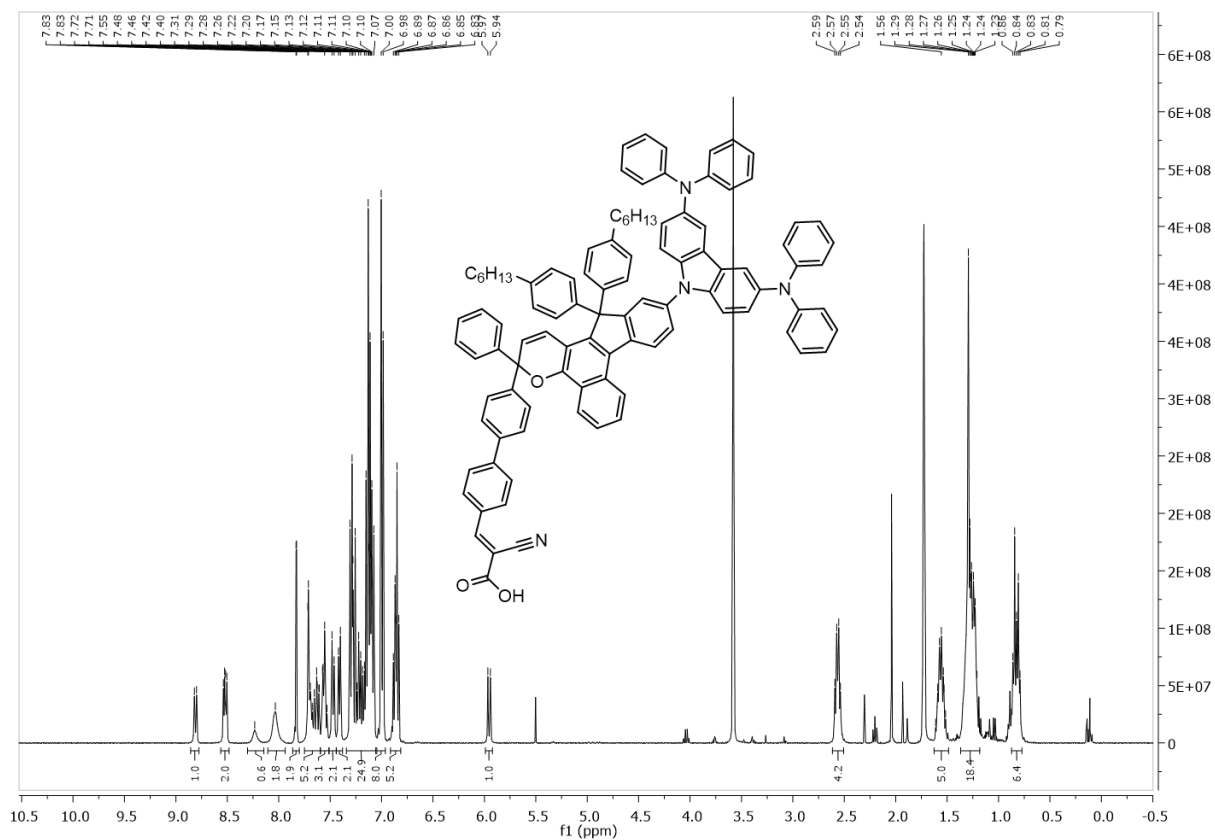
^{1}H and ^{13}C spectra of **SF4** in THF (D8).
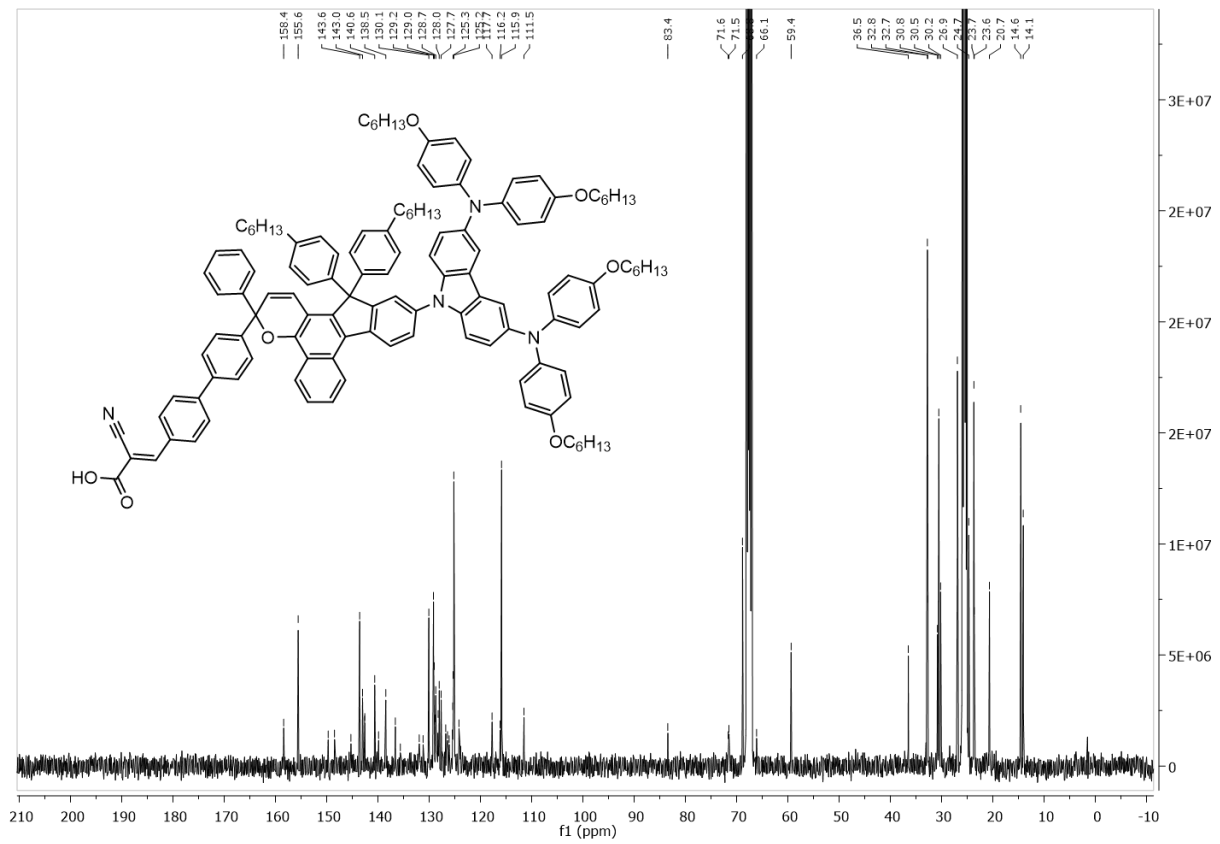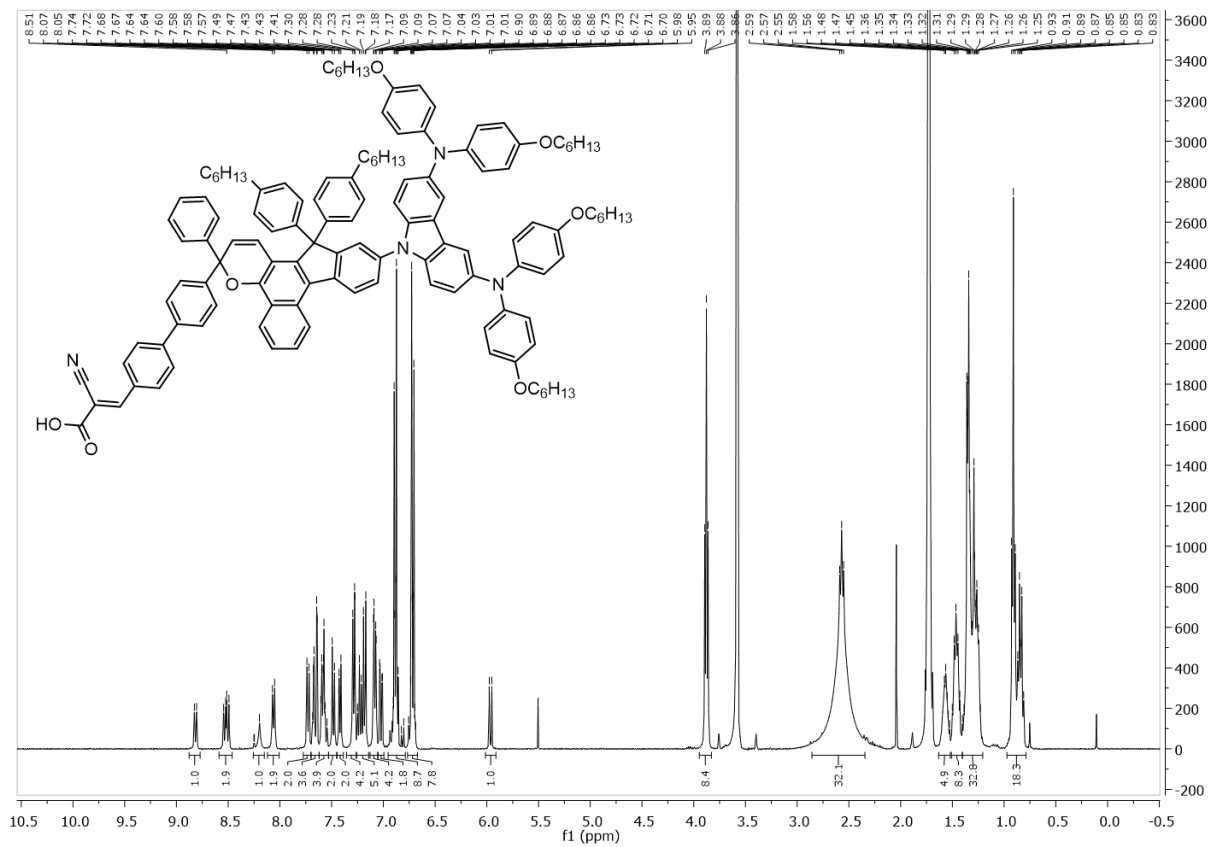
^{1}H and ^{13}C spectra of **SF5** in THF (D8).

