Supporting Information

Access to Spirocyclic Vinyl Sulfones via Radical Cyclization and Functional Group Migration

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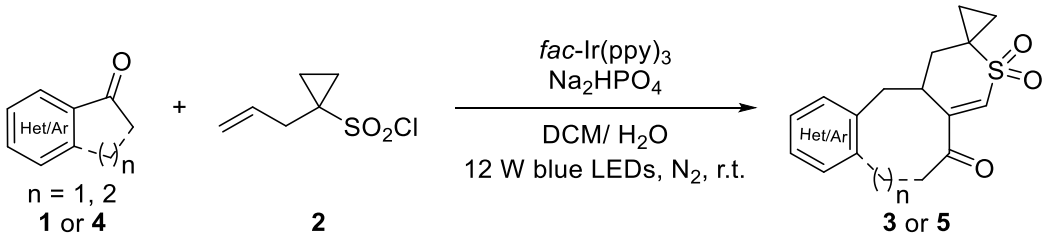
1. General experimental details

All reactions were maintained under nitrogen unless otherwise stated. Commercially available reagents were used without further purification. Infrared (FT-IR) spectra were recorded on a BRUKER VERTEX 70, ν_{max} in cm^{-1}. ^{1}H-NMR spectra were recorded on a BRUKER AVANCE III HD (400 MHz) spectrometer and a BRUKER AVANCE III HD (500 MHz) spectrometer. Chemical shifts are reported in ppm from tetramethylsilane with the solvent resonance as internal standard ($CDCl_3$: δ 7.26). Data are reported as follows: chemical shift, multiplicity (s = singlet, d = doublet, t = triplet, q = quadruplet, br = broad, m = multiplet), coupling constants (Hz) and integration. ^{13}C-NMR spectra were recorded on a Bruker AVANCE III HD (100 or 125 MHz) spectrometer with complete proton decoupling. Chemical shifts are reported in ppm from tetramethylsilane with the solvent resonance as the internal standard ($CDCl_3$: δ 77.16). ^{19}F-NMR spectra were recorded on a BRUKER AVANCE III HD (376 MHz) spectrometer. High resolution mass spectrometry (HRMS) was measured with a GCT Premier^{TM} and BRUKER micrOTF-Q III. Melting points were measured using INESA WRR and values are uncorrected.

Propargyl alcohol **1aa** and allylcyclopropane sulfonyl chloride **2** are commercially available reagents.

2. General procedure for the synthesis of spirocyclic vinyl sulfones

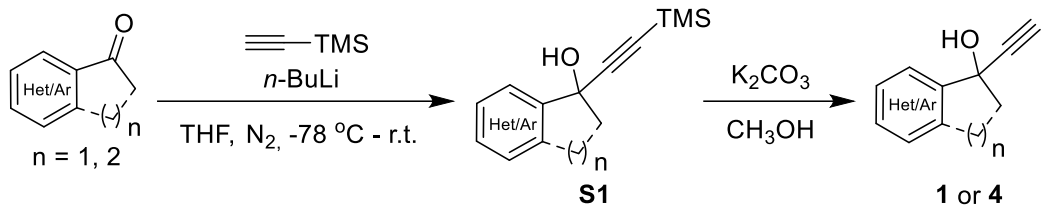


Propargyl alcohol **1** or **4** (0.2 mmol), Na_2HPO_4 (0.2 mmol), and *fac*-Ir(ppy)$_3$ (0.006 mmol, 3 mol %) were loaded in a reaction vial which was subjected to evacuation/ flushing with N_2 three times. Then allylcyclopropane sulfonyl chloride **2** (0.3 mmol) in CH_3CN (2 mL) and H_2O (0.2 mL) were added to the mixture via syringe. The reaction was irradiated with 12 W blue LEDs for about 12 hours. After reaction completion, the reaction mixture was directly concentrated in vacuo. Purification the residue by flash column chromatography on silica gel afforded the desired product **3** or **5**.

Gram-scale preparation:
Propargyl alcohol **1a** (5.0 mmol, 1.016 g), Na_2HPO_4 (5.0 mmol, 0.710 g), and *fac*-Ir(ppy)$_3$ (3 mol %, 100 mg) were loaded in a 100 mL round-bottom flask which was subjected to evacuation/ flushing with N_2 three times. Then allylcyclopropane sulfonyl chloride (7.5 mmol, 1.355 g) in CH_3CN (50 mL) and H_2O (5 mL) were added to the mixture. The reaction was irradiated with 12 W blue LEDs for 48 hours. After reaction completion, the reaction mixture was extracted with EtOAc, and the organic layers were

dried over anhydrous Na_2SO_4, and concentrated in vacuo. Purification the residue by flash column chromatography on silica gel afforded the desired product **3a** (76 % yield, 1.3203 g).

3. Synthesis of starting materials

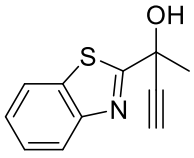


First step: To a solution of trimethylsilylacetylene (5.5 mmol, 1.1 equiv.) in anhydrous THF (11 mL, 0.5 M) was slowly added *n*-butyllithium (5.5 mmol, 1.1 equiv.) at -78 °C, then the mixture was stirred for 30 min at room temperature. Then ketone (5.0 mmol, 1.0 equiv.) in anhydrous THF (5 mL) was added dropwise via syringe and the mixture was stirred at room temperature for another 1 h. After reaction completion, the mixture was quenched by H_2O and extracted with EtOAc for three times. The combined organic extracts were washed by brine, dried over $MgSO_4$, filtered, concentrated, and purified by flash column chromatography on silica gel to give **S1**.

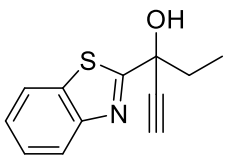
Second Step: A solution of **S1** (4.0 mmol, 1.0 equiv.) in CH_3OH (8 mL,0.5 M) was added K_2CO_3 (4.8 mmol, 1.2 equiv.) and stirred for 1 h at room temperature. After reaction completion, the crude reaction mixture was extracted with EtOAc, and the organic layers were dried over anhydrous Na_2SO_4, and concentrated in vacuo. Purification the residue by flash column chromatography on silica gel afforded the corresponding propargyl alcohol **1** or **4**.

4. Characterization of new starting materials and products

a. Starting materials

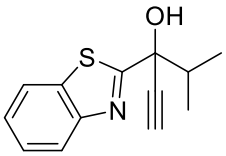


1a: yellow solid, m.p. 162-163 °C. ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.07-8.03 (m, 1H), 7.91-7.87 (m, 1H), 7.52-7.46 (m, 1H), 7.43-7.37 (m, 1H), 3.94 (br, 1H), 2.73 (s, 1H), 2.02 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 174.9, 152.7, 135.5, 126.3, 125.5, 123.5, 121.8, 84.9, 74.0, 68.9, 31.5. FT-IR: ν (cm^{-1}) 3232, 2212, 1651, 1633, 1364, 1155, 1036, 760. HRMS [ESI] calcd for $C_{11}H_{10}NOS$ $[M+H]^+$ 204.0478, found 204.0477.

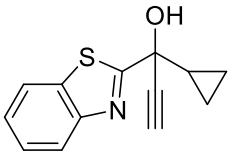


1b: yellow solid, m.p. 154-155 °C. ^{1}H NMR (500 MHz, $CDCl_3$) δ 8.05 (d, *J* = 8.0 Hz, 1H), 7.89 (d, *J* = 8.0 Hz, 1H), 7.52-7.47 (m, 1H), 7.43-7.38 (m, 1H), 3.80 (br, 1H), 2.74 (s, 1H), 2.31-2.16 (m, 2H), 1.11 (t, *J* = 7.0 Hz, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 174.4,

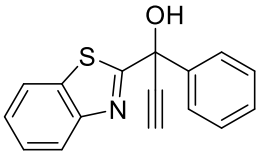
152.6, 135.5, 126.3, 125.4, 123.4, 121.8, 83.9, 74.8, 72.5, 37.2, 8.3. FT-IR: ν (cm^{-1}) 3242, 2102, 1651, 1633, 1315, 1180, 1057, 758. HRMS [ESI] calcd for $C_{12}H_{12}NOS$ $[M+H]^+$ 218.0643, found 218.0638.



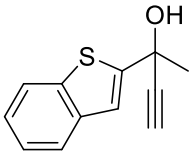
1c: yellow solid, m.p. 122-123 °C. ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.05 (d, *J* = 8.0 Hz, 1H), 7.88 (d, *J* = 8.0 Hz, 1H), 7.52-7.46 (m, 1H), 7.43-7.37 (m, 1H), 3.79 (s, 1H), 2.74 (s, 1H), 2.50-2.39 (m, 1H), 1.14 (d, *J* = 6.8 Hz, 3H), 1.04 (d, *J* = 6.4 Hz, 3H); ^{13}C NMR (125 MHz, $CDCl_3$) δ 174.5, 152.4, 135.5, 126.2, 125.4, 123.4, 121.8, 83.4, 75.6, 75.4, 40.2, 17.6, 16.5. FT-IR: ν (cm^{-1}) 3271, 2972, 2116, 1633, 1506, 1381, 1139, 1005. HRMS [ESI] calcd for $C_{13}H_{14}NOS$ $[M+H]^+$ 232.0791, found 232.0792.



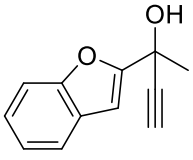
1d: yellow solid, m.p. 157-158 °C. ^{1}H NMR (400 MHz, d_6-DMSO) δ 8.08 (d, *J* = 7.6 Hz, 1H), 8.00 (d, *J* = 8.0 Hz, 1H), 7.54-7.48 (m, 1H), 7.46-7.40 (m, 1H), 7.07 (s, 1H), 3.64 (s, 1H), 1.60-1.52 (m, 1H), 0.71-0.63 (m, 2H), 0.59-0.52 (m, 1H), 0.49-0.42 (m, 1H); ^{13}C NMR (100 MHz, d_6-DMSO) δ 177.4, 153.4, 135.0, 126.6, 125.6, 123.3, 122.7, 83.9, 76.6, 71.4, 22.7, 2.8, 2.2. FT-IR: ν (cm^{-1}) 3289, 3065, 2116, 1636, 1450, 1386, 1155, 1051. HRMS [ESI] calcd for $C_{13}H_{12}NOS$ $[M+H]^+$ 230.0634, found 230.0643.



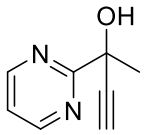
1e: yellow solid, m.p. 172-173 °C. ^{1}H NMR (500 MHz, d_6-DMSO) δ 8.08-8.05 (m, 1H), 7.98 (br, 1H), 7.96-7.93 (m, 1H), 7.75-7.71 (m, 2H), 7.49-7.45 (m, 1H), 7.43-7.36 (m, 3H), 7.33-7.28 (m, 1H), 3.98 (s, 1H); ^{13}C NMR (125 MHz, d_6-DMSO) δ 177.4, 153.4, 143.4, 135.1, 128.7, 128.6, 126.7, 126.4, 125.7, 123.3, 122.8, 85.2, 78.2, 72.7. FT-IR: ν (cm^{-1}) 3564, 3417, 2120, 1633, 1489, 1157, 1067, 984. HRMS [ESI] calcd for $C_{16}H_{11}NNaOS$ $[M+Na]^+$ 288.0454, found 288.0453.



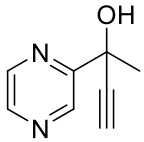
1f: yellow solid, m.p. 50-51 °C. ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.83-7.79 (m, 1H), 7.75-7.72 (m, 1H), 7.44 (s, 1H), 7.38-7.30 (m, 2H), 2.82 (br, 1H), 2.75 (s, 1H), 1.96 (s, 3H); ^{13}C NMR (125 MHz, $CDCl_3$) δ 150.1, 139.7, 139.2, 124.6, 124.5, 123.9, 122.5, 120.7, 86.0, 73.2, 67.6, 32.8. FT-IR: ν (cm^{-1}) 3291, 2985, 2116, 1653, 1369, 1155, 1069, 748. HRMS [ESI] calcd for $C_{12}H_{11}OS$ $[M+H]^+$ 203.0525, found 203.0519.



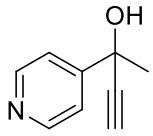
1g: yellow solid, m.p. 53-54 °C. ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.58-7.55 (m, 1H), 7.52-7.48 (m, 1H), 7.33-7.28 (m, 1H), 7.27-7.22 (m, 1H), 6.81 (s, 1H), 2.79 (br, 1H), 2.68 (s, 1H), 1.95 (s, 3H); ^{13}C NMR (125 MHz, $CDCl_3$) δ 158.1, 155.1, 127.8, 124.7, 123.0, 121.4, 111.5, 102.7, 84.7, 72.9, 65.2, 28.6. FT-IR: ν (cm^{-1}) 3292, 2993, 2120, 1651, 1454, 1373, 1141, 752. HRMS [ESI] calcd for $C_{12}H_{10}KO_2$ $[M+K]^+$ 225.0312, found 225.0314.



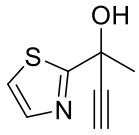
1h: yellow solid, m.p. 65-66 °C. ^{1}H NMR (500 MHz, $CDCl_3$) δ 8.80 (d, *J* = 5.0 Hz, 2H), 7.30 (dd, *J* = 5.0 Hz, 5.0 Hz, 1H), 5.13 (br, 1H), 2.54 (s, 1H), 1.90 (s, 3H); ^{13}C NMR (125 MHz, $CDCl_3$) δ 169.8, 157.4, 120.1, 86.4, 71.8, 69.6, 30.0. FT-IR: ν (cm^{-1}) 3291, 2986, 2112, 1634, 1508, 1404, 1153, 1086. HRMS [ESI] calcd for $C_8H_9N_2O$ $[M+H]^+$ 149.0709, found 149.0709.



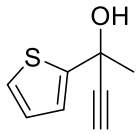
1i: yellow oil. ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.80 (s, 1H), 8.57-8.50 (m, 2H), 4.68 (br, 1H), 2.64 (s, 1H), 1.85 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 157.3, 143.9, 142.5, 142.3, 85.7, 73.3, 68.0, 31.5. FT-IR: ν (cm^{-1}) 3562, 3332, 2114, 1634, 1506, 1339, 1147, 1107. HRMS [ESI] calcd for $C_8H_9N_2O$ $[M+H]^+$ 149.0709, found 149.0705.



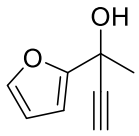
1j: yellow solid, m.p. 149-150 °C. ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.57-8.53 (m, 2H), 7.57-7.54 (m, 2H), 3.70 (br, 1H), 2.68 (s, 1H), 1.76 (s, 3H); ^{13}C NMR (100 MHz, d_6-DMSO) δ 155.3, 150.0, 120.4, 87.9, 75.3, 67.6, 33.3. FT-IR: ν (cm^{-1}) 3235, 1867, 1634, 1506, 1456, 1361, 1161, 1007. HRMS [ESI] calcd for $C_9H_{10}NO$ $[M+H]^+$ 148.0757, found 148.0752.



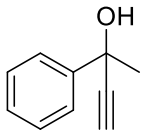
1k: yellow solid, m.p. 92-93 °C. ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.73 (s, 1H), 7.30 (s, 1H), 4.47 (br, 1H), 2.67 (s, 1H), 1.95 (s, 3H); ^{13}C NMR (125 MHz, $CDCl_3$) δ 174.6, 142.5, 119.9, 85.3, 73.4, 68.4, 31.7. FT-IR: ν (cm^{-1}) 3219, 2797, 2112, 1634, 1506, 1368, 1144, 1061. HRMS [ESI] calcd for C_7H_8NOS $[M+H]^+$ 154.0321, found 154.0320.



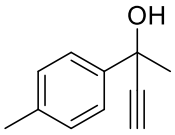
1l: yellow oil. ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.27-7.24 (m, 1H), 7.21-7.19 (m, 1H), 6.95 (dd, *J* = 5.0 Hz, 4.0 Hz, 1H), 2.71 (br, 1H), 2.68 (s, 1H), 1.90 (s, 3H); ^{13}C NMR (125 MHz, $CDCl_3$) δ 149.7, 126.7, 125.3, 124.2, 86.4, 72.6, 67.2, 33.0. FT-IR: ν (cm^{-1}) 3291, 2988, 2114, 1637, 1369, 1236, 1136, 926. HRMS [ESI] calcd for C_8H_7S $[M+H-H_2O]^+$ 135.0263, found 135.0260.



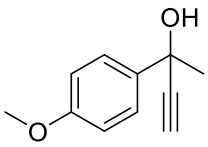
1m: yellow oil. ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.41-7.39 (m, 1H), 6.42-6.39 (m, 1H), 6.35-6.32 (m, 1H), 2.65 (br, 1H), 2.61 (s, 1H), 1.85 (s, 3H); ^{13}C NMR (125 MHz, $CDCl_3$) δ 155.7, 142.6, 110.3, 106.0, 85.1, 72.2, 64.7, 28.5. FT-IR: ν (cm^{-1}) 3294, 2993, 2118, 1633, 1373, 1339, 1159, 1010. HRMS [ESI] calcd for C_8H_7O $[M+H-H_2O]^+$ 119.0491, found 119.0486.



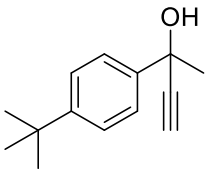
1n white solid, m.p. 47-48 °C. ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.69-7.65 (m, 2H), 7.41-7.35 (m, 2H), 7.34-7.29 (m, 1H), 2.68 (s, 1H), 2.44 (br, 1H), 1.80 (s, 3H); ^{13}C NMR (125 MHz, $CDCl_3$) δ 145.0, 128.4, 127.9, 124.9, 87.2, 73.1, 69.9, 33.1. FT-IR: ν (cm^{-1}) 3294, 2987, 2114, 1635, 1447, 1225, 1091, 764. HRMS [ESI] calcd for $C_{10}H_9$ $[M+H-H_2O]^+$ 129.0699, found 129.0695.



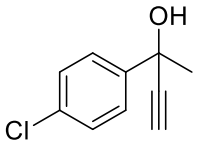
1o: white solid, m.p. 30-31 °C. ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.58-7.53 (m, 2H), 7.20-7.17 (m, 2H), 2.67 (s, 1H), 2.43 (br, 1H), 2.36 (s, 3H), 1.79 (s, 3H); ^{13}C NMR (125 MHz, $CDCl_3$) δ 142.2, 137.6, 129.0, 124.8, 87.4, 72.9, 69.7, 33.0, 21.1. FT-IR: ν (cm^{-1}) 3291, 2986, 2012, 1634, 1508, 1339, 1153, 1086. HRMS [ESI] calcd for $C_{11}H_{12}KO$ $[M+K]^+$ 199.0520, found 199.0520.



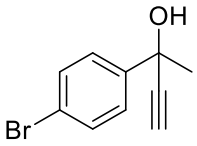
1p: white solid, m.p. 39-40 °C. ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.60-7.56 (m, 2H), 6.90-6.87 (m, 2H), 3.81 (s, 3H), 2.67 (s, 1H), 2.53-2.50 (m, 1H), 1.77 (s, 3H); ^{13}C NMR (125 MHz, $CDCl_3$) δ 159.2, 137.2, 126.2, 113.6, 87.4, 73.0, 69.5, 55.4, 33.0. FT-IR: ν (cm^{-1}) 3294, 2986, 2112, 1611, 1508, 1252, 1179, 1030. HRMS [ESI] calcd for $C_{11}H_{12}NaO$ $[M+Na]^+$ 199.0730, found 199.0730.



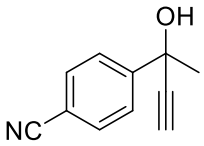
1q: white solid, m.p. 73-74 °C. ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.52-7.49 (m, 2H), 7.33-7.29 (m, 2H), 2.58 (s, 1H), 2.37 (br, 1H), 1.70 (s, 3H), 1.24 (s, 9H); ^{13}C NMR (125 MHz, $CDCl_3$) δ 150.9, 142.0, 125.3, 124.6, 87.4, 72.9, 69.7, 34.5, 32.9, 31.4. FT-IR: ν (cm^{-1}) 3305, 2964, 2114, 1634, 1506, 1361, 1157, 1086. HRMS [ESI] calcd for $C_{14}H_{18}NaO$ $[M+Na]^+$ 225.1250, found 225.1241.



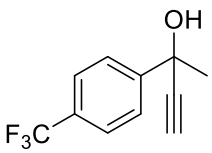
1r: yellow solid, m.p. 39-40 °C. ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.61-7.56 (m, 2H), 7.35-7.31 (m, 2H), 2.69 (s, 1H), 2.56 (br, 1H), 1.76 (s, 3H); ^{13}C NMR (125 MHz, $CDCl_3$) δ 143.6, 133.7, 128.5, 126.5, 86.8, 73.5, 69.4, 33.2. FT-IR: ν (cm^{-1}) 3298, 2988, 2114, 1636, 1489, 1396, 1153, 1094. HRMS [EI] calcd for $C_{10}H_9ClO$ $[M]^+$ 180.0337, found 180.0339.



1s: white solid, m.p. 42-43 °C. ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.54-7.50 (m, 2H), 7.50-7.46 (m, 2H), 2.68 (s, 1H), 2.59 (br, 1H), 1.75 (s, 3H); ^{13}C NMR (125 MHz, $CDCl_3$) δ 144.1, 131.4, 126.8, 121.9, 86.7, 73.5, 69.5, 33.2. FT-IR: ν (cm^{-1}) 3296, 2986, 2114, 1636, 1487, 1394, 1152, 1086. HRMS [ESI] calcd for $C_{10}H_{10}BrO$ $[M+H]^+$ 224.9910, found 224.9902.

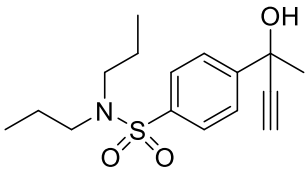


1t: yellow oil. ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.78-7.74 (m, 2H), 7.66-7.63 (m, 2H), 2.72 (s, 1H), 2.71 (br, 1H), 1.76 (s, 3H); ^{13}C NMR (125 MHz, $CDCl_3$) δ 150.2, 132.3, 125.8, 118.7, 111.6, 86.1, 74.0, 69.4, 33.3. FT-IR: ν (cm^{-1}) 3294, 2988, 2232, 2114, 1609, 1404, 1368, 1159. HRMS [ESI] calcd for $C_{11}H_9NNaO$ $[M+Na]^+$ 194.0576, found 194.0570.

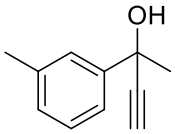


1u: yellow solid, m.p. 48-49 °C. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.80-7.75 (m, 2H), 7.65-7.60 (m, 2H), 2.71 (s, 1H), 2.64 (s, 1H), 1.78 (s, 3H); ^{13}C NMR (125 MHz, $CDCl_3$) δ 148.9, 130.1 (q, J = 32.1 Hz), 125.4, 125.4 (q, J = 3.8 Hz), 124.1 (q, J = 270.4 Hz), 86.5, 73.7, 69.6, 33.3; ^{19}F NMR (376 MHz, $CDCl_3$) δ -62.5. FT-IR: ν (cm^{-1}) 3306,

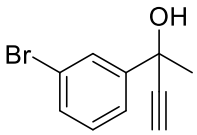
2989, 2118, 1620, 1414, 1371, 1165, 1070. HRMS [ESI] calcd for $C_{11}H_{10}F_3O$ $[M+H]^+$ 215.0678, found 215.0683.



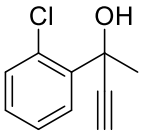
1v: yellow solid, m.p. 84-85 °C. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.78-7.75 (m, 4H), 3.05 (t, *J* = 7.6 Hz, 4H), 2.76 (s, 1H), 2.71 (s, 1H), 1.77 (s, 3H), 1.60-1.50 (m, 4H), 0.86 (t, *J* = 7.6 Hz, 6H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 149.4, 139.4, 127.2, 125.6, 86.4, 73.8, 69.5, 50.2, 33.4, 22.1, 11.2. FT-IR: ν (cm^{-1}) 3308, 2967, 2345, 1636, 1489, 1361, 1155, 1094. HRMS [ESI] calcd for $C_{16}H_{24}NO_3S$ $[M+H]^+$ 310.1471, found 310.1466.



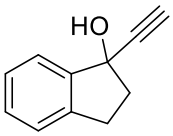
1w: colorless oil. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.50-7.44 (m, 2H), 7.29-7.24 (m, 1H), 7.15-7.10 (m, 1H), 2.67 (s, 1H), 2.42 (br, 1H), 2.39 (s, 3H), 1,79 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 145.0, 138.1, 128.6, 128.3, 125.5, 121.9, 87.4, 73.0, 69.8, 33.1, 21.6. FT-IR: ν (cm^{-1}) 3294, 2986, 2113, 1607, 1487, 1368, 1153, 1086. HRMS [ESI] calcd for $C_{11}H_{12}KO$ $[M+K]^+$ 199.0520, found 199.0515.



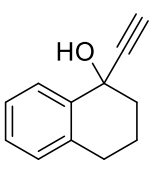
1x: colorless oil. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.83-7.80 (m, 1H), 7.60-7.56 (m, 1H), 7.46-7.41 (m, 1H), 7.27-7.21 (m, 1H), 2.70 (s, 1H), 2.54 (s, 1H), 1.77 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 147.3, 130.9, 130.0, 128.2, 123.6, 122.5, 86.6, 73.6, 69.4, 33.2. FT-IR: ν (cm^{-1}) 3296, 2986, 2115, 1636, 1472, 1338, 1155, 1074. HRMS [ESI] calcd for $C_{10}H_{10}BrO$ $[M+H]^+$ 224.9910, found 224.9907.



1y: yellow oil. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.80-7.76 (m, 1H), 7.42-7.37 (m, 1H), 7.31-7.21 (m, 2H), 3.31 (br, 1H), 2.64 (s, 1H), 1.95 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 140.7, 131.8, 131.4, 129.2, 127.0, 126.8, 86.2, 72.9, 68.9, 29.6. FT-IR: ν (cm^{-1}) 3296, 2986, 2114, 1636, 1431, 1371, 1155, 1097. HRMS [EI] calcd for $C_{10}H_9ClO$ $[M]^+$ 180.0337, found 180.0338.

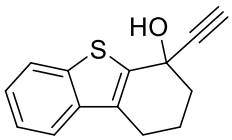


4a: white solid, m.p. 63-64 °C. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.54-7.49 (m, 1H), 7.31-7.23 (m, 3H), 3.16-3.06 (m, 1H), 2.96-2.86 (m, 1H), 2.63 (s, 1H), 2.61-2.51 (m, 1H), 2.47-2.39 (m, 1H), 2.37 (s, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 145.3, 143.1, 129.2, 127.2, 125.1, 123.2, 85.9, 76.2, 73.0, 43.1, 29.6. FT-IR: ν (cm^{-1}) 3291, 3022, 2988, 1634, 1474, 1338, 1157, 1042. HRMS [ESI] calcd for $C_{11}H_{10}KO$ $[M+K]^+$ 197.0363, found 197.0370.

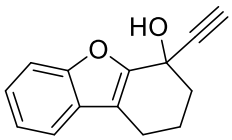


4b: yellow solid, m.p. 46-47 °C. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.80-7.75 (m, 1H), 7.28-7.20 (m, 2H), 7.13-7.08 (m, 1H), 2.89-2.75 (m, 2H), 2.60 (s, 1H), 2.36 (s, 1H), 2.25-2.20 (m, 2H), 2.09-1.99 (m, 1H), 1.99-1.88 (m, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 138.6, 136.1, 129.2, 128.3, 127.7, 126.6, 88.1, 72.4, 67.7, 38.9, 29.2, 19.1. FT-IR: ν (cm^{-1}) 3289, 2940, 2106,

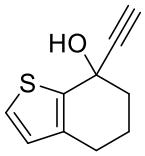
1636, 1489, 1362, 1161, 1086. HRMS [ESI] calcd for $C_{12}H_{12}NaO$ $[M+Na]^+$ 195.0780, found 195.0783.



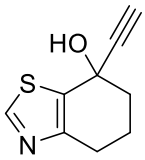
4c: white solid, m.p. 77-78 °C. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.85-7.79 (m, 1H), 7.65-7.59 (m, 1H), 7.40-7.31 (m, 2H), 2.86-2.73 (m, 2H), 2.68 (s, 1H), 2.63 (s, 1H), 2.40-2.26 (m, 2H), 2.20-2.06 (m, 2H); ^{13}C NMR (125 MHz, $CDCl_3$) δ 139.3, 139.3, 138.7, 132.1, 125.1, 124.2, 122.8, 121.9, 86.4, 73.2, 66.2, 39.7, 23.5, 19.3. FT-IR: ν (cm^{-1}) 3291, 2932, 2114, 1634, 1471, 1373, 1153, 1047. HRMS [ESI] calcd for $C_{14}H_{11}S$ $[M+H-H_2O]^+$ 211.0576, found 211.0571.



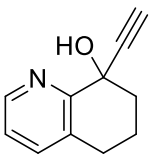
4d: yellow oil. ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.52-7.46 (m, 2H), 7.33-7.28 (m, 1H), 7.26-7.21 (m, 1H), 2.77 (s, 1H), 2.76-2.69 (m, 1H), 2.65 (s, 1H), 2.69-2.62 (m, 1H), 2.37-2.26 (m, 2H), 2.10-1.97 (m, 2H); ^{13}C NMR (125 MHz, $CDCl_3$) δ 154.7, 151.2, 127.7, 124.9, 122.7, 119.8, 115.8, 111.7, 84.4, 73.2, 64.0, 39.5, 20.6, 19.9. FT-IR: ν (cm^{-1}) 3291, 2947, 2114, 1634, 1452, 1250, 1134, 970. HRMS [ESI] calcd for $C_{14}H_{12}NaO_2$ $[M+Na]^+$ 235.0730, found 235.0734.



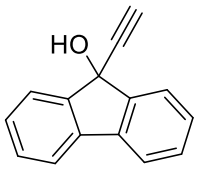
4e: yellow oil. ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.24 (d, *J* = 4.0 Hz, 1H), 6.74 (d, *J* = 4.0 Hz, 1H), 2.74-2.67 (m, 1H), 2.63 (s, 1H), 2.65-2.58 (m, 1H), 2.47 (s, 1H), 2.24-2.20 (m, 2H), 2.08-1.99 (m, 1H), 1.99-1.91 (m, 1H); ^{13}C NMR (125 MHz, $CDCl_3$) δ 138.6, 137.7, 127.2, 125.2, 87.1, 72.4, 65.5, 39.6, 25.4, 19.6. FT-IR: ν (cm^{-1}) 3289, 2936, 2112, 1651, 1454, 1319, 1159, 1089. HRMS [ESI] calcd for $C_{10}H_9S$ $[M+H-H_2O]^+$ 161.0419, found 161.0415.



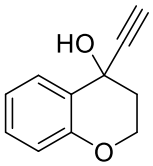
4f: yellow solid, m.p. 101-102 °C. ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.67 (s, 1H), 4.06 (s, 1H), 2.91-2.75 (m, 2H), 2.63 (s, 1H), 2.28-2.15 (m, 2H), 2.12-1.96 (m, 2H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 152.7, 152.6, 133.6, 86.7, 72.9, 65.1, 39.6, 26.4, 19.5. FT-IR: ν (cm^{-1}) 3287, 2949, 2110, 1651, 1454, 1359, 1265, 1085. HRMS [ESI] calcd for $C_9H_{10}NOS$ $[M+H]^+$ 180.0478, found 180.0473.



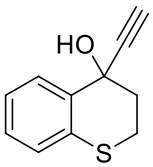
4g: yellow solid, m.p. 91-92 °C. ^{1}H NMR (500 MHz, $CDCl_3$) δ 8.45 (d, *J* = 4.5 Hz, 1H), 7.44 (d, *J* = 7.5 Hz, 1H), 7.16 (dd, *J* = 7.5 Hz, 4.5 Hz, 1H), 4.71 (s, 1H), 2.86-2.81 (m, 2H), 2.55 (s, 1H), 2.47-2.42 (m, 1H), 2.15-2.07 (m, 1H), 2.06-1.97 (m, 2H); ^{13}C NMR (125 MHz, $CDCl_3$) δ 156.8, 147.3, 137.6, 130.6, 123.2, 87. 6, 73.0, 68.0, 36.5, 27.9, 19.2. FT-IR: ν (cm^{-1}) 3286, 2949, 2104, 1573, 1445, 1329, 1169, 1086. HRMS [ESI] calcd for $C_{11}H_{12}NO$ $[M+H]^+$ 174.0914, found 174.0913.



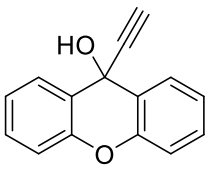
4h: white solid, m.p. 105-106 °C. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.73-7.68 (m, 2H), 7.64-7.59 (m, 2H), 7.44-7.32 (m, 4H), 2.70 (s, 1H), 2.47 (s, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 146.6, 139.1, 129.9, 128.7, 124.3, 120.3, 83.9, 74.6, 71.5. FT-IR: ν (cm^{-1}) 3290, 2989, 2112, 1633, 1506, 1365, 1158, 1059. HRMS [ESI] calcd for $C_{15}H_{11}O$ $[M+H]^+$ 207.0804, found 207.0810.



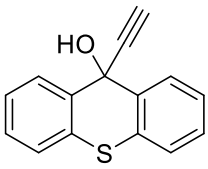
4i: white solid, m.p. 40-41 °C. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.68-7.64 (m, 1H), 7.25-7.20 (m, 1H), 6.98-6.93 (m, 1H), 6.86-6.82 (m, 1H), 4.34-4.29 (m, 2H), 2.71 (s, 1H), 2.64 (s, 1H), 2.41-2.33 (m, 1H), 2.32-2.26 (m, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 153.5, 130.3, 128.2, 124.6, 120.9, 117.3, 86.3, 73.1, 63.6, 62.2, 37.0. FT-IR: ν (cm^{-1}) 3289, 2926, 2117, 1633, 1456, 1373, 1159, 758. HRMS [ESI] calcd for $C_{11}H_{10}NaO_2$ $[M+Na]^+$ 197.0573, found 197.0582.



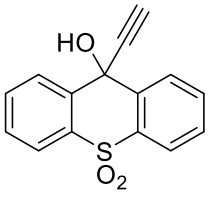
4j: yellow solid, m.p. 54-55 °C. ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.86-7.82 (m, 1H), 7.19-7.15 (m, 1H), 7.13-7.08 (m, 2H), 3.33-3.26 (m, 1H), 3.05-2.99 (m, 1H), 2.68 (s, 1H), 2.59-2.53 (m, 1H), 2.46 (s, 1H), 2.41-1.34 (m, 1H); ^{13}C NMR (125 MHz, $CDCl_3$) δ 134.7, 132.5, 128.8, 128.6, 126.8, 124.6, 86.5, 73.9, 66.4, 37.0, 22.2. FT-IR: ν (cm^{-1}) 3287, 2924, 2112, 1636, 1471, 1173, 1080, 1036. HRMS [ESI] calcd for $C_{11}H_{10}KOS$ $[M+K]^+$ 229.0084, found 229.0086.



4k: yellow solid, m.p. 63-64 °C. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.99-7.95 (m, 2H), 7.44-7.38 (m, 2H), 7.27-7.18 (m, 4H), 2.92 (s, 1H), 2.75 (s, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 149.6, 130.2, 128.6, 123.7, 123.3, 116.9, 85.1, 75.8, 64.0. FT-IR: ν (cm^{-1}) 3291, 2118, 1603, 1450, 1317, 1242, 1153, 756. HRMS [ESI] calcd for $C_{15}H_{10}NaO_2$ $[M+Na]^+$ 245.0573, found 245.0579.

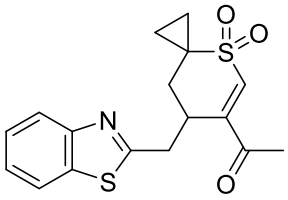


4l: yellow solid, m.p. 96-97 °C. ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.17-8.11 (m, 2H), 7.54-7.48 (m, 2H), 7.40-7.29 (m, 4H), 2.96 (s, 1H), 2.93 (s, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 136.0, 131.5, 128.2, 127.0, 126.7, 126.6, 82.7, 76.7, 70.5. FT-IR: ν (cm^{-1}) 3289, 2926, 2114, 1634, 1456, 1267, 1159, 1063. HRMS [ESI] calcd for $C_{15}H_{10}NaOS$ $[M+Na]^+$ 261.0345, found 261.0346.

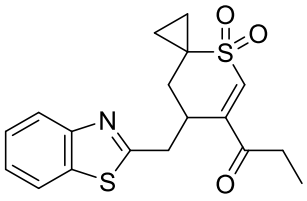


4m: yellow solid, m.p. 211-212 °C. ^{1}H NMR (400 MHz, d_6-DMSO) δ 8.17-8.13 (m, 2H), 8.10-8.06 (m, 2H), 7.86-7.80 (m, 2H), 7.75-7.68 (m, 2H), 3.76 (s, 1H), 3.37 (s, 1H); ^{13}C NMR (100 MHz, d_6-DMSO) δ 142.3, 135.4, 134.0, 130.0, 127.4, 123.7, 85.1, 77.6, 64.2. FT-IR: ν (cm^{-1}) 3258, 2920, 2114, 1445, 1292, 1163, 1136, 1063. HRMS [ESI] calcd for $C_{15}H_{14}NO_3S$ $[M+NH_4]^+$ 288.0689, found 288.0687.

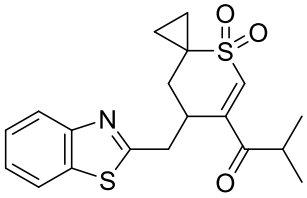
b. Products



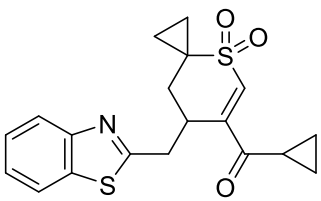
3a: yellow solid, m.p. 144-145 °C. ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.95 (d, *J* = 8.5 Hz, 1H), 7.84 (d, *J* = 8.0 Hz, 1H), 7.48-7.43 (m, 1H), 7.39-7.34 (m, 1H), 7.15 (s, 1H), 3.59-3.53 (m, 1H), 3.37-3.31 (m, 1H), 3.29-3.24 (m, 1H), 2.52 (dd, *J* = 15.5 Hz, 5.0 Hz, 1H), 2.46 (s, 3H), 2.08 (dd, *J* = 15.5 Hz, 5.0 Hz, 1H), 1.72-1.65 (m, 1H), 1.48-1.40 (m, 2H), 0.86-0.79 (m, 1H); ^{13}C NMR (125 MHz, $CDCl_3$) δ 197.3, 167.5, 153.0, 147.6, 135.4, 135.3, 126.2, 125.3, 122. 9, 121.7, 35.9, 35.3, 34.2, 31.0, 26.5, 13.3, 8.4. FT-IR: ν (cm^{-1}) 2924, 1688, 1435, 1362, 1296, 1211, 1125, 763. HRMS [ESI] calcd for $C_{17}H_{18}NO_3S_2$ $[M+H]^+$ 348.0723, found 348.0732.



3b: yellow solid, m.p. 106-107 °C. ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.95 (d, *J* = 8.0 Hz, 1H), 7.85 (d, *J* = 8.0 Hz, 1H), 7.48-7.44 (m, 1H), 7.40-7.35 (m, 1H), 7.11 (s, 1H), 3.61-3.55 (m, 1H), 3.37-3.30 (m, 1H), 3.28-3.23 (m, 1H), 2.90-2.81 (m, 1H), 2.78-2.69 (m, 1H), 2.52 (dd, *J* = 15.5 Hz, 5.0 Hz, 1H), 2.09 (dd, *J* = 15.5 Hz, 5.0 Hz, 1H), 1.72-1.65 (m, 1H), 1.48-1.41 (m, 2H), 1.14 (t, *J* = 7.5 Hz, 3H), 0.84-0.80 (m, 1H); ^{13}C NMR (125 MHz, $CDCl_3$) δ 200.1, 167. 6, 153.0, 147.5, 135.3, 134.2, 126.2, 125.3, 122.9, 121.7, 36.0, 35.3, 34.5, 31.8, 31.1, 13.2, 8.4, 7.9. FT-IR: ν (cm^{-1}) 2922, 1668, 1514, 1435, 1298, 1169, 1125, 762. HRMS [ESI] calcd for $C_{18}H_{20}NO_3S_2$ $[M+H]^+$ 362.0879, found 362.0877.

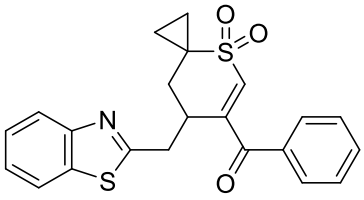


3c: yellow solid, m.p. 125-126 °C. ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.96 (d, *J* = 8.0 Hz, 1H), 7.85 (d, *J* = 8.0 Hz, 1H), 7.49-7.44 (m, 1H), 7.40-7.35 (m, 1H), 7.11 (s, 1H), 3.64-3.57 (m, 1H), 3.31-3.18 (m, 3H), 2.50 (dd, *J* = 15.5 Hz, 5.0 Hz, 1H), 2.10 (dd, *J* = 15.5 Hz, 5.0 Hz, 1H), 1.73-1.65 (m, 1H), 1.47-1.40 (m, 2H), 1.19 (d, *J* = 6.0 Hz, 3H), 1.18 (d, *J* = 6.5 Hz, 3H), 0.85-0.80 (m, 1H); ^{13}C NMR (125 MHz, $CDCl_3$) δ 203.9, 167.5, 153.0, 147.1, 135.3, 133.8, 126.2, 125.3, 122.9, 121.7, 36.0, 35.7, 35.3, 34.6, 30.9, 19.4, 18.5, 13.0, 8.5. FT-IR: ν (cm^{-1}) 2928, 2359, 1688, 1514, 1435, 1298, 1196, 1123. HRMS [ESI] calcd for $C_{19}H_{22}NO_3S_2$ $[M+H]^+$ 376.1036, found 376.1044.

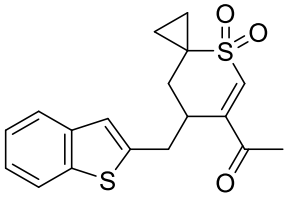


3d: yellow solid, m.p. 153-154 °C. ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.95 (d, *J* = 8.5 Hz, 1H), 7.84 (d, *J* = 8.0 Hz, 1H), 7.48-7.43 (m, 1H), 7.39-7.34 (m, 1H), 7.24 (s, 1H), 3.63-3.57 (m, 1H), 3.34-3.25 (m, 2H), 2.44 (dd, *J* = 15.5 Hz, 5.0 Hz, 1H), 2.37-2.31 (m, 1H), 2.19 (dd, *J* = 15.5 Hz, 5.5 Hz, 1H), 1.70-1.64 (m, 1H), 1.47-1.41 (m, 1H), 1.38-1.32 (m, 1H), 1.20-1.13 (m, 2H), 1.12-1.08 (m, 1H), 1.07-1.00 (m, 1H), 0.87-0.81 (m, 1H); ^{13}C NMR (125 MHz, $CDCl_3$) δ 200.0, 167.5, 153.0, 149.0, 135.3, 133.8, 126.2, 125.3, 122.9, 121.7, 36.1, 35.5, 34.8, 31.4, 18.2, 13.6, 12.7, 12.4, 8.9. FT-IR: ν (cm^{-1}) 2922, 2359,

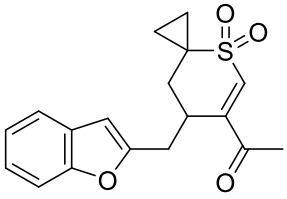
1688, 1506, 1456, 1298, 1163, 1125. HRMS [ESI] calcd for $C_{19}H_{20}NO_3S_2$ $[M+H]^+$ 374.0879, found 374.0877.



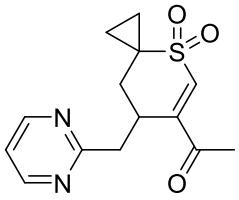
3e: white solid, m.p. 173-174 °C. ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.91-7.86 (m, 3H), 7.81 (d, *J* = 8.0 Hz, 1H), 7.66-7.61 (m, 1H), 7.52-7.47 (m, 2H), 7.46-7.41 (m, 1H), 7.38-7.33 (m, 1H), 6.76 (s, 1H), 3.83-3.76 (m, 1H), 3.44 (dd, *J* = 15.0 Hz, 9.0 Hz, 1H), 3.33 (dd, *J* = 15.0 Hz, 4.0 Hz, 1H), 2.65 (dd, *J* = 15.0 Hz, 8.0 Hz, 1H), 2.25 (dd, *J* = 15.0 Hz, 5.0 Hz, 1H), 1.70-1.64 (m, 1H), 1.50-1.43 (m, 1H), 1.23-1.17 (m, 1H), 0.97-0.91 (m, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 194.2, 166.7, 153.1, 148.3, 135.2, 135.0, 134.4, 134.2, 130.2, 128.9, 126.2, 125.3, 122.9, 121.6, 36.3, 36.0, 35.9, 32.5, 11.1, 10.2. FT-IR: ν (cm^{-1}) 2922, 1668, 1446, 1300, 1273, 1236, 1128, 762. HRMS [ESI] calcd for $C_{22}H_{20}NO_3S_2$ $[M+H]^+$ 410.0879, found 410.0878.



3f: yellow solid, m.p. 151-152 °C. ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.77 (d, *J* = 8.0 Hz, 1H), 7.69 (d, *J* = 7.5 Hz, 1H), 7.36-7.27 (m, 2H), 7.12 (s, 1H), 7.05 (s, 1H), 3.42-3.36 (m, 1H), 3.17 (dd, *J* = 15.0 Hz, 3.0 Hz, 1H), 3.00 (dd, *J* = 15.0 Hz, 11.0 Hz, 1H), 2.43 (s, 3H), 2.39 (dd, *J* = 15.5 Hz, 5.0 Hz, 1H), 2.12 (dd, *J* = 15.5 Hz, 5.5 Hz, 1H), 1.73-1.66 (m, 1H), 1.45-1.39 (m, 1H), 1.17-1.11 (m, 1H), 0.81-0.76 (m, 1H); ^{13}C NMR (125 MHz, $CDCl_3$) δ 197.4, 148.4, 141.6, 139.8, 139.5, 134.8, 124.5, 124.2, 123.1, 122.8, 122.3, 35.5, 35.4, 33.3, 31.1, 26.6, 12.9, 8.7. FT-IR: ν (cm^{-1}) 2920, 2359, 1688, 1435, 1296, 1221, 1125, 750. HRMS [ESI] calcd for $C_{18}H_{19}O_3S_2$ $[M+H]^+$ 347.0770, found 347.0761.

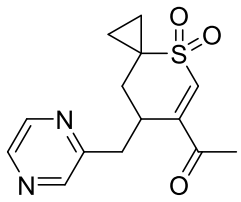


3g: white solid, m.p. 109-110 °C. ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.49 (d, *J* = 7.5 Hz, 1H), 7.41 (d, *J* = 8.0 Hz, 1H), 7.25-7.18 (m, 2H), 7.08 (s, 1H), 6.47 (s, 1H), 3.52-3.46 (m, 1H), 3.06-2.95 (m, 2H), 2.42 (s, 3H), 2.37 (dd, *J* = 15.5 Hz, 5.0 Hz, 1H), 2.16 (dd, *J* = 15.5 Hz, 5.5 Hz, 1H), 1.71-1.65 (m, 1H), 1.46-1.40 (m, 1H), 1.22-1.16 (m, 1H), 0.86-0.80 (m, 1H); ^{13}C NMR (125 MHz, $CDCl_3$) δ 197.4, 154.9, 154.8, 148.5, 134.7, 128.3, 124.0, 122.9, 120.6, 111.0, 104.7, 35.5, 33.4, 31.7, 31.1, 26.5, 12.6, 8.9. FT-IR: ν (cm^{-1}) 2924, 2357, 1694, 1454, 1362, 1298, 1211, 1125. HRMS [ESI] calcd for $C_{18}H_{19}O_4S$ $[M+H]^+$ 331.0999, found 331.0992.

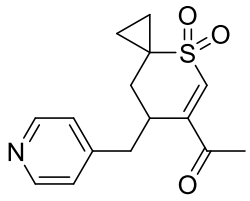


3h: yellow solid, m.p. 142-143 °C. ^{1}H NMR (500 MHz, $CDCl_3$) δ 8.64 (d, *J* = 4.0 Hz, 2H), 7.17-7.13 (m, 1H), 7.02 (s, 1H), 3.68-3.61 (m, 1H), 3.22 (dd, *J* = 14.0 Hz, 10.0 Hz, 1H), 3.11-3.05 (m, 1H), 2.43 (s, 3H), 2.38 (dd, *J* = 15.0 Hz, 4.5 Hz, 1H), 1.95 (dd, *J* = 15.0 Hz, 5.0 Hz, 1H), 1.64-1.57 (m, 1H), 1.42-1.35 (m, 1H), 1.30-1.23 (m, 1H), 0.82-0.75 (m, 1H); ^{13}C NMR (125 MHz, $CDCl_3$) δ 197.6, 168.0, 157.1, 149.4, 133.9, 119.2, 41.1, 35.5, 33.4, 31.6, 26.6, 12.5, 8.8. FT-

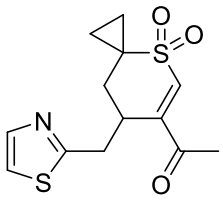
IR: ν (cm^{-1}) 2922, 2359, 1694, 1564, 1423, 1294, 1213, 1125. HRMS [ESI] calcd for $C_{14}H_{17}N_2O_3S$ $[M+H]^+$ 293.0954, found 293.0944.



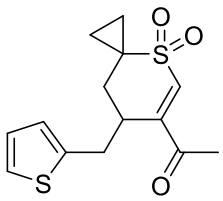
3i: yellow solid, m.p. 70-71 °C. ^{1}H NMR (500 MHz, $CDCl_3$) δ 8.49 (s, 1H), 8.48-8.46 (m, 1H), 8.45-8.43 (m, 1H), 7.09 (s, 1H), 3.50-3.44 (m, 1H), 3.07-2.96 (m, 2H), 2.45 (s, 3H), 2.34 (dd, *J* = 15.5 Hz, 5.0 Hz, 1H), 2.00 (dd, *J* = 15.5 Hz, 5.5 Hz, 1H), 1.69-1.63 (m, 1H), 1.45-1.39 (m, 1H), 1.37-1.31 (m, 1H), 0.85-0.79 (m, 1H); ^{13}C NMR (125 MHz, $CDCl_3$) δ 197.5, 154.3, 148.6, 145.1, 143.9, 143.1, 134.7, 36.8, 35.4, 33.9, 31.1, 26.5, 12.8, 8.7. FT-IR: ν (cm^{-1}) 2920, 1688, 1506, 1456, 1294, 1215, 1125, 1018. HRMS [ESI] calcd for $C_{14}H_{17}N_2O_3S$ $[M+H]^+$ 293.0954, found 293.0960.



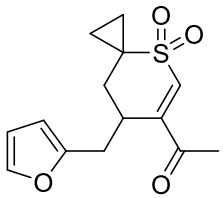
3j: yellow solid, m.p. 67-68 °C. ^{1}H NMR (500 MHz, $CDCl_3$) δ 8.54 (d, *J* = 4.5 Hz, 2H), 7.15 (d, *J* = 5.0 Hz, 2H), 7.13 (s, 1H), 3.37-3.30 (m, 1H), 2.99 (dd, *J* = 13.5 Hz, 3.0 Hz, 1H), 2.55 (dd, *J* = 13.5 Hz, 11.0 Hz, 1H), 2.44 (s, 3H), 2.24 (dd, *J* = 15.5 Hz, 5.0 Hz, 1H), 1.90 (dd, *J* = 15.5 Hz, 5.5 Hz, 1H), 1.72-1.66 (m, 1H), 1.44-1.38 (m, 1H), 1.04-0.98 (m, 1H), 0.79-0.72 (m, 1H); ^{13}C NMR (125 MHz, $CDCl_3$) δ 197.4, 150.2, 148.5, 147.5, 135.0, 124.1, 37.6, 35.3, 34.4, 31.2, 26.6, 12.7, 8.9. FT-IR: ν (cm^{-1}) 2922, 1688, 1603, 1506, 1456, 1294, 1213, 1125. HRMS [ESI] calcd for $C_{15}H_{18}NO_3S$ $[M+H]^+$ 292.1002, found 292.1010.



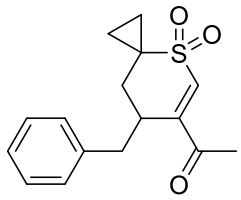
3k: red solid, m.p. 125-126 °C. ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.65 (d, *J* = 3.0 Hz, 1H), 7.24 (d, *J* = 3.0 Hz, 1H), 7.11 (s, 1H), 3.45-3.39 (m, 1H), 3.27 (dd, *J* = 14.5 Hz, 10.0 Hz, 1H), 3.15 (dd, *J* = 15.0 Hz, 5.0 Hz, 1H), 2.45 (dd, *J* = 15.0 Hz, 4.5 Hz, 1H), 2.44 (s, 3H), 2.05 (dd, *J* = 15.0 Hz, 5.0 Hz, 1H), 1.68-1.62 (m, 1H), 1.46-1.38 (m, 2H), 0.85-0.80 (m, 1H); ^{13}C NMR (125 MHz, $CDCl_3$) δ 197.3, 166.6, 147.8, 142.6, 135.1, 119.3, 35.2, 34.8, 34.7, 30.8, 26.5, 13.2, 8.4. FT-IR: ν (cm^{-1}) 2922, 2357, 1682, 1504, 1294, 1213, 1125, 1041. HRMS [ESI] calcd for $C_{13}H_{16}NO_3S_2$ $[M+H]^+$ 298.0566, found 298.0558.



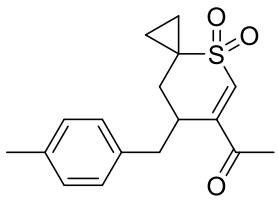
3l: white solid, m.p. 116-117 °C. ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.17 (d, *J* = 5.0 Hz, 1H), 7.07 (s, 1H), 6.93 (dd, *J* = 5.0 Hz, 3.5 Hz, 1H), 6.81 (d, *J* = 3.5 Hz, 1H), 3.32-3.27 (m, 1H), 3.06 (dd, *J* = 14.5 Hz, 3.5 Hz, 1H), 2.96 (dd, *J* = 14.5 Hz, 11.0 Hz, 1H), 2.40 (s, 3H), 2.33 (dd, *J* = 15.5 Hz, 5.0 Hz, 1H), 2.10 (dd, *J* = 15.5 Hz, 5.5 Hz, 1H), 1.70-1.64 (m, 1H), 1.44-1.38 (m, 1H), 1.14-1.09 (m, 1H), 0.82-0.77 (m, 1H); ^{13}C NMR (125 MHz, $CDCl_3$) δ 197.4, 148.7, 140.4, 134.5, 127.1, 126.2, 124.4, 36.0, 35.4, 32.4, 31.1, 26.6, 12.8, 8.7. FT-IR: ν (cm^{-1}) 2922, 2359, 1694, 1435, 1360, 1296, 1211, 1125. HRMS [ESI] calcd for $C_{14}H_{17}O_3S_2$ $[M+H]^+$ 297.0614, found 297.0622.



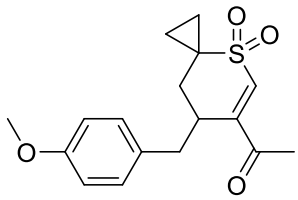
3m: brown oil. ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.32-7.30 (m, 1H), 7.03 (s, 1H), 6.29-6.26 (m, 1H), 6.06-6.04 (m, 1H), 3.37-3.30 (m, 1H), 2.90-2.79 (m, 2H), 2.38 (s, 3H), 2.33 (dd, *J* = 15.0 Hz, 5.0 Hz, 1H), 2.09 (dd, *J* = 15.5 Hz, 5.5 Hz, 1H), 1.68-1.62 (m, 1H), 1.44-1.38 (m, 1H), 1.20-1.14 (m, 1H), 0.86-0.80 (m, 1H); ^{13}C NMR (125 MHz, $CDCl_3$) δ 197.4, 151.9, 148.9, 141.9, 134.3, 110.4, 107.6, 35.5, 33.8, 31.7, 30.6, 26.6, 12.6, 8.8. FT-IR: ν (cm^{-1}) 2920, 2359, 1688, 1506, 1361, 1296, 1213, 1125. HRMS [ESI] calcd for $C_{14}H_{17}O_4S$ $[M+H]^+$ 281.0842, found 218.0844.



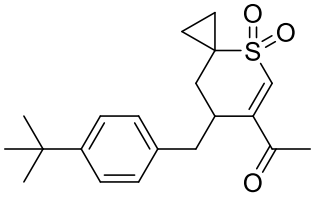
3n: yellow solid, m.p. 62-63 °C. ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.33-7.28 (m, 2H), 7.25-7.21 (m, 1H), 7.21-7.18 (m, 2H), 7.06 (s, 1H), 3.37-3.30 (m, 1H), 2.98 (dd, *J* = 14.0 Hz, 4.0 Hz, 1H), 2.55 (dd, *J* = 14.0 Hz, 11.0 Hz, 1H), 2.40 (s, 3H), 2.25 (dd, *J* = 15.5 Hz, 5.0 Hz, 1H), 1.94 (dd, *J* = 15.5 Hz, 5.0 Hz, 1H), 1.72-1.65 (m, 1H), 1.43-1.36 (m, 1H), 1.10-1.04 (m, 1H), 0.77-0.72 (m, 1H); ^{13}C NMR (125 MHz, $CDCl_3$) δ 197.7, 149.7, 138.3, 133.9, 128.9, 128.8, 126.9, 38.3, 35.4, 35.4, 31.2, 26.7, 12.8, 8.7. FT-IR: ν (cm^{-1}) 2920, 1690, 1454, 1296, 1267, 1211, 1126, 743. HRMS [ESI] calcd for $C_{16}H_{19}O_3S$ $[M+H]^+$ 291.1049, found 291.1052.



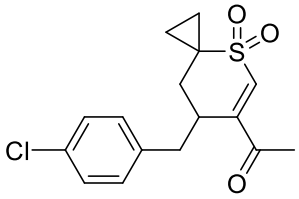
3o: yellow solid, m.p. 141-142 °C. ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.13-7.06 (m, 4H), 7.05 (s, 1H), 3.34-3.27 (m, 1H), 2.97-2.90 (m, 1H), 2.51 (dd, *J* = 12.5 Hz, 12.5 Hz, 1H), 2.40 (s, 3H), 2.32 (s, 3H), 2.25 (dd, *J* = 15.5 Hz, 5.0 Hz, 1H), 1.94 (dd, *J* = 15.5 Hz, 5.0 Hz, 1H), 1.70-1.64 (m, 1H), 1.43-1.36 (m, 1H), 1.10-1.04 (m, 1H), 0.77-0.71 (m, 1H); ^{13}C NMR (125 MHz, $CDCl_3$) δ 197.7, 149.8, 136.5, 135.1, 133.7, 129.5, 128.7, 37.8, 35.5, 35.4, 31.1, 26.7, 21.1, 12.8, 8.7. FT-IR: ν (cm^{-1}) 2922, 1684, 1506, 1456, 1296, 1211, 1126, 922. HRMS [ESI] calcd for $C_{17}H_{20}NaO_3S$ $[M+Na]^+$ 327.1025, found 327.1030.



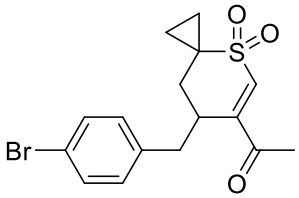
3p: white solid, m.p. 92-93 °C. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.12-7.07 (m, 2H), 7.03 (s, 1H), 6.86-6.81 (m, 2H), 3.78 (s, 3H), 3.31-3.23 (m, 1H), 2.91 (dd, *J* = 13.6 Hz, 4.0 Hz, 1H), 2.49 (dd, *J* = 13.6 Hz, 10.8 Hz, 1H), 2.39 (s, 3H), 2.23 (dd, *J* = 15.2 Hz, 5.2 Hz, 1H), 1.95 (dd, *J* = 15.2 Hz, 5.2 Hz, 1H), 1.71-1.63 (m, 1H), 1.42-1.35 (m, 1H), 1.09-1.02 (m, 1H), 0.78-0.70 (m, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 197.7, 158.5, 149.9, 133.7, 130.1, 129.8, 114.2, 55.3, 37.5, 35.7, 35.5, 31.2, 26.7, 12.8, 8.8. FT-IR: ν (cm^{-1}) 2922, 1695, 1508, 1456, 1296, 1211, 1125, 1034. HRMS [ESI] calcd for $C_{17}H_{20}NaO_4S$ $[M+Na]^+$ 343.0975, found 343.0984.



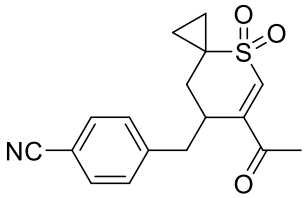
3q: white solid, m.p. 135-136 °C. ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.33-7.30 (m, 2H), 7.14-7.10 (m, 2H), 7.05 (s, 1H), 3.36-3.29 (m, 1H), 2.93 (dd, *J* = 13.5 Hz, 3.5 Hz, 1H), 2.54 (dd, *J* = 13.5 Hz, 11.0 Hz, 1H), 2.39 (s, 3H), 2.29 (dd, *J* = 15.5 Hz, 5.5 Hz, 1H), 1.95 (dd, *J* = 15.5 Hz, 5.5 Hz, 1H), 1.72-1.66 (m, 1H), 1.43-1.37 (m, 1H), 1.30 (s, 9H), 1.13-1.07 (m, 1H), 0.79-0.73 (m, 1H); ^{13}C NMR (125 MHz, $CDCl_3$) δ 197.6, 149.9, 149.8, 135.1, 133.7, 128.5, 125.7, 37.7, 35.4, 35.4, 34.5, 31.4, 31.1, 26.7, 13.0, 8.6. FT-IR: ν (cm^{-1}) 2961, 1694, 1558, 1456, 1362, 1298, 1209, 1126. HRMS [ESI] calcd for $C_{20}H_{26}NaO_3S$ $[M+Na]^+$ 369.1495, found 369.1485.



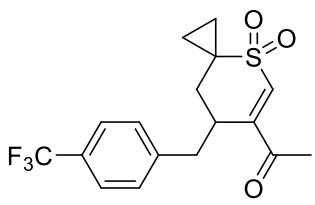
3r: white solid, m.p. 163-164 °C. ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.27 (d, *J* = 8.0 Hz, 2H), 7.13 (d, *J* = 8.0 Hz, 2H), 7.07 (s, 1H), 3.30-3.23 (m, 1H), 2.98-2.91 (m, 1H), 2.51 (dd, *J* = 12.0 Hz, 12.0 Hz, 1H), 2.40 (s, 3H), 2.11 (dd, *J* = 15.5 Hz, 5.5 Hz, 1H), 1.93 (dd, *J* = 15.5 Hz, 5.5 Hz, 1H), 1.70-1.63 (m, 1H), 1.42-1.35 (m, 1H), 1.05-0.99 (m, 1H), 0.77-0.71 (m, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 197.6, 149.2, 136.8, 134.3, 132.7, 130.2, 129.0, 37.7, 35.4, 35.3, 31.2, 26.7, 12.7, 8.9. FT-IR: ν (cm^{-1}) 2922, 1694, 1506, 1491, 1456, 1296, 1211, 1126. HRMS [ESI] calcd for $C_{16}H_{18}ClO_3S$ $[M+H]^+$ 325.0660, found 325.0666.



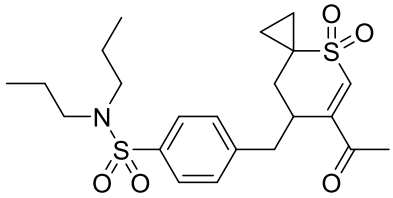
3s: white solid, m.p. 158-159 °C. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.44-7.40 (m, 2H), 7.08 (s, 1H), 7.09-7.05 (m, 2H), 3.31-3.22 (m, 1H), 2.93 (dd, *J* = 13.6 Hz, 3.6 Hz, 1H), 2.49 (dd, *J* = 13.6 Hz, 11.2 Hz, 1H), 2.41 (s, 3H), 2.20 (dd, *J* = 15.2 Hz, 5.2 Hz, 1H), 1.93 (dd, *J* = 15.2 Hz, 5.6 Hz, 1H), 1.70-1.63 (m, 1H), 1.42-1.35 (m, 1H), 1.05-0.98 (m, 1H), 0.78-0.70 (m, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 197.6, 149.2, 137.3, 134.3, 131.9, 130.5, 120.8, 37.7, 35.4, 35.2, 31.2, 26.7, 12.7, 8.9. FT-IR: ν (cm^{-1}) 2922, 1688, 1634, 1506, 1456, 1296, 1211, 1126. HRMS [ESI] calcd for $C_{17}H_{20}NaO_4S$ $[M+Na]^+$ 343.0975, found 343.0984.



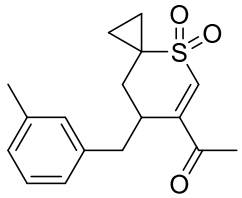
3t: white solid, m.p. 162-163 °C. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.59 (d, *J* = 8.0 Hz, 2H), 7.32 (d, *J* = 8.0 Hz, 2H), 7.13 (s, 1H), 3.34-3.26 (m, 1H), 3.03 (dd, *J* = 13.6 Hz, 3.6 Hz, 1H), 2.60 (dd, *J* = 13.6 Hz, 11.2 Hz, 1H), 2.41 (s, 3H), 2.20 (dd, *J* = 15.2 Hz, 5.2 Hz, 1H), 1.91 (dd, *J* = 15.2 Hz, 5.6 Hz, 1H), 1.71-1.63 (m, 1H), 1.42-1.34 (m, 1H), 1.04-0.96 (m, 1H), 0.79-0.71 (m, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 197.6, 148.6, 144.0, 134.9, 132.6, 129.7, 118.6, 110.9, 38.5, 35.4, 35.0, 31.3, 26.6, 12.7, 8.9. FT-IR: ν (cm^{-1}) 2922, 2228, 1684, 1506, 1456, 1296, 1211, 1125. HRMS [ESI] calcd for $C_{17}H_{18}NO_3S$ $[M+H]^+$ 316.1002, found 316.0993.



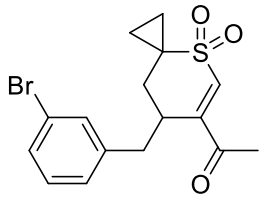
3u: white solid, m.p. 150-151 °C. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.56 (d, *J* = 8.0 Hz, 2H), 7.33 (d, *J* = 8.0 Hz, 2H), 7.11 (s, 1H), 3.37-3.28 (m, 1H), 3.05 (dd, *J* = 13.6 Hz, 2.4 Hz, 1H), 2.60 (dd, *J* = 13.6 Hz, 11.2 Hz, 1H), 2.42 (s, 3H), 2.21 (dd, *J* = 15.2 Hz, 5.6 Hz, 1H), 1.94 (dd, *J* = 15.2 Hz, 5.6 Hz, 1H), 1.72-1.65 (m, 1H), 1.44-1.36 (m, 1H), 1.07-0.99 (m, 1H), 0.79-0.71 (m, 1H); ^{13}C NMR (125 MHz, $CDCl_3$) δ 197.6, 148.9, 142.5 (q, J_{C-F} = 0.9 Hz), 134.6, 129.3 (q, J_{C-F} = 32.5 Hz), 129.2, 125.8 (q, J_{C-F} = 3.8 Hz), 124.1 (q, J_{C-F} = 270.3 Hz), 38.1, 35.4, 35.1, 31.2, 26.6, 12.7, 8.9; ^{19}F NMR (376 MHz, $CDCl_3$) δ -62.5 (s). FT-IR: ν (cm^{-1}) 2922, 2359, 1688, 1506, 1456, 1327, 1298, 1126. HRMS [ESI] calcd for $C_{17}H_{17}F_3NaO_3S$ $[M+Na]^+$ 381.0743, found 381.0737.



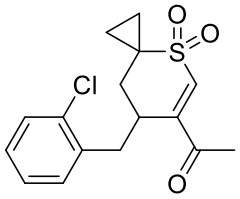
3v: yellow oil. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.72 (d, *J* = 8.0 Hz, 2H), 7.32 (d, *J* = 8.0 Hz, 2H), 7.11 (s, 1H), 3.35-3.26 (m, 1H), 3.09-3.00 (m, 5H), 2.60 (dd, *J* = 13.6 Hz, 11.2 Hz, 1H), 2.41 (s, 3H), 2.18 (dd, *J* = 15.2 Hz, 5.6 Hz, 1H), 1.91 (dd, *J* = 15.2 Hz, 5.6 Hz, 1H), 1.71-1.62 (m, 1H), 1.58-1.46 (m, 4H), 1.42-1.34 (m, 1H), 1.04-0.97 (m, 1H), 0.84 (t, *J* = 7.2 Hz, 6H), 0.77-0.70 (m, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 197.6, 148.8, 143.1, 139.0, 134.7, 129.4, 127.6, 49.9, 38.2, 35.4, 35.1, 31.3, 26.6, 22.0, 12.6, 11.2, 8.9. FT-IR: ν (cm^{-1}) 2967, 2876, 1686, 1506, 1373, 1298, 1155, 1126. HRMS [ESI] calcd for $C_{22}H_{32}NO_5S_2$ $[M+H]^+$ 454.1716, found 454.1723.



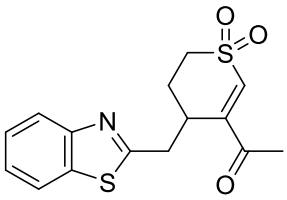
3w: white solid, m.p. 76-77 °C. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.22-7.16 (m, 1H), 7.07-6.96 (m, 4H), 3.37-3.28 (m, 1H), 2.95 (dd, *J* = 13.6 Hz, 3.2 Hz, 1H), 2.50 (dd, *J* = 12.8 Hz, 11.6 Hz, 1H), 2.40 (s, 3H), 2.33 (s, 3H), 2.25 (dd, *J* = 15.2 Hz, 5.2 Hz, 1H), 1.96 (dd, *J* = 15.2 Hz, 5.2 Hz, 1H), 1.72-1.64 (m, 1H), 1.44-1.36 (m, 1H), 1.12-1.04 (m, 1H), 0.79-0.71 (m, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 197.7, 149.8, 138.5, 138.1, 133.8, 129.5, 128.7, 127.6, 125.9, 38.3, 35.5, 35.4, 31.2, 26.7, 21.4, 12.8, 8.8. FT-IR: ν (cm^{-1}) 2922, 1694, 1609, 1506, 1456, 1296, 1211, 1126. HRMS [ESI] calcd for $C_{17}H_{20}NaO_3S$ $[M+Na]^+$ 327.1025, found 327.1030.



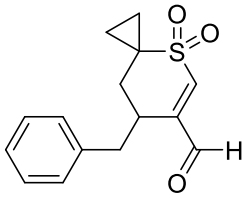
3x: white solid, m.p. 61-62 °C. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.39-7.33 (m, 2H), 7.21-7.11 (m, 2H), 7.08 (s, 1H), 3.33-3.25 (m, 1H), 2.97 (dd, *J* = 13.6 Hz, 3.6 Hz, 1H), 2.51 (dd, *J* = 13.6 Hz, 10.8 Hz, 1H), 2.41 (s, 3H), 2.24 (dd, *J* = 15.2 Hz, 5.2 Hz, 1H), 1.95 (dd, *J* = 15.2 Hz, 5.6 Hz, 1H), 1.72-1.65 (m, 1H), 1.44-1.36 (m, 1H), 1.07-1.00 (m, 1H), 0.80-0.73 (m, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 192.8, 144.3, 135.9, 129.7, 127.0, 125.6, 125.4, 122.8, 118.1, 33.3, 30.7, 30.5, 26.5, 21.9, 8.0, 4.1. FT-IR: ν (cm^{-1}) 2920, 1684, 1506, 1473, 1361, 1296, 1211, 1125. HRMS [ESI] calcd for $C_{16}H_{18}BrO_3S$ $[M+H]^+$ 369.0155, found 369.0163.



