

Electronic Supplementary Information

Palladium-Catalyzed Intramolecular Oxidative Annulation: Synthesis of *o*-Carboranoxazole

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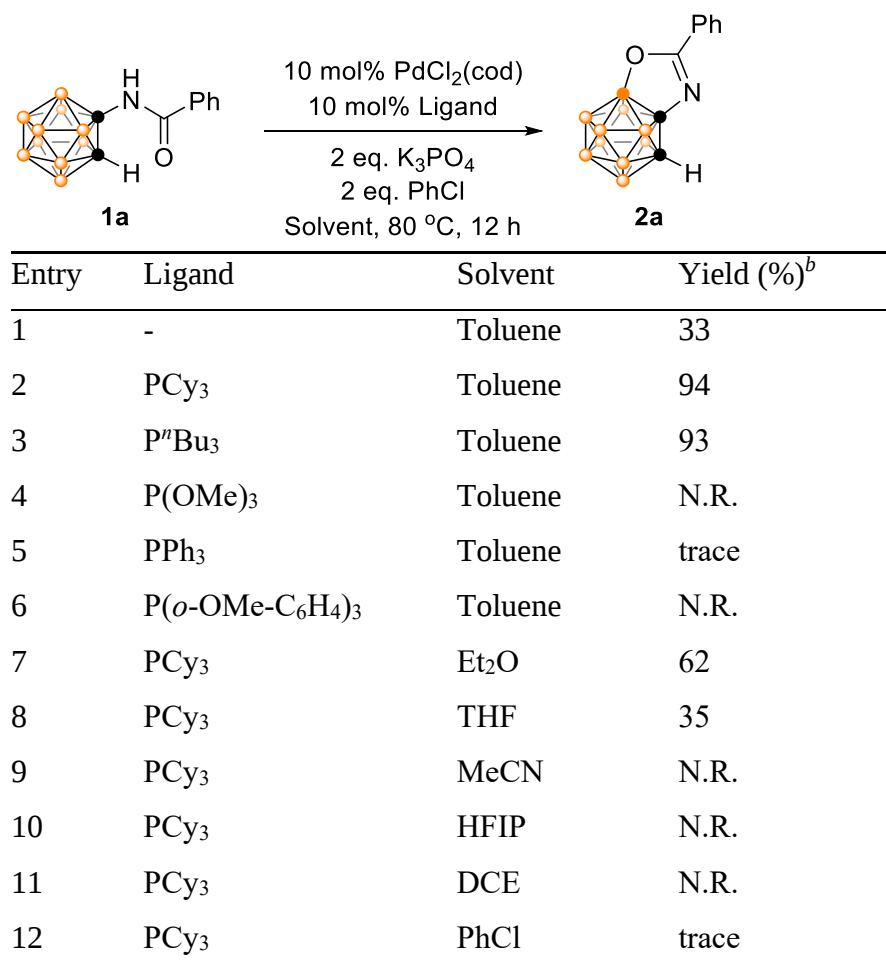
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General Procedures.

All reactions were carried out in oven-dried glassware under an atmosphere of dry N₂ with the rigid exclusion of air and moisture using standard Schlenk techniques or in a glovebox. Toluene was purified by solvent purification system prior to use. 1-Amino-*o*-carboranes were prepared according to literature procedures.¹ All other chemicals were purchased from either Aldrich or J&K Chemical Co. and used as received unless otherwise specified. ¹H NMR spectra were recorded on a Bruker/Agilent/Varian 400 spectrometer at 400 MHz. ¹³C{¹H}, ¹¹B and ¹⁹F NMR spectra were recorded on a Bruker/Agilent/Varian 400 spectrometer at 101, 128 and 376 MHz, respectively. All signals were reported in ppm unit with references to the residual solvent resonances of the deuterated solvents for proton and carbon chemical shifts, to external BF₃·OEt₂ (0.00) for boron chemical shifts and to external CFC₃ (0.00) for fluorine chemical shifts. Mass spectra were obtained on Thermo Fisher Scientific LTQ FTICR-MS spectrometer, Shanghai Institute of Organic Chemistry, CAS. The melting points of solid compounds were determined by a melting point apparatus without corrections (Shanghai INESA Physico-Optical Instrument Co., LTD).

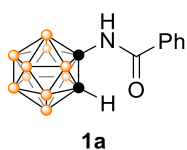
Table S1. Optimization of Reaction Solvents and Ligands^[a]



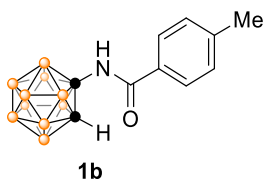
^a Reactions were conducted on 0.2 mmol scale in 4.0 mL of solvent. ^b Yield determined by ¹H NMR using 1,1,2,2-tetrachloroethane as the internal standard.

A Representative Procedure for the Preparation of Starting Materials 1a-z.

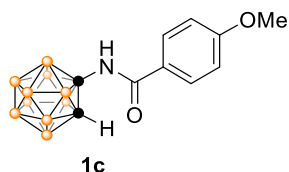
According to the literature procedure,² to a toluene solution (15 mL) of 1-amino-2-substituted-*o*-carborane (5.0 mmol) was added pyridine (1.2 mL, 15.0 mmol) and acyl chloride (15.0 mmol) successively under an atmosphere of dry nitrogen. The reaction flask was closed and the mixture was stirred at 80 °C for 12 h. After hydrolysis with water (20 mL) and extraction with diethyl ether (20 mL x 3), the organic portions were combined, dried over anhydrous Na₂SO₄ and concentrated to dryness in vacuo. The residue was subjected to flash column chromatography on silica gel (230-400 mesh) using *n*-hexane and ethyl acetate (3/1 in v/v) as eluent to give the products **1a-z**.



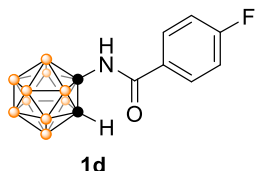
1a: White solid. 88% yield. M.p. = 162-163 °C. TLC: R_f = 0.30 (*n*-hexane:ethyl acetate = 10:1). ^1H NMR (CDCl_3 , 400 MHz): δ 7.66 (d, J = 8.0 Hz, 2H), 7.59 (t, J = 7.6 Hz, 1H), 7.48 (t, J = 7.6 Hz, 2H) (aromatic CH), 6.88 (s, 1H) (NH), 5.28 (s, 1H) (cage CH). $^{13}\text{C}\{^1\text{H}\}$ NMR (CDCl_3 , 101 MHz): δ 165.1 (C=O), 133.3, 131.9, 129.2, 127.2 (aromatic C), 78.8, 59.2 (cage C). ^{11}B NMR (CDCl_3 , 128 MHz): δ -4.1 (d, J = 153.6 Hz, 1B), -7.0 (d, J = 142.1 Hz, 1B), -10.9 (d, J = 149.8 Hz, 6B), -13.7 (d, J = 169.0 Hz, 2B) (BH). HRMS (DART) Calcd for $\text{C}_9\text{H}_{18}^{10}\text{B}_2^{11}\text{B}_8\text{NO}^+$ [$\text{M}+\text{H}^+$]: 264.2386, Found: 264.2386.



1b: White solid. 90% yield. M.p. = 156-157 °C. TLC: R_f = 0.32 (*n*-hexane:ethyl acetate = 10:1). ^1H NMR (CDCl_3 , 400 MHz): δ 7.55 (d, J = 8.0 Hz, 2H), 7.25 (d, J = 8.0 Hz, 2H) (aromatic CH), 6.95 (s, 1H) (NH), 5.24 (s, 1H) (cage CH), 2.41 (s, 3H) (CH_3). $^{13}\text{C}\{^1\text{H}\}$ NMR (CDCl_3 , 101 MHz): δ 165.8 (C=O), 144.1, 129.8, 129.5, 127.2 (aromatic C), 79.0, 59.8 (cage C), 21.7 (CH_3). ^{11}B NMR (CDCl_3 , 128 MHz): δ -4.1 (d, J = 153.6 Hz, 1B), -7.0 (d, J = 140.8 Hz, 1B), -10.9 (d, J = 148.5 Hz, 6B), -13.7 (d, J = 170.2 Hz, 2B) (BH). HRMS (ESI) Calcd for $\text{C}_{10}\text{H}_{18}^{10}\text{B}_2^{11}\text{B}_8\text{NO}^-$ [$\text{M}-\text{H}^+$]: 276.2397, Found: 276.2389.



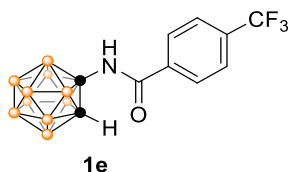
1c: White solid. 80% yield. M.p. = 150-151 °C. TLC: R_f = 0.15 (*n*-hexane:ethyl acetate = 10:1). ^1H NMR (CDCl_3 , 400 MHz): δ 7.64 (d, J = 9.2 Hz, 2H), 6.94 (d, J = 8.8 Hz, 2H) (aromatic CH), 6.79 (s, 1H) (NH), 5.28 (s, 1H) (cage CH), 3.86 (s, 3H) (OCH_3). $^{13}\text{C}\{^1\text{H}\}$ NMR (CDCl_3 , 101 MHz): δ 165.2 (C=O), 163.6, 129.3, 124.4, 114.4 (aromatic C), 79.1, 59.8 (cage C), 55.7 (OCH_3). ^{11}B NMR (CDCl_3 , 128 MHz): δ -4.1 (d, J = 144.6 Hz, 1B), -7.1 (d, J = 145.9 Hz, 1B), -10.9 (d, J = 148.5 Hz, 6B), -13.6 (d, J = 217.6 Hz, 2B) (BH). HRMS (ESI) Calcd for $\text{C}_{10}\text{H}_{18}^{10}\text{B}_2^{11}\text{B}_8\text{NO}_2^-$ [$\text{M}-\text{H}^+$]: 292.2355, Found: 292.2343.



1d

1d: White solid. 50% yield. M.p. = 164-165 °C. TLC: R_f = 0.31 (*n*-hexane:ethyl acetate = 10:1). ^1H NMR (CDCl_3 , 400 MHz): δ 7.69 (dd, J = 8.4, 4.8 Hz, 2H), 7.28 (t, J = 8.4 Hz, 2H) (aromatic CH), 6.84 (s, 1H) (NH), 5.24 (s, 1H) (cage CH).

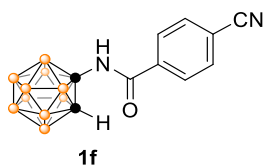
$^{13}\text{C}\{^1\text{H}\}$ NMR (CDCl_3 , 101 MHz): δ 164.7 (C=O), 165.7 (d, $^1J_{\text{C-F}}$ = 255.6 Hz), 129.9 (d, $^3J_{\text{C-F}}$ = 9.1 Hz), 128.6 (d, $^4J_{\text{C-F}}$ = 3.0 Hz), 116.4 (d, $^2J_{\text{C-F}}$ = 22.1 Hz) (aromatic C), 78.7, 59.7 (cage C). ^{11}B NMR (CDCl_3 , 128 MHz): δ -4.0 (d, J = 152.3 Hz, 1B), -6.9 (d, J = 147.2 Hz, 1B), -10.8 (d, J = 148.5 Hz, 6B), -13.6 (d, J = 175.4 Hz, 2B) (BH). ^{19}F NMR (377 MHz, CDCl_3): δ -104.6 (m, 1F). HRMS (ESI) Calcd for $\text{C}_9\text{H}_{15}^{10}\text{B}_2^{11}\text{B}_8\text{FNO}^-$ [M-H $^+$]: 280.2146, Found: 280.2139.



1e

1e: White solid. 78% yield. M.p. = 184-185 °C. TLC: R_f = 0.40 (*n*-hexane:ethyl acetate = 10:1). ^1H NMR (400 MHz, acetone- d_6): δ 7.78 (d, J = 8.4 Hz, 2H), 7.73 (d, J = 8.0 Hz, 2H) (aromatic CH), 6.97 (s, 1H) (NH), 5.22 (s, 1H) (cage CH).

$^{13}\text{C}\{^1\text{H}\}$ NMR (CDCl_3 , 101 MHz): δ 164.8 (C=O), 135.7, 134.8 (q, $^2J_{\text{C-F}}$ = 32.2 Hz), 127.8, 126.2 (q, $^3J_{\text{C-F}}$ = 4.0 Hz) (aromatic C), 123.4 (q, $^1J_{\text{C-F}}$ = 272.7 Hz) (CF_3), 78.4, 59.8 (cage C). ^{11}B NMR (CDCl_3 , 128 MHz): δ -3.9 (d, J = 156.2 Hz, 1B), -6.7 (d, J = 149.8 Hz, 1B), -10.8 (d, J = 145.9 Hz, 6B), -13.6 (d, J = 177.9 Hz, 2B) (BH). ^{19}F NMR (377 MHz, CDCl_3): δ -63.2 (s, 3F). HRMS (ESI) Calcd for $\text{C}_{10}\text{H}_{15}^{10}\text{B}_2^{11}\text{B}_8\text{F}_3\text{NO}^-$ [M-H $^+$]: 330.2114, Found: 330.2108.

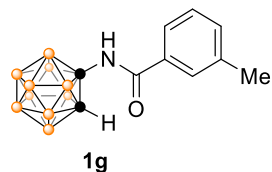


1f

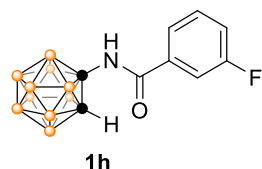
1f: White solid. 92% yield. M.p. = 159-160 °C. TLC: R_f = 0.10 (*n*-hexane:ethyl acetate = 10:1). ^1H NMR (400 MHz, acetone- d_6): δ 9.50 (s, 1H) (NH), 7.98 (d, J = 8.0 Hz, 2H), 7.91 (d, J = 8.4 Hz, 2H) (aromatic CH), 5.42 (s, 1H) (cage CH).

$^{13}\text{C}\{^1\text{H}\}$ NMR (acetone- d_6 , 101 MHz): δ 165.2 (C=O), 137.2, 132.3, 128.7, 117.7, 115.6 (aromatic C and CN), 79.9, 63.8 (cage C). ^{11}B NMR (THF, 128 MHz): δ -4.3 (d, J = 147.2 Hz, 1B), -6.9 (m, 1B), -11.1 (d, J = 152.3 Hz, 6B), -13.8 (m, 2B) (BH). HRMS (ESI) Calcd for

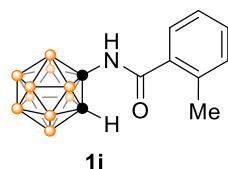
$\text{C}_{10}\text{H}_{15}^{10}\text{B}_2^{11}\text{B}_8\text{N}_2\text{O}^- [\text{M-H}^+]$: 287.2193, Found: 287.2186.



1g: White solid. 92% yield. M.p. = 157-159 °C. TLC: R_f = 0.35 (*n*-hexane:ethyl acetate = 10:1). ^1H NMR (CDCl_3 , 400 MHz): δ 7.47 (s, 1H), 7.44 (d, J = 7.2 Hz, 1H), 7.37 (m, 2H) (aromatic *CH*), 6.86 (s, 1H) (*NH*), 5.27 (s, 1H) (cage *CH*), 2.41 (s, 3H) (CH_3). $^{13}\text{C}\{^1\text{H}\}$ NMR (CDCl_3 , 101 MHz): δ 166.1 (C=O), 139.2, 134.0, 132.4, 129.0, 127.9, 124.2 (aromatic *C*), 78.9, 59.8 (cage *C*), 21.4 (CH_3). ^{11}B NMR (CDCl_3 , 128 MHz): δ -4.1 (d, J = 149.8 Hz, 1B), -7.1 (d, J = 139.5 Hz, 1B), -10.9 (d, J = 152.3 Hz, 6B), -13.7 (d, J = 171.5 Hz, 2B) (*BH*). HRMS (DART) Calcd for $\text{C}_{10}\text{H}_{20}^{10}\text{B}_2^{11}\text{B}_8\text{NO}^+ [\text{M}+\text{H}^+]$: 278.2543, Found: 278.2543.

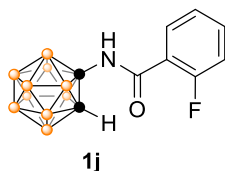


1h: White solid. 82% yield. M.p. = 147-148 °C. TLC: R_f = 0.30 (*n*-hexane:ethyl acetate = 10:1). ^1H NMR (CDCl_3 , 400 MHz): δ 7.43 (m, 3H), 7.30 (m, 1H) (aromatic *CH*), 6.91 (s, 1H) (*NH*), 5.22 (s, 1H) (cage *CH*). $^{13}\text{C}\{^1\text{H}\}$ NMR (CDCl_3 , 101 MHz): δ 164.6 (d, $^4J_{\text{C-F}}$ = 3.0 Hz) (C=O), 162.9 (d, $^1J_{\text{C-F}}$ = 249.6 Hz), 134.5 (d, $^3J_{\text{C-F}}$ = 7.0 Hz), 131.0 (d, $^3J_{\text{C-F}}$ = 8.1 Hz), 122.6 (d, $^4J_{\text{C-F}}$ = 3.0 Hz), 120.4 (d, $^2J_{\text{C-F}}$ = 21.1 Hz), 114.8 (d, $^2J_{\text{C-F}}$ = 23.1 Hz) (aromatic *C*) 78.5, 59.7 (cage *C*). ^{11}B NMR (CDCl_3 , 128 MHz): δ -4.0 (d, J = 142.1 Hz, 1B), -6.7 (d, J = 151.0 Hz, 1B), -10.8 (d, J = 151.0 Hz, 6B), -13.6 (d, J = 169.0 Hz, 2B) (*BH*). ^{19}F NMR (377 MHz, CDCl_3): δ -110.1 (m, 1F). HRMS (ESI) Calcd for $\text{C}_9\text{H}_{15}^{10}\text{B}_2^{11}\text{B}_8\text{FNO}^- [\text{M-H}^+]$: 280.2146, Found: 280.2139.

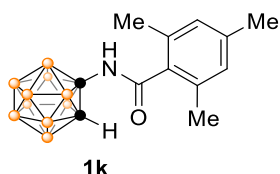


1i: White solid. 91% yield. M.p. = 157-159 °C. TLC: R_f = 0.30 (*n*-hexane:ethyl acetate = 10:1). ^1H NMR (CDCl_3 , 400 MHz): δ 7.43 (m, 1H), 7.30 (m, 3H) (aromatic *CH*), 6.74 (s, 1H) (*NH*), 5.32 (s, 1H) (cage *CH*), 2.44 (s, 3H) (CH_3). $^{13}\text{C}\{^1\text{H}\}$ NMR (CDCl_3 , 101 MHz): δ 168.1 (C=O), 136.7, 133.8, 131.7, 131.5, 126.7, 126.3 (aromatic *C*), 78.6, 59.4 (cage *C*), 19.8 (CH_3). ^{11}B NMR (CDCl_3 , 128 MHz): δ -4.1 (d, J = 151.0

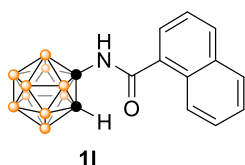
Hz, 1B), -7.0 (d, $J = 143.4$ Hz, 1B), -10.9 (d, $J = 147.2$ Hz, 6B), -13.6 (d, $J = 166.4$ Hz, 2B) (BH). HRMS (ESI) Calcd for $C_{10}H_{18}^{10}B_2^{11}B_8NO^-$ $[M-H^+]$: 276.2397, Found: 276.2389.



1j: White solid. 65% yield. M.p. = 121-122 °C. TLC: $R_f = 0.30$ (*n*-hexane:ethyl acetate = 10:1). 1H NMR ($CDCl_3$, 400 MHz): δ 8.01 (td, $J = 8.0, 2.0$ Hz, 1H), 7.57 (m, 1H), 7.31 (t, $J = 7.6$ Hz, 1H), 7.16 (dd, $J = 12.8, 8.4$ Hz, 1H) (aromatic CH), 7.64 (s, 1H) (NH), 5.18 (s, 1H) (cage CH). $^{13}C\{^1H\}$ NMR ($CDCl_3$, 101 MHz): δ 161.7 (d, $^3J_{C-F} = 3.0$ Hz) (C=O), 160.4 (d, $^1J_{C-F} = 247.6$ Hz), 135.2 (d, $^3J_{C-F} = 9.1$ Hz), 132.1 (d, $^4J_{C-F} = 1.0$ Hz), 125.5 (d, $^3J_{C-F} = 3.0$ Hz), 119.0 (d, $^2J_{C-F} = 10.1$ Hz), 116.5 (d, $^2J_{C-F} = 25.2$ Hz) (aromatic C), 78.4, 60.3 (cage C). ^{11}B NMR ($CDCl_3$, 128 MHz): δ -3.9 (d, $J = 149.8$ Hz, 1B), -6.8 (d, $J = 145.9$ Hz, 1B), -10.8 (d, $J = 151.0$ Hz, 6B), -13.7 (d, $J = 172.8$ Hz, 2B) (BH). ^{19}F NMR (377 MHz, $CDCl_3$): δ -112.6 (m, 1F). HRMS (ESI) Calcd for $C_9H_{15}^{10}B_2^{11}B_8FNO^-$ $[M-H^+]$: 280.2146, Found: 280.2139.

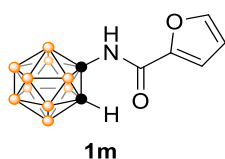


1k: White solid. 20% yield. M.p. = 231-232 °C. TLC: $R_f = 0.47$ (*n*-hexane:ethyl acetate = 10:1). 1H NMR ($CDCl_3$, 400 MHz): δ 6.85 (s, 2H) (aromatic CH), 6.54 (s, 1H) (NH), 5.41 (s, 1H) (cage CH), 2.28 (s, 3H), 2.22 (s, 6H) (CH_3). $^{13}C\{^1H\}$ NMR ($CDCl_3$, 101 MHz) δ 169.4 (C=O), 140.1, 134.1, 132.5, 128.6 (aromatic C), 78.3, 59.2 (cage C) 21.3, 18.9 (CH_3). ^{11}B NMR ($CDCl_3$, 128 MHz): δ -4.2 (d, $J = 151.0$ Hz, 1B), -6.9 (d, $J = 134.4$ Hz, 1B), -10.8 (d, $J = 143.4$ Hz, 6B), -13.6 (d, $J = 203.5$ Hz, 2B) (BH). HRMS (ESI) Calcd for $C_{12}H_{22}^{10}B_2^{11}B_8NO^-$ $[M-H^+]$: 304.2710, Found: 304.2704.

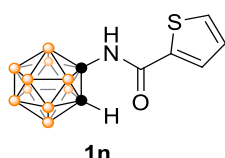


1l: White solid. 85% yield. M.p. = 188-189 °C. TLC: $R_f = 0.25$ (*n*-hexane:ethyl acetate = 10:1). 1H NMR ($CDCl_3$, 400 MHz): δ 8.13 (d, $J = 6.8$ Hz, 1H), 7.99 (d, $J = 8.0$ Hz, 1H), 7.90 (d, $J = 7.2$ Hz, 1H), 7.58 (m, 3H), 7.48 (t, $J = 7.2$ Hz, 1H) (aromatic

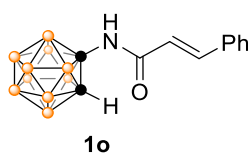
CH), 6.84 (s, 1H) (NH), 5.40 (s, 1H) (cage CH). $^{13}\text{C}\{^1\text{H}\}$ NMR (CDCl_3 , 101 MHz): δ 167.8 (C=O), 133.7, 132.4, 131.5, 129.7, 128.8, 128.1, 127.1, 125.7, 124.6, 124.4 (aromatic C), 78.6, 59.6 (cage C). ^{11}B NMR (CDCl_3 , 128 MHz): δ -5.0 (d, J = 145.9 Hz, 1B), -7.9 (d, J = 152.3 Hz, 1B), -11.9 (d, J = 129.3 Hz, 6B), -14.7 (d, J = 181.8 Hz, 2B) (BH). HRMS (ESI) Calcd for $\text{C}_{13}\text{H}_{18}^{10}\text{B}_2^{11}\text{B}_8\text{NO}^-$ $[\text{M}-\text{H}^+]$: 312.2397, Found: 312.2395.



1m: White solid. 82% yield. M.p. = 132-133 °C. TLC: R_f = 0.10 (n -hexane:ethyl acetate = 10:1). ^1H NMR (CDCl_3 , 400 MHz): δ 7.50 (d, J = 1.6 Hz, 1H), 7.20 (d, J = 3.6 Hz, 1H), 6.56 (dd, J = 3.6, 2.0 Hz, 1H) (aromatic CH), 7.12 (s, 1H) (NH), 5.11 (s, 1H) (cage CH). $^{13}\text{C}\{^1\text{H}\}$ NMR (CDCl_3 , 101 MHz): δ 155.9 (C=O), 145.5, 145.4, 145.4, 117.4, 113.2 (aromatic C), 78.3, 60.1 (cage C). ^{11}B NMR (CDCl_3 , 128 MHz): δ -4.0 (d, J = 151.0 Hz, 1B), -6.9 (d, J = 145.9 Hz, 1B), -10.8 (d, J = 148.5 Hz, 6B), -13.7 (d, J = 172.8 Hz, 2B) (BH). HRMS (ESI) Calcd for $\text{C}_7\text{H}_{14}^{10}\text{B}_2^{11}\text{B}_8\text{NO}_2^-$ $[\text{M}-\text{H}^+]$: 252.2033, Found: 252.2025.

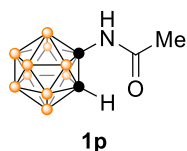


1n: White solid. 90% yield. M.p. = 151-152 °C. TLC: R_f = 0.15 (n -hexane:ethyl acetate = 10:1). ^1H NMR (CDCl_3 , 400 MHz): δ 7.61 (m, 1H), 7.50 (m, 1H), 7.12 (m, 1H) (aromatic CH), 6.79 (s, 1H) (NH), 5.18 (s, 1H) (cage CH). $^{13}\text{C}\{^1\text{H}\}$ NMR (CDCl_3 , 101 MHz): δ 160.0 (C=O), 136.3, 132.8, 129.8, 128.3 (aromatic C), 78.6, 60.0 (cage C). ^{11}B NMR (CDCl_3 , 128 MHz): δ -4.0 (d, J = 152.3 Hz, 1B), -6.9 (d, J = 148.5 Hz, 1B), -10.8 (d, J = 151.0 Hz, 6B), -13.6 (d, J = 167.7 Hz, 2B) (BH). HRMS (ESI) Calcd for $\text{C}_7\text{H}_{14}^{10}\text{B}_2^{11}\text{B}_8\text{NOS}^-$ $[\text{M}-\text{H}^+]$: 268.1805, Found: 268.1798.

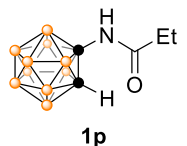


1o: White solid. 88% yield. M.p. = 116-117 °C. TLC: R_f = 0.23 (n -hexane:ethyl acetate = 10:1). ^1H NMR (CDCl_3 , 400 MHz): δ 7.67 (d, J = 16.0 Hz, 1H) (alkenyl CH), 7.46 (m, 2H), 7.37 (m, 3H) (aromatic CH), 6.40 (d, J = 16.0 Hz, H) (alkenyl CH), 5.11 (s, 1H) (cage CH).

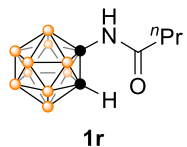
$^{13}\text{C}\{^1\text{H}\}$ NMR (CDCl_3 , 101 MHz): δ 164.3 ($\text{C}=\text{O}$), 145.2, 133.8, 131.0, 129.2, 128.3, 118.1 (aromatic C and alkenyl C), 78.8, 59.9 (cage C). ^{11}B NMR (CDCl_3 , 128 MHz): δ -4.0 (d, J = 147.2 Hz, 1B), -6.8 (d, J = 138.2 Hz, 1B), -10.8 (d, J = 151.0 Hz, 6B), -13.6 (d, J = 170.2 Hz, 2B) (BH). HRMS (ESI) Calcd for $\text{C}_{11}\text{H}_{18}^{10}\text{B}_2^{11}\text{B}_8\text{NO}^-$ [$\text{M}-\text{H}^+$]: 288.2397, Found: 288.2394.



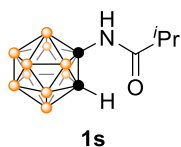
1p: is a known compound and its ^1H NMR data are the same as the reported one.² White solid. 76% yield. M.p. = 178-179 °C. ^1H NMR (CDCl_3 , 400 MHz): 6.50 (s, 1H) (NH), 5.07 (s, 1H) (cage CH), 1.99 (s, 3H) (CH_3).



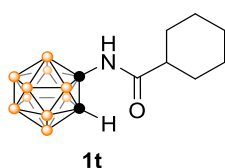
1q: White solid. 88% yield. M.p. = 129-131 °C. TLC: R_f = 0.10 (n -hexane:ethyl acetate = 10:1). ^1H NMR (CDCl_3 , 400 MHz): δ 6.40 (s, 1H) (NH), 5.09 (s, 1H) (cage CH), 2.18 (q, J = 7.6 Hz, 2H) (CH_2), 1.12 (t, J = 7.6 Hz, 3H) (CH_3). $^{13}\text{C}\{^1\text{H}\}$ NMR (CDCl_3 , 101 MHz): δ 172.2 ($\text{C}=\text{O}$), 78.5, 59.7 (cage C), 30.0 (CH_2), 9.1 (CH_3). ^{11}B NMR (CDCl_3 , 128 MHz): δ -4.1 (d, J = 147.2 Hz, 1B), -7.1 (d, J = 140.8 Hz, 1B), -11.0 (d, J = 151.0 Hz, 6B), -13.8 (d, J = 169.0 Hz, 2B) (BH). HRMS (ESI) Calcd for $\text{C}_5\text{H}_{16}^{10}\text{B}_2^{11}\text{B}_8\text{NO}^-$ [$\text{M}-\text{H}^+$]: 214.2241, Found: 214.2230.



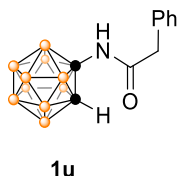
1r: White solid. 80% yield. M.p. = 116-117 °C. TLC: R_f = 0.16 (n -hexane:ethyl acetate = 10:1). ^1H NMR (CDCl_3 , 400 MHz): δ 6.57 (s, 1H) (NH), 5.08 (s, 1H) (cage CH), 2.13 (t, J = 7.2 Hz, 2H), 1.62 (m, 2H), 0.93 (t, J = 7.2 Hz, 3H) (alkyl H). $^{13}\text{C}\{^1\text{H}\}$ NMR (CDCl_3 , 101 MHz): δ 171.8 ($\text{C}=\text{O}$), 78.5, 59.8 (cage C), 38.7 (CH_2), 18.7 (CH_2), 13.5 (CH_3). ^{11}B NMR (CDCl_3 , 128 MHz): δ -4.2 (d, J = 147.2 Hz, 1B), -7.1 (d, J = 152.3 Hz, 1B), -11.0 (d, J = 147.2 Hz, 6B), -13.8 (d, J = 167.9 Hz, 2B) (BH). HRMS (DART) Calcd for $\text{C}_6\text{H}_{20}^{10}\text{B}_2^{11}\text{B}_8\text{NO}^-$ [$\text{M}+\text{H}^+$]: 230.2543, Found: 230.2541.



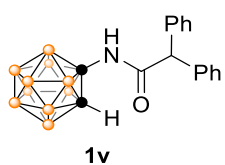
1s: White solid. 52% yield. M.p. = 151-152 °C. TLC: R_f = 0.18 (*n*-hexane:ethyl acetate = 10:1). ^1H NMR (CDCl_3 , 400 MHz): δ 6.31 (s, 1H) (NH), 5.14 (s, 1H) (cage CH), 2.26 (m, 1H), 1.12 (d, J = 6.8 Hz, 6H) (alkyl H). $^{13}\text{C}\{^1\text{H}\}$ NMR (CDCl_3 , 101 MHz): δ 175.5 (C=O), 78.6, 59.5 (cage C), 36.1 (CH), 19.1 (CH_3). ^{11}B NMR (CDCl_3 , 128 MHz): δ -4.2 (d, J = 144.6 Hz, 1B), -7.1 (d, J = 142.1 Hz, 1B), -11.0 (d, J = 152.3 Hz, 6B), -13.7 (d, J = 170.2 Hz, 2B) (BH). HRMS (ESI) Calcd for $\text{C}_6\text{H}_{18}^{10}\text{B}_2^{11}\text{B}_8\text{NO}^-$ [$\text{M}-\text{H}^+$]: 228.2397, Found: 228.2389.



1t: White solid. 88% yield. M.p. = 151-152 °C. TLC: R_f = 0.40 (*n*-hexane:ethyl acetate = 10:1). ^1H NMR (CDCl_3 , 400 MHz): δ 6.30 (s, 1H) (NH), 5.15 (s, 1H) (cage CH), 1.98 (m, 1H), 1.78 (m, 3H), 1.68 (m, 2H), 1.37 (m, 2H), 1.23 (m, 3H) (alkyl H). $^{13}\text{C}\{^1\text{H}\}$ NMR (CDCl_3 , 101 MHz): δ 174.7 (C=O), 78.7, 59.6 (cage C), 45.6 (CH), 29.2, 25.5, 25.4 (CH_2). ^{11}B NMR (CDCl_3 , 128 MHz): δ -4.3 (d, J = 145.9 Hz, 1B), -7.3 (d, J = 142.1 Hz, 1B), -11.1 (d, J = 152.3 Hz, 6B), -13.8 (d, J = 170.2 Hz, 2B) (BH). HRMS (ESI) Calcd for $\text{C}_9\text{H}_{22}^{10}\text{B}_2^{11}\text{B}_8\text{NO}^-$ [$\text{M}-\text{H}^+$]: 268.2710, Found: 268.2705.

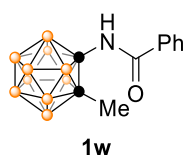


1u: White solid. 95% yield. M.p. = 153-154 °C. TLC: R_f = 0.18 (*n*-hexane:ethyl acetate = 10:1). ^1H NMR (CDCl_3 , 400 MHz): δ 7.37 (m, 3H), 7.18 (d, J = 7.6 Hz, 2H) (aromatic CH), 6.32 (s, 1H) (NH), 5.04 (s, 1H) (cage CH), 3.53 (s, 2H) (CH_2). $^{13}\text{C}\{^1\text{H}\}$ NMR (CDCl_3 , 101 MHz): δ 169.4 (C=O), 132.8, 129.6, 129.3, 128.4 (aromatic C), 78.4, 59.4 (cage C), 43.9 (CH_2). ^{11}B NMR (CDCl_3 , 128 MHz): δ -4.2 (d, J = 147.2 Hz, 1B), -7.1 (d, J = 140.8 Hz, 1B), -11.0 (d, J = 147.2 Hz, 6B), -13.8 (d, J = 167.8 Hz, 2B) (BH). HRMS (ESI) Calcd for $\text{C}_{10}\text{H}_{18}^{10}\text{B}_2^{11}\text{B}_8\text{NO}^-$ [$\text{M}-\text{H}^+$]: 276.2397, Found: 276.2392.

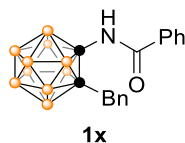


1v: White solid. 31% yield. M.p. = 126-128 °C. TLC: R_f = 0.29 (*n*-hexane:ethyl acetate = 10:1). ^1H NMR (CDCl_3 , 400 MHz): δ 7.36 (m, 6H), 7.18 (d, J = 6.8 Hz, 4H) (aromatic CH), 6.49 (s, 1H)

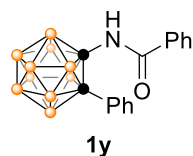
(NH), 5.13 (s, 1H) (cage CH), 4.82 (s, 1H) (CH). $^{13}\text{C}\{^1\text{H}\}$ NMR (CDCl_3 , 101 MHz): δ 170.7 (C=O), 137.6, 129.3, 128.7, 128.2 (aromatic C), 78.5, 59.3 (cage C), 59.1 (CH). ^{11}B NMR (CDCl_3 , 128 MHz): δ -4.1 (d, J = 148.5 Hz, 1B), -7.0 (d, J = 137.0 Hz, 1B), -10.9 (d, J = 143.4 Hz, 6B), -13.7 (d, J = 169.0 Hz, 2B) (BH). HRMS (ESI) Calcd for $\text{C}_{16}\text{H}_{22}^{10}\text{B}_2^{11}\text{B}_8\text{NO}^- [\text{M}-\text{H}^+]$: 352.2710, Found: 352.2703.



1w: White solid. 87% yield. M.p. = 147-148 °C. TLC: R_f = 0.17 (*n*-hexane:ethyl acetate = 10:1). ^1H NMR (CDCl_3 , 400 MHz): δ 8.12 (d, J = 7.2 Hz, 1H), 7.74 (d, J = 8.0 Hz, 1H), 7.62 (m, 1H), 7.50 (m, 2H) (aromatic CH), 7.05 (s, 1H) (NH), 2.04 (s, 3H) (CH_3). $^{13}\text{C}\{^1\text{H}\}$ NMR (CDCl_3 , 101 MHz): δ 165.5 (C=O), 133.3, 132.7, 129.3, 127.3 (aromatic C), 82.2, 78.8 (cage C), 22.5 (CH_3). ^{11}B NMR (CDCl_3 , 128 MHz): δ -7.1 (d, J = 143.4 Hz, 2B), -12.0 (m, 8B) (BH). HRMS (ESI) Calcd for $\text{C}_{10}\text{H}_{18}^{10}\text{B}_2^{11}\text{B}_8\text{NO}^- [\text{M}-\text{H}^+]$: 276.2397, Found: 276.2390.

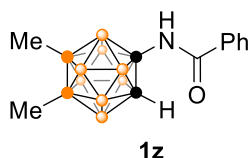


1x: White solid. 45% yield. M.p. = 149-150 °C. TLC: R_f = 0.18 (*n*-hexane:ethyl acetate = 10:1). ^1H NMR (CDCl_3 , 400 MHz): δ 7.79 (d, J = 7.2 Hz, 2H), 7.64 (t, J = 7.2 Hz, 1H), 7.53 (t, J = 8.0 Hz, 2H), 7.31 (m, 3H) (aromatic CH), 7.18 (s, 1H) (NH), 7.13 (m, 2H) (aromatic CH), 3.49 (s, 2H) (CH_2). $^{13}\text{C}\{^1\text{H}\}$ NMR (CDCl_3 , 101 MHz): δ 165.5 (C=O), 134.9, 133.4, 132.6, 130.3, 129.3, 128.8, 128.7, 128.2, 127.3 (aromatic C), 83.8, 83.4 (cage C), 40.7 (CH_2). ^{11}B NMR (CDCl_3 , 128 MHz): δ -5.0 (d, J = 90.9 Hz, 1B), -5.7 (d, J = 101.1 Hz, 1B), -11.4 (d, J = 134.4 Hz, 8B) (BH). HRMS (DART) Calcd for $\text{C}_{16}\text{H}_{24}^{10}\text{B}_2^{11}\text{B}_8\text{NO}^+ [\text{M}+\text{H}^+]$: 354.2856, Found: 354.2855.



1y: White solid. 85% yield. M.p. = 151-152 °C. TLC: R_f = 0.18 (*n*-hexane:ethyl acetate = 10:1). ^1H NMR (CDCl_3 , 400 MHz): δ 7.71 (d, J = 8.0 Hz, 2H), 7.47 (q, J = 7.6 Hz, 2H), 7.40 (m, 2H), 7.28 (m, 2H), 7.10 (d, J = 7.6 Hz, 2H) (aromatic CH), 6.91 (s, 1H) (NH). $^{13}\text{C}\{^1\text{H}\}$ NMR (CDCl_3 , 101 MHz): δ 166.1 (C=O), 133.0, 132.9, 131.4, 131.1, 130.4, 129.1, 129.0,

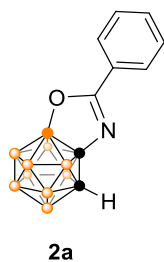
127.0 (aromatic C), 88.0, 85.5 (cage C). ^{11}B NMR (CDCl_3 , 128 MHz): δ -3.7 (d, J = 144.6 Hz, 1B), -4.8 (d, J = 137.0 Hz, 1B), -10.8 (m, 8B) (*BH*). HRMS (ESI) Calcd for $\text{C}_{15}\text{H}_{20}^{10}\text{B}_2^{11}\text{B}_8\text{NO}^-$ [$\text{M}-\text{H}^+$]: 338.2554, Found: 338.2548.



1z: White solid. 60% yield. M.p. = 156-157 °C. TLC: R_f = 0.29 (*n*-hexane:ethyl acetate = 10:1). ^1H NMR (CDCl_3 , 400 MHz): δ 7.66 (d, J = 7.2 Hz, 2H), 7.58 (t, J = 7.6 Hz, 1H), 7.47 (m, 2H) (aromatic *CH*), 6.81 (s, 1H) (*NH*), 5.05 (s, 1H) (cage *CH*), 0.23 (s, 3H), 0.20 (s, 3H) (cage B- CH_3). $^{13}\text{C}\{^1\text{H}\}$ NMR (CDCl_3 , 101 MHz): δ 165.9 ($\text{C}=\text{O}$), 133.1, 132.6, 129.2, 127.2 (aromatic C), 72.9, 52.9 (cage C), the $\text{B}_{\text{cage}}-\text{C}$ were not observed. ^{11}B NMR (CDCl_3 , 128 MHz): δ -5.0 (s, 1B) (*BC*), -2.3 (s, 1B) (*BC*), -9.9 (d, J = 151.0 Hz, 2B), -12.1 (d, J = 171.5 Hz, 2B), -14.8 (d, J = 148.5 Hz, 4B) (*BH*). HRMS (DART) Calcd for $\text{C}_{11}\text{H}_{22}^{10}\text{B}_2^{11}\text{B}_8\text{NO}^+$ [$\text{M}+\text{H}^+$]: 292.2699, Found: 292.2699.

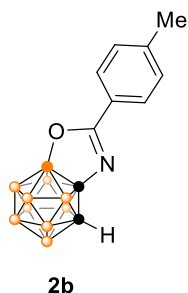
General procedure for the synthesis of 2.

To an oven-dried Schlenk flask equipped with a stir bar was sequentially added **1** (0.2 mmol), $\text{PdCl}_2(\text{cod})$ (4.3 mg, 0.015 mmol), PCy_3 (4.2 mg, 0.015 mmol), K_3PO_4 (85.0 mg, 0.4 mmol), PhCl (45.0 mg, 0.4 mmol), and toluene (4 mL). The flask was closed under an atmosphere of nitrogen, then stirred at 80 °C for 12 h. After hydrolysis with water (5 mL) and extraction with diethyl ether (10 mL x 3), the ether solutions were combined, dried over anhydrous Na_2SO_4 and concentrated to dryness in vacuo. The residue was subjected to flash column chromatography on silica gel (230-400 mesh) using *n*-hexane as eluent to give product **2**.

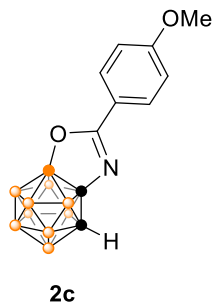


2a: White solid. 90% yield. M.p. = 126-127 °C. TLC: R_f = 0.22 (*n*-hexane:ethyl acetate = 10:1). ^1H NMR (CDCl_3 , 400 MHz): δ 8.08 (d, J = 8.0 Hz, 2H), 7.59 (t, J = 7.2 Hz, 1H), 7.48 (t, J = 8.0 Hz, 2H) (aromatic *CH*), 4.38 (s, 1H) (cage *CH*). $^{13}\text{C}\{^1\text{H}\}$ NMR (CDCl_3 , 101 MHz): δ 181.4 ($\text{C}=\text{N}$), 133.4, 128.9, 128.8, 128.7 (aromatic C),

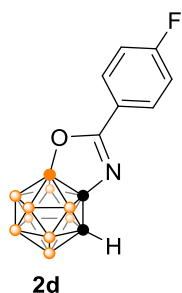
99.8, 56.8 (cage C). ^{11}B NMR (CDCl_3 , 128 MHz): δ 1.9 (s, 1B) (BO), -5.4 (d, J = 151.0 Hz, 1B), -10.2 (d, J = 171.5 Hz, 2B), -13.3 (d, J = 143.4 Hz, 2B), -14.1 (d, J = 120.3 Hz, 1B), -15.6 (d, J = 148.5 Hz, 1B), -16.6 (d, J = 96.0 Hz, 1B), -21.4 (d, J = 166.4 Hz, 1B) (BH). HRMS (ESI) Calcd for $\text{C}_9\text{H}_{16}^{10}\text{B}_2^{11}\text{B}_8\text{NO}^+$ [$\text{M}+\text{H}^+$]: 262.2230, Found: 262.2238.



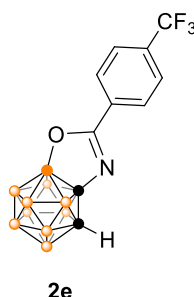
2b: White solid. 91% yield. M.p. = 182-183 °C. TLC: R_f = 0.22 (*n*-hexane:ethyl acetate = 10:1). ^1H NMR (CDCl_3 , 400 MHz): δ 7.95 (d, J = 8.4 Hz, 2H), 7.26 (d, J = 8.0 Hz, 2H) (aromatic CH), 4.35 (s, 1H) (cage CH), 2.42 (s, 3H) (CH_3). $^{13}\text{C}\{^1\text{H}\}$ NMR (CDCl_3 , 101 MHz): δ 181.7 (C=N), 144.2, 129.5, 128.8, 126.1 (aromatic C), 100.1, 56.9 (cage C), 21.9 (CH_3). ^{11}B NMR (CDCl_3 , 128 MHz): δ 1.9 (s, 1B) (BO), -5.5 (d, J = 152.3 Hz, 1B), -10.1 (d, J = 170.2 Hz, 2B), -13.4 (d, J = 135.7 Hz, 2B), -14.2 (d, J = 124.2 Hz, 1B), -15.7 (d, J = 156.2 Hz, 1B), -16.6 (d, J = 107.5 Hz, 1B), -21.4 (d, J = 166.4 Hz, 1B) (BH). HRMS (ESI) Calcd for $\text{C}_{10}\text{H}_{18}^{10}\text{B}_2^{11}\text{B}_8\text{NO}^+$ [$\text{M}+\text{H}^+$]: 276.2386, Found: 276.2388.



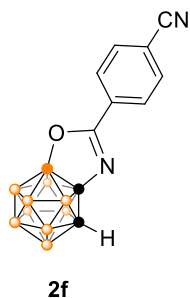
2c: White solid. 76% yield. M.p. = 188-190 °C. TLC: R_f = 0.1 (*n*-hexane:ethyl acetate = 10:1). ^1H NMR (CDCl_3 , 400 MHz): δ 8.01 (d, J = 8.0 Hz, 2H), 6.94 (d, J = 8.0 Hz, 2H) (aromatic CH), 4.34 (s, 1H) (cage CH), 3.87 (s, 3H) (OCH_3). $^{13}\text{C}\{^1\text{H}\}$ NMR (CDCl_3 , 101 MHz): δ 181.3 (C=N), 163.7, 130.8, 121.3, 114.1 (aromatic C), 100.3, 56.9 (cage C), 55.7 (OCH_3). ^{11}B NMR (acetone- d_6 , 128 MHz): δ 1.0 (s, 1B) (BO), -6.6 (d, J = 158.7 Hz, 1B), -11.0 (d, J = 171.5 Hz, 2B), -14.5 (d, J = 145.9 Hz, 2B), -15.3 (d, J = 113.9 Hz, 1B), -16.8 (d, J = 140.8 Hz, 1B), -17.6 (d, J = 99.8 Hz, 1B), -22.5 (d, J = 170.2 Hz, 1B) (BH). HRMS (ESI) Calcd for $\text{C}_{10}\text{H}_{18}^{10}\text{B}_2^{11}\text{B}_8\text{NO}_2^+$ [$\text{M}+\text{H}^+$]: 292.2335, Found: 292.2334.



2d: White solid. 90% yield. M.p. = 125-127 °C. TLC: R_f = 0.23 (*n*-hexane:ethyl acetate = 10:1). ^1H NMR (CDCl_3 , 400 MHz): δ 8.08 (dd, J = 8.8, 5.6 Hz, 2H), 7.14 (t, J = 8.4 Hz, 2H) (aromatic CH), 4.35 (s, 1H) (cage CH). $^{13}\text{C}\{^1\text{H}\}$ NMR (CDCl_3 , 101 MHz): δ 180.4 (C=N), 165.9 (d, $^1J_{\text{C-F}}$ = 254.6 Hz), 136.3 (d, $^3J_{\text{C-F}}$ = 9.1 Hz), 125.5 (d, $^4J_{\text{C-F}}$ = 3.0 Hz), 116.1 (d, $^2J_{\text{C-F}}$ = 22.1 Hz) (aromatic C), 56.9 (cage C). ^{11}B NMR (CDCl_3 , 128 MHz): δ 1.9 (s, 1B) (BO), -5.4 (d, J = 152.3 Hz, 1B), -10.2 (d, J = 171.5 Hz, 2B), -13.3 (d, J = 152.3 Hz, 2B), -14.1 (d, J = 111.4 Hz, 1B), -15.7 (d, J = 144.6 Hz, 1B), -16.6 (d, J = 111.4 Hz, 1B), -21.4 (d, J = 166.4 Hz, 1B) (BH). ^{19}F NMR (377 MHz, CDCl_3): δ -104.5 (m, 1F). HRMS (ESI) Calcd for $\text{C}_9\text{H}_{15}^{10}\text{B}_2^{11}\text{B}_8\text{FNO}^+$ [$\text{M}+\text{H}^+$]: 280.2135, Found: 280.2133.

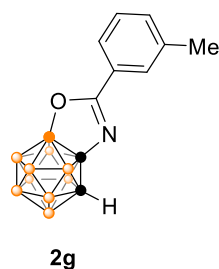


2e: White solid. 84% yield. M.p. = 109-111 °C. TLC: R_f = 0.28 (*n*-hexane:ethyl acetate = 10:1). ^1H NMR (CDCl_3 , 400 MHz): δ 8.19 (d, J = 8.4 Hz, 2H), 7.73 (d, J = 8.4 Hz, 2H) (aromatic CH), 4.38 (s, 1H) (cage CH). $^{13}\text{C}\{^1\text{H}\}$ NMR (CDCl_3 , 101 MHz): δ 179.9 (C=N), 134.8 (q, $^2J_{\text{C-F}}$ = 33.2 Hz), 131.9, 129.2, 125.9 (q, $^3J_{\text{C-F}}$ = 4.0 Hz) (aromatic C), 123.6 (q, $^1J_{\text{C-F}}$ = 272.7 Hz) (CF_3), 99.4, 57.0 (cage C). ^{11}B NMR (CDCl_3 , 128 MHz): δ 1.8 (s, 1B) (BO), -5.2 (d, J = 152.3 Hz, 1B), -10.4 (d, J = 171.5 Hz, 2B), -13.2 (d, J = 139.5 Hz, 2B), -14.0 (d, J = 130.6 Hz, 1B), -15.5 (d, J = 157.4 Hz, 1B), -16.5 (d, J = 112.6 Hz, 1B), -21.3 (d, J = 167.7 Hz, 1B) (BH). ^{19}F NMR (377 MHz, CDCl_3): δ -63.2 (s, 3F). HRMS (ESI) Calcd for $\text{C}_{10}\text{H}_{15}^{10}\text{B}_2^{11}\text{B}_8\text{F}_3\text{NO}^+$ [$\text{M}+\text{H}^+$]: 330.2103, Found: 330.2109.

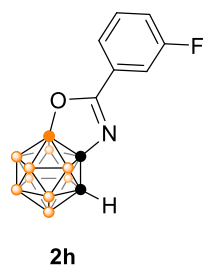


2f: White solid. 74% yield. M.p. = 179-181 °C. TLC: R_f = 0.1 (*n*-hexane:ethyl acetate = 10:1). ^1H NMR (CDCl_3 , 400 MHz): δ 8.18 (d, J = 8.0 Hz, 2H), 7.73 (d, J = 8.0 Hz, 2H) (aromatic CH), 4.40 (s, 1H) (cage CH). $^{13}\text{C}\{^1\text{H}\}$ NMR (CDCl_3 , 101 MHz): δ 179.4 (C=N), 132.6, 132.4, 129.2, 117.9, 116.6 (aromatic C and CN),

99.2, 57.0 (cage C). ^{11}B NMR (CDCl_3 , 128 MHz): δ 1.8 (s, 1B) (BO), -5.2 (d, J = 152.3 Hz, 1B), -10.4 (d, J = 172.8 Hz, 2B), -13.1 (d, J = 119.0 Hz, 2B), -13.9 (d, J = 148.5 Hz, 1B), -15.5 (d, J = 162.6 Hz, 1B), -16.4 (d, J = 108.8 Hz, 1B), -21.2 (d, J = 166.4 Hz, 1B) (BH). HRMS (DART) Calcd for $\text{C}_{10}\text{H}_{15}^{10}\text{B}_2^{11}\text{B}_8\text{N}_2\text{O}^+$ $[\text{M}+\text{H}^+]$: 287.2182, Found: 287.2182.

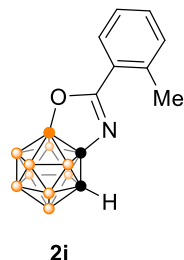


2g: White solid. 94% yield. M.p. = 117-118 °C. TLC: R_f = 0.24 (*n*-hexane:ethyl acetate = 10:1). ^1H NMR (CDCl_3 , 400 MHz): δ 7.90 (s, 1H), 7.87 (d, J = 7.6 Hz, 1H), 7.39 (d, J = 8.0 Hz, 1H), 7.35 (t, J = 7.2 Hz, 1H) (aromatic CH), 4.36 (s, 1H) (cage CH), 2.41 (s, 3H) (CH_3). $^{13}\text{C}\{^1\text{H}\}$ NMR (CDCl_3 , 101 MHz): δ 181.7 (C=N), 138.7, 134.2, 129.2, 128.8, 128.6, 125.9 (aromatic C), 99.9, 56.9 (cage C), 21.4 (CH_3). ^{11}B NMR (CDCl_3 , 128 MHz): δ 1.9 (s, 1B) (BO), -5.4 (d, J = 152.3 Hz, 1B), -10.2 (d, J = 171.5 Hz, 2B), -13.4 (d, J = 151.0 Hz, 2B), -14.1 (d, J = 111.4 Hz, 1B), -15.7 (d, J = 149.8 Hz, 1B), -16.6 (d, J = 102.4 Hz, 1B), -21.4 (d, J = 166.4 Hz, 1B) (BH). HRMS (ESI) Calcd for $\text{C}_{10}\text{H}_{18}^{10}\text{B}_2^{11}\text{B}_8\text{NO}^+$ $[\text{M}+\text{H}^+]$: 276.2386, Found: 276.2393.

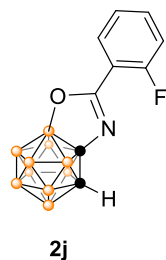


2h: White solid. 90% yield. M.p. = 119-121 °C. TLC: R_f = 0.23 (*n*-hexane:ethyl acetate = 10:1). ^1H NMR (CDCl_3 , 400 MHz): δ 7.87 (d, J = 8.0 Hz, 1H), 7.77 (dt, J = 9.6, 2.4 Hz, 1H), 7.45 (td, J = 8.0, 5.6 Hz, 1H), 7.28 (td, J = 8.4, 2.8 Hz, 1H) (aromatic CH), 4.37 (s, 1H) (cage CH). $^{13}\text{C}\{^1\text{H}\}$ NMR (CDCl_3 , 101 MHz): δ 180.2 (d, $^4J_{\text{C-F}}$ = 3.0 Hz) (C=N), 162.7 (d, $^1J_{\text{C-F}}$ = 247.6 Hz), 130.7 (d, $^3J_{\text{C-F}}$ = 8.1 Hz), 130.6 (d, $^4J_{\text{C-F}}$ = 8.1 Hz), 124.5 (d, $^3J_{\text{C-F}}$ = 11.1 Hz), 120.4 (d, $^2J_{\text{C-F}}$ = 21.1 Hz), 115.8 (d, $^2J_{\text{C-F}}$ = 23.1 Hz) (aromatic C), 99.5, 56.9 (cage C). ^{11}B NMR (CDCl_3 , 128 MHz): δ 1.8 (s, 1B) (BO), -5.3 (d, J = 151.0 Hz, 1B), -10.3 (d, J = 174.1 Hz, 2B), -13.3 (d, J = 136.9 Hz, 2B), -14.1 (d, J = 133.1 Hz, 1B), -15.6 (d, J = 152.3 Hz, 1B), -16.5 (d, J = 115.2 Hz, 1B), -21.3 (d, J = 167.7 Hz, 1B) (BH). ^{19}F NMR (377 MHz, CDCl_3): δ -111.6

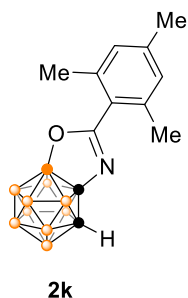
(m, 1F). HRMS (ESI) Calcd for $C_9H_{15}^{10}B_2^{11}B_8FNO^+$ $[M+H]^+$: 280.2146, Found: 280.2139.



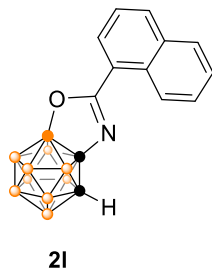
2i: White solid. 88% yield. M.p. = 135-137 °C. TLC: R_f = 0.32 (*n*-hexane:ethyl acetate = 10:1). 1H NMR ($CDCl_3$, 400 MHz): δ 7.87 (m, 2H), 7.37 (m, 2H), (aromatic *CH*), 4.36 (s, 1H) (cage *CH*), 2.41 (s, 3H) (CH_3). $^{13}C\{^1H\}$ NMR ($CDCl_3$, 101 MHz): δ 182.3 ($C=N$), 139.7, 132.3, 131.9, 130.5, 128.2, 126.1 (aromatic C), 99.9, 57.0 (cage C), 22.3 (CH_3). ^{11}B NMR ($CDCl_3$, 128 MHz): δ 1.5 (s, 1B) (*BO*), -5.4 (d, J = 147.2 Hz, 1B) -10.3, (d, J = 171.5 Hz, 2B), -13.4 (d, J = 138.2 Hz, 2B), -14.2 (d, J = 122.9 Hz, 1B), -15.6 (d, J = 161.3 Hz, 1B), -16.6 (d, J = 153.6 Hz, 1B), -21.5 (d, J = 167.7 Hz, 1B) (*BH*). HRMS (ESI) Calcd for $C_{10}H_{18}^{10}B_2^{11}B_8NO^+$ $[M+H]^+$: 276.2397, Found: 276.2390.



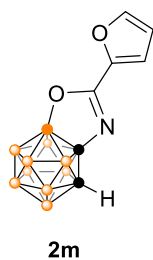
2j: White solid. 86% yield. M.p. = 90-92 °C. TLC: R_f = 0.15 (*n*-hexane:ethyl acetate = 10:1). 1H NMR ($CDCl_3$, 400 MHz): δ 8.05 (td, J = 7.6, 1.6 Hz, 1H), 7.56 (m, 1H), 7.23 (m, 2H) (aromatic *CH*), 4.45 (s, 1H) (cage *CH*). $^{13}C\{^1H\}$ NMR ($CDCl_3$, 101 MHz): δ 177.7 (d, $^3J_{C-F}$ = 7.0 Hz) ($C=N$), 161.6 (d, $^1J_{C-F}$ = 261.7 Hz), 134.9 (d, $^3J_{C-F}$ = 9.1 Hz), 131.5, 124.5 (d, $^3J_{C-F}$ = 4.0 Hz), 117.3 (d, $^2J_{C-F}$ = 21.1 Hz), 117.2 (d, $^2J_{C-F}$ = 22.1 Hz) (aromatic C), 99.5, 57.1 (cage C). ^{11}B NMR ($CDCl_3$, 128 MHz): δ 1.4 (s, 1B) (*BO*), -5.3 (d, J = 152.3 Hz, 1B), -10.4 (d, J = 167.7 Hz, 2B), -13.2 (d, J = 139.5 Hz, 2B), -14.1 (d, J = 128.0 Hz, 1B), -15.5 (d, J = 163.8 Hz, 1B), -16.5 (d, J = 154.88 Hz, 1B), -21.3 (d, J = 166.4 Hz, 1B) (*BH*). ^{19}F NMR (377 MHz, $CDCl_3$): δ -107.5 (m, 1F). HRMS (ESI) Calcd for $C_9H_{15}^{10}B_2^{11}B_8FNO^+$ $[M+H]^+$: 280.2135, Found: 280.2141.



2k: White solid. 90% yield. M.p. = 199-201 °C. TLC: R_f = 0.23 (*n*-hexane:ethyl acetate = 10:1). ^1H NMR (CDCl_3 , 400 MHz): δ 6.87 (s, 2H) (aromatic *CH*), 4.38 (s, 1H) (cage *CH*), 2.29 (s, 3H), 2.25 (s, 6H) (alkyl CH_3). $^{13}\text{C}\{^1\text{H}\}$ NMR (CDCl_3 , 101 MHz): δ 183.6 ($\text{C}=\text{N}$), 140.7, 137.4, 128.9, 126.8 (aromatic C), 99.3, 56.9 (cage C), 21.4, 20.00 (CH_3). ^{11}B NMR (CDCl_3 , 128 MHz): δ 1.6 (s, 1B) (*BO*), -5.3 (d, J = 156.2 Hz, 1B), -10.6 (d, J = 172.8 Hz, 2B), -13.3 (d, J = 135.7 Hz, 2B), -14.1 (d, J = 131.8 Hz, 1B), -15.6 (d, J = 169.0 Hz, 1B), -16.6 (d, J = 112.6 Hz, 1B), -21.5 (d, J = 167.0 Hz, 1B) (*BH*). HRMS (ESI) Calcd for $\text{C}_{12}\text{H}_{22}^{10}\text{B}_2^{11}\text{B}_8\text{NO}^+$ [$\text{M}+\text{H}^+$]: 304.2699, Found: 304.2694.

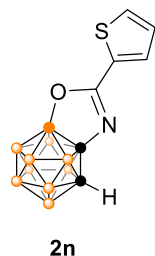


2l: White solid. 83% yield. M.p. = 145-147 °C. TLC: R_f = 0.27 (*n*-hexane:ethyl acetate = 10:1). ^1H NMR (CDCl_3 , 400 MHz): δ 8.96 (d, J = 8.8 Hz, 1H), 8.30 (d, J = 7.2 Hz, 1H), 8.06 (d, J = 8.0 Hz, 1H), 7.91 (d, J = 8.0 Hz, 1H), 7.64 (t, J = 7.6 Hz, 1H), 7.57 (t, J = 6.8 Hz, 1H), 7.55 (t, J = 7.6 Hz, 1H) (aromatic *CH*), 4.46 (s, 1H) (cage *CH*). $^{13}\text{C}\{^1\text{H}\}$ NMR (CDCl_3 , 101 MHz): δ 181.6 ($\text{C}=\text{N}$), 134.0, 133.9, 130.7, 130.7, 129.0, 128.2, 126.6, 125.8, 125.4, 124.8 (aromatic C), 99.9, 57.1 (cage C). ^{11}B NMR (CDCl_3 , 128 MHz): δ 1.5 (s, 1B) (*BO*), -5.3 (d, J = 152.3 Hz, 1B), -10.1 (d, J = 170.2 Hz, 2B), -13.2 (d, J = 139.5 Hz, 2B), -14.0 (d, J = 125.4 Hz, 1B), -15.4 (d, J = 163.8 Hz, 1B), -16.5 (d, J = 115.2 Hz, 1B), -21.3 (d, J = 166.4 Hz, 1B) (*BH*). HRMS (ESI) Calcd for $\text{C}_{13}\text{H}_{18}^{10}\text{B}_2^{11}\text{B}_8\text{NO}^+$ [$\text{M}+\text{H}^+$]: 312.2397, Found: 312.2395.

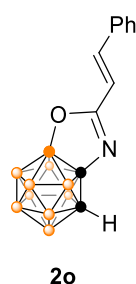


2m: White solid. 86% yield. M.p. = 184-186 °C. TLC: R_f = 0.10 (*n*-hexane:ethyl acetate = 10:1). ^1H NMR (CDCl_3 , 400 MHz): δ 7.60 (m, 1H), 7.24 (d, J = 3.6 Hz, 1H), 6.57 (dd, J = 3.6, 1.6 Hz, 1H) (aromatic *CH*), 4.37 (s, 1H) (cage *CH*). $^{13}\text{C}\{^1\text{H}\}$ NMR (CDCl_3 , 101 MHz): δ 172.1 ($\text{C}=\text{N}$), 146.9, 144.1, 117.8, 112.4 (aromatic C), 99.2, 57.0 (cage C). ^{11}B NMR (CDCl_3 , 128 MHz): δ 1.6 (s, 1B) (*BO*), -5.5 (d, J = 152.3 Hz,

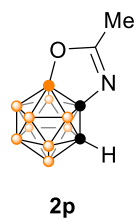
1B), -10.2 (d, $J = 171.5$ Hz, 2B), -13.4 (d, $J = 142.1$ Hz, 2B), -14.1 (d, $J = 115.2$ Hz, 1B), -15.7 (d, $J = 147.2$ Hz, 1B), -16.5 (d, $J = 90.9$ Hz, 1B), -21.3 (d, $J = 167.7$ Hz, 1B) (BH). HRMS (ESI) Calcd for $C_7H_{14}^{10}B_2^{11}B_8NO_2^+$ $[M+H]^+$: 252.2022, Found: 252.2021.



2n: White solid. 88% yield. M.p. = 161-162 °C. TLC: $R_f = 0.16$ (*n*-hexane:ethyl acetate = 10:1). 1H NMR ($CDCl_3$, 400 MHz): δ 7.84 (d, $J = 3.6$ Hz, 1H), 7.57 (d, $J = 4.8$ Hz, 1H), 7.13 (t, $J = 4.0$ Hz, 1H) (aromatic CH), 4.35 (s, 1H) (cage CH). $^{13}C\{^1H\}$ NMR ($CDCl_3$, 101 MHz): δ 176.5 (C=N), 132.9, 132.5, 131.7, 128.2 (aromatic C), 99.6, 56.8 (cage C). ^{11}B NMR ($CDCl_3$, 128 MHz): δ 1.8 (s, 1B) (BO), -5.5 (d, $J = 152.3$ Hz, 1B), -10.0 (d, $J = 172.8$ Hz, 2B), -13.3 (d, $J = 133.1$ Hz, 2B), -14.1 (d, $J = 131.8$ Hz, 1B), -15.7 (d, $J = 139.5$ Hz, 1B), -16.5 (d, $J = 98.6$ Hz, 1B), -21.3 (d, $J = 167.7$ Hz, 1B) (BH). HRMS (ESI) Calcd for $C_7H_{14}^{10}B_2^{11}B_8NOS^+$ $[M+H]^+$: 268.1805, Found: 268.1798.

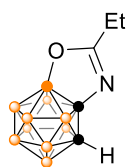


2o: White solid. 85% yield. M.p. = 152-153 °C. TLC: $R_f = 0.10$ (*n*-hexane:ethyl acetate = 10:1). 1H NMR ($CDCl_3$, 400 MHz): δ 7.75 (d, $J = 16.4$ Hz, 1H) (alkenyl CH), 7.54 (m, 2H), 7.41 (m, 3H) (aromatic CH), 6.67 (d, $J = 16.0$ Hz, 1H) (alkenyl CH), 4.31 (s, 1H) (cage CH). $^{13}C\{^1H\}$ NMR ($CDCl_3$, 101 MHz): δ 181.0 (C=N), 143.9, 134.3, 130.8, 129.2, 128.2, 116.4 (alkenyl & aromatic C), 99.7, 56.8 (cage C). ^{11}B NMR ($CDCl_3$, 128 MHz): δ 1.8 (s, 1B) (BO), -5.4 (d, $J = 151.0$ Hz, 1B), -10.2 (d, $J = 171.5$ Hz, 2B), -13.4 (d, $J = 134.4$ Hz, 2B), -14.1 (d, $J = 119.0$ Hz, 1B), -15.7 (d, $J = 144.6$ Hz, 1B), -16.5 (d, $J = 97.3$ Hz, 1B), -21.4 (d, $J = 162.6$ Hz, 1B) (BH). HRMS (ESI) Calcd for $C_{11}H_{18}^{10}B_2^{11}B_8NO^+$ $[M+H]^+$: 288.2386, Found: 288.2387.



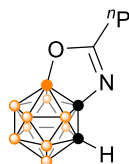
2p: White solid. 86% yield. M.p. = 82-84 °C. TLC: $R_f = 0.10$ (*n*-hexane:ethyl acetate = 10:1). 1H NMR ($CDCl_3$, 400 MHz): δ 4.25 (s, 1H) (cage CH), 2.25 (s, 3H) (CH_3). $^{13}C\{^1H\}$ NMR ($CDCl_3$, 101 MHz): δ 184.4 (C=N), 99.0, 56.6 (cage C), 18.6 (CH_3). ^{11}B NMR ($CDCl_3$,

128 MHz): δ 1.7 (s, 1B) (BO), -5.4 (d, J = 152.3 Hz, 1B), -10.4 (d, J = 171.5 Hz, 2B), -13.4 (d, J = 139.5 Hz, 2B), -14.3 (d, J = 139.5 Hz, 1B), -15.8 (d, J = 144.6 Hz, 1B), -16.7 (d, J = 162.6 Hz, 1B), -21.4 (d, J = 165.1 Hz, 1B) (BH). HRMS (ESI) Calcd for $C_4H_{14}^{10}B_2^{11}B_8NO^+$ [M+H⁺]: 200.2073, Found: 200.2067.



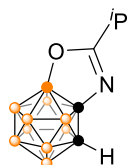
2q

2q: White solid. 80% yield. M.p. = 80-81 °C. TLC: R_f = 0.16 (*n*-hexane:ethyl acetate = 10:1). ¹H NMR (CDCl₃, 400 MHz): δ 4.27 (s, 1H) (cage CH), 2.54 (q, J = 7.6 Hz, 2H) (CH₂), 1.21 (t, J = 7.6 Hz, 3H) (CH₃). ¹³C{¹H} NMR (CDCl₃, 101 MHz): δ 188.5 (C=N), 99.5, 56.6 (cage C), 26.0 (CH₂), 10.2 (CH₃). ¹¹B NMR (CDCl₃, 128 MHz): δ 1.7 (s, 1B) (BO), -5.5 (d, J = 151.0 Hz, 1B), -10.4 (d, J = 170.2 Hz, 2B), -13.5 (d, J = 138.2 Hz, 2B), -14.4 (d, J = 137.0 Hz, 1B), -15.8 (d, J = 152.3 Hz, 1B), -16.8 (d, J = 110.1 Hz, 1B), -21.5 (d, J = 166.4 Hz, 1B) (BH). HRMS (ESI) Calcd for $C_5H_{16}^{10}B_2^{11}B_8NO^+$ [M+H⁺]: 214.2230, Found: 214.2226.



2r

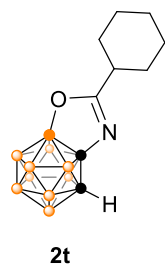
2r: White solid. 78% yield. M.p. = 128-130 °C. TLC: R_f = 0.17 (*n*-hexane:ethyl acetate = 10:1). ¹H NMR (CDCl₃, 400 MHz): δ 4.27 (s, 1H) (cage CH), 2.49 (t, J = 7.2 Hz, 2H), 1.71 (m, 2H) (CH₂), 0.95 (t, J = 7.2 Hz, 3H) (CH₃). ¹³C{¹H} NMR (CDCl₃, 101 MHz): δ 187.7 (C=N), 99.0, 56.6 (cage C), 34.2 (CH₂), 19.6 (CH₂), 13.6 (CH₃). ¹¹B NMR (THF, 128 MHz): δ 1.3 (s, 1B) (BO), -5.8 (d, J = 153.3 Hz, 1B), -10.7 (d, J = 171.5 Hz, 2B), -13.8 (d, J = 137.0 Hz, 2B), -14.6 (d, J = 134.4 Hz, 1B), -16.1 (d, J = 157.4 Hz, 1B), -17.0 (d, J = 152.3 Hz, 1B), -21.8 (d, J = 167.7 Hz, 1B) (BH). HRMS (ESI) Calcd for $C_6H_{18}^{10}B_2^{11}B_8NO^+$ [M+H⁺]: 228.2386, Found: 228.2383.



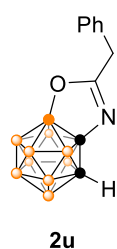
2s

2s: White solid. 86% yield. M.p. = 71-73 °C. TLC: R_f = 0.23 (*n*-hexane:ethyl acetate = 10:1). ¹H NMR (CDCl₃, 400 MHz): δ 4.28 (s, 1H) (cage CH), 2.77 (m, 1H) (CH), 1.21 (d, J = 7.2 Hz, 6H) (CH₃). ¹³C{¹H} NMR (CDCl₃, 101 MHz): δ 191.7 (C=N), 99.1, 56.7 (cage

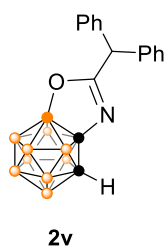
C), 32.3 (CH), 19.6 (CH₃), 19.5 (CH₃). ¹¹B NMR (CDCl₃, 128 MHz): δ 1.7 (s, 1B) (BO), -5.4 (d, *J* = 152.3 Hz, 1B) -10.4 (d, *J* = 171.5 Hz, 2B), -13.4 (d, *J* = 131.8 Hz, 2B), -14.3 (d, *J* = 138.2 Hz, 1B), -15.7 (d, *J* = 147.2 Hz, 1B), -16.7 (d, *J* = 117.8 Hz, 1B), -21.5 (d, *J* = 166.4 Hz, 1B) (BH). HRMS (ESI) Calcd for C₆H₁₈¹⁰B₂¹¹B₈NO⁺ [M+H⁺]: 228.2397, Found: 228.2389.



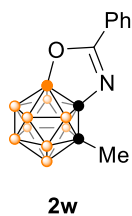
2t: White solid. 88% yield. M.p. = 118-120 °C. TLC: R_f = 0.22 (*n*-hexane:ethyl acetate = 10:1). ¹H NMR (CDCl₃, 400 MHz): δ 4.26 (s, 1H) (cage CH), 2.51 (m, *J* = m, 1H) (CH), 1.92 (m, 2H), 1.77 (m, 2H), 1.68 (m, 1H), 1.45 (m, 2H), 1.29 (m, 3H) (CH₂). ¹³C{¹H} NMR (CDCl₃, 101 MHz): δ 190.8 (C=N), 99.2, 56.7 (cage C), 41.3 (CH), 29.7, 29.6, 25.7, 25.4, 25.4 (CH₂). ¹¹B NMR (CDCl₃, 128 MHz): δ 1.6 (s, 1B) (BO), -5.5 (d, *J* = 152.3 Hz, 1B), -10.4 (d, *J* = 171.5 Hz, 2B), -13.5 (d, *J* = 135.7 Hz, 2B), -14.4 (d, *J* = 137.0 Hz, 1B), -15.8 (d, *J* = 154.9 Hz, 1B), -16.8 (d, *J* = 103.7 Hz, 1B), -21.6 (d, *J* = 166.4 Hz, 1B) (BH). HRMS (ESI) Calcd for C₉H₂₂¹⁰B₂¹¹B₈NO⁺ [M+H⁺]: 268.2699, Found: 268.2703.



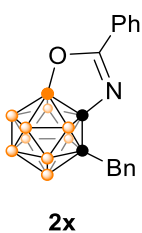
2u: Colorless oil. 76% yield. TLC: R_f = 0.1 (*n*-hexane:ethyl acetate = 10:1). ¹H NMR (CDCl₃, 400 MHz): δ 7.30 (m, 3H), 7.20 (d, *J* = 6.4 Hz, 2H) (aromatic CH), 4.21 (s, 1H) (cage CH), 3.77 (s, 2H) (CH₂). ¹³C{¹H} NMR (CDCl₃, 101 MHz): δ 185.4 (C=N), 133.6, 129.1, 129.0, 127.7 (aromatic CH), 98.9, 56.7 (cage C), 38.8 (CH₂). ¹¹B NMR (CDCl₃, 128 MHz): δ 1.7 (s, 1B) (BO), -5.3 (d, *J* = 152.3 Hz, 1B), -10.5 (d, *J* = 171.5 Hz, 2B), -13.3 (d, *J* = 140.8 Hz, 2B), -14.3 (d, *J* = 140.8 Hz, 1B), -15.7 (d, *J* = 163.8 Hz, 1B), -16.7 (d, *J* = 116.5 Hz, 1B), -21.3 (d, *J* = 169.0 Hz, 1B) (BH). HRMS (ESI) Calcd for C₁₀H₁₈¹⁰B₂¹¹B₈NO⁺ [M+H⁺]: 276.2386, Found: 276.2392.



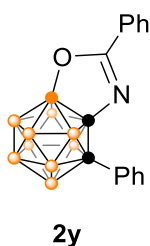
2v: White solid. 74% yield. M.p. = 128-130 °C. TLC: R_f = 0.15 (*n*-hexane:ethyl acetate = 10:1). ^1H NMR (CDCl_3 , 400 MHz): δ 7.26 (m, 10H) (aromatic *CH*), 5.25 (s, 1H) (*CH*), 4.25 (s, 1H) (cage *CH*). $^{13}\text{C}\{^1\text{H}\}$ NMR (CDCl_3 , 101 MHz): δ 186.8 (*C=N*), 138.0, 137.9, 129.0, 128.9, 128.9, 128.8, 127.8, 127.8 (aromatic *C*), 98.8, 56.8 (cage *C*), 54.5 (*CH*). ^{11}B NMR (CDCl_3 , 128 MHz): δ 1.7 (s, 1B) (*BO*), -5.2 (d, J = 152.3 Hz, 1B), -10.6 (d, J = 144.6 Hz, 2B), -13.2 (d, J = 144.6 Hz, 2B), -14.2 (d, J = 137.0 Hz, 1B), -15.6 (d, J = 165.1 Hz, 1B), -16.6 (d, J = 113.9 Hz, 1B), -21.3 (d, J = 163.8 Hz, 1B) (*BH*). RMS (ESI) Calcd for $\text{C}_{16}\text{H}_{22}^{10}\text{B}_2^{11}\text{B}_8\text{NO}^+$ [$\text{M}+\text{H}^+$]: 352.2699, Found: 352.2697.



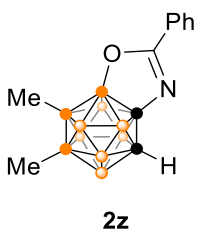
2w: White solid. 78% yield. M.p. = 75-77 °C. TLC: R_f = 0.2 (*n*-hexane:ethyl acetate = 80:1). ^1H NMR (CDCl_3 , 400 MHz): δ 8.13 (d, J = 6.8 Hz, 2H), 7.58 (m, 1H), 7.47 (t, J = 7.6 Hz, 2H) (aromatic *CH*), 2.26 (s, 3H) (CH_3). $^{13}\text{C}\{^1\text{H}\}$ NMR (CDCl_3 , 101 MHz): δ 181.4 (*C=N*), 133.3, 129.0, 128.8, 128.8 (aromatic *C*), 102.1, 72.3 (cage *C*), 21.0 (CH_3). ^{11}B NMR (CDCl_3 , 128 MHz): δ 2.5 (s, 1B) (*BO*), -7.7 (d, J = 201.0 Hz, 1B), -9.2 (d, J = 158.7 Hz, 2B), -15.4 (m, 5B), -18.3 (d, J = 167.7 Hz, 1B) (*BH*). HRMS (ESI) Calcd for $\text{C}_{10}\text{H}_{18}^{10}\text{B}_2^{11}\text{B}_8\text{NO}^+$ [$\text{M}+\text{H}^+$]: 276.2397, Found: 276.2390.



