# Supplementary Information

## Functionalized porphyrin-fullerene dyads: a pathway to enhanced the performance of perovskite solar cells

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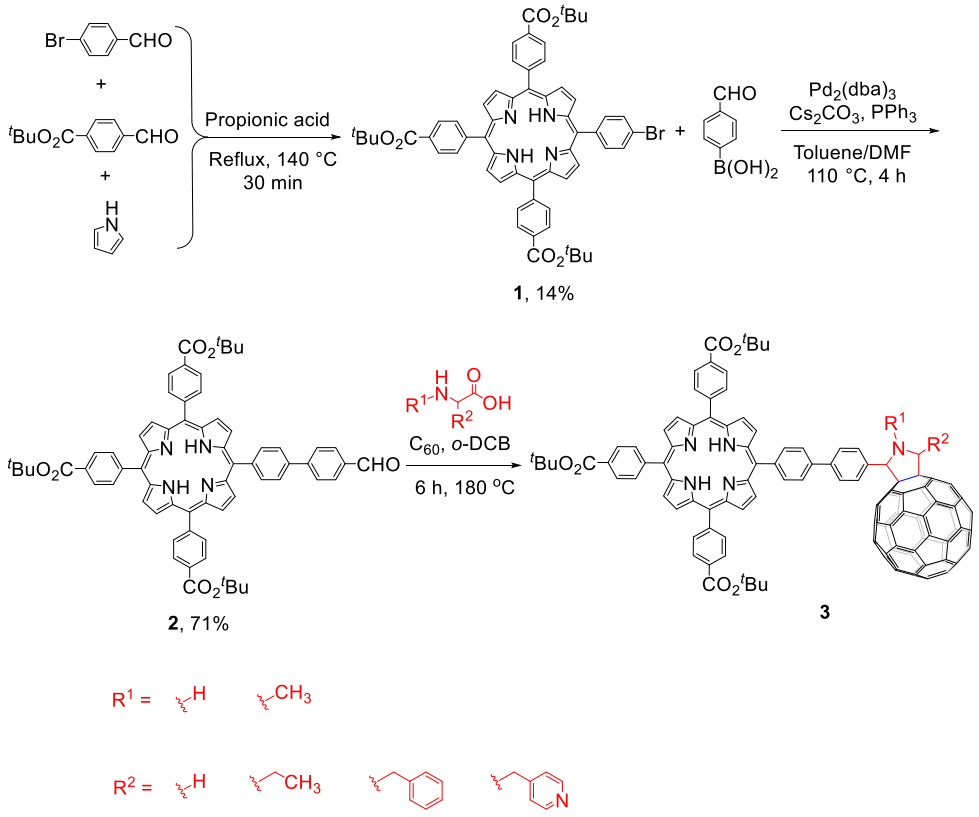
## 1. General information

All chemicals were obtained commercially and used without further purification. NMR spectra were recorded on a 400 and 500 MHz NMR spectrometer (400 or 500 MHz for $^{1}$H NMR; 101 or 126 MHz for $^{13}$C{$^{1}$H} NMR). $^{1}$H NMR and $^{13}$C{$^{1}$H} NMR chemical shifts were determined relative to internal TMS at $\delta$ 0.00 ppm. Data for $^{1}$H NMR and $^{13}$C{$^{1}$H} NMR are reported as follows: chemical shift ($\delta$, ppm), multiplicity (s = singlet, d = doublet, t = triplet, m = multiplet). IR spectra were obtained on a Thermo Scientific Nicolet 6700 instrument. High-resolution mass spectra (HRMS) were measured with MALDI-TOF. UV-vis spectra were obtained on a MAPADA UV-1800PC instrument. Cyclic voltammetry (CV) and differential pulse voltammetry (DPV) measurements were performed under an argon atmosphere using a Shanghai Chenhua CHI620E workstation.

## 2. Synthetic route of dyads 3a-e




## 3. Synthesis and spectral data of compounds 1, 2 and 3a-e

Synthesis and spectral data of compound **1**: A mixture of 4-bromobenzaldehyde (200 mg, 1.08 mmol) and *tert*-butyl 4-formylbenzoate (670 mg, 3.24 mmol) was dissolved in 30 mL of propionic acid and then heated to reflux at 140 °C. Subsequently, pyrrole (0.3 mL, 4.32 mmol) was added dropwise to the refluxing reaction mixture. After that, the solution was maintained at reflux for 30 min and then cooled down to room temperature. After the solvent had been evaporated in vacuo, the residue was purified by silica gel column chromatography using dichloromethane and petroleum ether in a ratio of 1:1 (v/v) as the eluent to give some unidentified products and the targeted product **1** (149.2 mg, 14%): red solid; m.p. > 300 ºC. $^{1}$H NMR (400 MHz, $CDCl_3$) $\delta$ 8.86–8.80 (m, 8H), 8.40 (d, $J$ = 8.1 Hz, 6H), 8.27 (d, $J$ = 8.1 Hz, 6H), 8.07 (d, $J$ = 8.2 Hz, 2H), 7.90 (d, $J$ = 8.2 Hz, 2H), 1.76 (s, 27H), –2.82 (s, 2H); $^{13}$C{$^{1}$H} NMR (101 MHz, $CDCl_3$) $\delta$ 165.9, 146.2, 140.9, 135.8, 134.4, 131.6, 130.0, 127.8, 122.6, 119.49, 119.46, 119.1, 81.5, 28.4; FT-IR $\nu$/cm$^{-1}$ (KBr) 2976, 2929, 1716, 1606, 1476, 1340, 1367, 1294, 1253, 1163, 1116, 1022, 967, 847, 798, 763, 722; UV-Vis ($CHCl_3$) $\lambda_{max}$/nm (log $\varepsilon$)

421 (5.65), 516 (3.39), 551 (4.31), 591 (4.00), 646 (3.62); HRMS (ESI) *m*/*z* calcd for $C_{59}H_{54}{}^{79}BrN_4O_6$ $[M+H]^+$ 993.3221, found 993.3209.

Synthesis and spectral data of compound **2**: Porphyrin **1** (62.9 mg, 0.063 mmol) was treated with (4-formylphenyl)boronic acid (57.0 mg, 0.379 mmol) in the presence of $Pd_2(dba)_3$ (6.0 mg, 0.006 mmol), $Cs_2CO_3$ (82.0 mg, 0.253 mmol), and $PPh_3$ (25.0 mg, 0.095 mmol) in the solution of toluene/DMF (2:1) under an argon atmosphere. The reaction mixture was refluxed at 110 °C for 12 h and then cooled down to room temperature. After the solvent had been evaporated in vacuo, the residue was purified by silica gel column chromatography using ethyl acetate and petroleum ether in a ratio of 1:10 (v/v) as the eluent to give product **2** (45.8 mg, 71%): pink solid; m.p. > 300 ºC. $^1$H NMR (400 MHz, $CDCl_3$) $\delta$ 10.14 (s, 1H), 8.93 (d, $J$ = 4.8 Hz, 2H), 8.87–8.80 (m, 6H), 8.40 (d, $J$ = 8.1 Hz, 6H), 8.33 (d, $J$ = 7.9 Hz, 2H), 8.28 (d, $J$ = 8.1 Hz, 6H), 8.09 (d, $J$ = 8.4 Hz, 2H), 8.06 (d, $J$ = 8.4 Hz, 2H), 8.03 (d, $J$ = 7.9 Hz, 2H), 1.76 (s, 27H), –2.77 (s, 2H); $^{13}$C{$^1$H} NMR (101 MHz, $CDCl_3$) $\delta$ 191.9, 165.9, 146.7, 146.23, 146.19, 142.2, 139.1, 135.5, 135.2, 134.4, 131.6, 130.5, 127.9, 127.8, 125.8, 119.9, 119.5, 119.4, 81.5, 28.4; FT-IR $\nu$/cm$^{-1}$ (KBr) 2976, 2928, 1715, 1605, 1475, 1393, 1368, 1294, 1255, 1166, 1116, 1020, 966, 847, 799, 763, 731; UV-Vis ($CHCl_3$) $\lambda_{max}$/nm (log $\varepsilon$) 421 (5.60), 516 (4.24), 552 (3.95), 591 (3.68), 646 (3.51); MALDI-TOF MS *m*/*z* calcd for $C_{66}H_{58}N_4O_7$ $[M]^-$ 1018.4311, found 1018.4303.

General procedure for fullerene-porphyrin dyads **3**: A mixture of compound **2** (0.03 mmol), $C_{60}$ (0.03 mmol), and an amino acid (0.09 mmol) was dissolved in 15 mL of *o*-DCB. Then, the solution was heated to reflux at 180 °C for 6 h. After the solvent had been evaporated in vacuo, the residue was separated on a silica gel column with $CS_2$ as the eluent to give unreacted $C_{60}$, and subsequent elution with ethyl acetate/petroleum ether/carbon disulfide (1:2:2 v/v) as an eluent to give the desired product **3**.

Synthesis and spectral data of **3a**: Following the general procedure, the reaction of compound **2** (30.6 mg, 0.03 mmol) with $C_{60}$ (21.6 mg, 0.03 mmol) and sarcosine (8.0 mg, 0.09 mmol) afforded the recovered $C_{60}$ (4.6 mg, 21%) and **3a** (17.1 mg, 32%): amorphous purple-brown solid; m.p. > 300 ºC. $^1$H NMR (500 MHz, 1:1 $CS_2$/$CDCl_3$) $\delta$ 8.85 (d, $J$ = 4.7 Hz, 2H), 8.77–8.71 (m, 6H), 8.33 (d, $J$ = 7.9 Hz, 6H), 8.23–8.18 (m, 8H), 7.97–7.89 (m, 6H), 4.96 (s, 1H), 4.95 (d, $J$ = 9.0 Hz, 1H), 4.23 (d, $J$ = 9.0 Hz, 1H), 2.87 (s, 3H), 1.72 (s, 27H), -2.89 (s, 2H); $^{13}$C{$^1$H} NMR (126 MHz, 1:1 $CS_2$/$CDCl_3$) $\delta$ 164.9, 155.8, 153.5, 153.0, 152.8, 146.9, 146.4, 146.1, 145.94, 145.90, 145.88, 145.84, 145.77, 145.7, 145.5, 145.4, 145.24, 145.20, 145.1, 145.03, 145.02, 144.96, 144.9, 144.84, 144.81, 144.7, 144.31, 144.25, 144.03, 143.97, 142.8, 142.6, 142.3, 142.23, 142.22, 142.19, 141.91, 141.89, 141.81, 141.78, 141.71, 141.66, 141.64, 141.63, 141.5, 141.34, 141.26, 140.9, 140.6, 139.90, 139.86, 139.70, 139.67, 139.3, 136.7, 136.3, 136.2, 135.6, 135.4, 135.0, 134.2 , 131.3, 127.7, 125.3, 120.1, 119.2, 119.0, 80.5, 76.9, 69.9, 68.7, 39.9, 28.1; FT-IR $\nu$/cm$^{-1}$ (KBr) 2975, 1716, 1605, 1558, 1474, 1455, 1392, 1367, 1295, 1253, 1165, 1184, 1114, 1020, 1005, 994, 982, 965, 867, 846, 798, 763, 725, 527; UV-Vis ($CHCl_3$) $\lambda_{max}$/nm (log $\varepsilon$) 258 (4.99), 314 (4.66), 421 (5.56), 516 (4.21), 553 (3.89), 593 (3.60), 646 (3.51), 704 (2.60); MALDI-TOF MS *m*/*z* calcd for $C_{128}H_{63}N_5O_6$ $[M]^-$ 1766.4817, found 1766.4801.

Synthesis and spectral data of **3b**: Following the general procedure, the reaction of compound **2** (30.6 mg, 0.03 mmol) with $C_{60}$ (21.6 mg, 0.03 mmol) and *N*-glycine (6.7 mg, 0.09 mmol) afforded the recovered $C_{60}$ (7.2 mg, 33%) and **3b** (11.0 mg, 21%): amorphous purple-brown colour solid; m.p. > 300 ºC. $^1$H NMR (400 MHz, 1:1 $CS_2$/$CDCl_3$) $\delta$ 8.89 (d, $J$ = 5.0 Hz, 2H), 8.80–8.74 (m, 6H), 8.39–8.32 (m, 6H), 8.23 (d, $J$ = 7.9 Hz, 4H), 8.20–8.12 (m, 4H), 7.93 (d, *J*

= 8.0 Hz, 2H), 7.85 (d, *J* = 7.9 Hz, 2H), 7.58 (d, *J* = 7.8 Hz, 2H), 4.98 (s, 1H), 4.19 (d, *J* = 9.9 Hz, 1H), 3.89 (d, *J* = 9.9 Hz, 1H), 2.48 (s, 1H), 1.73 (s, 27H), -2.84 (s, 2H); $^{13}C\{^{1}H\}$ NMR (101 MHz, 1:1 $CS_2/CDCl_3$) $\delta$ 165.3, 154.9, 152.8, 152.5, 152.0, 146.40, 146.37, 146.03, 145.99, 145.6, 145.54, 145.48, 145.44, 145.38, 145.3, 145.2, 145.1, 144.7, 144.64, 144.57, 144.5, 144.41, 144.39, 144.2, 144.1, 143.7, 143.6, 143.5, 142.2, 142.10, 142.07, 142.0, 141.9, 141.8, 141.7, 141.6, 141.4, 141.35, 141.32, 141.2, 141.1, 141.0, 140.9, 140.3, 139.6, 139.4, 139.3, 139.2, 139.0, 136.6, 135.9, 134.948, 134.946, 134.3, 134.2, 131.4, 128.5, 127.8, 127.3, 125.3, 120.2, 119.3, 119.2, 80.9, 77.3, 76.3, 72.0, 61.0, 28.2; FT-IR $\nu$/cm$^{-1}$ (KBr) 2974, 2923, 1716, 1606, 1465, 1392, 1367, 1293, 1253, 1165, 1115, 1020, 966, 846, 799, 765, 727, 527; UV-Vis ($CHCl_3$) $\lambda_{max}$/nm (log $\varepsilon$) 259 (5.13), 315 (4.83), 422 (5.57), 517 (4.22), 552 (3.87), 592 (3.64), 646 (3.45), 698 (2.60); MALDI-TOF MS *m*/*z* calcd for $C_{127}H_{61}N_5O_6$ $[M]^-$ 1752.4661, found 1752.4642.

Synthesis and spectral data of **3c**: Following the general procedure, the reaction of compound **2** (30.6 mg, 0.03 mmol) with $C_{60}$ (21.6 mg, 0.03 mmol) and 2-aminobutyric acid (9.3 mg, 0.09 mmol) afforded the recovered $C_{60}$ (5.1 mg, 24%) and **3c** (15.1 mg, 28%): amorphous purple-brown solid; m.p. > 300 ºC. $^{1}H$ NMR (400 MHz, 1:1 $CS_2/CDCl_3$) $\delta$ 8.85 (d, *J* = 4.6 Hz, 2H), 8.80–8.72 (m, 6H), 8.34 (d, *J* = 8.4 Hz, 6H), 8.20 (d, *J* = 8.4 Hz, 6H), 8.17–8.11 (m, 3H), 7.90 (d, *J* = 8.1 Hz, 2H), 7.83 (d, *J* = 8.0 Hz, 2H), 7.72 (d, *J* = 7.8 Hz, 1H), 5.29 (s, 1H), 4.25 (d, *J* = 10.0 Hz, 1H), 2.82 (s, 1H), 2.61–2.40 (m, 1H), 2.16–2.00 (m, 1H), 1.71 (s, 30H), -2.87 (s, 2H); $^{13}C\{^{1}H\}$ NMR (101 MHz, 1:1 $CS_2/CDCl_3$) $\delta$ 165.0, 152.9, 152.8, 152.7, 152.6, 146.1, 146.0, 145.9, 145.53, 145.46, 145.3, 145.2, 145.12, 145.09, 145.0, 144.9, 144.8, 144.7, 144.5, 144.45, 144.44, 144.39, 144.34, 144.30, 144.25, 144.13, 144.09, 143.7, 143.6, 143.4, 143.3, 142.2, 142.1, 141.9, 141.8, 141.73, 141.68, 141.6, 141.5, 141.4, 141.3, 141.21, 141.18, 141.12, 141.09, 140.9, 140.8, 140.3, 139.6, 139.3, 139.1, 138.94, 138.90, 136.7, 136.2, 136.0, 135.0, 134.9, 134.8, 134.2, 131.3, 128.7, 127.7, 127.2, 125.2, 120.1, 119.2, 119.1, 80.6, 77.7, 75.5, 75.0, 72.9, 28.1, 26.6, 13.0; FT-IR $\nu$/cm$^{-1}$ (KBr) 2967, 2908, 1710, 1601, 1560, 1454, 1392, 1360, 1289, 1159, 1109, 962, 844, 794, 759, 721, 521; UV-Vis ($CHCl_3$) $\lambda_{max}$/nm (log $\varepsilon$) 259 (5.10), 315 (4.83), 422 (5.59), 517 (4.26), 552 (3.95), 591 (3.72), 647 (3.56), 701 (2.70); MALDI-TOF MS *m*/*z* calcd for $C_{129}H_{65}N_5O_6$ $[M]^-$ 1780.4974, found 1780.4966.

Synthesis and spectral data of **3d**: Following the general procedure, the reaction of compound **2** (30.6 mg, 0.03 mmol) with $C_{60}$ (21.6 mg, 0.03 mmol) and phenylalanine (14.8 mg, 0.09 mmol) afforded the recovered $C_{60}$ (6.3 mg, 29%) and **3d** (13.6 mg, 25%): amorphous purple-brown solid; m.p. > 300 ºC. $^{1}H$ NMR (500 MHz, 1:1 $CS_2/CDCl_3$) $\delta$ 8.87 (d, *J* = 4.7 Hz, 2H), 8.83–8.75 (m, 6H), 8.40–8.32 (m, 7H), 8.27–8.19 (m, 8H), 7.98–7.91 (m, 3H), 7.88 (d, *J* = 7.9 Hz, 2H), 7.58 (d, *J* = 7.4 Hz, 2H), 7.45 (t, *J* = 7.5 Hz, 2H), 7.34 (t, *J* = 7.4 Hz, 1H), 5.61 (s, 1H), 4.92 (d, *J* = 9.8 Hz, 1H), 3.95 (d, *J* = 13.0 Hz, 1H), 3.45 (dd, *J* = 13.0, 9.8 Hz, 1H), 2.91 (s, 1H), 1.74 (s, 27H), -2.84 (s, 2H); $^{13}C\{^{1}H\}$ NMR (126 MHz, 1:1 $CS_2/CDCl_3$) $\delta$ 165.6, 153.2, 153.0, 152.8, 146.5, 146.3, 146.2, 146.1, 145.90, 145.87, 145.71, 145.66, 145.64, 145.59, 145.52, 145.50, 145.4, 145.3, 145.19, 145.16, 145.1, 144.93, 144.87, 144.85, 144.8, 144.7, 144.6, 144.5, 144.1, 144.0, 143.8, 143.7, 142.6, 142.4, 142.2, 142.1, 142.03, 141.96, 141.9, 141.71, 141.69, 141.63, 141.57, 141.5, 141.45, 141.44, 141.2, 141.1, 141.0, 140.4, 139.78, 139.76, 139.5, 139.31, 139.30, 139.1, 137.2, 137.1, 136.6, 135.8, 135.4, 135.0, 134.3, 131.4, 129.2, 129.10, 129.06, 127.8, 127.3, 127.0, 125.3, 120.3, 119.3, 119.2, 81.1, 77.3, 74.6, 74.5, 72.1, 39.9, 28.3; FT-IR $\nu$/cm$^{-1}$ (KBr) 2967, 2923, 1710, 1604, 1555, 1471, 1456, 1398, 1363, 1298, 1245, 1162, 1106, 1030, 959, 847, 792, 759, 724, 524; UV-Vis ($CHCl_3$) $\lambda_{max}$/nm (log $\varepsilon$) 259 (5.11), 314 (4.85), 421 (5.60), 517 (4.26), 553 (3.90), 592 (3.78), 647 (3.56), 702 (2.60); MALDI-TOF MS *m*/*z* calcd for $C_{134}H_{67}N_5O_6$ $[M]^-$ 1842.5130, found 1842.5122.