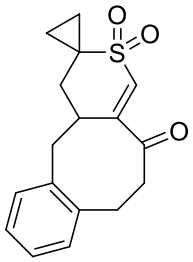
3y: white solid, m.p. 69-70 °C. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.36-7.32 (m, 1H), 7.25-7.14 (m, 3H), 7.01 (s, 1H), 3.54-3.46 (m, 1H), 3.03 (dd, *J* = 13.6 Hz, 5.6 Hz, 1H), 2.87 (dd, *J* = 13.6 Hz, 5.6 Hz, 1H), 2.32 (s, 3H), 2.21 (dd, *J* = 15.2 Hz, 5.6 Hz, 1H), 2.09 (dd, *J* = 15.2 Hz, 6.0 Hz, 1H), 1.70-1.62 (m, 1H), 1.43-1.36 (m, 1H), 1.12-1.05 (m, 1H), 0.81-0.74 (m, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 197.6, 150.1, 135.7, 134.3, 133.5, 130.8, 130.0, 128.4, 127.1, 36.3, 35.6, 34.0, 32.4, 26.7, 12.4, 9.1. FT-IR: ν (cm^{-1}) 2924, 1694, 1633, 1506, 1473, 1296, 1211, 1125. HRMS [ESI] calcd for $C_{16}H_{18}ClO_3S$ $[M+H]^+$ 325.0660, found 325.0652.



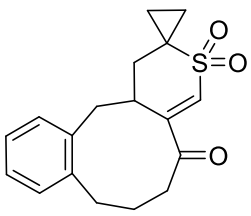
3z: white solid, m.p. 133-134 °C. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.99-7.95 (m, 1H), 7.88-7.84 (m, 1H), 7.51-7.45 (m, 1H), 7.42-7.36 (m, 1H), 7.04 (s, 1H), 3.54-3.43 (m, 2H), 3.31 (dd, *J* = 14.8 Hz, 4.0 Hz, 1H), 3.23-3.16 (m, 2H), 2.50-2.42 (m, 1H), 2.45 (s, 3H), 2.42-2.36 (m, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 196.8, 167.0, 153.1, 147.2, 135.4, 135.3, 126.3, 125.4, 122.9, 121.7, 46.7, 35.2, 32.5, 26.2, 23.9. FT-IR: ν (cm^{-1}) 2922, 1688, 1514, 1435, 1358, 1296, 1215, 1126. HRMS [ESI] calcd for $C_{15}H_{16}NO_3S_2$ $[M+H]^+$ 322.0566, found 322.0572.



3aa: yellow solid, m.p. 75-76 °C. ^{1}H NMR (400 MHz, $CDCl_3$) δ 9.57 (s, 1H), 7.35-7.30 (m, 2H), 7.25-7.19 (m, 3H), 7.13 (s, 1H), 3.23-3.15 (m, 2H), 2.55 (dd, *J* = 14.0 Hz, 12.0 Hz, 1H), 2.29 (dd, *J* = 15.6 Hz, 5.2 Hz, 1H), 1.95 (dd, *J* = 15.6 Hz, 4.8 Hz, 1H), 1.75-1.67 (m, 1H), 1.46-1.38 (m, 1H), 1.13-1.07 (m, 1H), 0.79-0.72 (m, 1H); ^{13}C NMR (125 MHz, $CDCl_3$) δ 191.2, 148.9, 142.0, 138.1, 128.9, 128.8, 127.0, 37.7, 36.1, 34.3, 31.0, 12.8, 8.7. FT-IR: ν (cm^{-1}) 2922, 1697, 1558, 1456, 1417, 1361, 1298, 1138. HRMS [ESI] calcd for $C_{15}H_{17}O_3S$ $[M+H]^+$ 277.0893, found 277.0895.

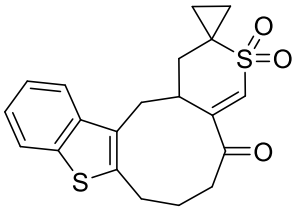


5a: yellow oil. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.25-7.15 (m, 3H), 7.10-7.06 (m, 1H), 6.29 (s, 1H), 3.21-3.13 (m, 1H), 3.08-3.01 (m, 1H), 3.00-2.86 (m, 4H), 2.67-2.54 (m, 2H), 2.26-2.18 (m, 1H), 1.65-1.58 (m, 1H), 1.47-1.40 (m, 1H), 1.05-0.98 (m, 1H), 0.97-0.90 (m, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 204.6, 154.2, 138.3, 135.4, 131.4, 130.1, 128.3, 127.6, 125.1, 46.0, 38.4, 37.8, 36.4, 34.4, 29.8, 10.6, 10.4. FT-IR: ν (cm^{-1}) 2920, 2849, 1697, 1558, 1456, 1294, 1230, 1120. HRMS [ESI] calcd for $C_{17}H_{19}O_3S$ $[M+H]^+$ 303.1049, found 303.1042.

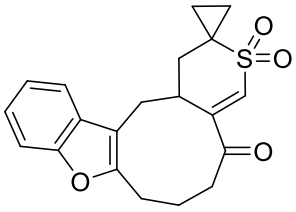


5b: white solid, m.p. 172-173 °C. ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.21-7.17 (m, 2H), 7.13-7.07 (m, 2H), 6.42 (s, 1H), 3.28-3.19 (m, 1H), 2.90-2.76 (m, 4H), 2.75-2.68 (m, 1H), 2.51-2.39 (m, 2H), 2.33-2.24 (m, 1H), 2.16-2.04 (m, 2H), 1.66 (dd, *J* = 10.5 Hz, 5.0 Hz, 1H), 1.45-1.39 (m, 1H), 1.07-0.96 (m, 2H); ^{13}C NMR (125 MHz, $CDCl_3$) δ 204.3, 153.0, 131.7, 130.7, 129.6, 128.5, 127.8,

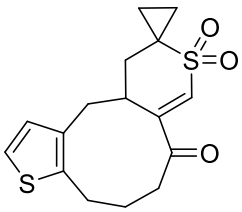
127.3, 125.2, 38.2, 37.1, 36.9, 30.0, 18.9, 12.8, 12.6, 11.0, 9.9. FT-IR: ν (cm^{-1}) 2920, 1694, 1633, 1506, 1418, 1294, 1142, 1121. HRMS [ESI] calcd for $C_{18}H_{21}O_3S$ $[M+H]^+$ 317.1206, found 317.1196.



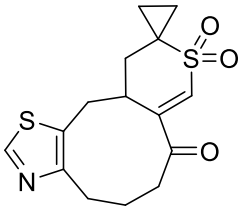
5c: yellow solid, m.p. 203-204 °C. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.79-7.75 (m, 1H), 7.64-7.60 (m, 1H), 7.38-7.30 (m, 2H), 6.39 (s, 1H), 3.50-3.42 (m, 1H), 3.40-3.30 (m, 1H), 3.29-3.11 (m, 1H), 2.92-2.84 (m, 2H), 2.83-2.73 (m, 1H), 2.45-2.34 (m, 2H), 2.32-2.18 (m, 2H), 1.99-1.85 (m, 1H), 1.67-1.59 (m, 1H), 1.45-1.38 (m, 1H), 1.05-0.95 (m, 2H); ^{13}C NMR (125 MHz, $CDCl_3$) δ 204.6, 152.7, 139.1, 135.7, 131.9, 128.4, 124.8, 124.4, 122.6, 121.7, 38.2, 37.7, 37.2, 34.9, 30.7, 24.5, 22.9, 11.4, 9.6. FT-IR: ν (cm^{-1}) 2924, 2359, 1695, 1506, 1456, 1296, 1202, 1121. HRMS [ESI] calcd for $C_{20}H_{21}O_3S_2$ $[M+H]^+$ 373.0927, found 373.0922.



5d: white solid, m.p. 176-177 °C. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.45-7.40 (m, 2H), 7.31-7.26 (m, 1H), 7.24-7.29 (m, 1H), 6.37 (d, *J* = 1.6 Hz, 1H), 3.49-3.41 (m, 1H), 3.25-3.12 (m, 2H), 2.78-2.65 (m, 3H), 2.58-2.49 (m, 1H), 2.42-2.26 (m, 2H), 2.23-2.13 (m, 1H), 1.95 (dd, *J* = 15.2 Hz, 5.2 Hz, 1H), 1.65-1.58 (m, 1H), 1.45-1.39 (m, 1H), 1.04-0.97 (m, 2H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 204.8, 154.6, 153.0, 150.8, 128.3, 128.2, 124.7, 122.6, 119.1, 115.6, 111.3, 38.3, 37.4, 37.2, 34.9, 29.0, 24.6, 20.1, 11.4, 9.6. FT-IR: ν (cm^{-1}) 2926, 1695, 1616, 1506, 1456, 1296, 1123, 1032. HRMS [ESI] calcd for $C_{20}H_{21}O_4S$ $[M+H]^+$ 357.1155, found 357.1153.

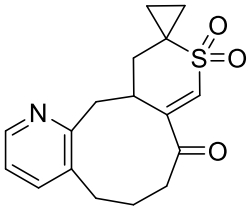


5e: yellow solid, m.p. 157-158 °C. ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.18 (d, *J* = 5.5 Hz, 1H), 6.73 (d, *J* = 5.5 Hz, 1H), 6.40 (d, *J* = 1.5 Hz, 1H), 3.39-3.32 (m, 1H), 3.30-3.22 (m, 1H), 3.16-3.02 (m, 1H), 2.73-2.57 (m, 3H), 2.50-2.37 (m, 2H), 2.23-2.15 (m, 1H), 2.12-2.02 (m, 1H), 1.94-1.86 (m, 1H), 1.64-1.58 (m, 1H), 1.43-1.38 (m, 1H), 1.03-0.94 (m, 2H); ^{13}C NMR (125 MHz, $CDCl_3$) δ 204.3, 152.9, 138.0, 134.4, 128.9, 128.3, 125.1, 39.0, 37.9, 37.0, 34.9, 30.1, 26.0, 24.9, 11.3, 9.6. FT-IR: ν (cm^{-1}) 2920, 2849, 1696, 1506, 1456, 1296, 1152, 1123. HRMS [ESI] calcd for $C_{16}H_{19}O_3S_2$ $[M+H]^+$ 323.0770, found 323.0768.

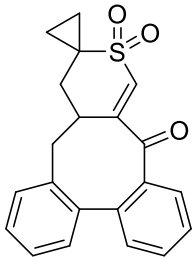


5f: yellow solid, m.p. 145-146 °C. ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.66 (s, 1H), 6.43 (d, *J* = 1.6 Hz, 1H), 3.42-3.34 (m, 1H), 3.31-3.24 (m, 1H), 3.02-2.92 (m, 1H), 2.86-2.76 (m, 2H), 2.75-2.68 (m, 1H), 2.47-2.40 (m, 2H), 2.31-2.23 (m, 1H), 2.22-2.14 (m, 1H), 1.93-1.86 (m, 1H), 1.63-1.57 (m, 1H), 1.41-1.36 (m, 1H), 1.01-0.93 (m, 2H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 204.6, 152.9, 152.4, 152.2, 129.0, 128.4, 38.2, 37.8, 36.8, 34.4, 28.6, 25.5, 25.0, 11.3, 9.6. FT-IR: ν (cm^{-1})

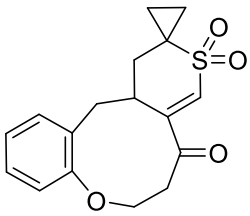
2926, 2855, 1689, 1603, 1454, 1346, 1152, 1072. HRMS [ESI] calcd for $C_{15}H_{18}NO_3S_2$ $[M+H]^+$ 324.0723, found 324.0724.



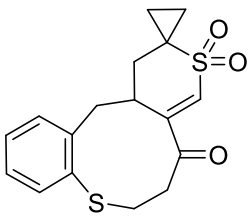
5g: yellow oil. ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.44 (dd, *J* = 4.8 Hz, 1.6 Hz, 1H), 7.40 (dd, *J* = 7.6 Hz, 1.2 Hz, 1H), 7.12 (dd, *J* = 7.6 Hz, 4.8 Hz, 1H), 6.38 (d, *J* = 1.6 Hz, 1H), 3.41-3.32 (m, 1H), 3.15-2.65 (m, 5H), 2.57-2.48 (m, 1H), 2.41-2.22 (m, 2H), 2.14-1.98 (m, 2H), 1.60-1.54 (m, 1H), 1.42-1.36 (m, 1H), 1.05-0.95 (m, 2H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 204.6, 156.8, 153.3, 148.3, 138.5, 134.1, 127.4, 122.7, 38.7, 38.6, 37.3, 35.9, 30.2, 25.7, 22.7, 11.4, 9.4. FT-IR: ν (cm^{-1}) 2924, 2865, 1701, 1574, 1454, 1296, 1197, 1123. HRMS [ESI] calcd for $C_{17}H_{20}NO_3S$ $[M+H]^+$ 318.1158, found 318.1164.



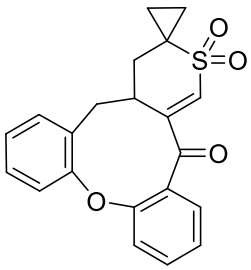
5h: yellow solid, m.p. 164-165 ºC. ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.08-8.04 (m, 1H), 7.67-7.62 (m, 1H), 7.53-7.48 (m, 1H), 7.44-7.41 (m, 2H), 7.39-7.35 (m, 1H), 7.27-7.22 (m, 2H), 6.37 (s, 1H), 3.27-3.15 (m, 2H), 3.07 (dd, *J* = 14.8 Hz, 9.6 Hz, 1H), 2.58-2.52 (m, 1H), 1.78 (dd, *J* = 14.8 Hz, 5.6 Hz, 1H), 1.59-1.54 (m, 1H), 1.42-1.36 (m, 1H), 0.99-0.89 (m, 2H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 194.7, 152.4, 141.6, 139.6, 135.7, 133.9, 133.0, 130.8, 130.1, 130.1, 129.5, 128.5, 128.2, 127.9, 38.1, 36.6, 35.7, 33.0, 11.2, 9.3. FT-IR: ν (cm^{-1}) 2924, 2357, 1694, 1591, 1477, 1296, 1231, 1123. HRMS [ESI] calcd for $C_{21}H_{19}O_3S$ $[M+H]^+$ 351.1049, found 351.1052.



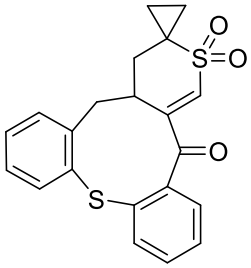
5i: yellow solid, m.p. 164-165 ºC. ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.27-7.22 (m, 1H), 7.04-7.01 (m, 2H), 6.95-6.92 (m, 1H), 6.58 (s, 1H), 4.74-4.69 (m, 1H), 4.22-4.15 (m, 1H), 3.46 (dd, *J* = 14.0 Hz, 4.0 Hz, 1H), 3.43-3.36 (m, 1H), 3.10-3.03 (m, 2H), 2.81 (dd, *J* = 15.0 Hz, 11.0 Hz, 1H), 2.31 (dd, *J* = 14.0 Hz, 4.0 Hz, 1H), 1.63 (dd, *J* = 15.0 Hz, 5.0 Hz, 1H), 1.54-1.49 (m, 1H), 1.38-1.33 (m, 1H), 0.98-0.89 (m, 2H); ^{13}C NMR (125 MHz, $CDCl_3$) δ 200.5, 158.3, 150.8, 132.3, 129.9, 129.1, 127.6, 123.5, 118.9, 69.7, 40.8, 36.9, 35.9, 32.4, 32.1, 11.6, 8.9. FT-IR: ν (cm^{-1}) 2924, 1699, 1506, 1489, 1456, 1296, 1248, 1124. HRMS [ESI] calcd for $C_{17}H_{19}O_4S$ $[M+H]^+$ 319.0999, found 319.1007.



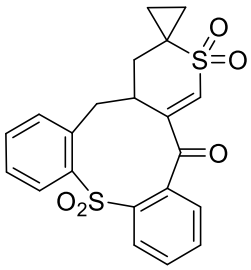
5j: yellow solid, m.p. 174-175 ºC. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.59-7.54 (m, 1H), 7.34-7.28 (m, 1H), 7.25-7.16 (m, 2H), 6.59 (s, 1H), 3.39-3.31 (m, 1H), 3.30-3.05 (m, 5H), 2.69-2.58 (m, 2H), 2.34-2.22 (m, 1H), 1.68-1.60 (m, 1H), 1.45-1.37 (m, 1H), 1.10-1,03 (m, 1H), 0.98-0.92 (m, 1H); ^{13}C NMR (125 MHz, $CDCl_3$) δ 201.6, 152.2, 143.1, 137.6, 134.4, 130.7, 129.8, 128.5, 55.2, 39.9, 38.2, 37.7, 36.4, 34.4, 10.7, 10.3. FT-IR: ν (cm^{-1}) 2920, 2849, 1697, 1506, 1456, 1296, 1219, 1121. HRMS [ESI] calcd for $C_{17}H_{19}O_3S_2$ $[M+H]^+$ 335.0770, found 335.0764.



5k: yellow solid, m.p. 164-165 °C. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.62-7.55 (m, 1H), 7.47-7.42 (m, 1H), 7.40-7.35 (m, 1H), 7.29-7.23 (m, 1H), 7.15-7.09 (m, 2H), 7.06-7.00 (m, 1H), 6.71-6.64 (m, 1H), 6.23 (s, 1H), 3.68-3.55 (m, 1H), 3.27-3.19 (m, 1H), 3.00-2.87 (m, 1H), 2.76-2.68 (m, 1H), 2.01-1.92 (m, 1H), 1.82-1.74 (m, 1H), 1.55-1.47 (m, 1H), 1.20-1.12 (m, 1H), 0.93-0.85 (m, 1H); ^{13}C NMR (125 MHz, $CDCl_3$) δ 195.2, 158.7, 158.6, 158.3, 155.2, 133.7, 131.3, 129.7, 129.3, 129.2, 126.8, 125.2, 124.9, 123.0, 121.0, 38.6, 37.9, 36.0, 35.8, 14.1, 8.4. FT-IR: ν (cm^{-1}) 2922, 2850, 1695, 1636, 1456, 1296, 1227, 1126. HRMS [ESI] calcd for $C_{21}H_{19}O_4S$ $[M+H]^+$ 367.0999, found 367.0992.



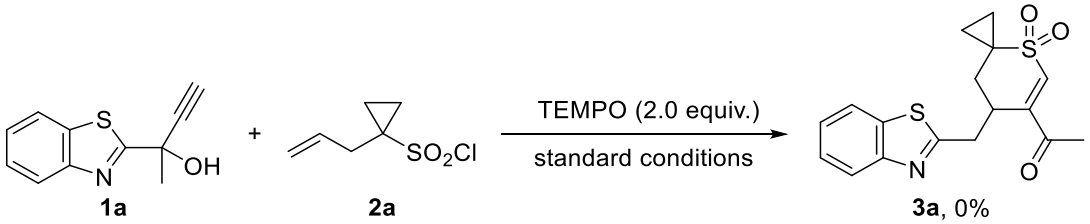
5l: yellow solid, m.p. 156-157 °C. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.69-7.65 (m, 1H), 7.49-7.43 (m, 1H), 7.35-7.27 (m, 2H), 7.27-7.17 (m, 3H), 7.11-7.05 (m, 1H), 6.31 (s, 1H), 4.15-4.06 (m, 1H), 3.45-3.36 (m, 1H), 3.04 (dd, *J* = 15.2 Hz, 4.4 Hz, 1H), 2.74-2.68 (m, 1H), 2.06-1.99 (m, 1H), 1.86-1.78 (m, 1H), 1.54-1.46 (m, 1H), 1.24-1.18 (m, 1H), 0.95-0.87 (m, 1H); ^{13}C NMR (125 MHz, $CDCl_3$) δ 196.1, 152.6, 142.3, 139.5, 139.4, 136.7, 135.4, 133.0, 131.8, 130.3, 130.3, 130.2, 128.9, 127.8, 127.7, 40.4, 38.0, 35.7, 35.4, 13.8, 8.2. FT-IR: ν (cm^{-1}) 2924, 2850, 1695, 1506, 1456, 1296, 1224, 1126. HRMS [ESI] calcd for $C_{21}H_{19}O_3S_2$ $[M+H]^+$ 383.0770, found 383.0763.



5m: white solid, m.p. 157-158 °C. ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.31 (d, *J* = 8.0 Hz, 1H), 7.77-7.70 (m, 1H), 7.66-7.60 (m, 1H), 7.58-7.48 (m, 2H), 7.35-7.28 (m, 3H), 6.40 (s, 1H), 4.93-4.84 (m, 1H), 3.52-3.42 (m, 1H), 3.16 (dd, *J* = 15.2 Hz, 5.2 Hz, 1H), 2.73 (dd, *J* = 12.4 Hz, 3.6 Hz, 1H), 1.94 (dd, *J* = 15.2 Hz, 2.4 Hz, 1H), 1.89-1.82 (m, 1H), 1.55-1.48 (m, 1H), 1.28-1.21 (m, 1H), 0.96-0.89 (m, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 195.2, 150.5, 141.6, 140.0, 138.4, 136.8, 135.2, 133.8, 133.1, 133.0, 131.9, 131.5, 129.2, 129.1, 126.3, 38.0, 37.5, 35.2, 34.9, 14.4, 7.8. FT-IR: ν (cm^{-1}) 2920, 2851, 1682, 1516, 1436, 1298, 1264, 1126. HRMS [ESI] calcd for $C_{21}H_{19}O_5S_2$ $[M+H]^+$ 415.0668 found 415.0666.

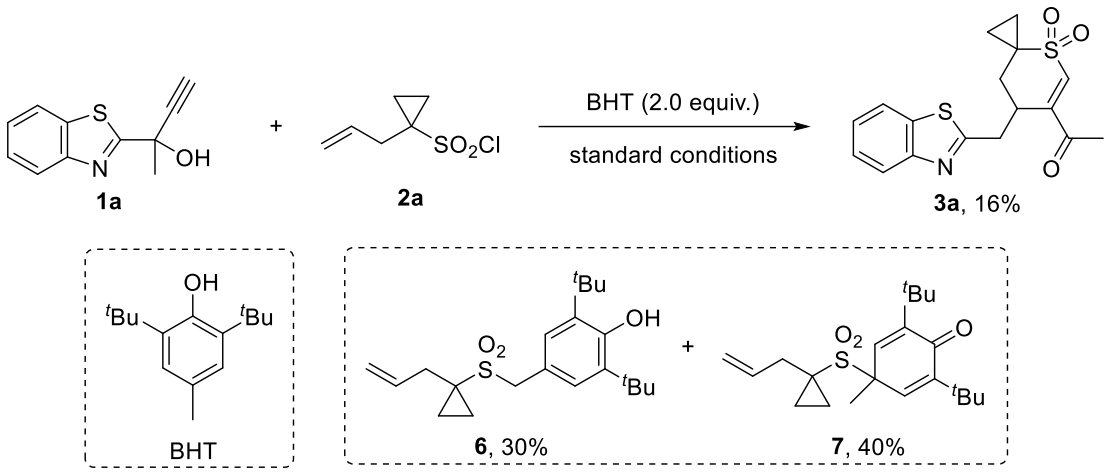
5. Mechanistic studies

a) Radical trapping experiments

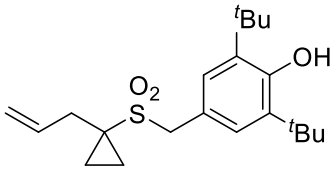


Propargyl alcohol **1a** (0.2 mmol, 40.7 mg), Na_2HPO_4 (0.2 mmol, 28.4 mg), TEMPO

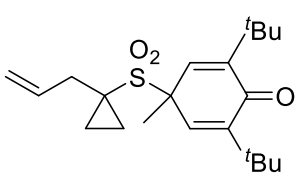
(0.6 mmol, 93.8 mg), and *fac*-Ir(ppy)$_3$ (3 mol %, 4.0 mg) were loaded in a reaction vial which was subjected to evacuation/ flushing with N_2 three times. Then allylcyclopropane sulfonyl chloride **2a** (0.3 mmol, 55.9 mg) in CH_3CN (2 mL) and H_2O (0.2 mL) were added to the mixture via syringe. The reaction was irradiated with 12 W blue LEDs. No desired product **3a** was detected by TLC.



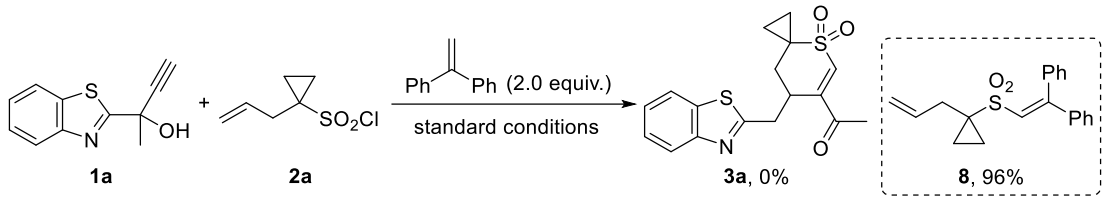
Propargyl alcohol **1a** (0.2 mmol, 40.7 mg), Na_2HPO_4 (0.2 mmol, 28.4 mg), BHT (0.4 mmol, 88.1 mg), and *fac*-Ir(ppy)$_3$ (3 mol %, 4 mg) were loaded in a reaction vial which was subjected to evacuation/ flushing with N_2 three times. Then allylcyclopropane sulfonyl chloride **2a** (0.3 mmol, 55.9 mg) in CH_3CN (2 mL) and H_2O (0.2 mL) were added to the mixture via syringe. The reaction was irradiated with 12 W blue LEDs. After reaction completion, the reaction mixture was concentrated in vacuo. Purification the residue by flash column chromatography on silica gel afforded the desired product **3a** in a 16% yield, radical trapping adducts **6** in a 30% yield and **7** in a 40% yield.



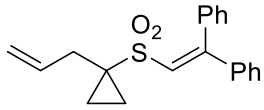
6: yellow solid, m.p. 64-65 ^oC. ^1H NMR (500 MHz, $CDCl_3$) δ 7.17 (s, 2H), 5.75-5.65 (m, 1H), 5.31 (s, 1H), 5.17-5.09 (m, 2H), 4.21 (s, 2H), 2.61 (d, J = 7.5 Hz, 2H), 1.44 (s, 18H), 1.18-1.14 (m, 2H), 0.75-0.71 (m, 2H); ^{13}C NMR (125 MHz, $CDCl_3$) δ 154.4, 136.3, 132.6, 127.7, 119.4, 118.7, 58.1, 37.8, 34.9, 34.3, 30.3, 9.2. FT-IR: ν (cm^{-1}) 3320, 2967, 2868, 1634, 1471, 1417, 1236, 1109. HRMS [ESI] calcd for $C_{21}H_{32}NaO_3S$ $[M+Na]^+$ 387.1964, found 387.1968.



7: white solid, m.p. 115-116 ^oC. ^1H NMR (500 MHz, $CDCl_3$) δ 6.74 (s, 2H), 5.53-5.42 (m, 1H), 5.02 (d, J = 10.0 Hz, 1H), 4.90 (d, J = 17.0 Hz, 1H), 2.48 (d, J = 7.0 Hz, 2H), 1.65 (s, 3H), 1.34-1.31 (m, 2H), 1.25 (s, 18H), 0.77-0.73 (m, 2H); ^{13}C NMR (125 MHz, $CDCl_3$) δ 184.6, 149.5, 136.9, 131.4, 119.7, 66.8, 39.5, 35.4, 34.7, 29.1, 21.0, 10.0. FT-IR: ν (cm^{-1}) 2961, 2869, 1634, 1417, 1305, 1294, 1246, 1132. HRMS [ESI] calcd for $C_{21}H_{33}O_3S$ $[M+H]^+$ 365.2145, found 365.2147.



Propargyl alcohol **1a** (0.2 mmol, 40.7 mg), Na_2HPO_4 (0.2 mmol, 28.4 mg), and *fac*-$Ir(ppy)_3$ (3 mol %, 4 mg) were loaded in a reaction vial which was subjected to evacuation/ flushing with N_2 three times. Then allylcyclopropane sulfonyl chloride **2a** (0.3 mmol, 55.9 mg) in CH_3CN (2 mL), 1,1-diphenylethylene (0.4 mmol, 72.1 mg), and H_2O (0.2 mL) were added to the mixture via syringe. The reaction was irradiated with 12 W blue LEDs. No desired product **3a** was detected by TLC. The reaction mixture was concentrated in vacuo. Purification the residue by flash column chromatography on silica gel afforded the radical trapping adduct **8** in a 96% yield.



8: yellow oil. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.43-7.31 (m, 8H), 7.29-7.24 (m, 2H), 6.77 (s, 1H), 5.81-5.69 (m, 1H), 5.17-5.10 (m, 2H), 2.68 (d, *J* = 7.2 Hz, 2H), 1.23-1.19 (m, 2H), 0.78-0.74 (m, 2H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 155.5, 139.8, 136.1, 132.9, 130.2, 129.9, 129.2, 128.7, 128.3, 127.8, 124.9, 119.2, 40.9, 34.9, 9.9. FT-IR: ν (cm^{-1}) 3059, 2920, 1607, 1489, 1445, 1301, 1123, 923. HRMS [ESI] calcd for $C_{20}H_{21}O_3S$ $[M+H]^+$ 325.1257, found 325.1252.

b) Quantum yield measurements

Determination of the light intensity at 456 nm

The photon flux of the kessil light (40 W, λ_{max} = 456 nm) was determined by standard ferrioxalate actinometry following a modified literature procedure of Yoon[1] and Glorius[2]. A 0.15 M solution of ferrioxalate was prepared by dissolving potassium ferrioxalate hydrate (0.737 g) in H_2SO_4 (10 mL of a 0.05 M solution). A buffered solution of 1,10-phenanthroline was prepared by dissolving 1,10-phenanthroline (5.0 mg) and sodium acetate (1.13 g) in H_2SO_4 (5.0 mL of a 0.5 M solution). Both solutions were stored in the dark. To determine the photon flux of the LED, the ferrioxalate solution (3.0 mL) was placed in a cuvette and irradiated for 60 seconds at λ_{max} = 456 nm. After irradiation, the phenanthroline solution (0.525 mL) was added to the cuvette and the mixture was allowed to stir in the dark for 1 h to allow the ferrous ions to completely coordinate to the phenanthroline. The absorbance of the solution was measured at 510 nm. The same procedure was repeated two more times. A nonirradiated sample was also prepared and the absorbance at 510 nm was measured. The average of the absorption of the irradiated and non-irradiated samples was determined and used to calculate the generated amount of Fe(II) according to the Lambert-Beer law (equation 1),

$$\textbf{mol } Fe^{2+} = (V \times \Delta A510nm)/ (l \times \varepsilon) \qquad (1)$$

where V is the total volume ($3.525*10^{-3}$ L), ΔA510nm the difference between absorbance of irradiated samples and the non-irradiated (control) ones (at $\lambda = 510$ nm), l is the path length of the cuvette (1.0 cm), and ε is the molar attenuation coefficient of the ferrioxalate actinometer $\lambda = 510$ nm ($11100\ L \cdot mol^{-1} \cdot cm^{-1}$)[3]. The photonflux can be calculated using equation 2,

$$\textbf{photo flux} = \text{mol } Fe^{2+} / (\Phi_F \times t \times f) \qquad (2)$$

where Φ is the quantum yield of the ferrioxalate actinometer (1.11 at $\lambda = 436$ nm)[4] and t is the irradiation time (60 s). The fraction of light absorbed at $\lambda = 456$ nm by the actinometer (f) is calculated by using equation 3. A456nm is the absorbance of the ferrioxalate solution at $\lambda = 456$ nm.

$$f = 1 - 10^{-}A_{456\,nm} \qquad (3)$$

The absorbance (A_{456nm}) of the ferrioxalate solution was measured to be > 3 indicating that > 99.9% of the photons are absorbed ($f > 0.999$). The photon flux was therefore calculated to be $5.3*10^{-9}$ einstein s^{-1} as an average of three experiments.

Determination of the quantum yield

1a **2a** **3a**

The reaction mixture was stirred and irradiated by blue LED ($\lambda_{max} = 456$ nm) for 3600 s. The yield of product was determined by ^{1}H NMR analysis using toluene as an internal standard. The yield of 3a was determined to be 15.5% (0.0155×10^{-3} mol of **3a**). The reaction quantum yield (Φ) was determined using equation 4 where the photon flux is 5.3×10^{-9} einsteins s^{-1} (determined by actinometry as described above), t is the reaction time (3600 s) and f is the fraction of incident light absorbed by the catalyst, determined using (equation 3).

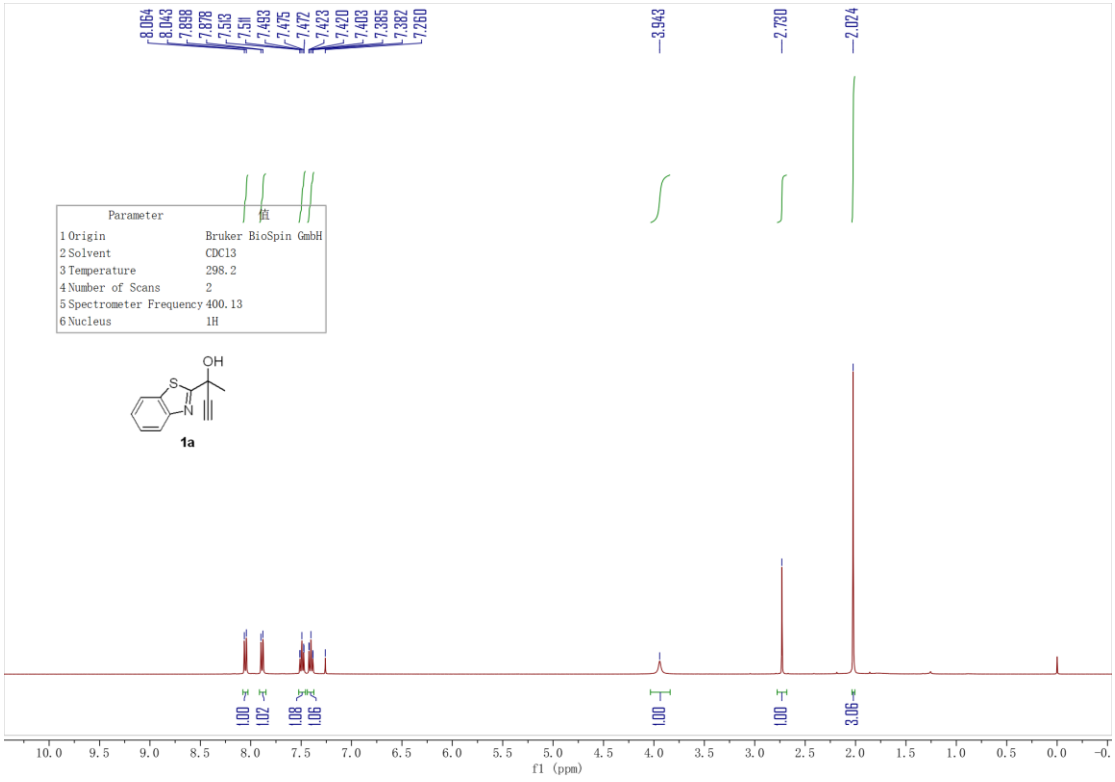
$$\text{Quantum Yield} = \text{moles of product formed} / (\text{flux} \times f \times t) \qquad (4)$$
$$= 0.0155 \times 10^{-3} / (5.3 \times 10^{-9} \times 1 \times 3600) = 0.81$$

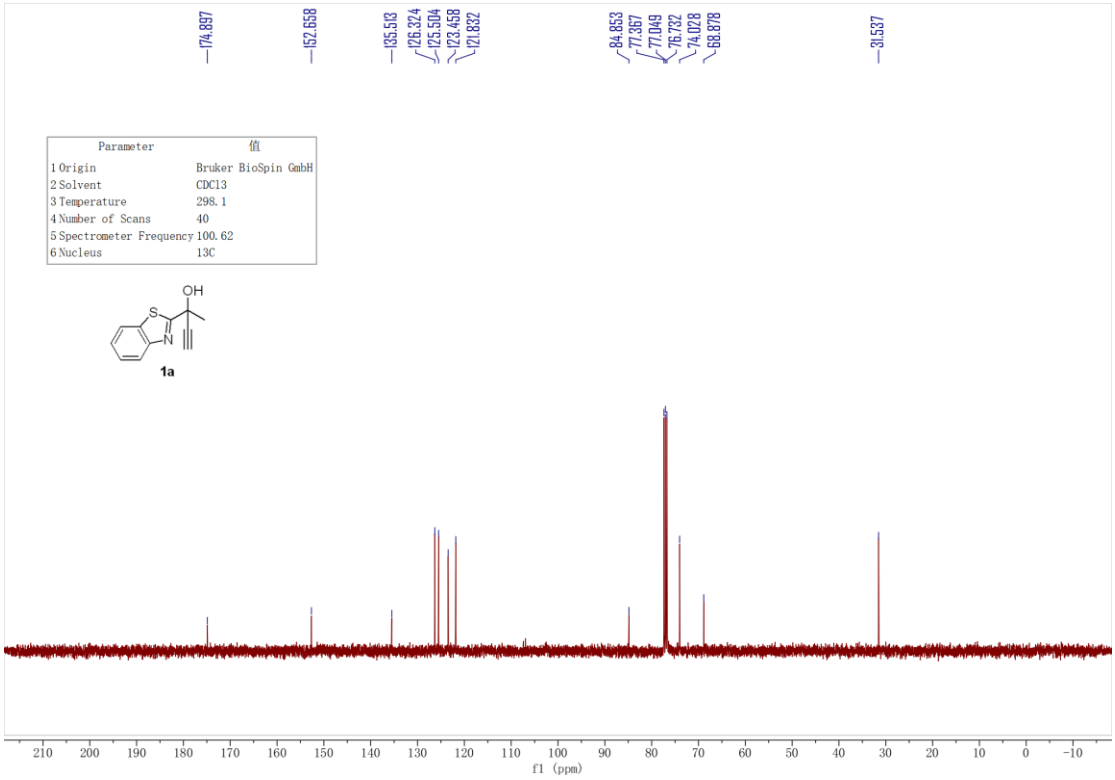
Conclusion: Although the light on/off experiments showed that the product formation occurred only during the periods of constant light irradiation. Typical lifetime of radical chain process can be on the second or sub-second timescale, which means chain processes can terminate faster than the timescale of the analytical measurement used. The quantum yield measurement ($\Phi < 1$) indicated that the reaction mainly proceeded via a photocatalytic pathway, but the contribution of radical chain process could not be ruled out.

1. M. A. Cismesia, T. P. Yoon, *Chem. Sci.* **2015**, *6*, 5426-5434.
2. L. Quach, S. Dutta, P. M. Pflüger, F. Sandfort, P. Belotti, F. Glorius, *ACS Catal*.

2022, *12*, 2499-2504.
3. I. P. Pozdnyakov, O. V. Kel, V. F. Plyusnin, V. P. Grivin, N. M. Bazhin, *J. Phys. Chem. A,* **2008**, *112*, 8316-8322.
4. A. Dewanji, L. Dalsen, J. A. Rossi-Ashton, E. Gasson, G. E. M. Crisenza, D. J. Procter, *Nat. Chem.* **2023**, *15*, 43-52.