Closing kinetic
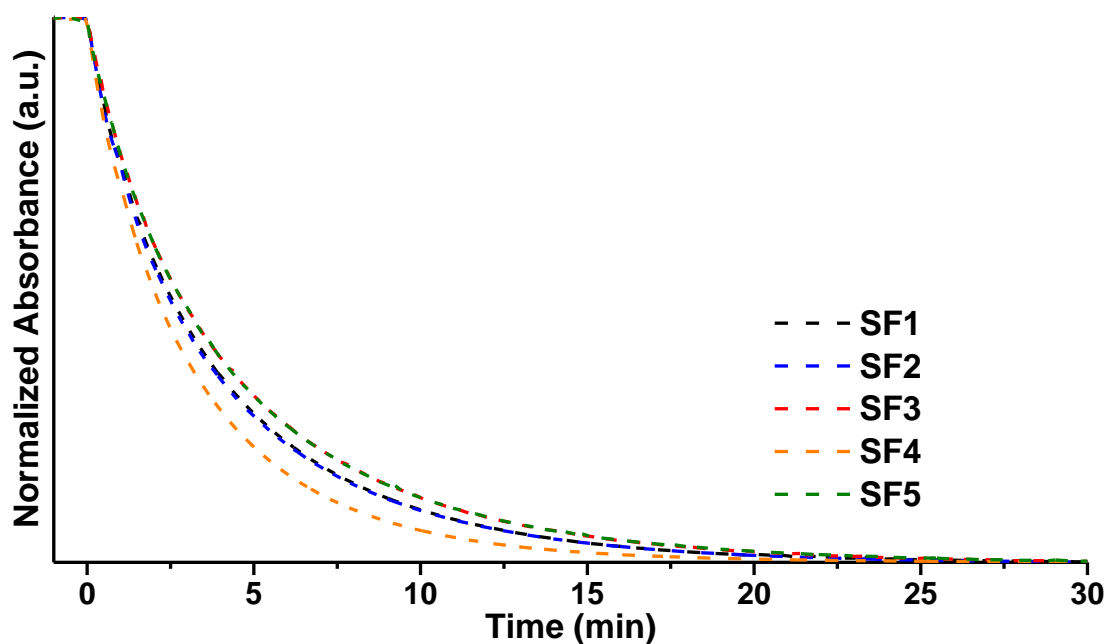
Figure S0-1: discoloration kinetic measurement for the five carbazole dyes

        To measure the closing kinetic, we follow the evolution of the absorbance of the λ_{max} of each dye after reaching their respective PSS at 25°C. The kinetic values presented in the main text were obtained by a mono-exponential fitting of the curves in figure S1.

