Electronic Supplementary Information

Copper-mediated synthesis of fullerooxazoles from [60]fullerene and *N*-hydroxybenzimidoyl cyanides

Qing-Song Liu,[a] Wen-Jie Qiu,[a] Wen-Qiang Lu[a] and Guan-Wu Wang*[a,b]

[a]Hefei National Laboratory for Physical Sciences at Microscale and Department of Chemistry, University of Science and Technology of China, Hefei, Anhui 230026, P. R. China
E-mail: gwang@ustc.edu.cn; Fax: +86 551 3607864; Tel: +86 551 3607864
[b]State Key Laboratory of Applied Organic Chemistry, Lanzhou University, Lanzhou, Gansu 730000, P. R. China

Table of Contents

1. General information

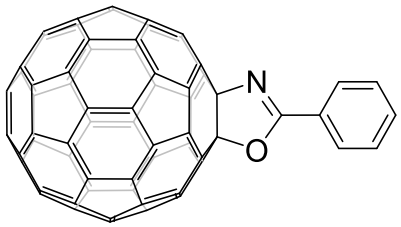
Anhydrous 1,2-dichlorobenzene (1,2-$C_6H_4Cl_2$) was freshly distilled, *N*-hydroxybenzimidoyl cyanides **1a**–**r** were synthesized by the literature procedure.[1] Other chemicals were purchased from commercial sources and used as received. ^{1}H NMR and ^{13}C NMR spectra were recorded on a Bruker ASCEND III–400 or a Bruker ASCEND III–500 or a JEOL JNM-ECZ600R/SI spectrometer at room temperature. ^{1}H NMR chemical shifts were determined relative to TMS. ^{13}C NMR chemical shifts were determined relative to TMS or residual DMSO (δ 39.03 ppm). Abbreviations for signal couplings are: s, singlet; d, doublet; t, triplet; m, multiplet. High resolution mass spectra were obtained on a Bruker UltrafleXtreme MALDI-TOF/TOF instrument. UV-vis spectra were obtained on a SHIMADZU UV-3600PLUS instrument. IR spectra were obtained on a Thermo Scientific Nicolet 6700 instrument. Electrochemical reaction was performed under an argon atmosphere at 0 °C using a Shanghai Chenhua CHI630D workstation.

2. General procedure for the reaction of C_{60} with substrates 1

A mixture of C_{60} (0.05 mmol), **1** (0.15 mmol) (0.25 mmol for **1c**, **1f** and **1m**), $CuBr_2$ (0.05 mmol) and Na_2HPO_4 (0.10 mmol) was completely dissolved in anhydrous 1,2-$C_6H_4Cl_2$ (6 mL) and the reaction was performed in a sealed tube. After being stirred in an oil bath at 150 °C (160 °C for **1i**) for 1 h, the resulting solution was evaporated in vacuo and subsequently separated on a silica gel column (300–400 mesh) with carbon disulfide (CS_2) as the eluent to give recovered C_{60} and then the desired products **2**.

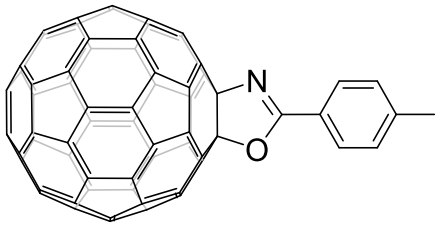
Products **2a**–**c**, **2g**–**j**, **2p** and **2q** were known compounds, and their spectra were consistent with those reported in the literature.[2a–f]

3. Synthesis and spectral data of compounds 2a–r and 3a



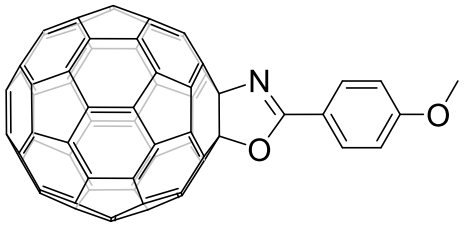
2a

Synthesis and spectral data of 2a: by following the general procedure, the reaction of C_{60} (36.8 mg, 0.05 mmol) with **1a** (21.9 mg, 0.15 mmol), $CuBr_2$ (11.4 mg, 0.05 mmol) and Na_2HPO_4 (14.5 mg, 0.10 mmol) at 150 °C for 1 h afforded recovered C_{60} (16.8 mg, 46%) and **2a**[2a,c–f] (12.7 mg, 30%): amorphous brown solid; ^{1}H NMR (400 MHz, CS_2 with DMSO-d_6 as the external deuterium lock) δ 8.44–8.37 (m, 2H), 7.70–7.64 (m, 1H), 7.64–7.58 (m, 2H).



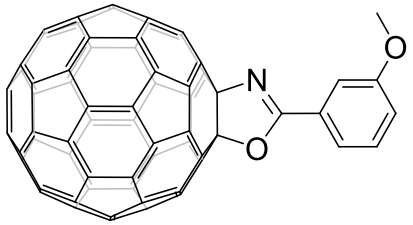
2b

Synthesis and spectral data of 2b: by following the general procedure, the reaction of C_{60} (36.3 mg, 0.05 mmol) with **1b** (24.3 mg, 0.15 mmol), $CuBr_2$ (11.0 mg, 0.05 mmol) and Na_2HPO_4 (14.2 mg, 0.10 mmol) at 150 °C for 1 h afforded recovered C_{60} (20.9 mg, 58%) and **2b**[2a,e,f] (11.0 mg, 26%): amorphous brown solid; ^{1}H NMR (400 MHz, 1:1 CS_2/$CDCl_3$) δ 8.35 (d, J = 8.0 Hz, 2H), 7.43 (d, J = 8.0 Hz, 2H), 2.55 (s, 3H).



2c

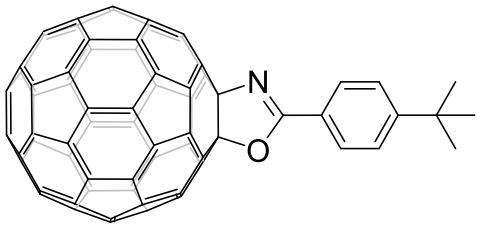
Synthesis and spectral data of 2c: by following the general procedure, the reaction of C_{60} (35.9 mg, 0.05 mmol) with **1c** (44.3 mg, 0.25 mmol), $CuBr_2$ (11.8 mg, 0.05 mmol) and Na_2HPO_4 (14.5 mg, 0.10 mmol) at 150 °C for 1 h afforded recovered C_{60} (16.9 mg, 47%) and **2c**[2a–f] (10.4 mg, 24%): amorphous brown solid; ^{1}H NMR (500 MHz, 1:1 CS_2/$CDCl_3$) δ 8.38 (d, J = 8.9 Hz, 2H), 7.10 (d, J = 8.9 Hz, 2H), 3.96 (s, 3H).



2d

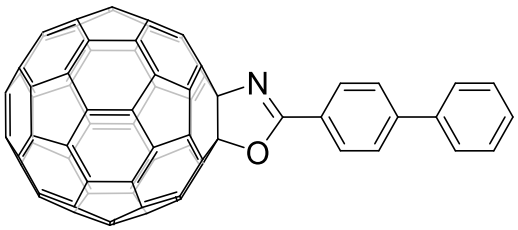
Synthesis and spectral data of 2d: by following the general procedure, the reaction of C_{60} (35.9 mg, 0.05 mmol) with **1d** (26.6 mg, 0.15 mmol), $CuBr_2$ (11.1 mg, 0.05 mmol) and Na_2HPO_4 (14.5 mg, 0.10 mmol) at 150 °C for 1 h afforded recovered C_{60} (15.2 mg, 42%) and **2d** (9.8 mg, 22%): amorphous brown solid; ^{1}H NMR (400 MHz, CS_2 with DMSO-d_6 as the external deuterium lock) δ 7.96 (d, J = 7.6 Hz, 1H), 7.89 (dd, J = 2.6, 1.6 Hz, 1H), 7.48 (t, J = 7.9 Hz, 1H), 7.15 (ddd, J = 8.3, 2.7, 1.0 Hz, 1H), 3.96 (s, 3H); ^{13}C NMR (101 MHz, CS_2 with DMSO-d_6 as the external deuterium lock and reference, all 2C unless indicated) δ 164.40 (1C, *C*=N), 159.04 (1C, aryl *C*), 147.55 (1C), 147.49, 147.14 (1C), 145.75 (4C), 145.61, 145.46, 145.40, 145.12, 144.98, 144.83, 144.59, 144.48, 144.22, 143.97, 143.65, 143.02, 142.18, 142.15, 142.07, 141.75 (4C), 141.66, 141.51, 141.39 (4C), 139.85, 139.01, 137.21, 135.51, 129.30 (1C, aryl *C*), 127.56 (1C,

aryl *C*), 121.20 (1C, aryl *C*), 118.85 (1C, aryl *C*), 112.85 (1C, aryl *C*), 96.71 (1C, sp^3-*C* of C_{60}), 91.62 (1C, sp^3-*C* of C_{60}), 54.64 (1C); FT-IR ν/cm^{-1} (KBr) 1641, 1580, 1512, 1489, 1461, 1431, 1327, 1042, 983, 936, 786, 715, 526; UV-vis (CHCl3) λ_{max} nm (log ε) 257 (5.03), 316 (4.56), 418 (3.34), 453 (3.09), 684 (1.97); MALDI-TOF MS *m/z* calcd for $C_{68}H_7NO_2$ $[M]^-$ 869.0482, found 869.0474.



2e

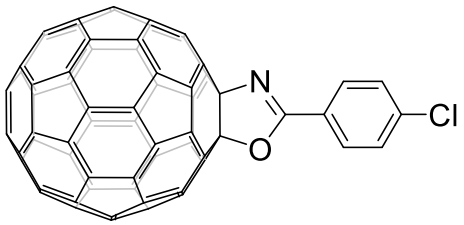
Synthesis and spectral data of 2e: by following the general procedure, the reaction of C_{60} (36.3 mg, 0.05 mmol) with **1e** (30.5 mg, 0.15 mmol), $CuBr_2$ (11.5 mg, 0.05 mmol) and Na_2HPO_4 (14.0 mg, 0.10 mmol) at 150 ºC for 1 h afforded recovered C_{60} (18.3 mg, 50%) and **2e** (8.5 mg, 19%): amorphous brown solid; ^{1}H NMR (400 MHz, CS_2 with DMSO-d_6 as the external deuterium lock) δ 8.30 (d, J = 8.4 Hz, 2H), 7.59 (d, J = 8.4 Hz, 2H), 1.46 (s, 9H); ^{13}C NMR (101 MHz, CS_2 with DMSO-d_6 as the external deuterium lock and reference, all 2C unless indicated) δ 164.37 (1C, *C*=N), 154.85 (1C, aryl *C*), 147.70, 147.56 (1C), 147.14 (1C), 145.75, 145.74, 145.60, 145.46, 145.40, 145.12, 145.04, 144.86, 144.59, 144.48, 144.26, 143.99, 143.66, 143.21, 142.17, 142.16, 142.06, 141.77 (4C), 141.66, 141.52, 141.40 (4C), 139.82, 139.00, 137.23, 135.49, 128.72 (aryl *C*), 125.23 (aryl *C*), 123.67 (1C, aryl *C*), 96.58 (1C, sp^3-*C* of C_{60}), 91.72 (1C, sp^3-*C* of C_{60}), 34.26 (1C), 30.80 (3C); FT-IR ν/cm^{-1} (KBr) 1640, 1324, 1111, 1085, 984, 932, 843, 774, 686, 661, 603, 576, 563, 525; UV-vis ($CHCl_3$) λ_{max} nm (log ε) 256 (5.08), 316 (4.62), 419 (3.45), 456 (3.23), 680 (2.27); MALDI-TOF MS *m/z* calcd for $C_{71}H_{13}NO$ $[M]^-$ 895.1003, found 895.1001.



2f

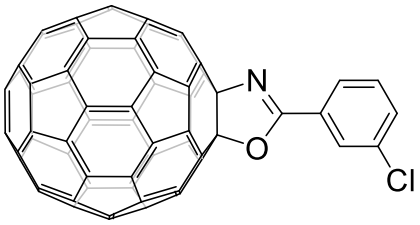
Synthesis and spectral data of 2f: by following the general procedure, the reaction of C_{60} (35.5 mg, 0.05 mmol) with **1f** (53.5 mg, 0.25 mmol), $CuBr_2$ (11.3 mg, 0.05 mmol) and Na_2HPO_4 (14.3 mg, 0.10 mmol) at 150 ºC for 1 h afforded recovered C_{60} (17.3 mg, 49%) and **2f** (10.6 mg, 23%): amorphous brown solid; ^{1}H NMR (400 MHz, CS_2 with DMSO-d_6 as the external deuterium lock) δ 8.46 (dd, J = 8.3, 1.6 Hz, 2H), 7.79 (dd, J = 8.3, 1.6 Hz, 2H), 7.69–7.61 (m, 2H), 7.50–7.41 (m, 2H), 7.41–7.34 (m, 1H); ^{13}C NMR (101 MHz, CS_2 with DMSO-d_6 as the external deuterium lock and reference, all 2C unless indicated) δ 164.46 (1C, *C*=N), 147.74 (3C), 147.31 (1C), 145.93 (4C), 145.78,

145.64, 145.58, 145.31, 145.20, 145.02, 144.77 (3C including 1 aryl *C*), 144.66, 144.41, 144.16, 143.83, 143.26, 142.35 (4C), 142.24, 141.94 (4C), 141.84, 141.69, 141.57 (4C), 140.02, 139.58 (1C, aryl *C*), 139.19, 137.41, 135.68, 129.52 (aryl *C*), 128.81 (aryl *C*), 127.97 (1C, aryl *C*), 127.13 (aryl *C*), 127.02 (aryl *C*), 125.39 (1C, aryl *C*), 96.89 (1C, sp^3-*C* of C_{60}), 91.91 (1C, sp^3-*C* of C_{60}); FT-IR ν/cm^{-1} (KBr) 1638, 1511, 1322, 1088, 982, 931, 847, 766, 730, 694, 661, 603, 575, 563, 525; UV-vis ($CHCl_3$) λ_{max} nm (log ε) 258 (5.04), 314 (4.75), 413 (3.52), 454 (3.22), 689 (2.34); MALDI-TOF MS *m*/*z* calcd for $C_{73}H_9NO$ $[M]^-$ 915.0690, found 915.0684.



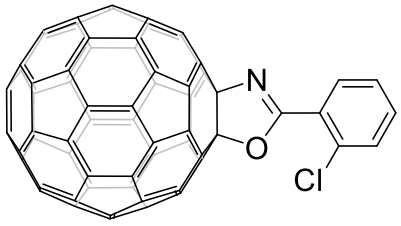
2g

Synthesis and spectral data of 2g: by following the general procedure, the reaction of C_{60} (35.8 mg, 0.05 mmol) with **1g** (27.4 mg, 0.15 mmol), $CuBr_2$ (11.1 mg, 0.05 mmol) and Na_2HPO_4 (14.5 mg, 0.10 mmol) at 150 °C for 1 h afforded recovered C_{60} (15.6 mg, 44%) and **2g**[2b–d,f] (12.6 mg, 29%): amorphous brown solid; ^{1}H NMR (500 MHz, 1:1 CS_2/$CDCl_3$) δ 8.40 (d, J = 8.5 Hz, 2H), 7.60 (d, J = 8.5 Hz, 2H).



2h

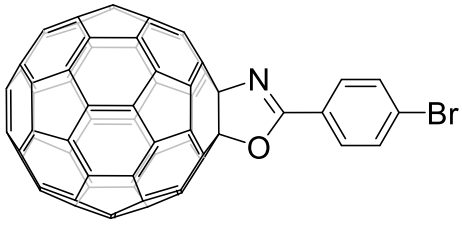
Synthesis and spectral data of 2h: by following the general procedure, the reaction of C_{60} (36.1 mg, 0.05 mmol) with **1h** (27.6 mg, 0.15 mmol), $CuBr_2$ (11.4 mg, 0.05 mmol) and Na_2HPO_4 (14.5 mg, 0.10 mmol) at 150 °C for 1 h afforded recovered C_{60} (10.1 mg, 28%) and **2h**[2e] (9.4 mg, 21%): amorphous brown solid; ^{1}H NMR (500 MHz, 1:1 CS_2/$CDCl_3$) δ 8.46 (t, J = 2.0 Hz, 1H), 8.36 (dt, J = 8.0, 1.3 Hz, 1H), 7.69–7.62 (m, 1H), 7.58 (t, J = 8.0 Hz, 1H).



2i

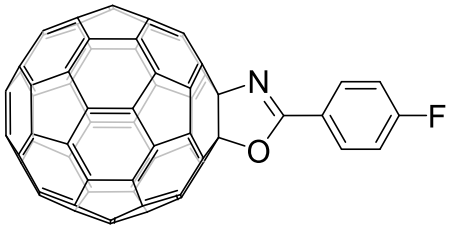
Synthesis and spectral data of 2i: by following the general procedure, the reaction of

C_{60} (36.2 mg, 0.05 mmol) with **1i** (27.2 mg, 0.15 mmol), $CuBr_2$ (11.1 mg, 0.05 mmol) and Na_2HPO_4 (14.1 mg, 0.10 mmol) at 160 ºC for 1 h afforded recovered C_{60} (16.2 mg, 45%) and **2i**[2e,f] (8.0 mg, 18%): amorphous brown solid; ^{1}H NMR (500 MHz, 1:1 CS_2/$CDCl_3$) δ 8.37 (d, J = 7.6 Hz, 1H), 7.67 (d, J = 8.0 Hz, 1H), 7.59 (dd, J = 8.0, 7.6 Hz, 1H), 7.54 (t, J = 7.5 Hz, 1H).



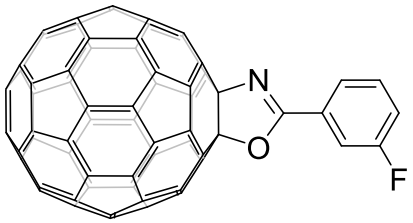
2j

Synthesis and spectral data of 2j: by following the general procedure, the reaction of C_{60} (36.2 mg, 0.05 mmol) with **1j** (34.4 mg, 0.15 mmol), $CuBr_2$ (11.2 mg, 0.05 mmol) and Na_2HPO_4 (14.2 mg, 0.10 mmol) at 150 ºC for 1 h afforded recovered C_{60} (13.6 mg, 38%) and **2j**[2a] (11.7 mg, 25%): amorphous brown solid; ^{1}H NMR (400 MHz, CS_2 with DMSO-d_6 as the external deuterium lock) δ 8.30 (d, J = 8.4 Hz, 2H), 7.75 (d, J = 8.4 Hz, 2H).



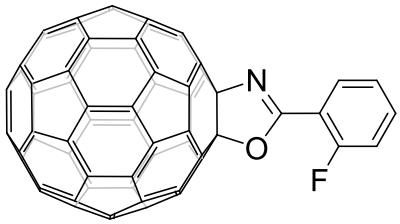
2k

Synthesis and spectral data of 2k: by following the general procedure, the reaction of C_{60} (36.0 mg, 0.05 mmol) with **1k** (25.0 mg, 0.15 mmol), $CuBr_2$ (11.3 mg, 0.05 mmol) and Na_2HPO_4 (14.2 mg, 0.10 mmol) at 150 ºC for 1 h and afforded recovered C_{60} (16.8 mg, 47%) and **2k** (13.1 mg, 31%): amorphous brown solid; ^{1}H NMR (500 MHz, CS_2 with DMSO-d_6 as the external deuterium lock) δ 8.44 (dd, J = 8.4, 5.5 Hz, 2H), 7.28 (t, J = 8.3 Hz, 2H); ^{13}C NMR (126 MHz, CS_2 with DMSO-d_6 as the external deuterium lock, all 2C unless indicated) δ 164.29 (1C, aryl *C*, d, J = 255.5 Hz), 163.06 (1C, *C*=N), 147.10 (1C), 146.90, 146.68 (1C), 145.29 (4C), 145.15, 145.00, 144.95, 144.67, 144.48, 144.33, 144.13, 144.02, 143.68, 143.50, 143.17, 142.41, 141.72, 141.69, 141.61, 141.28, 141.25, 141.18, 141.04, 140.92, 140.87, 139.37, 138.55, 136.75, 135.00, 130.61 (aryl *C*, d, J = 8.8 Hz), 122.24 (1C, aryl *C*, d, J = 3.2 Hz), 114.93 (aryl *C*, d, J = 21.8 Hz), 96.41 (1C, sp^3-*C* of C_{60}), 91.16 (1C, sp^3-*C* of C_{60}); FT-IR ν/cm^{-1} (KBr) 1638, 1604, 1510, 1459, 1426, 1341, 1270, 1178, 748, 563, 527; UV-vis ($CHCl_3$) λ_{max} nm (log ε) 256 (5.01), 317 (4.56), 416 (3.52), 458 (3.27), 684 (2.65); MALDI-TOF MS *m*/*z* calcd for $C_{67}H_4NOF$ $[M]^-$ 857.0282, found 857.0286.



2l

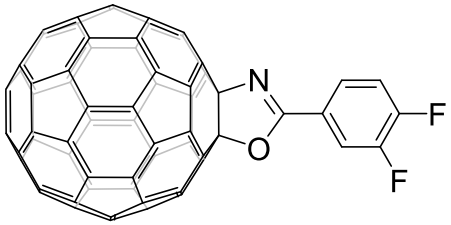
Synthesis and spectral data of 2l: by following the general procedure, the reaction of C_{60} (35.7 mg, 0.05 mmol) with **1l** (22.2 mg, 0.15 mmol), $CuBr_2$ (11.5 mg, 0.05 mmol) and Na_2HPO_4 (14.6 mg, 0.10 mmol) at 150 °C for 1 h afforded recovered C_{60} (13.0 mg, 36%) and **2l** (11.5 mg, 27%): amorphous brown solid; ^{1}H NMR (500 MHz, CS_2 with DMSO-d_6 as the external deuterium lock) δ 8.25–8.20 (m, 1H), 8.13–8.06 (m, 1H), 7.61 (td, J = 7.9, 5.6 Hz, 1H), 7.38–7.32 (m, 1H); ^{13}C NMR (126 MHz, CS_2 with DMSO-d_6 as the external deuterium lock and reference, all 2C unless indicated) δ 163.05 (1C, *C*=N, d, J = 3.0 Hz), 161.56 (1C, aryl *C*, d, J = 248.8 Hz), 147.11 (1C), 146.69 (3C), 145.32 , 145.31, 145.17, 145.02, 144.96, 144.70, 144.49, 144.33, 144.15, 144.03, 143.68, 143.49, 143.17, 142.24, 141.74, 141.69, 141.62, 141.30, 141.23, 141.20, 141.06, 140.93, 140.87, 139.39, 138.58, 136.74, 135.05, 129.39 (1C, aryl *C*, J = 7.7 Hz), 128.20 (1C, aryl *C*, d, J = 8.2 Hz), 123.91 (1C, aryl *C*, d, J = 3.1 Hz), 118.34 (1C, aryl *C*, d, J = 21.1 Hz), 115.24 (1C, aryl *C*, d, J = 23.5 Hz), 96.46 (1C, sp^3-*C* of C_{60}), 91.10 (1C, sp^3-*C* of C_{60}); FT-IR ν/cm^{-1} (KBr) 1644, 1452, 1316, 1086, 982, 936, 883, 848, 789, 713, 564, 526; UV-vis ($CHCl_3$) λ_{max} nm (log ε) 256 (5.11), 316 (4.67), 412 (3.62), 454 (3.36), 683 (2.61); MALDI-TOF MS m/z calcd for $C_{67}H_4NOF$ [M]$^-$ 857.0282, found 857.0285.



2m

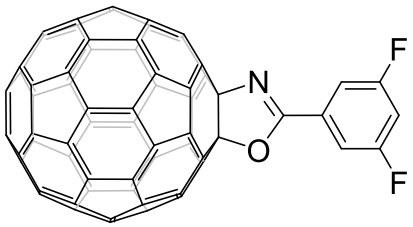
Synthesis and spectral data of 2m: by following the general procedure, the reaction of C_{60} (36.2 mg, 0.05 mmol) with **1m** (37.0 mg, 0.25 mmol), $CuBr_2$ (11.1 mg, 0.05 mmol) and Na_2HPO_4 (14.5 mg, 0.10 mmol) at 150 °C for 1 h afforded recovered C_{60} (11.4 mg, 31%) and **2m** (10.4 mg, 24%): amorphous brown solid; ^{1}H NMR (500 MHz, 1:1 CS_2/$CDCl_3$) δ 8.45 (td, J = 7.4, 1.6 Hz, 1H), 7.72–7.62 (m, 1H), 7.42 (t, J = 7.6 Hz, 1H), 7.35 (dd, J = 10.1, 8.9 Hz, 1H); ^{13}C NMR (126 MHz, 1:1 CS_2/$CDCl_3$, all 2C unless indicated) δ 162.81 (1C, *C*=N, d, J = 5.4 Hz), 161.62 (1C, aryl *C*, d, J = 261.6 Hz), 148.15 (1C), 147.74 (1C), 147.53, 146.34 (4C), 146.22, 146.04, 145.99, 145.76, 145.60, 145.40, 145.16, 145.06, 144.78, 144.50, 144.19, 143.22, 142.73, 142.68, 142.62, 142.31, 142.20 (4C), 142.06, 141.94, 141.88, 140.34, 139.58, 137.79, 136.25, 134.18 (1C, aryl *C*, d, J = 8.7 Hz), 131.95 (1C, aryl *C*), 124.32 (1C, aryl *C*, d, J = 3.8 Hz), 117.14 (1C, aryl *C*, d, J = 21.6 Hz), 115.16 (1C, aryl *C*, d, J = 10.2 Hz), 97.01 (1C, sp^3-

C of C_{60}), 91.98 (1C, sp^3-*C* of C_{60}); FT-IR ν/cm^{-1} (KBr) 1641, 1495, 1456, 1330, 1229, 1066, 982, 932, 822, 763, 740, 658, 603, 563, 526; UV-vis ($CHCl_3$) λ_{max} nm (log ε) 256 (5.02), 317 (4.57), 417 (3.53), 454 (3.30), 684 (2.52); MALDI-TOF MS *m*/*z* calcd for $C_{67}H_4NOF$ $[M]^-$ 857.0282, found 857.0289.