6. ^{1}H, ^{13}C, and ^{19}F NMR spectra

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68.878
31.537
Parameter 值
1 Origin Bruker BioSpin GmbH
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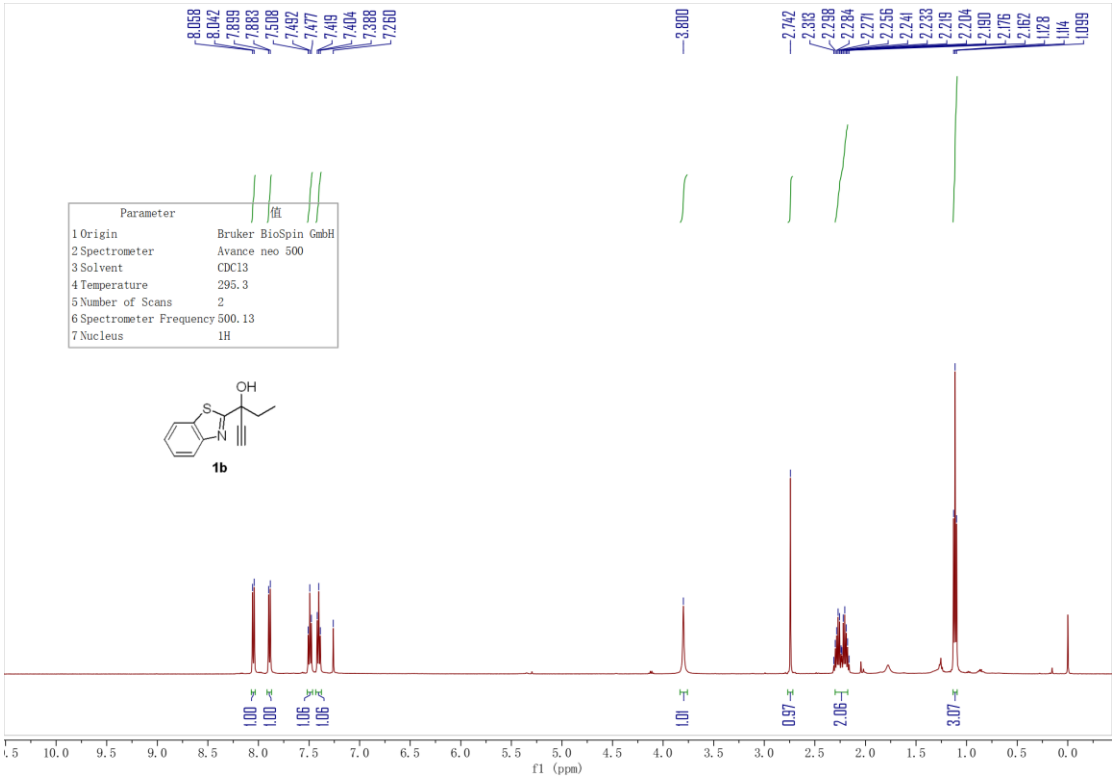
3 Temperature 298.1
4 Number of Scans 40
5 Spectrometer Frequency 100.62
6 Nucleus 13C
OH
S
N
1a
f1 (ppm)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2.313
2.298
2.284
2.271
2.256
2.241
2.233
2.219
2.204
2.190
2.176
2.162
1.128
1.114
1.099
Parameter 值
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2 Spectrometer Avance neo 500
3 Solvent CDCl3
4 Temperature 295.3
5 Number of Scans 2
6 Spectrometer Frequency 500.13
7 Nucleus 1H
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1b
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1.00
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1.06
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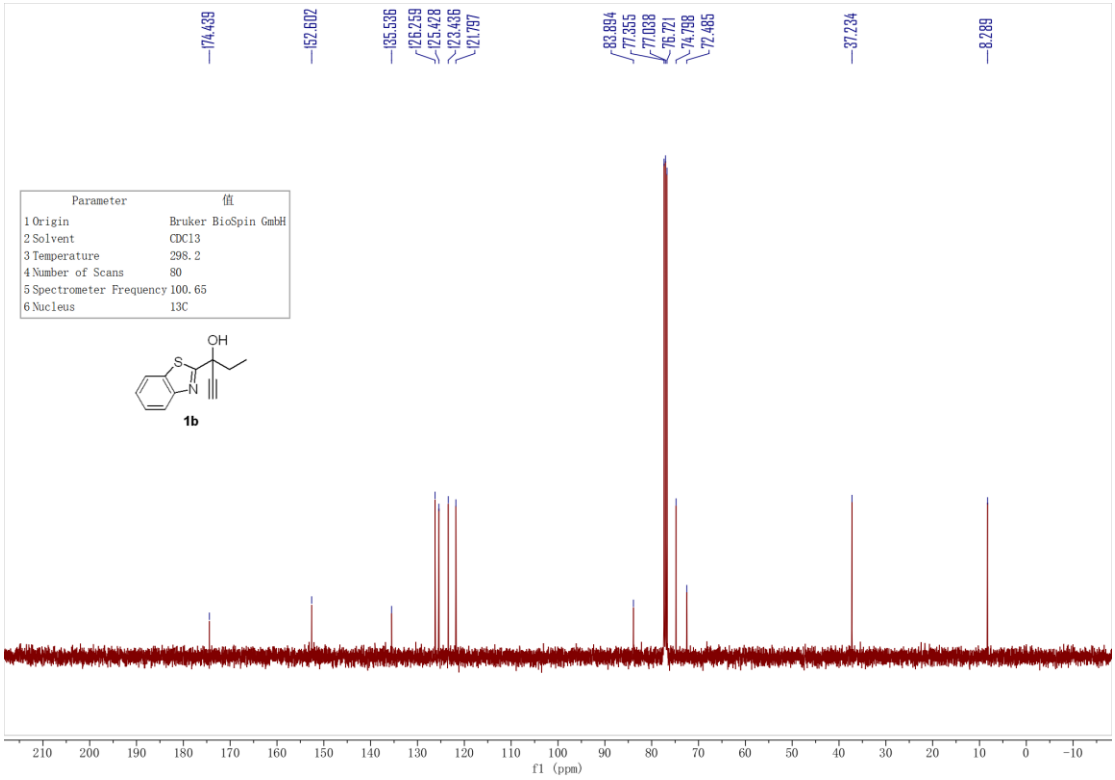
f1 (ppm)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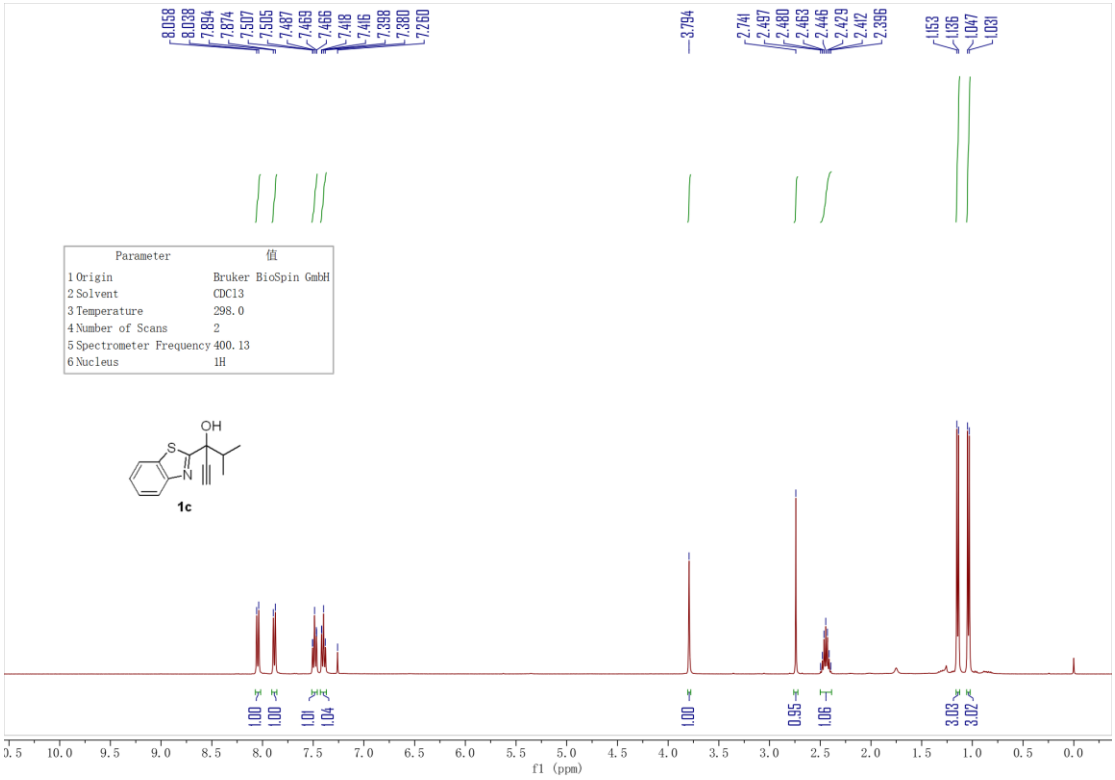
N
1b
f1 (ppm)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7.260
3.794
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2.480
2.463
2.446
2.429
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2.396
1.153
1.136
1.047
1.031
Parameter 值
1 Origin Bruker BioSpin GmbH
2 Solvent CDCl3
3 Temperature 298.0
4 Number of Scans 2
5 Spectrometer Frequency 400.13
6 Nucleus 1H
OH
S
N
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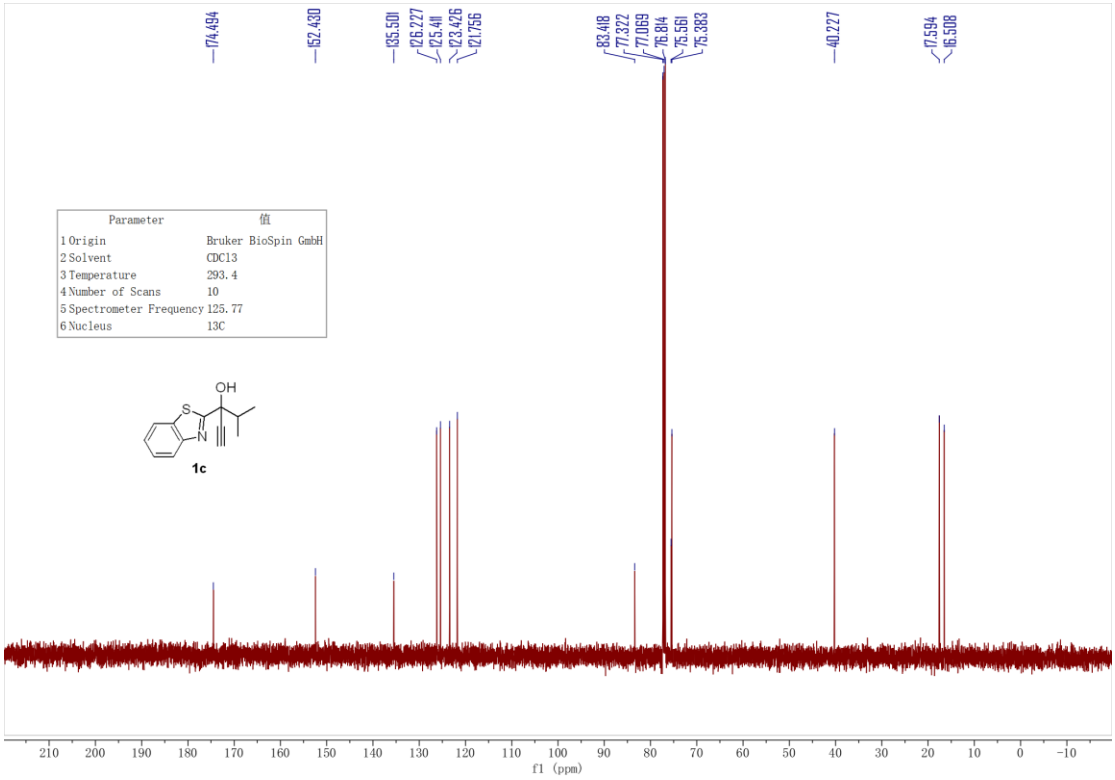
3.02
f1 (ppm)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4 Number of Scans 10
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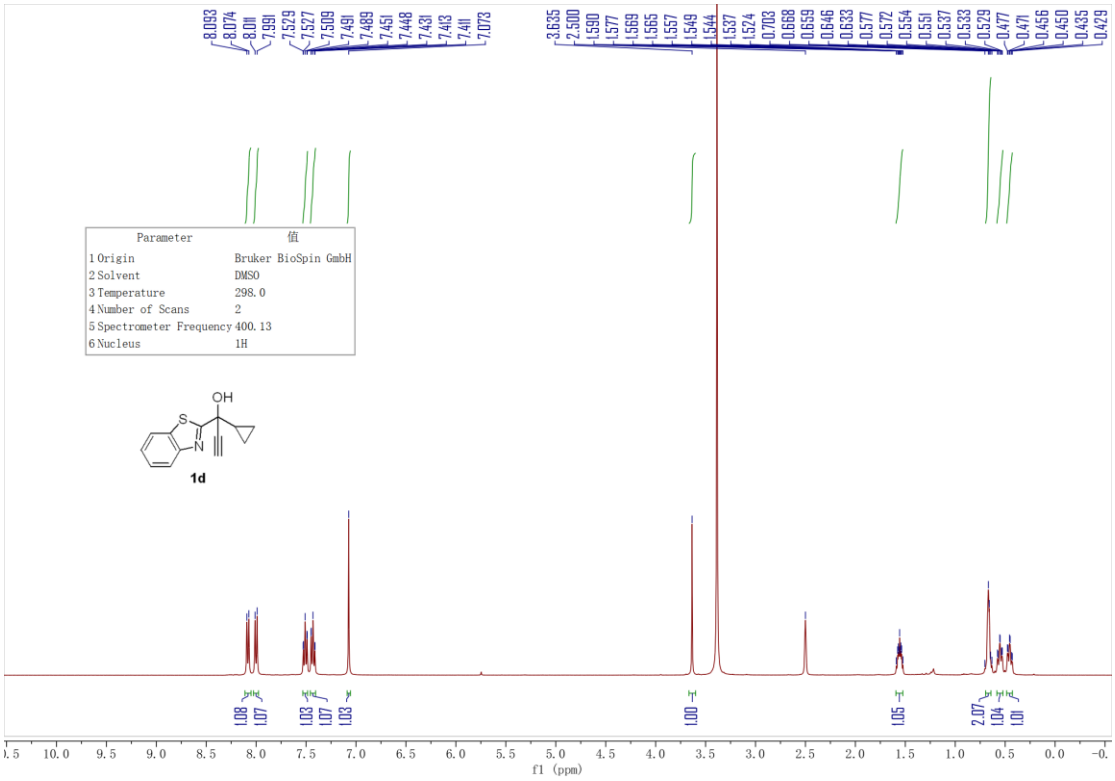
6 Nucleus 13C
OH
S
N
1c
f1 (ppm)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1.577
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1.549
1.544
1.537
1.524
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0.668
0.659
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0.577
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0.537
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1.07
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1.05
2.07
1.04
1.01
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5 Spectrometer Frequency 400.13
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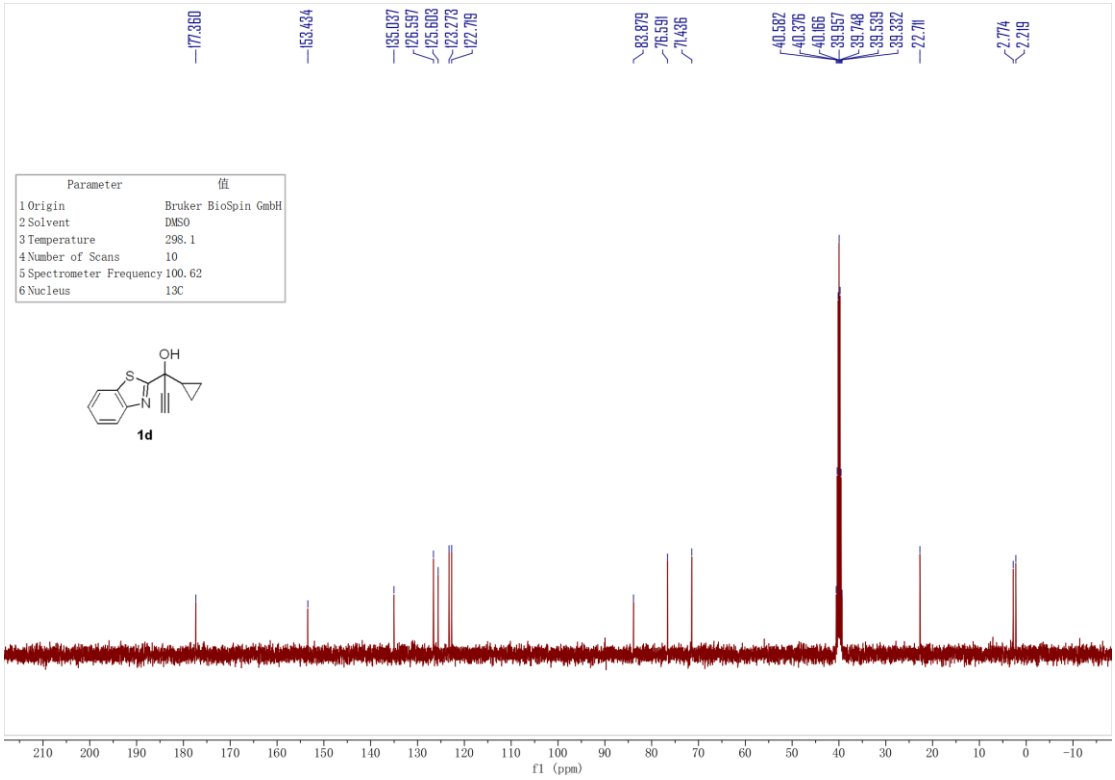
OH
S
N
1d
f1 (ppm)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39.332
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2.219
Parameter 值
1 Origin Bruker BioSpin GmbH
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4 Number of Scans 10
5 Spectrometer Frequency 100.62
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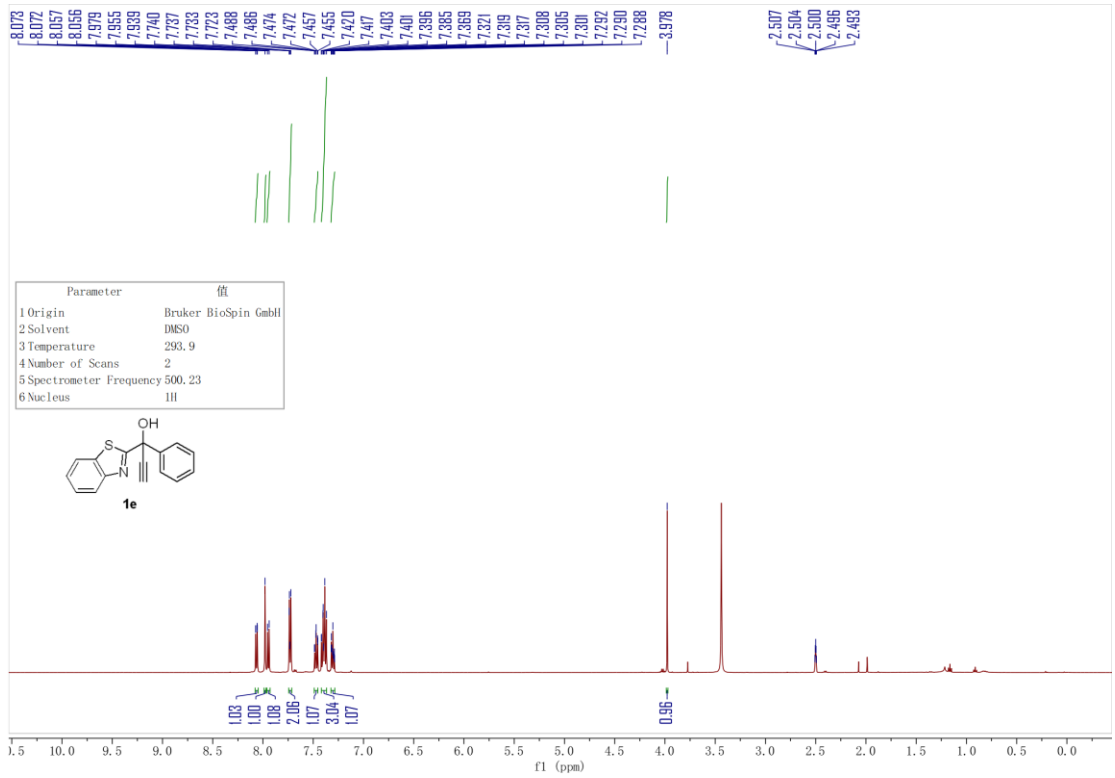
OH
S
N
1d
f1 (ppm)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7.472
7.457
7.455
7.420
7.417
7.403
7.401
7.396
7.385
7.369
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7.317
7.308
7.305
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2.507
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2.496
2.493
Parameter 值
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3 Temperature 293.9
4 Number of Scans 2
5 Spectrometer Frequency 500.23
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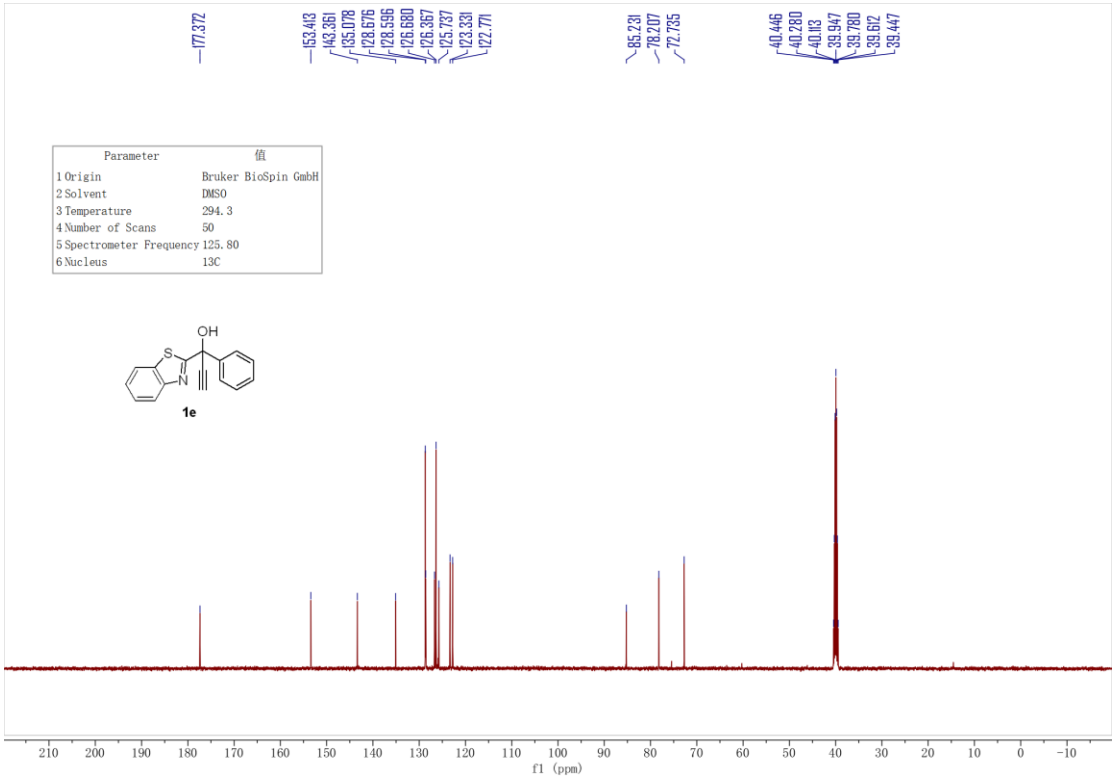
f1 (ppm)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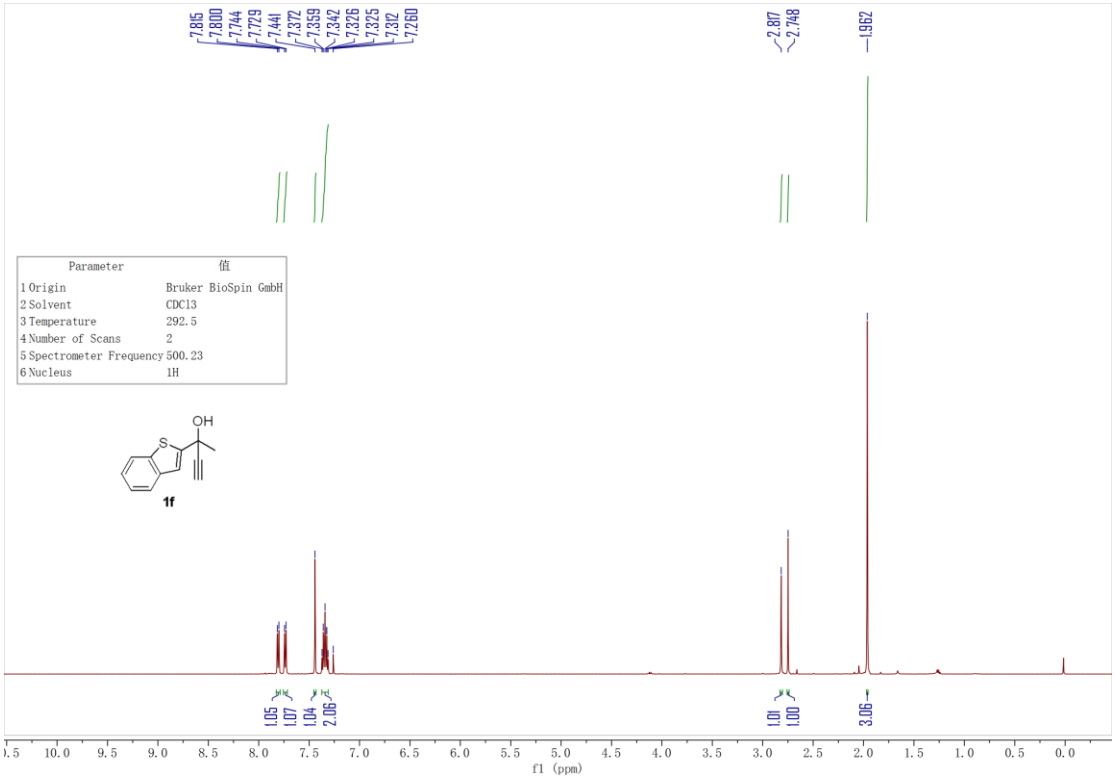
S
N
1e
f1 (ppm)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7.260
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2.748
1.962
Parameter 值
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2 Solvent CDCl3
3 Temperature 292.5
4 Number of Scans 2
5 Spectrometer Frequency 500.23
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S
1f
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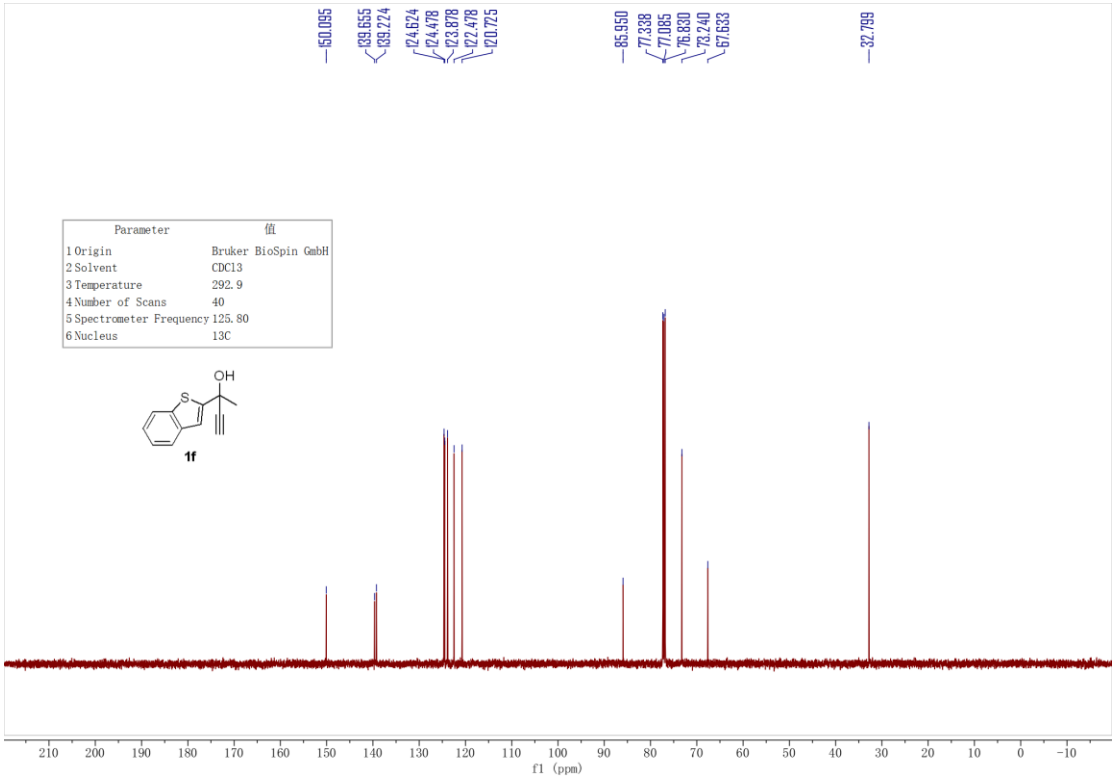
1.07
1.04
2.06
1.01
1.00
3.06
f1 (ppm)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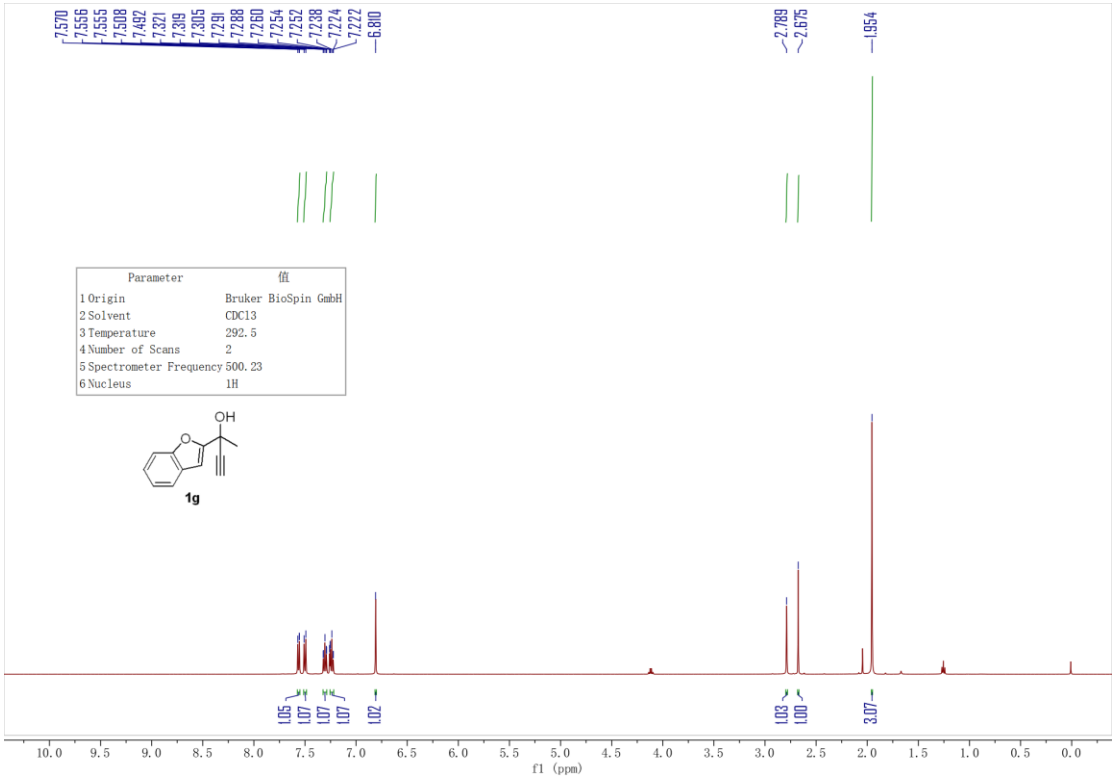
OH
S
1f
f1 (ppm)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6.810
2.789
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Parameter 值
1 Origin Bruker BioSpin GmbH
2 Solvent CDCl3
3 Temperature 292.5
4 Number of Scans 2
5 Spectrometer Frequency 500.23
6 Nucleus 1H
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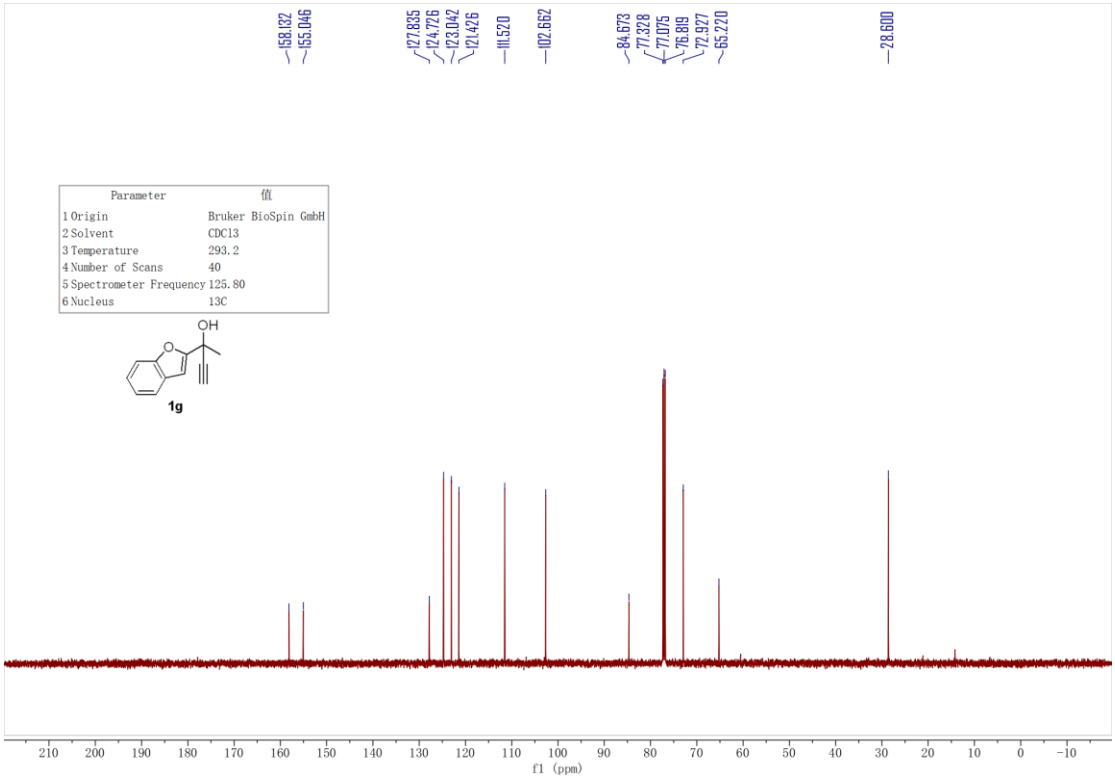
f1 (ppm)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Parameter 值
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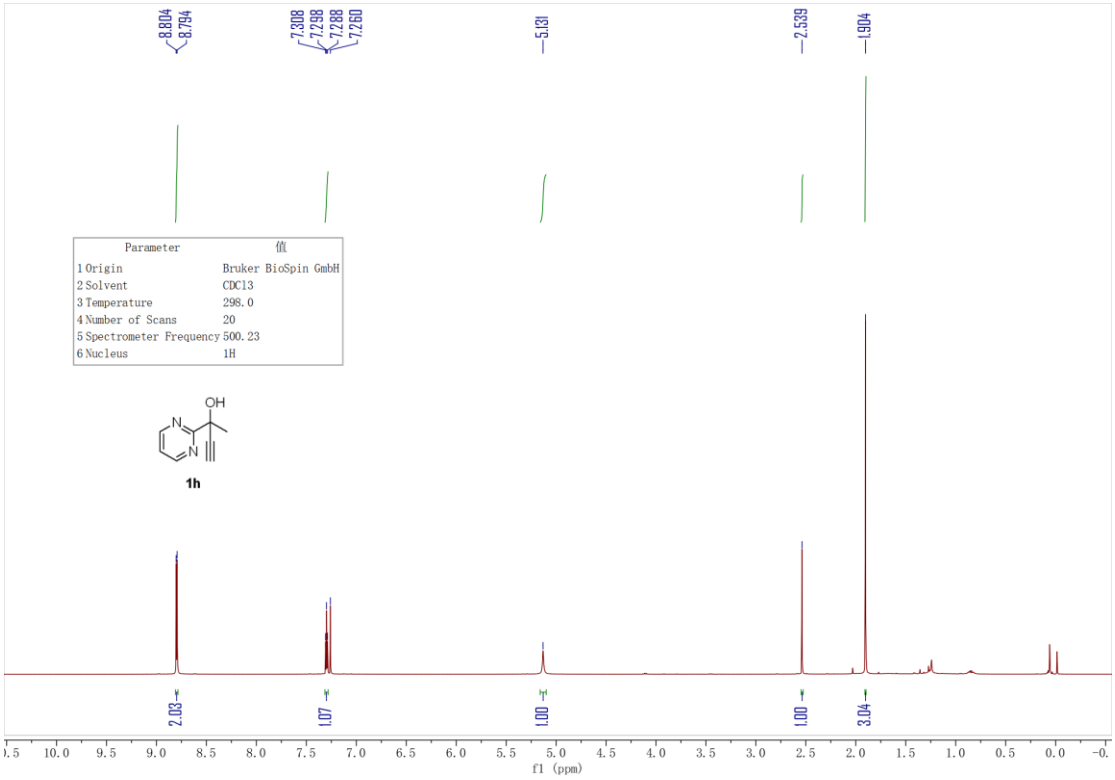
6 Nucleus 13C
OH
1g
f1 (ppm)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N
1h
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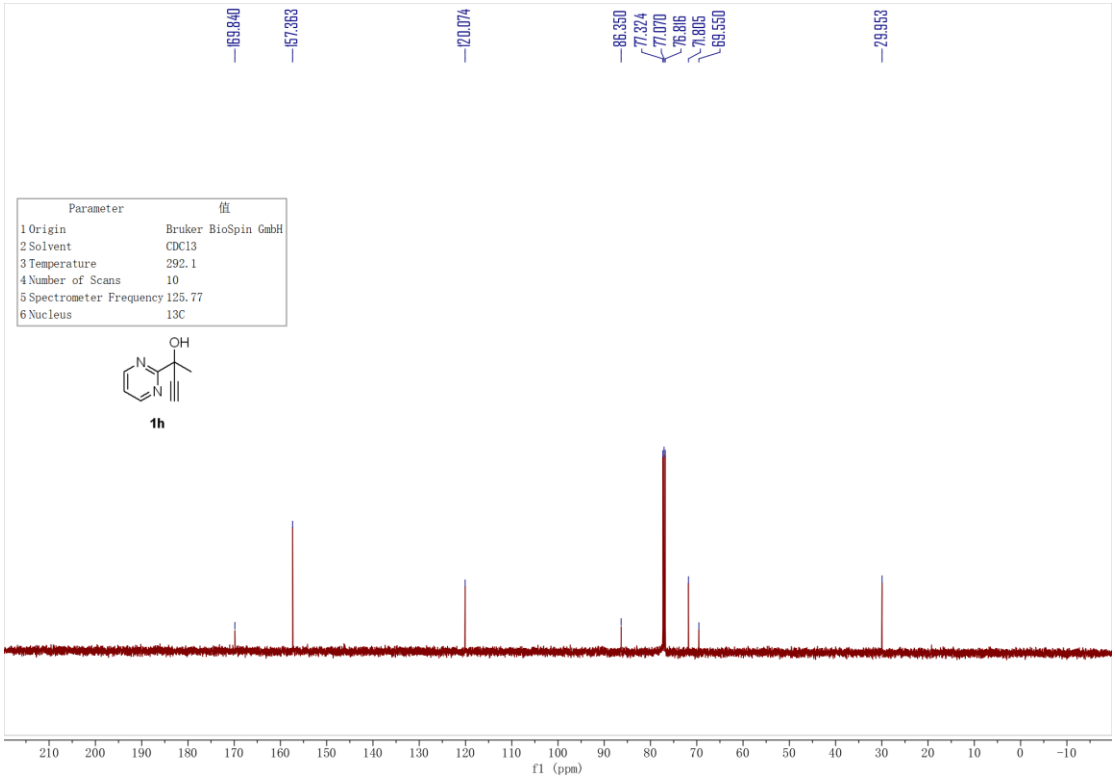
f1 (ppm)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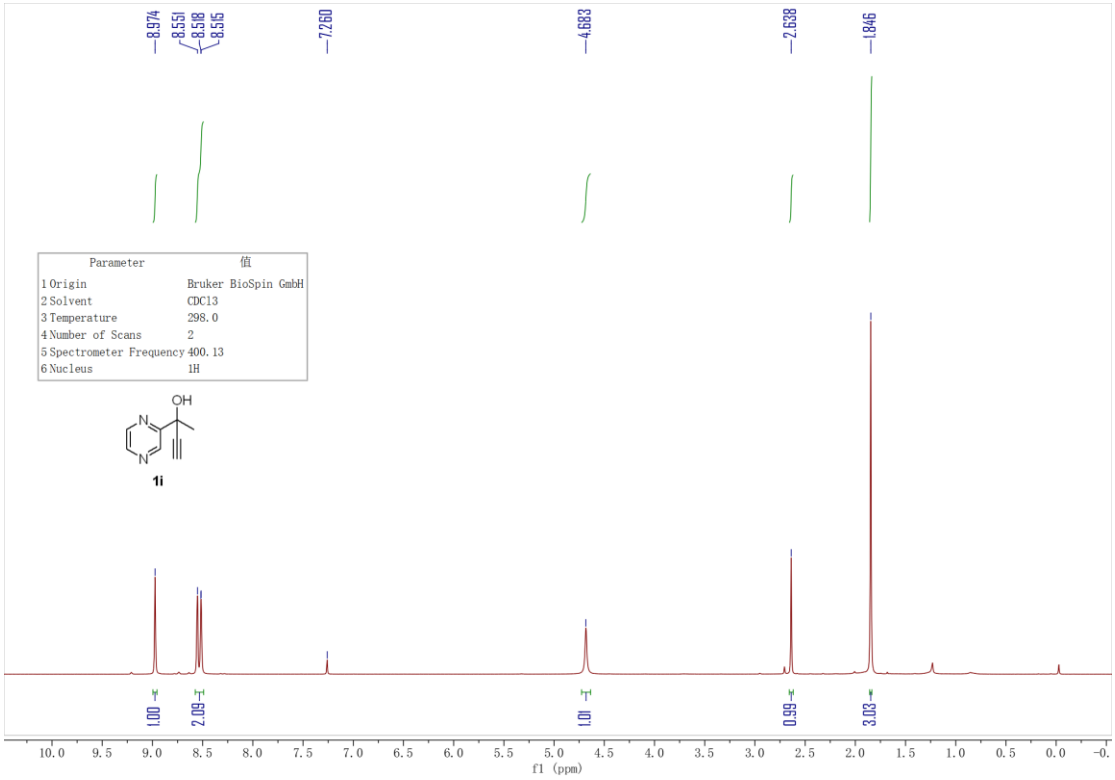
1h
f1 (ppm)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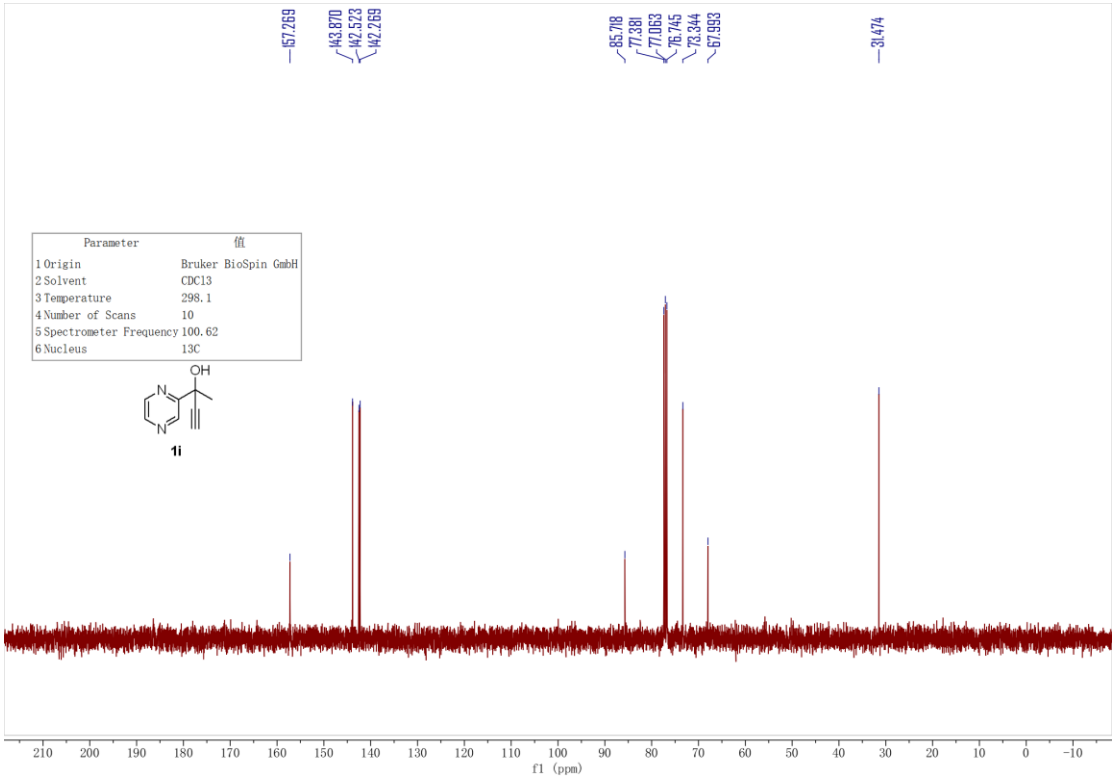
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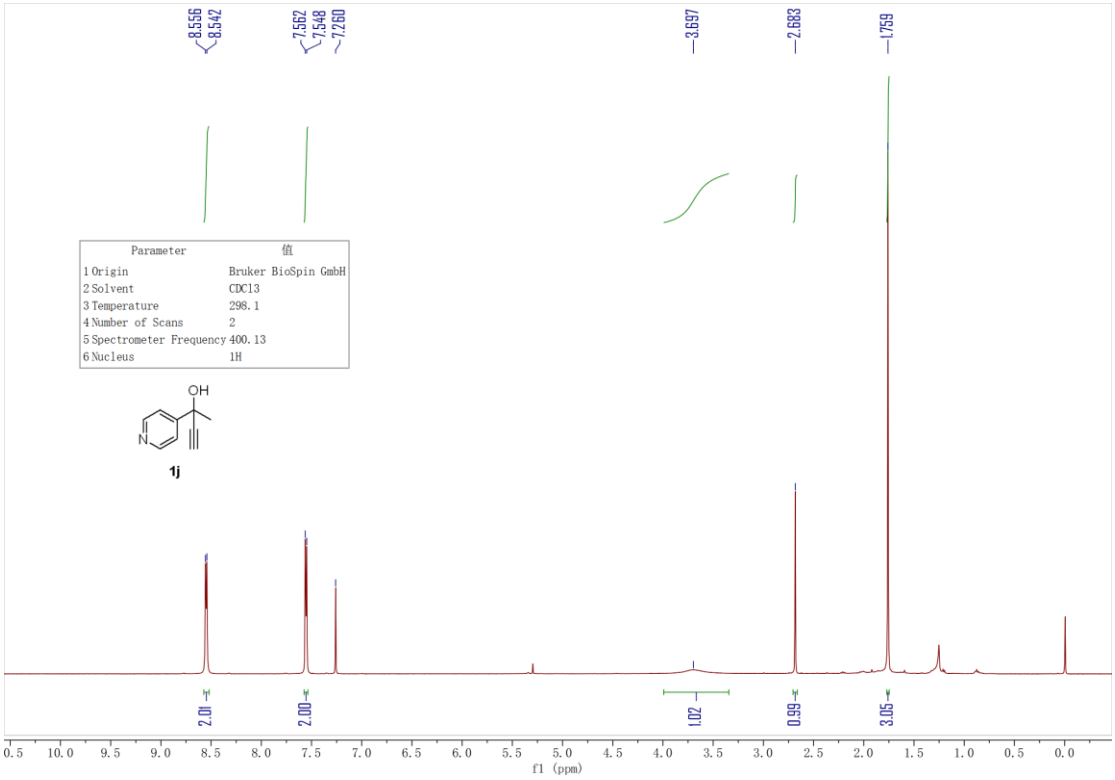
f1 (ppm)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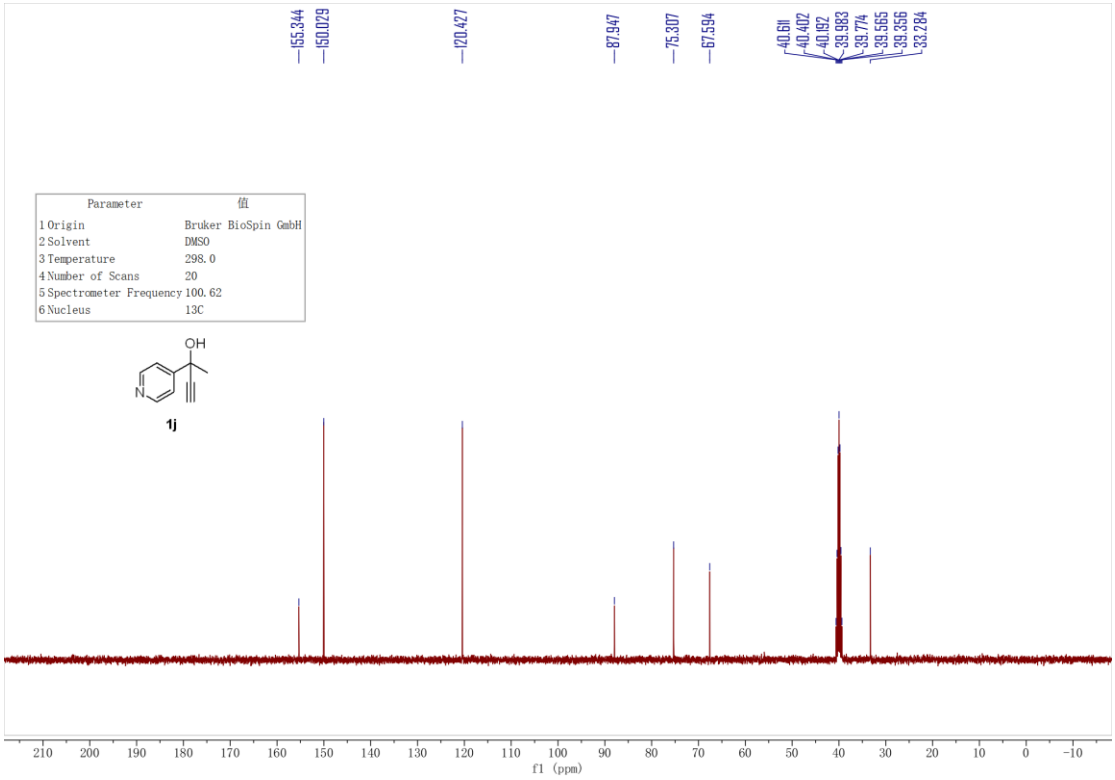
f1 (ppm)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Parameter 值
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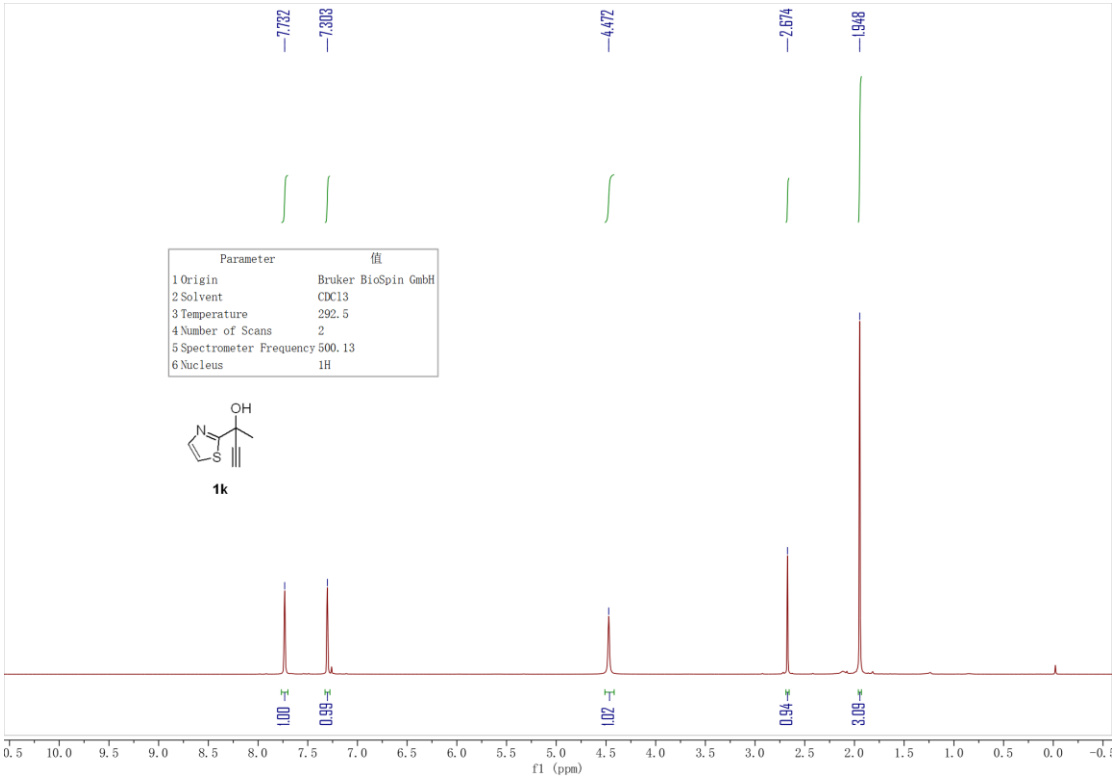
N
1j
f1 (ppm)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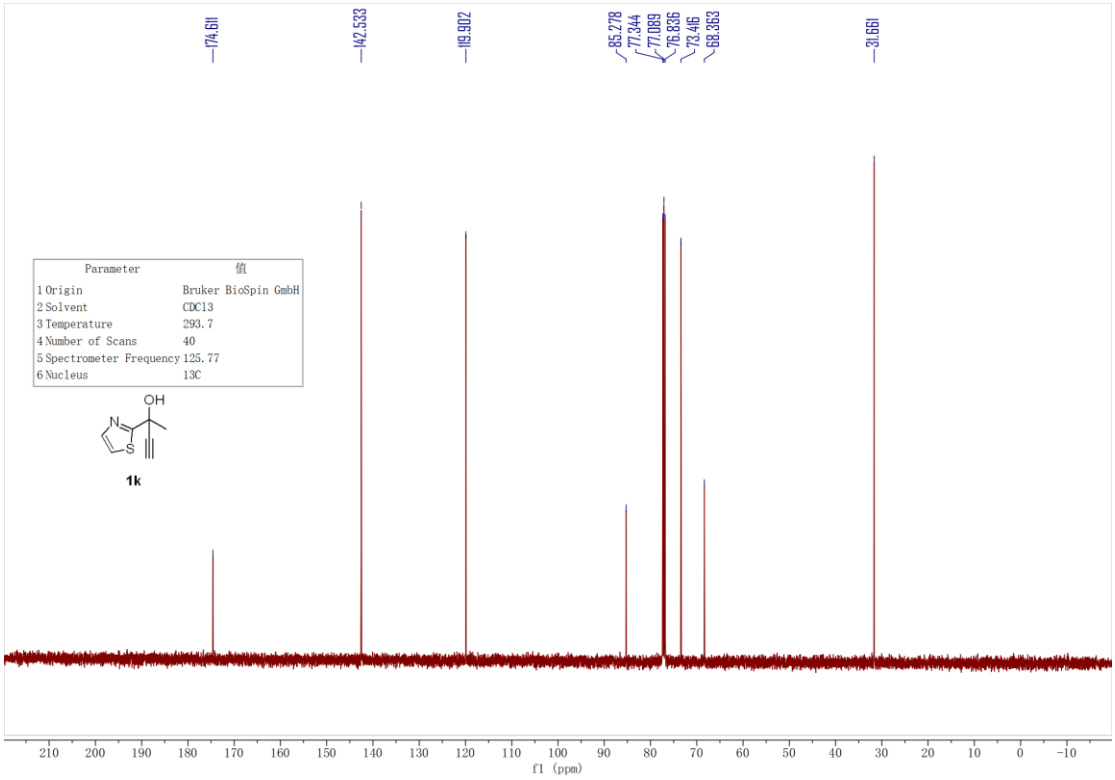
f1 (ppm)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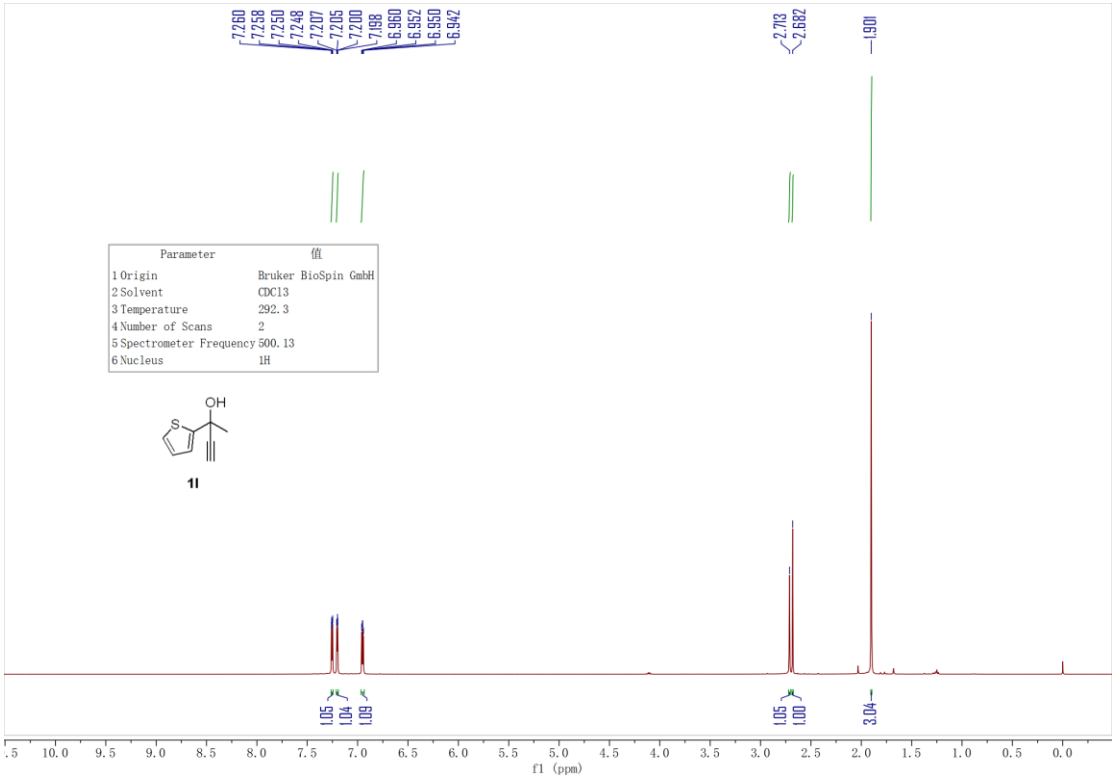
N
S
1k
f1 (ppm)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2.682
1.901
Parameter 值
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2 Solvent CDCl3
3 Temperature 292.3
4 Number of Scans 2
5 Spectrometer Frequency 500.13
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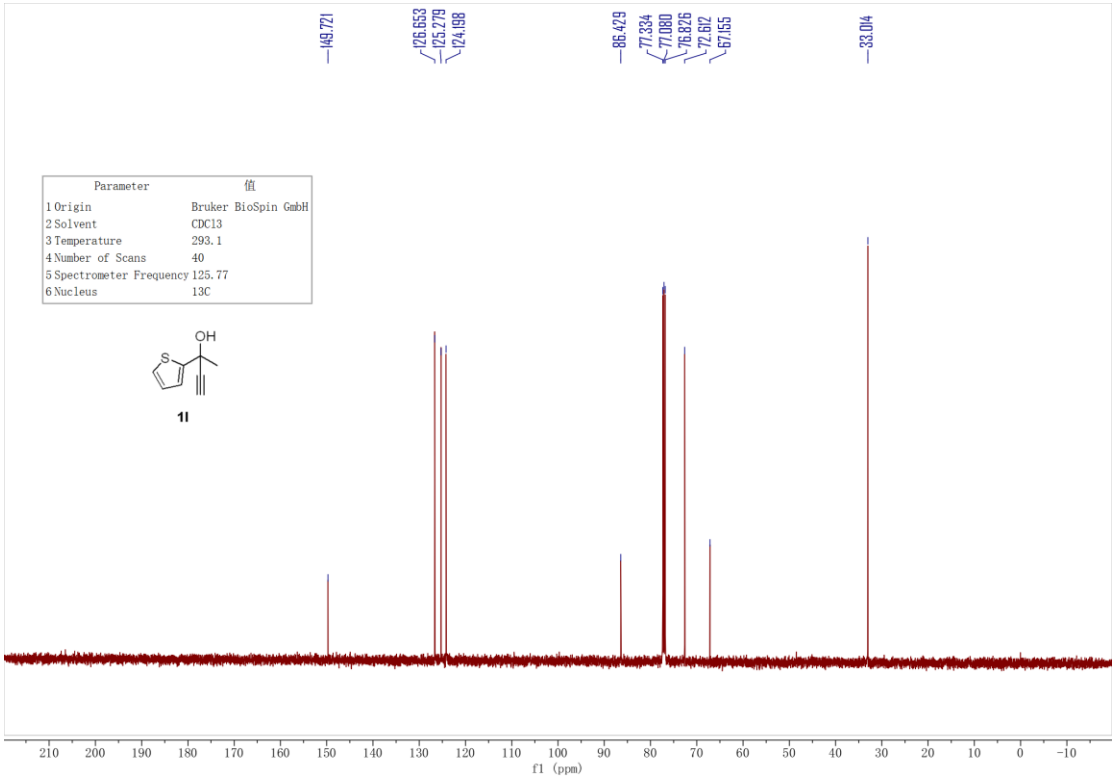
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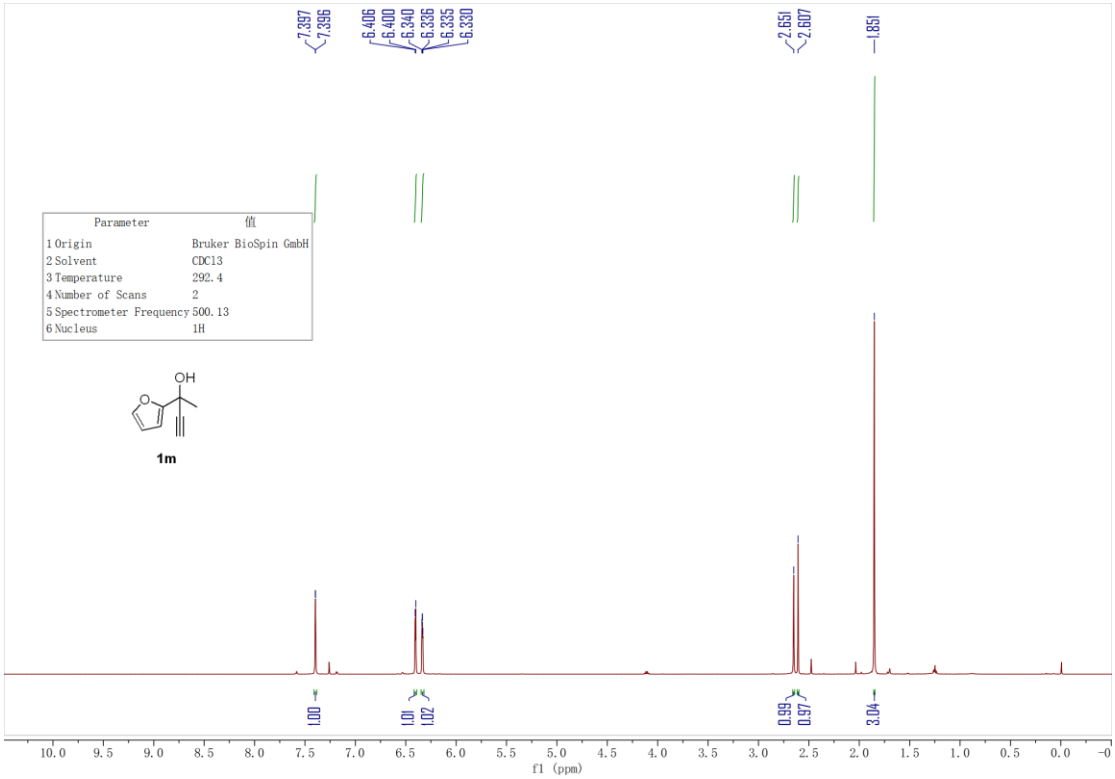
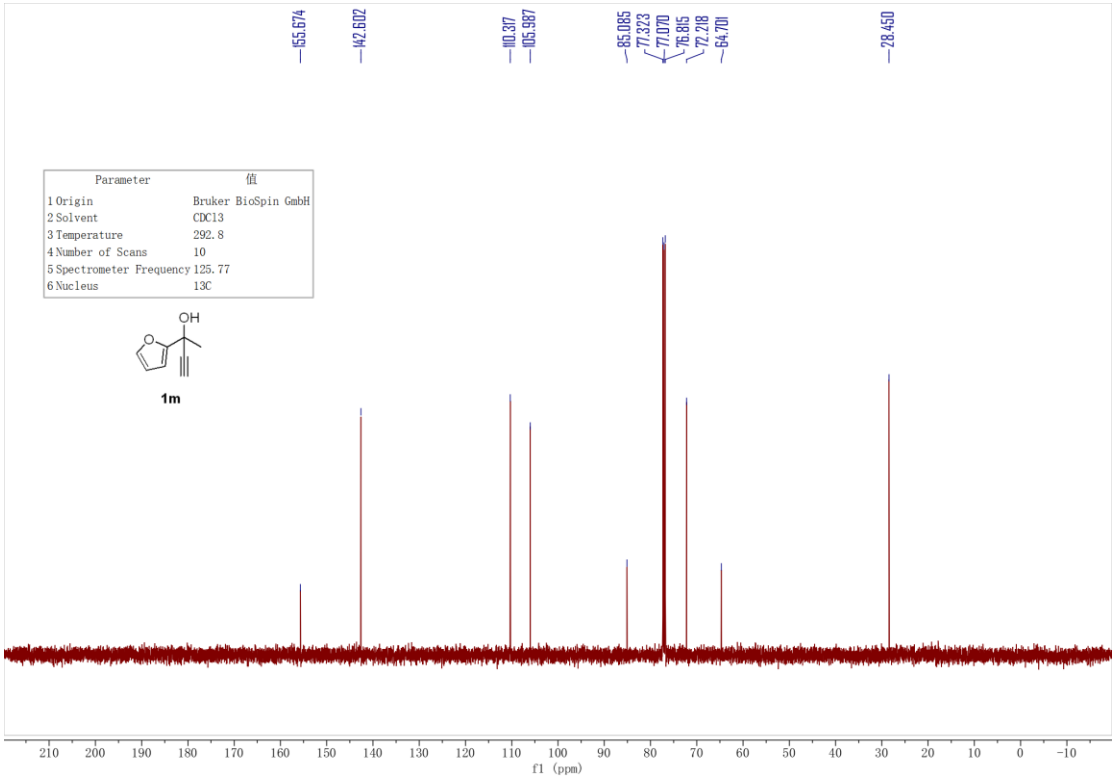
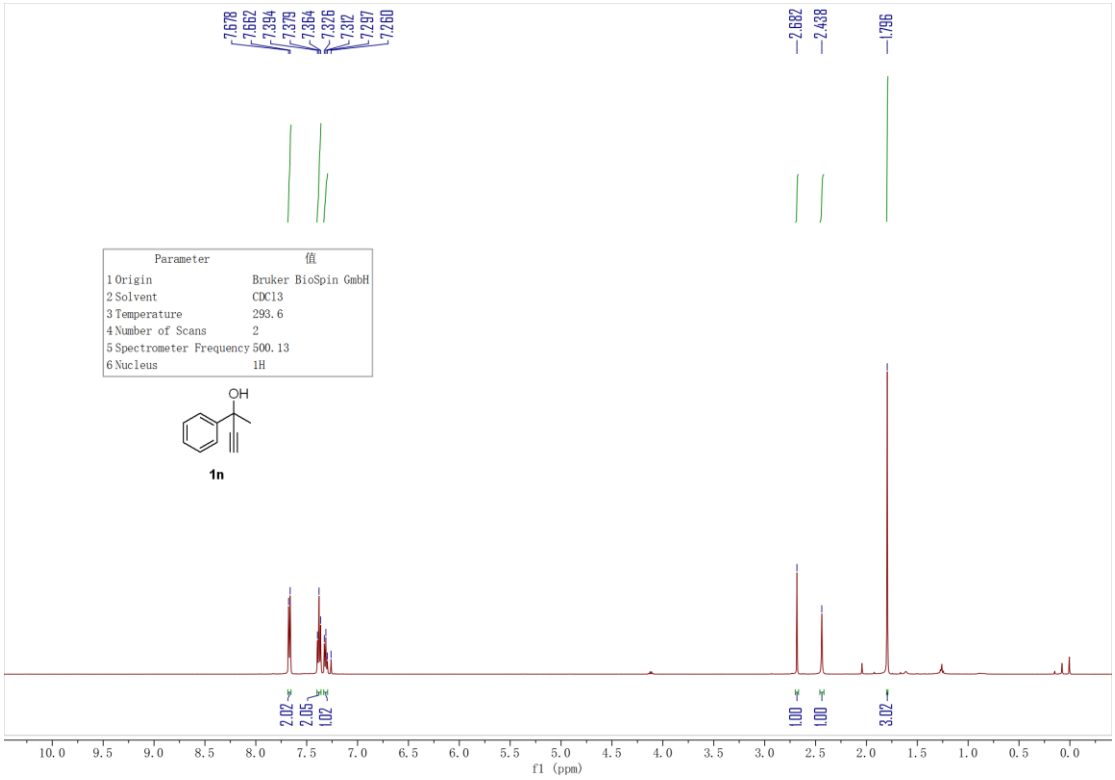
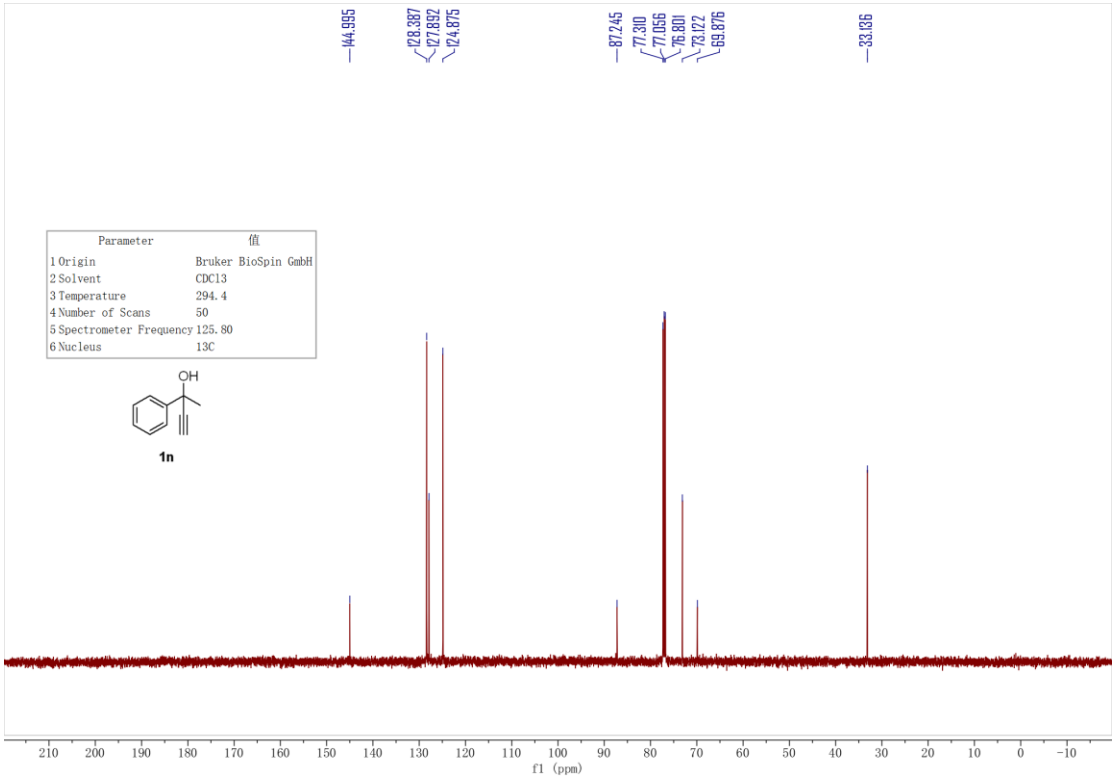
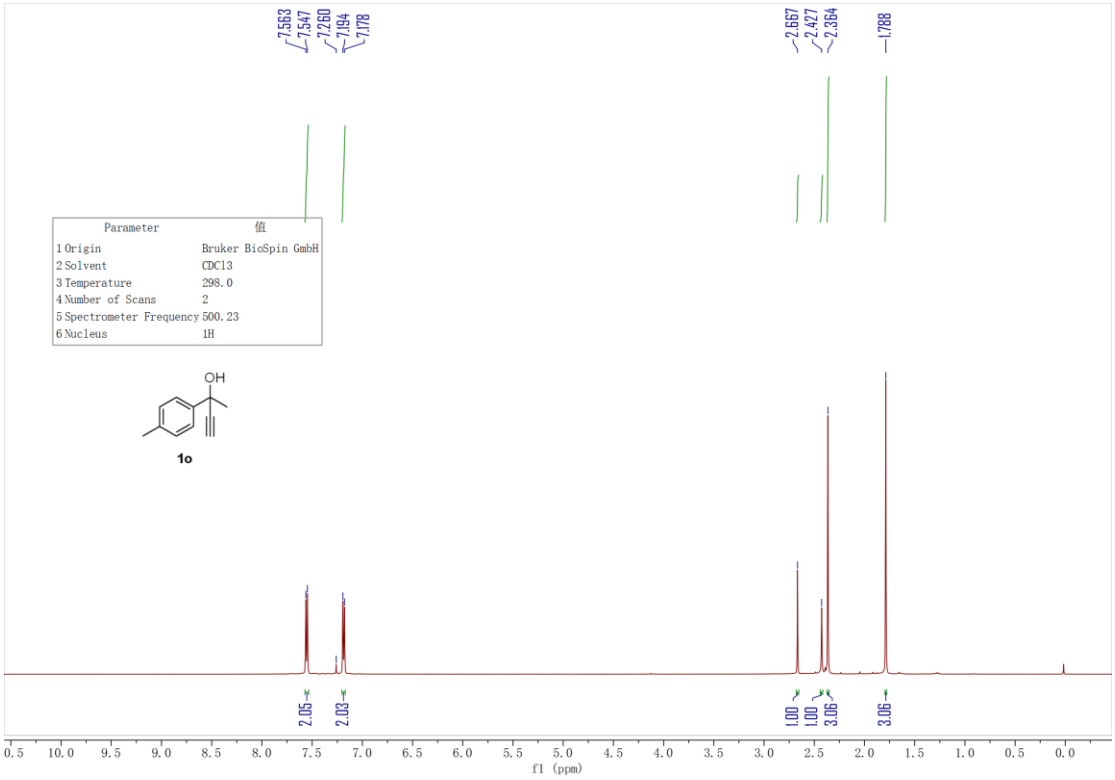
126.653
125.279
124.198
86.429
77.334
77.080
76.826
72.612
67.155
33.014
Parameter 值
1 Origin Bruker BioSpin GmbH
2 Solvent CDCl3
3 Temperature 293.1
4 Number of Scans 40
5 Spectrometer Frequency 125.77
6 Nucleus 13C
OH
S
1l
f1 (ppm)

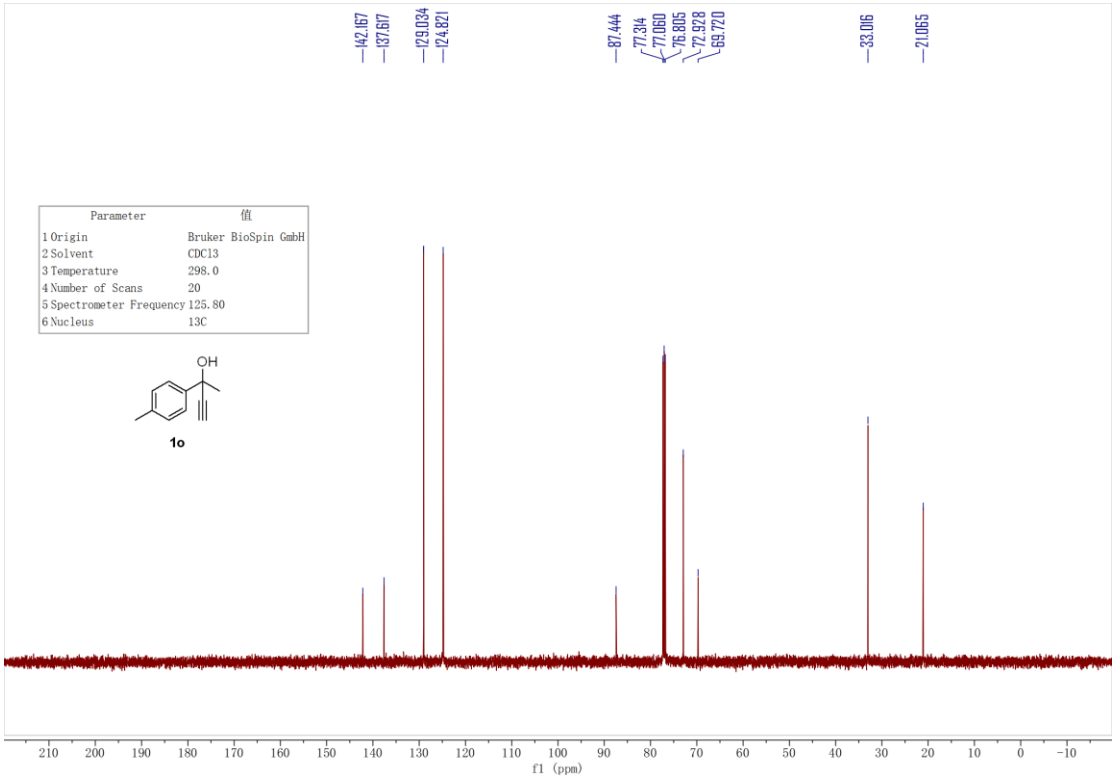

7.397
7.396
6.406
6.400
6.340
6.336
6.335
6.330
2.651
2.607
1.851
Parameter 值
1 Origin Bruker BioSpin GmbH
2 Solvent CDCl3
3 Temperature 292.4
4 Number of Scans 2
5 Spectrometer Frequency 500.13
6 Nucleus 1H
OH
O
1m
1.00
1.01
1.02
0.99
0.97
3.04
f1 (ppm)

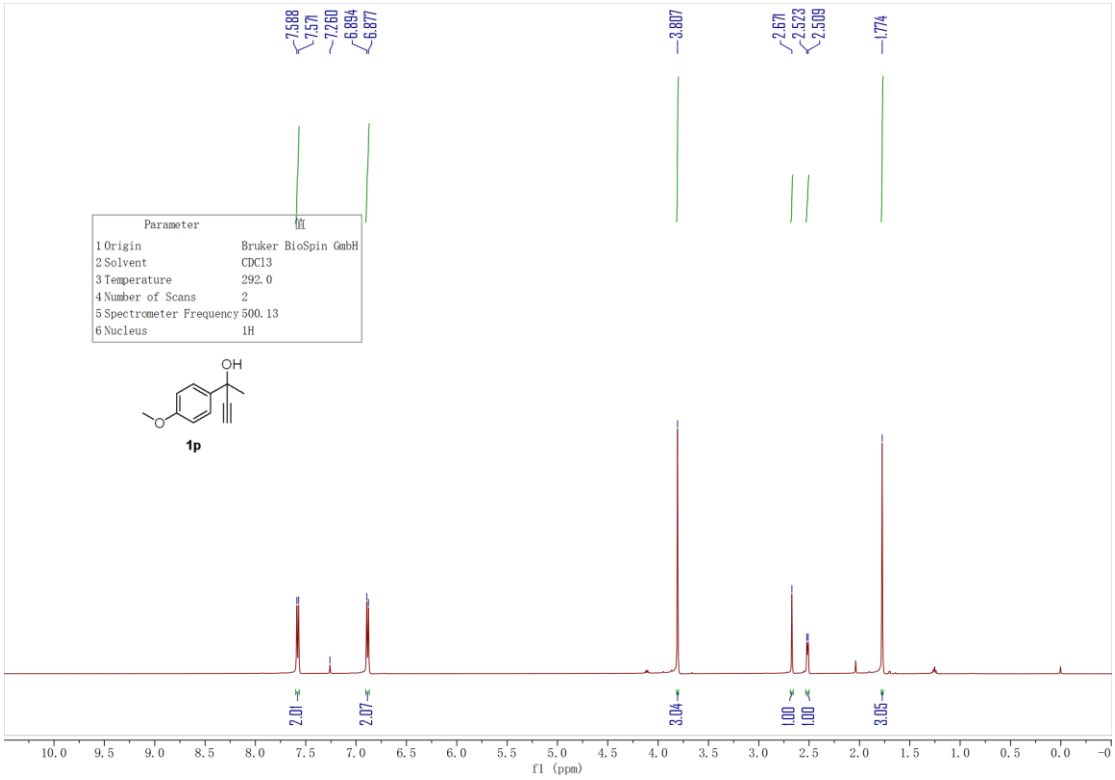

155.674
142.602
110.317
105.987
85.085
77.323
77.070
76.815
72.218
64.701
28.450
Parameter 值
1 Origin Bruker BioSpin GmbH
2 Solvent CDCl3
3 Temperature 292.8
4 Number of Scans 10
5 Spectrometer Frequency 125.77
6 Nucleus 13C
OH
1m
f1 (ppm)

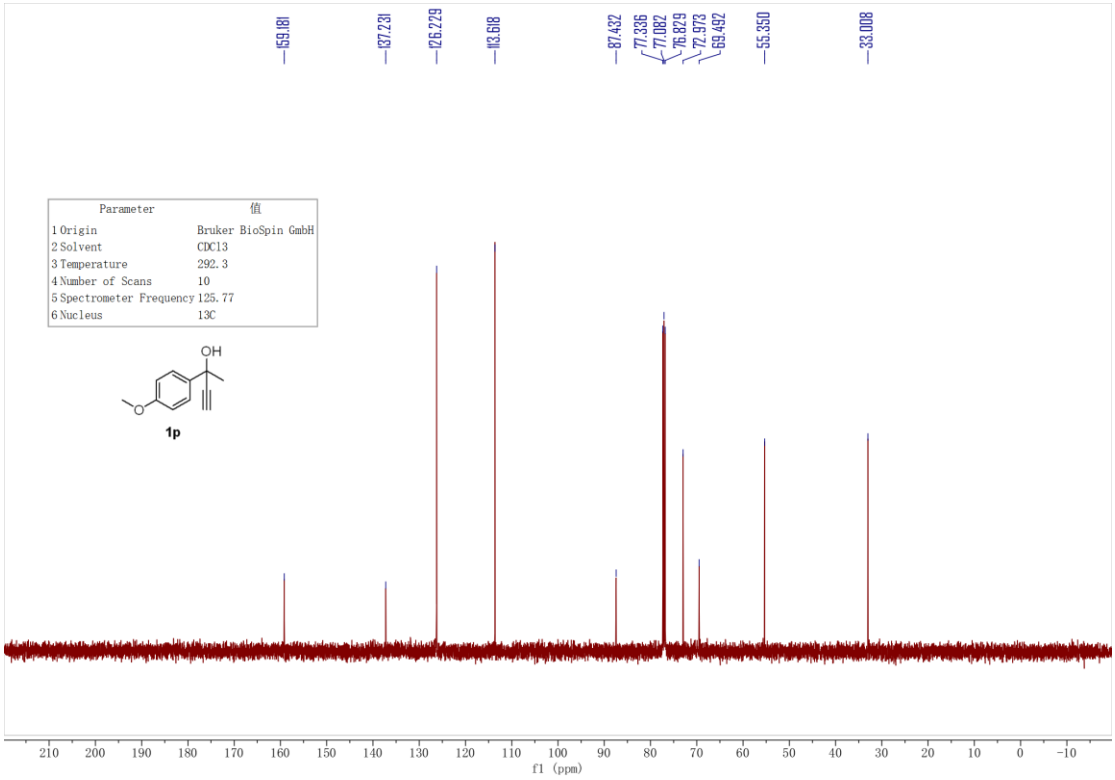

7.678
7.662
7.394
7.379
7.364
7.326
7.312
7.297
7.260
2.682
2.438
1.796
Parameter 值
1 Origin Bruker BioSpin GmbH
2 Solvent CDCl3
3 Temperature 293.6
4 Number of Scans 2
5 Spectrometer Frequency 500.13
6 Nucleus 1H
OH
1n
2.02
2.05
1.02
1.00
1.00
3.02
f1 (ppm)

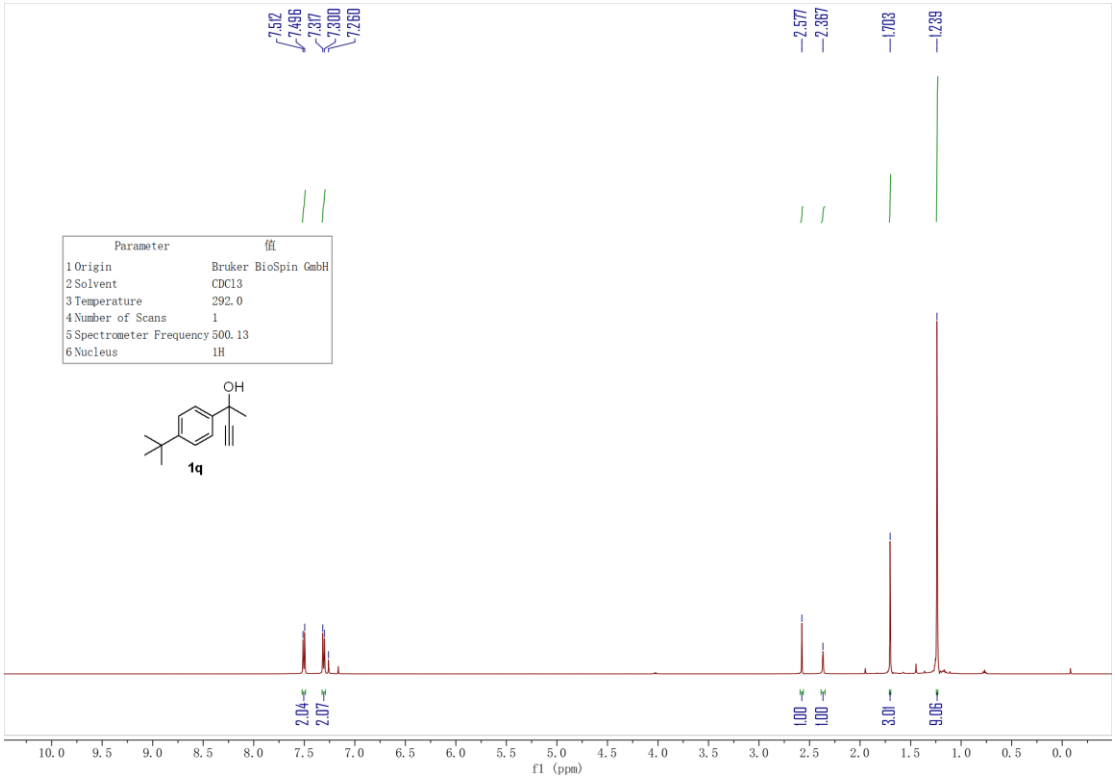

144.995
128.387
127.892
124.875
87.245
77.310
77.056
76.801
73.122
69.876
33.186
Parameter 值
1 Origin Bruker BioSpin GmbH
2 Solvent CDCl3
3 Temperature 294.4
4 Number of Scans 50
5 Spectrometer Frequency 125.80
6 Nucleus 13C
OH
1n
f1 (ppm)

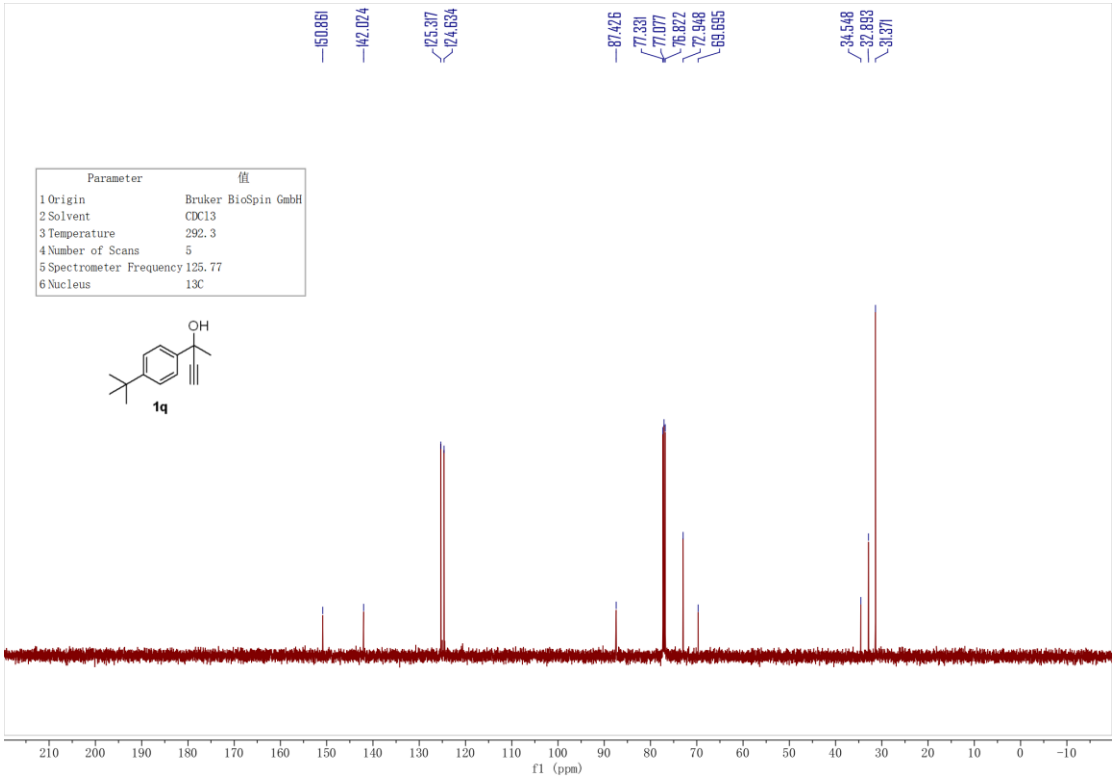

7.563
7.547
7.260
7.194
7.178
2.667
2.427
2.364
1.788
Parameter 值
1 Origin Bruker BioSpin GmbH
2 Solvent CDCl3
3 Temperature 298.0
4 Number of Scans 2
5 Spectrometer Frequency 500.23
6 Nucleus 1H
OH
1o
2.05
2.03
1.00
1.00
3.06
3.06
f1 (ppm)

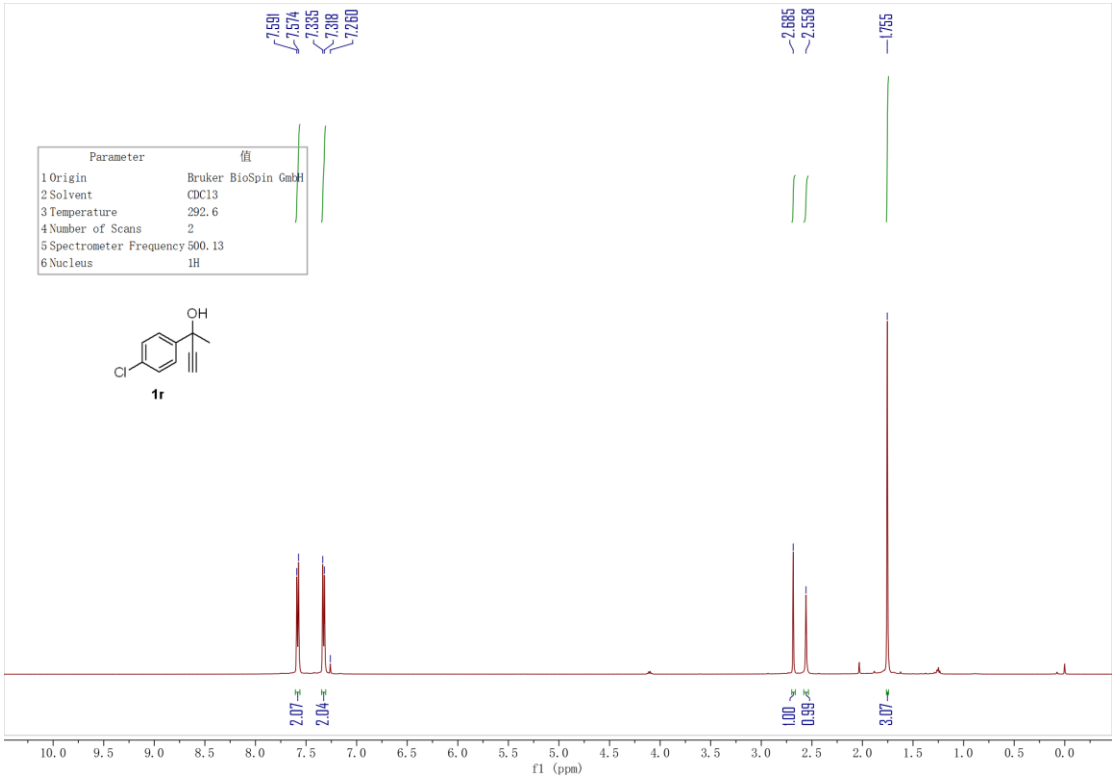

142.167
137.617
129.034
124.821
87.444
77.314
77.060
76.805
72.928
69.720
33.016
21.065
Parameter 值
1 Origin Bruker BioSpin GmbH
2 Solvent CDCl3
3 Temperature 298.0
4 Number of Scans 20
5 Spectrometer Frequency 125.80
6 Nucleus 13C
OH
1o
f1 (ppm)

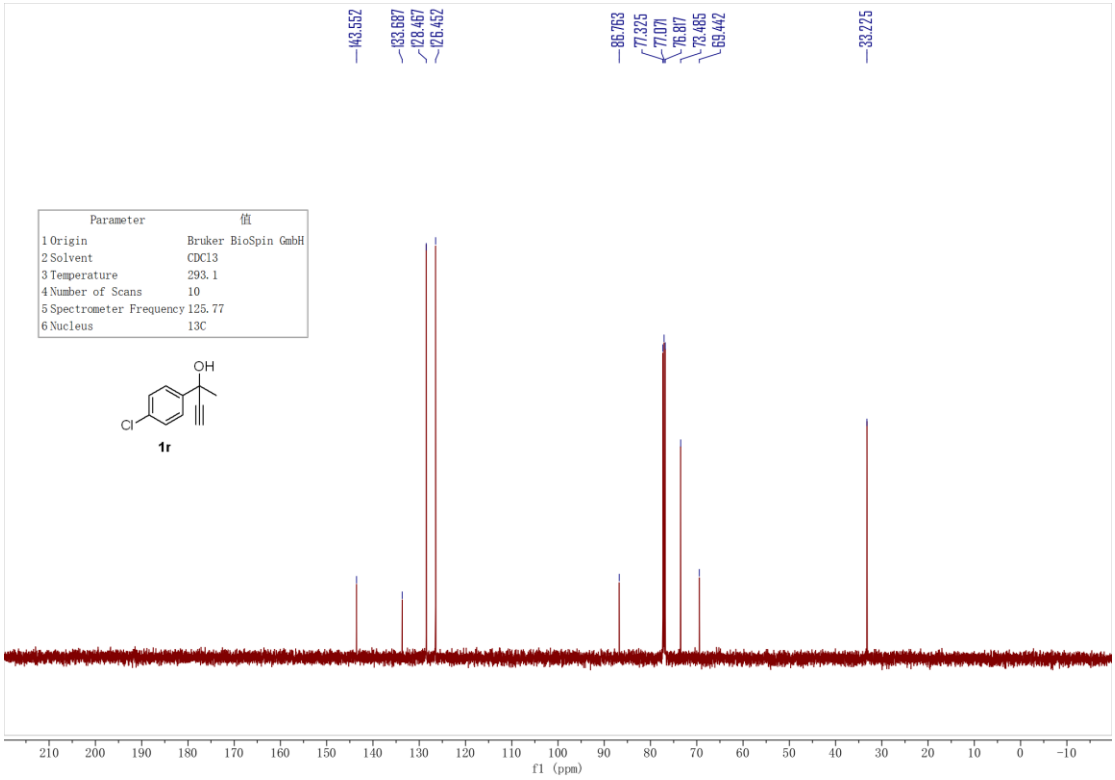

7.588
7.571
7.260
6.894
6.877
3.807
2.671
2.523
2.509
1.774
Parameter 值
1 Origin Bruker BioSpin GmbH
2 Solvent CDCl3
3 Temperature 292.0
4 Number of Scans 2
5 Spectrometer Frequency 500.13
6 Nucleus 1H
OH
1p
2.01
2.07
3.04
1.00
1.00
3.05
f1 (ppm)

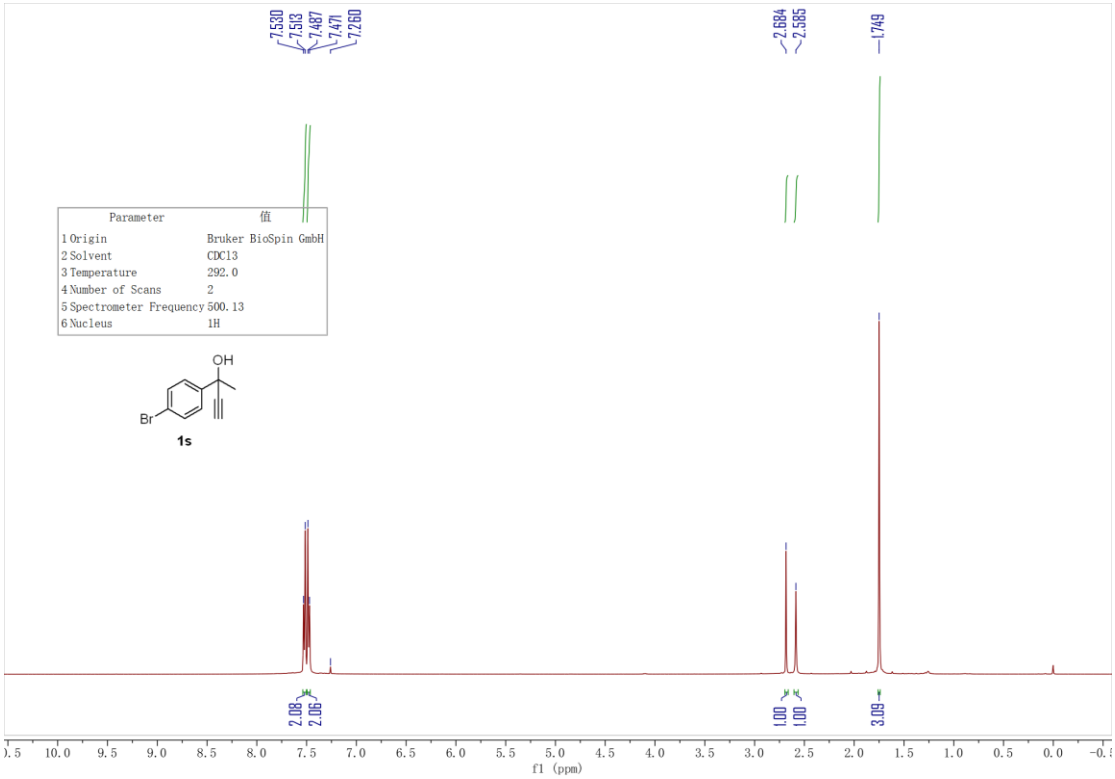

159.181
137.231
126.229
113.618
87.432
77.336
77.082
76.829
72.973
69.492
55.350
33.008
Parameter 值
1 Origin Bruker BioSpin GmbH
2 Solvent CDCl3
3 Temperature 292.3
4 Number of Scans 10
5 Spectrometer Frequency 125.77
6 Nucleus 13C
OH
O
1p
f1 (ppm)

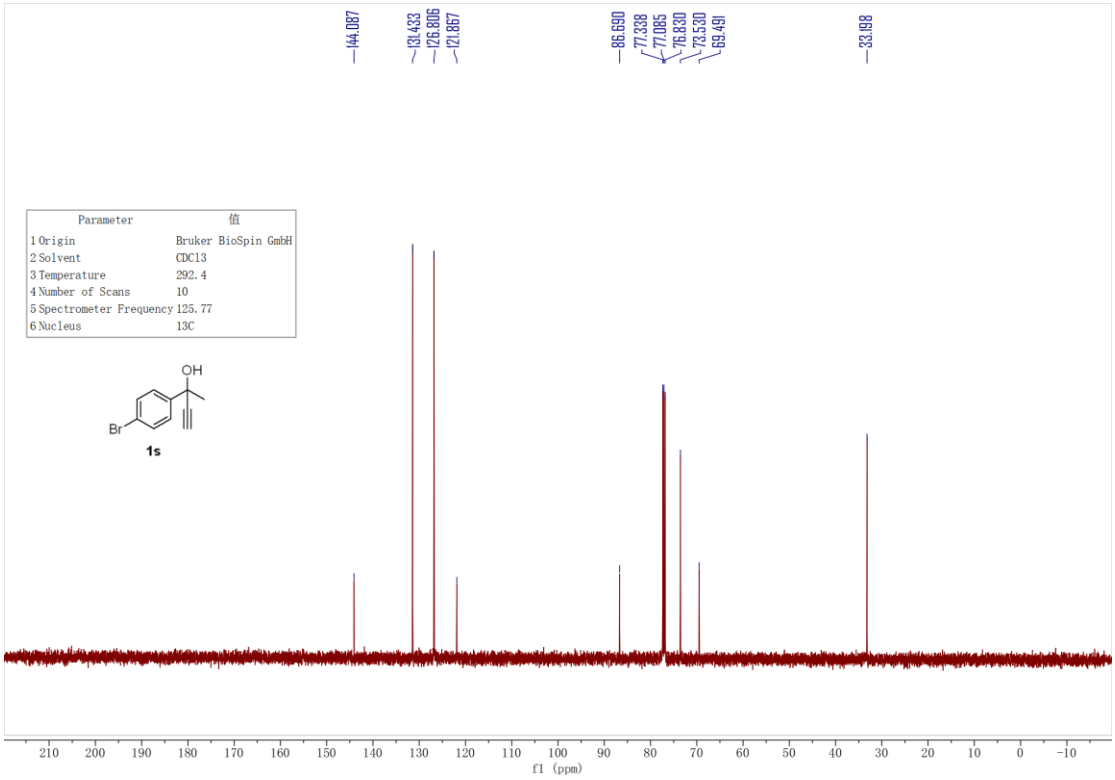

7.512
7.496
7.317
7.300
7.260
2.577
2.367
1.703
1.239
Parameter 值
1 Origin Bruker BioSpin GmbH
2 Solvent CDCl3
3 Temperature 292.0
4 Number of Scans 1
5 Spectrometer Frequency 500.13
6 Nucleus 1H
OH
1q
2.04
2.07
1.00
1.00
3.01
9.06
f1 (ppm)


150.861
142.024
125.397
124.634
87.426
77.331
77.077
76.822
72.948
69.695
34.548
32.893
31.371
Parameter 值
1 Origin Bruker BioSpin GmbH
2 Solvent CDCl3
3 Temperature 292.3
4 Number of Scans 5
5 Spectrometer Frequency 125.77
6 Nucleus 13C
OH
1q
f1 (ppm)


7.591
7.574
7.335
7.318
7.260
2.685
2.558
1.755
Parameter 值
1 Origin Bruker BioSpin GmbH
2 Solvent CDCl3
3 Temperature 292.6
4 Number of Scans 2
5 Spectrometer Frequency 500.13
6 Nucleus 1H
OH
Cl
1r
2.07
2.04
1.00
0.99
3.07
f1 (ppm)