Synthesis and spectral data of **3e**: Following the general procedure, the reaction of compound **2** (30.6 mg, 0.03 mmol) with $C_{60}$ (21.6 mg, 0.03 mmol) and 4-pyridylalanine (14.9 mg, 0.09 mmol) afforded the recovered $C_{60}$ (6.2 mg, 29%) and **3e** (14.5 mg, 26%): amorphous purple-brown solid; m.p. > 300 ºC. $^{1}$H NMR (500 MHz, 1:1 $CS_2$/$CDCl_3$) $\delta$ 8.85 (d, $J$ = 4.7 Hz, 2H), 8.81–8.73 (m, 6H), 8.66–8.55 (m, 2H), 8.41–8.30 (m, 7H), 8.27–8.19 (m, 7H), 8.18 (d, $J$ = 7.8 Hz, 2H), 7.92 (d, $J$ = 7.7 Hz, 2H), 7.88–7.82 (m, 3H), 7.46 (s, 1H), 5.53 (s, 1H), 4.83 (d, $J$ = 10.9 Hz, 1H), 3.87 (d, $J$ = 13.3 Hz, 1H), 3.46–3.34 (m, 1H), 2.83 (s, 1H), 1.73 (s, 27H), -2.84 (s, 2H); $^{13}$C{$^{1}$H} NMR (126 MHz, 1:1 $CS_2$/$CDCl_3$) $\delta$ 165.4, 152.7, 152.6, 152.3, 151.9, 150.2, 146.3, 146.2, 146.12, 146.10, 146.0, 145.8, 145.6, 145.5, 145.44, 145.37, 145.24, 145.16, 145.0, 144.92, 144.87, 144.8, 144.74, 144.66, 144.61, 144.52, 144.47, 144.4, 144.2, 143.8, 143.6, 143.49, 143.45, 142.4, 142.11, 142.09, 141.9, 141.8, 141.7, 141.6, 141.43, 141.37, 141.35, 141.31, 141.25, 141.2, 141.1, 141.0, 140.9, 140.6, 139.7, 139.6, 139.4, 139.2, 139.1, 137.0, 136.6, 136.2, 135.6, 135.0, 134.3, 131.4, 129.0, 127.8, 127.3, 125.3, 124.5, 120.2, 119.3, 119.2, 81.0, 77.3, 74.7, 74.5, 71.0, 39.2, 28.2; FT-IR $\nu$/cm$^{-1}$ (KBr) 2917, 2843, 1710, 1607, 1554, 1472, 1451, 1391, 1363, 1292, 1248, 1162, 1114, 1012, 965, 842, 794, 765, 721, 524; UV-Vis ($CHCl_3$) $\lambda_{max}$/nm (log $\varepsilon$) 258 (5.15), 315 (4.86), 422 (5.58), 517 (4.24), 553 (3.95), 592 (3.67), 647 (3.56), 696 (2.90); MALDI-TOF MS $m/z$ calcd for $C_{133}H_{66}N_6O_6$ $[M]^-$ 1843.5083, found 1843.5077.

## 4. Device fabrication

The perovskite precursor solution was prepared by dissolving $CH_3NH_3I$ and $PbI_2$ in a mixture of solvents DMF/DMSO (1.0 mL, 7:3, v/v) with a chemical formula of $MAPbI_3$ and 0.1 wt % **3a** was doped into the perovskite precursor solution. 10 mg of $NiO_x$ nanoparticles were dispersed in a mixture of solvents $H_2O$/IPA (3:1, v/v) by ultra-sonification. 2PACz was dissolved in ethanol with a concentration of 0.3 mg/mL. The ITO/$NiO_x$ substrates were then transferred into a nitrogen-filled glove box for the deposition of the 2PACz layer, and the 2PACz layer was spin-coated at 4000 rpm for 30 s. For the preparation of the perovskite film, 25 μL of precursor solution was spin-coated onto the ITO/$NiO_x$ substrate at 3500 rpm for 30 s. During the last 20 s of the spinning process, 200 μL of chlorobenzene was dropped onto the perovskite layer and then annealed at 100 °C for 10 min. $PC_{61}BM$ in chlorobenzene (20 mg $mL^{-1}$) was then spin-coated on the perovskite film at 2000 rpm for 30 s. Then, cathode buffer layer BCP (0.5 mg $mL^{-1}$ in isopropanol) was spin-coated on the $PC_{61}BM$ electron-transport layer. Finally, an 80-nm thickness of Ag anode was deposited by thermal evaporation under a pressure of $10^{-6}$ Torr. The active area of the device was 0.04 $cm^2$, which was defined by a shadow mask.

