Electronic Supplementary Information

Electrochemical regioselective alkylations of [60]fulleroindoline with bulky alkyl bromides

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1. General methods

All electrochemical reactions were performed under argon atmosphere using a SHANGHAI CHENHUA CHI630D workstation. Tetra-*n*-butylammonium perchlorate (TBAP) was recrystallized from absolute ethanol and dried in a vacuum at 313 K prior to use. Compound **1** was synthesized according to the procedures developed by our group.[1] Other chemicals were obtained commercially and used without further purification. Controlled potential electrolysis (CPE) was carried out on a potentiostat/galvanostat using an "H" type cell which consisted of two platinum gauze electrodes (serving as working and counter electrodes, respectively) separated by a sintered glass frit. The saturated calomel electrode (SCE) was used as reference electrode and separated from the bulk of the solution by a fritted-glass bridge of low porosity, which contained the solvent/supporting electrolyte mixture. NMR spectra were recorded on a 400 or 500 MHz NMR spectrometer (400 MHz for ^{1}H NMR; 101 or 126 MHz for ^{13}C NMR). ^{1}H NMR chemical shifts were determined relative to TMS or residual $CDCl_2CDCl_2$ (δ 5.92 ppm). ^{13}C NMR chemical shifts were determined relative to residual $CDCl_3$ (δ 77.16 ppm), residual $CDCl_2CDCl_2$ (δ 72.86 ppm) or external d_6-DMSO (δ 39.52 ppm). Data for ^{1}H NMR and ^{13}C NMR are reported as follows: chemical shift (δ, ppm), multiplicity (s = singlet, d = doublet, t = triplet, m = multiplet). High-resolution mass spectra (HRMS) were measured with MALDI-TOF in a positive or negative mode.

Synthesis of the dianion $\mathbf{1}^{2-}$: 17.3 mg (0.020 mmol) of **1** was electroreduced by CPE at –1.1 V vs SCE in 15.0 mL of ODCB solution containing 0.1 M TBAP under an argon atmosphere at room temperature. The potentiostat was turned off when the theoretical number of coulombs required for full conversion of **1** into $\mathbf{1}^{2-}$ was reached. The electrolysis was terminated after about 2.5 h, and a dark-green solution of $\mathbf{1}^{2-}$ was obtained.

2. Experimental procedures and spectral data for compounds 3a–e.

Synthesis of compound 3a in the absence of trifluoroacetic acid (TFA): After the electrolysis of **1** (17.3 mg, 0.020 mmol), the dianion $\mathbf{1}^{2-}$ reacted with 2,4,6-tris(bromomethyl)mesitylene (16.0 mg, 0.040 mmol) at 25 °C for 10 min, the resulting mixture was directly filtered through a silica gel (200–300 mesh) plug with CS_2/CH_2Cl_2 (1:1 v/v) to remove the supporting electrolyte and insoluble materials, and then evaporated in vacuo to remove the solvent. Next, the residue was further separated on a silica gel column (300–400 mesh) with CS_2/CH_2Cl_2 (4:1 v/v) as the eluent to afford product **3a** (9.3 mg, 39%) as an amorphous brown solid along with unreacted **1** (4.1 mg, 24%). ^{1}H NMR (400 MHz, 1:1 $CS_2/CDCl_3$) δ 8.10 (d, J = 7.8 Hz, 1H), 7.39 (s, 1H), 7.25 (d, J = 7.8 Hz, 1H), 5.94 (s, 1H), 4.68 (d, J = 14.2 Hz, 1H), 4.50–4.35 (m, 5H), 2.80 (s, 3H), 2.61 (s, 6H), 2.36 (s, 6H); ^{13}C NMR (101 MHz, 1:1 $CS_2/CDCl_3$ with $Cr(acac)_3$ as relaxation reagent, all 1C unless indicated) δ 167.65 (*C*=*O*), 156.08, 154.59, 150.90, 149.52, 149.31, 148.83, 148.63, 148.10 (2C), 147.82, 147.53, 147.46, 147.23, 146.95 (2C), 146.73, 146.64, 146.17, 146.11 (3C), 145.89, 145.77, 145.59, 145.16,

145.13, 145.00, 144.53 (4C), 144.19 (2C), 144.01, 143.77, 143.70, 143.42, 143.33, 143.23, 142.96, 142.60, 142.20, 141.99, 141.92, 141.78, 141.30, 141.27, 141.20, 141.04, 140.95, 140.15, 140.07, 139.87 (2C), 138.34, 137.91, 137.59, 137.19, 136.19, 136.15, 133.83, 133.36, 133.19, 132.19, 128.44, 125.65, 125.01, 115.44, 83.63 (sp^3-*C* of C_{60}), 62.51 (sp^3-*C* of C_{60}), 58.46 (sp^3-*C* of C_{60}), 56.53 (sp^3-*C* of C_{60}), 41.14, 30.42 (2C), 26.80, 22.17, 18.19, 18.00, 15.07; UV-vis ($CHCl_3$) λ_{max}/nm (log ε) 246 (5.26), 320 (4.72), 448 (3.91), 520 (3.35), 706 (2.60); FT-IR ν/cm^{-1} (KBr) 1669, 1498, 1439, 1360, 1342, 1301, 1249, 1203, 1093, 1048, 858, 812, 789, 613, 599, 532; MALDI-TOF MS *m/z* calcd for $C_{81}H_{24}NO^{79}Br_2$ $[M–H]^-$ 1184.0230, found 1184.0215.

Synthesis of compound 3a in the presence of TFA: After the electrolysis of **1** (17.3 mg, 0.020 mmol), the dianion $\mathbf{1}^{2-}$ reacted with 2,4,6-tris(bromomethyl)mesitylene (16.0 mg, 0.040 mmol) at 25 °C for 10 min, then TFA (3.0 μL, 0.040 mmol) was added, and the reaction mixture was stirred at 25 °C for 10 min, the resulting mixture was directly filtered through a silica gel (200–300 mesh) plug with CS_2/CH_2Cl_2 (1:1 v/v) to remove the supporting electrolyte and insoluble materials, and then evaporated in vacuo to remove the solvent. Next, the residue was further separated on a silica gel column (300–400 mesh) with CS_2/CH_2Cl_2 (4:1 v/v) as the eluent to afford product **3a** (12.1 mg, 51%) as an amorphous brown solid along with unreacted **1** (2.3 mg, 13%).

Synthesis of compound 3b: After the electrolysis of **1** (17.3 mg, 0.020 mmol), the dianion $\mathbf{1}^{2-}$ reacted with 2,4,6-tris(bromomethyl)mesitylene (40.0 mg, 0.100 mmol) at 25 °C for 5 h, the resulting mixture was directly filtered through a silica gel (200–300 mesh) plug with CS_2/CH_2Cl_2 (1:1 v/v) to remove the supporting electrolyte and insoluble materials, and then evaporated in vacuo to remove the solvent. Next, the residue was further separated on a silica gel column (300–400 mesh) with CS_2/CH_2Cl_2 (4:1 v/v) as the eluent to afford product **3b** (13.9 mg, 46%) as an amorphous brown solid along with unreacted **1** (2.5 mg, 14%). ^{1}H NMR (400 MHz, 1:1 $CS_2/CDCl_3$) δ 8.11 (d, J = 7.7 Hz, 1H), 7.38 (s, 1H), 7.33 (d, J = 7.7 Hz, 1H), 4.69 (d, J = 13.5 Hz, 1H), 4.67 (d, J = 14.2 Hz, 1H), 4.47–4.30 (m, 9H), 4.11 (d, J = 13.5 Hz, 1H), 2.78 (s, 3H), 2.64 (s, 3H), 2.58 (s, 3H), 2.38 (s, 3H), 2.36 (s, 3H), 2.30 (s, 3H), 2.28 (s, 3H), 2.10 (s, 3H); ^{13}C NMR (101 MHz, 1:1 $CS_2/CDCl_3$, all 1C unless indicated) δ 168.78 (*C*=*O*), 155.68, 155.50, 152.04, 150.74, 149.98, 149.77, 148.81, 148.32, 148.06, 148.01, 147.71 (2C), 146.73, 146.72, 146.53, 146.44, 146.31, 146.25, 146.16, 146.08, 145.94, 145.89, 145.81, 145.59, 145.48, 145.14, 145.07, 144.77 (2C), 144.73, 144.63, 144.30, 144.26, 144.06, 143.76, 143.67, 143.65, 143.10, 142.99, 142.92, 142.13, 142.06, 142.04, 141.81, 141.04, 141.02, 140.84 (2C), 140.48, 140.36, 140.20, 139.52, 139.45, 139.26, 138.59, 138.43, 138.39, 138.03, 137.75, 136.46, 136.28, 136.08, 136.01, 133.68, 133.48, 133.43, 133.29, 132.91, 132.53, 132.23, 129.66, 125.89, 125.68, 116.77, 89.07 (sp^3-*C* of C_{60}), 64.35 (sp^3-*C* of C_{60}), 63.15 (sp^3-*C* of C_{60}), 58.74 (sp^3-*C* of C_{60}), 41.02, 37.63, 30.71, 30.56 (2C), 30.45, 25.58, 22.23, 18.37, 18.12, 17.86, 17.82, 15.19, 15.09; UV-vis ($CHCl_3$) λ_{max}/nm (log ε) 247 (5.22), 324 (4.69), 450 (3.94), 523 (3.60), 708 (3.35); FT-IR ν/cm^{-1} (KBr) 1668, 1498, 1441, 1366, 1340, 1297, 1250, 1203, 1101, 1011, 852, 789, 740, 618, 563, 527; MALDI-TOF MS *m/z* calcd for $C_{93}H_{39}NO^{79}Br_2{}^{81}Br_2$ $[M]^-$ 1504.9730, found 1504.9713.

Synthesis of compound 3c in the absence of TFA: After the electrolysis of **1** (17.3 mg, 0.020 mmol), the dianion $\mathbf{1}^{2-}$ reacted with diphenylbromomethane (10.0 mg, 0.040 mmol) at 25 °C for 1 h, the resulting mixture was directly filtered through a silica gel (200–300 mesh) plug with CS_2/CH_2Cl_2 (1:1 v/v) to remove the supporting electrolyte and insoluble materials, and then evaporated in vacuo to remove the solvent. Next, the residue was further separated on a silica gel column (300–400 mesh) with CS_2/CH_2Cl_2 (4:1 v/v) as the eluent to afford product **3c** (9.1 mg, 44%) as an amorphous brown solid along with unreacted **1** (4.3 mg, 25%). ^{1}H NMR (400 MHz, 1:1 $CS_2/CDCl_3$) δ 8.25 (d, J = 7.7 Hz, 1H), 8.08 (d, J = 7.8 Hz, 2H), 7.47 (t, J = 7.7 Hz, 2H), 7.42–7.32 (m, 5H), 7.15–7.07 (m, 3H), 5.87 (s, 1H), 5.58 (s, 1H), 2.79 (s, 3H), 2.63 (s, 3H); ^{13}C NMR (101 MHz, CS_2 with DMSO-d_6 as external reference and $Cr(acac)_3$ as relaxation reagent, all 1C unless indicated) δ 166.27 (*C*=*O*), 155.74, 154.10, 151.25, 149.59, 149.25, 149.17, 148.71, 148.64, 148.14, 147.99, 147.72, 147.55, 147.38, 147.12, 147.03, 146.93, 146.91, 146.61, 146.17, 145.96 (2C), 145.80, 145.76, 145.65, 145.21, 145.13, 145.11, 144.66, 144.60, 144.51, 144.33, 144.23, 144.20, 144.14, 143.65, 143.38, 143.30, 143.24, 142.97, 142.71, 142.56, 142.51, 141.97, 141.80, 141.61, 141.29 (2C), 141.21, 141.01, 140.55, 139.88, 139.84, 139.79 (2C), 139.77, 139.74, 138.31, 138.15, 137.95, 137.55, 134.37, 130.20 (2C), 129.43 (2C), 128.90 (2C), 128.07 (2C), 127.63, 127.24, 125.83, 124.79, 115.37, 83.49 (sp^3-*C* of C_{60}), 64.07, 62.47 (sp^3-*C* of C_{60}), 62.37 (sp^3-*C* of C_{60}), 56.36 (sp^3-*C* of C_{60}), 26.72, 22.42; UV-vis ($CHCl_3$) λ_{max}/nm (log ε) 251 (5.09), 321 (4.62), 448 (3.78), 519 (3.24), 709 (2.48); FT-IR ν/cm^{-1} (KBr) 1670, 1497, 1449, 1438, 1367, 1340, 1300, 1247, 1028, 969, 857, 785, 745, 701, 617, 603, 565, 528; MALDI-TOF MS *m/z* calcd for $C_{82}H_{21}NO$ $[M]^-$ 1035.1629, found 1035.1622.

Synthesis of compound 3c in the presence of TFA: After the electrolysis of **1** (17.3 mg, 0.020 mmol), the dianion $\mathbf{1}^{2-}$ reacted with diphenylbromomethane (10.0 mg, 0.040 mmol) at 25 °C for 1 h, then TFA (3.0 μL, 0.040 mmol) was added, and the reaction mixture was stirred at 25 °C for 10 min, the resulting mixture was directly filtered through a silica gel (200–300 mesh) plug with CS_2/CH_2Cl_2 (1:1 v/v) to remove the supporting electrolyte and insoluble materials, and then evaporated in vacuo to remove the solvent. Next, the residue was further separated on a silica gel column (300–400 mesh) with CS_2/CH_2Cl_2 (4:1 v/v) as the eluent to afford product **3c** (12.0 mg, 58%) as an amorphous brown solid along with unreacted **1** (2.9 mg, 17%).

Synthesis of compounds 3d and 3e: After the electrolysis of **1** (17.3 mg, 0.020 mmol), the dianion $\mathbf{1}^{2-}$ reacted with diphenylbromomethane (197.6 mg, 0.80 mmol) and NaH (57–63% oil dispersion, 4.0 mg, 0.100 mmol) at 25 °C for 10 h, the resulting mixture was directly filtered through a silica gel (200–300 mesh) plug with CS_2/CH_2Cl_2 (1:1 v/v) to remove the supporting electrolyte and insoluble materials, and then evaporated in vacuo to remove the solvent. Next, the residue was further separated on a silica gel column (300–400 mesh) with CS_2/CH_2Cl_2 (4:1 v/v) as the eluent to afford product **3d** (3.0 mg, 13%) and **3e** (8.3 mg, 35%) as amorphous brown solids along with unreacted **1** (3.2 mg, 18%).