143.552
133.687
128.467
126.452
86.763
77.325
77.071
76.817
73.485
69.442
33.225
Parameter 值
1 Origin Bruker BioSpin GmbH
2 Solvent CDCl3
3 Temperature 293.1
4 Number of Scans 10
5 Spectrometer Frequency 125.77
6 Nucleus 13C
OH
Cl
1r
f1 (ppm)


7.530
7.513
7.487
7.471
7.260
2.684
2.665
1.749
Parameter 值
1 Origin Bruker BioSpin GmbH
2 Solvent CDCl3
3 Temperature 292.0
4 Number of Scans 2
5 Spectrometer Frequency 500.13
6 Nucleus 1H
OH
Br
1s
2.08
2.06
1.00
1.00
3.09
f1 (ppm)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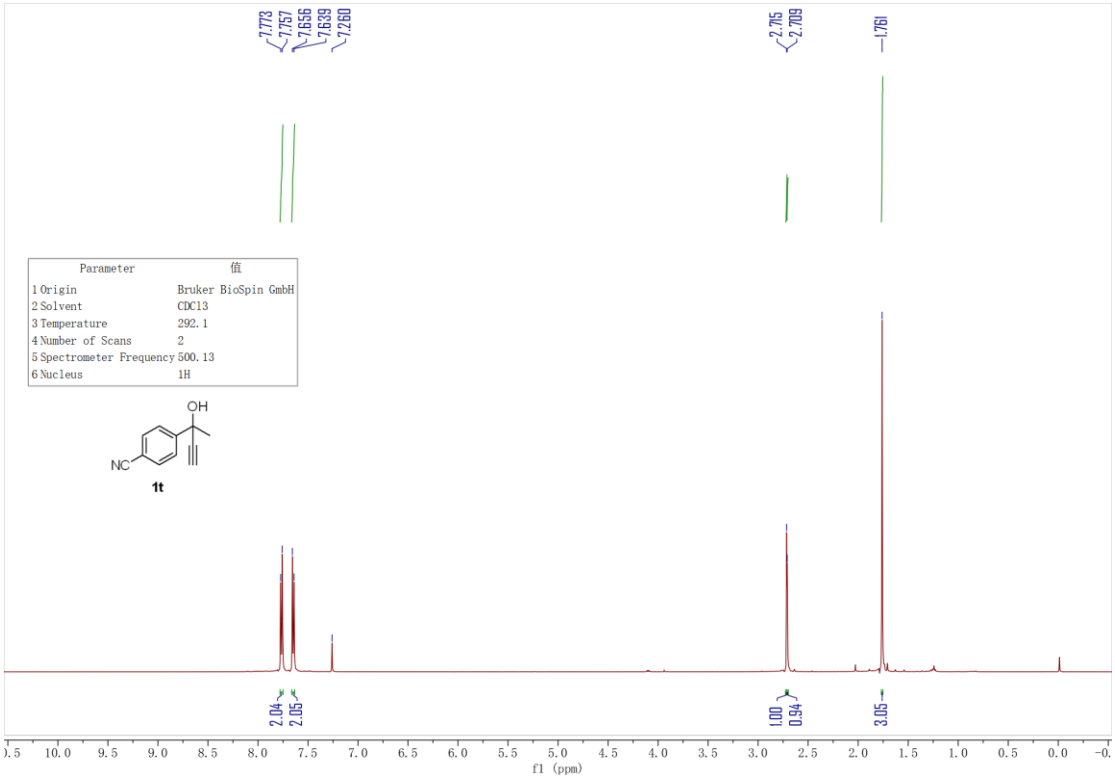
121.867
86.690
77.338
77.085
76.830
73.530
69.491
33.198
Parameter 值
1 Origin Bruker BioSpin GmbH
2 Solvent CDCl3
3 Temperature 292.4
4 Number of Scans 10
5 Spectrometer Frequency 125.77
6 Nucleus 13C
OH
Br
1s
f1 (ppm)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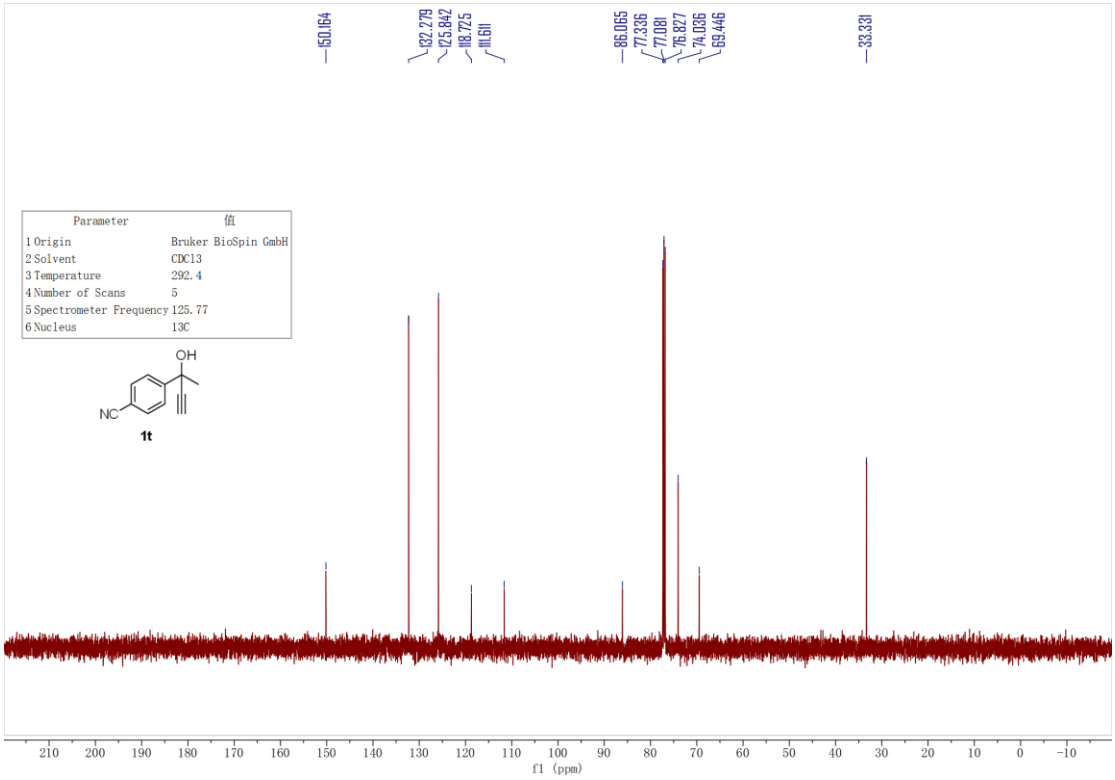
7.757
7.656
7.639
7.260
2.715
2.709
1.761
Parameter 值
1 Origin Bruker BioSpin GmbH
2 Solvent CDCl3
3 Temperature 292.1
4 Number of Scans 2
5 Spectrometer Frequency 500.13
6 Nucleus 1H
OH
NC
1t
2.04
2.05
1.00
0.94
3.05
f1 (ppm)


150.164
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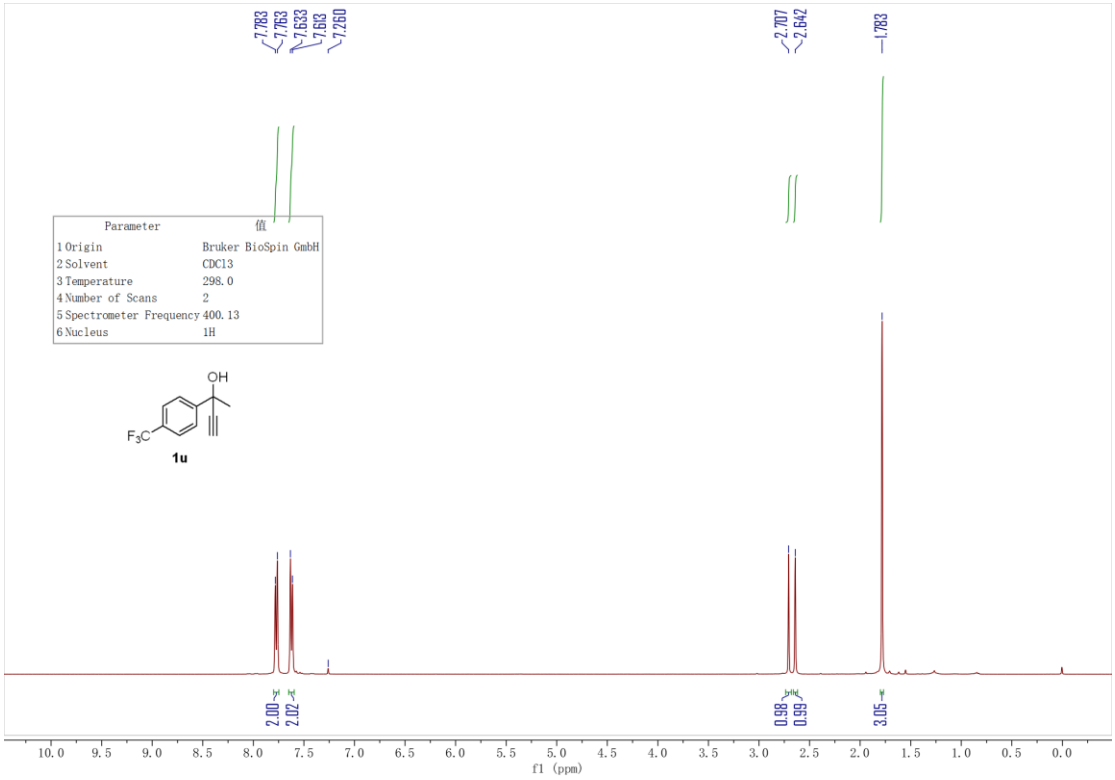
125.842
118.725
111.611
86.065
77.336
77.081
76.827
74.036
69.446
33.331
Parameter 值
1 Origin Bruker BioSpin GmbH
2 Solvent CDCl3
3 Temperature 292.4
4 Number of Scans 5
5 Spectrometer Frequency 125.77
6 Nucleus 13C
OH
NC
1t
f1 (ppm)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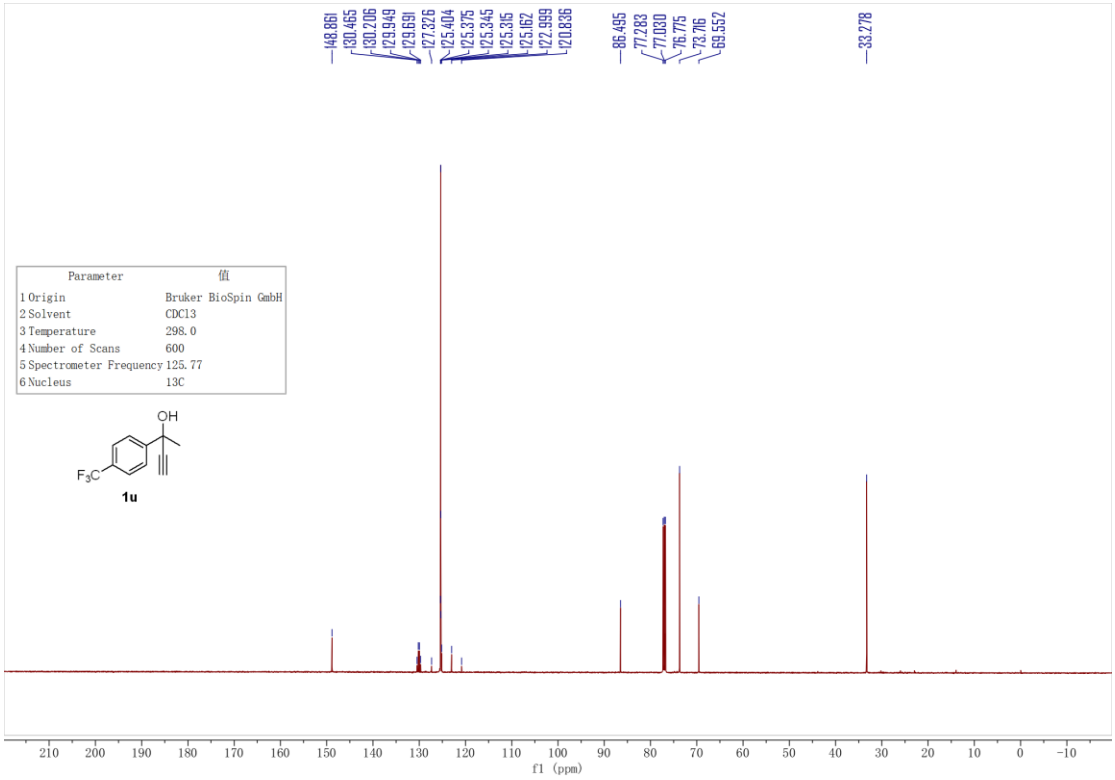
7.763
7.633
7.613
7.260
2.707
2.642
1.783
Parameter 值
1 Origin Bruker BioSpin GmbH
2 Solvent CDCl3
3 Temperature 298.0
4 Number of Scans 2
5 Spectrometer Frequency 400.13
6 Nucleus 1H
OH
F3C
1u
2.00
2.02
0.98
0.99
3.05
f1 (ppm)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125.375
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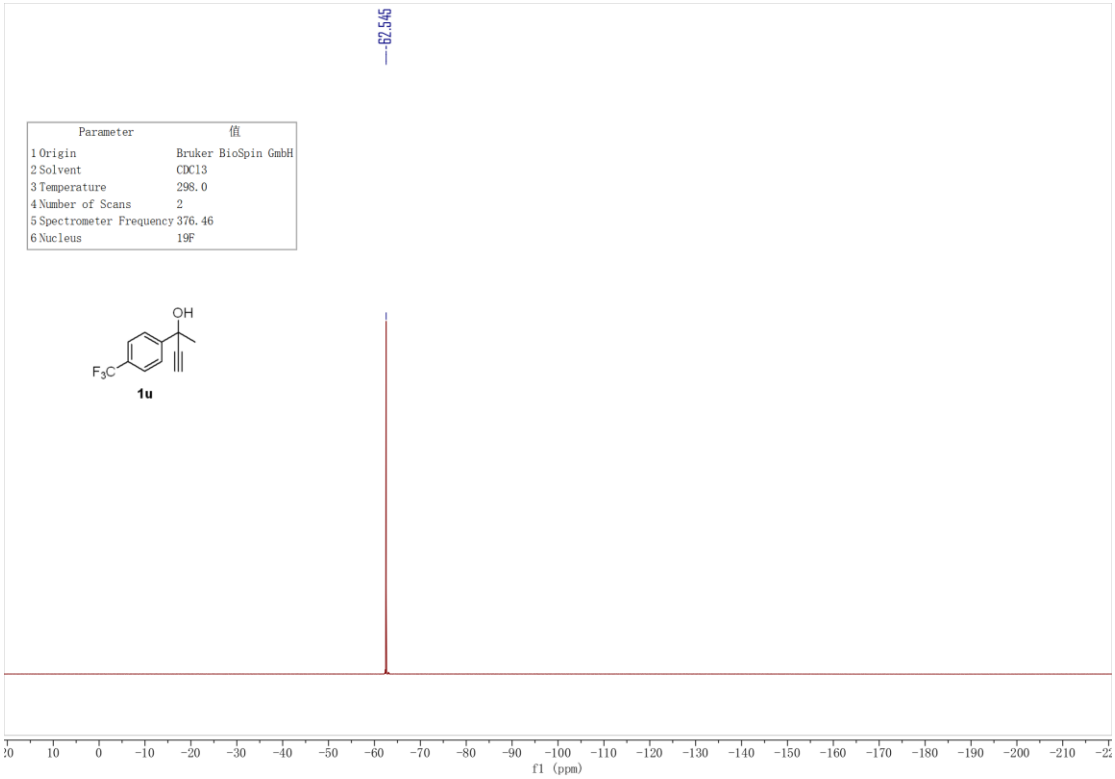
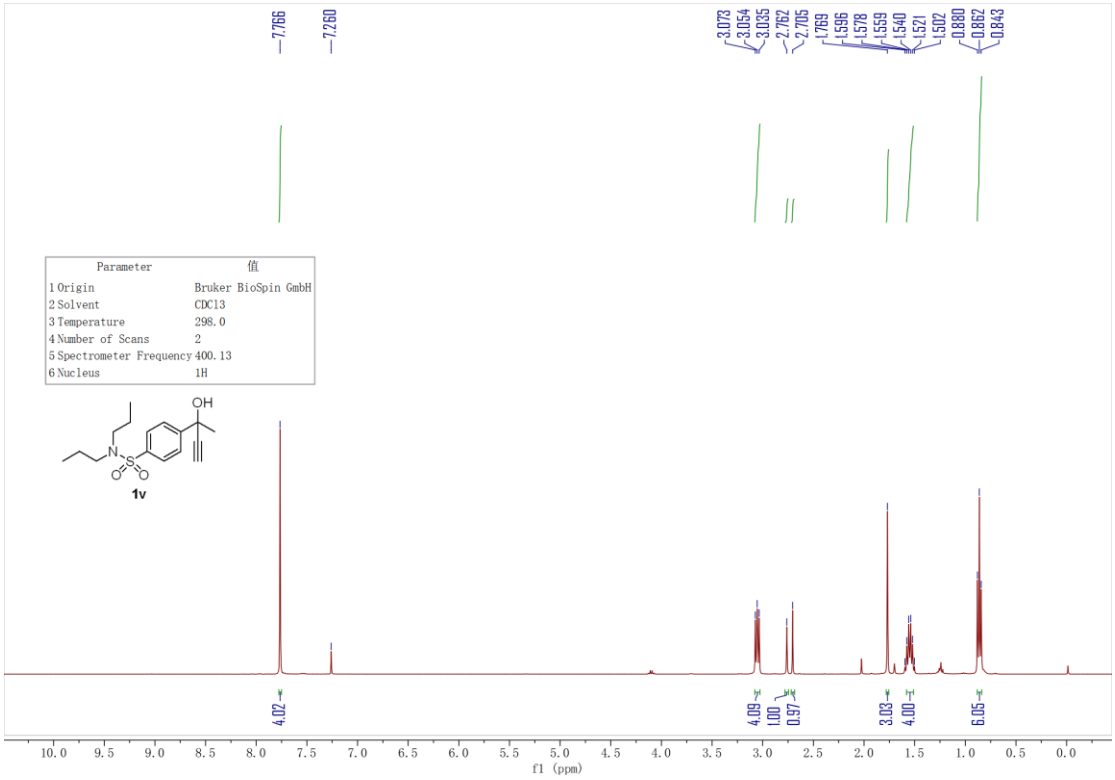
125.315
125.162
122.999
120.836
86.495
77.283
77.030
76.775
73.716
69.552
33.278
Parameter 值
1 Origin Bruker BioSpin GmbH
2 Solvent CDCl3
3 Temperature 298.0
4 Number of Scans 600
5 Spectrometer Frequency 125.77
6 Nucleus 13C
OH
F3C
1u
f1 (ppm)


62.545
Parameter 值
1 Origin Bruker BioSpin GmbH
2 Solvent CDCl3
3 Temperature 298.0
4 Number of Scans 2
5 Spectrometer Frequency 376.46
6 Nucleus 19F
OH
F3C
1u
f1 (ppm)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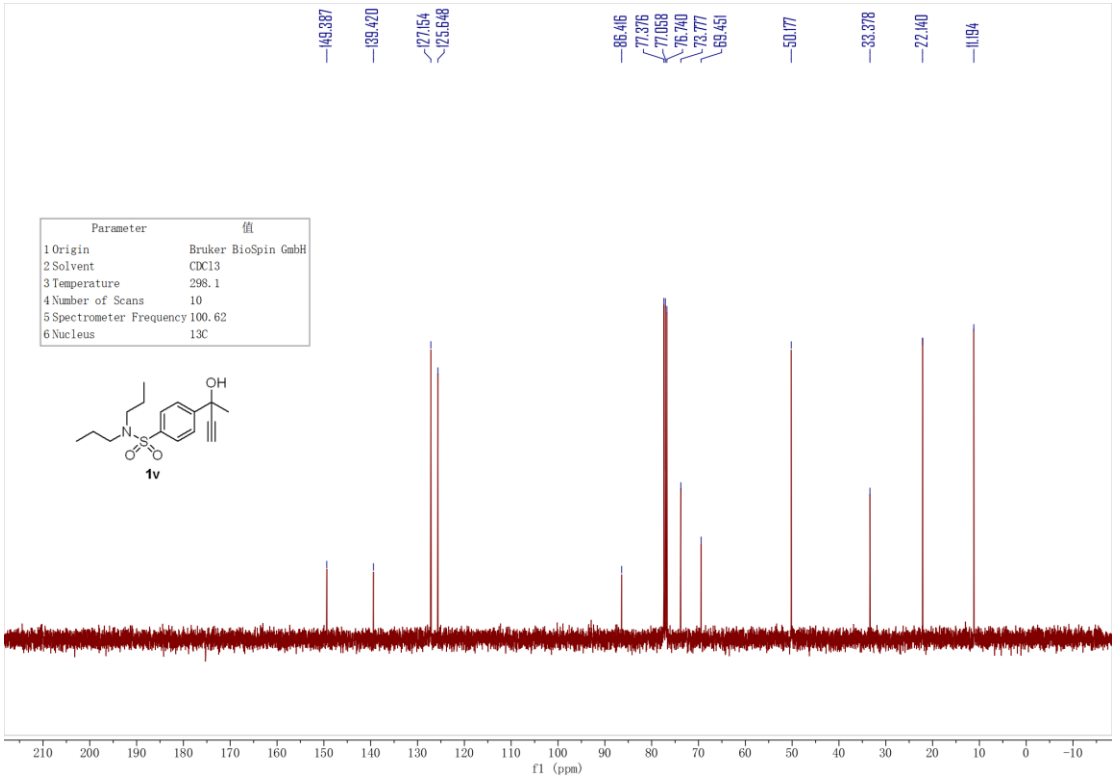
2.762
2.705
1.769
1.596
1.578
1.559
1.540
1.521
1.502
0.880
0.862
0.843
Parameter 值
1 Origin Bruker BioSpin GmbH
2 Solvent CDCl3
3 Temperature 298.0
4 Number of Scans 2
5 Spectrometer Frequency 400.13
6 Nucleus 1H
OH
1v
4.02
4.09
1.00
0.97
3.03
4.00
6.05
f1 (ppm)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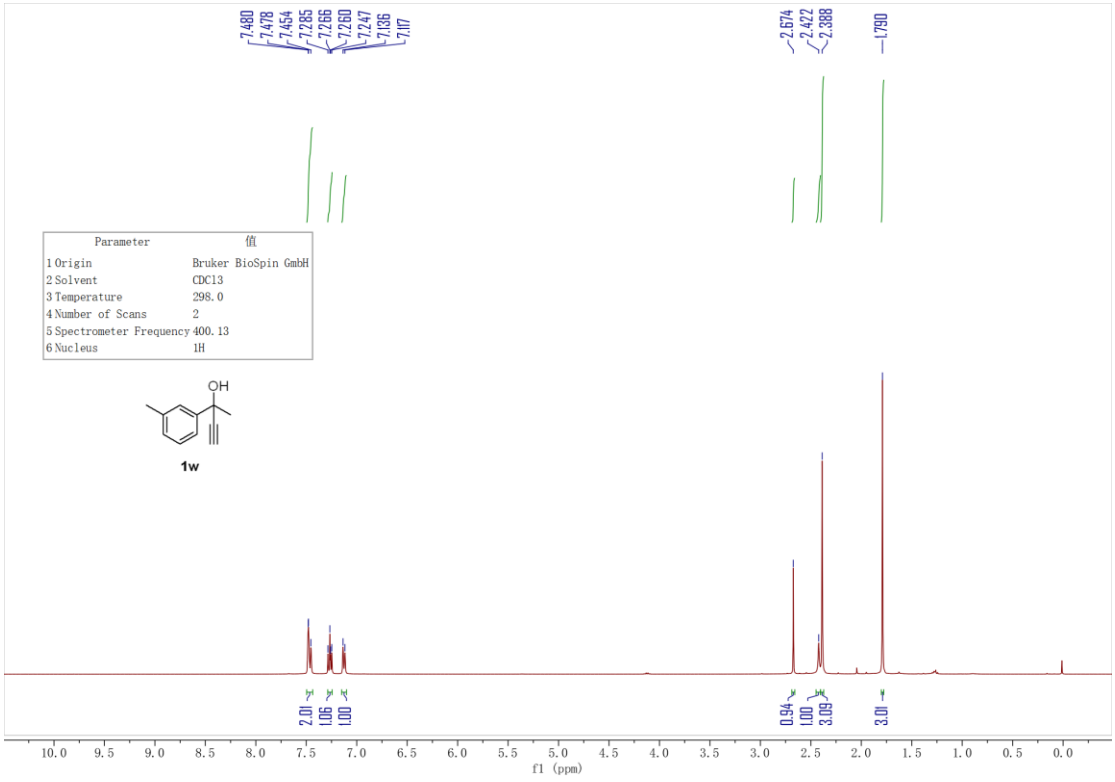
71.376
77.058
76.740
73.777
69.451
50.177
33.378
22.140
11.194
Parameter 值
1 Origin Bruker BioSpin GmbH
2 Solvent CDCl3
3 Temperature 298.1
4 Number of Scans 10
5 Spectrometer Frequency 100.62
6 Nucleus 13C
OH
1v
f1 (ppm)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7.260
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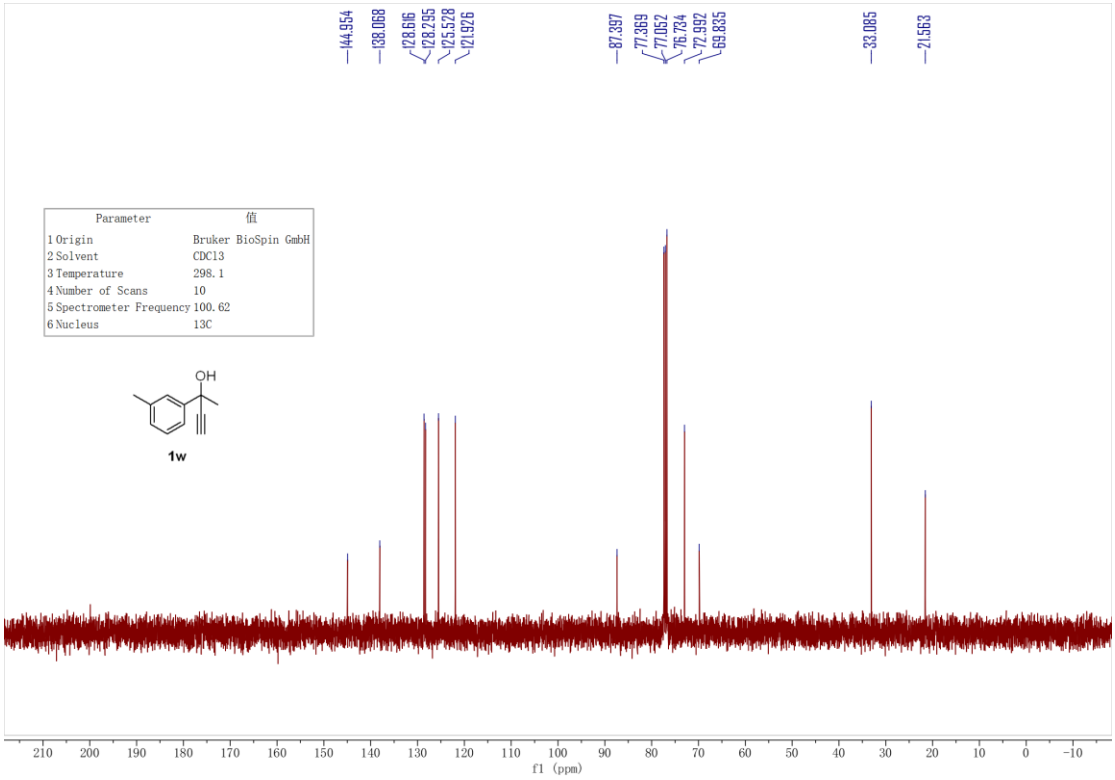
7.136
7.117
2.674
2.422
2.388
1.790
Parameter 值
1 Origin Bruker BioSpin GmbH
2 Solvent CDCl3
3 Temperature 298.0
4 Number of Scans 2
5 Spectrometer Frequency 400.13
6 Nucleus 1H
OH
1w
2.01
1.06
1.00
0.94
1.00
3.09
3.01
f1 (ppm)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128.295
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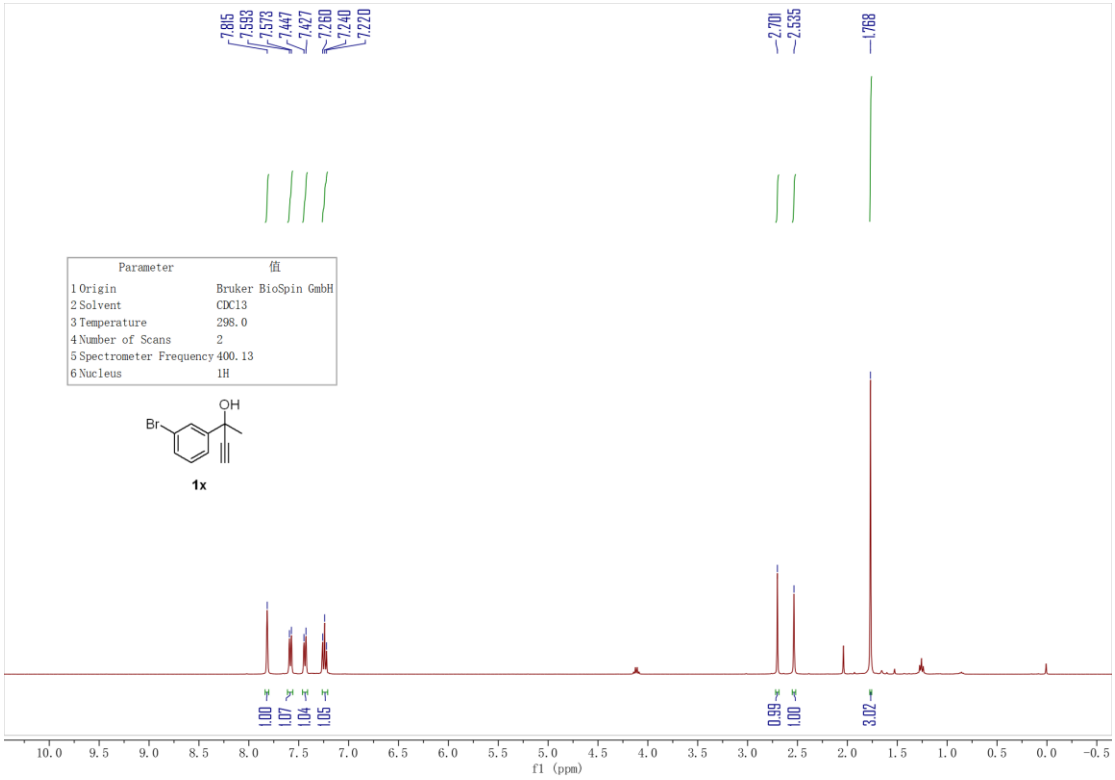
121.926
87.397
77.369
77.052
76.734
72.992
69.835
33.085
21.563
Parameter 值
1 Origin Bruker BioSpin GmbH
2 Solvent CDCl3
3 Temperature 298.1
4 Number of Scans 10
5 Spectrometer Frequency 100.62
6 Nucleus 13C
OH
1w
f1 (ppm)


7.895
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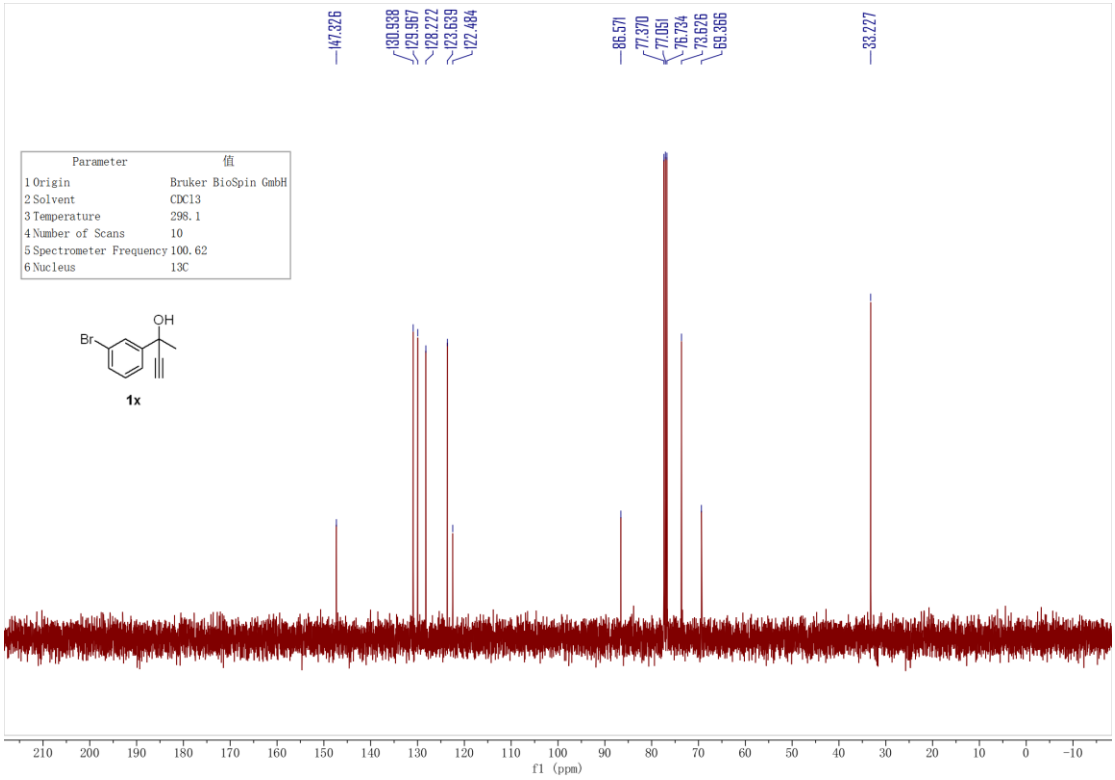
7.573
7.447
7.427
7.260
7.240
7.220
2.701
2.535
1.768
Parameter 值
1 Origin Bruker BioSpin GmbH
2 Solvent CDCl3
3 Temperature 298.0
4 Number of Scans 2
5 Spectrometer Frequency 400.13
6 Nucleus 1H
OH
Br
1x
1.00
1.07
1.04
1.05
0.99
1.00
3.02
f1 (ppm)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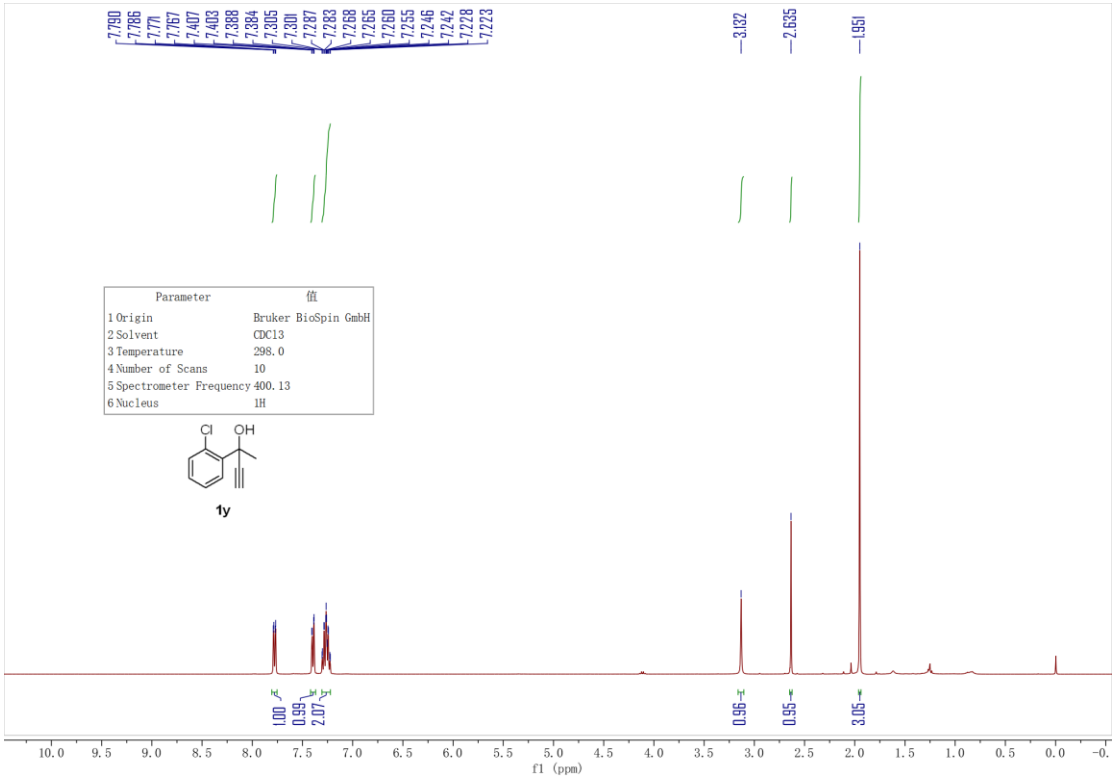
86.571
77.370
77.051
76.734
73.626
69.366
33.227
Parameter 值
1 Origin Bruker BioSpin GmbH
2 Solvent CDCl3
3 Temperature 298.1
4 Number of Scans 10
5 Spectrometer Frequency 100.62
6 Nucleus 13C
OH
Br
1x
f1 (ppm)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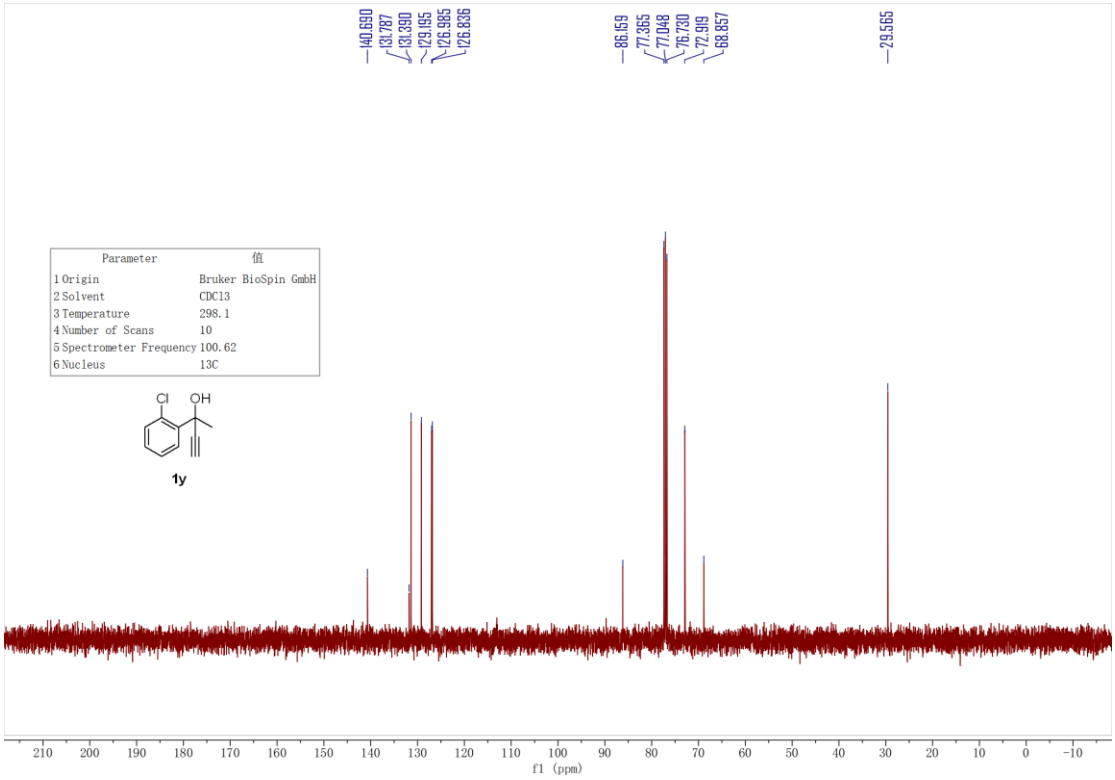
7.268
7.265
7.260
7.255
7.246
7.242
7.228
7.223
3.632
2.635
1.951
Parameter 值
1 Origin Bruker BioSpin GmbH
2 Solvent CDCl3
3 Temperature 298.0
4 Number of Scans 10
5 Spectrometer Frequency 400.13
6 Nucleus 1H
Cl OH
1y
1.00
0.99
2.07
0.96
0.95
3.05
f1 (ppm)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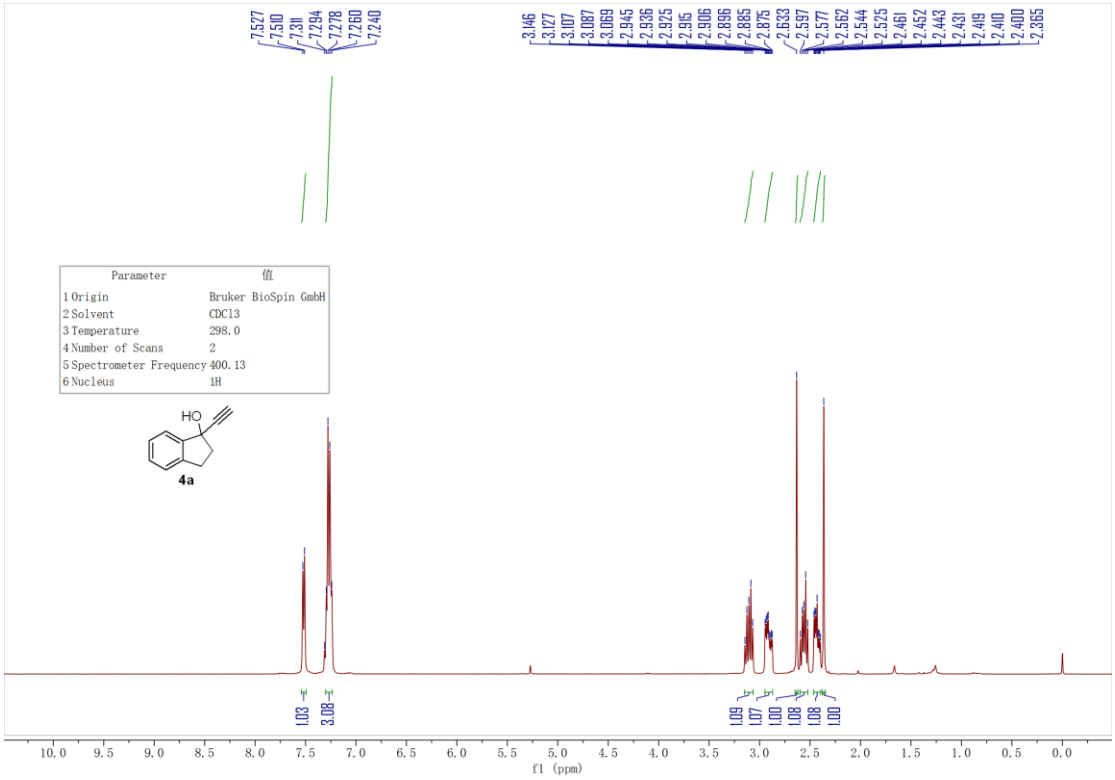
86.159
77.365
77.048
76.730
72.919
68.857
29.565
Parameter 值
1 Origin Bruker BioSpin GmbH
2 Solvent CDCl3
3 Temperature 298.1
4 Number of Scans 10
5 Spectrometer Frequency 100.62
6 Nucleus 13C
Cl OH
1y
f1 (ppm)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7.240
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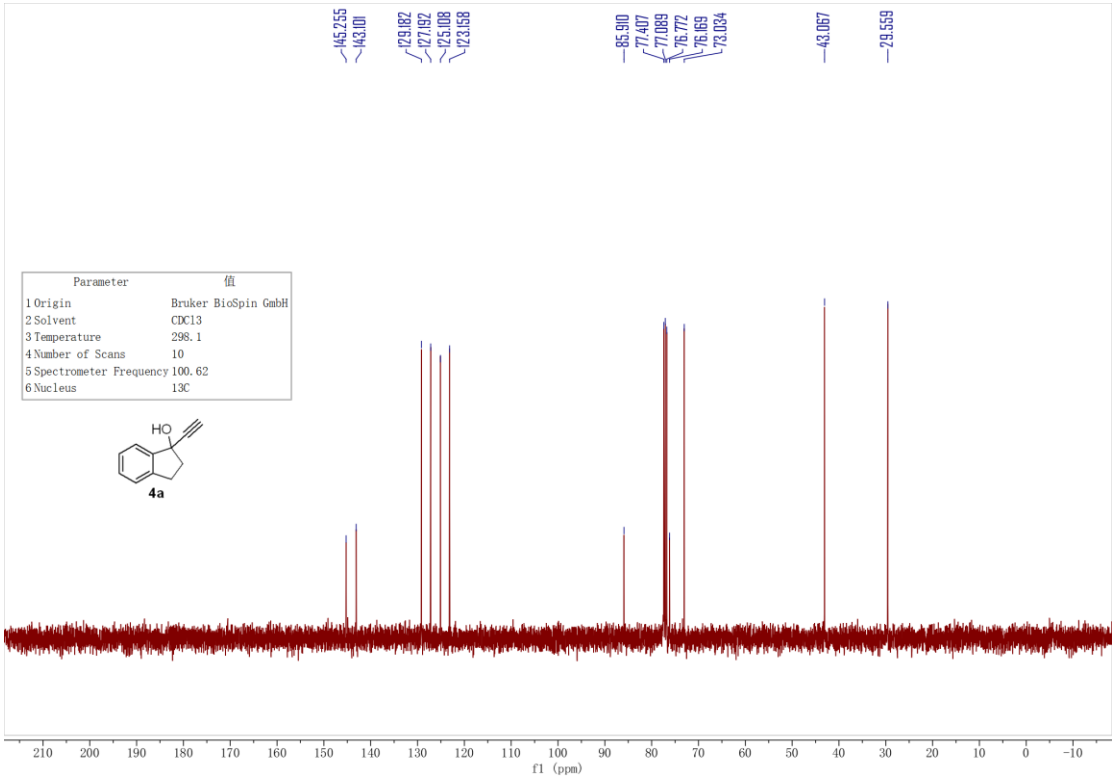
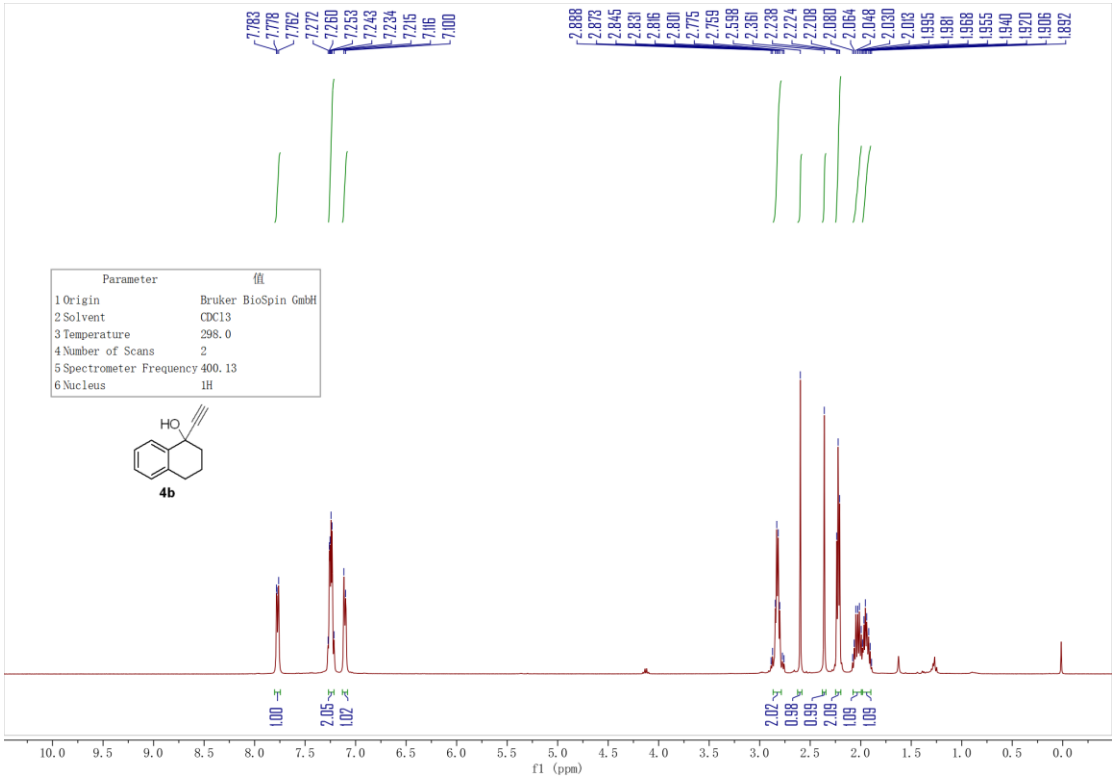
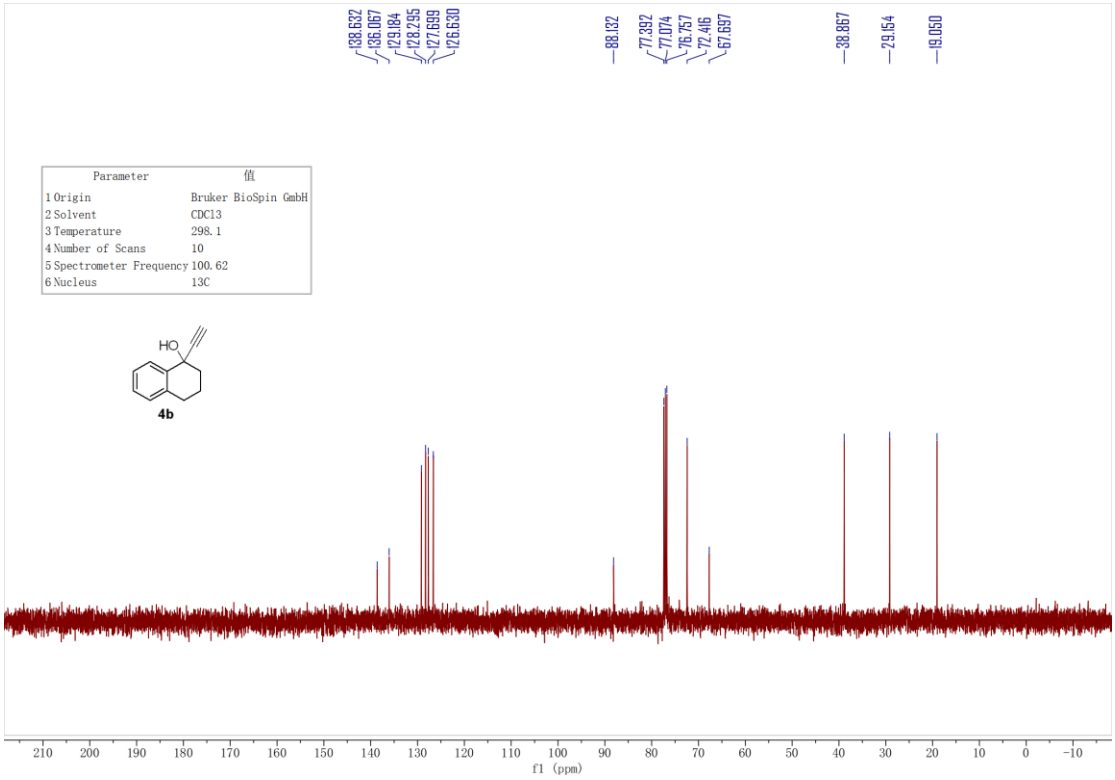
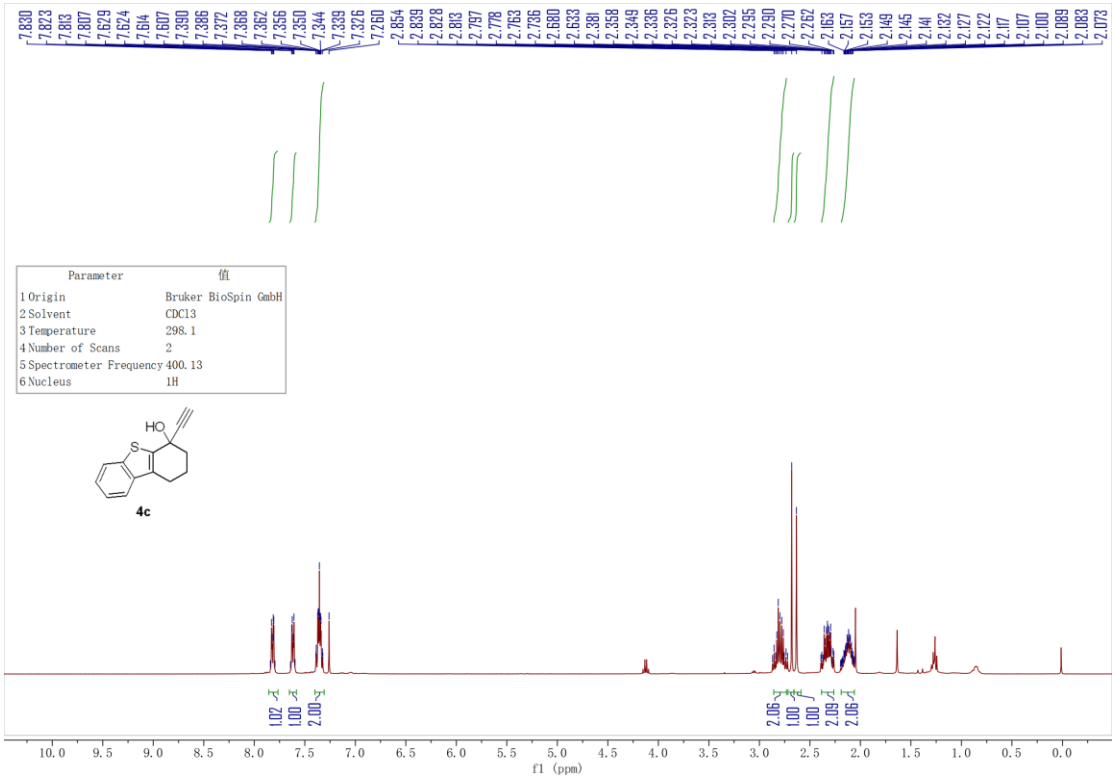
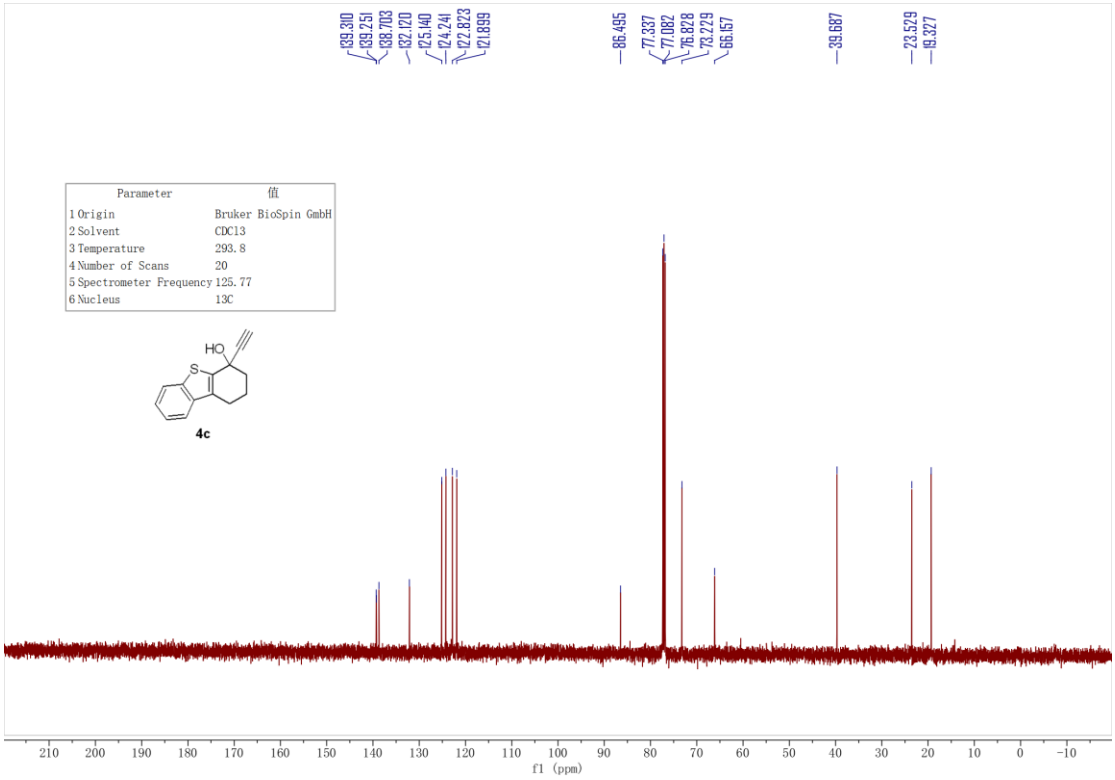
3.069
2.945
2.936
2.925
2.915
2.906
2.896
2.885
2.875
2.633
2.597
2.577
2.562
2.544
2.525
2.461
2.452
2.443
2.431
2.419
2.410
2.400
2.365
Parameter 值
1 Origin Bruker BioSpin GmbH
2 Solvent CDCl3
3 Temperature 298.0
4 Number of Scans 2
5 Spectrometer Frequency 400.13
6 Nucleus 1H
HO
4a
1.03
3.08
1.09
1.07
1.00
1.08
1.08
1.00
10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)

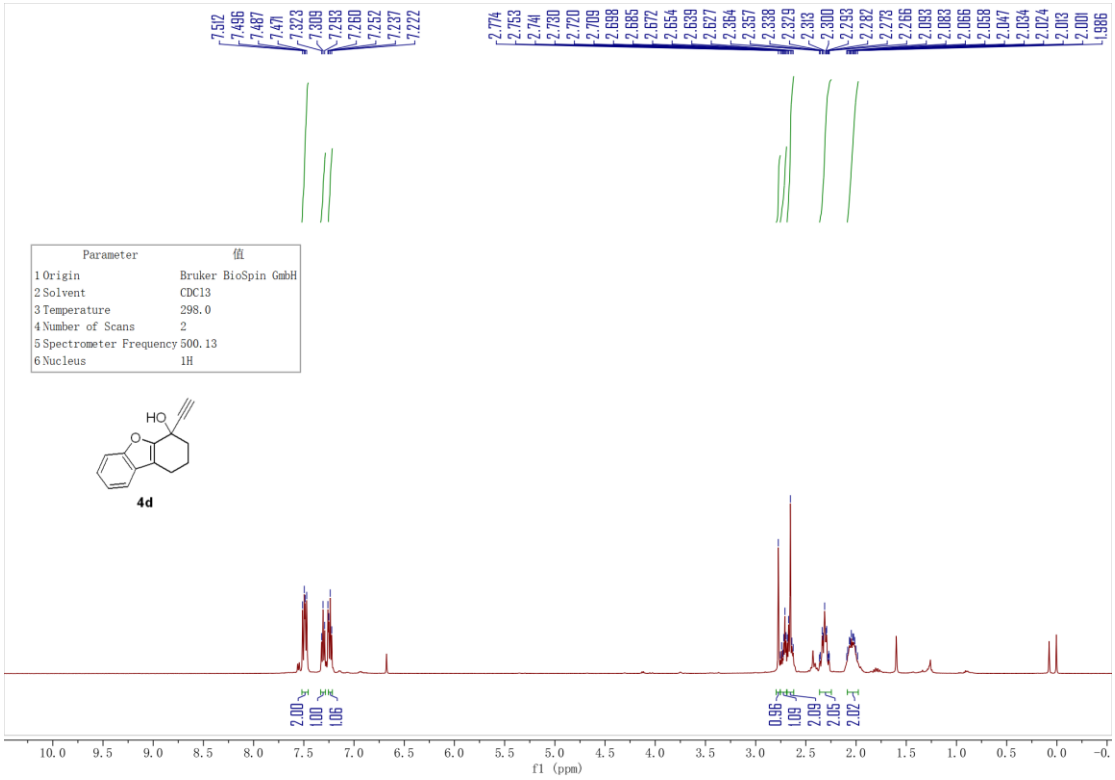

145.255
143.101
129.182
127.192
125.108
123.158
85.910
77.407
77.089
76.772
76.169
73.034
43.067
29.559
Parameter 值
1 Origin Bruker BioSpin GmbH
2 Solvent CDCl3
3 Temperature 298.1
4 Number of Scans 10
5 Spectrometer Frequency 100.62
6 Nucleus 13C
HO
4a
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)

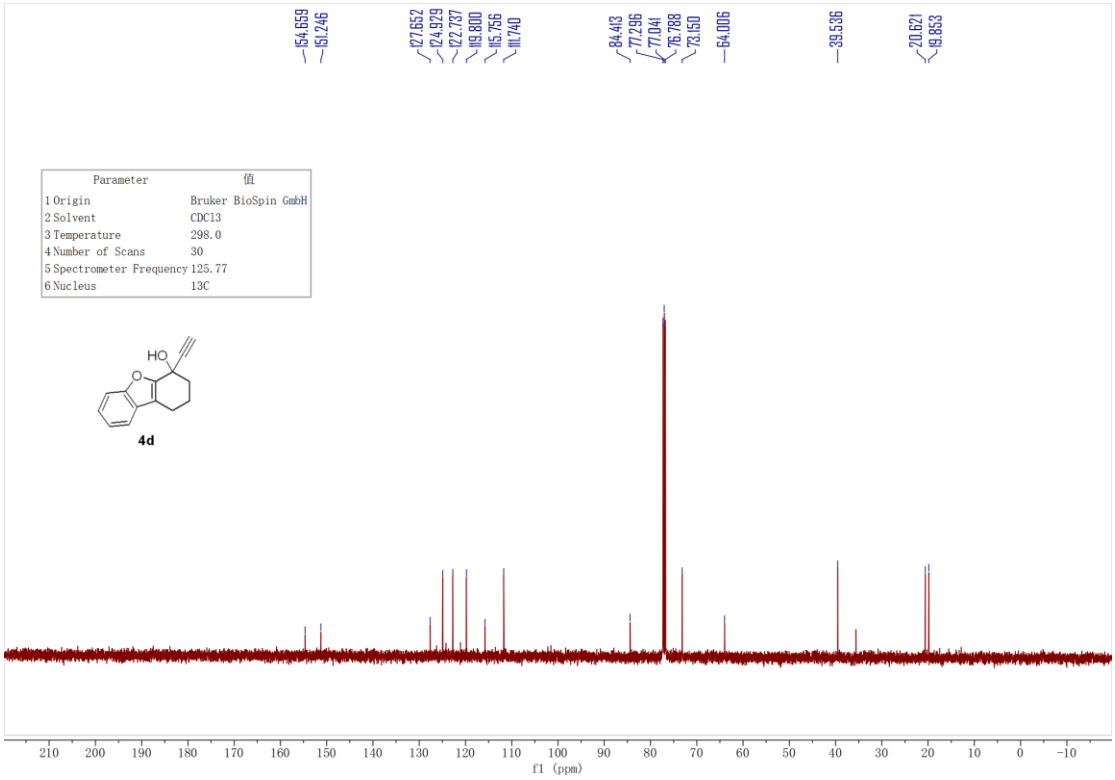

7.783
7.778
7.762
7.272
7.260
7.253
7.243
7.234
7.215
7.116
7.100
2.888
2.873
2.845
2.831
2.816
2.801
2.775
2.759
2.598
2.361
2.238
2.224
2.208
2.080
2.064
2.048
2.030
2.013
1.995
1.981
1.968
1.955
1.940
1.920
1.906
1.892
Parameter 值
1 Origin Bruker BioSpin GmbH
2 Solvent CDCl3
3 Temperature 298.0
4 Number of Scans 2
5 Spectrometer Frequency 400.13
6 Nucleus 1H
HO
4b
1.00
2.05
1.02
2.02
0.98
0.99
2.09
1.09
1.09
f1 (ppm)

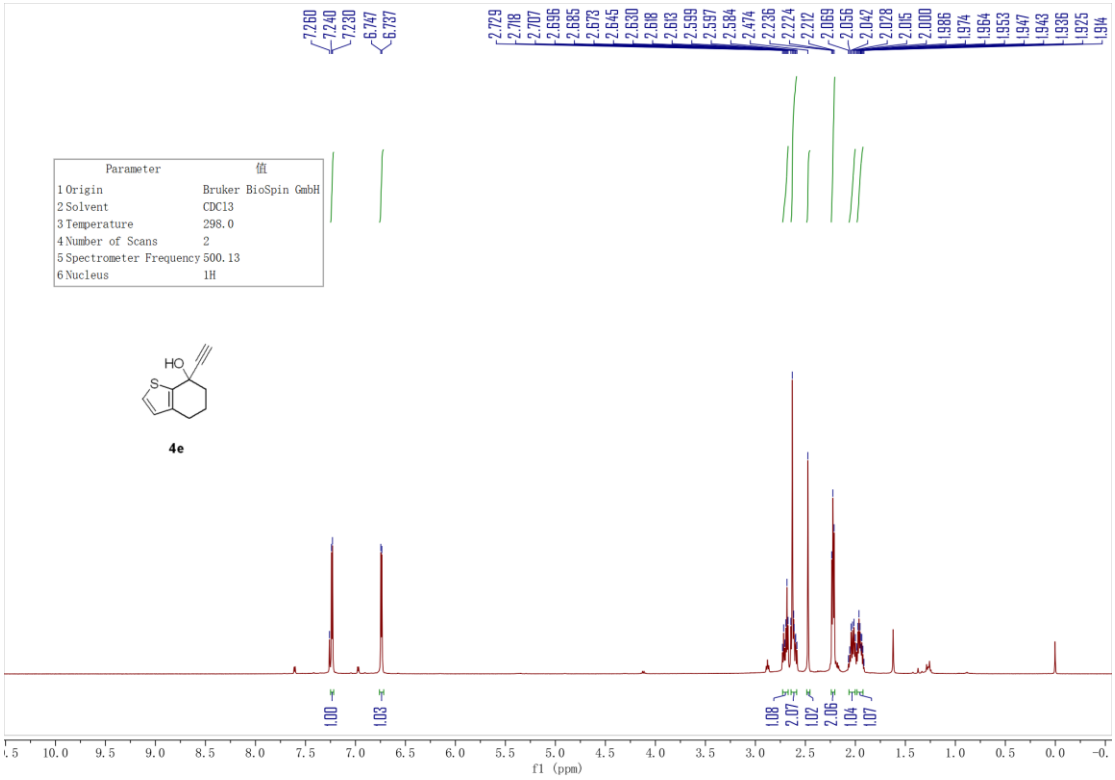

138.632
136.067
129.184
128.295
127.699
126.630
88.132
77.392
77.074
76.757
72.416
67.697
38.867
29.154
19.050
Parameter 值
1 Origin Bruker BioSpin GmbH
2 Solvent CDCl3
3 Temperature 298.1
4 Number of Scans 10
5 Spectrometer Frequency 100.62
6 Nucleus 13C
HO
4b
f1 (ppm)

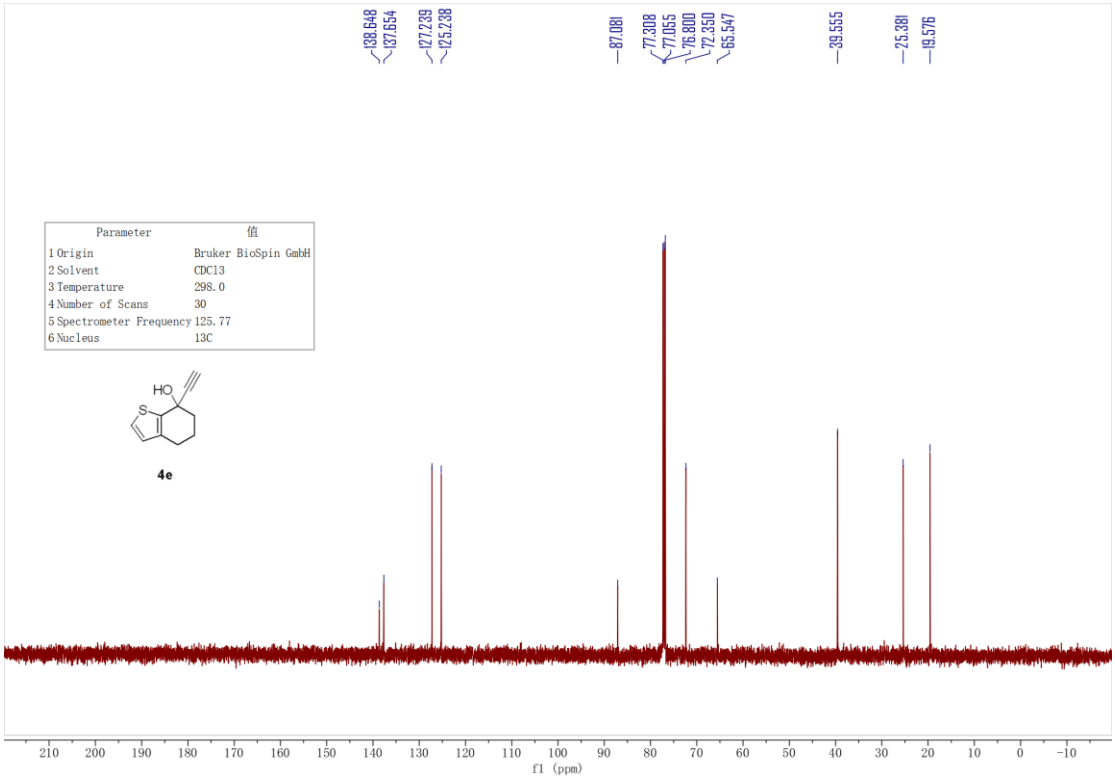

7.830
7.823
7.813
7.807
7.629
7.624
7.614
7.607
7.390
7.386
7.372
7.368
7.362
7.356
7.350
7.344
7.339
7.326
7.260
2.854
2.839
2.828
2.813
2.797
2.778
2.763
2.736
2.680
2.633
2.381
2.358
2.349
2.336
2.326
2.323
2.313
2.302
2.295
2.290
2.270
2.262
2.163
2.157
2.153
2.149
2.145
2.141
2.132
2.127
2.122
2.117
2.107
2.100
2.089
2.083
2.073
Parameter 值
1 Origin Bruker BioSpin GmbH
2 Solvent CDCl3
3 Temperature 298.1
4 Number of Scans 2
5 Spectrometer Frequency 400.13
6 Nucleus 1H
HO
S
4c
1.02
1.00
2.00
2.06
1.00
1.00
2.09
2.06
10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)