## 5. UV-Vis spectra of compounds 1, 2 and 3a-e

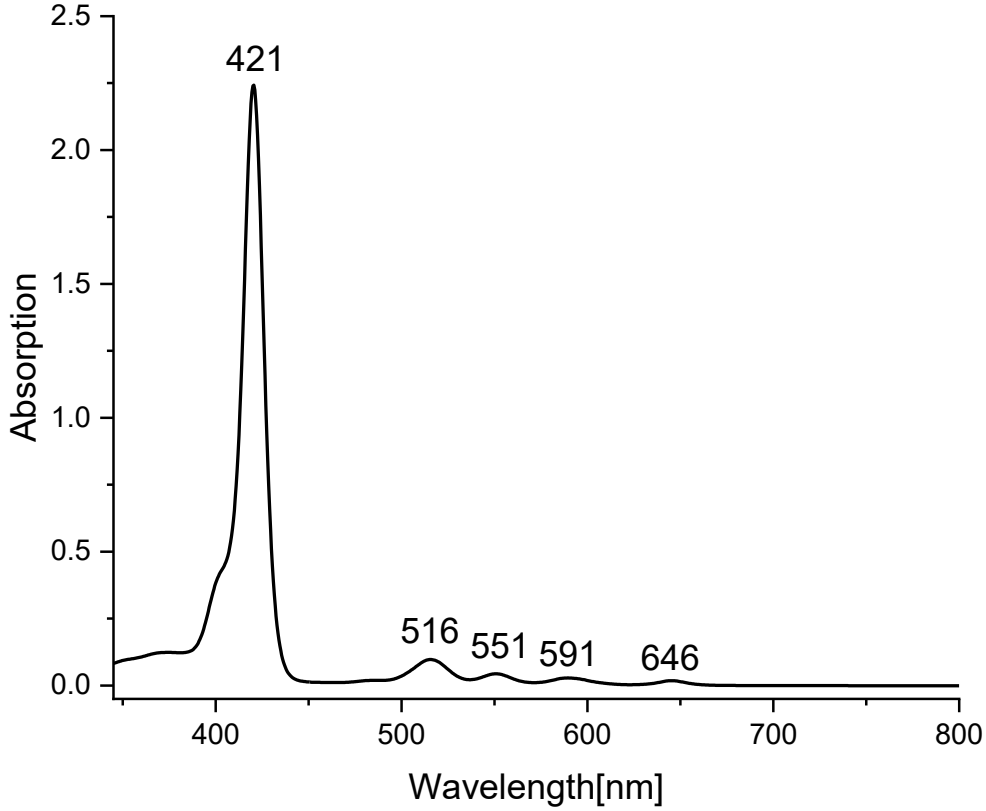



**Figure S1** UV-Vis absorption of compound **1** ($5\times10^{-6}$ mol/L in $CHCl_3$)

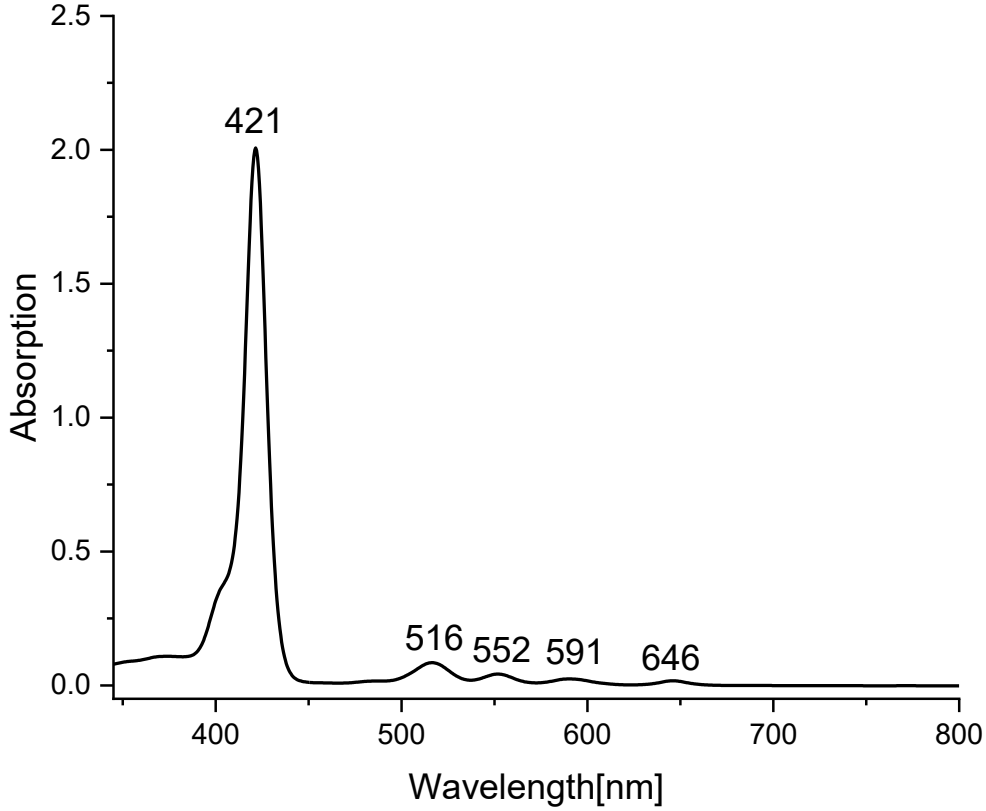



**Figure S2** UV-Vis absorption of compound **2** ($5\times10^{-6}$ mol/L in $CHCl_3$)

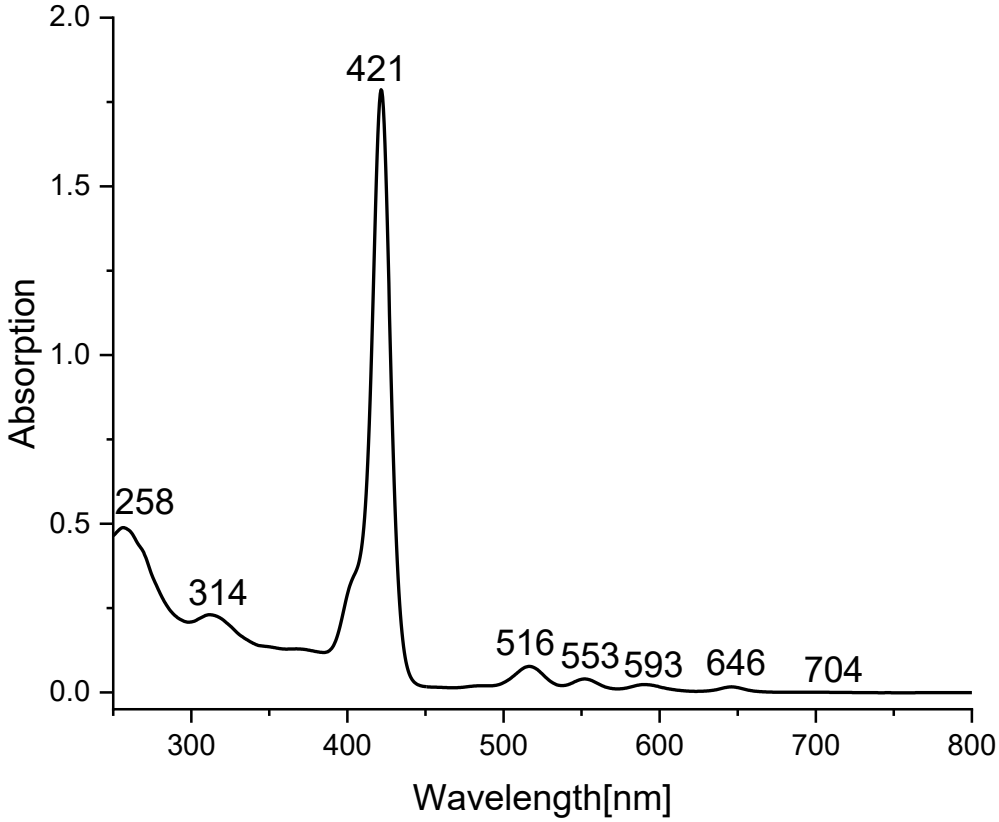



**Figure S3** UV-Vis absorption of compound **3a** ($5\times10^{-6}$ mol/L in $CHCl_3$)

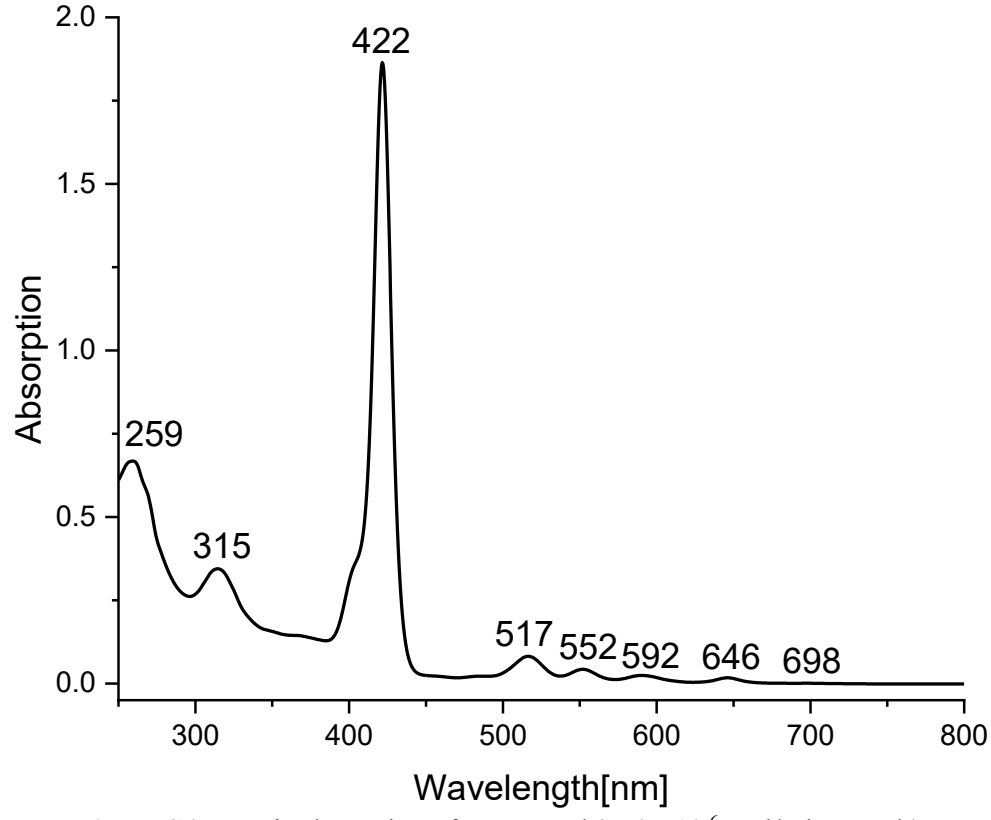



**Figure S4** UV-Vis absorption of compound **3b** ($5\times10^{-6}$ mol/L in $CHCl_3$)

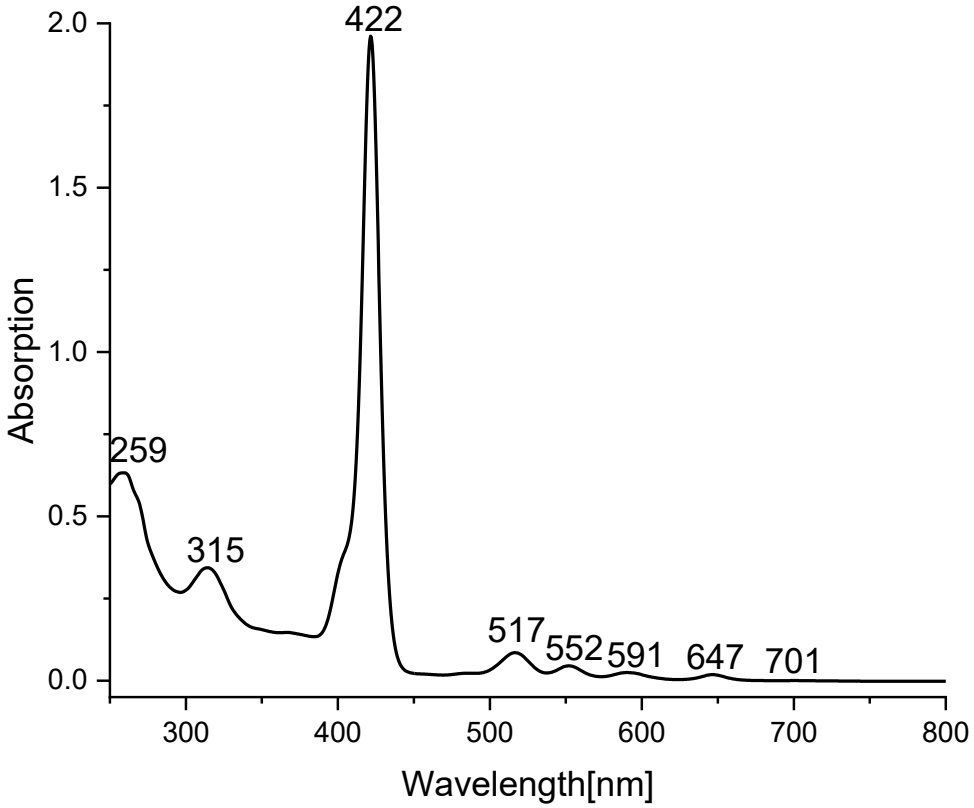



**Figure S5** UV-Vis absorption of compound **3c** ($5\times10^{-6}$ mol/L in $CHCl_3$)

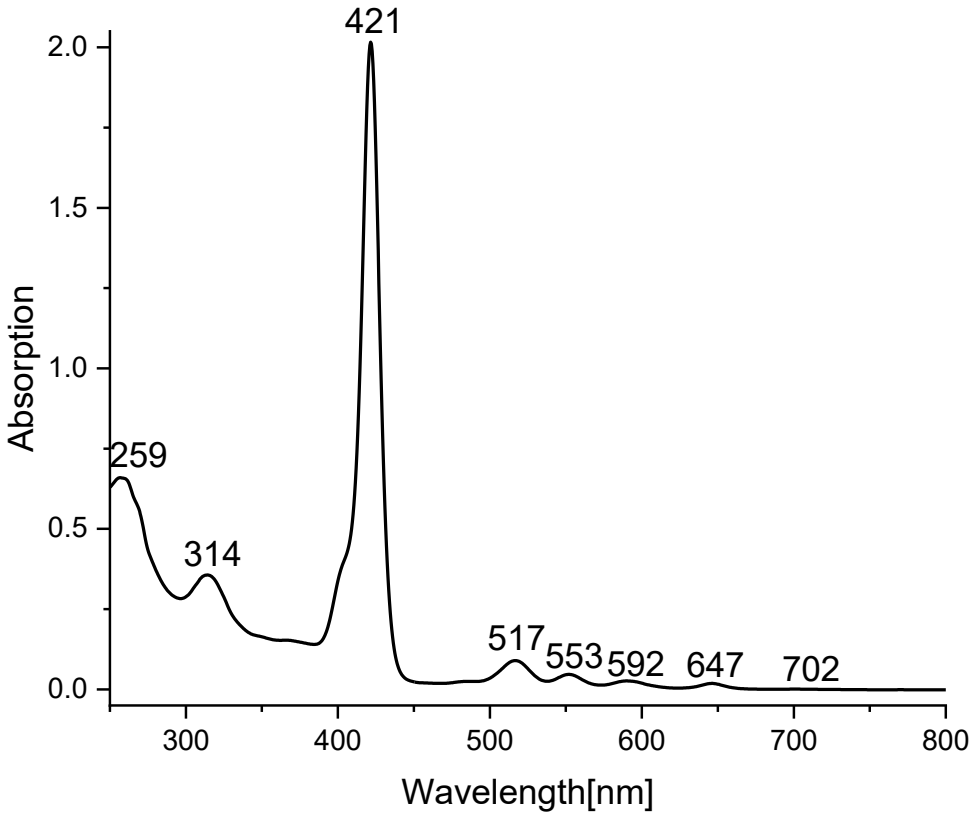



**Figure S6** UV-Vis absorption of compound **3d** ($5\times10^{-6}$ mol/L in $CHCl_3$)

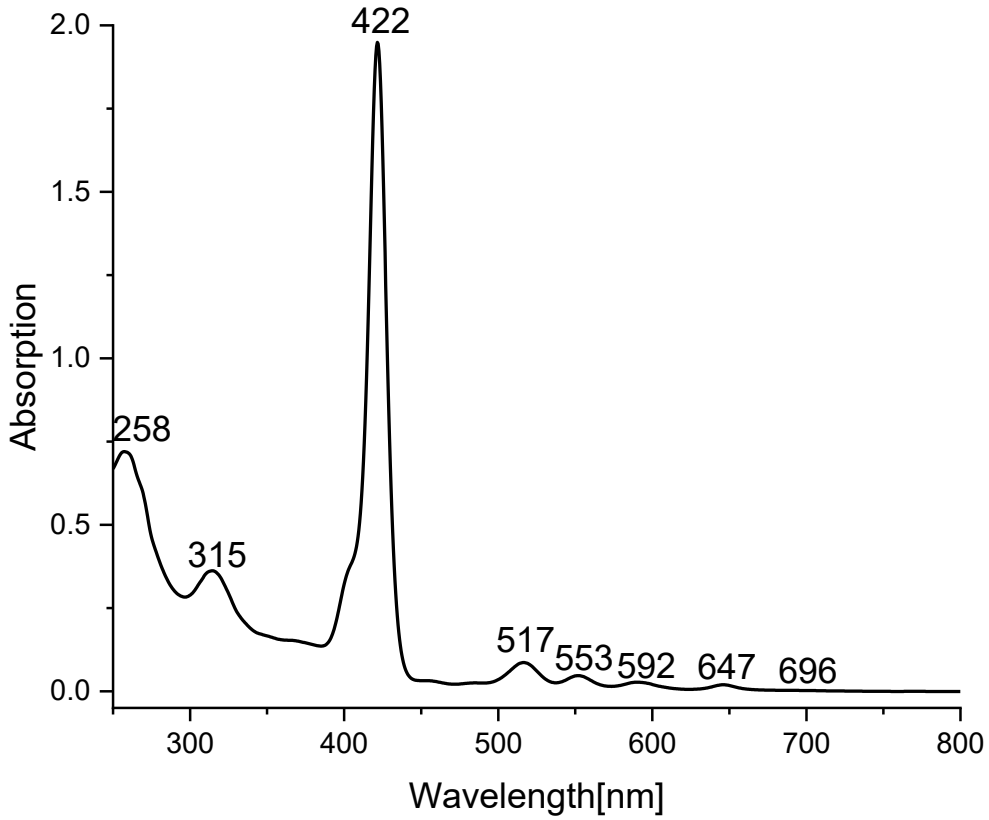