DFT calculation
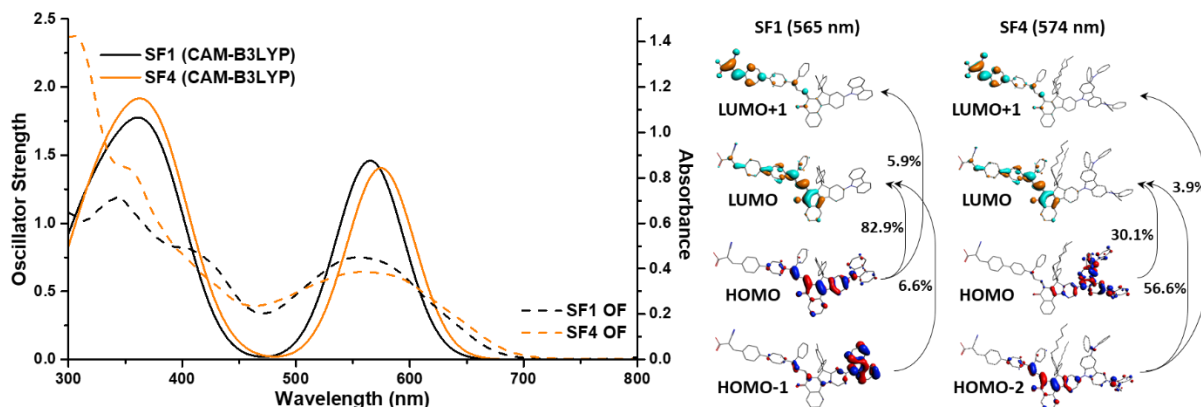
Comparison of UV-visible absorption spectrum for SF1 and SF4 a under continuous irradiation (Xenon lamp, 200 W, 300-600 nm). Concentration: 2 x 10-5 mol.L-1 in toluene at 25°C with the TD-DFT calculated spectra at the CAM-B3LYP level of theory (left). Calculated electronic transitions for SF1 and SF4 (right).