2n

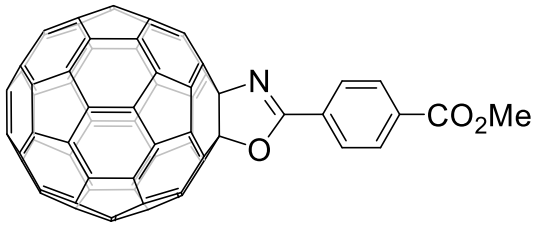
Synthesis and spectral data of 2n: by following the general procedure, the reaction of C_{60} (35.8 mg, 0.05 mmol) with **1n** (27.8 mg, 0.15 mmol), $CuBr_2$ (11.2 mg, 0.05 mmol) and Na_2HPO_4 (14.2 mg, 0.10 mmol) at 150 °C for 1 h afforded recovered C_{60} (13.2 mg, 37%) and **2n** (11.1 mg, 26%): amorphous brown solid; ^{1}H NMR (500 MHz, 1:1 CS_2/$CDCl_3$) δ 8.34–8.28 (m, 1H), 8.28–8.24 (m, 1H), 7.47–7.40 (m, 1H); ^{13}C NMR (126 MHz, 1:1 CS_2/$CDCl_3$, all 2C unless indicated) δ 163.93 (1C, *C*=N), 153.23 (1C, aryl *C*, dd, *J* = 256.9, 12.7 Hz), 150.34 (1C, aryl *C*, dd, *J* = 250.9, 13.1 Hz), 148.18 (1C), 147.77 (1C), 147.36, 146.37 (4C), 146.23, 146.07, 146.02, 145.77, 145.39, 145.35, 145.19, 145.09, 144.61, 144.49, 144.19, 143.01, 142.77, 142.71, 142.66, 142.30, 142.21, 142.19, 142.08, 141.95, 141.83, 140.41, 139.61, 137.81, 136.19, 126.01 (1C, aryl *C*, dd, *J* = 7.1, 3.7 Hz), 123.88 (1C, aryl *C*, dd, *J* = 6.4, 3.8 Hz), 118.60 (1C, aryl *C*, d, *J* = 19.6 Hz), 117.85 (1C, aryl *C*, d, *J* = 17.9 Hz), 97.84 (1C, sp^3-*C* of C_{60}), 91.95 (1C, sp^3-*C* of C_{60}); FT-IR ν/cm^{-1} (KBr) 1646, 1512, 1438, 1339, 1323, 1268, 1195, 1141, 1080, 983, 937, 823, 794, 776, 720, 563, 526; UV-vis ($CHCl_3$) λ_{max} nm (log ε) 256 (5.07), 317 (4.61), 416 (3.45), 452 (3.20), 683 (2.42); MALDI-TOF MS *m*/*z* calcd for $C_{67}H_3NOF_2$ $[M]^-$ 875.0188, found 875.0182.



2o

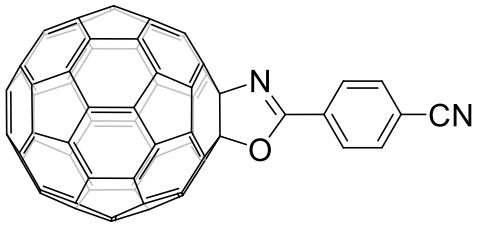
Synthesis and spectral data of 2o: by following the general procedure, the reaction of C_{60} (35.8 mg, 0.05 mmol) with **1o** (27.3 mg, 0.15 mmol), $CuBr_2$ (11.9 mg, 0.05 mmol) and Na_2HPO_4 (14.1 mg, 0.10 mmol) at 150 °C for 1 h afforded recovered C_{60} (14.2 mg, 40%) and **2o** (8.8 mg, 20%): amorphous brown solid; ^{1}H NMR (500 MHz, 1:1 CS_2/$CDCl_3$) δ 8.03–7.96 (m, 2H), 7.12 (tt, *J* = 8.5, 2.4 Hz, 1H); ^{13}C NMR (126 MHz, 1:1 CS_2/$CDCl_3$, all 2C unless indicated) δ 163.89 (1C, *C*=N, t, *J* = 3.6 Hz), 162.99 (aryl *C*, dd, *J* = 250.7, 12.1 Hz), 148.19 (1C), 147.77 (1C), 147.13, 146.39, 146.37, 146.24, 146.08, 146.02, 145.79, 145.38, 145.33, 145.19, 145.09, 144.60, 144.48, 144.18,

142.81, 142.77, 142.70, 142.66, 142.30, 142.21, 142.16, 142.08, 141.95, 141.81, 140.42, 139.63, 137.80, 136.23, 129.92 (1C, aryl *C*, t, *J* = 10.2 Hz), 112.31 (aryl *C*, dd, *J* = 20.9, 6.9 Hz), 107.88 (1C, aryl *C*, t, *J* = 25.1 Hz), 97.88 (1C, sp^3-*C* of C_{60}), 91.89 (1C, sp^3-*C* of C_{60}); FT-IR ν/cm^{-1} (KBr) 1648, 1619, 1593, 1437, 1354, 1123, 987, 938, 873, 853, 717, 561, 526; UV-vis ($CHCl_3$) λ_{max} nm (log ε) 254 (5.06), 318 (4.59), 415 (3.48), 457 (3.22), 682 (2.50); MALDI-TOF MS *m*/*z* calcd for $C_{67}H_3NOF_2$ $[M]^-$ 875.0188, found 875.0185.



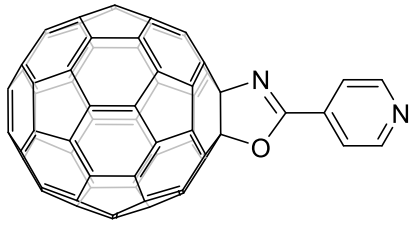
2p

Synthesis and spectral data of 2p: by following the general procedure, the reaction of C_{60} (35.7 mg, 0.05 mmol) with **1p** (30.7 mg, 0.15 mmol), $CuBr_2$ (11.2 mg, 0.05 mmol) and Na_2HPO_4 (14.3 mg, 0.10 mmol) at 150 °C for 1 h afforded recovered C_{60} (10.8 mg, 30%) and **2p**[2b,e] (10.1 mg, 23%): amorphous brown solid; ^{1}H NMR (500 MHz, 1:1 CS_2/$CDCl_3$) δ 8.54 (d, *J* = 7.8 Hz, 2H), 8.29 (d, *J* = 7.8 Hz, 2H), 4.00 (s, 3H).



2q

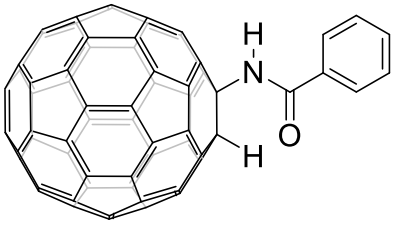
Synthesis and spectral data of 2q: by following the general procedure, the reaction of C_{60} (35.6 mg, 0.05 mmol) with **1q** (25.4 mg, 0.15 mmol), $CuBr_2$ (12.4 mg, 0.05 mmol) and Na_2HPO_4 (14.4 mg, 0.10 mmol) at 150 °C for 1 h afforded recovered C_{60} (9.7 mg, 27%) and **2q**[2b] (10.4 mg, 24%): amorphous brown solid; ^{1}H NMR (500 MHz, 1:1 CS_2/$CDCl_3$) δ 8.59 (d, *J* = 8.3 Hz, 2H), 7.93 (d, *J* = 8.3 Hz, 2H).



2r

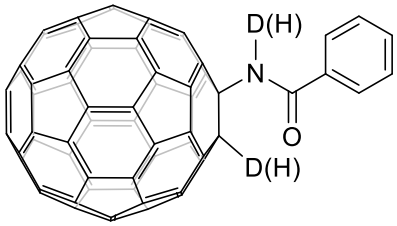
Synthesis and spectral data of 2r: by following the general procedure, the reaction of C_{60} (36.1 mg, 0.05 mmol) with **1r** (22.4 mg, 0.15 mmol), $CuBr_2$ (11.5 mg, 0.05 mmol) and Na_2HPO_4 (14.4 mg, 0.10 mmol) at 150 °C for 1 h afforded recovered C_{60} (24.9 mg,

69%) and **2r** (4.7 mg, 14%): amorphous brown solid; ^{1}H NMR (500 MHz, 1:1 CS_2/$CDCl_3$) δ 8.95 (d, J = 6.0 Hz, 2H), 8.28 (d, J = 6.0 Hz, 2H); ^{13}C NMR (151 MHz, 1:1 CS_2/$CDCl_3$, all 2C unless indicated) δ 164.14 (1C, *C*=N), 150.63 (aryl *C*), 148.15 (1C), 147.74 (1C), 146.97, 146.37 (4C), 146.22, 146.05, 146.00, 145.77, 145.36, 145.29, 145.17, 145.08, 144.57, 144.44, 144.15, 142.76, 142.69 (4C), 142.65, 142.28, 142.19, 142.13, 142.06, 141.93, 141.79, 140.42, 139.63, 137.72, 136.19, 134.13 (1C, aryl *C*), 122.44 (aryl *C*), 97.76 (1C, sp^3-*C* of C_{60}), 91.91 (1C, sp^3-*C* of C_{60}); FT-IR ν/cm^{-1} (KBr) 1648, 1592, 1556, 1408, 1333, 1099, 991, 981, 930, 831, 773, 563, 526; UV-vis ($CHCl_3$) λ_{max} nm (log ε) 255 (5.04), 317 (4.58), 416 (3.49), 449 (3.26), 684 (2.39); MALDI-TOF MS m/z calcd for $C_{66}H_4N_2O$ $[M]^-$ 840.0329, found 840.0315.



3a

Synthesis and spectral data of 3a: 16.8 mg (0.02 mmol) of **2a** was electroreduced by controlled potential electrolysis (CPE) at –1.07 V vs saturated calomel electrode (SCE) in 15 mL of 1,2-$C_6H_4Cl_2$ containing 0.1 M *n*-butylammonium perchlorate (TBAP) under an argon atmosphere at 0 °C. 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 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. The electrolysis was terminated when the theoretical number of coulombs required for a full conversion of **2a** to $\mathbf{2a}^{2-}$ was reached. Then, the dianionic $\mathbf{2a}^{2-}$ was reacted with trifluoroacetic acid (7.6 μL, 0.10 mmol) at 0 °C for 10 min. The reaction mixture was 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. After evaporation in vacuo, the residue was separated on a silica gel (300–400 mesh) column with CS_2/CH_2Cl_2 (4:1, v/v) to afford product **3a** (8.5 mg, 50%) as an amorphous brown solid; ^{1}H NMR (400 MHz, $CDCl_2CDCl_2$) δ 8.52 (s, 1H), 8.23–8.14 (m, 2H), 7.68–7.63 (m, 1H), 7.63–7.56 (m, 2H), 6.91 (s, 1H); ^{13}C NMR (151 MHz, 2:1 $CDCl_2CDCl_2$/CS_2, all 2C unless indicated) δ 166.99 (1C, *C*=O), 151.84, 147.98, 146.90 (1C), 146.15 (1C), 145.59, 145.48, 145.23, 145.09, 145.06, 145.03, 144.64, 144.37, 144.24, 144.20 (4C), 143.88, 143.33, 142.05, 141.62, 141.51, 141.35, 141.17, 141.00, 140.81, 140.50, 140.17, 139.25, 138.74, 137.64, 135.45, 132.40 (1C, aryl *C*), 131.67 (1C, aryl *C*), 128.09 (aryl *C*), 126.47 (aryl *C*), 71.75 (1C, sp^3-*C* of C_{60}), 59.53 (1C, sp^3-*C* of C_{60}); FT-IR ν/cm^{-1} (KBr) 3416, 1668, 1639, 1577, 1515, 1464, 1427, 1269, 1250, 707, 688, 551, 527; UV-vis ($CHCl_3$) λ_{max} nm (log ε) 258 (5.03), 328 (4.52), 405 (3.77), 431 (3.62), 697 (2.87); MALDI-TOF MS m/z calcd for $C_{67}H_7NO$ $[M]^-$ 841.0533, found 841.0541.



3a-D

Synthesis and spectral data of 3a-D: 8.4 mg (0.01 mmol) of **2a** was electroreduced by controlled potential electrolysis (CPE) at –1.07 V vs saturated calomel electrode (SCE) in 15 mL of 1,2-$C_6H_4Cl_2$ containing 0.1 M *n*-butylammonium perchlorate (TBAP) under an argon atmosphere at 0 °C. The electrolysis was terminated when the theoretical number of coulombs required for a full conversion of **2a** to **2a**$^{2-}$ was reached. Then, the dianionic **2a**$^{2-}$ was reacted with CF_3CO_2D (73.2 μL, 1.00 mmol) at 0 °C for 10 min. After removal of volatiles in vacuo, the residue was dissolved in CS_2. Subsequent filtration to remove TBAP and insoluble impurities. Evaporation of the resulting filtrate to remove CS_2 and then washing with methanol provided product **3a**-D along with decomposition product C_{60} as an amorphous brown solid (Figure S1); ^{1}H NMR (500 MHz, $CDCl_2CDCl_2$) δ 8.54 (s, 0.85H), 8.20 (d, J = 7.6 Hz, 2H), 7.69–7.64 (m, 1H), 7.64–7.57 (m, 2H), 6.91 (s, 0.44H). The ^{1}H NMR spectrum of **3a**-D showed all expected signals of **3a** except that the fullerenyl proton at 6.91 ppm had an integral of 0.44 and the amide proton at 8.54 ppm had an integral of 0.85, hinting partial H-D exchange during the workup process.

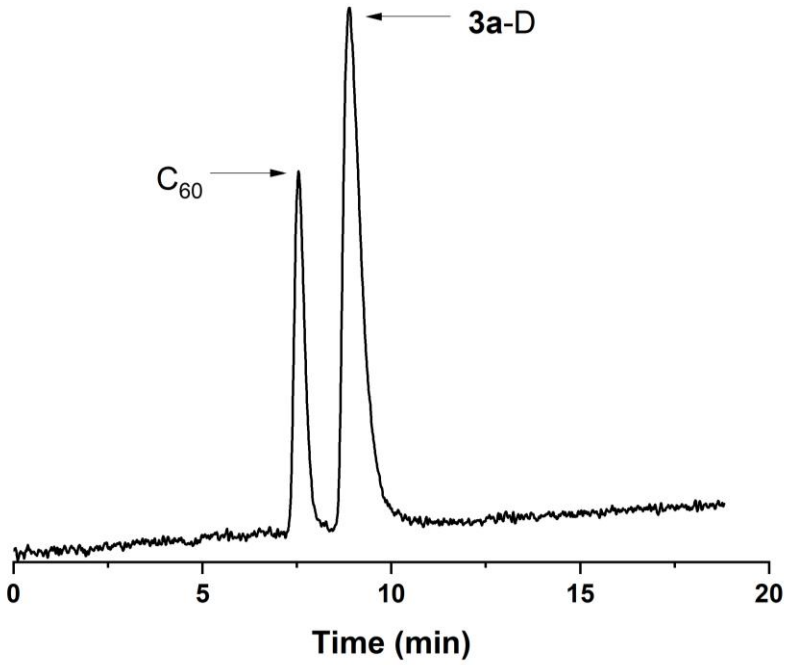


Figure S1. Reaction of **2a**$^{2-}$ and CF_3COOD.

4. Attempted reaction of $2a^{2-}$ with MeI or D_2O

Attempted reaction of $2a^{2-}$ with MeI: 8.4 mg (0.01 mmol) of **2a** was electroreduced by controlled potential electrolysis (CPE) at –1.07 V vs saturated calomel electrode (SCE) in 15 mL of 1,2-$C_6H_4Cl_2$ containing 0.1 M *n*-butylammonium perchlorate (TBAP) under an argon atmosphere at 0 °C. The electrolysis was terminated when the theoretical number of coulombs required for a full conversion of **2a** to $\mathbf{2a}^{2-}$ was reached. Then, the dianionic $\mathbf{2a}^{2-}$ was reacted with MeI (32.0 μL, 0.50 mmol) at 0 °C for 6 h. It was found that **2a** was partially decomposed to C_{60} (Figure S2).

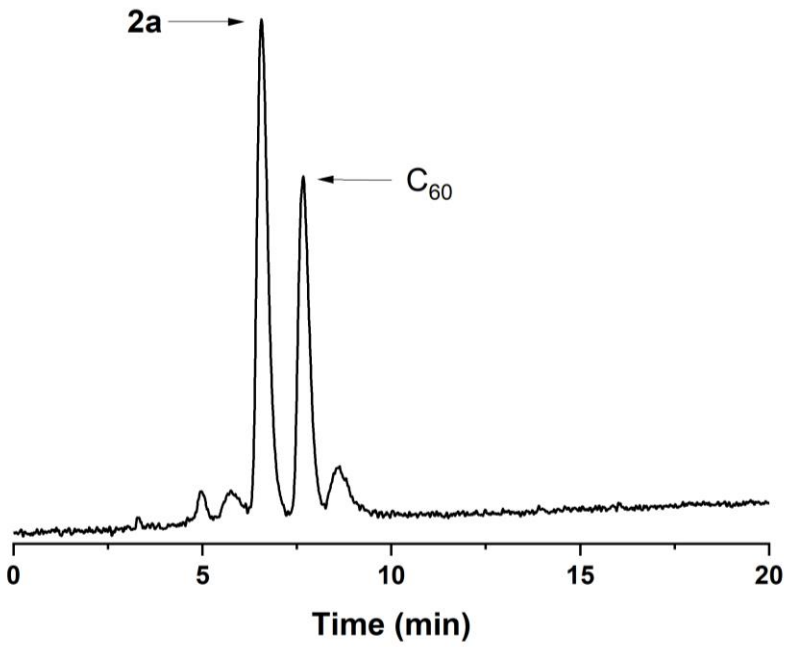


Figure S2. Reaction of $\mathbf{2a}^{2-}$ and MeI.

Attempted reaction of $2a^{2-}$ with D_2O: 8.4 mg (0.01 mmol) of **2a** was electroreduced by controlled potential electrolysis (CPE) at –1.07 V vs saturated calomel electrode (SCE) in 15 mL of 1,2-$C_6H_4Cl_2$ containing 0.1 M *n*-butylammonium perchlorate (TBAP) under an argon atmosphere at 0 °C. The electrolysis was terminated when the theoretical number of coulombs required for a full conversion of **2a** to $\mathbf{2a}^{2-}$ was reached. Then, the dianionic $\mathbf{2a}^{2-}$ was reacted with D_2O (10.0 μL, 0.50 mmol) at 0 °C for 6 h, It was found that **2a** was partially decomposed to C_{60} (Figure S3).

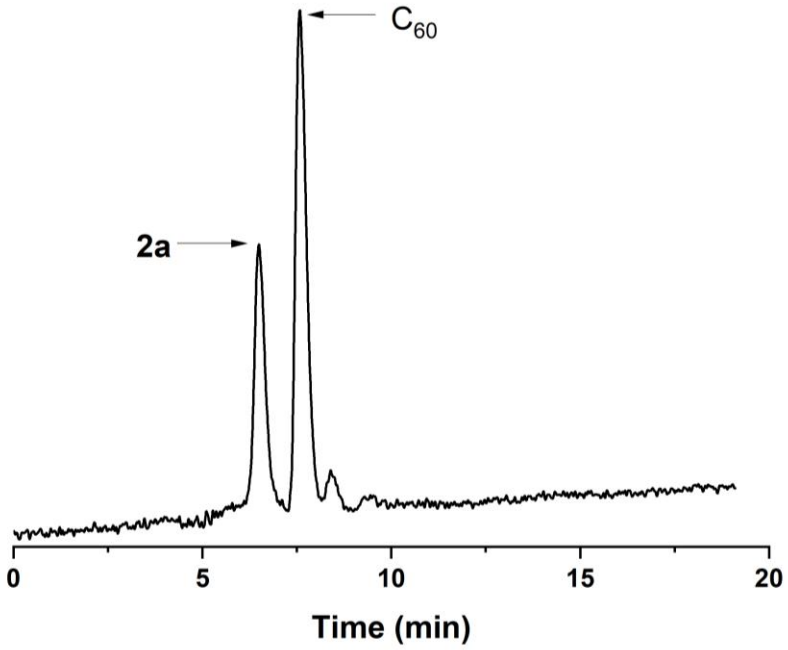
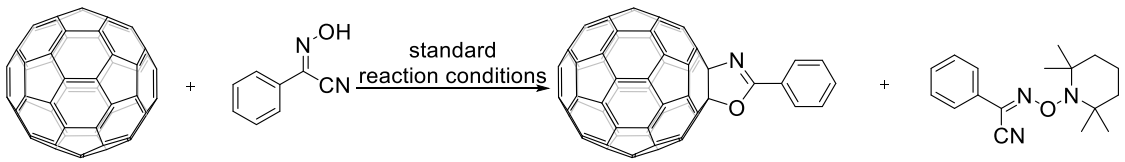


Figure S3. Reaction of $\mathbf{2a}^{2-}$ and D_2O.

5. Control experiments

A mixture of C_{60} (36.1 mg, 0.05 mmol), **1a** (21.8 mg, 0.15 mmol) and $CuBr_2$ (11.4 mg, 0.05 mmol), Na_2HPO_4 (14.4 mg, 0.10 mmol) and TEMPO (3.9 mg, 0.025 mmol) was completely dissolved in 1,2-$C_6H_4Cl_2$. After being stirred in an oil bath at 150 ºC for 1 h, the resulting solution was evaporated in vacuo and subsequently separated on a silica gel column (300–400 mesh) with CS_2 as the eluent to give recovered C_{60} (24.5 mg, 68%) and the product **2a** (4.4 mg, 10%). While adding 1 equiv. of TEMPO (7.8 mg, 0.05 mmol), there was no desired product, and the radical coupling product **4** between TEMPO and **1a** radical was successfully detected by ESI-MS. ESI-MS *m*/*z* calcd for $C_{17}H_{24}N_3O$ $[M+H]^+$ 286.1914, found 286.1919.



1a	additive	2a	recovered C_{60}	4
	TEMPO (0.5 equiv)	10%	68%	
	TEMPO (1 equiv)	0%	97%	

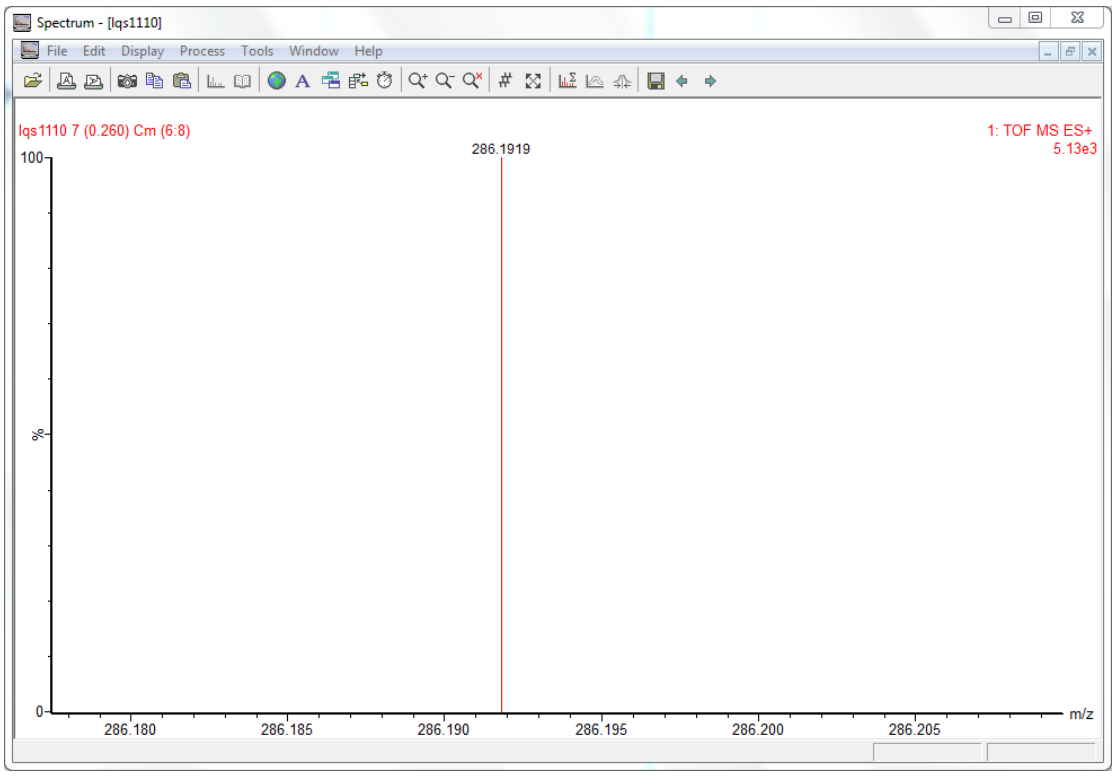
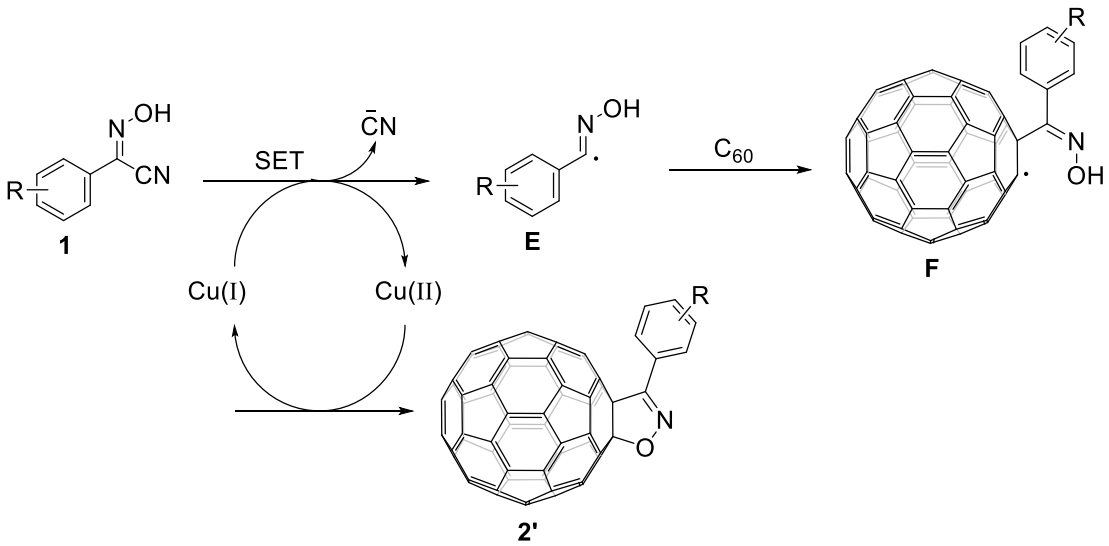


Figure S4. HRMS of product **4**.

6. Reaction mechanism leading to fulleroisoxazoles



Scheme S1. Reaction mechanism for the formation of fulleroisoxazoles **2'**.

7. References

1 A. J. Neel and R. Zhao, *Org. Lett.*, 2018, **20**, 2024−2027.

2 (*a*) F.-B. Li, T.-X. Liu and G.-W. Wang, *J. Org. Chem.*, 2008, **73**, 6417–6420; (*b*) Y. Takeda, S. Enokijima, T. Nagamachi, K. Nakayama and S. Minakata, *Asian J. Org. Chem.*, 2013, **2**, 91–97; (*c*) H.-T. Yang, W.-L. Ren, C.-P. Dong, Y. Yang, X.-Q. Sun and C.-B. Miao, *Tetrahedron Lett.*, 2013, **54**, 6799–6803; (*d*) H.-T. Yang, X.-C. Liang, Y.-H. Wang, Y. Yang, X.-Q. Sun and C.-B. Miao, *Org. Lett.*, 2013, **15**, 4650–4653; (*e*) T.-X. Liu, Y. Liu, D. Chao, P. Zhang, Q. Liu, L. Shi, Z. Zhang and G. Zhang, *J. Org. Chem.*, 2014, **79**, 11084−11090; (*f*) X.-F. Zhang, F.-B. Li, J.-L. Shi, J. Wu and L. Liu, *New J. Chem.*, 2016, **40**, 1626–1632.