2x: White solid. 72% yield. M.p. = 71-72 °C. TLC: R_f = 0.26 (*n*-hexane:ethyl acetate = 10:1). ^1H NMR (CDCl_3 , 400 MHz): δ 8.17 (d, J = 7.6 Hz, 2H), 7.59 (t, J = 8.0 Hz, 1H), 7.49 (t, J = 8.0 Hz, 2H), 7.31 (m, 5H) (aromatic *CH*), 3.80 (m, 2H) (CH_2). $^{13}\text{C}\{^1\text{H}\}$ NMR (CDCl_3 , 101 MHz): δ 181.4 (*C=N*), 135.4, 133.3, 130.5, 129.0, 128.9, 128.8, 128.7, 128.1 (aromatic *C*), 102.8 (cage *C*), 39.5 (CH_2). ^{11}B NMR (CDCl_3 , 128 MHz): δ 2.5 (s, 1B) (*BO*), -8.2 (d, J = 167.7 Hz, 2B), -9.9 (d, J = 216.3 Hz, 1B), -13.7 (m, 5B), -19.2 (d, J = 163.8 Hz, 1B) (*BH*). HRMS (ESI) Calcd for $\text{C}_{16}\text{H}_{22}^{10}\text{B}_2^{11}\text{B}_8\text{NO}^+$ [$\text{M}+\text{H}^+$]: 352.2699, Found: 352.2707.

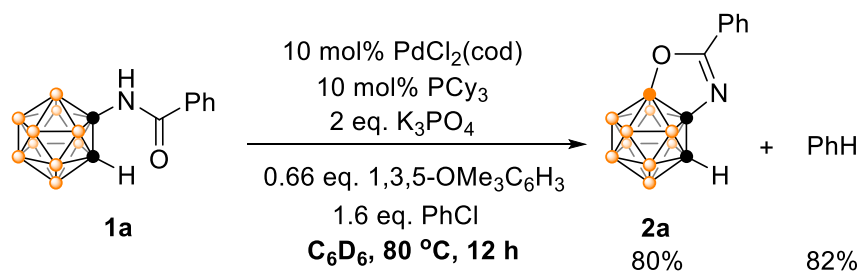


2y: Colorless oil. 64% yield. TLC: $R_f = 0.25$ (*n*-hexane:ethyl acetate = 10:1). ^1H NMR (CDCl_3 , 400 MHz): δ 8.15 (d, $J = 7.6$ Hz, 2H), 7.89 (d, $J = 7.2$ Hz, 2H), 7.59 (t, $J = 7.6$ Hz, 1H), 7.46 (m, 5H) (aromatic CH). $^{13}\text{C}\{^1\text{H}\}$ NMR (CDCl_3 , 101 MHz): δ 180.9 ($\text{C}=\text{N}$), 133.3, 131.6, 130.1, 129.4, 128.9, 128.9, 128.8, 128.7 (aromatic C), 103.7, 78.9 (cage C). ^{11}B NMR (CDCl_3 , 128 MHz): δ 2.6 (s, 1B) (BO), -7.5 (d, $J = 176.6$ Hz, 2B), -9.3 (d, $J = 212.5$ Hz, 1B), -13.3 (m, 5B), -18.0 (d, $J = 166.4$ Hz, 1B) (BH). HRMS (ESI) Calcd for $\text{C}_{15}\text{H}_{20}^{10}\text{B}_2^{11}\text{B}_8\text{NO}^+$ [$\text{M}+\text{H}^+$]: 338.2543, Found: 338.2548.



2z: White solid. 75% yield. M.p. = 165-166 °C. TLC: $R_f = 0.18$ (*n*-hexane:ethyl acetate = 10:1). ^1H NMR (CDCl_3 , 400 MHz): δ 8.08 (d, $J = 8.0$ Hz, 2H), 7.57 (t, $J = 7.6$ Hz, 1H), 7.46 (t, $J = 7.6$ Hz, 2H) (aromatic CH), 4.19 (s, 1H) (cage CH), 0.45 (s, 3H), 0.23 (s, 3H) (CH_3). $^{13}\text{C}\{^1\text{H}\}$ NMR (CDCl_3 , 101 MHz): δ 181.1 ($\text{C}=\text{N}$), 133.1, 128.9, 128.8, 128.7 (aromatic C), 94.3, 50.3 (cage C), the $\text{B}_{\text{cage}}\text{-C}$ were not observed. ^{11}B NMR (CDCl_3 , 128 MHz): δ 4.8 (s, 1B) (BO), 0.9 (s, 1B) (BC), -2.9 (s, 1B) (BC), -11.5 (d, $J = 153.6$ Hz, 4B), -16.8 (d, $J = 161.3$ Hz, 2B), -20.8 (d, $J = 165.1$ Hz, 1B) (BH). HRMS (ESI) Calcd for $\text{C}_{11}\text{H}_{20}^{10}\text{B}_2^{11}\text{B}_8\text{NO}^+$ [$\text{M}+\text{H}^+$]: 290.2543, Found: 290.2541.

Preliminary mechanistic study.



1a (13.1 mg, 0.05 mmol), PdCl₂(cod) (1.4 mg, 10 mol%), PCy₃ (1.4 mg, 10 mol%), K₃PO₄ (21.1 mg, 0.1 mmol), PhCl (9.0 mg, 0.8 mmol), and 1,3,5-trimethoxybenzene (internal standard, 5.5 mg, 0.033 mmol) were mixed in C₆D₆ (2 mL) in a J. Young valve NMR tube in glovebox. The tube was closed and heated at 80 °C (bath temperature) for 12 h. The reaction was then monitored by ¹H NMR.

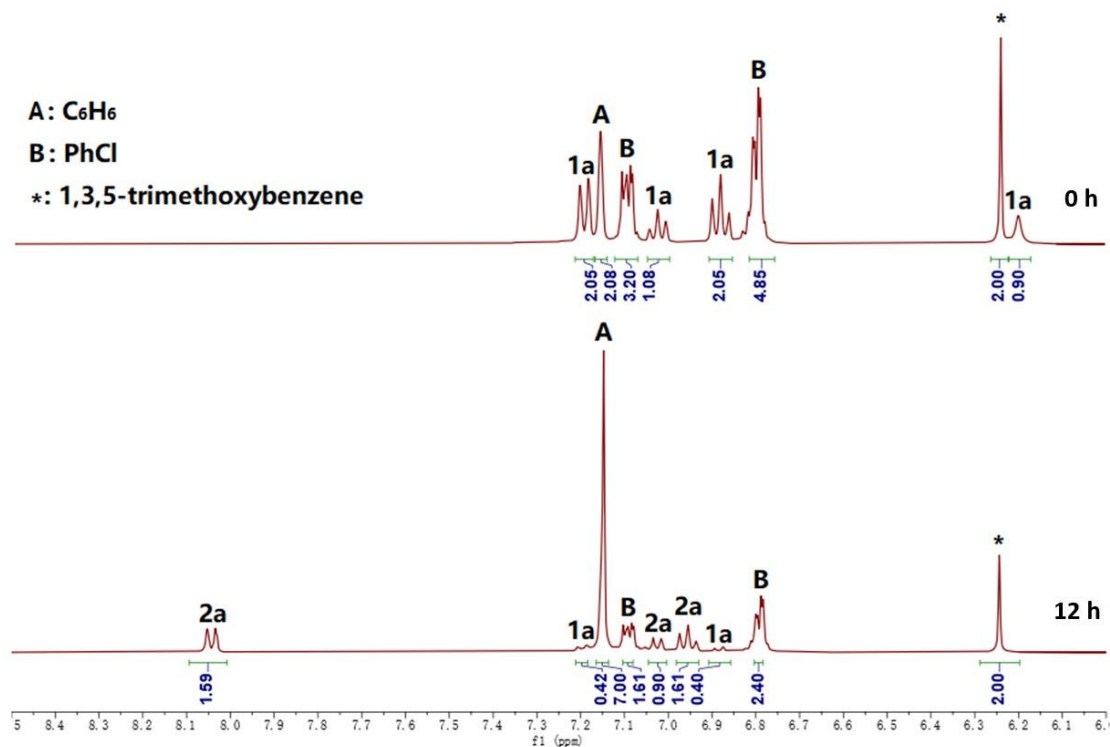


Figure S1. ¹H NMR spectra of the control experiment

X-ray Structure Determination. The data of **2b**, **2m**, and **2t** were collected at 213 K on a Bruker APEX DUO diffractometer. An empirical absorption correction was applied using the SADABS program.³ All structures were solved by direct methods and subsequent Fourier difference techniques and refined anisotropically for all non-

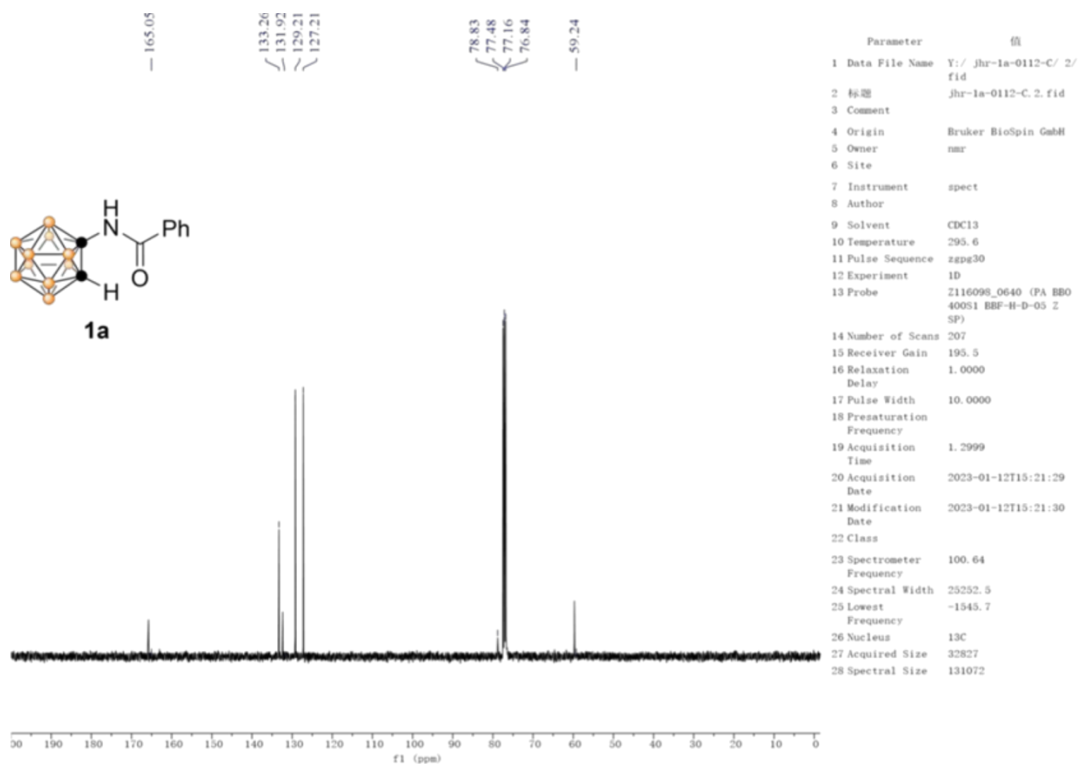
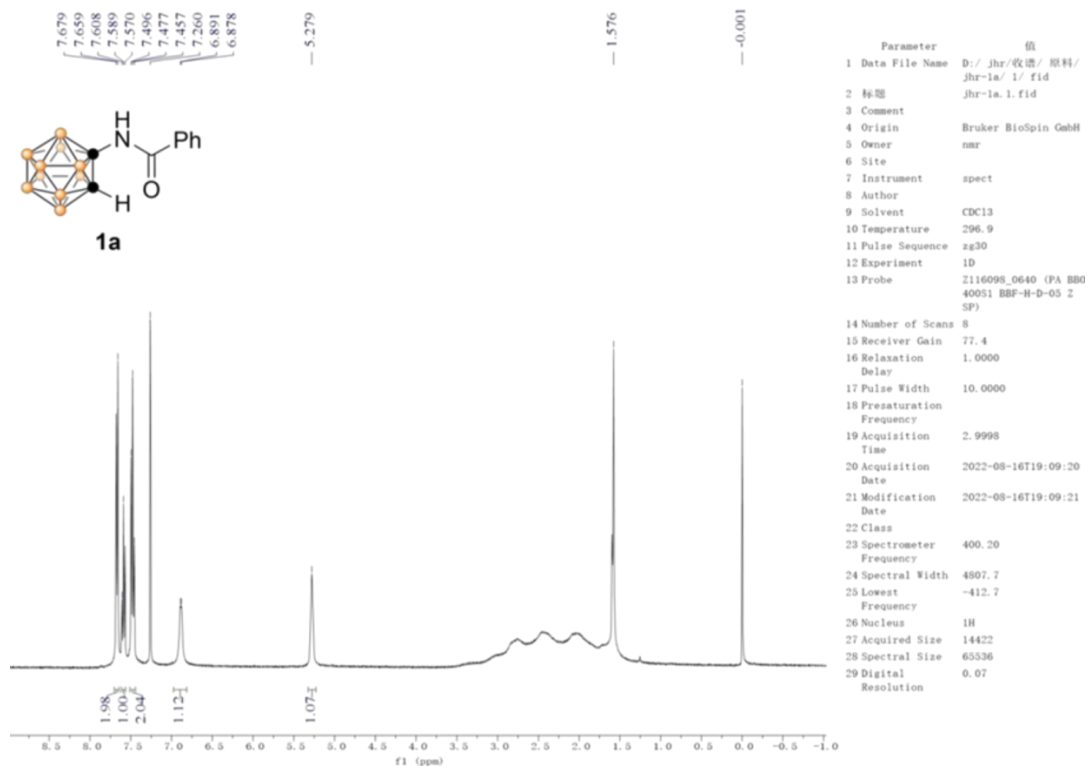
hydrogen atoms by full-matrix least-squares on F^2 using the SHELXTL program package⁴. All hydrogen atoms were geometrically fixed using the riding model. Crystal data and details of data collection and structure refinements were given in Table S2. CCDC 2417342-2417344 (**2b**, **2m** and **2t**) contains the supplementary crystallographic data for this paper. These data can be obtained free of charge from The Cambridge Crystallographic Data Centre via www.ccdc.cam.ac.uk/data_request/cif.

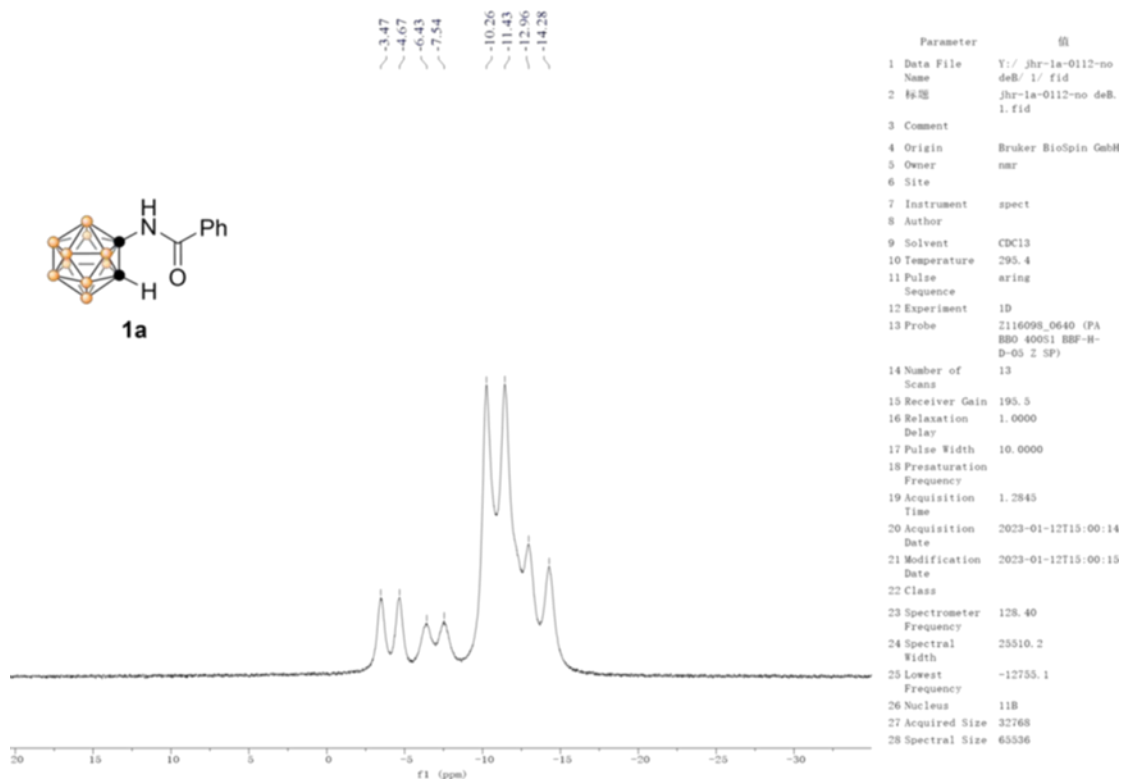
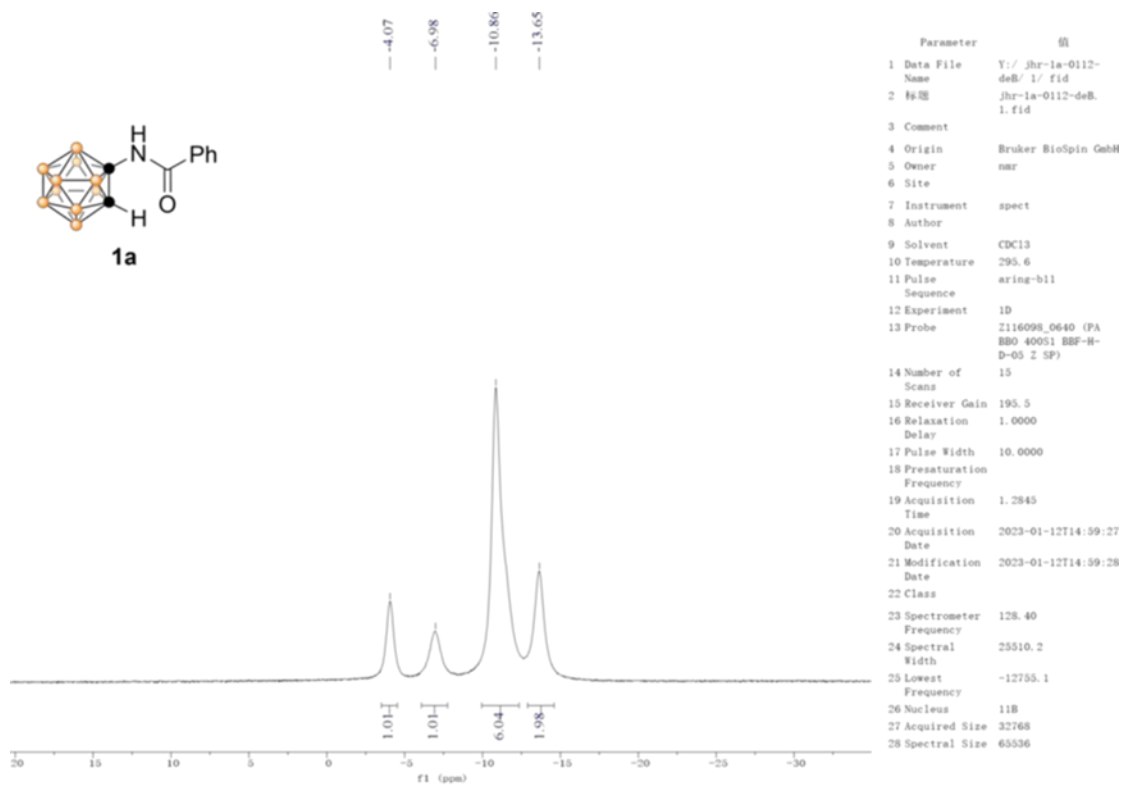
Table S2. Crystal Data and Summary of Data Collection and Refinements.

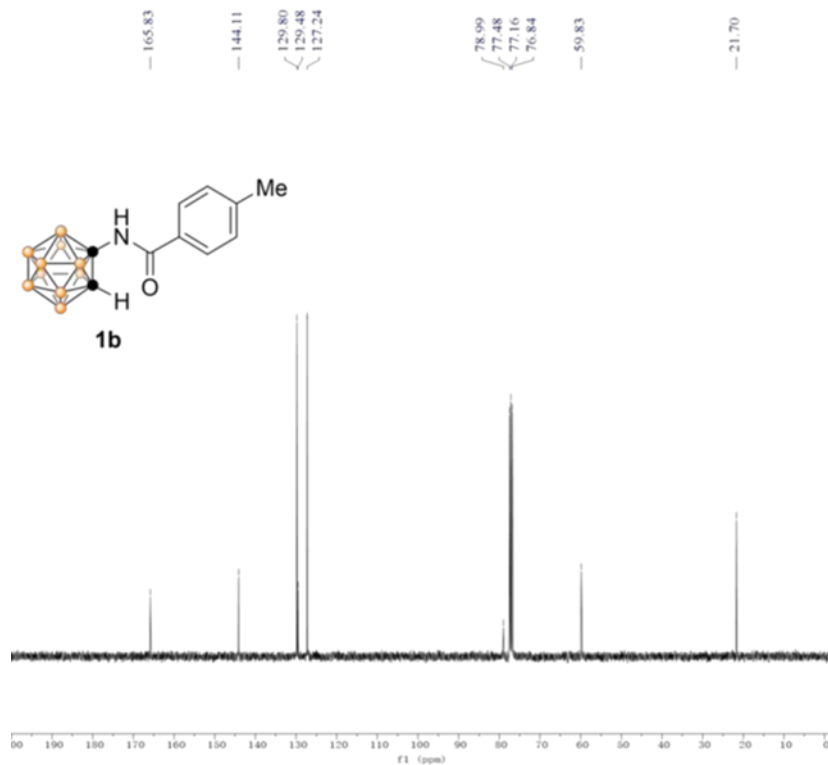
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formula	C ₁₀ H ₁₇ B ₁₀ NO	C ₇ H ₁₄ B ₁₀ NO ₂	C ₉ H ₂₁ B ₁₀ NO
crystal size (mm ³)	0.07x0.07x0.05	0.07x0.07x0.05	0.07x0.07x0.05
fw	275.35	252.29	267.37
crystal system	monoclinic	monoclinic	monoclinic
space group	<i>P</i> 2 ₁ /c	<i>P</i> 2 ₁ /c	<i>P</i> 2 ₁ /n
<i>a</i> , Å	11.486(1)	6.759(1)	11.687(1)
<i>b</i> , Å	19.564(1)	20.968(1)	11.014(1)
<i>c</i> , Å	6.782(1)	9.278(1)	12.611(1)
β , deg	95.718(2)	98.688(2)	110.678(2)
<i>V</i> , Å ³	1516.3(1)	1299.7(1)	1518.7(1)
<i>Z</i>	4	4	4
<i>D</i> _{calcd} , Mg/m ³	1.206	1.289	1.169
radiation (λ) Å	1.34139	1.34139	1.34139
2 θ range, deg	7.8 to 110.1	9.2 to 109.9	7.7 to 109.8
μ , mm ⁻¹	0.304	0.360	0.289
<i>F</i> (000)	568	516	560
no. of obsd reflns	2849	2458	2886
no. of params refnd	200	181	190
goodness of fit	1.081	1.047	1.060
R1	0.0678	0.0450	0.0443
wR2	0.1797	0.1202	0.1209

References

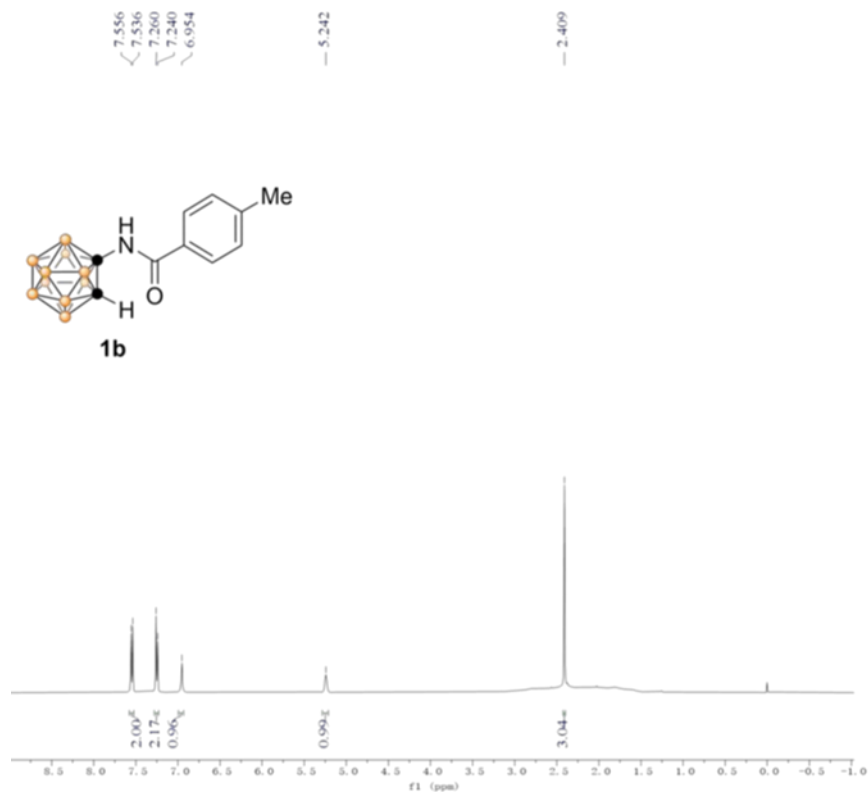
1. N. Yong, Y. Wang, J. Miao, Y. Li and Z. Zhang, *J. Organomet. Chem.*, 2015, **798**, 182-188.
2. R. Cheng, J. Zhang, H. Zhang, Z. Qiu and Z. Xie, *Nat. Commun.*, 2021, **12**, 7146.
3. Sheldrick, G. M. *SADABS: Program for Empirical Absorption Correction of Area Detector Data*. University of Göttingen: Germany, 1996.
4. Sheldrick, G. M. *SHELXTL 5.10 for Windows NT: Structure Determination Software Programs*. Bruker Analytical X-ray Systems, Inc., Madison, Wisconsin, USA, 1997.



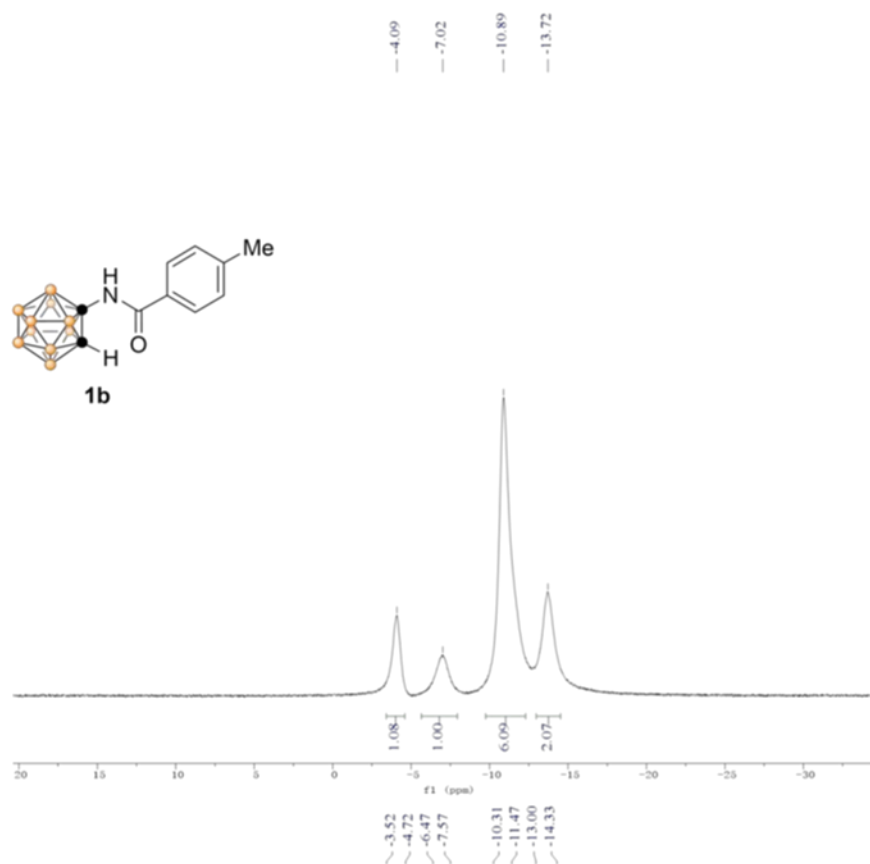




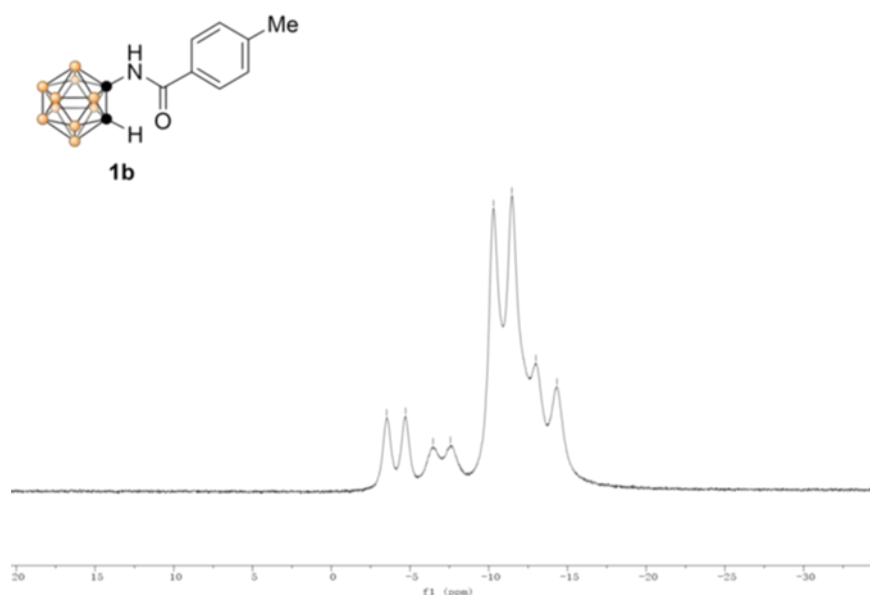
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5 Owner	nmr
6 Site	
7 Instrument	spect
8 Author	
9 Solvent	CDCl3
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11 Pulse Sequence	zgpg30
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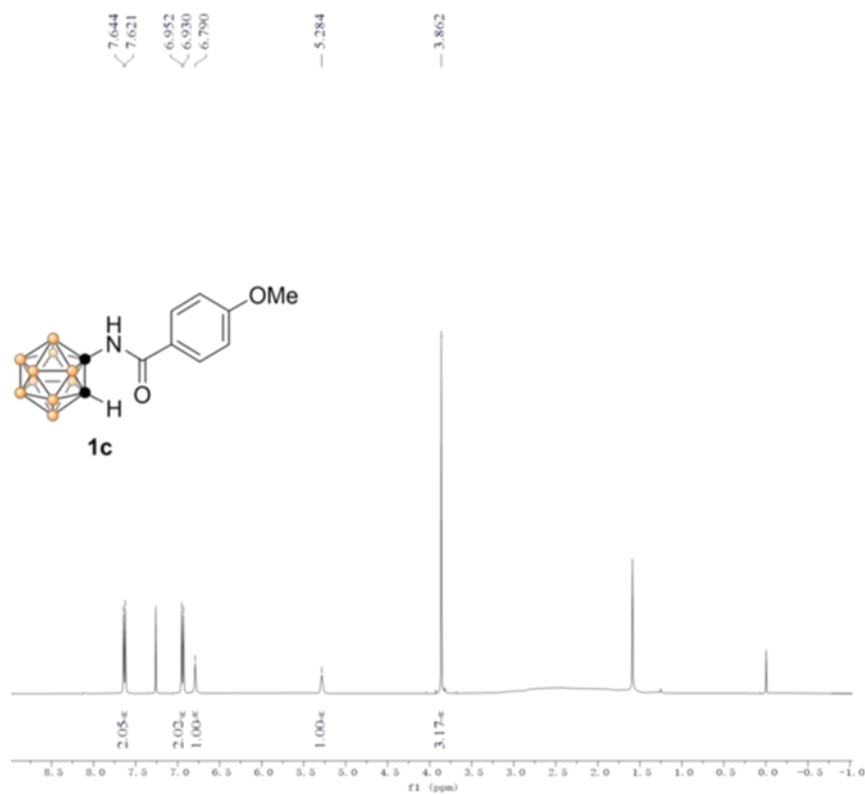
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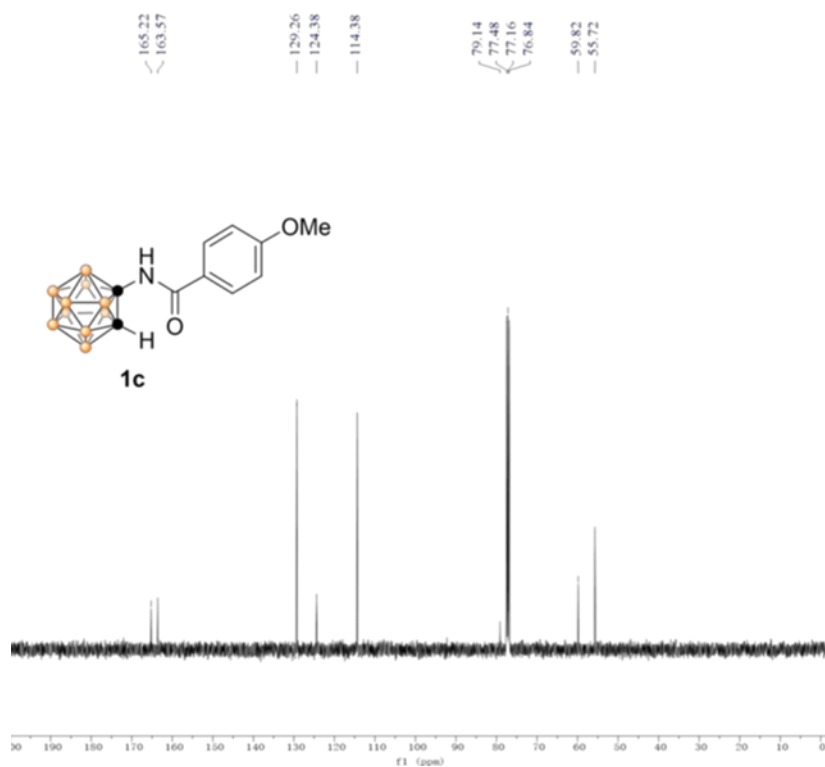
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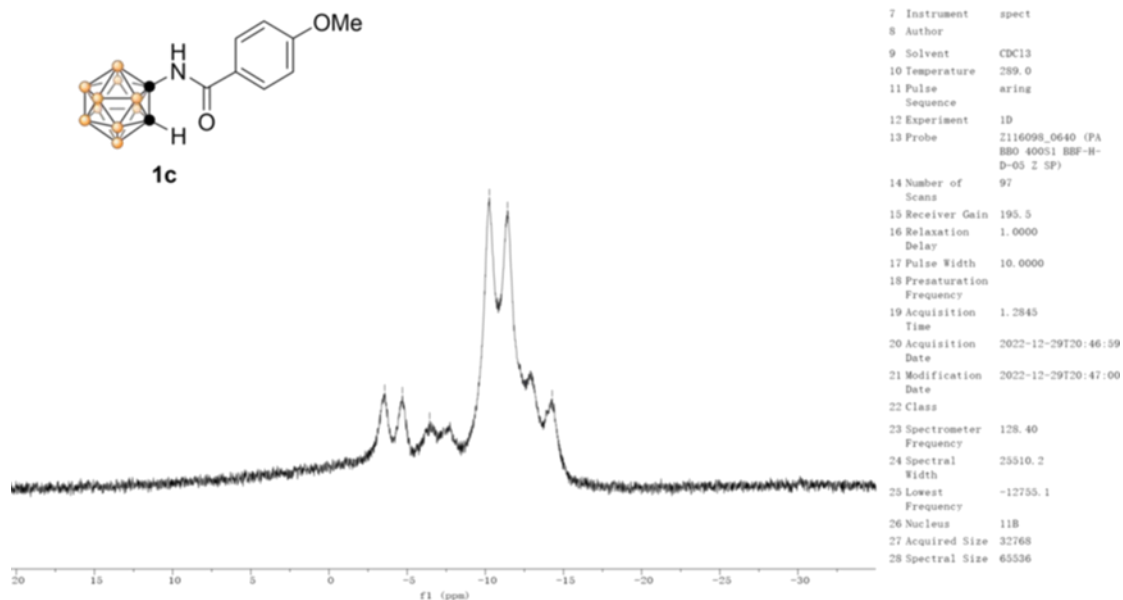
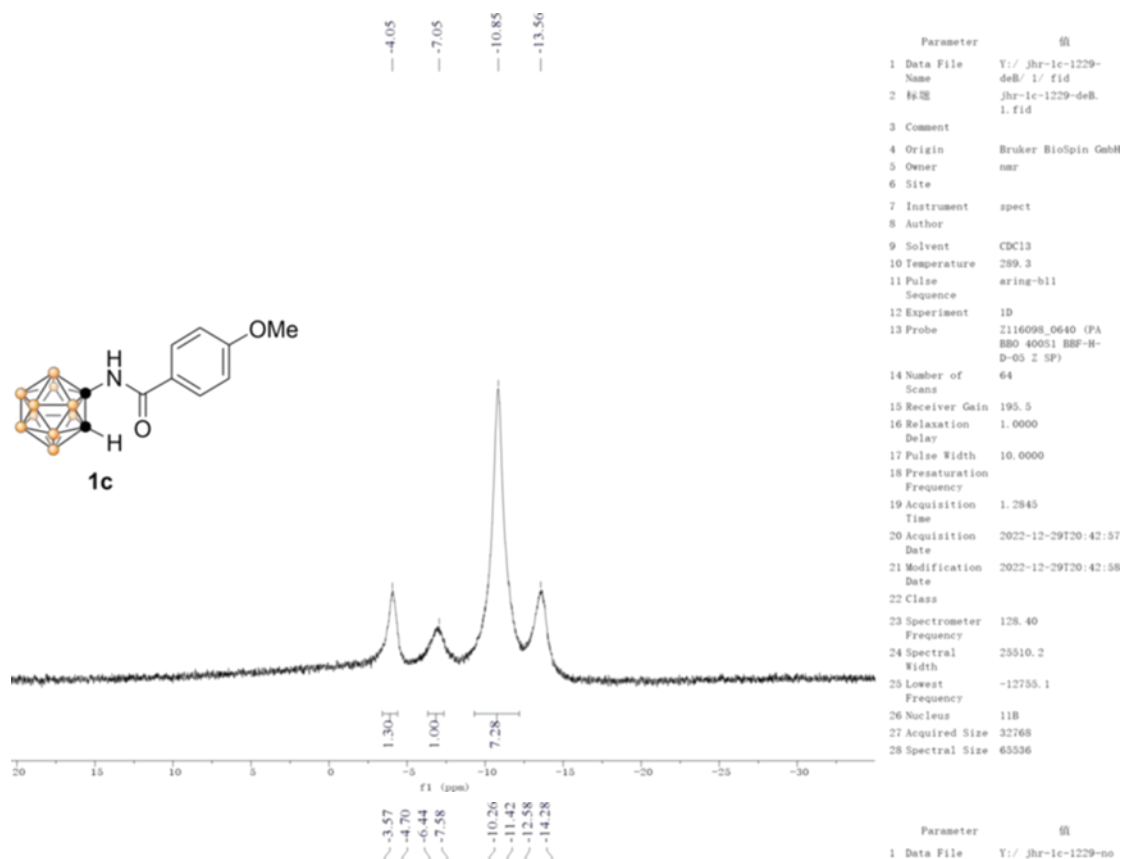
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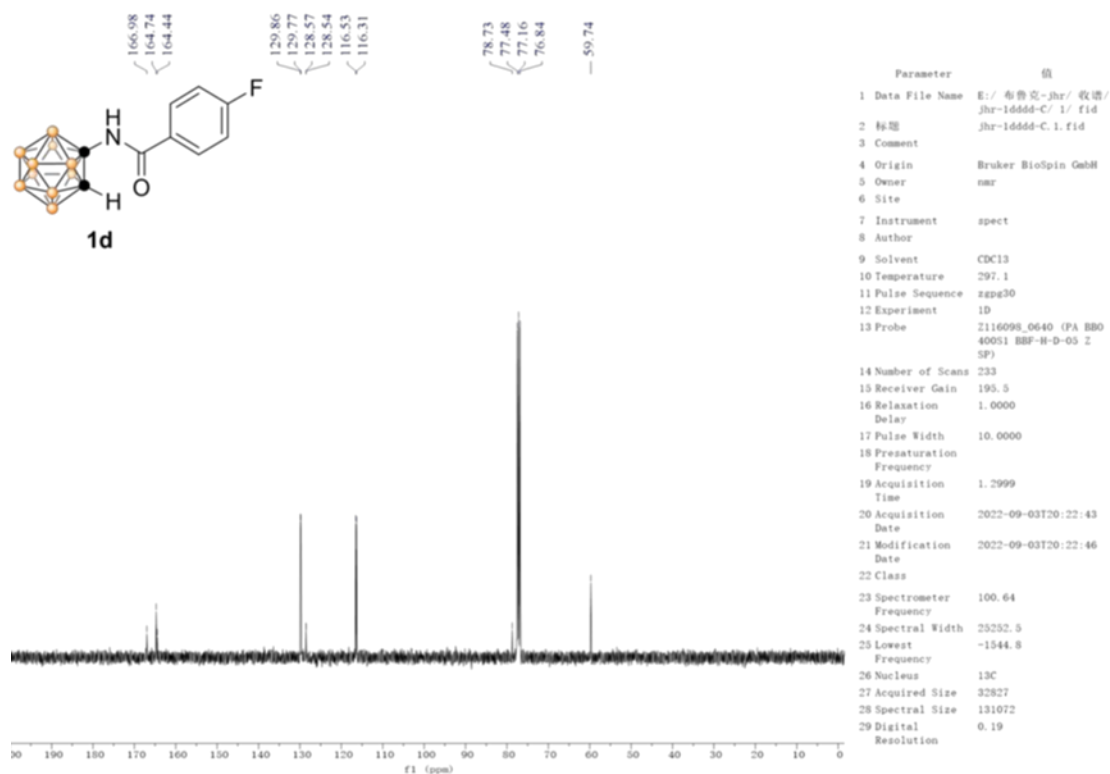
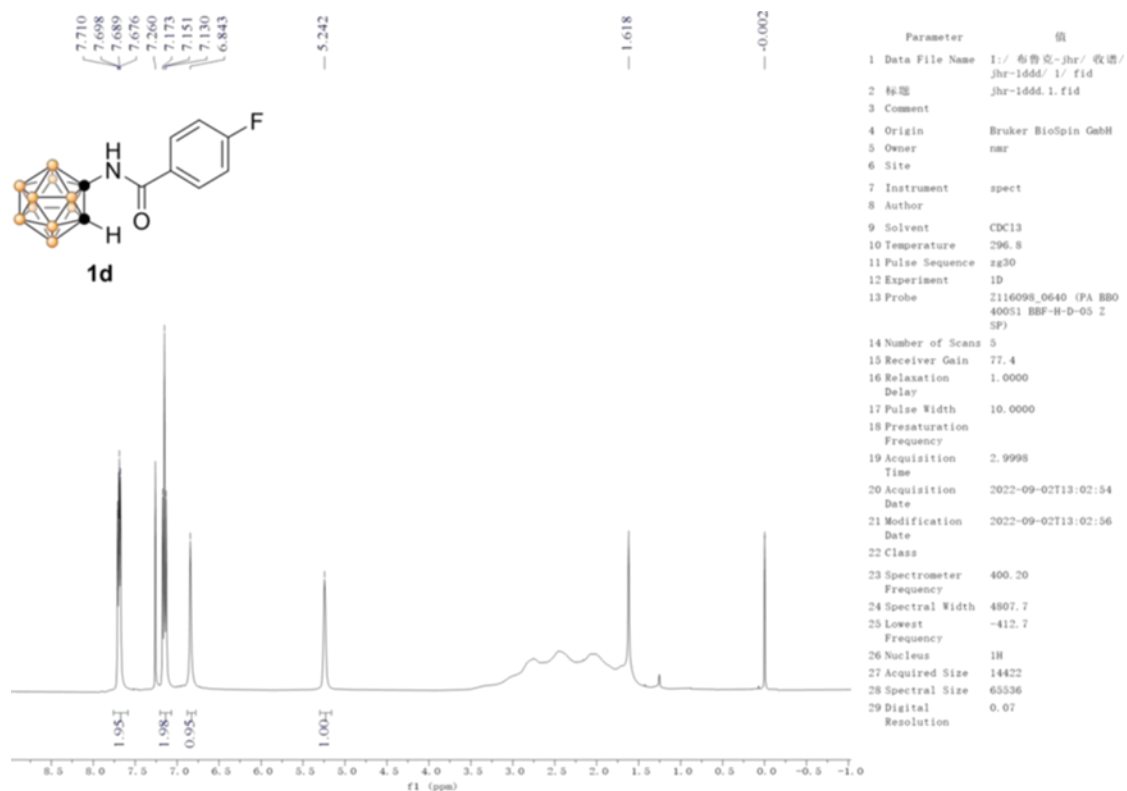


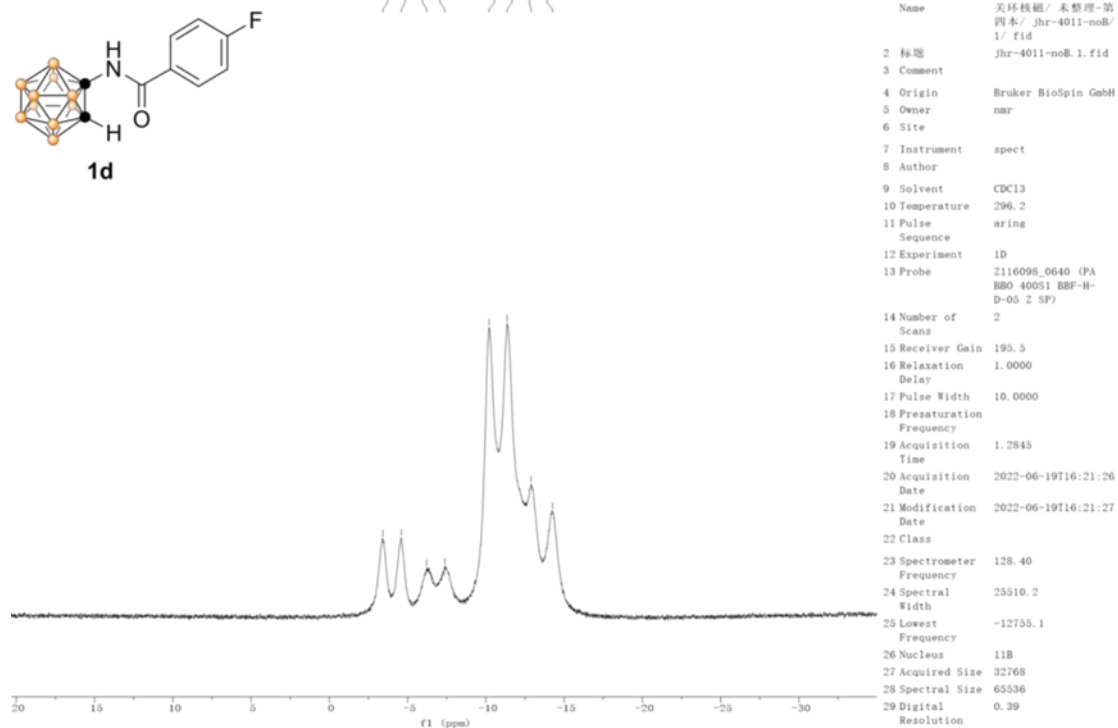
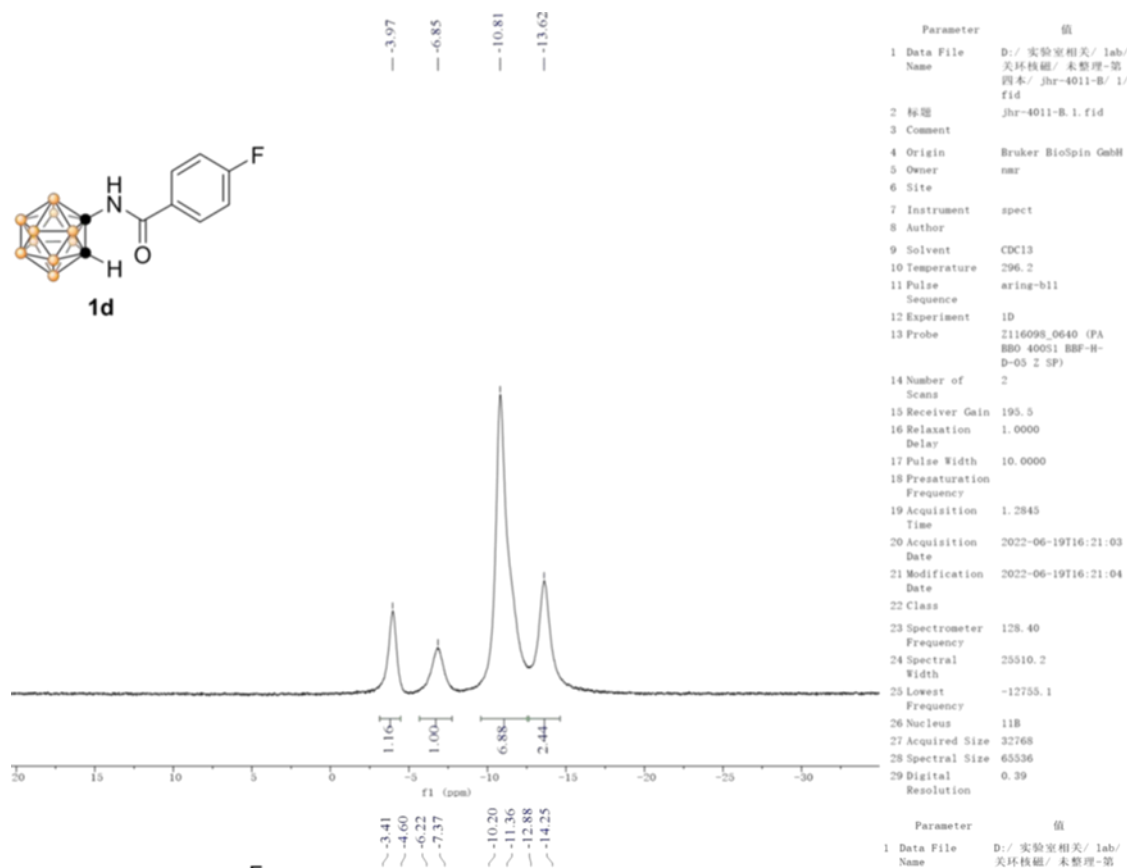
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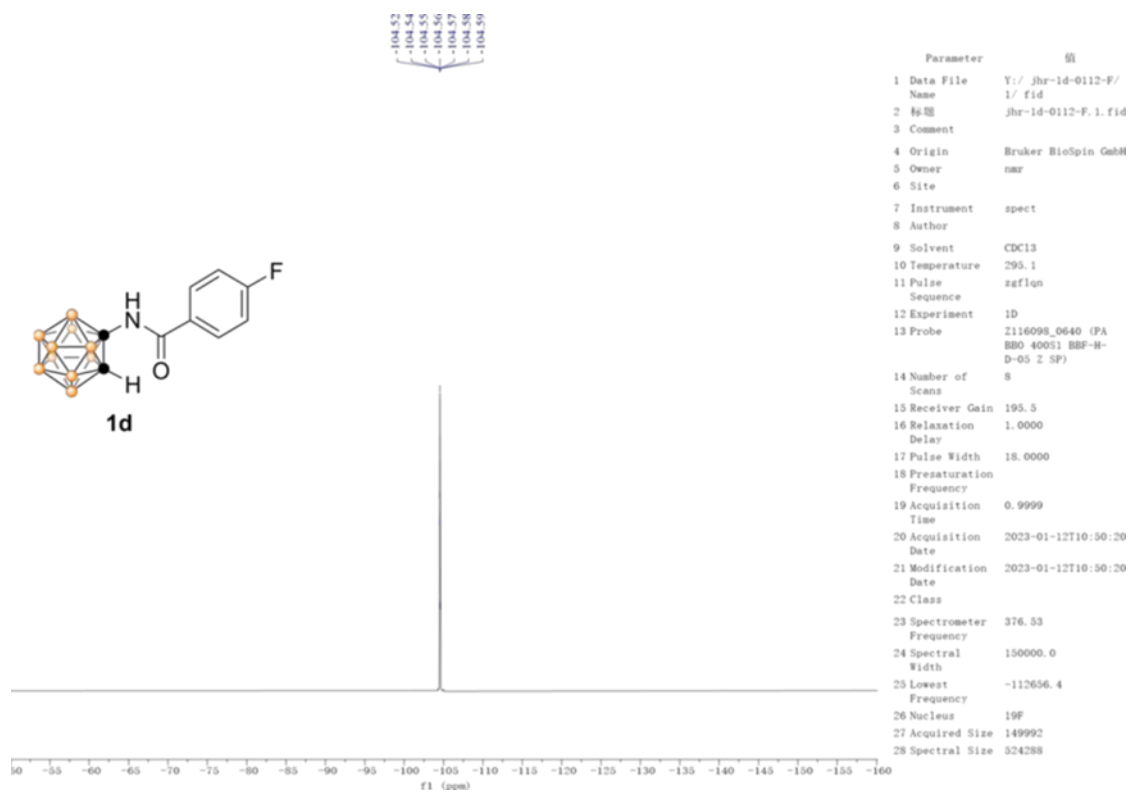


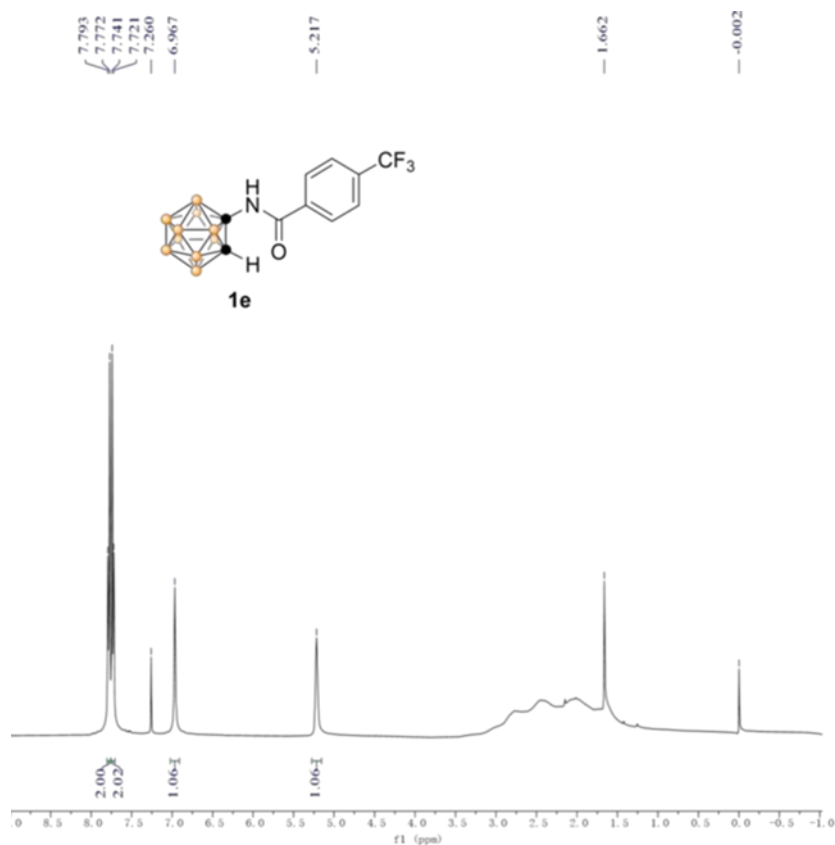
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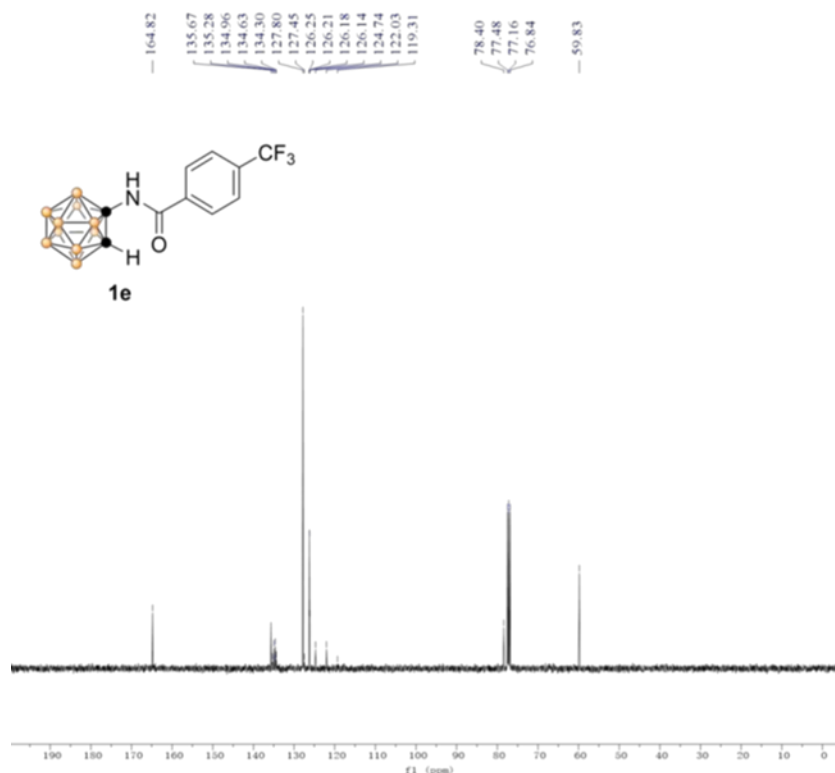




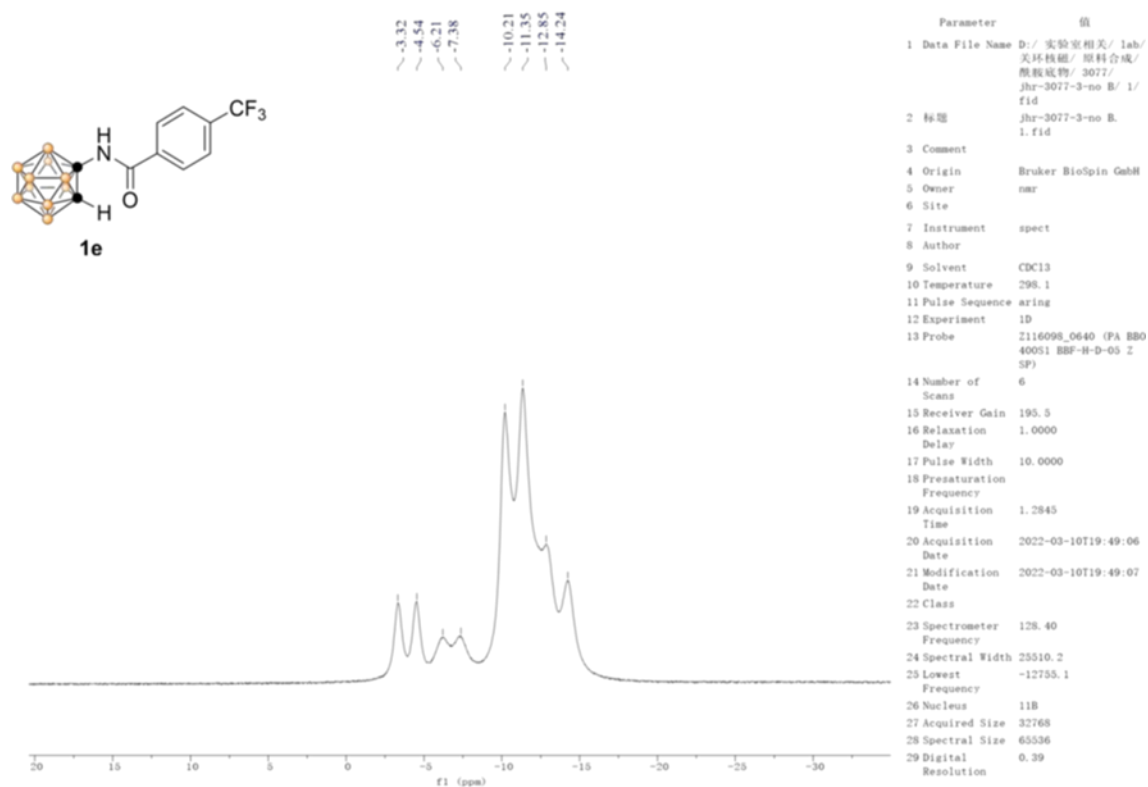
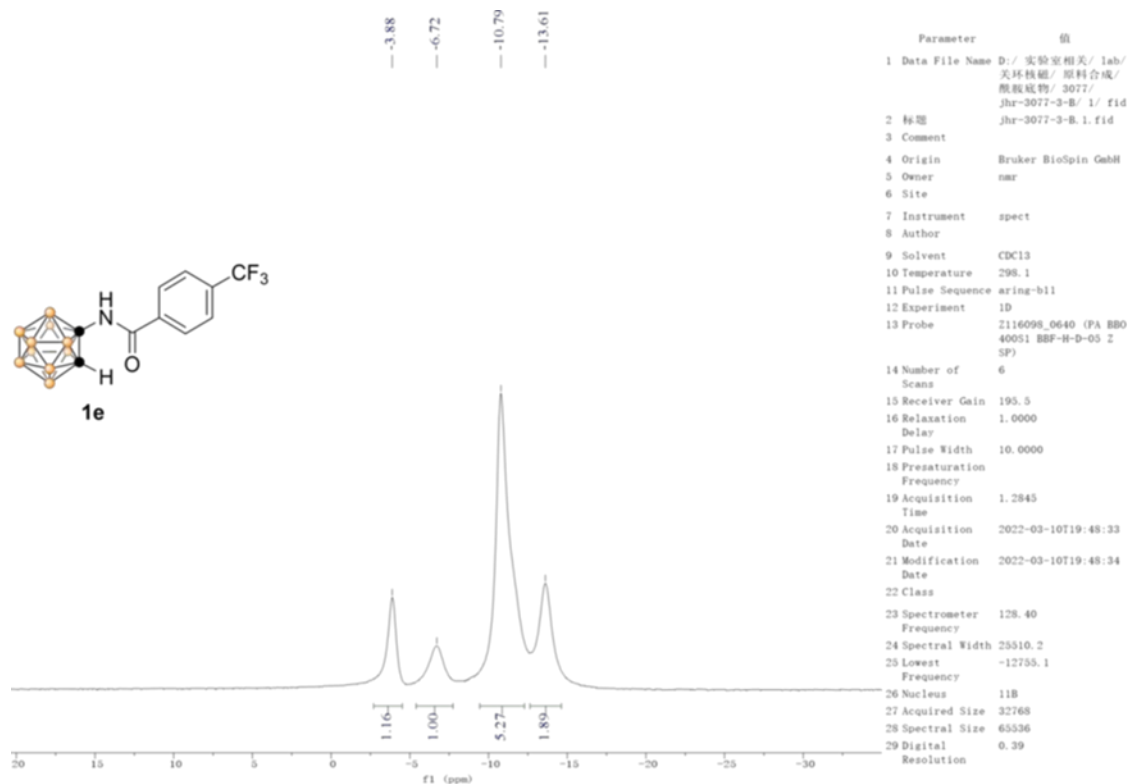


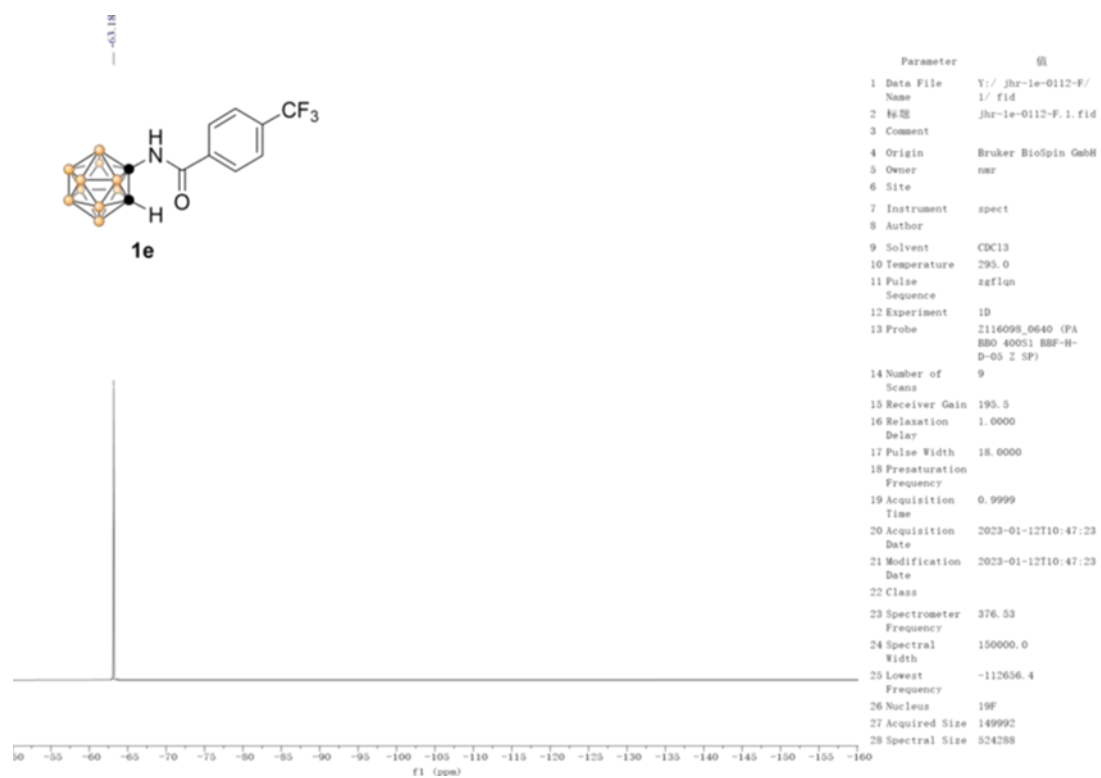


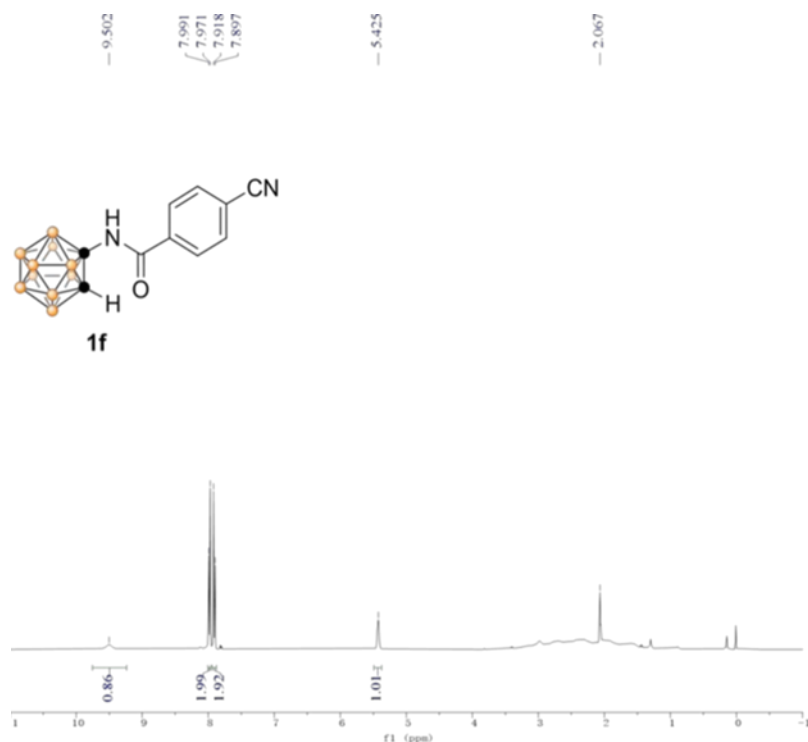
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2 标题	jhr-1e.4.f1d
3 Comment	
4 Origin	Bruker BioSpin GmbH
5 Owner	nmr
6 Site	
7 Instrument	spect
8 Author	
9 Solvent	CDCl3
10 Temperature	297.0
11 Pulse Sequence	zg30
12 Experiment	1D
13 Probe	Z116098_0640 (PA BB0 400S1 BPF-H-D-05 Z SP)
14 Number of Scans	5
15 Receiver Gain	77.4
16 Relaxation Delay	1.0000
17 Pulse Width	10.0000
18 Presaturation Frequency	
19 Acquisition Time	2.9998
20 Acquisition Date	2022-08-16T19:17:45
21 Modification Date	2022-08-16T19:17:46
22 Class	
23 Spectrometer Frequency	400.20
24 Spectral Width	4807.7
25 Lowest Frequency	-412.7
26 Nucleus	1H
27 Acquired Size	14422
28 Spectral Size	65536
29 Digital Resolution	0.07



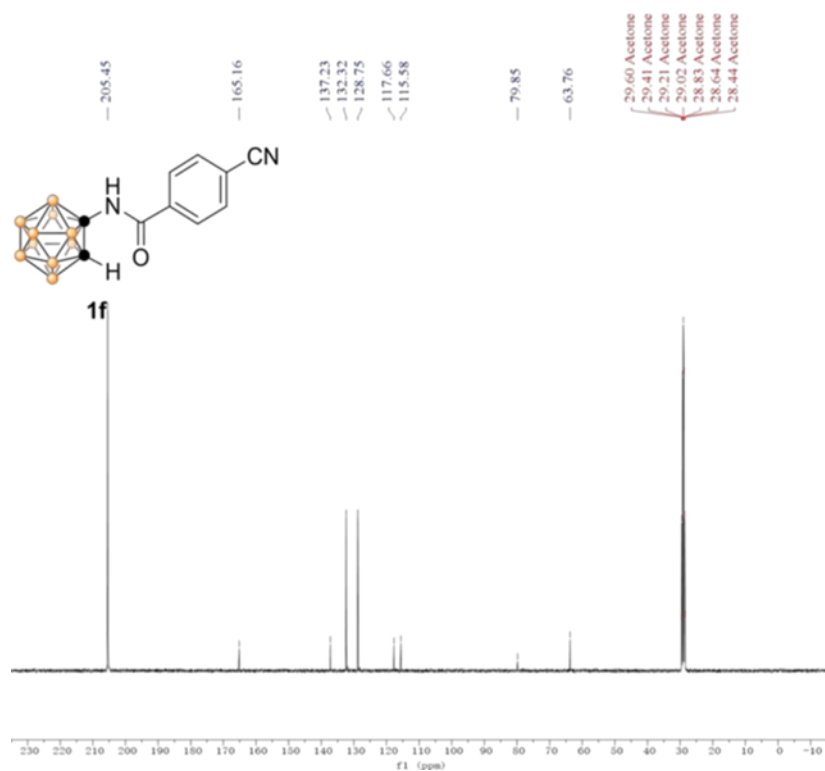
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1 Data File Name	E:/ 布鲁克-jhr/ 收通/ jhr-lee-C/ 1/ f1d
2 标题	jhr-lee-C.1.f1d
3 Comment	
4 Origin	Bruker BioSpin GmbH
5 Owner	nmr
6 Site	
7 Instrument	spect
8 Author	
9 Solvent	CDCl3
10 Temperature	297.2
11 Pulse Sequence	zgpg30
12 Experiment	1D
13 Probe	Z116098_0640 (PA BB0 400S1 BPF-H-D-05 Z SP)
14 Number of Scans	71
15 Receiver Gain	195.5
16 Relaxation Delay	1.0000
17 Pulse Width	10.0000
18 Presaturation Frequency	
19 Acquisition Time	1.2999
20 Acquisition Date	2022-08-17T19:38:01
21 Modification Date	2022-08-17T19:38:04
22 Class	
23 Spectrometer Frequency	100.64
24 Spectral Width	25252.5
25 Lowest Frequency	-1546.6
26 Nucleus	13C
27 Acquired Size	32827
28 Spectral Size	131072
29 Digital Resolution	0.19



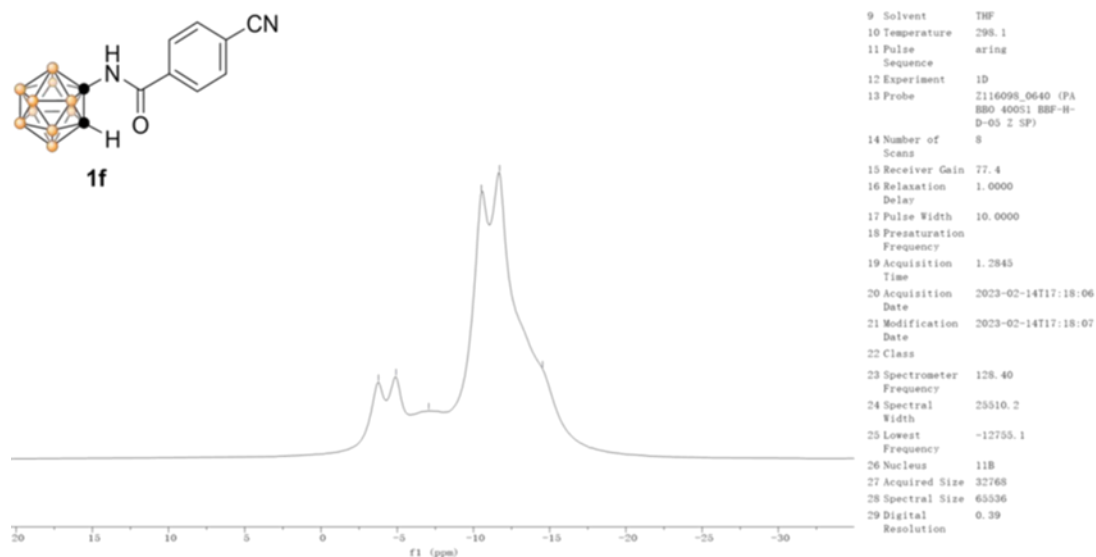
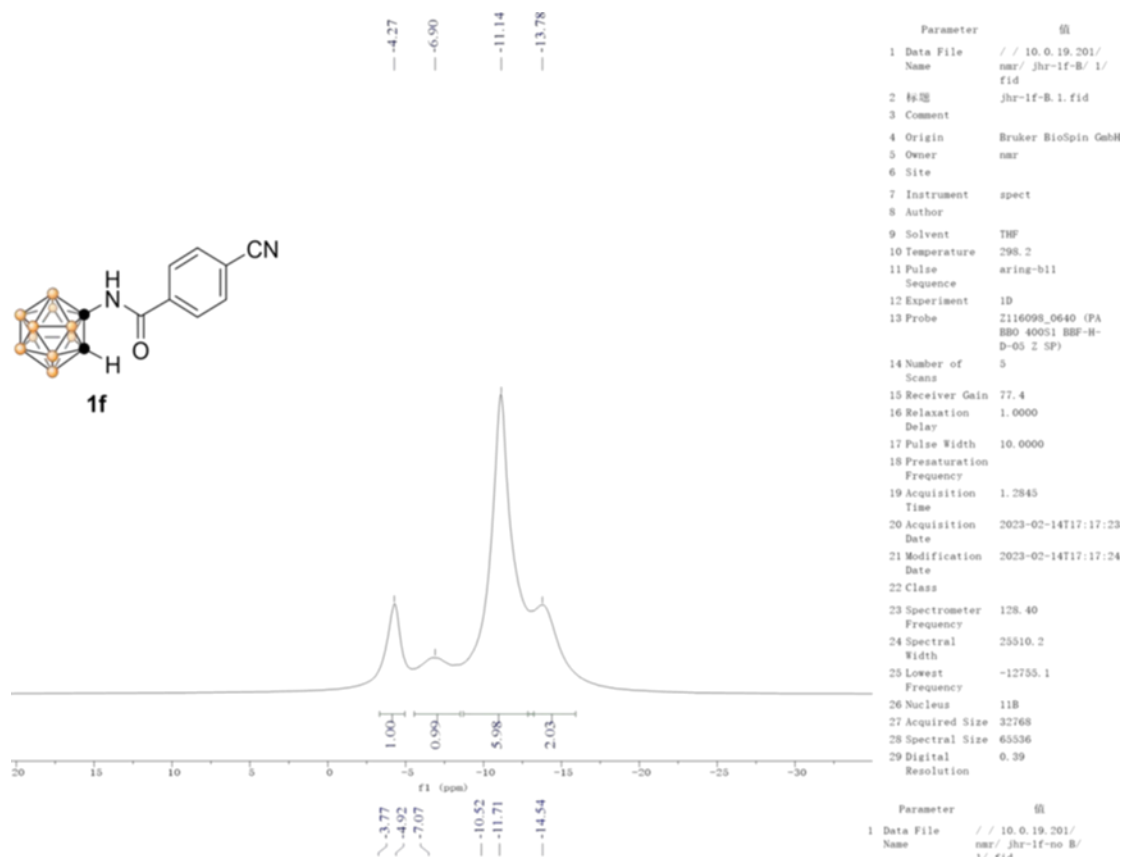


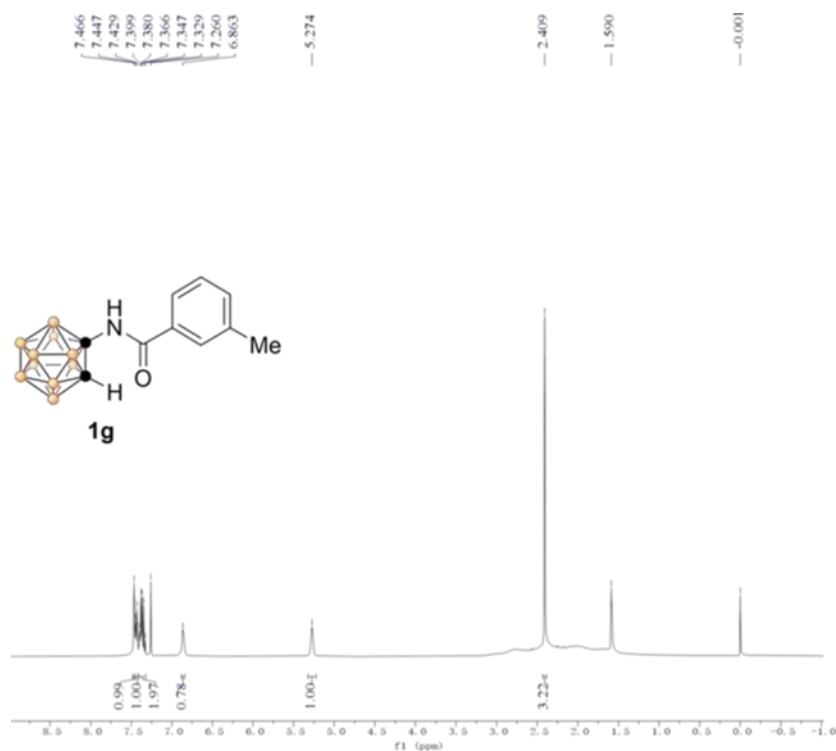


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1 Data File Name	Y:/ jhr-1f-0111-d-acetone/ 1/ f1d
2 标题	jhr-1f-0111-d-acetone.1.f1d
3 Comment	
4 Origin	Bruker BioSpin GmbH
5 Owner	nmr
6 Site	
7 Instrument	spect
8 Author	
9 Solvent	Acetone
10 Temperature	294.9
11 Pulse Sequence	zg30
12 Experiment	1D
13 Probe	2116098_0640 (PA BB0 400S1 BBF-H-D-05 2 SF)
14 Number of Scans	22
15 Receiver Gain	56.7
16 Relaxation Delay	1.0000
17 Pulse Width	10.0000
18 Presaturation Frequency	
19 Acquisition Time	2.9998
20 Acquisition Date	2023-01-11T12:47:33
21 Modification Date	2023-01-11T12:47:34
22 Class	
23 Spectrometer Frequency	400.20
24 Spectral Width	4807.7
25 Lowest Frequency	-402.8
26 Nucleus	1H
27 Acquired Size	14422
28 Spectral Size	65536