Compounds 3d: ^{1}H NMR (400 MHz, TCE-d_2) δ 8.13 (d, J = 7.6 Hz, 2H), 7.91 (d, J = 7.7 Hz, 1H), 7.54 (t, J = 7.6 Hz, 2H), 7.51–7.45 (m, 2H), 7.40 (t, J = 7.3 Hz, 2H), 7.33

(d, J = 7.8 Hz, 2H), 7.17 (d, J = 7.7 Hz, 1H), 7.13–7.03 (m, 4H), 7.02–6.93 (m, 4H), 6.92–6.81 (m, 3H), 6.03 (s, 1H), 5.51 (s, 1H), 2.47 (s, 3H), 2.26 (s, 3H); ^{13}C NMR (126 MHz, TCE-d_2, all 1C unless indicated) δ 168.39 (*C*=*O*), 154.77, 152.92, 150.73, 150.20, 149.42, 148.78, 148.48, 147.76, 147.37, 147.03, 146.91, 146.89, 146.84, 146.83, 145.89, 145.74, 145.48, 145.45, 145.20, 144.97, 144.91, 144.85, 144.65, 144.63, 144.55, 143.99, 143.87, 143.75, 143.56 (2C), 143.54, 143.31, 143.16, 143.13, 142.86, 142.61, 142.54, 142.38, 142.22, 142.04, 141.98, 141.94, 141.13 (2C), 140.82, 140.42, 140.34, 140.23, 139.96, 139.77, 139.61, 139.47, 139.33, 138.72, 138.40, 137.50, 137.45, 137.25, 136.71, 136.07, 134.10, 132.89, 129.36 (2C), 128.62 (2C), 128.15 (2C), 128.05, 127.14 (2C), 127.10 (2C), 126.60, 126.47, 126.29, 125.62, 124.52, 123.94, 122.93, 116.39, 88.04 (sp^3-*C* of C_{60}), 66.38, 63.69 (sp^3-*C* of C_{60}), 62.56 (sp^3-*C* of C_{60}), 61.50, 56.79 (sp^3-*C* of C_{60}), 25.23, 20.78; UV-vis ($CHCl_3$) λ_{max}/nm (log ε) 252 (5.08), 323 (4.66), 454 (3.78), 522 (3.27), 709 (2.43); FT-IR ν/cm^{-1} (KBr) 1665, 1497, 1449, 1364, 1338, 1297, 1244, 1032, 849, 746, 701, 638, 618, 598, 527; MALDI-TOF MS *m/z* calcd for $C_{95}H_{31}NONa$ $[M+Na]^+$ 1224.2298, found 1224.2289.

Compounds 3e: ^{1}H NMR (400 MHz, TCE-d_2) δ 7.93 (d, J = 7.8 Hz, 1H), 7.50–7.35 (m, 8H), 7.34–7.23 (m, 4H), 7.19–7.05 (m, 8H), 6.97 (d, J = 7.5 Hz, 2H), 5.15 (s, 1H), 4.31 (s, 1H), 2.81 (s, 3H), 2.63 (s, 3H); ^{13}C NMR (101 MHz, TCE-d_2, all 1C unless indicated) δ 168.12 (*C*=*O*), 155.37, 152.65, 151.57, 150.72, 148.55, 147.79, 147.75, 147.39, 147.08, 146.70, 146.60, 146.45, 146.33, 146.19, 146.06, 145.86, 145.54, 145.51 (2C), 145.40, 145.24, 145.03, 144.93, 144.66, 144.58, 144.49, 144.43, 144.32 (2C), 144.04, 143.95, 143.64, 143.34, 142.84, 142.58, 142.31, 142.16, 141.95, 141.59, 141.52, 141.44, 141.21, 141.15, 141.01, 140.77, 140.45, 140.41, 140.34, 140.08, 139.93, 139.69, 139.62, 138.94, 138.45, 138.36, 138.20, 137.66, 137.62, 137.51 (2C), 136.80, 132.03, 129.19 (2C), 128.59 (2C), 128.19 (2C), 128.03 (2C), 127.79 (2C), 127.60 (2C), 127.53 (2C), 127.37 (2C), 126.78, 126.45, 126.33 (2C), 126.07, 125.98, 124.29, 114.85, 75.48 (sp^3-*C* of C_{60}), 64.46 (sp^3-*C* of C_{60}), 62.85 (sp^3-*C* of C_{60}), 62.21, 61.00 (sp^3-*C* of C_{60}), 59.01, 26.59, 21.36; UV-vis ($CHCl_3$) λ_{max}/nm (log ε) 262 (4.94), 322 (4.62), 427 (3.95), 487 (3.47), 614 (3.00), 682 (2.69); FT-IR ν/cm^{-1} (KBr) 1674, 1496, 1450, 1423, 1367, 1341, 1302, 1243, 1027, 960, 856, 745, 702, 617, 596, 529; MALDI-TOF MS *m/z* calcd for $C_{95}H_{31}NONa$ $[M+Na]^+$ 1224.2298, found 1224.2295.

3. ^{1}H NMR and ^{13}C NMR spectra of compounds 3a–e.

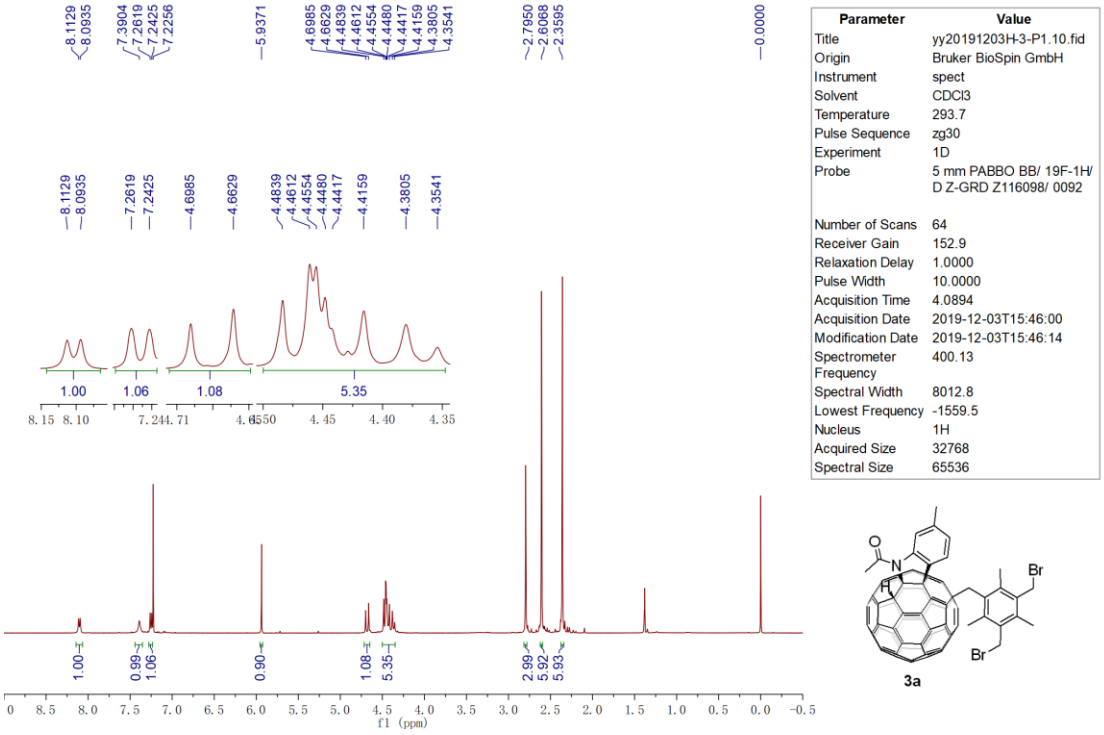


Figure S1. ^{1}H NMR (400 MHz, 1:1 CS_2/$CDCl_3$) of compound 3a.

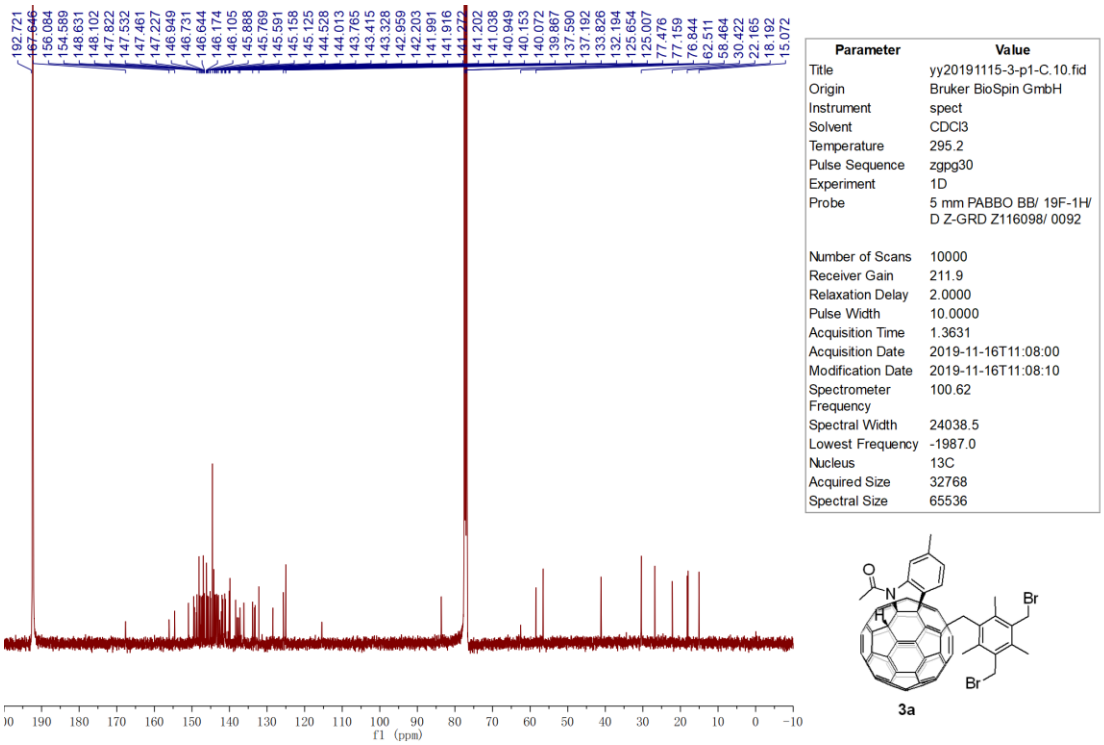


Figure S2. ^{13}C NMR (101 MHz, 1:1 CS_2/$CDCl_3$ with $Cr(acac)_3$ as relaxation reagent) of compound 3a.

Figure S3. Expanded ^{13}C NMR (101 MHz, 1:1 $CS_2/CDCl_3$ with $Cr(acac)_3$ as relaxation reagent) of compound 3a.

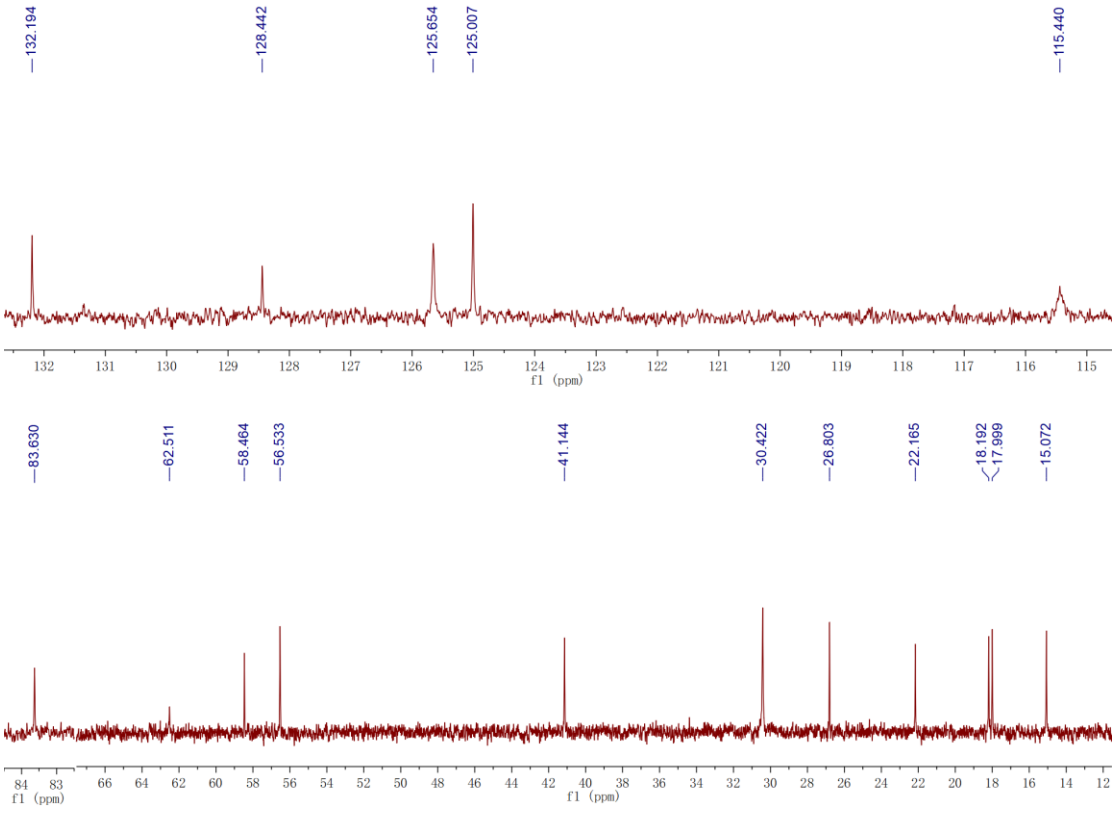


Figure S4. Expanded ^{13}C NMR (101 MHz, 1:1 $CS_2/CDCl_3$ with $Cr(acac)_3$ as relaxation reagent) of compound 3a.