8. NMR spectra of compounds 2a–r and 3a

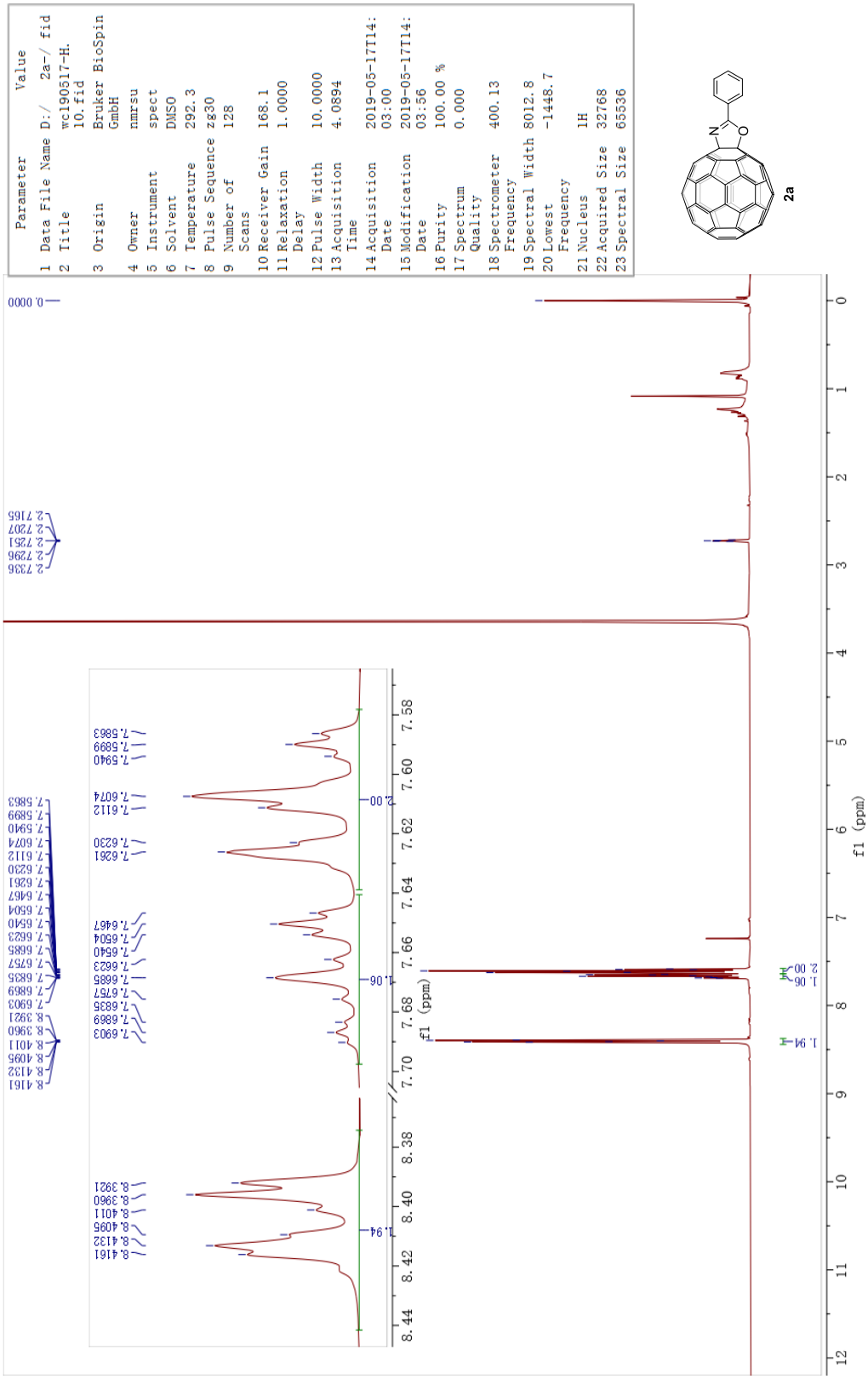


Figure S5. ^{1}H NMR (400 MHz, CS_2/DMSO-d_6) of **2a**.

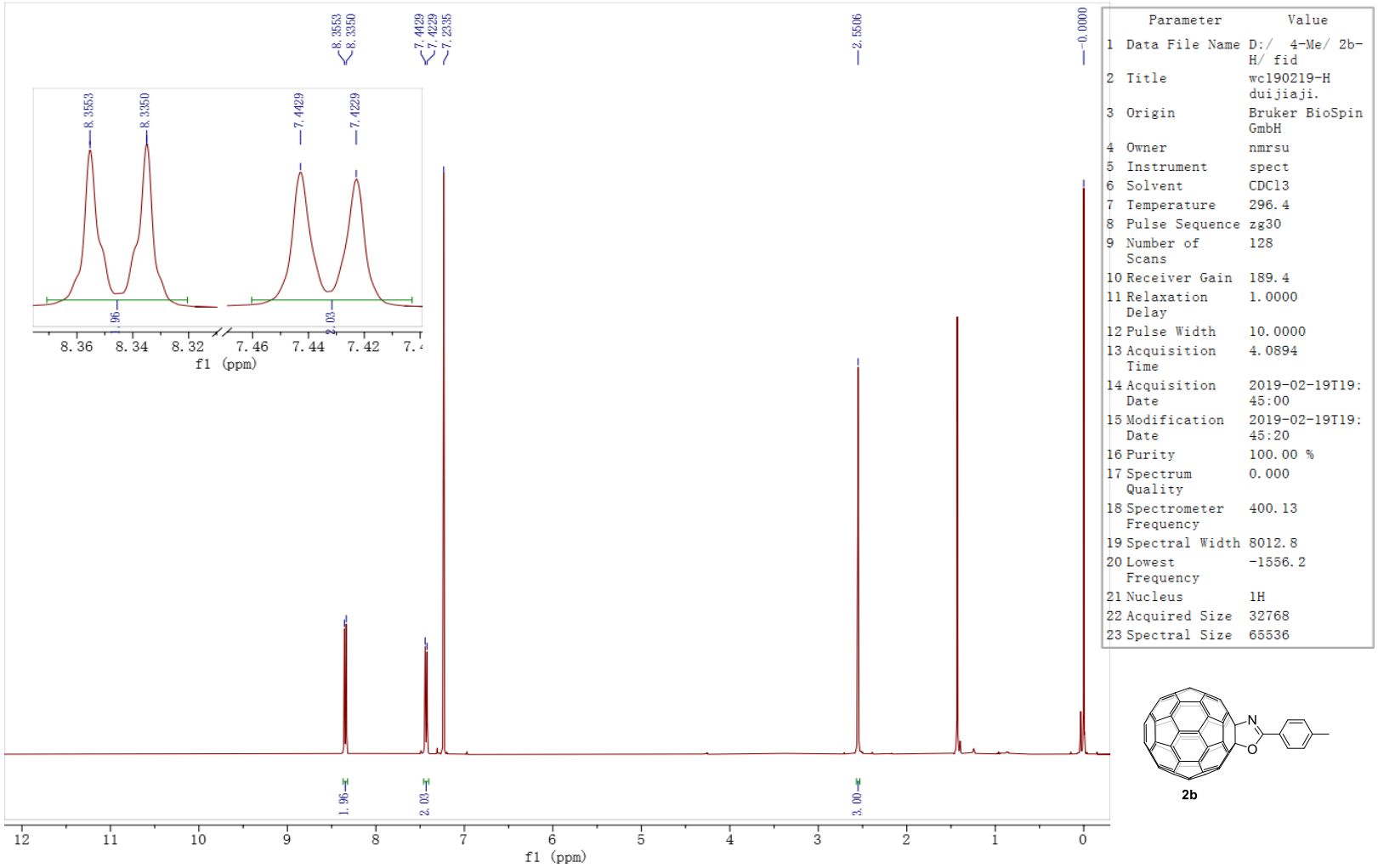


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Figure S6. ^{1}H NMR (400 MHz, 1:1 CS_2/$CDCl_3$) of **2b**.

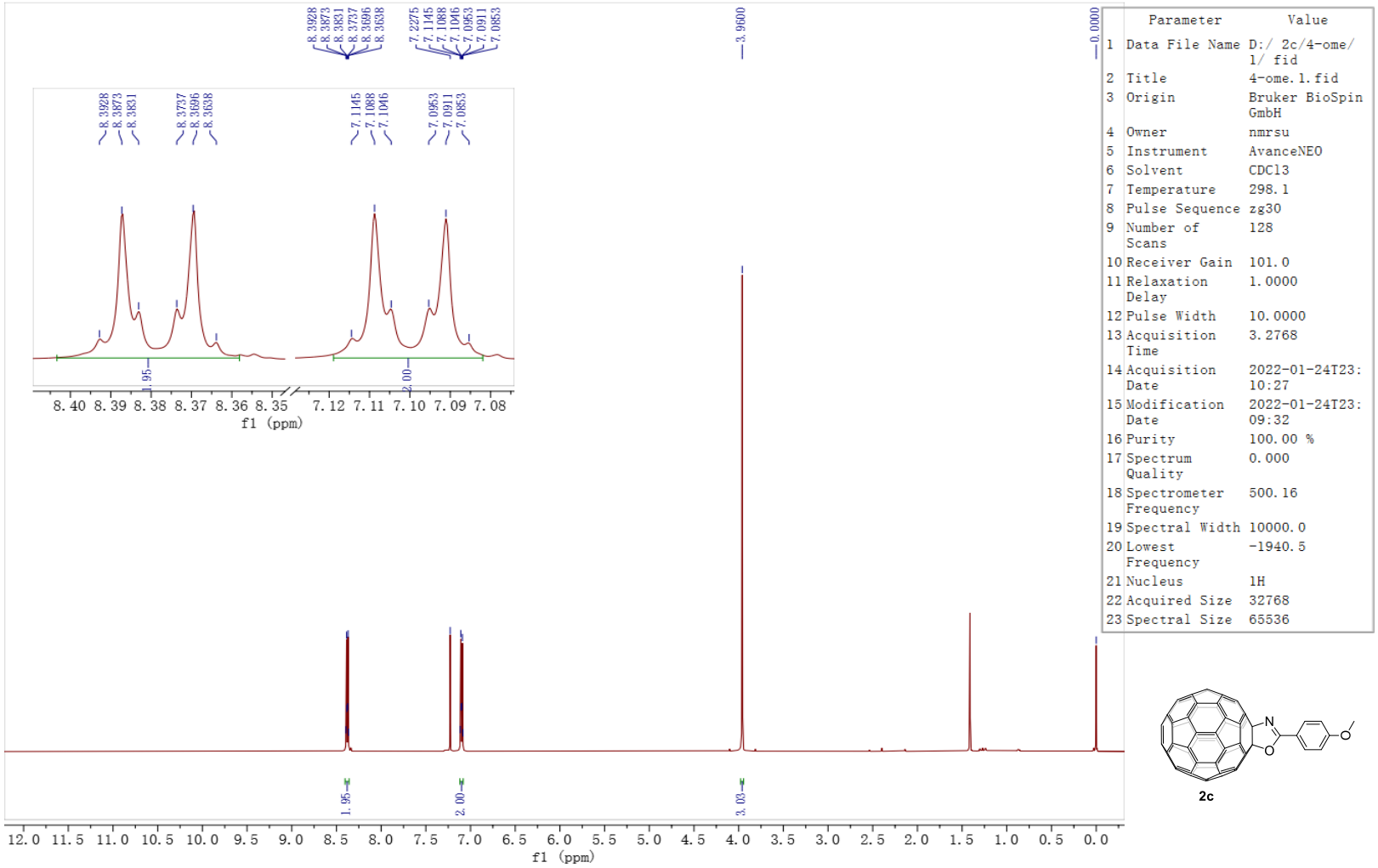


Figure S7. ^{1}H NMR (500 MHz, 1:1 CS_2/$CDCl_3$) of **2c**.

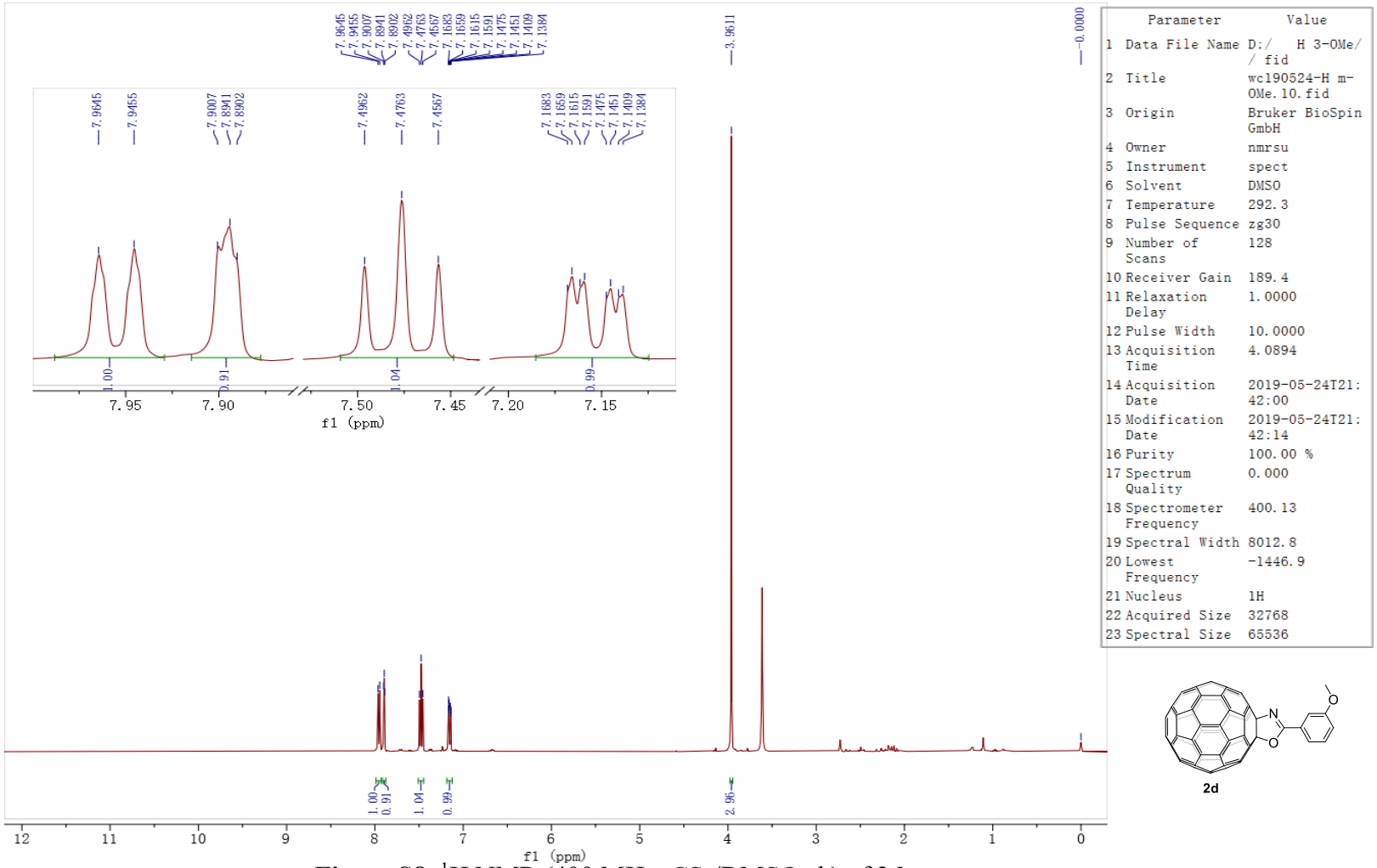


Figure S8. ^{1}H NMR (400 MHz, CS_2/DMSO-d_6) of **2d**.

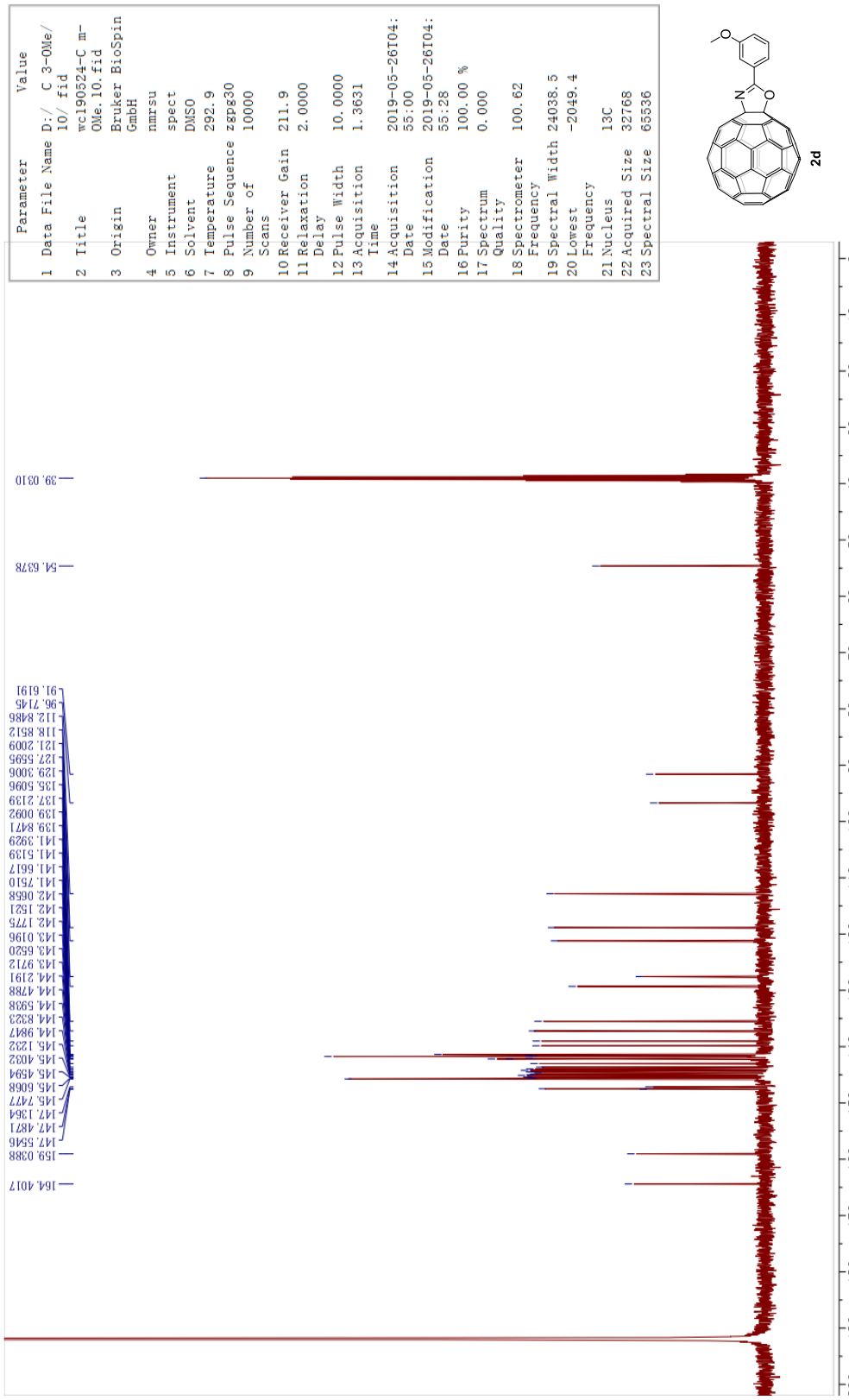


Figure S9. ^{13}C NMR (101 MHz, CS_2/DMSO-d_6) of **2d**.

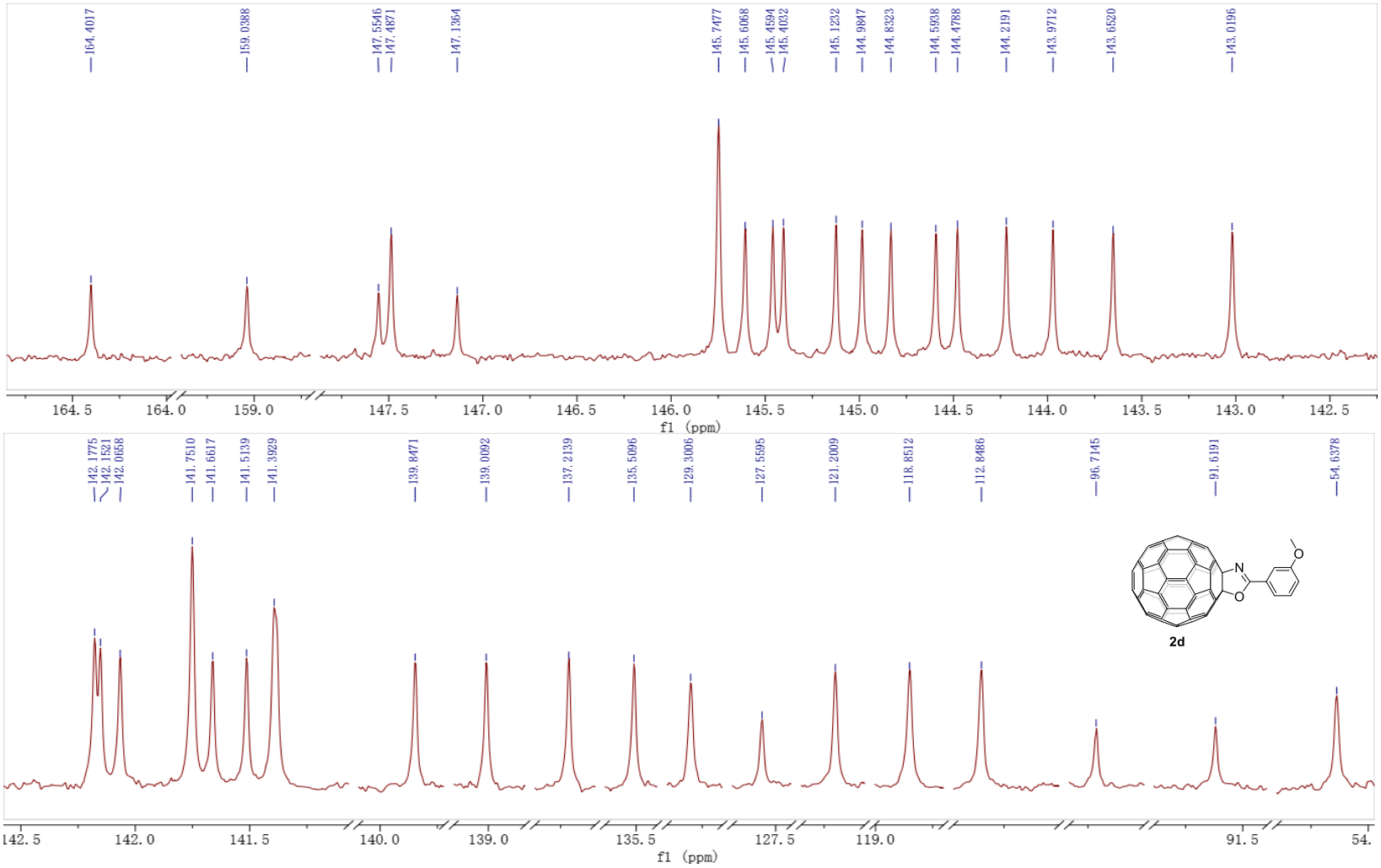
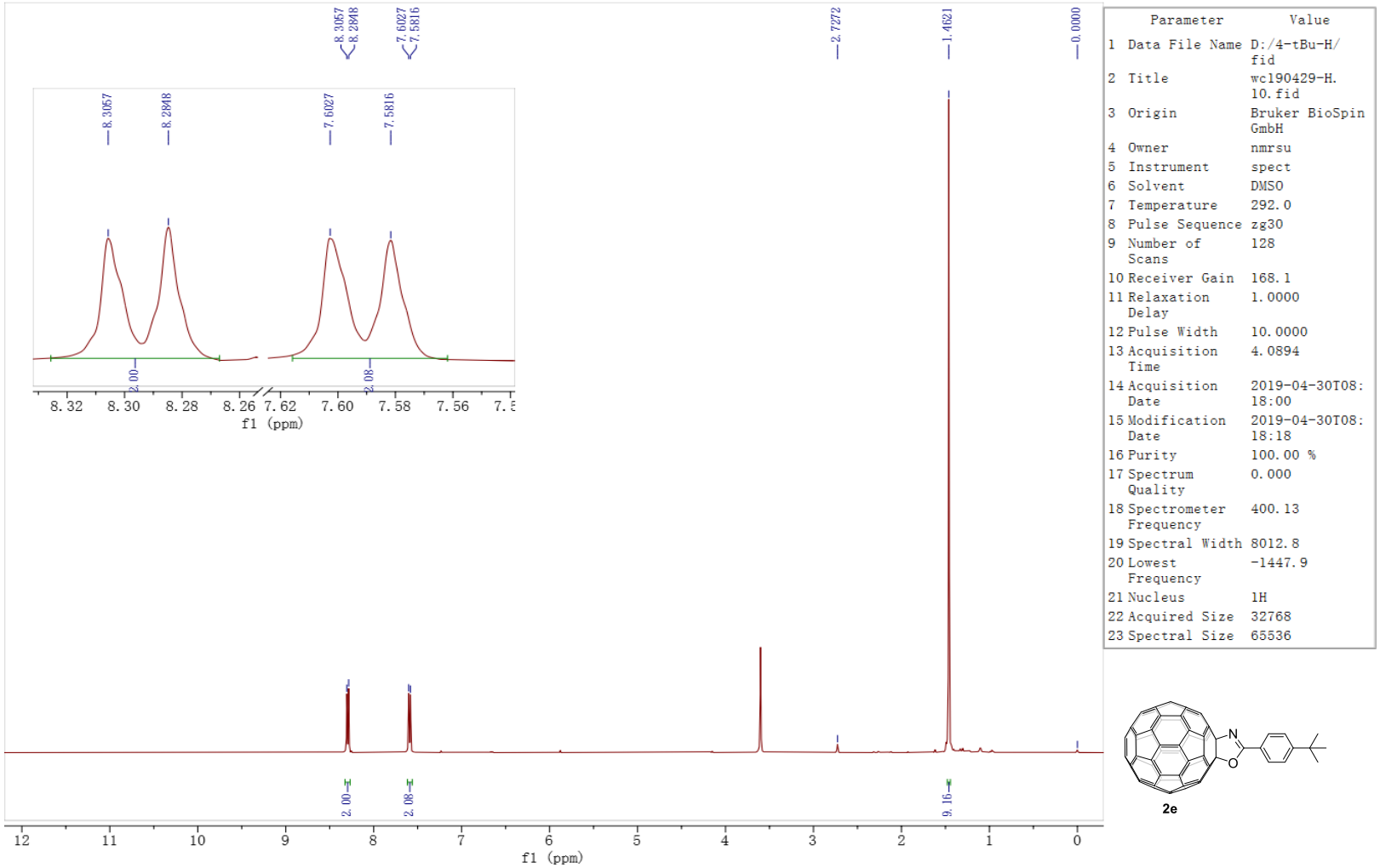


Figure S10. Expanded ^{13}C NMR (101 MHz, CS_2/DMSO-d_6) of **2d**.



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22	Acquired Size	32768
23	Spectral Size	65536

Figure S11. ^{1}H NMR (400 MHz, CS_2/DMSO-d_6) of **2e**.