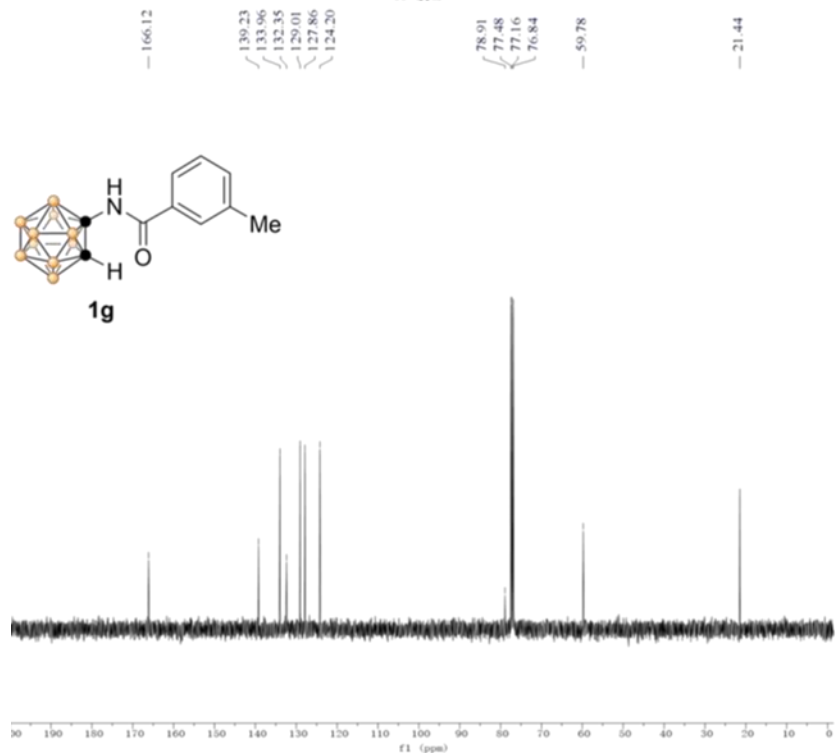


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1 Data File Name	Y:/ jhr-1f-0111-d-acetone-C/ 1/ f1d
2 标题	jhr-1f-0111-d-acetone-C.1.f1d
3 Comment	
4 Origin	Bruker BioSpin GmbH
5 Owner	nmr
6 Site	
7 Instrument	spect
8 Author	
9 Solvent	Acetone
10 Temperature	295.0
11 Pulse Sequence	zgpg30
12 Experiment	1D
13 Probe	2116098_0640 (PA BB0 400S1 BBF-H-D-05 2 SF)
14 Number of Scans	159
15 Receiver Gain	195.5
16 Relaxation Delay	1.0000
17 Pulse Width	10.0000
18 Presaturation Frequency	
19 Acquisition Time	1.2999
20 Acquisition Date	2023-01-11T12:56:13
21 Modification Date	2023-01-11T12:56:14
22 Class	
23 Spectrometer Frequency	100.64
24 Spectral Width	25252.5
25 Lowest Frequency	-1556.9
26 Nucleus	13C
27 Acquired Size	32827
28 Spectral Size	131072

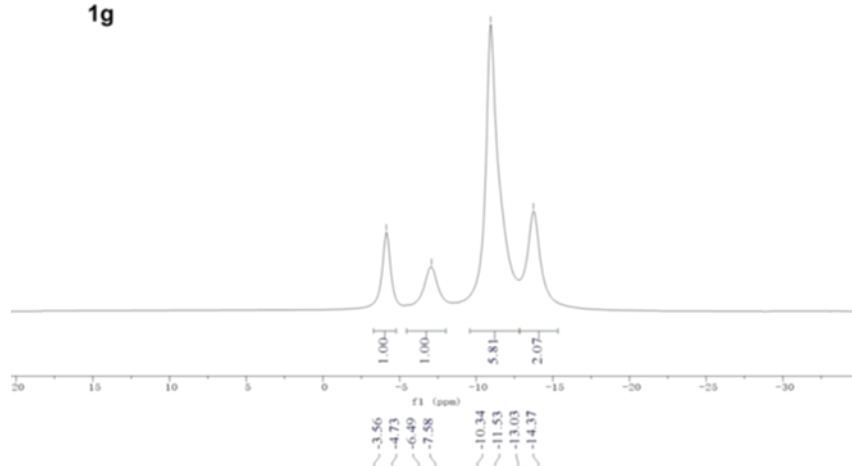




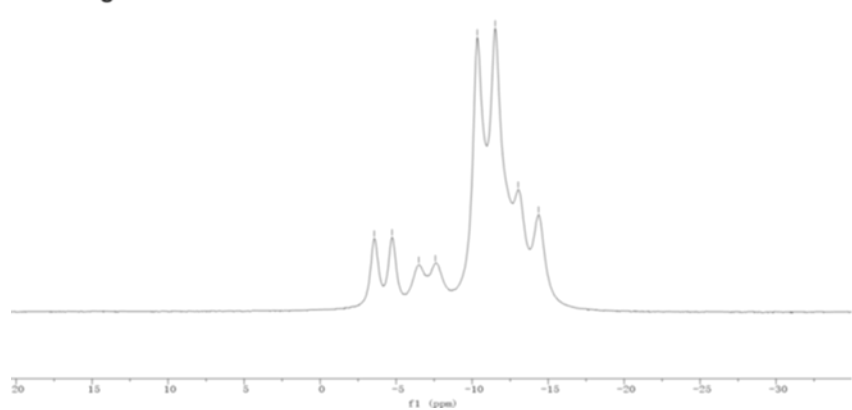
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2 标题	jhr-1g.6.fid
3 Comment	
4 Origin	Bruker BioSpin GmbH
5 Owner	nmr
6 Site	
7 Instrument	spect
8 Author	
9 Solvent	CDCl3
10 Temperature	297.1
11 Pulse Sequence	zg30
12 Experiment	1D
13 Probe	Z116098_0640 (PA BB0 400S1 BRF-H-D-05 Z SP)
14 Number of Scans	5
15 Receiver Gain	77.4
16 Relaxation Delay	1.0000
17 Pulse Width	10.0000
18 Presaturation Frequency	
19 Acquisition Time	2.9998
20 Acquisition Date	2022-08-16T19:23:46
21 Modification Date	2022-08-16T19:23:46
22 Class	
23 Spectrometer Frequency	400.20
24 Spectral Width	4907.7
25 Lowest Frequency	-412.9
26 Nucleus	1H
27 Acquired Size	14422
28 Spectral Size	65536
29 Digital Resolution	0.07



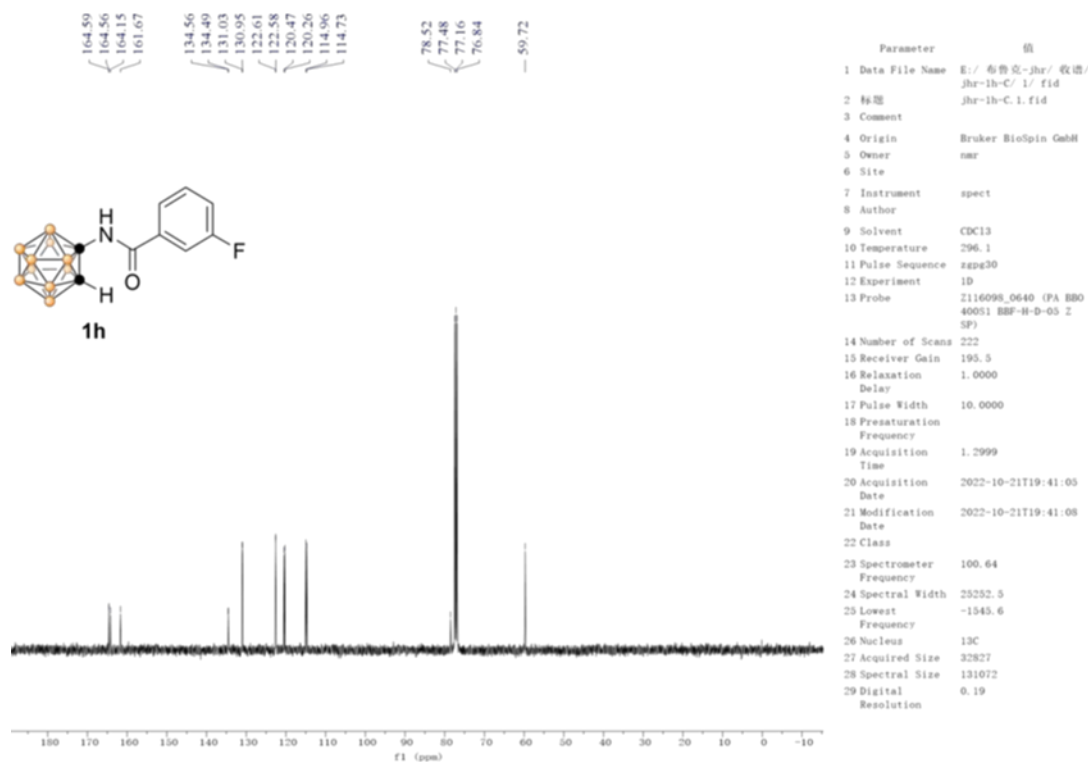
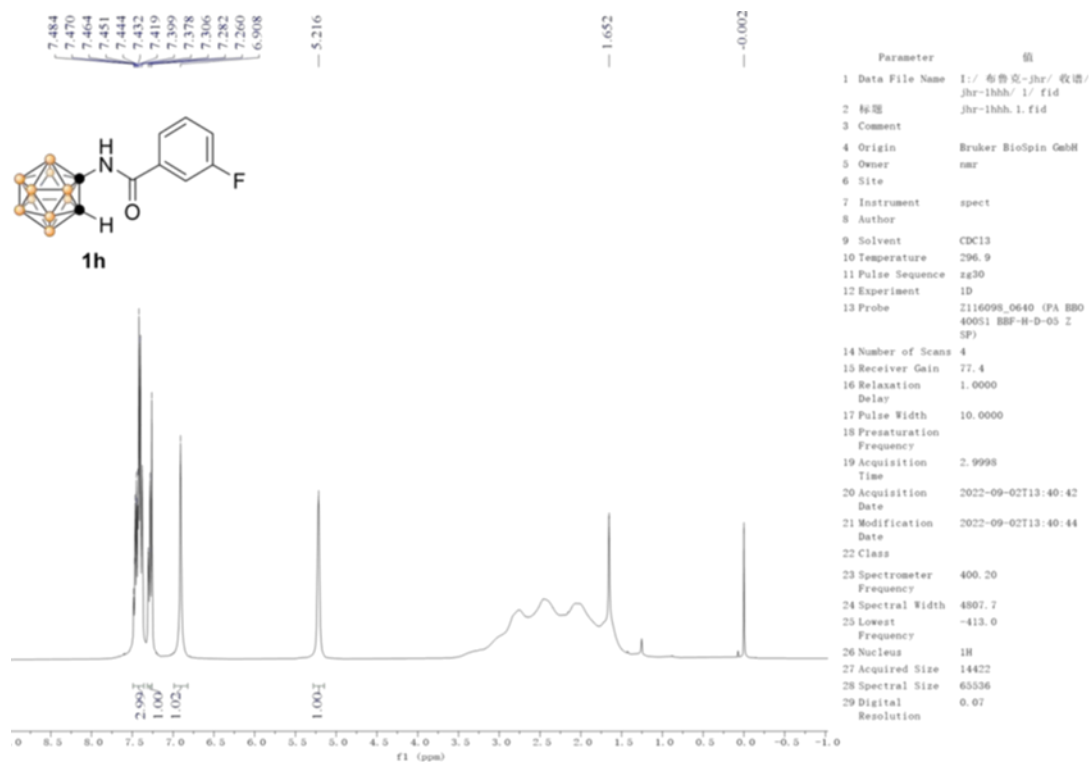
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2 标题	jhr-1g-C.1.fid
3 Comment	
4 Origin	Bruker BioSpin GmbH
5 Owner	nmr
6 Site	
7 Instrument	spect
8 Author	
9 Solvent	CDCl3
10 Temperature	297.2
11 Pulse Sequence	zgpg30
12 Experiment	1D
13 Probe	Z116098_0640 (PA BB0 400S1 BRF-H-D-05 Z SP)
14 Number of Scans	16
15 Receiver Gain	195.5
16 Relaxation Delay	1.0000
17 Pulse Width	10.0000
18 Presaturation Frequency	
19 Acquisition Time	1.2999
20 Acquisition Date	2022-08-17T19:41:29
21 Modification Date	2022-08-17T19:41:29
22 Class	
23 Spectrometer Frequency	100.64
24 Spectral Width	25252.5
25 Lowest Frequency	-1547.7
26 Nucleus	13C
27 Acquired Size	32827
28 Spectral Size	131072
29 Digital Resolution	0.19

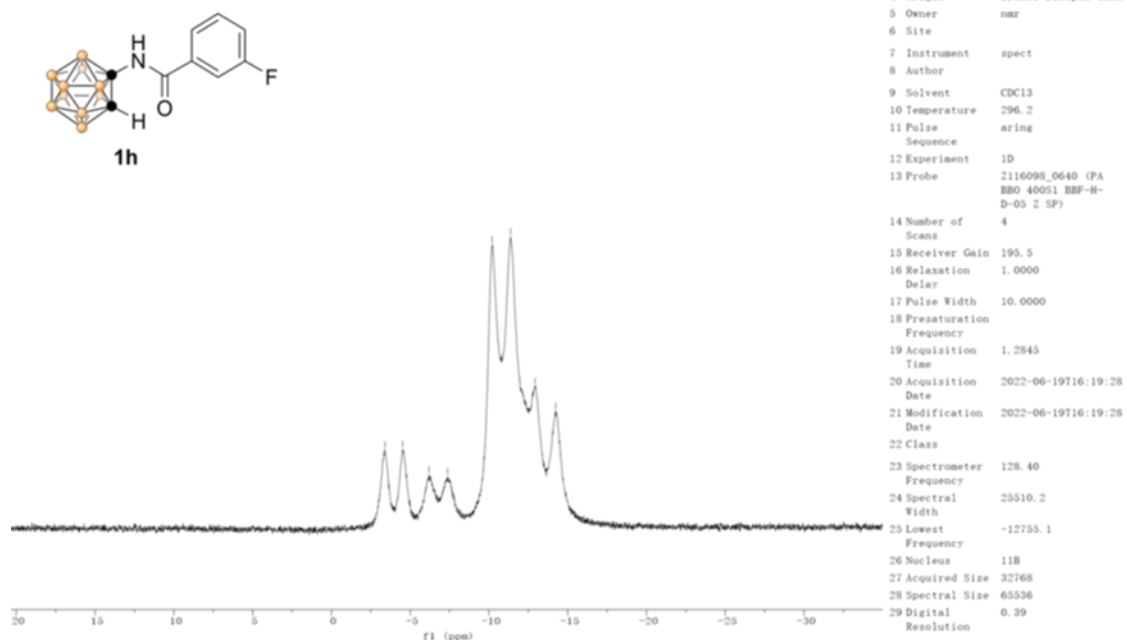
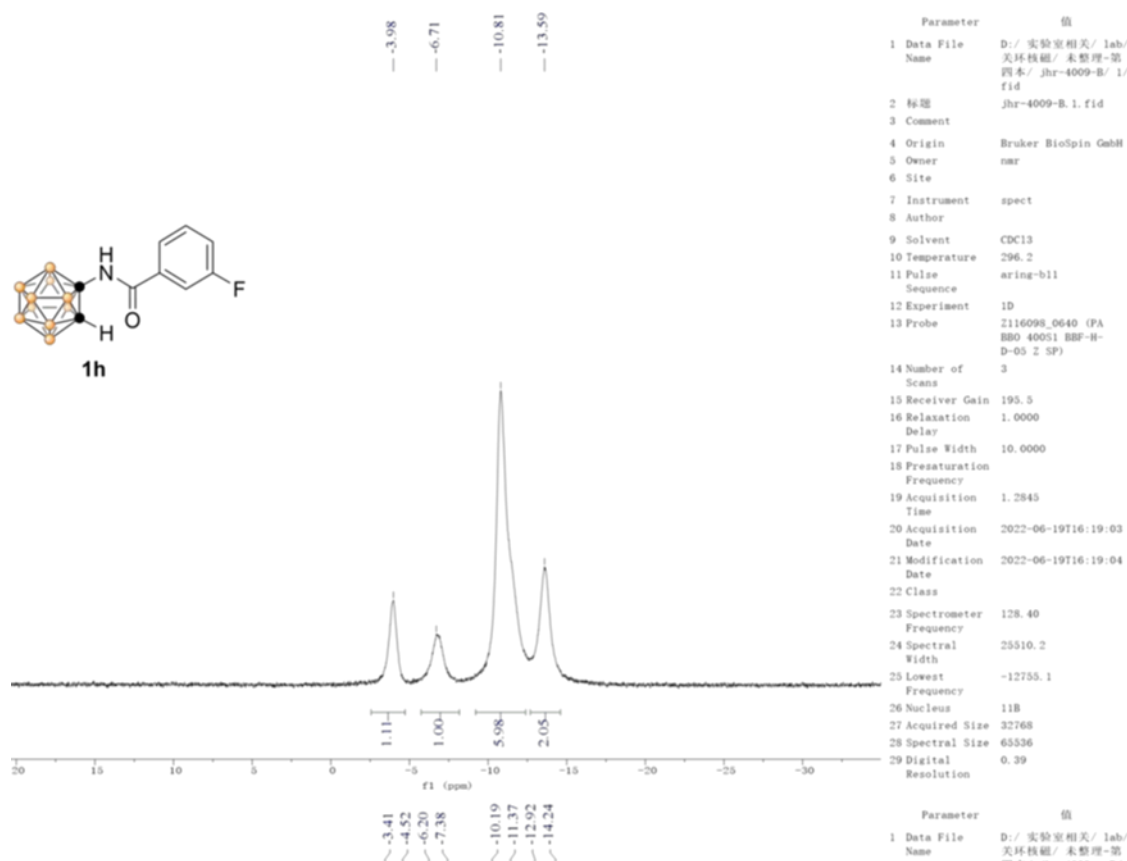


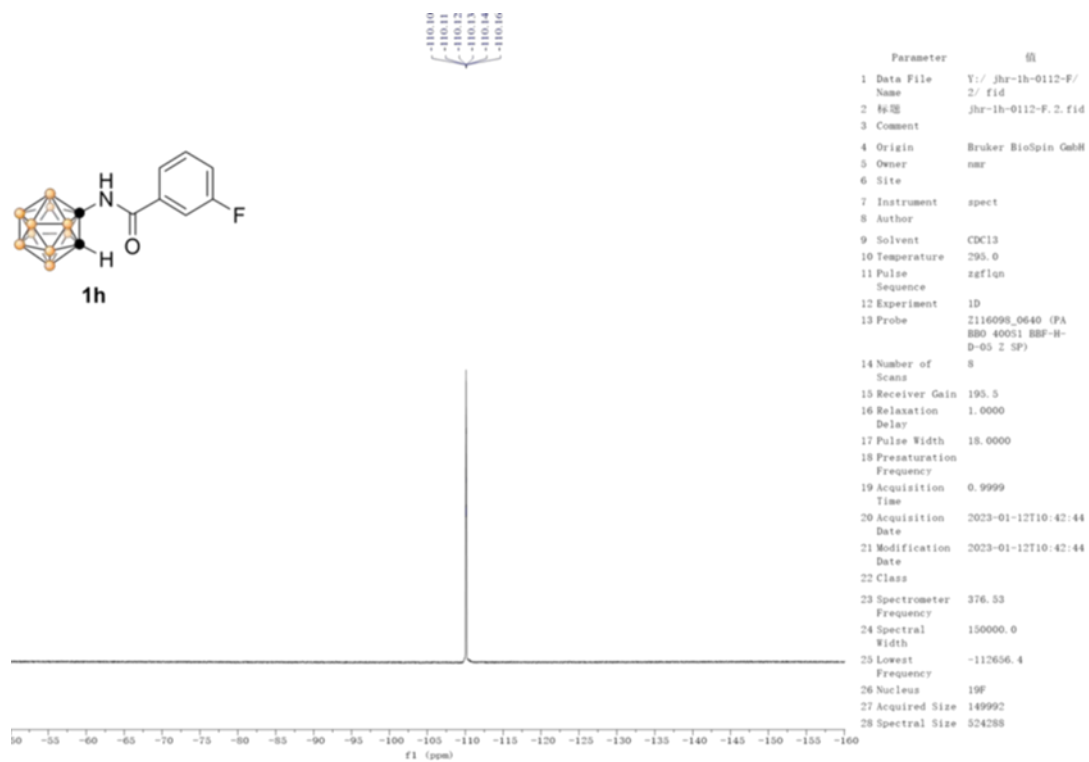
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2 标题	jhr-1g-0112-deB.1.f1d
3 Comment	
4 Origin	Bruker BioSpin GmbH
5 Owner	nmr
6 Site	
7 Instrument	spect
8 Author	
9 Solvent	C6D6
10 Temperature	295.0
11 Pulse Sequence	aring-b11
12 Experiment	1D
13 Probe	211609S_0640 (PA BB0 400S1 BBF-H- D-03 2 SP)
14 Number of Scans	8
15 Receiver Gain	195.5
16 Relaxation Delay	1.0000
17 Pulse Width	10.0000
18 Presaturation Frequency	
19 Acquisition Time	1.2845
20 Acquisition Date	2023-01-12T09:46:20
21 Modification Date	2023-01-12T09:46:21
22 Class	
23 Spectrometer Frequency	128.40
24 Spectral Width	23510.2
25 Lowest Frequency	-12735.1
26 Nucleus	1H
27 Acquired Size	32768
28 Spectral Size	65336

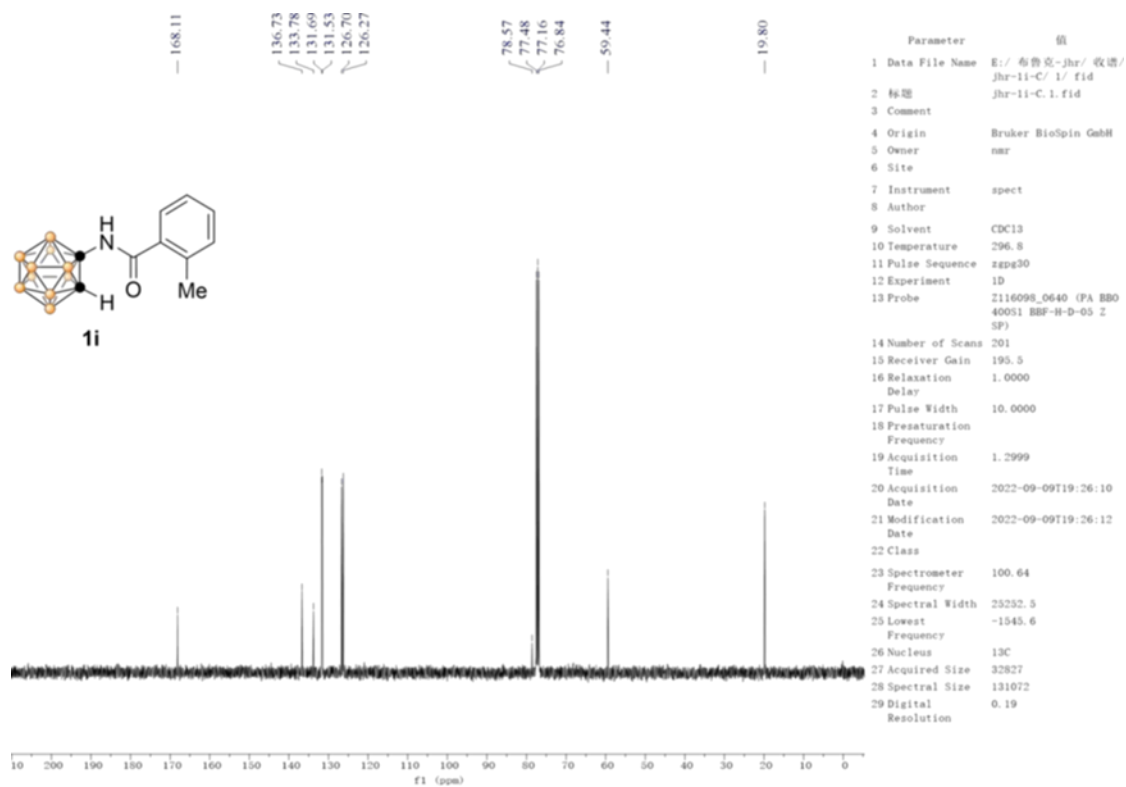
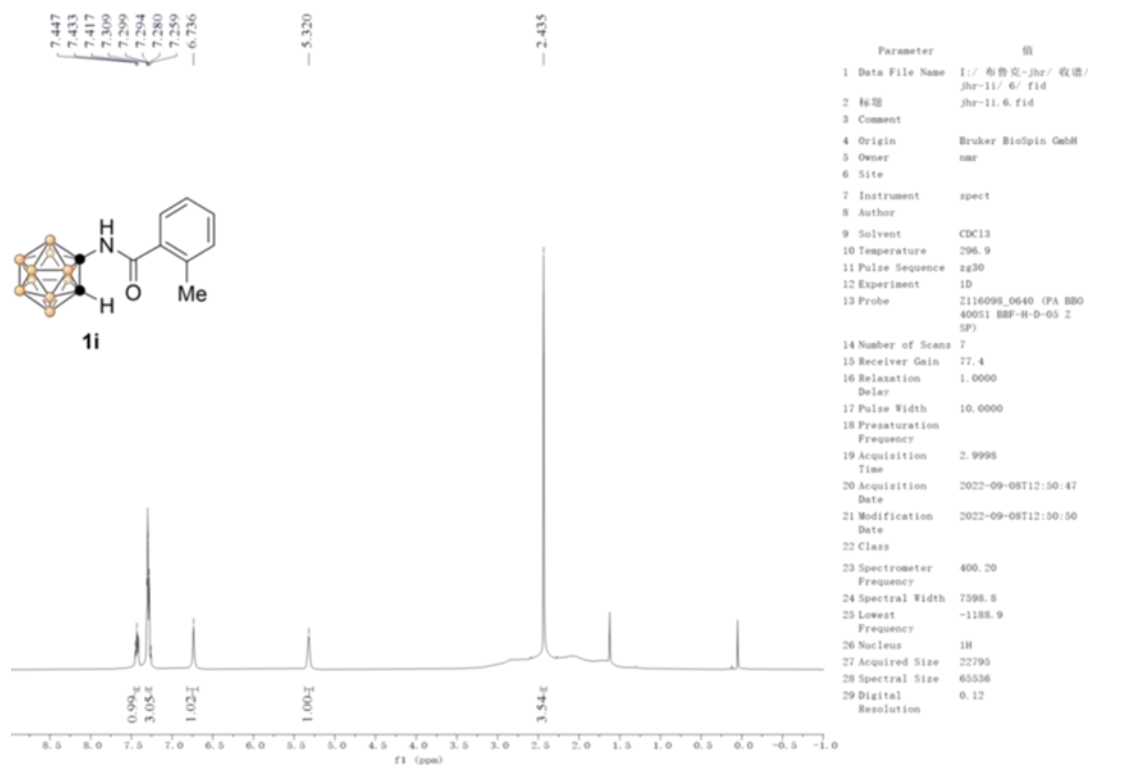


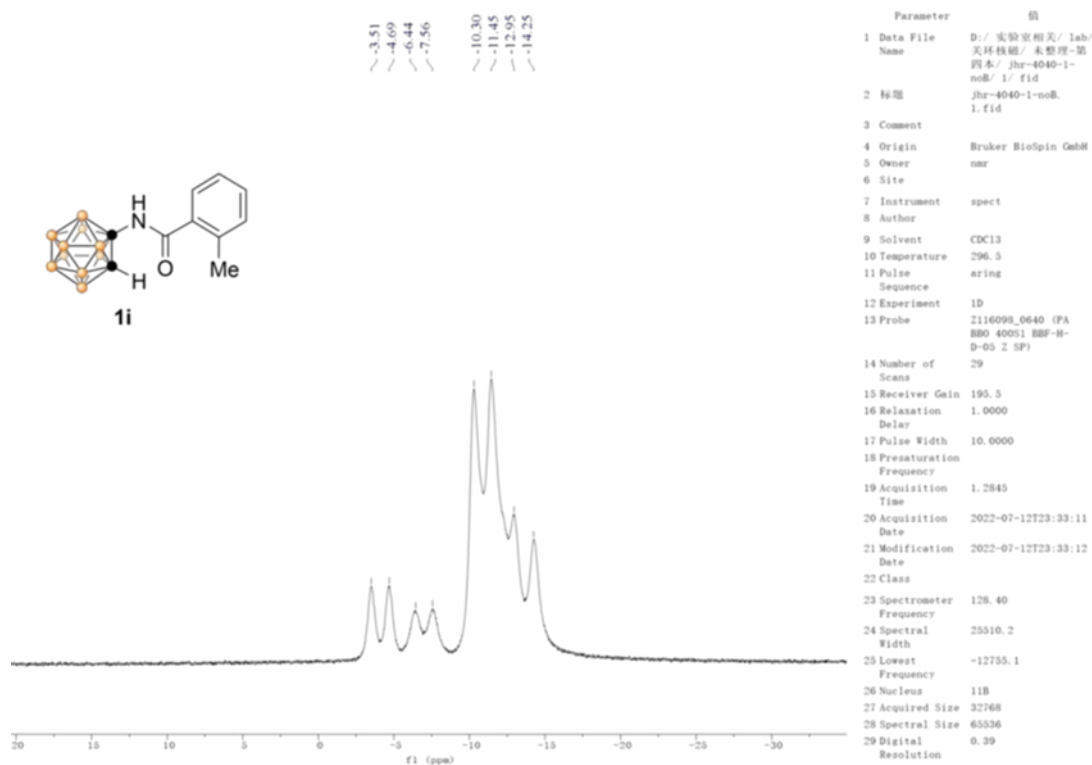
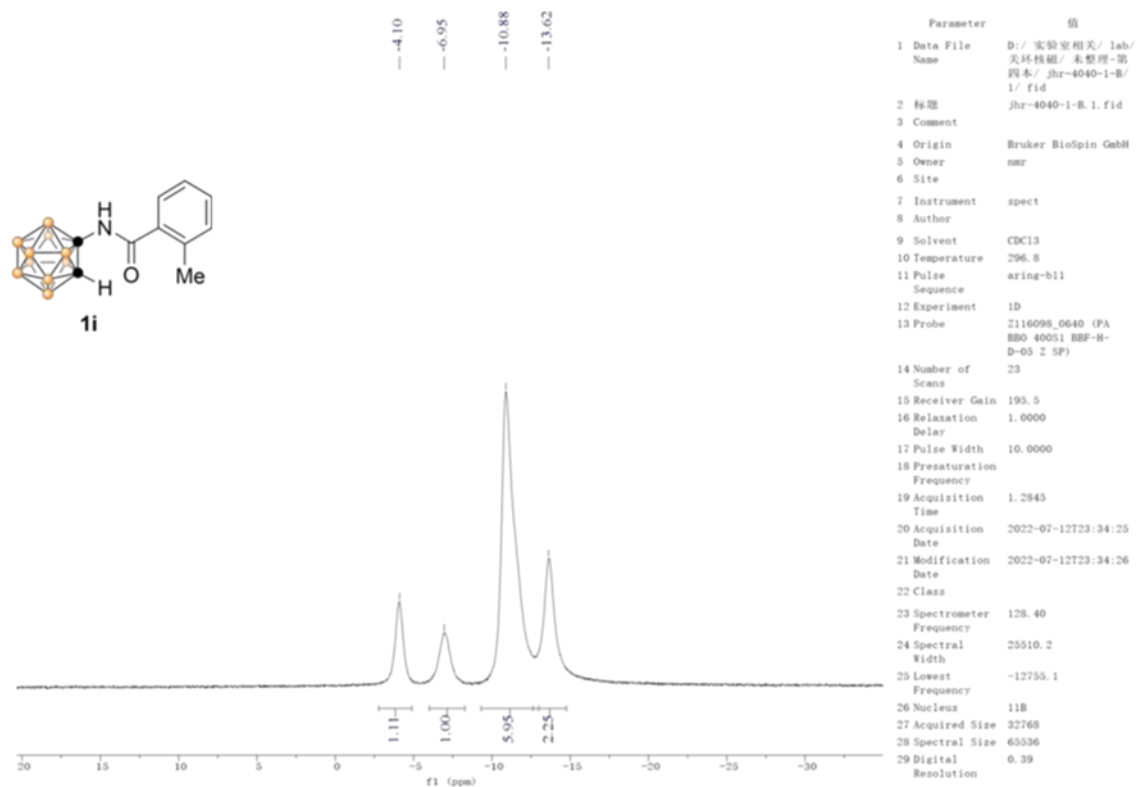
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2 标题	jhr-1g-0112-no deB. 1.fid
3 Comment	
4 Origin	Bruker BioSpin GmbH
5 Owner	nmr
6 Site	
7 Instrument	spect
8 Author	
9 Solvent	C6D6
10 Temperature	295.0
11 Pulse Sequence	aring
12 Experiment	1D
13 Probe	216098_0640 (PA RBO 400S1 BRF-H- D-05 2 SP)
14 Number of Scans	11
15 Receiver Gain	195.5
16 Relaxation Delay	1.0000
17 Pulse Width	10.0000
18 Presaturation Frequency	
19 Acquisition Time	1.2845
20 Acquisition Date	2023-01-12T09:45:42
21 Modification Date	2023-01-12T09:45:43
22 Class	
23 Spectrometer Frequency	128.40
24 Spectral Width	25510.2
25 Lowest Frequency	-12755.1
26 Nucleus	1H
27 Acquired Size	32768
28 Spectral Size	65356

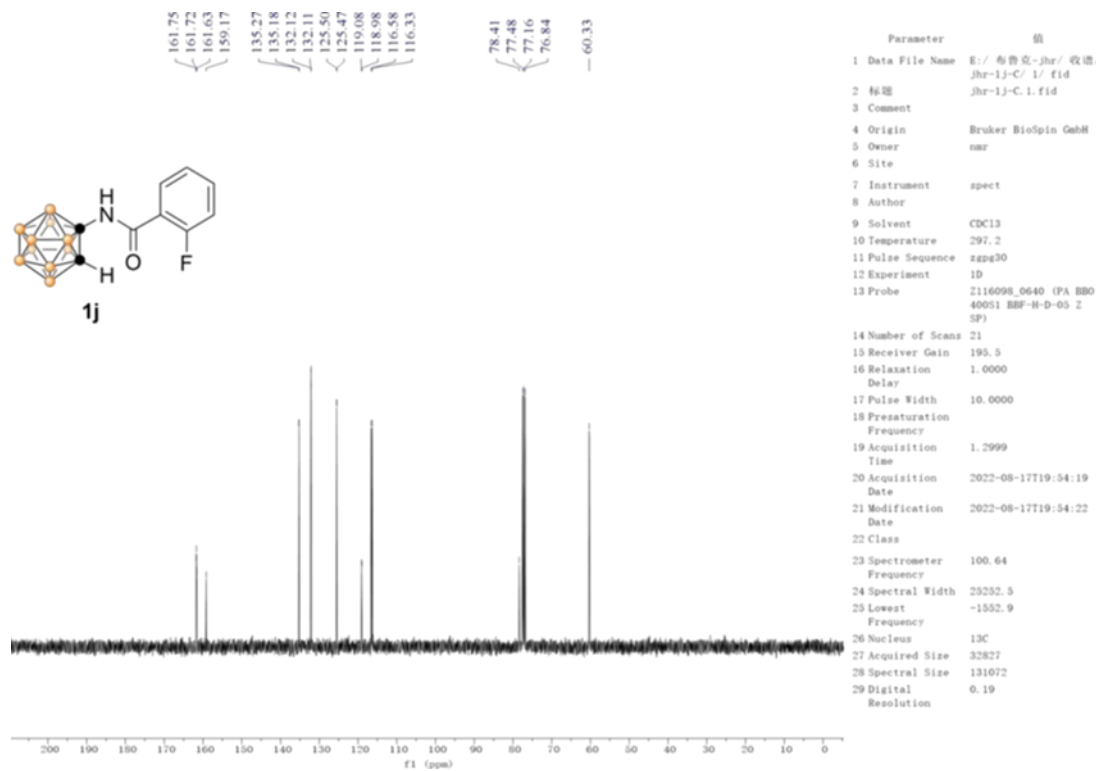
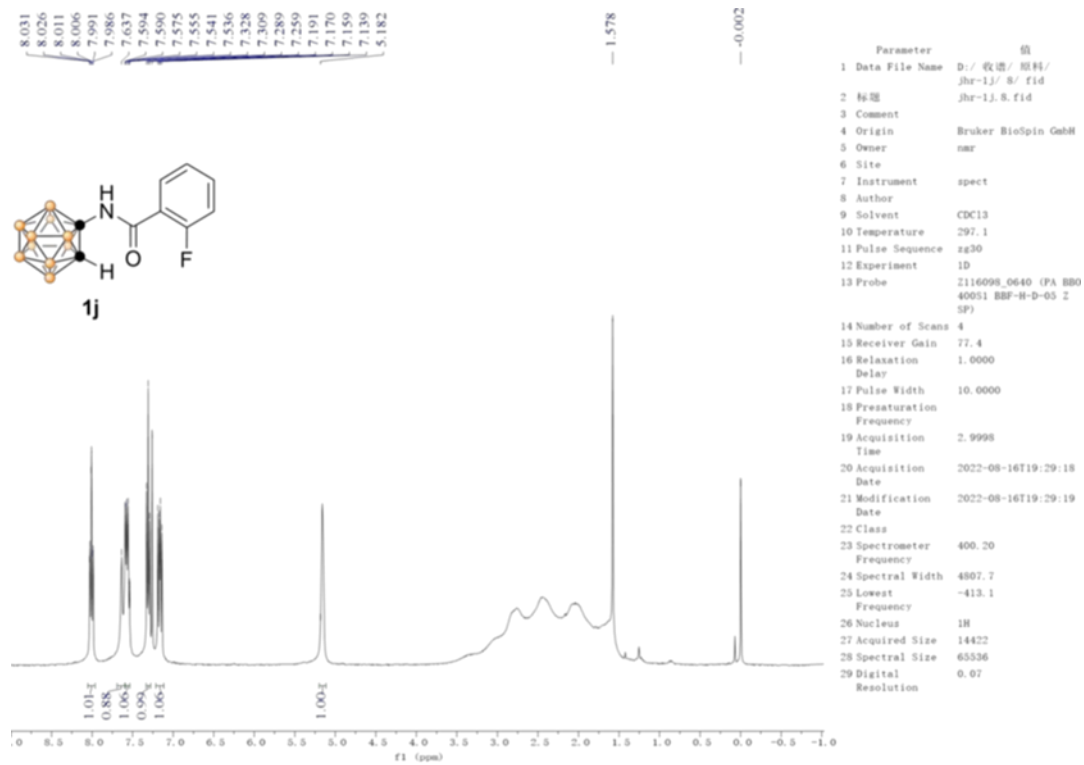


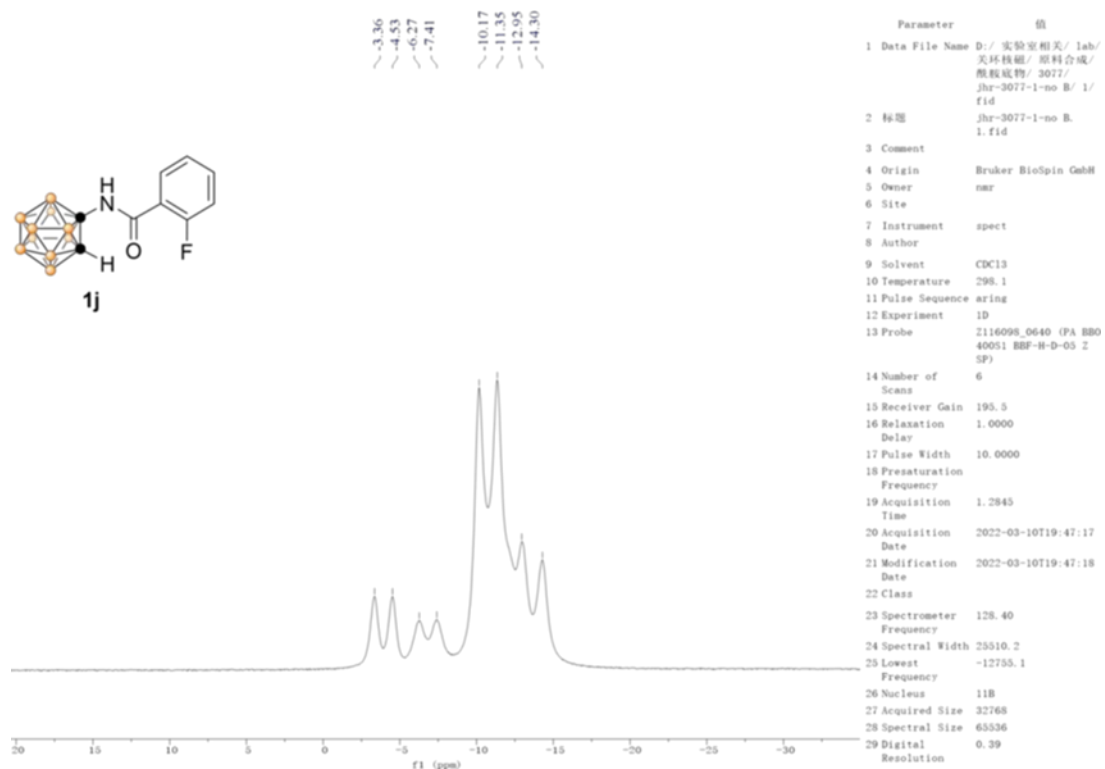
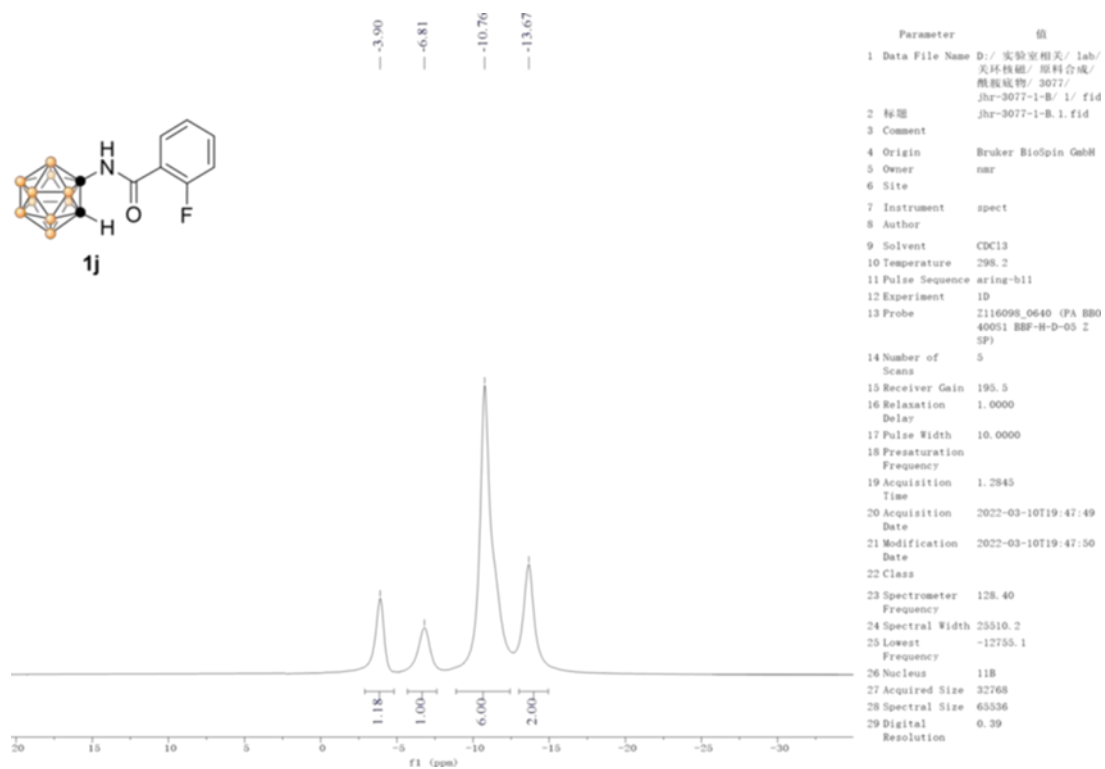


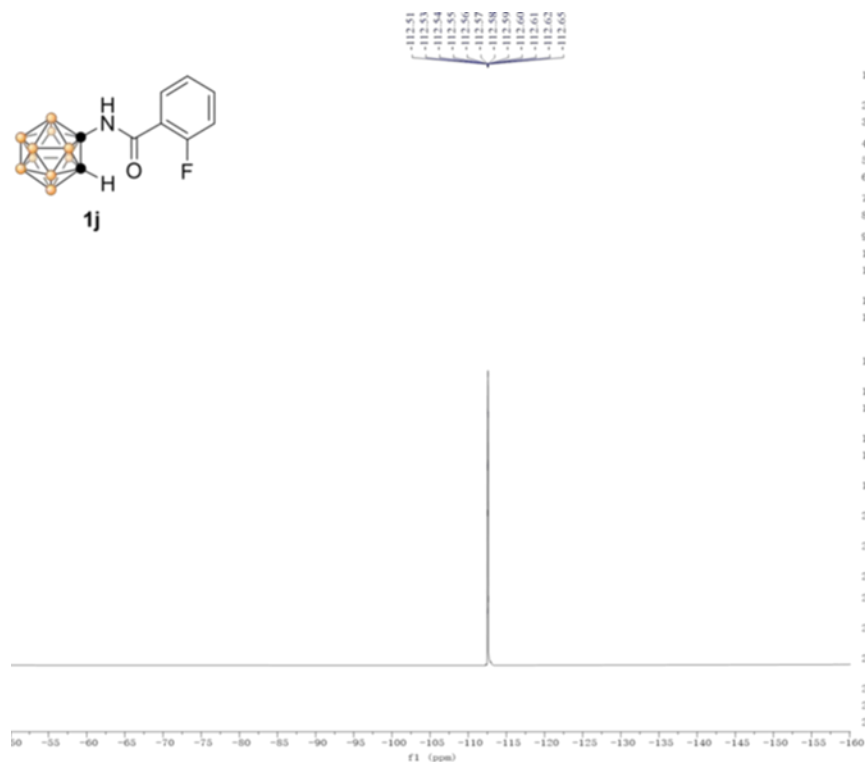
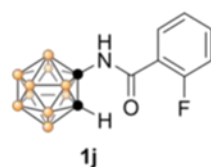




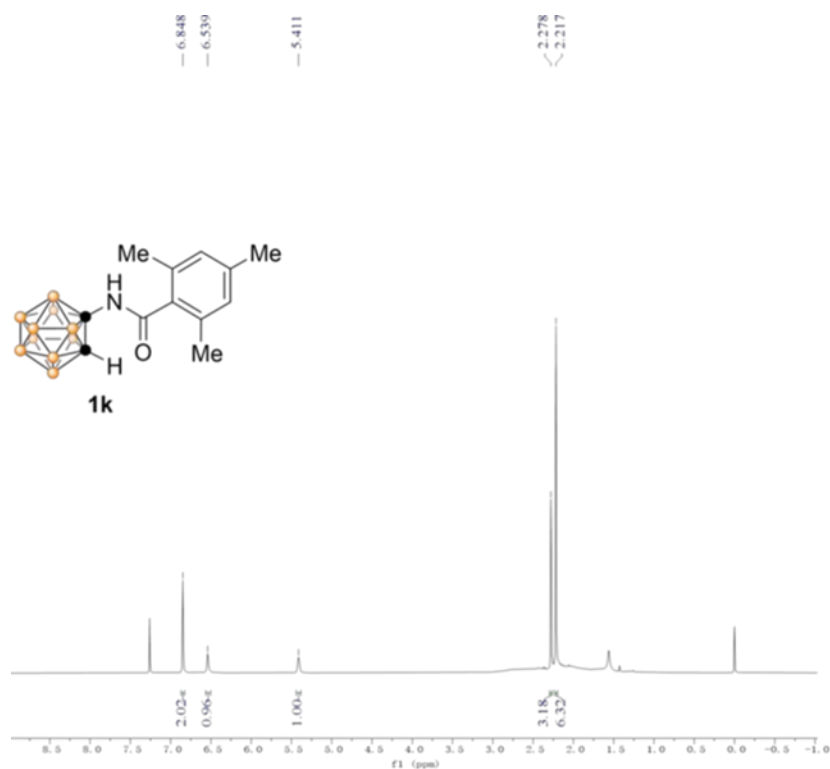




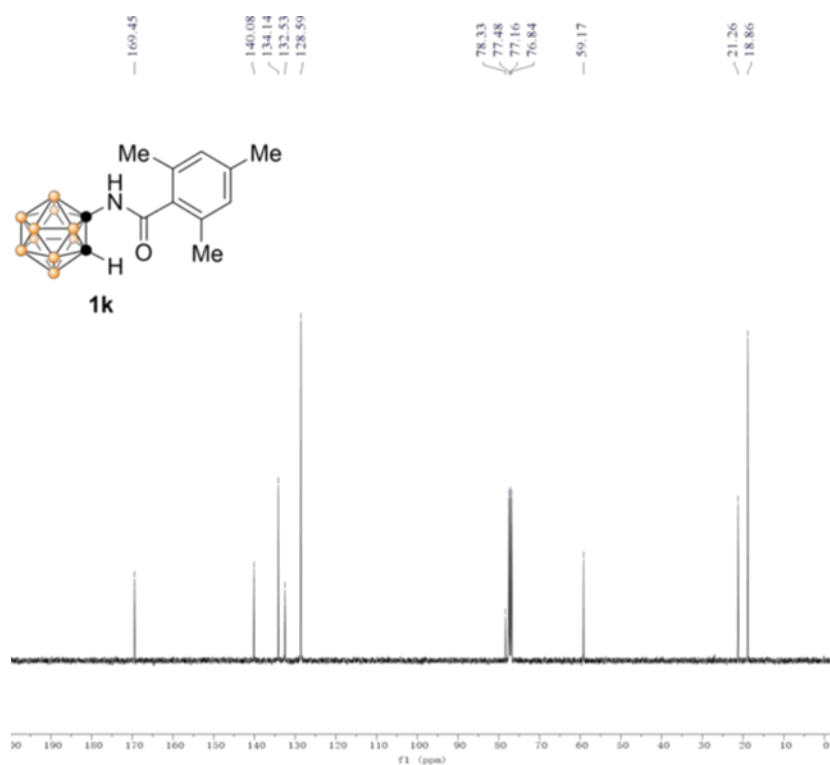




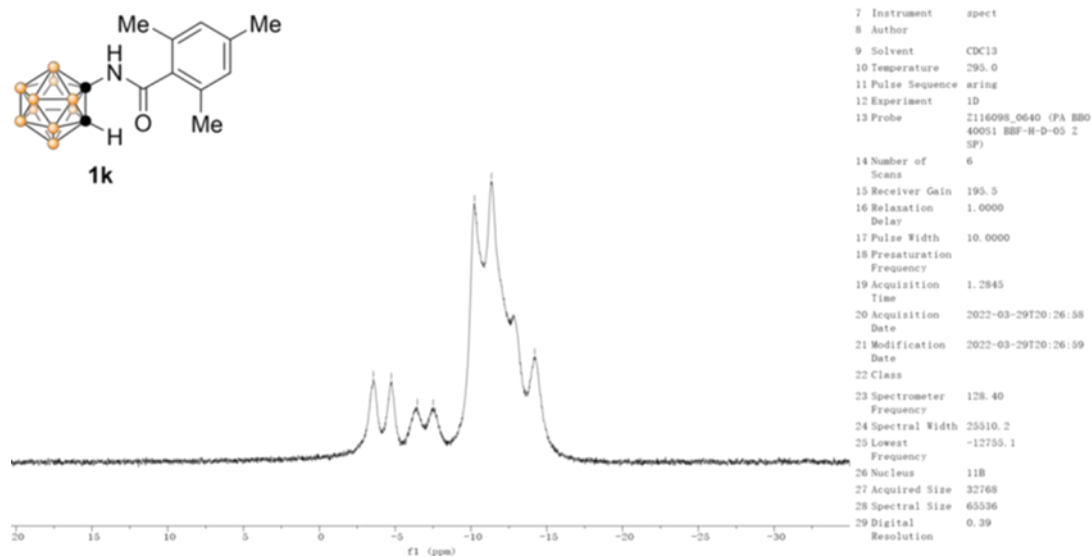
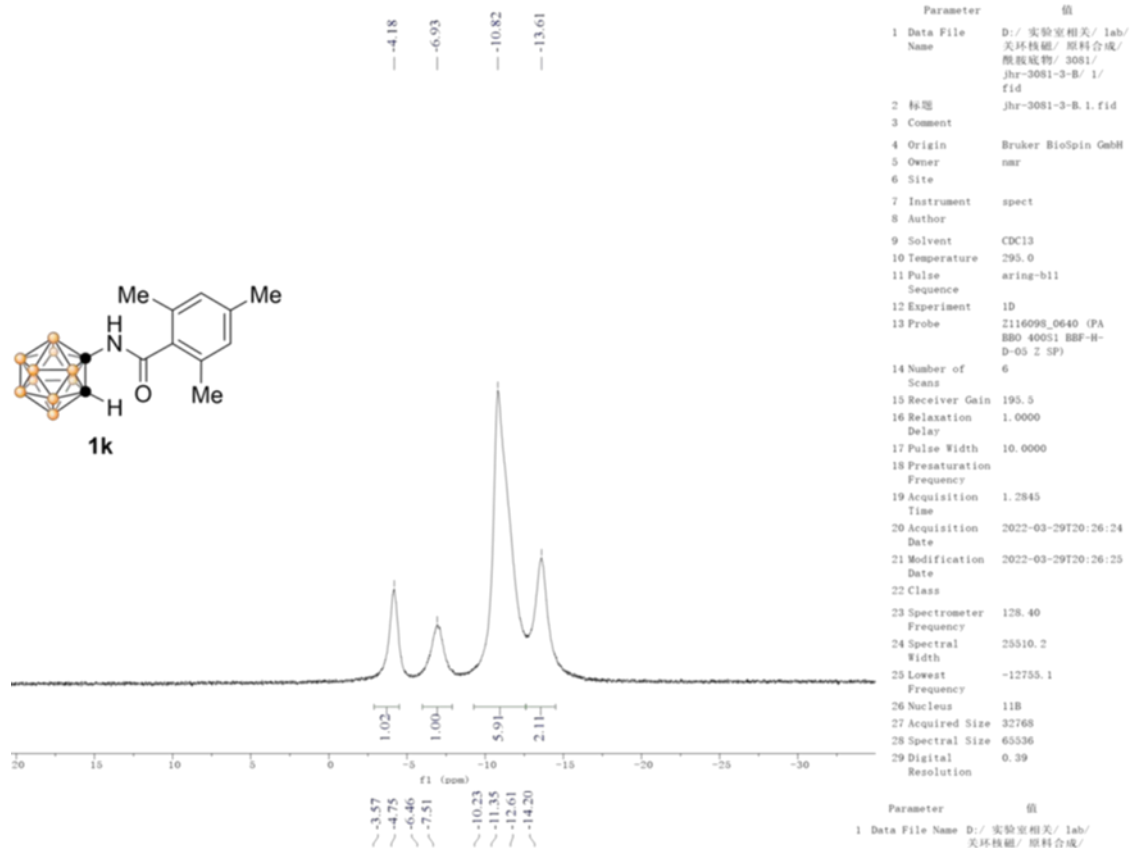
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Name	1/ f1d
2 标题	jhr-1j-0112-F.1.f1d
3 Comment	
4 Origin	Bruker BioSpin GmbH
5 Owner	nmr
6 Site	
7 Instrument	spect
8 Author	
9 Solvent	CDCl3
10 Temperature	295.1
11 Pulse Sequence	zgfgqn
12 Experiment	1D
13 Probe	2116098_0640 (PA BBO 400S1 BBSF-H- D-05 Z SP)
14 Number of Scans	15
15 Receiver Gain	195.5
16 Relaxation Delay	1.0000
17 Pulse Width	18.0000
18 Presaturation Frequency	
19 Acquisition Time	0.9999
20 Acquisition Date	2023-01-12T10:45:08
21 Modification Date	2023-01-12T10:45:08
22 Class	
23 Spectrometer Frequency	376.53
24 Spectral Width	150000.0
25 Lowest Frequency	-112656.4
26 Nucleus	19F
27 Acquired Size	149992
28 Spectral Size	524288

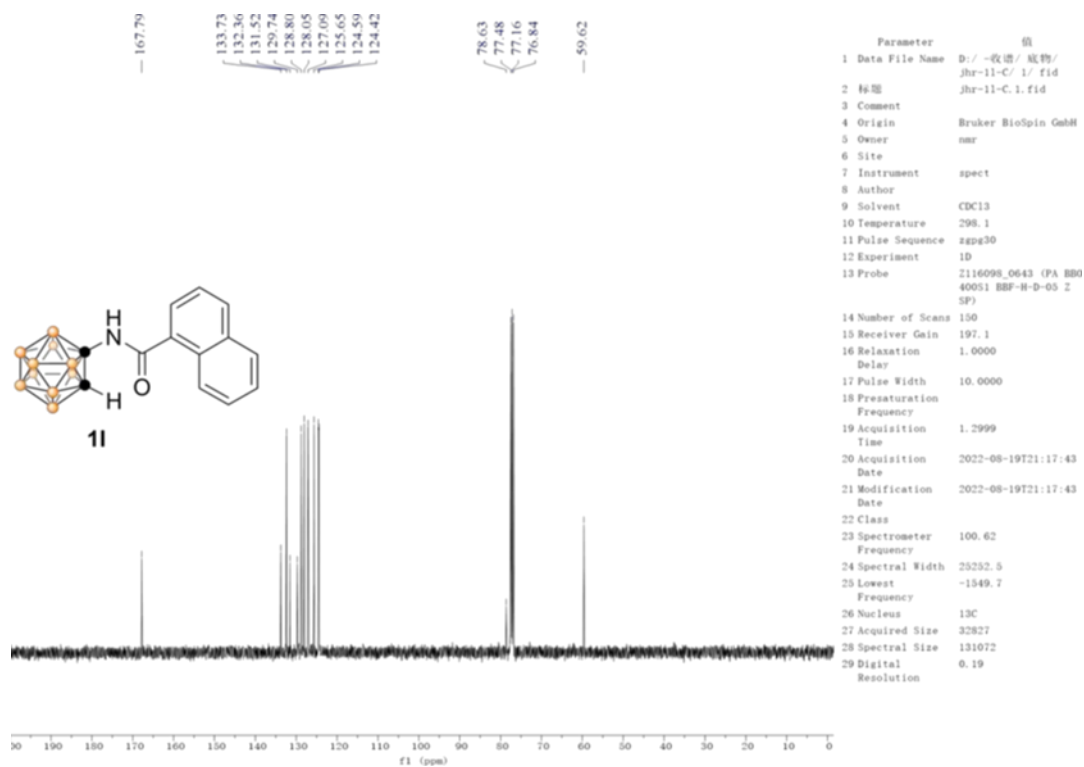
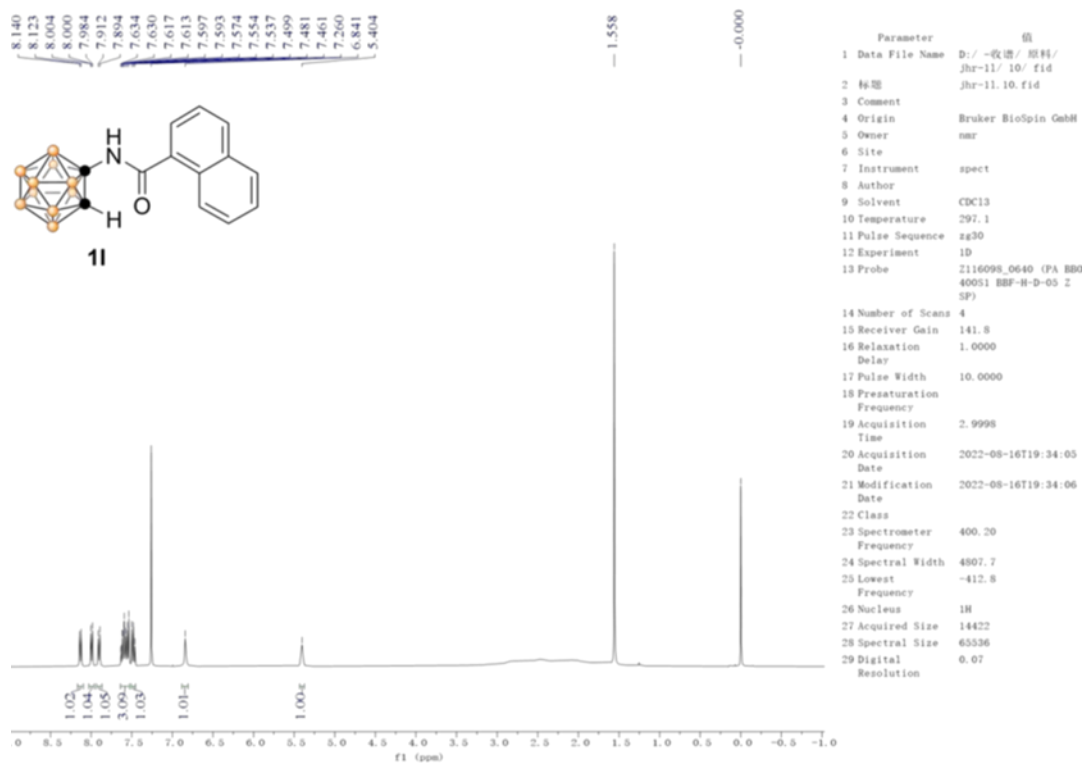


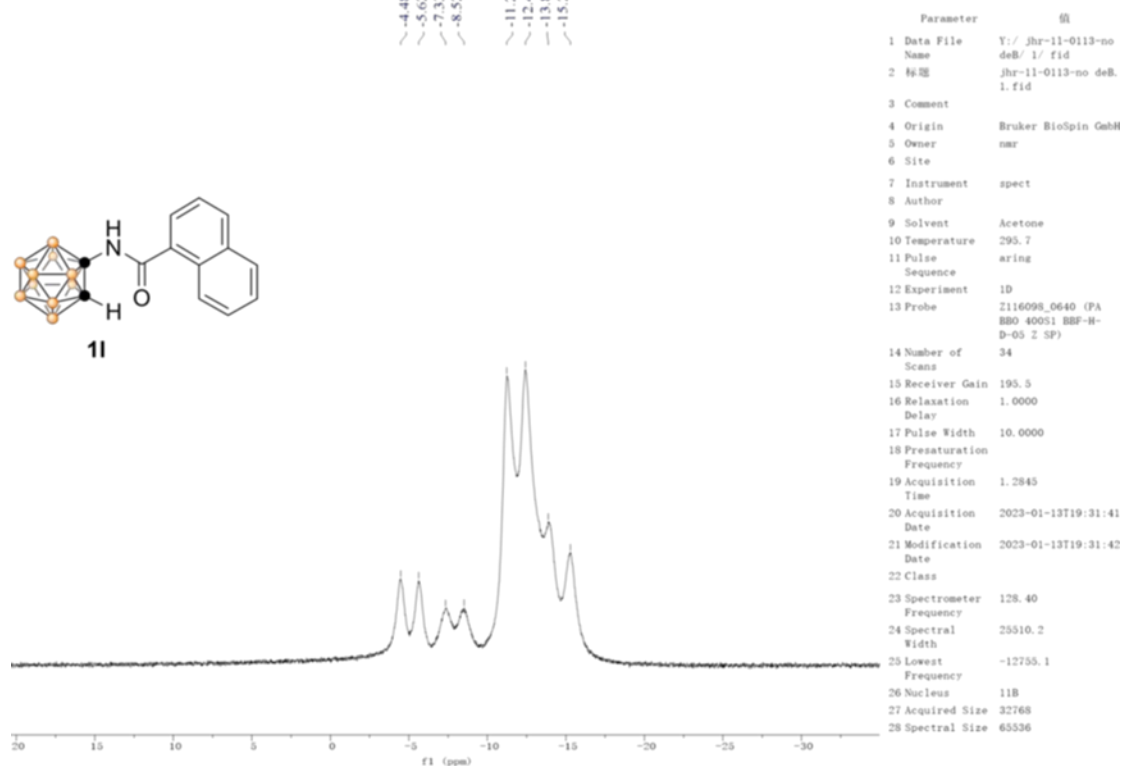
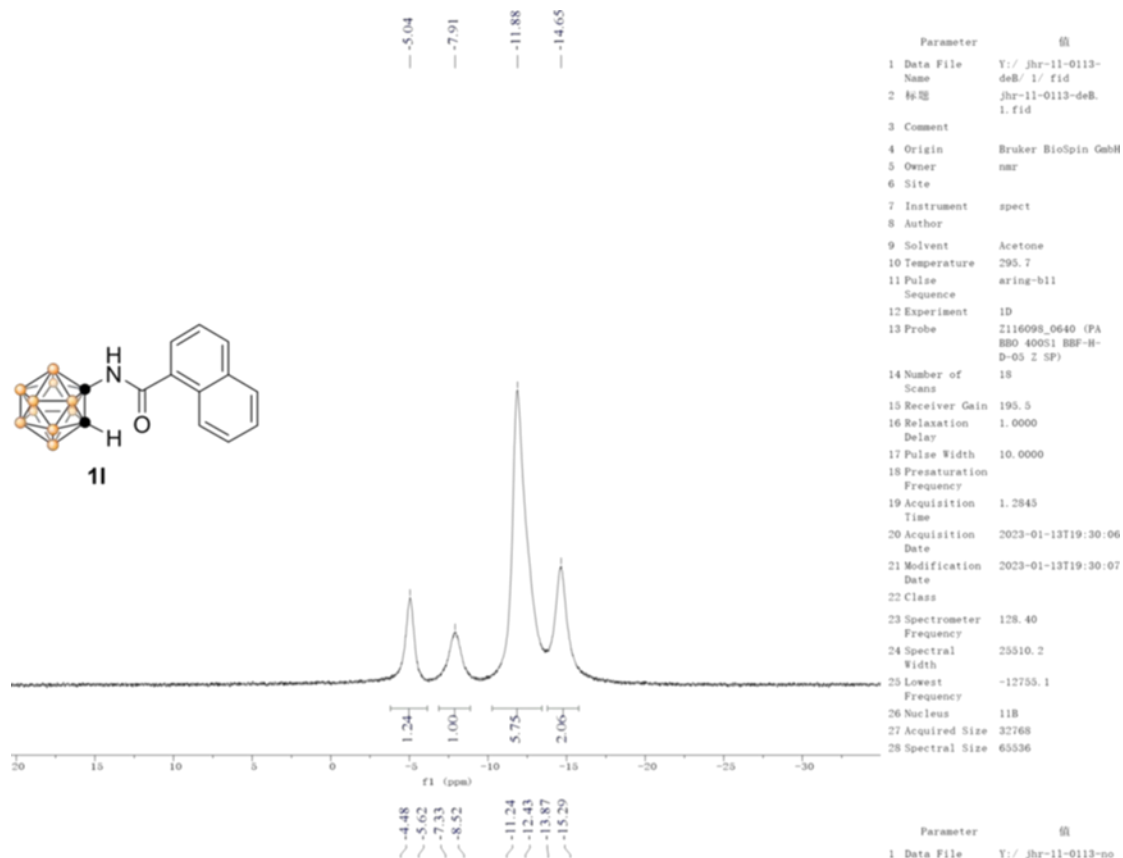
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1 Data File Name	D:/ 收谱/ 原料/ jhr-1k/ 9/ f1d
2 标题	jhr-1k.9.f1d
3 Comment	
4 Origin	Brucker Biospin GmbH
5 Owner	nmr
6 Site	
7 Instrument	spect
8 Author	
9 Solvent	CDCl3
10 Temperature	297.1
11 Pulse Sequence	zg30
12 Experiment	1D
13 Probe	2116098_0640 (PA BBO 400S1 BPF-H-D-05 Z 5P)
14 Number of Scans	4
15 Receiver Gain	77.4
16 Relaxation Delay	1.0000
17 Pulse Width	10.0000
18 Presaturation Frequency	
19 Acquisition Time	2.9998
20 Acquisition Date	2022-08-16T19:31:40
21 Modification Date	2022-08-16T19:31:40
22 Class	
23 Spectrometer Frequency	400.20
24 Spectral Width	4807.7
25 Lowest Frequency	-412.9
26 Nucleus	1H
27 Acquired Size	14422
28 Spectral Size	65536
29 Digital Resolution	0.07

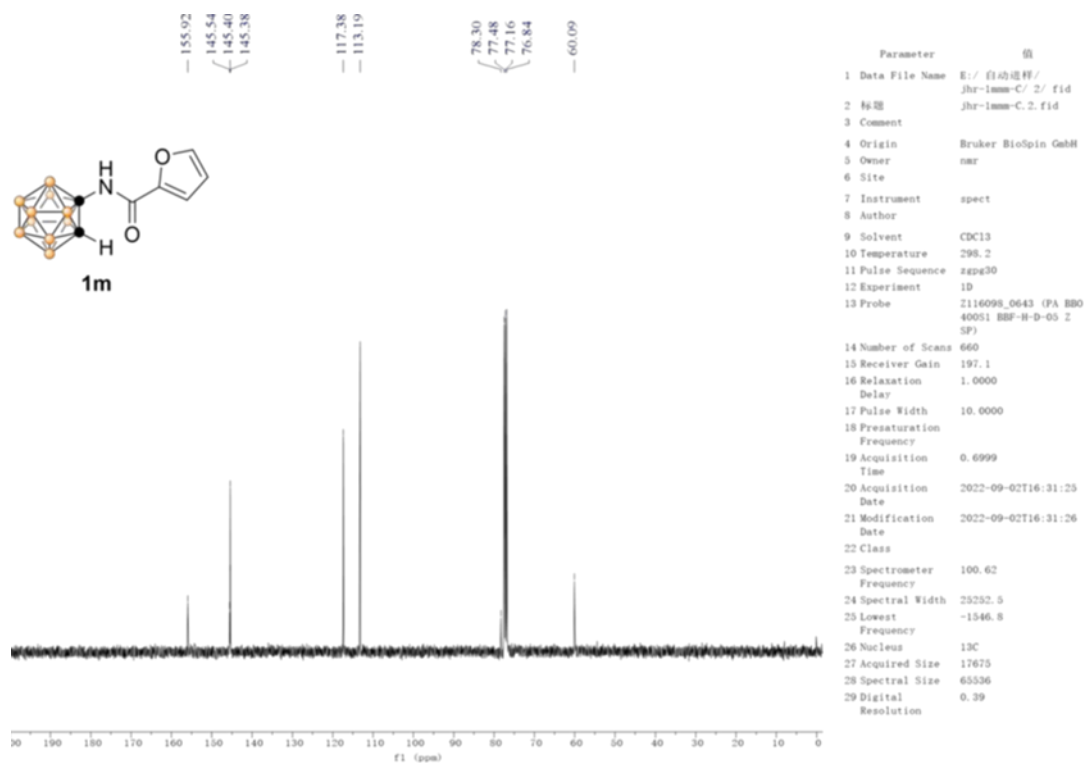
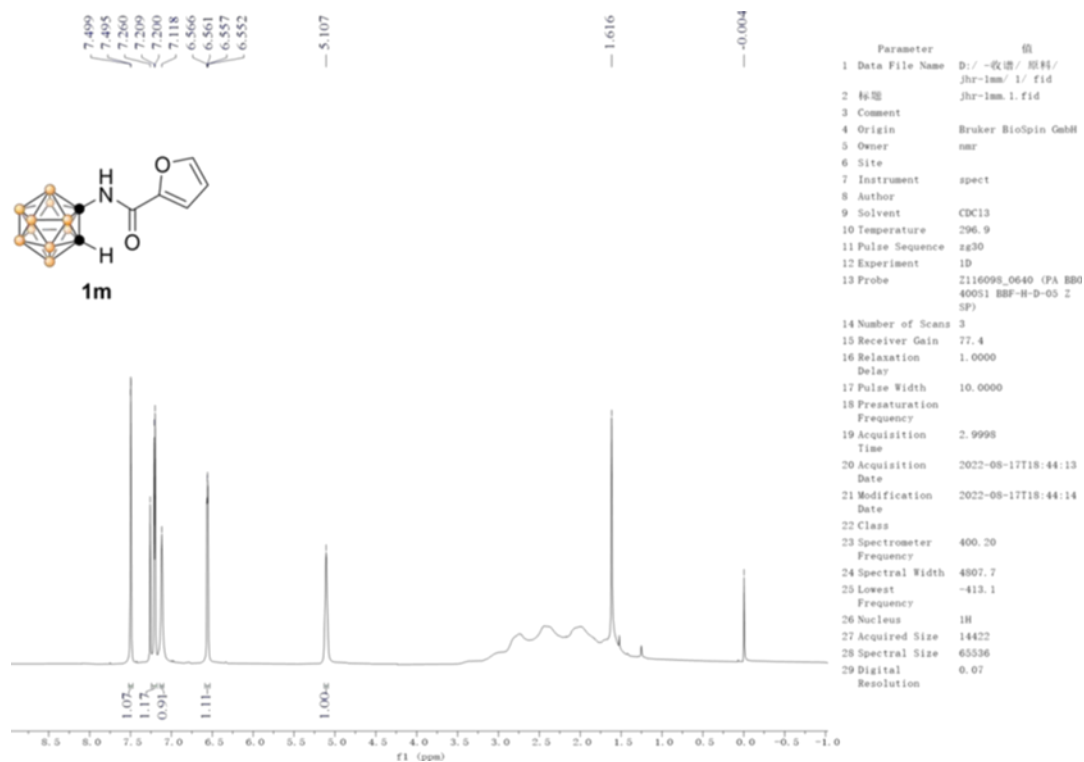


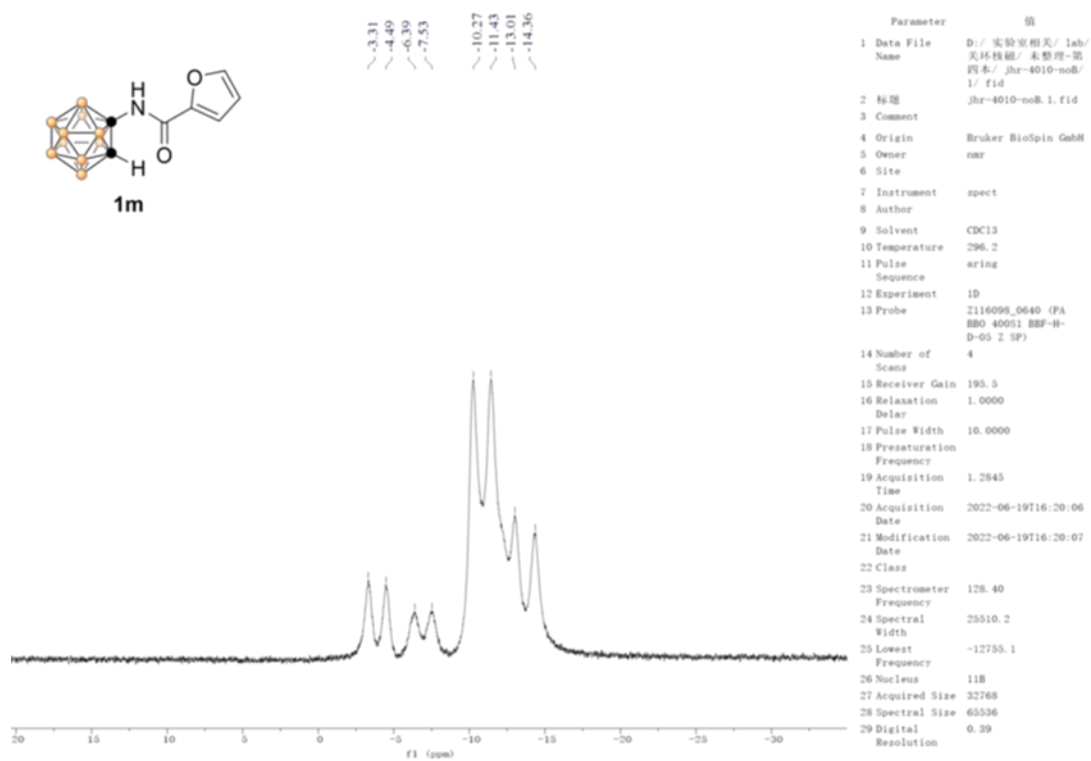
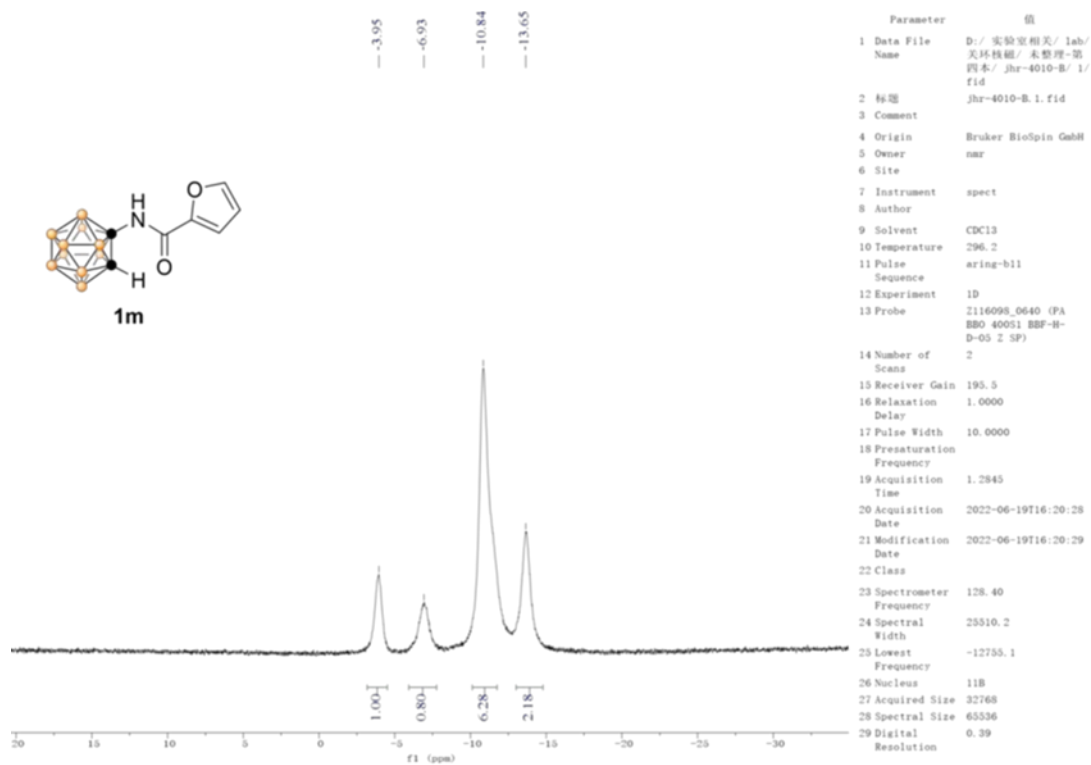
Parameter	值
1 Data File Name	D:/ 收谱/ 产物/ jhr-1k-C/ 1/ f1d
2 标题	jhr-1k-C.1.f1d
3 Comment	
4 Origin	Brucker Biospin GmbH
5 Owner	nmr
6 Site	
7 Instrument	spect
8 Author	
9 Solvent	CDCl3
10 Temperature	298.2
11 Pulse Sequence	zgpg30
12 Experiment	1D
13 Probe	2116098_0643 (PA BBO 400S1 BPF-H-D-05 Z 5P)
14 Number of Scans	150
15 Receiver Gain	197.1
16 Relaxation Delay	1.0000
17 Pulse Width	10.0000
18 Presaturation Frequency	
19 Acquisition Time	1.2999
20 Acquisition Date	2022-08-19T20:20:52
21 Modification Date	2022-08-19T20:20:52
22 Class	
23 Spectrometer Frequency	100.62
24 Spectral Width	23252.5
25 Lowest Frequency	-1550.6
26 Nucleus	13C
27 Acquired Size	32827
28 Spectral Size	131072
29 Digital Resolution	0.19