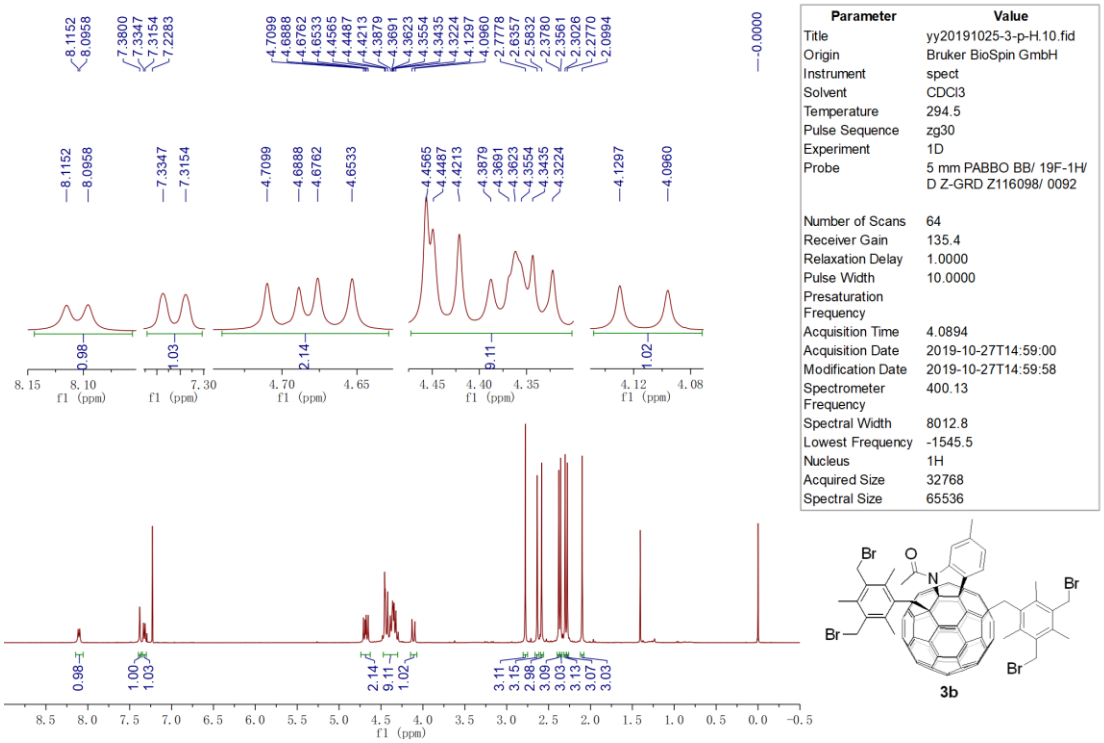


Figure S5. ^{1}H NMR (400 MHz, 1:1 CS_2/$CDCl_3$) of compound 3b.

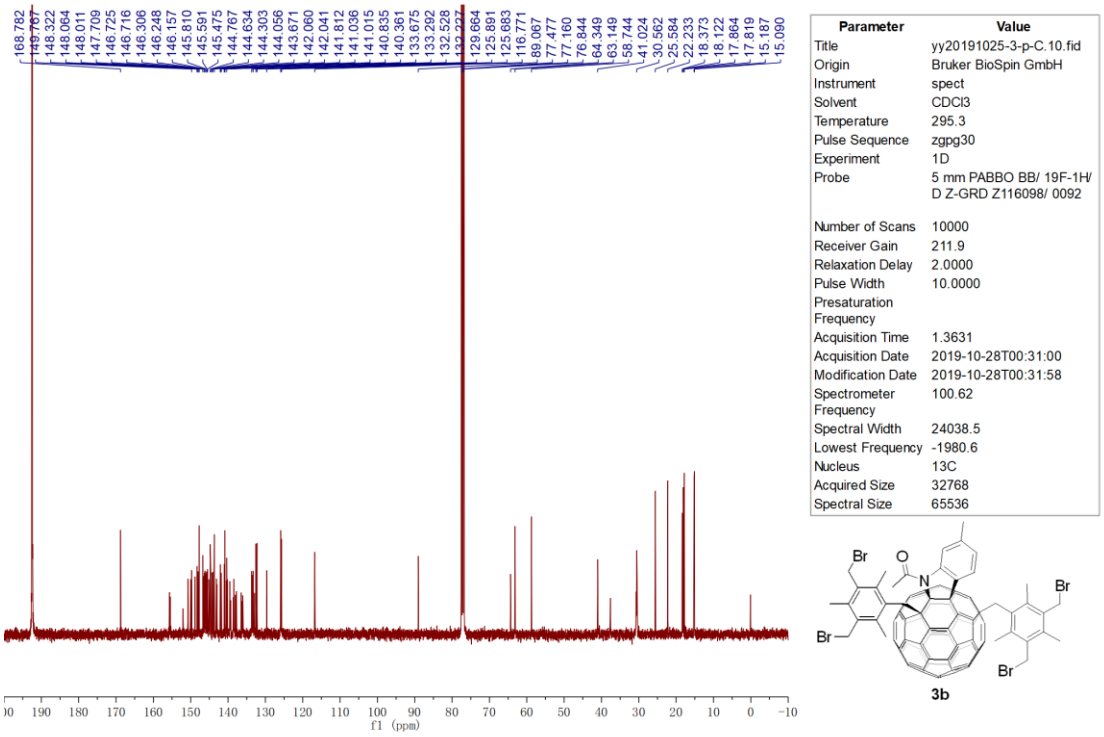


Figure S6. ^{13}C NMR (101 MHz, 1:1 CS_2/$CDCl_3$) of compound 3b.

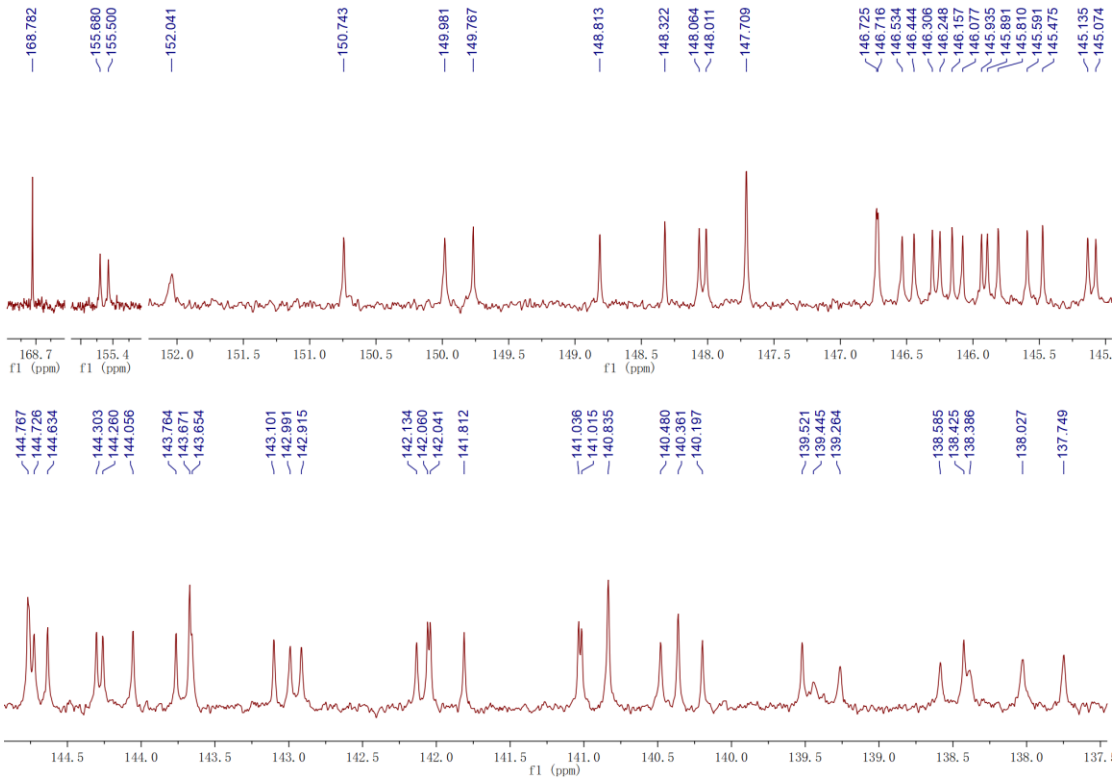


Figure S7. Expanded ^{13}C NMR (101 MHz, 1:1 $CS_2/CDCl_3$) of compound 3b.

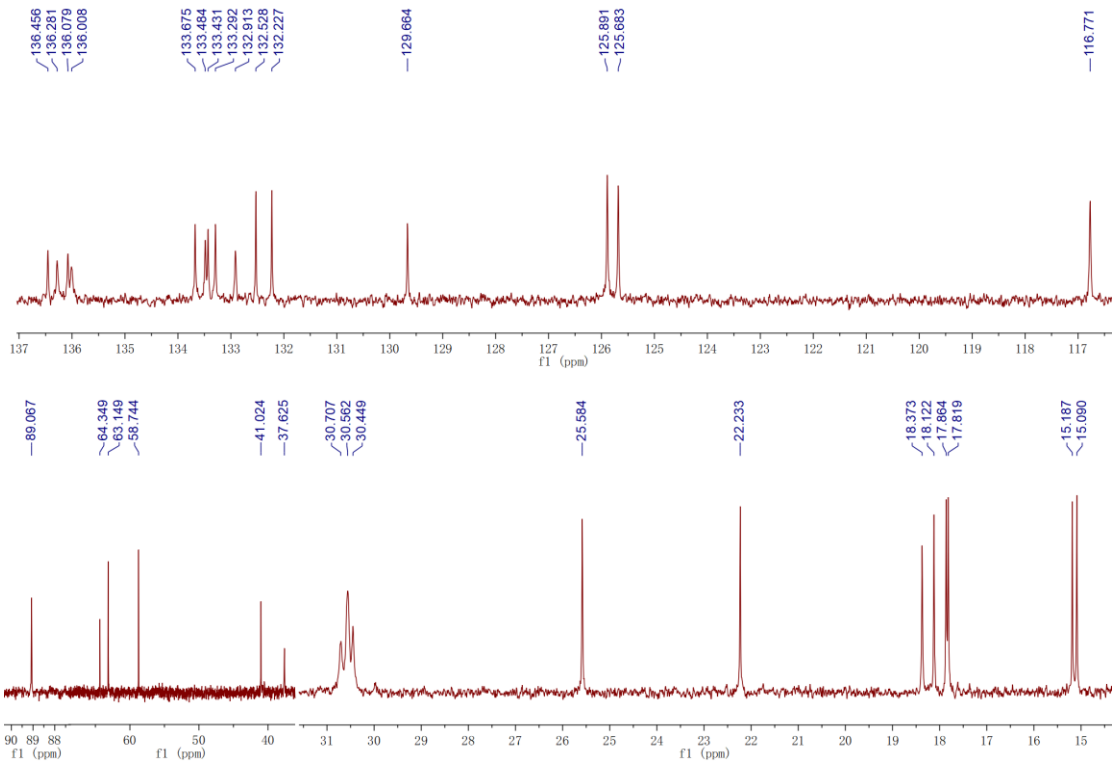


Figure S8. Expanded ^{13}C NMR (101 MHz, 1:1 $CS_2/CDCl_3$) of compound 3b.

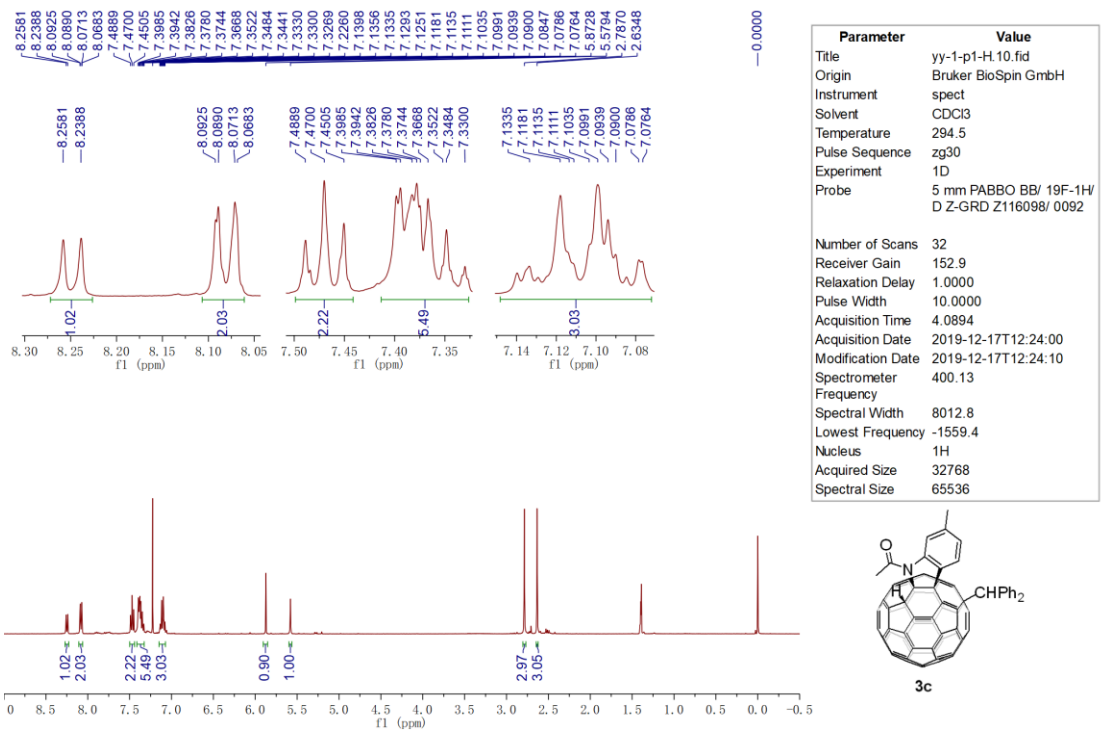


Figure S9. ^{1}H NMR (400 MHz, 1:1 CS_2/$CDCl_3$) of compound 3c.

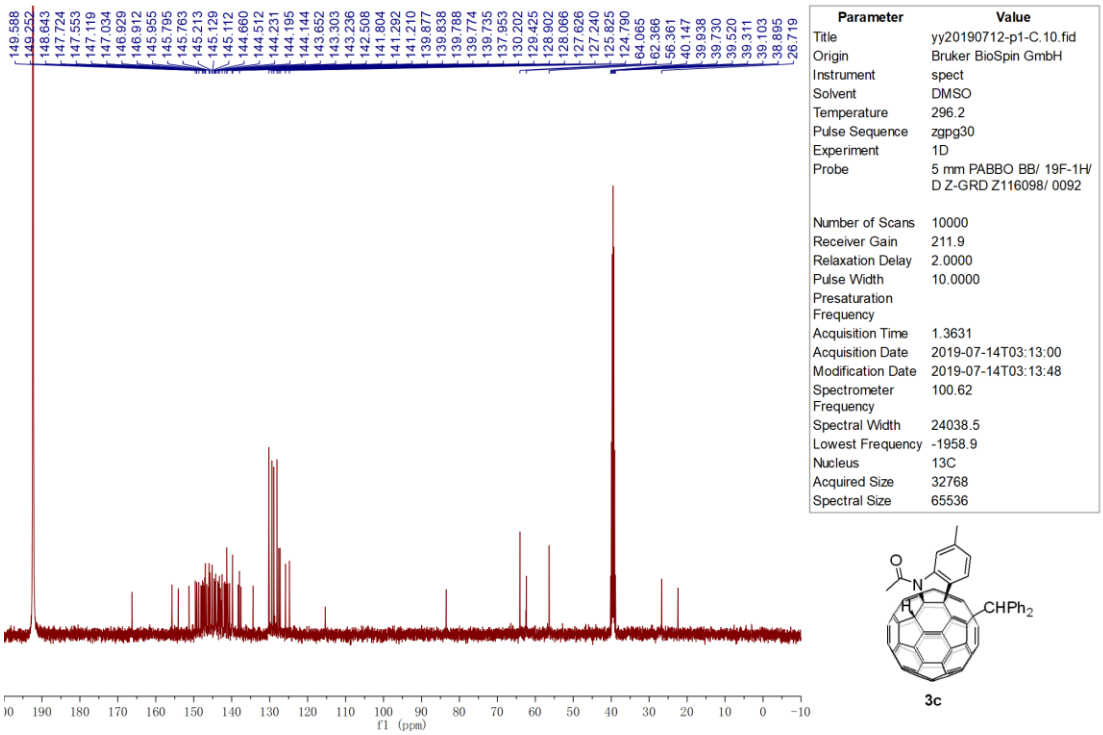


Figure S10. ^{13}C NMR (101MHz, CS_2/DMSO-d_6 with $Cr(acac)_3$ as relaxation reagent) of compound 3c.