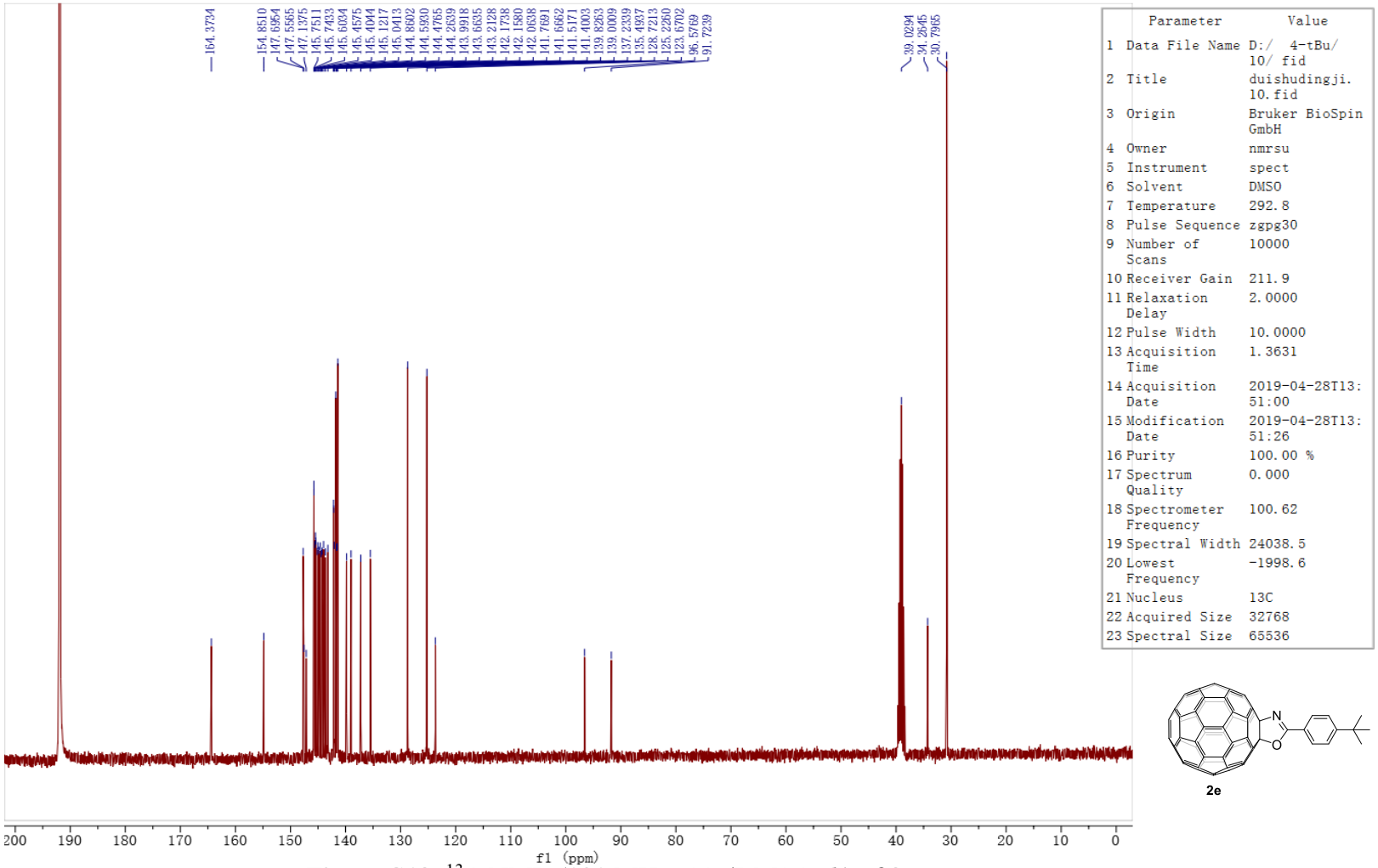


Figure S12. ^{13}C NMR (101 MHz, CS_2/DMSO-d_6) of **2e**.

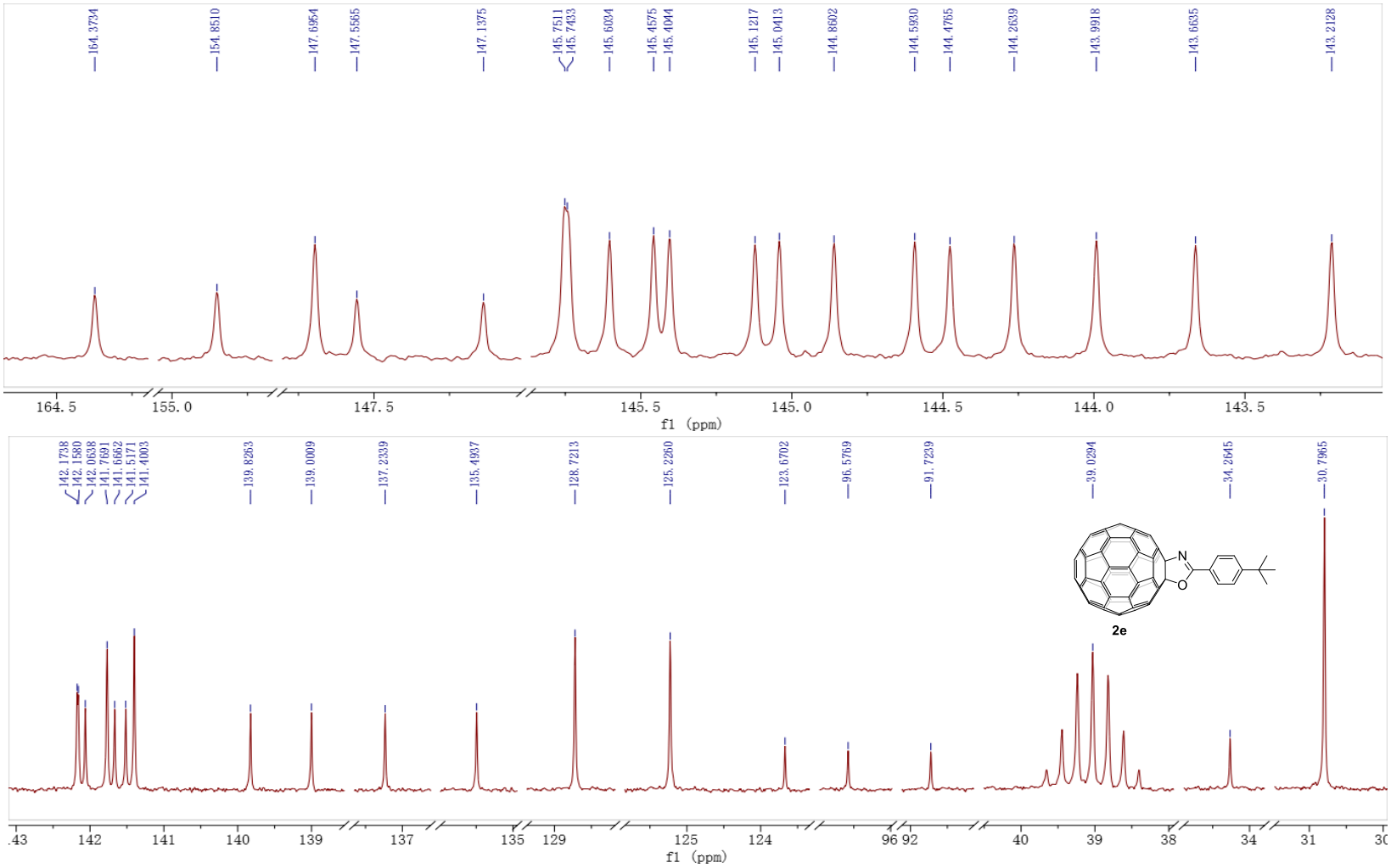


Figure S13. Expanded ^{13}C NMR (101 MHz, CS_2/DMSO-d_6) of **2e**.

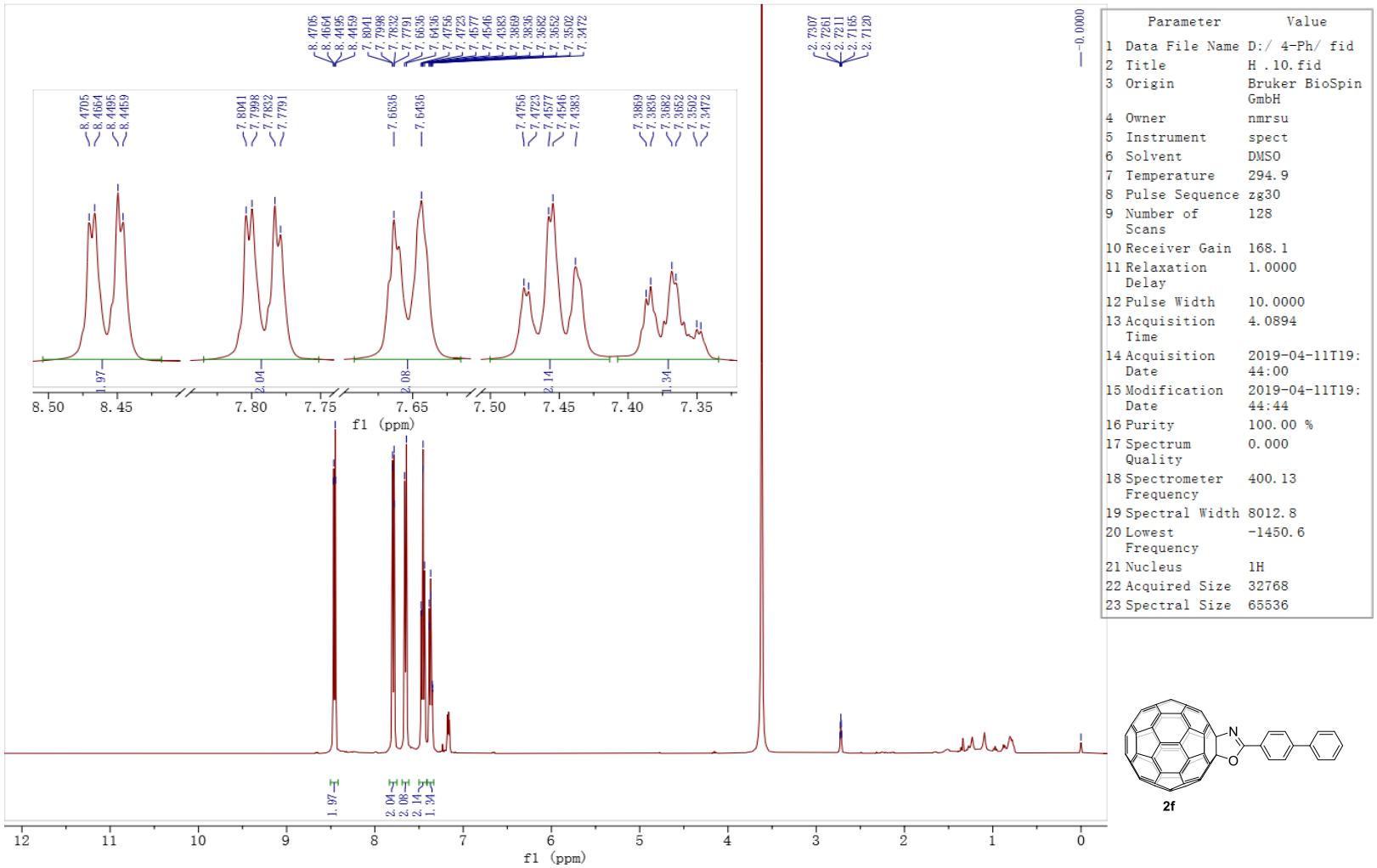


Figure S14. ^{1}H NMR (400 MHz, CS_2/DMSO-d_6) of **2f**.

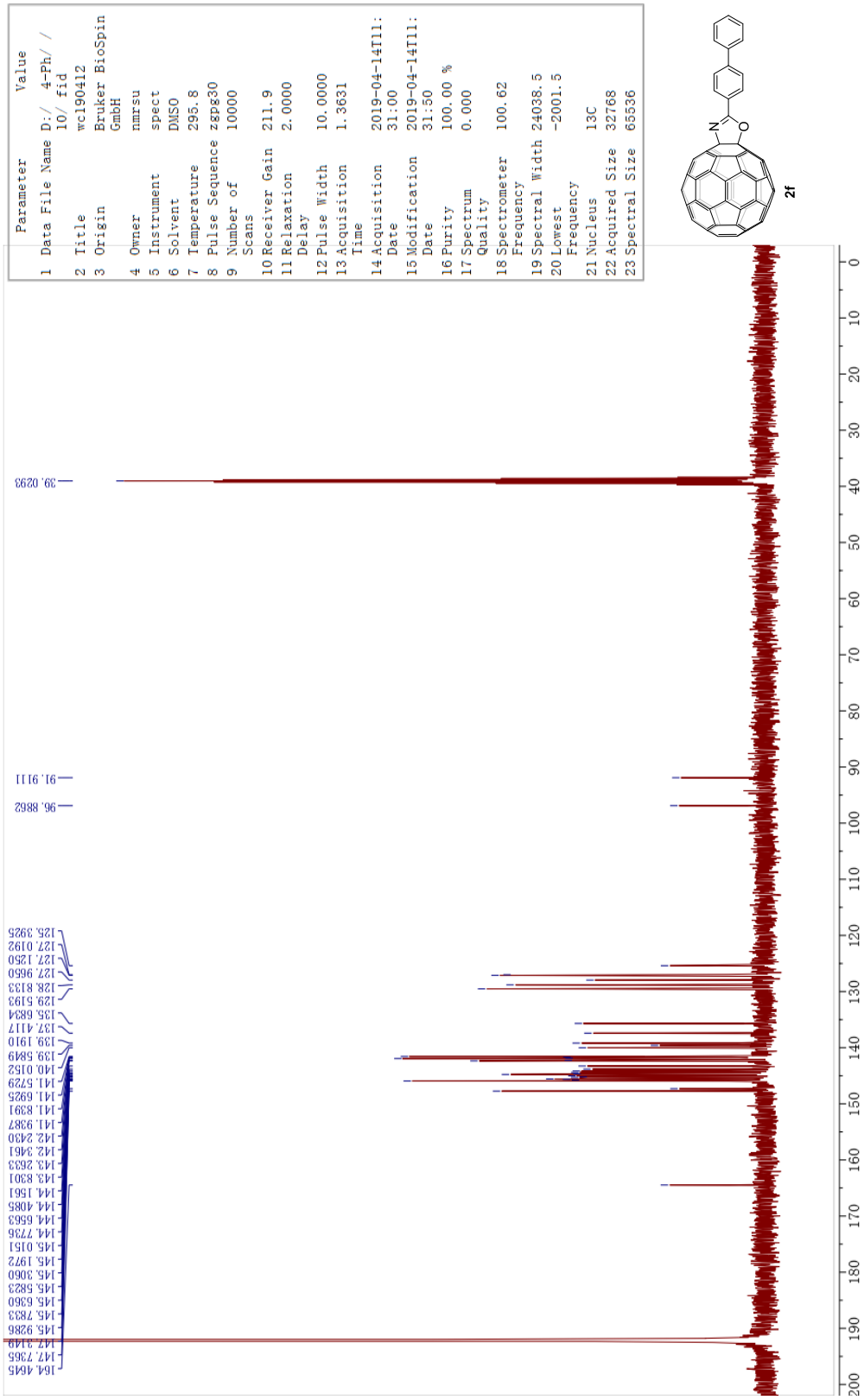


Figure S15. ^{13}C NMR (101 MHz, CS_2/DMSO-d_6) of **2f**.

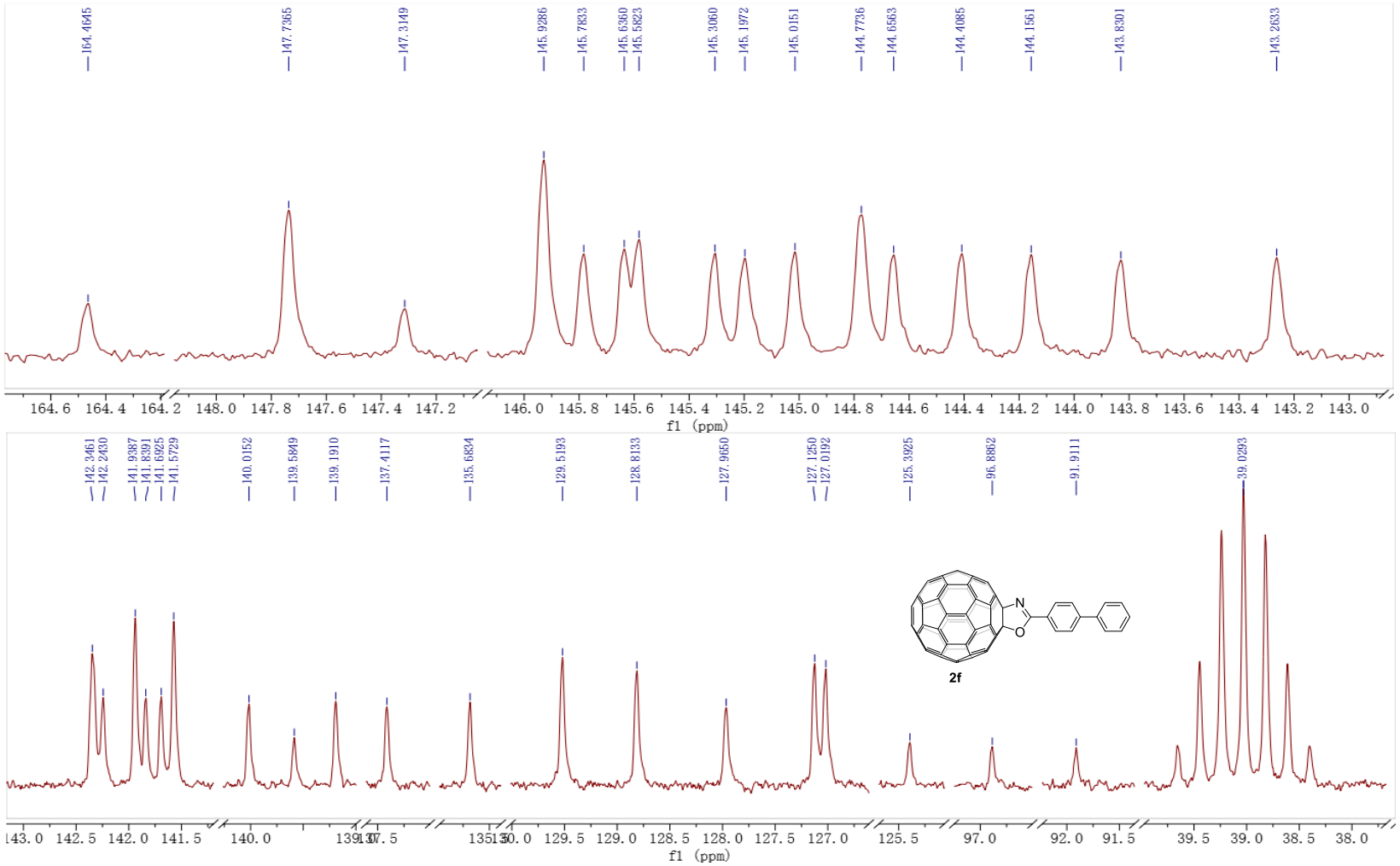


Figure S16. Expanded ^{13}C NMR (101 MHz, CS_2/DMSO-d_6) of **2f**.

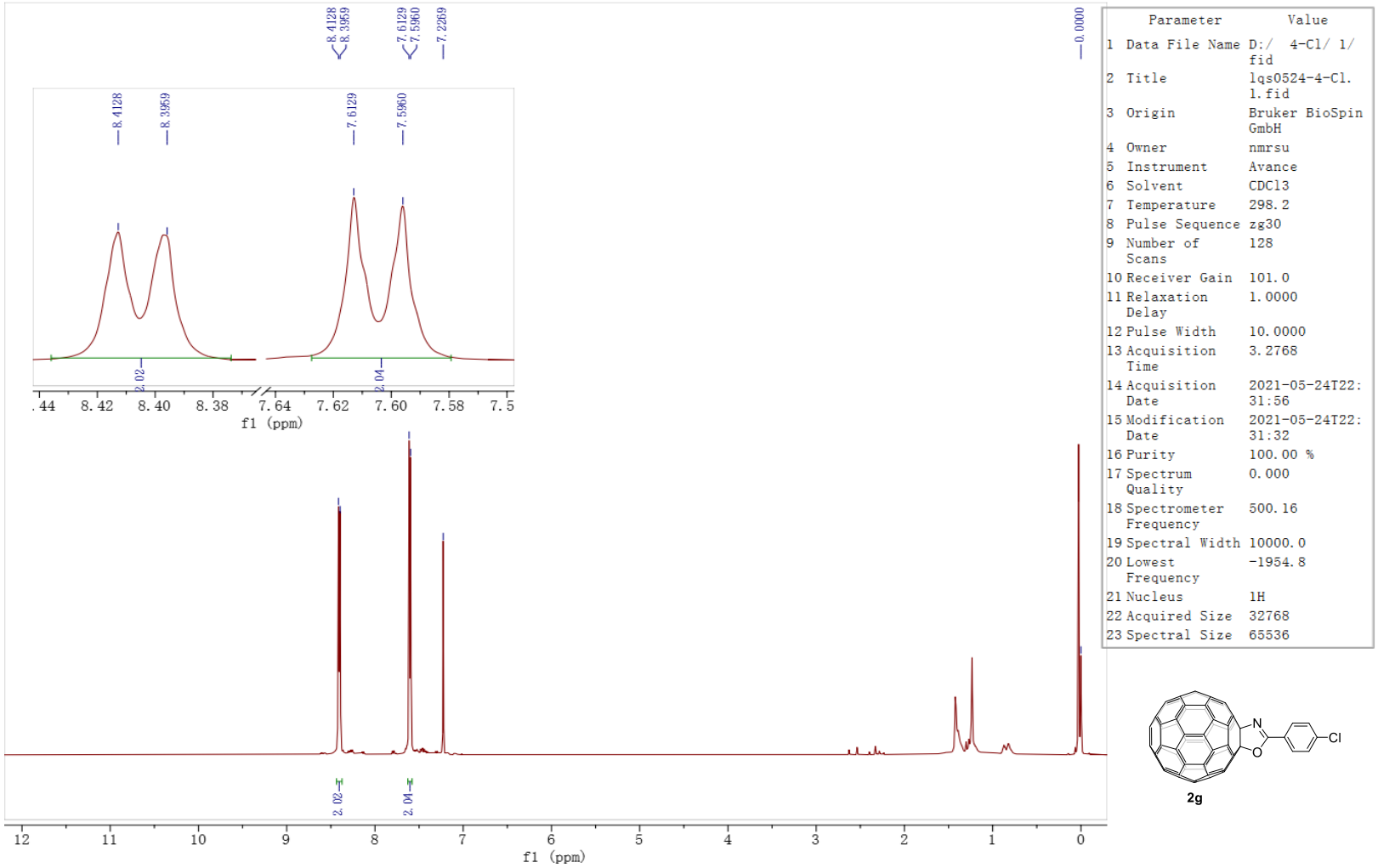


Figure S17. ^{1}H NMR (500 MHz, 1:1 $CS_2/CDCl_3$) of **2g**.

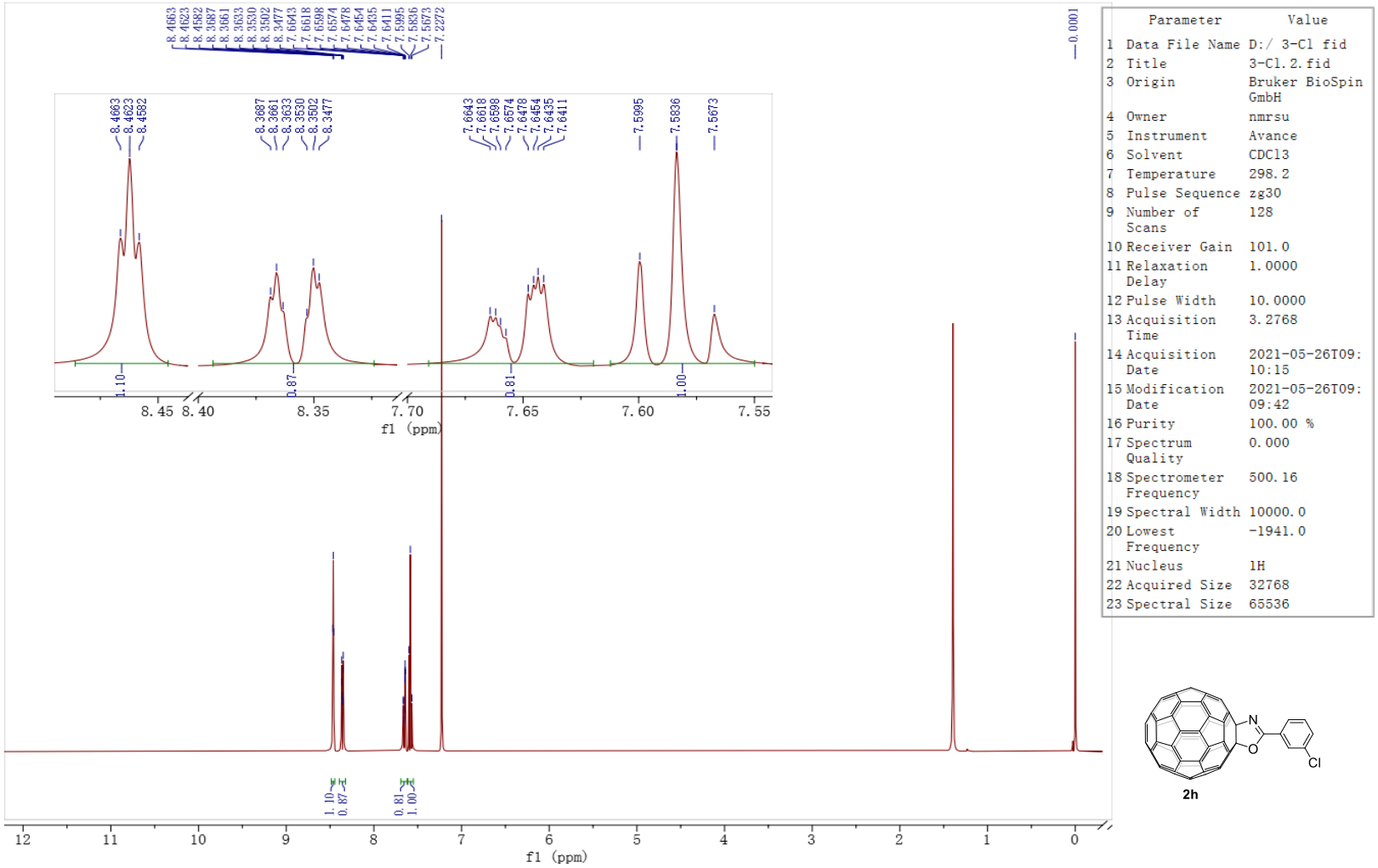


Figure S18. ^{1}H NMR (500 MHz, 1:1 $CS_2/CDCl_3$) of **2h**.