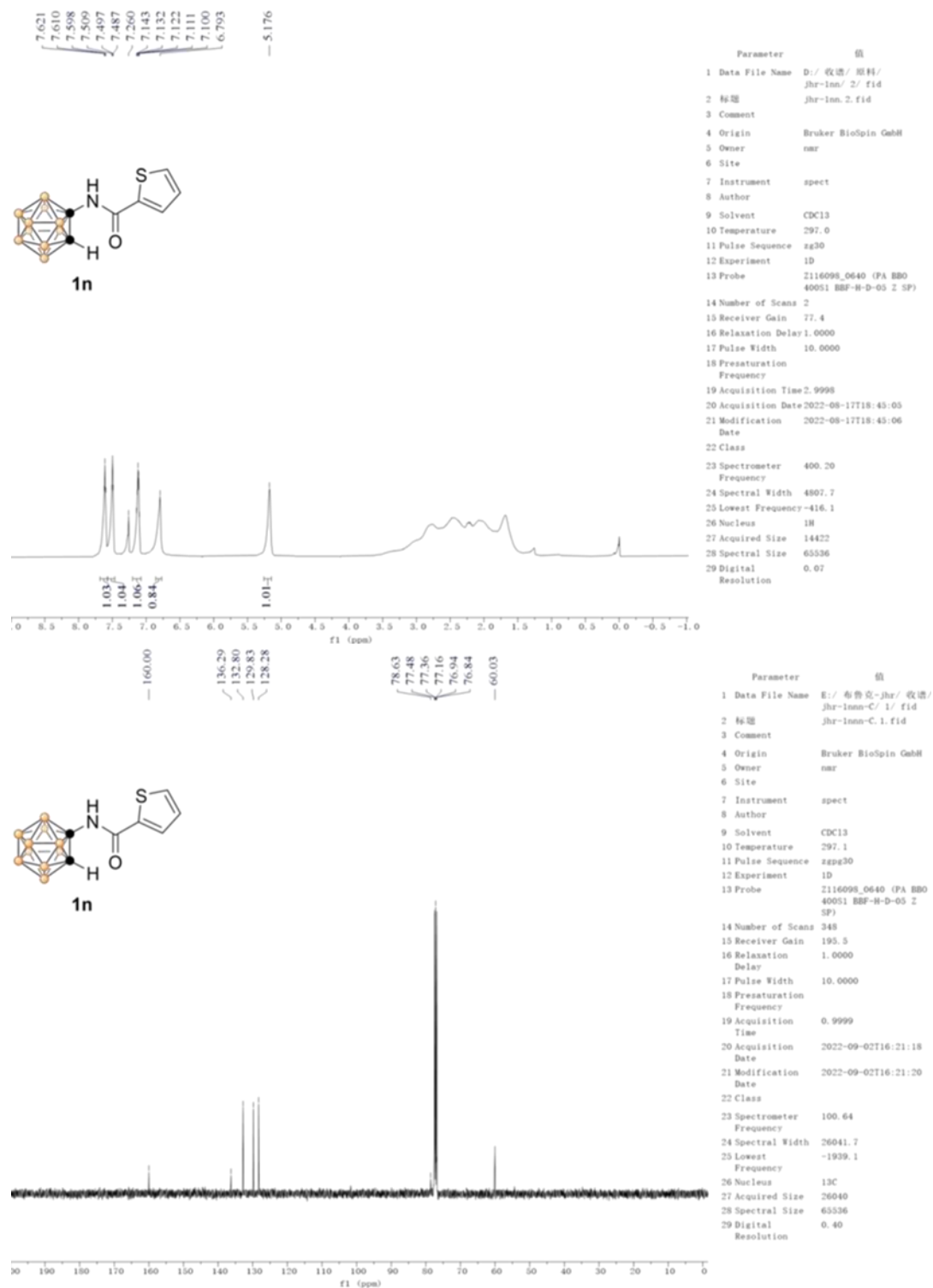




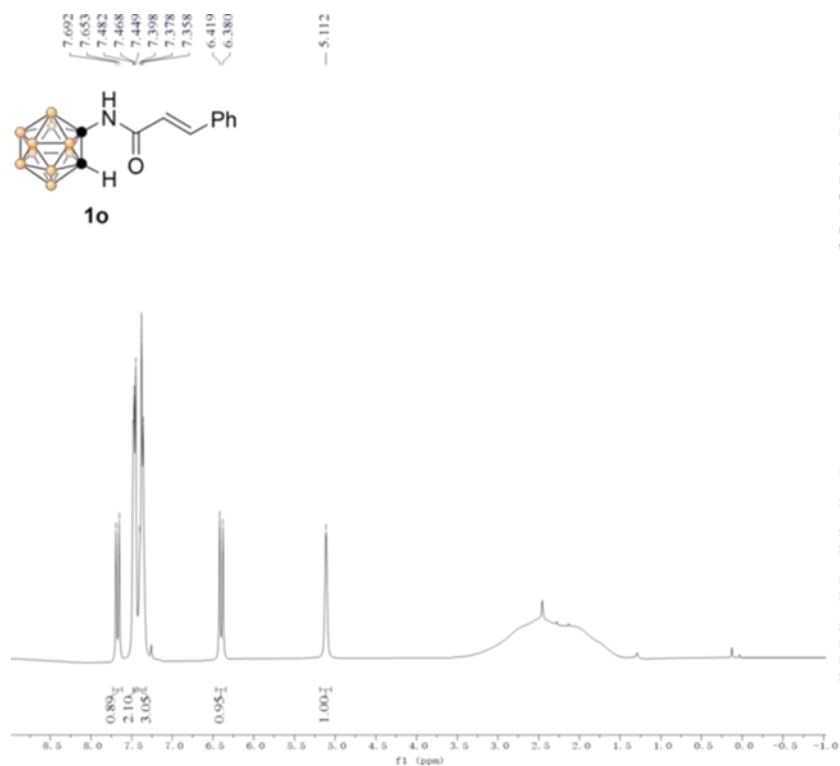




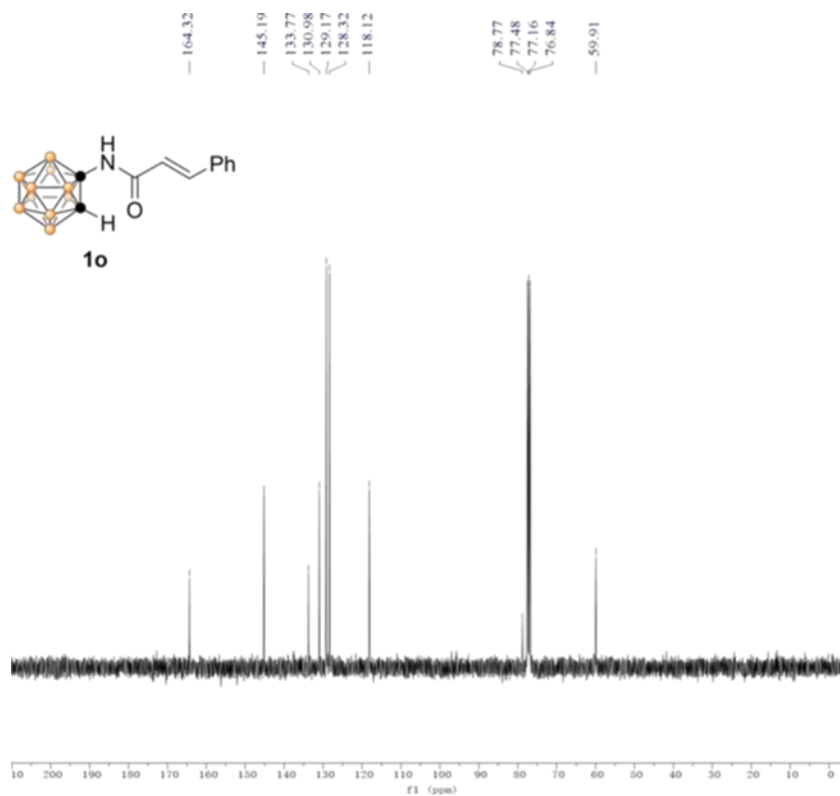




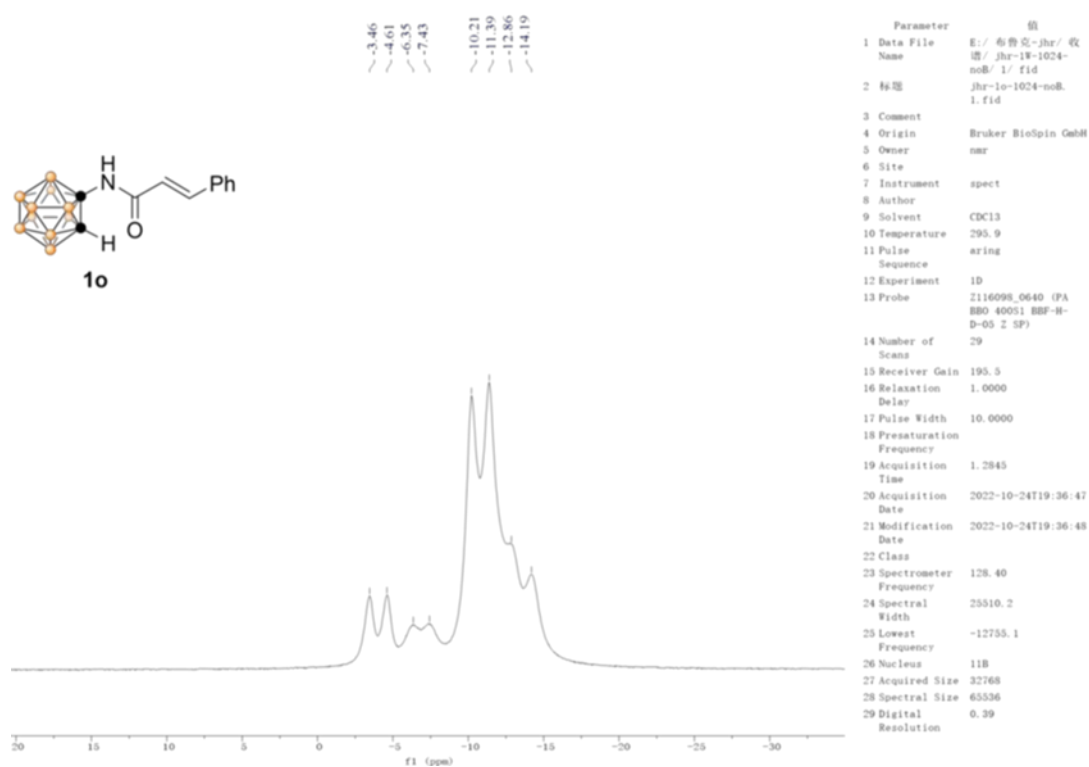
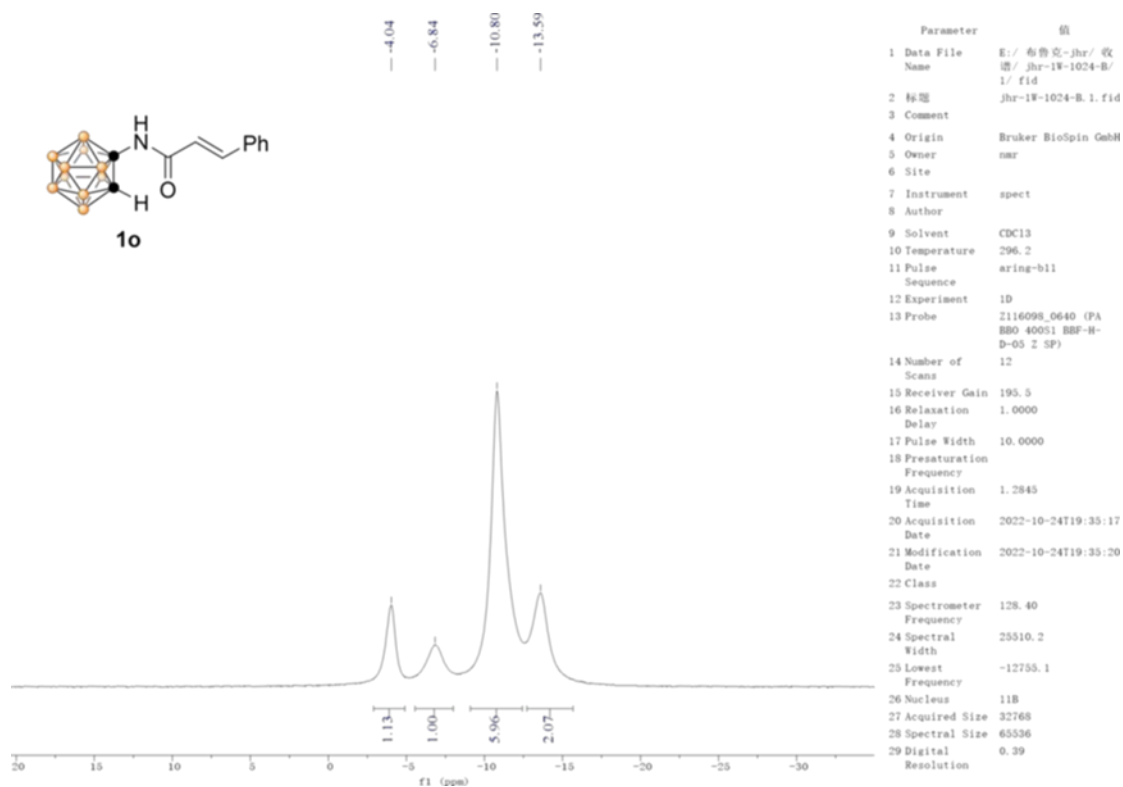


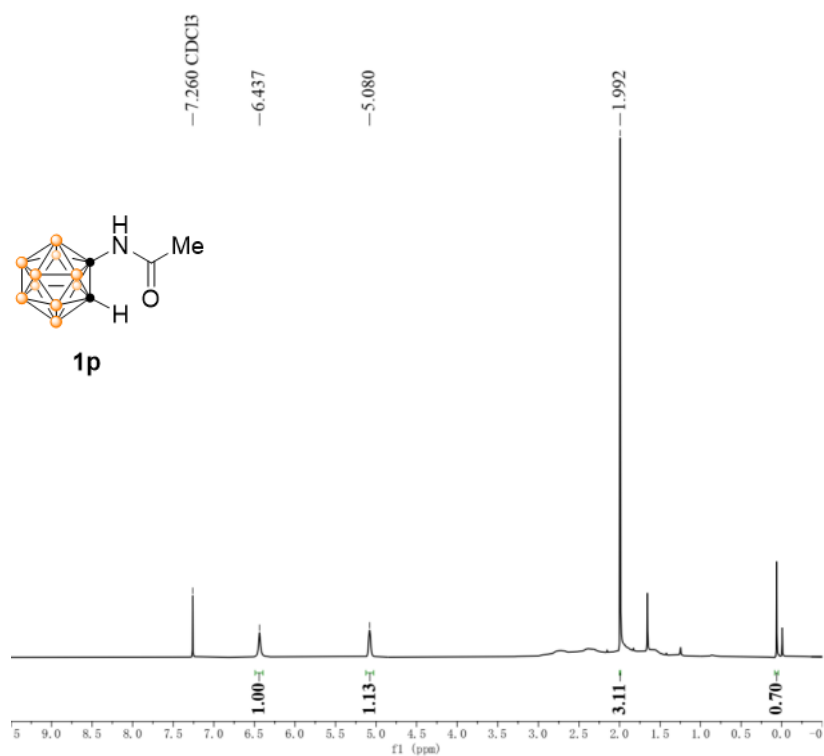


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1 Data File Name	C:/Users/17336/AppData/Local/Temp/BNZ_63ef213e3806cc06/cyy-jhr-1w.fid/ fid
2 标题	cyy-jhr-1w
3 Comment	
4 Origin	Varian
5 Owner	
6 Site	
7 Instrument	vnmr5
8 Author	
9 Solvent	CDCl3
10 Temperature	25.0
11 Pulse Sequence	s2pul
12 Experiment	1D
13 Probe	4nuc
14 Number of Scans	12
15 Receiver Gain	34
16 Relaxation Delay	1.0000
17 Pulse Width	7.7000
18 Presaturation Frequency	
19 Acquisition Time	3.0000
20 Acquisition Date	2023-02-17T11:24:34
21 Modification Date	2023-02-17T03:23:00
22 Class	
23 Spectrometer Frequency	399.72
24 Spectral Width	7375.8
25 Lowest Frequency	-1185.6
26 Nucleus	1H
27 Acquired Size	22727
28 Spectral Size	65536
29 Digital Resolution	0.12

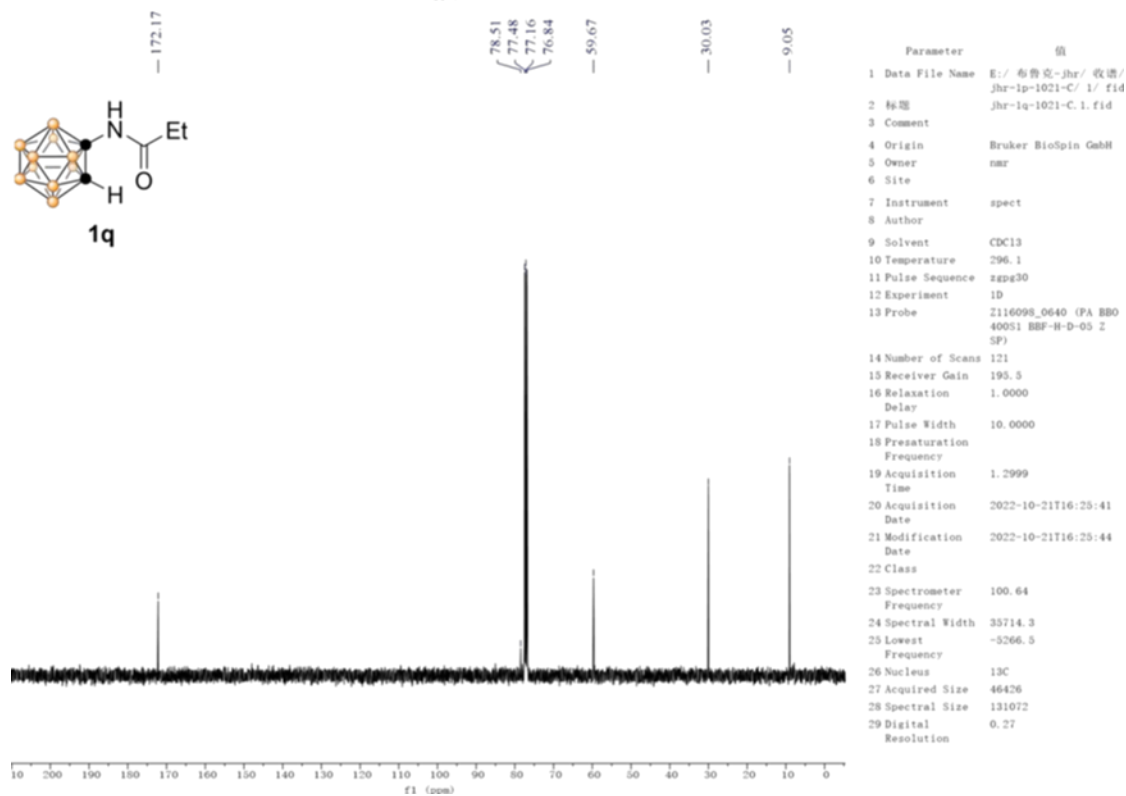
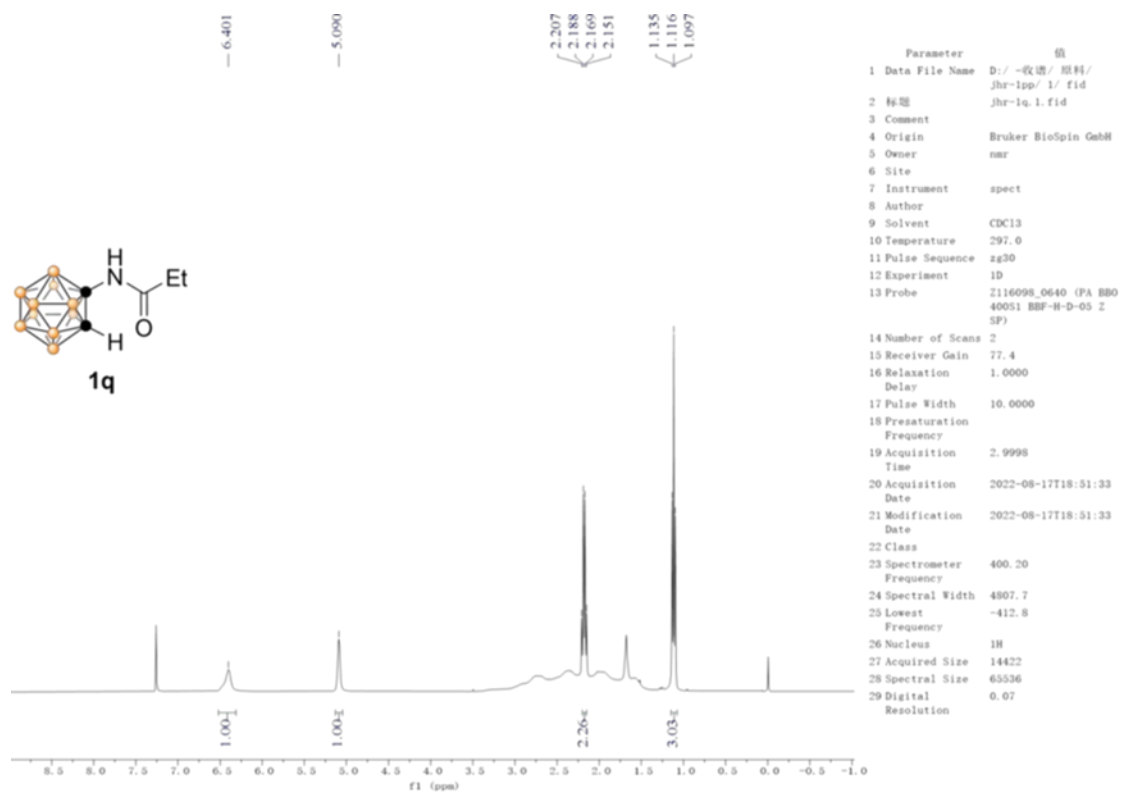


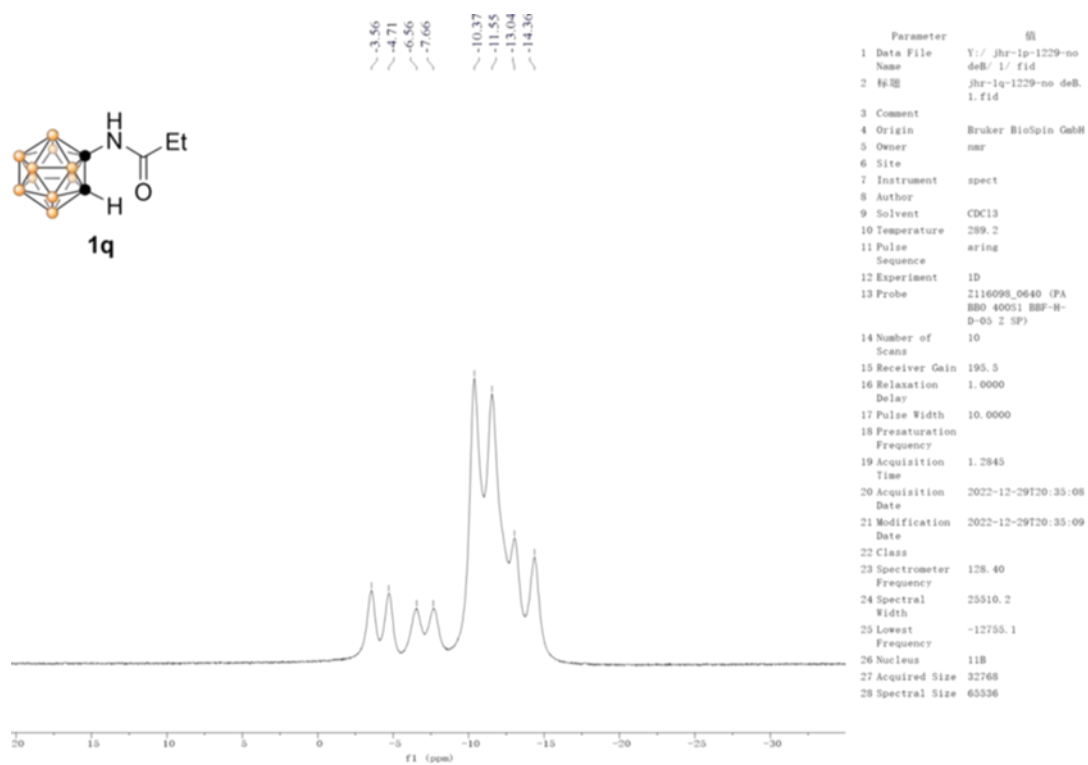
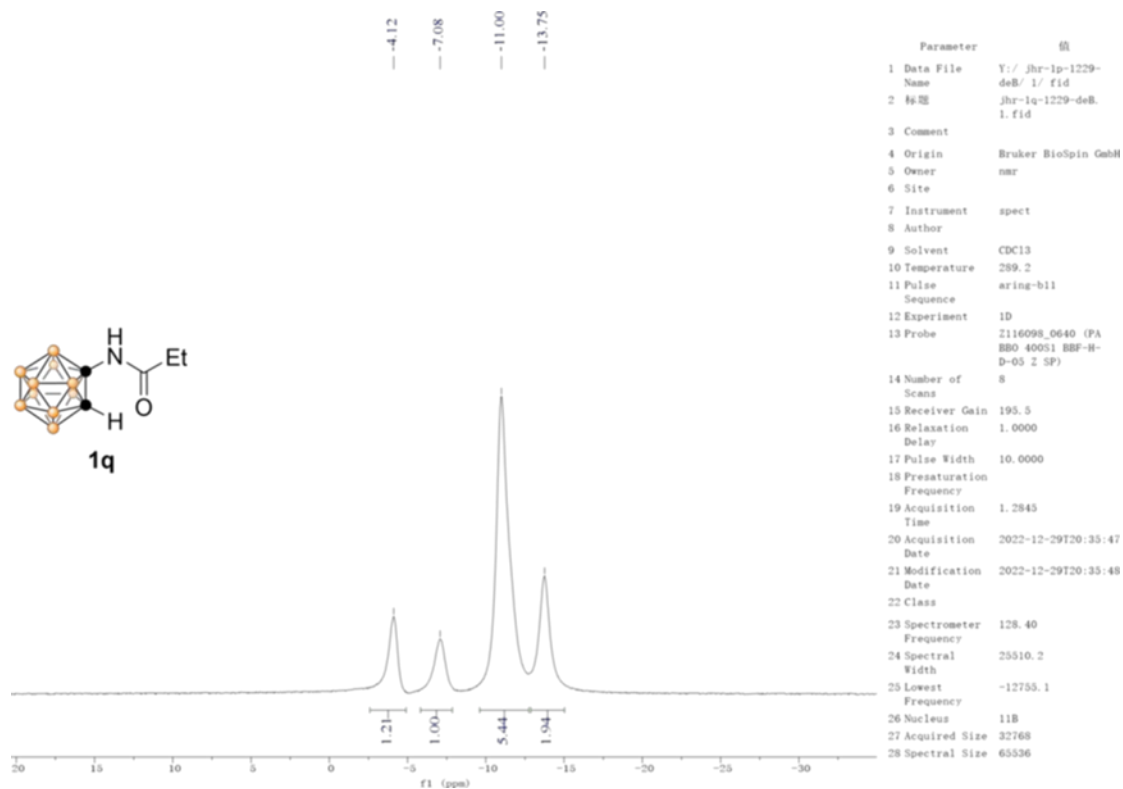
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1 Data File Name	E:/ 布鲁克-jhr/ 收谱/jhr-1w-1024-C/ 1/ fid
2 标题	jhr-1w-1024-C.1.fid
3 Comment	
4 Origin	Bruker BioSpin GmbH
5 Owner	nar
6 Site	
7 Instrument	spect
8 Author	
9 Solvent	CDCl3
10 Temperature	296.2
11 Pulse Sequence	zgpg30
12 Experiment	1D
13 Probe	Z16098_0640 (PA BB040051 BRF-H-D-05 Z SP)
14 Number of Scans	63
15 Receiver Gain	195.5
16 Relaxation Delay	1.0000
17 Pulse Width	10.0000
18 Presaturation Frequency	
19 Acquisition Time	1.2999
20 Acquisition Date	2022-10-24T19:14:16
21 Modification Date	2022-10-24T19:14:18
22 Class	
23 Spectrometer Frequency	100.64
24 Spectral Width	23252.5
25 Lowest Frequency	-1547.3
26 Nucleus	13C
27 Acquired Size	32827
28 Spectral Size	131072
29 Digital Resolution	0.19

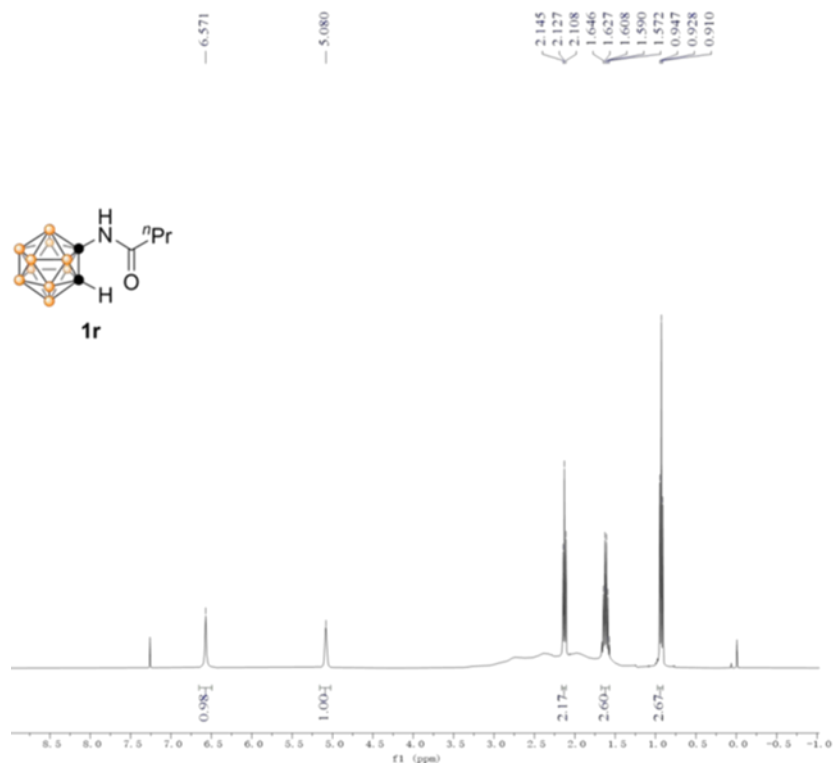




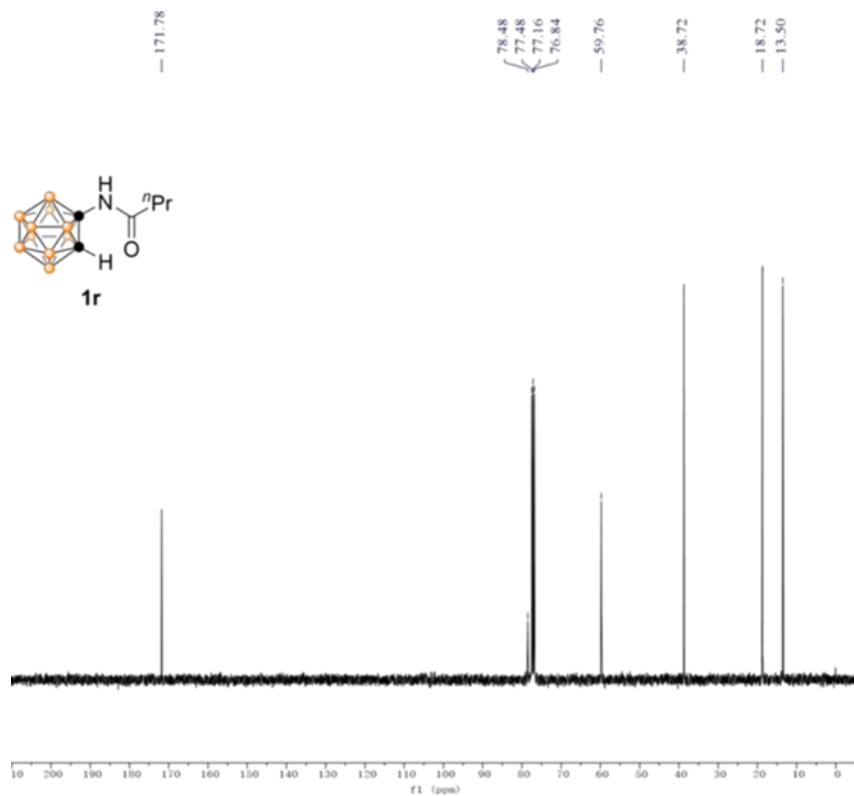
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zyt-1-q-h/ 4/ fid	
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Comment	
Origin	Brucker BioSpin GmbH
Owner	nmr
Site	
Instrument	spect
Author	
Solvent	CDCl3
Temperature	291.2
Pulse Sequence	zg30
Experiment	1D
Probe	Z116098_0640 (PA BB0 400SI BBF-H-D-05 Z SP)
Number of Scans	3
Receiver Gain	77.4
Relaxation Delay	1.0000
Pulse Width	10.0000
Presaturation	
Frequency	
Acquisition	2.9998
Time	
Acquisition Date	2025-02-10T12:38:46
Modification	2025-02-10T12:38:47
Date	
Class	
Spectrometer	400.20
Frequency	
Spectral Width	4807.7
Lowest	-412.7
Frequency	
Nucleus	1H
Acquired Size	14422
Spectral Size	65536
...	...



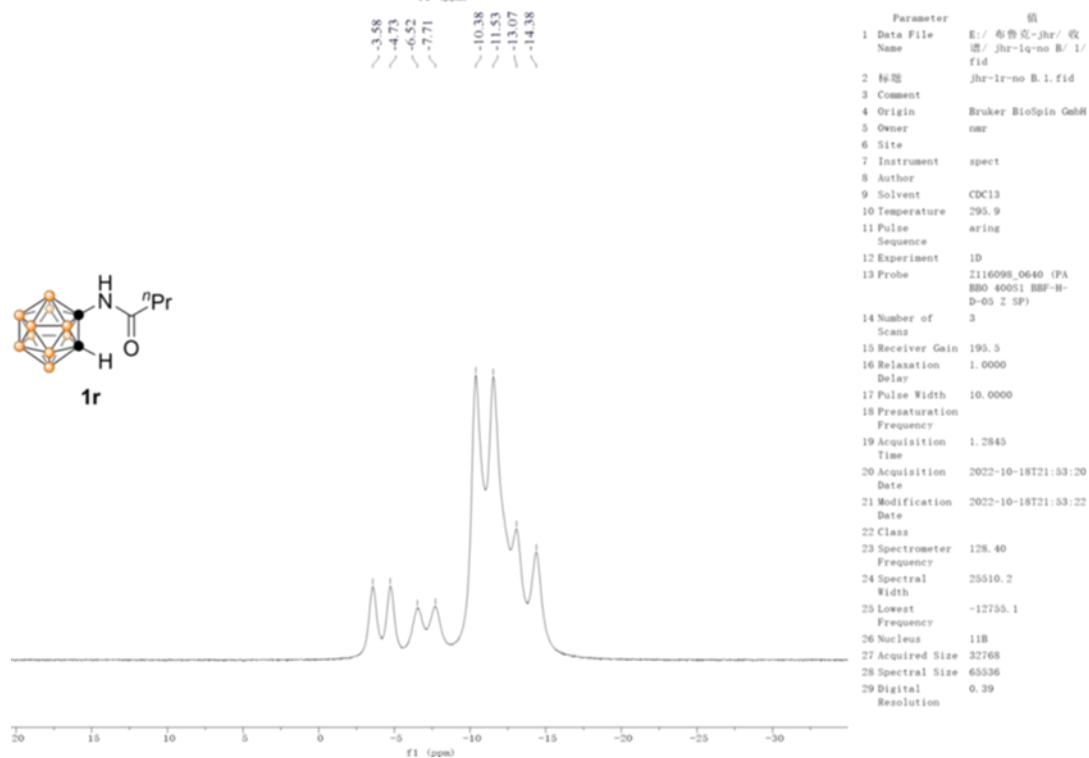
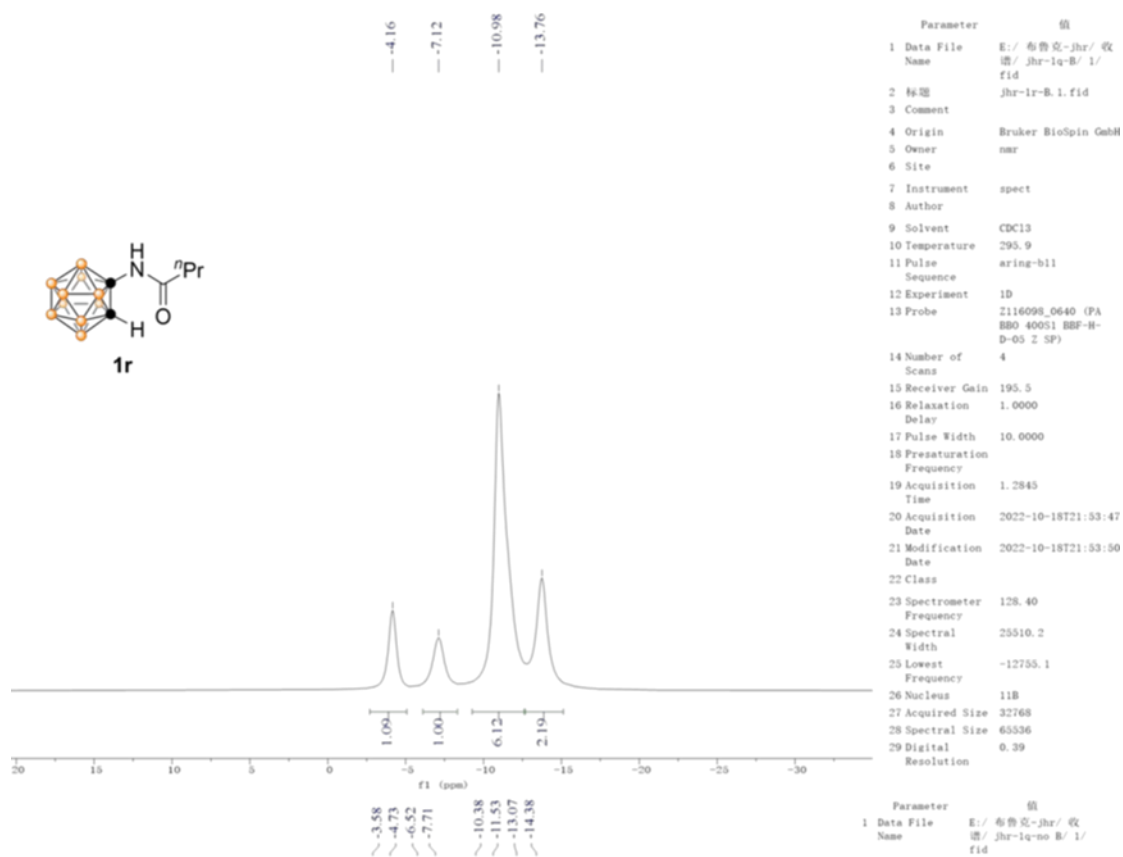


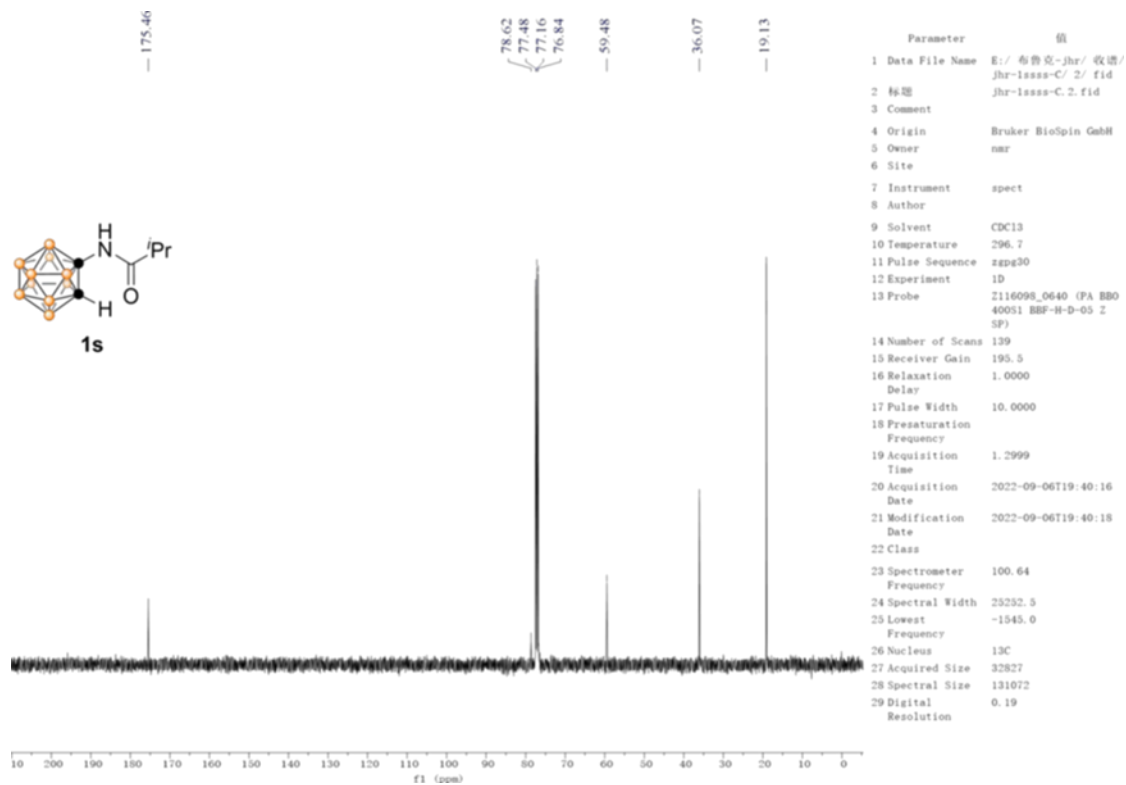
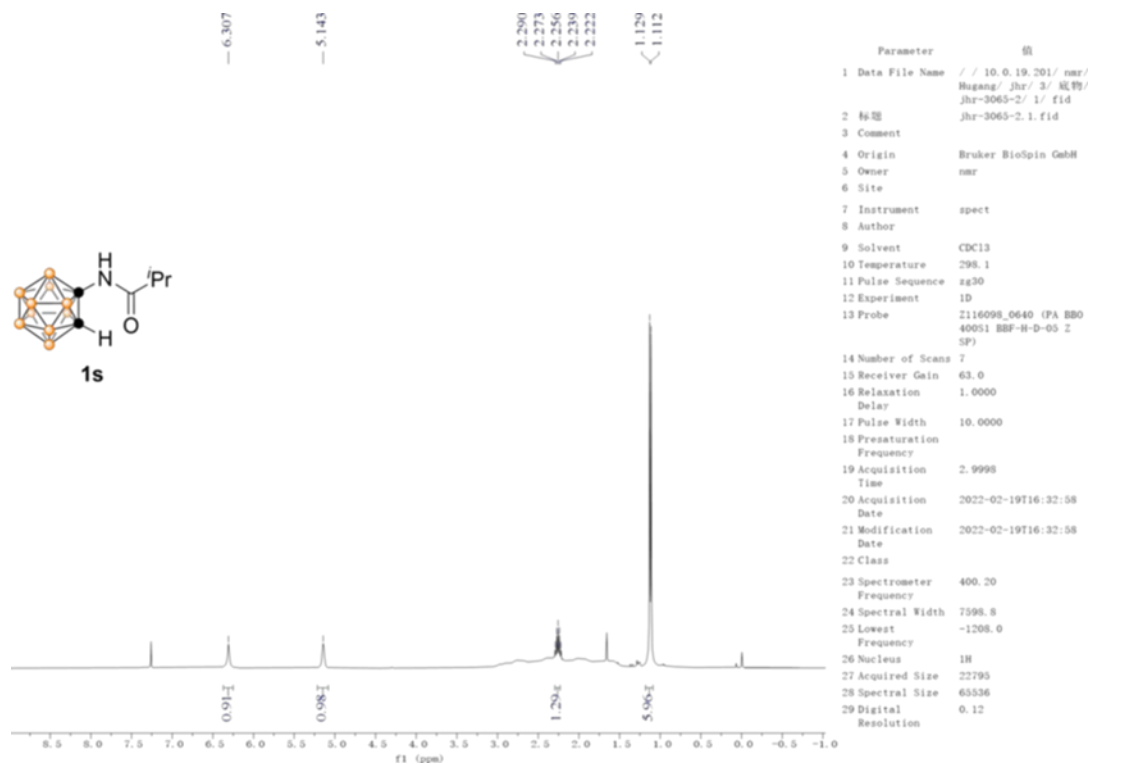


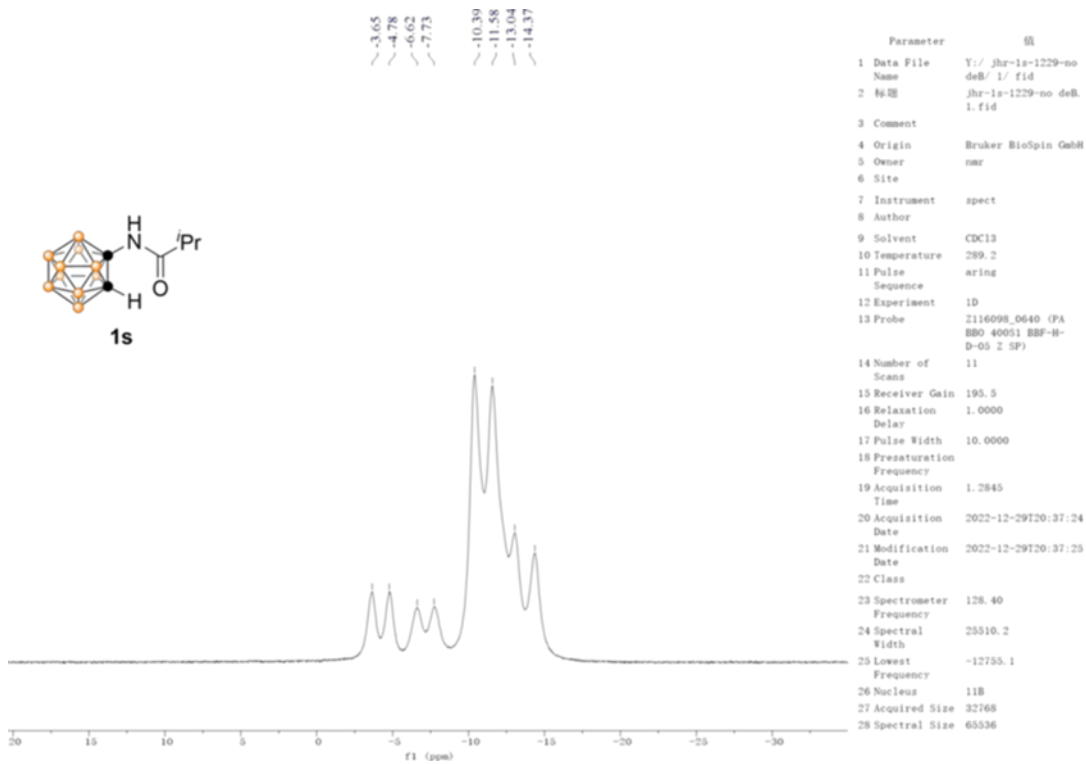
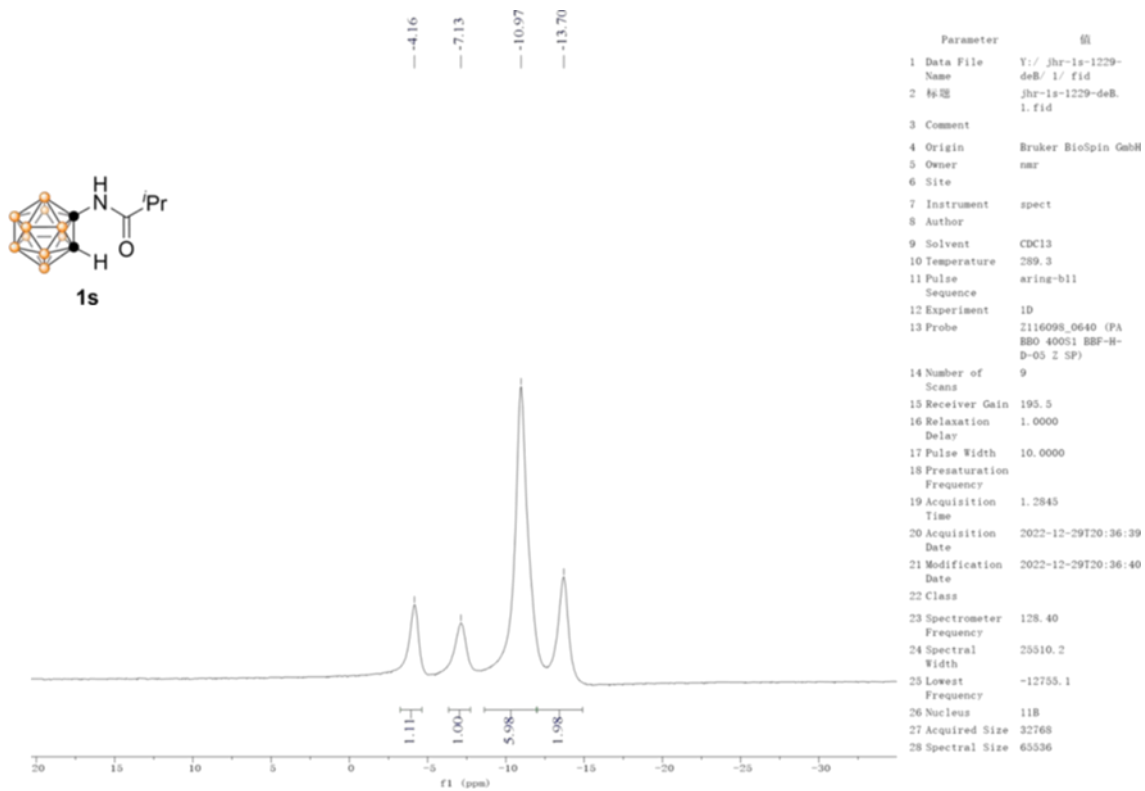
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2 标题	jhr-1r-1018.1.fid
3 Comment	
4 Origin	Bruker BioSpin GmbH
5 Owner	nmr
6 Site	
7 Instrument	spect
8 Author	
9 Solvent	CDCl3
10 Temperature	295.9
11 Pulse Sequence	zg30
12 Experiment	1D
13 Probe	2116095_0640 (PA BB0 400SI BHF-W-D-05 Z SP)
14 Number of Scans	5
15 Receiver Gain	38.4
16 Relaxation Delay	1.0000
17 Pulse Width	10.0000
18 Presaturation Frequency	
19 Acquisition Time	2.9998
20 Acquisition Date	2022-10-18T21:43:41
21 Modification Date	2022-10-18T21:43:42
22 Class	
23 Spectrometer Frequency	400.20
24 Spectral Width	4807.7
25 Lowest Frequency	-412.3
26 Nucleus	¹ H
27 Acquired Size	14422
28 Spectral Size	65536
29 Digital Resolution	0.07

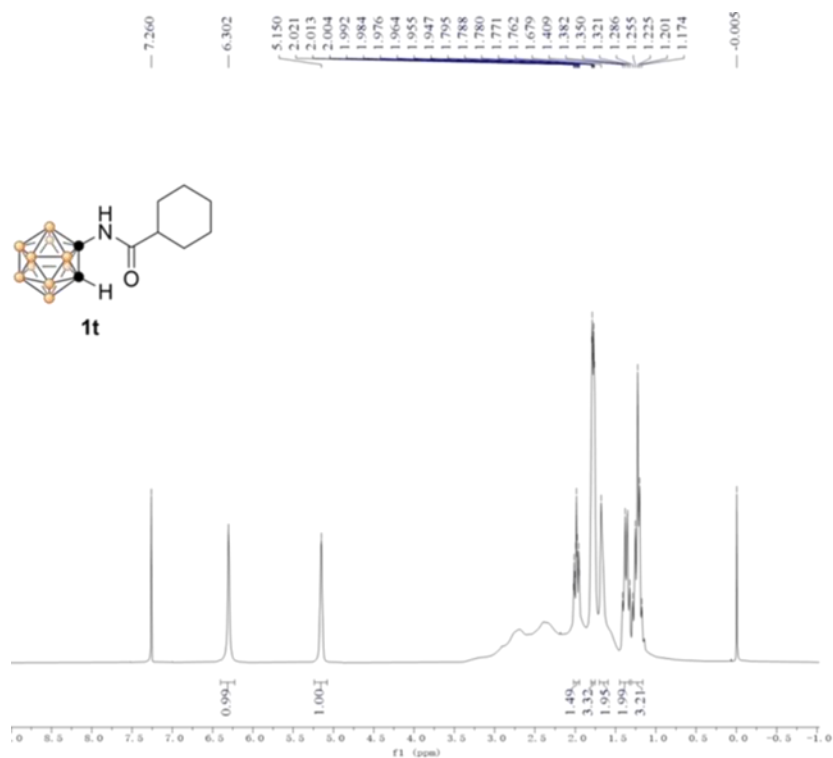


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1 Data File Name	E:/ 布鲁克-jhr/ 收谱/ jhr-1q-1018-C/ 1/ f1d
2 标题	jhr-1r-1018-C.1.fid
3 Comment	
4 Origin	Bruker BioSpin GmbH
5 Owner	nmr
6 Site	
7 Instrument	spect
8 Author	
9 Solvent	CDCl3
10 Temperature	296.1
11 Pulse Sequence	zgpg30
12 Experiment	1D
13 Probe	2116095_0640 (PA BB0 400SI BHF-W-D-05 Z SP)
14 Number of Scans	97
15 Receiver Gain	195.5
16 Relaxation Delay	1.0000
17 Pulse Width	10.0000
18 Presaturation Frequency	
19 Acquisition Time	1.2999
20 Acquisition Date	2022-10-19T13:04:53
21 Modification Date	2022-10-19T13:04:56
22 Class	
23 Spectrometer Frequency	100.64
24 Spectral Width	23252.5
25 Lowest Frequency	-1547.9
26 Nucleus	¹³ C
27 Acquired Size	32827
28 Spectral Size	131072
29 Digital Resolution	0.19

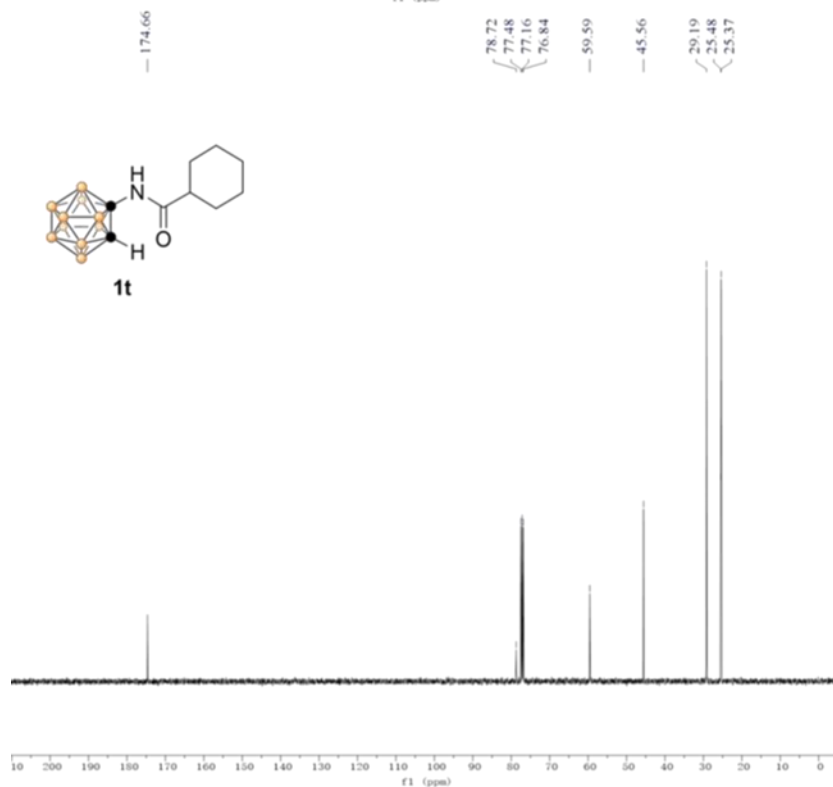




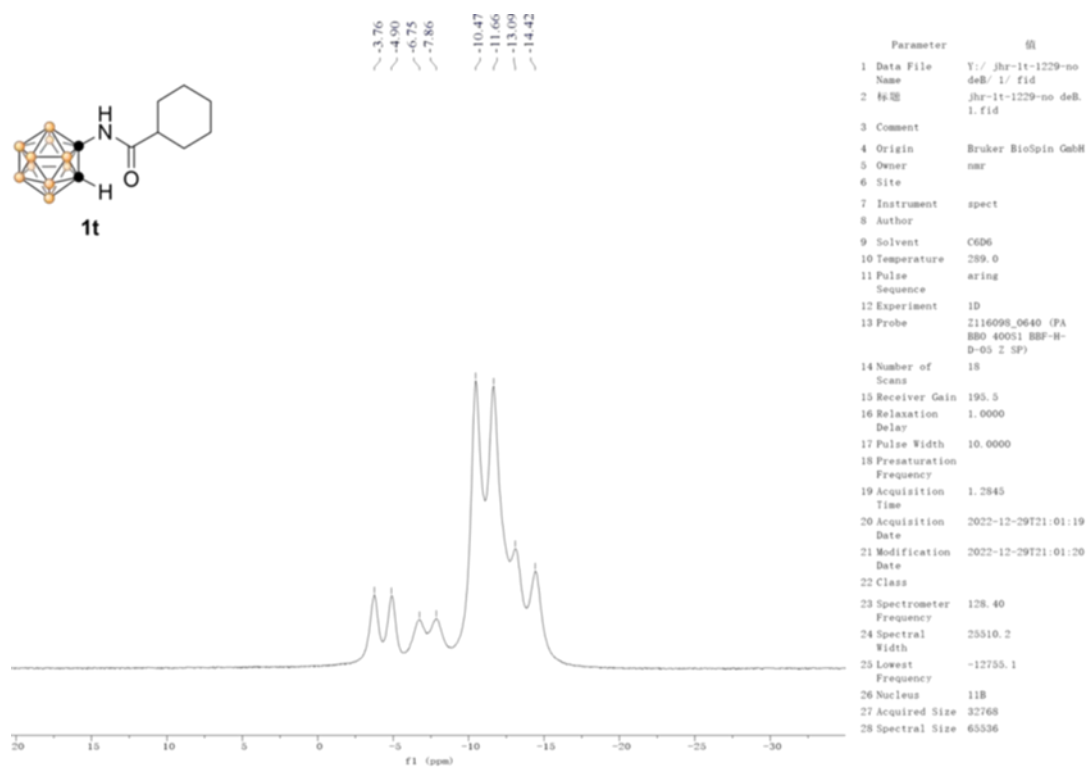
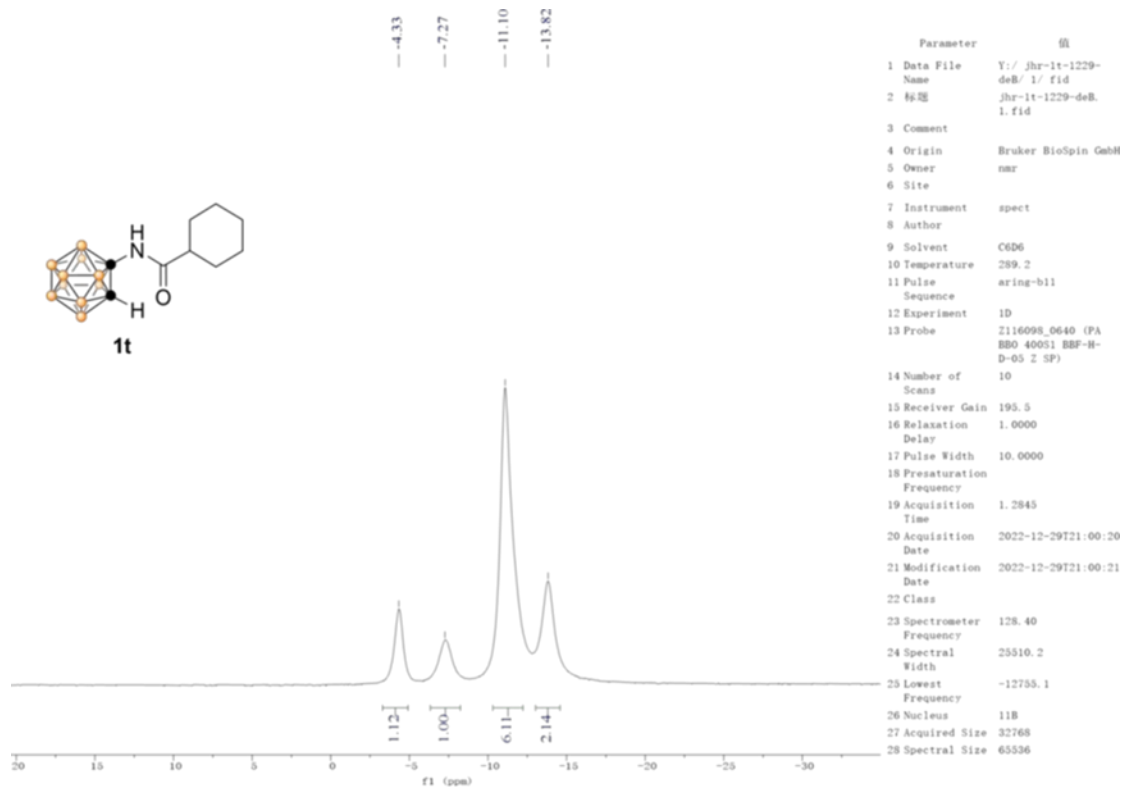


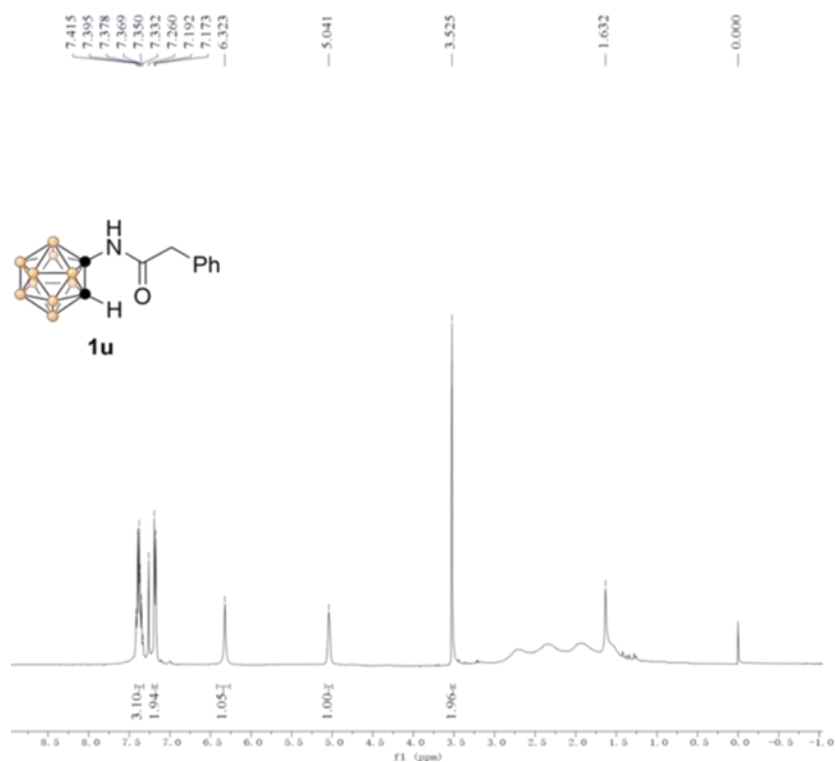


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2 标题	jhr-1ttt.1.fid
3 Comment	
4 Origin	Bruker BioSpin GmbH
5 Owner	nmr
6 Site	
7 Instrument	spect
8 Author	
9 Solvent	CDCl3
10 Temperature	296.5
11 Pulse Sequence	zg30
12 Experiment	1D
13 Probe	Z116098_0640 (PA BB0 400S1 BBF-H-D-05 Z SP)
14 Number of Scans	10
15 Receiver Gain	63.0
16 Relaxation Delay	1.0000
17 Pulse Width	10.0000
18 Presaturation Frequency	
19 Acquisition Time	2.9998
20 Acquisition Date	2022-09-06T19:31:13
21 Modification Date	2022-09-06T19:31:16
22 Class	
23 Spectrometer Frequency	400.20
24 Spectral Width	4807.7
25 Lowest Frequency	-412.7
26 Nucleus	1H
27 Acquired Size	14422
28 Spectral Size	65536
29 Digital Resolution	0.07

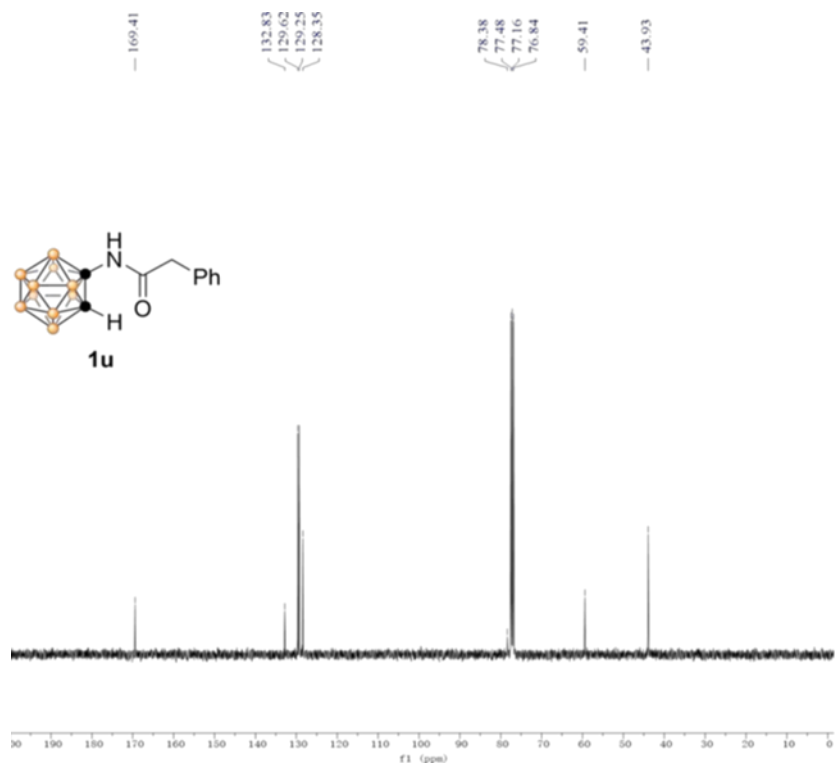


Parameter	值
1 Data File Name	D:/ -收谱/ 底物/ jhr-1t-C/ 1/ fid
2 标题	jhr-1t-C.1.fid
3 Comment	
4 Origin	Bruker BioSpin GmbH
5 Owner	nmr
6 Site	
7 Instrument	spect
8 Author	
9 Solvent	CDCl3
10 Temperature	298.1
11 Pulse Sequence	zgpg30
12 Experiment	1D
13 Probe	Z116098_0643 (PA BB0 400S1 BBF-H-D-05 Z SP)
14 Number of Scans	150
15 Receiver Gain	197.1
16 Relaxation Delay	1.0000
17 Pulse Width	10.0000
18 Presaturation Frequency	
19 Acquisition Time	1.2999
20 Acquisition Date	2022-08-19T21:27:43
21 Modification Date	2022-08-19T21:27:43
22 Class	
23 Spectrometer Frequency	100.62
24 Spectral Width	25252.5
25 Lowest Frequency	-1549.7
26 Nucleus	13C
27 Acquired Size	32827
28 Spectral Size	131072
29 Digital Resolution	0.19

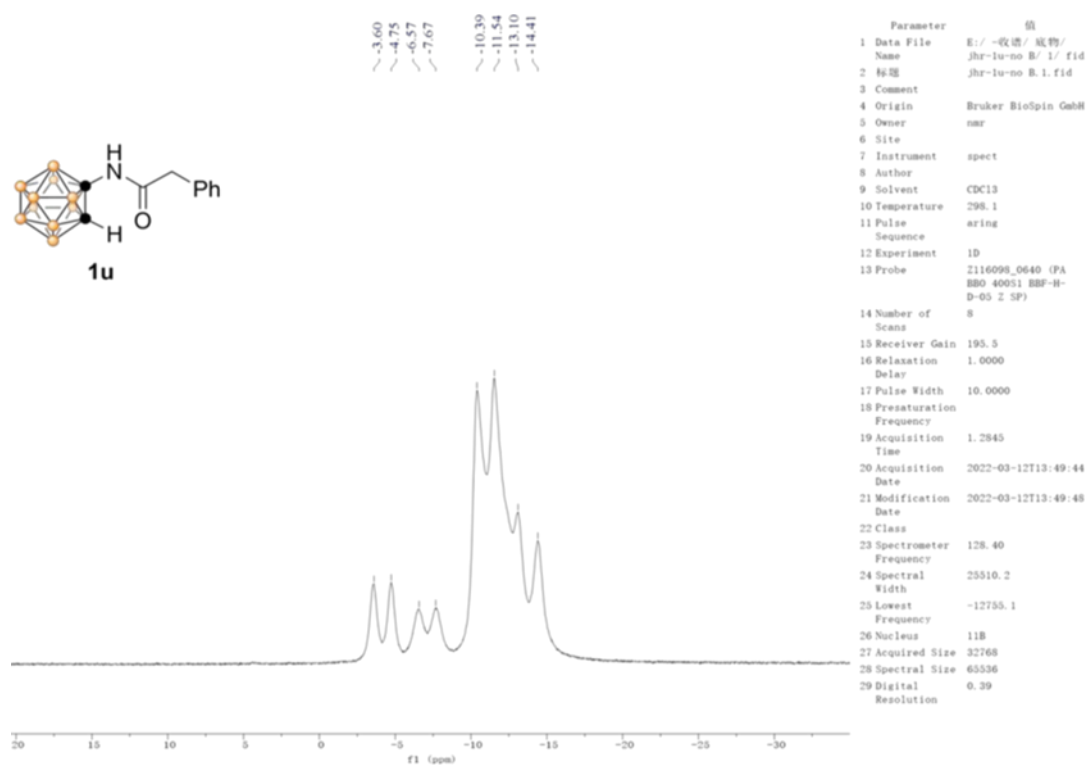
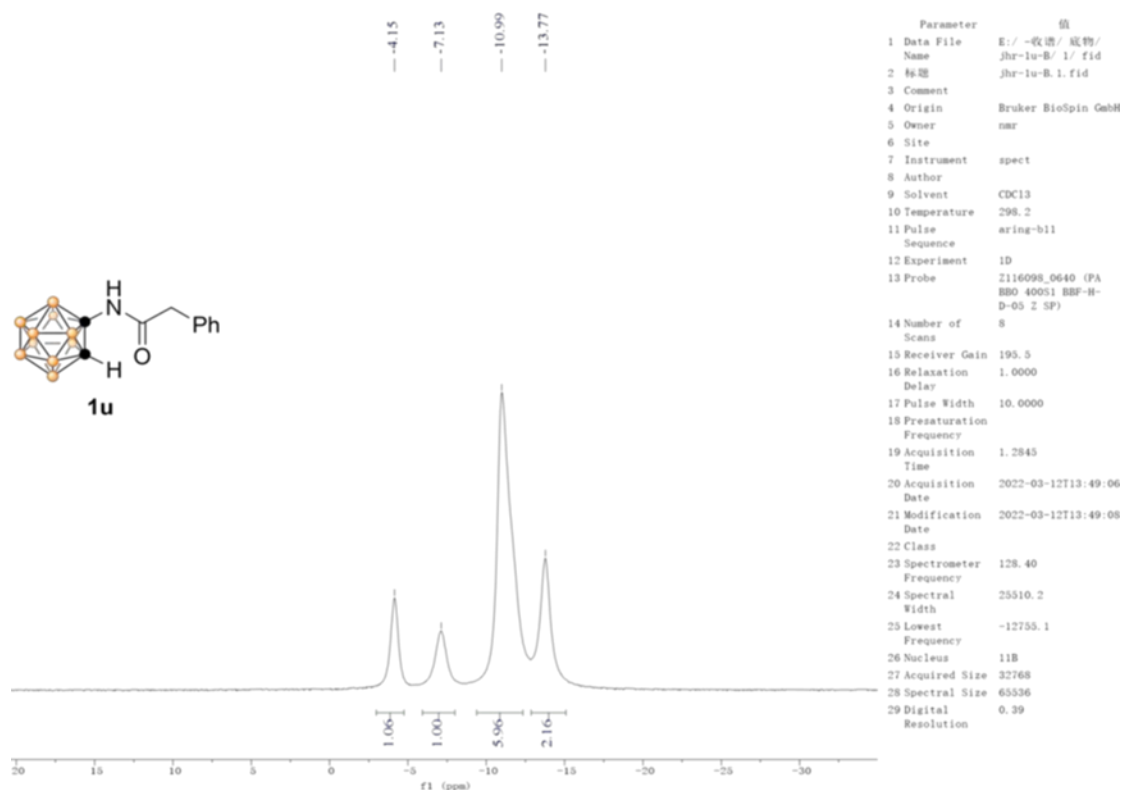


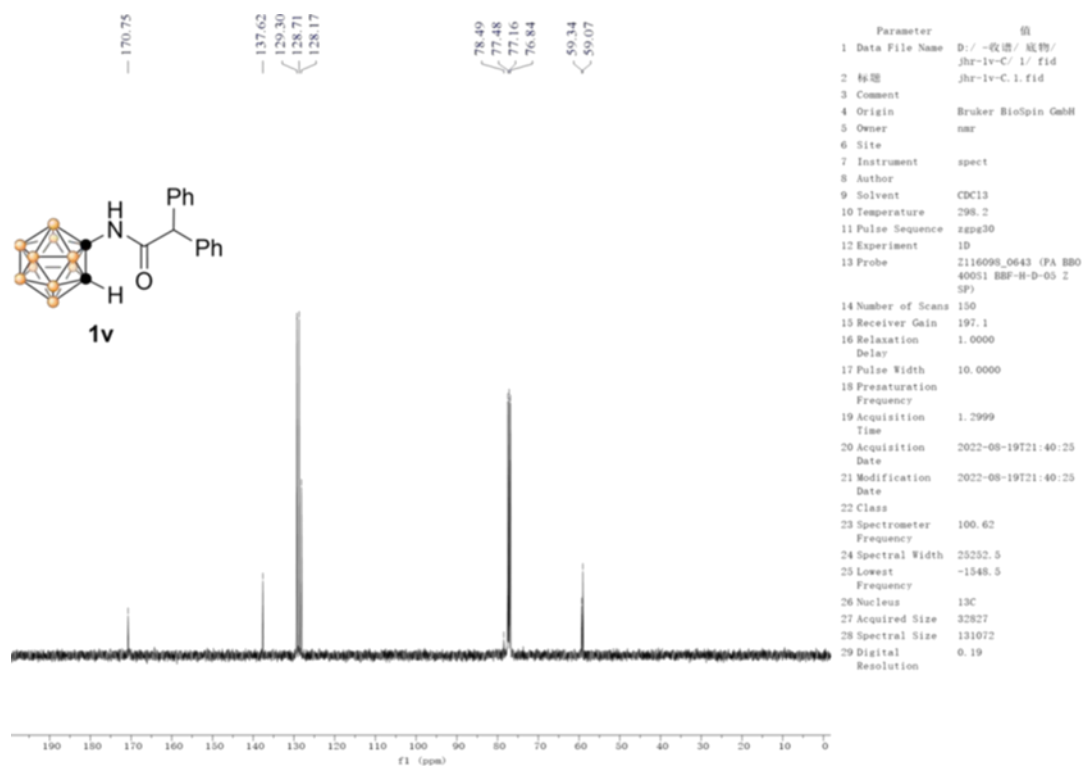
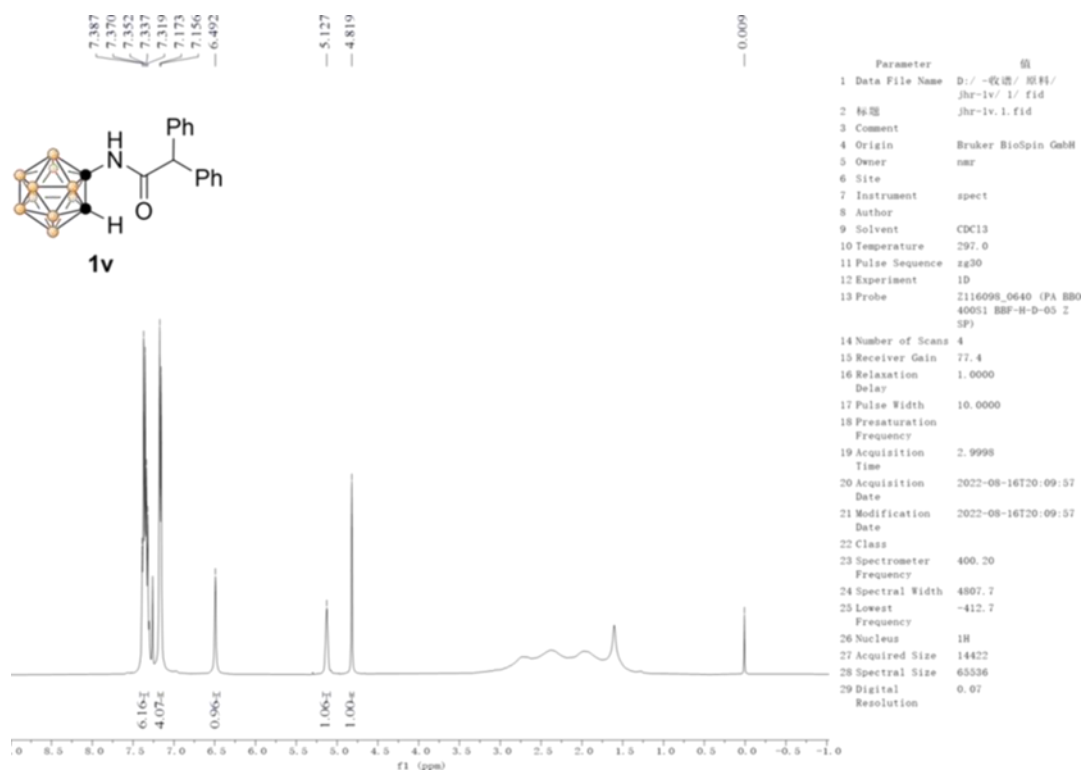