Figure S11. Expanded ^{13}C NMR (101 MHz, CS_2/DMSO-d_6 with $Cr(acac)_3$ as relaxation reagent) of compound 3c.

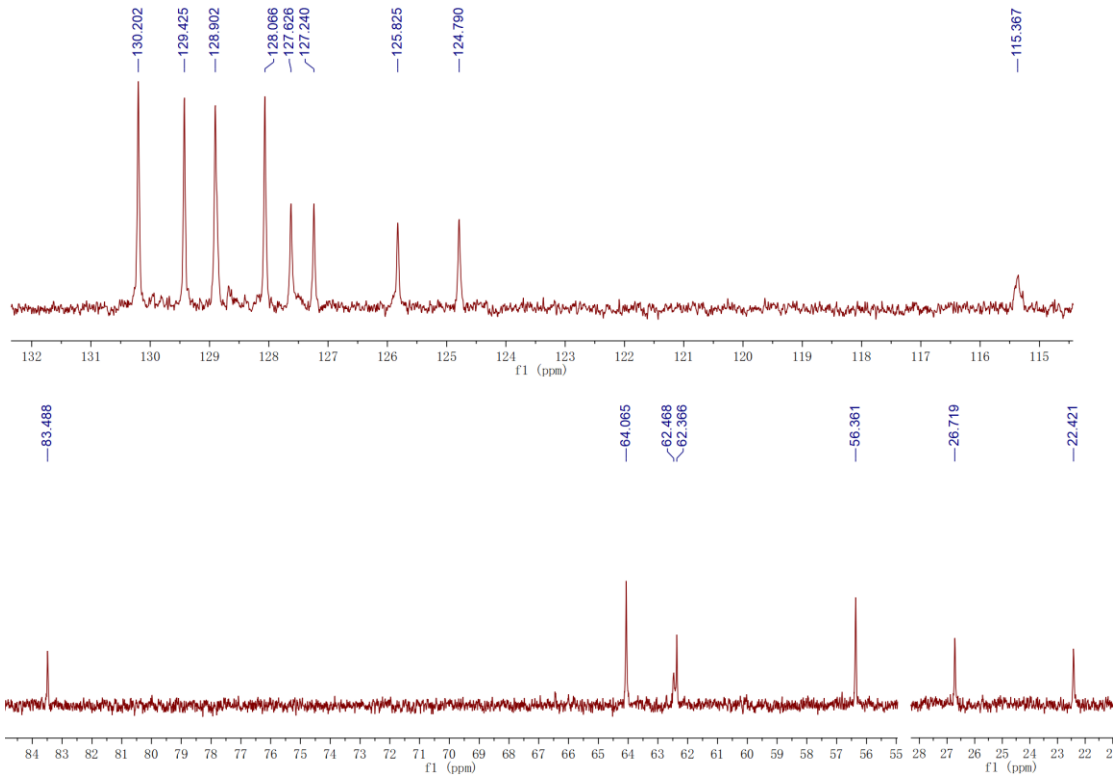


Figure S12. Expanded ^{13}C NMR (101 MHz, CS_2/DMSO-d_6 with $Cr(acac)_3$ as relaxation reagent) of compound 3c.

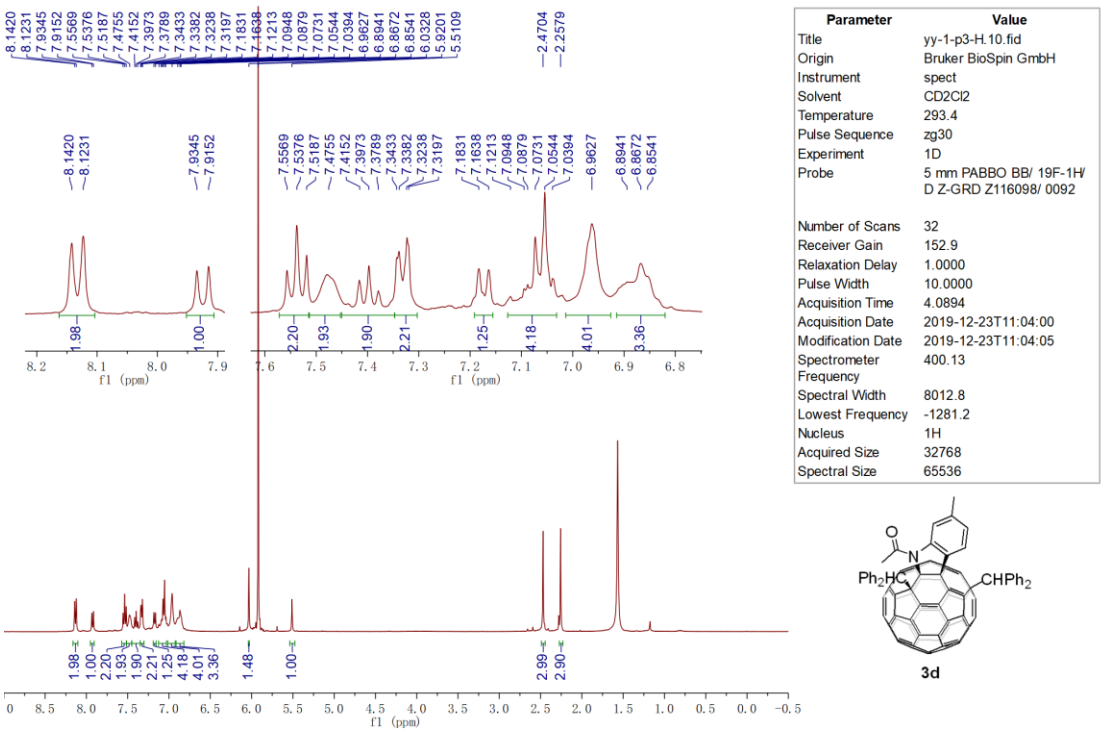


Figure S13. ^{1}H NMR (400 MHz, TCE-d_2) of compound 3d.

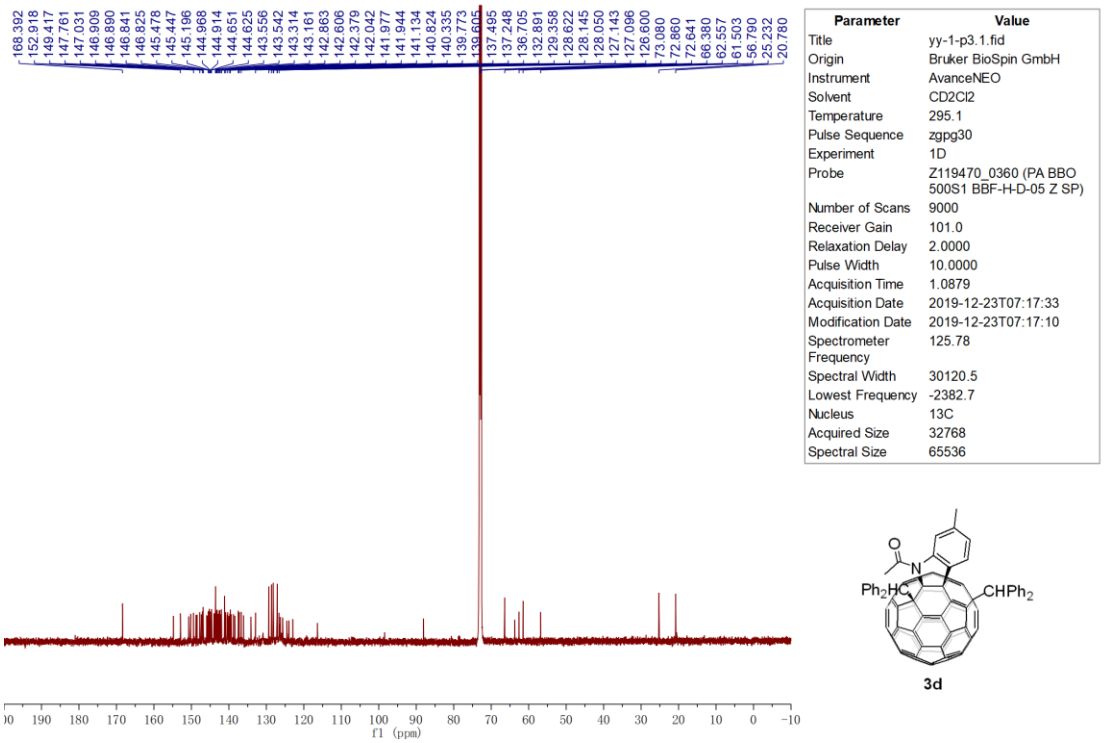


Figure S14. ^{13}C NMR (126 MHz, TCE-d_2) of compound 3d.

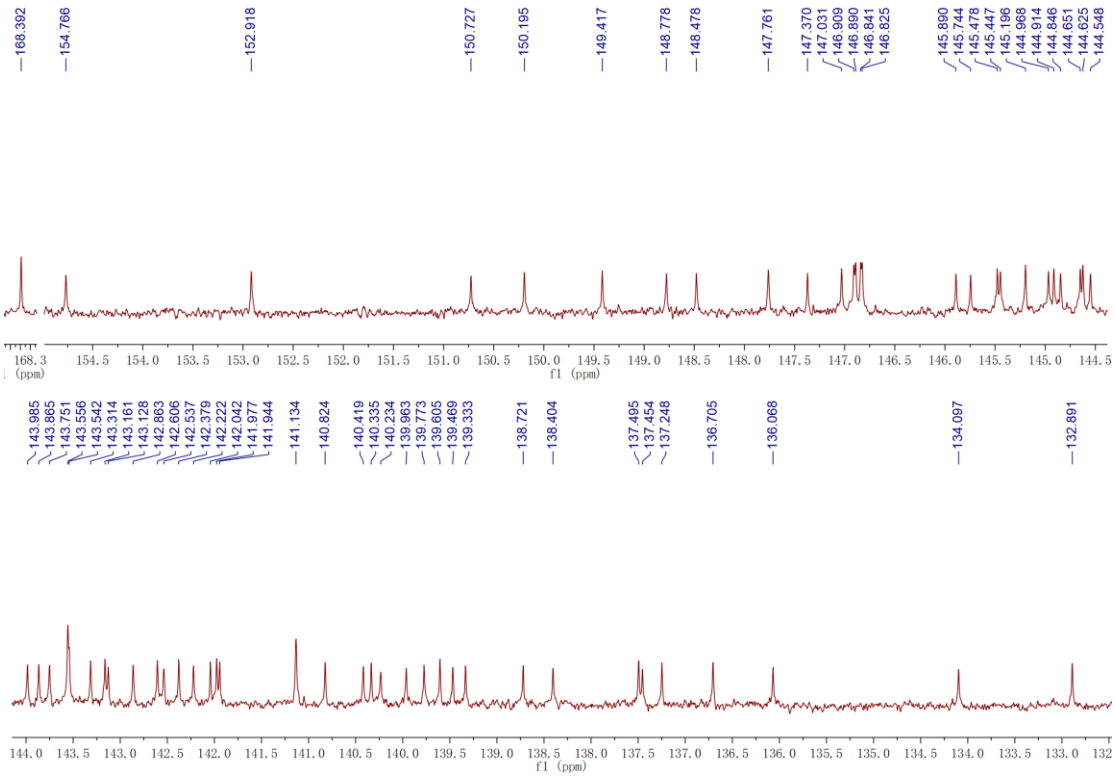


Figure S15. Expanded ^{13}C NMR (126 MHz, TCE-d_2) of compound 3d.

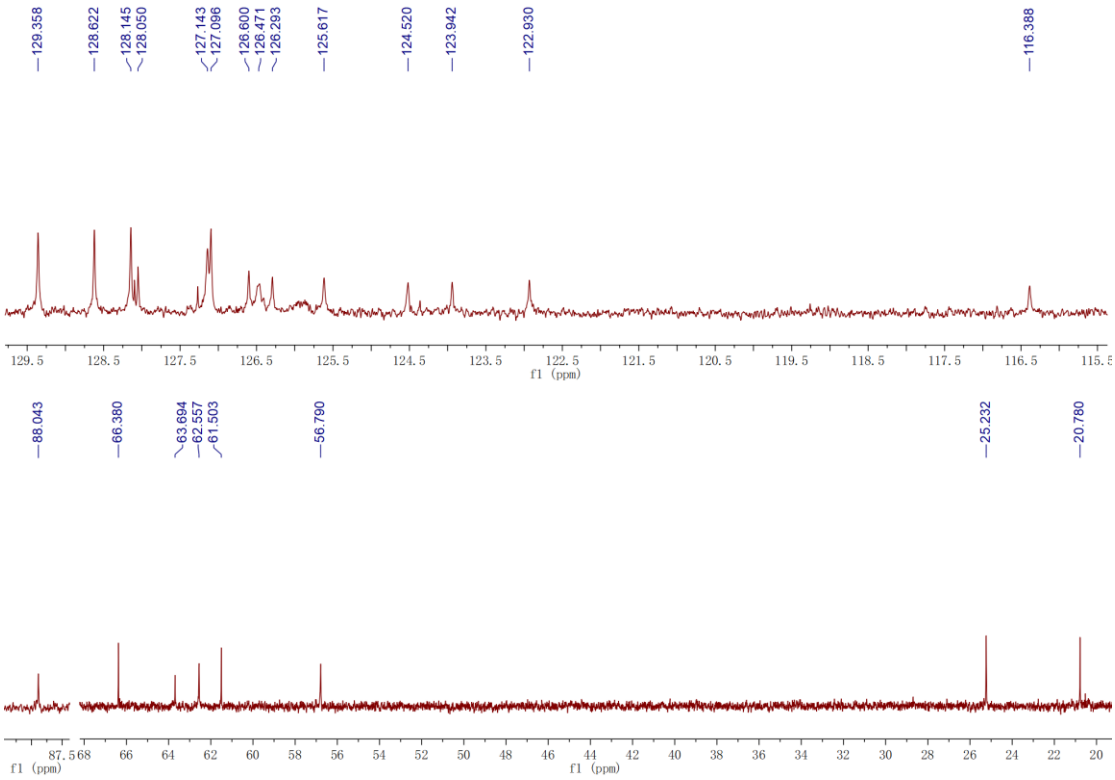


Figure S16. Expanded ^{13}C NMR (126 MHz, TCE-d_2) of compound 3d.