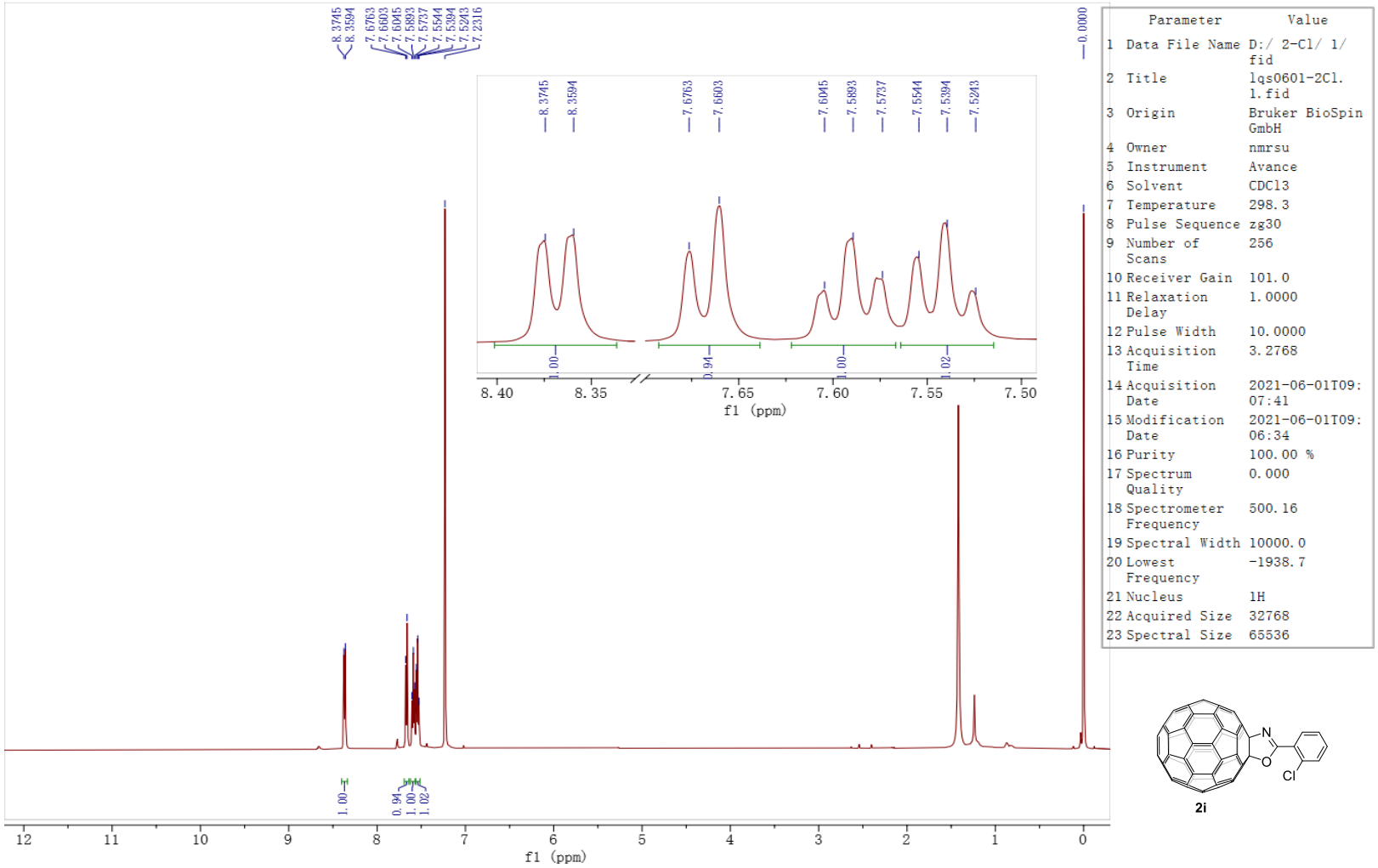
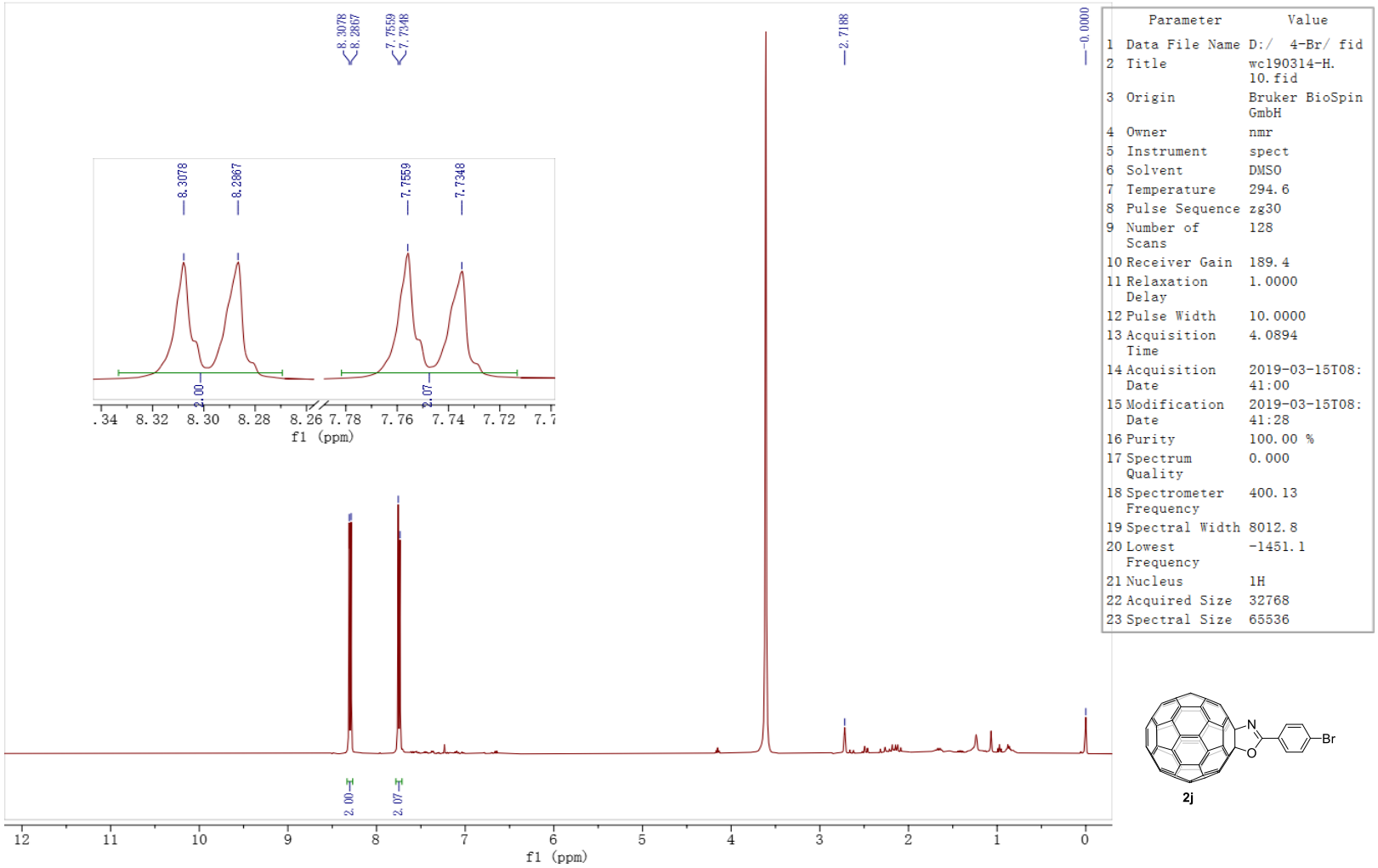


Figure S19. ^{1}H NMR (500 MHz, 1:1 $CS_2/CDCl_3$) of **2i**.



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4	Owner	nmr
5	Instrument	spect
6	Solvent	DMSO
7	Temperature	294. 6
8	Pulse Sequence	zg30
9	Number of Scans	128
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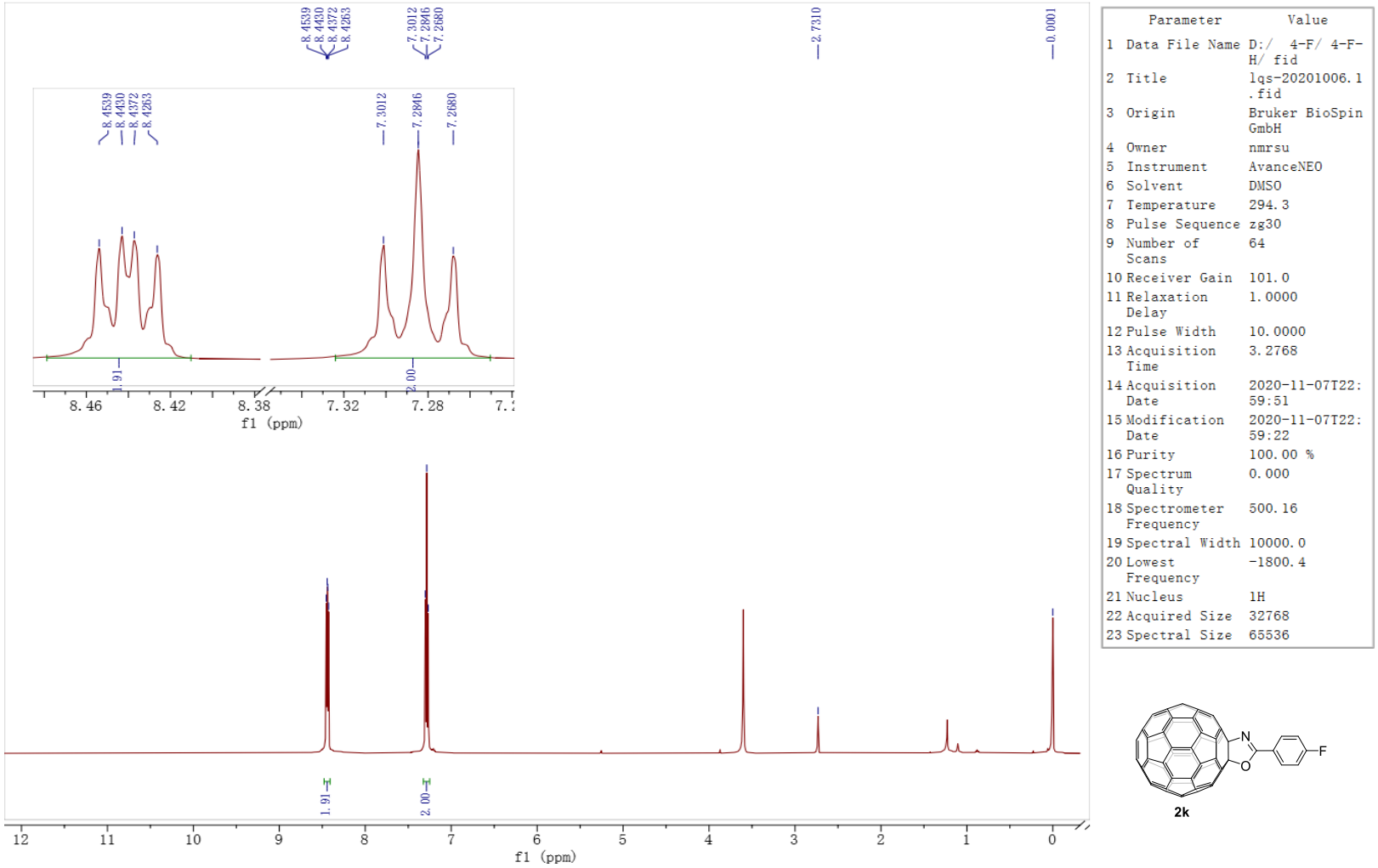
11	Relaxation Delay	1. 0000
12	Pulse Width	10. 0000
13	Acquisition Time	4. 0894
14	Acquisition Date	2019-03-15T08: 41:00
15	Modification Date	2019-03-15T08: 41:28
16	Purity	100. 00 %
17	Spectrum Quality	0. 000
18	Spectrometer Frequency	400. 13
19	Spectral Width	8012. 8
20	Lowest Frequency	-1451. 1
21	Nucleus	1H
22	Acquired Size	32768
23	Spectral Size	65536

Figure S20. ^{1}H NMR (400 MHz, CS_2/DMSO-d_6) of **2j**.



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4	Owner	nmrsu
5	Instrument	AvanceNEO
6	Solvent	DMSO
7	Temperature	294.3
8	Pulse Sequence	zg30
9	Number of Scans	64
10	Receiver Gain	101.0
11	Relaxation Delay	1.0000
12	Pulse Width	10.0000
13	Acquisition Time	3.2768
14	Acquisition Date	2020-11-07T22:59:51
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16	Purity	100.00 %
17	Spectrum Quality	0.000
18	Spectrometer Frequency	500.16
19	Spectral Width	10000.0
20	Lowest Frequency	-1800.4
21	Nucleus	1H
22	Acquired Size	32768
23	Spectral Size	65536

Figure S21. ^{1}H NMR (500 MHz, CS_2/DMSO-d_6) of **2k**.

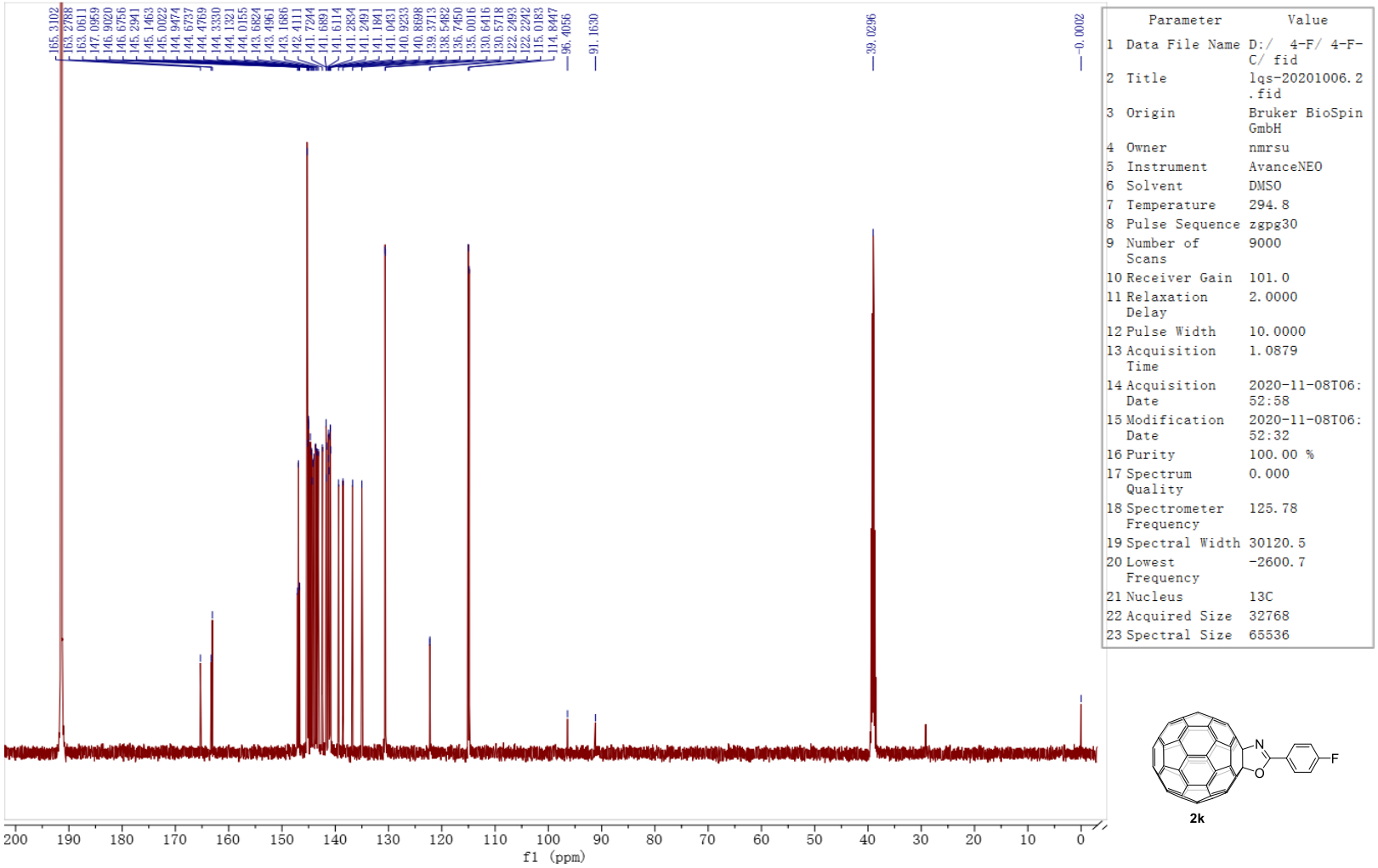


Figure S22. ^{13}C NMR (126 MHz, CS_2/DMSO-d_6) of **2k**.

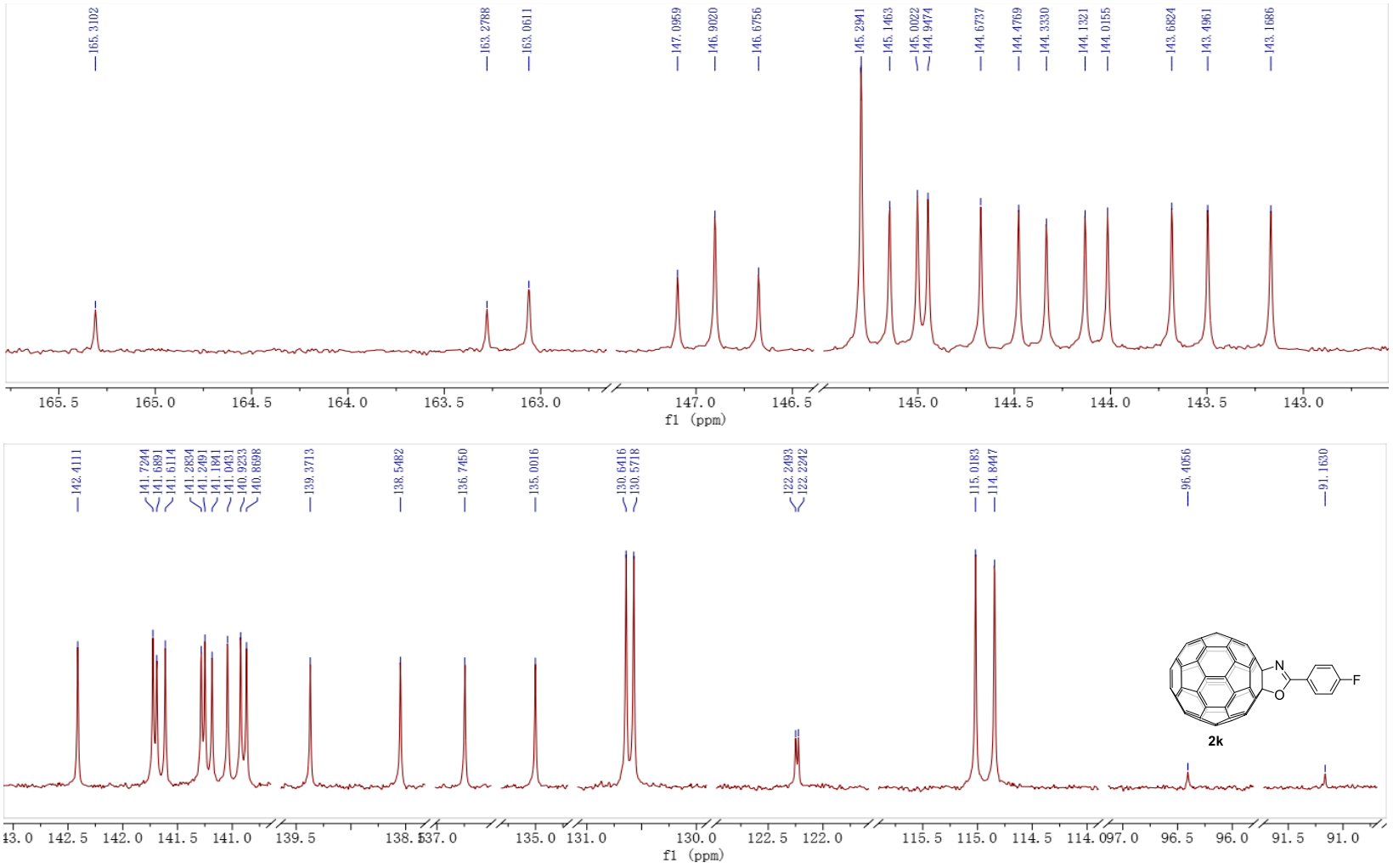


Figure S23. Expanded ^{13}C NMR (126 MHz, CS_2/DMSO-d_6) of **2k**.

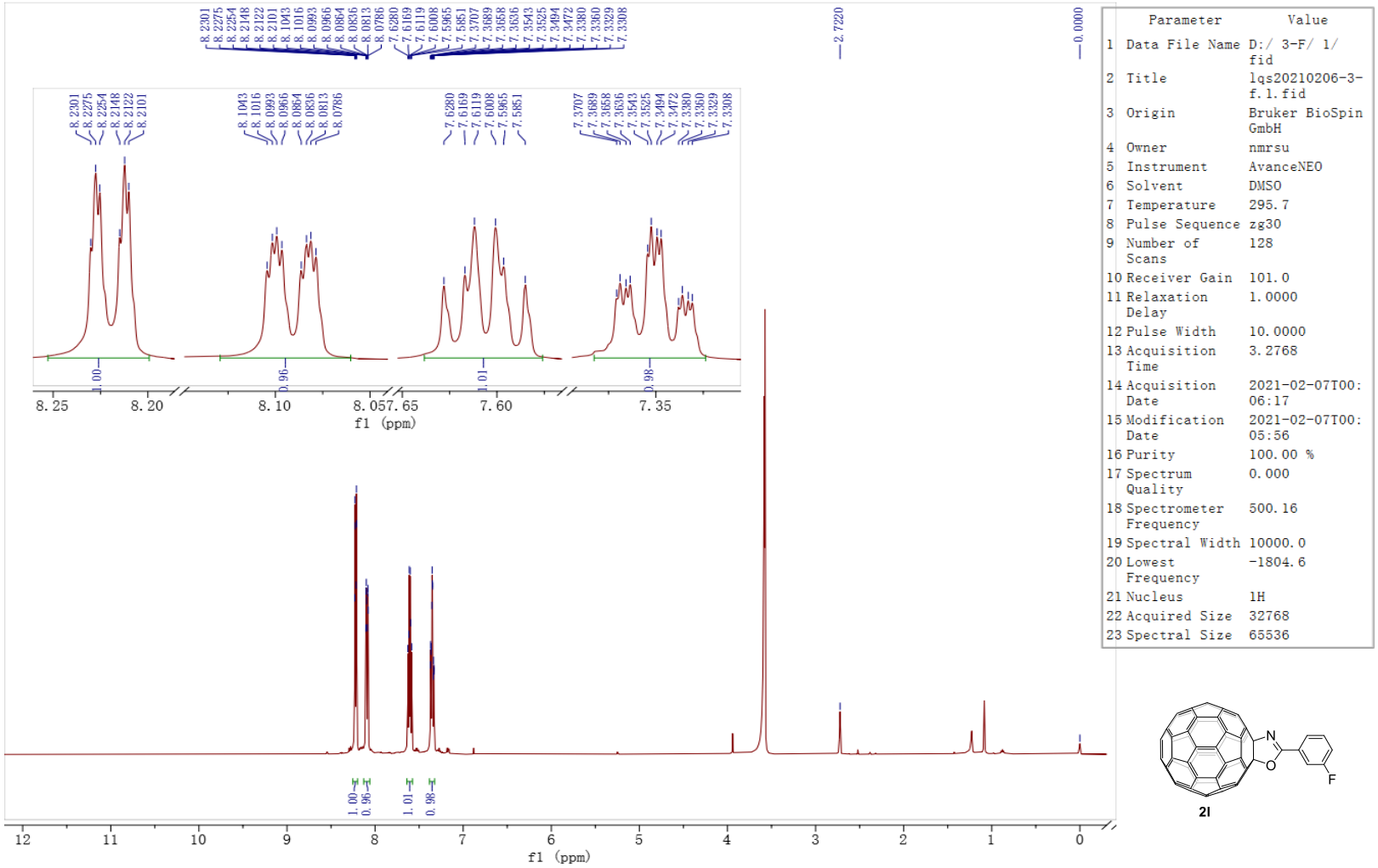


Figure S24. ^{1}H NMR (500 MHz, CS_2/DMSO-d_6) of **2l**.

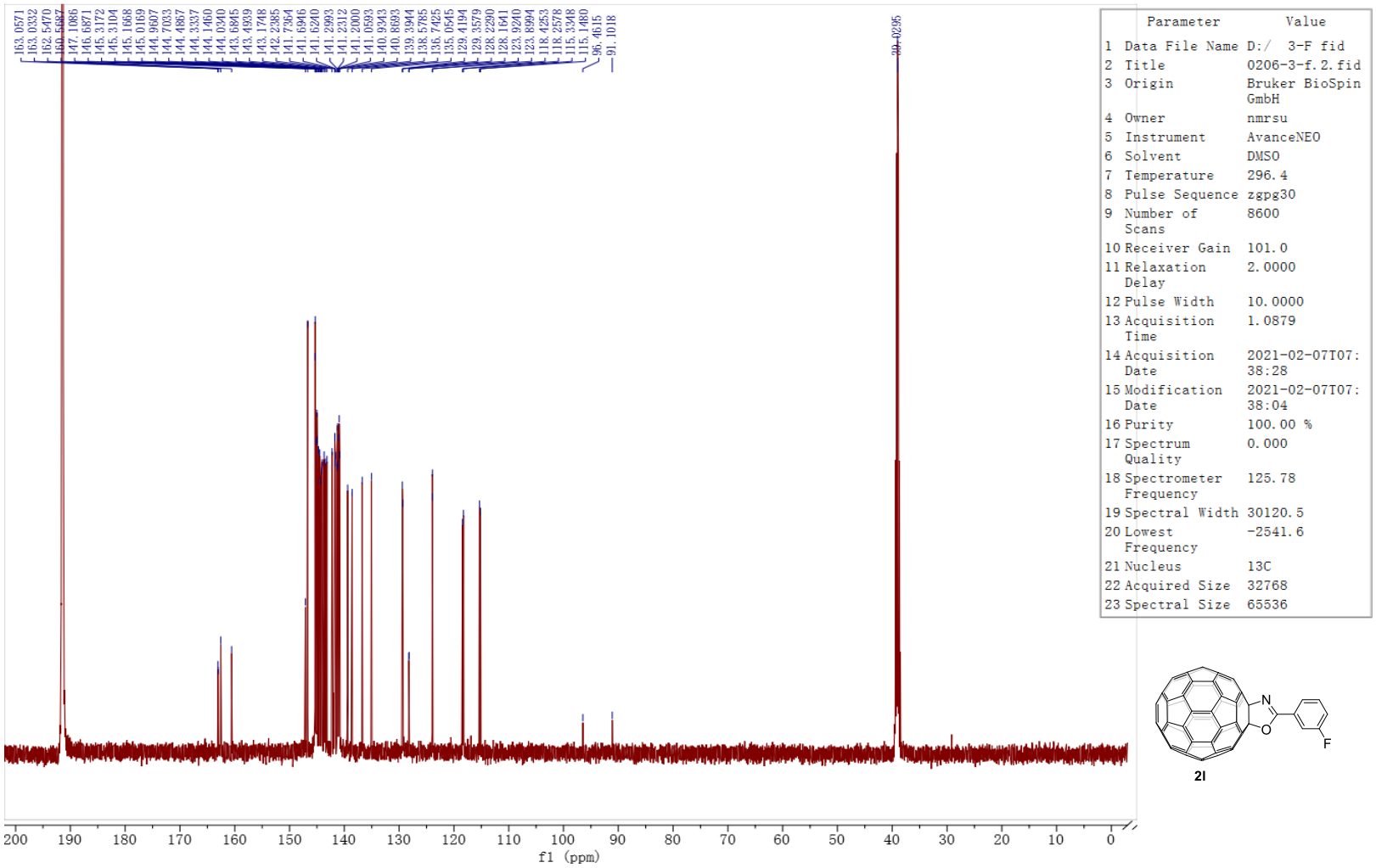


Figure S25. ^{13}C NMR (126 MHz, CS_2/DMSO-d_6) of **2l**.