Comparison absorption SF1 and NP1.
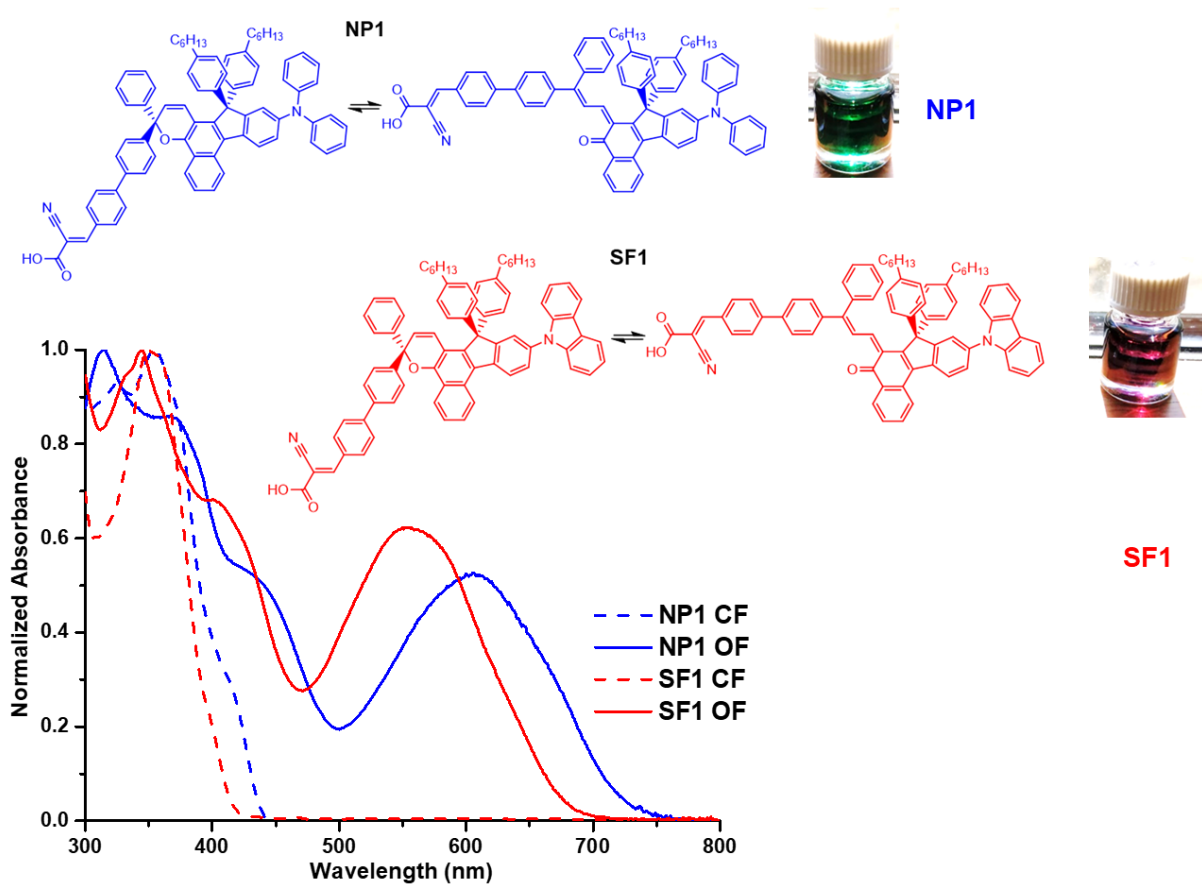
Cyclic Voltammetry:
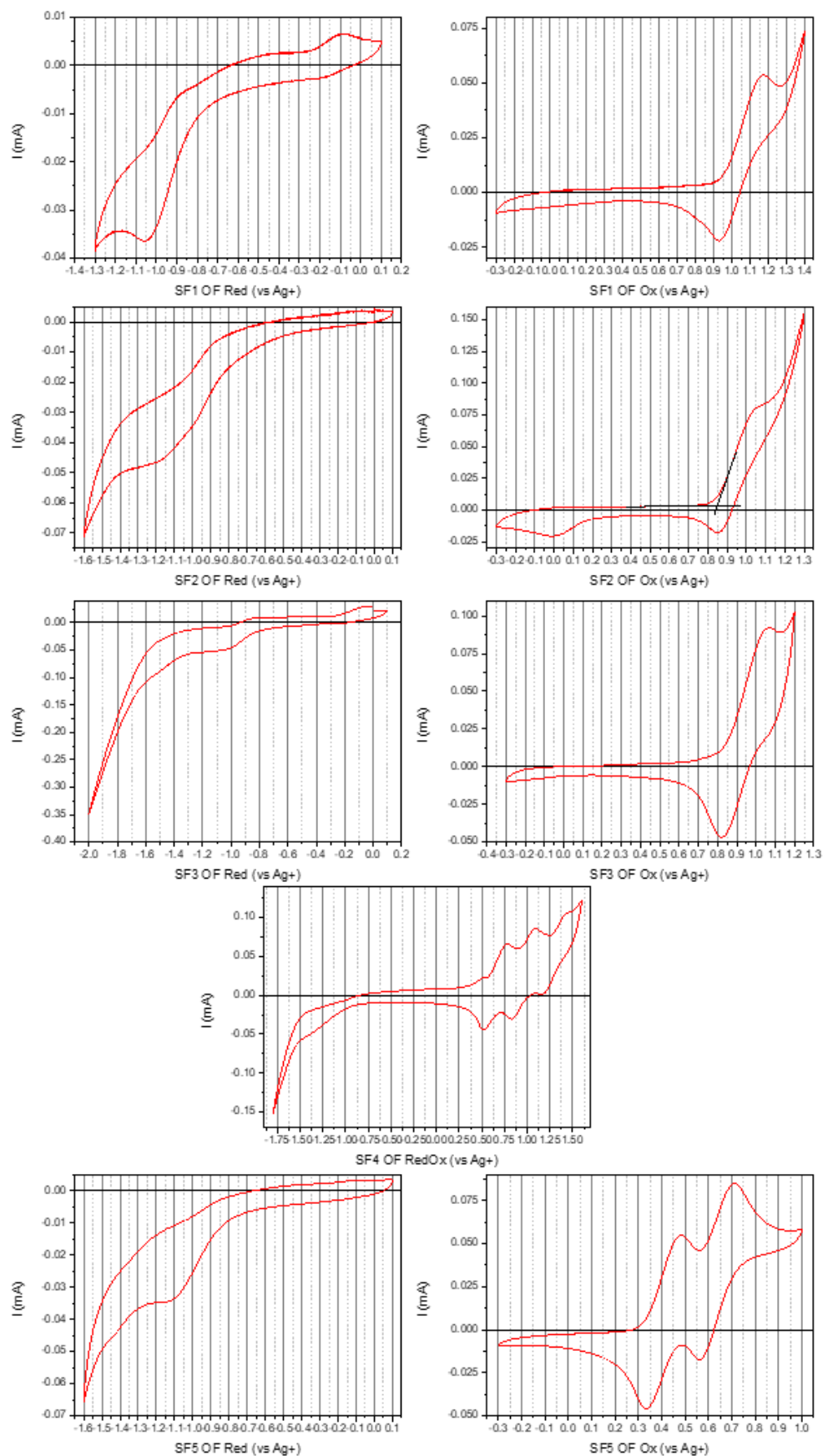
Cyclic voltammetry shows two successive oxidation peaks separated by around 200 mV. The first onset at 0.41 V vs. AgCl/Ag (ca. 0.63 V vs. NHE) is ascribed to the two-electron process thioate oxidation into the corresponding disulfide form (Figure Sx). This value lies between the redox potential of di-iodide anion radical/iodide in acetonitrile ($E°''(I_2^-/I^-)$ = 0.79V vs. NHE) and of tri-iodide/iodide redox couple ($E°''(I_3^-/I^-)$ = 0.35 V vs. NHE).[5–7]
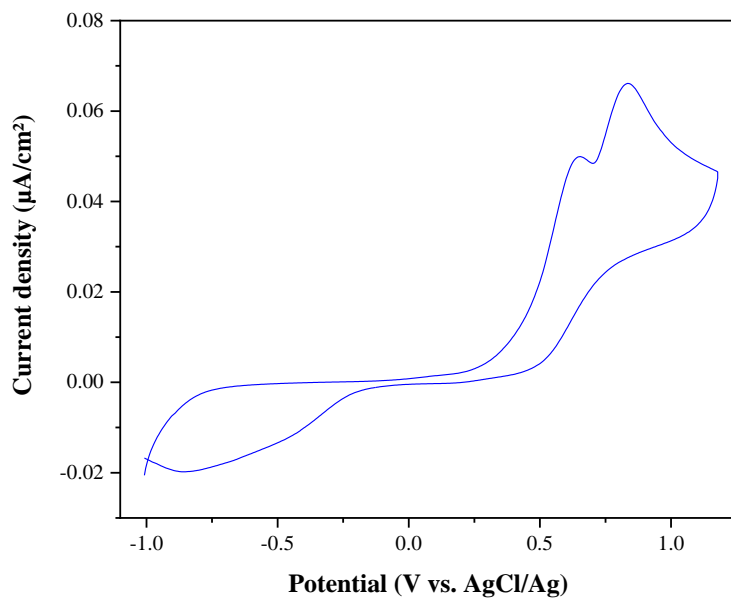
Cyclic voltamperogram recorded at 100 mV/s scan rate of the CH_3-S-SO_3^- TMA^+ with I^- in acetonitrile. The working electrode is a glassy carbon, Pt wire counter-electrode and AgCl/Ag quasi-reference electrode. The electrolyte contains 0.01 M of tetrabutylammonium hexafluorophosphate ($TBAPF_6$) as a supporting salt.