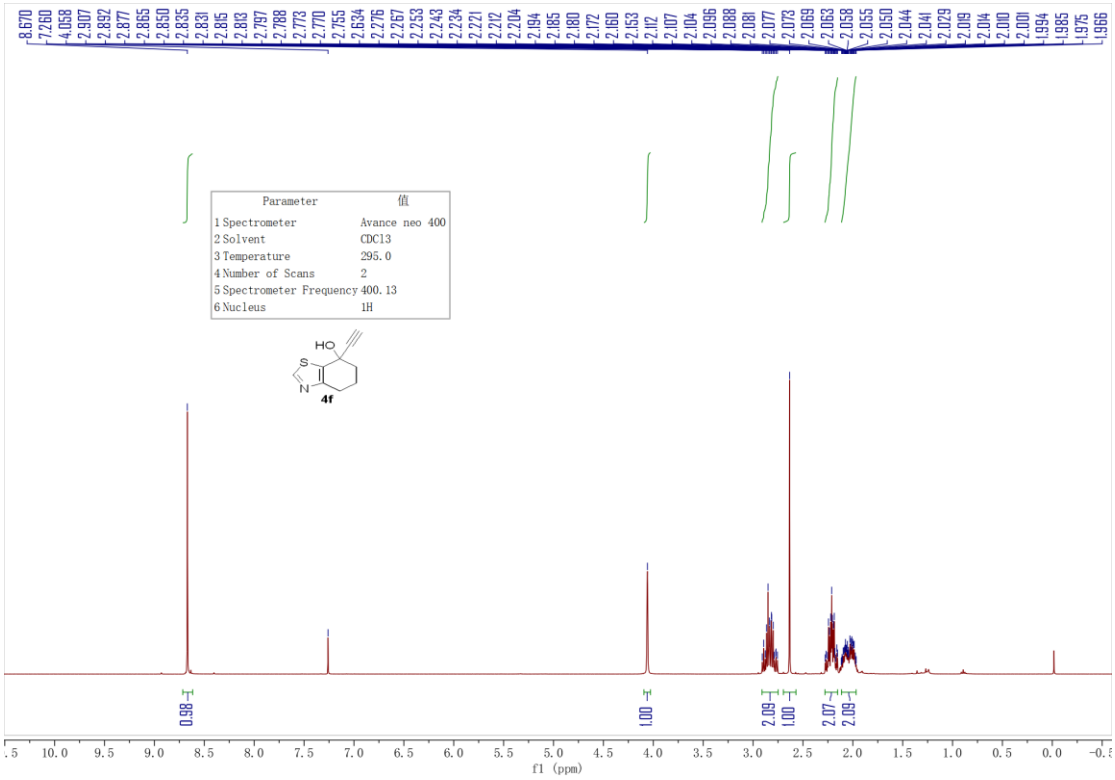

139.310
139.251
138.703
132.120
125.140
124.241
122.823
121.899
86.495
77.337
77.082
76.828
73.229
66.157
39.687
23.529
19.327
Parameter 值
1 Origin Bruker BioSpin GmbH
2 Solvent CDCl3
3 Temperature 293.8
4 Number of Scans 20
5 Spectrometer Frequency 125.77
6 Nucleus 13C
HO
S
4c
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)

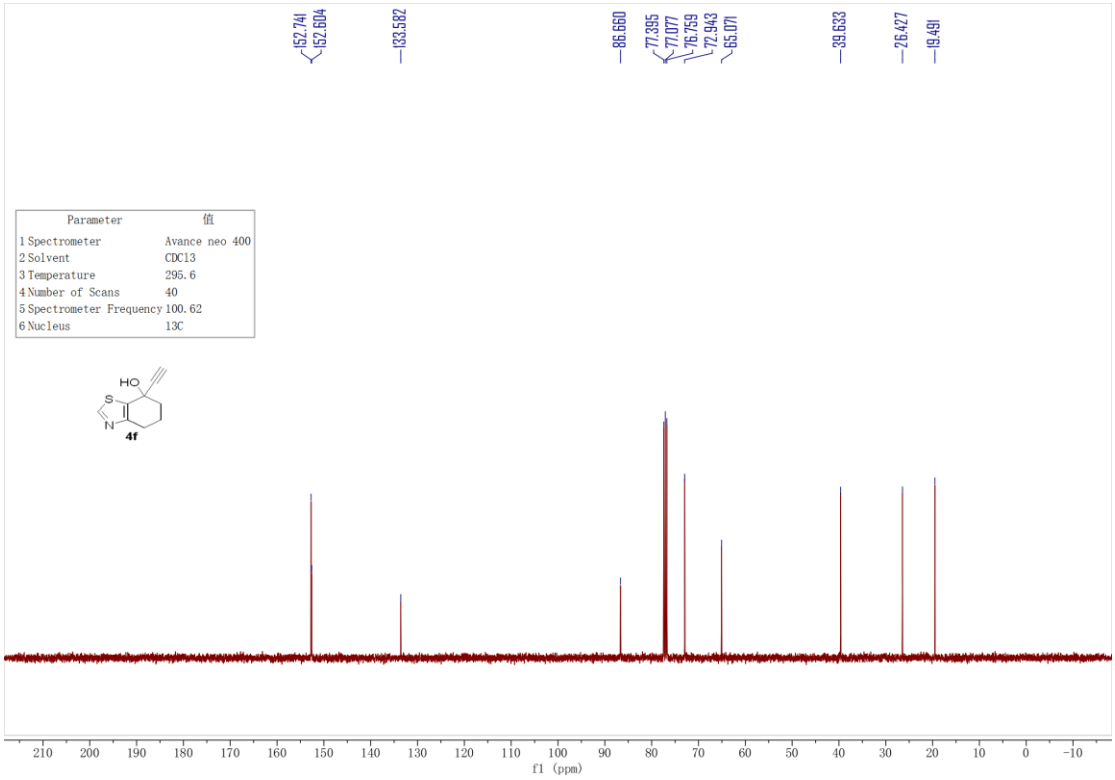

7.512
7.496
7.487
7.471
7.323
7.309
7.293
7.260
7.252
7.237
7.222
2.774
2.753
2.741
2.730
2.720
2.709
2.698
2.685
2.672
2.654
2.639
2.627
2.364
2.357
2.338
2.329
2.313
2.300
2.293
2.282
2.273
2.266
2.093
2.083
2.066
2.058
2.047
2.034
2.024
2.013
2.001
1.986
Parameter 值
1 Origin Bruker BioSpin GmbH
2 Solvent CDCl3
3 Temperature 298.0
4 Number of Scans 2
5 Spectrometer Frequency 500.13
6 Nucleus 1H
HO
4d
2.00
1.00
1.06
0.96
1.09
2.09
2.05
2.02
10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.
f1 (ppm)

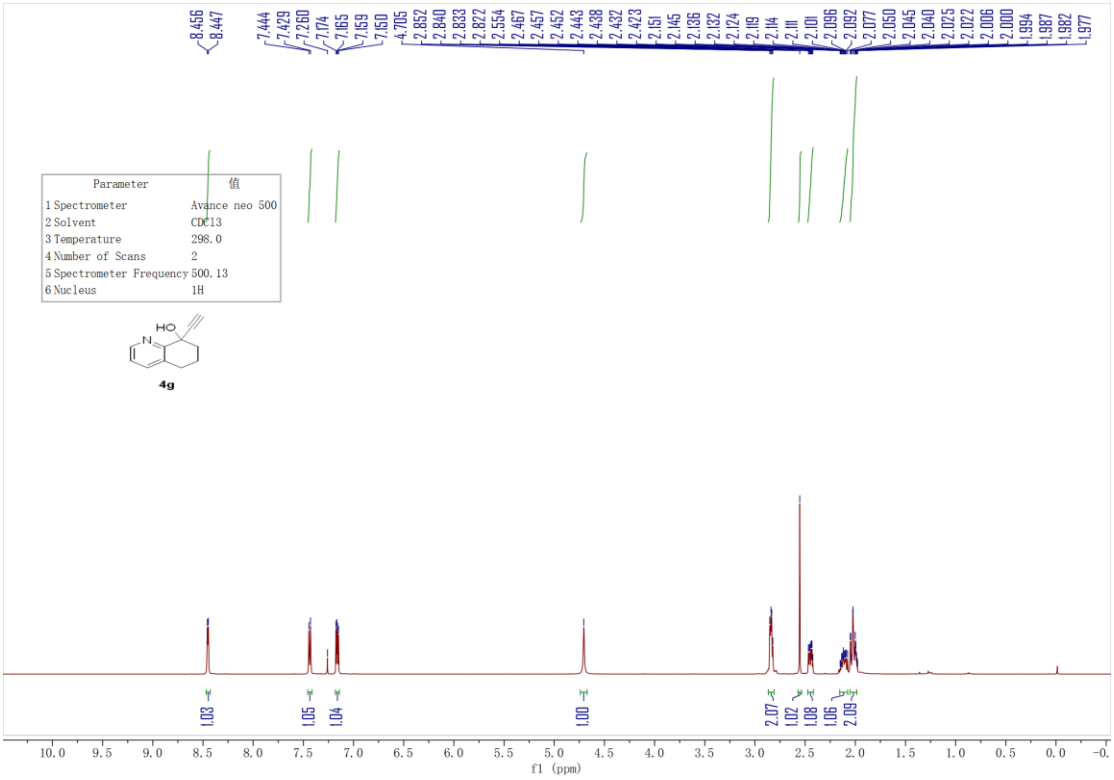

154.659
151.246
127.652
124.929
122.737
119.800
115.756
111.740
84.413
77.296
77.041
76.788
73.150
64.006
39.536
20.621
19.853
Parameter 值
1 Origin Bruker BioSpin GmbH
2 Solvent CDCl3
3 Temperature 298.0
4 Number of Scans 30
5 Spectrometer Frequency 125.77
6 Nucleus 13C
HO
4d
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)

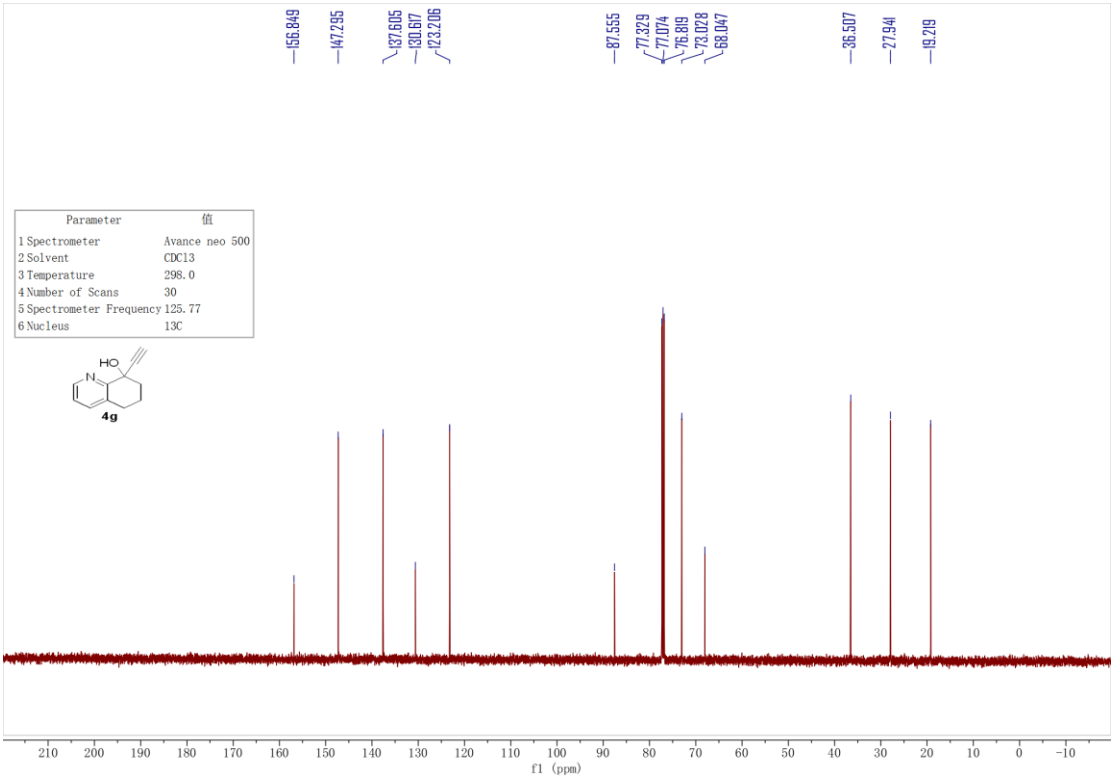

7.260
7.240
7.230
6.747
6.737
2.729
2.718
2.707
2.696
2.685
2.673
2.645
2.630
2.618
2.613
2.599
2.597
2.584
2.474
2.236
2.224
2.212
2.069
2.056
2.042
2.028
2.005
2.000
1.986
1.974
1.964
1.953
1.947
1.943
1.936
1.925
1.914
Parameter 值
1 Origin Bruker BioSpin GmbH
2 Solvent CDCl3
3 Temperature 298.0
4 Number of Scans 2
5 Spectrometer Frequency 500.13
6 Nucleus 1H
HO
S
4e
1.00
1.03
1.08
2.07
1.02
2.06
1.04
1.07
f1 (ppm)

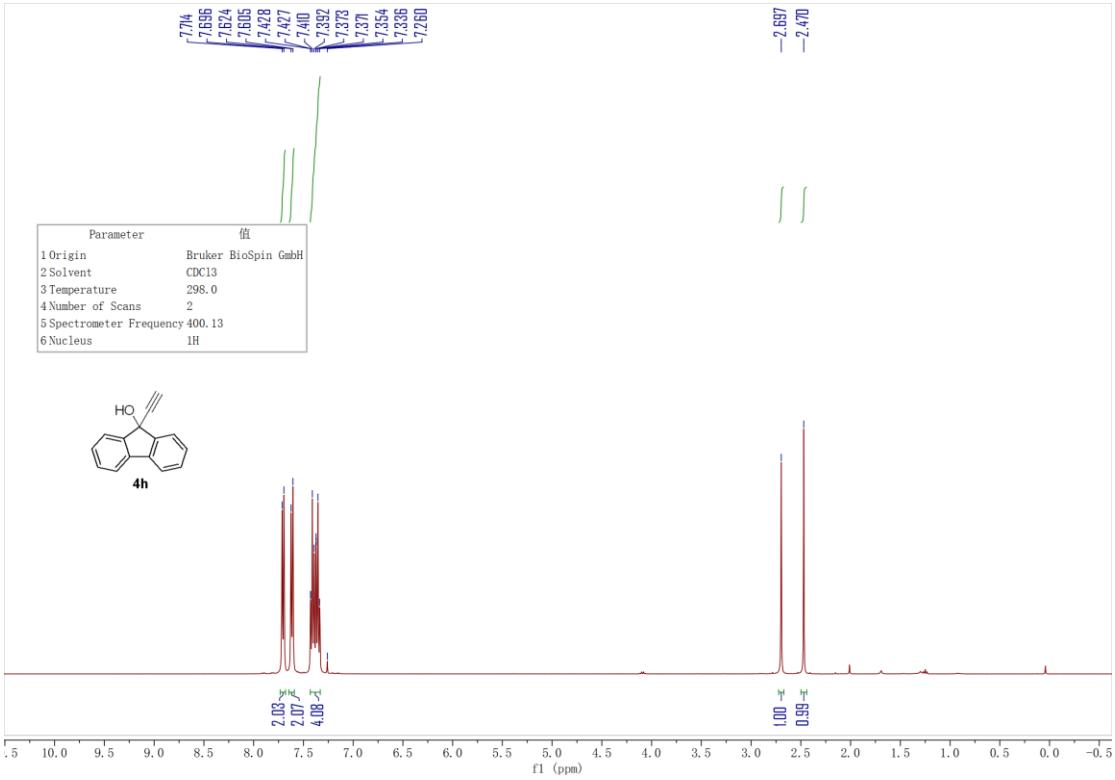

138.648
137.654
127.239
125.238
87.081
77.308
77.055
76.800
72.350
65.547
39.555
25.381
19.576
Parameter 值
1 Origin Bruker BioSpin GmbH
2 Solvent CDCl3
3 Temperature 298.0
4 Number of Scans 30
5 Spectrometer Frequency 125.77
6 Nucleus 13C
HO
S
4e
f1 (ppm)


8.670
7.260
4.058
2.907
2.892
2.877
2.865
2.850
2.835
2.831
2.805
2.803
2.797
2.788
2.773
2.770
2.755
2.634
2.276
2.267
2.253
2.243
2.234
2.221
2.212
2.204
2.194
2.165
2.180
2.172
2.160
2.153
2.112
2.107
2.104
2.096
2.088
2.081
2.077
2.073
2.069
2.063
2.058
2.055
2.050
2.044
2.041
2.029
2.009
2.004
2.000
2.001
1.994
1.985
1.975
1.966
Parameter 值
1 Spectrometer Avance neo 400
2 Solvent CDC13
3 Temperature 295.0
4 Number of Scans 2
5 Spectrometer Frequency 400.13
6 Nucleus 1H
HO
S
N
4f
0.98
1.00
2.09
1.00
2.07
2.09
f1 (ppm)


152.741
152.604
133.582
86.660
77.395
77.077
76.759
72.943
65.071
39.633
26.427
19.491
Parameter 值
1 Spectrometer Avance neo 400
2 Solvent CDC13
3 Temperature 295.6
4 Number of Scans 40
5 Spectrometer Frequency 100.62
6 Nucleus 13C
HO
S
N
4f
f1 (ppm)


8.456
8.447
7.444
7.429
7.260
7.174
7.165
7.159
7.150
4.705
2.852
2.840
2.833
2.822
2.554
2.467
2.457
2.452
2.443
2.438
2.432
2.423
2.151
2.145
2.136
2.132
2.124
2.119
2.114
2.111
2.101
2.096
2.092
2.077
2.050
2.045
2.040
2.025
2.022
2.006
2.000
1.994
1.987
1.982
1.977
Parameter 值
1 Spectrometer Avance neo 500
2 Solvent CDC13
3 Temperature 298.0
4 Number of Scans 2
5 Spectrometer Frequency 500.13
6 Nucleus 1H
HO
N
4g
1.03
1.05
1.04
1.00
2.07
1.02
1.08
1.06
2.09
10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.
f1 (ppm)


156.849
147.295
137.605
130.617
123.206
87.555
77.329
77.074
76.819
73.028
68.047
36.507
27.941
19.219
Parameter 值
1 Spectrometer Avance neo 500
2 Solvent CDC13
3 Temperature 298.0
4 Number of Scans 30
5 Spectrometer Frequency 125.77
6 Nucleus 13C
HO
N
4g
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)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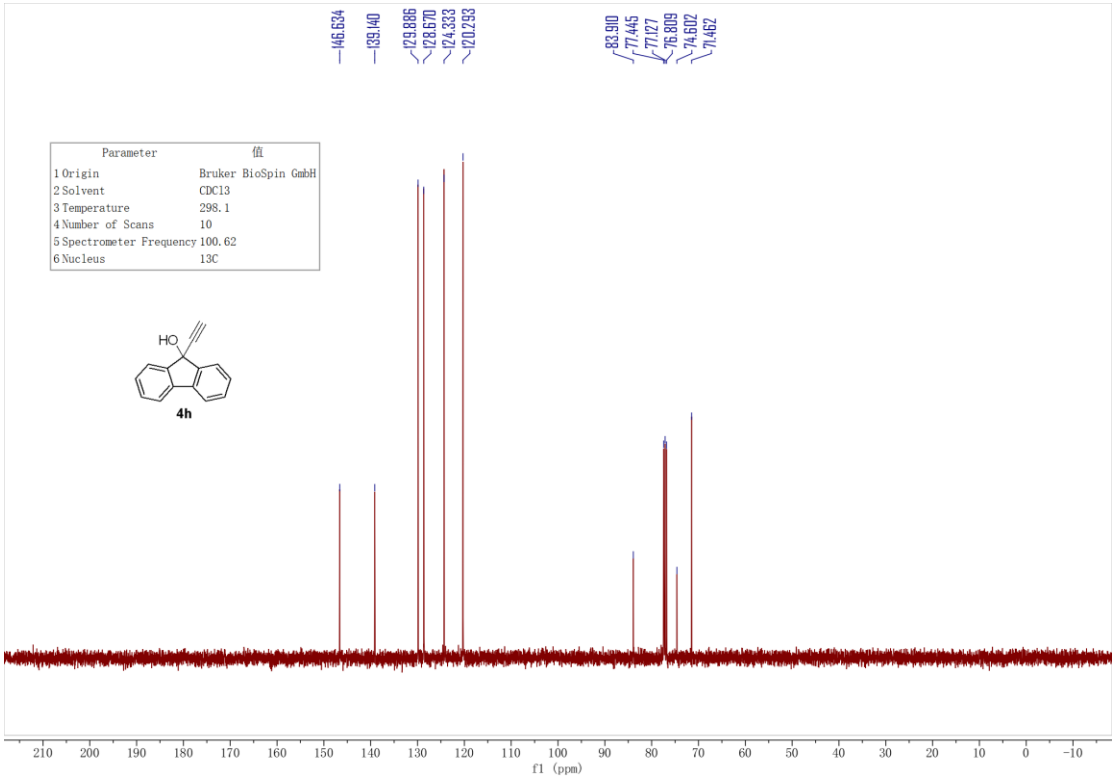
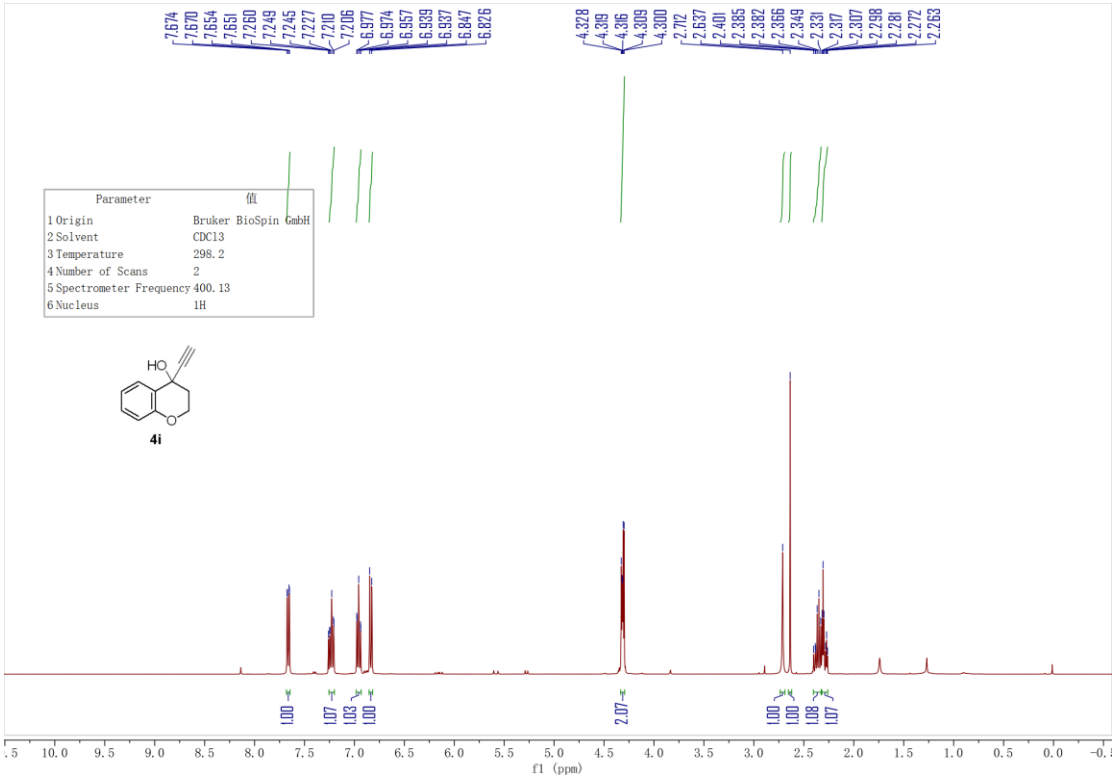
7.696
7.624
7.605
7.428
7.427
7.410
7.392
7.373
7.371
7.354
7.336
7.260
2.697
2.470
Parameter 值
1 Origin Bruker BioSpin GmbH
2 Solvent CDCl3
3 Temperature 298.0
4 Number of Scans 2
5 Spectrometer Frequency 400.13
6 Nucleus 1H
HO
4h
2.03
2.07
4.08
1.00
0.99
f1 (ppm)


146.634
139.140
129.886
128.670
124.333
120.293
83.910
77.445
77.127
76.809
74.602
71.462
Parameter 值
1 Origin Bruker BioSpin GmbH
2 Solvent CDCl3
3 Temperature 298.1
4 Number of Scans 10
5 Spectrometer Frequency 100.62
6 Nucleus 13C
HO
4h
f1 (ppm)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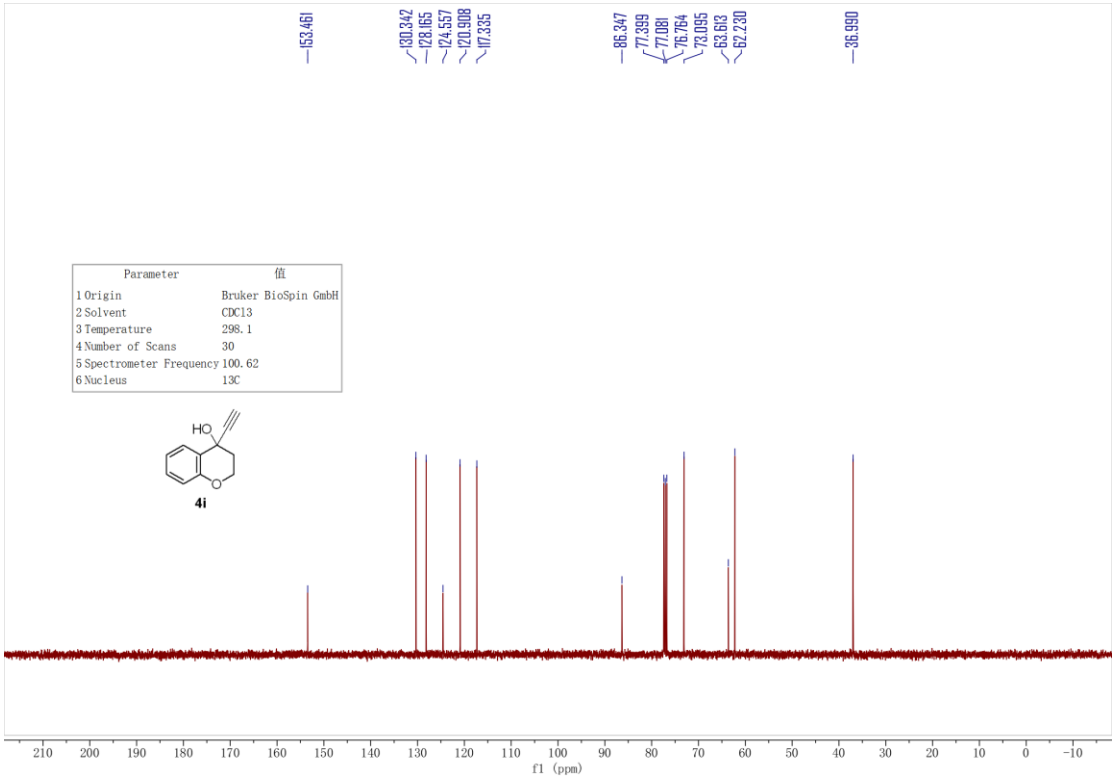
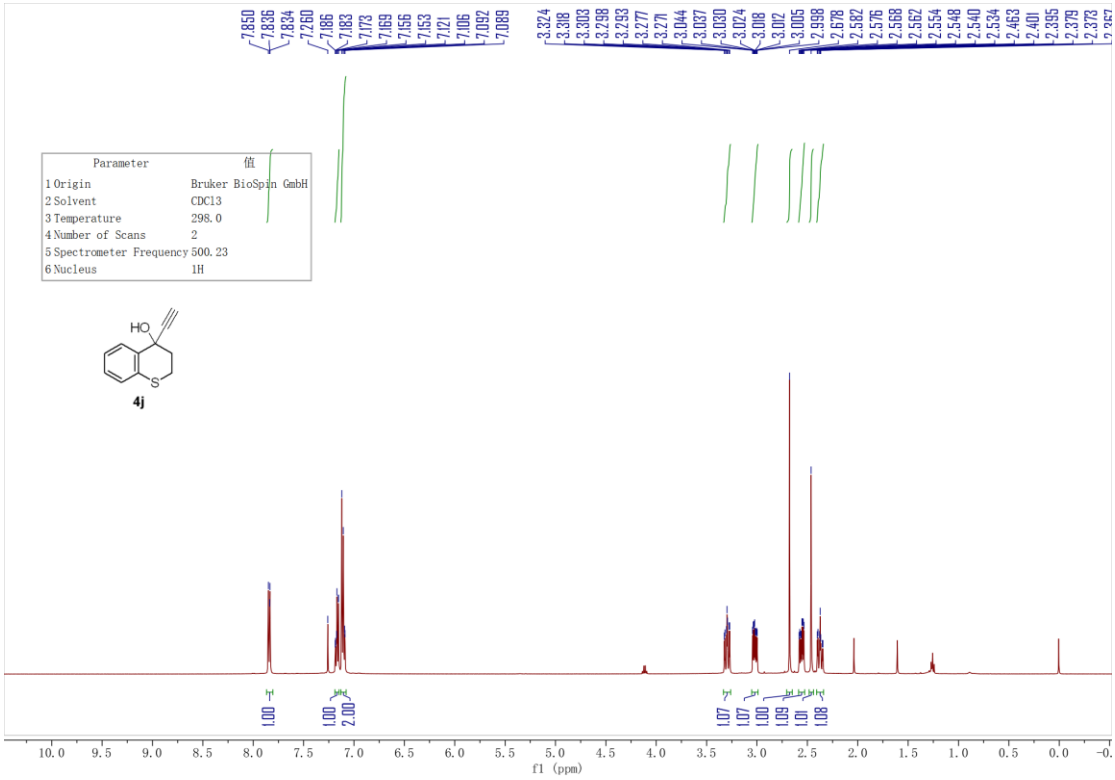
7.654
7.651
7.260
7.249
7.245
7.227
7.210
7.206
6.977
6.974
6.957
6.939
6.937
6.847
6.826
4.328
4.319
4.316
4.309
4.300
2.712
2.637
2.401
2.385
2.382
2.366
2.349
2.331
2.317
2.307
2.298
2.281
2.272
2.263
Parameter 值
1 Origin Bruker BioSpin GmbH
2 Solvent CDCl3
3 Temperature 298.2
4 Number of Scans 2
5 Spectrometer Frequency 400.13
6 Nucleus 1H
HO
4i
1.00
1.07
1.03
1.00
2.07
1.00
1.00
1.08
1.07
f1 (ppm)


153.461
130.342
128.165
124.557
120.908
117.335
86.347
77.399
77.081
76.764
73.095
63.613
62.230
36.990
Parameter 值
1 Origin Bruker BioSpin GmbH
2 Solvent CDCl3
3 Temperature 298.1
4 Number of Scans 30
5 Spectrometer Frequency 100.62
6 Nucleus 13C
HO
4i
f1 (ppm)


7.850
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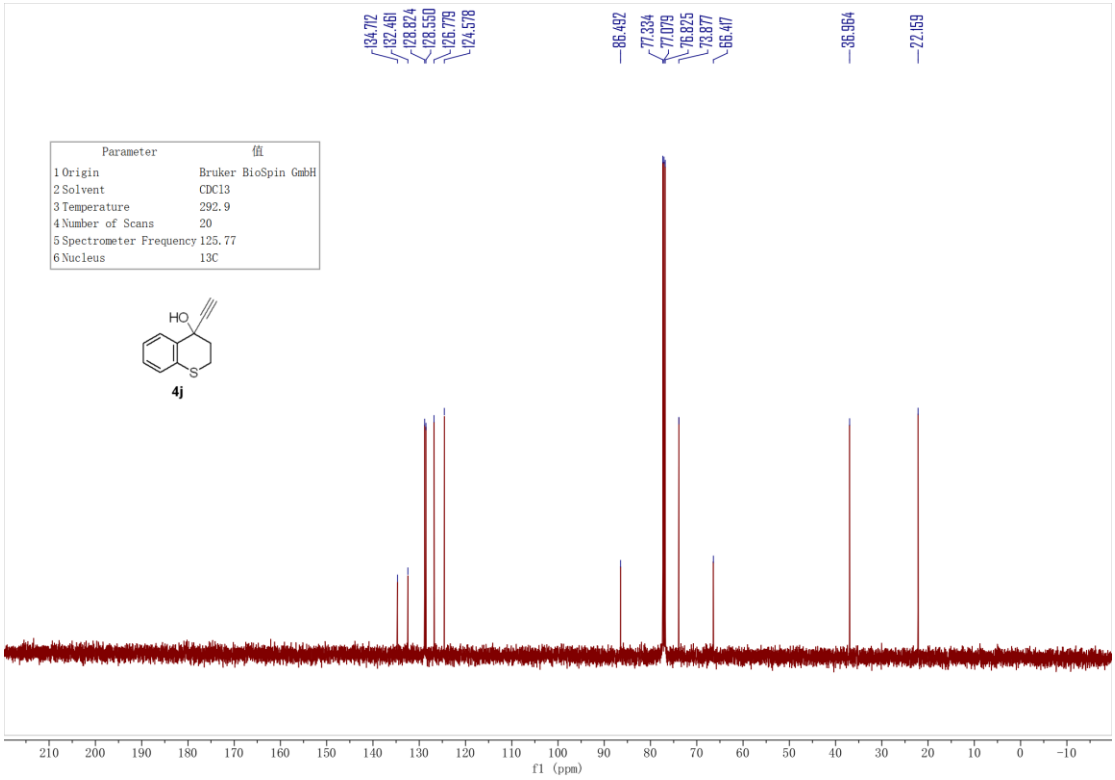
7.834
7.260
7.186
7.183
7.173
7.169
7.156
7.153
7.121
7.106
7.092
7.089
3.324
3.318
3.303
3.298
3.293
3.277
3.271
3.044
3.037
3.030
3.024
3.018
3.012
3.005
2.998
2.678
2.582
2.576
2.568
2.562
2.554
2.548
2.540
2.534
2.463
2.401
2.395
2.379
2.373
Parameter 值
1 Origin Bruker BioSpin GmbH
2 Solvent CDCl3
3 Temperature 298.0
4 Number of Scans 2
5 Spectrometer Frequency 500.23
6 Nucleus 1H
HO
S
4j
1.00
1.00
2.00
1.07
1.07
1.00
1.09
1.01
1.08
f1 (ppm)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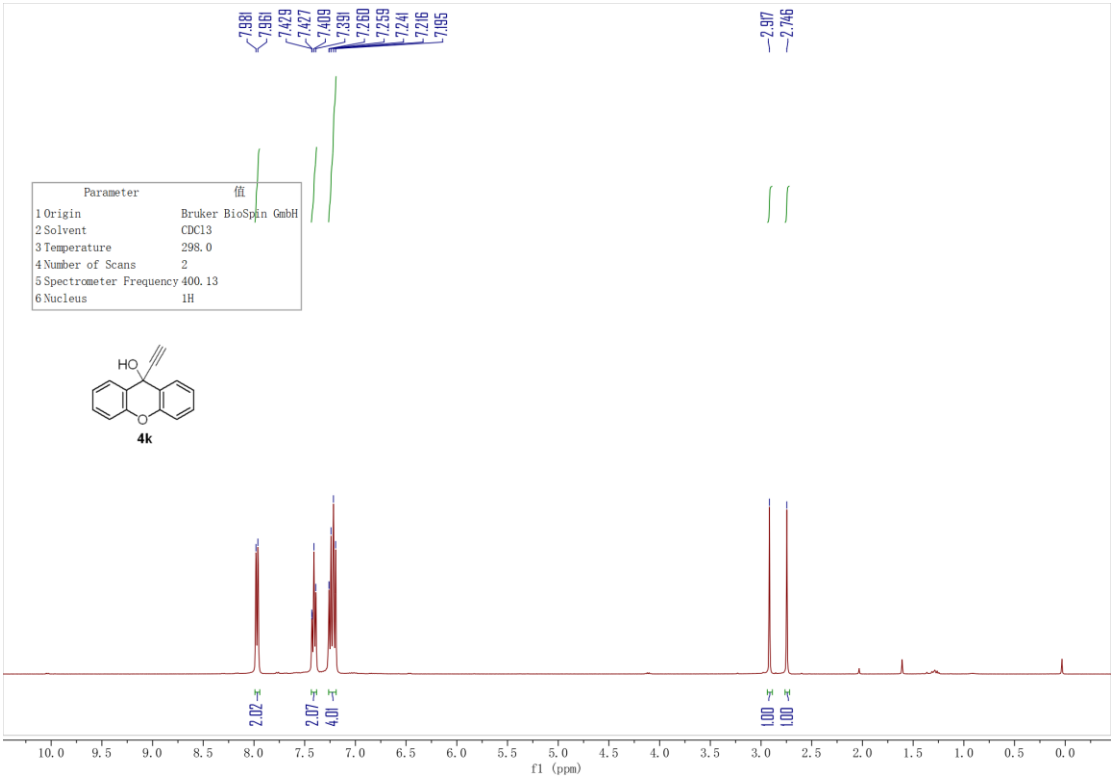
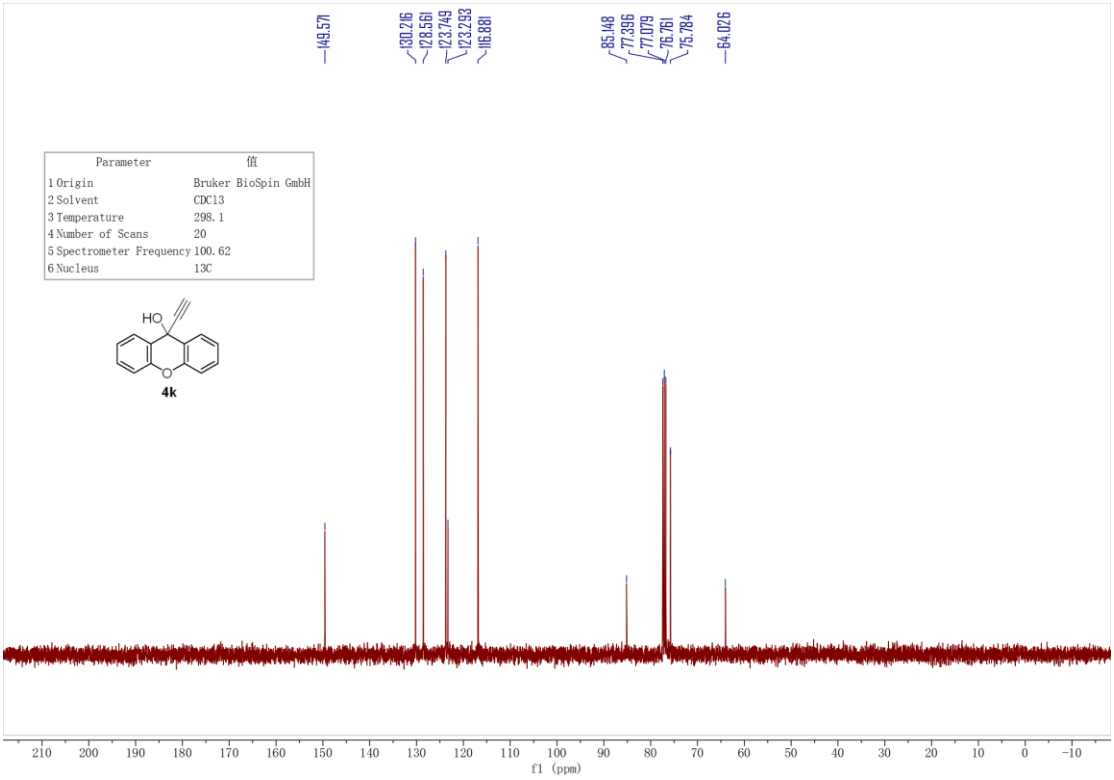
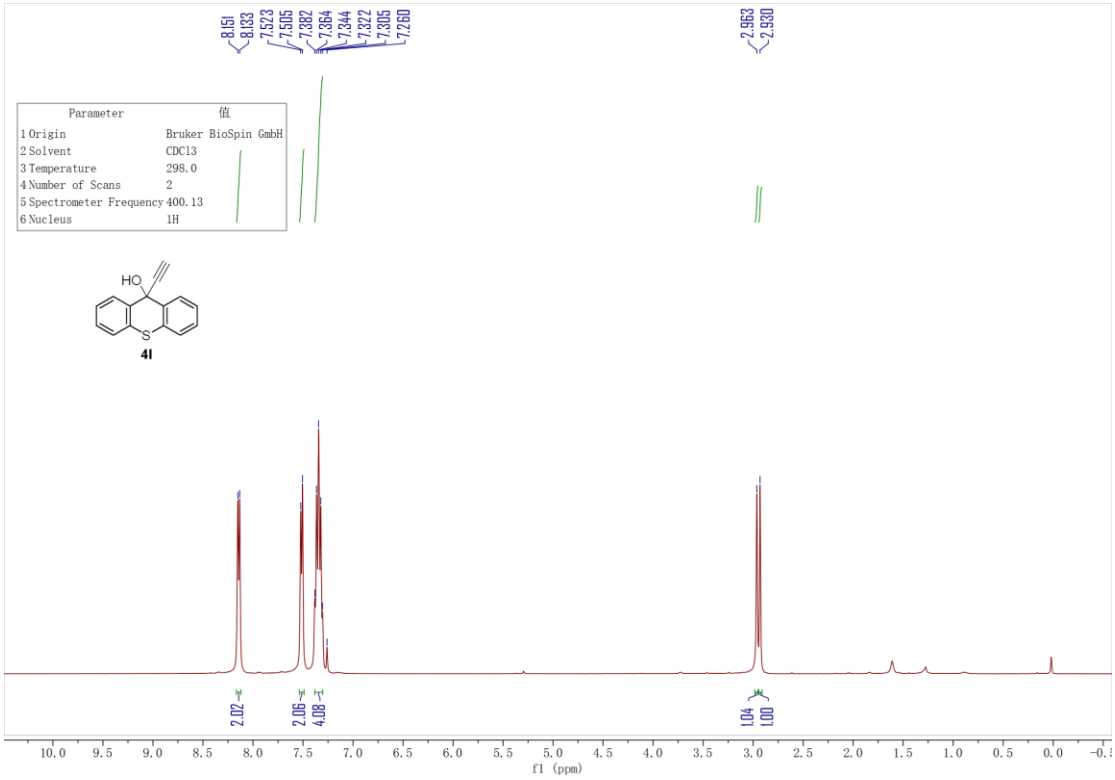
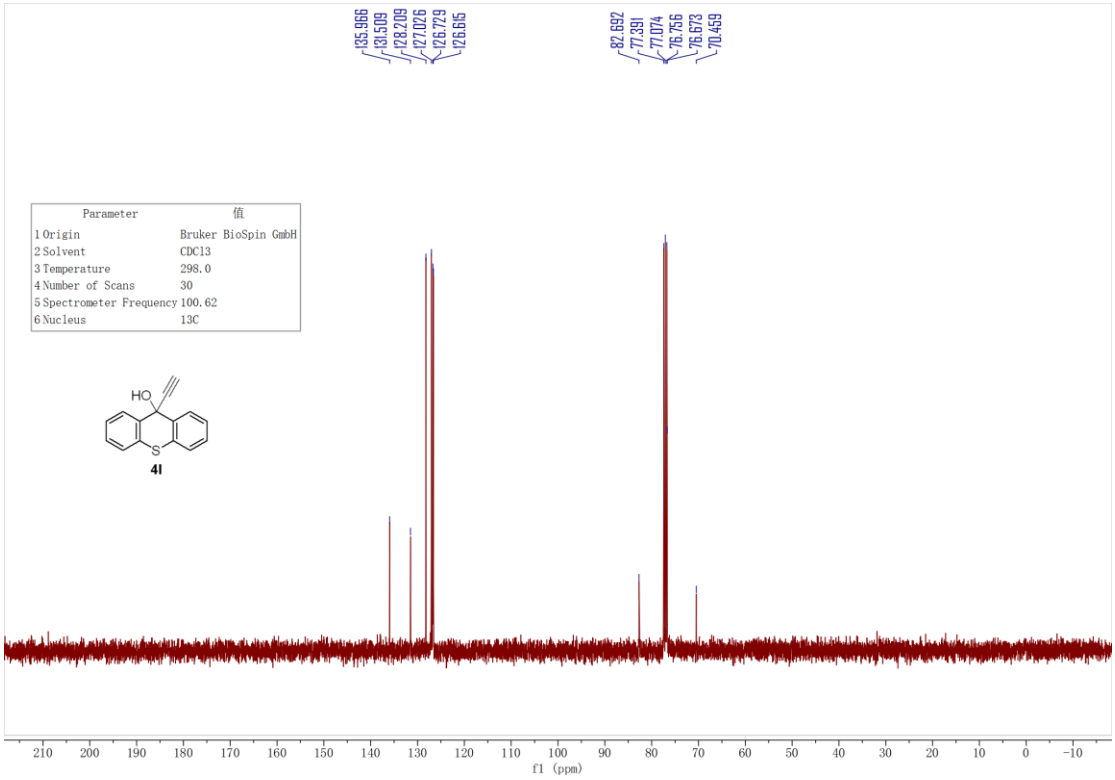
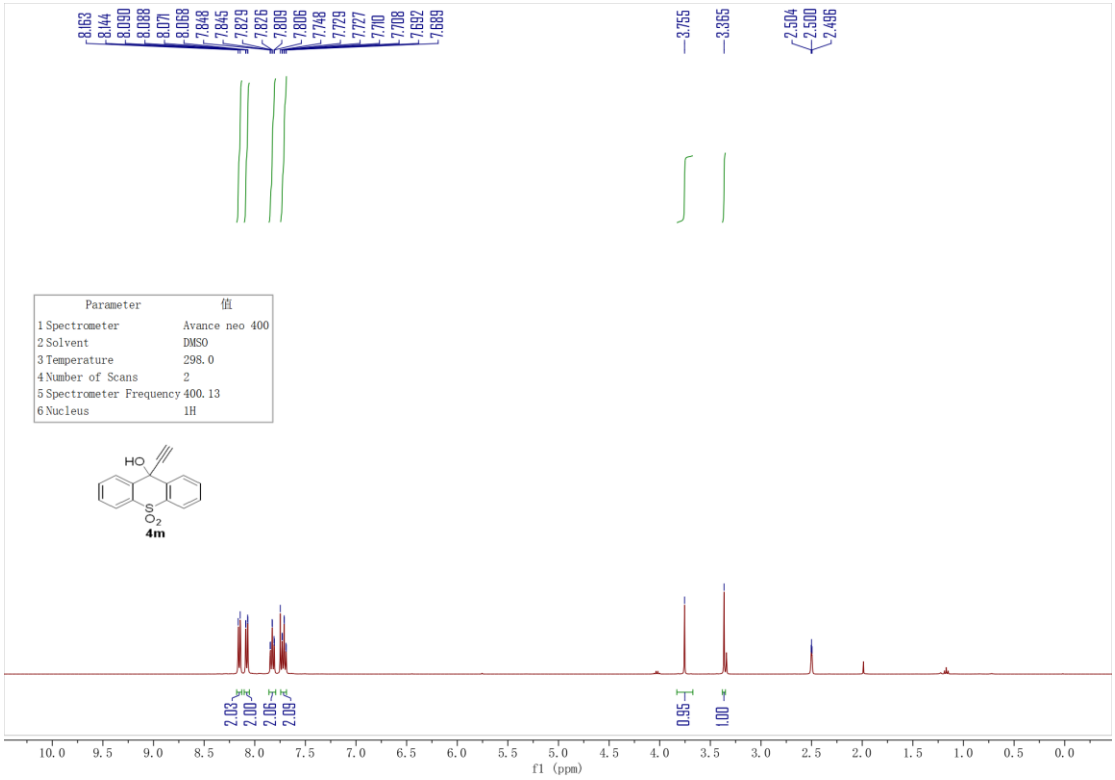
132.461
128.824
128.550
126.779
124.578
86.492
77.334
77.079
76.825
73.877
66.417
36.964
22.159
Parameter 值
1 Origin Bruker BioSpin GmbH
2 Solvent CDCl3
3 Temperature 292.9
4 Number of Scans 20
5 Spectrometer Frequency 125.77
6 Nucleus 13C
HO
S
4j
f1 (ppm)


7.981
7.961
7.429
7.427
7.409
7.391
7.260
7.259
7.241
7.216
7.195
2.997
2.746
Parameter 值
1 Origin Bruker BioSpin GmbH
2 Solvent CDCl3
3 Temperature 298.0
4 Number of Scans 2
5 Spectrometer Frequency 400.13
6 Nucleus 1H
HO
4k
2.02
2.07
4.01
1.00
1.00
f1 (ppm)


149.571
130.216
128.561
123.749
123.293
116.881
85.148
77.396
77.079
76.761
75.784
64.026
Parameter 值
1 Origin Bruker BioSpin GmbH
2 Solvent CDCl3
3 Temperature 298.1
4 Number of Scans 20
5 Spectrometer Frequency 100.62
6 Nucleus 13C
HO
4k
f1 (ppm)


8.151
8.133
7.523
7.505
7.382
7.364
7.344
7.322
7.305
7.260
2.963
2.930
Parameter 值
1 Origin Bruker BioSpin GmbH
2 Solvent CDCl3
3 Temperature 298.0
4 Number of Scans 2
5 Spectrometer Frequency 400.13
6 Nucleus 1H
HO
S
4l
2.02
2.06
4.08
1.04
1.00
f1 (ppm)


135.966
131.509
128.209
127.026
126.729
126.695
82.692
77.391
77.074
76.756
76.673
70.459
Parameter 值
1 Origin Bruker BioSpin GmbH
2 Solvent CDCl3
3 Temperature 298.0
4 Number of Scans 30
5 Spectrometer Frequency 100.62
6 Nucleus 13C
HO
S
4l
f1 (ppm)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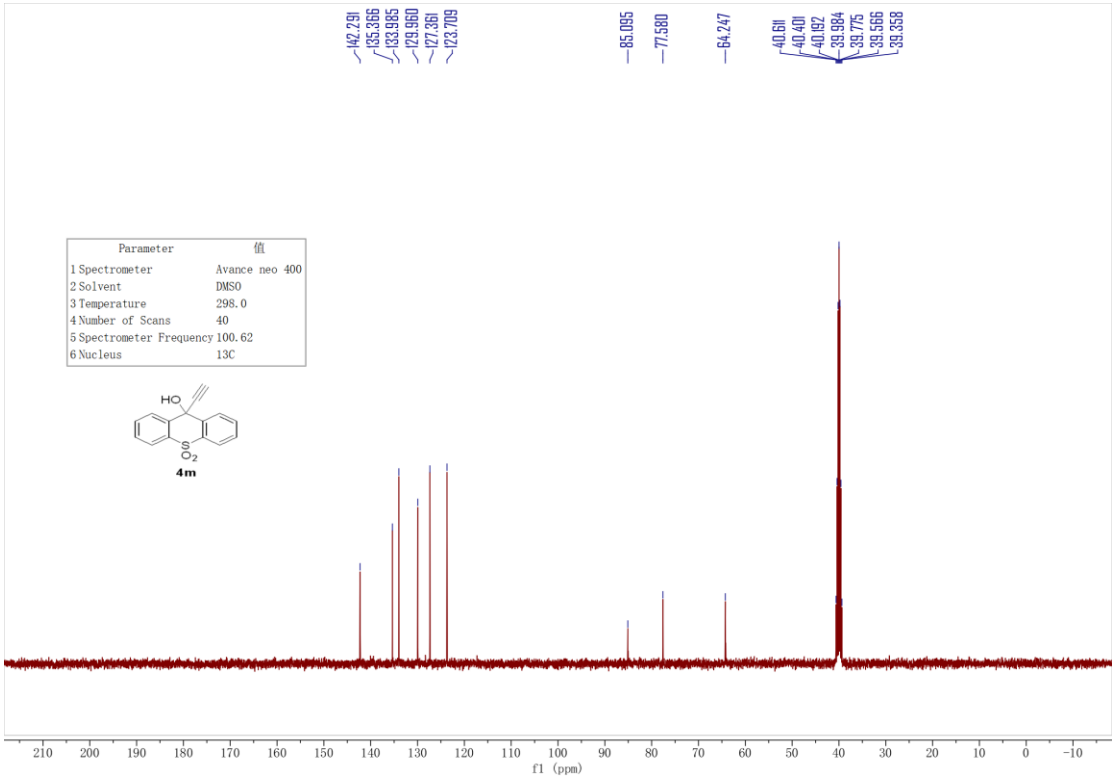
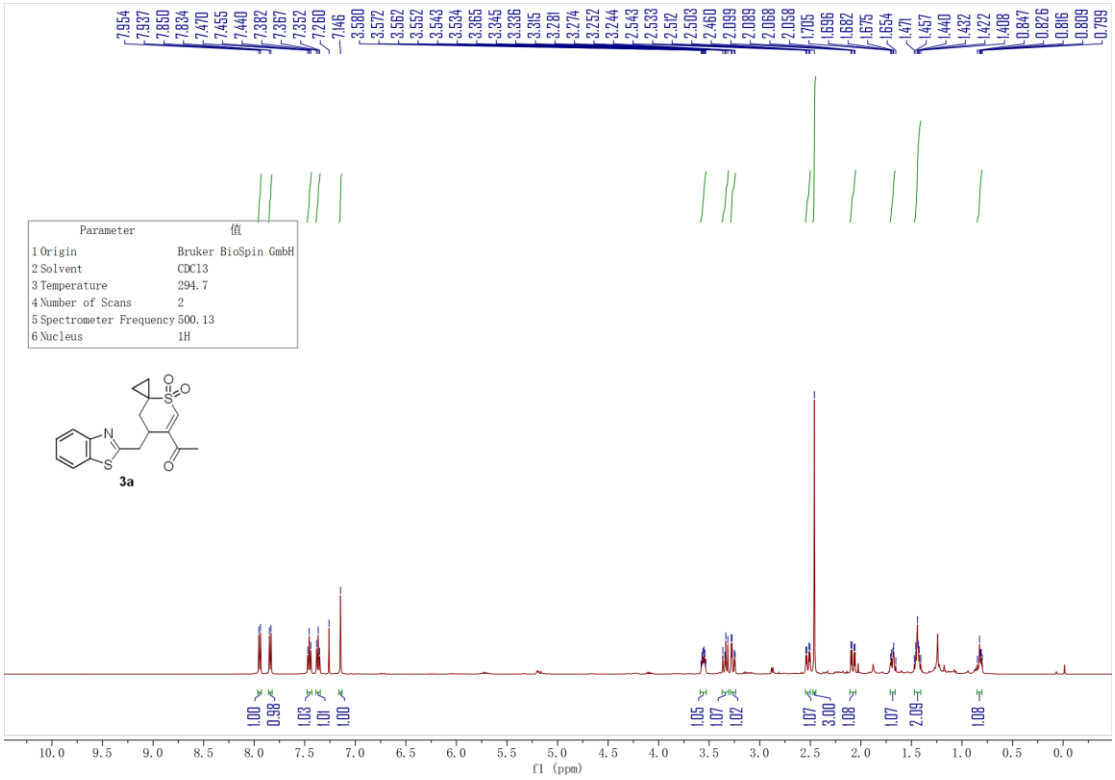
8.088
8.071
8.068
8.068
7.848
7.845
7.829
7.826
7.809
7.806
7.748
7.729
7.727
7.710
7.708
7.692
7.689
3.755
3.365
2.504
2.500
2.496
Parameter 值
1 Spectrometer Avance neo 400
2 Solvent DMSO
3 Temperature 298.0
4 Number of Scans 2
5 Spectrometer Frequency 400.13
6 Nucleus 1H
HO
S
O2
4m
2.03
2.00
2.06
2.09
0.95
1.00
10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)


142.291
135.366
133.985
129.960
127.361
123.709
85.095
77.580
64.247
40.611
40.401
40.192
39.984
39.775
39.566
39.358
Parameter 值
1 Spectrometer Avance neo 400
2 Solvent DMSO
3 Temperature 298.0
4 Number of Scans 40
5 Spectrometer Frequency 100.62
6 Nucleus 13C
HO
S
O2
4m
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)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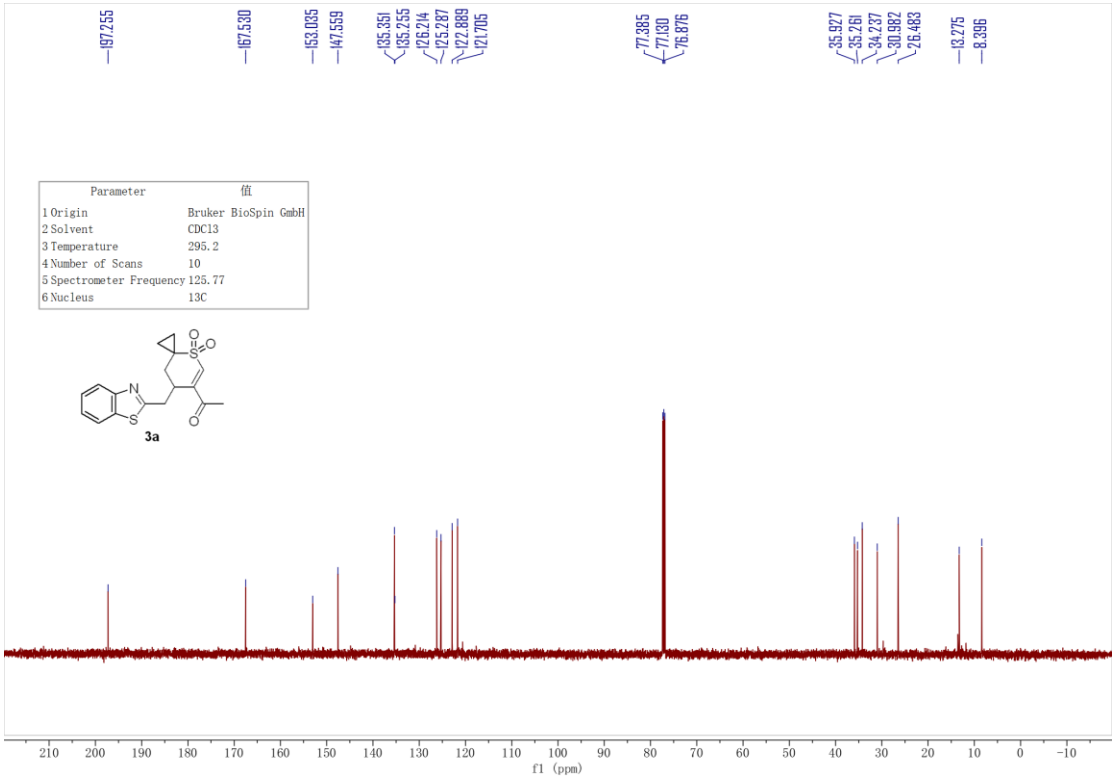
7.937
7.850
7.834
7.470
7.455
7.440
7.382
7.367
7.352
7.260
7.146
3.580
3.572
3.562
3.552
3.543
3.534
3.365
3.345
3.336
3.315
3.281
3.274
3.252
3.244
2.543
2.533
2.512
2.503
2.460
2.099
2.089
2.068
2.058
1.705
1.696
1.682
1.675
1.654
1.471
1.457
1.440
1.432
1.422
1.408
0.847
0.826
0.816
0.809
0.799
Parameter 值
1 Origin Bruker BioSpin GmbH
2 Solvent CDCl3
3 Temperature 294.7
4 Number of Scans 2
5 Spectrometer Frequency 500.13
6 Nucleus 1H
3a
1.00
0.98
1.03
1.01
1.00
1.05
1.07
1.02
1.07
3.00
1.08
1.07
2.09
1.08
f1 (ppm)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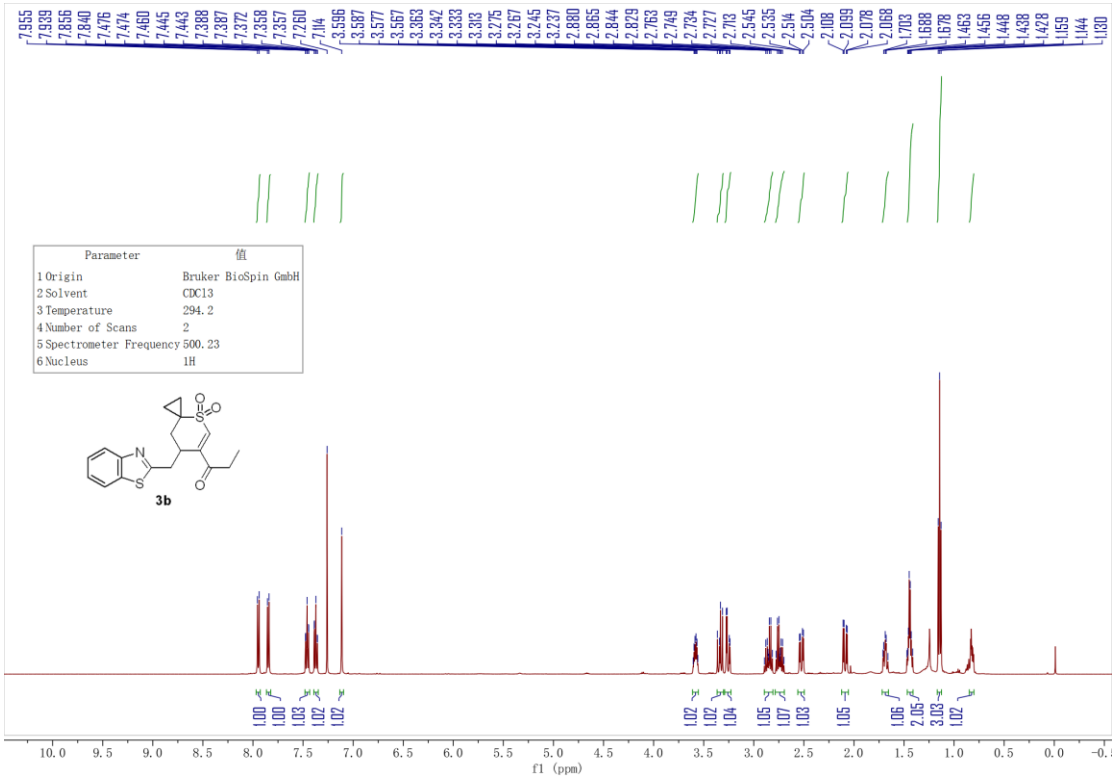
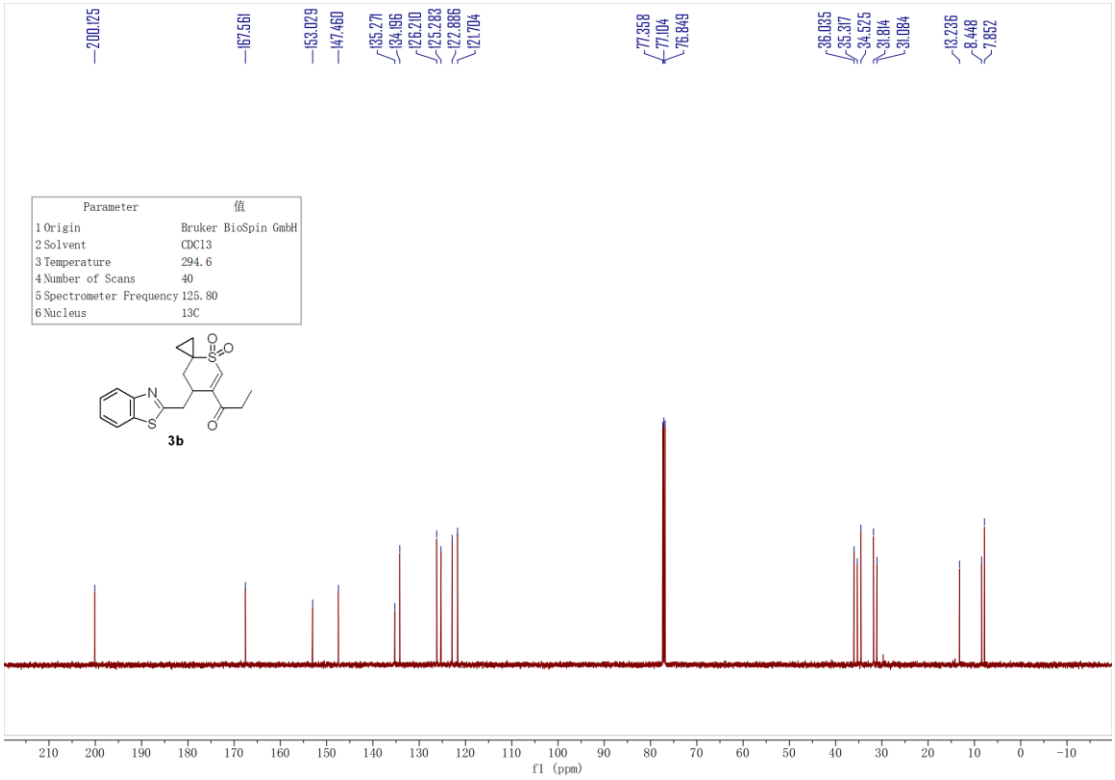
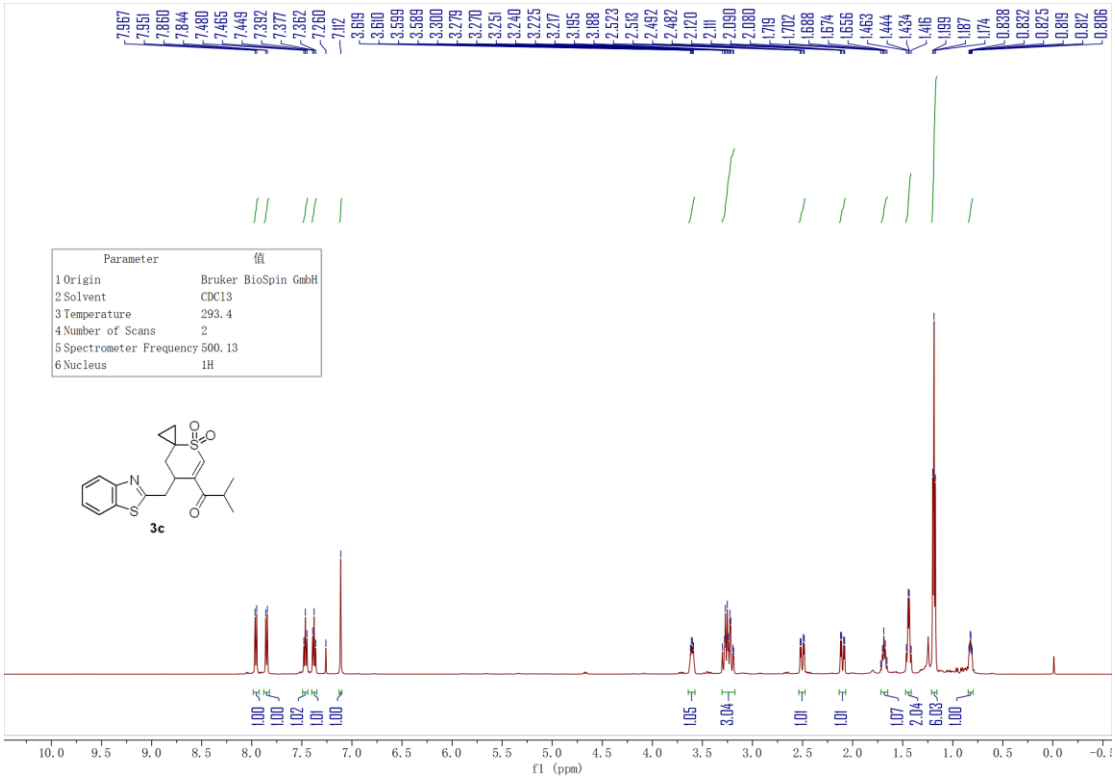
153.035
147.559
135.351
135.255
126.214
125.287
122.889
121.705
77.385
77.130
76.876
35.927
35.261
34.237
30.982
26.483
13.275
8.396
Parameter 值
1 Origin Bruker BioSpin GmbH
2 Solvent CDCl3
3 Temperature 295.2
4 Number of Scans 10
5 Spectrometer Frequency 125.77
6 Nucleus 13C
3a
f1 (ppm)


Parameter 值
1 Origin Bruker BioSpin GmbH
2 Solvent CDCl3
3 Temperature 294.2
4 Number of Scans 2
5 Spectrometer Frequency 500.23
6 Nucleus 1H
3b
f1 (ppm)