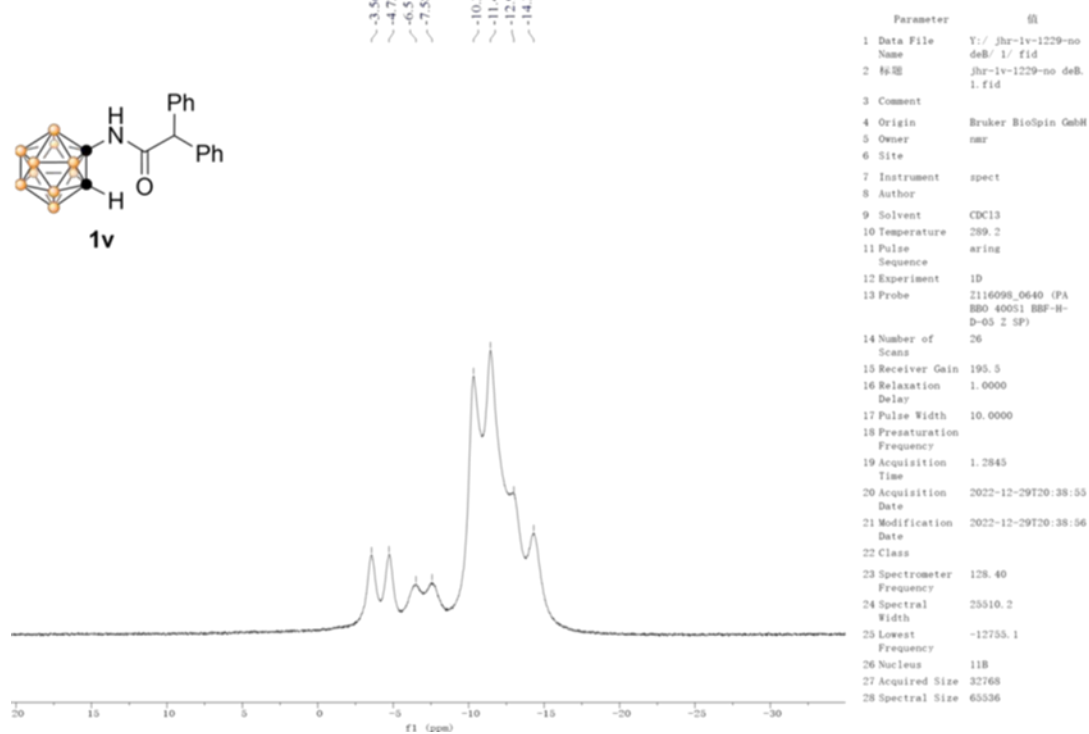
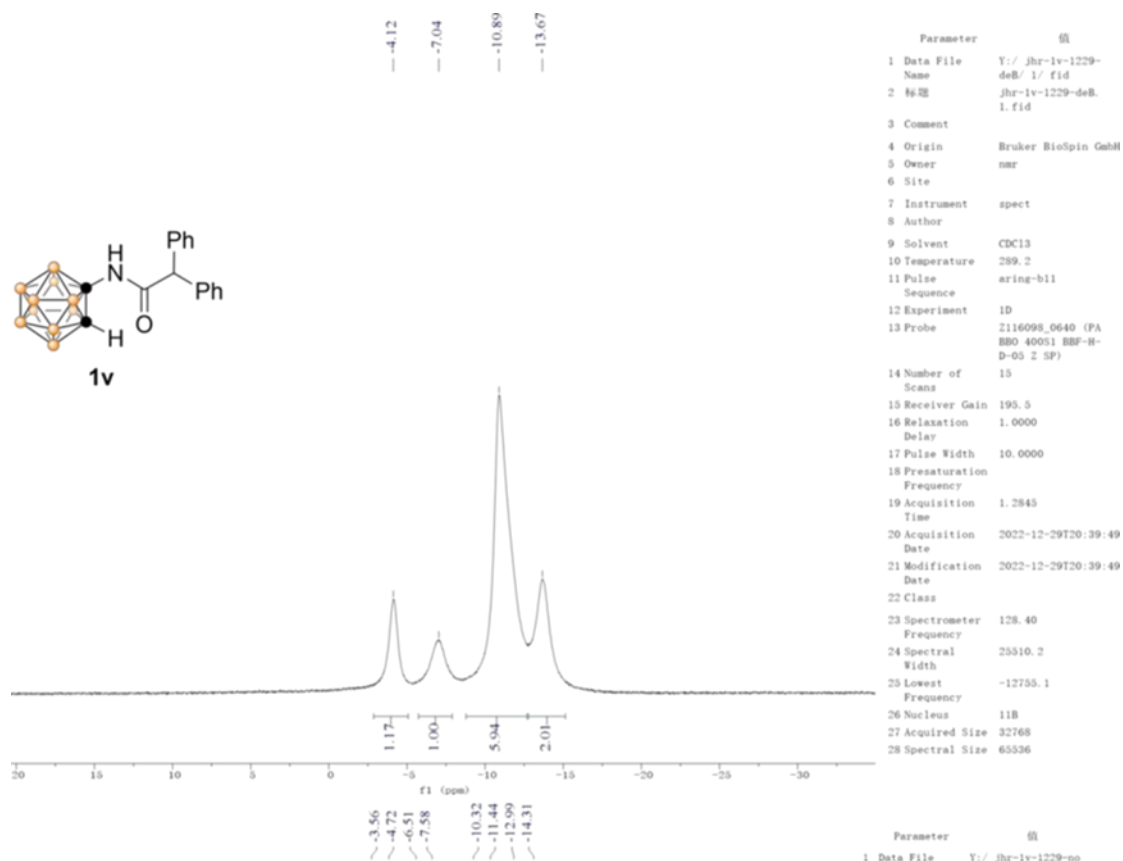
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3 Comment	
4 Origin	Bruker BioSpin GmbH
5 Owner	nar
6 Site	
7 Instrument	spect
8 Author	
9 Solvent	CDCl3
10 Temperature	296.9
11 Pulse Sequence	zg30
12 Experiment	1D
13 Probe	Z116098_0640 (PA BB0 40051 BRF-H-D-05 Z SP)
14 Number of Scans	7
15 Receiver Gain	77.4
16 Relaxation Delay	1.0000
17 Pulse Width	10.0000
18 Presaturation Frequency	
19 Acquisition Time	2.9998
20 Acquisition Date	2022-09-08T13:01:37
21 Modification Date	2022-09-08T13:01:40
22 Class	
23 Spectrometer Frequency	400.20
24 Spectral Width	7598.8
25 Lowest Frequency	-1208.1
26 Nucleus	1H
27 Acquired Size	22795
28 Spectral Size	65536
29 Digital Resolution	0.12



Parameter	值
1 Data File Name	E:/ 布鲁克-jhr/ 收谱/ jhr-lu-C/ 1/ fid
2 标题	jhr-lu-C.1.fid
3 Comment	
4 Origin	Bruker BioSpin GmbH
5 Owner	nar
6 Site	
7 Instrument	spect
8 Author	
9 Solvent	CDCl3
10 Temperature	296.9
11 Pulse Sequence	zgpg30
12 Experiment	1D
13 Probe	Z116098_0640 (PA BB0 40051 BRF-H-D-05 Z SP)
14 Number of Scans	218
15 Receiver Gain	195.5
16 Relaxation Delay	1.0000
17 Pulse Width	10.0000
18 Presaturation Frequency	
19 Acquisition Time	1.2999
20 Acquisition Date	2022-09-09T19:48:21
21 Modification Date	2022-09-09T19:48:24
22 Class	
23 Spectrometer Frequency	100.64
24 Spectral Width	23252.5
25 Lowest Frequency	-1545.4
26 Nucleus	13C
27 Acquired Size	32827
28 Spectral Size	131072
29 Digital Resolution	0.19



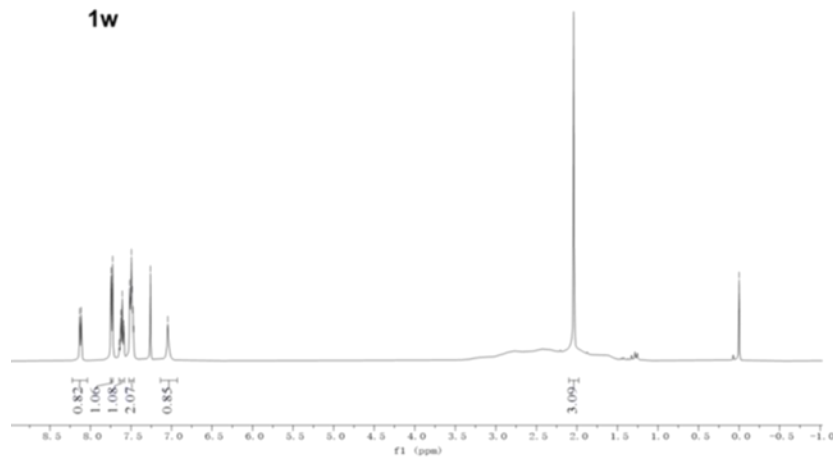




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8.113
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7.642
7.624
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7.513
7.505
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7.485
7.475
7.466
7.260
7.046

2.039

0.000



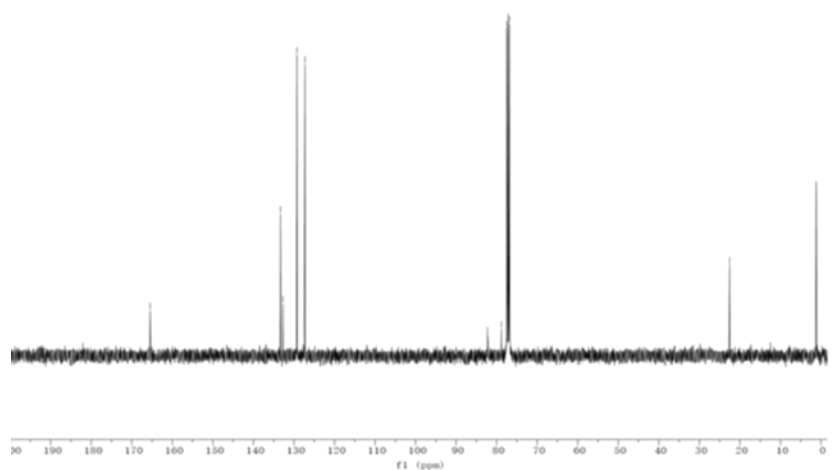
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3 Comment	
4 Origin	Braker Biospin GmbH
5 Owner	nmr
6 Site	
7 Instrument	spect
8 Author	
9 Solvent	CDCl3
10 Temperature	296.7
11 Pulse Sequence	zg30
12 Experiment	1D
13 Probe	2116098_0640 (PA BBO 400S1 BPF-H-D-05 Z SP)
14 Number of Scans	6
15 Receiver Gain	77.4
16 Relaxation Delay	1.0000
17 Pulse Width	10.0000
18 Presaturation Frequency	
19 Acquisition Time	2.9998
20 Acquisition Date	2022-09-09T18:40:03
21 Modification Date	2022-09-09T18:40:06
22 Class	
23 Spectrometer Frequency	400.20
24 Spectral Width	4807.7
25 Lowest Frequency	-412.0
26 Nucleus	1H
27 Acquired Size	14422
28 Spectral Size	65536
29 Digital Resolution	0.07

165.47

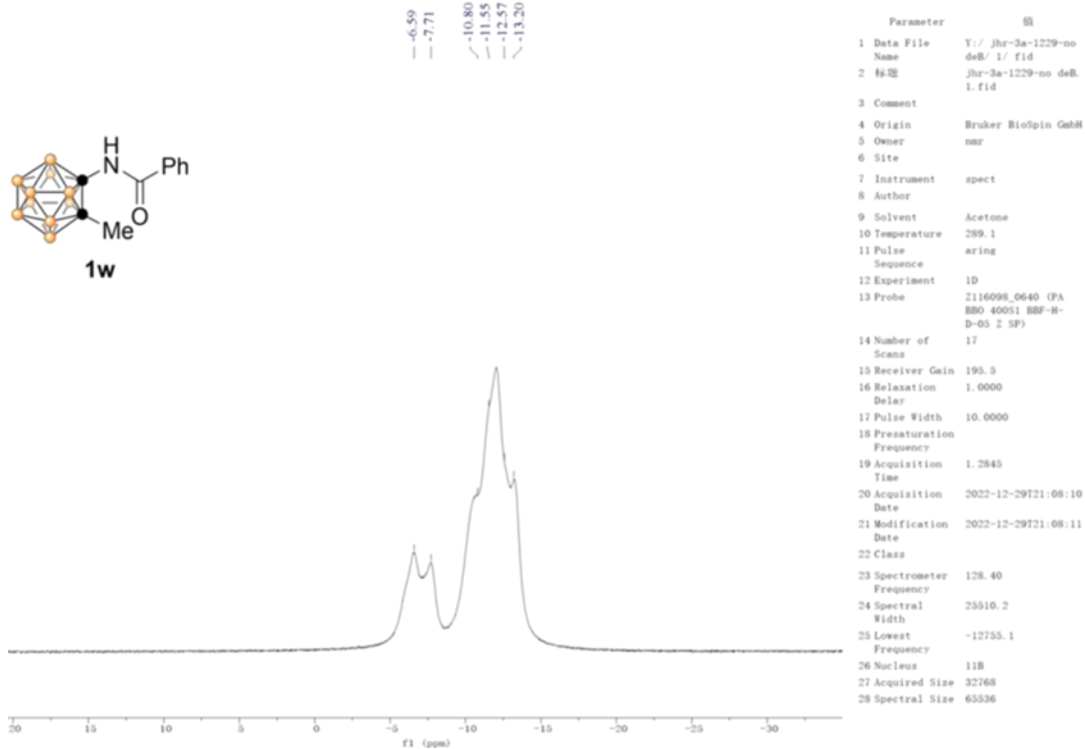
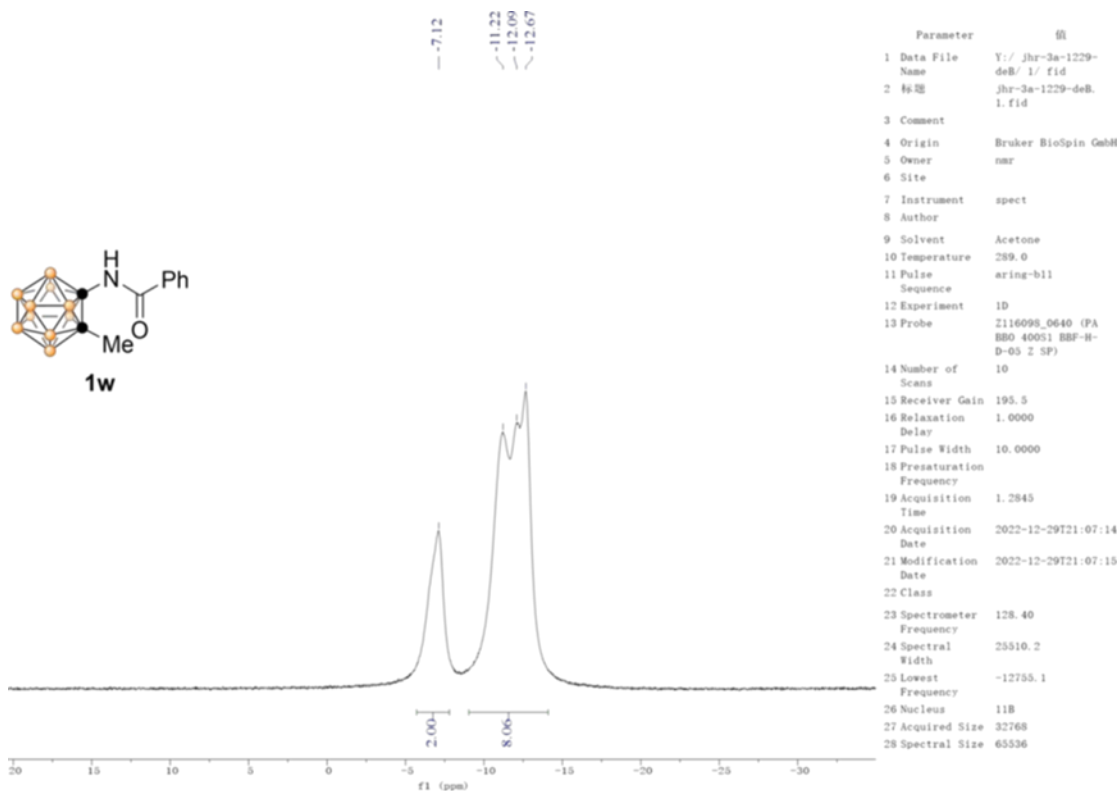
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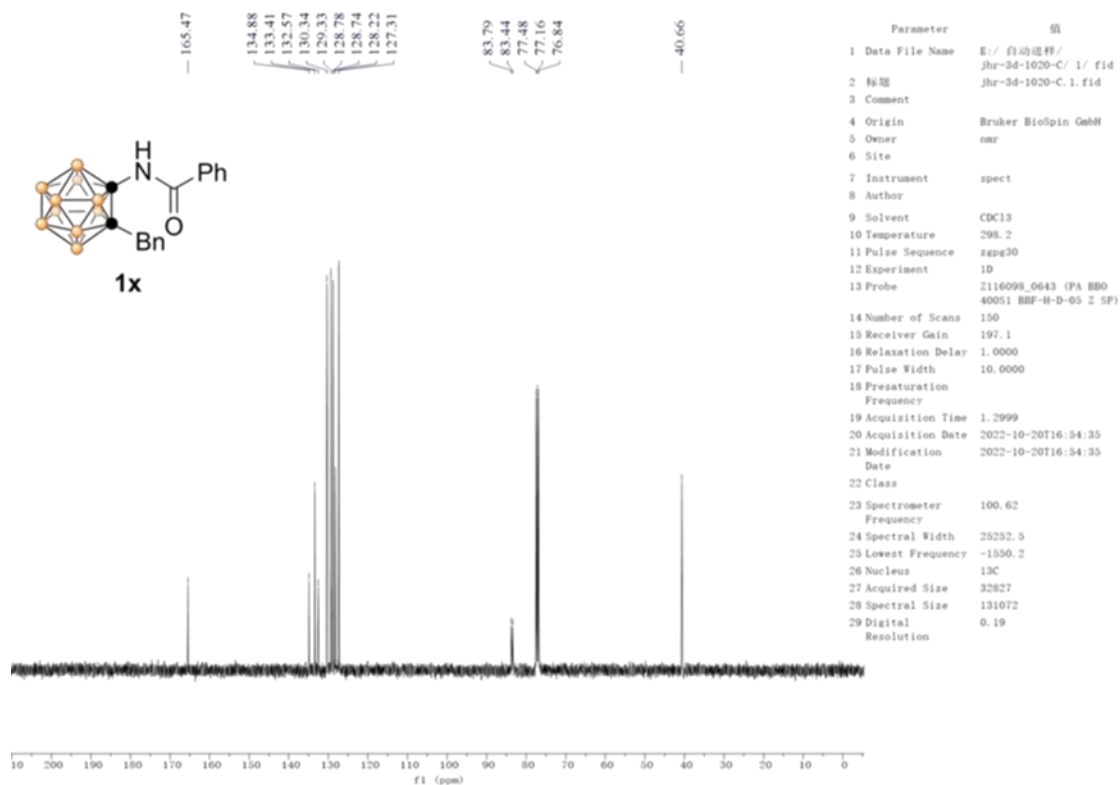
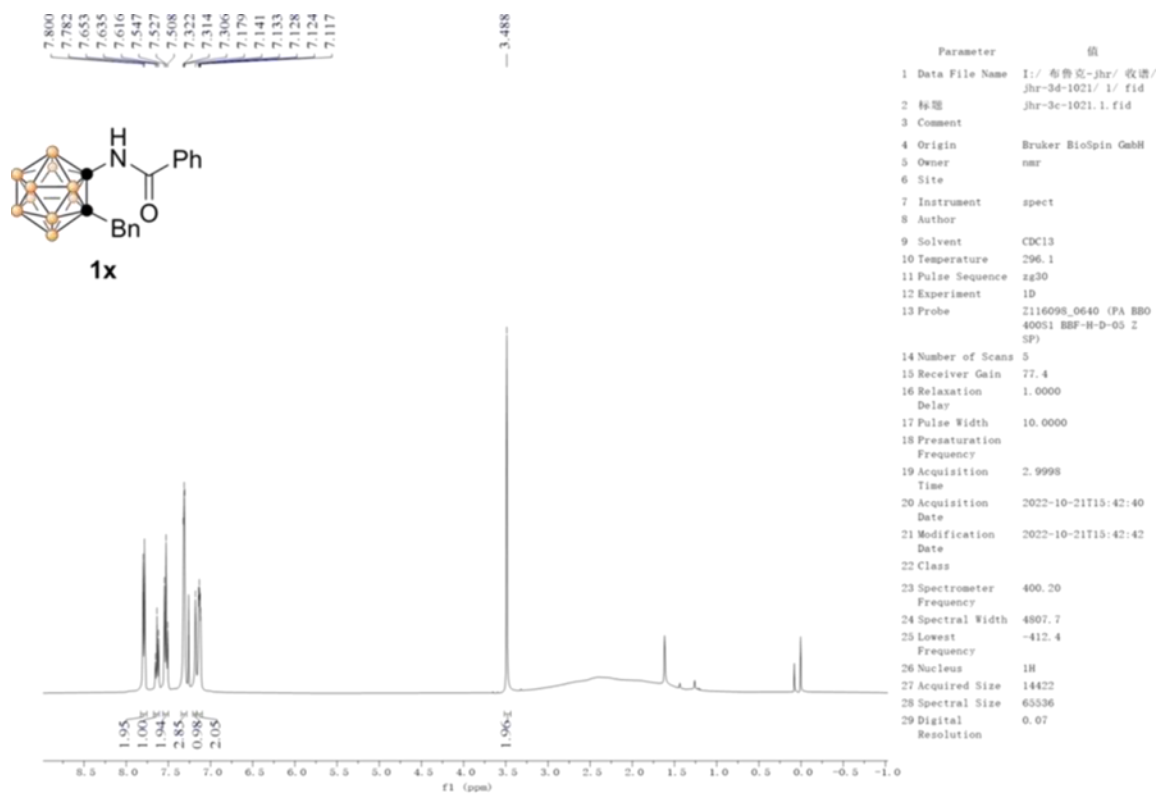
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77.16
76.84

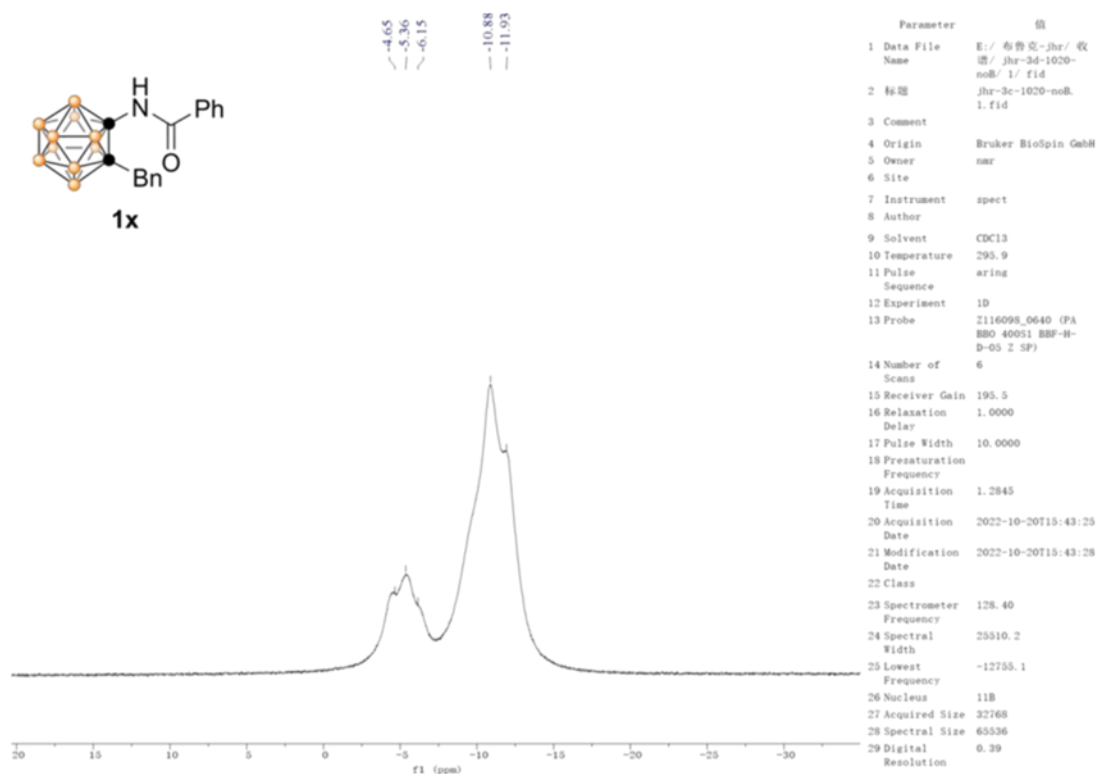
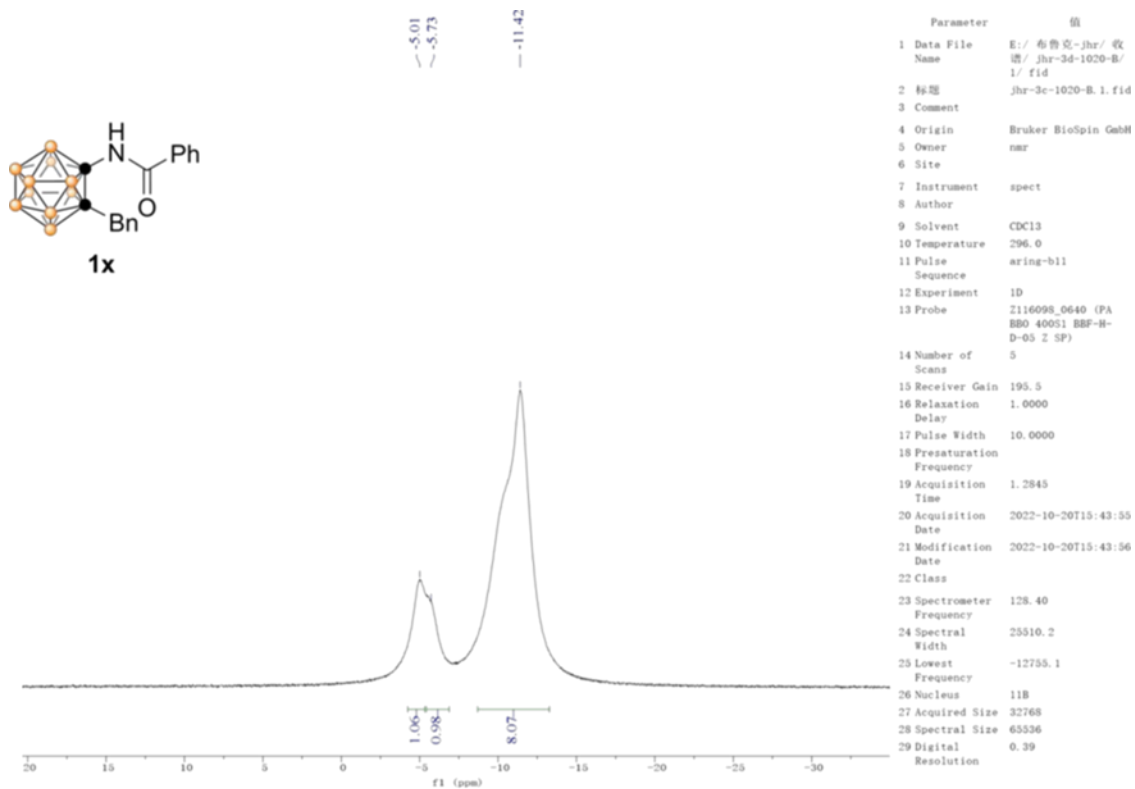
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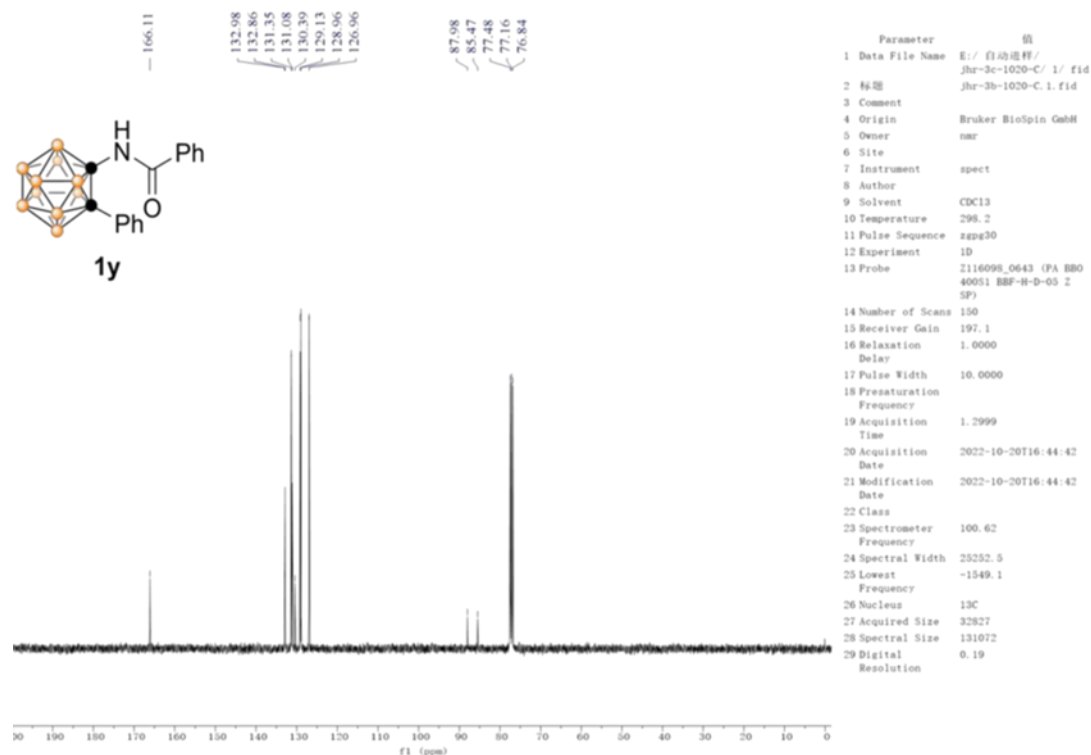
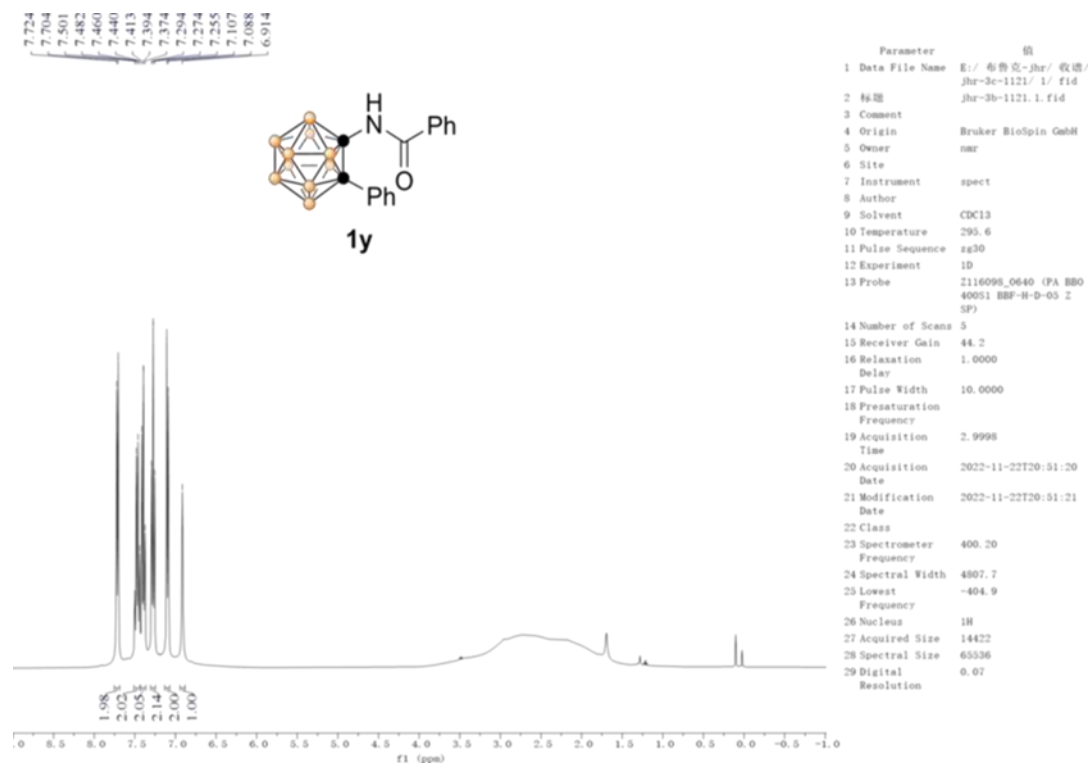


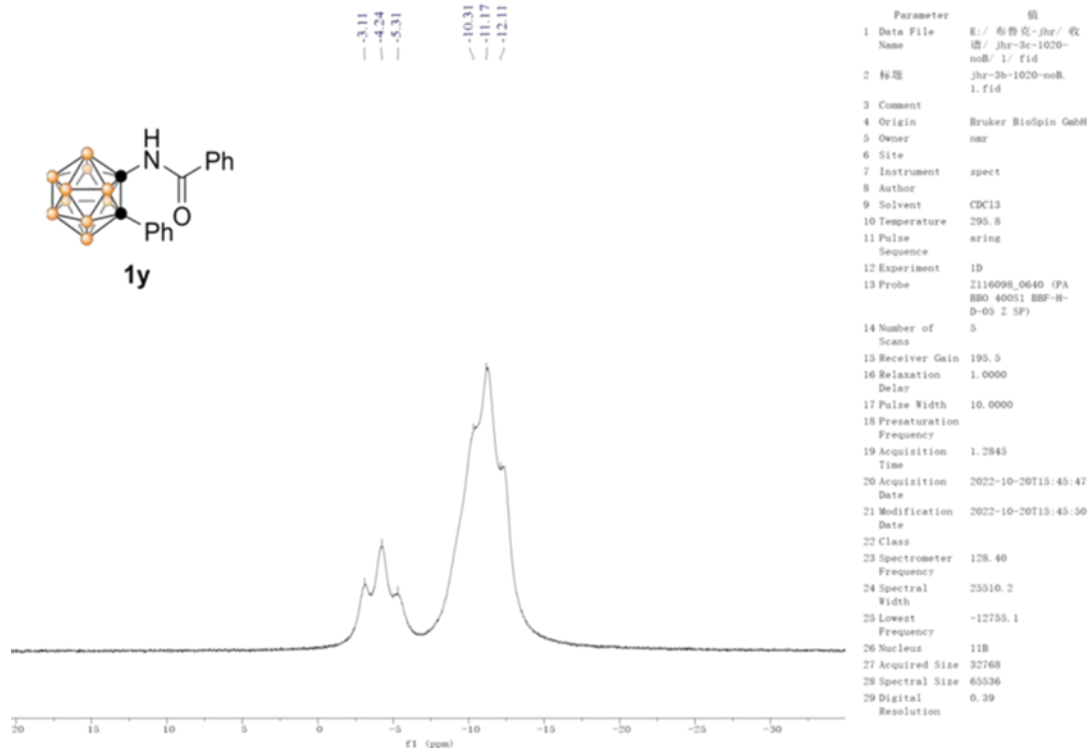
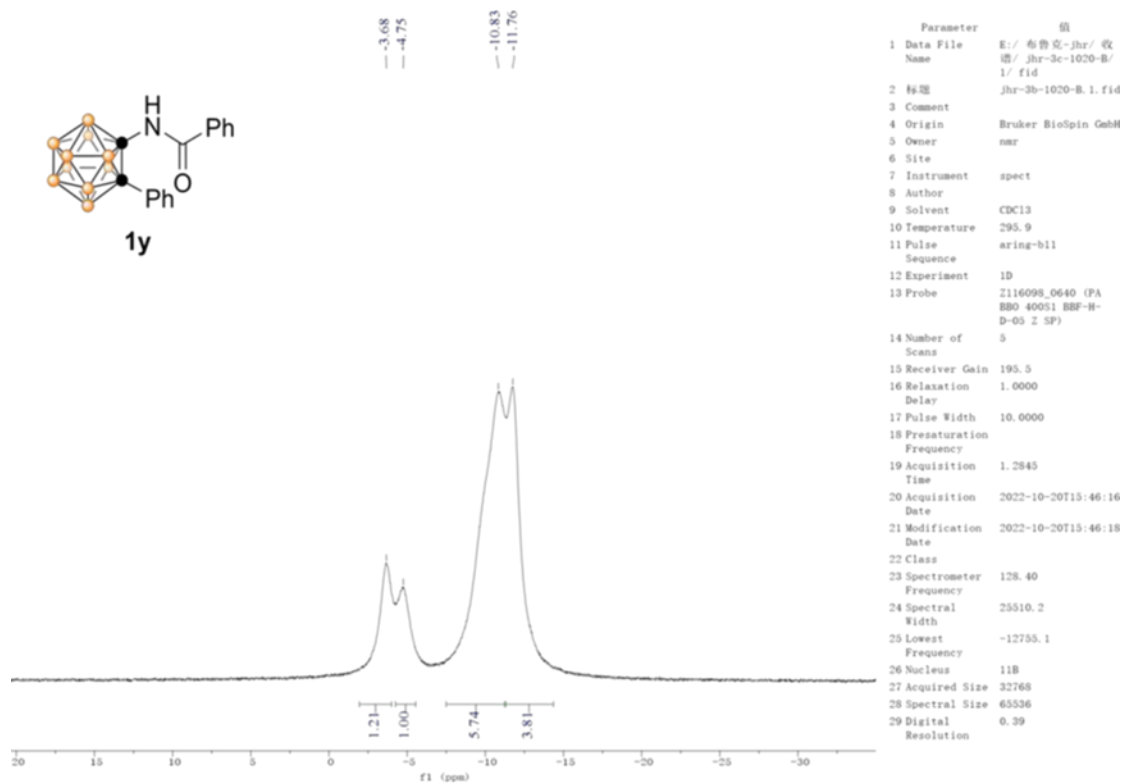
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2 标题	jhr-3a-1121-C.1.f1d
3 Comment	
4 Origin	Braker Biospin GmbH
5 Owner	nmr
6 Site	
7 Instrument	spect
8 Author	
9 Solvent	CDCl3
10 Temperature	295.7
11 Pulse Sequence	zgpg30
12 Experiment	1D
13 Probe	2116098_0640 (PA BBO 400S1 BPF-H-D-05 Z SP)
14 Number of Scans	108
15 Receiver Gain	195.5
16 Relaxation Delay	1.0000
17 Pulse Width	10.0000
18 Presaturation Frequency	
19 Acquisition Time	1.2999
20 Acquisition Date	2022-11-22T20:40:16
21 Modification Date	2022-11-22T20:40:17
22 Class	
23 Spectrometer Frequency	100.64
24 Spectral Width	25252.5
25 Lowest Frequency	-1546.0
26 Nucleus	13C
27 Acquired Size	32827
28 Spectral Size	131072
29 Digital Resolution	0.19

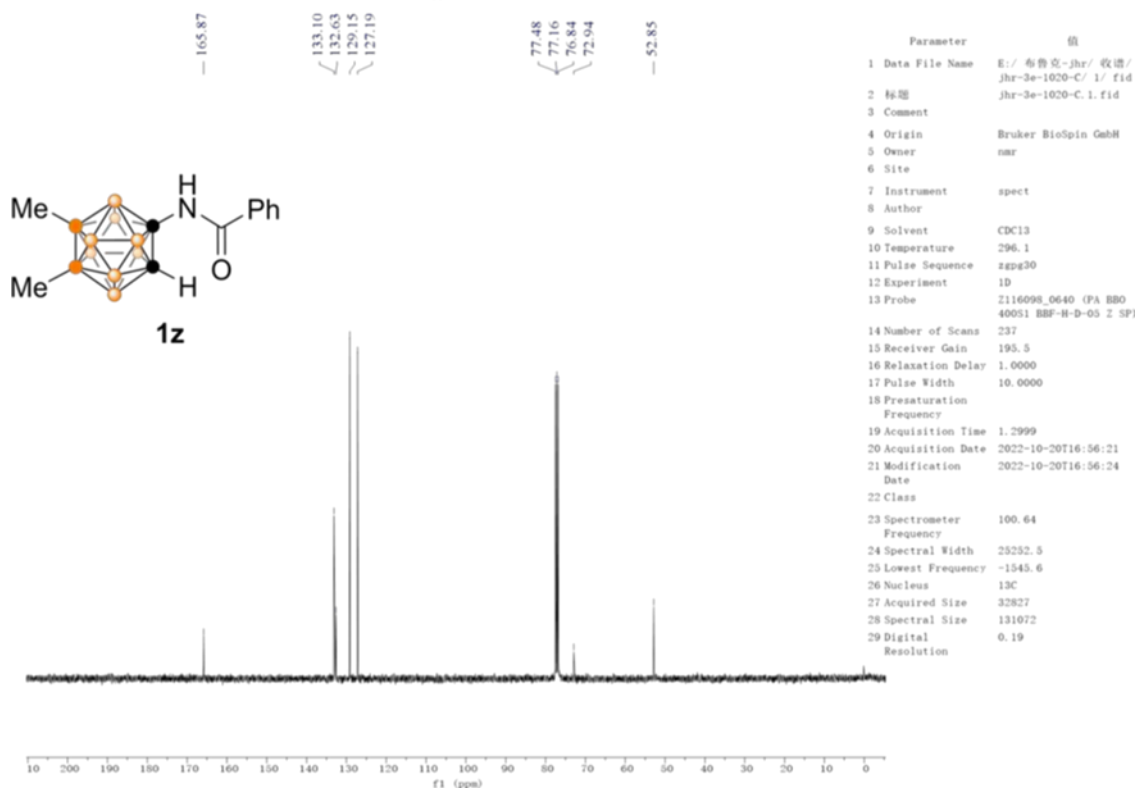
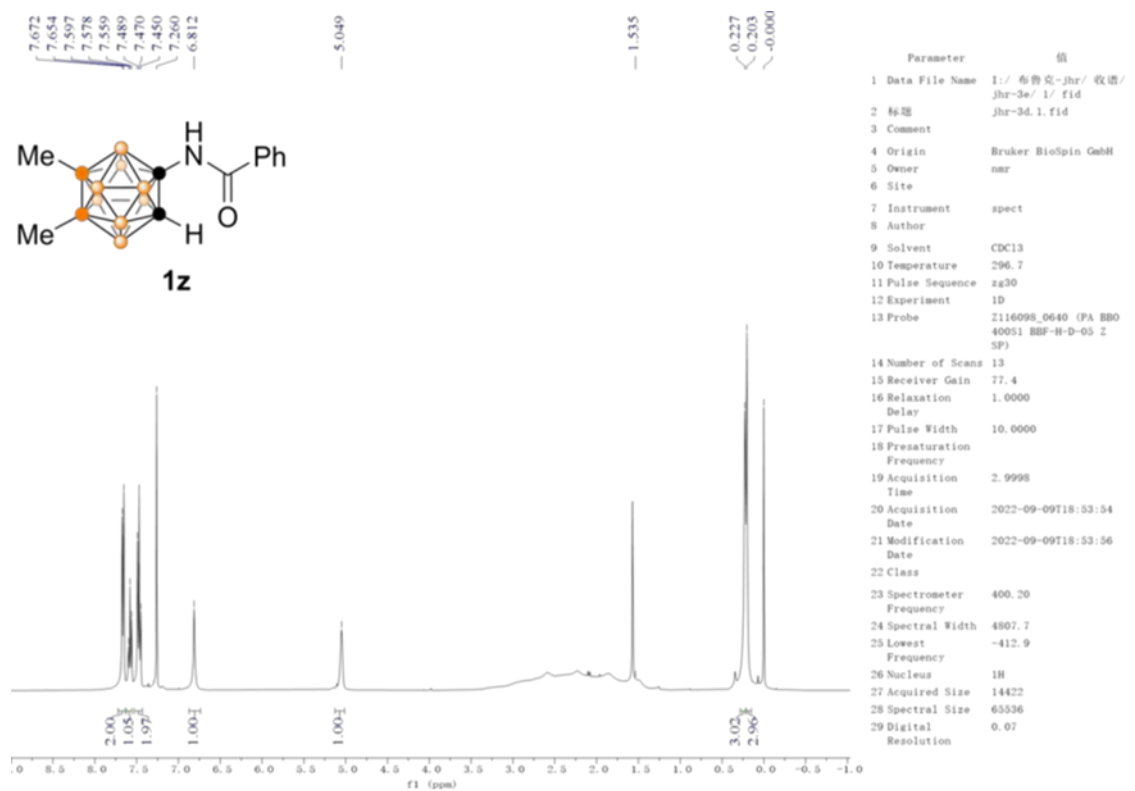


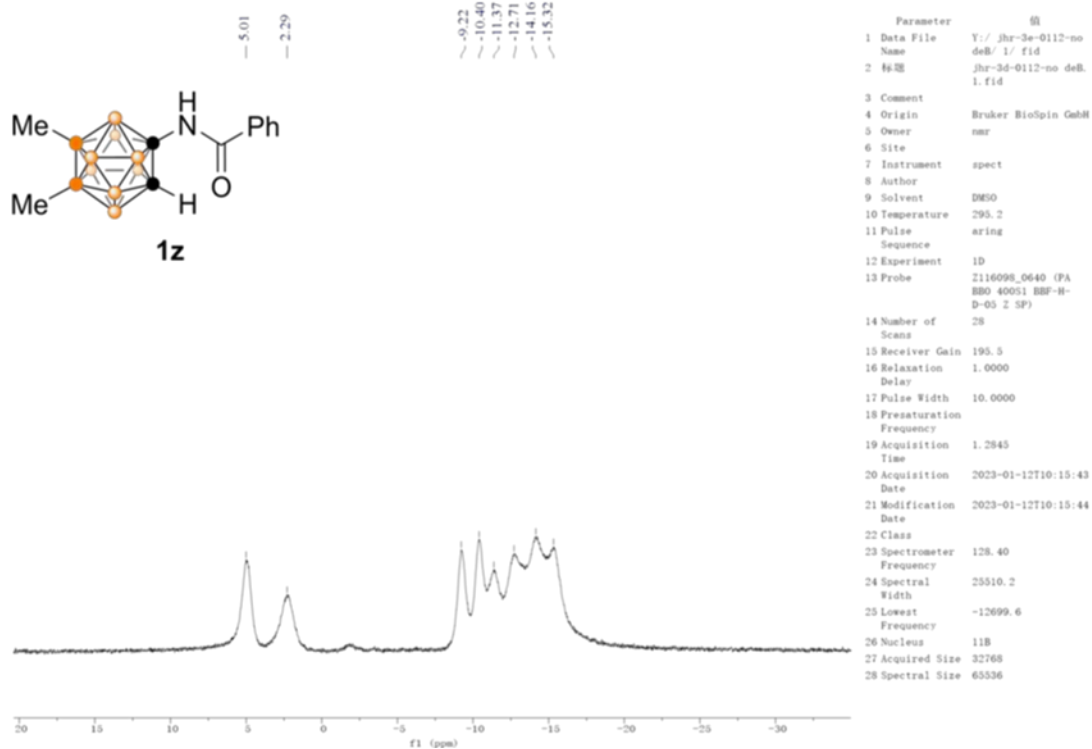
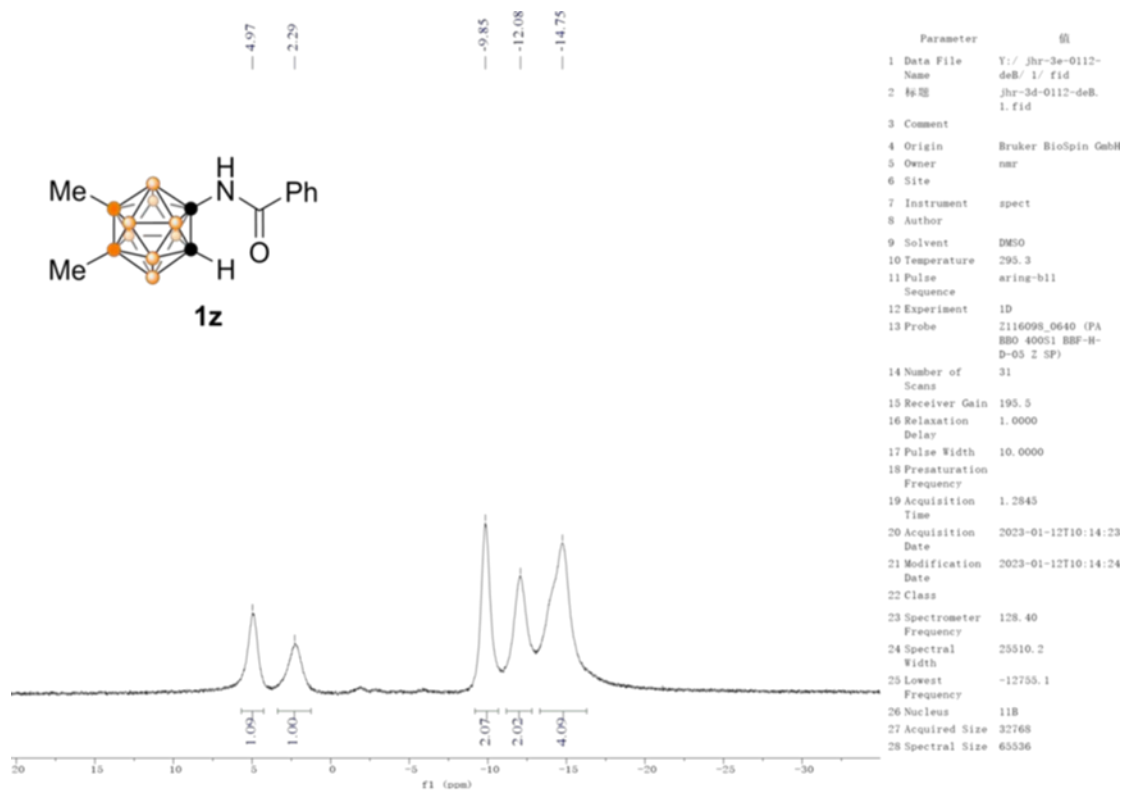


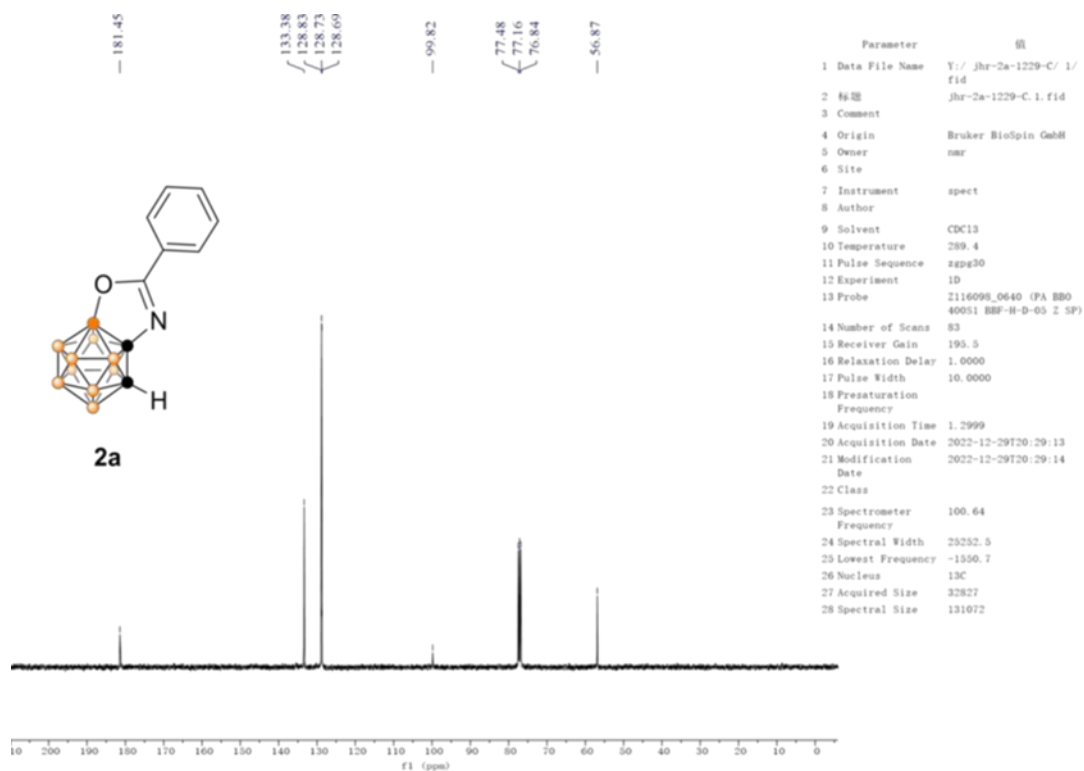
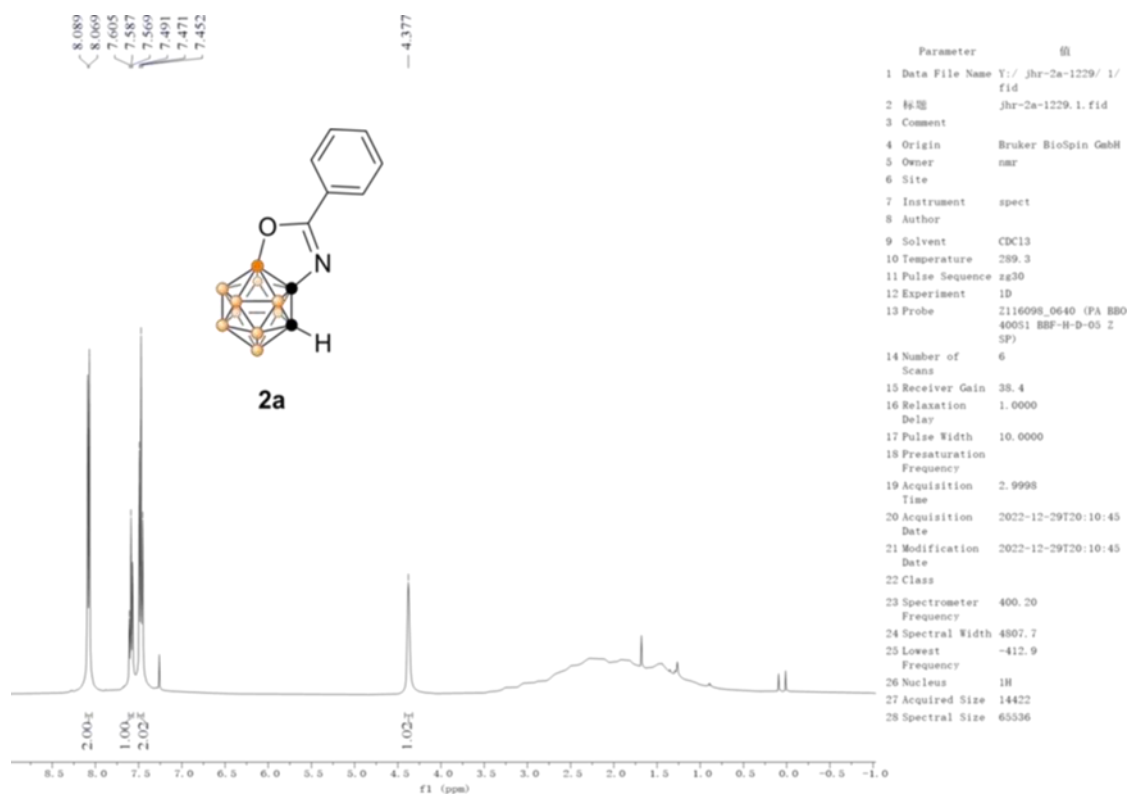


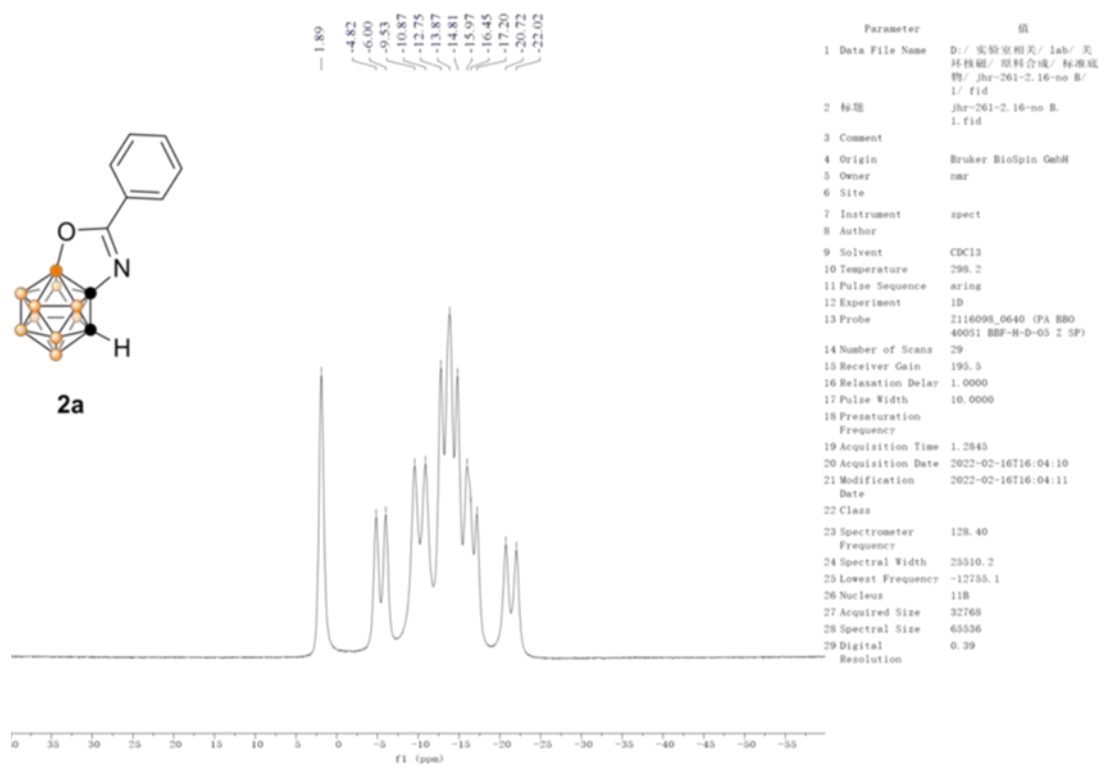
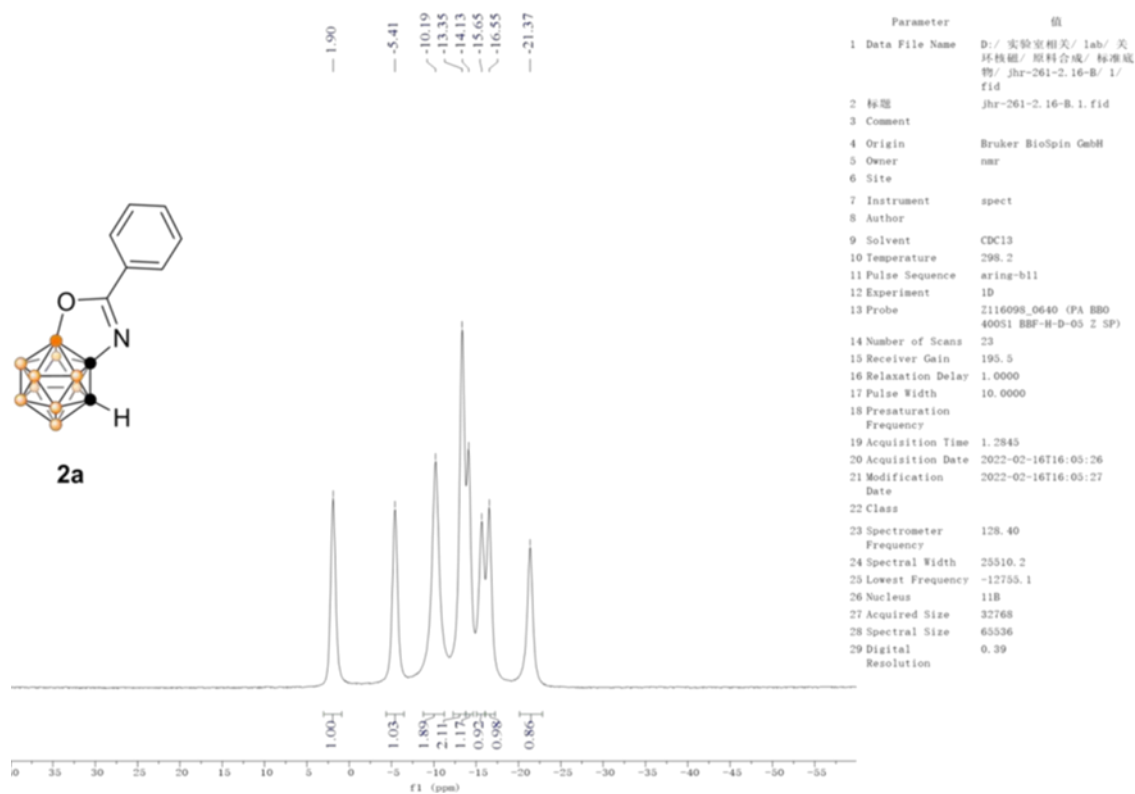


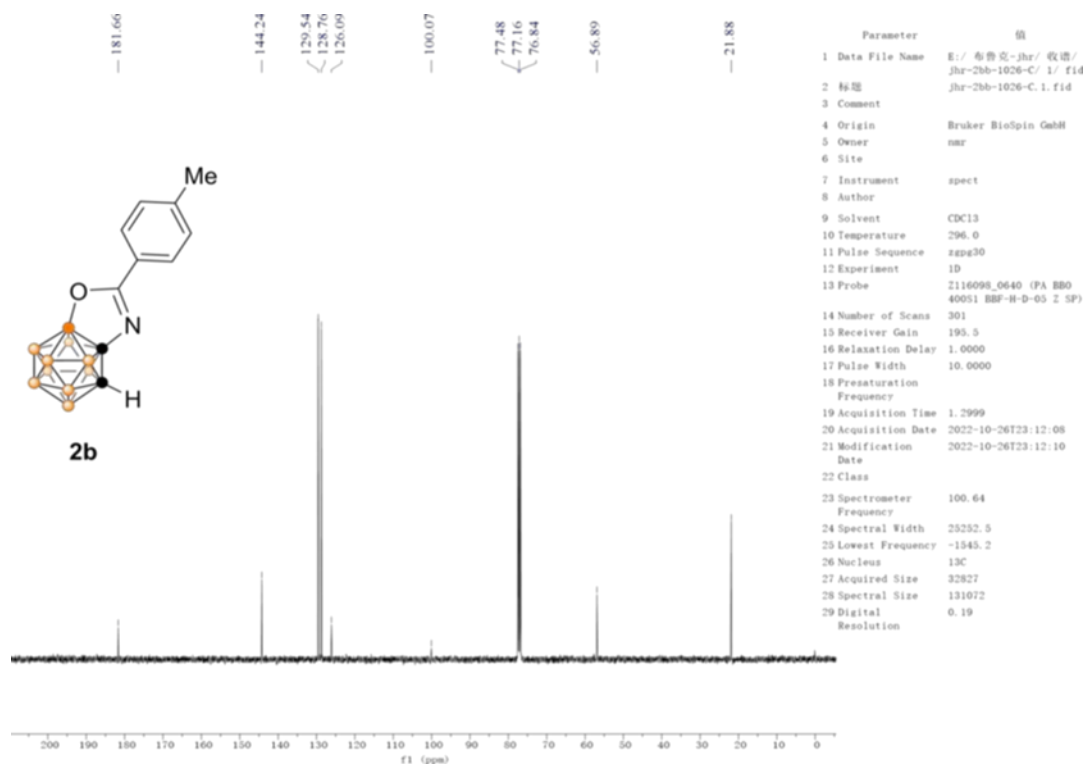
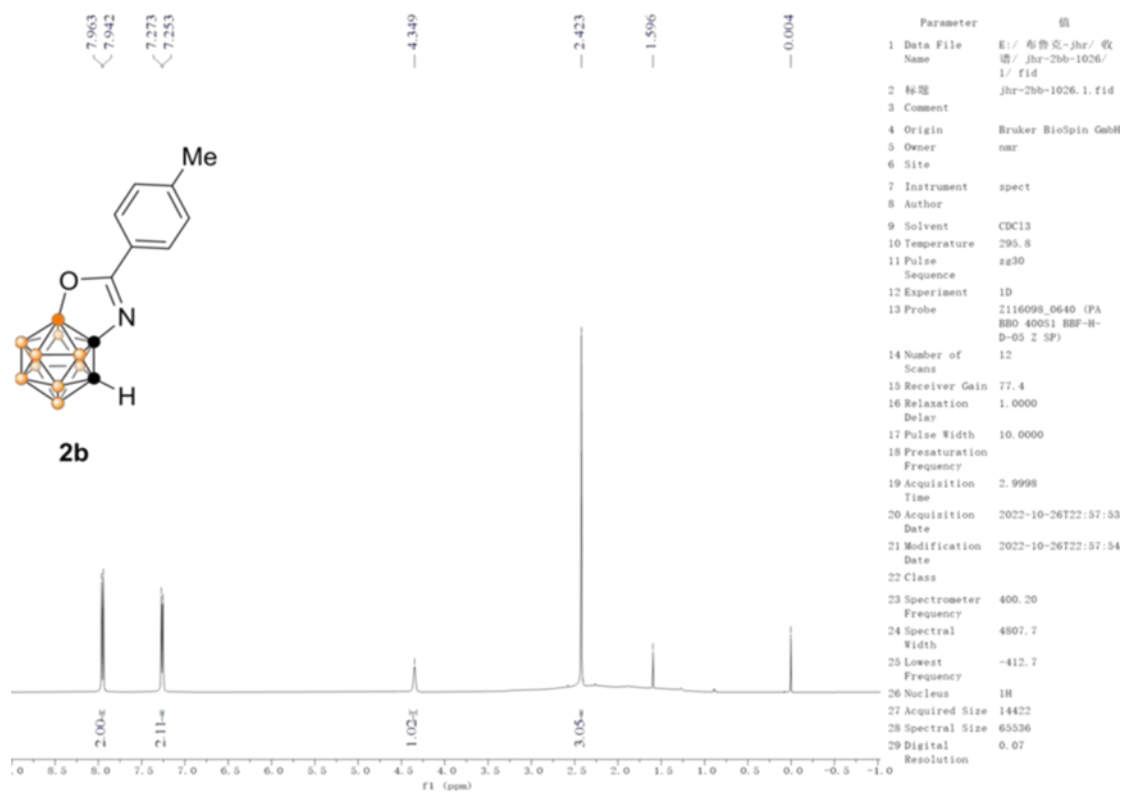


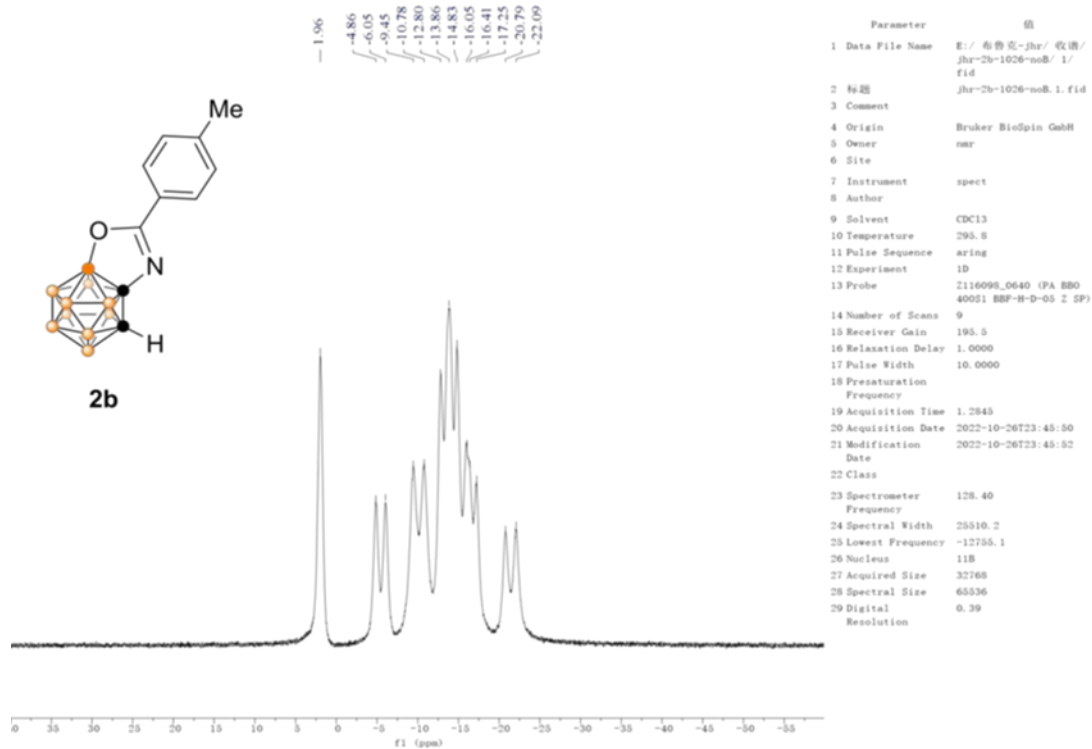
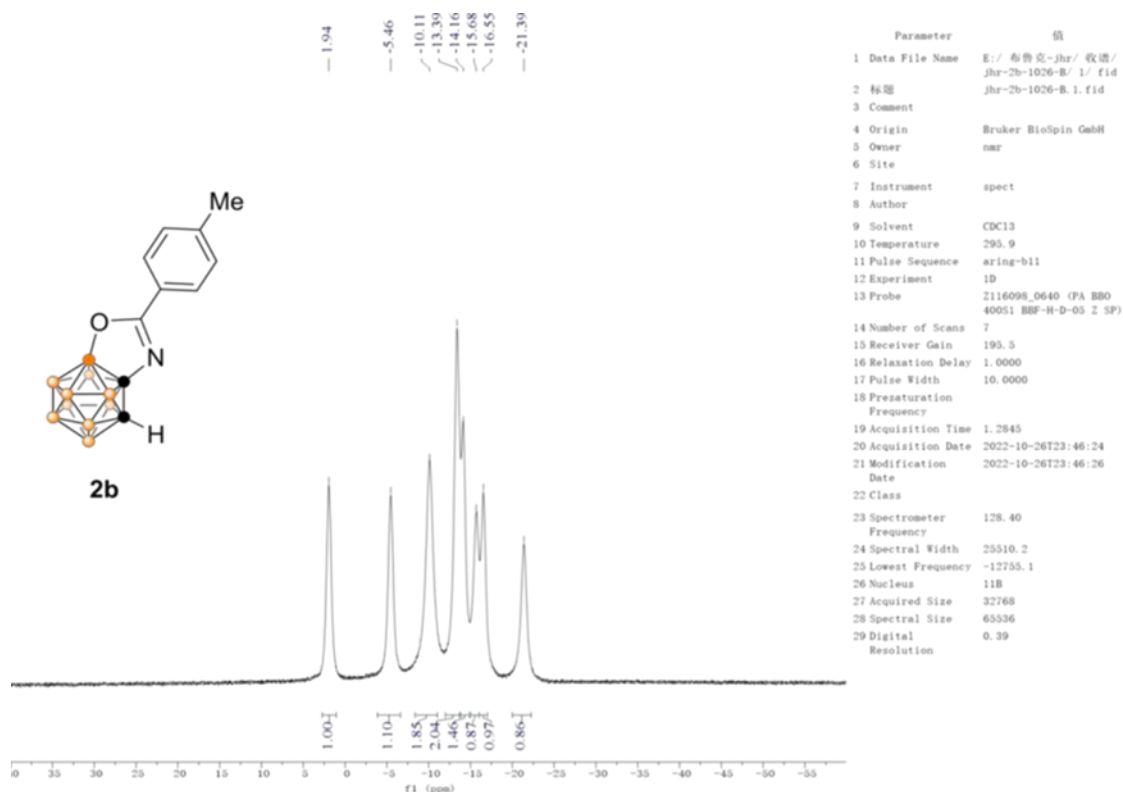


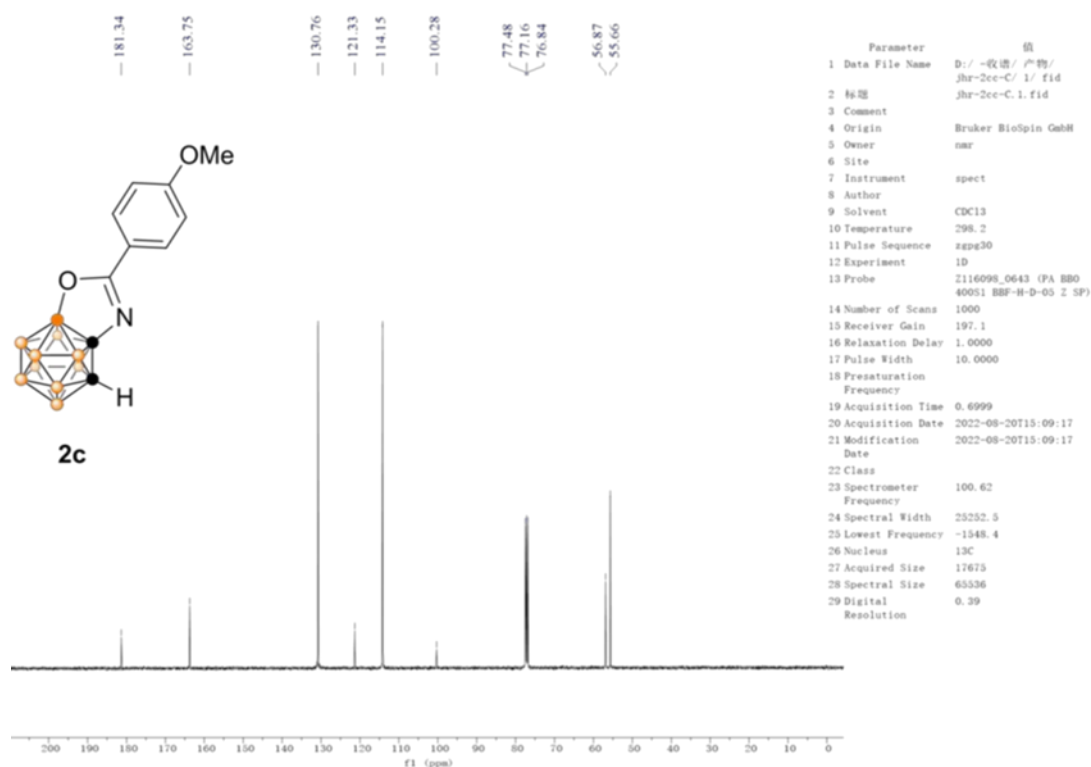
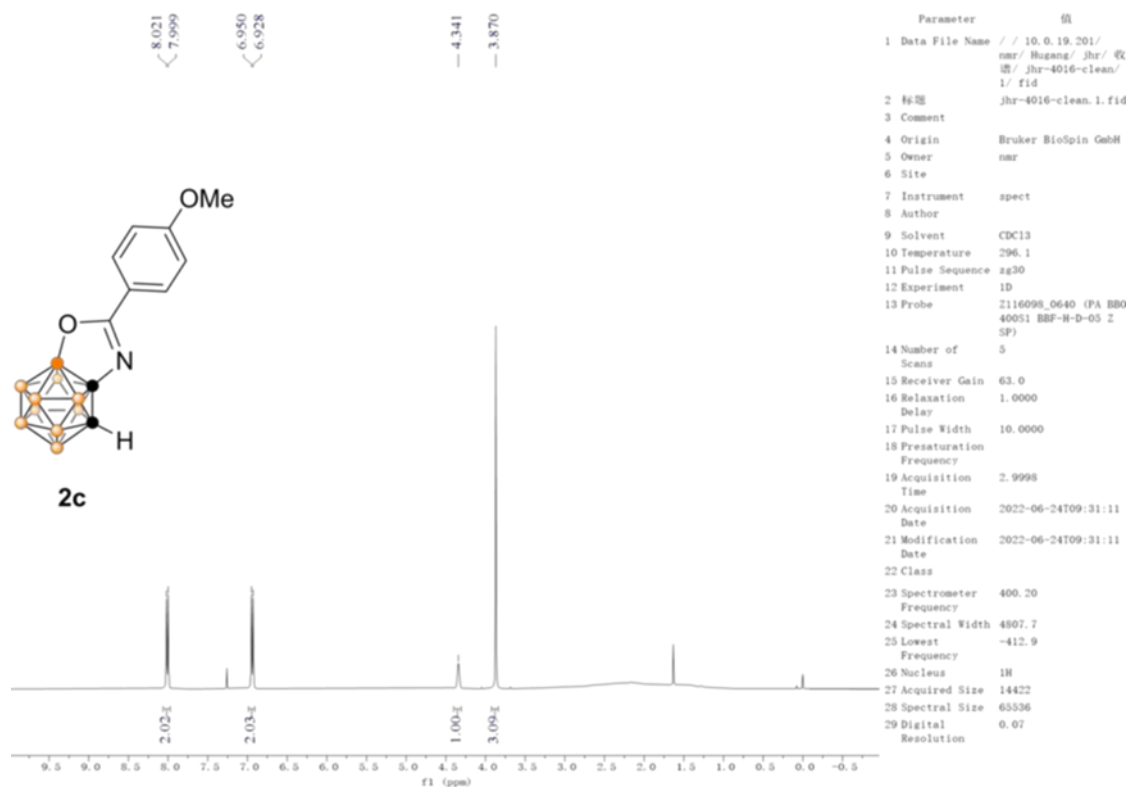