Impedance Spectroscopy

Dyes	α		β	
	Before LS	**After LS**	**Before LS**	**After LS**
SF1	0.26	0.25	0.52	0.47
SF2	0.27	0.25	0.57	0.60
SF3	0.28	0.27	0.36	0.43
SF4	0.29	0.27	0.58	0.59
SF5	0.28	0.25	0.46	0.49

Table S1: α and β values obtained from fitting the EIS results of the SF1-5 solar cells to the equivalent circuit described in the main text.
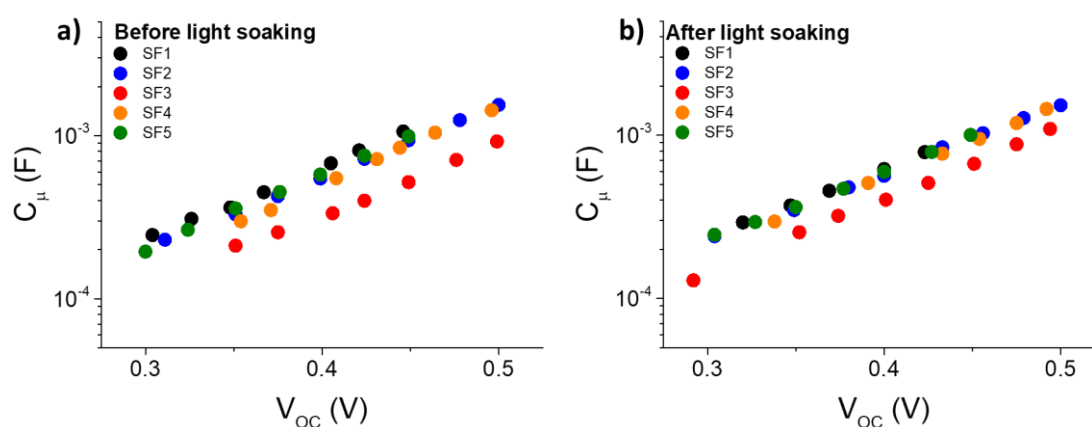
The electrochemical impedance spectroscopy (EIS) measurements were done using an Autolab PGSTAT30 FRA2 potentiostat controlled by the NOVA 2.1 software. The studies were conducted on complete solar cells using red (655 nm) LED before and after 15 minutes of device activation under 1 Sun (AM1.5G at 100 mW.cm^{-2}) to probe the photostationary state. These measurements were conducted with the applied potential equal to the generated open-circuit voltage under continuous illumination using Thorlabs LED in a wide range of DC light intensities. The impedance spectra were obtained by applying a 10 mV sinusoidal voltage perturbation in the $10^5 - 10^{-1}$ Hz frequency range. The resulting spectra were analyzed and modelled using ZView Software (Scribner).

Cell fabrication and characterization

- 0.36 cm² TiO_2 (Solaronix Ti-Nanoxide T/SP) 13 μm mesoporous TiO_2 + 4 μm TiO_2 light scattering layer (Solaronix, Ti-Nanoxide R/SP) for opaque cells or 13 μm TiO_2 for transparent cells.

- Cleaned with absolute ethanol and dried under an argon flux.

- Immersion into a freshly prepared 40 mmol.L^{-1} $TiCl_4$ aqueous solution at 70°C for 20 minutes (in oven).

- Rinsed with distilled water followed by absolute ethanol and dried under an argon flux.

- The photoanodes are then sintered under air at 500°C for 20 minutes and cooled down to 80°C (with the platinum counter-electrodes).

- Sensitization through immersion in a dyeing bath solution overnight at room temperature with a dye concentration of 0.5 mM and CDCA 5 mM in a one to one volume mix of chloroform and terbutanol (7 mL solutions).

- Drilled counter electrodes are coated with a thin layer of an ethanolic solution of $PtH2Cl6$ (Plastisol, Solaronix) and charred under air at 500°C (with the photoanodes).

- After sensitization, photoanodes are rinsed with DCM, absolute ethanol and dried under argon flux.

- Cells are assembled with a surlyn thermoglueing polymer (60 μm thick) using a heating press at 105 °C for 15 seconds on one side (photoanode on bottom) and 5 seconds on the other.

- Electrolyte (optimized homemade) is introduced via the pre-drilled hole using a vacuum pump.

- Injection hole is then sealed with a surlyn thermoplastic polymer and a thin glass cover using heat (welding iron).

- Contacts along the cell edges are made with tin using a sonic welding iron.

$TiCl_4$ solution: 100 mL distilled water cooled with ice under strong stirring, $TiCl_4$ (4 mmol, 758.7 mg, 0.44 mL) is added extremely slowly (dropwise) and stirred 10 minutes (then kept at 4°C for 1 week maximum).

Homemade Electrolyte: I_2 90 mmol.L^{-1}, LiI 0.5 mol.L^{-1} in acetonitrile (2 mL acetonitrile + 22.8 mg I_2 + 133.9 mg LiI).