Parameter 值
1 Origin Bruker BioSpin GmbH
2 Solvent CDCl3
3 Temperature 294.6
4 Number of Scans 40
5 Spectrometer Frequency 125.80
6 Nucleus 13C
3b
f1 (ppm)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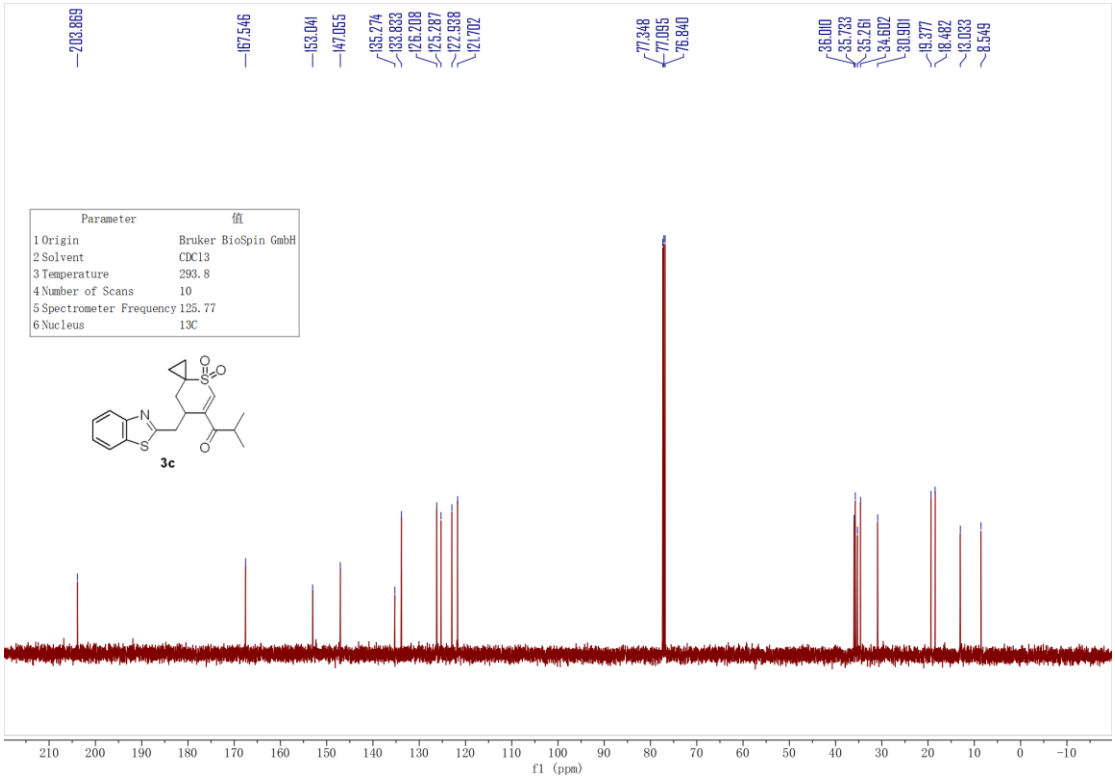
7.951
7.860
7.844
7.480
7.465
7.449
7.392
7.377
7.362
7.260
7.112
3.693
3.610
3.599
3.589
3.300
3.279
3.270
3.251
3.240
3.225
3.217
3.195
3.188
2.523
2.513
2.492
2.482
2.120
2.111
2.090
2.080
1.719
1.702
1.688
1.674
1.656
1.463
1.444
1.434
1.416
1.199
1.187
1.174
0.838
0.832
0.825
0.819
0.812
0.806
Parameter 值
1 Origin Bruker BioSpin GmbH
2 Solvent CDCl3
3 Temperature 293.4
4 Number of Scans 2
5 Spectrometer Frequency 500.13
6 Nucleus 1H
3c
1.00
1.00
1.02
1.01
1.00
1.05
3.04
1.01
1.01
1.07
2.04
6.03
1.00
f1 (ppm)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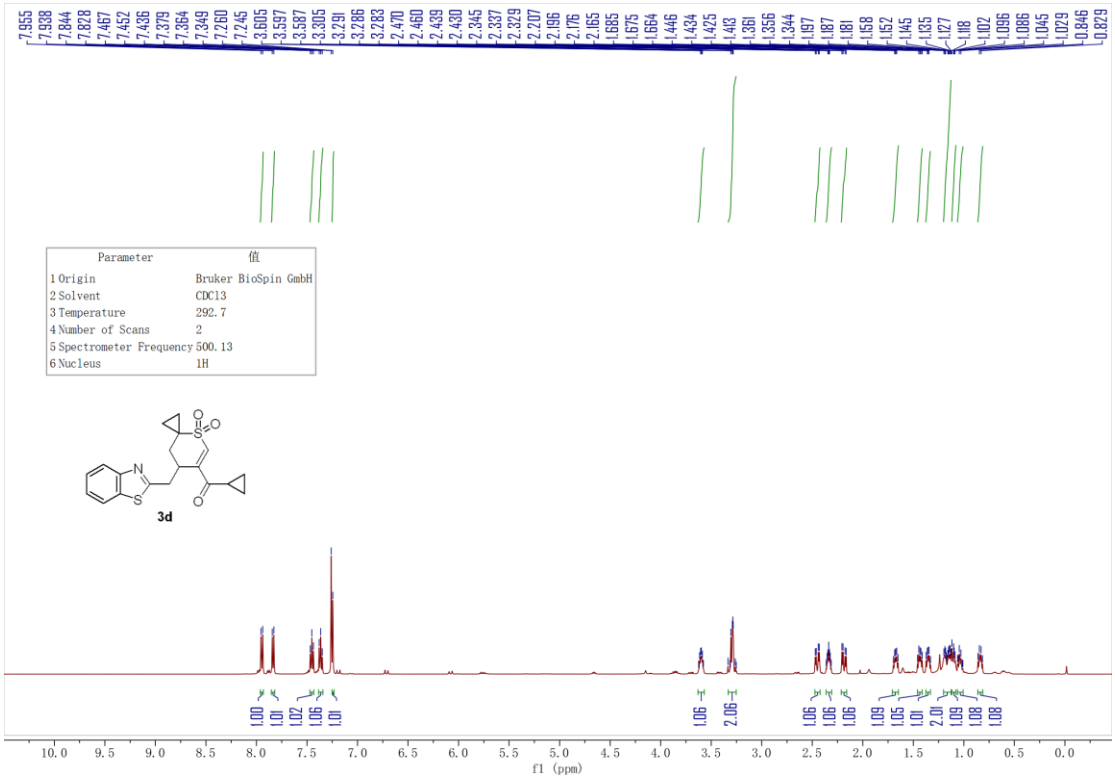
167.546
153.041
147.055
135.274
133.833
126.208
125.287
122.938
121.702
77.348
77.095
76.840
36.010
35.733
35.261
34.602
30.901
19.377
18.482
18.033
8.549
Parameter 值
1 Origin Bruker BioSpin GmbH
2 Solvent CDCl3
3 Temperature 293.8
4 Number of Scans 10
5 Spectrometer Frequency 125.77
6 Nucleus 13C
3c
f1 (ppm)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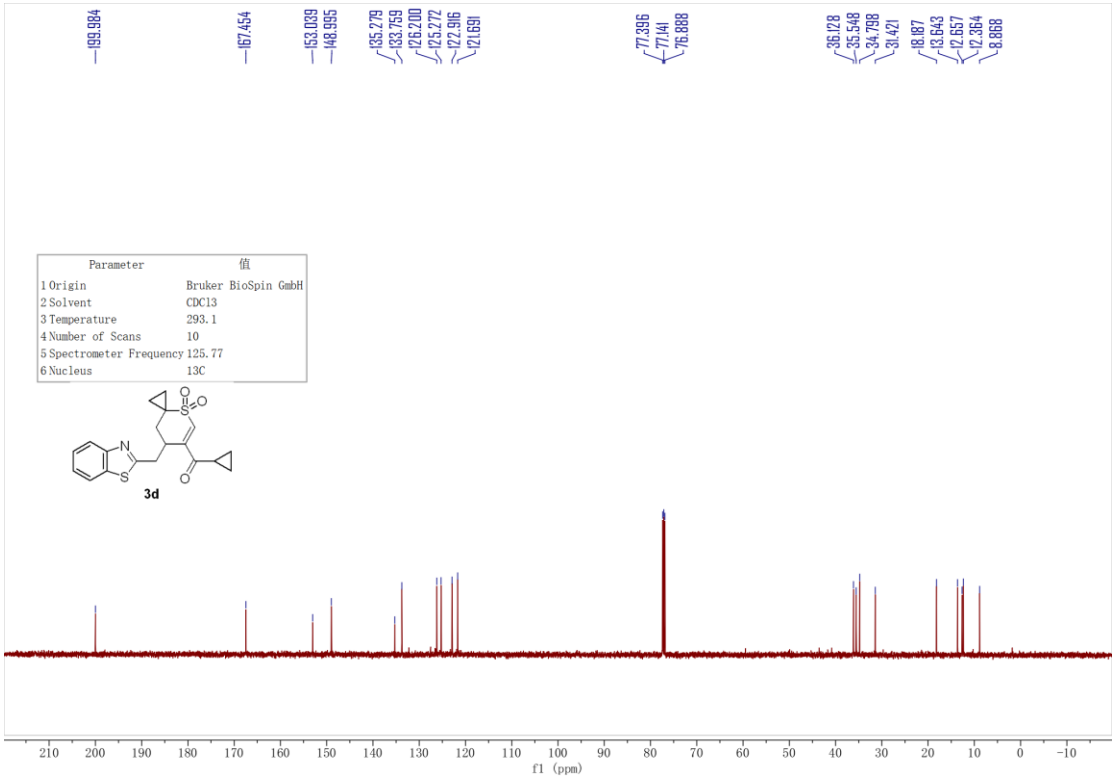
7.938
7.844
7.828
7.467
7.452
7.436
7.379
7.364
7.349
7.260
7.245
3.605
3.597
3.587
3.305
3.291
3.286
3.283
2.470
2.460
2.439
2.430
2.345
2.337
2.329
2.207
2.196
2.176
2.165
1.685
1.675
1.664
1.446
1.434
1.425
1.413
1.361
1.356
1.344
1.197
1.187
1.181
1.158
1.152
1.145
1.135
1.127
1.118
1.102
1.096
1.086
1.045
1.029
0.846
0.829
Parameter 值
1 Origin Bruker BioSpin GmbH
2 Solvent CDCl3
3 Temperature 292.7
4 Number of Scans 2
5 Spectrometer Frequency 500.13
6 Nucleus 1H
3d
1.00 1.01 1.02 1.06 1.01 1.06 2.06 1.06 1.06 1.06 1.09 1.05 1.01 2.01 1.09 1.08 1.08
10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)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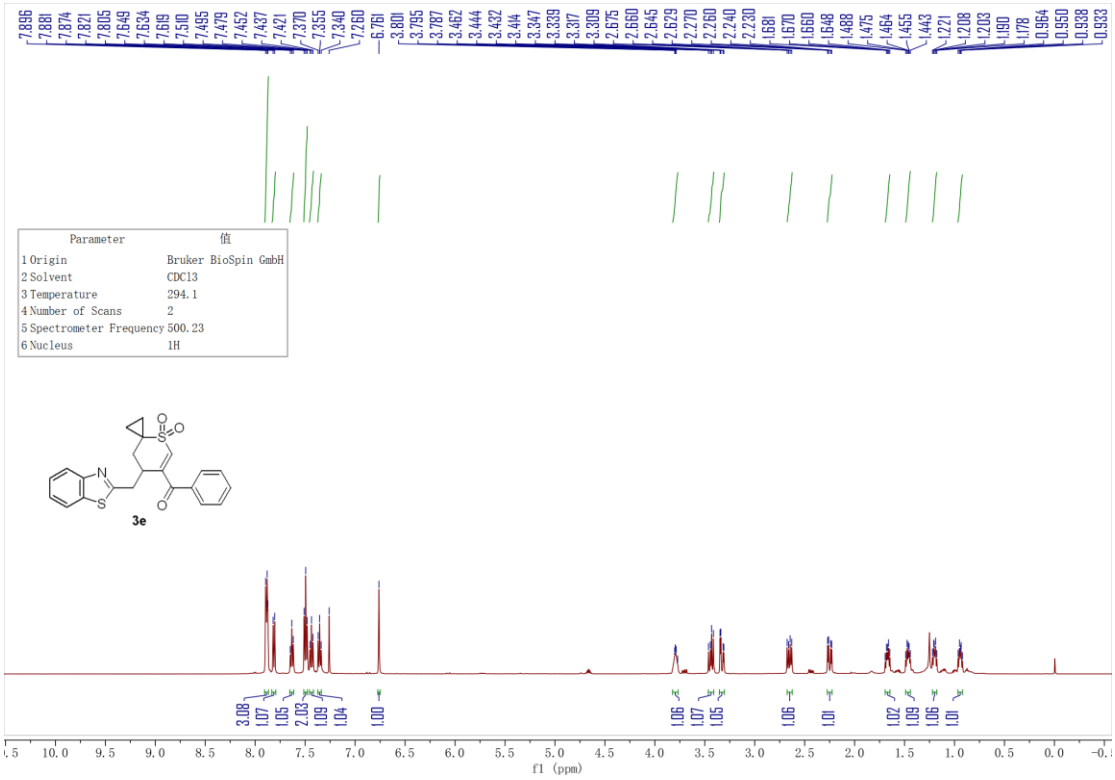
153.039
148.995
135.279
133.759
126.200
125.272
122.916
121.691
77.396
77.141
76.888
36.128
35.548
34.798
31.421
18.187
13.643
12.657
12.364
8.868
Parameter 值
1 Origin Bruker BioSpin GmbH
2 Solvent CDCl3
3 Temperature 293.1
4 Number of Scans 10
5 Spectrometer Frequency 125.77
6 Nucleus 13C
3d
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)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7.874
7.821
7.805
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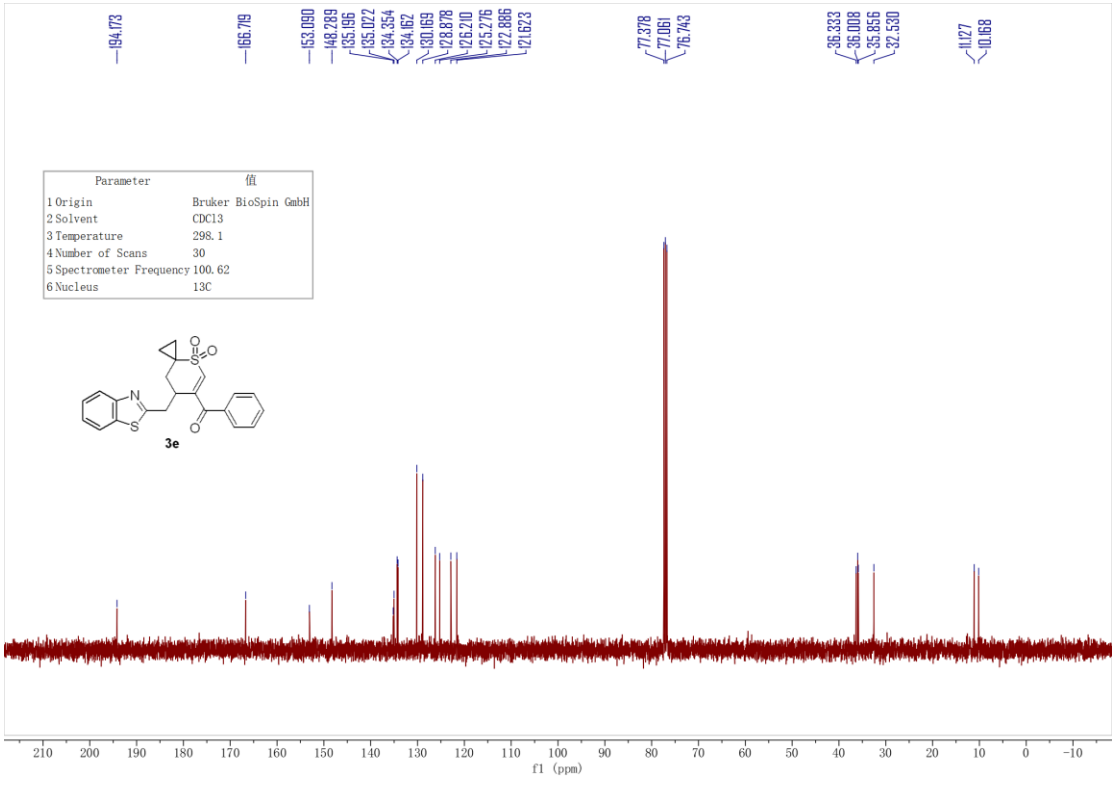
7.634
7.619
7.510
7.495
7.479
7.452
7.437
7.421
7.370
7.355
7.340
7.260
6.761
3.801
3.795
3.787
3.462
3.444
3.432
3.344
3.347
3.339
3.317
3.309
2.675
2.660
2.645
2.629
2.270
2.260
2.240
2.230
1.681
1.670
1.660
1.648
1.488
1.475
1.464
1.455
1.443
1.221
1.208
1.203
1.190
1.178
0.964
0.950
0.938
0.933
Parameter 值
1 Origin Bruker BioSpin GmbH
2 Solvent CDCl3
3 Temperature 294.1
4 Number of Scans 2
5 Spectrometer Frequency 500.23
6 Nucleus 1H
3e
3.08
1.07
1.05
2.03
1.09
1.04
1.00
1.06
1.07
1.05
1.06
1.01
1.02
1.09
1.06
1.01
f1 (ppm)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166.719
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148.289
135.196
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134.354
134.162
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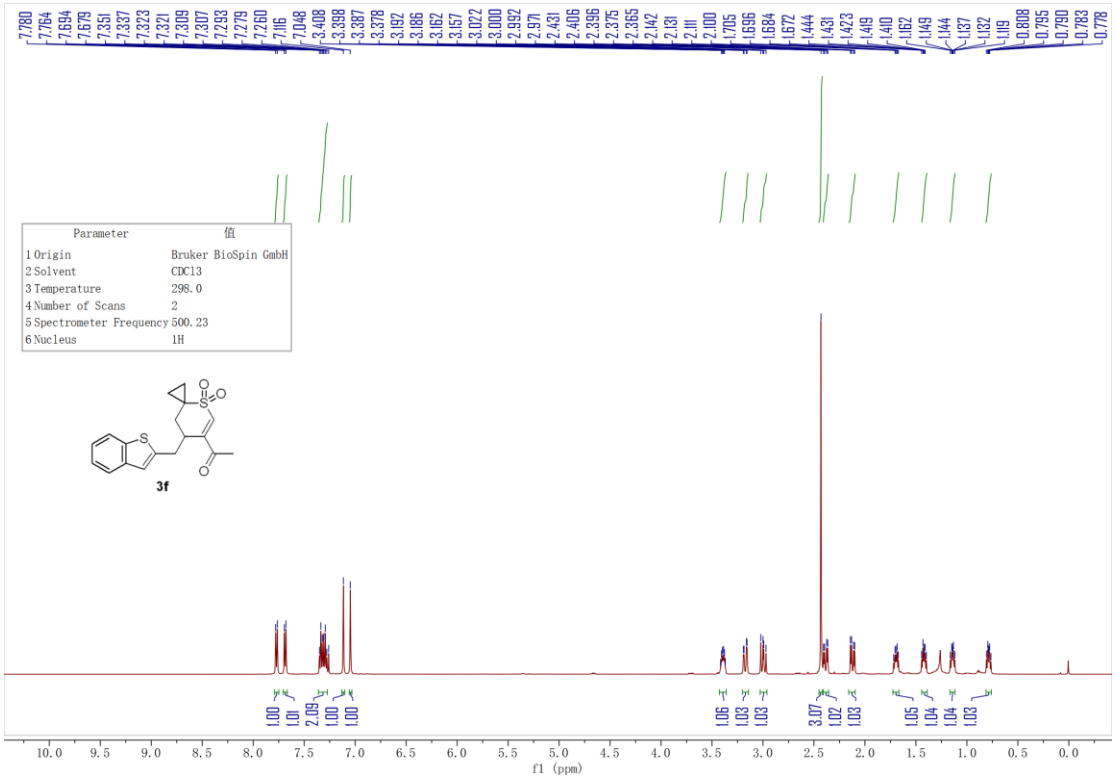
128.878
126.210
125.276
122.866
121.623
77.378
77.061
76.743
36.333
36.008
35.856
32.530
11.127
10.668
Parameter 值
1 Origin Bruker BioSpin GmbH
2 Solvent CDCl3
3 Temperature 298.1
4 Number of Scans 30
5 Spectrometer Frequency 100.62
6 Nucleus 13C
3e
f1 (ppm)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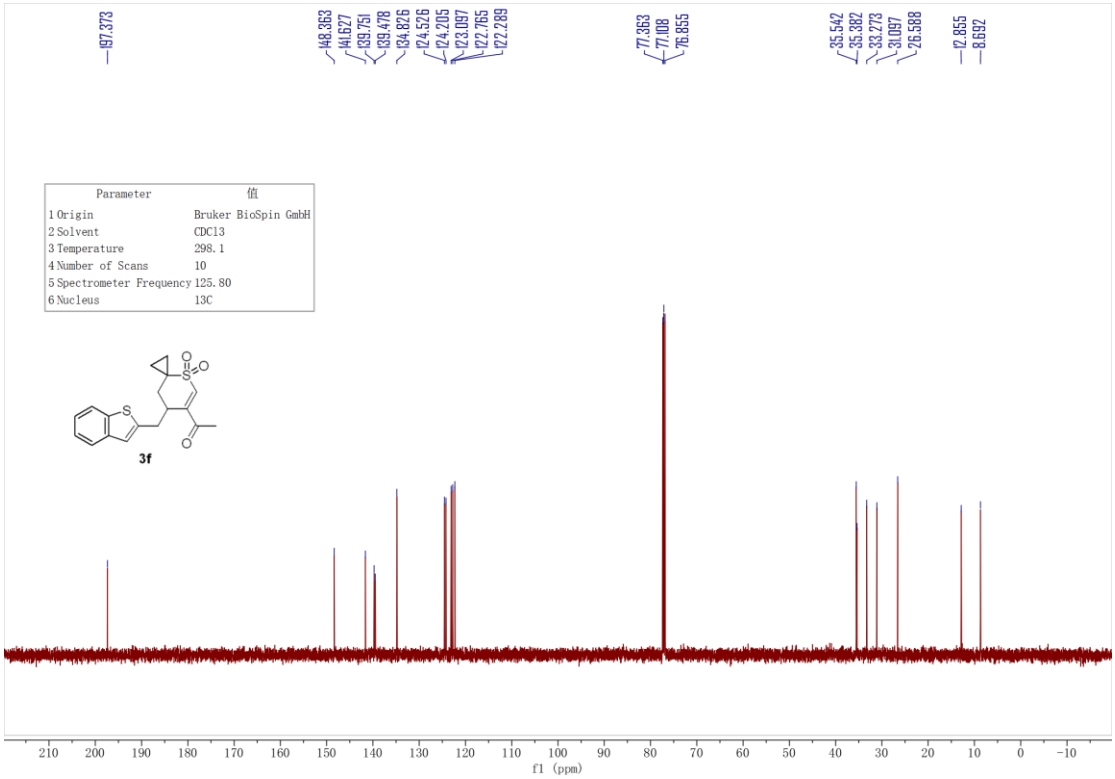
7.764
7.694
7.679
7.351
7.337
7.323
7.321
7.309
7.307
7.293
7.279
7.260
7.116
7.048
3.408
3.398
3.387
3.378
3.192
3.185
3.162
3.157
3.022
3.000
2.992
2.971
2.431
2.406
2.396
2.375
2.365
2.142
2.131
2.111
2.100
1.705
1.696
1.684
1.672
1.444
1.431
1.423
1.419
1.410
1.162
1.149
1.144
1.137
1.132
1.119
0.808
0.795
0.790
0.783
0.778
Parameter 值
1 Origin Bruker BioSpin GmbH
2 Solvent CDCl3
3 Temperature 298.0
4 Number of Scans 2
5 Spectrometer Frequency 500.23
6 Nucleus 1H
3f
1.00
1.01
2.09
1.00
1.00
1.06
1.03
1.03
3.07
1.02
1.03
1.05
1.04
1.04
1.03
f1 (ppm)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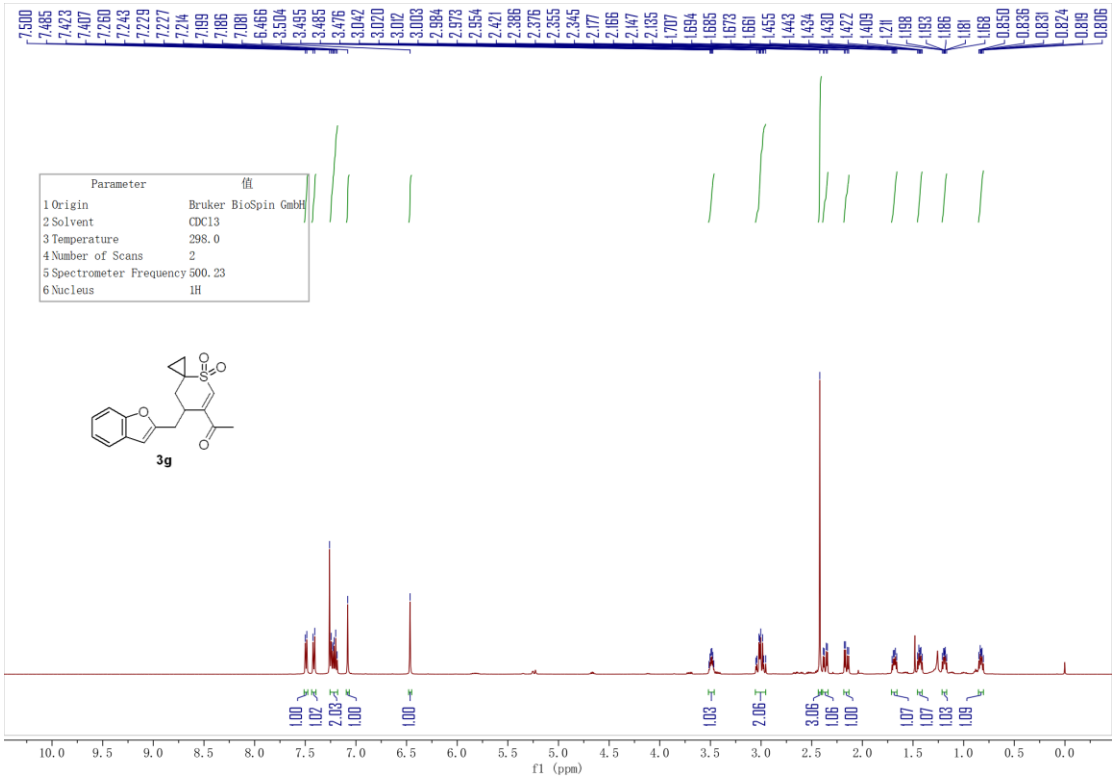
124.205
123.097
122.765
122.289
77.363
77.108
76.855
35.542
35.382
33.273
31.097
26.588
12.855
8.692
Parameter 值
1 Origin Bruker BioSpin GmbH
2 Solvent CDCl3
3 Temperature 298.1
4 Number of Scans 10
5 Spectrometer Frequency 125.80
6 Nucleus 13C
3f
f1 (ppm)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7.423
7.407
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7.243
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7.227
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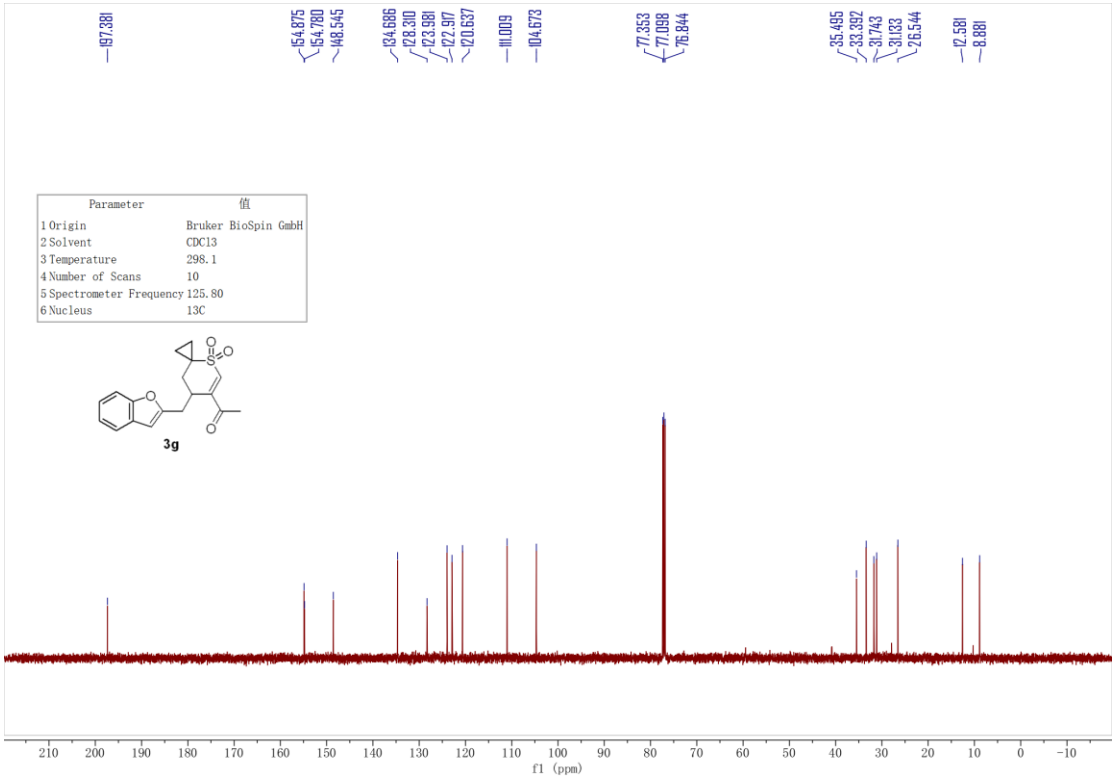
7.199
7.186
7.081
6.466
3.504
3.495
3.485
3.476
3.042
3.020
3.012
3.003
2.984
2.973
2.954
2.421
2.386
2.376
2.355
2.345
2.177
2.166
2.147
2.135
1.707
1.694
1.685
1.673
1.661
1.455
1.443
1.434
1.430
1.422
1.409
1.211
1.198
1.193
1.186
1.181
1.168
0.850
0.836
0.831
0.824
0.819
0.806
Parameter 值
1 Origin Bruker BioSpin GmbH
2 Solvent CDCl3
3 Temperature 298.0
4 Number of Scans 2
5 Spectrometer Frequency 500.23
6 Nucleus 1H
3g
1.00
1.02
2.03
1.00
1.00
1.03
2.06
3.06
1.06
1.00
1.07
1.07
1.03
1.09
f1 (ppm)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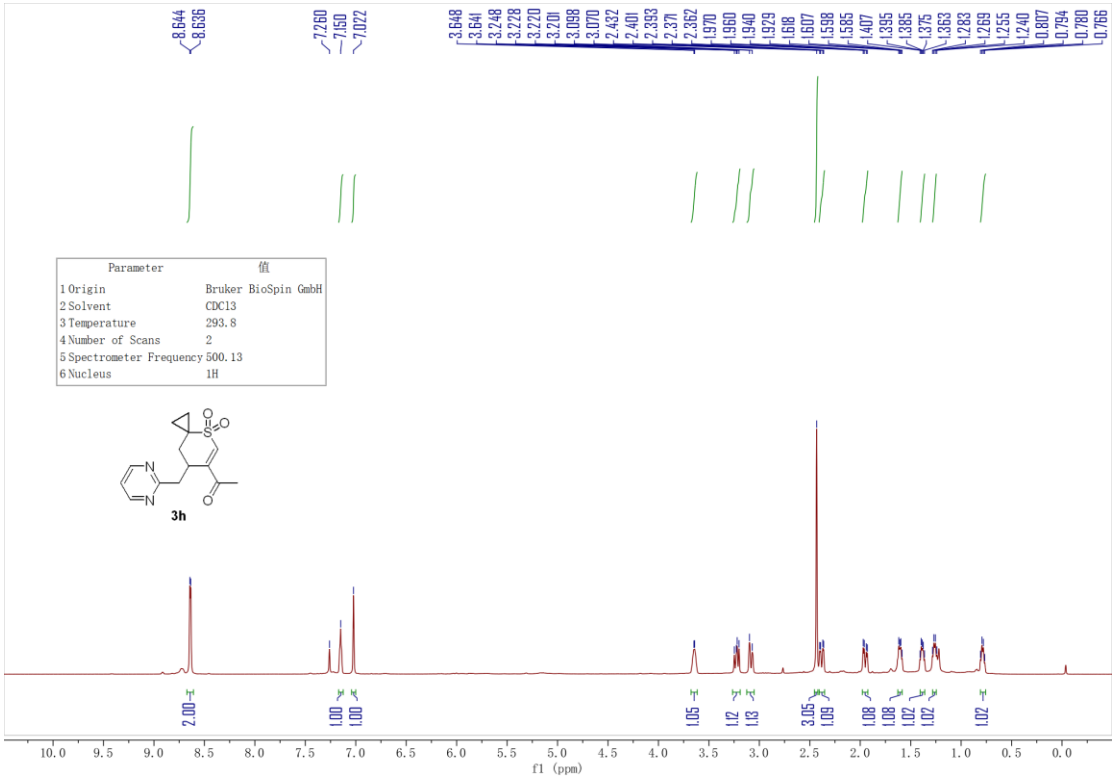
77.098
76.844
35.495
33.392
31.743
31.033
26.544
12.581
8.881
Parameter 值
1 Origin Bruker BioSpin GmbH
2 Solvent CDCl3
3 Temperature 298.1
4 Number of Scans 10
5 Spectrometer Frequency 125.80
6 Nucleus 13C
3g
f1 (ppm)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3.248
3.228
3.220
3.201
3.098
3.070
2.432
2.401
2.393
2.371
2.362
1.970
1.960
1.940
1.929
1.618
1.607
1.598
1.585
1.407
1.395
1.385
1.375
1.363
1.283
1.269
1.255
1.240
0.807
0.794
0.780
0.766
Parameter 值
1 Origin Bruker BioSpin GmbH
2 Solvent CDCl3
3 Temperature 293.8
4 Number of Scans 2
5 Spectrometer Frequency 500.13
6 Nucleus 1H
3h
2.00
1.00
1.00
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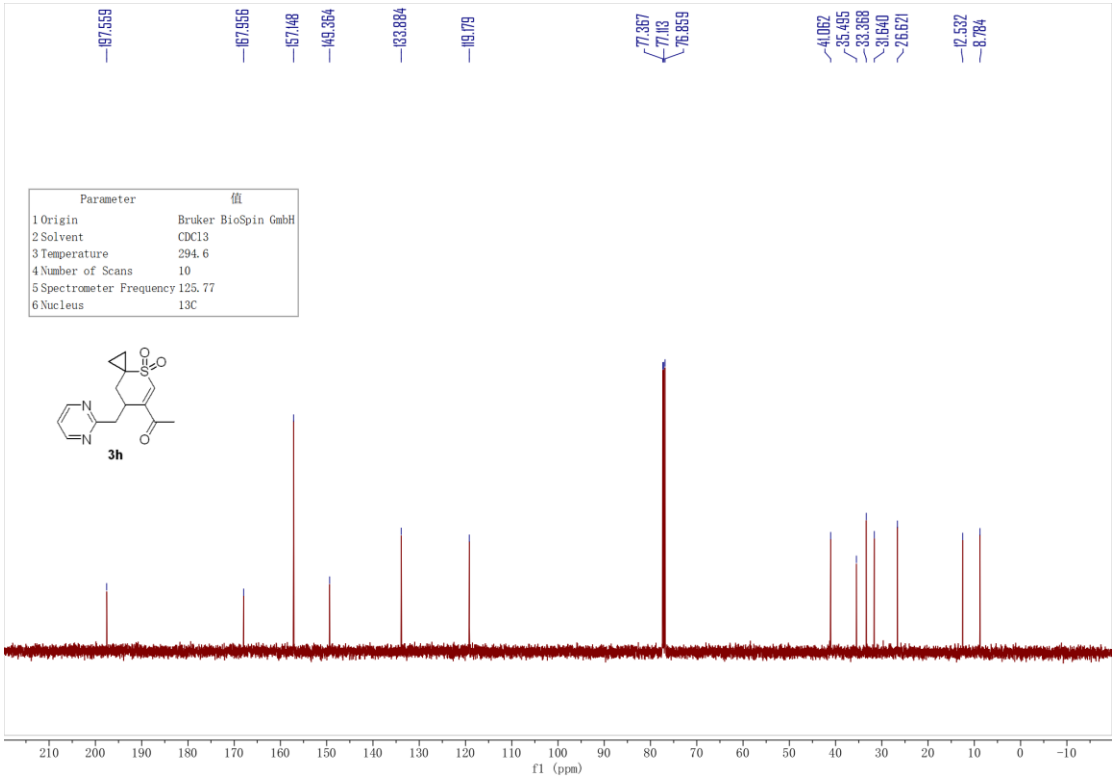
3.05
1.09
1.08
1.08
1.02
1.02
1.02
f1 (ppm)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77.367
77.113
76.859
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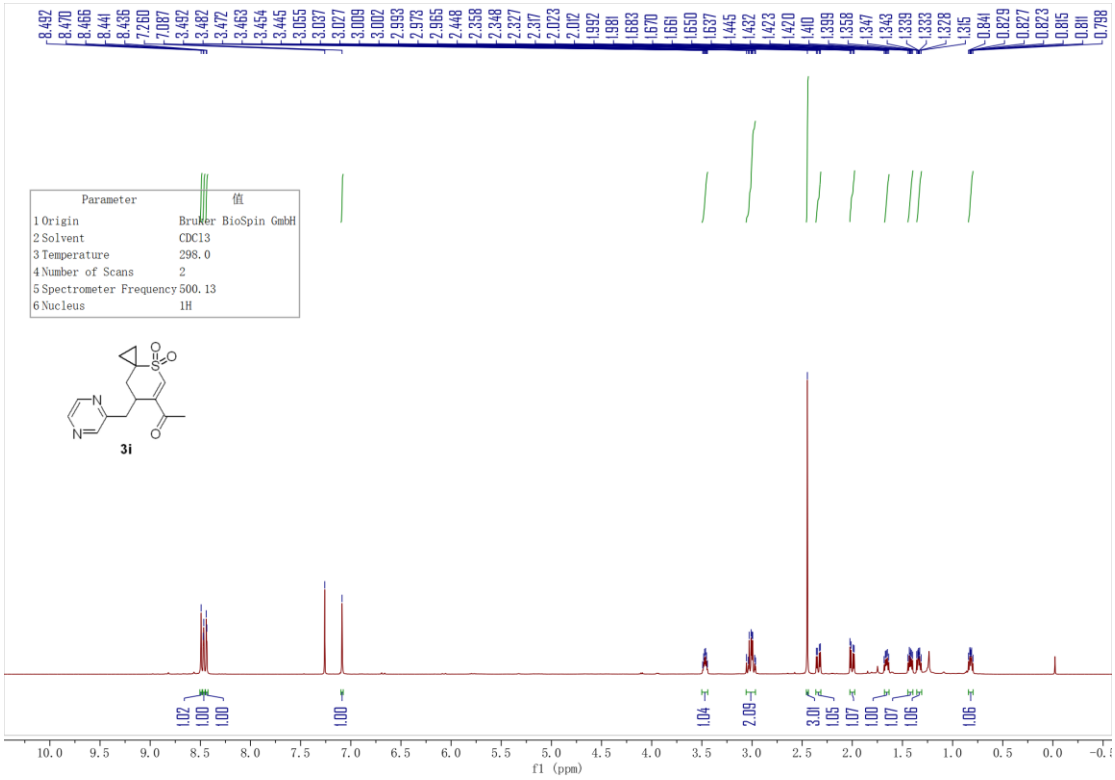
35.495
33.368
31.640
26.621
12.532
8.784
Parameter 值
1 Origin Bruker BioSpin GmbH
2 Solvent CDCl3
3 Temperature 294.6
4 Number of Scans 10
5 Spectrometer Frequency 125.77
6 Nucleus 13C
3h
f1 (ppm)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3.445
3.055
3.037
3.027
3.009
3.002
2.993
2.973
2.965
2.448
2.358
2.348
2.327
2.317
2.023
2.002
1.992
1.981
1.683
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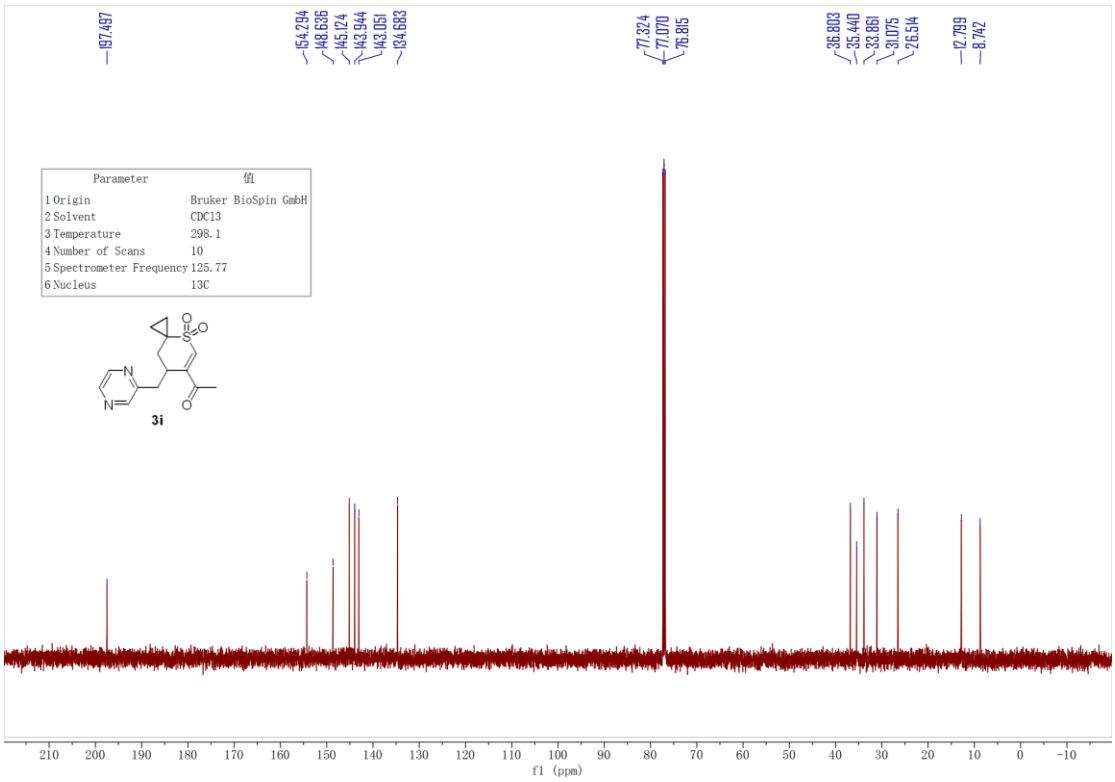
1.661
1.650
1.637
1.445
1.432
1.423
1.420
1.410
1.399
1.358
1.347
1.343
1.339
1.333
1.328
1.315
0.844
0.829
0.827
0.823
0.815
0.811
0.798
Parameter 值
1 Origin Bruker BioSpin GmbH
2 Solvent CDCl3
3 Temperature 298.0
4 Number of Scans 2
5 Spectrometer Frequency 500.13
6 Nucleus 1H
3i
1.02
1.00
1.00
1.00
1.04
2.09
3.01
1.05
1.07
1.00
1.07
1.06
1.06
f1 (ppm)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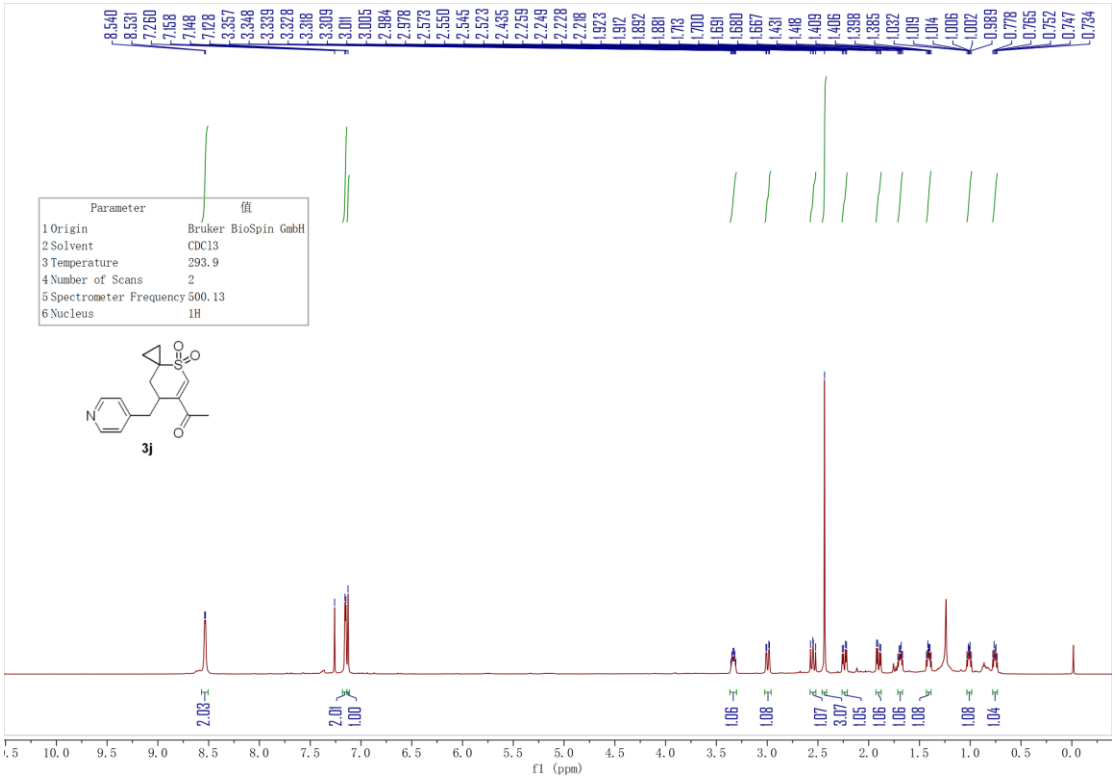
35.440
33.861
31.075
26.514
12.799
8.742
Parameter 值
1 Origin Bruker BioSpin GmbH
2 Solvent CDCl3
3 Temperature 298.1
4 Number of Scans 10
5 Spectrometer Frequency 125.77
6 Nucleus 13C
3i
f1 (ppm)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7.128
3.357
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3.328
3.318
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3.011
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2.259
2.249
2.228
2.218
1.923
1.912
1.892
1.881
1.713
1.700
1.691
1.680
1.667
1.431
1.418
1.409
1.406
1.398
1.385
1.032
1.019
1.014
1.006
1.002
0.989
0.778
0.765
0.752
0.747
0.734
Parameter 值
1 Origin Bruker BioSpin GmbH
2 Solvent CDCl3
3 Temperature 293.9
4 Number of Scans 2
5 Spectrometer Frequency 500.13
6 Nucleus 1H
3j
2.03
2.01
1.00
1.06
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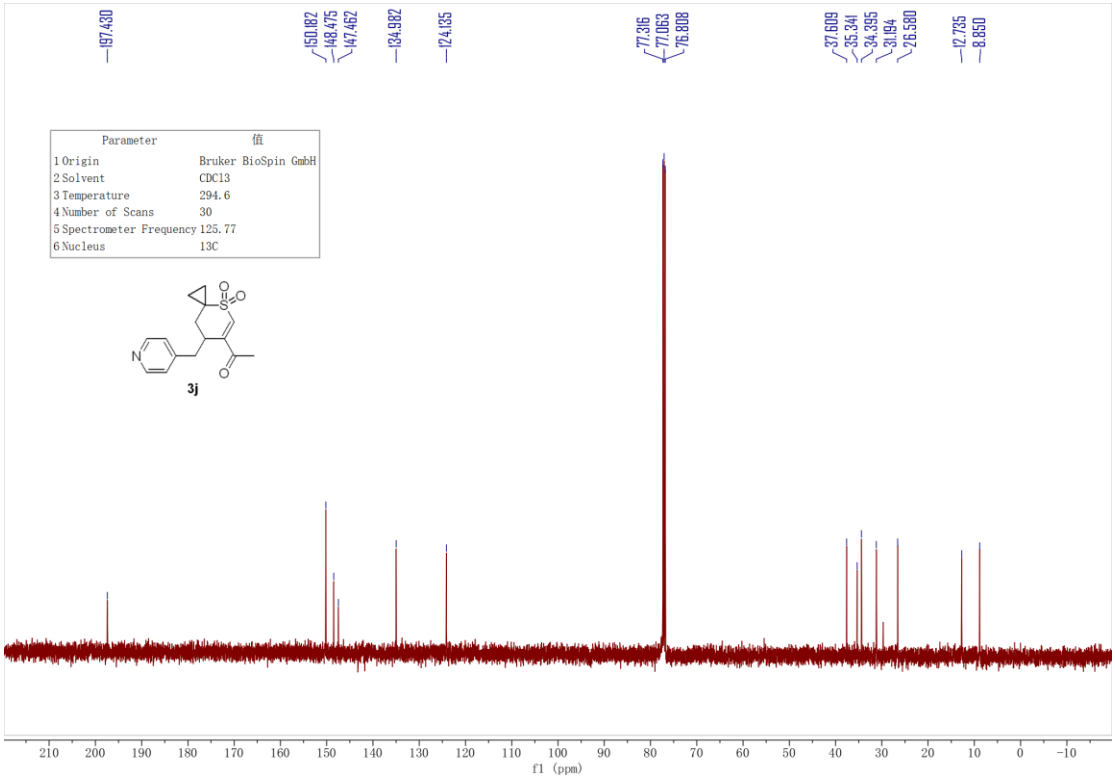
1.06
1.06
1.08
1.08
1.04
f1 (ppm)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77.316
77.063
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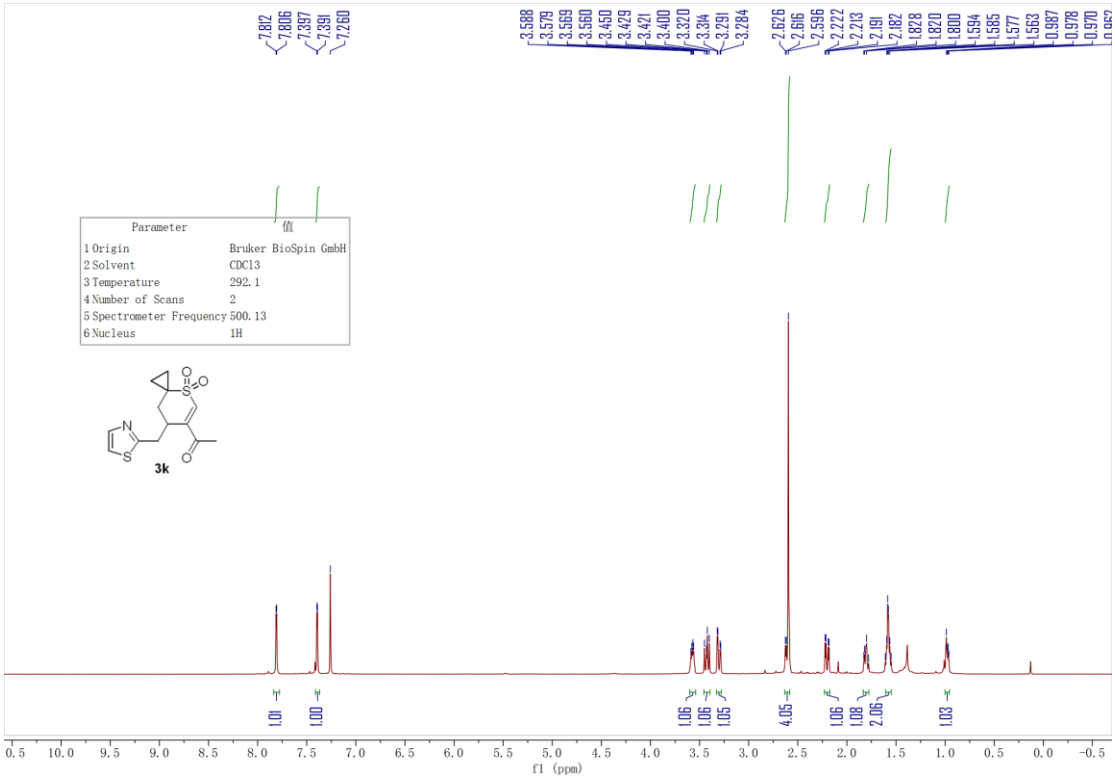
35.341
34.395
31.194
26.580
12.735
8.850
Parameter 值
1 Origin Bruker BioSpin GmbH
2 Solvent CDCl3
3 Temperature 294.6
4 Number of Scans 30
5 Spectrometer Frequency 125.77
6 Nucleus 13C
3j
f1 (ppm)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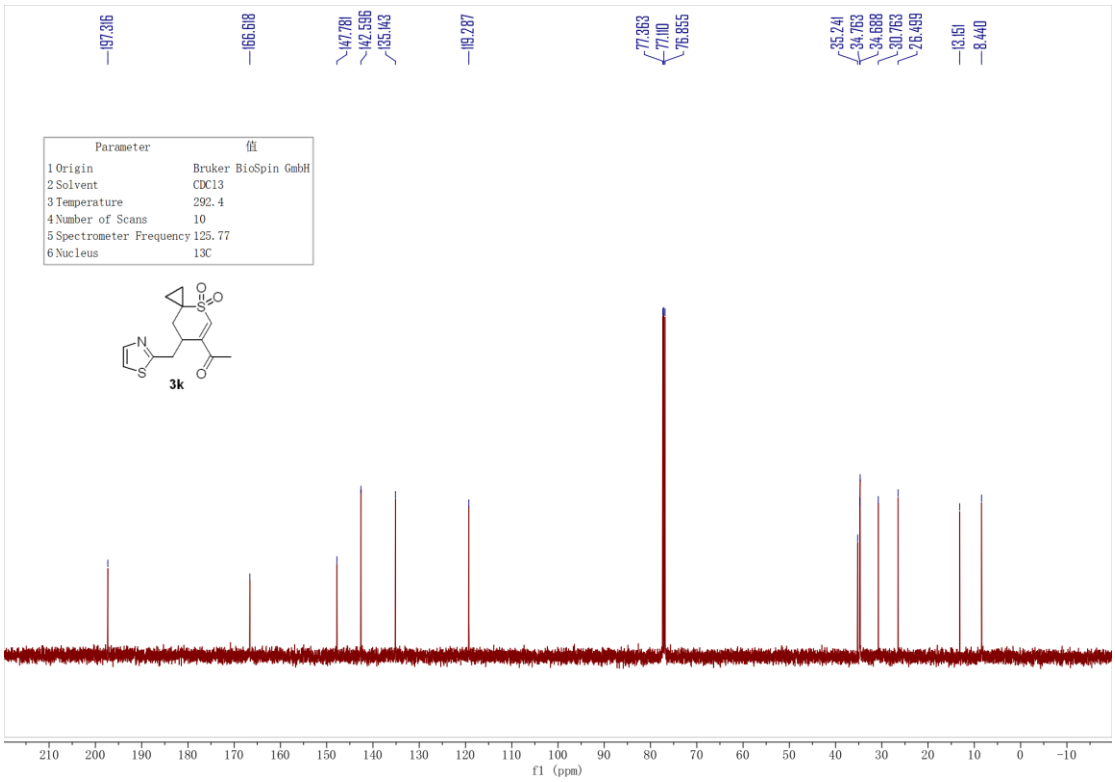
7.806
7.397
7.391
7.260
3.588
3.579
3.569
3.560
3.450
3.429
3.421
3.400
3.320
3.314
3.291
3.284
2.626
2.616
2.596
2.222
2.213
2.191
2.182
1.828
1.820
1.800
1.594
1.585
1.577
1.563
0.987
0.978
0.970
Parameter 值
1 Origin Bruker BioSpin GmbH
2 Solvent CDCl3
3 Temperature 292.1
4 Number of Scans 2
5 Spectrometer Frequency 500.13
6 Nucleus 1H
3k
1.01
1.00
1.06
1.06
1.05
4.05
1.06
1.08
2.06
1.03
f1 (ppm)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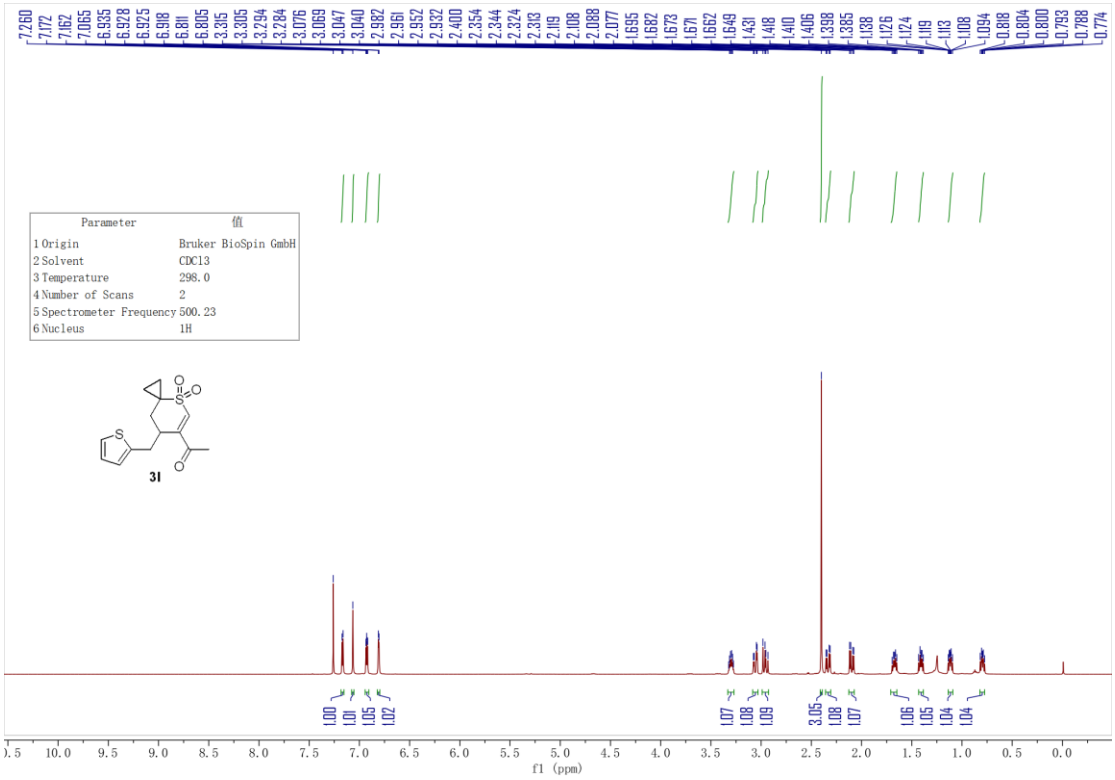
166.618
147.781
142.595
135.143
119.287
77.363
77.110
76.855
35.241
34.763
34.688
30.763
26.499
13.151
8.440
Parameter 值
1 Origin Bruker BioSpin GmbH
2 Solvent CDCl3
3 Temperature 292.4
4 Number of Scans 10
5 Spectrometer Frequency 125.77
6 Nucleus 13C
3k
f1 (ppm)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7.172
7.162
7.065
6.935
6.928
6.925
6.918
6.811
6.805
3.395
3.305
3.294
3.284
3.076
3.069
3.047
3.040
2.982
2.961
2.952
2.932
2.400
2.354
2.344
2.324
2.313
2.119
2.108
2.088
2.077
1.695
1.682
1.673
1.671
1.662
1.649
1.431
1.418
1.410
1.406
1.398
1.385
1.138
1.126
1.124
1.119
1.113
1.108
1.094
0.818
0.804
0.800
0.793
0.788
0.774
Parameter 值
1 Origin Bruker BioSpin GmbH
2 Solvent CDCl3
3 Temperature 298.0
4 Number of Scans 2
5 Spectrometer Frequency 500.23
6 Nucleus 1H
3l
1.00
1.01
1.05
1.02
1.07
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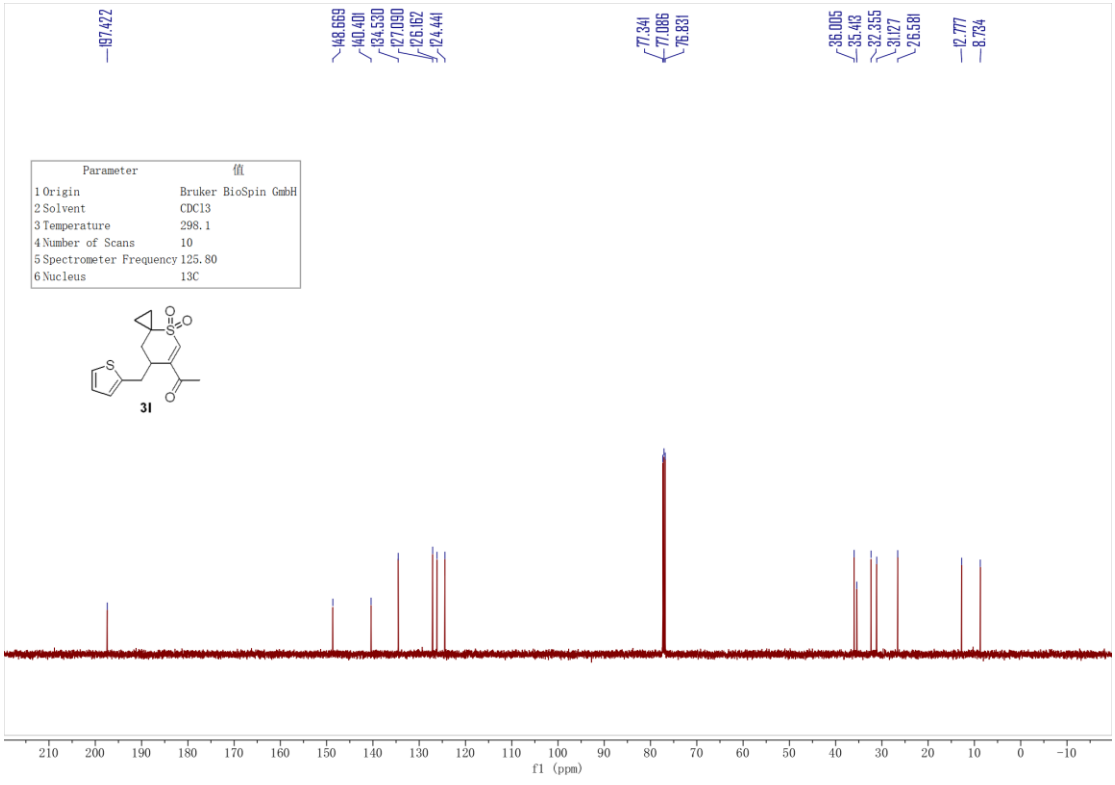
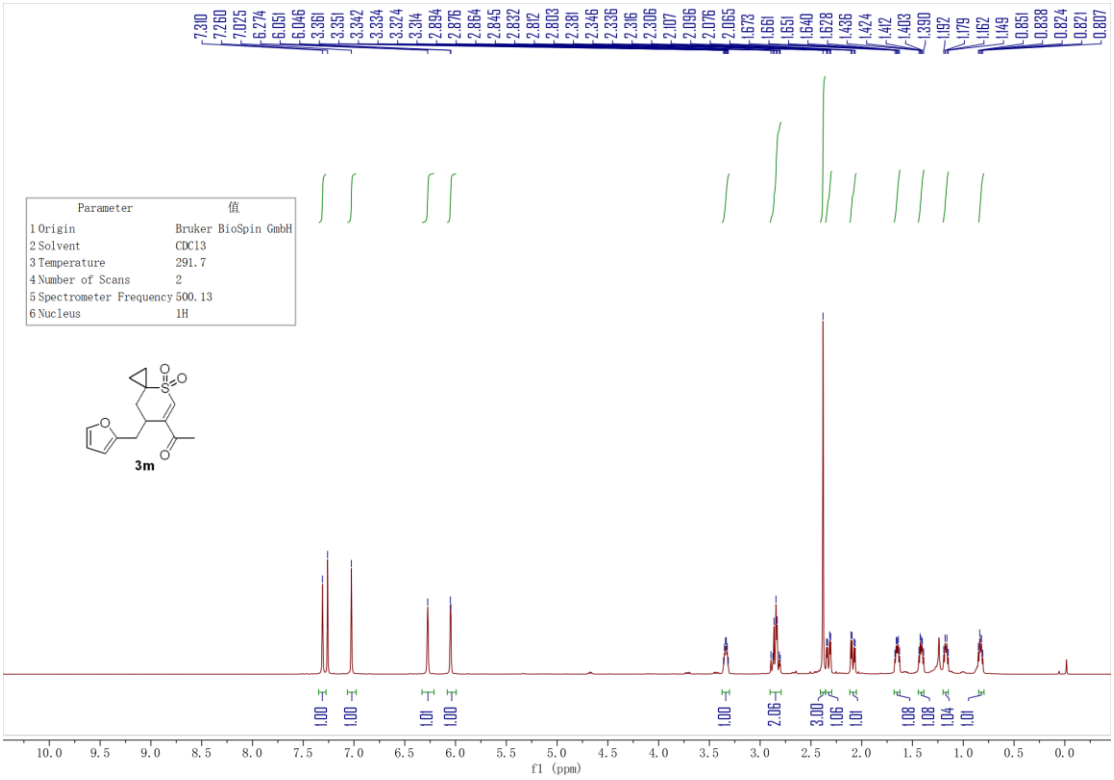
1.09
3.05
1.08
1.07
1.06
1.05
1.04
1.04
f1 (ppm)