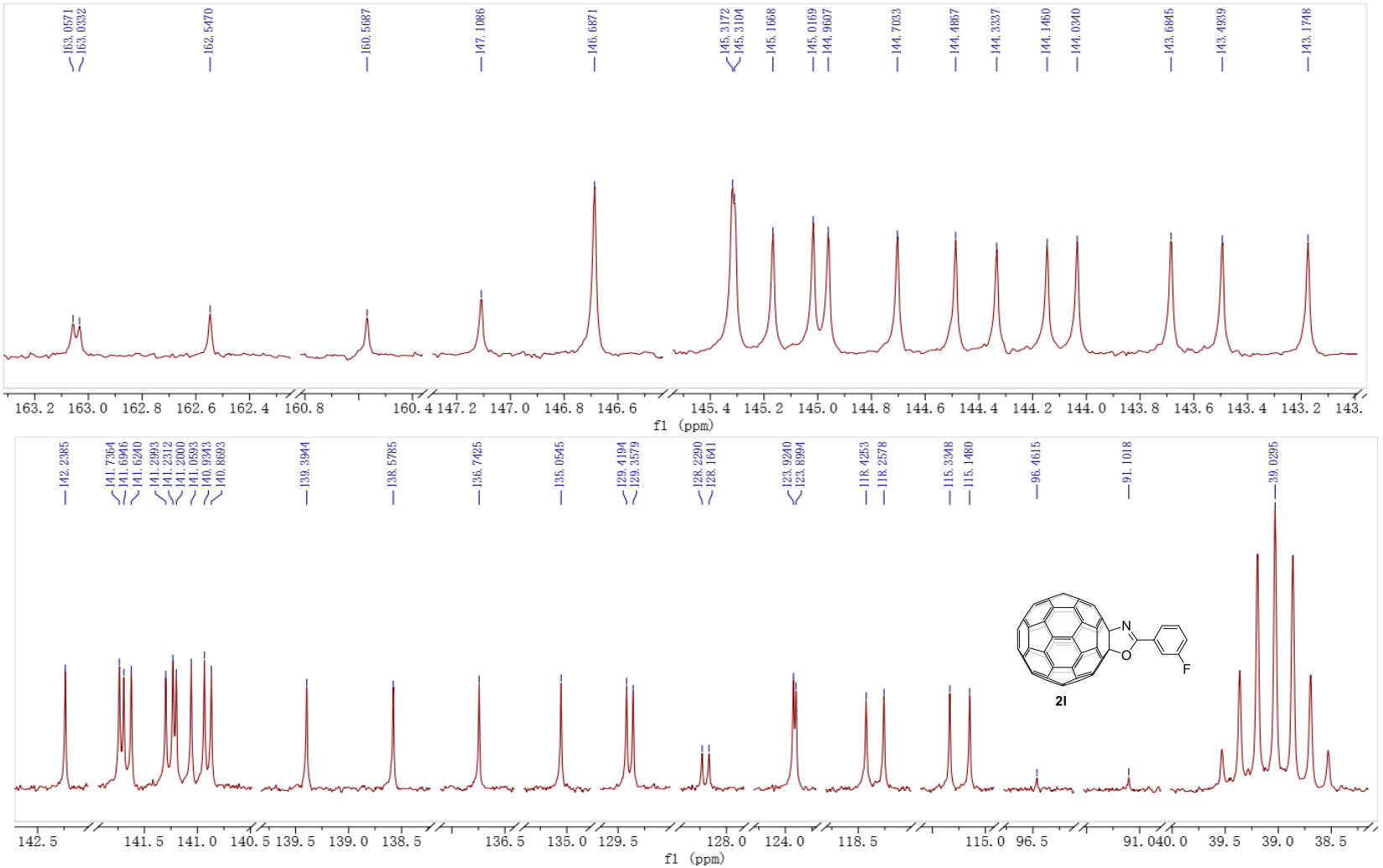


Figure S26. Expanded ^{13}C NMR (126 MHz, CS_2/DMSO-d_6) of **2l**.

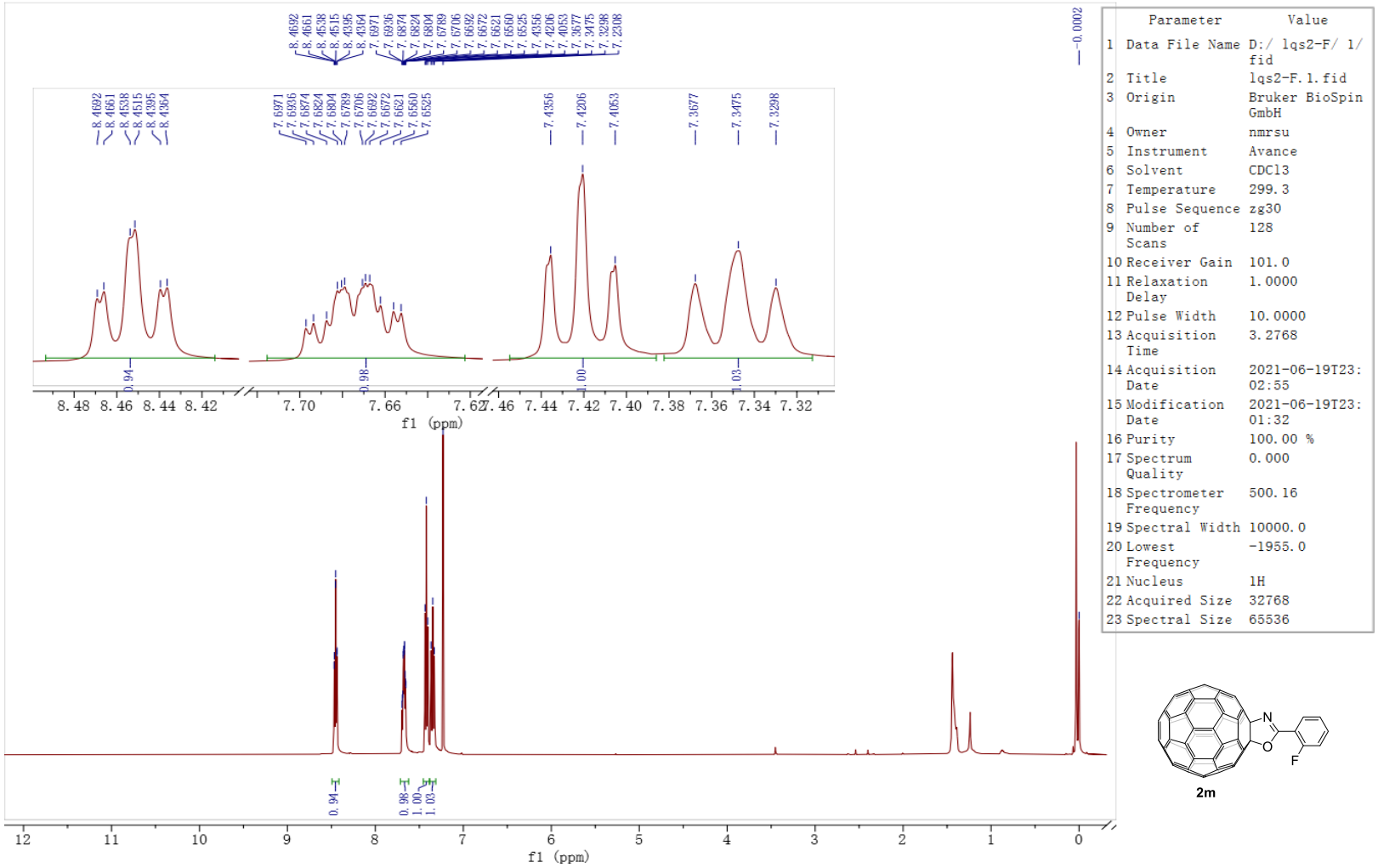


Figure S27. ^{1}H NMR (500 MHz, 1:1 CS_2/$CDCl_3$) of **2m**.

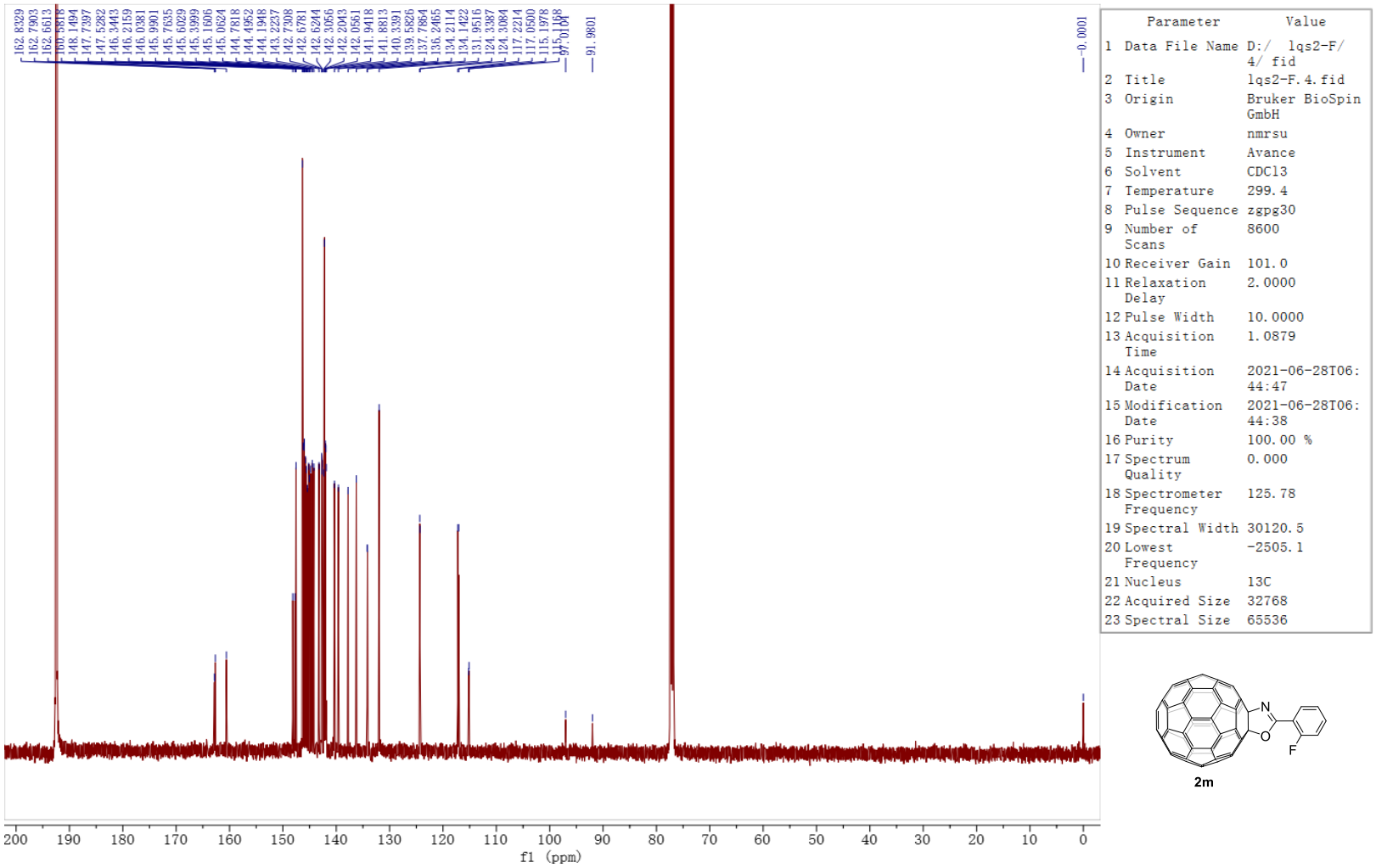


Figure S28. ^{13}C NMR (126 MHz, 1:1 $CS_2/CDCl_3$) of **2m**.

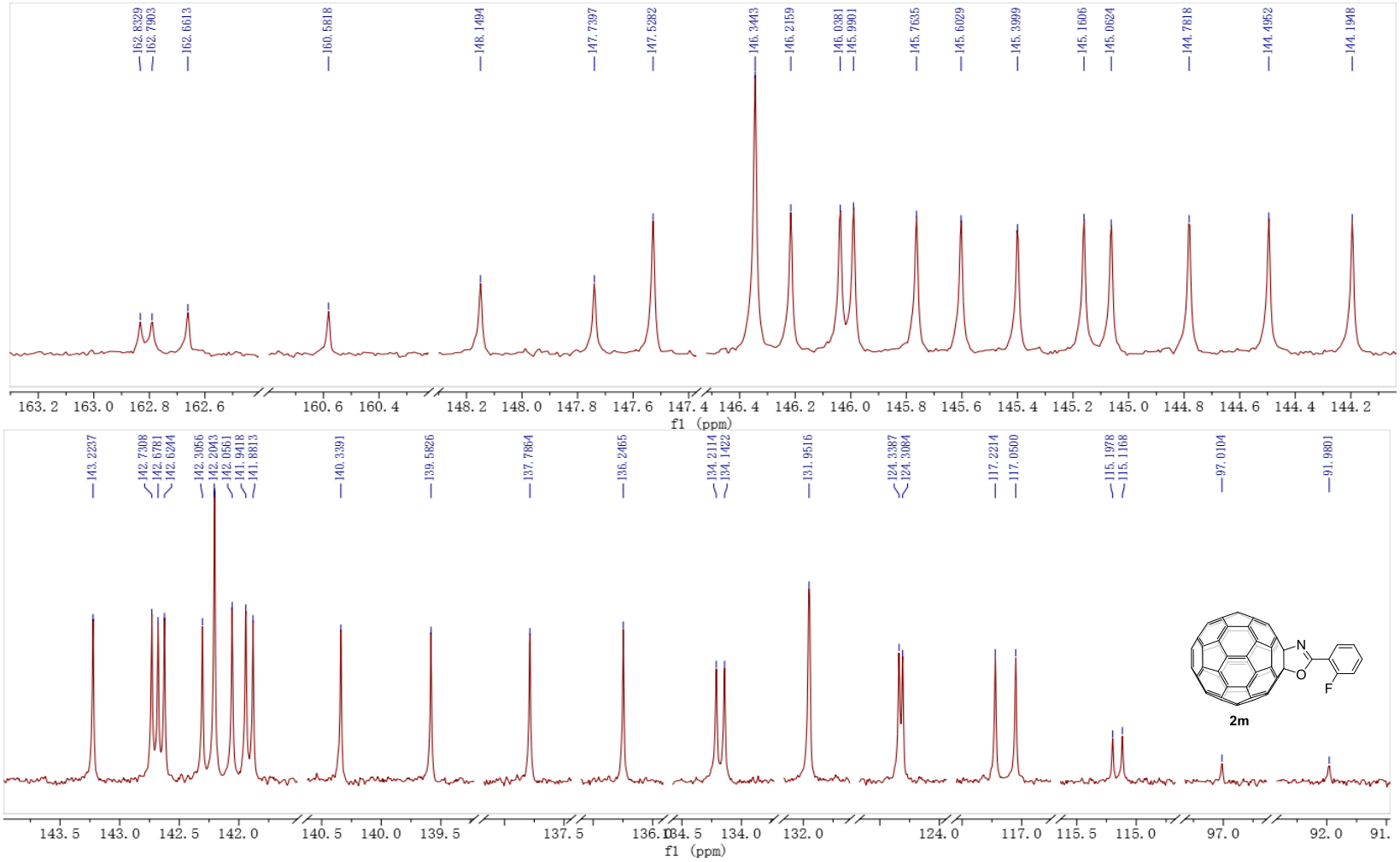


Figure S29. Expanded ^{13}C NMR (126 MHz, 1:1 $CS_2/CDCl_3$) of **2m**.

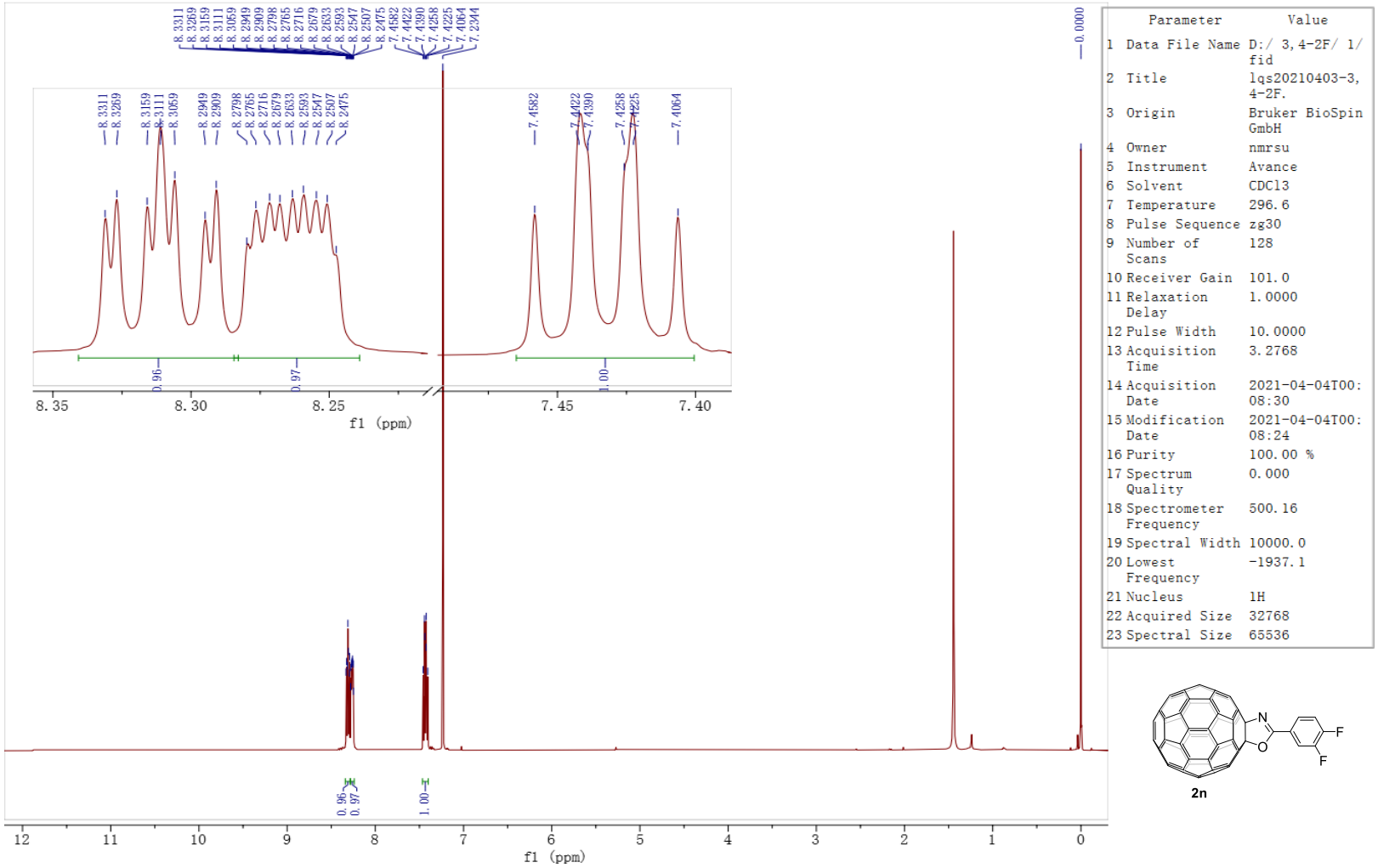


Figure S30. ^{1}H NMR (500 MHz, 1:1 $CS_2/CDCl_3$) of **2n**.

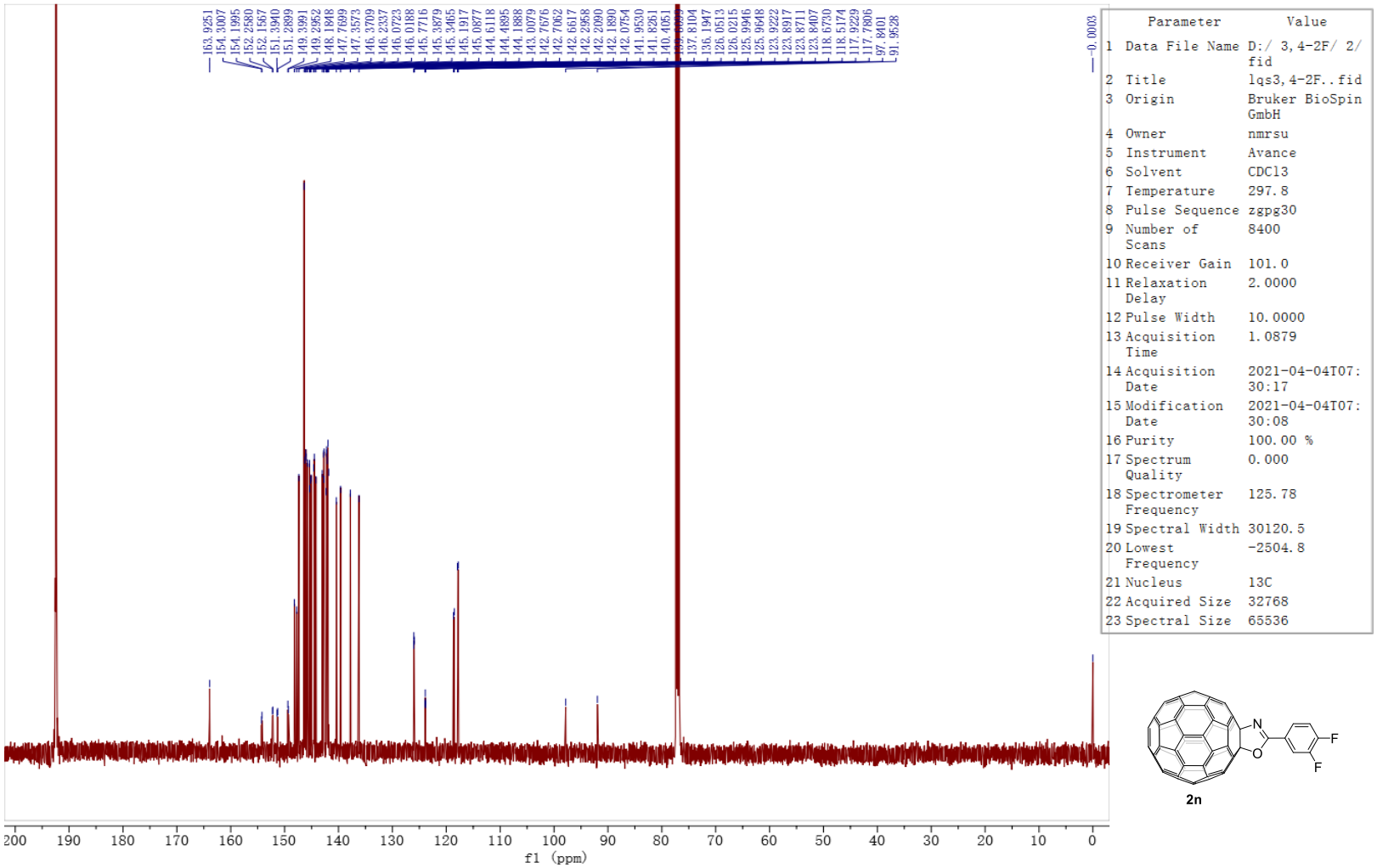


Figure S31. ^{13}C NMR (126 MHz, 1:1 $CS_2/CDCl_3$) of **2n**.

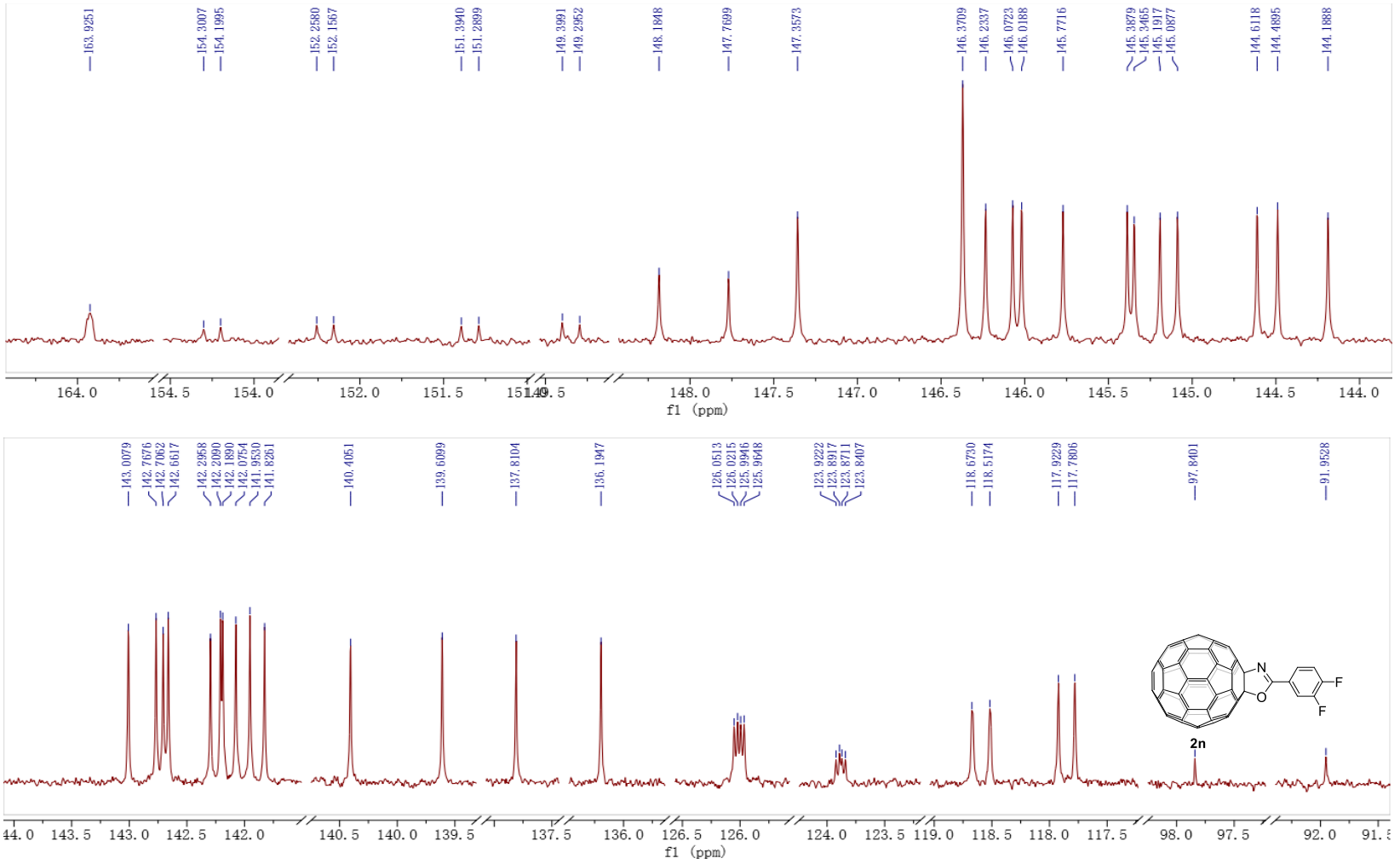


Figure S32. Expanded ^{13}C NMR (126 MHz, 1:1 $CS_2/CDCl_3$) of **2n**.