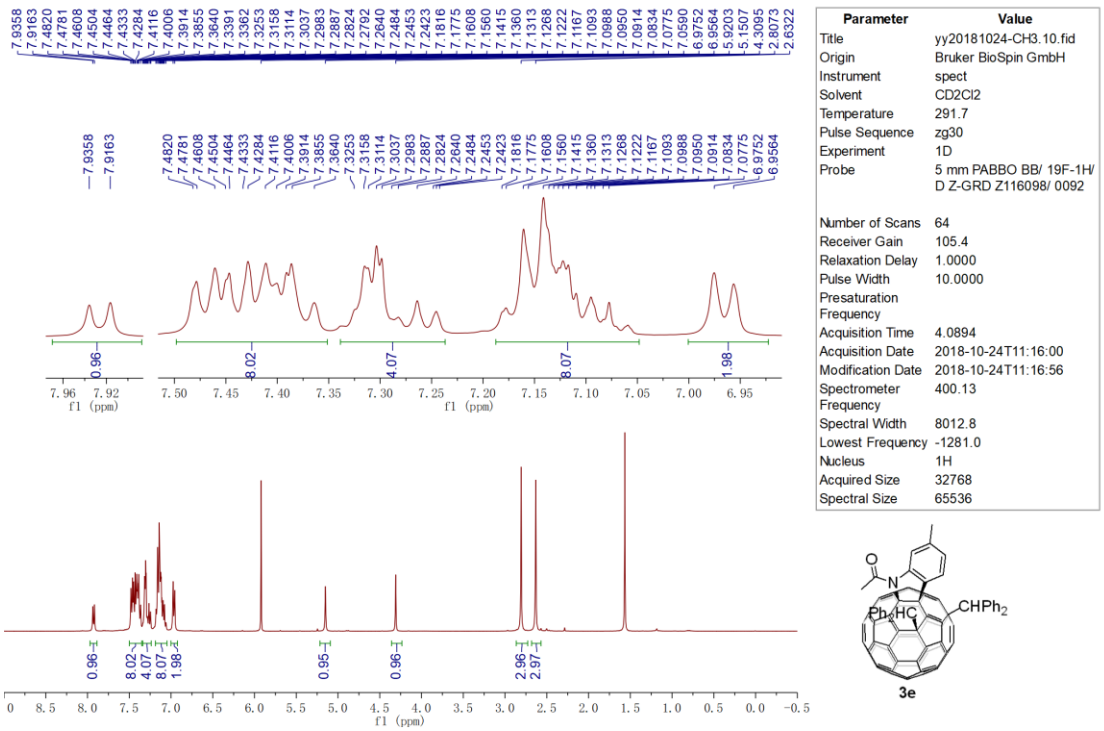


Figure S17. ^{1}H NMR (400 MHz, TCE-d_2) of compound 3e.

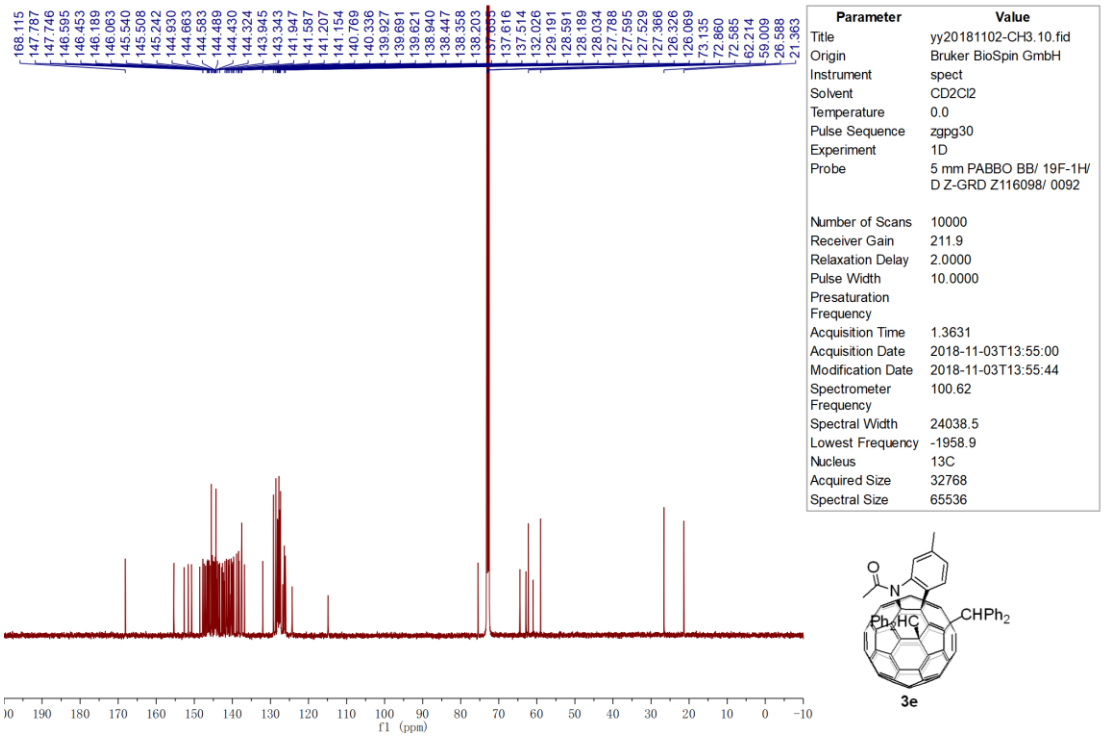


Figure S18. ^{13}C NMR (101 MHz, TCE-d_2) of compound 3e.

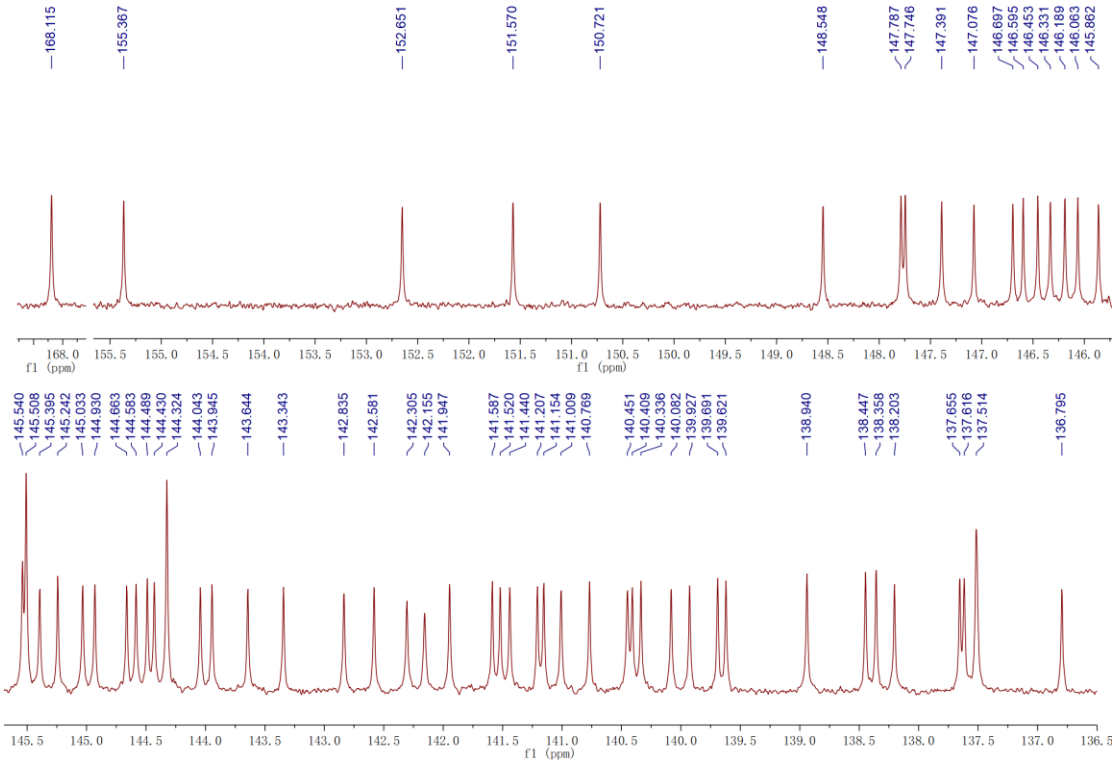


Figure S19. Expanded ^{13}C NMR (101 MHz, TCE-d_2) of compound 3e.

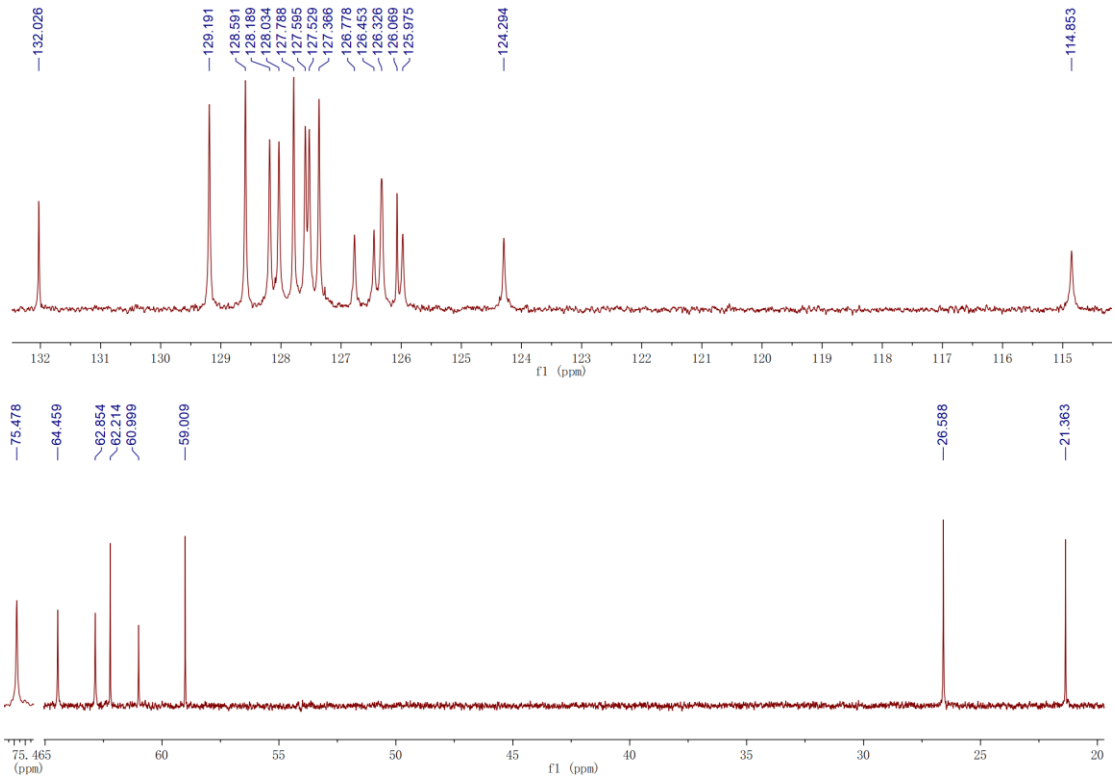


Figure S20. Expanded ^{13}C NMR (101 MHz, TCE-d_2) of compound 3e.

4. UV-vis spectra of compounds 3a–3e.

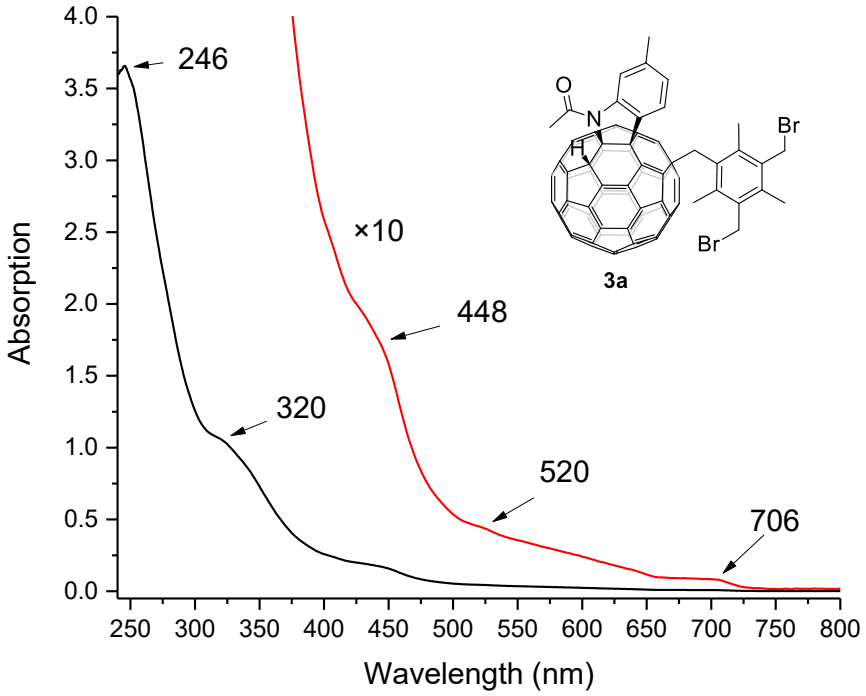


Figure S21. UV-vis absorption of compound 3a in $CHCl_3$.