197.422
148.669
140.401
134.530
127.090
126.162
124.441
71.341
77.086
76.831
36.005
35.413
32.355
31.127
26.581
12.777
8.734
Parameter 值
1 Origin Bruker BioSpin GmbH
2 Solvent CDCl3
3 Temperature 298.1
4 Number of Scans 10
5 Spectrometer Frequency 125.80
6 Nucleus 13C
3l
f1 (ppm)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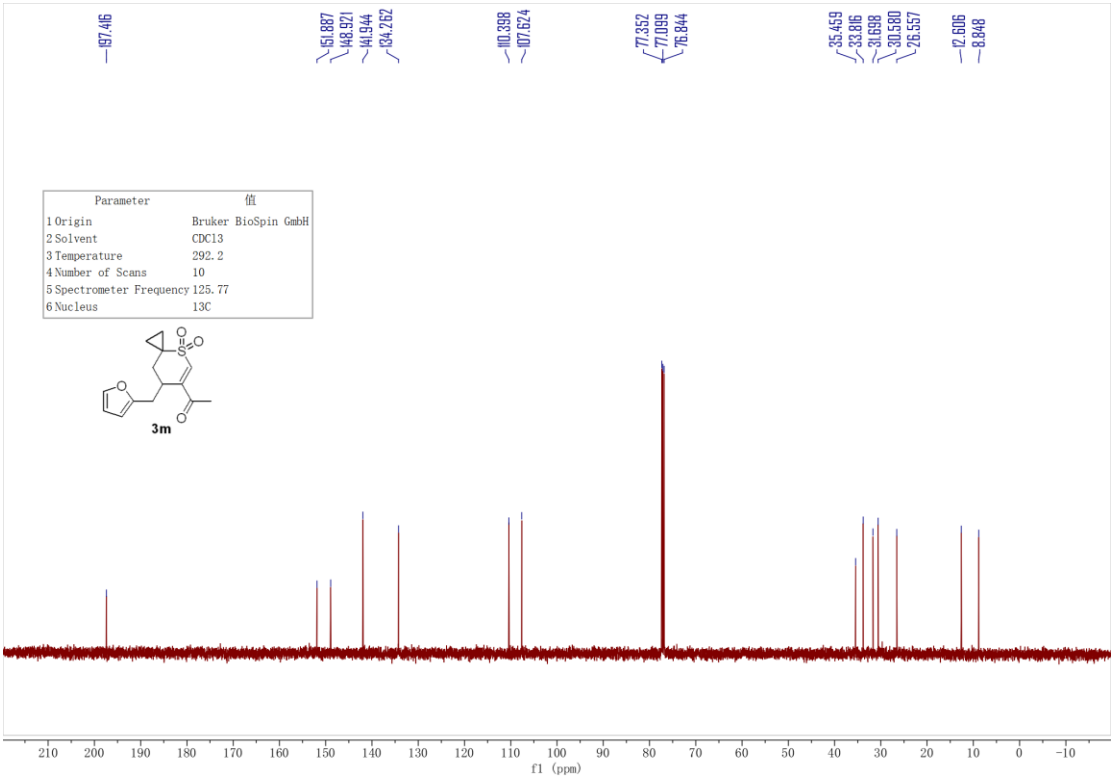
7.260
7.025
6.274
6.051
6.046
3.361
3.351
3.342
3.334
3.324
3.314
2.894
2.876
2.864
2.845
2.832
2.812
2.803
2.381
2.346
2.336
2.316
2.306
2.107
2.096
2.076
2.065
1.673
1.661
1.651
1.640
1.628
1.436
1.424
1.412
1.403
1.390
1.192
1.179
1.162
1.149
0.851
0.838
0.824
0.821
0.807
Parameter 值
1 Origin Bruker BioSpin GmbH
2 Solvent CDCl3
3 Temperature 291.7
4 Number of Scans 2
5 Spectrometer Frequency 500.13
6 Nucleus 1H
3m
1.00
1.00
1.01
1.00
1.00
2.06
3.00
1.06
1.01
1.08
1.08
1.04
1.01
f1 (ppm)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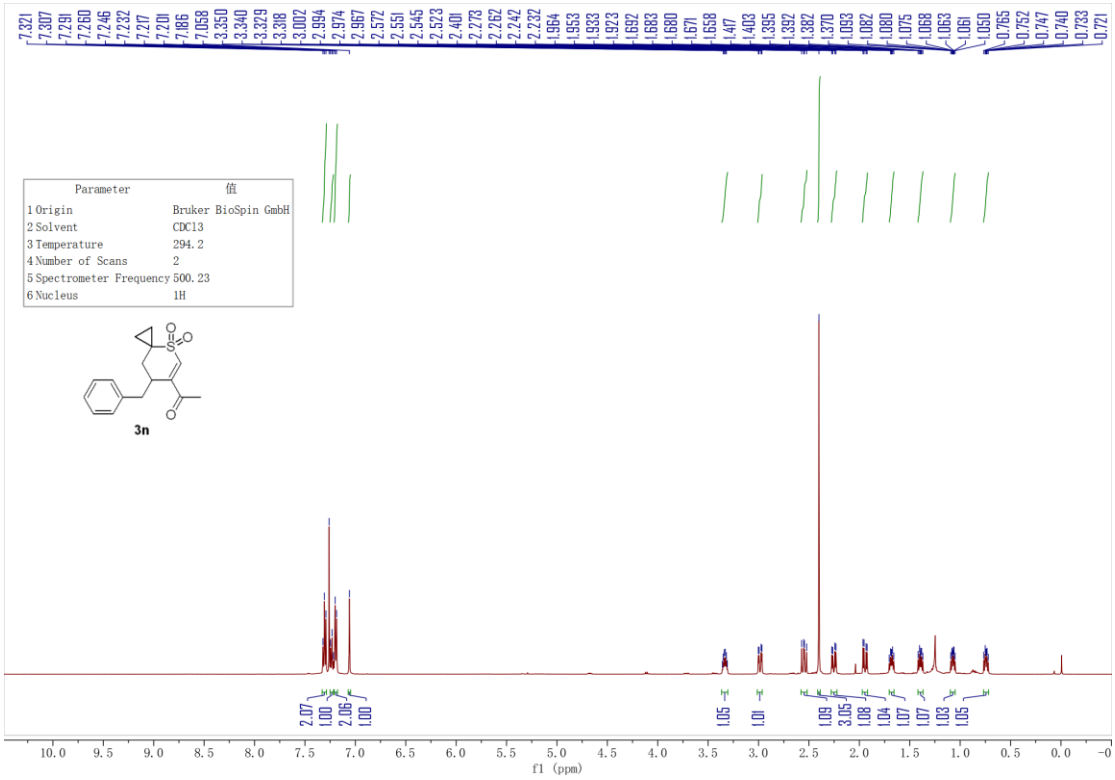
151.887
148.921
141.944
134.262
110.398
107.624
77.352
77.099
76.844
35.459
33.816
31.698
30.580
26.557
12.606
8.848
Parameter 值
1 Origin Bruker BioSpin GmbH
2 Solvent CDCl3
3 Temperature 292.2
4 Number of Scans 10
5 Spectrometer Frequency 125.77
6 Nucleus 13C
3m
f1 (ppm)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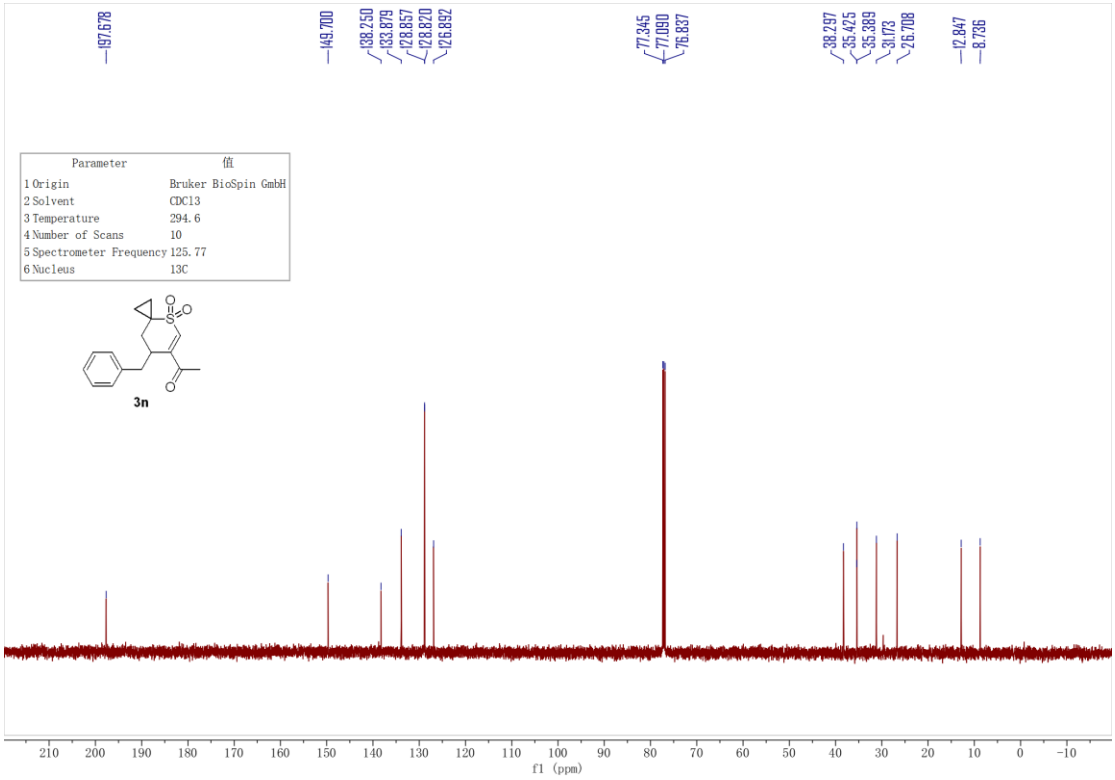
7.307
7.291
7.260
7.246
7.232
7.217
7.201
7.185
7.058
3.350
3.340
3.329
3.308
3.002
2.994
2.974
2.967
2.572
2.551
2.545
2.523
2.401
2.273
2.262
2.242
2.232
1.964
1.953
1.933
1.923
1.692
1.683
1.680
1.671
1.658
1.447
1.403
1.395
1.392
1.382
1.370
1.093
1.082
1.080
1.075
1.068
1.063
1.061
1.050
0.765
0.752
0.747
0.740
0.733
0.721
Parameter 值
1 Origin Bruker BioSpin GmbH
2 Solvent CDC13
3 Temperature 294.2
4 Number of Scans 2
5 Spectrometer Frequency 500.23
6 Nucleus 1H
3n
2.07
1.00
2.06
1.00
1.05
1.01
1.09
3.05
1.08
1.04
1.07
1.07
1.03
1.05
f1 (ppm)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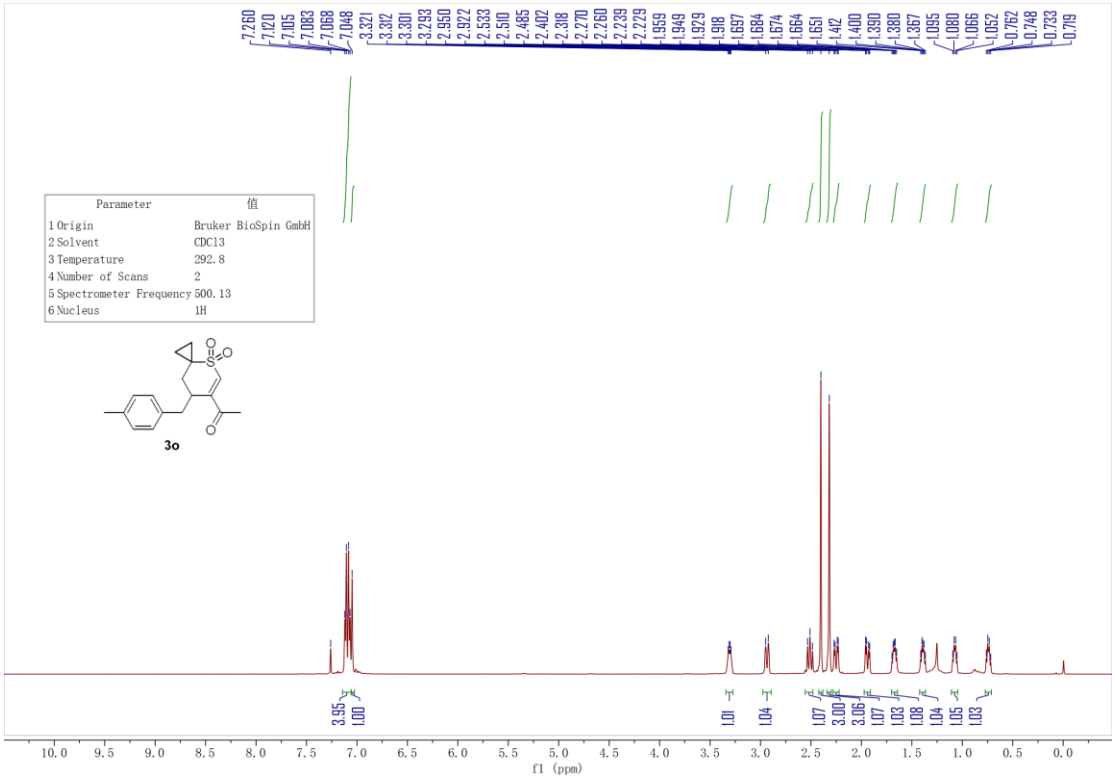
149.700
138.250
133.879
128.857
128.820
126.892
77.345
77.090
76.837
38.297
35.425
35.389
31.173
26.708
12.847
8.736
Parameter 值
1 Origin Bruker BioSpin GmbH
2 Solvent CDC13
3 Temperature 294.6
4 Number of Scans 10
5 Spectrometer Frequency 125.77
6 Nucleus 13C
3n
f1 (ppm)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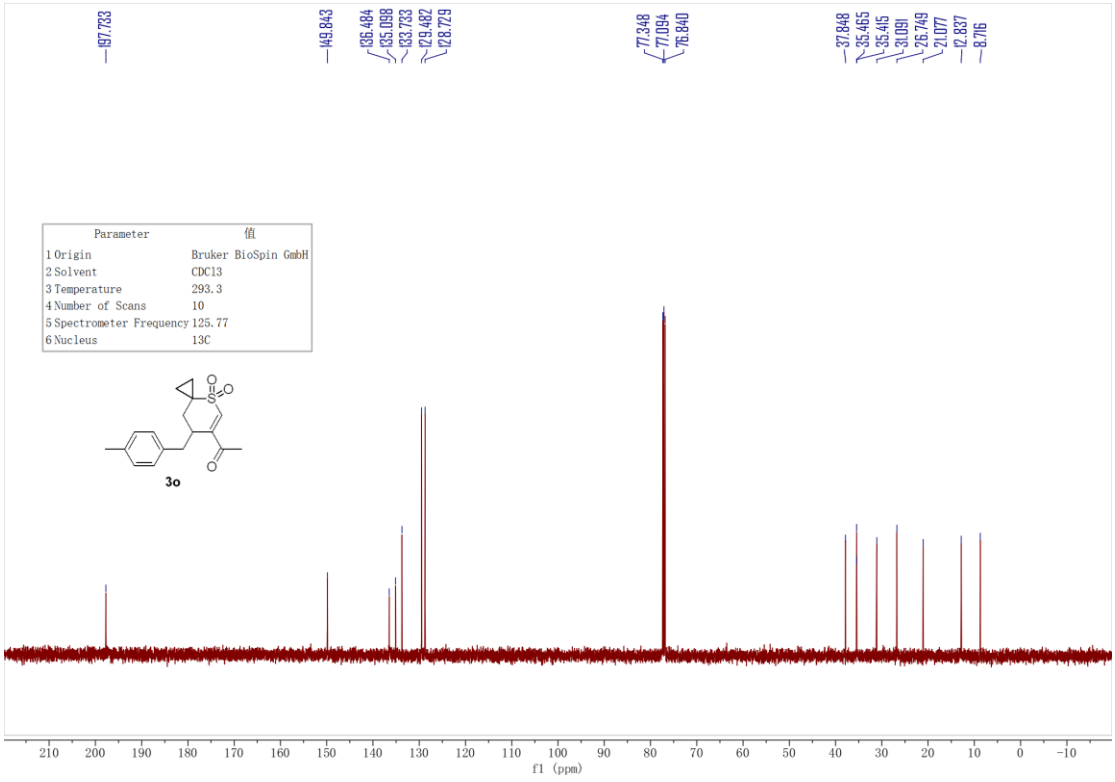
7.120
7.105
7.083
7.068
7.048
3.321
3.312
3.301
3.293
2.950
2.922
2.533
2.510
2.485
2.407
2.398
2.270
2.260
2.239
2.229
1.959
1.949
1.929
1.918
1.697
1.684
1.674
1.664
1.651
1.412
1.400
1.390
1.380
1.367
1.095
1.080
1.066
1.052
0.762
0.748
0.733
0.719
Parameter 值
1 Origin Bruker BioSpin GmbH
2 Solvent CDCl3
3 Temperature 292.8
4 Number of Scans 2
5 Spectrometer Frequency 500.13
6 Nucleus 1H
3o
3.95
1.00
1.01
1.04
1.07
3.00
3.06
1.07
1.03
1.08
1.04
1.05
1.03
10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)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136.484
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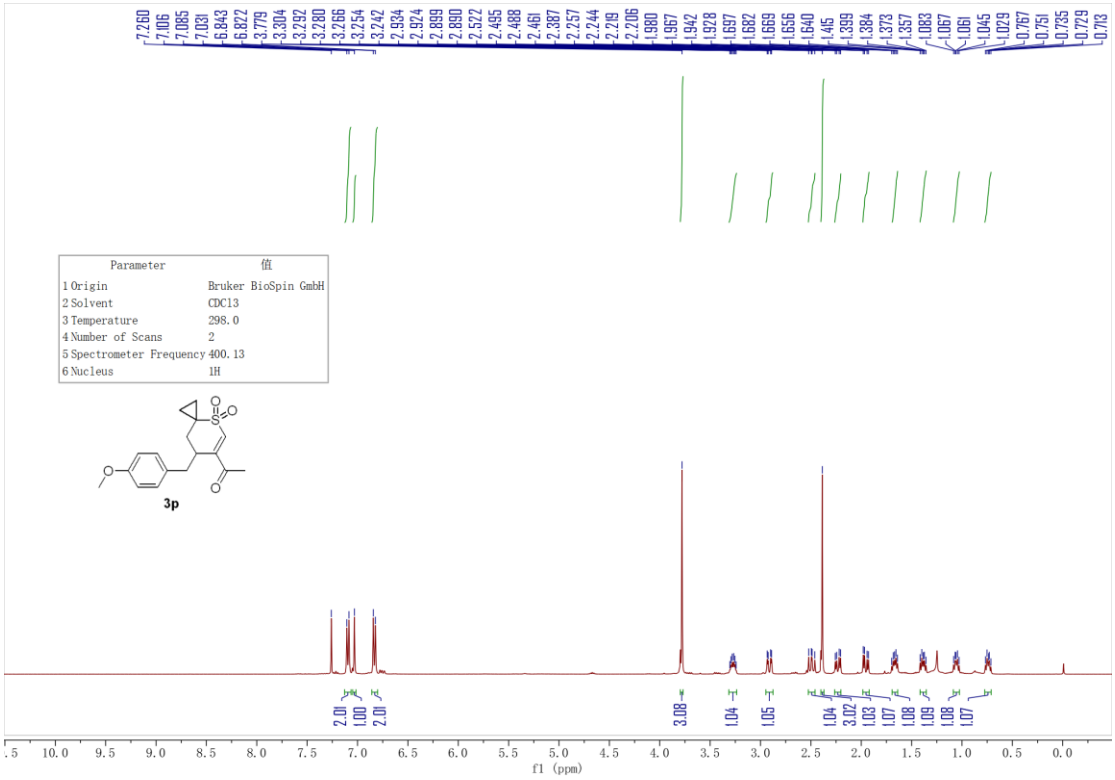
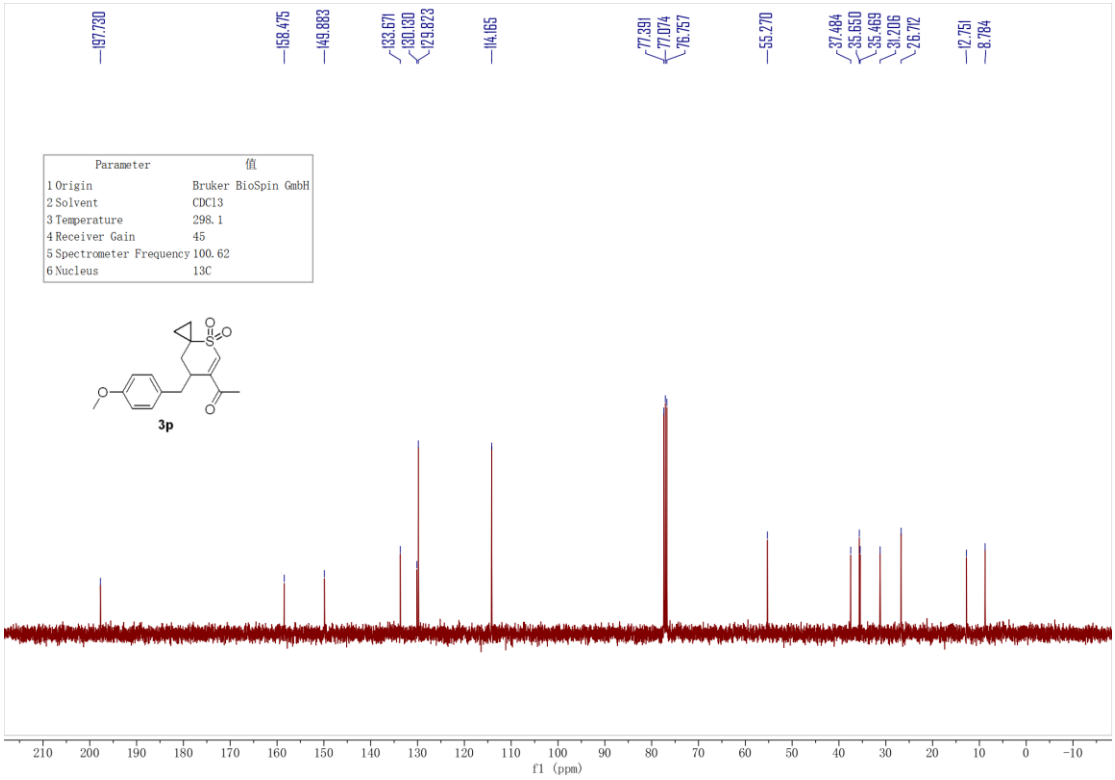
129.482
128.729
77.348
77.094
76.840
37.848
35.465
35.415
31.091
26.749
21.077
12.837
8.716
Parameter 值
1 Origin Bruker BioSpin GmbH
2 Solvent CDCl3
3 Temperature 293.3
4 Number of Scans 10
5 Spectrometer Frequency 125.77
6 Nucleus 13C
3o
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)


7.260
7.106
7.085
7.031
6.843
6.822
3.779
3.304
3.292
3.280
3.266
3.254
3.242
2.934
2.924
2.899
2.890
2.522
2.495
2.488
2.461
2.387
2.257
2.244
2.219
2.206
1.980
1.967
1.942
1.928
1.697
1.682
1.669
1.656
1.640
1.445
1.399
1.384
1.373
1.357
1.083
1.067
1.061
1.045
1.029
0.767
0.751
0.735
0.729
0.713
Parameter 值
1 Origin Bruker BioSpin GmbH
2 Solvent CDCl3
3 Temperature 298.0
4 Number of Scans 2
5 Spectrometer Frequency 400.13
6 Nucleus 1H
3p
2.01
1.00
2.01
3.08
1.04
1.05
1.04
3.02
1.03
1.07
1.08
1.09
1.08
1.07
f1 (ppm)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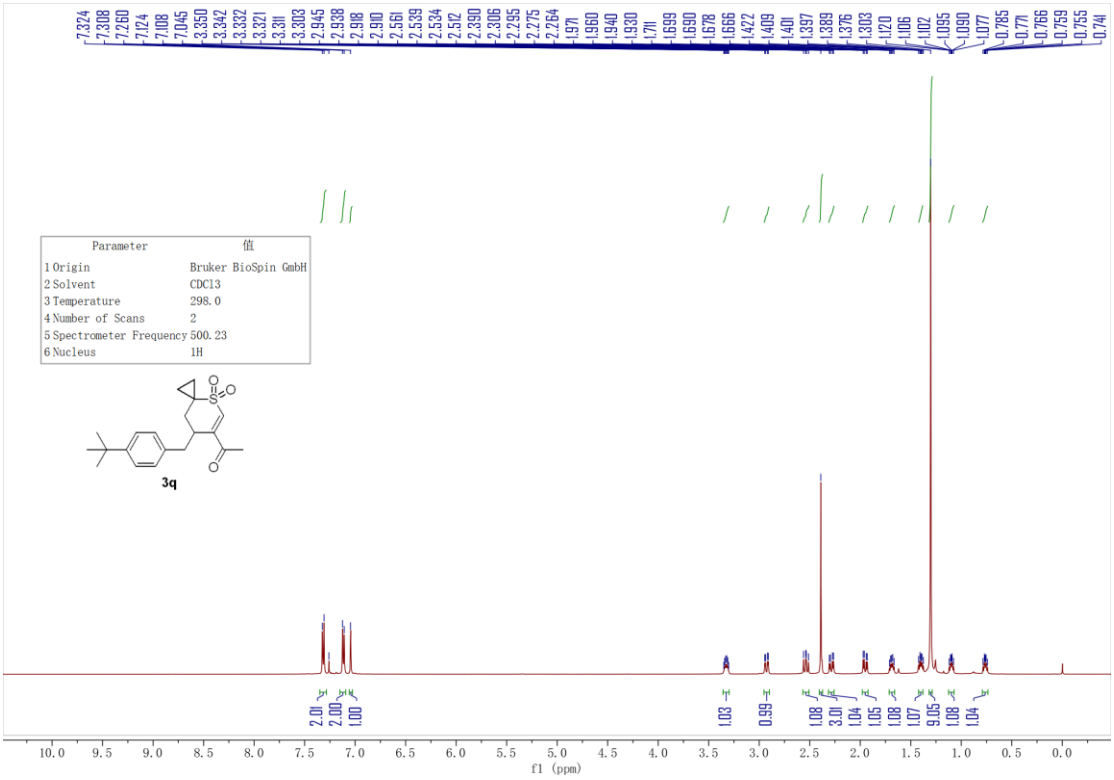
158.475
149.883
133.671
130.130
129.823
114.165
77.391
77.074
76.757
55.270
37.484
35.650
35.469
31.206
26.712
12.751
8.784
Parameter 值
1 Origin Bruker BioSpin GmbH
2 Solvent CDCl3
3 Temperature 298.1
4 Receiver Gain 45
5 Spectrometer Frequency 100.62
6 Nucleus 13C
3p
f1 (ppm)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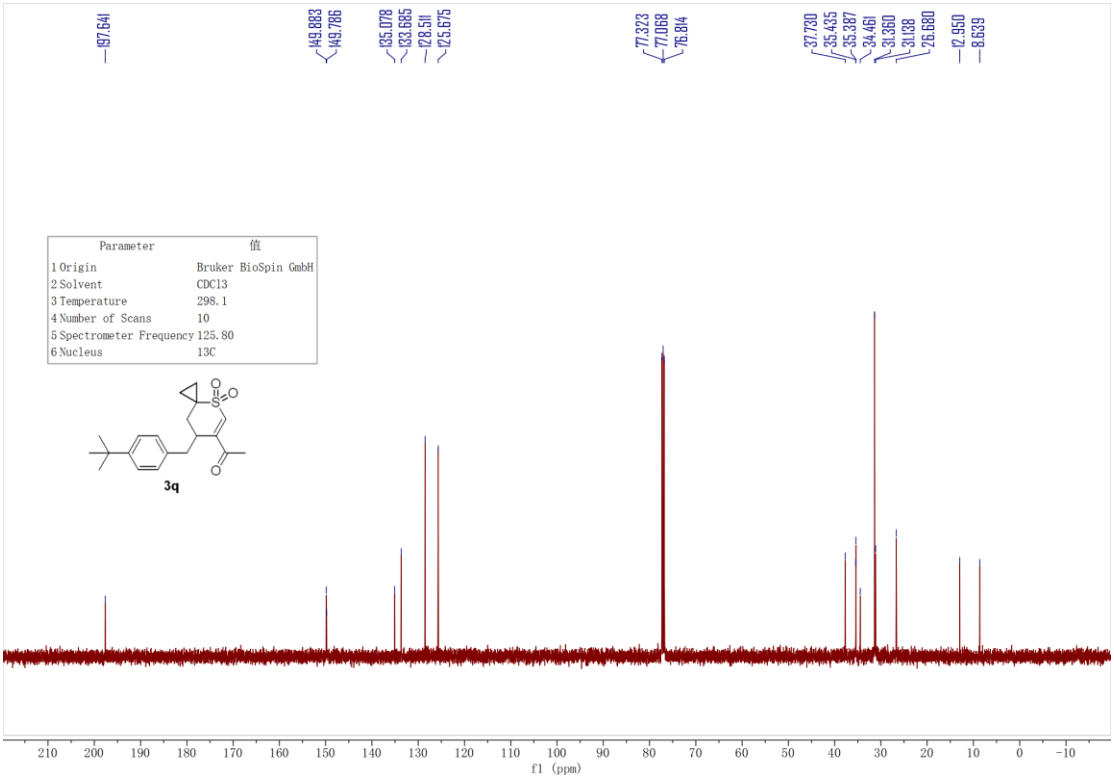
7.308
7.260
7.124
7.108
7.045
3.350
3.342
3.332
3.321
3.311
3.303
2.945
2.938
2.918
2.910
2.561
2.539
2.534
2.512
2.390
2.306
2.295
2.275
2.264
1.971
1.960
1.940
1.930
1.711
1.699
1.690
1.678
1.666
1.422
1.409
1.401
1.397
1.389
1.376
1.303
1.120
1.106
1.102
1.095
1.090
1.077
0.785
0.771
0.766
0.759
0.755
0.744
Parameter 值
1 Origin Bruker BioSpin GmbH
2 Solvent CDCl3
3 Temperature 298.0
4 Number of Scans 2
5 Spectrometer Frequency 500.23
6 Nucleus 1H
3q
2.01
2.00
1.00
1.03
0.99
1.08
3.01
1.04
1.05
1.08
1.07
9.05
1.08
1.04
f1 (ppm)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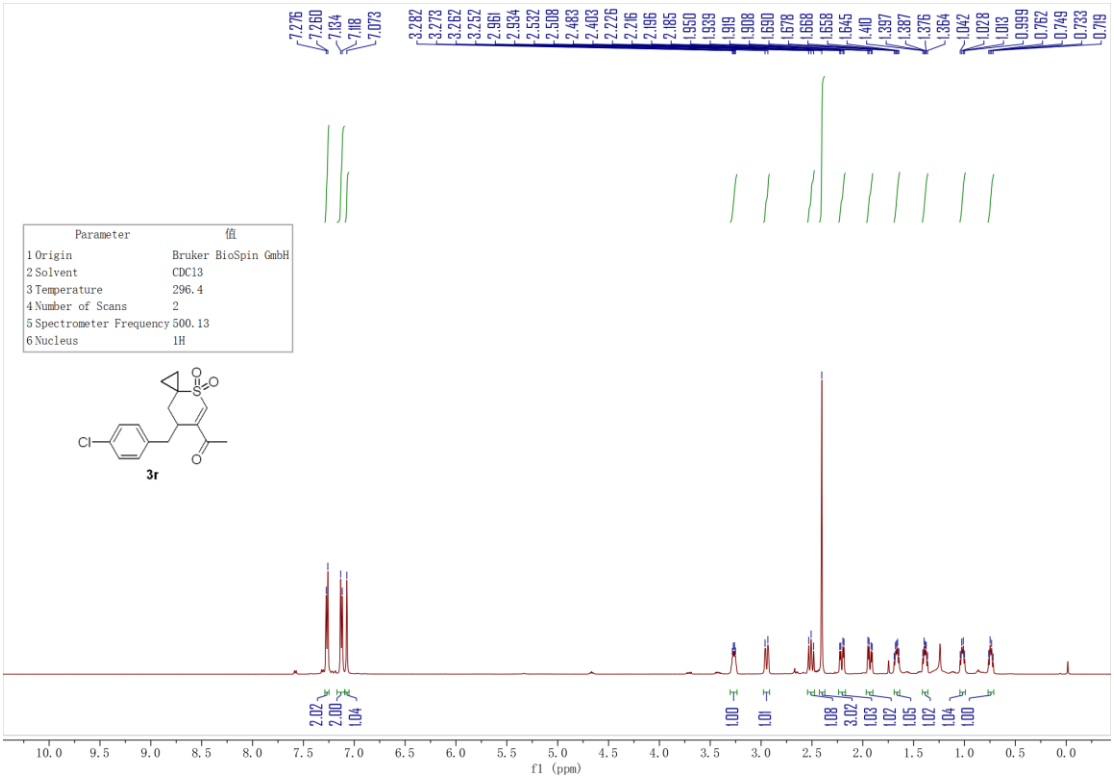
125.675
77.323
77.068
76.814
37.730
35.435
35.387
34.461
31.360
31.138
26.680
12.950
8.639
Parameter 值
1 Origin Bruker BioSpin GmbH
2 Solvent CDCl3
3 Temperature 298.1
4 Number of Scans 10
5 Spectrometer Frequency 125.80
6 Nucleus 13C
3q
f1 (ppm)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7.184
7.118
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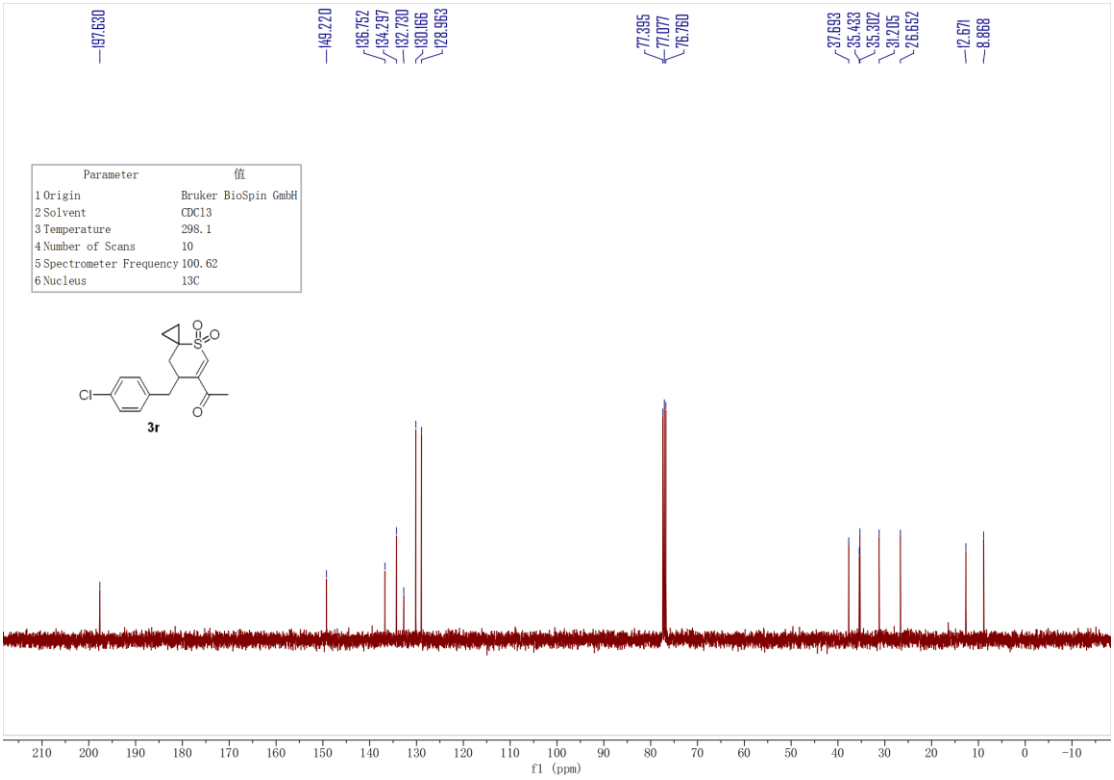
3.282
3.273
3.262
3.252
2.961
2.934
2.532
2.508
2.483
2.403
2.226
2.216
2.196
2.185
1.950
1.939
1.919
1.908
1.690
1.678
1.668
1.658
1.645
1.410
1.397
1.387
1.376
1.364
1.042
1.028
1.013
0.999
0.762
0.749
0.733
0.719
Parameter 值
1 Origin Bruker BioSpin GmbH
2 Solvent CDCl3
3 Temperature 296.4
4 Number of Scans 2
5 Spectrometer Frequency 500.13
6 Nucleus 1H
Cl
O
S
O
O
3r
2.02
2.00
1.04
1.00
1.01
1.08
3.02
1.03
1.02
1.05
1.02
1.04
1.00
10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)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134.297
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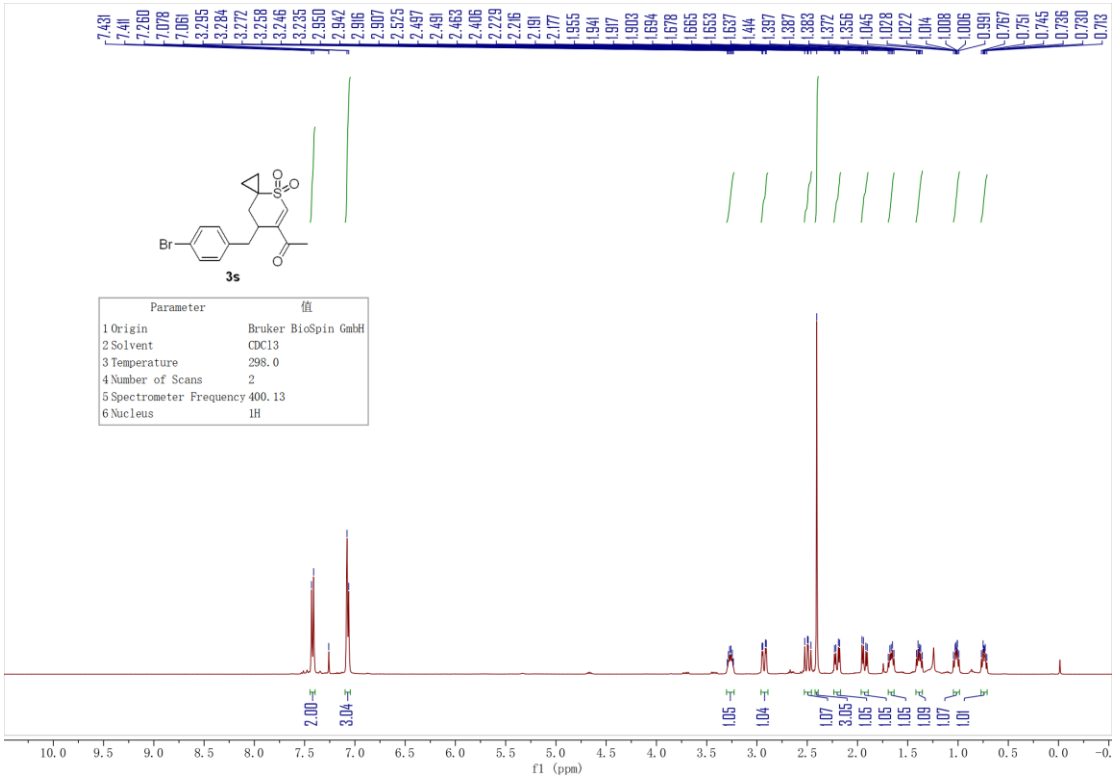
130.166
128.963
77.395
77.077
76.760
37.693
35.433
35.302
31.205
26.652
12.671
8.868
Parameter 值
1 Origin Bruker BioSpin GmbH
2 Solvent CDCl3
3 Temperature 298.1
4 Number of Scans 10
5 Spectrometer Frequency 100.62
6 Nucleus 13C
Cl
O
S
O
O
3r
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)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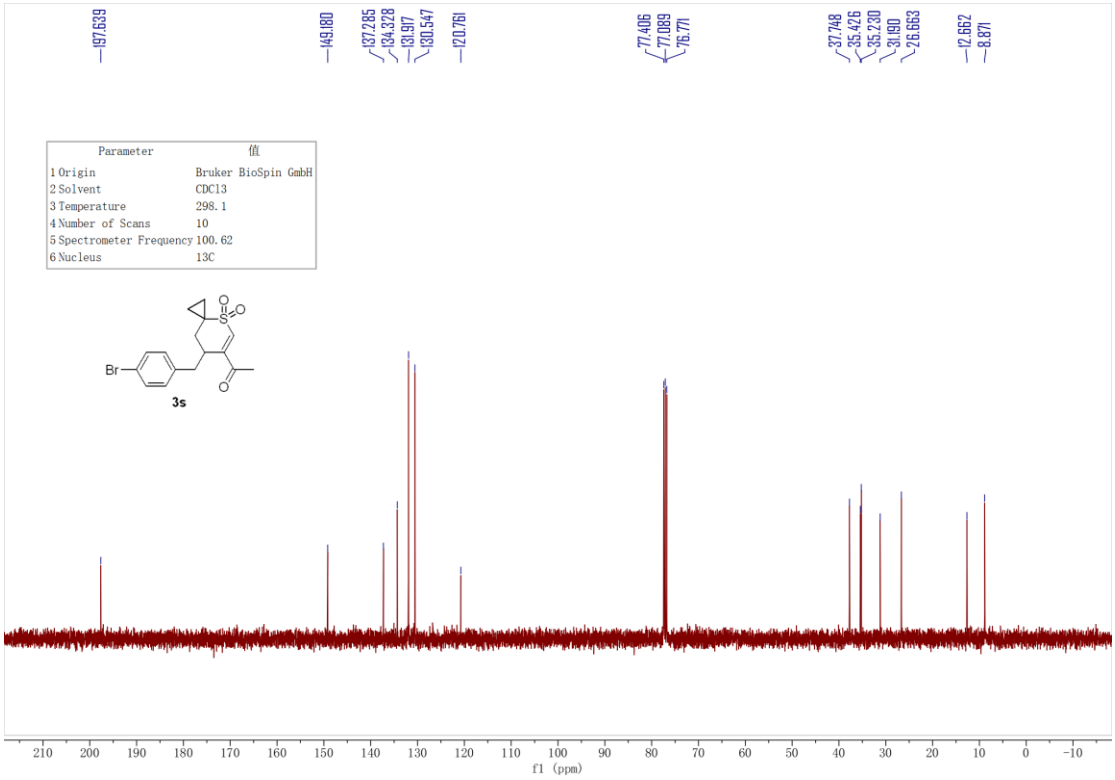
3.295
3.284
3.272
3.258
3.246
3.235
2.950
2.942
2.916
2.907
2.525
2.497
2.491
2.463
2.406
2.229
2.216
2.191
2.177
1.955
1.941
1.917
1.903
1.694
1.678
1.665
1.653
1.637
1.414
1.397
1.387
1.383
1.372
1.356
1.045
1.028
1.022
1.014
1.008
1.006
0.991
0.767
0.751
0.745
0.736
0.730
0.713
Br
O
S
O
O
3s
Parameter 值
1 Origin Bruker BioSpin GmbH
2 Solvent CDCl3
3 Temperature 298.0
4 Number of Scans 2
5 Spectrometer Frequency 400.13
6 Nucleus 1H
2.00
3.04
1.05
1.04
1.07
3.05
1.05
1.05
1.05
1.09
1.07
1.01
f1 (ppm)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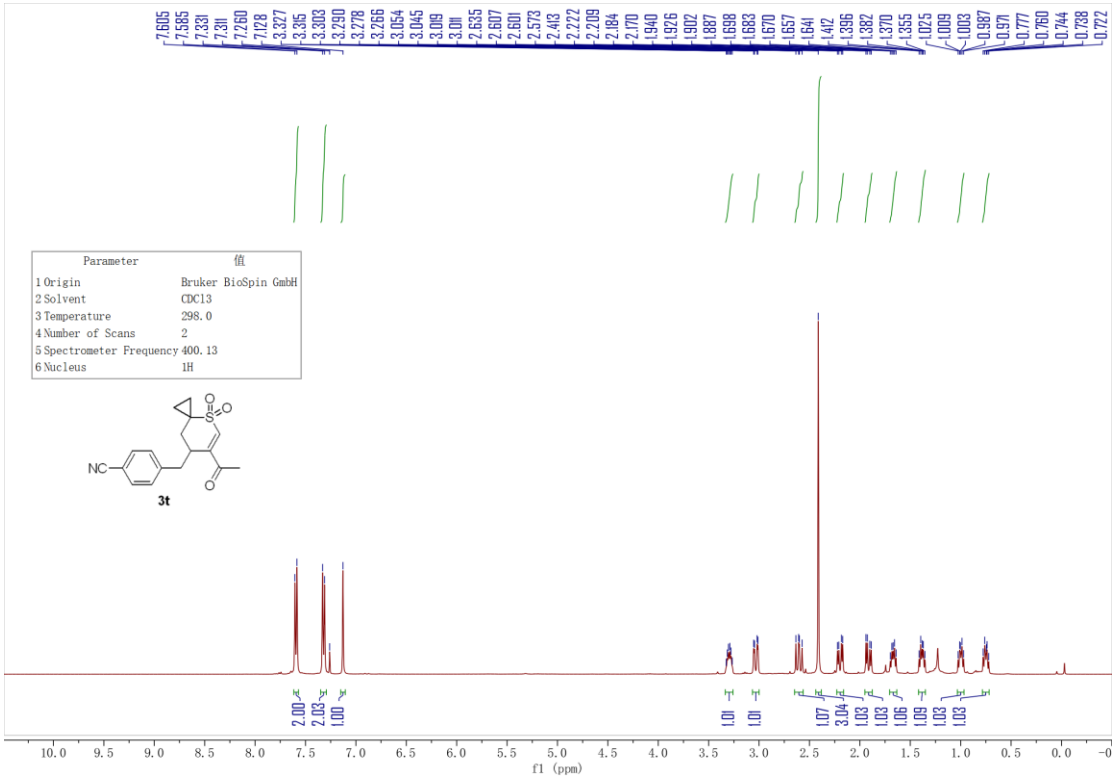
120.761
77.406
77.089
76.771
37.748
35.426
35.230
31.190
26.663
12.662
8.871
Parameter 值
1 Origin Bruker BioSpin GmbH
2 Solvent CDCl3
3 Temperature 298.1
4 Number of Scans 10
5 Spectrometer Frequency 100.62
6 Nucleus 13C
Br
O
S
O
O
3s
f1 (ppm)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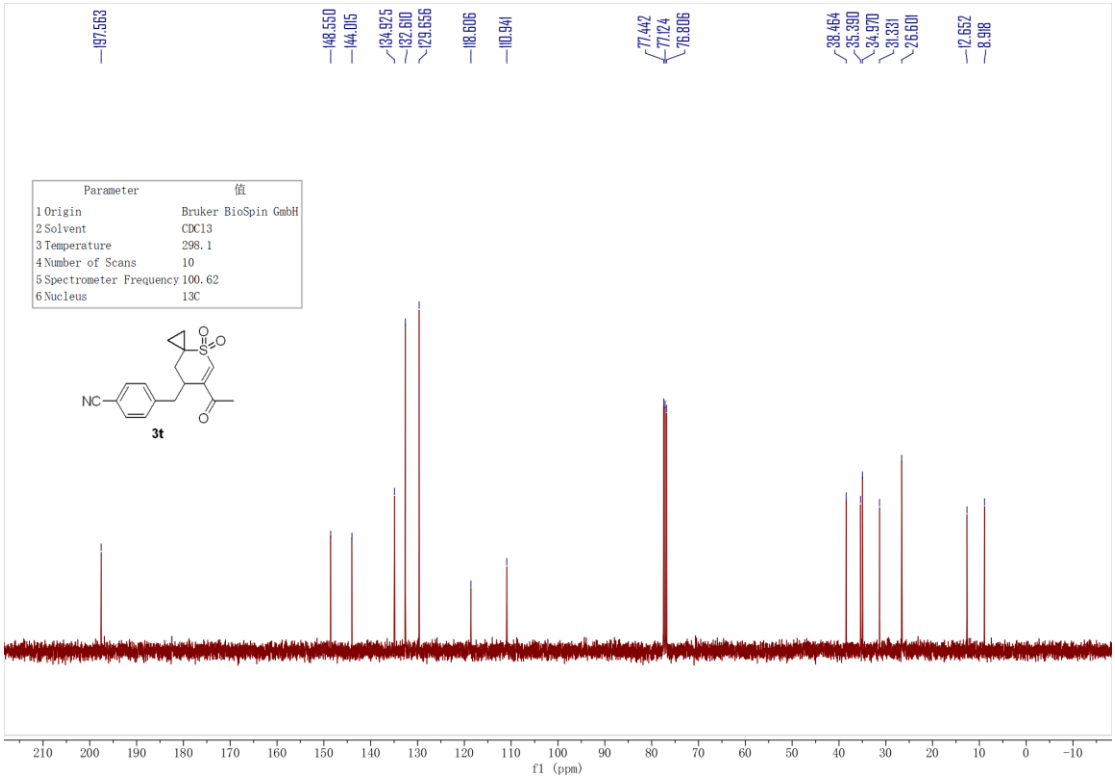
7.311
7.260
7.128
3.327
3.315
3.303
3.290
3.278
3.266
3.054
3.045
3.019
3.011
2.635
2.607
2.601
2.573
2.443
2.222
2.209
2.184
2.170
1.940
1.926
1.902
1.887
1.698
1.683
1.670
1.657
1.641
1.412
1.396
1.382
1.370
1.355
1.025
1.009
1.003
0.987
0.971
0.777
0.760
0.744
0.738
0.722
Parameter 值
1 Origin Bruker BioSpin GmbH
2 Solvent CDCl3
3 Temperature 298.0
4 Number of Scans 2
5 Spectrometer Frequency 400.13
6 Nucleus 1H
NC
3t
2.00
2.03
1.00
1.01
1.01
1.07
3.04
1.03
1.03
1.06
1.09
1.03
1.03
f1 (ppm)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134.925
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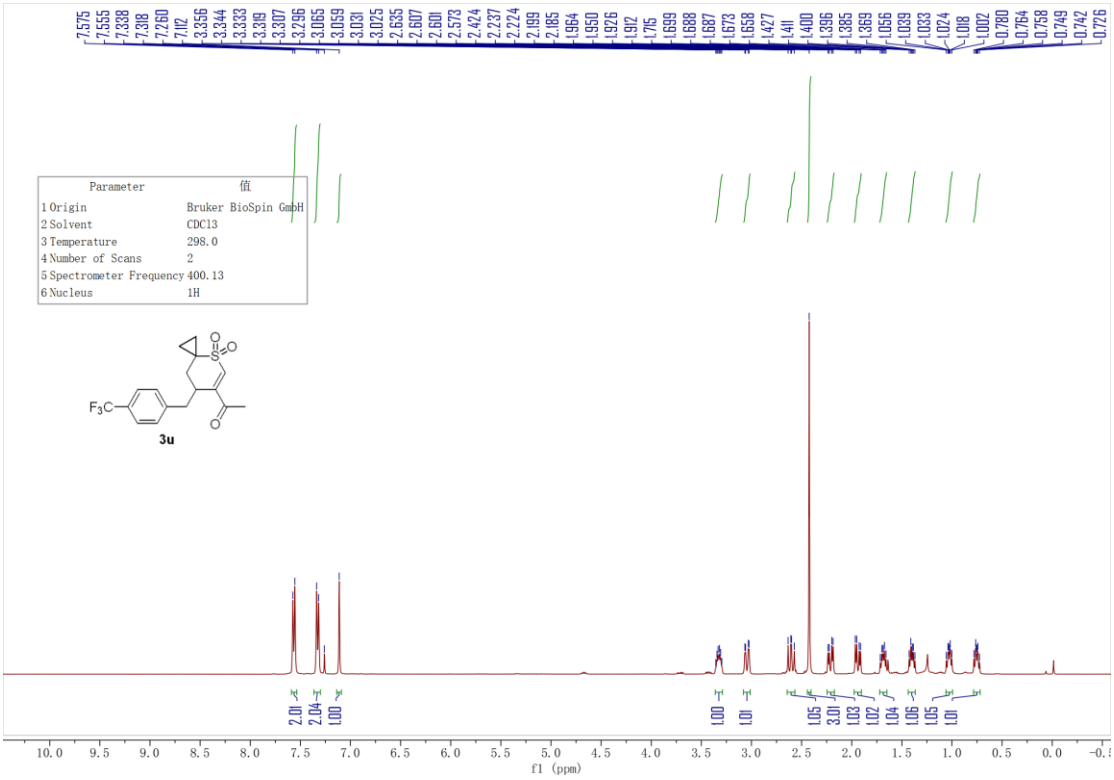
129.656
118.606
110.941
77.442
77.124
76.806
38.464
35.390
34.970
31.331
26.601
12.652
8.918
Parameter 值
1 Origin Bruker BioSpin GmbH
2 Solvent CDCl3
3 Temperature 298.1
4 Number of Scans 10
5 Spectrometer Frequency 100.62
6 Nucleus 13C
NC
3t
f1 (ppm)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7.555
7.338
7.318
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7.112
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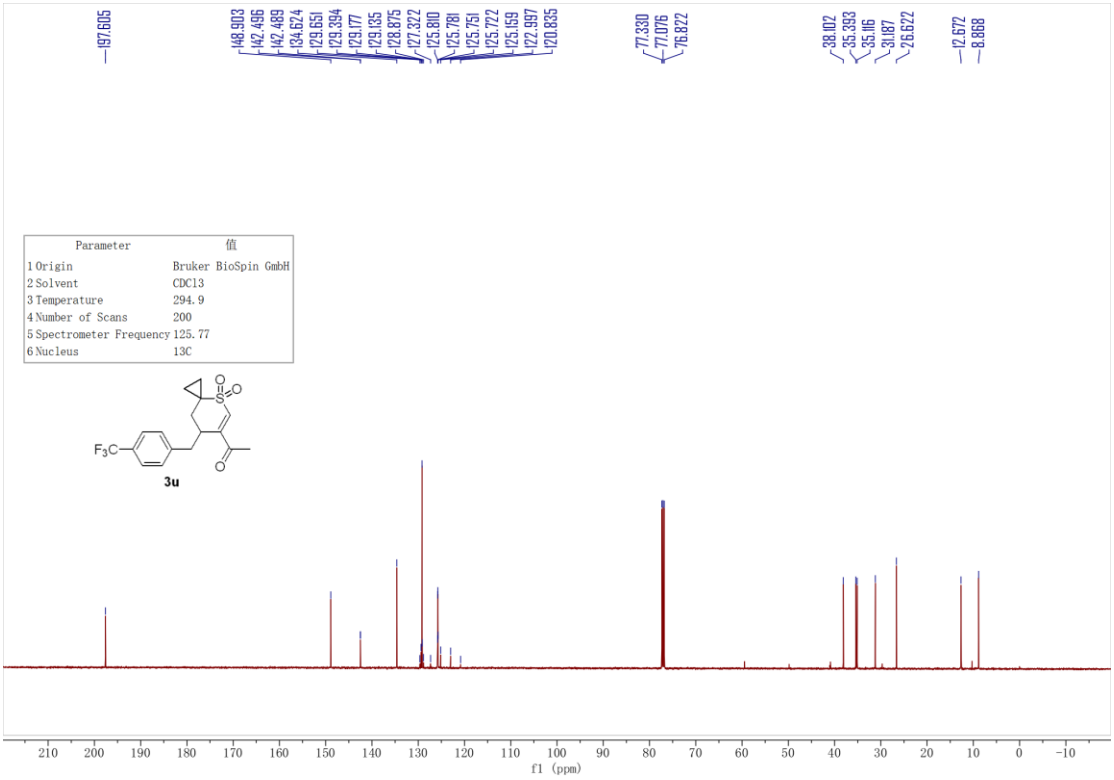
3.344
3.333
3.319
3.307
3.296
3.065
3.059
3.031
3.025
2.635
2.607
2.601
2.573
2.424
2.237
2.224
2.199
2.185
1.964
1.950
1.926
1.912
1.765
1.699
1.688
1.687
1.673
1.658
1.427
1.411
1.400
1.396
1.385
1.369
1.056
1.039
1.033
1.024
1.018
1.002
0.780
0.764
0.758
0.749
0.742
0.726
Parameter 值
1 Origin Bruker BioSpin GmbH
2 Solvent CDCl3
3 Temperature 298.0
4 Number of Scans 2
5 Spectrometer Frequency 400.13
6 Nucleus 1H
F3C
3u
2.01
2.04
1.00
1.00
1.01
1.05
3.01
1.03
1.02
1.04
1.06
1.05
1.01
f1 (ppm)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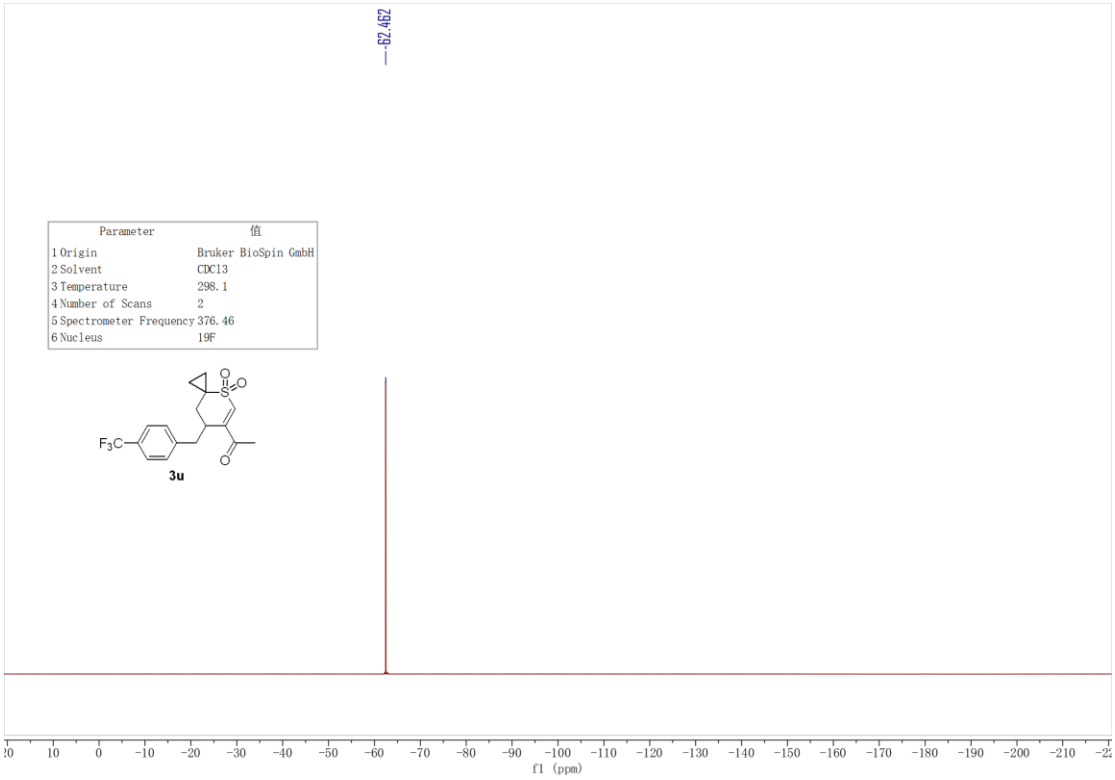
142.496
142.489
134.624
129.651
129.394
129.177
129.135
128.875
127.322
125.810
125.781
125.751
125.722
125.159
122.997
120.835
77.330
77.076
76.822
38.102
35.393
35.116
31.187
26.622
12.672
8.868
Parameter 值
1 Origin Bruker BioSpin GmbH
2 Solvent CDCl3
3 Temperature 294.9
4 Number of Scans 200
5 Spectrometer Frequency 125.77
6 Nucleus 13C
F3C
3u
f1 (ppm)


-62.462
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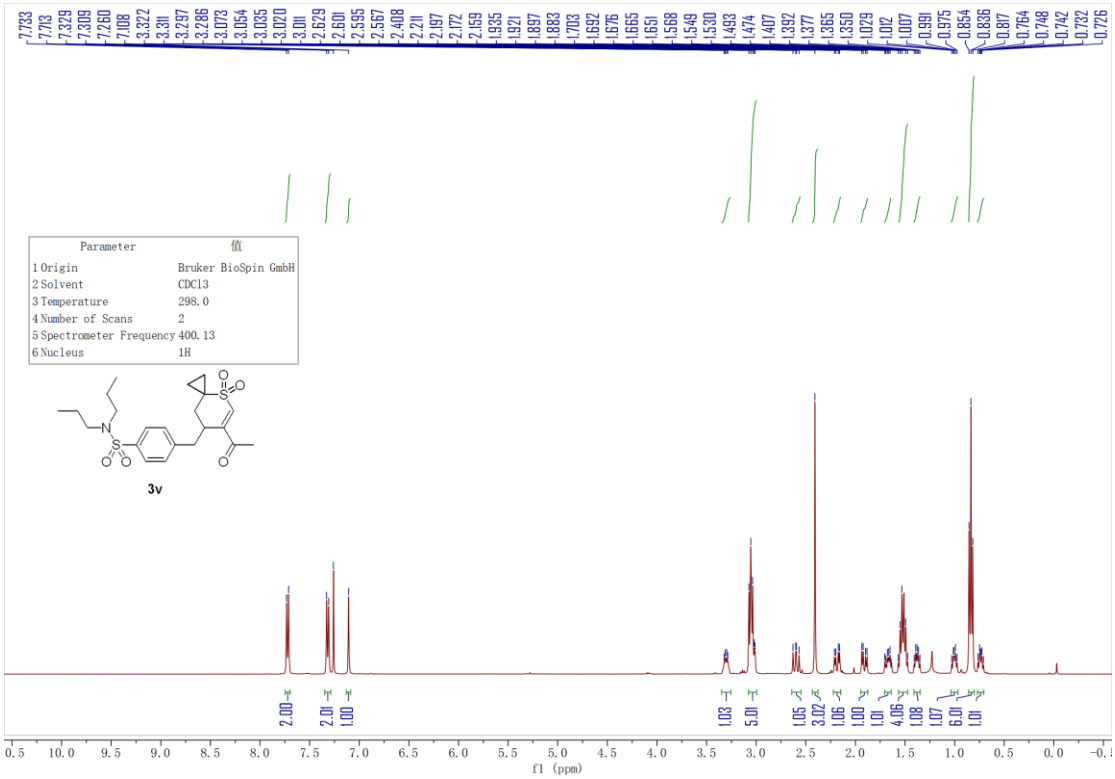
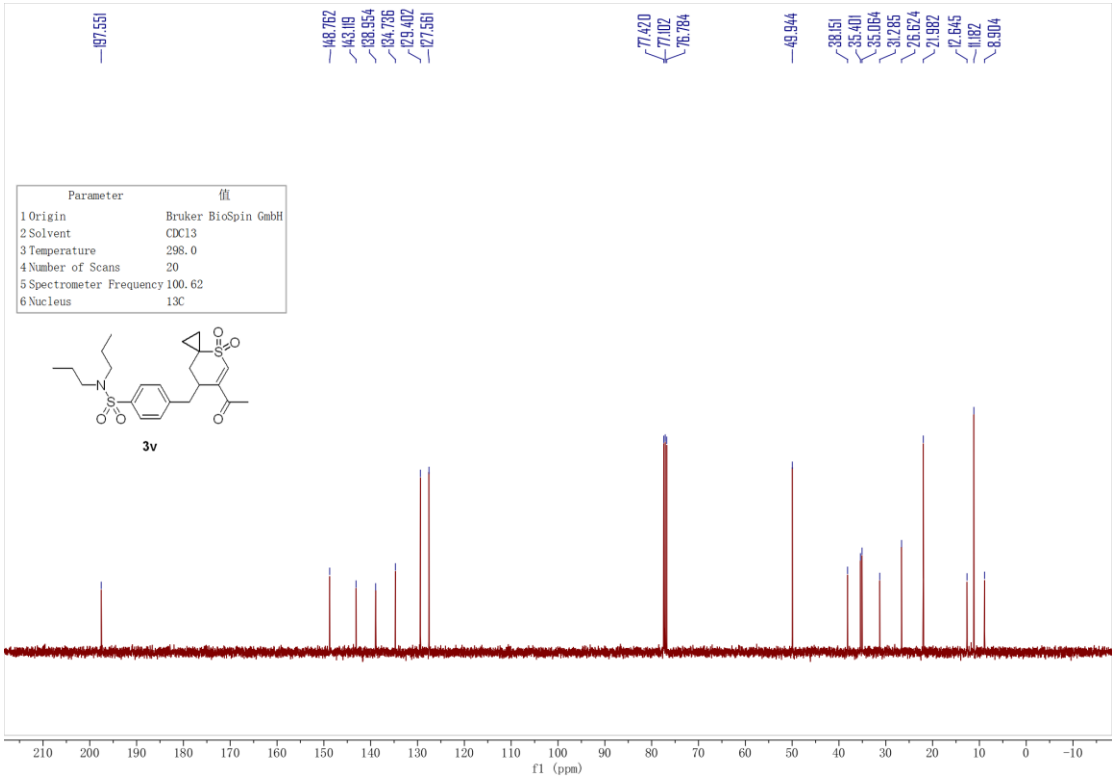
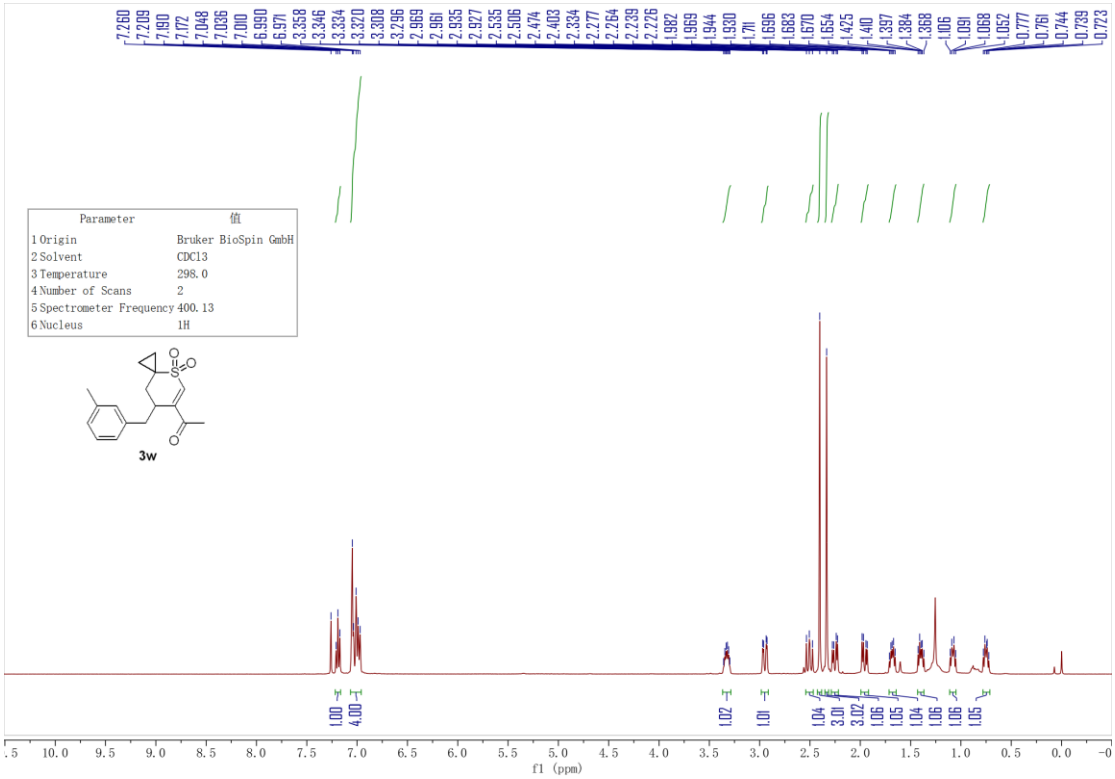
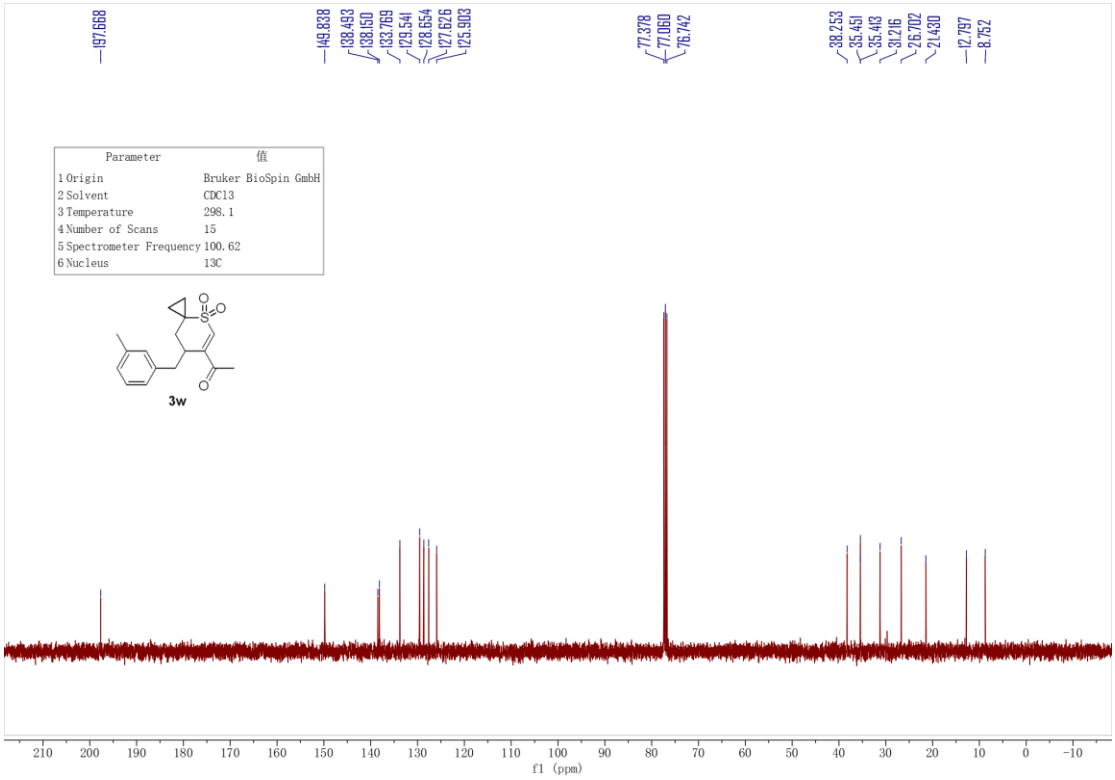
1 Origin Bruker BioSpin GmbH
2 Solvent CDCl3
3 Temperature 298.1
4 Number of Scans 2
5 Spectrometer Frequency 376.46
6 Nucleus 19F
F3C
3u
f1 (ppm)


Parameter 值
1 Origin Bruker BioSpin GmbH
2 Solvent CDCl3
3 Temperature 298.0
4 Number of Scans 2
5 Spectrometer Frequency 400.13
6 Nucleus 1H
3v
2.00
2.01
1.00
1.03
5.01
1.05
3.02
1.06
1.00
1.01
4.06
1.08
1.07
6.01
1.01
f1 (ppm)


197.561
148.762
143.119
138.954
134.736
129.402
127.561
77.420
77.102
76.784
49.944
38.151
35.401
35.054
31.285
26.624
21.982
12.645
11.182
8.904
Parameter 值
1 Origin Bruker BioSpin GmbH
2 Solvent CDCl3
3 Temperature 298.0
4 Number of Scans 20
5 Spectrometer Frequency 100.62
6 Nucleus 13C
3v
f1 (ppm)