**Figure S7** UV-Vis absorption of compound **3e** ($5\times10^{-6}$ mol/L in $CHCl_3$)

## 6. CVs and DPVs of compounds 1, 2 and 3a-e

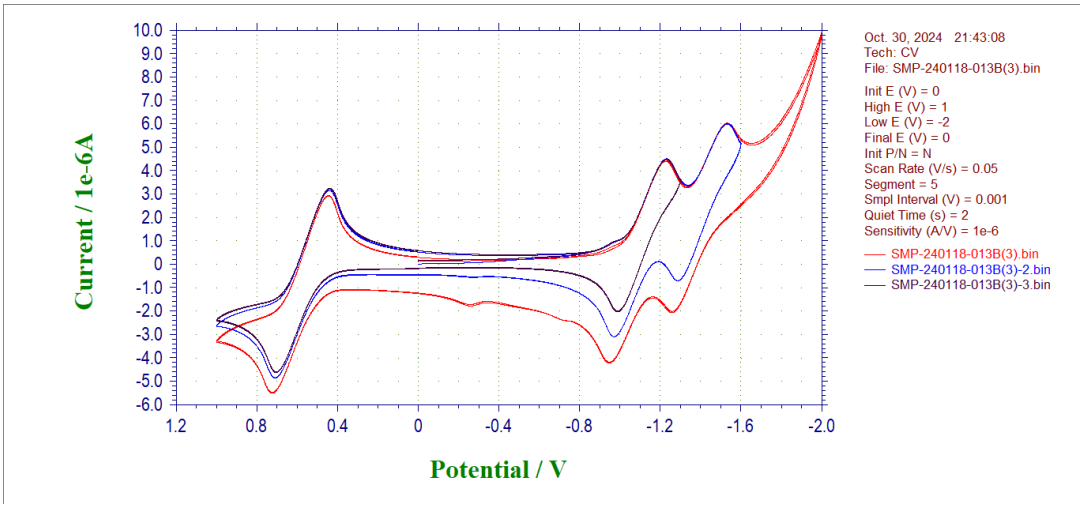



**Figure S8** CV of compound **1**

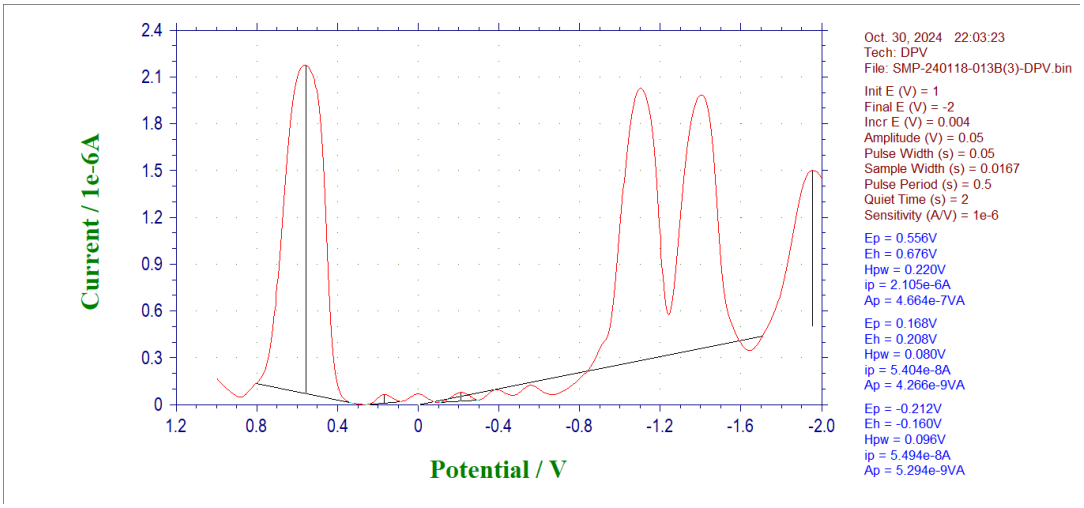



**Figure S9** DPV of compound **1**

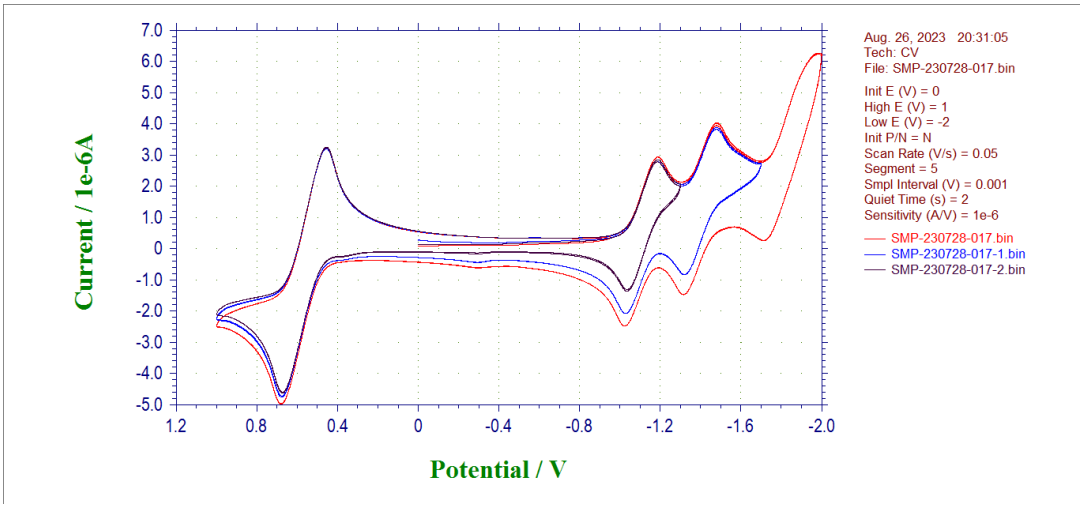



**Figure S10** CV of compound **2**

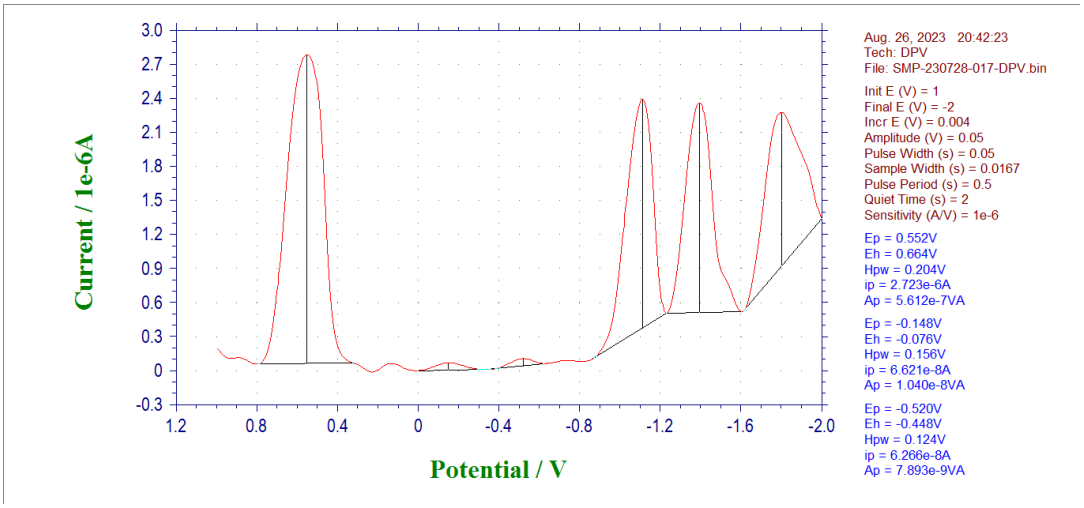



**Figure S11** DPV of compound **2**

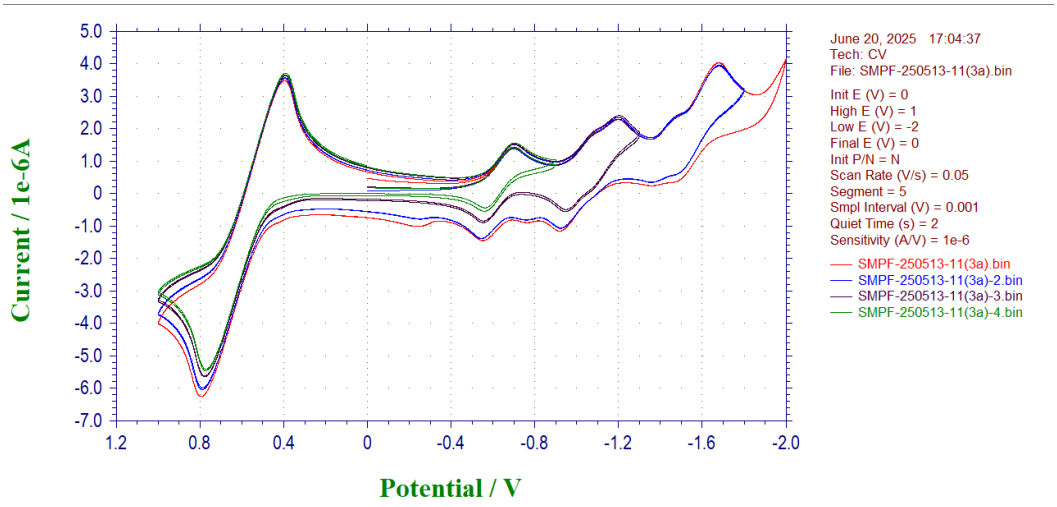



**Figure S12** CV of compound **3a**

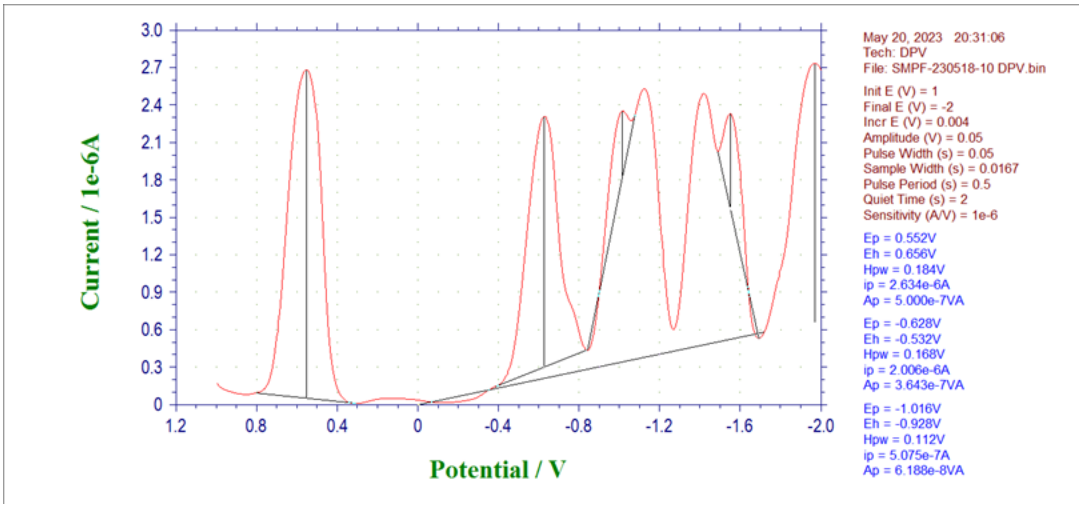



**Figure S13** DPV of compound **3a**

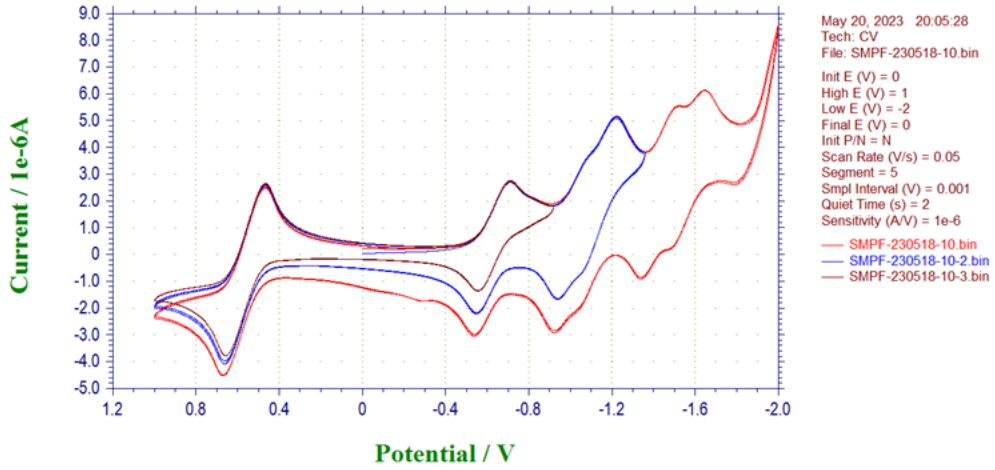



**Figure S14** CV of compound **3b**

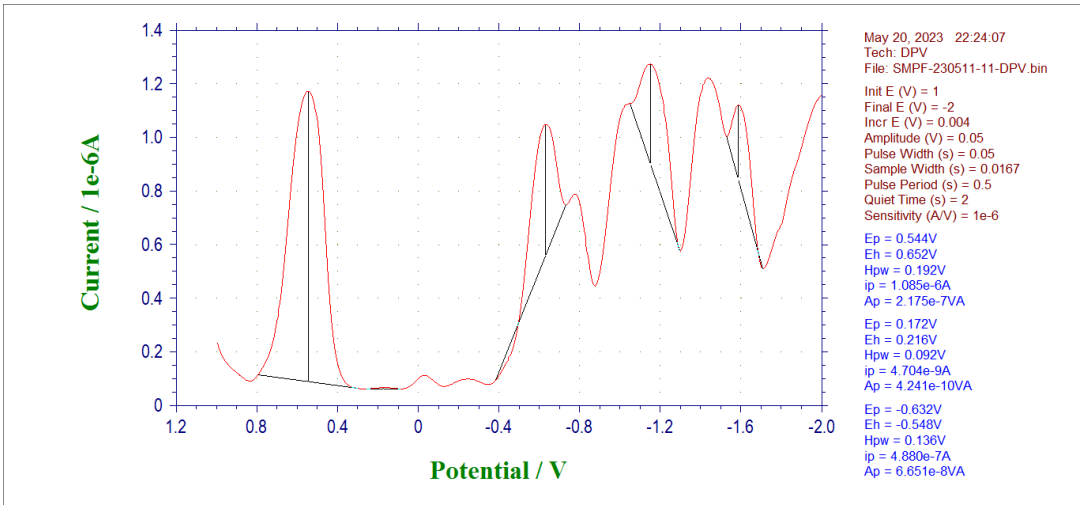



**Figure S15** DPV of Compound **3b**

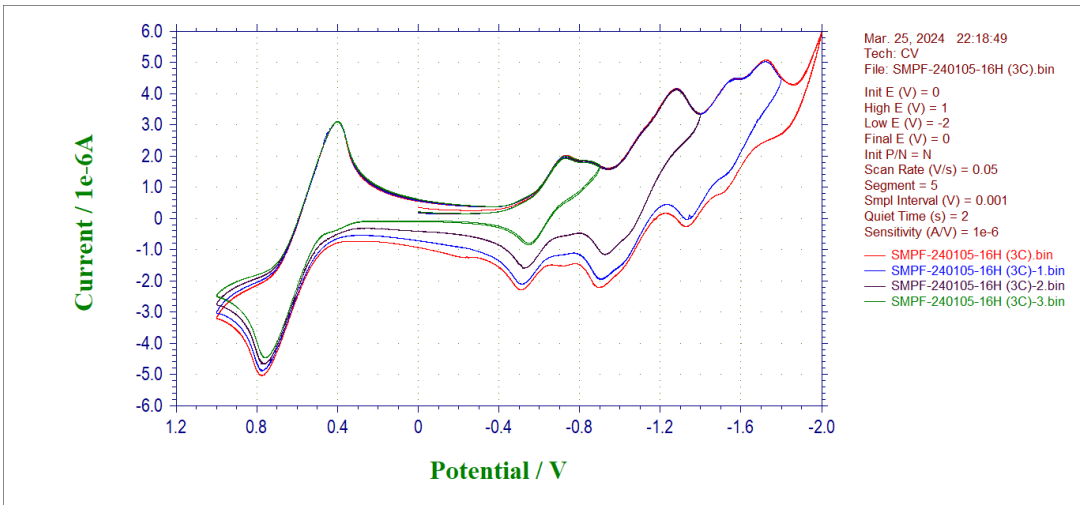



**Figure S16** CV of compound **3c**

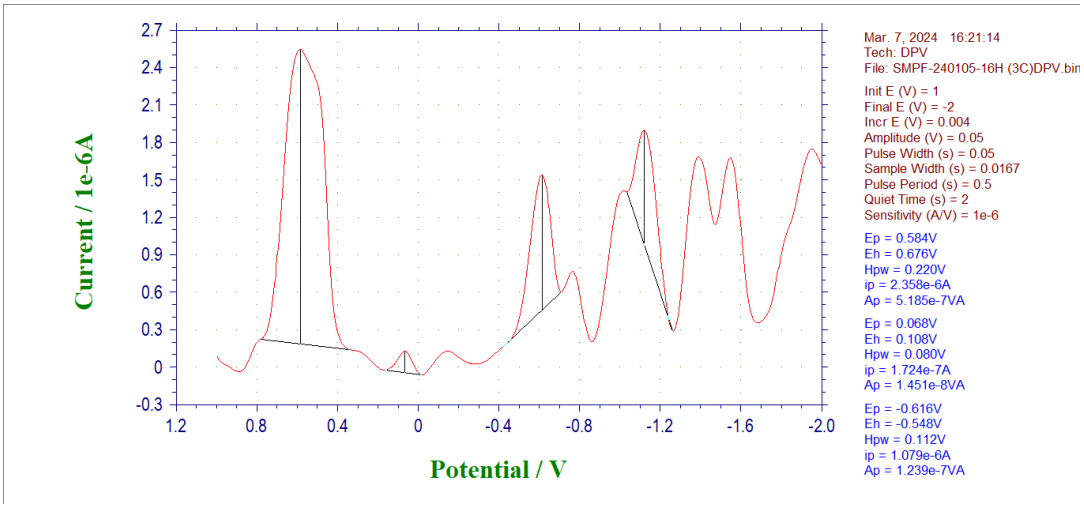



**Figure S17** DPV of compound **3c**

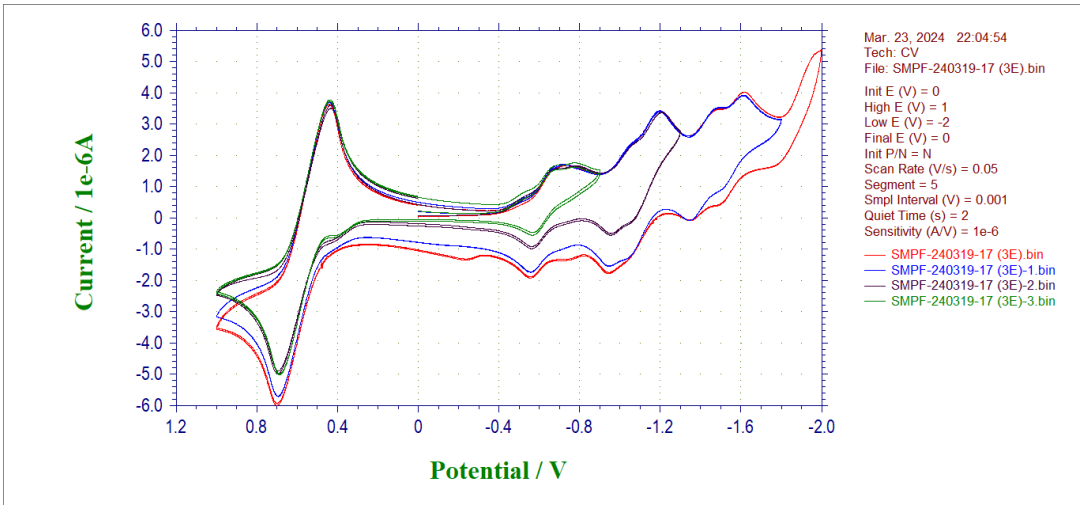