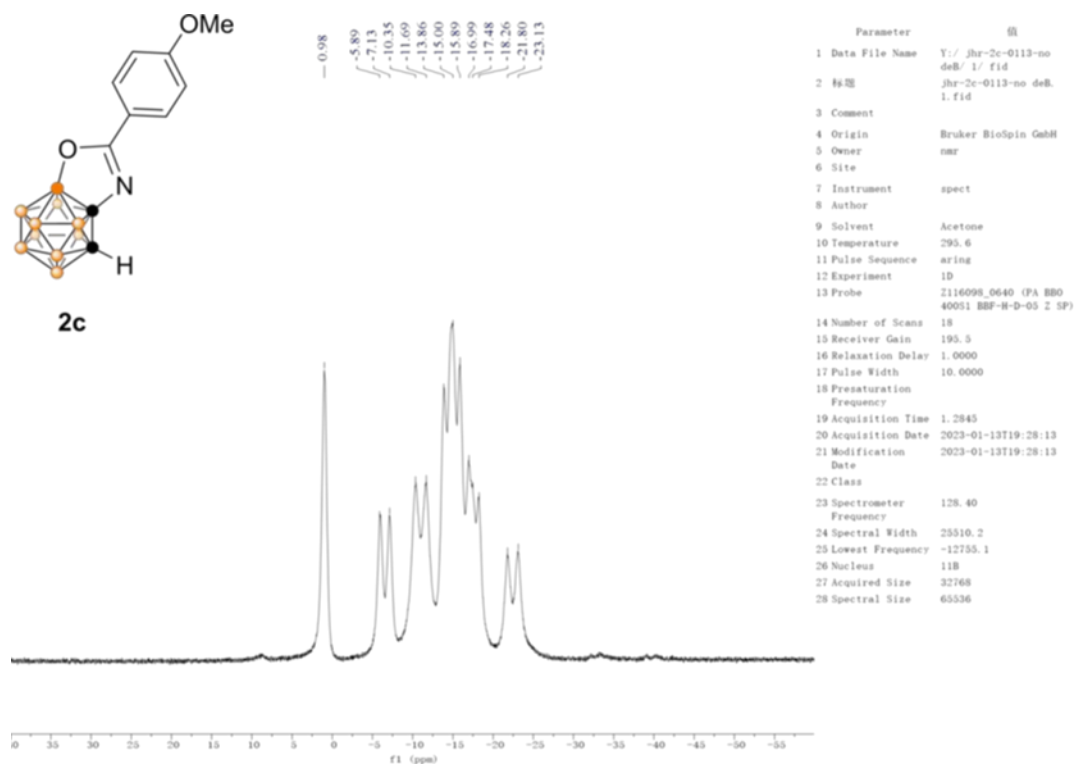
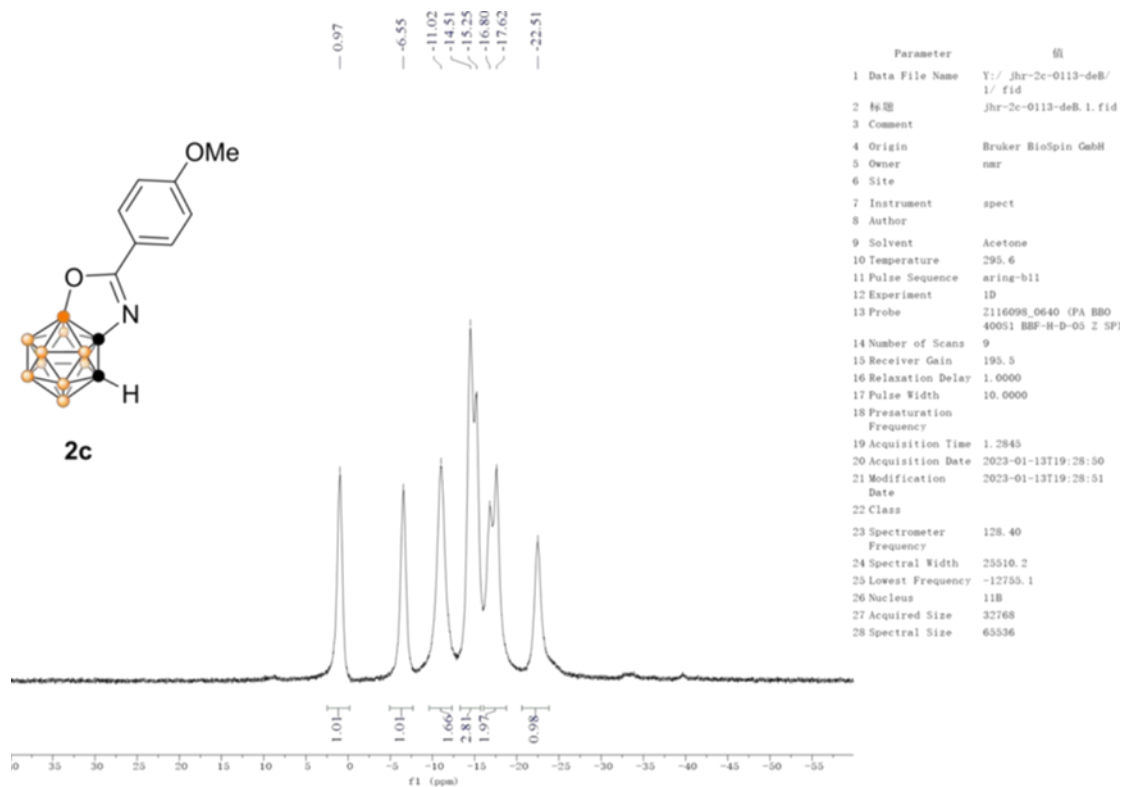


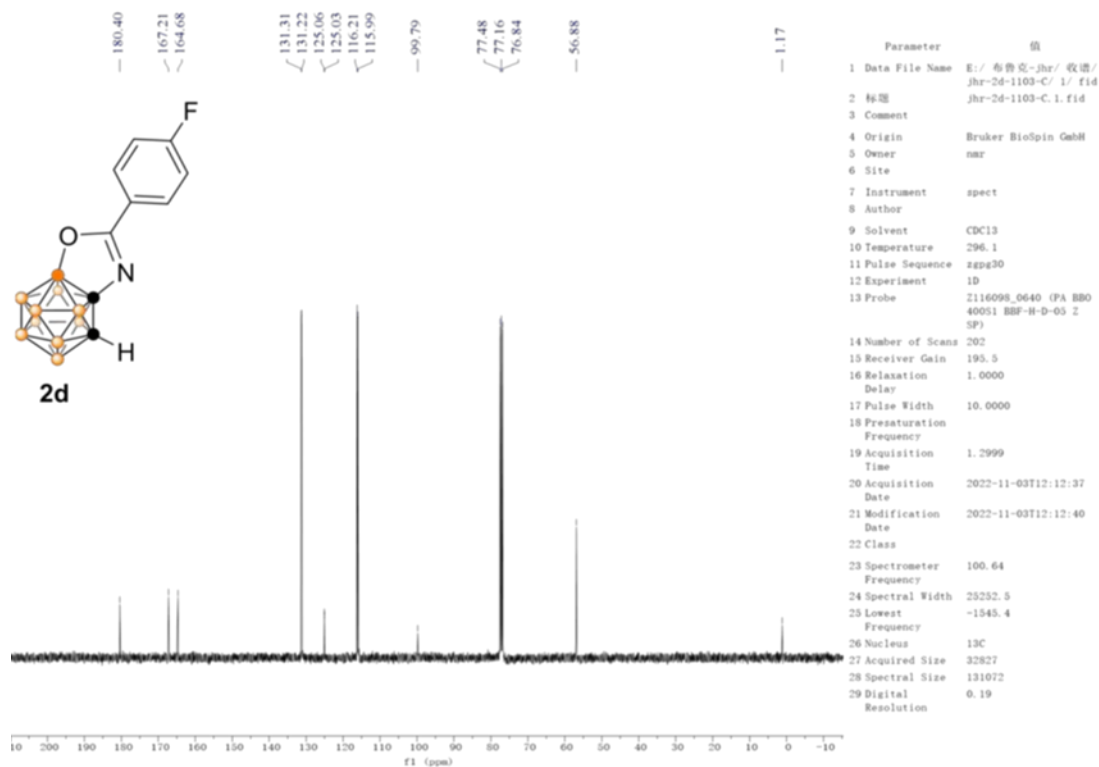
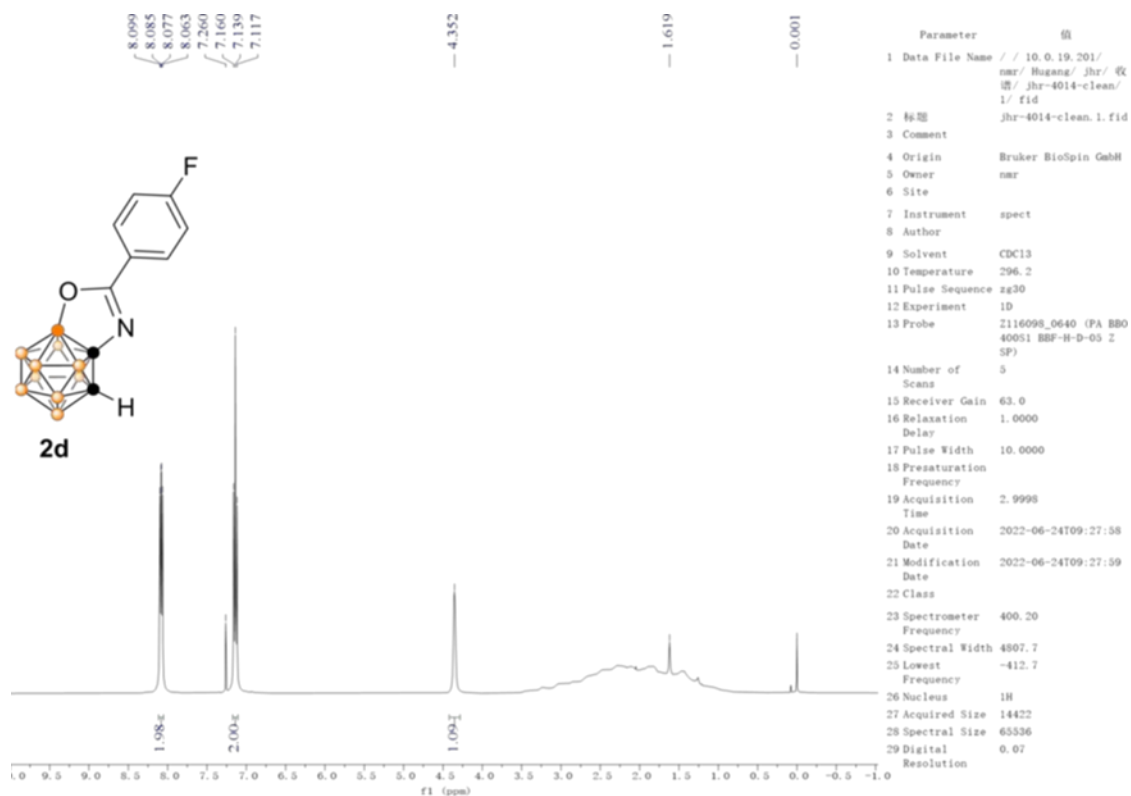


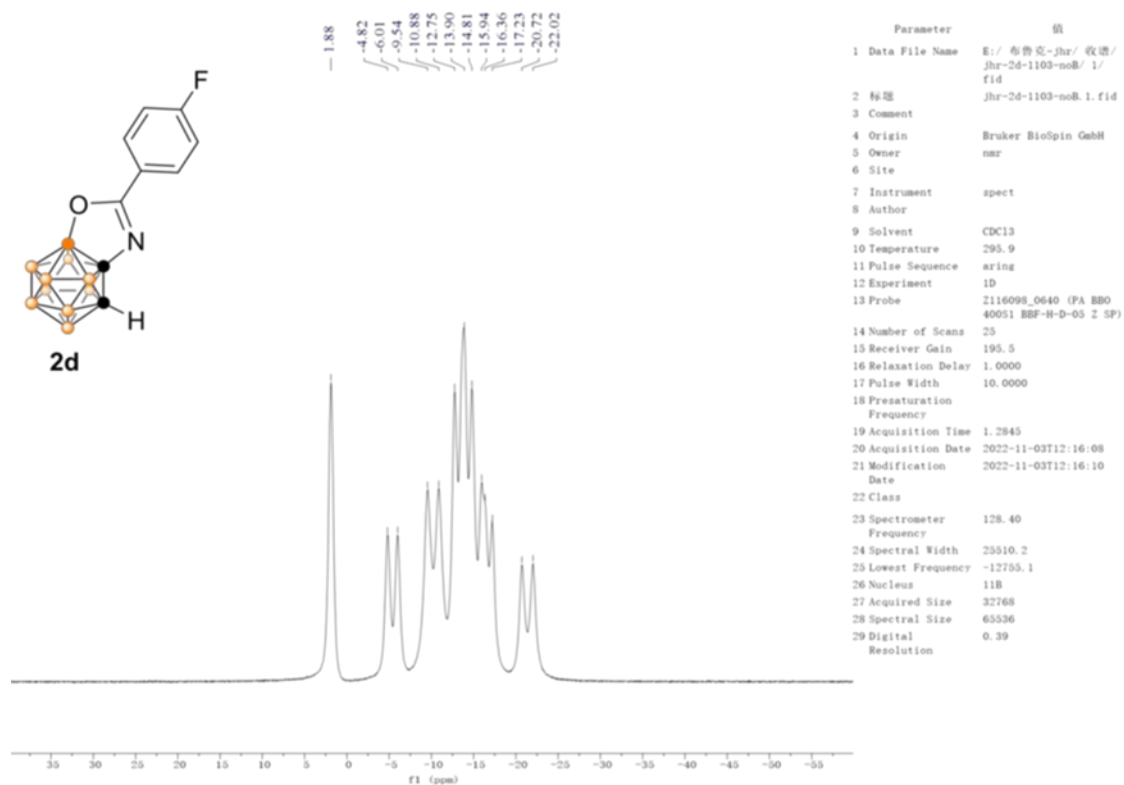
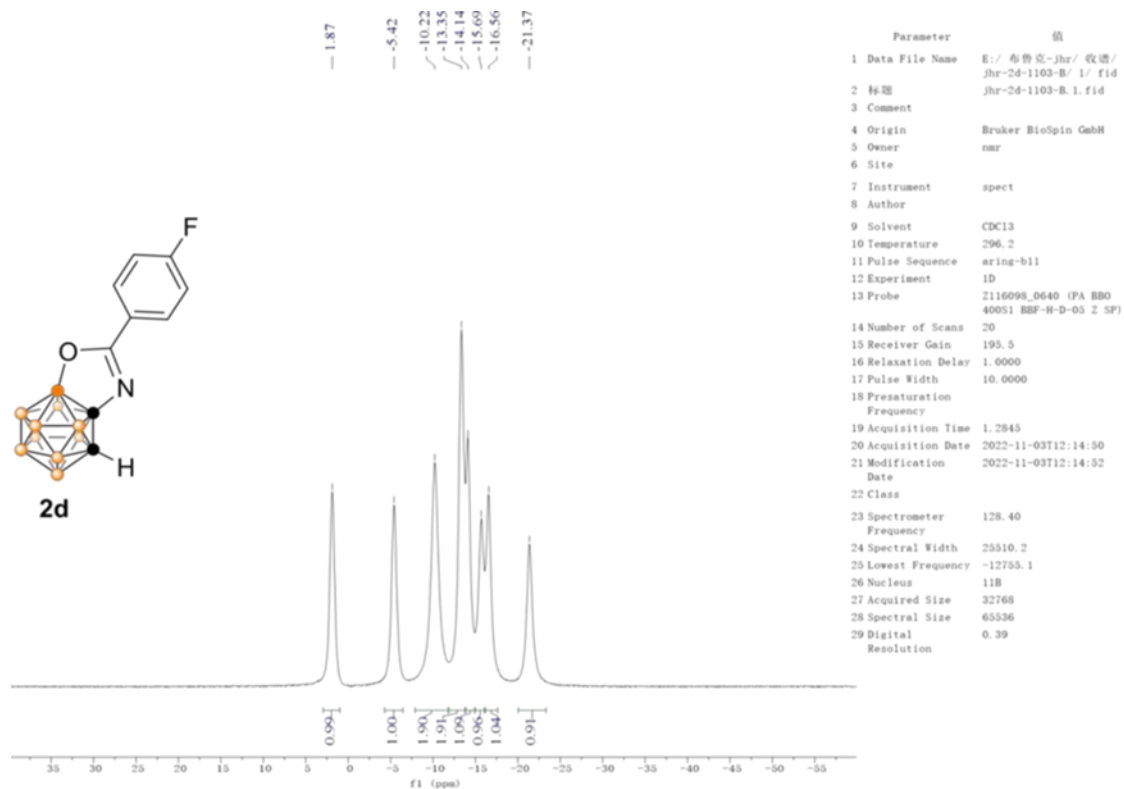






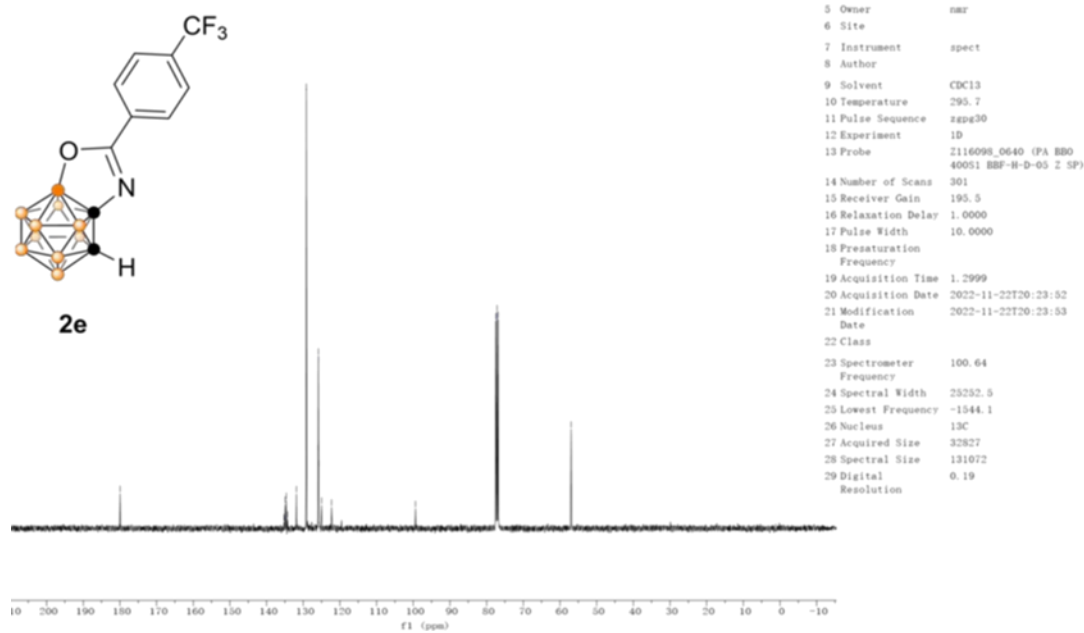
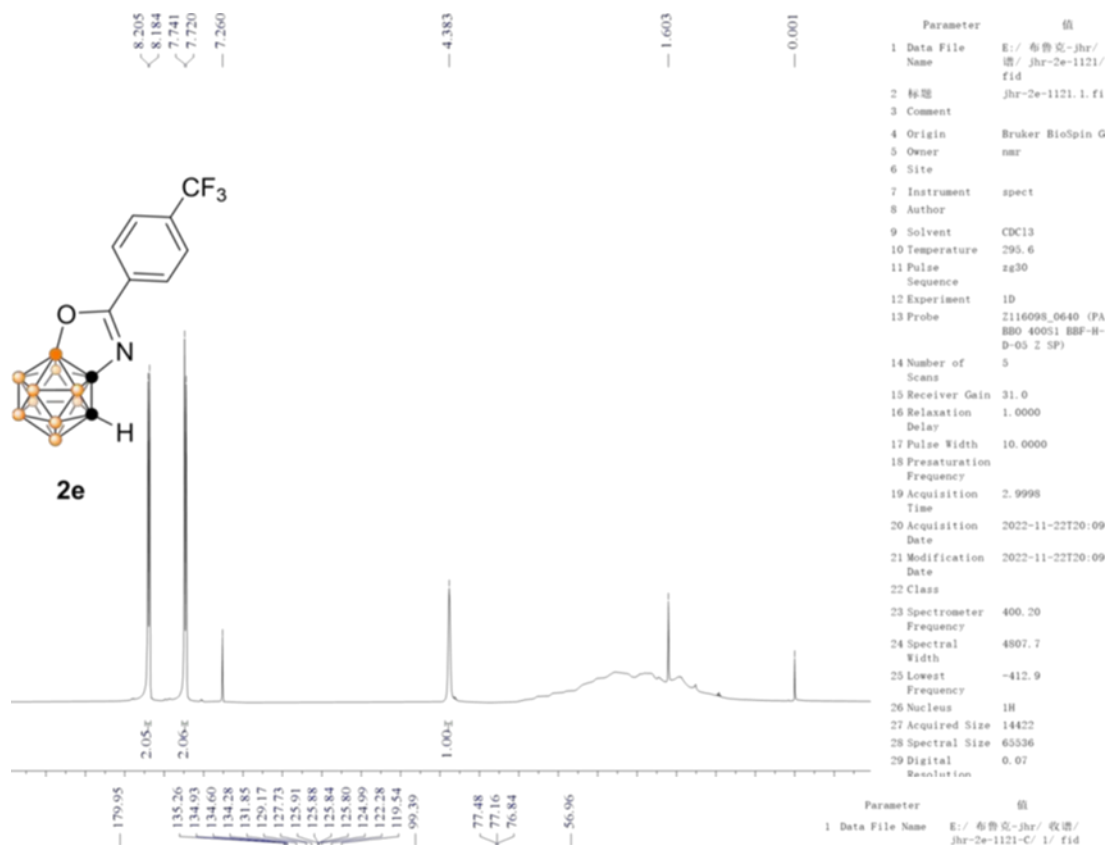


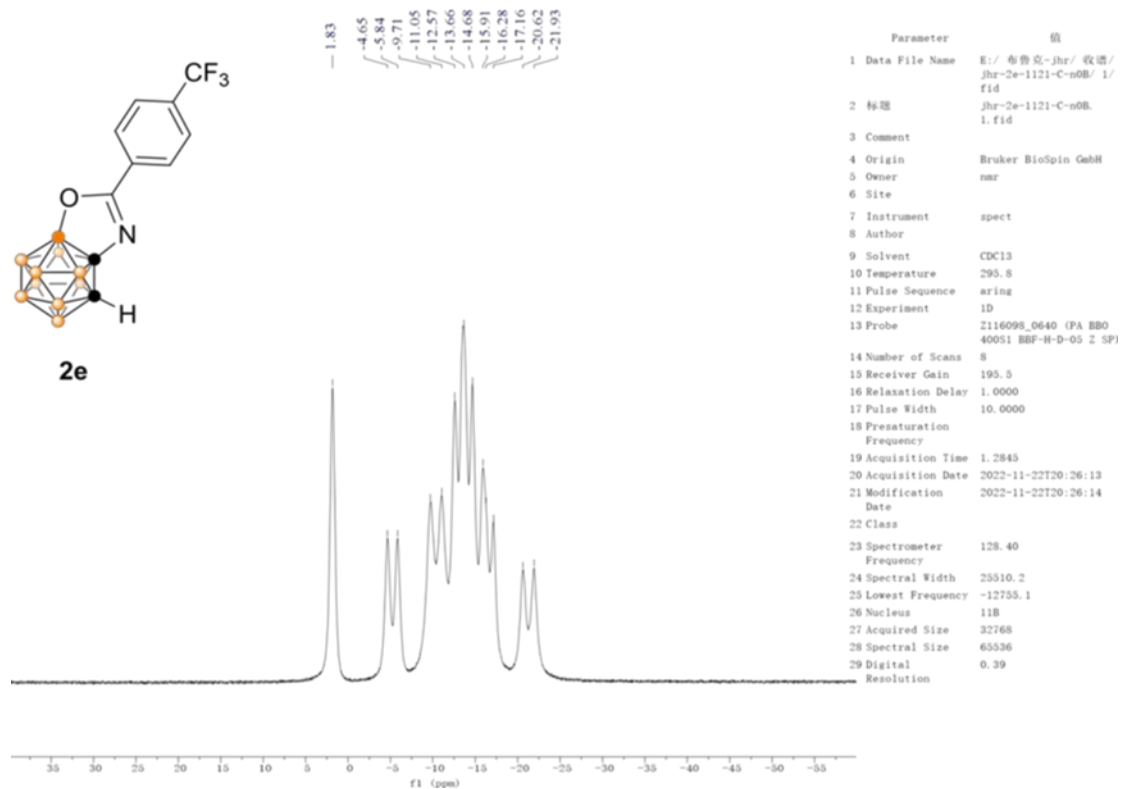
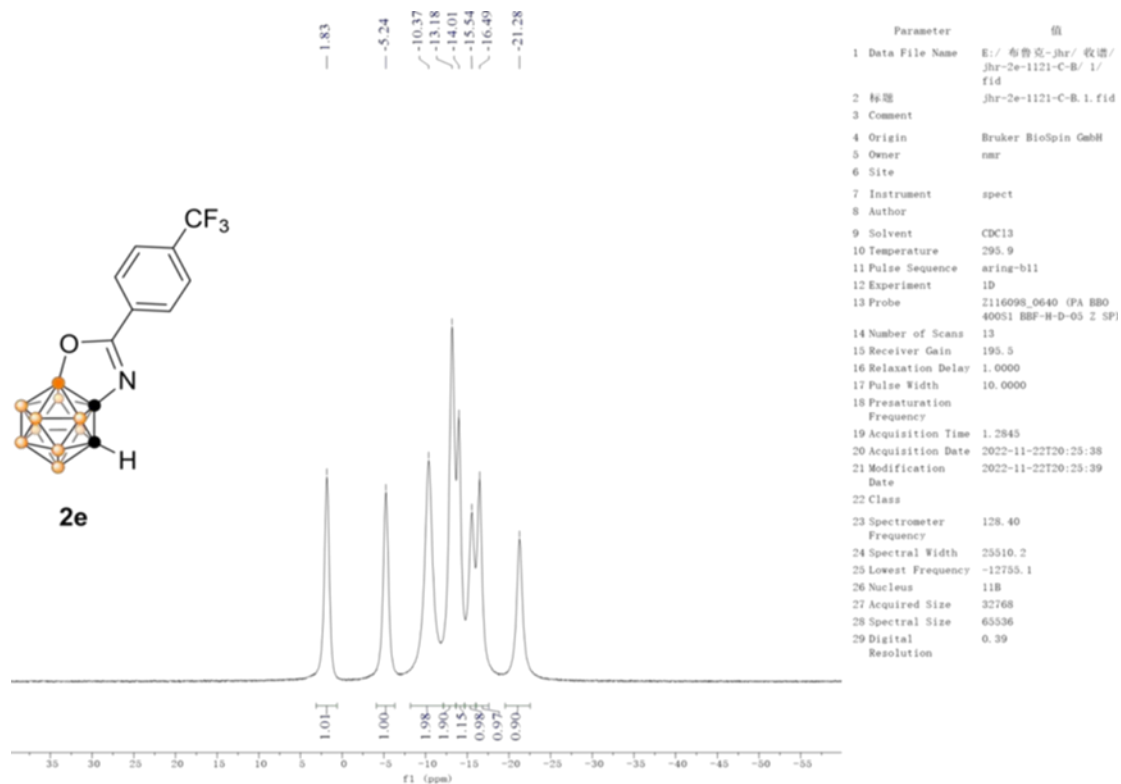


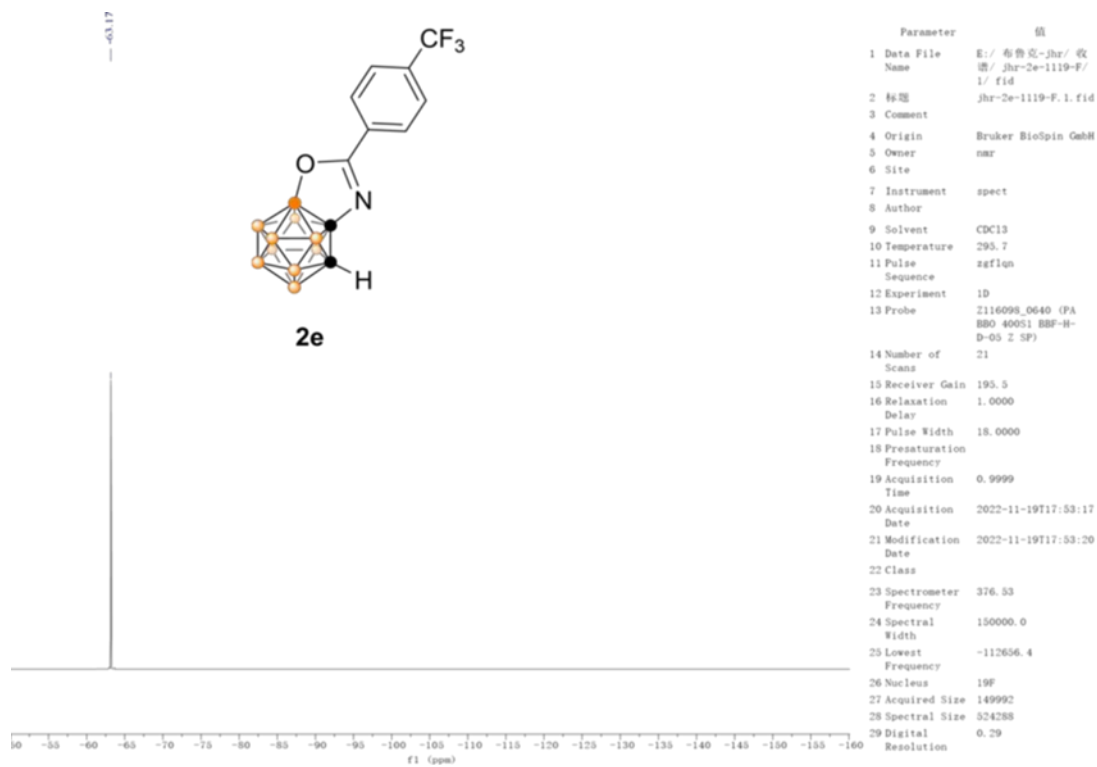


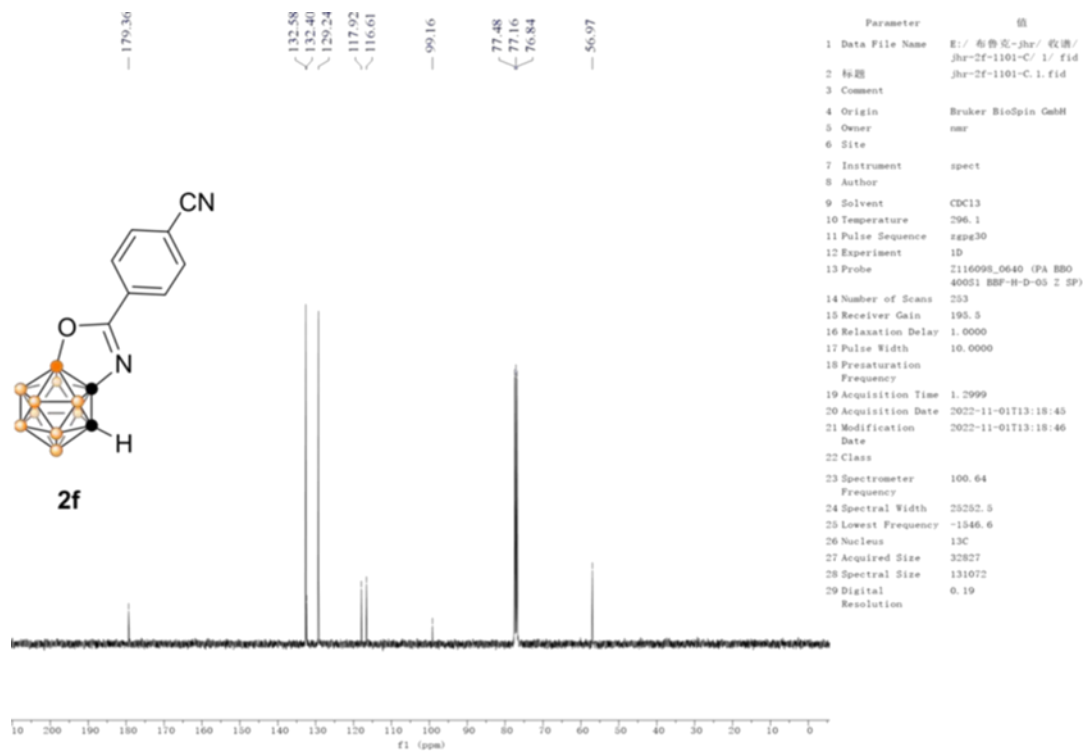
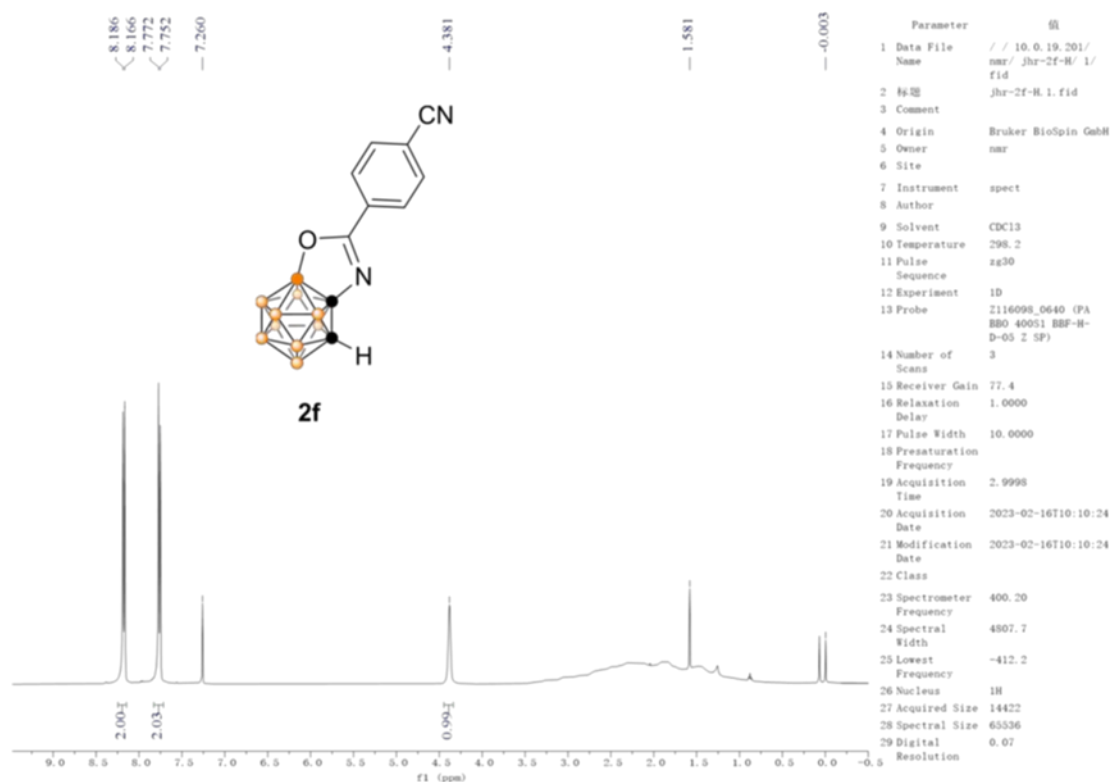


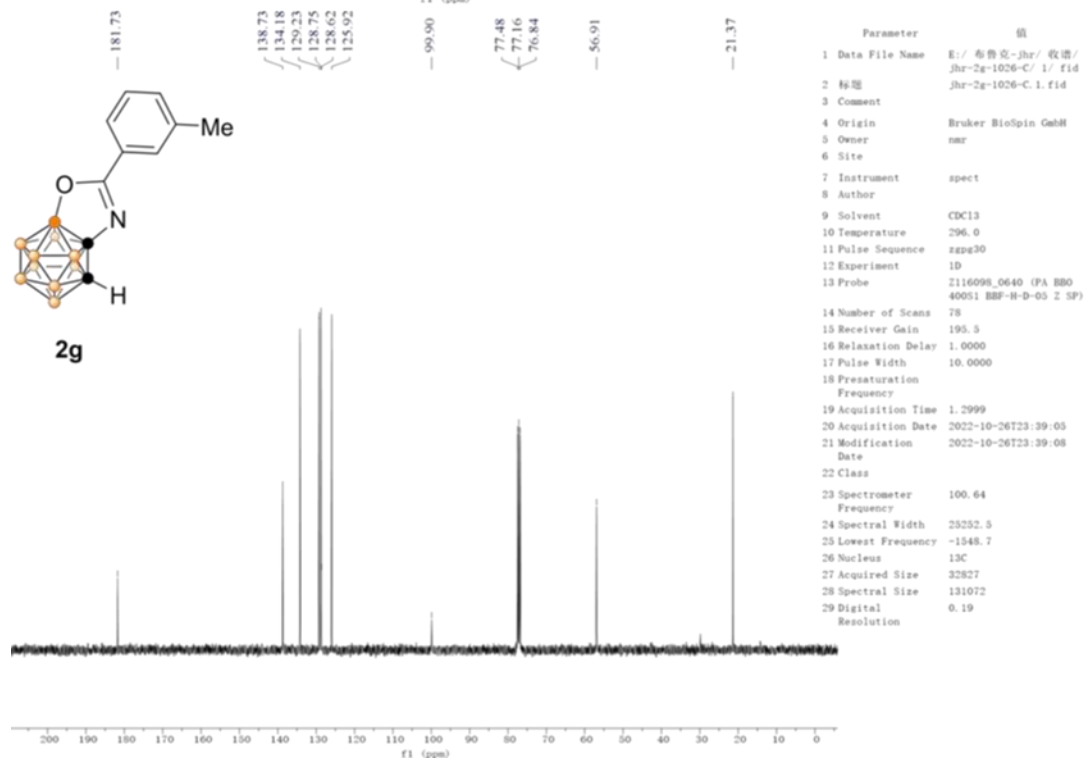
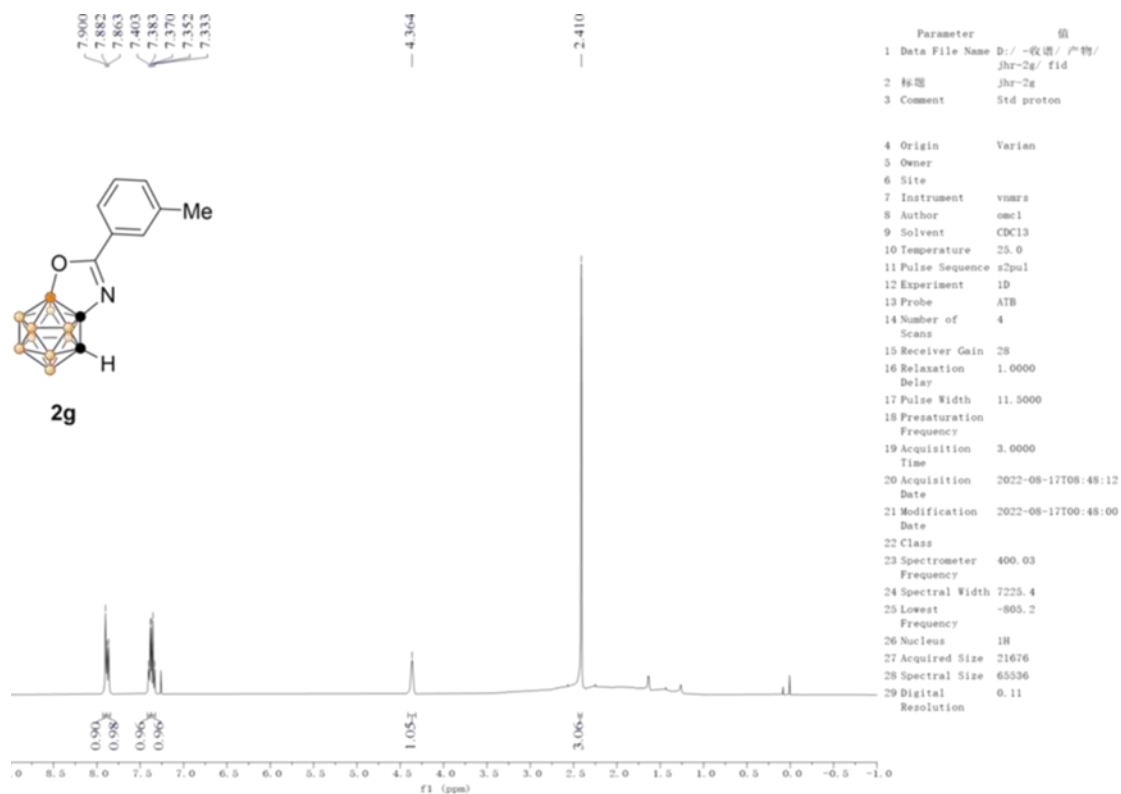
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2 标题	jhr-24-1103-F.1.fid
3 Comment	
4 Origin	Brucker BioSpin GmbH
5 Owner	nmr
6 Site	
7 Instrument	spect
8 Author	
9 Solvent	CDC13
10 Temperature	295.8
11 Pulse Sequence	zgpg30
12 Experiment	1D
13 Probe	2116098_0640 (PA BBO 400SI BRF-N- D-05 2 SP)
14 Number of Scans	9
15 Receiver Gain	195.5
16 Relaxation Delay	1.0000
17 Pulse Width	18.0000
18 Presaturation Frequency	
19 Acquisition Time	0.9999
20 Acquisition Date	2022-11-03T12:18:23
21 Modification Date	2022-11-03T12:18:26
22 Class	
23 Spectrometer Frequency	376.83
24 Spectral Width	75000.0
25 Lowest Frequency	-75156.4
26 Nucleus	19F
27 Acquired Size	74996
28 Spectral Size	262144
29 Digital Resolution	0.29

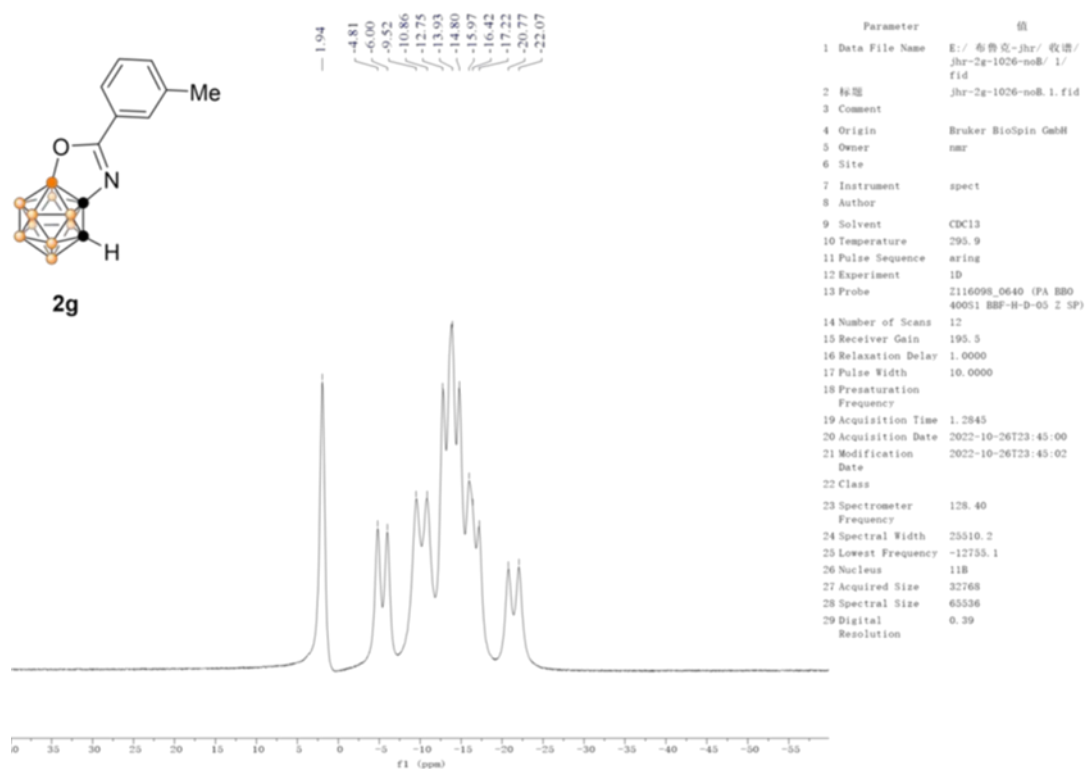
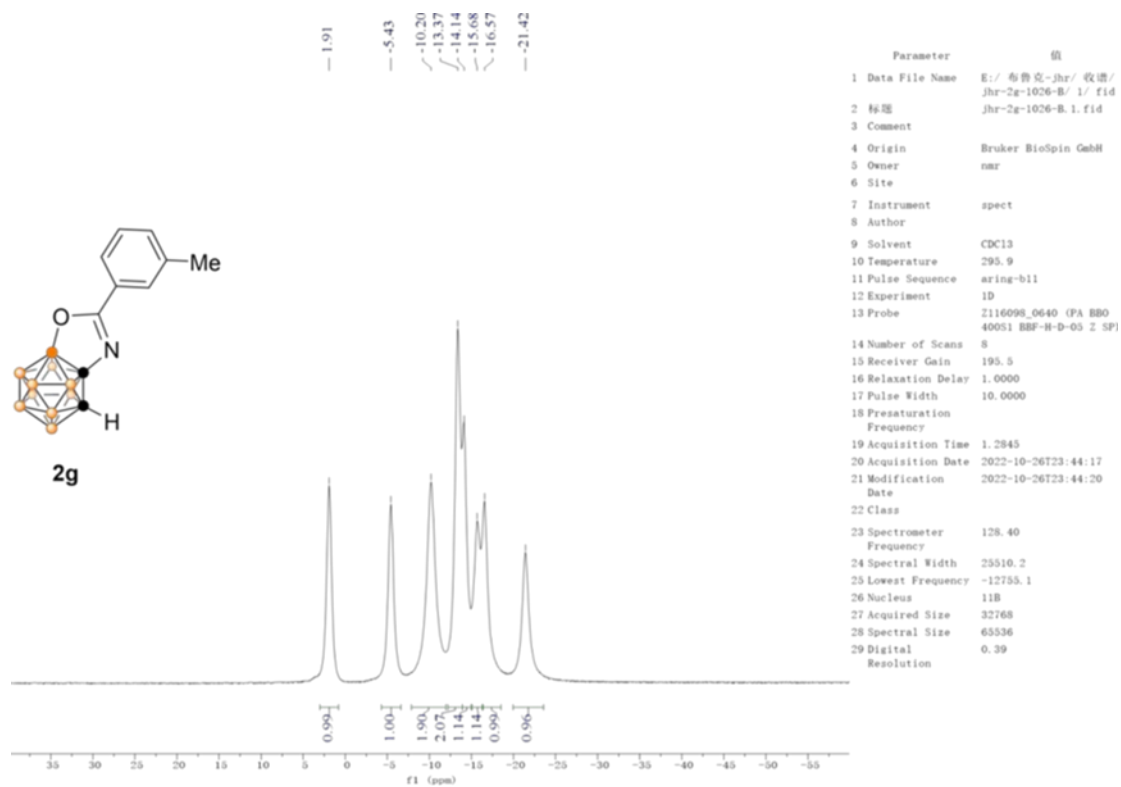


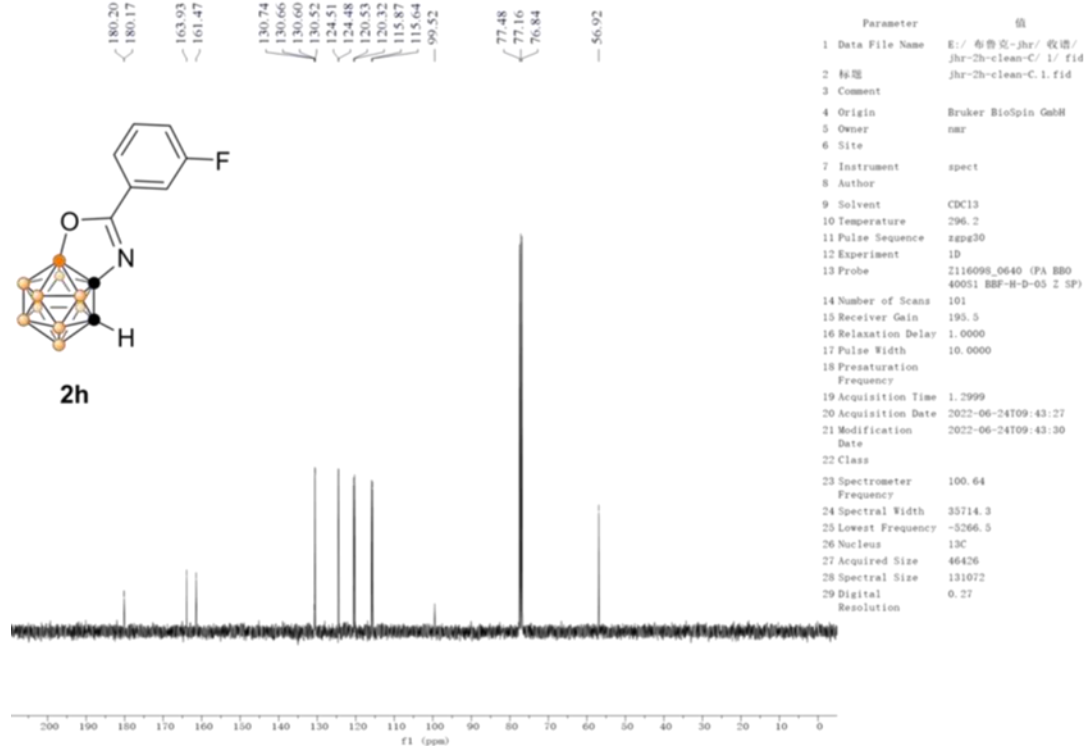
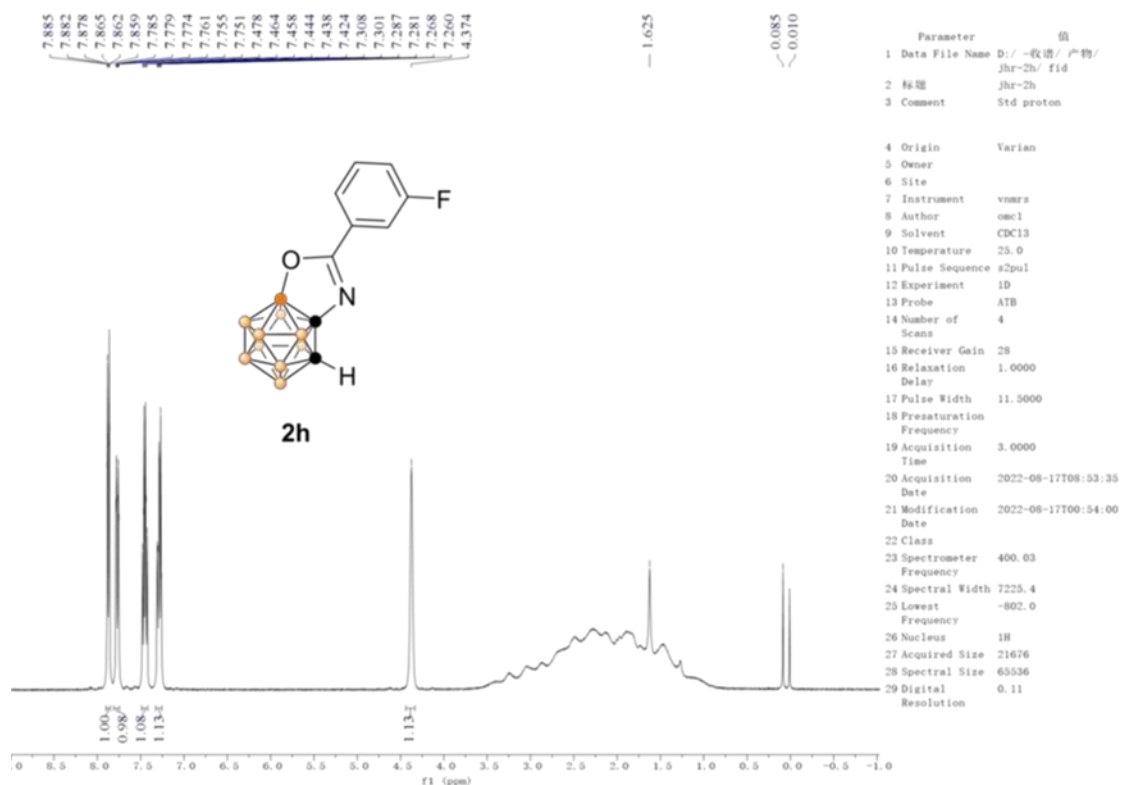


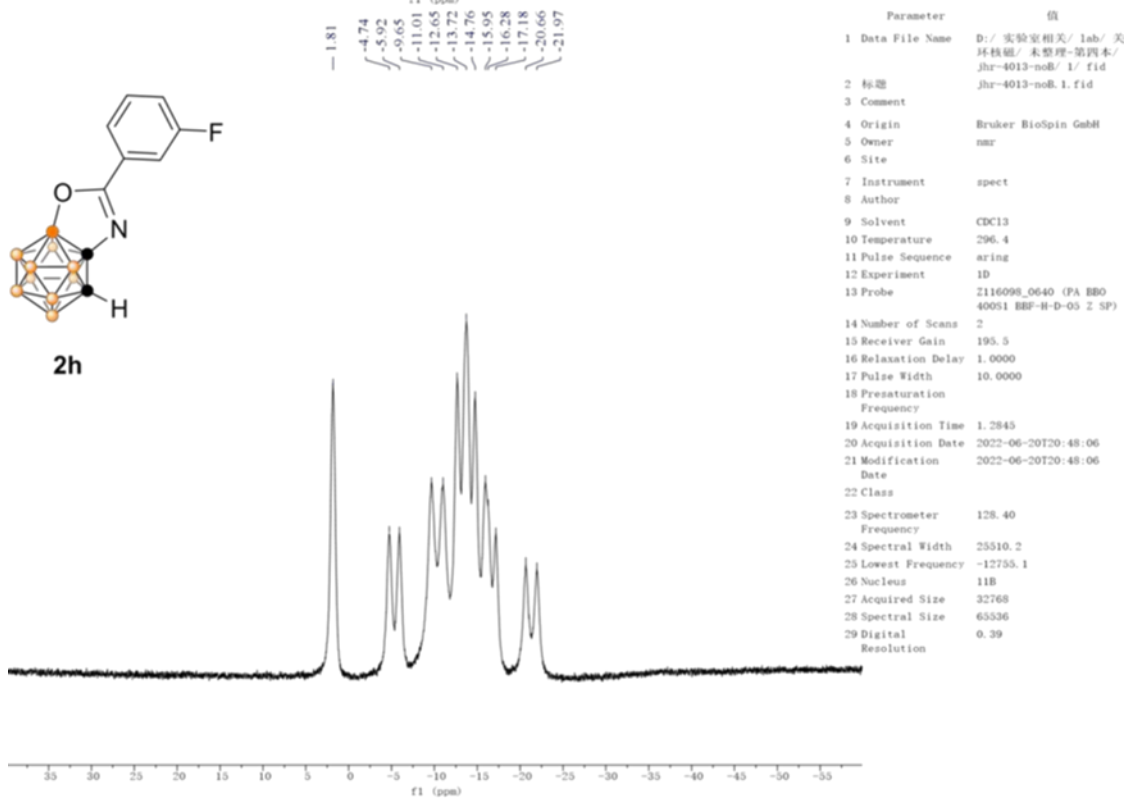
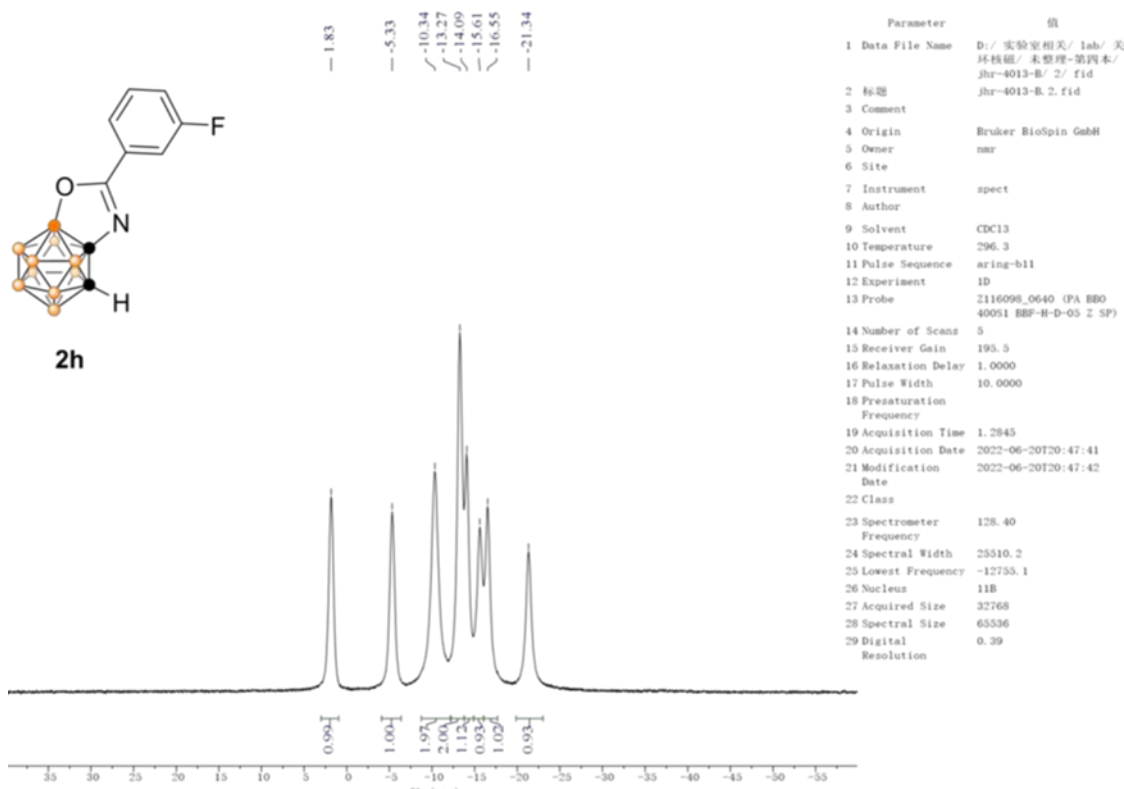


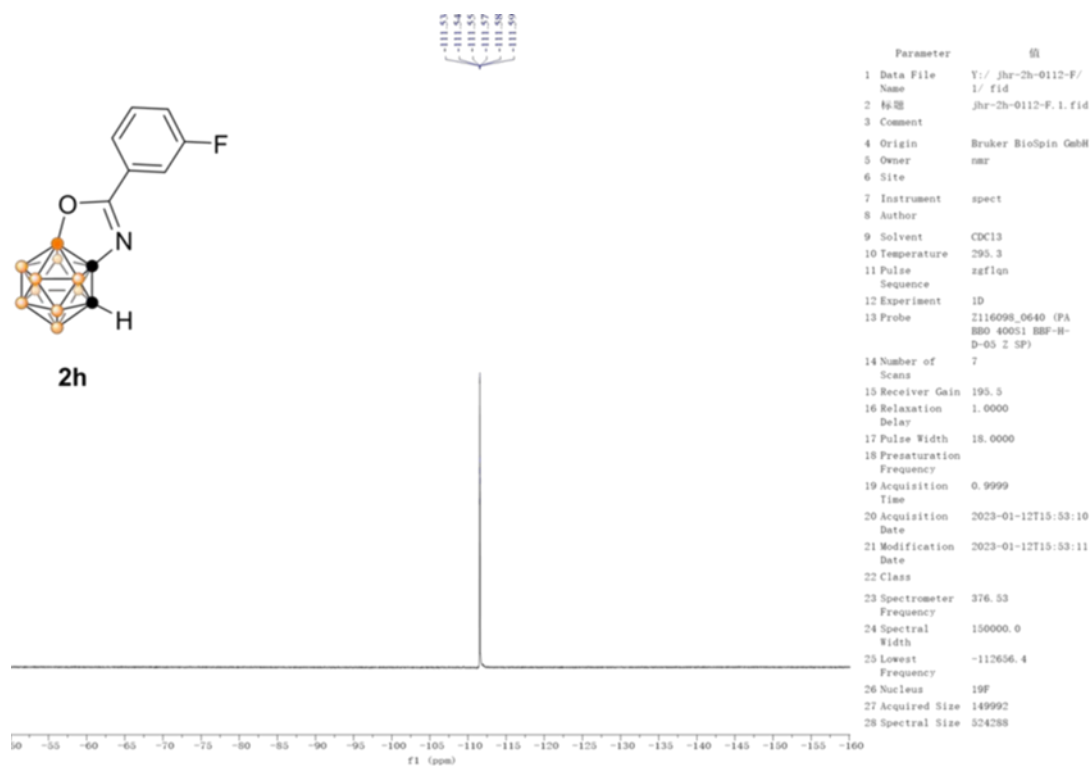


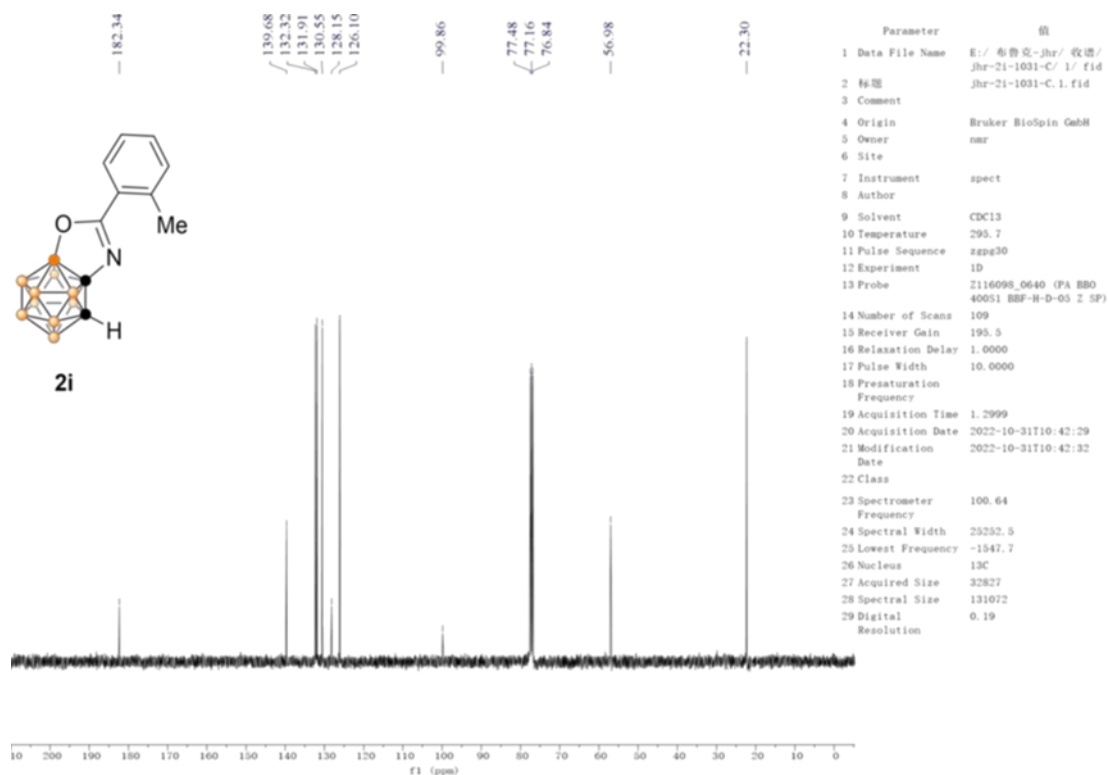
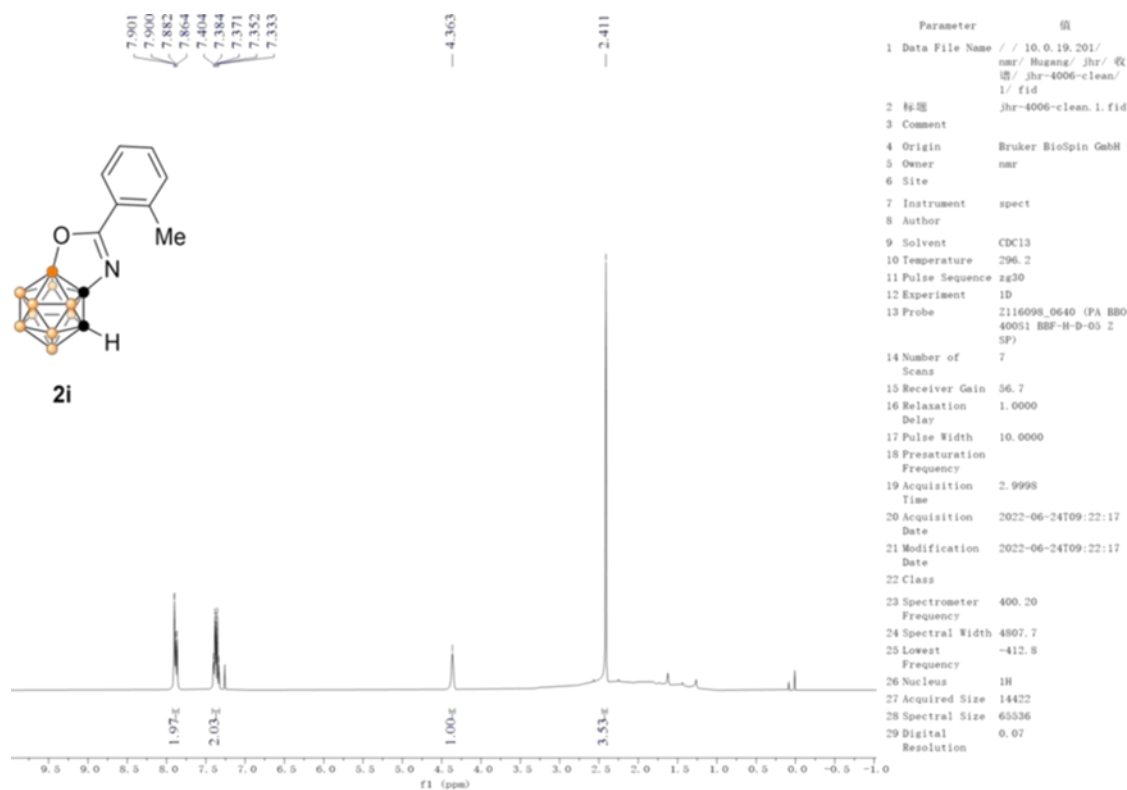


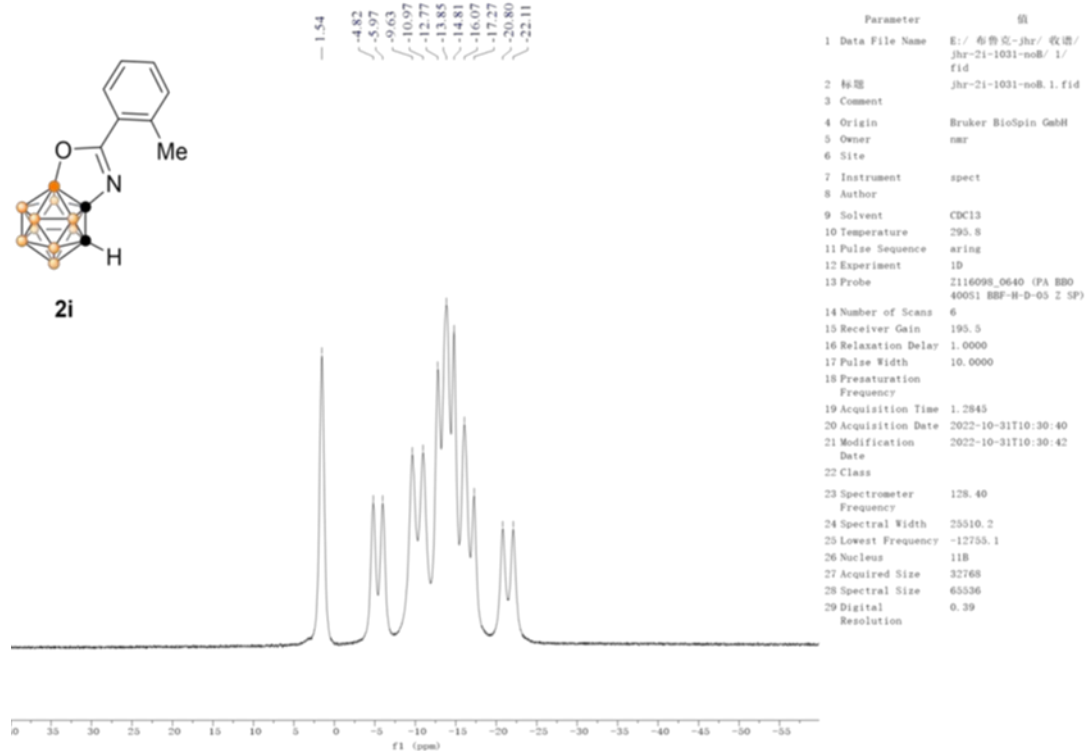
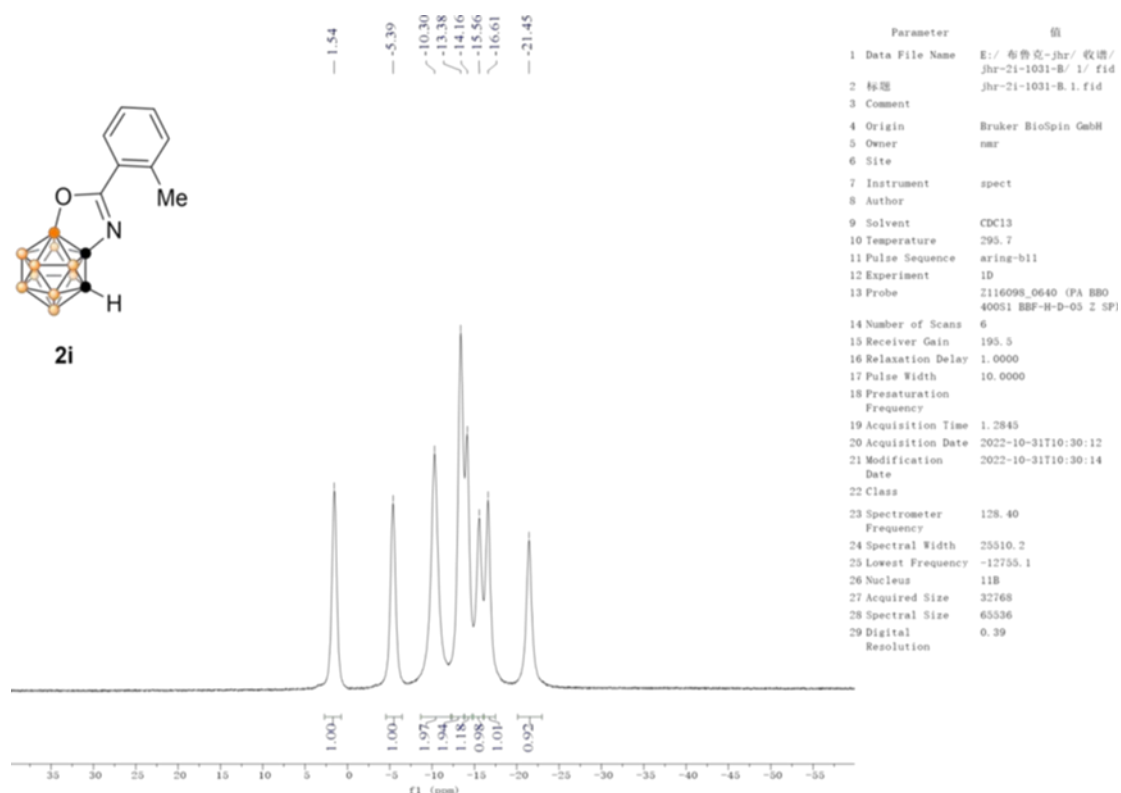


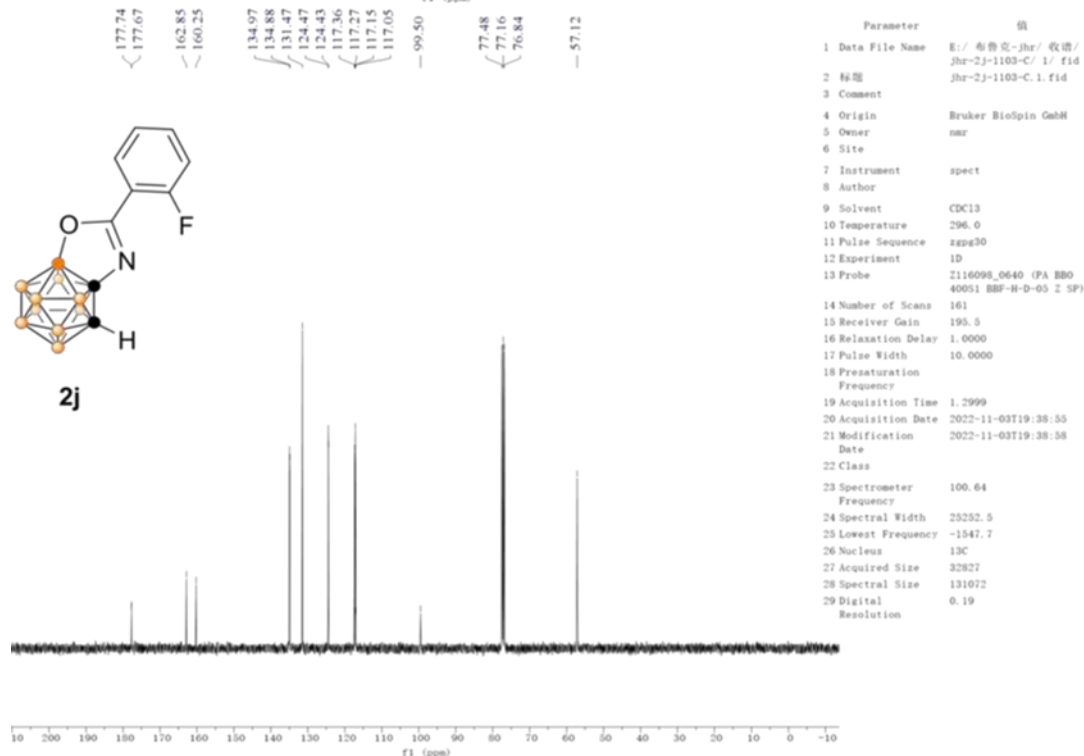
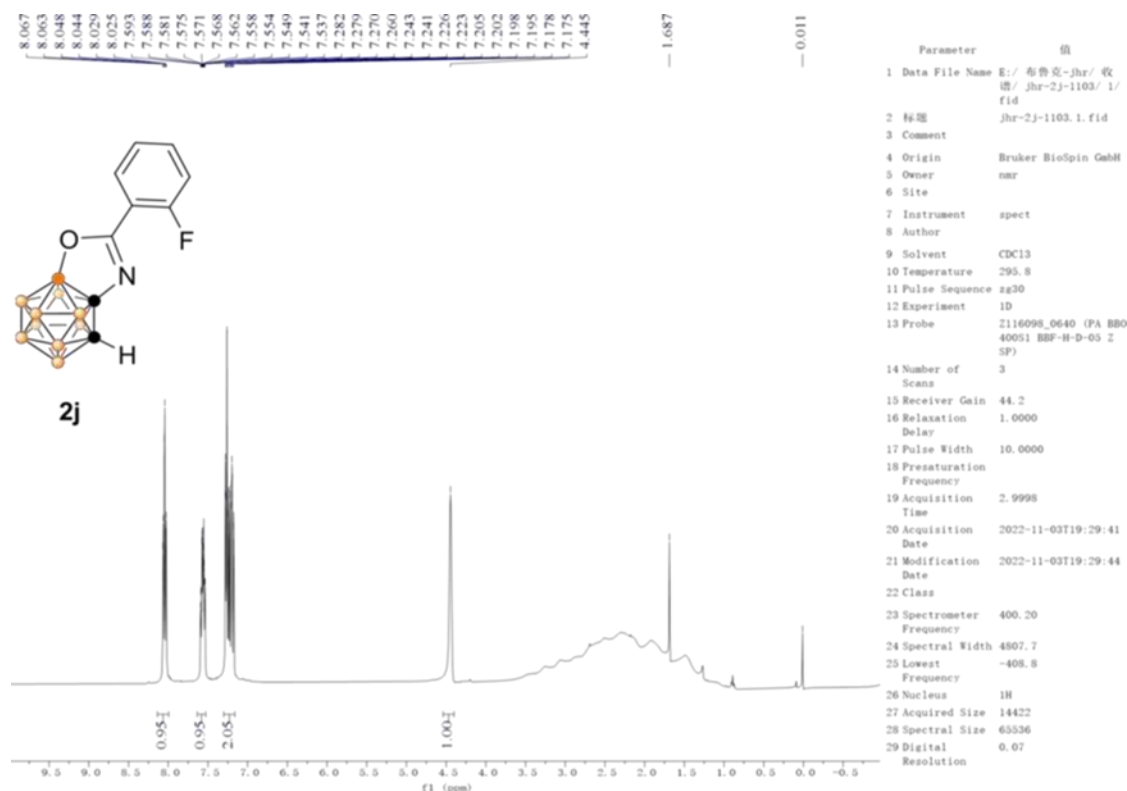


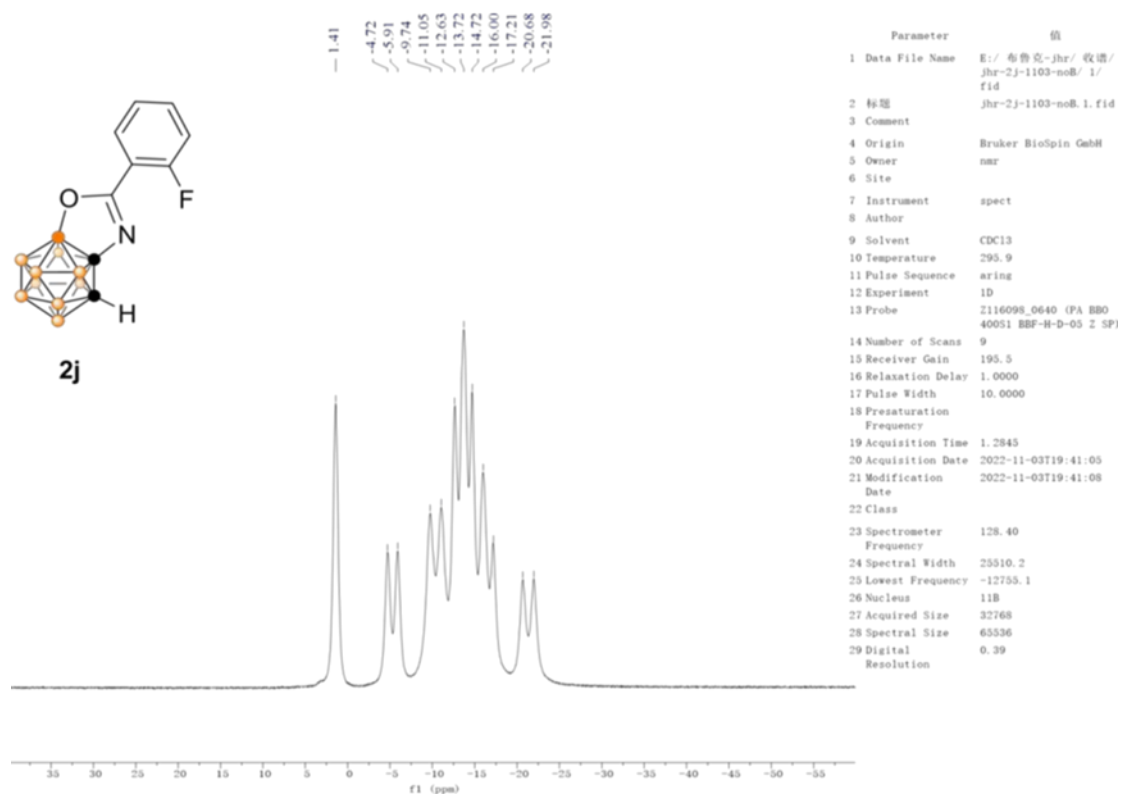
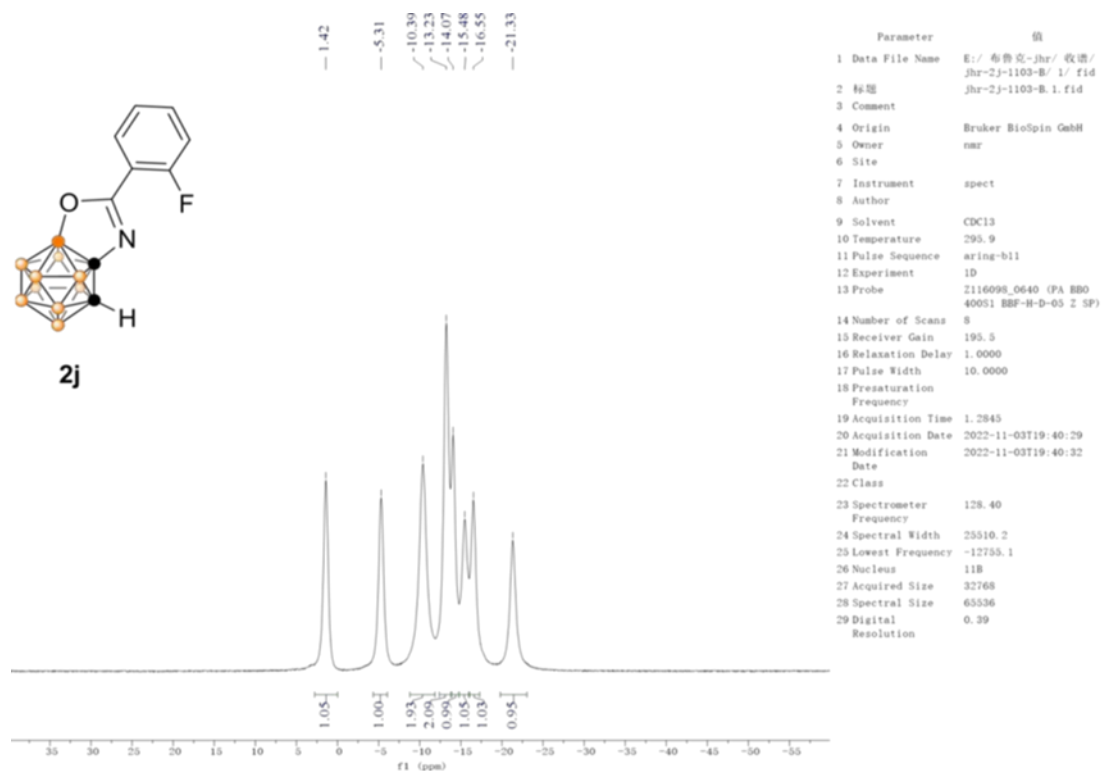