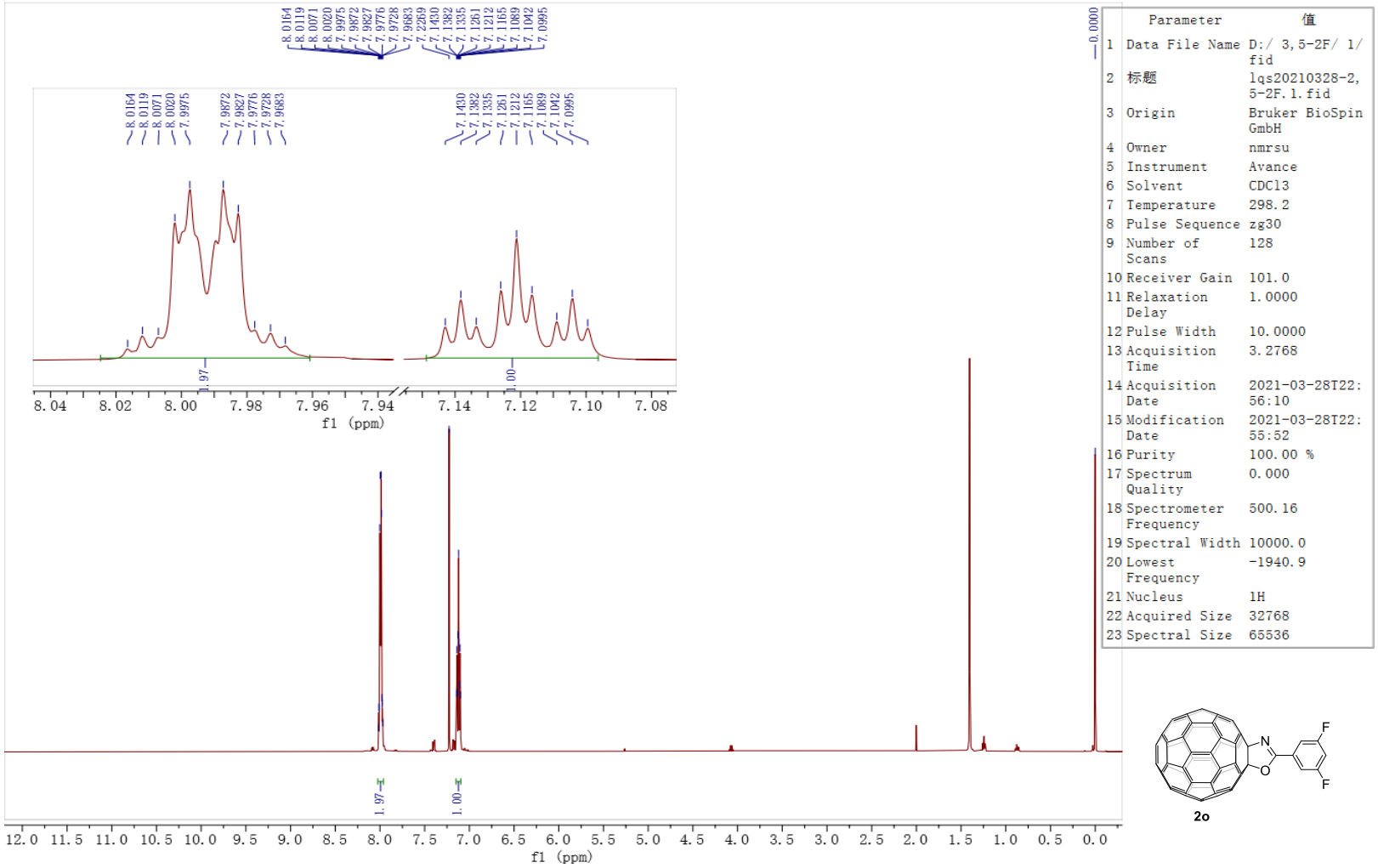


Figure S33. ^{1}H NMR (500 MHz, 1:1 $CS_2/CDCl_3$) of **2o**.

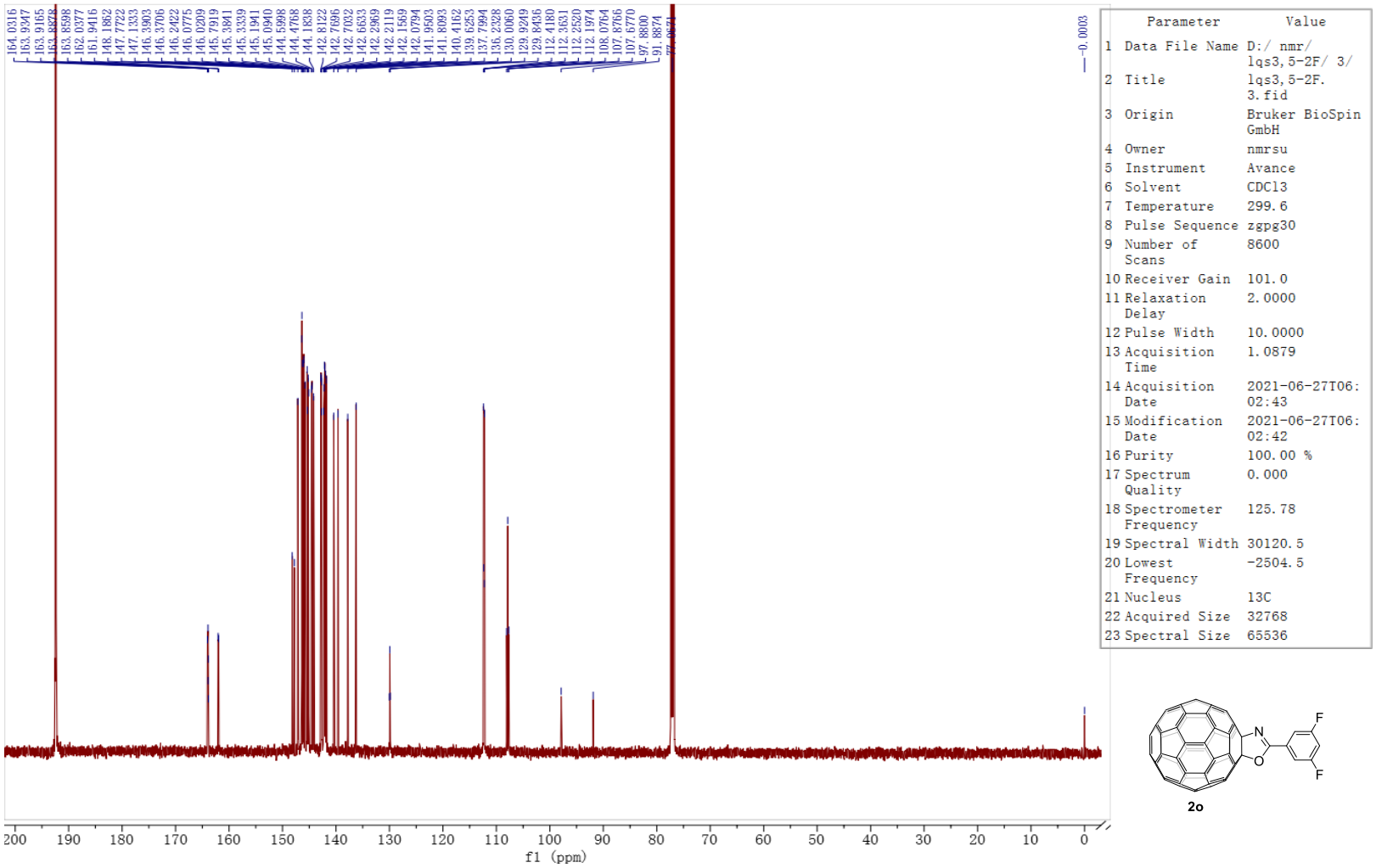


Figure S34. ^{13}C NMR (126 MHz, 1:1 $CS_2/CDCl_3$) of **2o**.

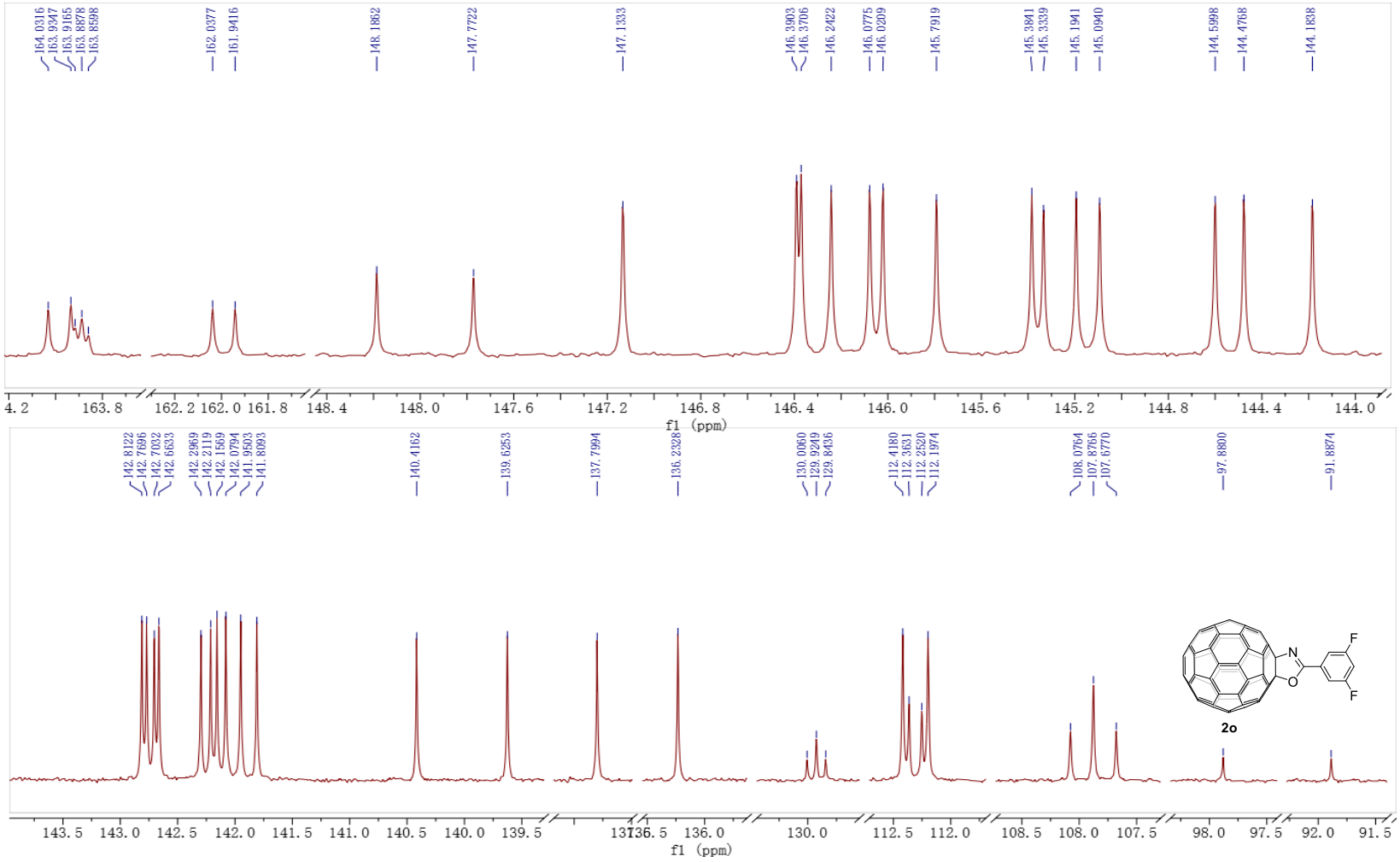


Figure S35. Expanded ^{13}C NMR (126 MHz, 1:1 $CS_2/CDCl_3$) of **2o**.

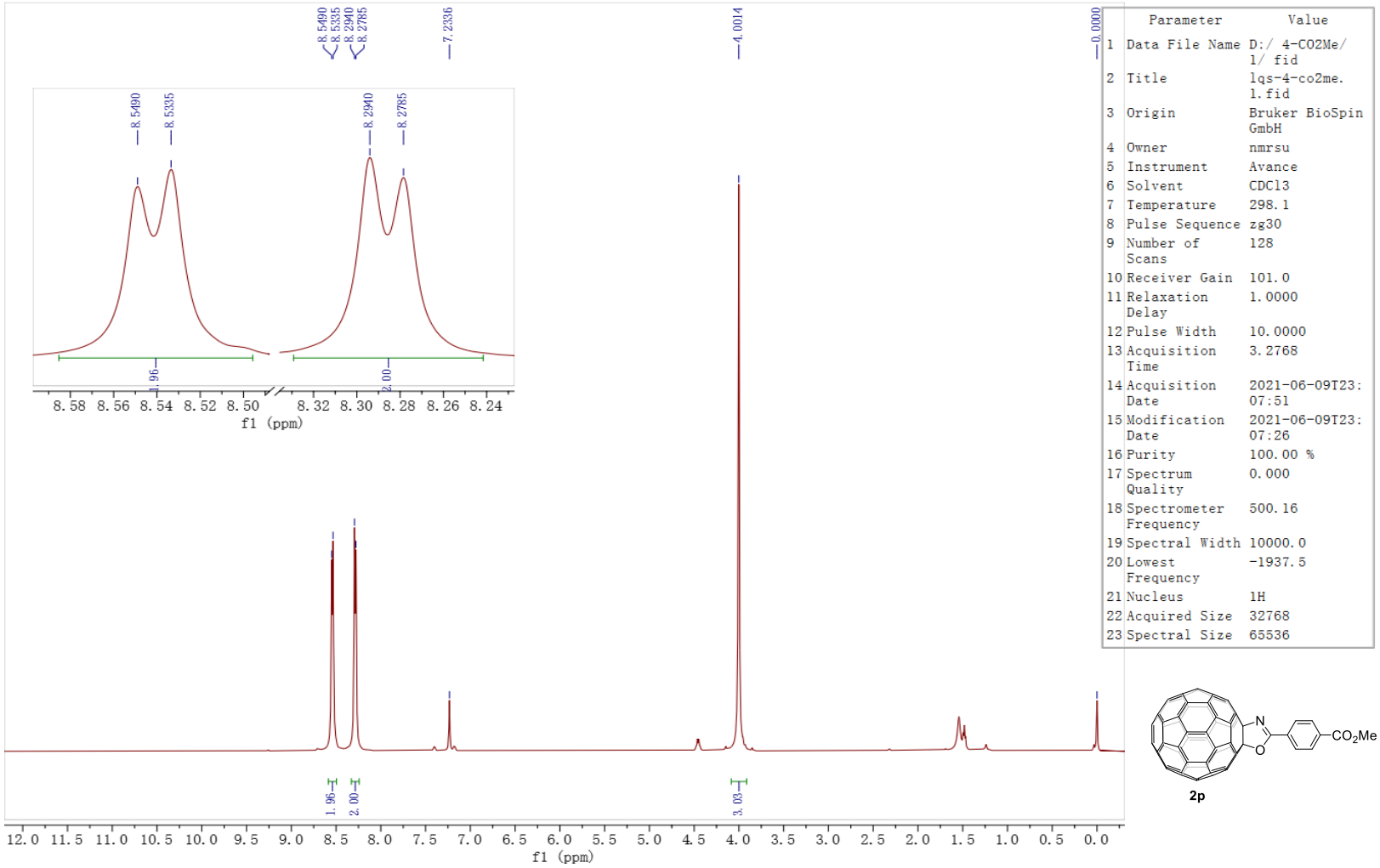


Figure S36. ^{1}H NMR (500 MHz, 1:1 $CS_2/CDCl_3$) of **2p**.

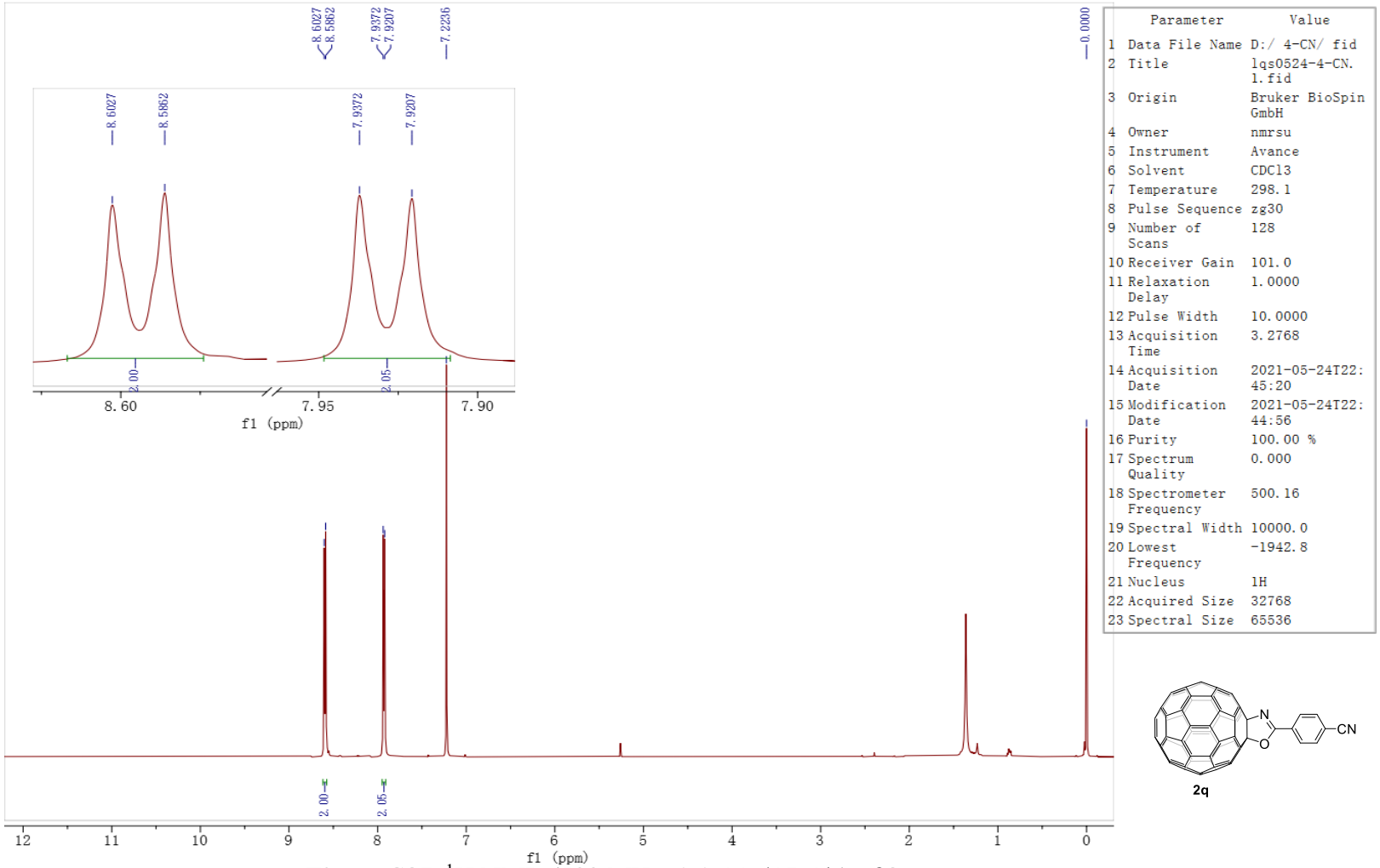


Figure S37. ^{1}H NMR (500 MHz, 1:1 $CS_2/CDCl_3$) of **2q**.

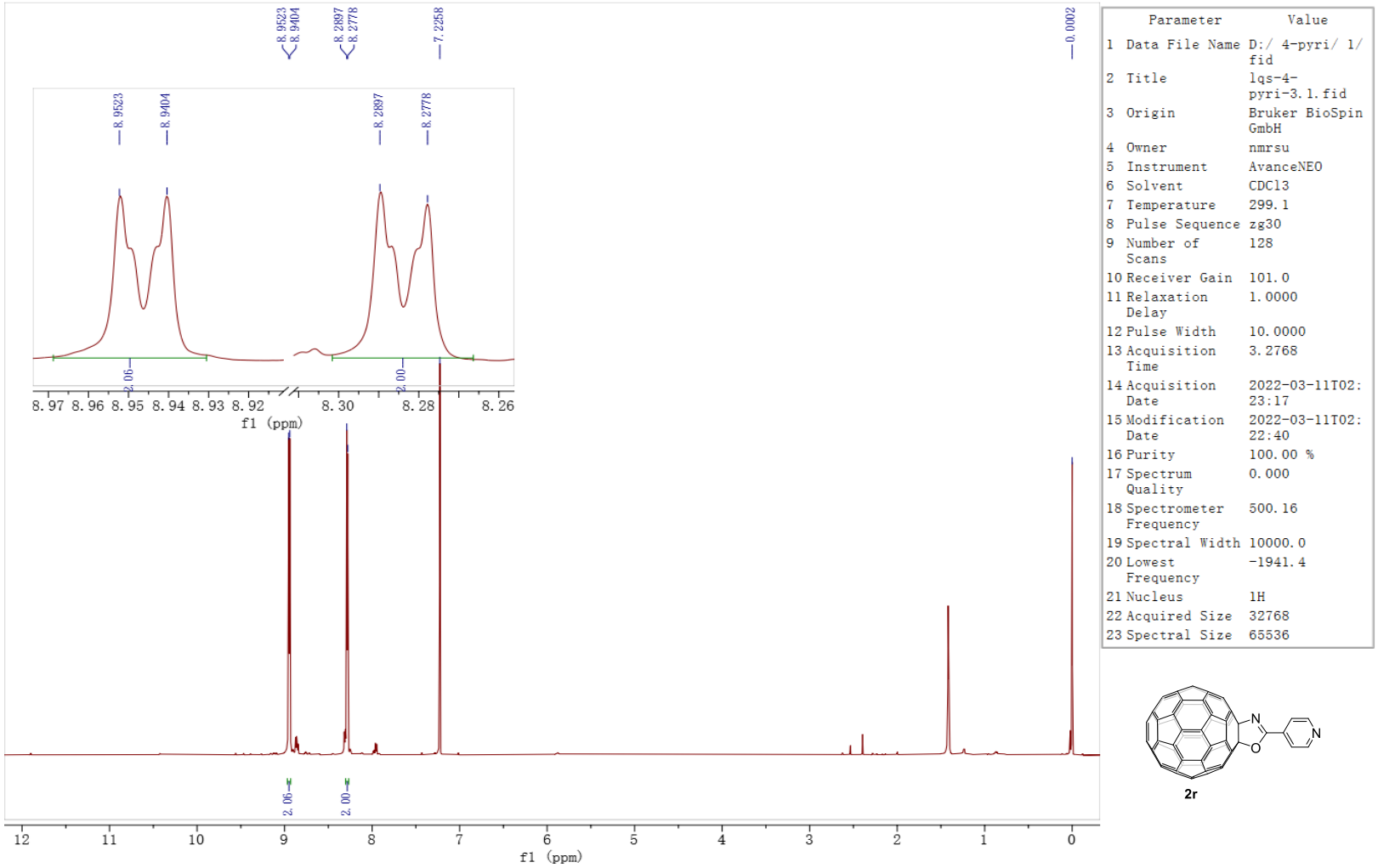
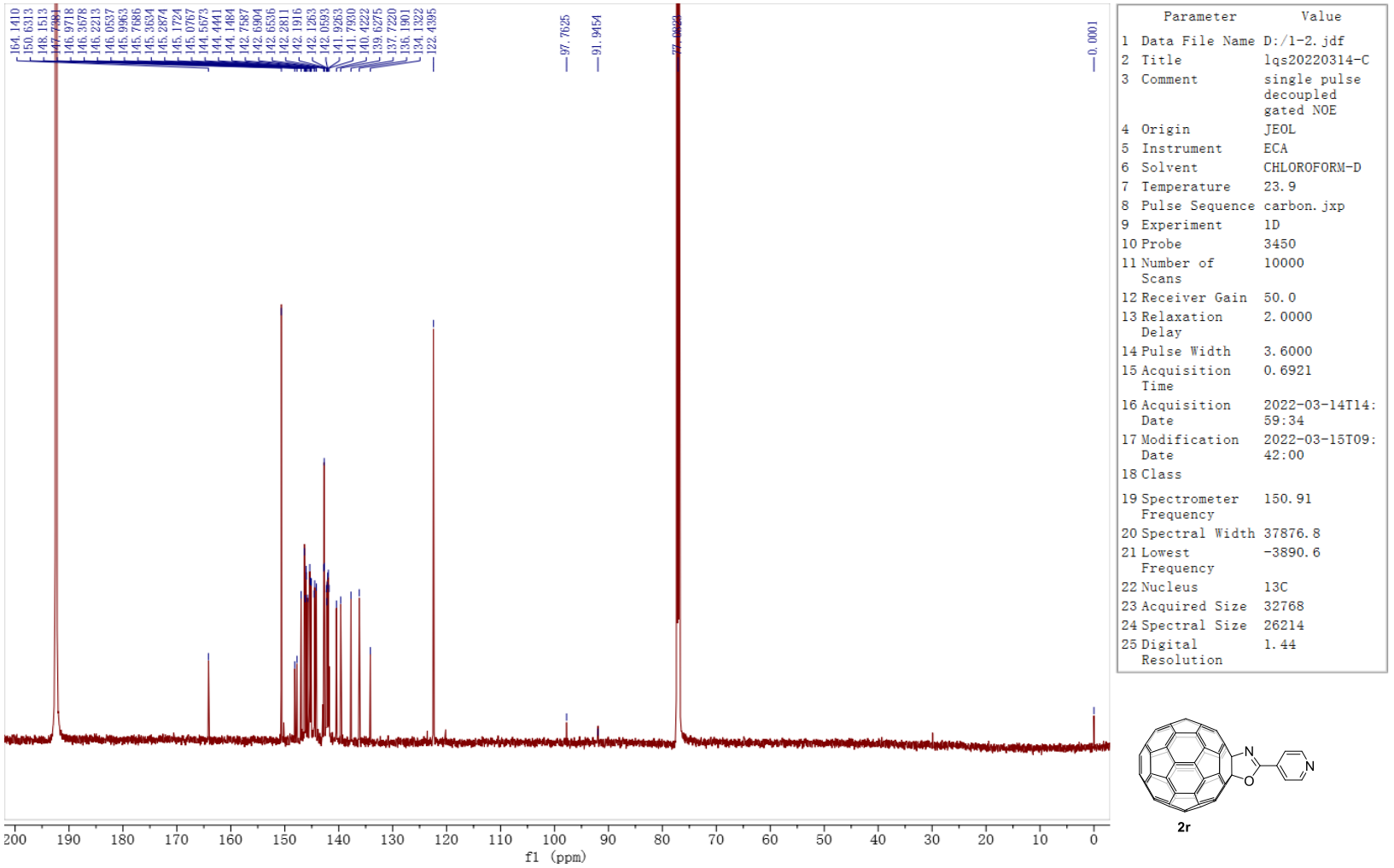


Figure S38. ^{1}H NMR (500 MHz, 1:1 $CS_2/CDCl_3$) of **2r**.