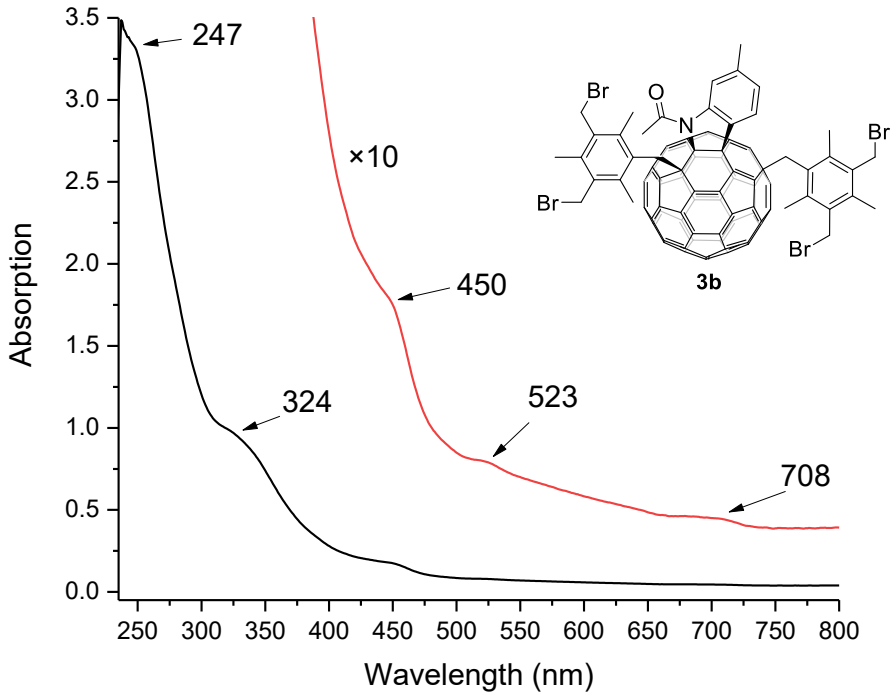


Figure S22. UV-vis absorption of compound 3b in $CHCl_3$.

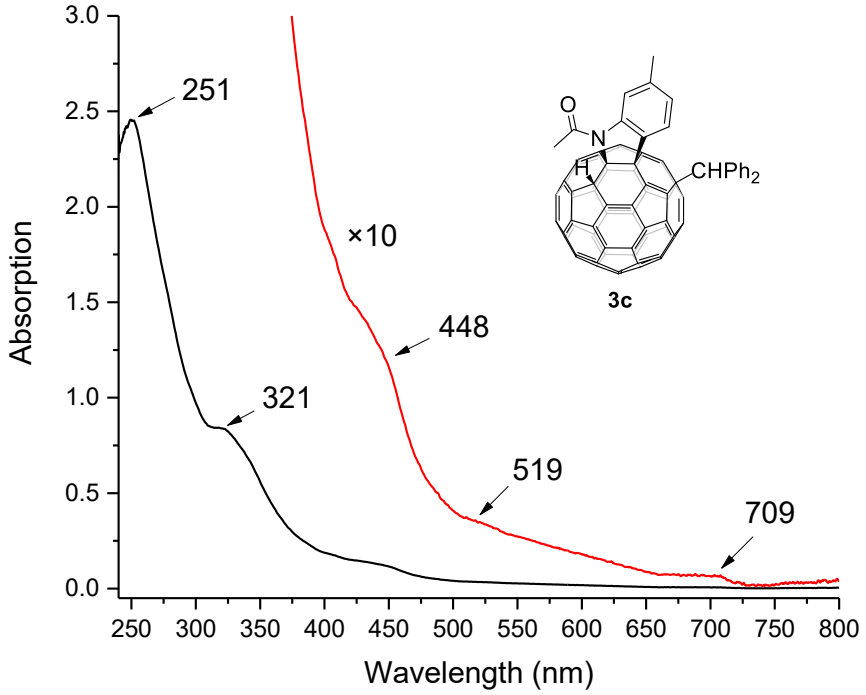


Figure S23. UV-vis absorption of compound 3c in $CHCl_3$.

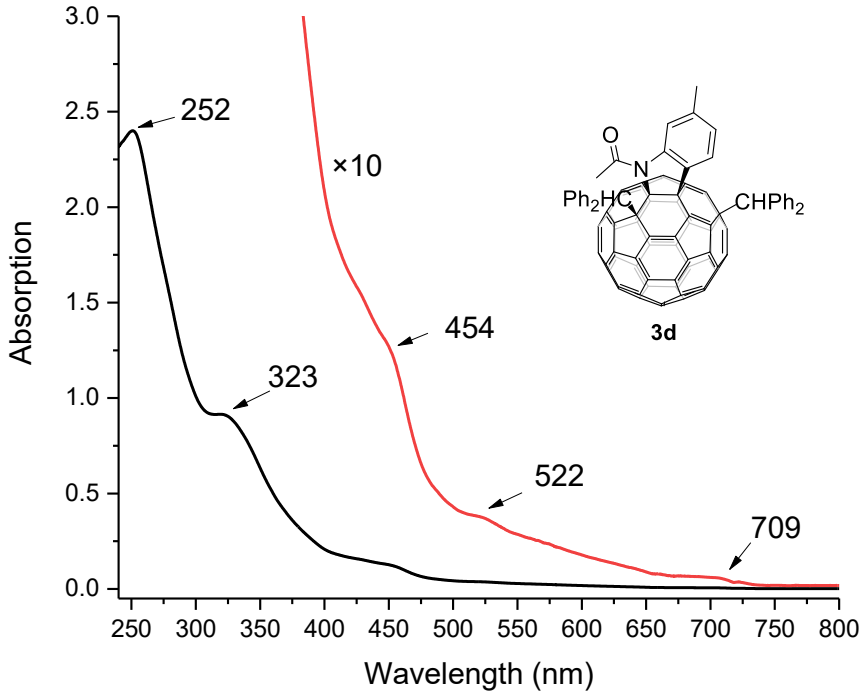


Figure S24. UV-vis absorption of compound 3d in $CHCl_3$.

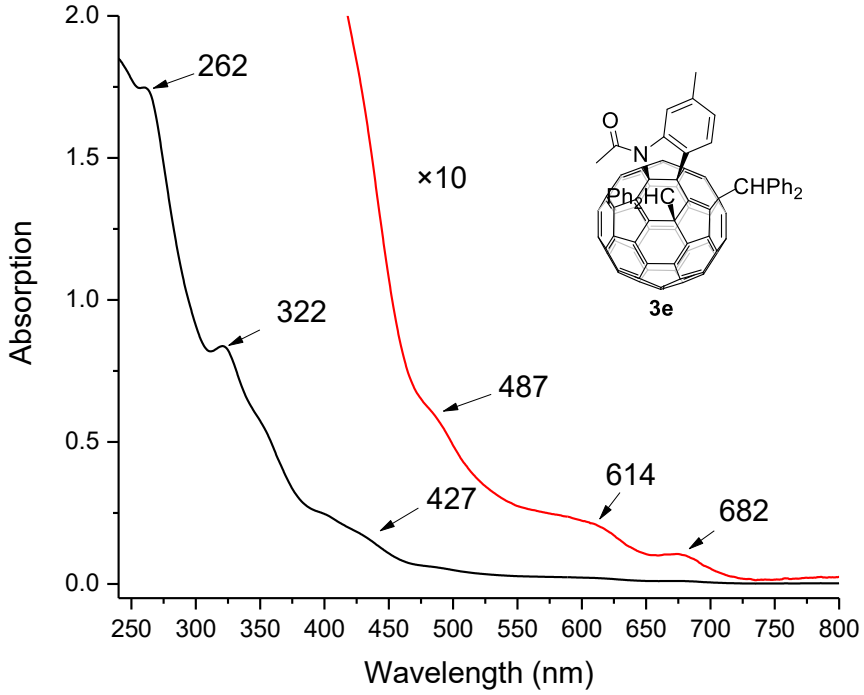


Figure S25. UV-vis absorption of compound 3e in $CHCl_3$.

5. Single-crystal X-ray crystallography of compound 3d.

Black block crystals of **3d** was obtained through slow diffusion of hexane into a carbon disulfide solution of **3d** at 4 ºC. The X-ray diffraction of **3d** was performed at 173 K using the wavelength of 0.71073 Å with a CCD detector at the beamline BL17B of the Shanghai Synchrotron Radiation Facility (SSRF). The multiscan method was used for absorption corrections. The structure was solved by direct method and refined with full-matrix least-squares refinement using the SHELXL-2016/6 within OLEX2.

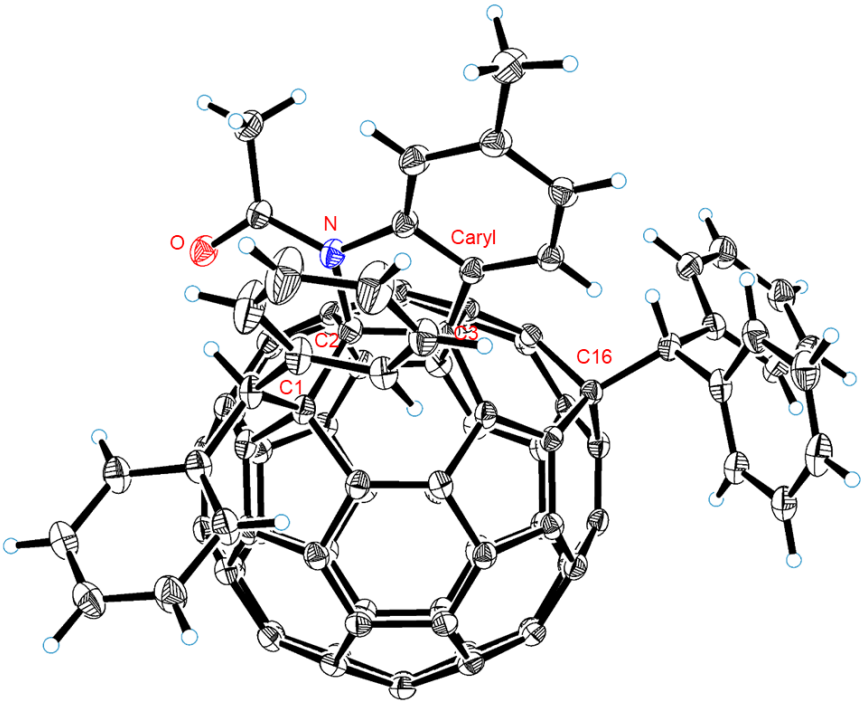
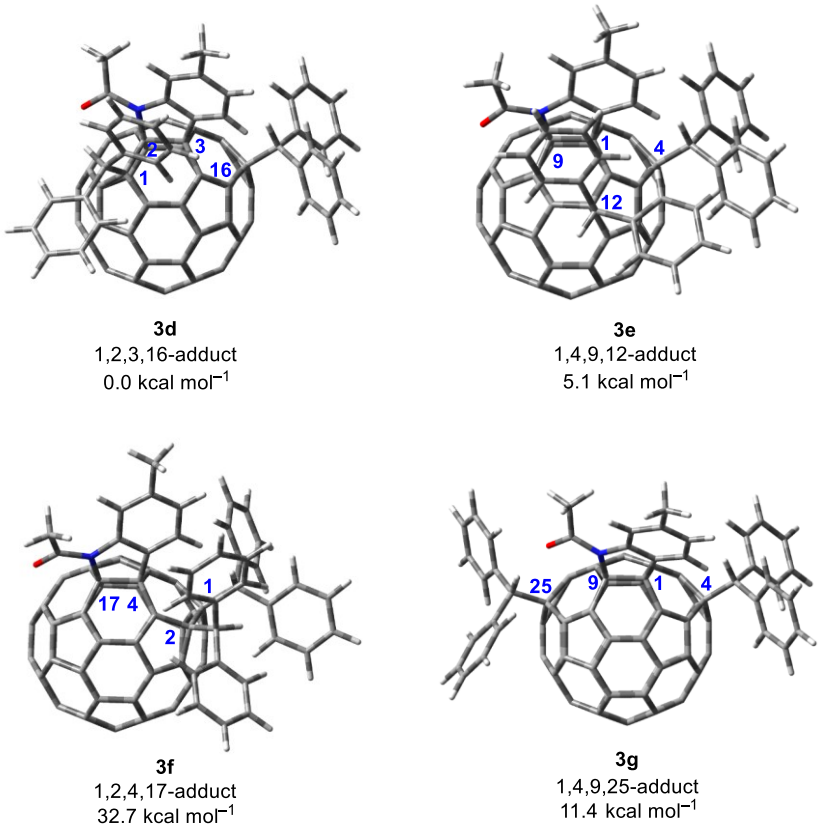


Figure S26. ORTEP diagram for product 3d with thermal ellipsoids shown at 30% probability, the solvent CS_2 molecule is omitted for clarity.

Table S1. Crystal data and structure refinement for compound 3d.

Identification code	1992595
Empirical formula	$C_{96}H_{31}NOS_2$
Formula weight	1278.34
Temperature/K	173(2)
Crystal system	monoclinic
Space group	$P2_1/n$
a/Å	10.205
b/Å	23.555
c/Å	23.364
α/°	90
β/°	95.62
γ/°	90
Volume/Å^3	5589.2
Z	4
ρ_{calc} g/cm^3	1.519
μ/mm^{-1}	0.160
F(000)	2616.0
Crystal size/mm^3	0.03 × 0.04 × 0.03
Radiation	synchrotron (λ = 0.71073)
2Θ range for data collection/°	4.368 to 50.084
Index ranges	$0 \le h \le 12$, $0 \le k \le 28$, $-26 \le l \le 26$
Reflections collected	9603
Independent reflections	9603 [R_{int} = 0.047, R_{sigma} = 0.0434]
Data/restraints/parameters	9603/36/888
Goodness-of-fit on F^2	1.082
Final R indexes [I>=2σ (I)]	R_1 = 0.1151, wR_2 = 0.2902
Final R indexes [all data]	R_1 = 0.1196, wR_2 = 0.2931
Largest diff. peak/hole / e Å^{-3}	1.66/-1.62

6. Calculated energies for products 3d–g.



3d
1,2,3,16-adduct
0.0 kcal mol^{-1}

3e
1,4,9,12-adduct
5.1 kcal mol^{-1}

3f
1,2,4,17-adduct
32.7 kcal mol^{-1}

3g
1,4,9,25-adduct
11.4 kcal mol^{-1}

Figure S27. Relative energies of the possible four products 3d–g.