Characterization

Current-voltage curve

Before measurements, the AM 1.5 G simulator (Newport class AAA) was calibrated using a reference silicon photodiode equipped with an infrared-cut-off filter (KG3; Schott). This reference photodiode consisted of a readout device and a 2 cm × 2 cm calibrated solar cell made from monocrystalline silicon with a KG3 window. The cell was also equipped with a thermocouple assembled in accordance with IEC 60904-2. The certification is accredited by the National Institute of Standards and Technology to the ISO-17025 standard and is traceable to the National Renewable Energy Laboratory. The spectral mismatch factor M of the solar simulator was found at 1.08 using a reference dye sensitized solar cell fabricated with YKP-88.[8]

The current–voltage characteristics of the cells were measured under dark and under the AM 1.5 G (1,000 W×m −2) irradiation condition, which was achieved by applying an external potential bias to the cell while measuring the generated photocurrent with a Keithley model 2400 digital source meter. Measurement for the cells was from +0.7 to −0.2 V, divided into 45 points, with a speed of 20 mV×s $^{-1}$. The devices were masked before the measurements to attain an illuminated active area of 0.36 cm²

Effect of CDCA on the performances of the cells

	J_{SC}	V_{OC}	FF	PCE	J_{SC}	V_{OC}	FF	PCE
	mA.cm^{-2}	V		%	mA.cm^{-2}	V		%
SF1	2.47	0.52	0.68	**0.87**	2.78	0.48	0.67	**0.89**
SF2	5.41	0.45	0.68	**1.68**	5.24	0.47	0.67	**1.67**
SF3	4.29	0.48	0.66	**1.36**	4.27	0.52	0.74	**1.63**
SF4	8.14	0.51	0.68	**2.81**	7.93	0.52	0.73	**3.04**
	No CDCA co-adsorption				**10 CDCA : Dye co-adsorption**			

Python program:

Library colour-science: https://www.colour-science.org/

Sun AM1.5G: https://www.nrel.gov/grid/solar-resource/spectra-am1.5.html

Photopic response: https://cie.co.at/datatable/cie-spectral-luminous-efficiency-photopic-vision
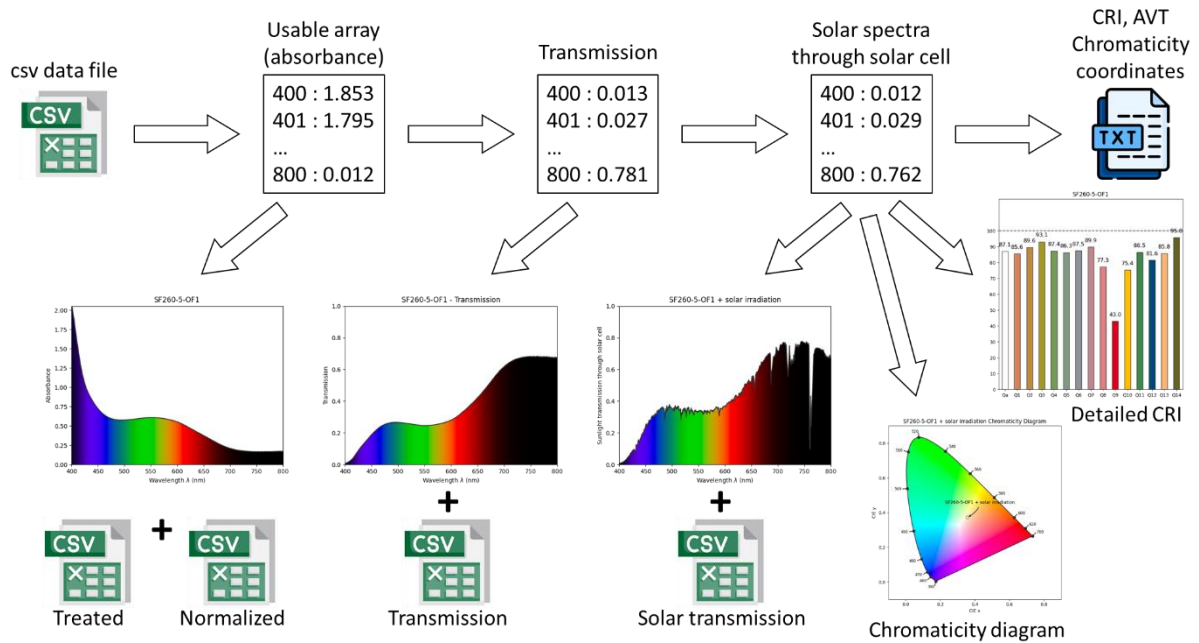
Figure S0-1: Working principle of the python program used to obtain the CRI and the AVT values