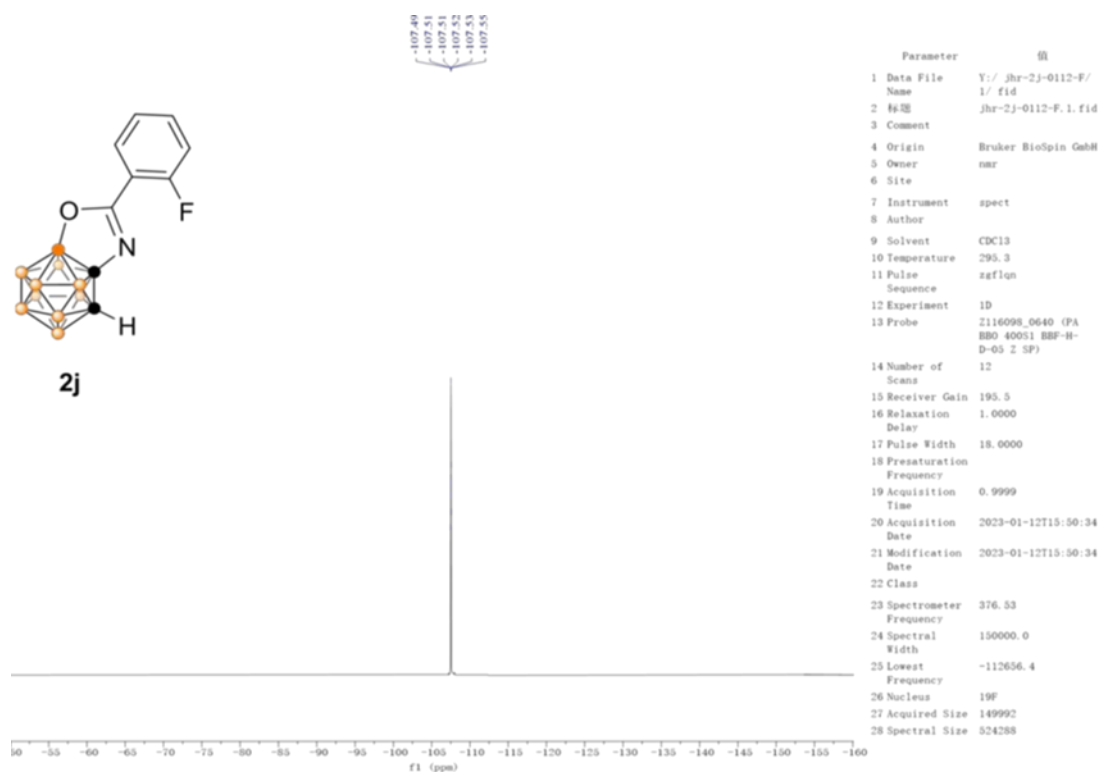


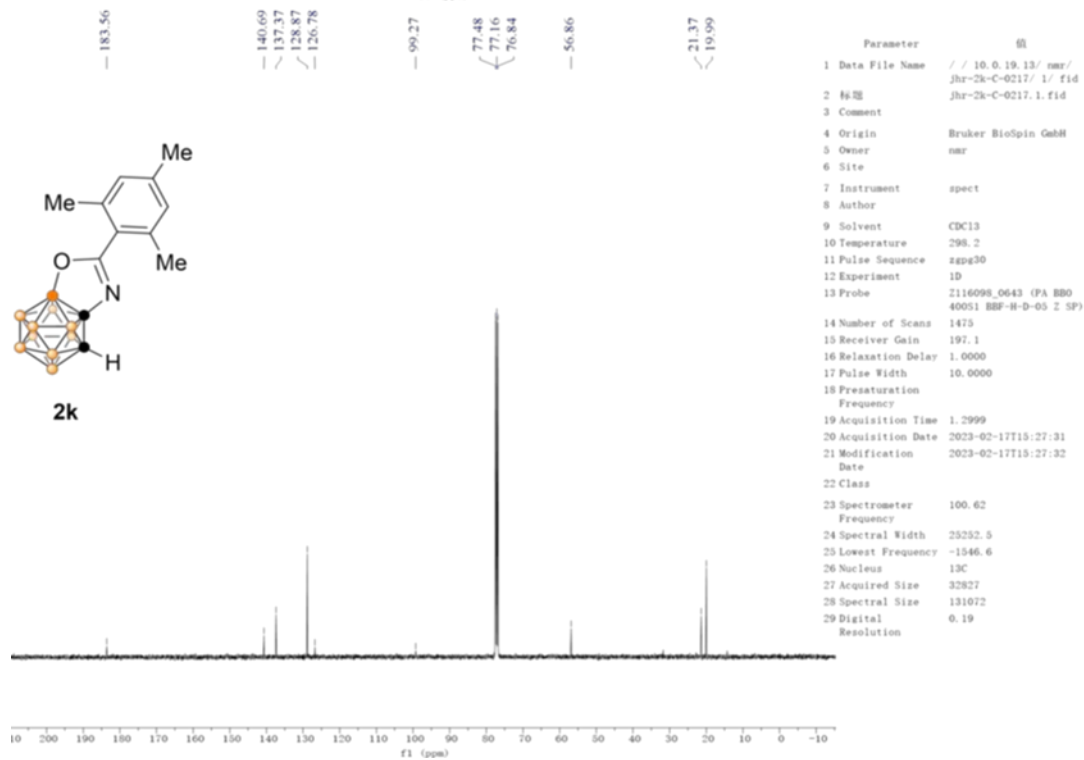
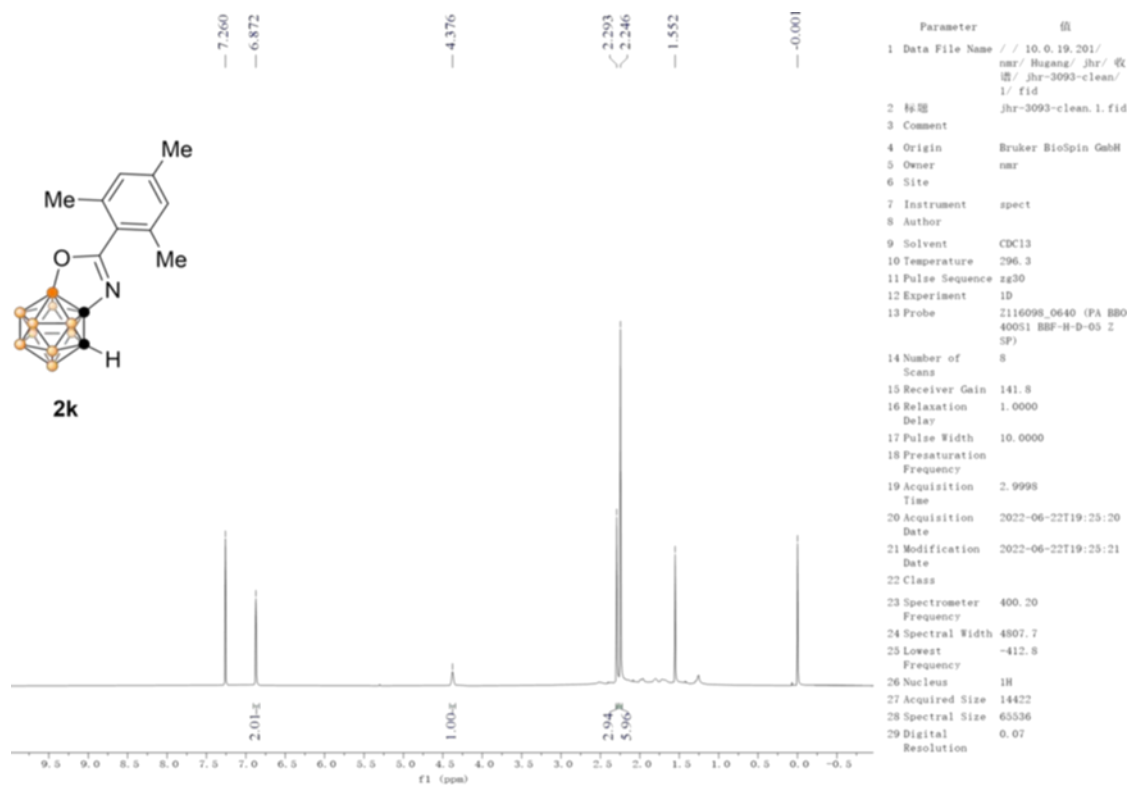


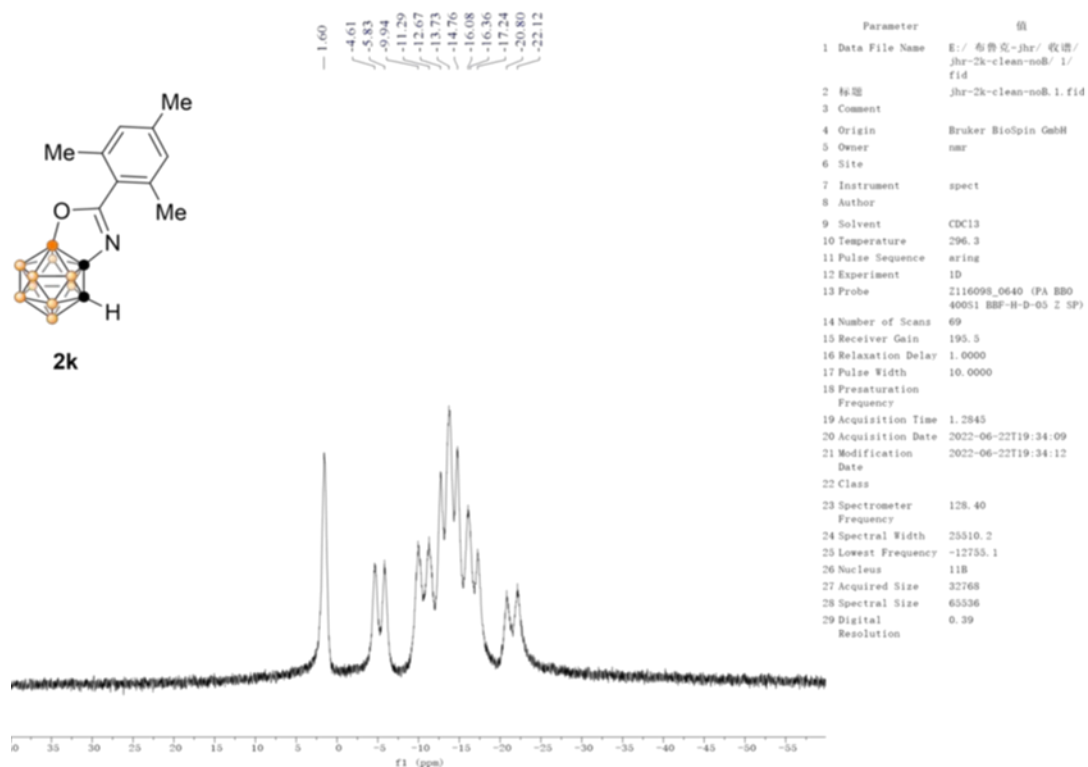
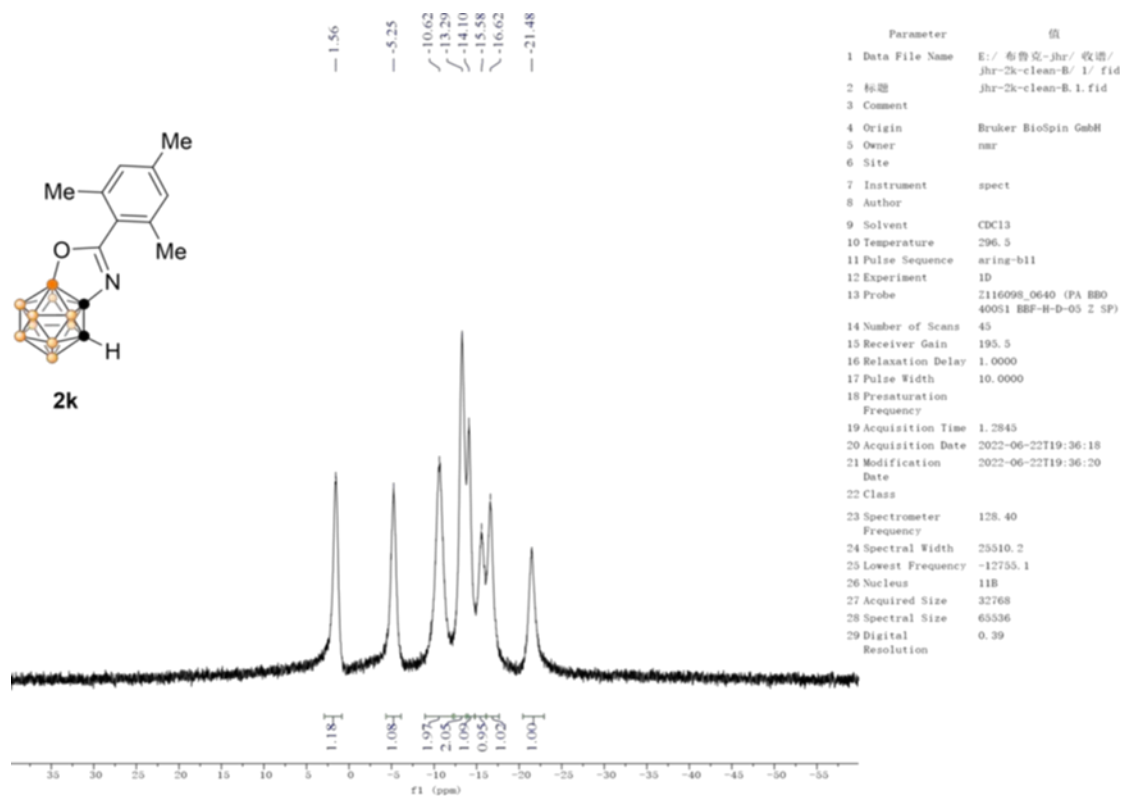


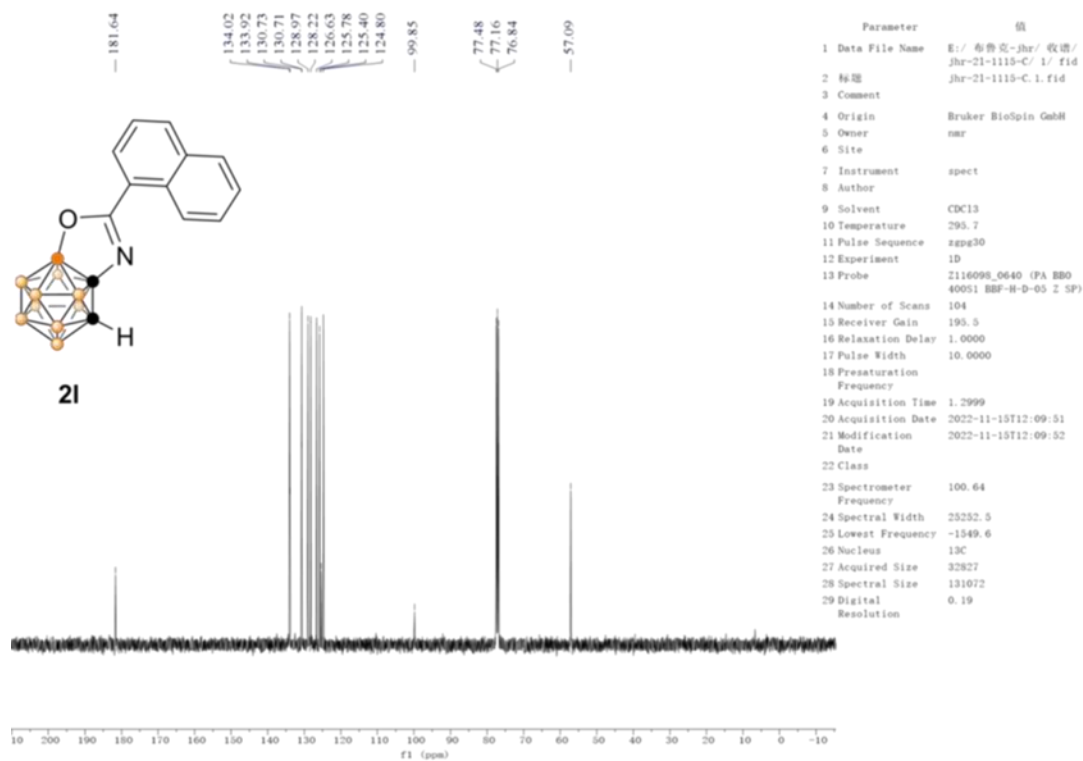
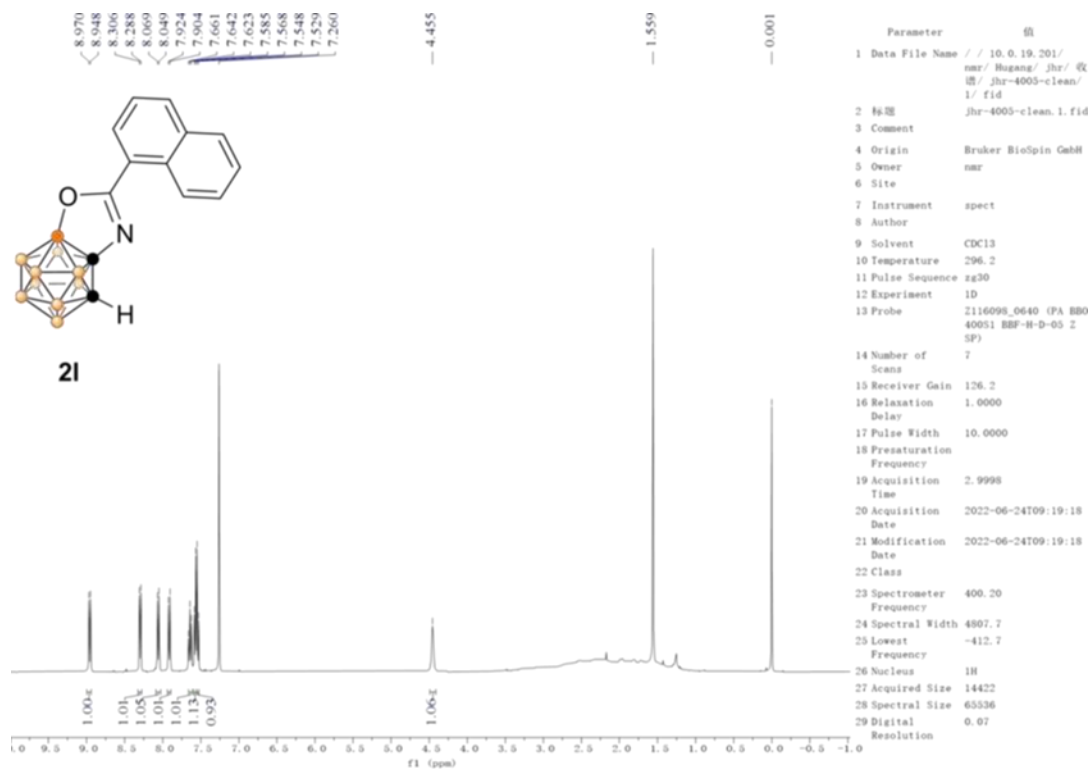


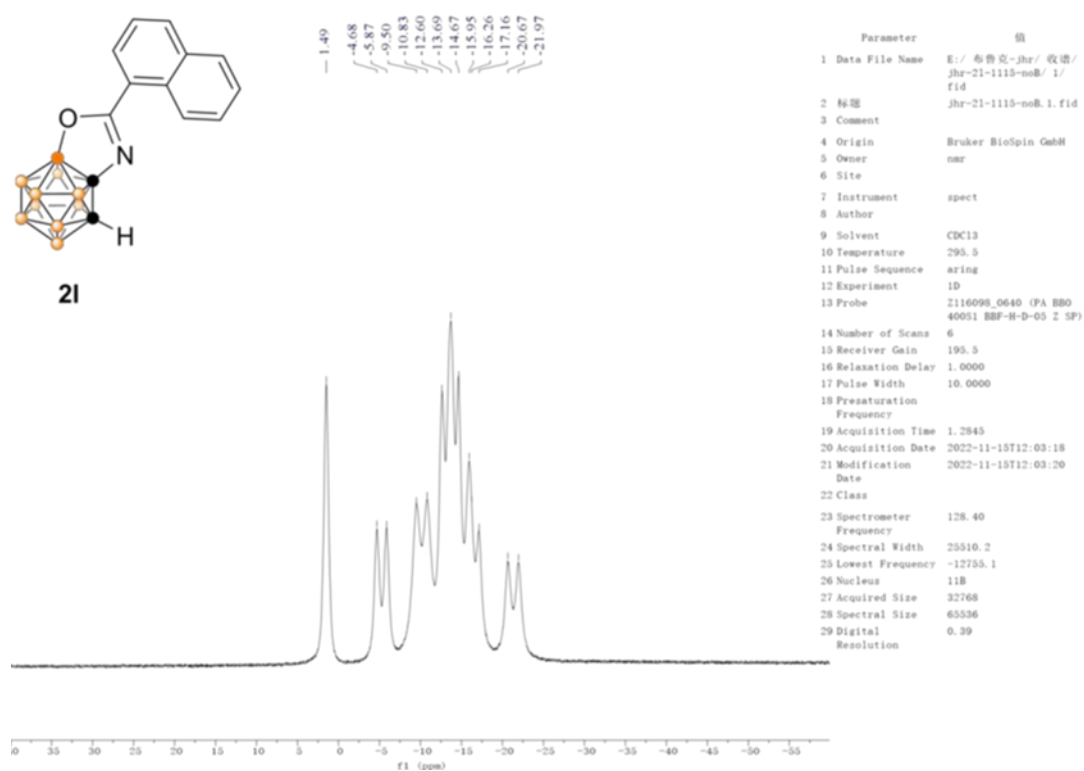
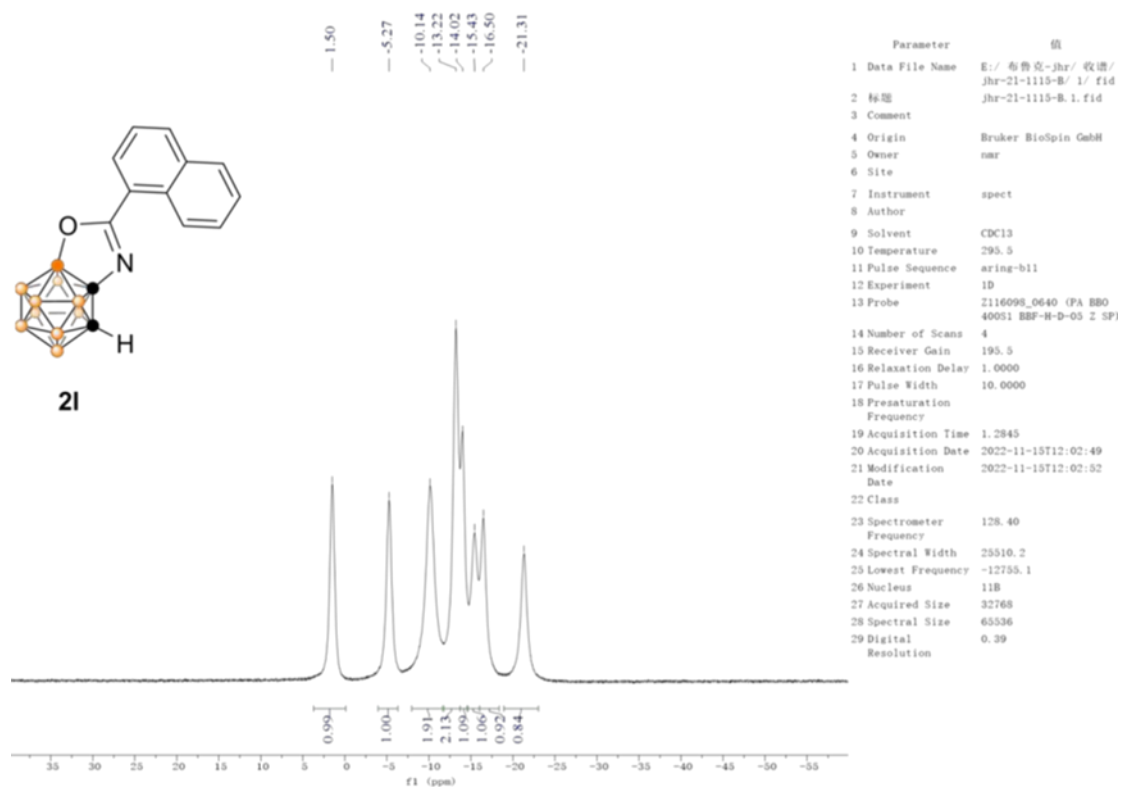


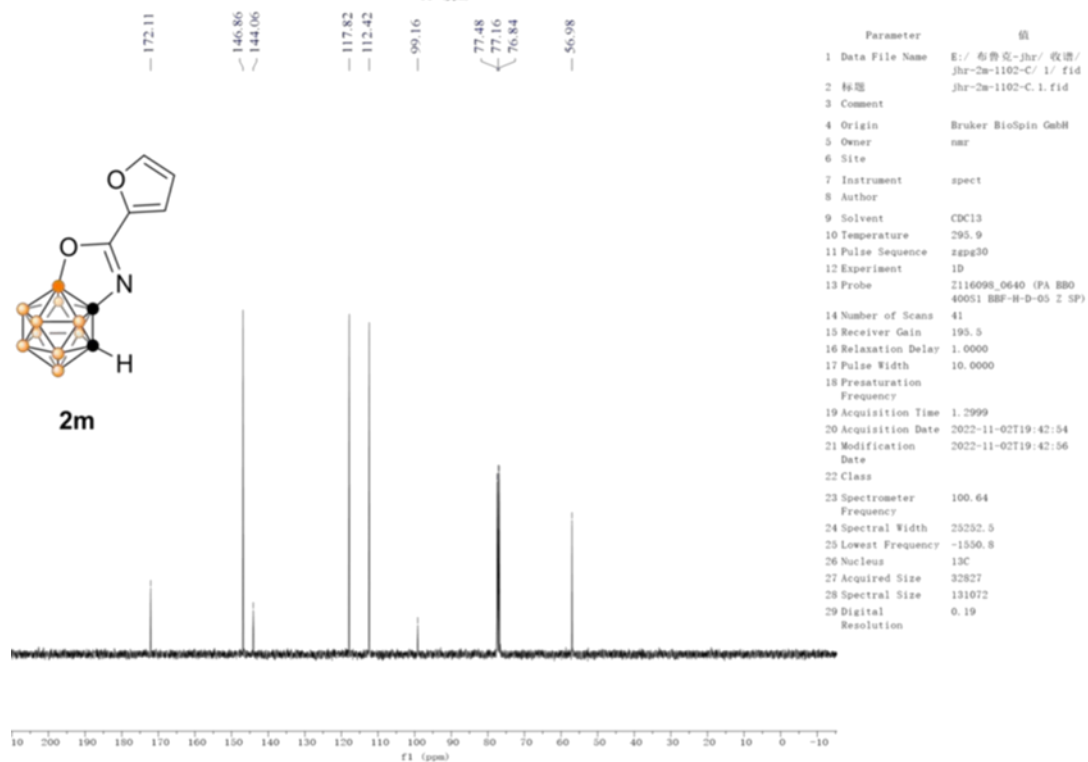
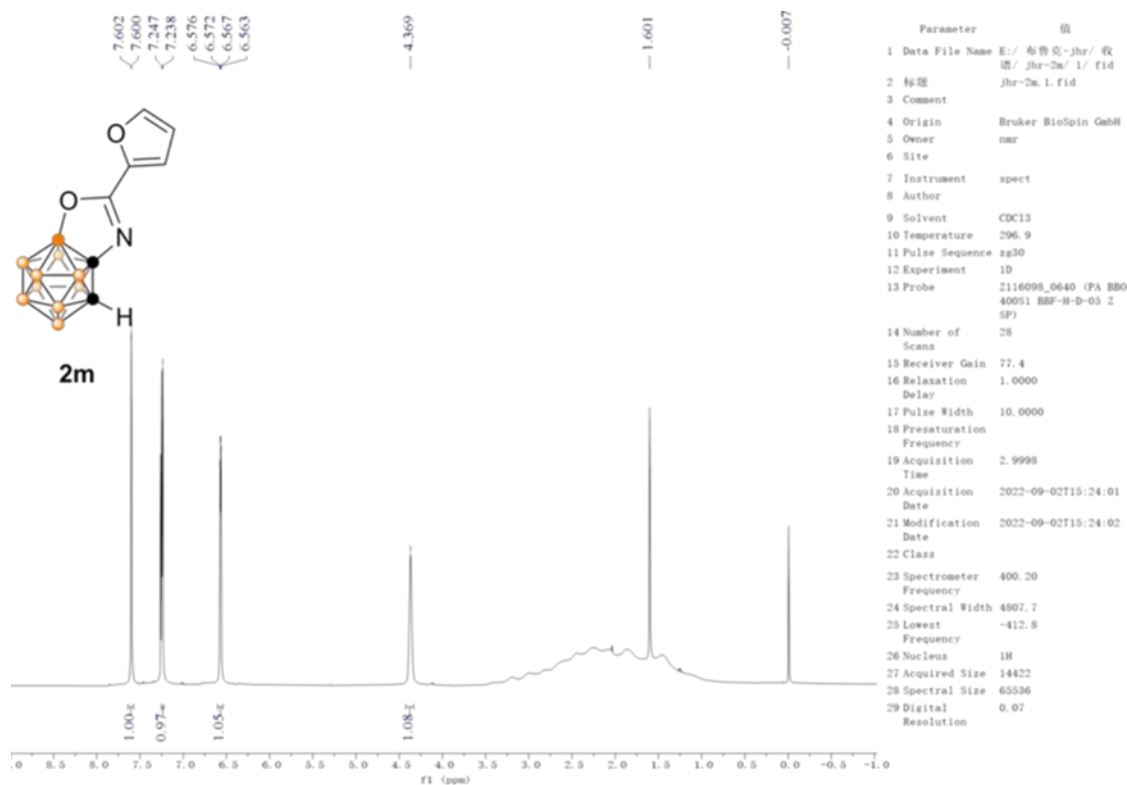


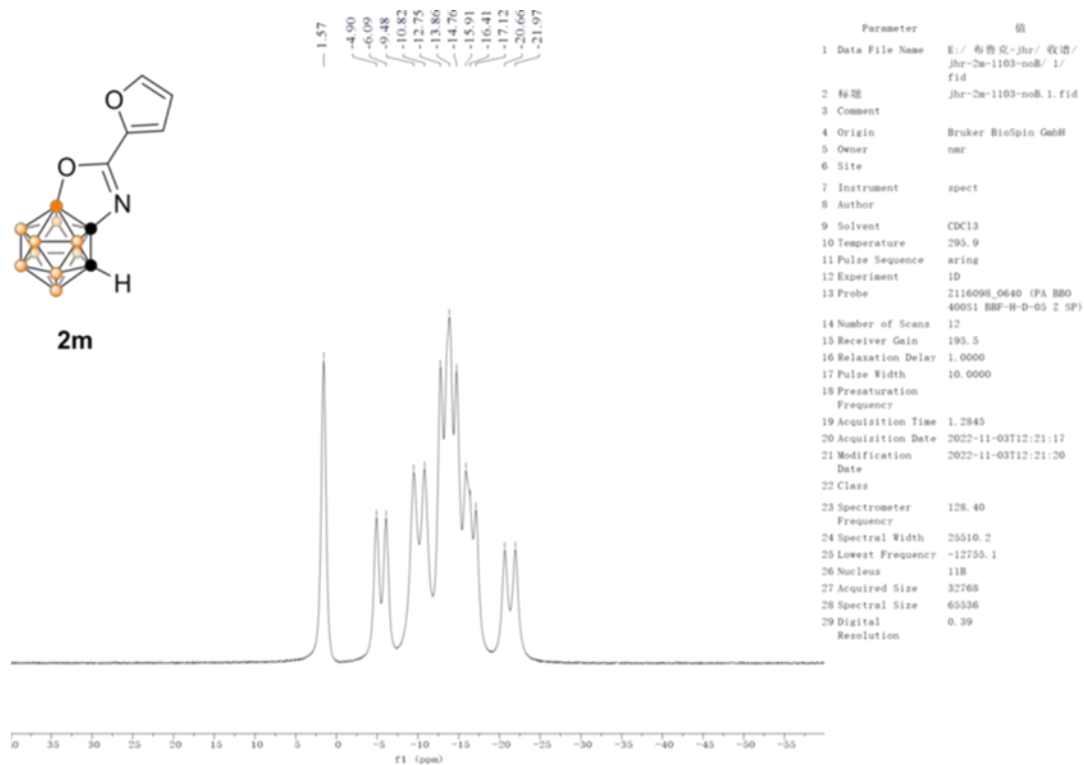
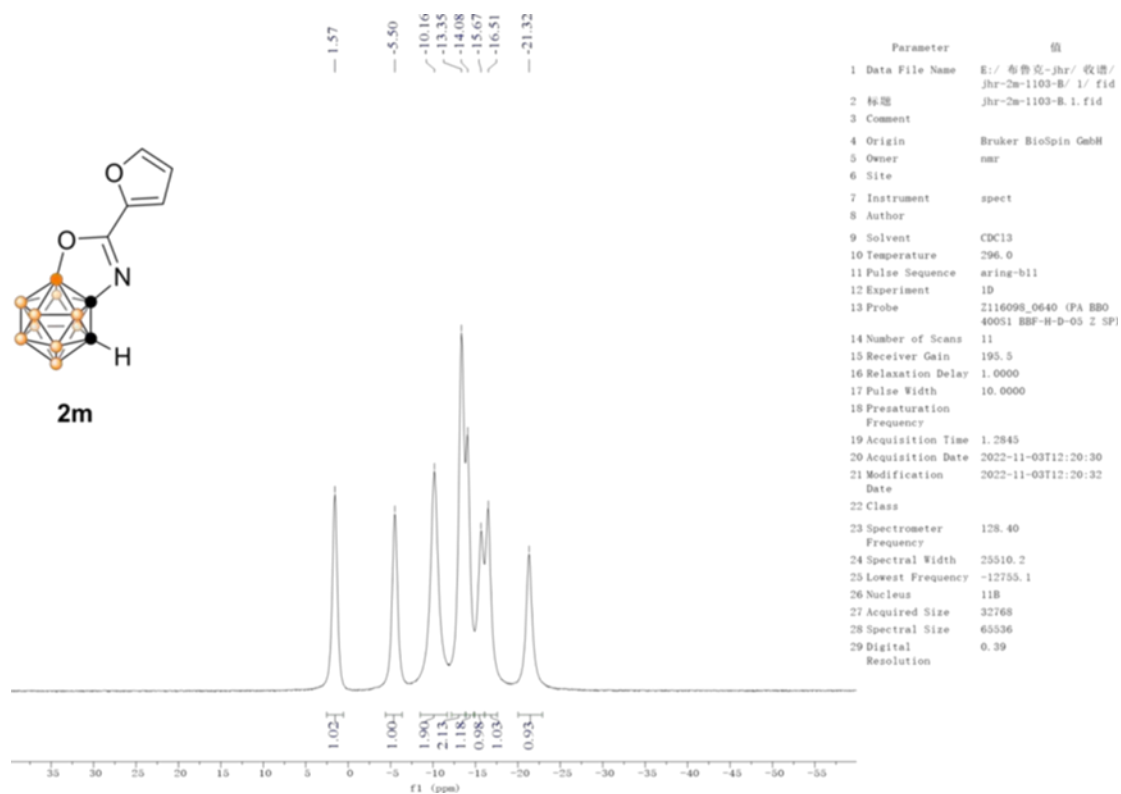


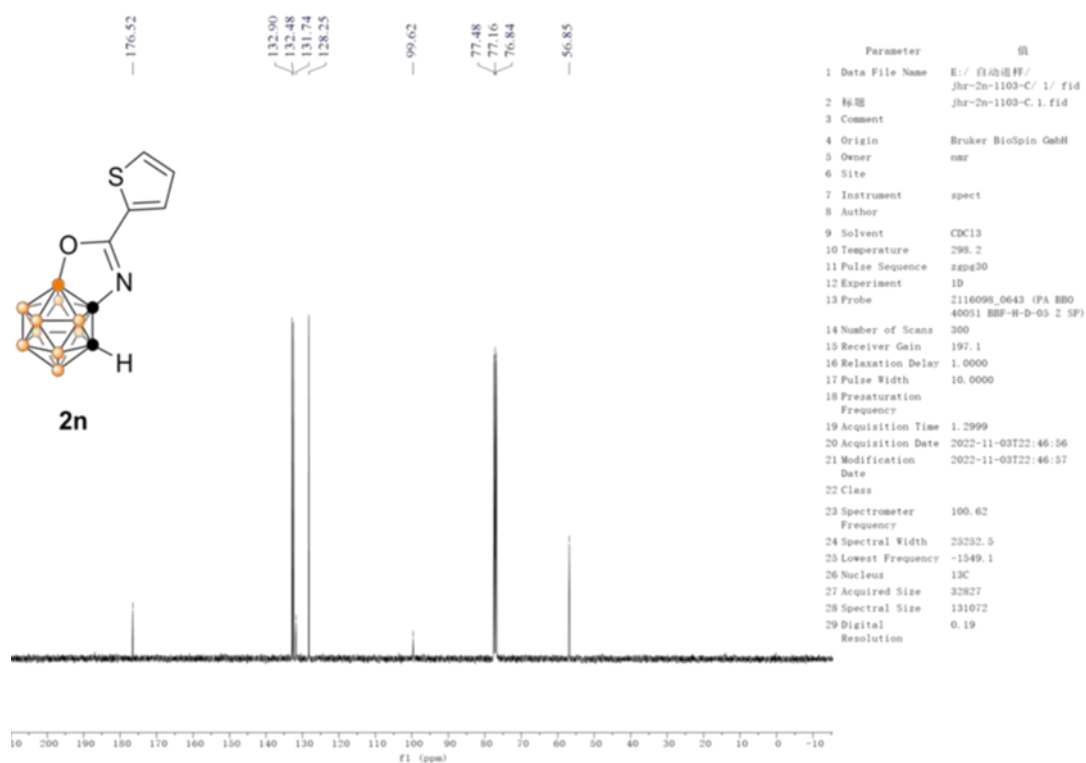
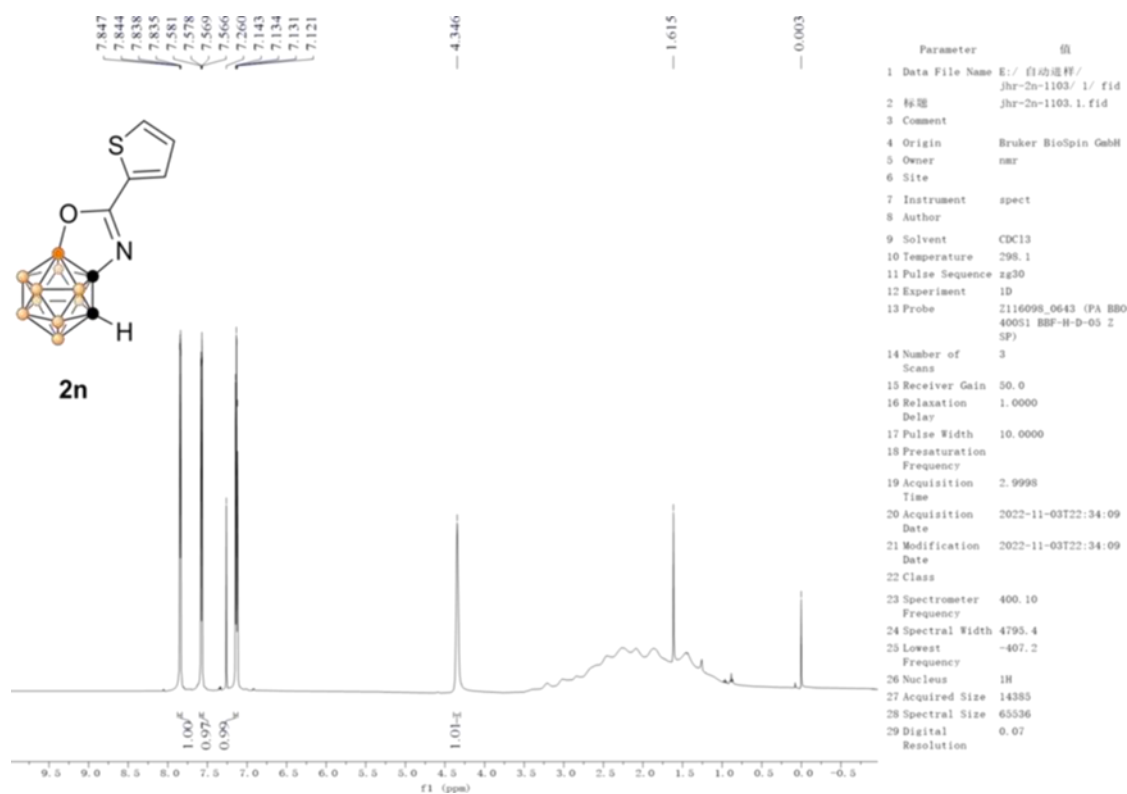


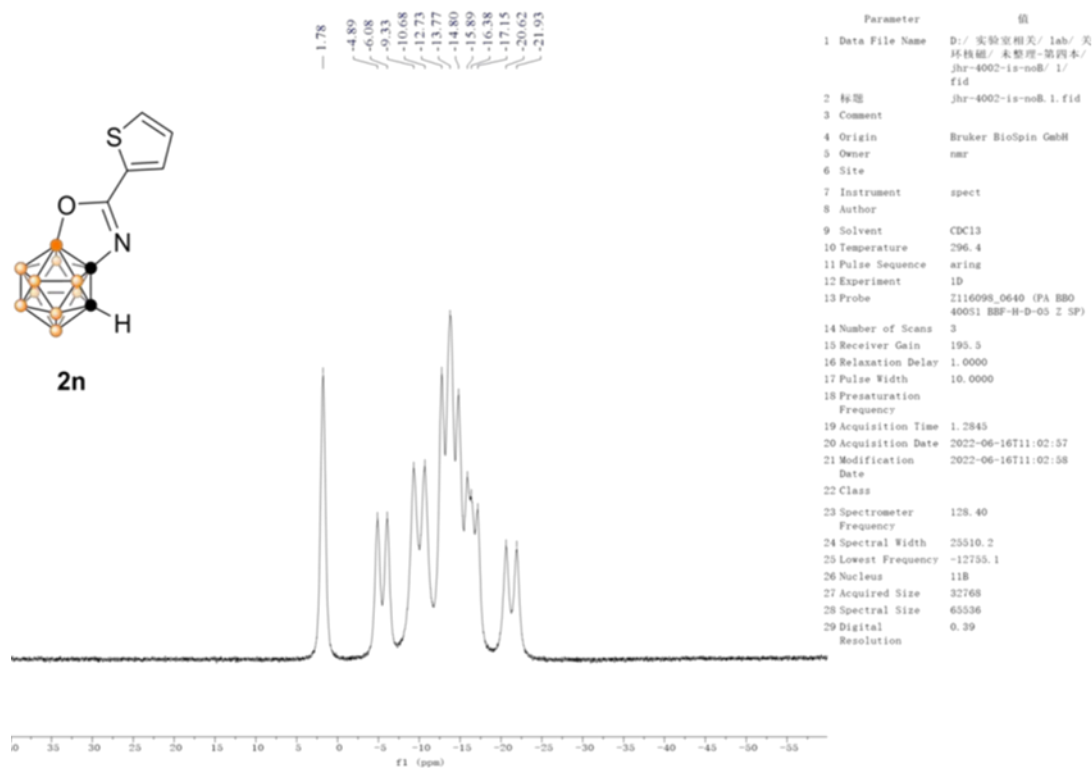
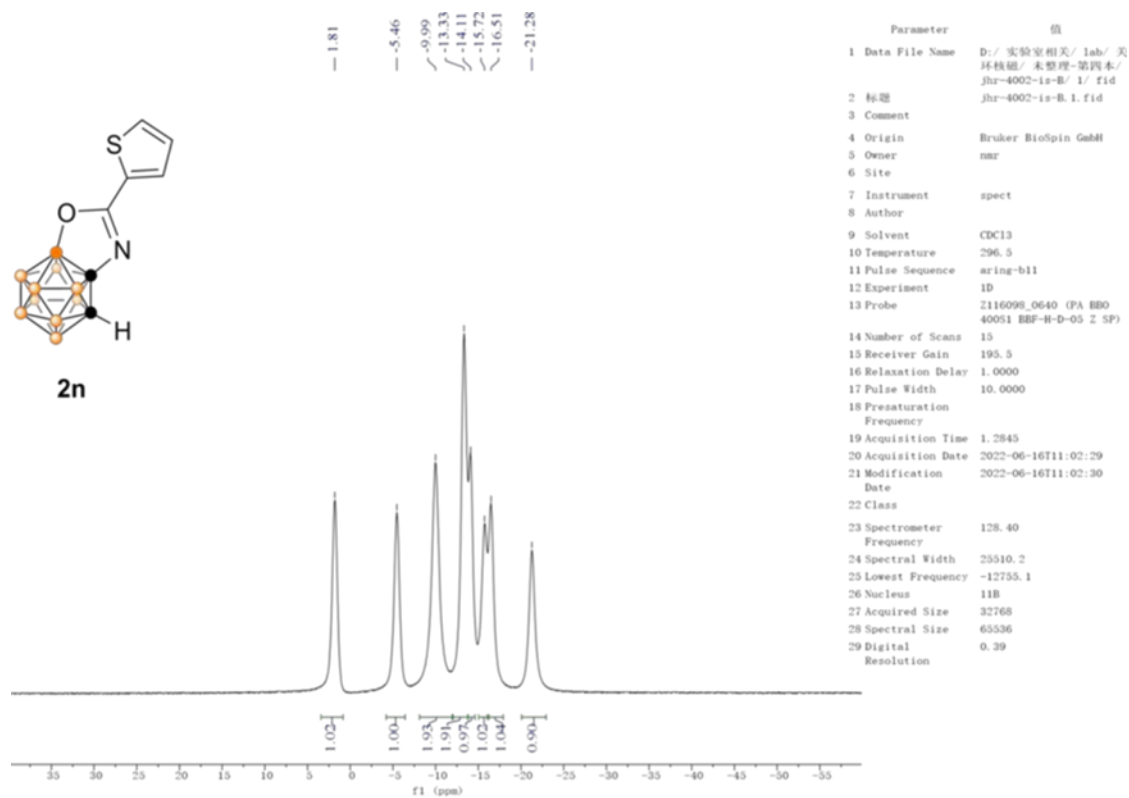


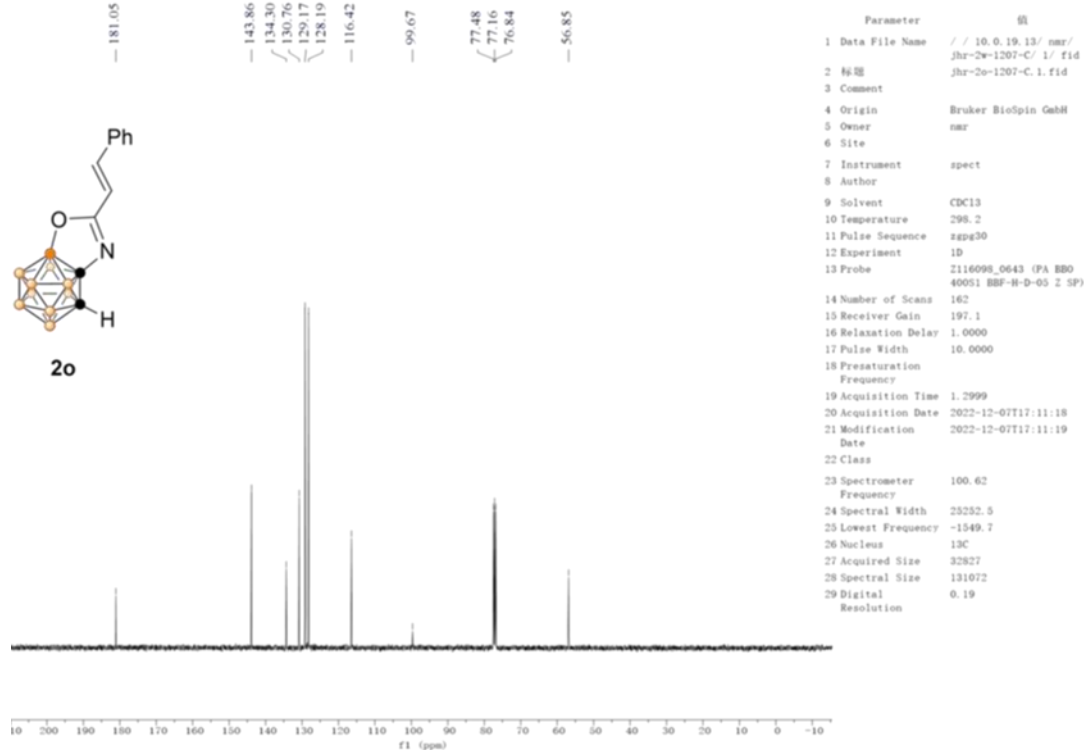
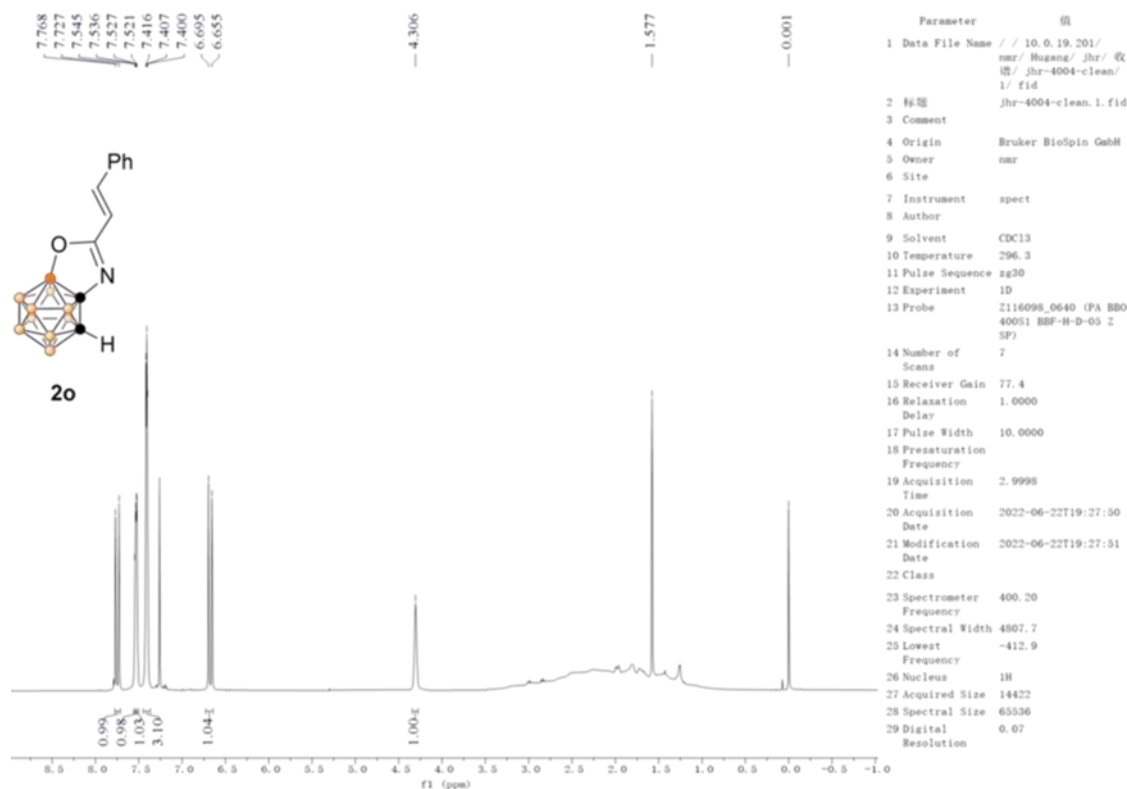


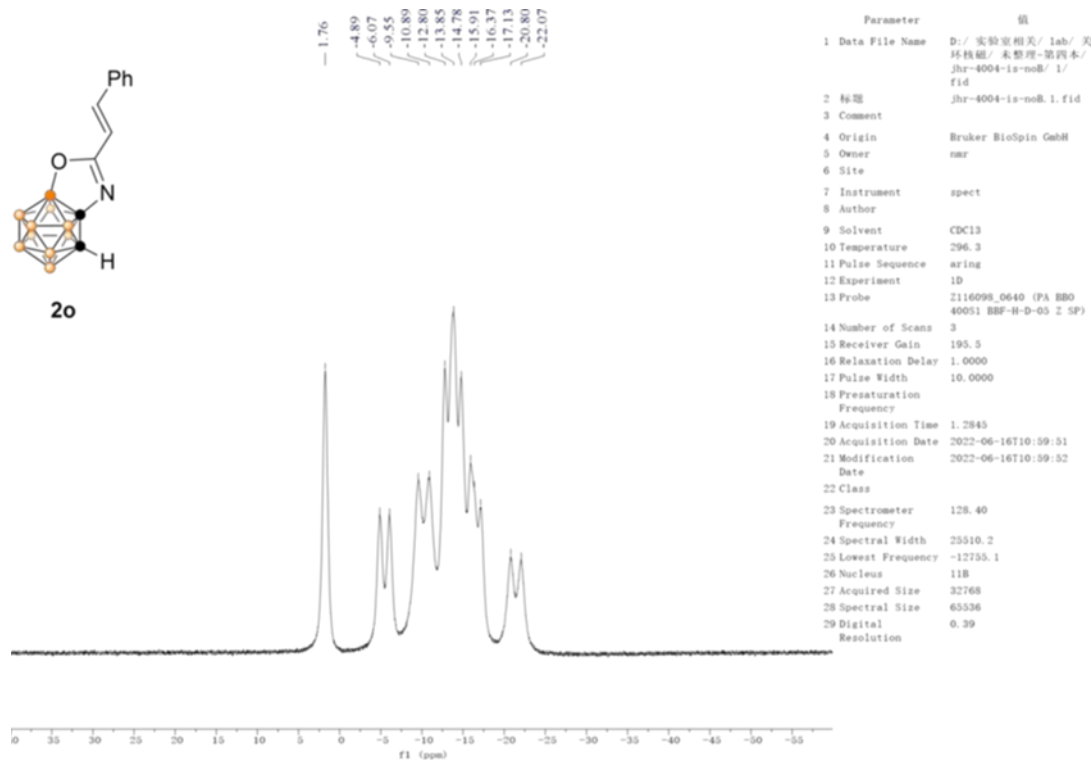
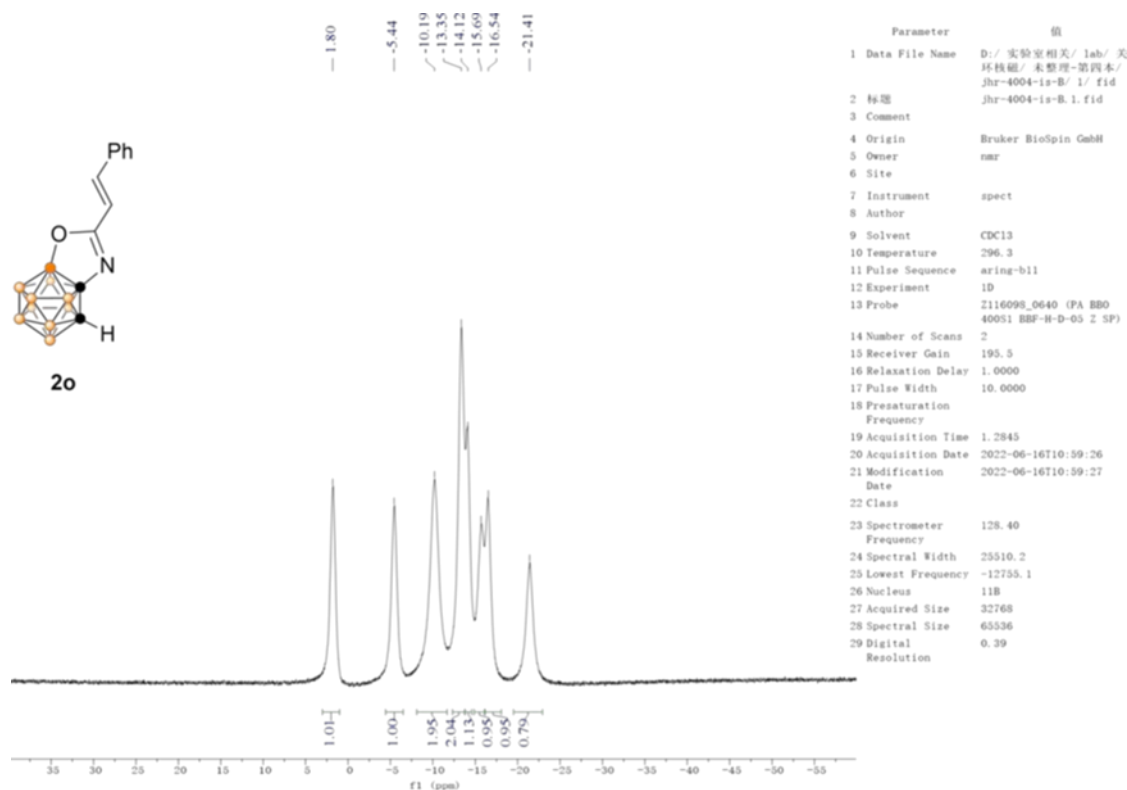


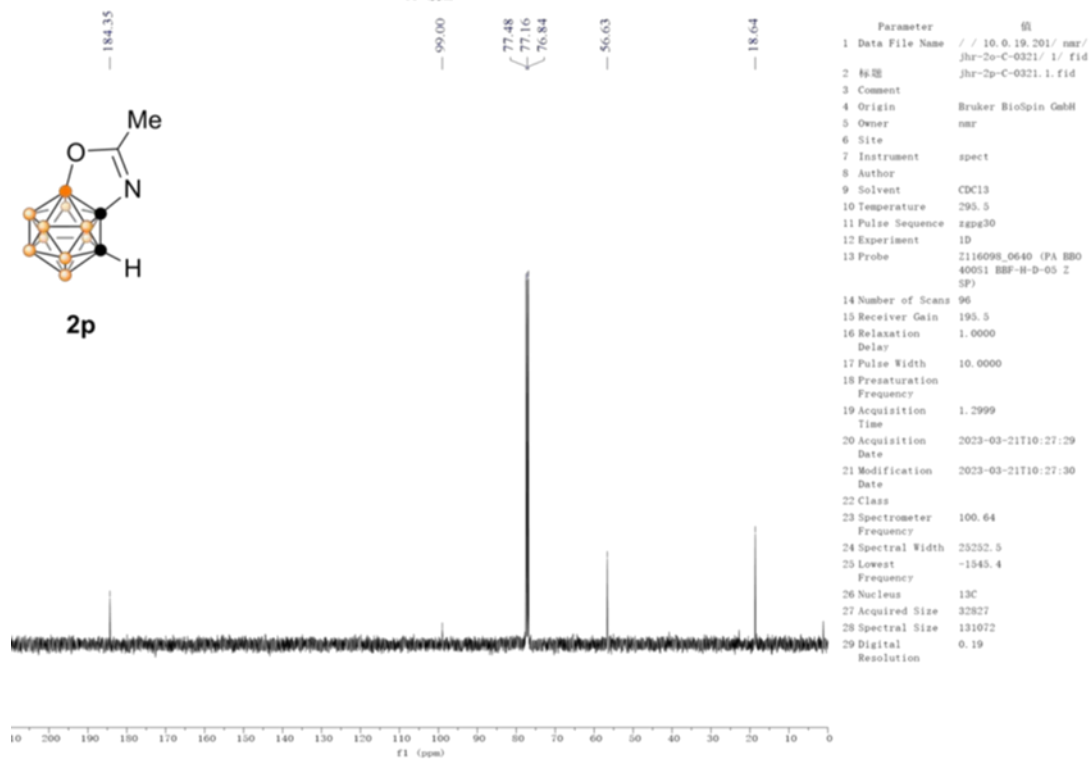
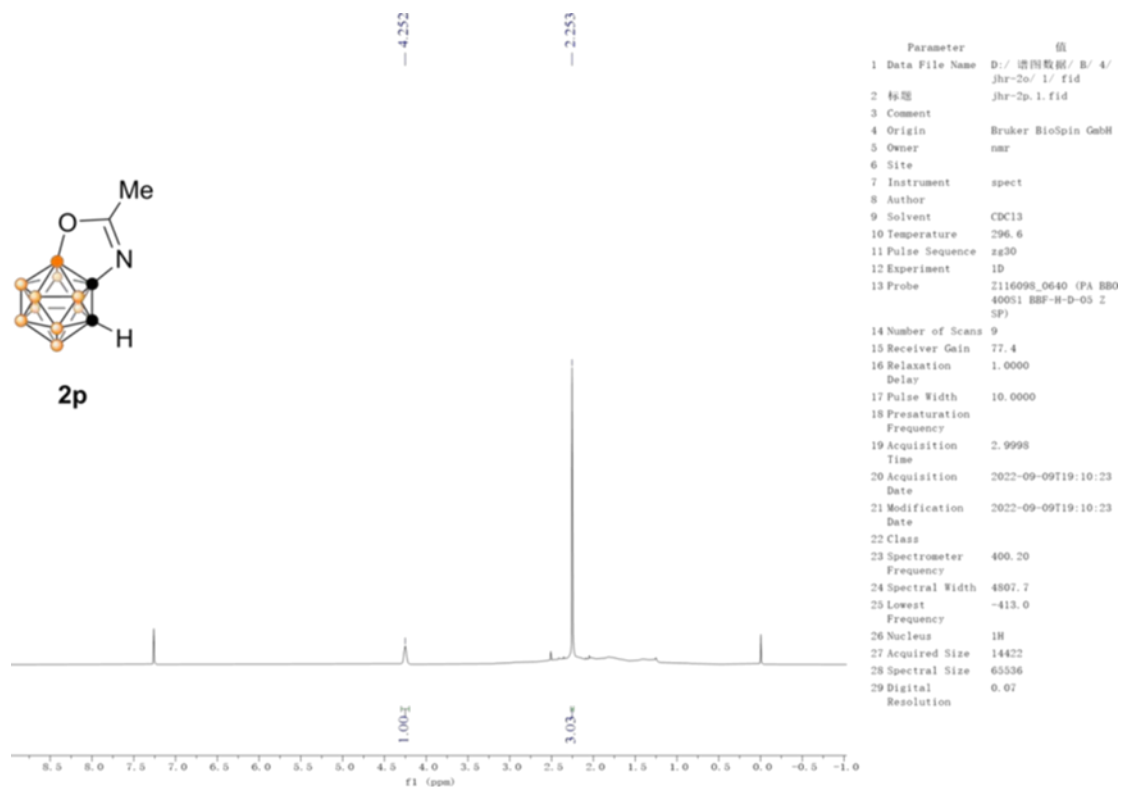


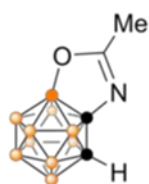




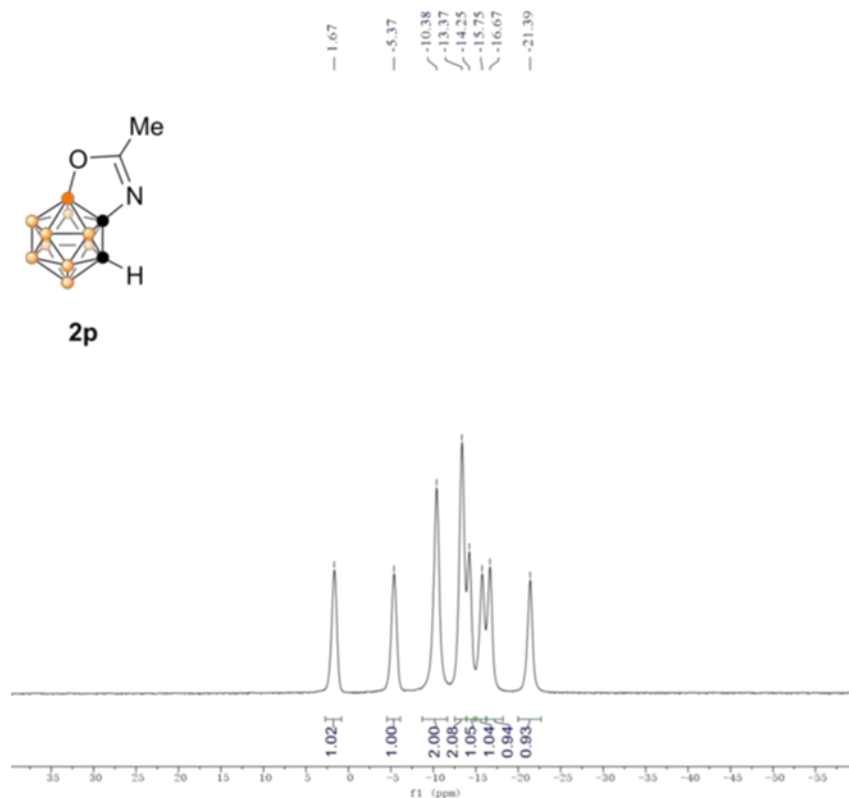




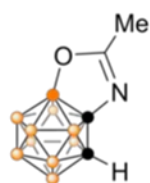




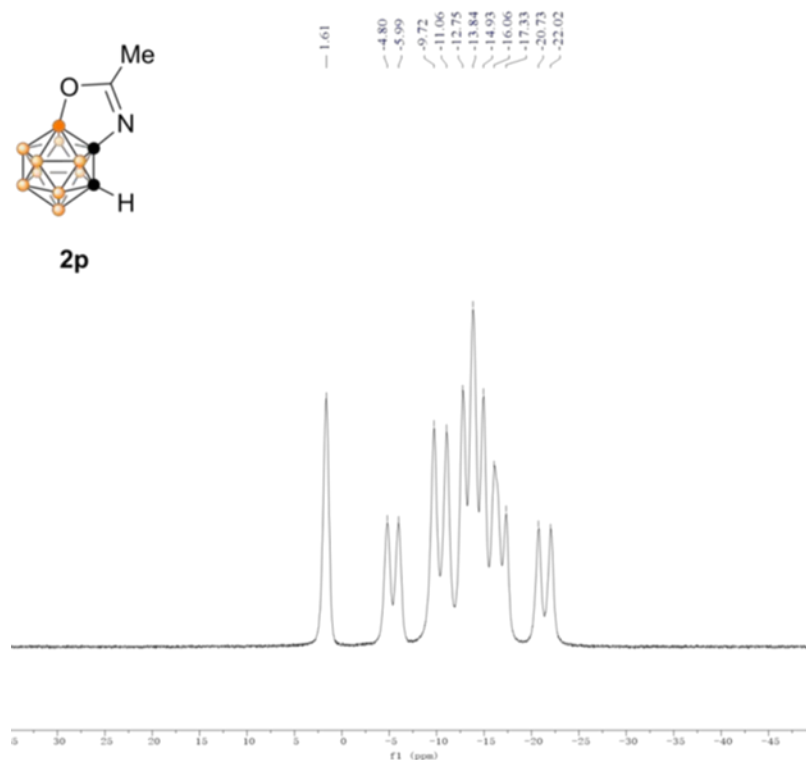
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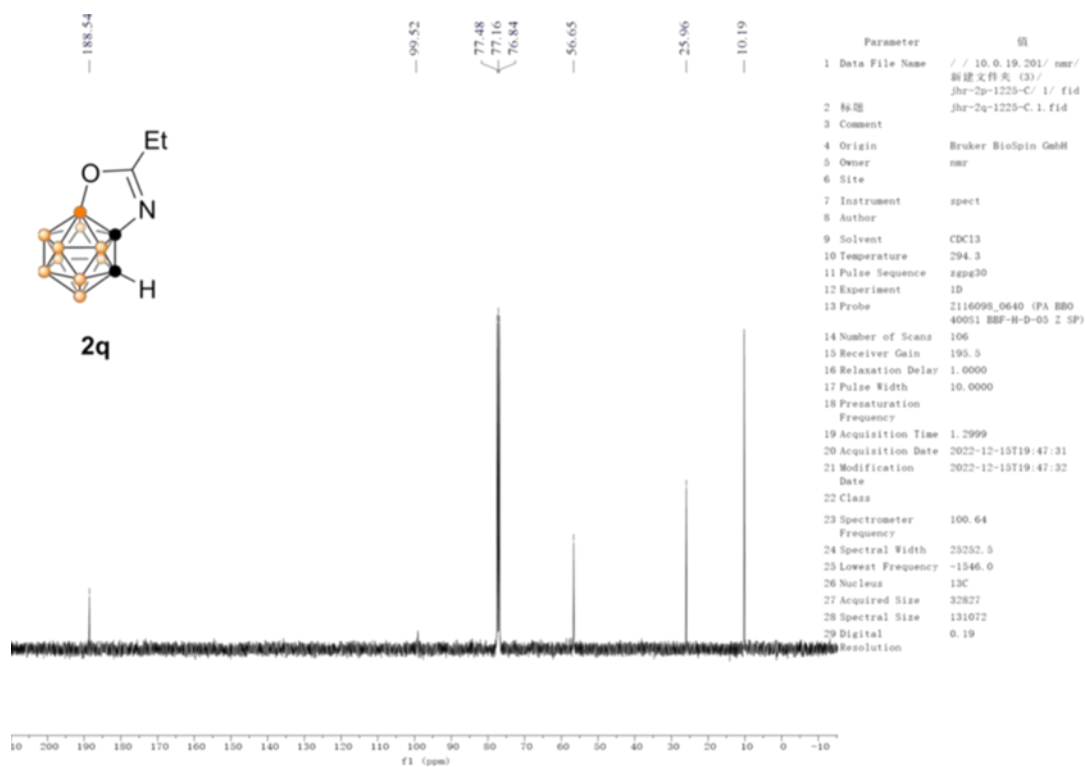
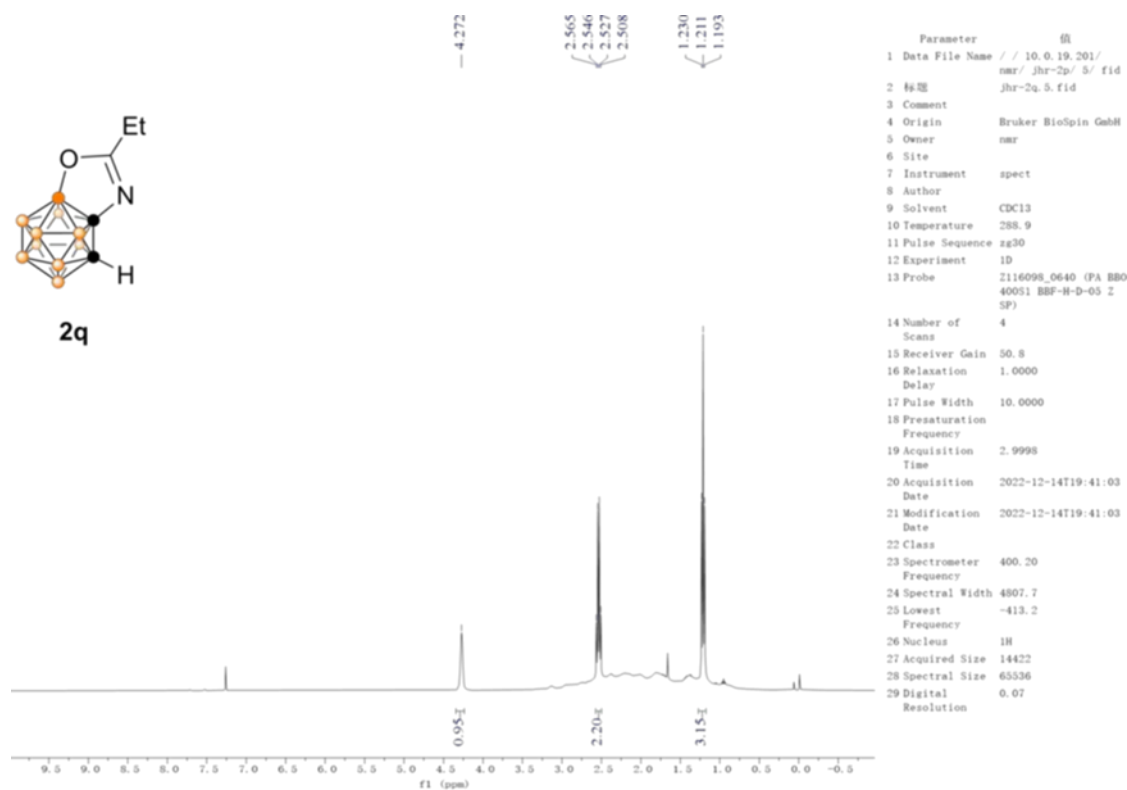
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4 Origin	Bruker BioSpin GmbH
5 Owner	nmz
6 Site	
7 Instrument	spect
8 Author	
9 Solvent	CDCl3
10 Temperature	293.5
11 Pulse Sequence	aring-b11
12 Experiment	1D
13 Probe	2116098_0640 (PA BBO 400S1 BPF-H-D-03 Z SP)
14 Number of Scans	14
15 Receiver Gain	195.5
16 Relaxation Delay	1.0000
17 Pulse Width	10.0000
18 Presaturation Frequency	
19 Acquisition Time	1.2845
20 Acquisition Date	2023-03-21T10:19:34
21 Modification Date	2023-03-21T10:19:34
22 Class	
23 Spectrometer Frequency	128.40
24 Spectral Width	25510.2
25 Lowest Frequency	-12755.1
26 Nucleus	11B
27 Acquired Size	32768
28 Spectral Size	65536
29 Digital Resolution	0.39

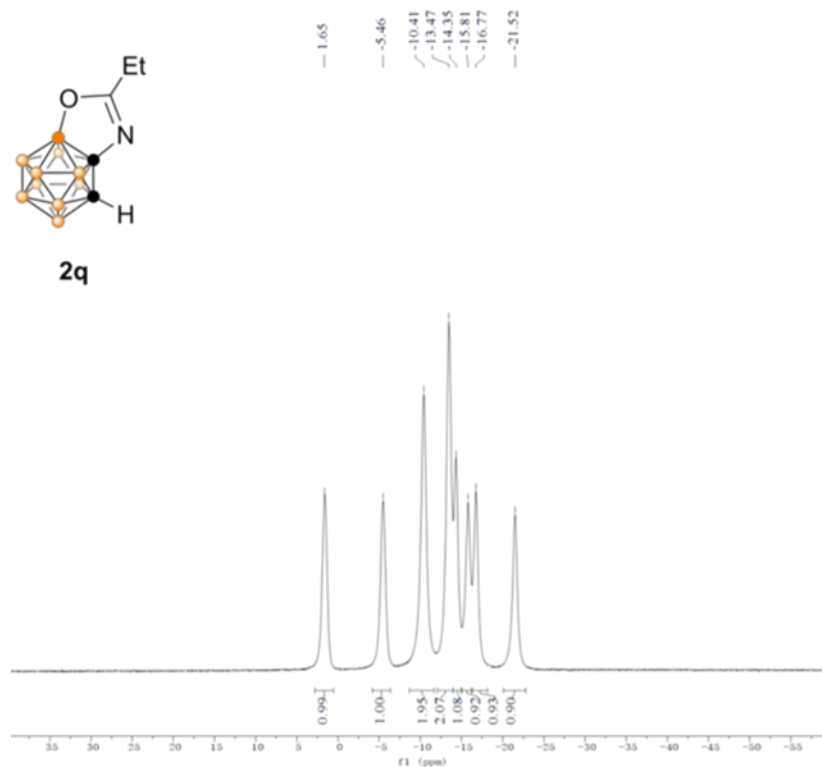
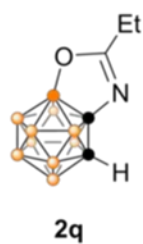


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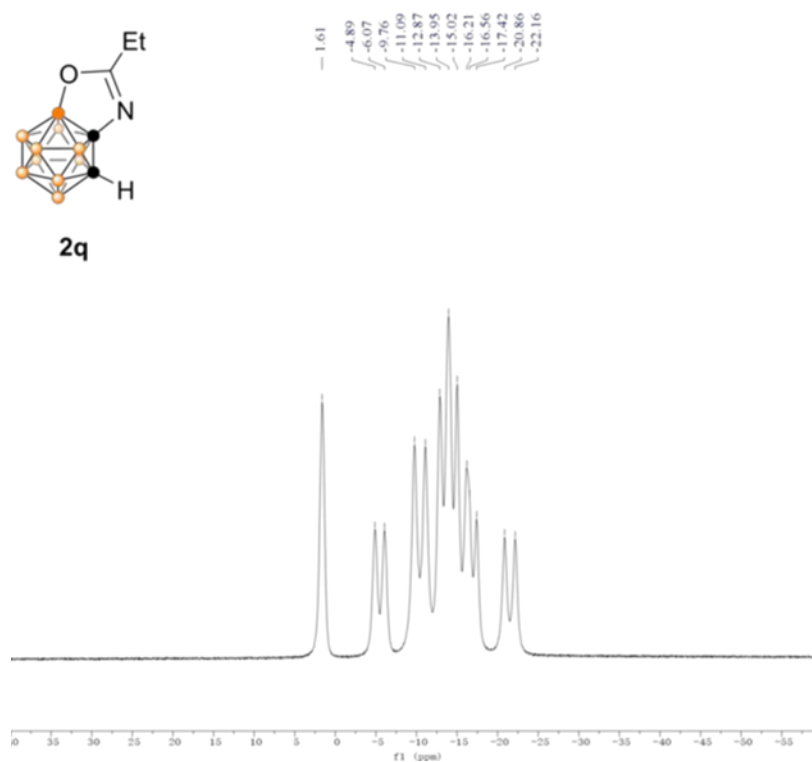
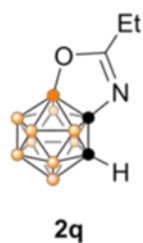


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2 标题	jhr-2p-no deB-0321.1.fid
3 Comment	
4 Origin	Bruker BioSpin GmbH
5 Owner	nmz
6 Site	
7 Instrument	spect
8 Author	
9 Solvent	CDCl3
10 Temperature	293.4
11 Pulse Sequence	aring
12 Experiment	1D
13 Probe	2116098_0640 (PA BBO 400S1 BPF-H-D-03 Z SP)
14 Number of Scans	8
15 Receiver Gain	195.5
16 Relaxation Delay	1.0000
17 Pulse Width	10.0000
18 Presaturation Frequency	
19 Acquisition Time	1.2845
20 Acquisition Date	2023-03-21T10:20:12
21 Modification Date	2023-03-21T10:20:13
22 Class	
23 Spectrometer Frequency	128.40
24 Spectral Width	25510.2
25 Lowest Frequency	-12755.1
26 Nucleus	11B
27 Acquired Size	32768
28 Spectral Size	65536
29 Digital Resolution	0.39