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7	Temperature	23.9
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9	Experiment	1D
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12	Receiver Gain	50.0
13	Relaxation Delay	2.0000
14	Pulse Width	3.6000
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16	Acquisition Date	2022-03-14T14:59:34
17	Modification Date	2022-03-15T09:42:00
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20	Spectral Width	37876.8
21	Lowest Frequency	-3890.6
22	Nucleus	13C
23	Acquired Size	32768
24	Spectral Size	26214
25	Digital Resolution	1.44

2r

Figure S39. ^{13}C NMR (151 MHz, 1:1 $CS_2/CDCl_3$) of **2r**.

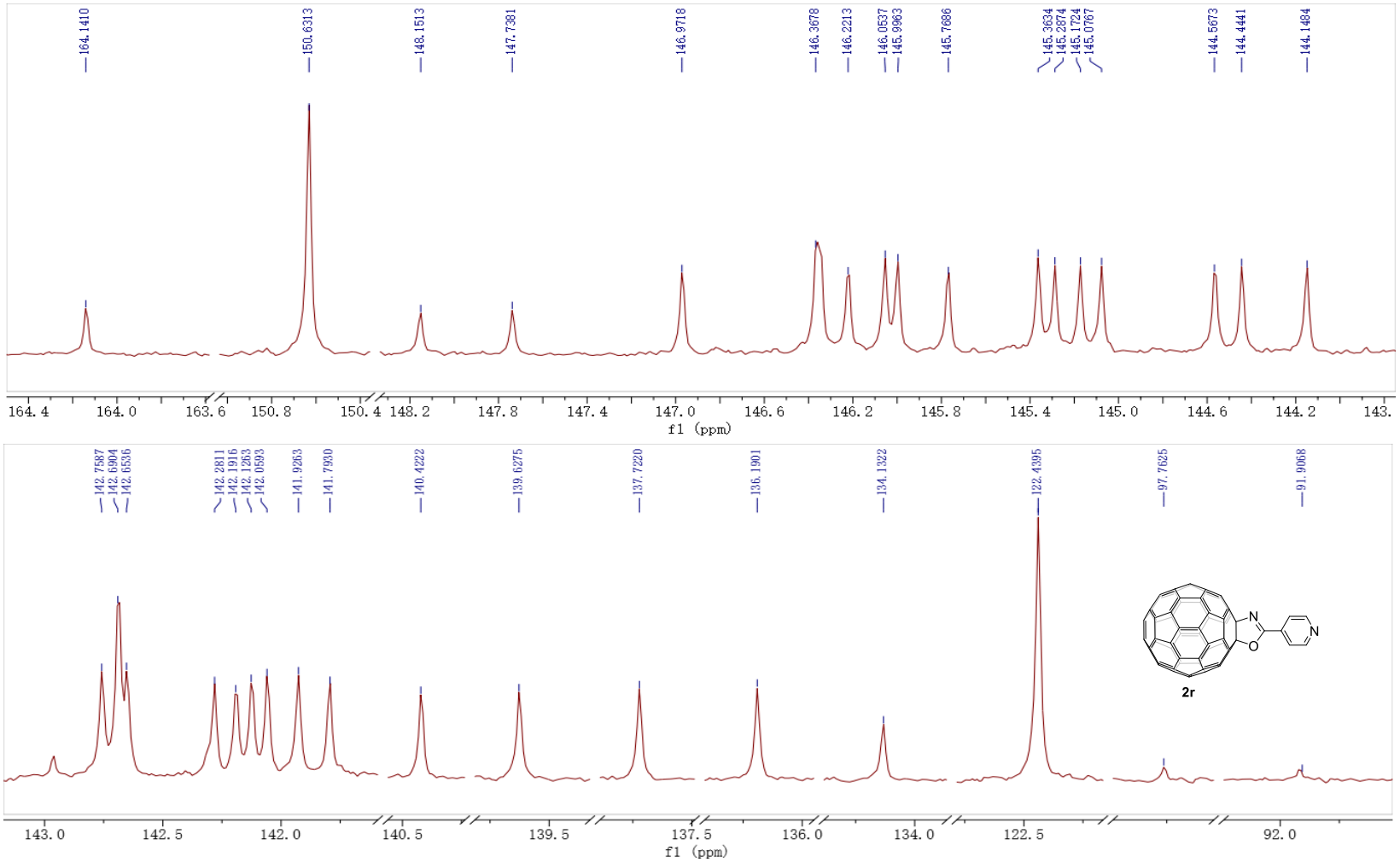

Figure S40. Expanded ^{13}C NMR (151 MHz, 1:1 $CS_2/CDCl_3$) of **2r**.

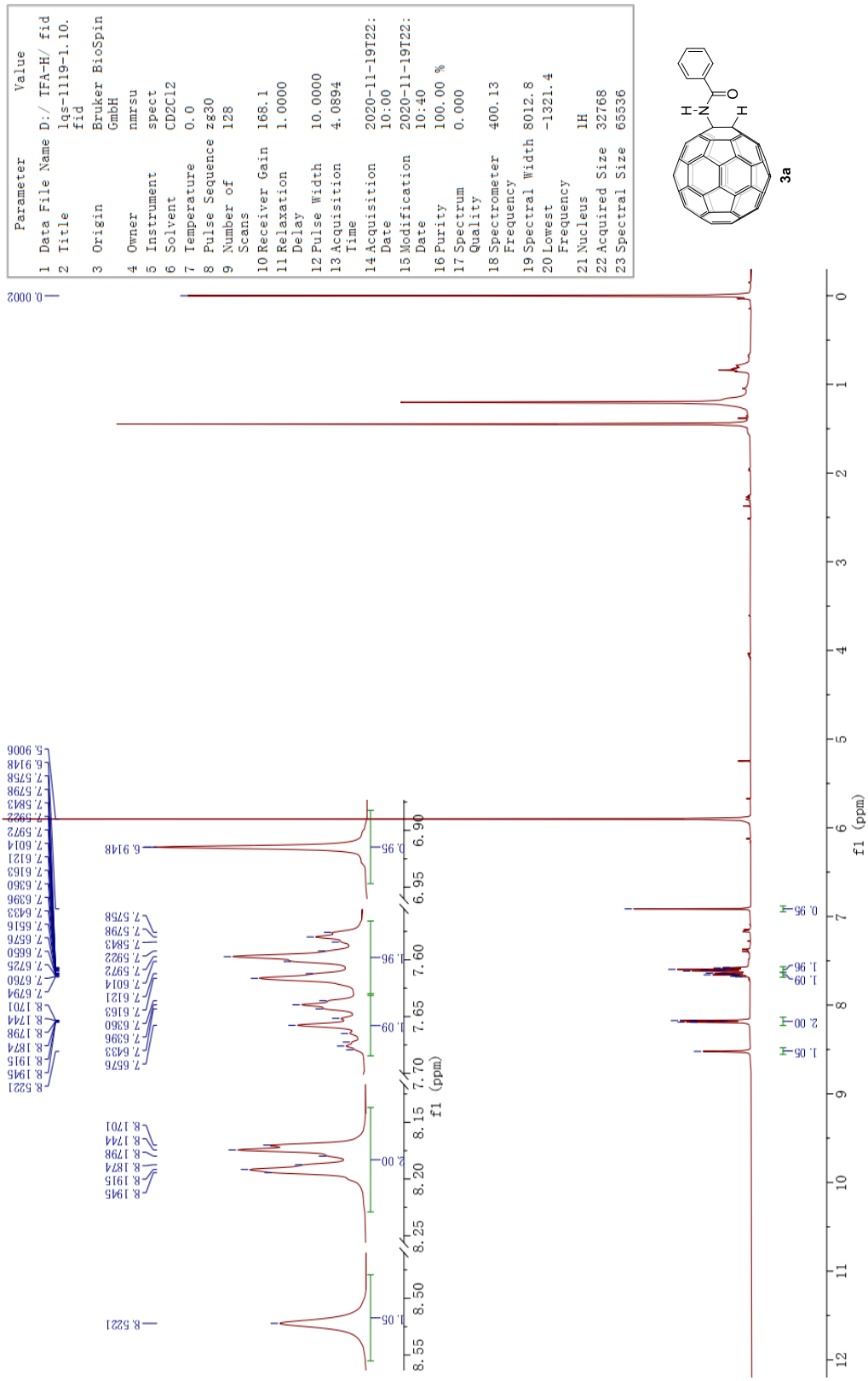

Figure S41. ^{1}H NMR (400 MHz, $CDCl_2CDCl_2$) of **3a**.

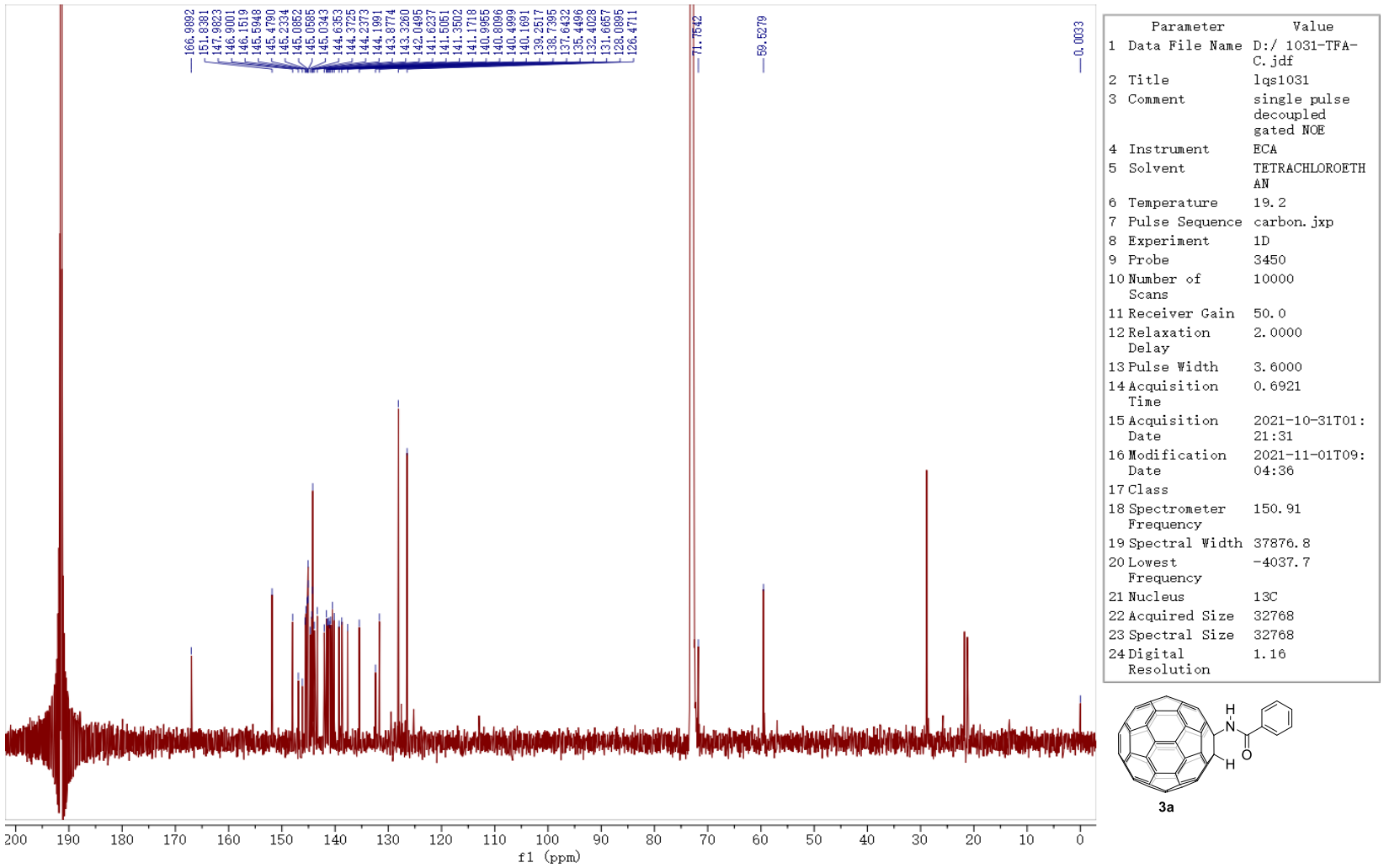

Figure S42. ^{13}C NMR (151 MHz, 2:1 $CDCl_2CDCl_2/CS_2$) of **3a**.

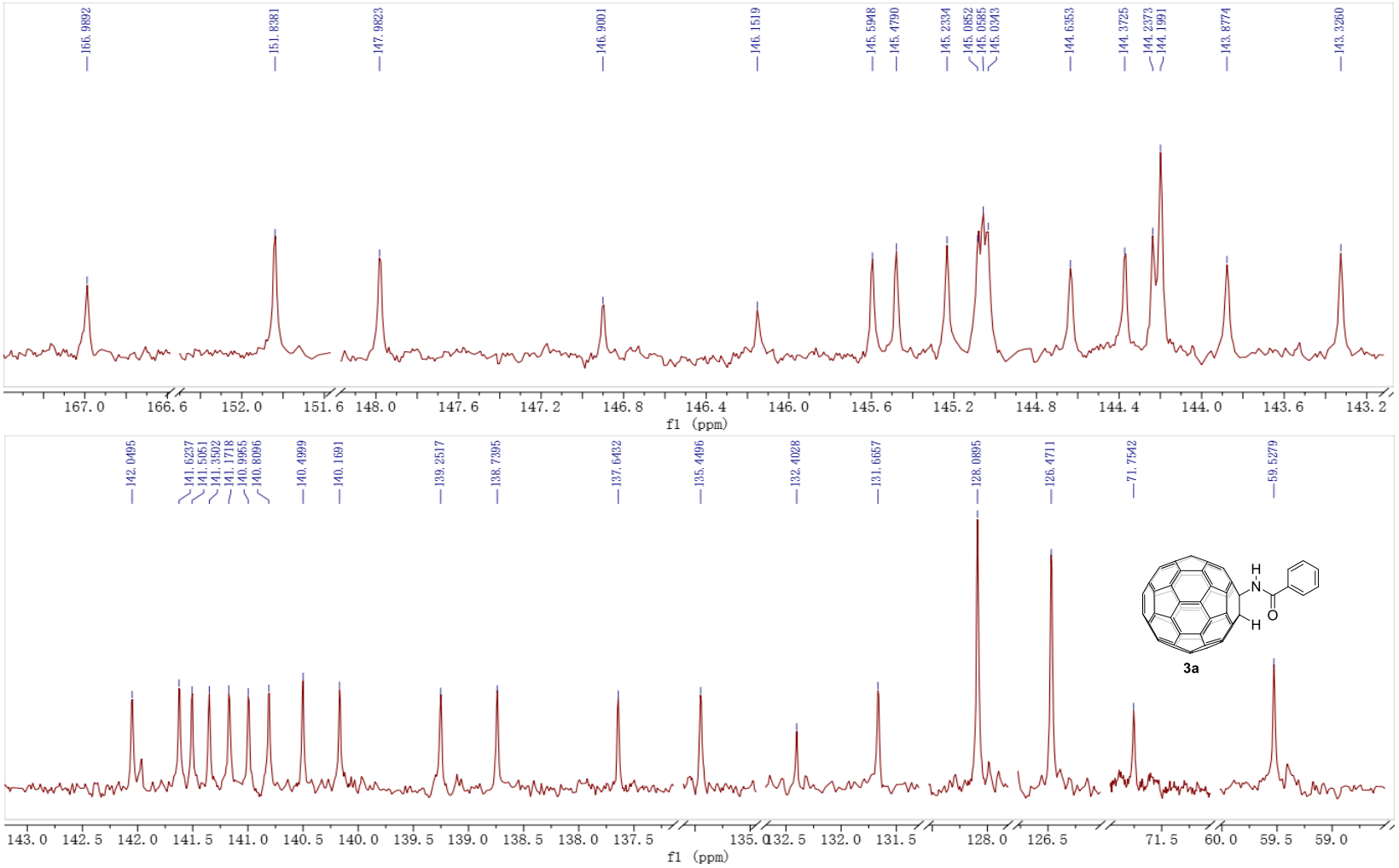

Figure S43. Expanded ^{13}C NMR (151 MHz, 2:1 $CDCl_2CDCl_2/CS_2$) of **3a**.

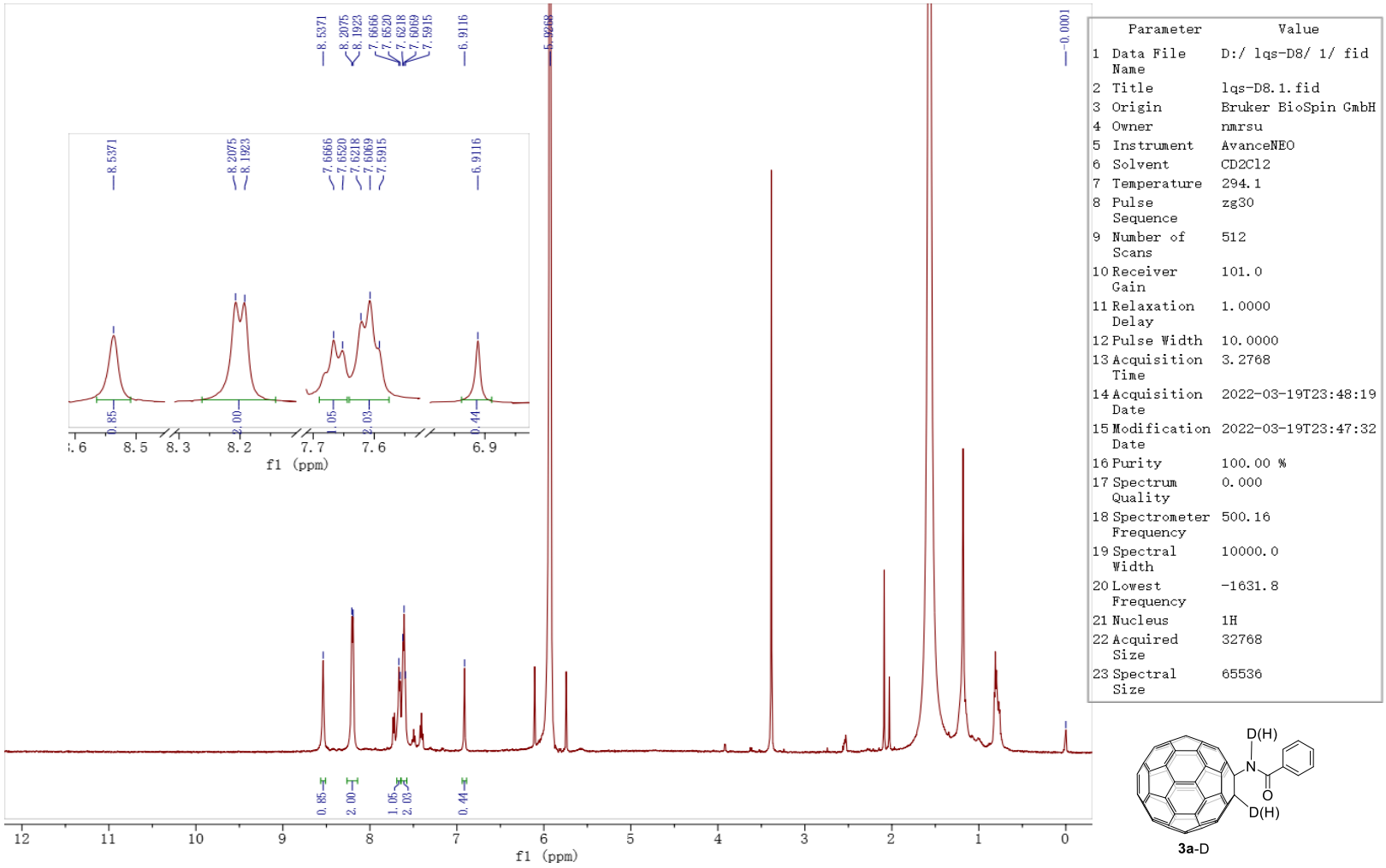

Figure S44. ^{1}H NMR (500 MHz, $CDCl_2CDCl_2$) of **3a**-D.

9. UV-vis Spectra of Compounds 2d–f, 2k–o, 2r and 3a

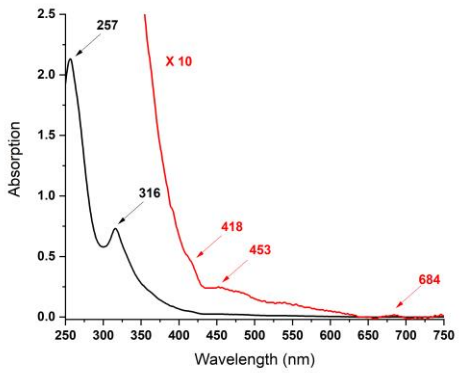

Figure S45. UV-vis absorption of compound **2d**.

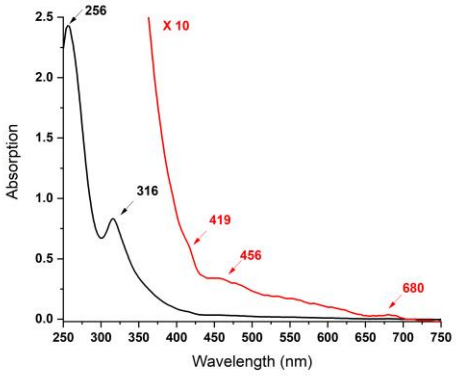

Figure S46. UV-vis absorption of compound **2e**.

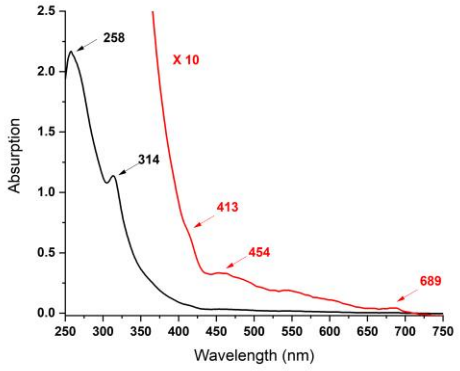

Figure S47. UV-vis absorption of compound **2f**.

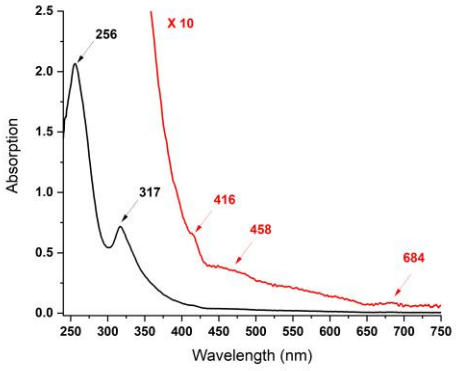

Figure S48. UV-vis absorption of compound **2k**.

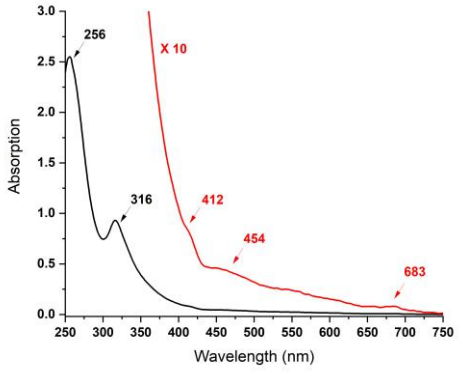

Figure S49. UV-vis absorption of compound **2l**.

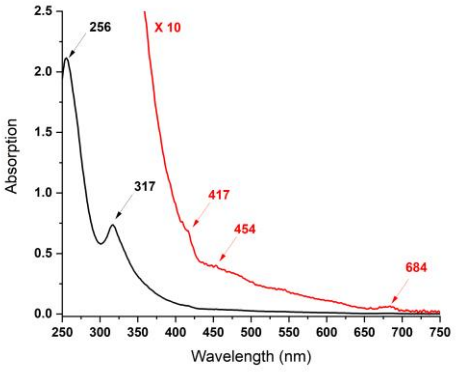

Figure S50. UV-vis absorption of compound **2m**.

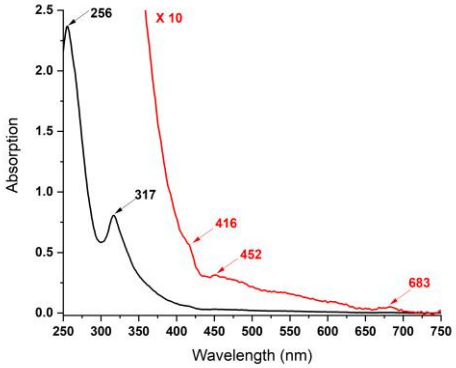

Figure S51. UV-vis absorption of compound **2n**.

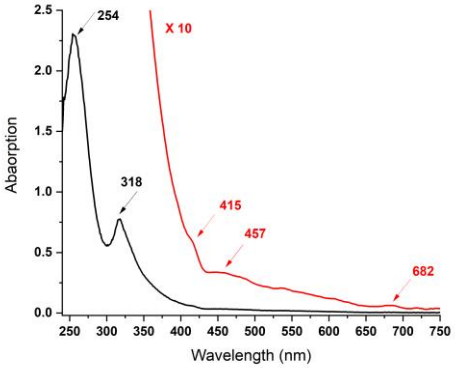

Figure S52. UV-vis absorption of compound **2o**.

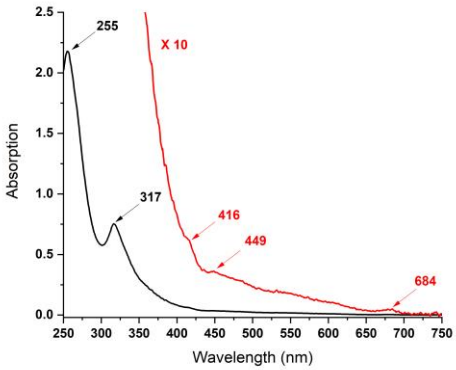

Figure S53. UV-vis absorption of compound **2r**.

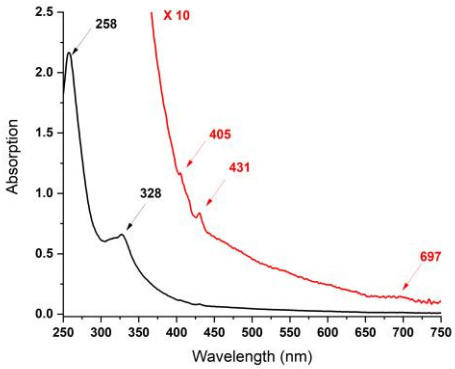

Figure S54. UV-vis absorption of compound **3a**.