GitHub of the program: https://github.com/Samuel-Fauvel/CRI-AVT-Solar-Cells

Program:

```python
import math
import colour
import numpy as np
import pandas as pd
from colour.plotting.common import render as render


def isfloat(num):
    try:
        float(num)
        return True
    except ValueError:
        return False


def csv_to_usable(csv_values_raw):
    is_data = isfloat(csv_values_raw[0][0])
    z = 0
    while not is_data:
        f = np.delete(csv_values_raw, [0, z], 0)
        z += 1
        is_data = isfloat(f[0][0])
    spectral_distrib = {}
    i = len(f) - 1
    j = 0
    if float(f[i][0]) > float(f[j][0]):
        while j <= i:
            spectral_distrib[float(f[i][0])] = float(f[i][1])
            j += 1
    elif float(f[i][0]) < float(f[j][0]):
        while i > 0:
            spectral_distrib[float(f[i][0])] = float(f[i][1])
            i -= 1
    return spectral_distrib
```

```python
def csv_to_transmission(csv_values_raw):
    is_data = isfloat(csv_values_raw[0][0])
    z = 0
    while not is_data:
        f = np.delete(csv_values_raw, [0, z], 0)
        z += 1
        is_data = isfloat(f[0][0])
    spectral_distrib_transmission = {}
    i = len(f) - 1
    j = 0
    if float(f[i][0]) > float(f[j][0]):
        while j <= i:
            k = -float(f[i][1])
            l = math.pow(10, k)
            spectral_distrib_transmission[float(f[i][0])] = float(k)
            j += 1
    elif float(f[i][0]) < float(f[j][0]):
        while i > 0:
            m = -float(f[i][1])
            n = math.pow(10, m)
            spectral_distrib_transmission[float(f[i][0])] = float(n)
            i -= 1
    return spectral_distrib_transmission



def sd_to_csv(sd, title):
    a = np.asarray(sd.values)
    b = np.asarray(sd.wavelengths)
    data = {'Wavelength': b, 'Absorbance': a}
    c = pd.DataFrame(data=data)
    c.to_csv(title + '.csv', columns=('Wavelength', 'Absorbance'), sep=',', index=False)
    return 0



def sun_filter_400_800(spectre_transmission, sun_400_800):
```

```python
    spectre_filter = spectre_transmission.interpolate(colour.SpectralShape(400, 800, 1))
    a = np.asarray(spectre_filter.values)
    b = np.asarray(spectre_filter.wavelengths)
    data = {'Wavelength': b, 'Absorbance': a}
    c = pd.DataFrame(data=data)
    d = c.values
    sun_to_filter = sun_400_800
    filtered_sun = {}


    i = 0
    for i in range(len(d)):
        actual_row = d[i]
        transmission_value = actual_row[1]
        actual_wavelength = actual_row[0]
        filtered_value = transmission_value * sun_to_filter[actual_wavelength]
        filtered_sun[actual_wavelength] = filtered_value
        i = + 1


    return filtered_sun



def png_spectrum_400_800(spectre, file_title):
    max_abs = max(spectre.values)
    min_abs = 0
    bonding_box = [400, 800, min_abs, max_abs]
    settings = {
        'filename': file_title,
        'standalone': True,
        'bounding_box': bonding_box,
        "tight_layout": False,
        'title': file_title,
        'x_label': 'Wavelength $\\lambda$ (nm)',
        'y_label': 'Absorbance',
    }
    render(**settings)
    colour.plotting.plot_single_sd(spectre, **settings)
```

```python
        return 0



def png_transmission_400_800(spectre_transmission, file_title):
    bonding_box = [400, 800, 0, 1]
    settings = {
        'filename': file_title,
        'standalone': True,
        'bounding_box': bonding_box,
        "tight_layout": False,
        'title': file_title,
        'x_label': 'Wavelength $\\lambda$ (nm)',
        'y_label': 'Transmission',
    }
    render(**settings)
    colour.plotting.plot_single_sd(spectre_transmission, **settings)
    return 0



def png_sun_filtered_spectrum(sun_filteredspectrum, file_title):
    max_abs = max(sun_filteredspectrum.values)
    if max_abs <= 1:
        bonding_box = [400, 800, 0, 1]
    else:
        max_abs_margin = max_abs + 0.1
        bonding_box = [400, 800, 0, max_abs_margin]

    settings = {
        'filename': file_title,
        'standalone': True,
        'bounding_box': bonding_box,
        "tight_layout": False,
        'title': file_title,
        'x_label': 'Wavelength $\\lambda$ (nm)',
        'y_label': 'Sunlight transmission through solar cell',
    }
```

```python
        render(**settings)
        colour.plotting.plot_single_sd(sun_filtered_spectrum, **settings)
        return 0




def png_chromaticity_diagram(spectre, file_title):
    settings = {
        'filename': file_title + " Chromaticity Diagram",
        'standalone': True,
        'title': file_title + " Chromaticity Diagram",
    }
    render(**settings)
    colour.plotting.plot_single_sd(spectre, **settings)
    spectre_msds = colour.MultiSpectralDistributions(spectre)
    colour.plotting.plot_sds_in_chromaticity_diagram_CIE1931(spectre_msds, **settings)
    return 0




def png_color_sample(RGB, title):
    colour_sample = colour.plotting.common.ColourSwatch(RGB, title)

    settings = {
        'filename': title + " Colour Sample",
        'standalone': True,
        'title': title,
    }
    colour.plotting.common.plot_single_colour_swatch(colour_sample, **settings)




def png_CRI_detailed(spectrum, file_title):
    settings = {
        'filename': file_title + " CRI",
        'standalone': True,
        'title': file_title,
    }
    render(**settings)
```

```
colour.plotting.quality.plot_single_sd_colour_rendering_index_bars(spectrum, **settings)
```

##########

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"https://www.nrel.gov/grid/solar-resource/spectra-am1.5.html, AM 1.5 G"

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"https://cie.co.at/datatable/cie-spectral-luminous-efficiency-photopic-vision, Photopic response"

##########

"Extract the data from the csv file (spectrum.csv)"

```
csv = pd.read_csv("spectrum.csv")
title = csv.columns[0]
title_transmission = title + " - Transmission"
title_normalized = title + " - Normalized"
title_sun = title + " + solar irradiation"
csv_values_raw = csv.values
csv_sd = csv_to_usable(csv_values_raw)
```