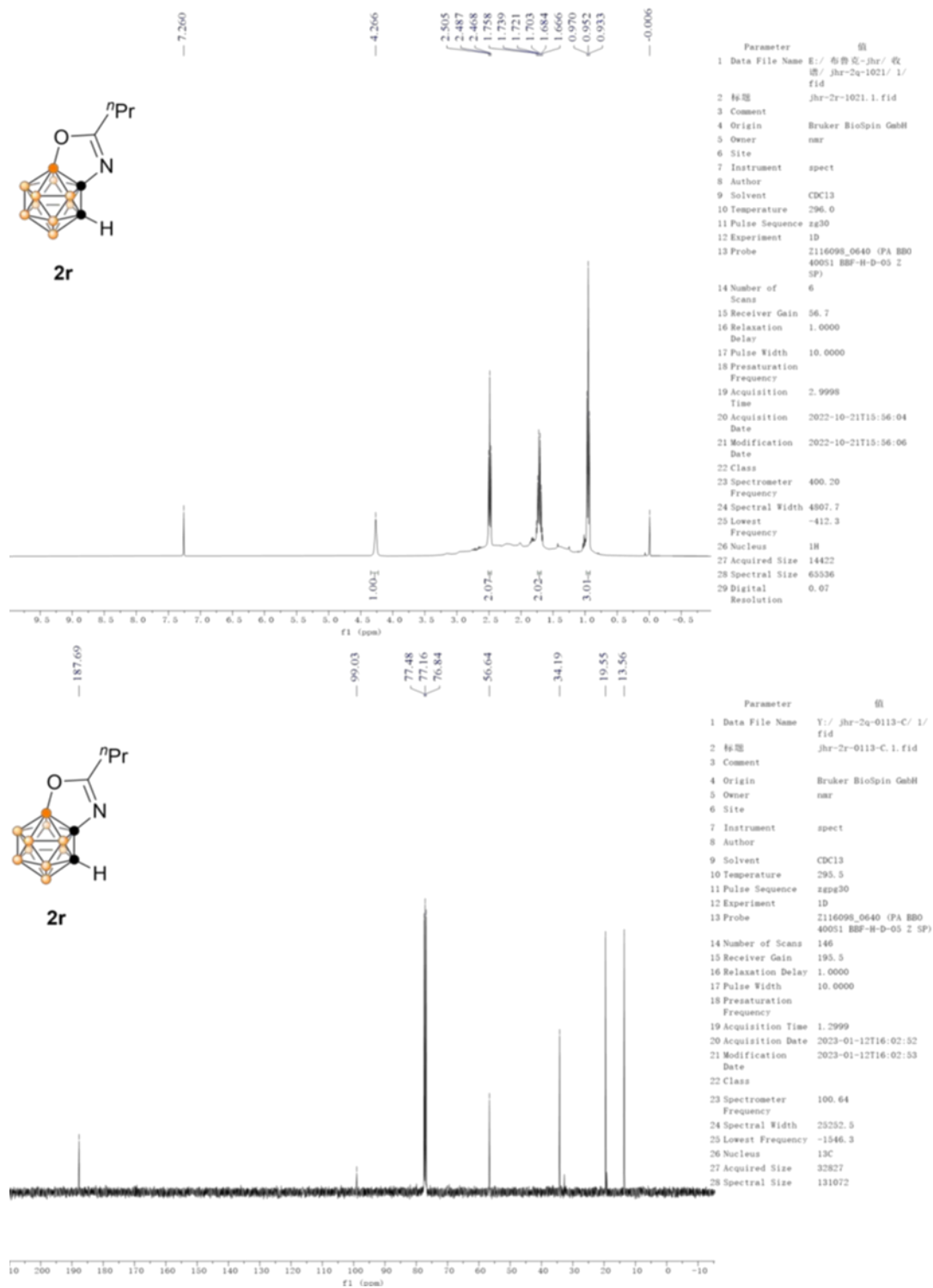


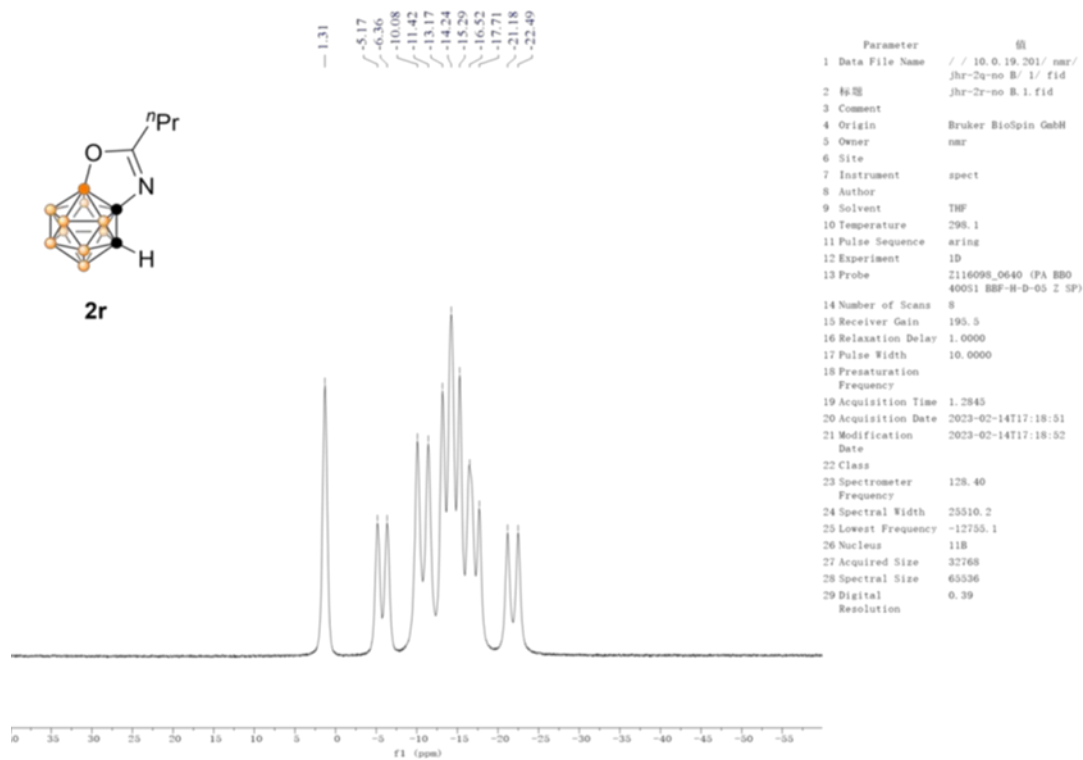
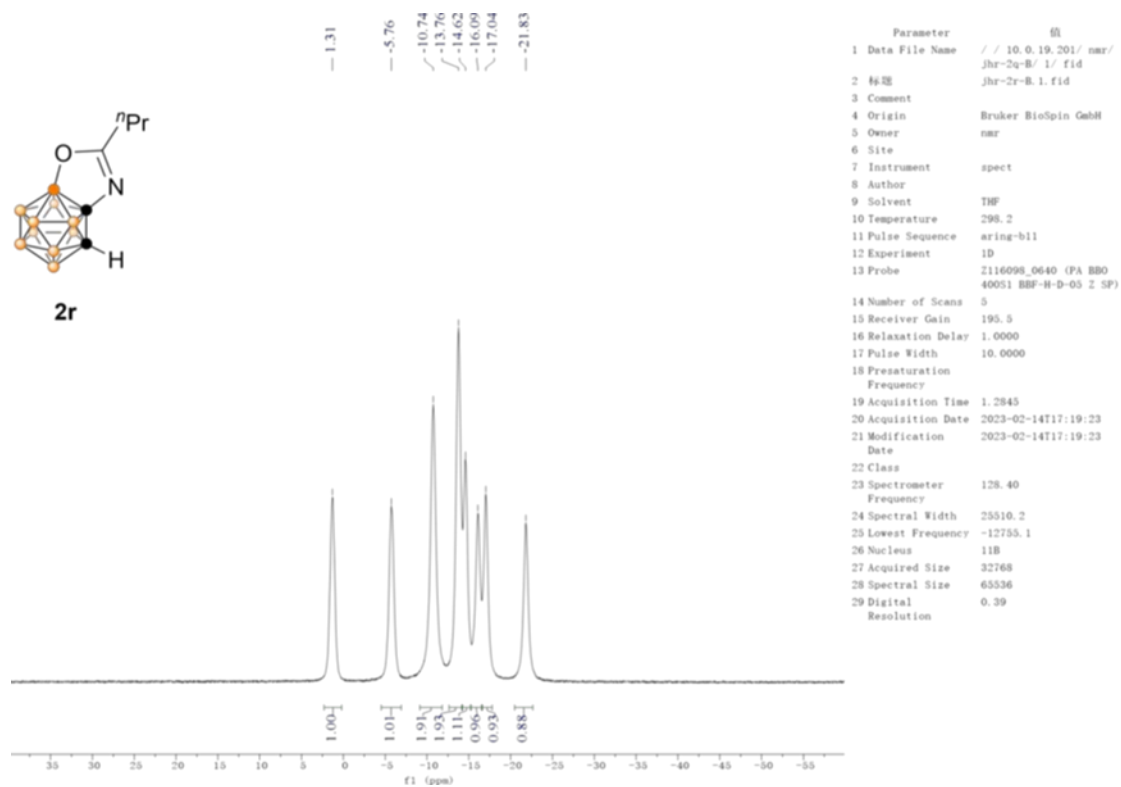


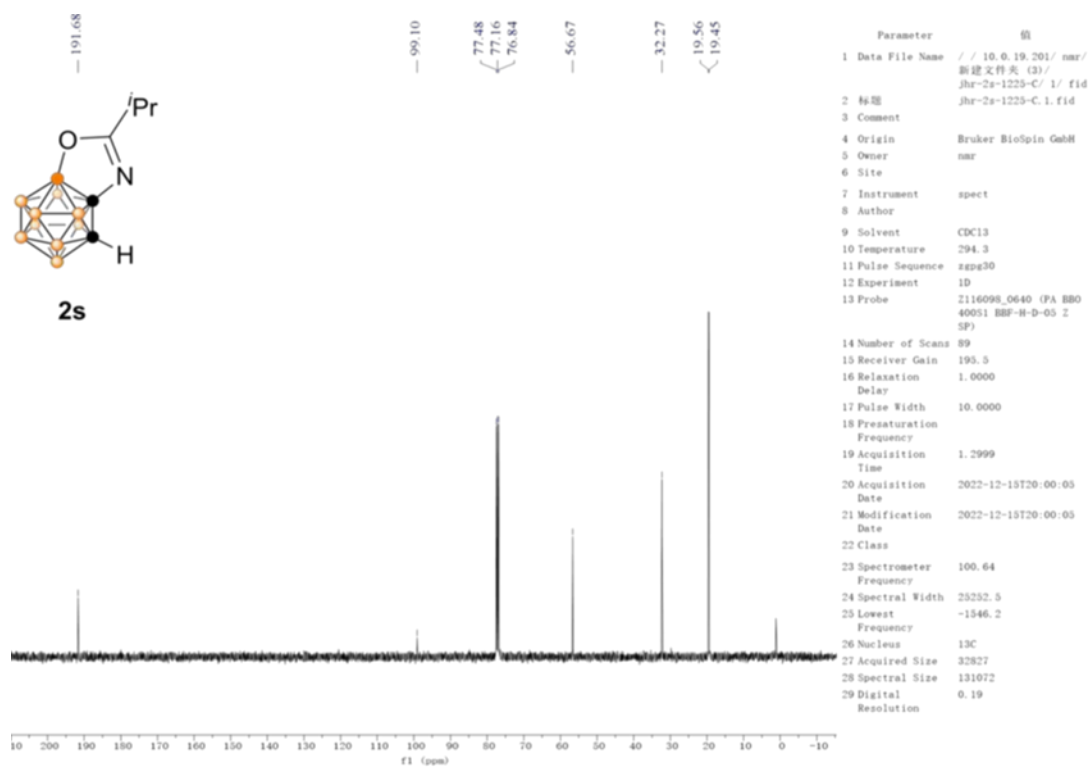
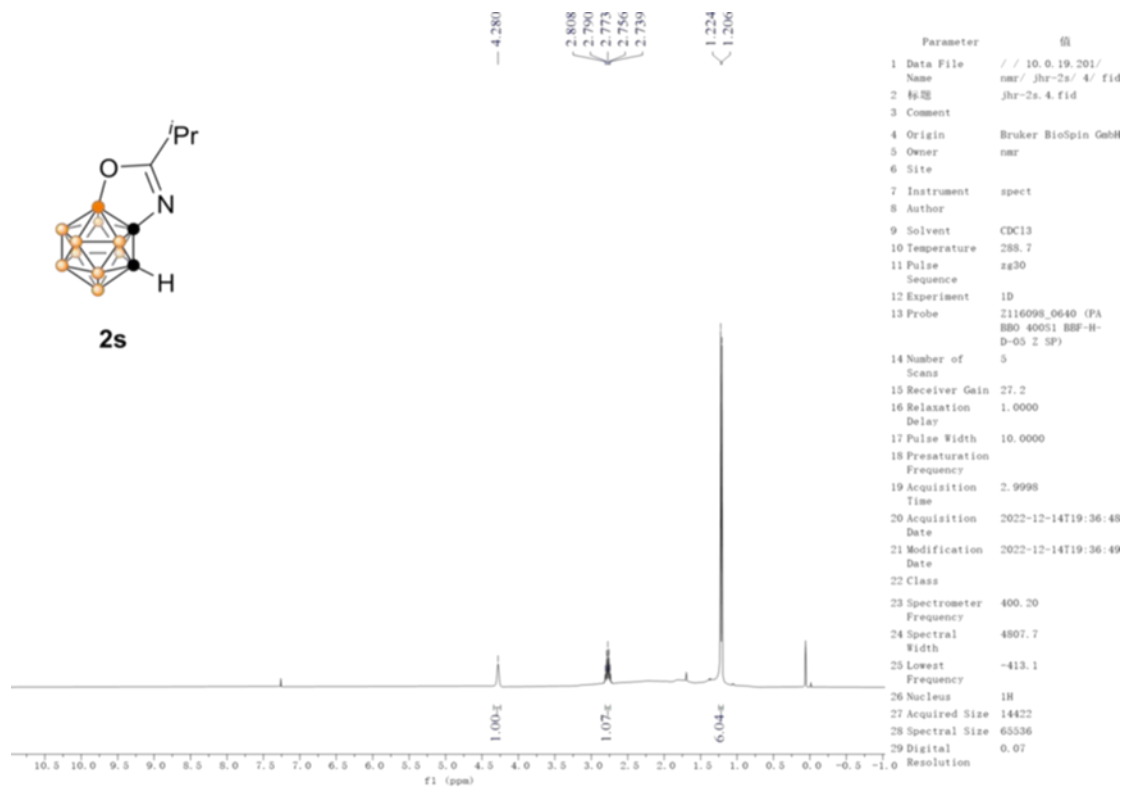
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2 标题	jhr-2q-1223-deB.1.fid
3 Comment	
4 Origin	Bruker BioSpin GmbH
5 Owner	nar
6 Site	
7 Instrument	spect
8 Author	
9 Solvent	CDCl3
10 Temperature	294.5
11 Pulse Sequence	aring-b11
12 Experiment	1D
13 Probe	2116095_0640 (PA BBO 400S1 BBF-H-D-03 2 SP)
14 Number of Scans	7
15 Receiver Gain	195.5
16 Relaxation Delay	1.0000
17 Pulse Width	10.0000
18 Presaturation Frequency	
19 Acquisition Time	1.2845
20 Acquisition Date	2022-12-15T20:26:23
21 Modification Date	2022-12-15T20:26:26
22 Class	
23 Spectrometer Frequency	128.40
24 Spectral Width	25510.2
25 Lowest Frequency	-12755.1
26 Nucleus	1H
27 Acquired Size	32768
28 Spectral Size	65536
29 Digital Resolution	0.39

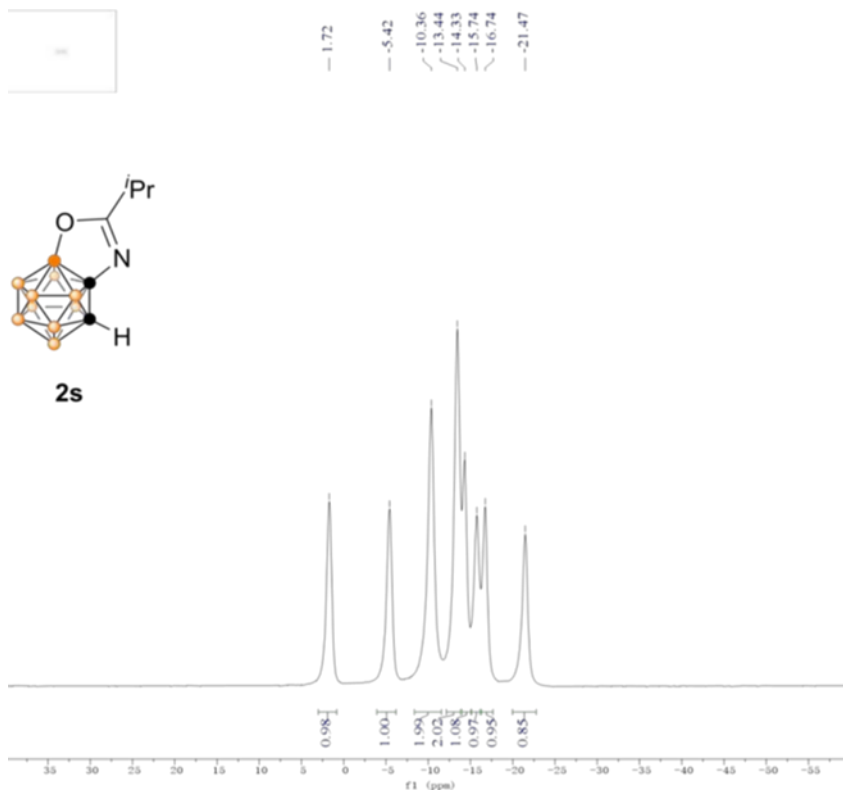
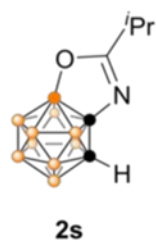


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2 标题	jhr-2q-1223-no deB. 1.fid
3 Comment	
4 Origin	Bruker BioSpin GmbH
5 Owner	nar
6 Site	
7 Instrument	spect
8 Author	
9 Solvent	CDCl3
10 Temperature	294.4
11 Pulse Sequence	aring
12 Experiment	1D
13 Probe	2116095_0640 (PA BBO 400S1 BBF-H-D-03 2 SP)
14 Number of Scans	7
15 Receiver Gain	195.5
16 Relaxation Delay	1.0000
17 Pulse Width	10.0000
18 Presaturation Frequency	
19 Acquisition Time	1.2845
20 Acquisition Date	2022-12-15T20:27:29
21 Modification Date	2022-12-15T20:27:30
22 Class	
23 Spectrometer Frequency	128.40
24 Spectral Width	25510.2
25 Lowest Frequency	-12755.1
26 Nucleus	1H
27 Acquired Size	32768
28 Spectral Size	65536
29 Digital Resolution	0.39

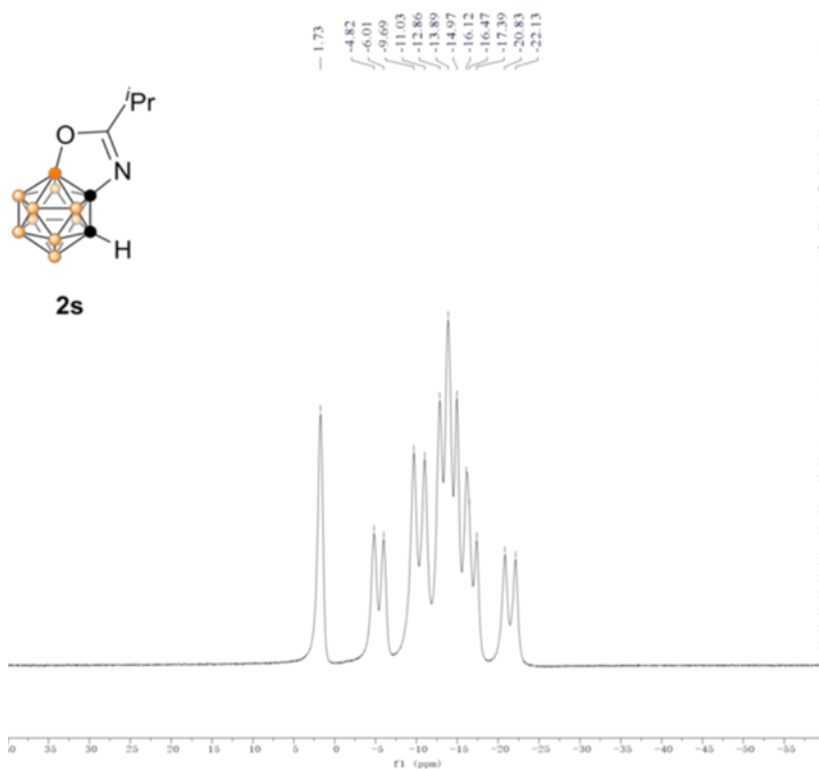




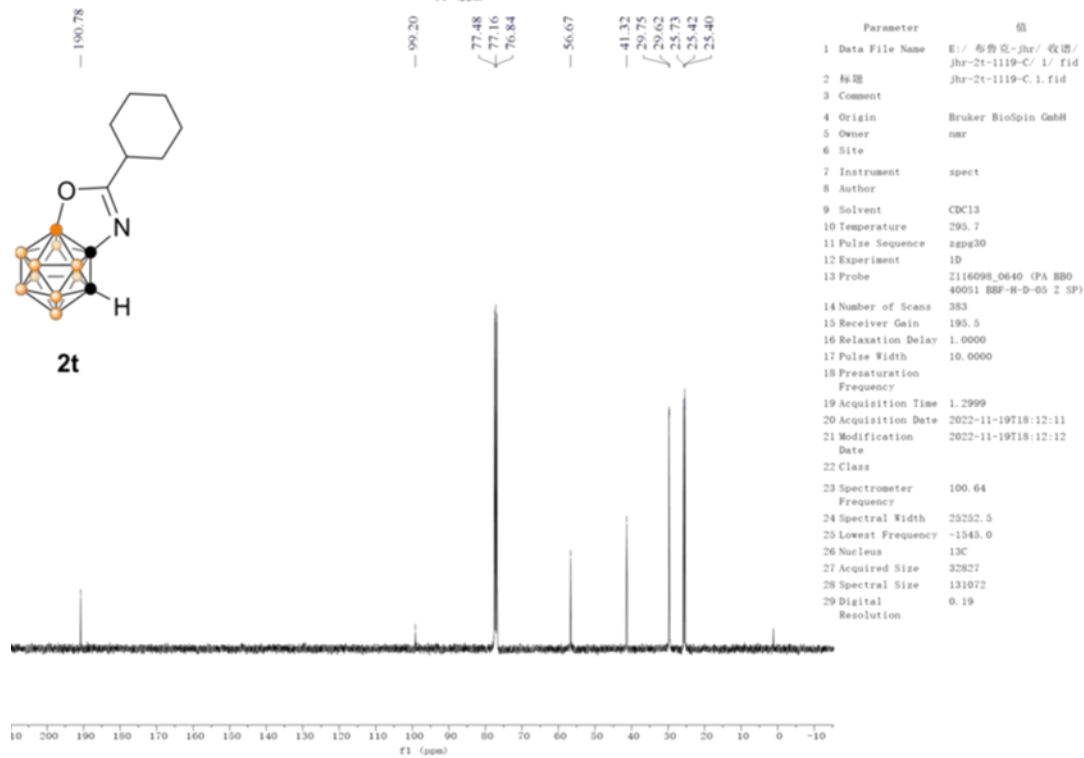
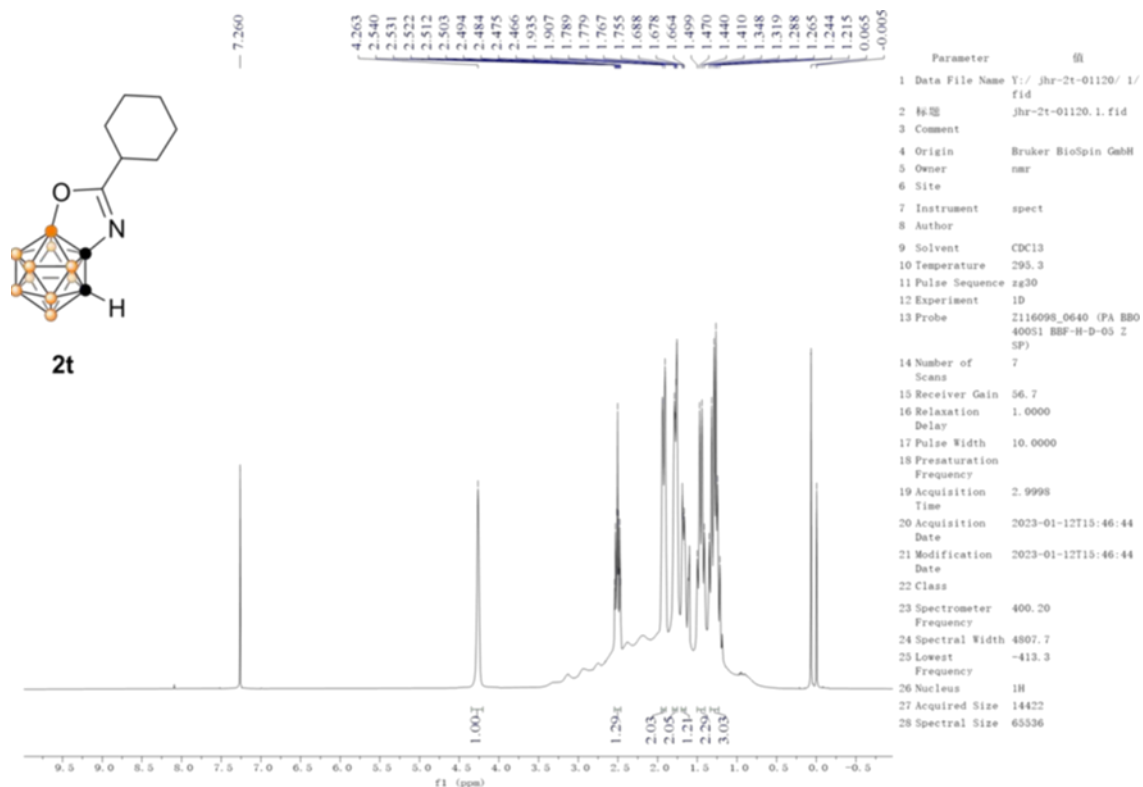


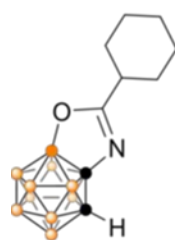


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2 标题	jhr-2s-1225-deB.1.fid
3 Comment	
4 Origin	Bruker BioSpin GmbH
5 Owner	nmr
6 Site	
7 Instrument	spect
8 Author	
9 Solvent	CDCl3
10 Temperature	294.4
11 Pulse Sequence	aring-b11
12 Experiment	1D
13 Probe	Z116098_0640 (PA BB0 400S1 BBF-H-D-05 2 SP)
14 Number of Scans	15
15 Receiver Gain	195.5
16 Relaxation Delay	1.0000
17 Pulse Width	10.0000
18 Presaturation Frequency	
19 Acquisition Time	1.2845
20 Acquisition Date	2022-12-15T20:39:43
21 Modification Date	2022-12-15T20:39:46
22 Class	
23 Spectrometer Frequency	128.40
24 Spectral Width	25510.2
25 Lowest Frequency	-12755.1
26 Nucleus	1H
27 Acquired Size	32768
28 Spectral Size	65536
29 Digital Resolution	0.39

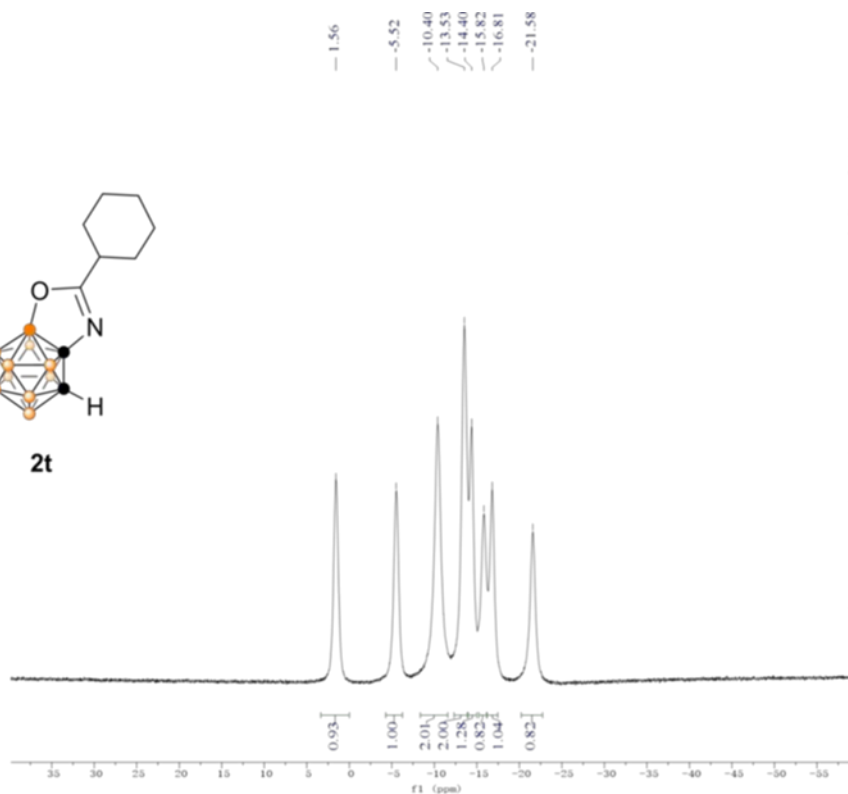


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2 标题	jhr-2s-1225-no deB0.1.fid
3 Comment	
4 Origin	Bruker BioSpin GmbH
5 Owner	nmr
6 Site	
7 Instrument	spect
8 Author	
9 Solvent	CDCl3
10 Temperature	294.4
11 Pulse Sequence	aring
12 Experiment	1D
13 Probe	Z116098_0640 (PA BB0 400S1 BBF-H-D-05 2 SP)
14 Number of Scans	7
15 Receiver Gain	195.5
16 Relaxation Delay	1.0000
17 Pulse Width	10.0000
18 Presaturation Frequency	
19 Acquisition Time	1.2845
20 Acquisition Date	2022-12-15T20:40:20
21 Modification Date	2022-12-15T20:40:21
22 Class	
23 Spectrometer Frequency	128.40
24 Spectral Width	25510.2
25 Lowest Frequency	-12755.1
26 Nucleus	1H
27 Acquired Size	32768
28 Spectral Size	65536
29 Digital Resolution	0.39

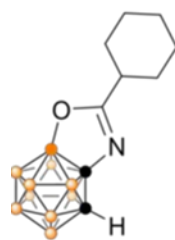




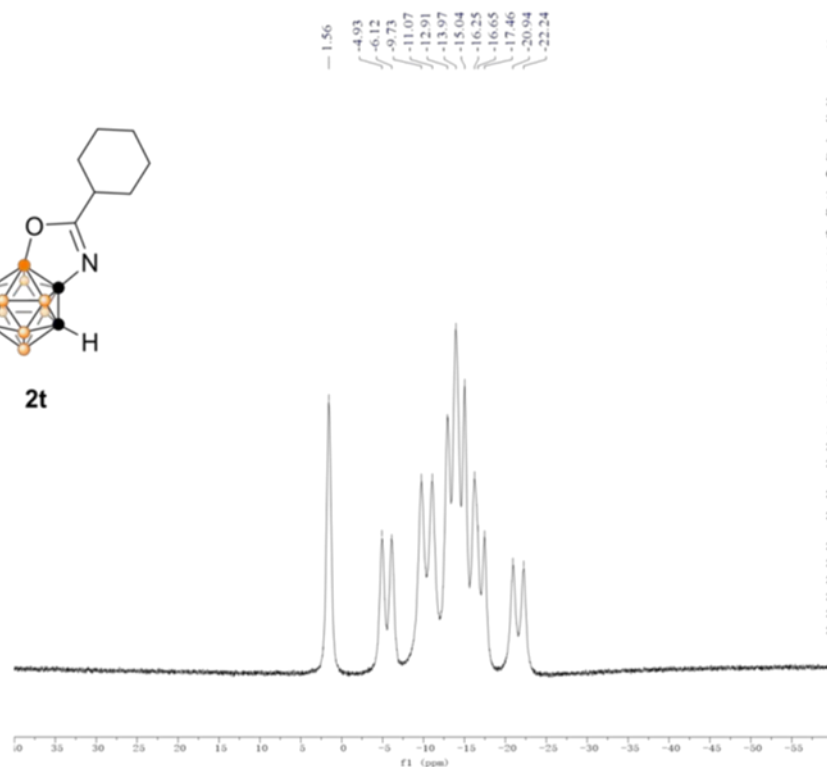
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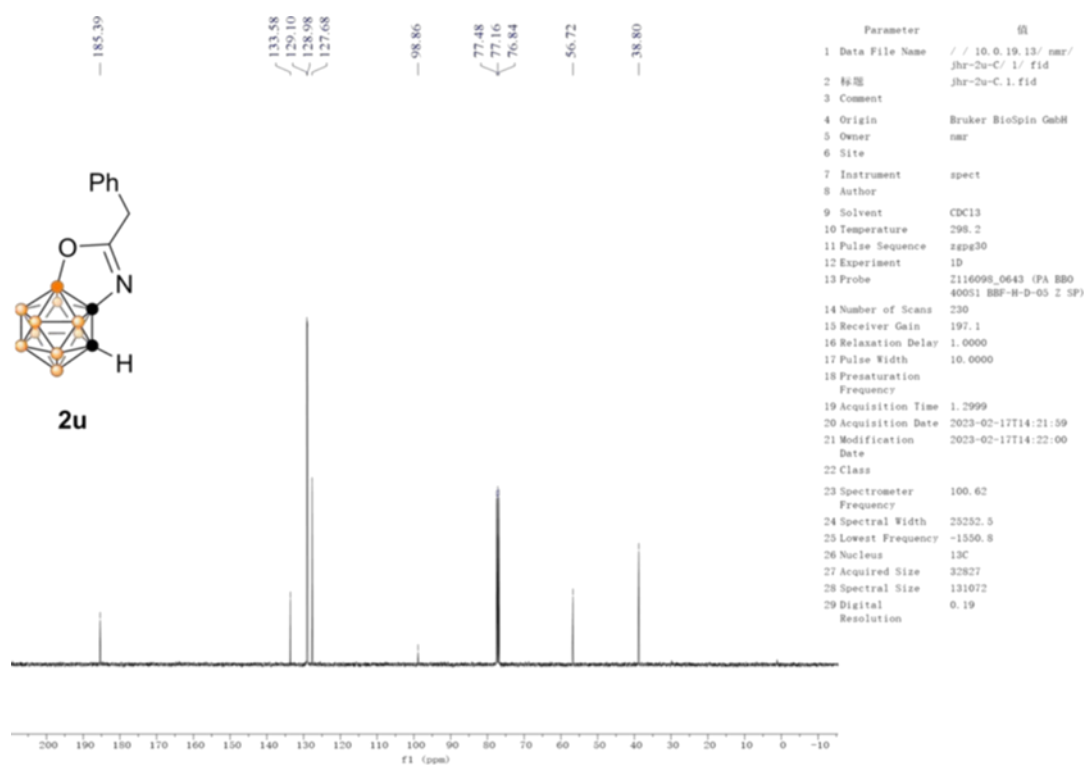
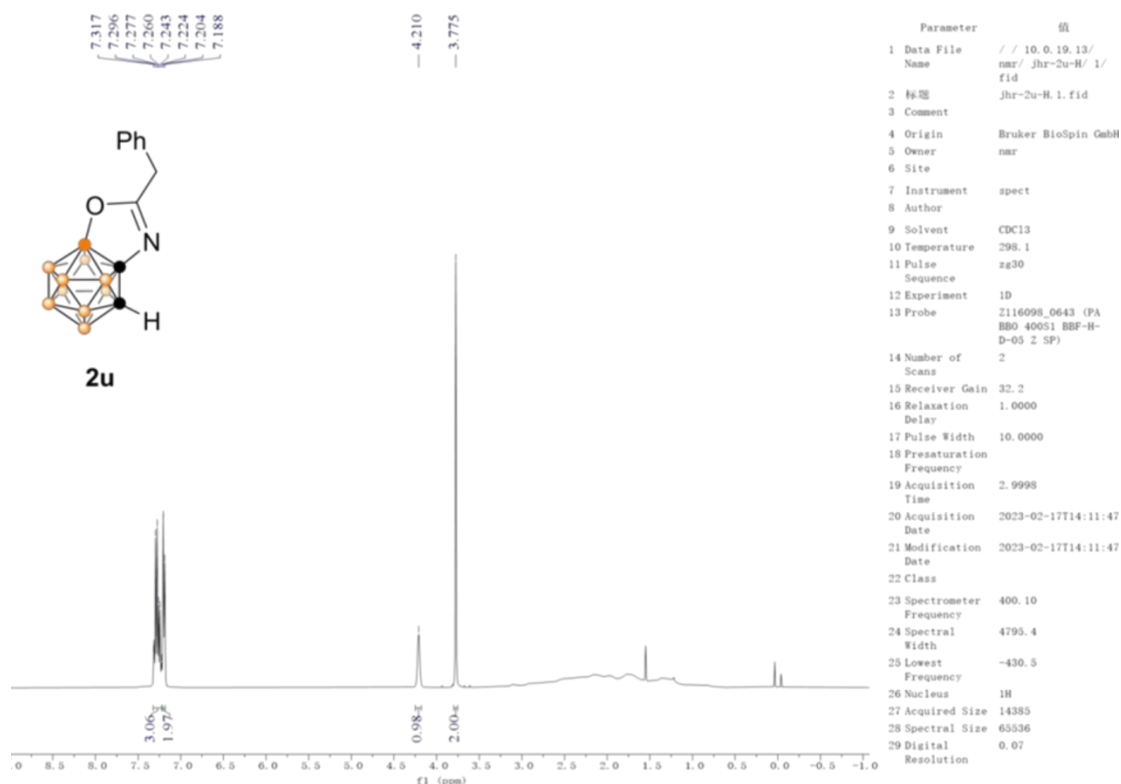
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1 Data File Name	D:/ 实验室相关/ 1ab/ 关
2 标题	标题/ 未整理-第四本/
3 Comment	jhr-4007-is-B. 1. fid
4 Origin	Bruker BioSpin GmbH
5 Owner	nmr
6 Site	
7 Instrument	spect
8 Author	
9 Solvent	CDCl3
10 Temperature	296.2
11 Pulse Sequence	aring-b11
12 Experiment	1D
13 Probe	Z116098_0640 (PA BB0 40051 BBP-H-D-05 2 SP)
14 Number of Scans	2
15 Receiver Gain	193.5
16 Relaxation Delay	1.0000
17 Pulse Width	10.0000
18 Presaturation	Frequency
19 Acquisition Time	1.2845
20 Acquisition Date	2022-06-19T16:17:05
21 Modification	2022-06-19T16:17:06
22 Class	
23 Spectrometer	128.40
24 Spectral Width	25510.2
25 Lowest Frequency	-12755.1
26 Nucleus	11B
27 Acquired Size	32768
28 Spectral Size	65536
29 Digital	0.39
Resolution	

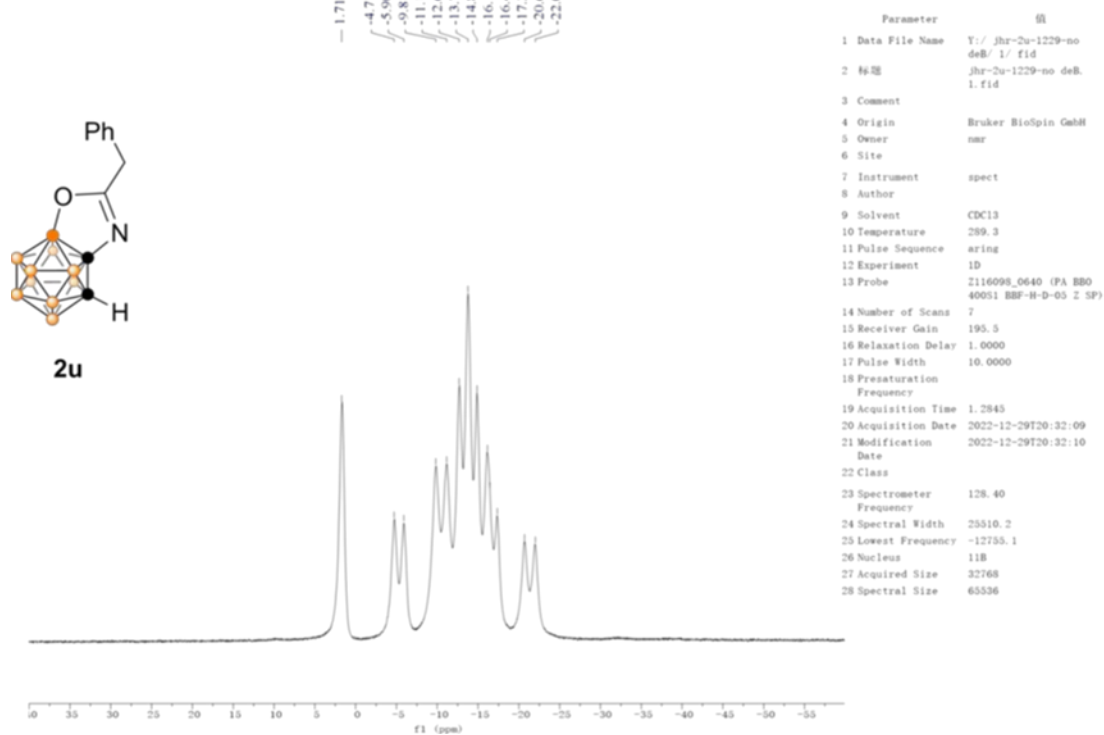
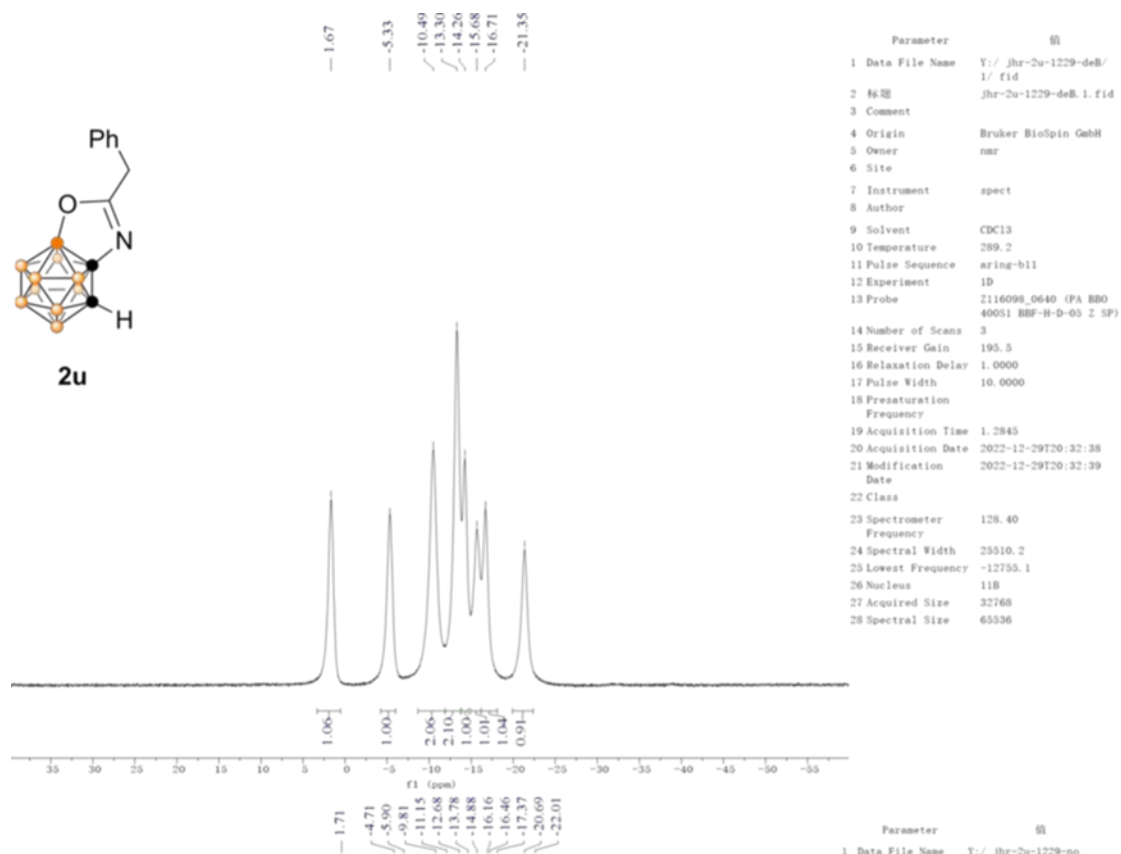


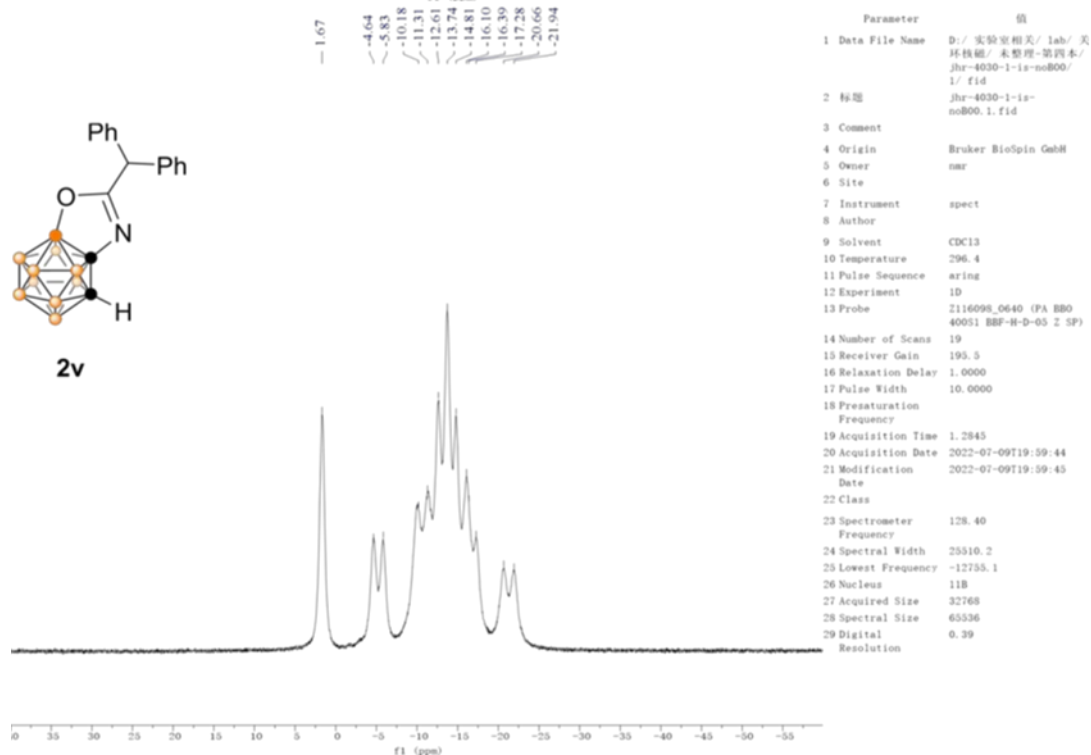
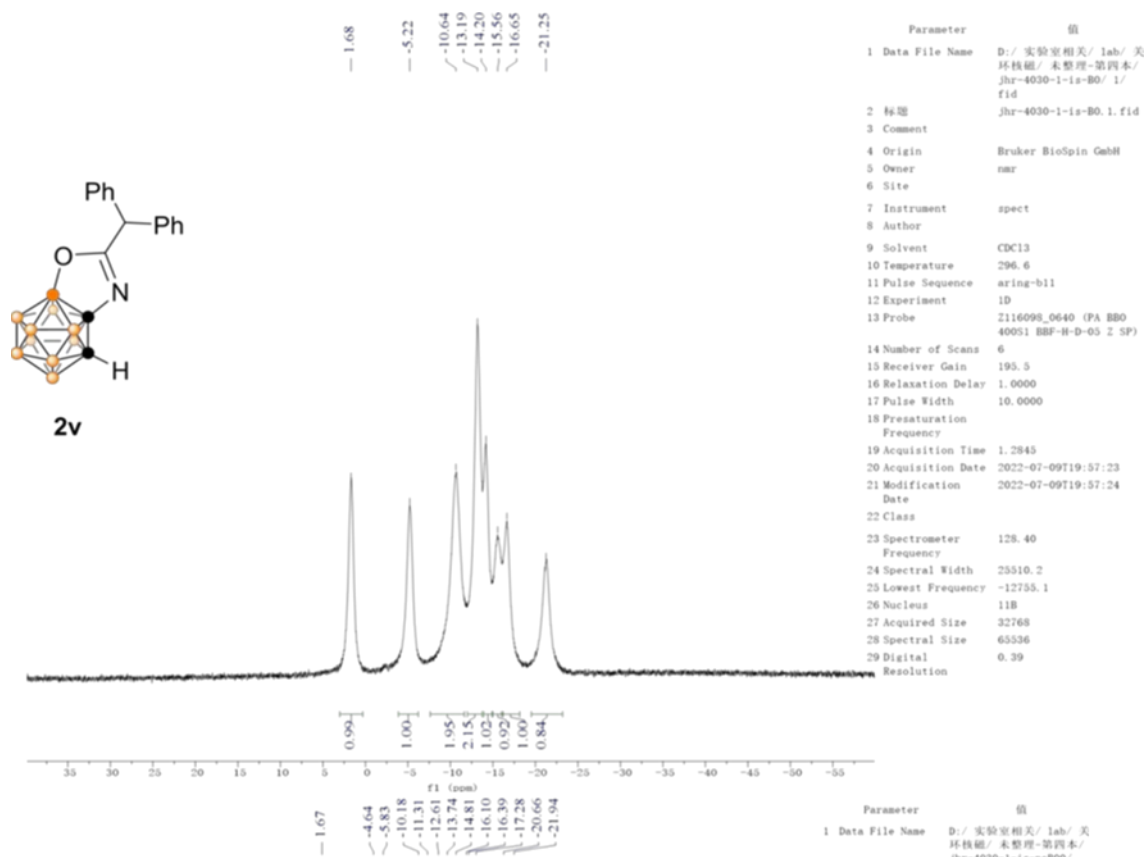
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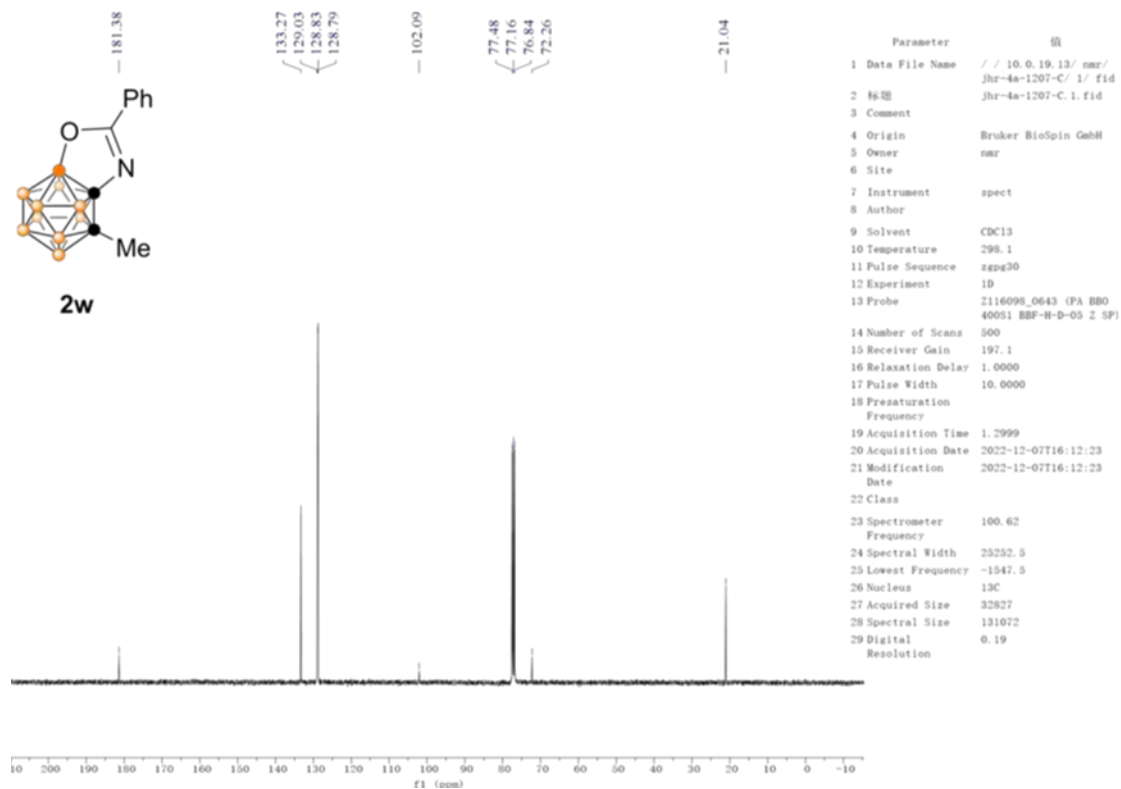
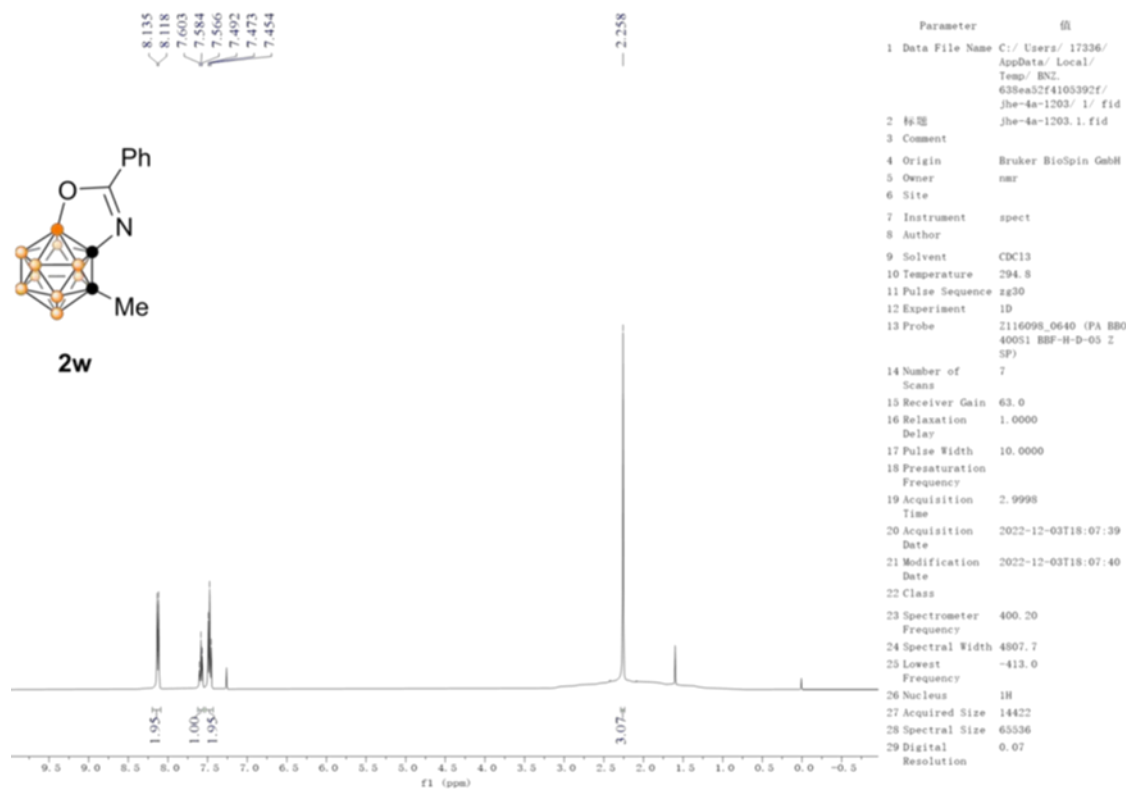


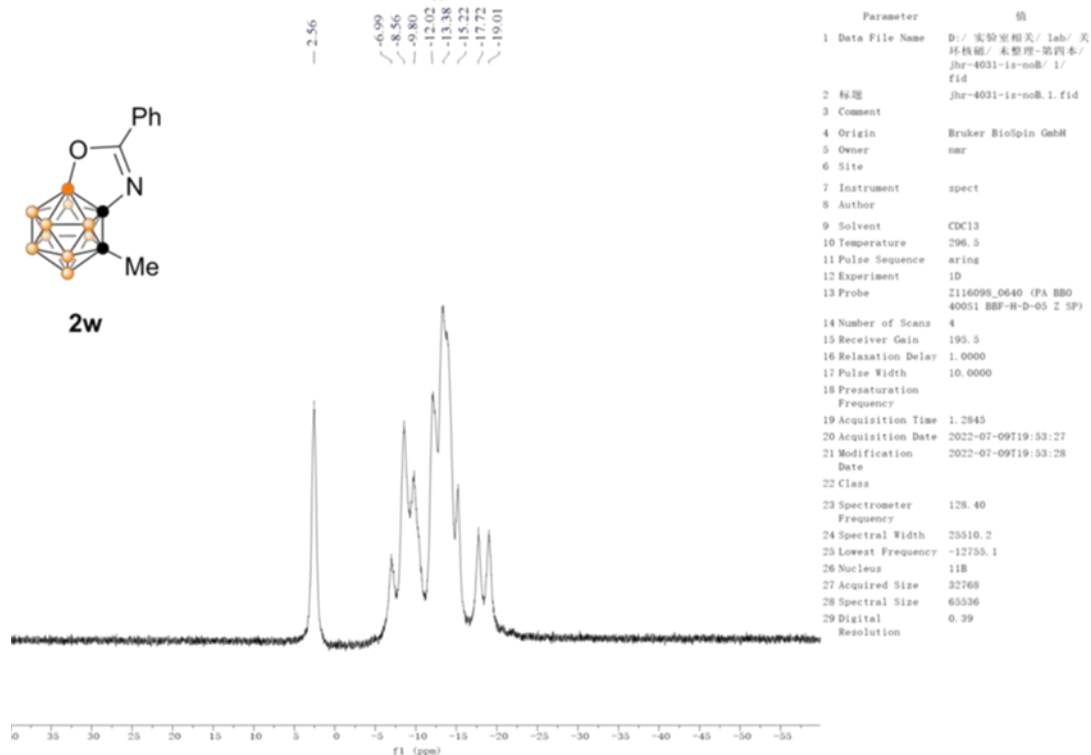
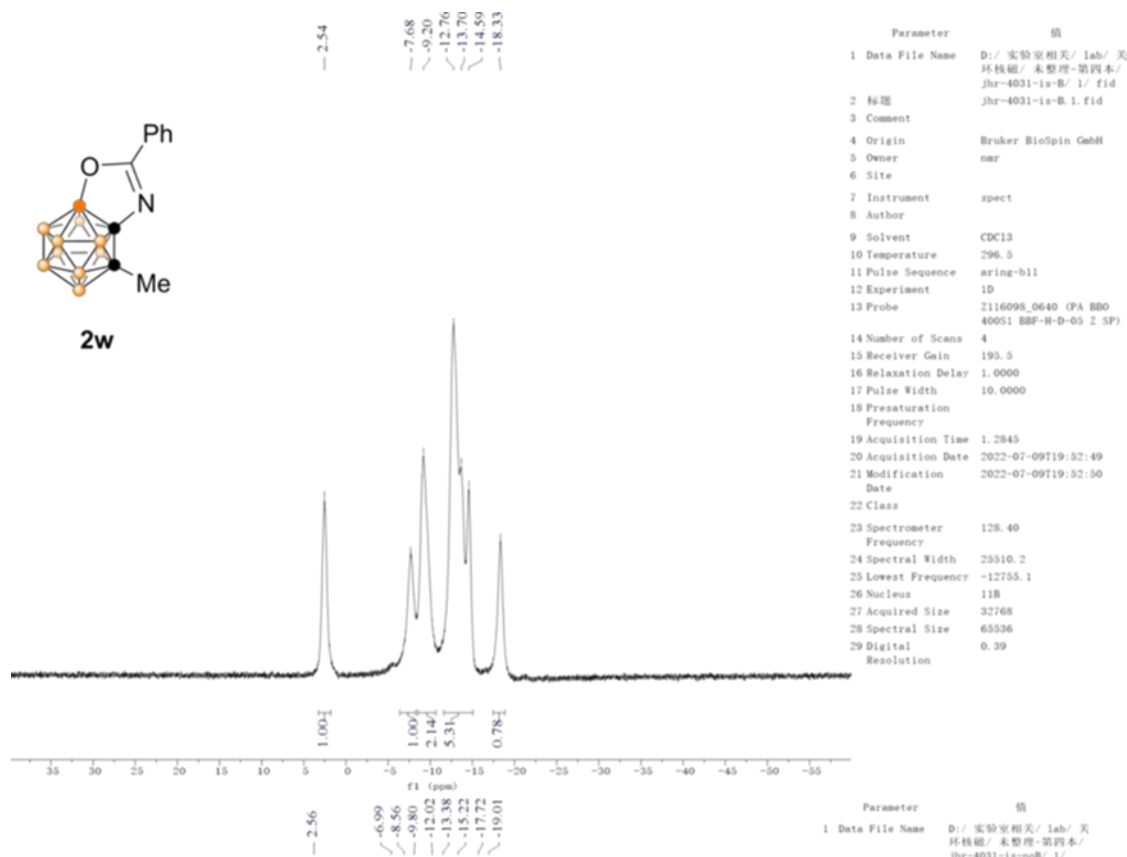
Parameter	值
1 Data File Name	D:/ 实验室相关/ 1ab/ 关
2 标题	标题/ 未整理-第四本/
3 Comment	jhr-4007-is-noB. 1. fid
4 Origin	Bruker BioSpin GmbH
5 Owner	nmr
6 Site	
7 Instrument	spect
8 Author	
9 Solvent	CDCl3
10 Temperature	296.2
11 Pulse Sequence	aring
12 Experiment	1D
13 Probe	Z116098_0640 (PA BB0 40051 BBP-H-D-05 2 SP)
14 Number of Scans	2
15 Receiver Gain	193.5
16 Relaxation Delay	1.0000
17 Pulse Width	10.0000
18 Presaturation	Frequency
19 Acquisition Time	1.2845
20 Acquisition Date	2022-06-19T16:17:32
21 Modification	2022-06-19T16:17:33
22 Class	
23 Spectrometer	128.40
24 Spectral Width	25510.2
25 Lowest Frequency	-12755.1
26 Nucleus	11B
27 Acquired Size	32768
28 Spectral Size	65536
29 Digital	0.39
Resolution	

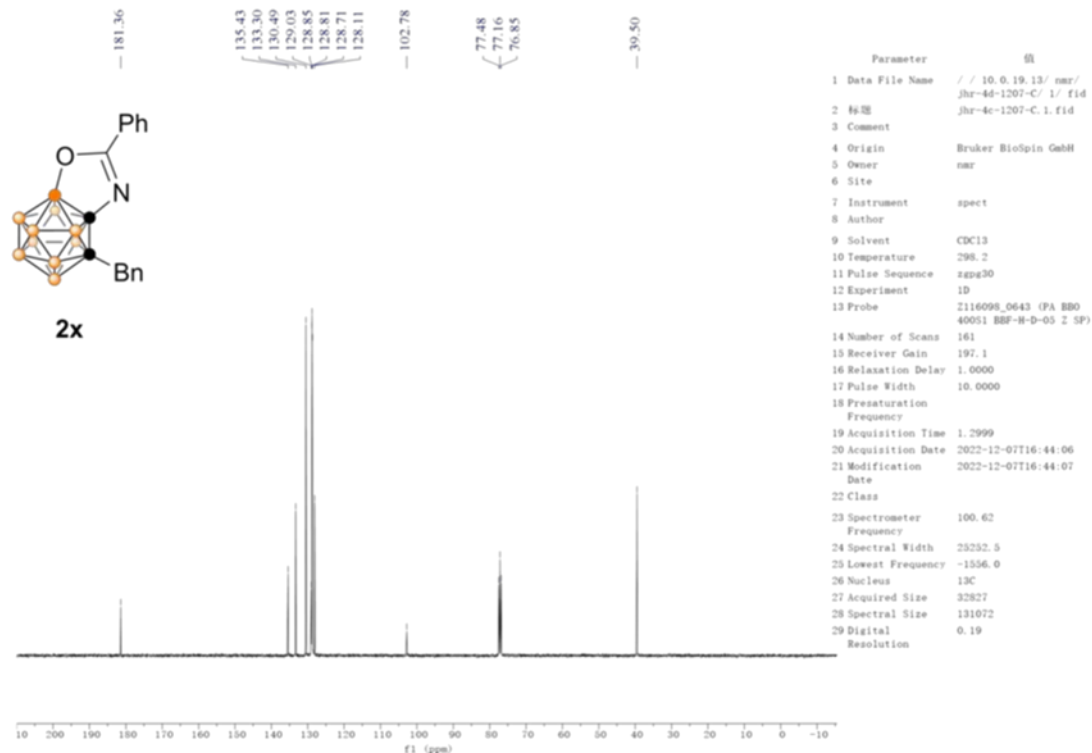
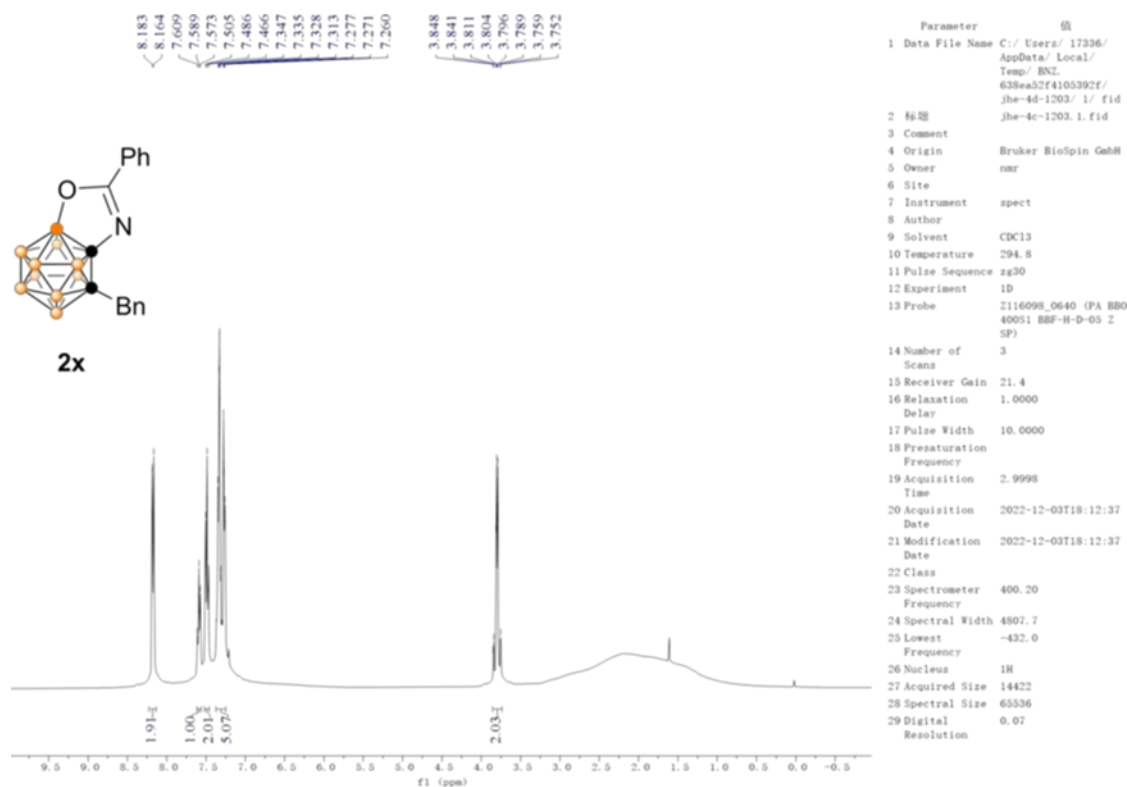


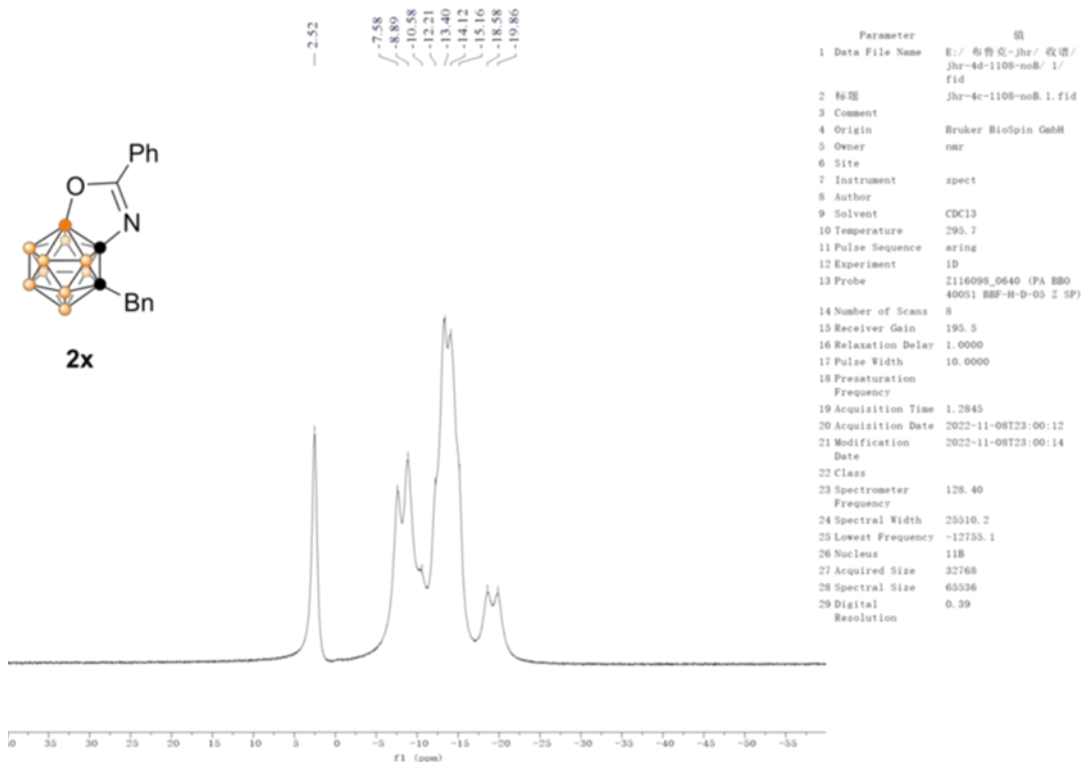
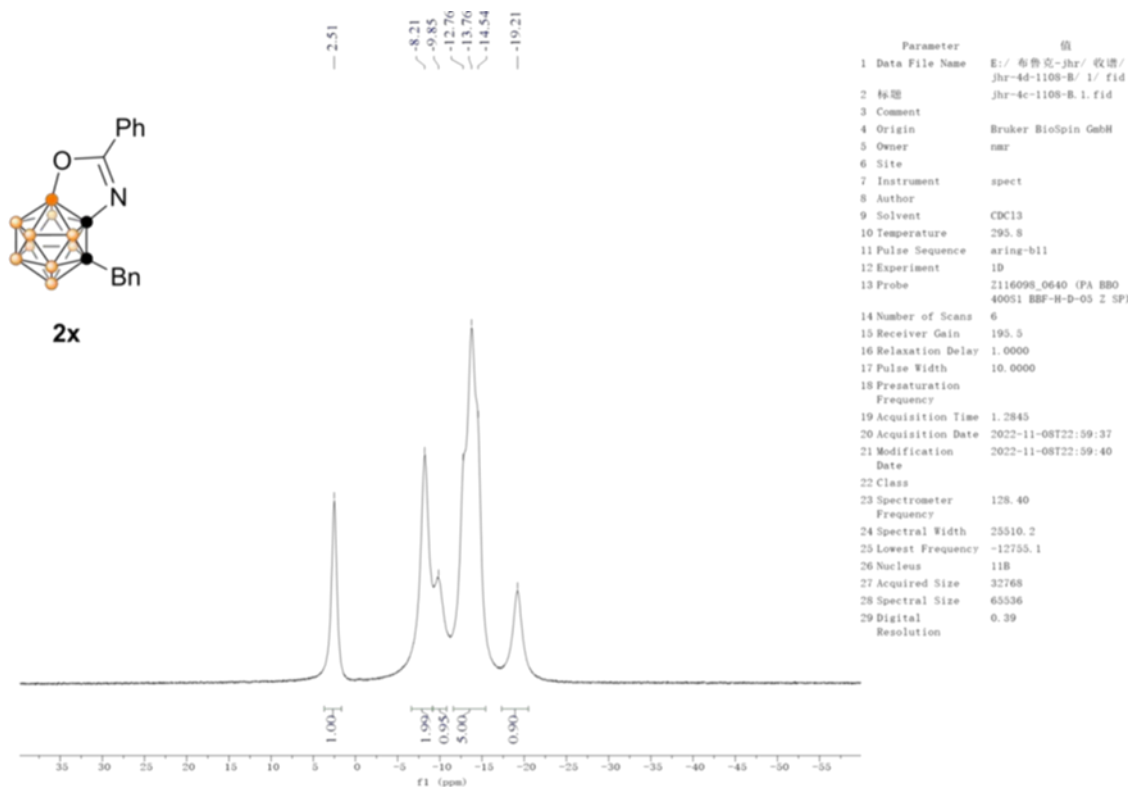




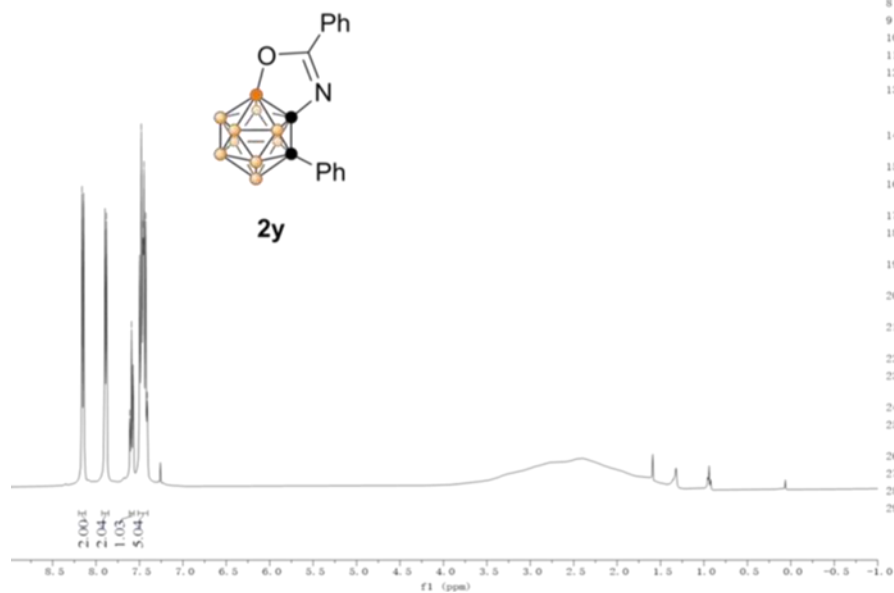






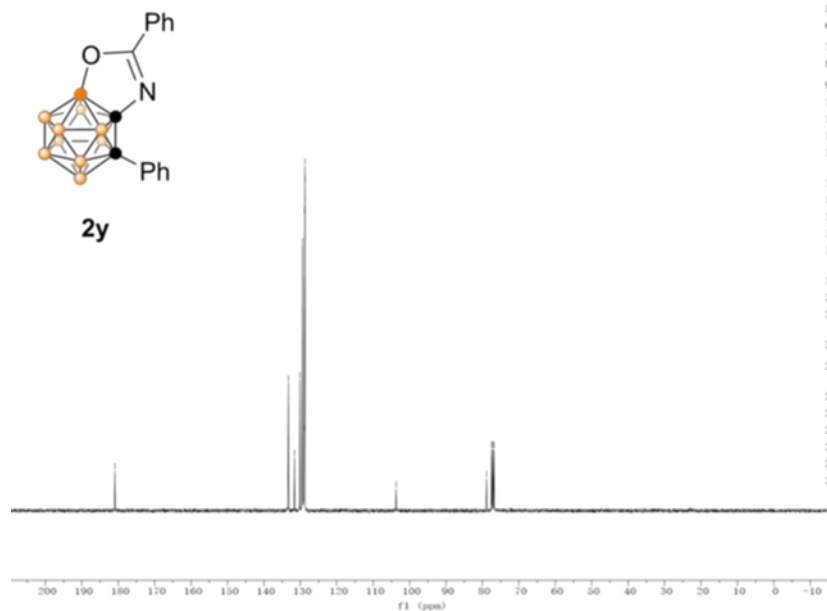


8.162
8.143
7.899
7.881
7.611
7.592
7.574
7.498
7.480
7.459
7.454
7.447
7.428
7.412



Parameter	值
1 Data File Name	// 10.0.19.201/ nmr/ jhr-4c-1103/ 17/ fid
2 标题	jhr-4b-1103.17.fid
3 Comment	
4 Origin	Bruker BioSpin GmbH
5 Owner	nmr
6 Site	
7 Instrument	spect
8 Author	
9 Solvent	CDCl3
10 Temperature	294.6
11 Pulse Sequence	zg30
12 Experiment	1D
13 Probe	Z116098_0640 (PA BBO 400S1 BRF-H-D-05 Z SP)
14 Number of Scans	6
15 Receiver Gain	21.4
16 Relaxation Delay	1.0000
17 Pulse Width	10.0000
18 Presaturation Frequency	
19 Acquisition Time	2.9998
20 Acquisition Date	2022-11-30T19:22:17
21 Modification Date	2022-11-30T19:22:18
22 Class	
23 Spectrometer Frequency	400.20
24 Spectral Width	7598.8
25 Lowest Frequency	-1208.1
26 Nucleus	1H
27 Acquired Size	22795
28 Spectral Size	65536
29 Digital Resolution	0.12

180.94
133.28
131.63
130.14
129.37
128.94
128.88
128.75
128.74
103.72
78.88
77.48
77.16
76.84



Parameter	值
1 Data File Name	// 10.0.19.13/ nmr/ jhr-4c-1207-C/ 2/ fid
2 标题	jhr-4b-1207-C.2.fid
3 Comment	
4 Origin	Bruker BioSpin GmbH
5 Owner	nmr
6 Site	
7 Instrument	spect
8 Author	
9 Solvent	CDCl3
10 Temperature	298.2
11 Pulse Sequence	zgpg30
12 Experiment	1D
13 Probe	Z116098_0643 (PA BBO 400S1 BRF-H-D-05 Z SP)
14 Number of Scans	113
15 Receiver Gain	197.1
16 Relaxation Delay	1.0000
17 Pulse Width	10.0000
18 Presaturation Frequency	
19 Acquisition Time	1.2999
20 Acquisition Date	2022-12-07T16:53:46
21 Modification Date	2022-12-07T16:53:47
22 Class	
23 Spectrometer Frequency	100.62
24 Spectral Width	25252.5
25 Lowest Frequency	-1555.6
26 Nucleus	13C
27 Acquired Size	32827
28 Spectral Size	131072
29 Digital Resolution	0.19