**Figure S18** CV of compound **3d**

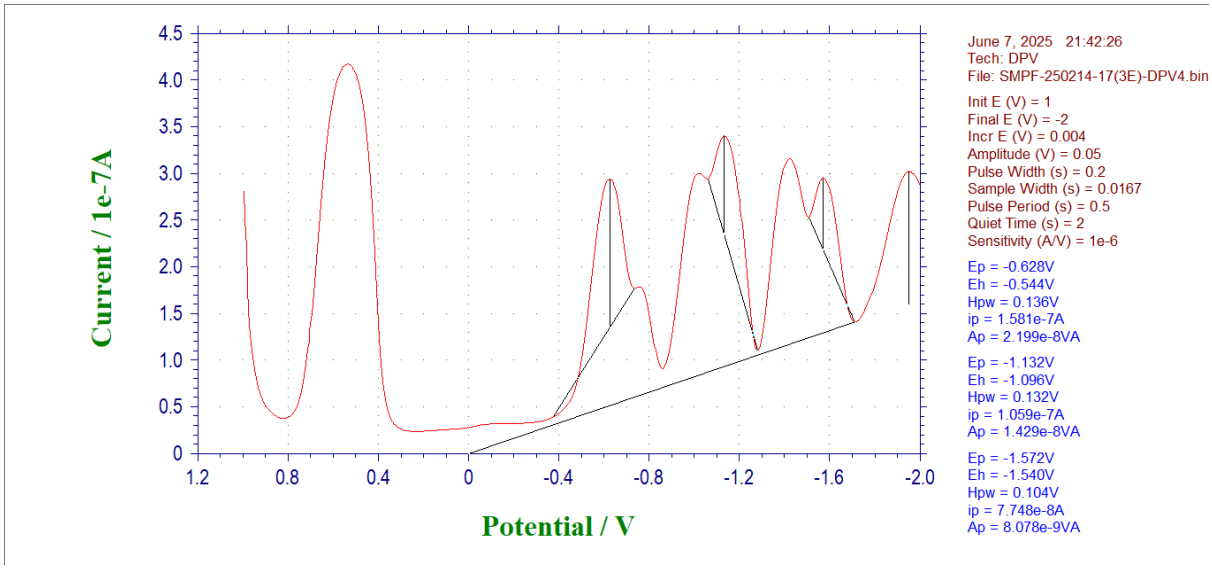



**Figure S19** DPV of compound **3d**

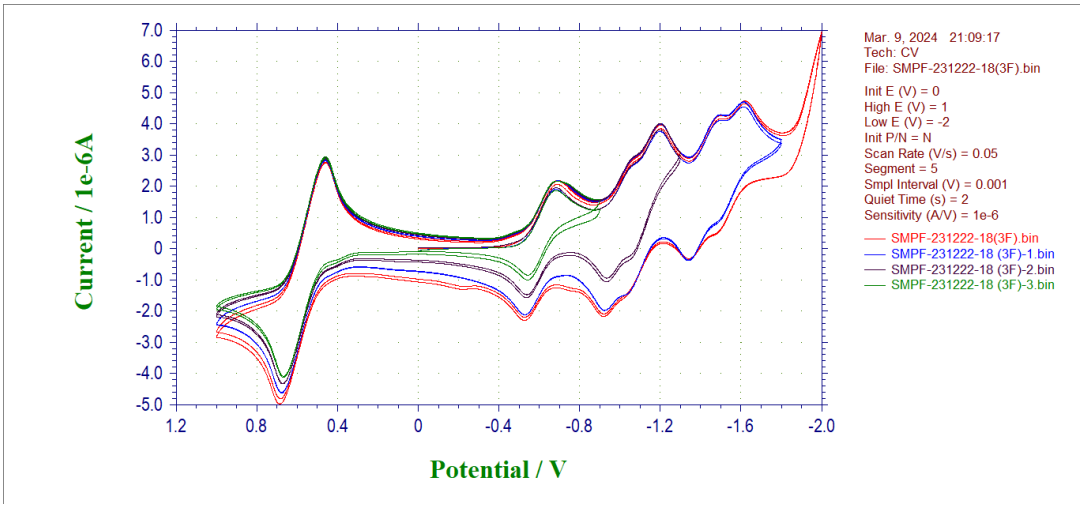



**Figure S20** CV of compound **3e**

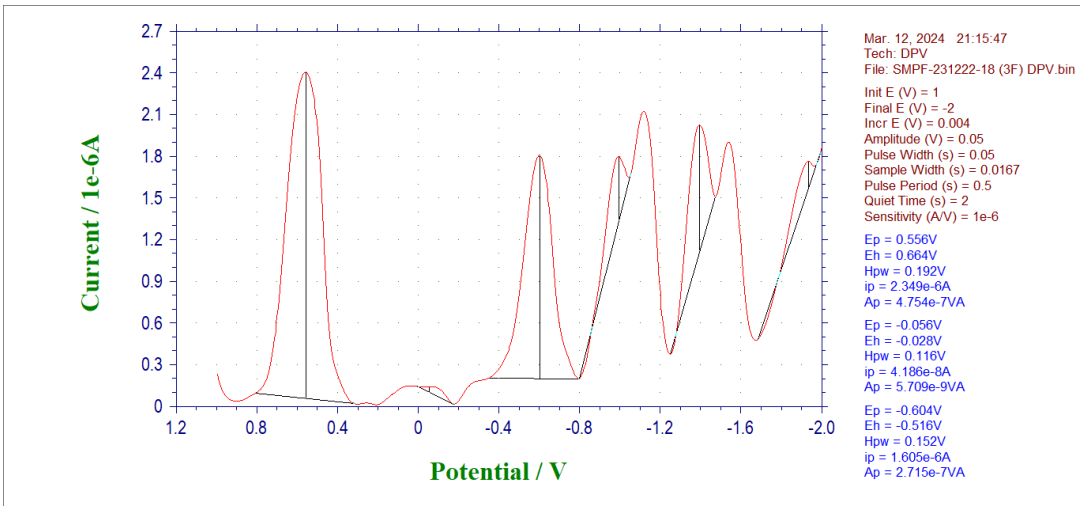



**Figure S21** DPV of compound **3e**

## 7. NMR spectra of compounds 1, 2, and 3a-e

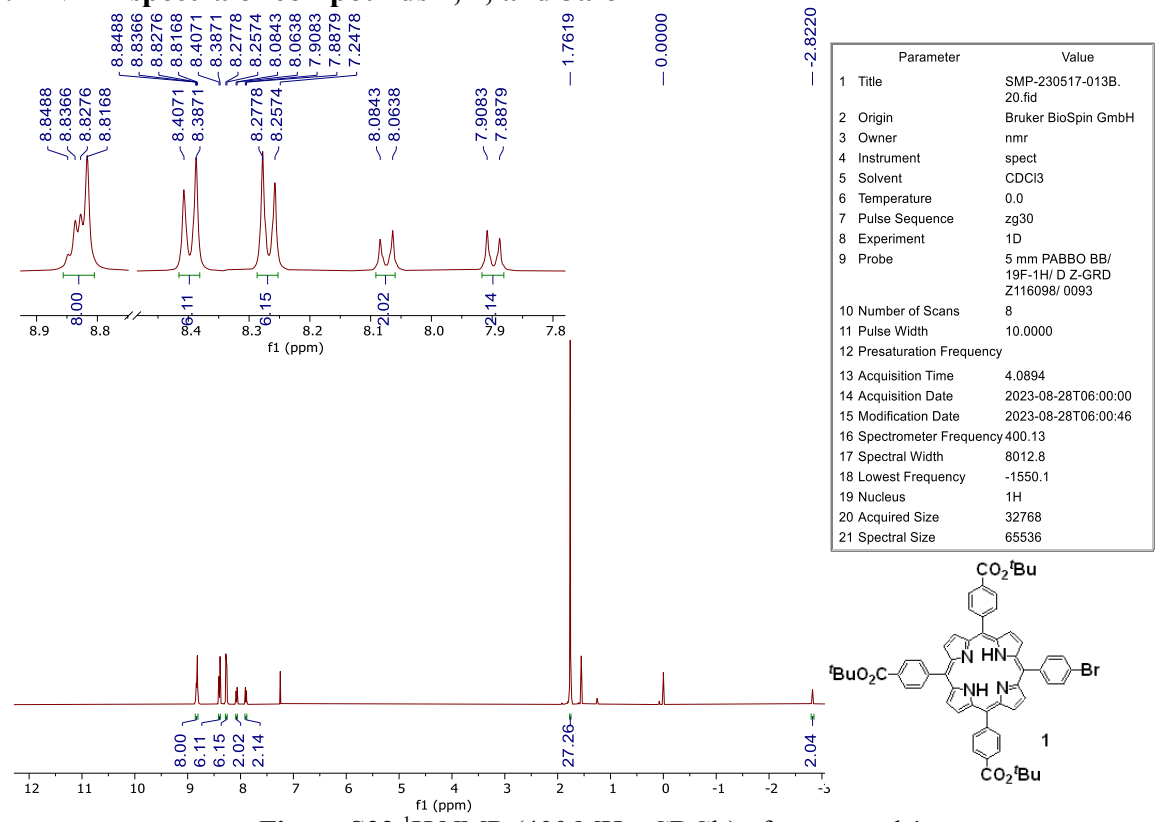



**Figure S22** $^{1}$H NMR (400 MHz, $CDCl_3$) of compound **1**

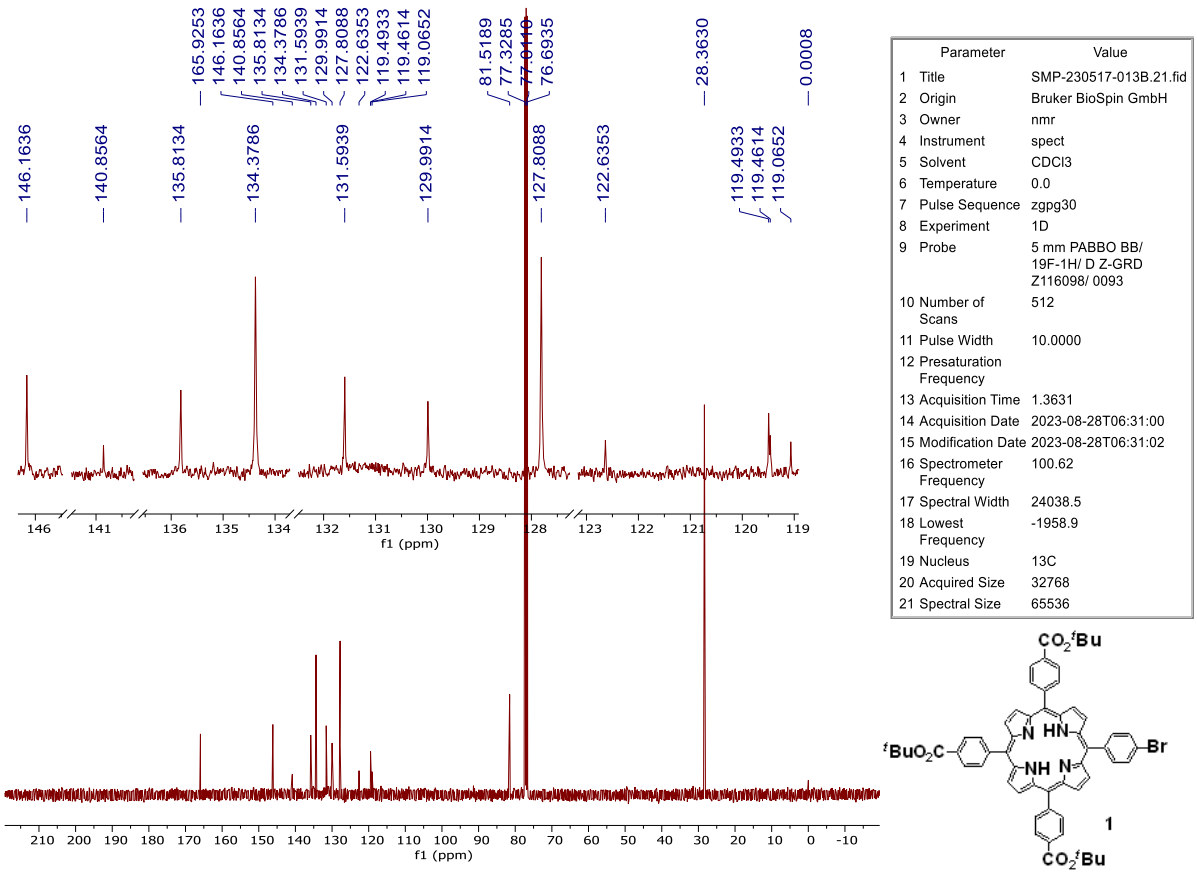



**Figure S23** $^{13}$C{$^{1}$H} NMR (101 MHz, $CDCl_3$) of compound **1**

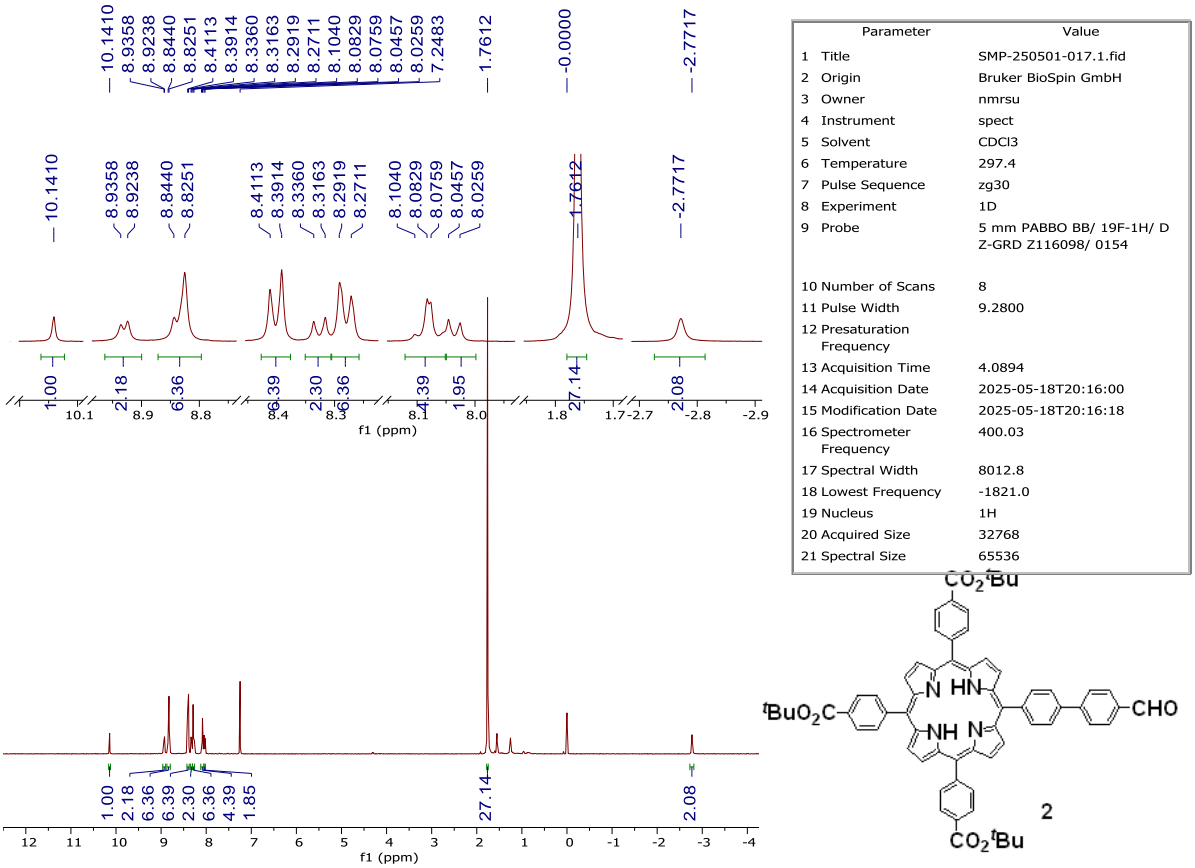



**Figure S24** $^{1}$H NMR (400 MHz, $CDCl_3$) of compound **2**

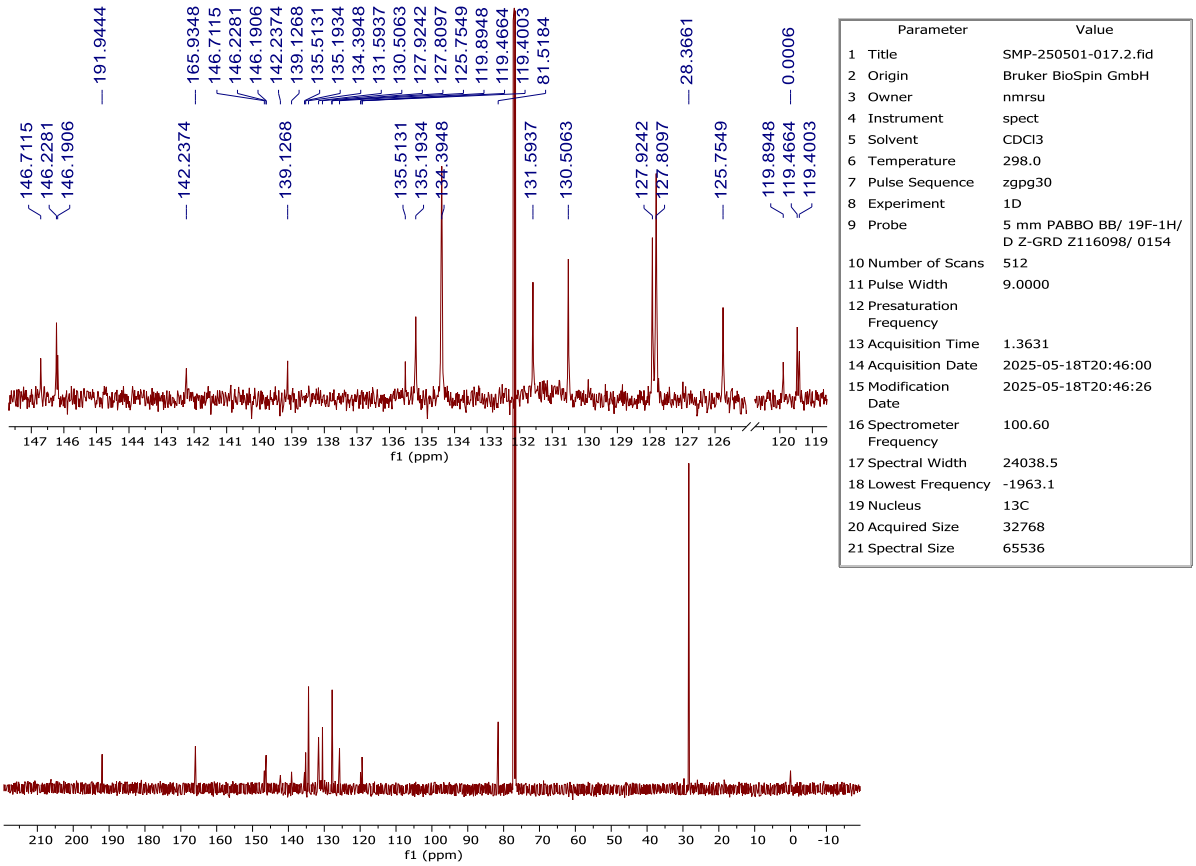



**Figure S25** $^{13}C\{^{1}H\}$ NMR (101 MHz, $CDCl_3$) of compound **2**

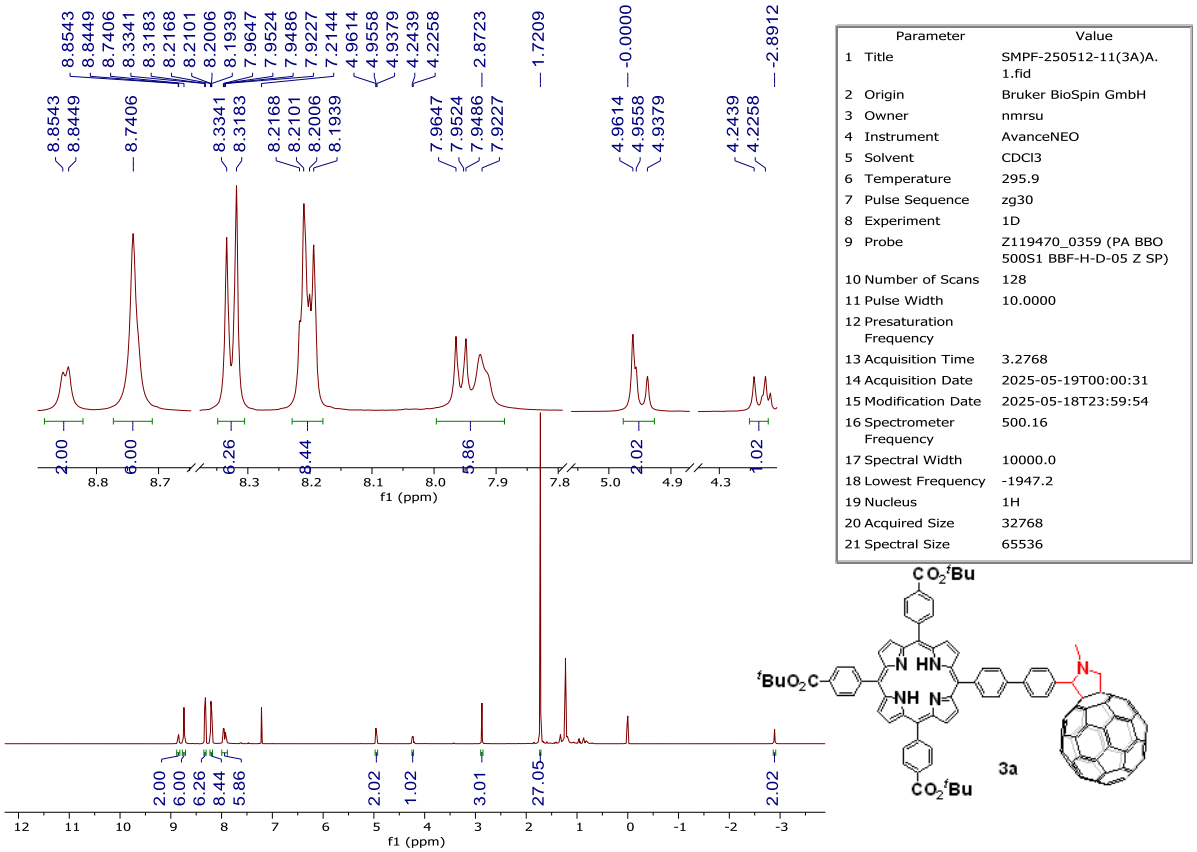



**Figure S26** $^{1}$H NMR (500 MHz, $CS_2/CDCl_3$) of compound **3a**

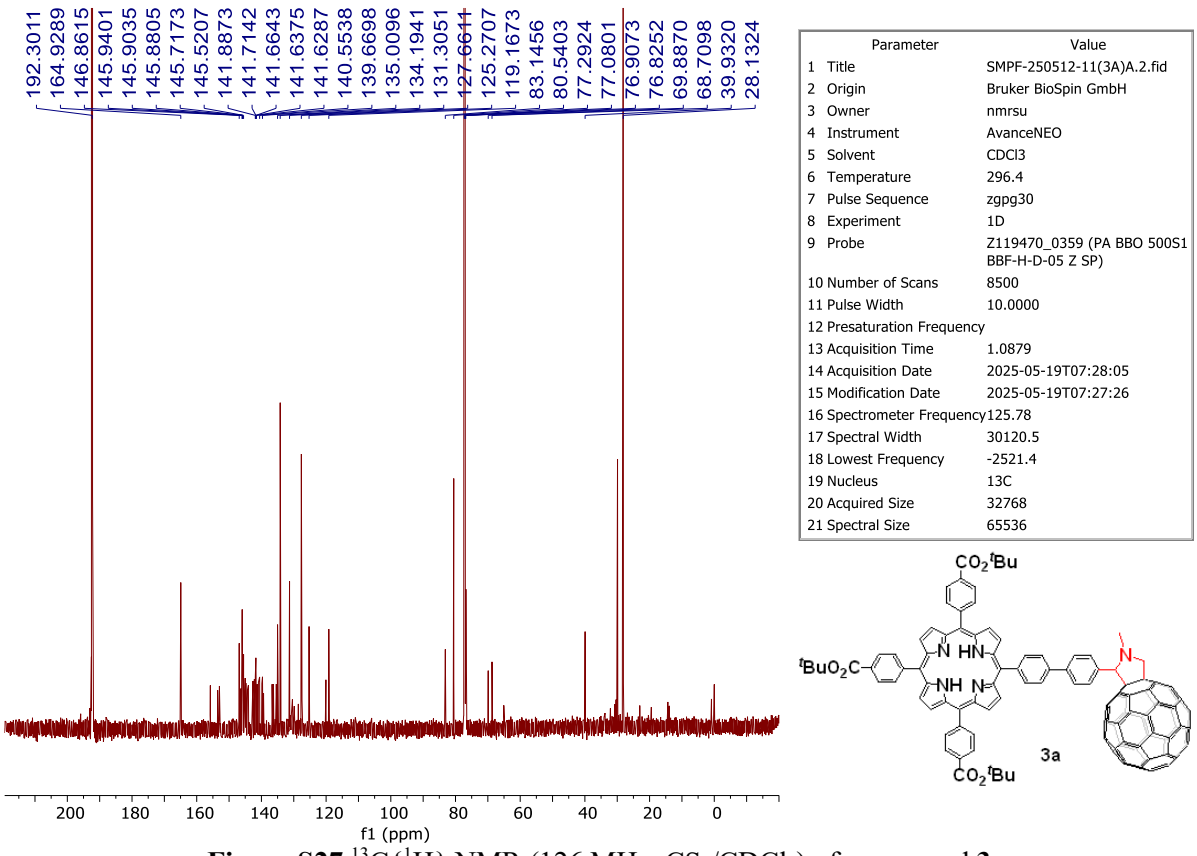