7. The xyz coordinates and energies for the lowest energy structures of INT-1 and 3d–g

INT-1

-1 1

C	-3.86905200	2.14699200	1.68886700
C	-4.21848000	0.91996300	2.38045600
C	-3.30905600	0.31777800	3.23829600
C	-2.00027800	0.91068000	3.43551000
C	-1.66696600	2.07339300	2.75963600
C	-2.60906100	2.70138100	1.87911800
C	-4.45189900	2.10823900	0.36591200
C	-5.13327000	0.84081500	0.21903100
C	-5.00409900	0.10773200	1.46734800
C	-4.83864500	-1.26981500	1.45254700
C	-3.13495500	-1.12530800	3.22077400
C	-1.03065300	-0.16183200	3.57256100
C	0.23131100	0.00809700	2.99462000
C	0.59888300	1.21323700	2.31535200
C	-0.34278200	2.23559600	2.13945300
C	-0.45112600	3.04369900	0.98206700

C	-1.84561200	3.24843800	0.75989900
C	-2.43556200	3.25414000	-0.50828000
C	-3.71088000	2.62575500	-0.70082400
C	-5.12495600	0.15507000	-0.99270600
C	-4.37792400	0.70150800	-2.10924000
C	-3.69085100	1.90010900	-1.96743400
C	-2.36898000	2.04542100	-2.52862600
C	-1.58362800	2.85427600	-1.62291400
C	-0.24012700	2.58962300	-1.44483800
C	0.52379200	2.92678900	-0.16381200
C	1.59028700	1.72029000	-0.02142800
C	1.40162200	0.82346200	1.17482400
C	-1.72274600	-1.40864900	3.42897200
C	0.93693700	-2.52203900	-0.18881900
C	0.21747700	-3.01508700	0.87583300
C	-1.08189500	-3.61091300	0.67763300
C	-1.63723800	-3.67874100	-0.59647800
C	-0.90780100	-3.13320800	-1.71166600
C	0.67783900	-1.30813700	-2.17209500
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C	1.92774700	-1.34015300	-0.07980400
C	1.60326600	-0.53542900	1.16420900
C	0.84836700	-1.09107900	2.27590200
C	0.18888200	-2.30281300	2.17487900
C	-1.91141100	-3.26491100	1.81674200
C	-3.25992900	-2.99876800	1.63326800
C	-3.83383800	-3.04841800	0.29866900
C	-3.04590100	-3.39371200	-0.79247200
C	-3.18322400	-2.66087900	-2.03741800
C	-1.86204200	-2.50411500	-2.61022900
C	-1.52650300	-1.32811300	-3.26660400
C	-0.22585200	-0.72105800	-3.04826600
C	1.33464000	0.85576600	-1.26817600
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C	-0.39149300	0.70639500	-3.02703400
C	-1.78418100	0.99961700	-3.23426300
C	-2.49550000	-0.25517700	-3.38172900
C	-3.76191500	-0.40287300	-2.82673300
C	-4.11290600	-1.63005400	-2.14257500
C	-4.94365000	-1.28267500	-1.00392900
C	-4.81038200	-1.98487600	0.18951100
C	-1.11877600	-2.46980300	2.74123900
C	-3.88548200	-1.89992400	2.35032900
C	0.33696900	-2.54389000	-1.49246900

C	2.92084300	2.43721700	0.03027000
C	2.77602700	3.81169400	-0.20028400
C	3.90771100	4.62968100	-0.16204500
C	5.16610400	4.07269100	0.10083200
C	5.28372300	2.71113000	0.36155900
C	4.15187200	1.89538400	0.34478100
H	3.85281700	5.69961800	-0.30302700
H	6.25543000	2.28850500	0.60301700
H	4.22145800	0.84768800	0.62392300
C	0.82924800	5.32676700	-0.72319000
O	-0.38087900	5.43811300	-0.76996900
C	1.70904400	6.50871400	-1.08433700
H	1.04703400	7.26346000	-1.50795400
H	2.19505800	6.92383700	-0.19661300
H	2.47904000	6.23974500	-1.81187300
C	3.44955900	-1.72275400	-0.24924000
N	1.42041300	4.13066100	-0.37450900
C	6.37622200	4.97461600	0.12422300
H	6.56229300	5.41357700	-0.86225400
H	6.23982100	5.80188900	0.82891200
H	7.27267600	4.42375600	0.42087500
C	3.65124900	-2.71912200	-1.38172600
C	3.55137700	-4.09808100	-1.18030100
C	3.89583800	-2.25022400	-2.67428300
C	3.69050700	-4.98284500	-2.24476400
H	3.36562700	-4.48237500	-0.18134400
C	4.03553700	-3.13254500	-3.74223200
H	3.96073200	-1.17774200	-2.84379000
C	3.93307800	-4.50374700	-3.52997800
H	3.60646100	-6.05139600	-2.06886100
H	4.22081600	-2.74537100	-4.73991300
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C	3.60591000	-2.97744700	1.98340200
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H	7.20171900	-1.64982200	2.50010800
H	3.86541800	-3.98747900	3.85873400
H	6.17742600	-3.14457800	4.20353000

3d

0 1

C	0.62837600	-4.25738900	-0.66648600
C	-0.39728700	-4.39074500	-1.68522400
C	-0.47878900	-3.46925800	-2.71638000
C	0.45798600	-2.36249100	-2.76801600
C	1.42009900	-2.21779600	-1.77436700
C	1.51625200	-3.18496300	-0.70579200
C	0.06097300	-4.65740800	0.59461800
C	-1.32470700	-5.03058400	0.37180100
C	-1.60803600	-4.86719200	-1.04020100
C	-2.84605300	-4.38766300	-1.44909500
C	-1.77285700	-2.97081000	-3.15006100
C	-0.24923700	-1.19865900	-3.24329400
C	0.04843000	0.03992800	-2.69062300
C	1.04503300	0.16121500	-1.65804800
C	1.74602700	-0.92576700	-1.22170000
C	2.42976400	-1.06876200	0.14570600
C	1.92492100	-2.49261000	0.48777800
C	1.36692300	-2.87137000	1.67889200
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C	-2.29299800	-4.71072700	1.31471800
C	-1.92011100	-4.00028400	2.52572900
C	-0.59919400	-3.62797500	2.72526700
C	-0.28929000	-2.32205600	3.26604600
C	0.90469700	-1.83962700	2.62486600
C	1.03199700	-0.51893000	2.30093800
C	1.96203700	0.04000300	1.22754100
C	1.13650400	1.31637500	0.66618000
C	0.59847300	1.20285600	-0.73057700
C	-1.62281300	-1.56462300	-3.47924600
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C	-4.46789600	0.19459800	0.86669400
C	-2.51701900	1.35770300	1.80928800
C	-1.32164300	1.85693100	1.19258000
C	-1.62310400	2.34540200	-0.22898700
C	-0.60229500	1.69193600	-1.14144300
C	-0.99725100	0.97121200	-2.36424500
C	-2.30767400	0.63397200	-2.60377200
C	-3.83771800	-1.13215200	-2.49825500

C	-3.98623700	-2.47812000	-2.19778700
C	-4.56362700	-2.87617200	-0.92444800
C	-4.97929000	-1.91258100	-0.01700100
C	-4.70166200	-2.07959000	1.39742600
C	-4.38727800	-0.77631400	1.94558800
C	-3.40716400	-0.65206900	2.91929300
C	-2.45789900	0.44362700	2.85352700
C	-0.09385100	1.39696300	1.58978500
C	-0.02594900	0.38878200	2.60227100
C	-1.17536000	-0.05229500	3.26719700
C	-1.31348700	-1.44330800	3.60110600
C	-2.69403700	-1.82612000	3.38521700
C	-2.99130400	-3.07623200	2.85567400
C	-4.01631200	-3.20562600	1.84193200
C	-3.58456600	-4.21410300	0.89098800
C	-3.85533800	-4.05290400	-0.46369600
C	-2.63374200	-0.66125900	-3.15199000
C	-2.92852600	-3.41632200	-2.52540600
C	-3.54955800	1.24187600	0.79700200
C	2.12551500	2.45169000	0.80462400
C	3.21974100	2.06301400	1.57600600
C	4.28322800	2.93613600	1.76949700
C	4.23791200	4.21176700	1.19408200
C	3.14569000	4.58152600	0.41058500
C	2.09046500	3.69397600	0.19932600
H	5.18001700	2.63795200	2.29557200
H	3.13331700	5.55815700	-0.06553500
H	1.27656400	3.95185200	-0.47338400
C	3.79134400	0.01429700	2.91603800
O	3.67490500	-1.19631700	3.01659100
C	4.67256500	0.78408300	3.87286300
H	4.77891300	0.16320900	4.76247600
H	5.66527200	0.92845100	3.43413300
H	4.25926100	1.75916400	4.13692900
C	-1.61421400	3.92243000	-0.25288600
N	3.09995100	0.70306800	1.93858600
C	5.40779300	5.14076900	1.39072800
H	5.46176500	5.49659700	2.42523500
H	6.34789000	4.62348900	1.17037600
H	5.33713300	6.01443500	0.73814700
C	-2.79677000	4.48093900	0.52577000
C	-4.04214100	4.68620400	-0.07304100
C	-2.65620700	4.74715600	1.88939800
C	-5.12158400	5.14159300	0.67733600

H	-4.16896900	4.49573300	-1.13486800
C	-3.73441900	5.20350400	2.64288900
H	-1.69129500	4.58613400	2.36527400
C	-4.97195500	5.40046700	2.03751500
H	-6.08280200	5.29614900	0.19672500
H	-3.60509800	5.40565400	3.70175100
H	-5.81544600	5.75555900	2.62152800
H	-0.71674500	4.18775500	0.31797600
C	-1.44700400	4.54891100	-1.62394400
C	-0.58210900	5.63991600	-1.75173500
C	-2.13641300	4.11230600	-2.75796400
C	-0.40266700	6.27594900	-2.97634300
H	-0.04938800	5.99908500	-0.87294300
C	-1.95820100	4.74475300	-3.98560700
H	-2.82086600	3.27278600	-2.68741600
C	-1.09002600	5.82668300	-4.10014000
H	0.27509000	7.12095000	-3.05130900
H	-2.50027400	4.38721600	-4.85581700
H	-0.95063700	6.31582800	-5.05913100
C	4.01206800	-1.14067100	-0.00508900
H	4.34482800	-1.47099200	0.97995900
C	4.44186200	-2.23801100	-0.97357800
C	4.75026000	-3.50377300	-0.46978600
C	4.52641800	-2.02718900	-2.35159200
C	5.11585800	-4.54225100	-1.32120000
H	4.68453700	-3.67729100	0.60224200
C	4.88683200	-3.06458400	-3.20679000
H	4.31269100	-1.04333500	-2.76122300
C	5.18053000	-4.32568200	-2.69472800
H	5.34891300	-5.51991000	-0.91025700
H	4.94167500	-2.88463200	-4.27612800
H	5.46362500	-5.13377600	-3.36219500
C	4.76015300	0.14899100	-0.31250600
C	6.00499100	0.32705100	0.30510800
C	4.32939700	1.12694600	-1.21193400
C	6.79941600	1.43445400	0.02486000
H	6.36037400	-0.43095200	1.00152300
C	5.11859700	2.24310700	-1.48832000
H	3.37149100	1.03024100	-1.71013500
C	6.35893400	2.39878200	-0.88007000
H	7.76724000	1.53965000	0.50748600
H	4.75324800	2.99220800	-2.18438600
H	6.97649300	3.26278300	-1.10756900

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C	3.15741200	-3.27474100	1.66532500
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C	2.76302900	-1.55516500	3.37505100
C	1.33911800	-1.70898200	3.17667600
C	0.87030300	-2.58801500	2.23274200
C	1.78301000	-3.40229600	1.47707200
C	4.03132400	-3.25765300	0.51585400
C	5.08128400	-2.28626800	0.76290800
C	4.84973400	-1.70585600	2.07470300
C	5.09398100	-0.35685300	2.28659000
C	3.02344100	-0.14377700	3.59304500
C	0.71007200	-0.37737100	3.30236100
C	-0.35422500	-0.03964100	2.49590000
C	-1.13089800	-1.03908600	1.63146400
C	-0.23719800	-2.20955800	1.33216200
C	-0.05388600	-2.78792200	0.11968700
C	1.22690700	-3.52190400	0.15581600
C	2.05962300	-3.52666500	-0.93252900
C	3.48376000	-3.37580500	-0.75885000
C	5.55386100	-1.49418200	-0.27335700
C	4.99683400	-1.63075100	-1.60756500
C	3.97955700	-2.54430400	-1.84092000
C	2.85487100	-2.17935400	-2.68140400
C	1.66092400	-2.77143800	-2.13532700
C	0.45939600	-2.10174600	-2.18674700
C	-0.67694000	-2.30499300	-1.17383200
C	-1.36737300	-0.85603000	-1.04385300
C	-1.28639900	-0.22549100	0.33577000
C	1.75796400	0.56816700	3.55209300
C	0.56060000	2.90005700	-0.23156900
C	1.09390800	3.01221200	1.02920500
C	2.51396100	3.16698300	1.21840900
C	3.37037400	3.20008600	0.12309500
C	2.82323300	3.05652900	-1.20038100
C	0.94772600	1.92161800	-2.31529600
C	-0.25264500	1.33414000	-1.79083000
C	-0.72407800	2.10941900	-0.55640800
C	-0.97548200	1.07760300	0.53573700
C	-0.39650100	1.24013500	1.88409600
C	0.58497200	2.18070300	2.14044200
C	2.89034300	2.43992900	2.41764400

C	4.09694200	1.76125100	2.46454200
C	4.98300600	1.77800700	1.31472100
C	4.63099700	2.48414500	0.17044700
C	4.86384400	1.90280900	-1.13695900
C	3.74714900	2.25846000	-1.98755500
C	3.26188400	1.34587200	-2.91328200
C	1.83136600	1.18217300	-3.08792500
C	-0.52599900	0.01168600	-1.99808700
C	0.41266300	-0.78633600	-2.73757900
C	1.55758400	-0.21166700	-3.30527900
C	2.80691700	-0.92323200	-3.27491700
C	3.86895700	0.03366900	-3.02881900
C	4.93662700	-0.31003100	-2.20941800
C	5.44514300	0.64231400	-1.24380200
C	5.82222800	-0.08531100	-0.04922100
C	5.59537600	0.47212200	1.20336600
C	1.69232800	1.83993800	2.97798400
C	4.16683800	0.43943500	3.06711700
C	1.44903700	2.88574300	-1.35714600
C	-2.77870700	-1.11104600	-1.53089400
C	-2.93384400	-2.42813700	-1.97526700
C	-4.13530200	-2.81587000	-2.56661000
C	-5.20177700	-1.91223600	-2.63488700
C	-5.05603100	-0.62605500	-2.12154700
C	-3.83790900	-0.22331000	-1.57608000
H	-4.29141100	-3.80819700	-2.96315700
H	-5.89136500	0.06718200	-2.15606600
H	-3.72981300	0.77821800	-1.17127600
C	-1.49599500	-4.51342800	-1.90585700
O	-0.39439800	-4.95349600	-1.63539200
C	-2.57497900	-5.42288300	-2.44516900
H	-2.17491800	-6.43528400	-2.39891300
H	-3.48856600	-5.35635800	-1.85022700
H	-2.80747900	-5.17908800	-3.48589300
C	-1.96261400	2.99408500	-0.95444100
N	-1.76046100	-3.16790000	-1.72779300
C	-6.50955600	-2.36853100	-3.23100800
H	-6.36244500	-2.79793600	-4.22692900
H	-6.97317000	-3.14187100	-2.60757200
H	-7.21665500	-1.54034400	-3.31963500
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C	-1.01220100	5.25192400	-1.65368000
C	-1.72594600	3.71914300	-3.36354600
C	-0.61359200	6.15640000	-2.63237600