"Transform the csv absorbance to transmission data"

```
csv_sd_transmission = csv_to_transmission(csv_values_raw)
spectre_raw_transmission = colour.SpectralDistribution(csv_sd_transmission,
name=title_transmission)
spectre_raw_transmission_copy = spectre_raw_transmission.copy()
spectre_temp_transmission = spectre_raw_transmission_copy.interpolate(colour.SpectralShape(400,
800, 1))
```

```python
spectre_transmission = spectre_temp_transmission.copy().extrapolate(colour.SpectralShape(400,
800, 1),

                                    extrapolator_kwargs={'method': 'Constant', })


"Transform the transmission data to sun filtered light"
sun_filtered_spectrum_data = sun_filter_400_800(spectre_transmission, sun_400_800)
sun_filtered_spectrum = colour.SpectralDistribution(sun_filtered_spectrum_data, name=title_sun)


"Transform the raw absorbance data into usable SpectralDistribution class"


spectre_raw = colour.SpectralDistribution(csv_sd, name=title)
spectre_raw_copy = spectre_raw.copy()
spectre_temp = spectre_raw_copy.interpolate(colour.SpectralShape(400, 800, 1))
spectre = spectre_temp.copy().extrapolate(colour.SpectralShape(400, 800, 1),
                        extrapolator_kwargs={'method': 'Constant', })
spectre_norma = spectre.copy().normalise()


"AVT calculation from 400 to 750 nm"


spectre_transmission_AVT = spectre_transmission.copy()


spectre_AVT_abs = spectre_transmission_AVT.interpolate(colour.SpectralShape(400, 750, 1))
AVT_spectre_values = np.asarray(spectre_AVT_abs.values)
AVT_spectre_wavelengths = np.asarray(spectre_AVT_abs.wavelengths)
data = {'Wavelength': AVT_spectre_wavelengths, 'Transmission': AVT_spectre_values}
AVT_array = pd.DataFrame(data=data)
AVT_data = AVT_array.values


i = 0
AVT_cumul_1 = 0
AVT_cumul_2 = 0
for i in range(len(AVT_data)):
    actual_row = AVT_data[i]
    actual_wavelength = actual_row[0]
    transmission_value = actual_row[1]
    sun_value = sun_400_800[actual_wavelength]
```

```python
        photopic_response_value = photopic_response_400_800[actual_wavelength]


    AVT_cumul_1 = AVT_cumul_1 + (transmission_value * sun_value * photopic_response_value)
    AVT_cumul_2 = AVT_cumul_2 + (sun_value * photopic_response_value)


    i = + 1


AVT = AVT_cumul_1 / AVT_cumul_2


"Transform transmission spectrum to XYZ, xy and RGB"
XYZ = colour.colorimetry.tristimulus_values.sd_to_XYZ(sun_filtered_spectrum)
xy = colour.models.cie_xyy.XYZ_to_xy(XYZ)
RGB = colour.models.rgb.common.XYZ_to_sRGB(XYZ)


"Create a png file with a colour sample"
png_color_sample(RGB, title)


"Create a png file with the chromaticity diagram"
png_chromaticity_diagram(spectre_transmission, title_transmission)
png_chromaticity_diagram(sun_filtered_spectrum, title_sun)


"Calculate the CRI value"
CRI = colour.colour_rendering_index(sun_filtered_spectrum)


"Create a txt file with the CRI value, the AVT value, the XYZ coordinates, the xy coordinates and the RGB values"


text = "CRI = " + str(CRI) + "\nAVT (from 400 to 750 nm) = " + str(AVT) \
    + "\n\nXYZ coordinates :\n" + "X=" + str(XYZ[0]) + " Y=" + str(XYZ[1]) + " Z=" + str(XYZ[2]) \
    + "\n\nxy coordinates :\n" + "x=" + str(xy[0]) + " y=" + str(xy[1]) \
    + "\n\nRGB values :\n" + "R=" + str(RGB[0]) + " G=" + str(RGB[1]) + " B=" + str(RGB[2])
name_note = 'CRI-AVT and coordinate values ' + title
note = open(name_note, "w")
note.write(text)
note.close()
```

"Create png files with the absorbance and transmission spectra from 400 to 800 nm"

```
png_spectrum_400_800(spectre, title)
png_transmission_400_800(spectre_transmission, title_transmission)
png_sun_filtered_spectrum(sun_filtered_spectrum, title_sun)
```

"Create a png file with the detailed CRI values"

```
png_CRI_detailed(sun_filtered_spectrum, title)
```

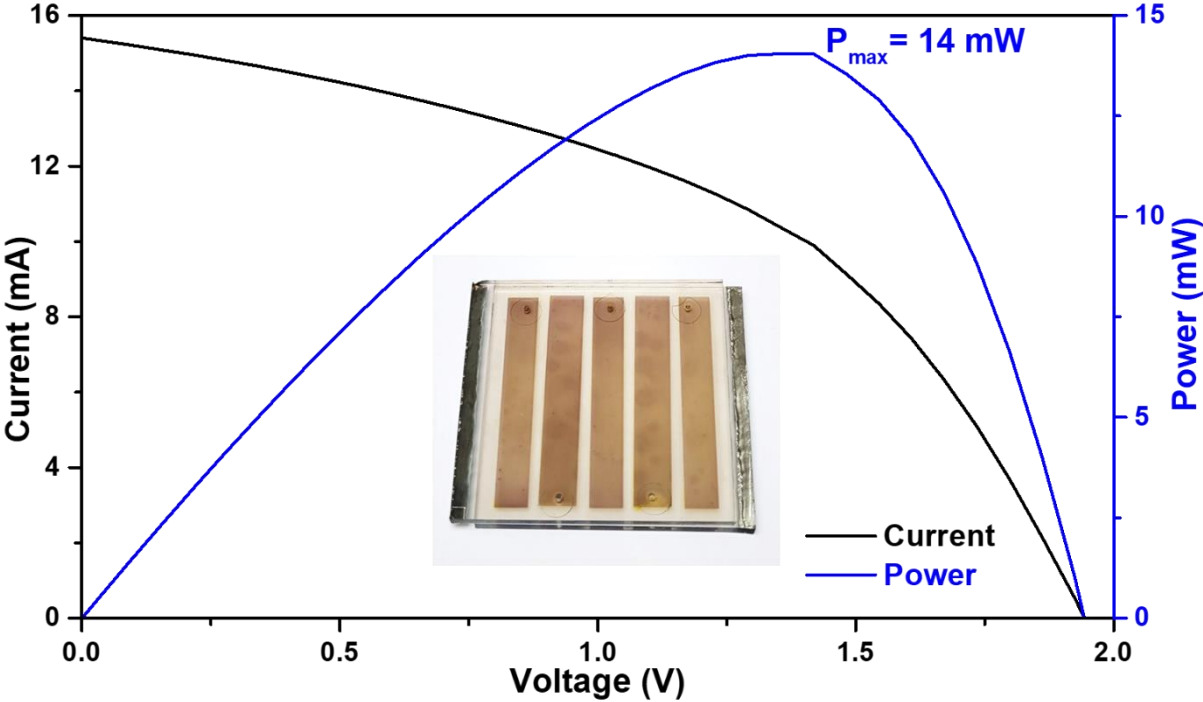"Create csv files with treated data of the spectrum"

```
sd_to_csv(spectre, title)
sd_to_csv(spectre_norma, title_normalized)
sd_to_csv(spectre_transmission, title_transmission)
sd_to_csv(sun_filtered_spectrum, title_sun)
```

Photovoltaic performances W-type module with SF4

Picture of a translucent solar cell (25 cm²):

Taken 21/04/2023, in Aubonne (rainy day)

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