**Figure S27** $^{13}C\{^{1}H\}$ NMR (126 MHz, $CS_2/CDCl_3$) of compound **3a**

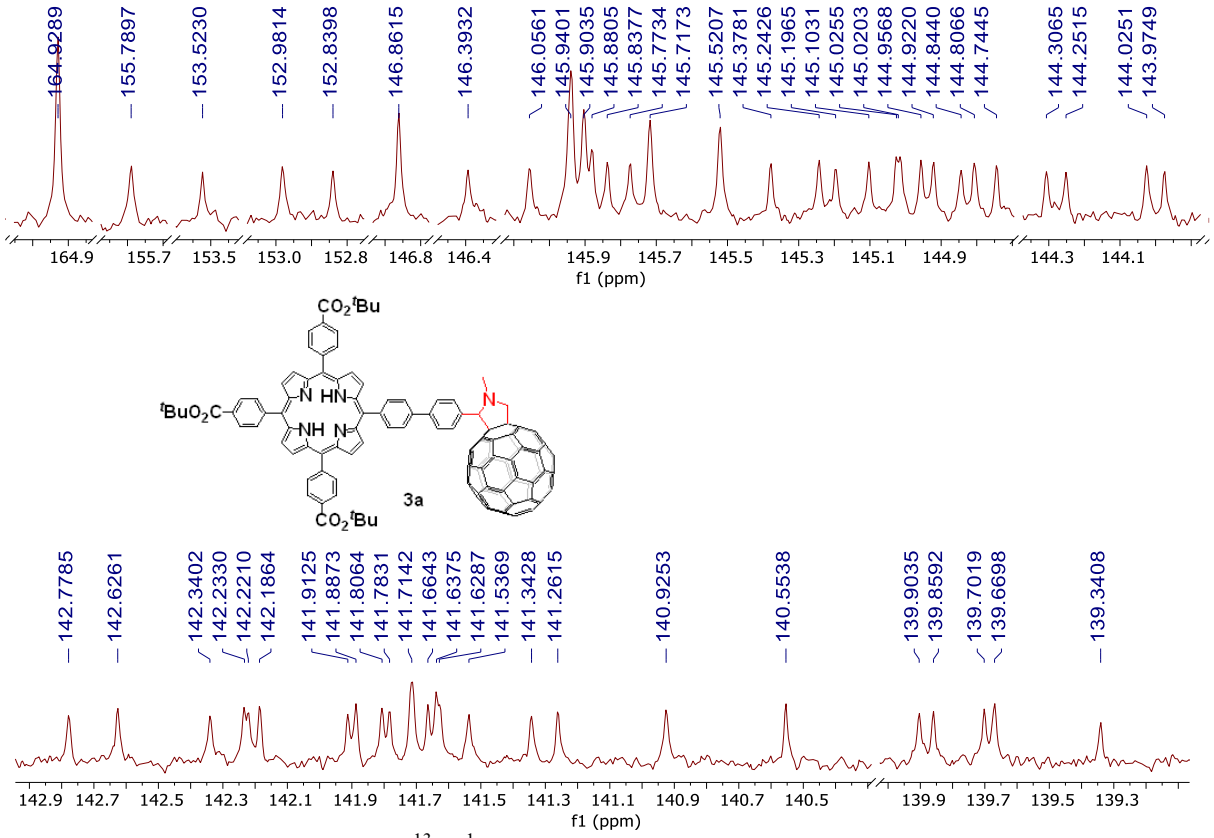



**Figure S28** Expanded $^{13}C\{^{1}H\}$ NMR (126 MHz, $CS_2/CDCl_3$) of compound **3a**

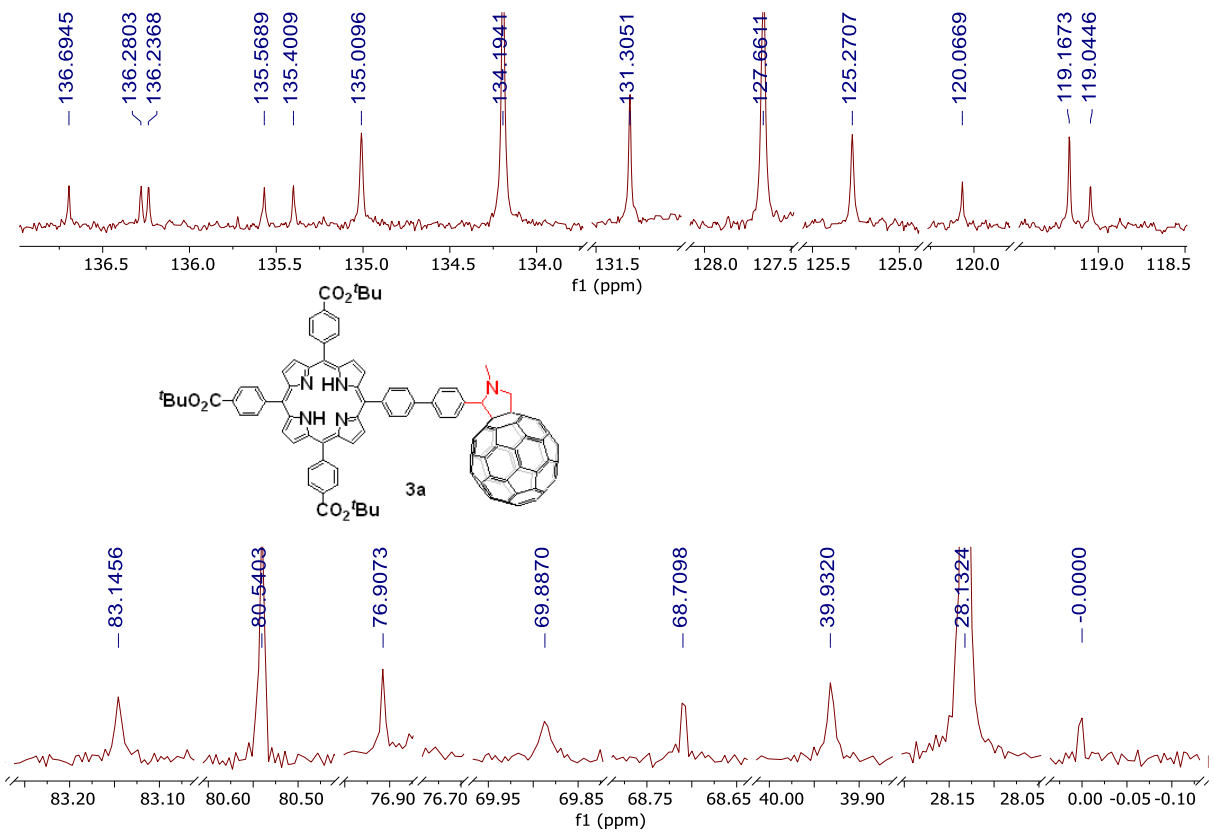



**Figure S29** Expanded $^{13}C\{^{1}H\}$ NMR (126 MHz, $CS_2/CDCl_3$) of compound **3a**

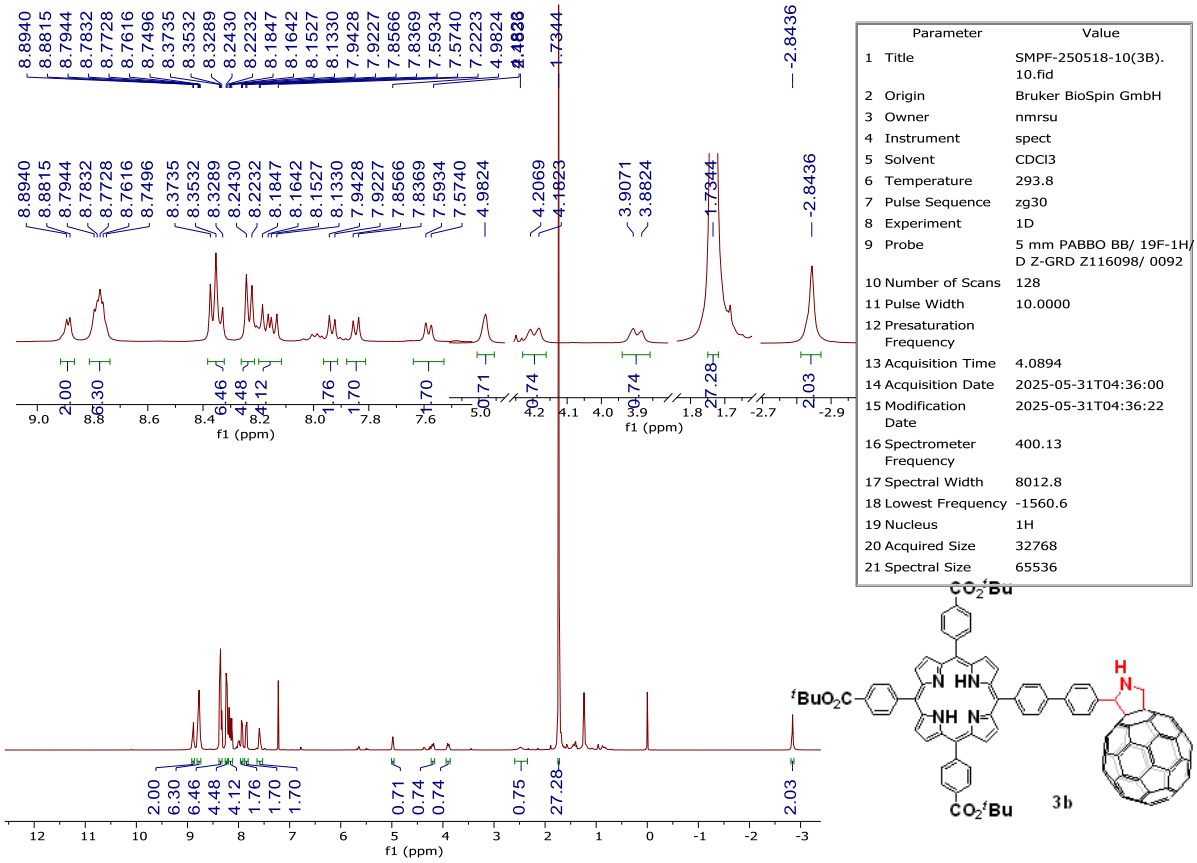



**Figure S30** $^{1}$H NMR (400 MHz, $CS_2$/$CDCl_3$) of compound **3b**

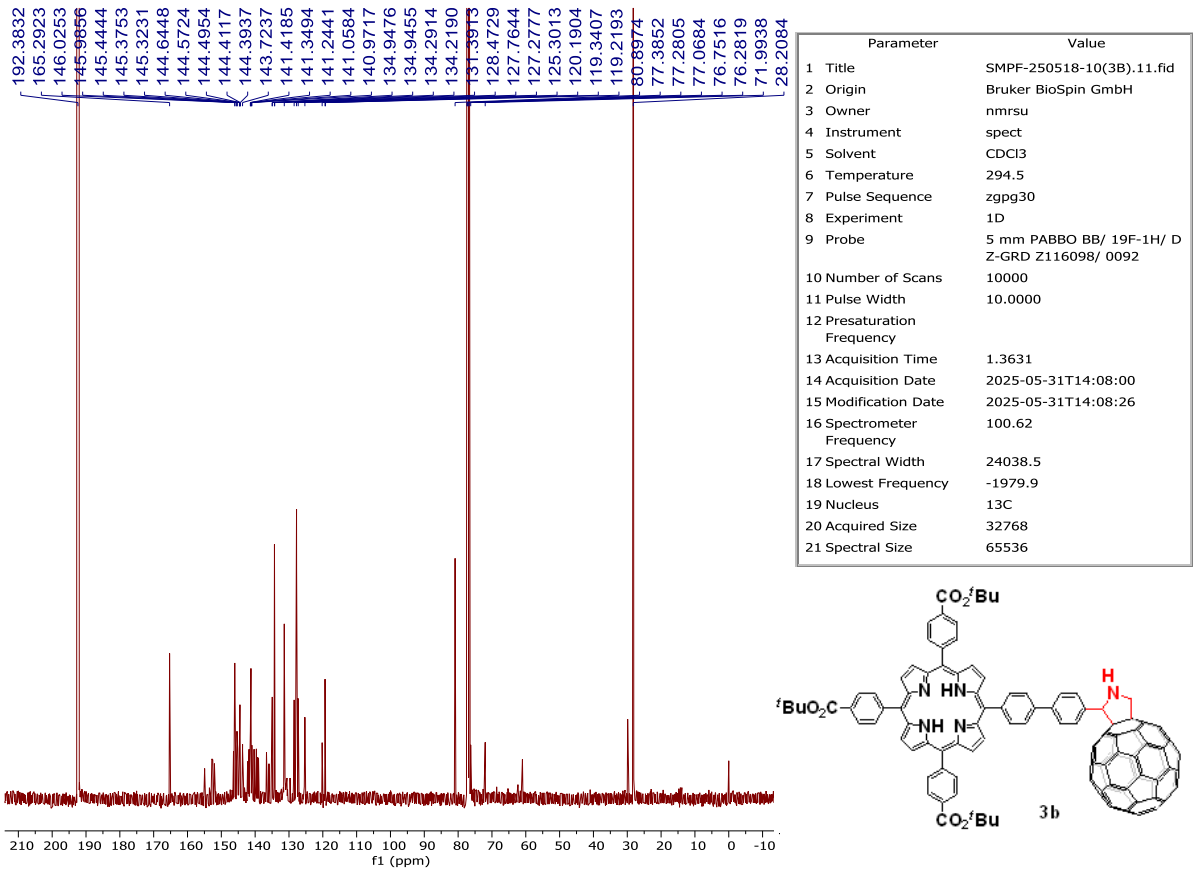



**Figure S31** $^{13}$C{$^{1}$H} NMR (101 MHz, $CS_2$/$CDCl_3$) of compound **3b**

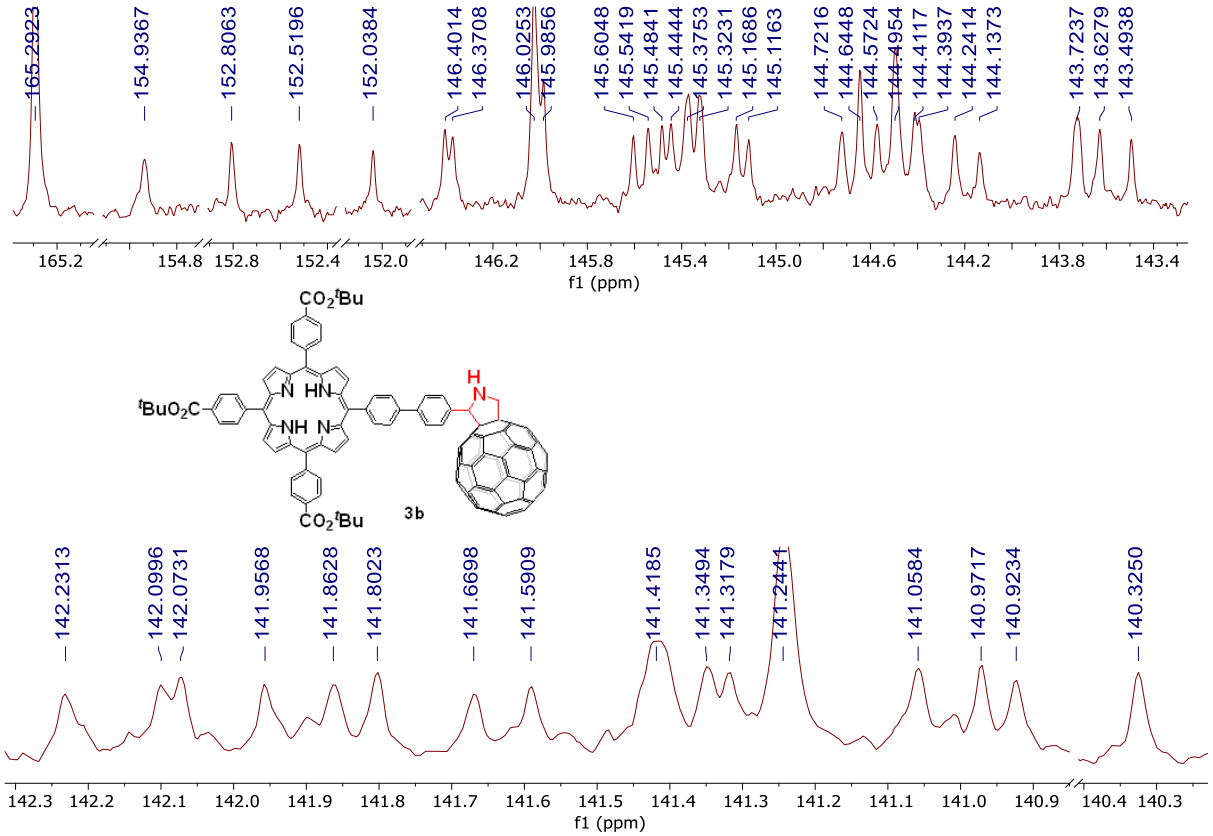



**Figure S32** Expanded $^{13}C\{^{1}H\}$ NMR (101 MHz, $CS_2/CDCl_3$) of compound **3b**

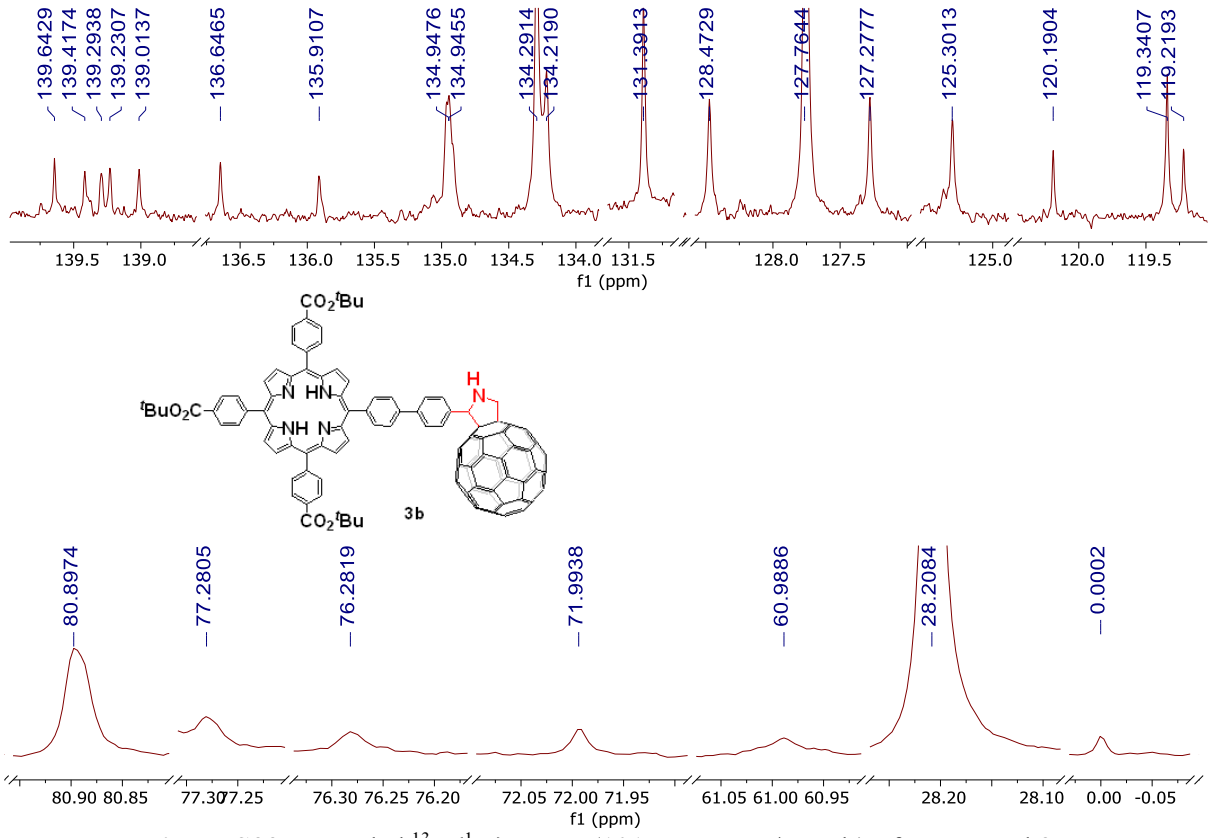



**Figure S33** Expanded $^{13}C\{^{1}H\}$ NMR (101 MHz, $CS_2/CDCl_3$) of compound **3b**

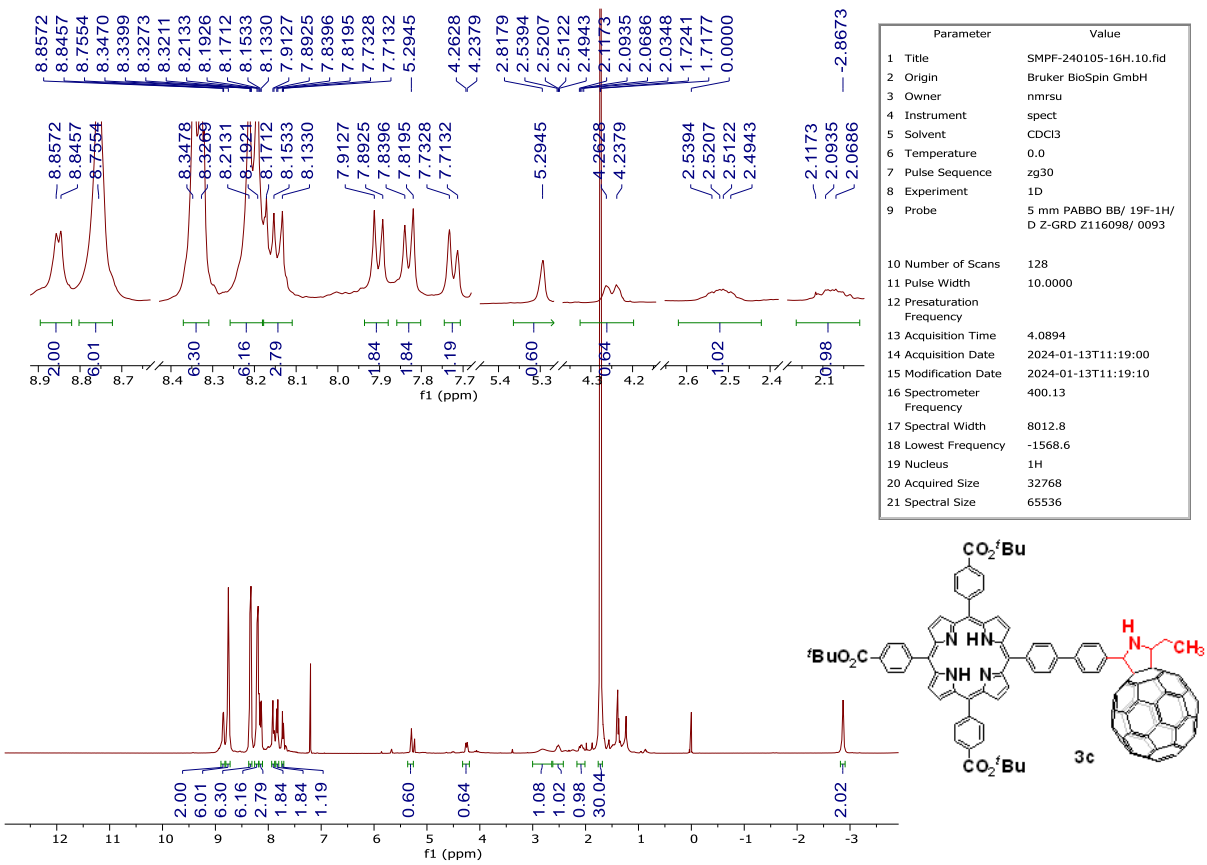