H	-0.89689300	5.50335200	-0.60226800
C	-1.33165400	4.62444100	-4.34544000
H	-2.15318700	2.76004700	-3.64970300
C	-0.77164800	5.84495700	-3.98105500
H	-0.18160100	7.10872100	-2.34015400
H	-1.46305300	4.37474200	-5.39381900
H	-0.46172000	6.55272200	-4.74376600
H	-2.63453000	2.29368800	-1.45897100
C	-2.77032100	3.65512600	0.14992000
C	-4.10913300	3.95218100	-0.13927000
C	-2.24444100	4.09012600	1.36594400
C	-4.89179300	4.68438000	0.74586300
H	-4.52634400	3.63187600	-1.09231000
C	-3.03108700	4.81256400	2.26346800
H	-1.21121300	3.88640100	1.61960800
C	-4.35077000	5.12216500	1.95447000
H	-5.92229300	4.91525600	0.49254000
H	-2.60104100	5.13875000	3.20557800
H	-4.95645400	5.69629900	2.64904400
C	-2.43647800	-1.50965800	2.40700000
H	-2.01207200	-2.06027000	3.25746300
C	-3.18268300	-0.33188700	2.99975900
C	-3.23697900	-0.19698300	4.38943300
C	-3.78492200	0.65615600	2.21429600
C	-3.88002900	0.88585100	4.98214200
H	-2.76240800	-0.94972700	5.01449700
C	-4.43288200	1.73721400	2.80181200
H	-3.74473500	0.58791300	1.13160600
C	-4.48013000	1.85792600	4.18758100
H	-3.90759600	0.96910200	6.06443900
H	-4.89089700	2.49042900	2.16960100
H	-4.97847400	2.70861300	4.64313900
C	-3.29256500	-2.52055700	1.64913400
C	-2.84328300	-3.84504900	1.56236100
C	-4.54446100	-2.21764800	1.10468300
C	-3.60194200	-4.82645100	0.93195700
H	-1.89614500	-4.12110100	2.01662900
C	-5.31225000	-3.19943600	0.48486400
H	-4.94647000	-1.21486000	1.18173900
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H	-3.22751300	-5.84533800	0.88480100
H	-6.28305100	-2.93373000	0.07586700
H	-5.44883300	-5.27307600	-0.08758500

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C	-2.26962100	0.43379300	3.43698000
C	-2.03497500	1.68730600	2.92612800
C	-3.08879000	2.40582800	2.26386300
C	-5.03639900	1.93357900	0.85386600
C	-5.71403600	0.67381600	0.59980000
C	-5.44146500	-0.21349200	1.71629500
C	-5.24030200	-1.56831100	1.49319800
C	-3.36907600	-1.59935300	3.08453700
C	-1.25967700	-0.62604200	3.30451600
C	-0.08877200	-0.37494400	2.62101900
C	0.21574800	0.94631900	2.04937100
C	-0.78141400	1.98982000	2.20461900
C	-1.03379900	2.88464300	1.20728600
C	-2.47558200	3.13232700	1.17570200
C	-3.13978400	3.24160300	-0.02454900
C	-4.43140600	2.61986900	-0.19627800
C	-5.77887400	0.16369500	-0.68797800
C	-5.16261300	0.88486000	-1.78623800
C	-4.49668800	2.07756100	-1.54188300
C	-3.23370800	2.35162800	-2.19655700
C	-2.38078400	3.06510300	-1.27651200
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C	-0.14591400	3.01139200	-0.00487300
C	0.99101000	1.84914400	-0.16400700
C	1.01943000	0.81962600	0.95874900
C	-1.94125500	-1.86604900	3.09924900
C	0.38053700	-2.40719000	-0.82344200
C	-0.22208200	-3.08345900	0.20459200
C	-1.52887300	-3.67116400	0.04898700
C	-2.20592700	-3.58083200	-1.16215800
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C	-0.11974900	-0.92470400	-2.54054900
C	0.74118800	-0.24521200	-1.60798000
C	1.41691300	-1.26013700	-0.66227500
C	1.51959200	-0.65823100	0.84448300
C	0.51255400	-1.34461500	1.77877400
C	-0.13452700	-2.53809800	1.57553100
C	-2.25265000	-3.50232700	1.29557800

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C	-4.31949900	-3.14456500	0.01503100
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C	-3.90107400	-2.41709600	-2.29334200
C	-2.64366300	-2.13922700	-2.95457000
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C	-1.09657000	-0.25910100	-3.26044400
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C	-3.39422600	0.17373500	-3.34107200
C	-4.59852100	-0.09106100	-2.70305200
C	-4.85709800	-1.41203500	-2.16638900
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C	-1.38989500	-2.80325500	2.22617000
C	-4.18788000	-2.27817800	2.19524500
C	-0.35314300	-2.25987800	-2.04772200
C	2.21956500	2.67117800	-0.52035000
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C	2.93612000	4.95861200	-0.84191200
C	4.15731100	4.50136100	-1.34075200
C	4.38060700	3.12830600	-1.46703800
C	3.40852500	2.21965800	-1.07089700
H	2.75493000	6.02431900	-0.82218800
H	5.32218900	2.76783600	-1.87170100
H	3.59201900	1.15612500	-1.16968200
C	0.00583000	5.46680700	0.25987400
O	-1.20812800	5.51586600	0.29640600
C	0.84092200	6.69271200	0.56080000
H	0.22244800	7.33886900	1.18420000
H	1.77283100	6.45299100	1.07603500
H	1.07124000	7.23552300	-0.36078200
C	2.81343000	-1.67022400	-1.31621500
N	0.64891700	4.26938800	0.00141100
C	5.22650200	5.48522700	-1.74235600
H	4.80973100	6.48040500	-1.91827100
H	5.98406500	5.57604600	-0.95547000
H	5.73816900	5.16253600	-2.65344300
C	2.72140600	-1.75376000	-2.84066900
C	2.33030900	-2.93894500	-3.46948700
C	3.01230300	-0.64145700	-3.63297300
C	2.20247900	-3.00097700	-4.85325300

H	2.12072900	-3.81941400	-2.86727800
C	2.89221200	-0.70184700	-5.01875500
H	3.31421800	0.29181100	-3.16354400
C	2.48056000	-1.88087000	-5.63289700
H	1.88720900	-3.92784800	-5.32264100
H	3.12011900	0.17549700	-5.61623000
H	2.38204000	-1.92893300	-6.71297100
H	3.47944300	-0.82797100	-1.09206500
C	3.54538500	-2.92628100	-0.82937200
C	4.84407000	-3.10931300	-1.32985600
C	3.03871700	-3.89637000	0.03398200
C	5.60604700	-4.21601900	-0.98156000
H	5.25105900	-2.36980200	-2.01648400
C	3.79900300	-5.01649100	0.38003300
H	2.05528500	-3.78381300	0.47159100
C	5.08145100	-5.18333800	-0.12459500
H	6.60786500	-4.32782600	-1.38471100
H	3.37640600	-5.75483700	1.05522800
H	5.66979200	-6.05424800	0.14610200
C	2.96720200	-0.83057500	1.54987400
H	3.39577000	-1.70659500	1.07161900
C	4.00556600	0.27418700	1.37753600
C	3.86718800	1.57242300	1.88556300
C	5.23106200	-0.06958900	0.79557900
C	4.91385900	2.48525900	1.81726000
H	2.92628500	1.89600000	2.31686500
C	6.27536900	0.84770700	0.70681900
H	5.37412000	-1.08113000	0.41939700
C	6.12218900	2.12974900	1.22519400
H	4.77318200	3.48737300	2.21133100
H	7.21322200	0.55087400	0.24639300
H	6.93526800	2.84716400	1.16491000
C	2.90342500	-1.22706700	3.03033500
C	3.20090000	-2.54973500	3.36917000
C	2.59382100	-0.33849800	4.06559500
C	3.17323800	-2.98118300	4.69286100
H	3.46458900	-3.25263600	2.58298300
C	2.55726200	-0.76701900	5.38805300
H	2.36827400	0.69928700	3.84982100
C	2.84529000	-2.09100200	5.70927900
H	3.41171000	-4.01461800	4.92609000
H	2.30638500	-0.05884600	6.17202800
H	2.82037100	-2.42191900	6.74289200

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C	0.79299300	-0.96449400	-3.63905800
C	1.37861200	0.14744700	-3.03468700
C	2.55646200	0.00210500	-2.22783400
C	3.63146800	-1.64354900	-0.73713500
C	3.32290800	-3.03808200	-0.55103000
C	2.63727200	-3.51180200	-1.73675500
C	1.60777600	-4.43168600	-1.61462800
C	0.29285100	-3.23356900	-3.31651000
C	-0.64762900	-1.11243500	-3.63004200
C	-1.42462600	-0.14017600	-3.01280400
C	-0.79659500	0.99059200	-2.36842200
C	0.56399000	1.14863900	-2.37873200
C	1.29537400	1.65915300	-1.20209000
C	2.45924900	0.95156000	-1.10153400
C	3.24663700	0.72237400	0.17362400
C	3.54532500	-0.77222800	0.31631600
C	2.96589500	-3.51687100	0.70651400
C	2.88107400	-2.59945100	1.81312000
C	3.14704600	-1.24836400	1.60234600
C	2.33545200	-0.22217700	2.22273200
C	2.25438900	0.91194400	1.34120800
C	1.05875600	1.58705000	1.23564400
C	0.58817000	2.32825100	-0.02669400
C	-1.01715100	2.11956300	-0.03628700
C	-1.56140700	1.28577200	-1.16084900
C	-0.96047100	-2.50885300	-3.43160500
C	-3.34551400	-1.44512300	0.39864400
C	-3.24369600	-2.31666700	-0.66003900
C	-2.65893900	-3.62350700	-0.48571300
C	-2.19028600	-4.02399100	0.76162000
C	-2.26618800	-3.10623400	1.86827200
C	-2.17830500	-0.68201500	2.27384500
C	-2.31084600	0.43506600	1.38300700
C	-3.29756500	0.09207300	0.25662100
C	-2.60989400	0.43024500	-1.05199700
C	-2.54298900	-0.51222700	-2.18320100
C	-2.85280100	-1.83905600	-2.00680400
C	-1.91800500	-3.96006400	-1.68587400

C	-0.72524600	-4.66011500	-1.58918400
C	-0.22140600	-5.05679600	-0.28586000
C	-0.94011200	-4.75136300	0.86373300
C	-0.24691900	-4.28311400	2.04911300
C	-1.06692800	-3.26493000	2.67116800
C	-0.47038000	-2.15320900	3.25297800
C	-1.04384400	-0.83548600	3.05897600
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C	-0.07798200	1.15554500	1.99843800
C	0.03053900	0.10937000	2.92031700
C	1.27040100	-0.60215200	3.03241900
C	0.97026300	-2.00909300	3.23662300
C	1.75599500	-2.98733100	2.64162000
C	1.13748300	-4.14714000	2.03463800
C	1.88521500	-4.47311600	0.83430500
C	1.21836300	-4.91692700	-0.30170400
C	-2.04033700	-2.85948700	-2.62519100
C	0.40581000	-4.28217600	-2.41757200
C	-2.81132600	-1.83825000	1.67184900
C	-1.56466200	3.52426400	-0.18255200
C	-0.53609300	4.45864800	-0.16975600
C	-0.79548100	5.79511100	-0.46612500
C	-2.11100300	6.20354900	-0.71208200
C	-3.13518700	5.25647300	-0.71520100
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H	-0.00051600	6.52514800	-0.54815500
H	-4.15046700	5.56484900	-0.94836200
H	-3.64209000	3.16719400	-0.59726200
C	1.82814000	4.40539800	0.59843400
O	2.84738900	3.75366500	0.73923000
C	1.78756900	5.84746000	1.05861300
H	2.59726100	5.95575400	1.78006900
H	1.98431100	6.52681600	0.22434500
H	0.83647500	6.12095100	1.51831200
C	-4.66248900	0.84084000	0.51425300
N	0.70409700	3.82443900	0.06374000
C	-2.39830400	7.65677600	-0.99338300
H	-2.40033900	8.24152200	-0.06704200
H	-1.64067300	8.08960900	-1.65343000
H	-3.37451100	7.78194500	-1.46793300
C	-5.38177700	0.25570600	1.72146900
C	-6.24503400	-0.83622400	1.60617800
C	-5.13917000	0.78863700	2.98917200
C	-6.84633100	-1.38475800	2.73456600

H	-6.45416700	-1.25680300	0.62666900
C	-5.73956600	0.24214300	4.12027300
H	-4.46426000	1.63605200	3.08935700
C	-6.59492900	-0.84814100	3.99500200
H	-7.51640600	-2.23242100	2.62799100
H	-5.54062300	0.67135000	5.09752700
H	-7.06589300	-1.27653800	4.87432300
H	-4.35793100	1.85243500	0.80568800
C	-5.56302600	1.00028700	-0.69550200
C	-6.21620600	2.22402300	-0.87275000
C	-5.80602500	-0.02101700	-1.61717700
C	-7.08020100	2.43003100	-1.94316800
H	-6.04981100	3.02205400	-0.15123000
C	-6.66852800	0.18169800	-2.69140300
H	-5.32336500	-0.98577300	-1.49795300
C	-7.30691000	1.40702900	-2.85974300
H	-7.57474000	3.38944200	-2.06120300
H	-6.83923000	-0.62287600	-3.40011100
H	-7.97739700	1.56354500	-3.69900600
C	4.60672100	1.54106500	0.20949800
H	4.29772300	2.57489700	0.10472600
C	5.31485600	1.44710000	1.55109100
C	5.39748800	2.61519600	2.31863500
C	5.87697400	0.27738600	2.07938700
C	6.02935500	2.62173300	3.55833700
H	4.94432100	3.52431400	1.93474600
C	6.50878200	0.28120000	3.32007600
H	5.81569500	-0.65904100	1.53684500
C	6.59119400	1.45364800	4.06431200
H	6.07941700	3.54326800	4.13087200
H	6.93479000	-0.64063300	3.70459900
H	7.08448100	1.45481700	5.03163000
C	5.42995800	1.23651000	-1.03654700
C	5.17750600	2.02279000	-2.16810600
C	6.37851200	0.21780500	-1.14528600
C	5.82687300	1.78786000	-3.37425400
H	4.44548600	2.82469000	-2.09489800
C	7.03623400	-0.01880800	-2.35139500
H	6.62522800	-0.39645300	-0.28772000
C	6.75966500	0.75859900	-3.47087800
H	5.60617800	2.40995000	-4.23642200
H	7.77007900	-0.81700200	-2.41167200
H	7.27131100	0.56877200	-4.40943000

E = -3767.24151264

7. Reference

1 B. Zhu and G.-W. Wang, *Org. Lett.*, 2009, **11**, 4334.