**Figure S34** $^{1}$H NMR (400 MHz, $CS_2/CDCl_3$) of compound **3c**

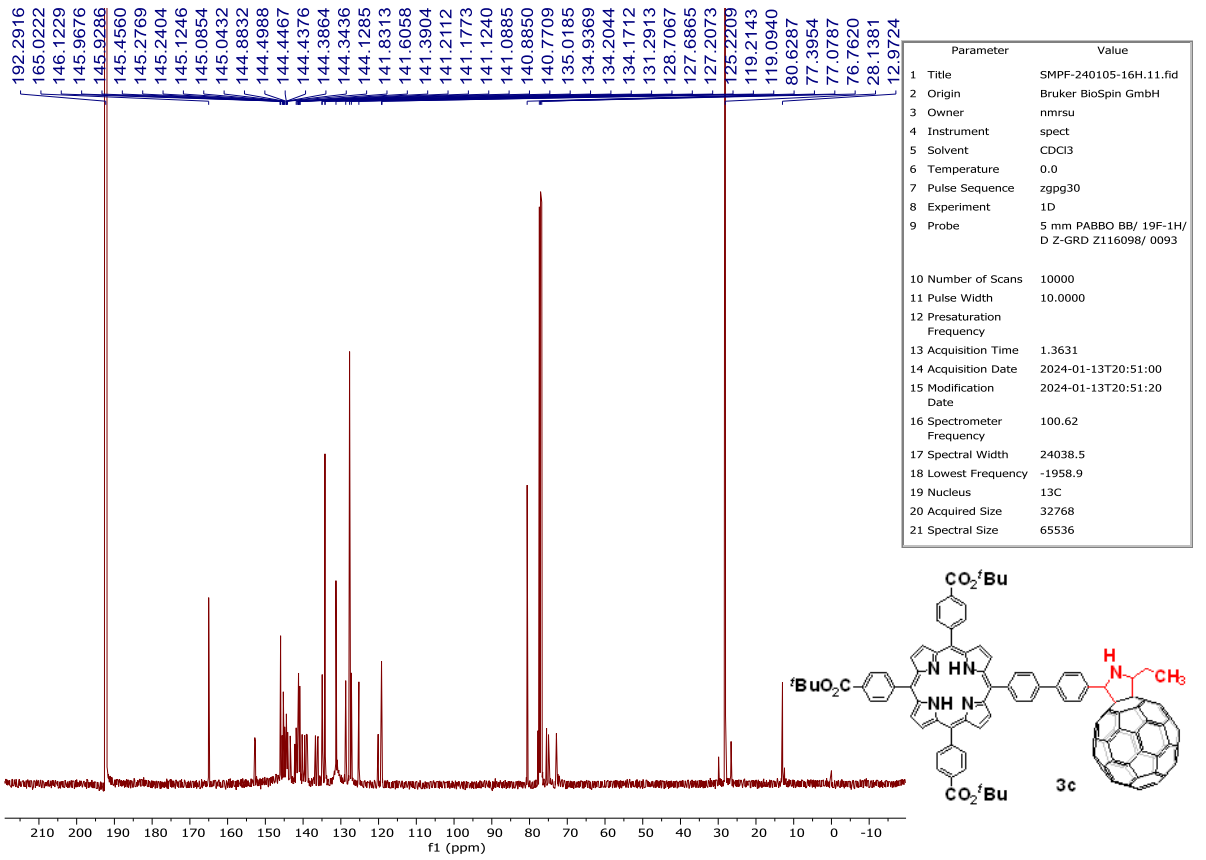



**Figure S35** $^{13}C\{^{1}H\}$ NMR (101 MHz, $CS_2/CDCl_3$) of compound **3c**

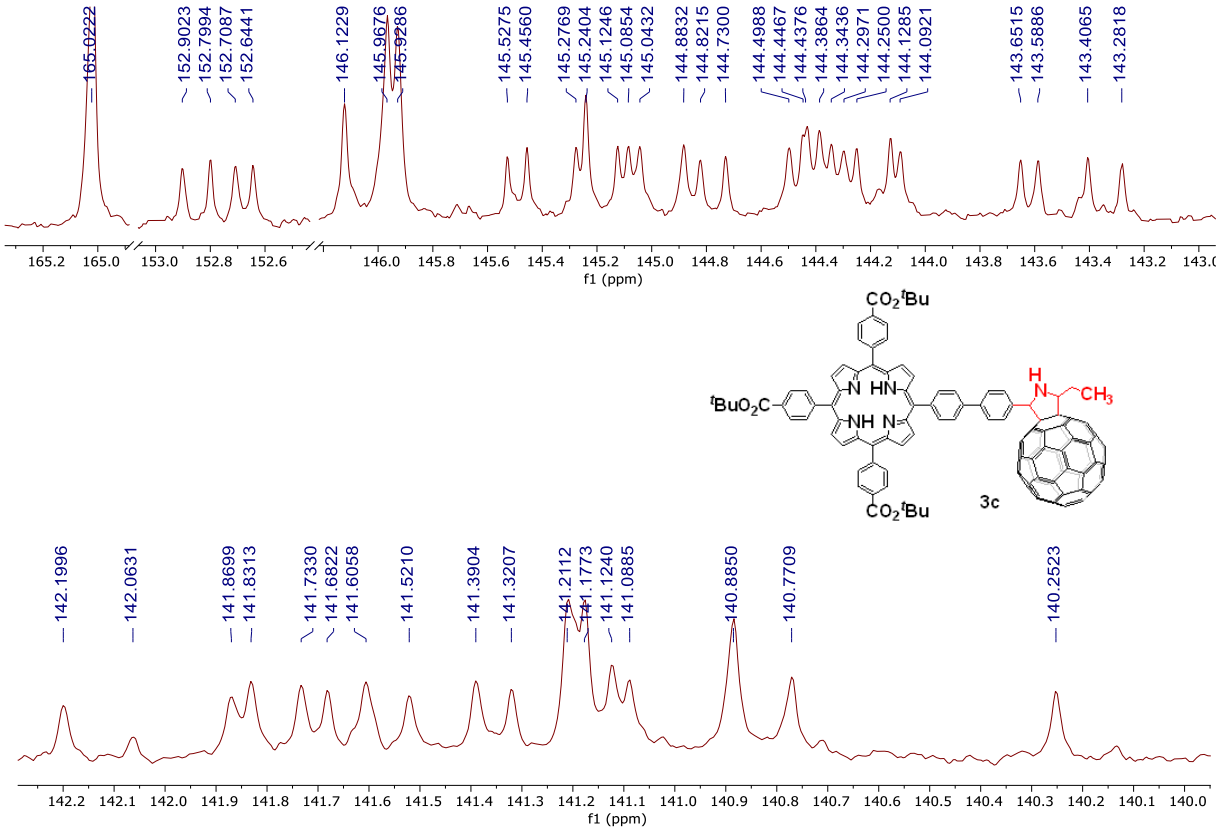



**Figure S36** Expanded $^{13}C\{^{1}H\}$ NMR (101 MHz, $CS_2/CDCl_3$) of compound **3c**

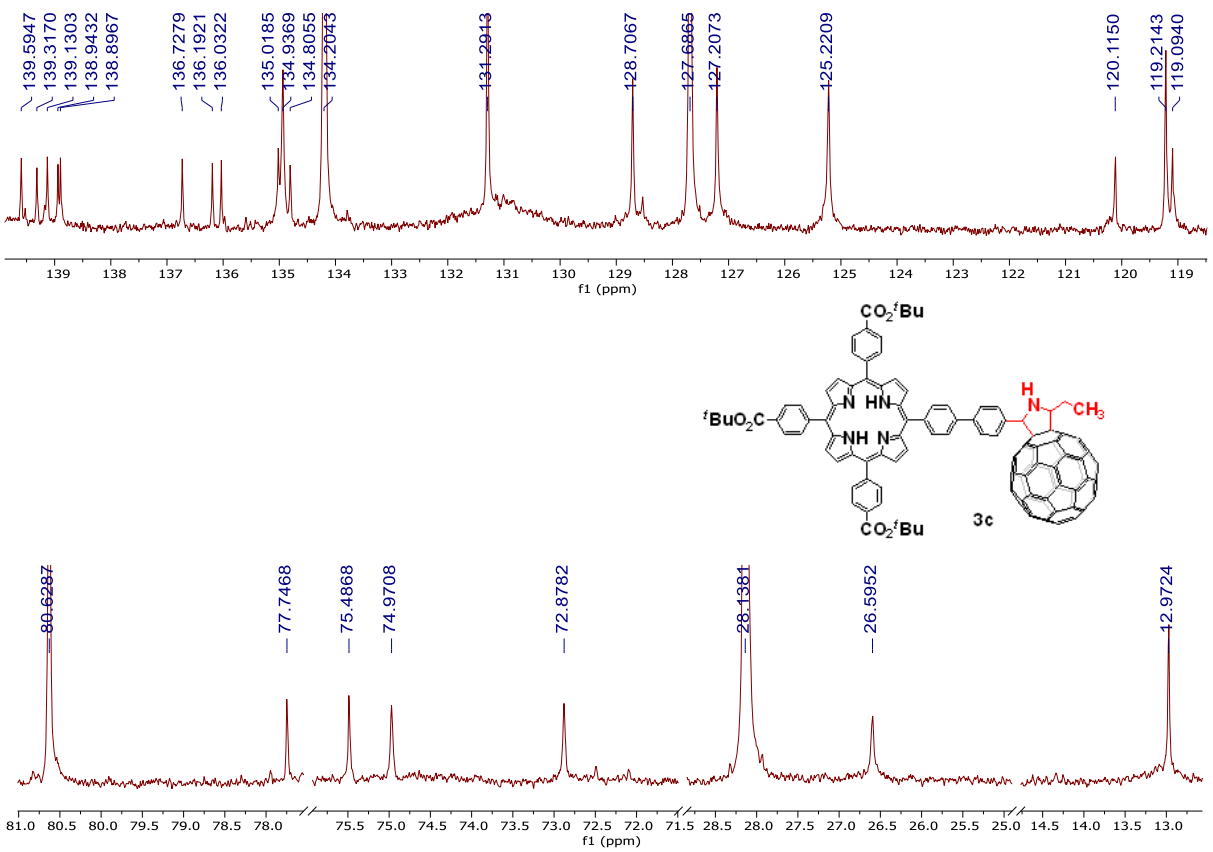



**Figure S37** Expanded $^{13}C\{^{1}H\}$ NMR (101 MHz, $CS_2/CDCl_3$) of compound **3c**

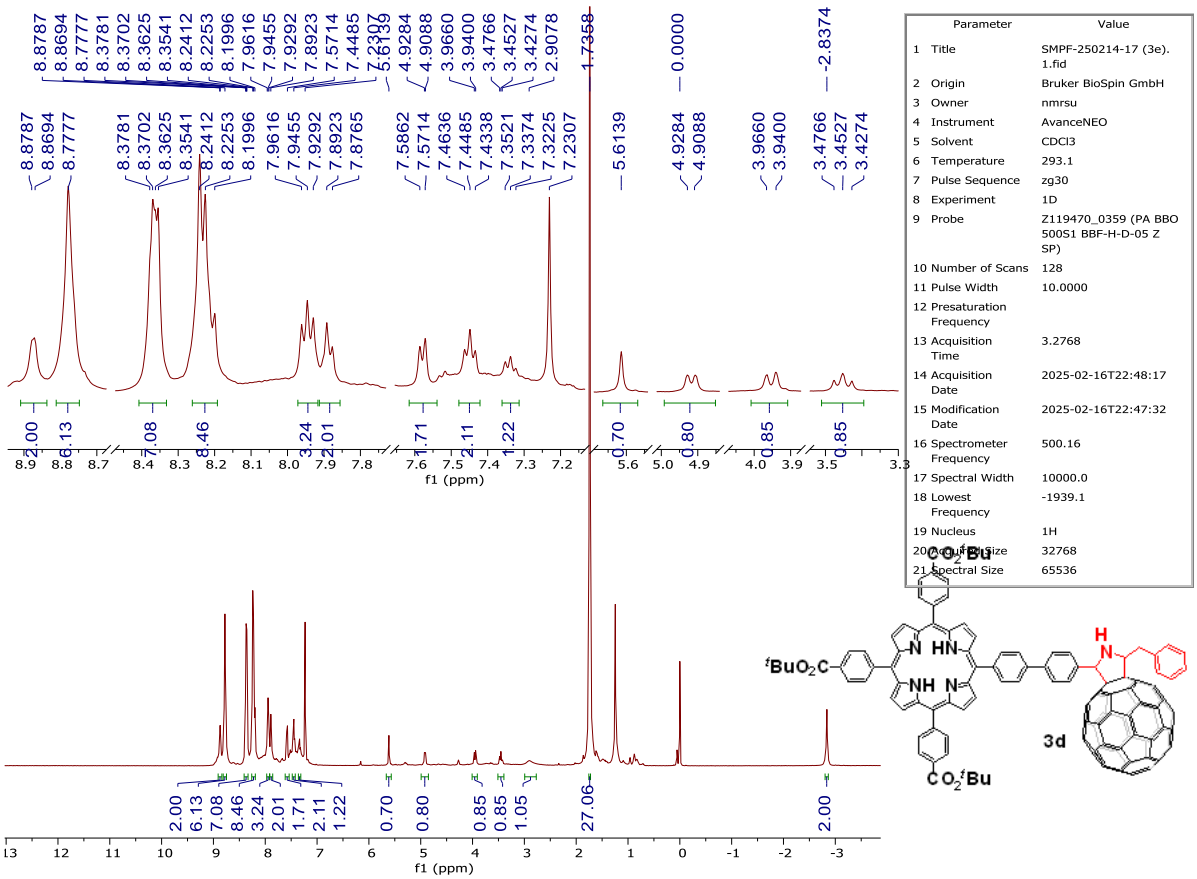



**Figure S38** $^{1}$H NMR (500 MHz, $CS_2/CDCl_3$) of compound **3d**

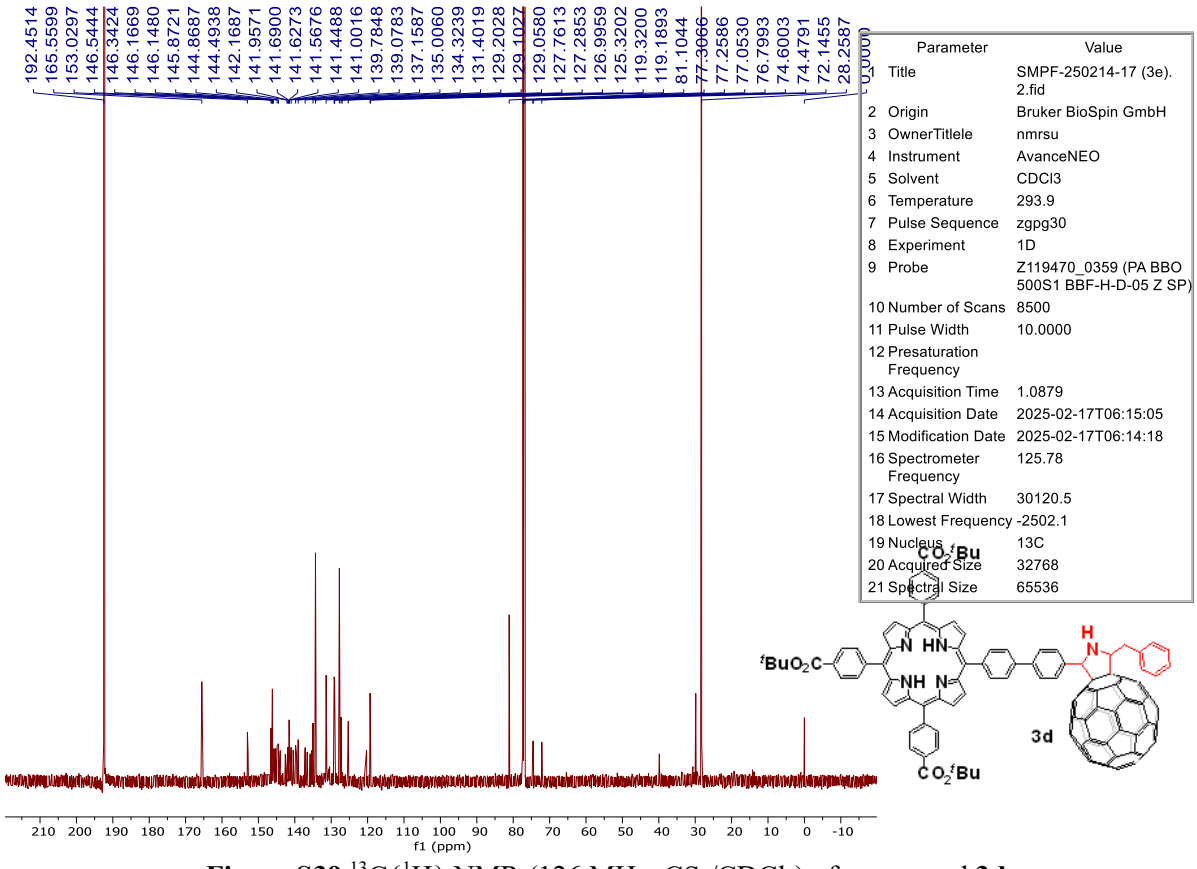



**Figure S39** $^{13}C\{^{1}H\}$ NMR (126 MHz, $CS_2/CDCl_3$) of compound **3d**

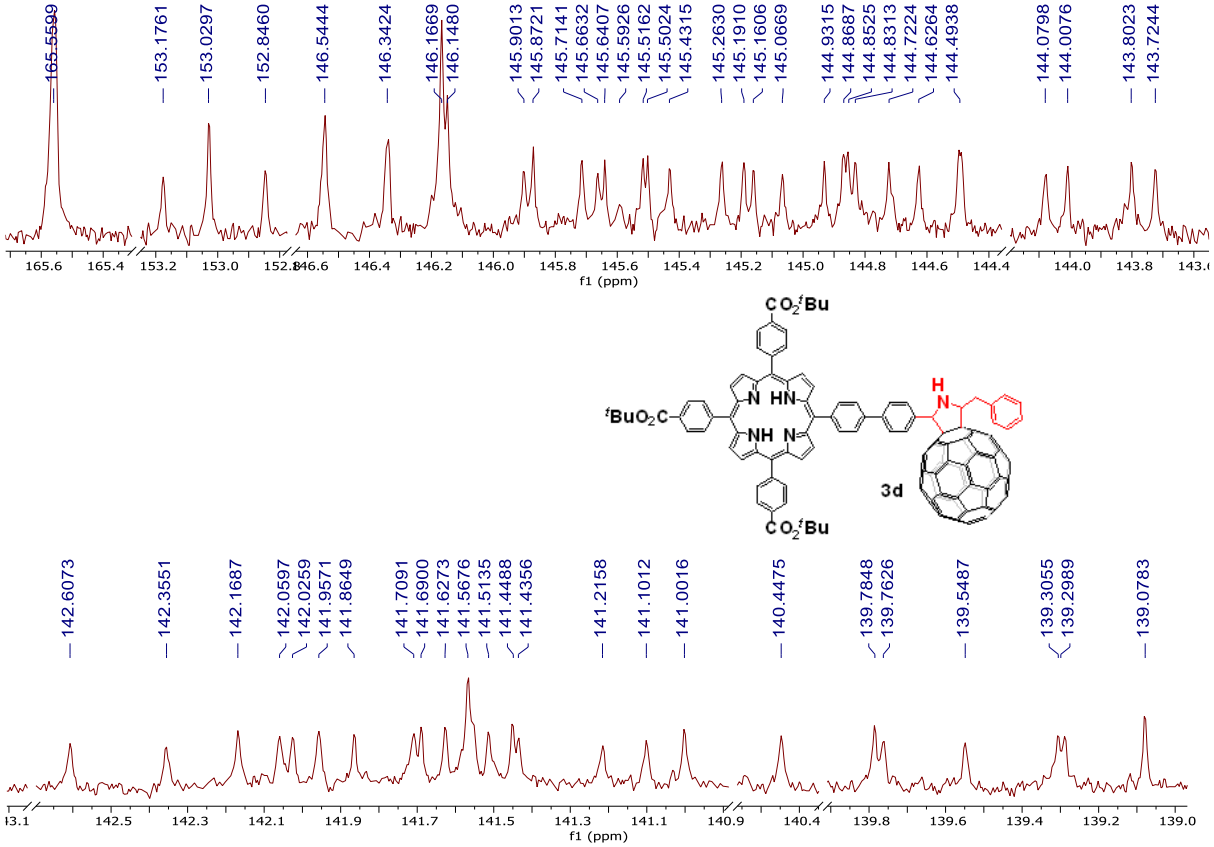



**Figure S40** Expanded $^{13}C\{^{1}H\}$ NMR (126 MHz, $CS_2/CDCl_3$) of compound **3d**

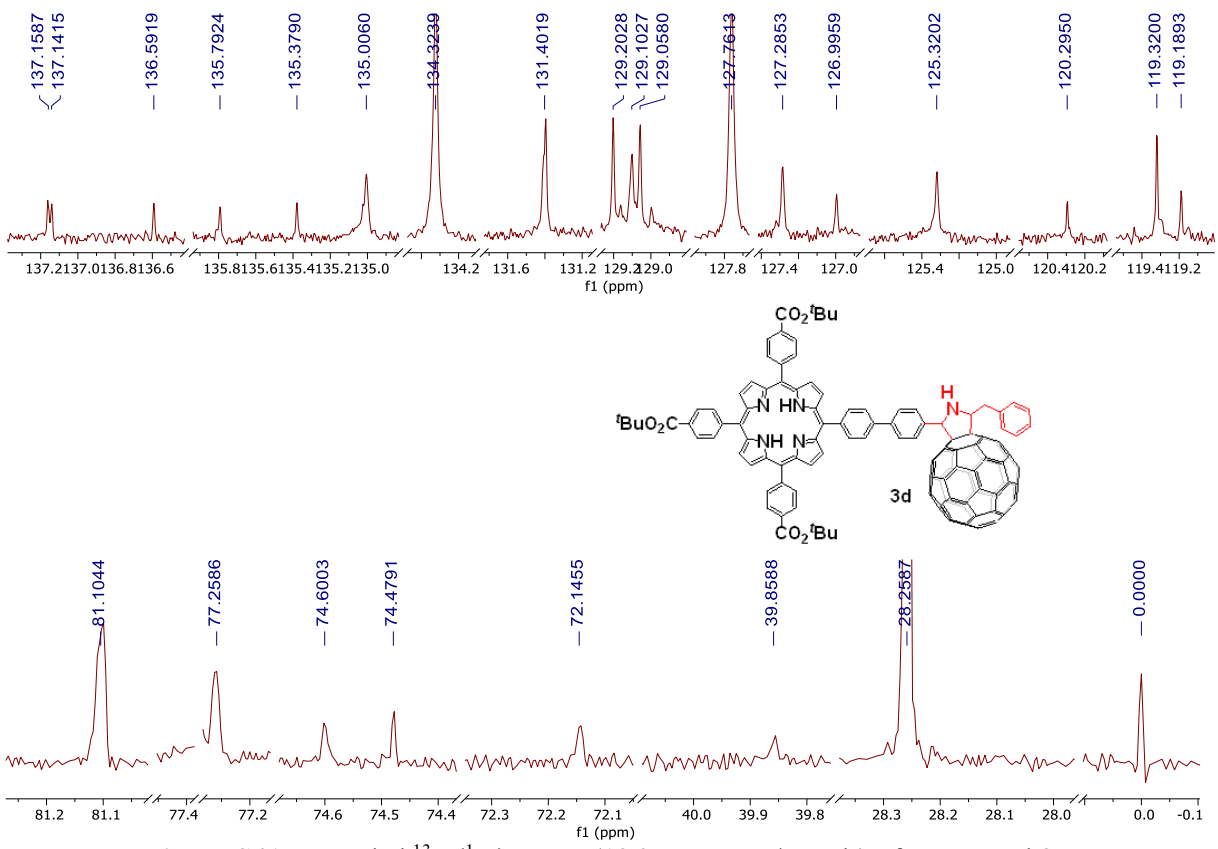
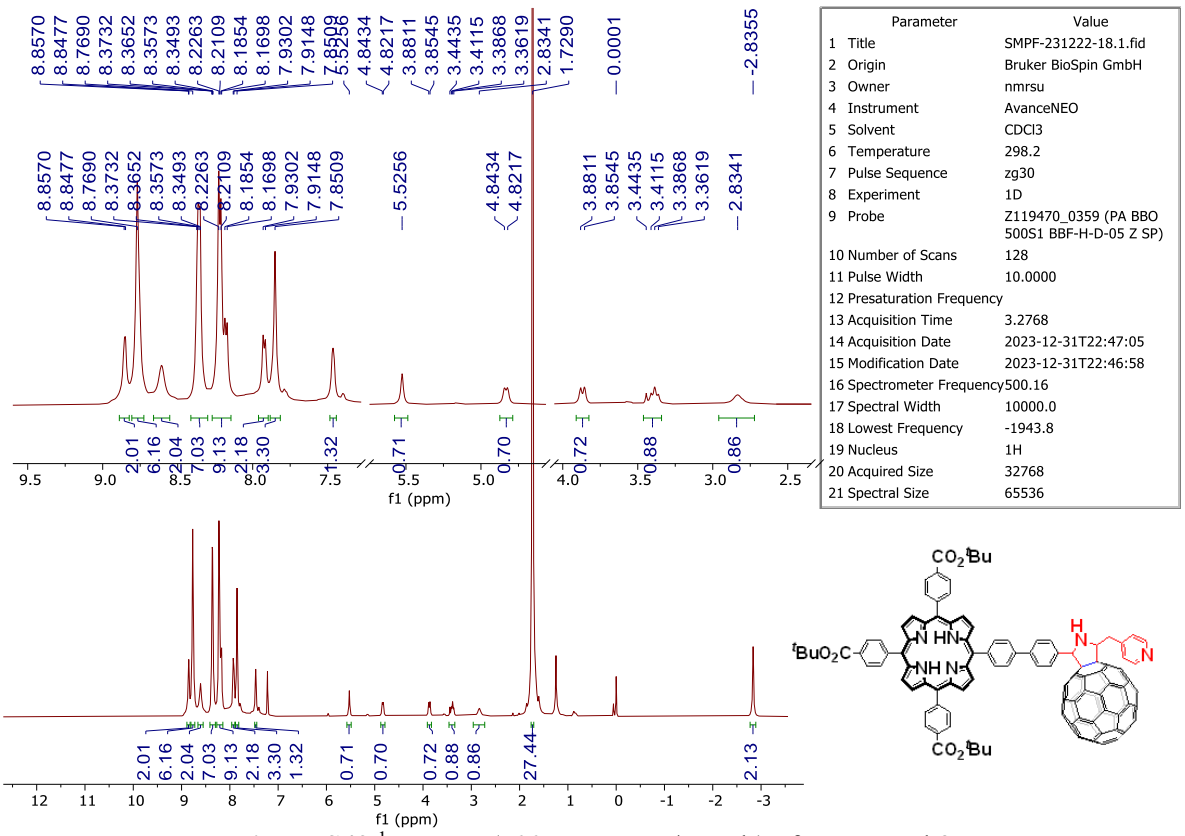



**Figure S41** Expanded $^{13}C\{^{1}H\}$ NMR (126 MHz, $CS_2/CDCl_3$) of compound **3d**

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| 6 Temperature | 298.2 |
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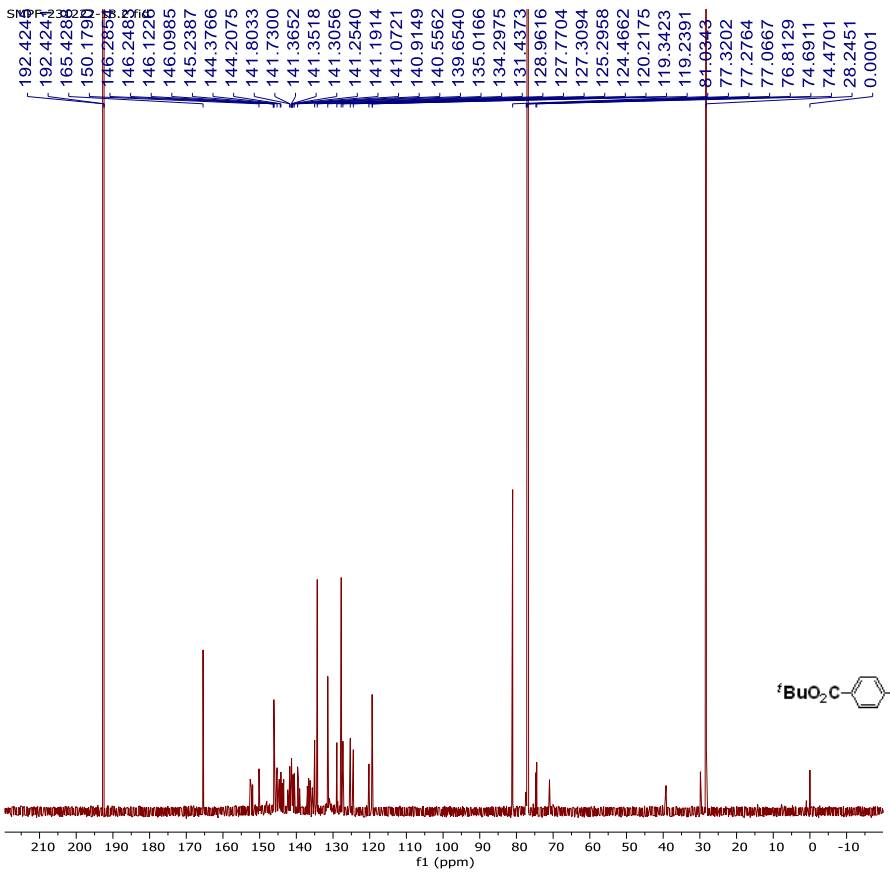
**Figure S42** $^{1}$H NMR (500 MHz, $CS_2$/$CDCl_3$) of compound **3e**




| Parameter | Value |
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| 3 Owner | nmrsu |
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| 6 Temperature | 298.2 |
| 7 Pulse Sequence | zgpg30 |
| 8 Experiment | 1D |
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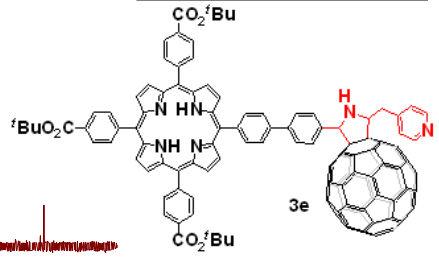


**Figure S43** $^{13}$C{$^{1}$H} NMR (126 MHz, $CS_2$/$CDCl_3$) of compound **3e**

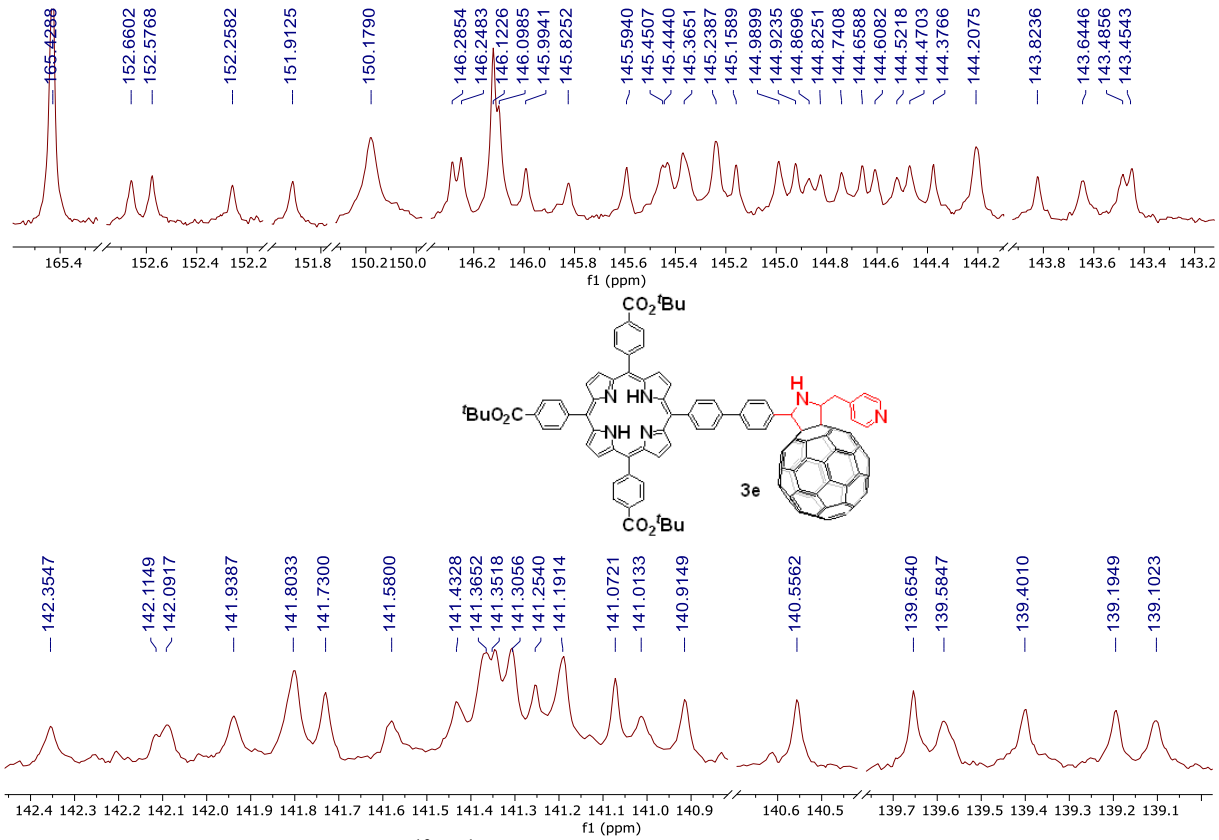


**Figure S44** Expanded $^{13}C\{^1H\}$ NMR (126 MHz, $CS_2/CDCl_3$) of compound **3e**

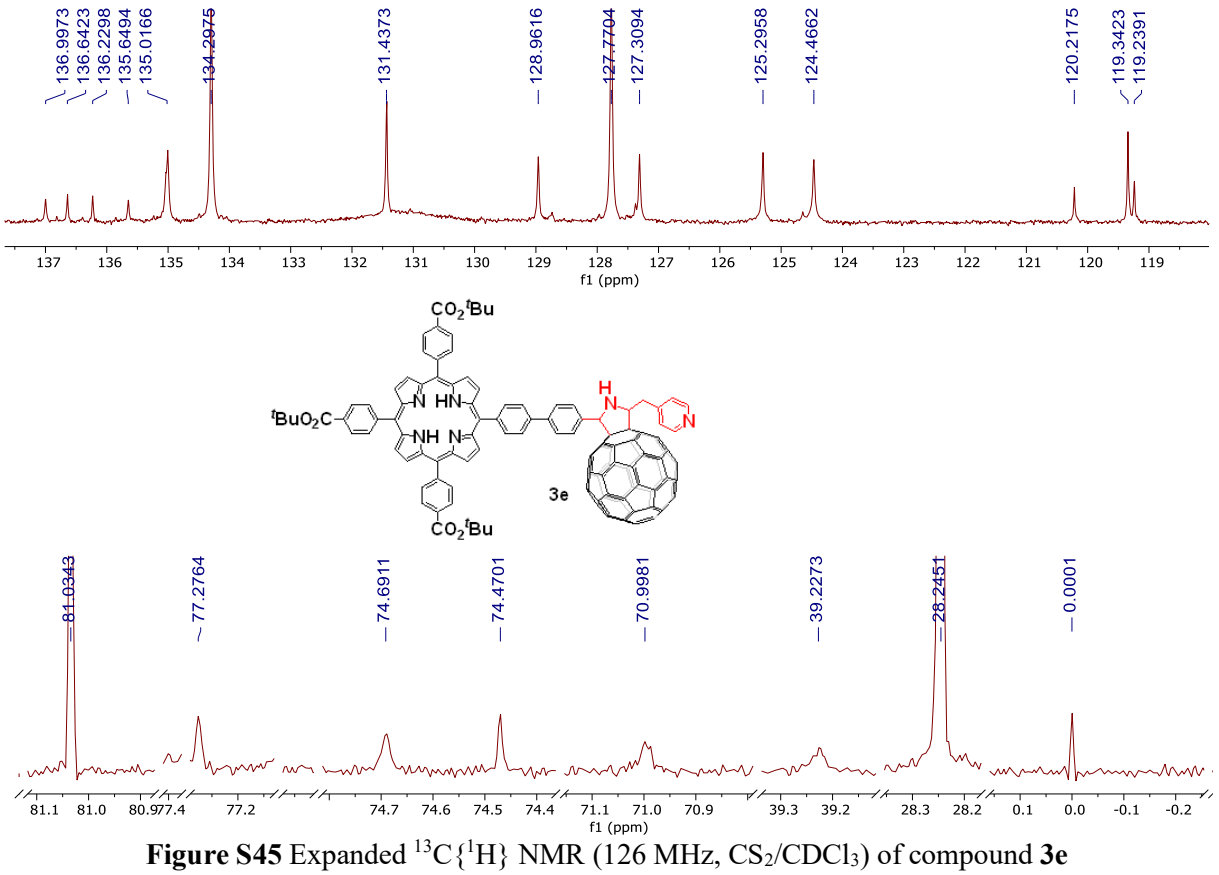


**Figure S45** Expanded $^{13}C\{^1H\}$ NMR (126 MHz, $CS_2/CDCl_3$) of compound **3e**