7.260
7.209
7.190
7.172
7.048
7.036
7.010
6.990
6.971
3.358
3.346
3.334
3.320
3.308
3.296
2.969
2.961
2.935
2.927
2.535
2.506
2.474
2.403
2.334
2.277
2.264
2.239
2.226
1.982
1.969
1.944
1.930
1.711
1.696
1.683
1.670
1.654
1.425
1.410
1.397
1.384
1.368
1.106
1.091
1.068
1.052
0.777
0.761
0.744
0.739
0.723
Parameter 值
1 Origin Bruker BioSpin GmbH
2 Solvent CDCl3
3 Temperature 298.0
4 Number of Scans 2
5 Spectrometer Frequency 400.13
6 Nucleus 1H
3w
1.00
4.00
1.02
1.01
1.04
3.01
3.02
1.06
1.05
1.04
1.06
1.06
1.05
f1 (ppm)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138.150
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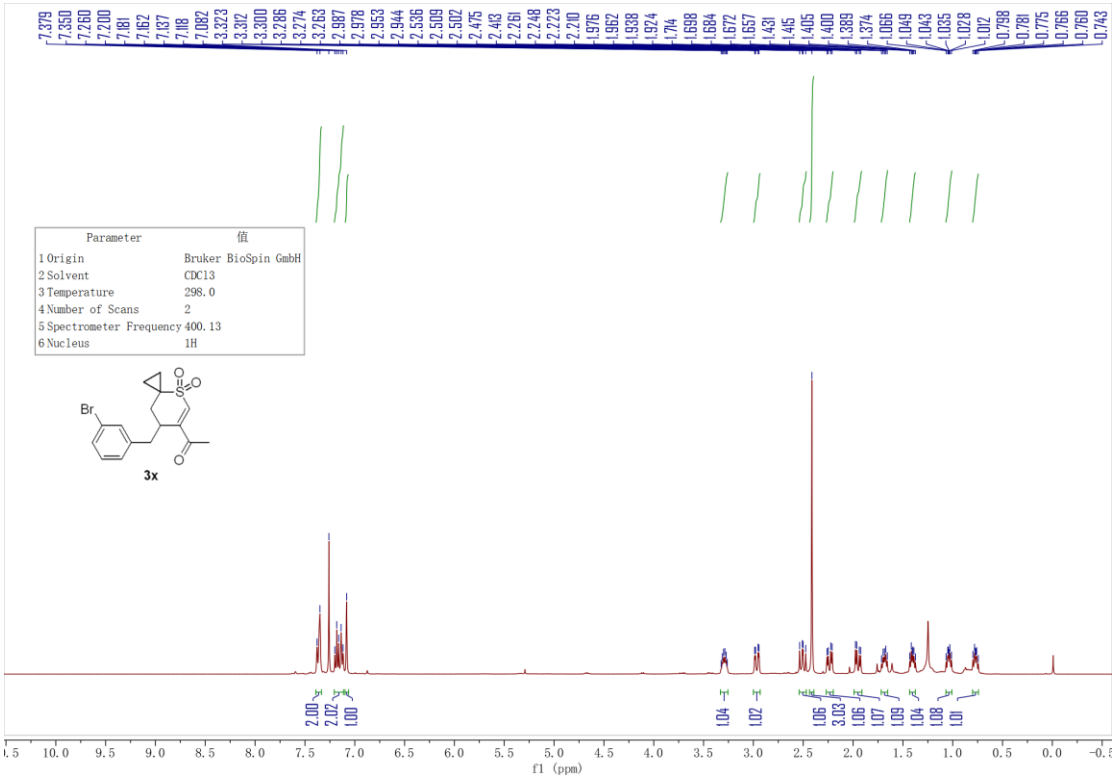
129.541
128.654
127.625
125.903
77.378
77.060
76.742
38.253
35.451
35.443
31.216
26.702
21.430
12.797
8.752
Parameter 值
1 Origin Bruker BioSpin GmbH
2 Solvent CDCl3
3 Temperature 298.1
4 Number of Scans 15
5 Spectrometer Frequency 100.62
6 Nucleus 13C
3w
f1 (ppm)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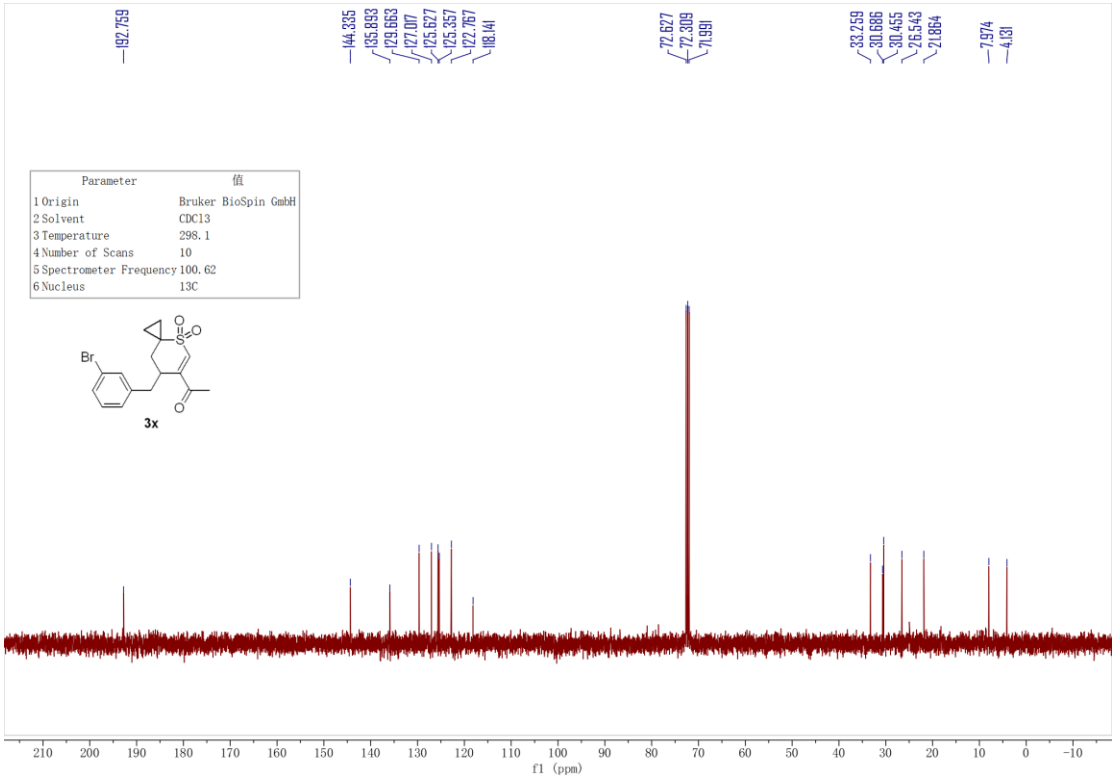
7.350
7.260
7.200
7.181
7.162
7.137
7.118
7.082
3.323
3.312
3.300
3.286
3.274
3.263
2.987
2.978
2.953
2.944
2.536
2.509
2.502
2.475
2.463
2.261
2.248
2.223
2.210
1.976
1.962
1.938
1.924
1.774
1.698
1.684
1.672
1.657
1.431
1.445
1.405
1.400
1.389
1.374
1.066
1.049
1.043
1.035
1.028
1.012
0.798
0.781
0.775
0.766
0.760
0.743
Parameter 值
1 Origin Bruker BioSpin GmbH
2 Solvent CDCl3
3 Temperature 298.0
4 Number of Scans 2
5 Spectrometer Frequency 400.13
6 Nucleus 1H
Br
3x
2.00
2.02
1.00
1.04
1.02
1.06
3.03
1.06
1.07
1.09
1.04
1.08
1.01
f1 (ppm)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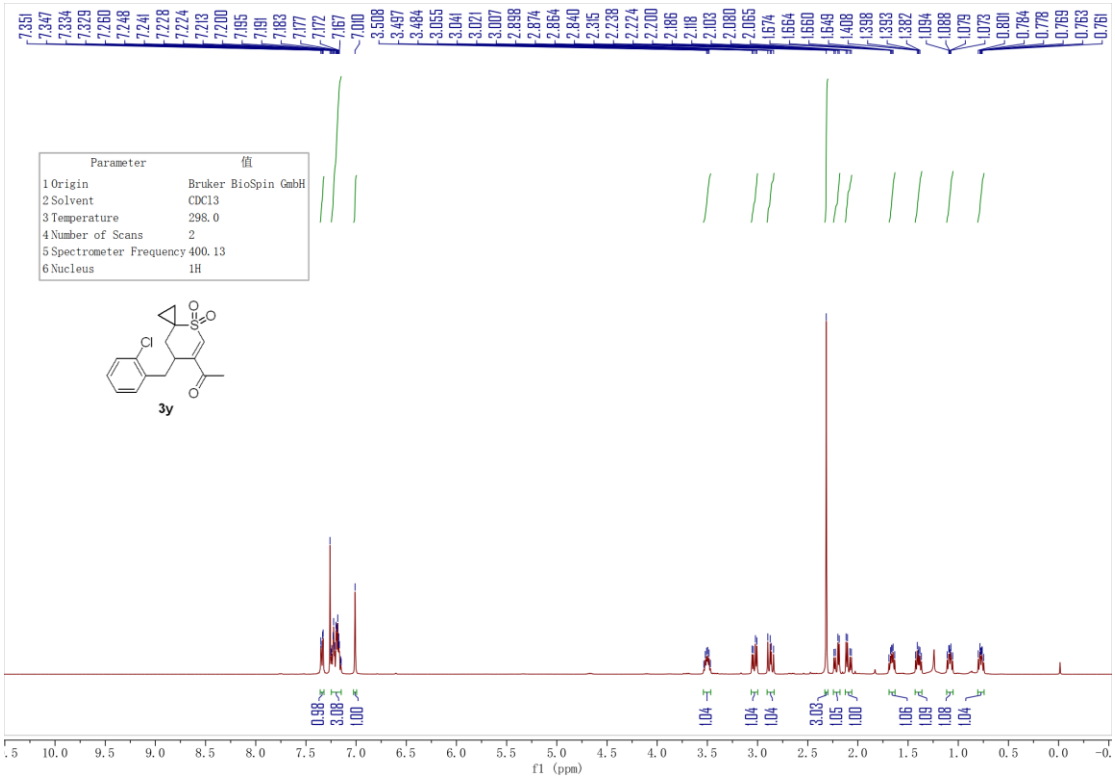
135.893
129.663
127.107
125.627
125.357
122.767
118.141
72.627
72.309
71.991
33.259
30.686
30.455
26.543
21.864
7.974
4.131
Parameter 值
1 Origin Bruker BioSpin GmbH
2 Solvent CDCl3
3 Temperature 298.1
4 Number of Scans 10
5 Spectrometer Frequency 100.62
6 Nucleus 13C
Br
O
S
O
O
3x
f1 (ppm)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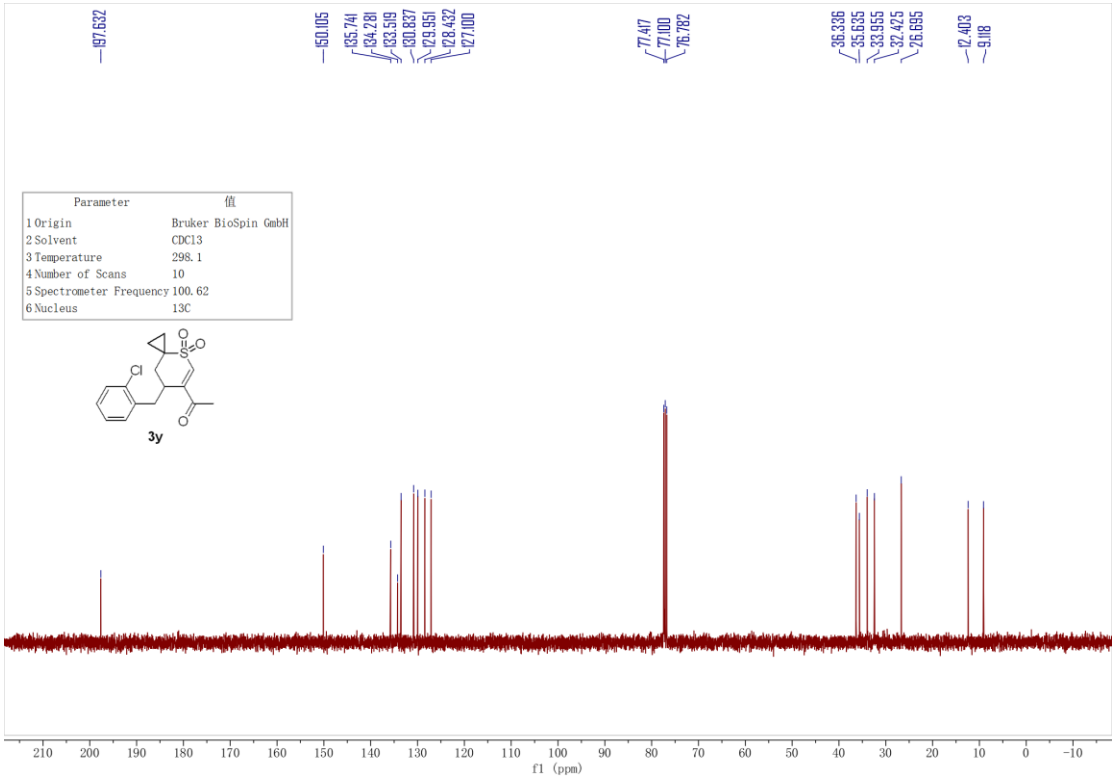
7.347
7.334
7.329
7.260
7.248
7.241
7.228
7.224
7.213
7.200
7.195
7.191
7.183
7.177
7.172
7.167
7.010
3.508
3.497
3.484
3.055
3.041
3.021
3.007
2.898
2.874
2.864
2.840
2.345
2.238
2.224
2.200
2.186
2.118
2.103
2.080
2.065
1.674
1.664
1.660
1.649
1.408
1.398
1.393
1.382
1.094
1.088
1.079
1.073
0.801
0.784
0.778
0.769
0.763
0.761
Parameter 值
1 Origin Bruker BioSpin GmbH
2 Solvent CDCl3
3 Temperature 298.0
4 Number of Scans 2
5 Spectrometer Frequency 400.13
6 Nucleus 1H
Cl
O
S
O
O
3y
0.98
3.08
1.00
1.04
1.04
1.04
3.03
1.05
1.00
1.06
1.09
1.08
1.04
f1 (ppm)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133.519
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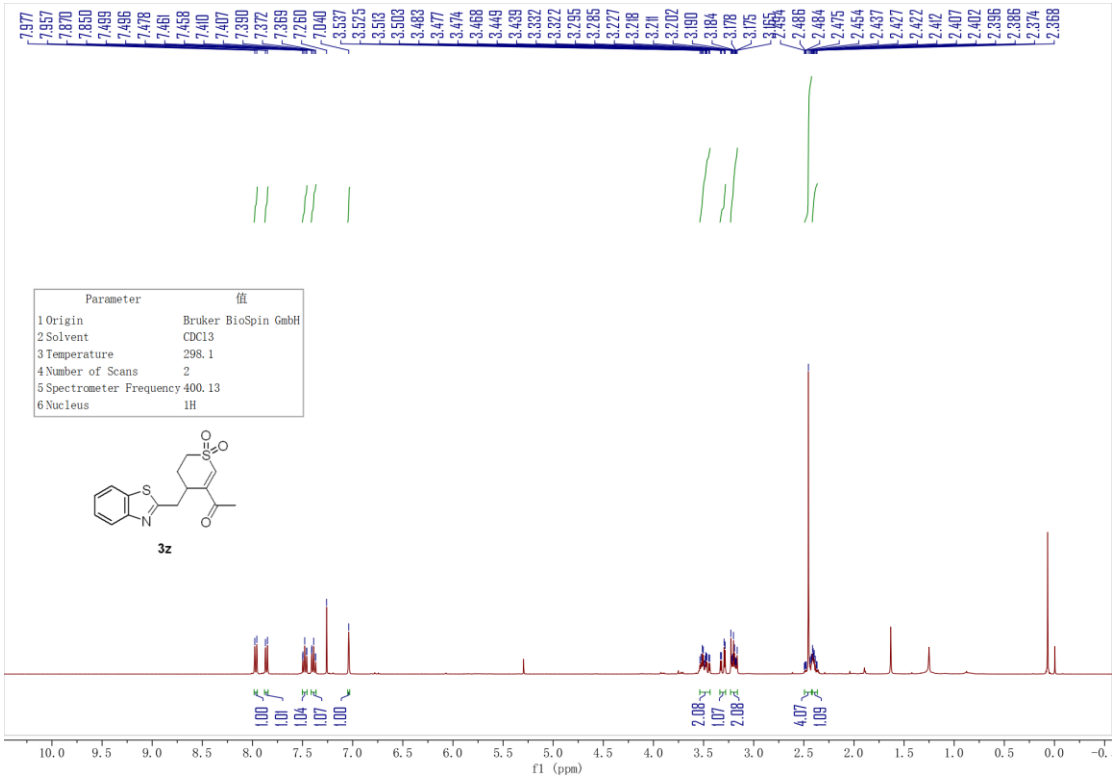
129.951
128.432
127.100
77.417
77.100
76.782
36.336
35.635
33.955
32.425
26.655
12.403
9.118
Parameter 值
1 Origin Bruker BioSpin GmbH
2 Solvent CDCl3
3 Temperature 298.1
4 Number of Scans 10
5 Spectrometer Frequency 100.62
6 Nucleus 13C
3y
f1 (ppm)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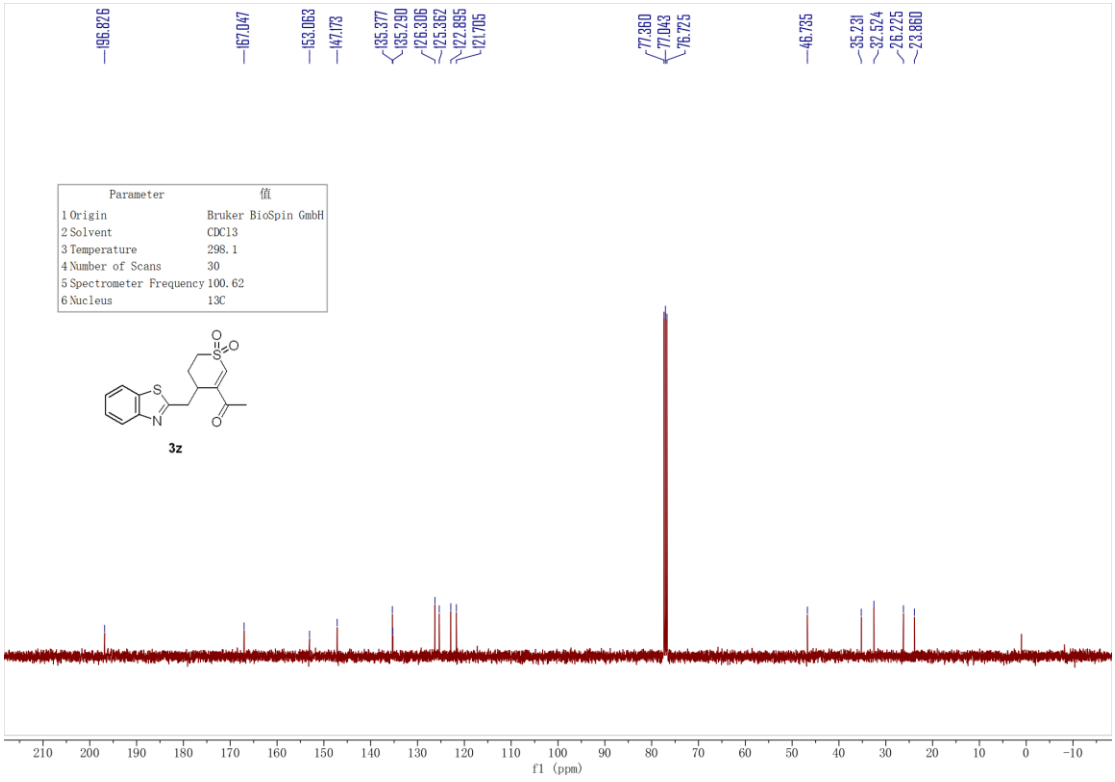
7.461
7.458
7.410
7.407
7.390
7.372
7.369
7.260
7.040
3.537
3.525
3.513
3.503
3.483
3.477
3.474
3.468
3.449
3.439
3.332
3.322
3.295
3.285
3.227
3.218
3.211
3.202
3.190
3.184
3.178
3.175
3.165
2.494
2.486
2.484
2.475
2.454
2.437
2.427
2.422
2.412
2.407
2.402
2.396
2.386
2.374
2.368
Parameter 值
1 Origin Bruker BioSpin GmbH
2 Solvent CDCl3
3 Temperature 298.1
4 Number of Scans 2
5 Spectrometer Frequency 400.13
6 Nucleus 1H
3z
1.00
1.01
1.04
1.07
1.00
2.08
1.07
2.08
4.07
1.09
f1 (ppm)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125.362
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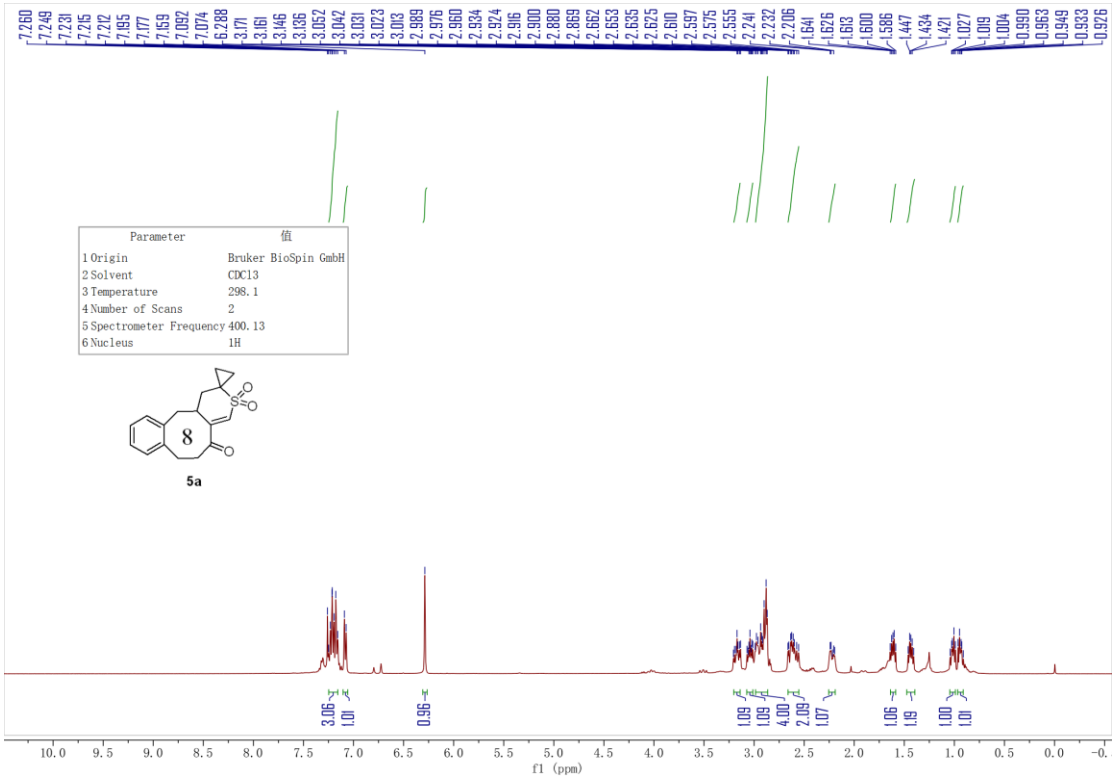
121.705
77.360
77.043
76.725
46.735
35.231
32.524
26.225
23.860
Parameter 值
1 Origin Bruker BioSpin GmbH
2 Solvent CDCl3
3 Temperature 298.1
4 Number of Scans 30
5 Spectrometer Frequency 100.62
6 Nucleus 13C
3z
f1 (ppm)


Parameter 值
1 Origin Bruker BioSpin GmbH
2 Solvent CDCl3
3 Temperature 298.1
4 Number of Scans 2
5 Spectrometer Frequency 400.13
6 Nucleus 1H
5a
3.06
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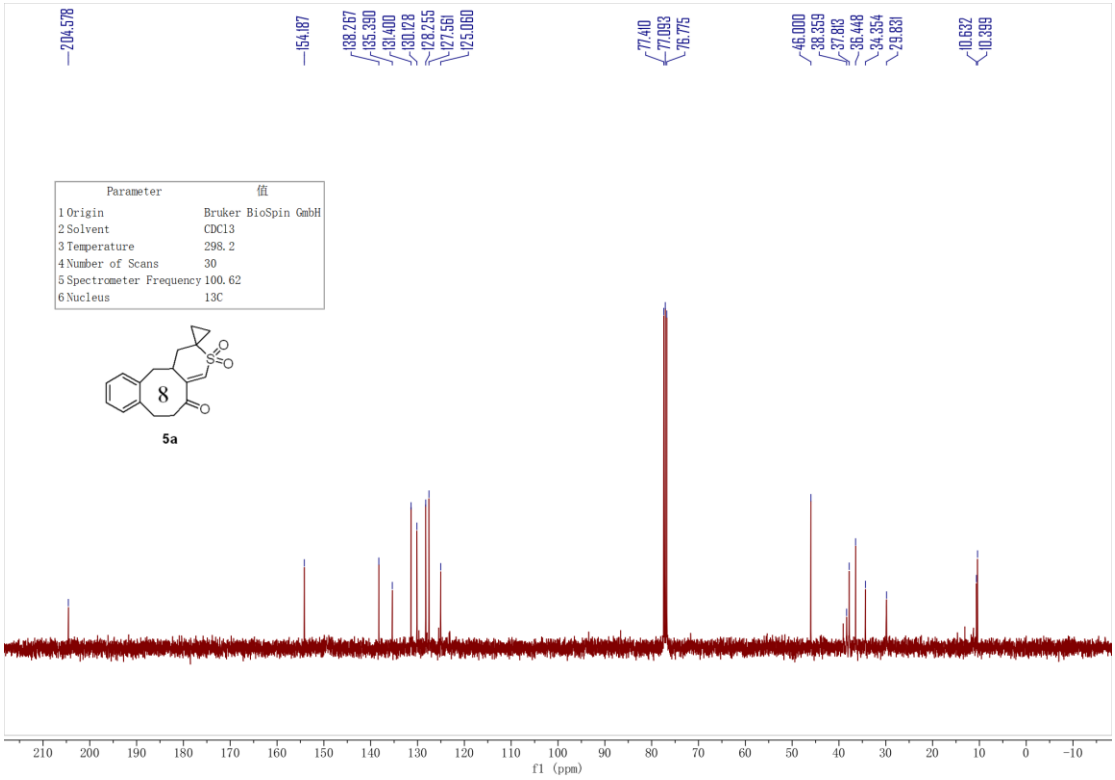
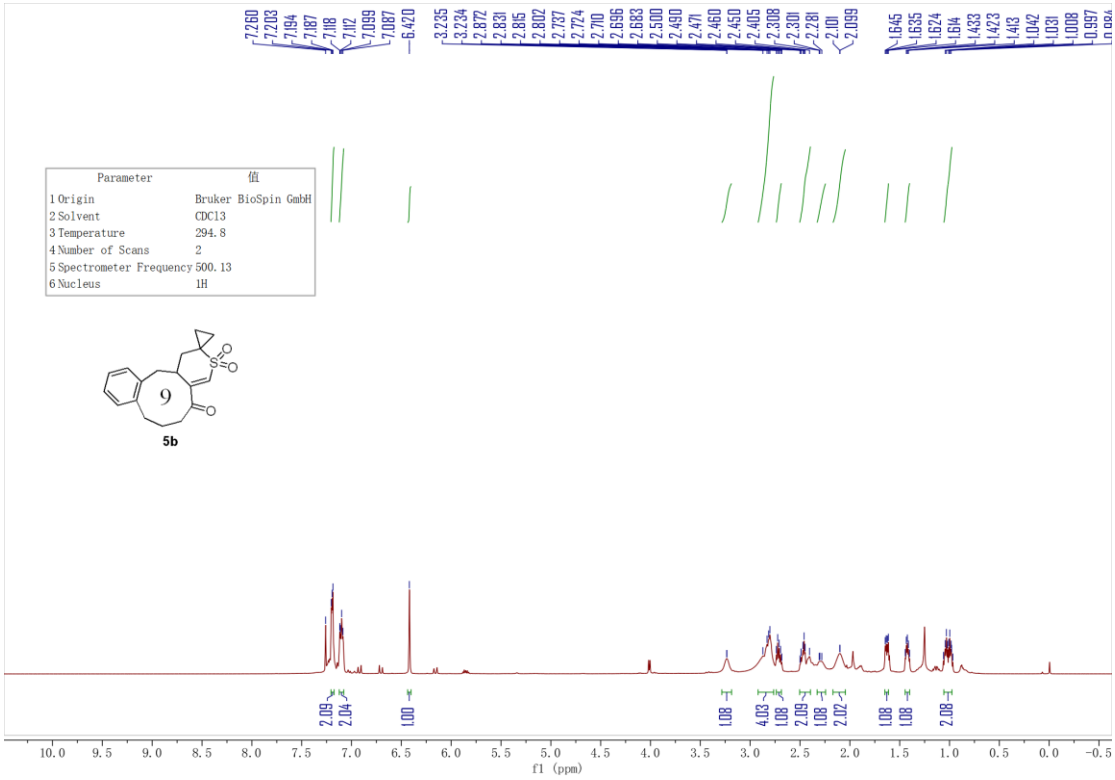
1.09
1.03
4.00
2.09
1.07
1.06
1.19
1.00
1.01
f1 (ppm)


204.578
154.187
138.267
135.390
131.400
130.128
128.255
127.561
125.060
77.410
77.093
76.775
46.000
38.359
37.813
36.448
34.354
29.831
10.632
10.399
Parameter 值
1 Origin Bruker BioSpin GmbH
2 Solvent CDCl3
3 Temperature 298.2
4 Number of Scans 30
5 Spectrometer Frequency 100.62
6 Nucleus 13C
8
5a
f1 (ppm)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7.187
7.118
7.112
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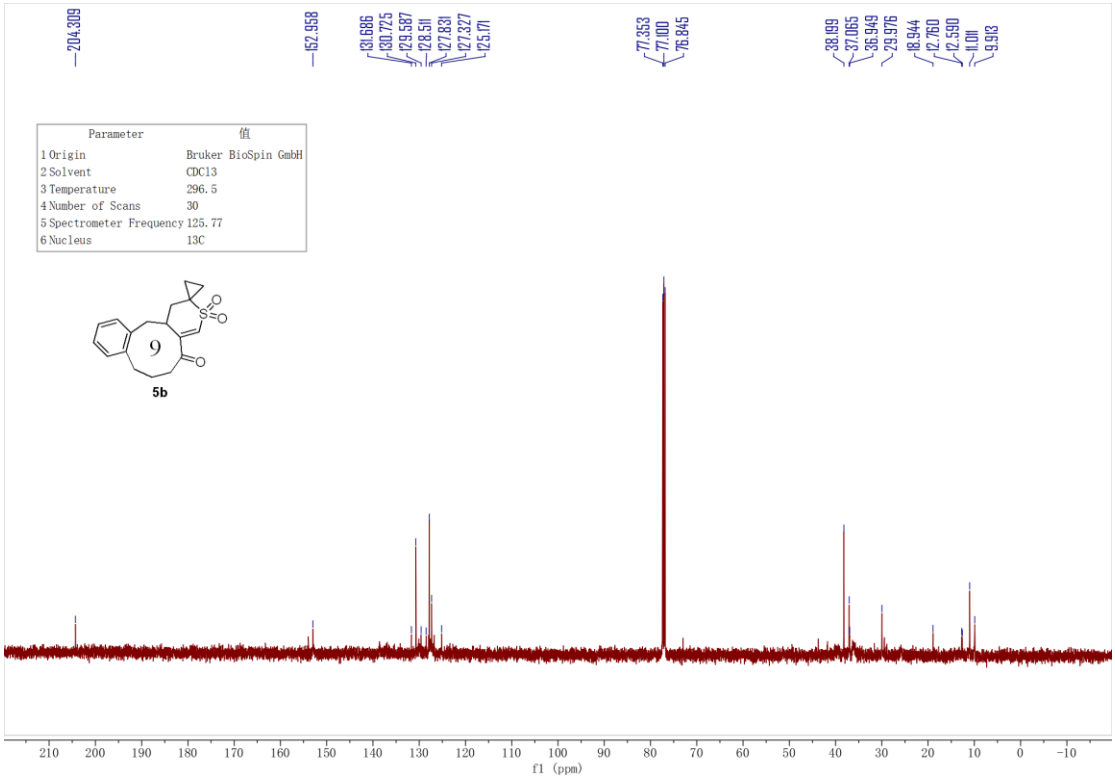
7.087
6.420
3.235
3.234
2.872
2.831
2.815
2.802
2.737
2.724
2.710
2.696
2.683
2.500
2.490
2.471
2.460
2.450
2.405
2.308
2.301
2.281
2.101
2.099
1.645
1.635
1.624
1.614
1.433
1.423
1.413
1.042
1.031
1.008
0.997
Parameter 值
1 Origin Bruker BioSpin GmbH
2 Solvent CDCl3
3 Temperature 294.8
4 Number of Scans 2
5 Spectrometer Frequency 500.13
6 Nucleus 1H
9
5b
2.09
2.04
1.00
1.08
4.03
1.08
2.09
1.08
2.02
1.08
1.08
2.08
f1 (ppm)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127.327
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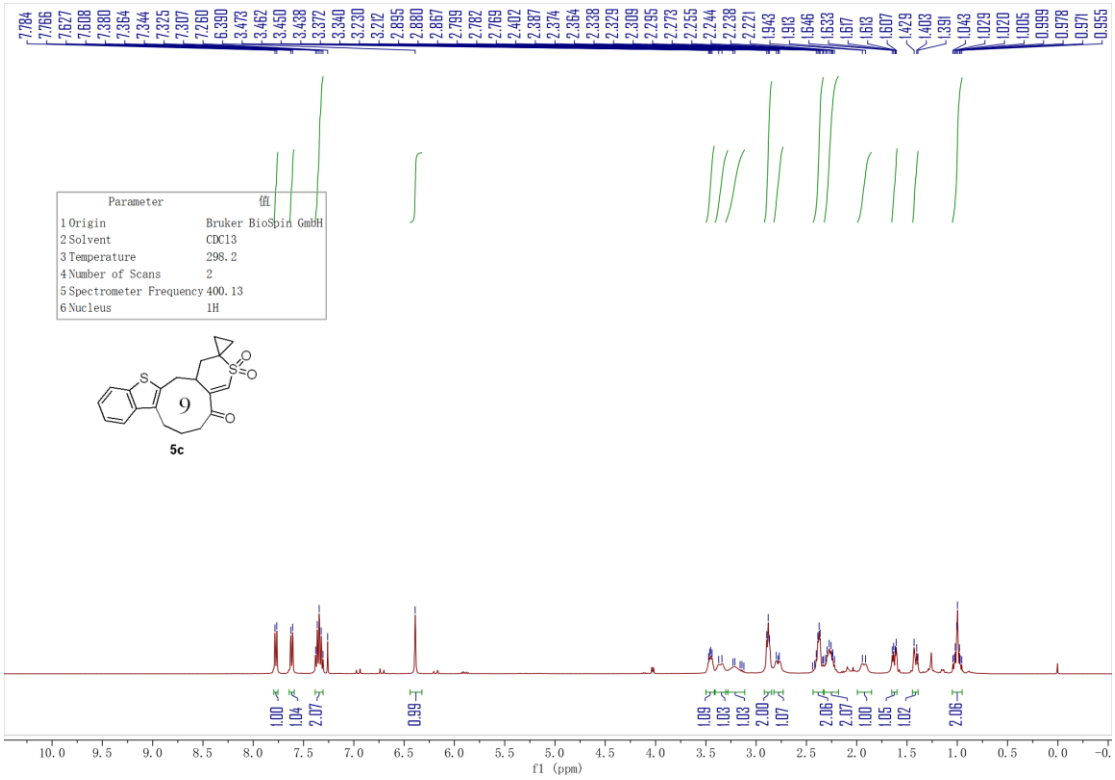
77.353
77.100
76.845
38.199
37.065
36.949
29.976
18.944
12.760
12.590
11.011
9.913
Parameter 值
1 Origin Bruker BioSpin GmbH
2 Solvent CDCl3
3 Temperature 296.5
4 Number of Scans 30
5 Spectrometer Frequency 125.77
6 Nucleus 13C
9
5b
f1 (ppm)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7.325
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7.260
6.390
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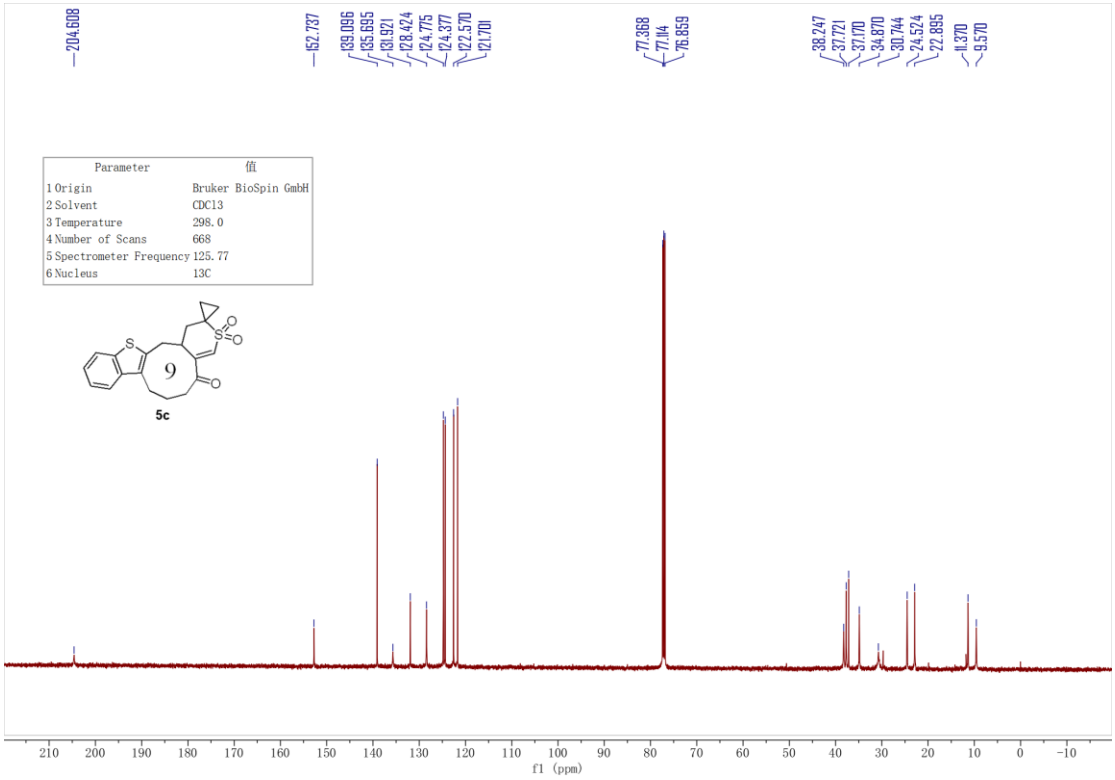
3.462
3.450
3.438
3.372
3.340
3.230
3.212
2.895
2.880
2.867
2.799
2.782
2.769
2.402
2.387
2.374
2.364
2.338
2.329
2.309
2.295
2.273
2.255
2.244
2.238
2.221
1.943
1.918
1.646
1.633
1.617
1.613
1.607
1.429
1.403
1.391
1.043
1.029
1.020
1.005
0.999
0.978
0.971
0.955
Parameter 值
1 Origin Bruker BioSpin GmbH
2 Solvent CDCl3
3 Temperature 298.2
4 Number of Scans 2
5 Spectrometer Frequency 400.13
6 Nucleus 1H
9
5c
1.00
1.04
2.07
0.99
1.09
1.03
1.03
2.00
1.07
2.06
2.07
1.00
1.05
1.02
2.06
f1 (ppm)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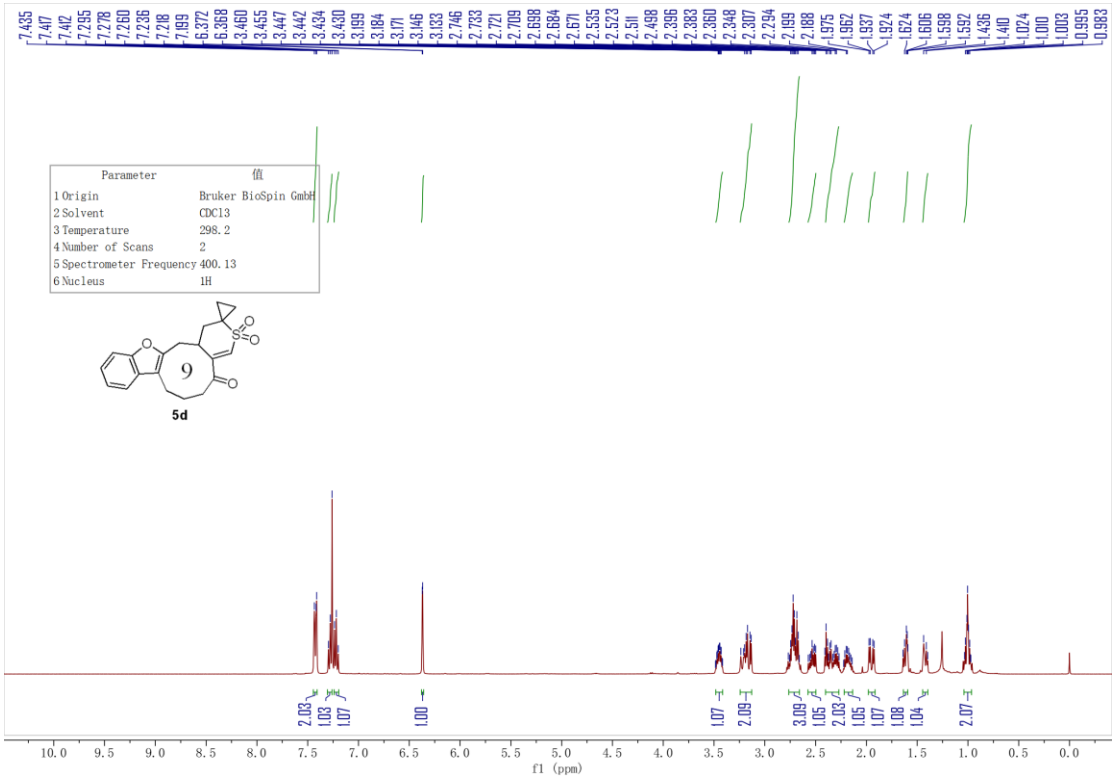
124.377
122.570
121.701
77.368
77.114
76.859
38.247
37.721
37.170
34.870
30.744
24.524
22.895
11.370
9.570
Parameter 值
1 Origin Bruker BioSpin GmbH
2 Solvent CDCl3
3 Temperature 298.0
4 Number of Scans 668
5 Spectrometer Frequency 125.77
6 Nucleus 13C
5c
f1 (ppm)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7.236
7.218
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6.372
6.368
3.460
3.455
3.447
3.442
3.434
3.430
3.199
3.184
3.171
3.146
3.133
2.746
2.733
2.721
2.709
2.698
2.684
2.671
2.535
2.523
2.511
2.498
2.396
2.383
2.360
2.348
2.307
2.294
2.199
2.188
1.975
1.962
1.937
1.924
1.624
1.606
1.598
1.592
1.436
1.410
1.024
1.010
1.003
0.995
0.983
Parameter 值
1 Origin Bruker BioSpin GmbH
2 Solvent CDCl3
3 Temperature 298.2
4 Number of Scans 2
5 Spectrometer Frequency 400.13
6 Nucleus 1H
5d
2.03
1.03
1.07
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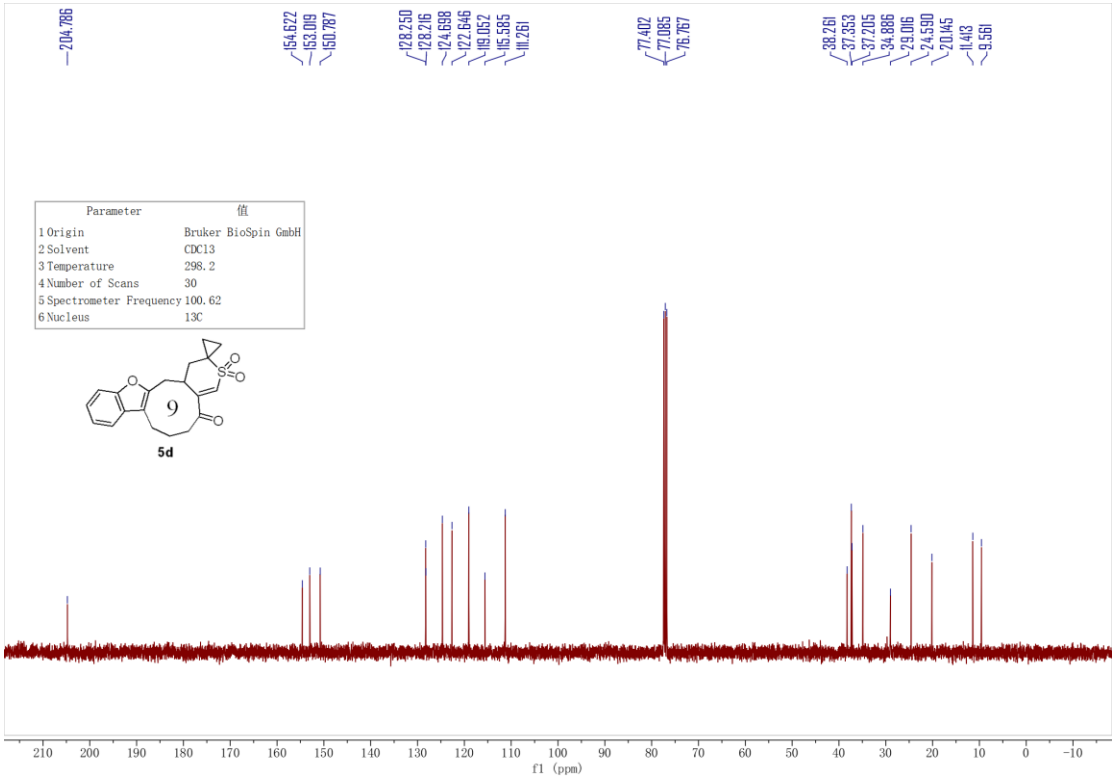
1.07
1.08
1.04
2.07
f1 (ppm)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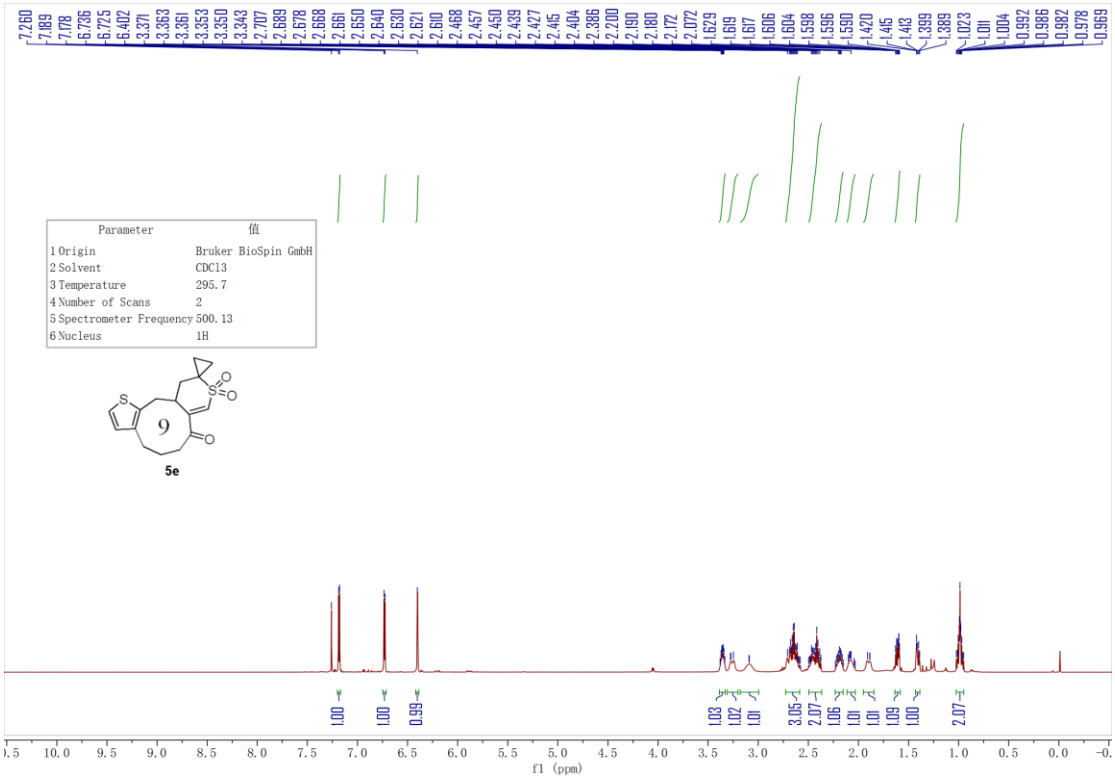
111.261
77.402
77.085
76.767
38.261
37.353
37.205
34.886
29.016
24.590
20.445
11.413
9.561
Parameter 值
1 Origin Bruker BioSpin GmbH
2 Solvent CDCl3
3 Temperature 298.2
4 Number of Scans 30
5 Spectrometer Frequency 100.62
6 Nucleus 13C
5d
f1 (ppm)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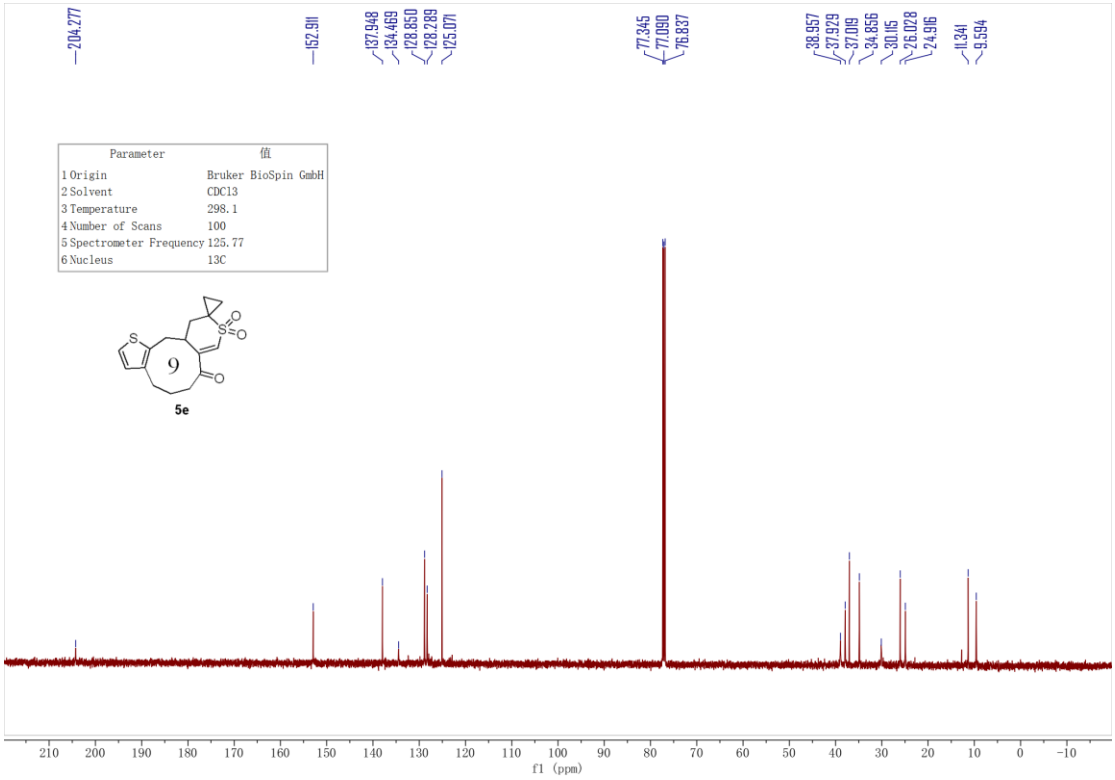
2.707
2.689
2.678
2.668
2.661
2.650
2.640
2.630
2.621
2.610
2.468
2.457
2.450
2.439
2.427
2.415
2.404
2.386
2.200
2.190
2.180
2.172
2.072
1.629
1.619
1.617
1.606
1.604
1.598
1.596
1.590
1.420
1.415
1.413
1.389
1.023
1.011
1.004
0.992
0.986
0.982
0.978
0.969
Parameter 值
1 Origin Bruker BioSpin GmbH
2 Solvent CDCl3
3 Temperature 295.7
4 Number of Scans 2
5 Spectrometer Frequency 500.13
6 Nucleus 1H
5e
1.00
1.00
0.99
1.03
1.02
1.01
3.05
2.07
1.06
1.01
1.01
1.09
1.00
2.07
f1 (ppm)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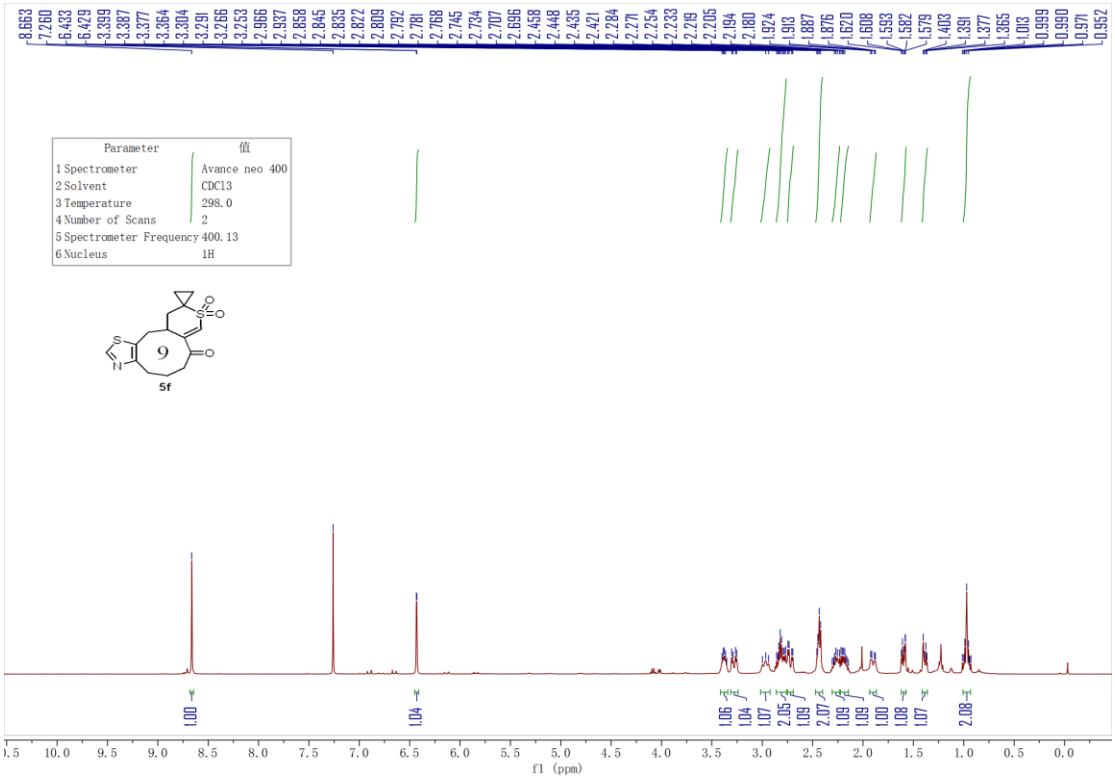
137.948
134.469
128.850
128.289
125.071
77.345
77.090
76.837
38.957
37.929
37.019
34.856
30.115
26.028
24.916
11.341
9.594
Parameter 值
1 Origin Bruker BioSpin GmbH
2 Solvent CDCl3
3 Temperature 298.1
4 Number of Scans 100
5 Spectrometer Frequency 125.77
6 Nucleus 13C
5e
f1 (ppm)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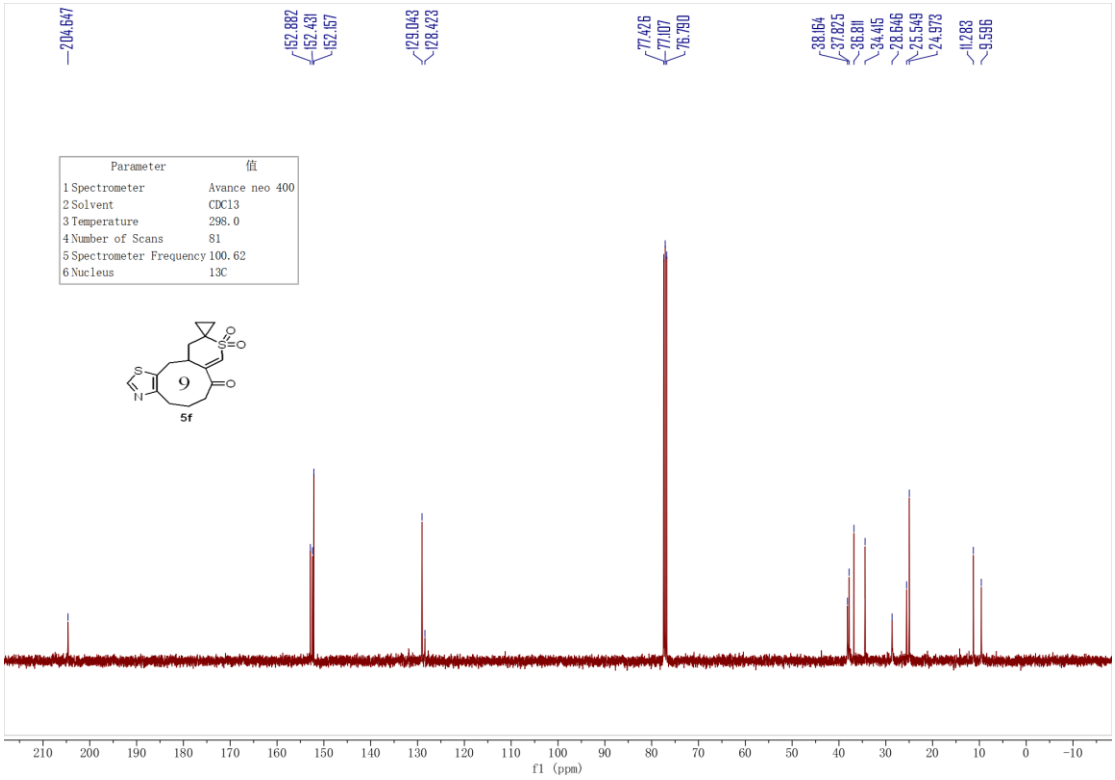
7.260
6.433
6.429
3.399
3.387
3.377
3.364
3.304
3.291
3.266
3.253
2.966
2.937
2.858
2.845
2.835
2.822
2.809
2.792
2.781
2.768
2.745
2.734
2.707
2.696
2.458
2.448
2.435
2.421
2.284
2.271
2.254
2.233
2.219
2.205
2.194
2.180
1.974
1.913
1.887
1.876
1.620
1.608
1.593
1.582
1.579
1.403
1.391
1.377
1.365
1.013
0.999
0.990
0.971
0.952
Parameter 值
1 Spectrometer Avance neo 400
2 Solvent CDCl3
3 Temperature 298.0
4 Number of Scans 2
5 Spectrometer Frequency 400.13
6 Nucleus 1H
5f
1.00
1.04
1.06
1.04
1.07
2.05
1.09
2.07
1.09
1.09
1.00
1.08
1.07
2.08
f1 (ppm)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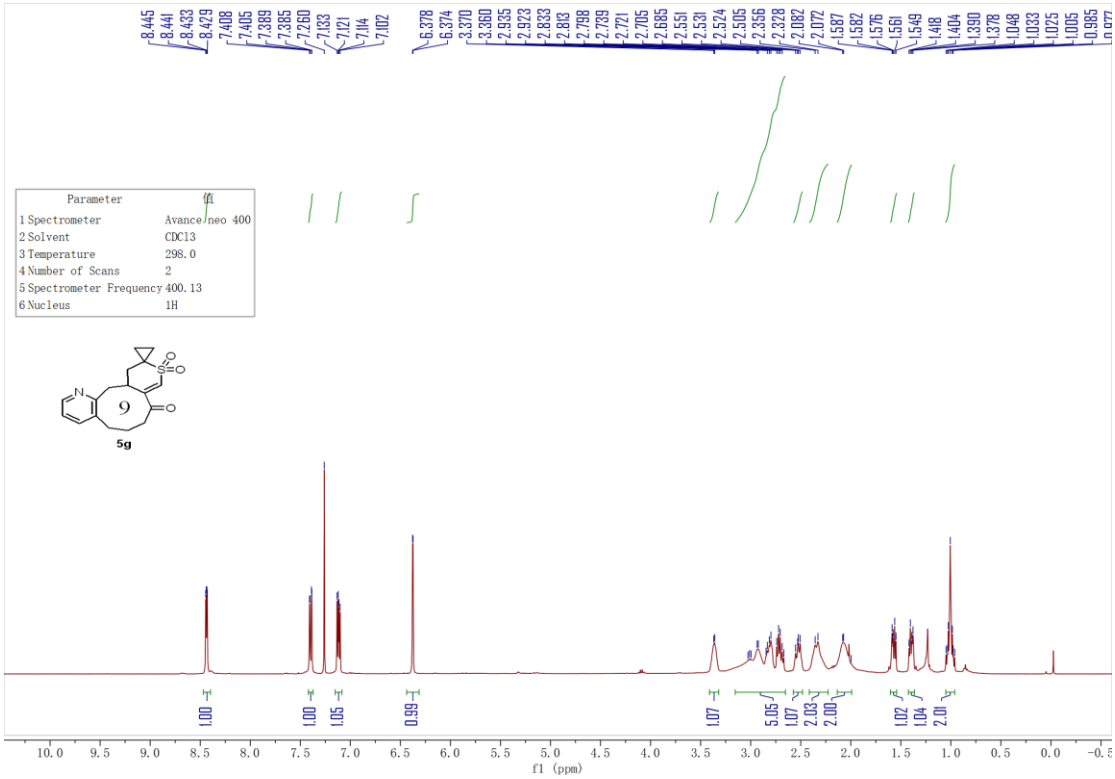
152.431
152.157
129.043
128.423
77.426
77.107
76.790
38.164
37.825
36.811
34.415
28.646
25.549
24.973
11.283
9.596
Parameter
1 Spectrometer Avance neo 400
2 Solvent CDCl3
3 Temperature 298.0
4 Number of Scans 81
5 Spectrometer Frequency 100.62
6 Nucleus 13C
5f
f1 (ppm)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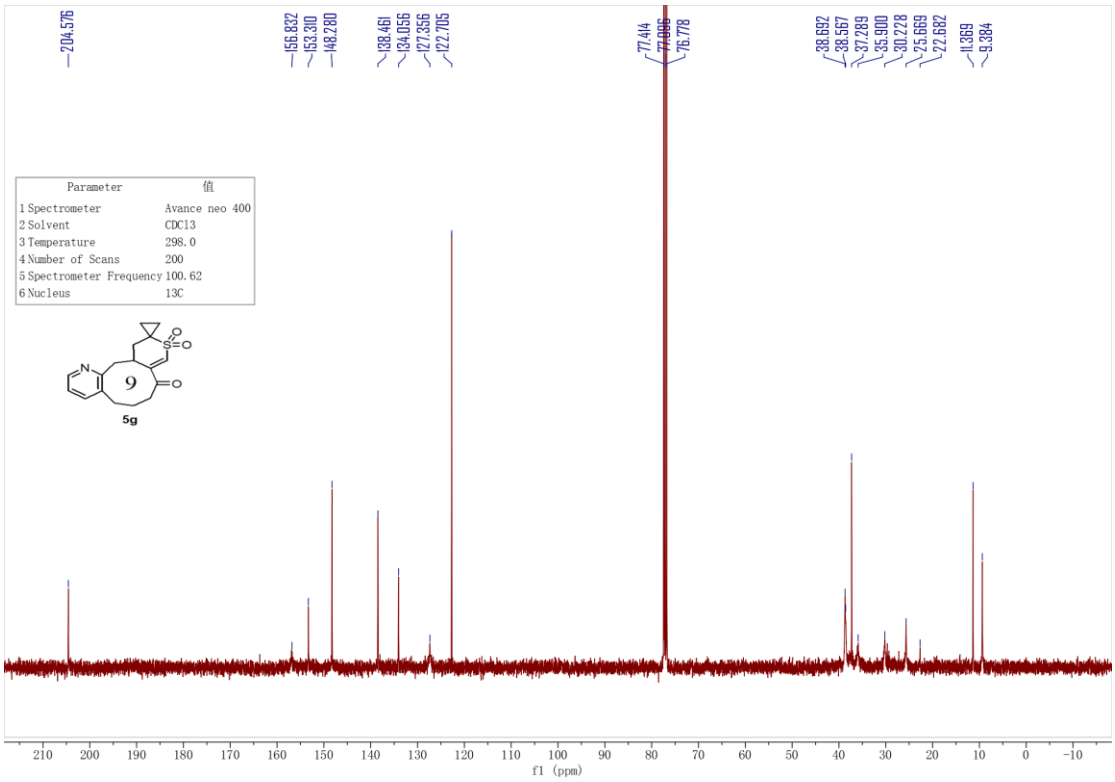
8.441
8.433
8.429
7.408
7.405
7.389
7.385
7.260
7.133
7.121
7.114
7.102
6.378
6.374
3.370
3.360
2.935
2.923
2.833
2.813
2.798
2.739
2.721
2.705
2.685
2.551
2.531
2.524
2.505
2.356
2.328
2.082
2.072
1.587
1.582
1.576
1.561
1.549
1.418
1.404
1.390
1.378
1.048
1.033
1.025
1.005
0.985
Parameter
1 Spectrometer Avance neo 400
2 Solvent CDCl3
3 Temperature 298.0
4 Number of Scans 2
5 Spectrometer Frequency 400.13
6 Nucleus 1H
5g
1.00
1.00
1.05
0.99
1.07
5.05
1.07
2.03
2.00
1.02
1.04
2.01
f1 (ppm)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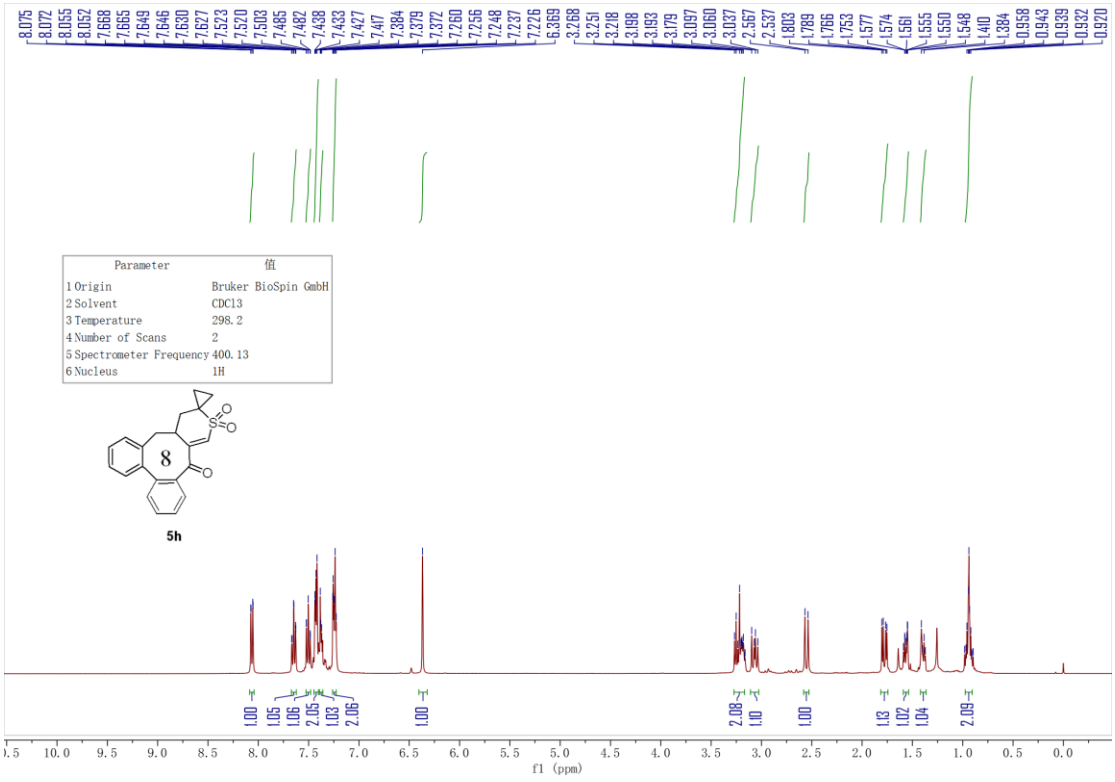
148.780
138.461
134.056
127.356
122.705
77.414
77.096
76.778
38.692
38.567
37.289
35.900
30.728
25.669
22.682
11.369
9.384
Parameter 值
1 Spectrometer Avance neo 400
2 Solvent CDCl3
3 Temperature 298.0
4 Number of Scans 200
5 Spectrometer Frequency 100.62
6 Nucleus 13C
9
5g
f1 (ppm)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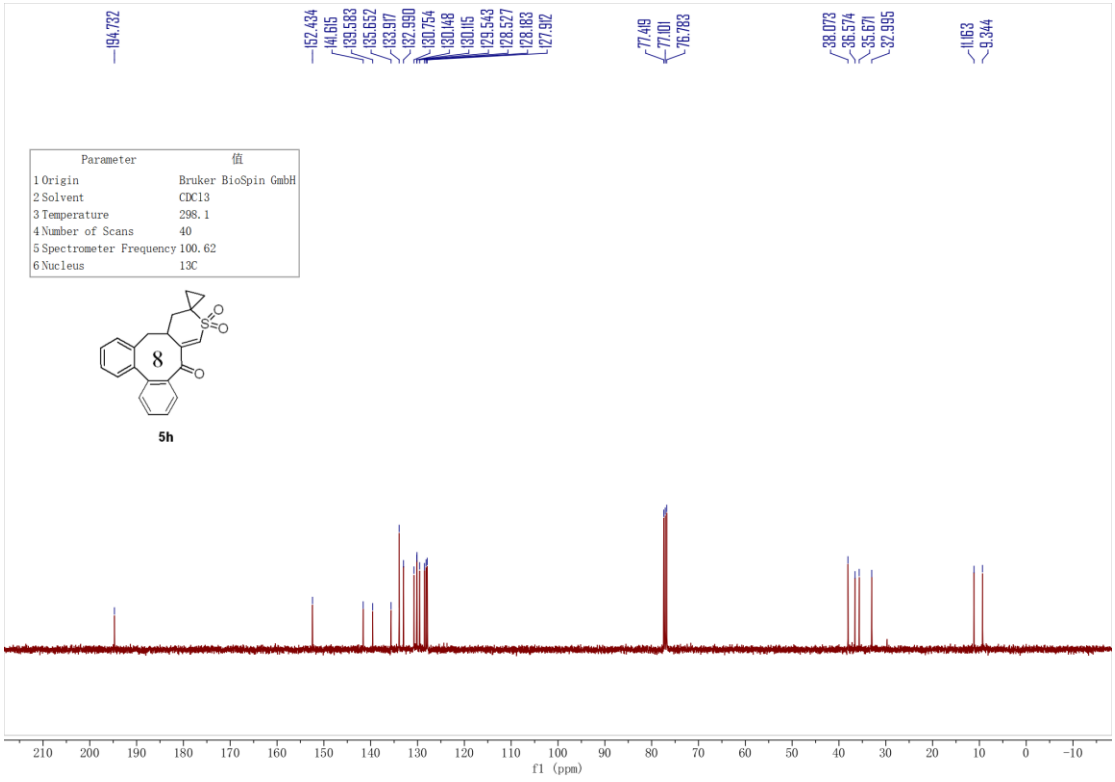
8.072
8.055
8.052
7.668
7.665
7.649
7.646
7.630
7.627
7.523
7.520
7.503
7.485
7.482
7.438
7.433
7.427
7.417
7.384
7.379
7.372
7.260
7.256
7.248
7.237
7.226
6.369
3.268
3.251
3.218
3.198
3.193
3.179
3.097
3.060
3.037
2.567
2.537
1.803
1.789
1.766
1.753
1.577
1.574
1.561
1.555
1.550
1.548
1.410
1.384
0.958
0.943
0.939
0.932
0.920
Parameter 值
1 Origin Bruker BioSpin GmbH
2 Solvent CDCl3
3 Temperature 298.2
4 Number of Scans 2
5 Spectrometer Frequency 400.13
6 Nucleus 1H
8
5h
1.00
1.05
1.06
2.05
1.03
2.06
1.00
2.08
1.10
1.00
1.13
1.02
1.04
2.09
f1 (ppm)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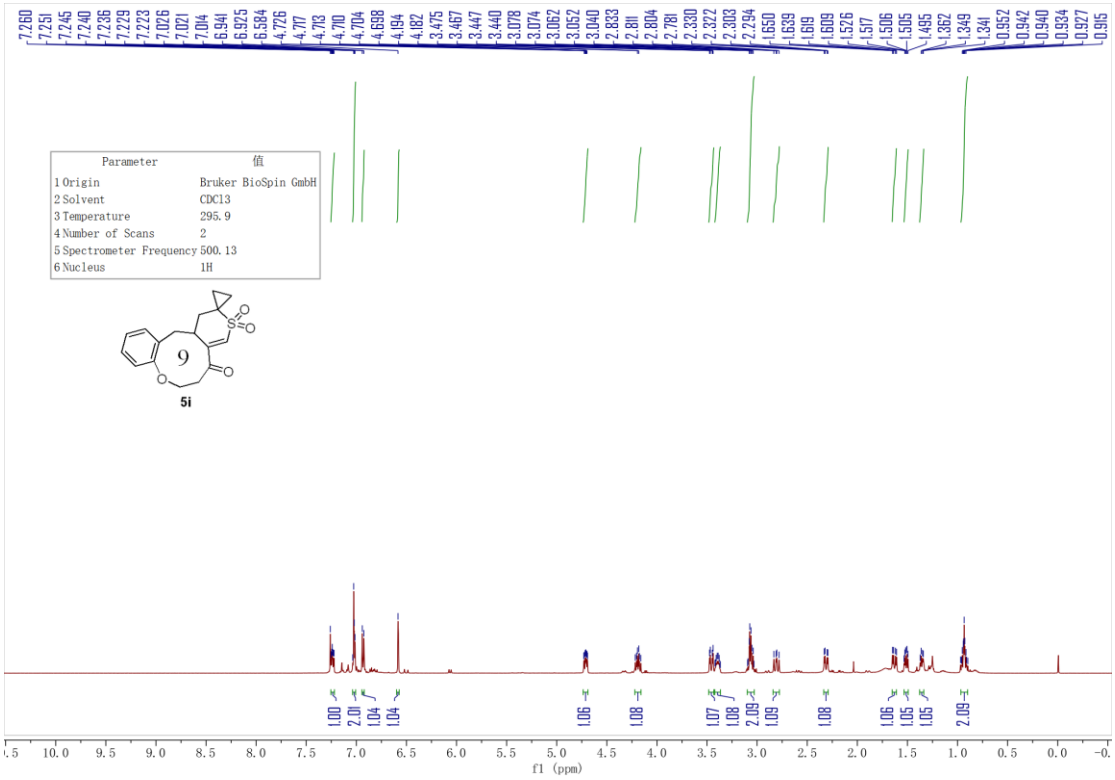
141.615
139.583
135.652
133.917
132.990
130.754
130.148
130.115
129.543
128.527
128.183
127.912
77.419
77.101
76.783
38.073
36.574
35.671
32.995
11.163
9.344
Parameter 值
1 Origin Bruker BioSpin GmbH
2 Solvent CDCl3
3 Temperature 298.1
4 Number of Scans 40
5 Spectrometer Frequency 100.62
6 Nucleus 13C
8
S
O
O
O
5h
f1 (ppm)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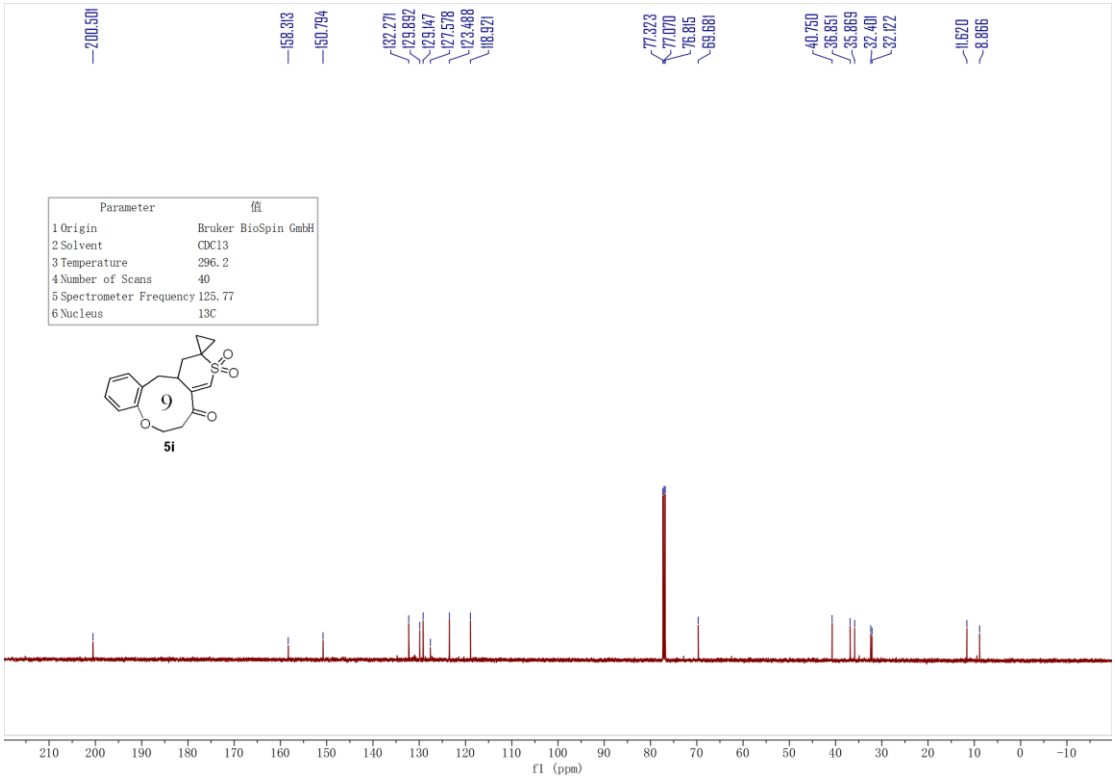
7.251
7.245
7.240
7.236
7.229
7.223
7.026
7.021
7.014
6.941
6.925
6.584
4.726
4.717
4.713
4.710
4.704
4.698
4.194
4.182
3.475
3.467
3.447
3.440
3.078
3.074
3.062
3.052
3.040
2.833
2.811
2.804
2.781
2.330
2.322
2.303
2.294
1.650
1.639
1.619
1.609
1.576
1.517
1.506
1.505
1.495
1.362
1.349
1.341
0.952
0.942
0.940
0.934
0.927
0.915
Parameter 值
1 Origin Bruker BioSpin GmbH
2 Solvent CDCl3
3 Temperature 295.9
4 Number of Scans 2
5 Spectrometer Frequency 500.13
6 Nucleus 1H
9
S
O
O
O
O
5i
1.00
2.01
1.04
1.04
1.06
1.08
1.07
1.08
2.09
1.09
1.08
1.06
1.05
1.05
2.09
f1 (ppm)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150.794
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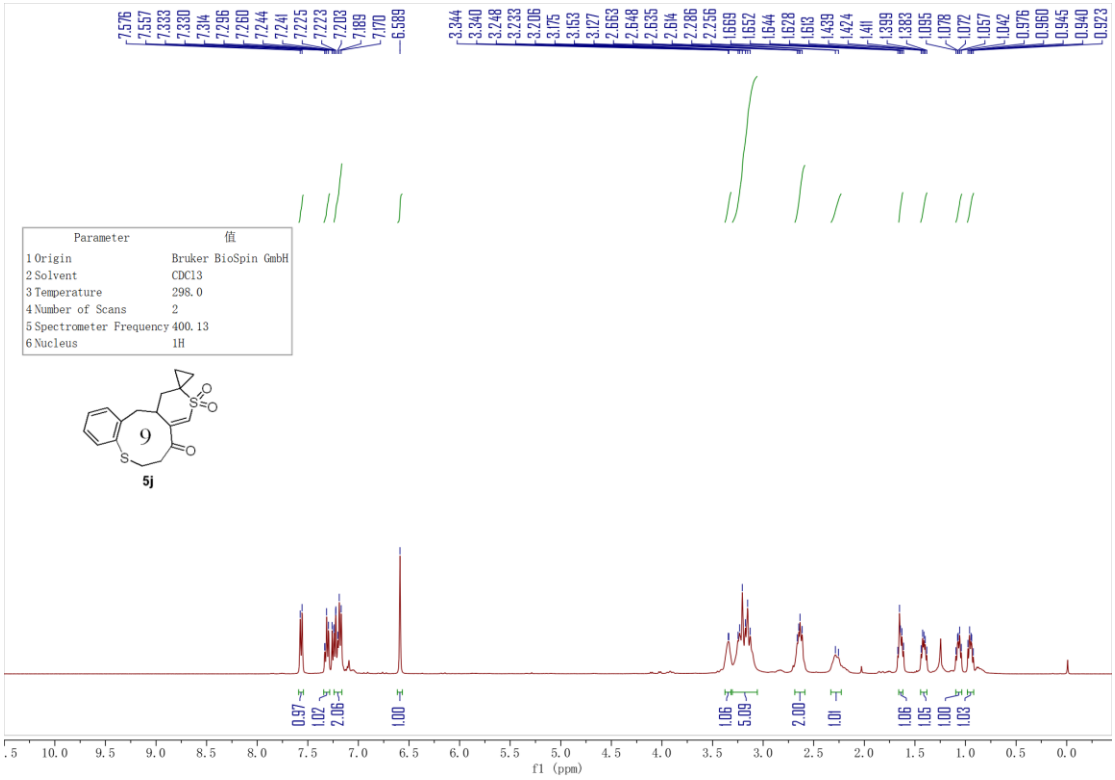
127.578
123.488
118.921
77.323
77.070
76.815
69.681
40.750
36.851
35.869
32.401
32.122
11.620
8.866
Parameter 值
1 Origin Bruker BioSpin GmbH
2 Solvent CDCl3
3 Temperature 296.2
4 Number of Scans 40
5 Spectrometer Frequency 125.77
6 Nucleus 13C
5i
f1 (ppm)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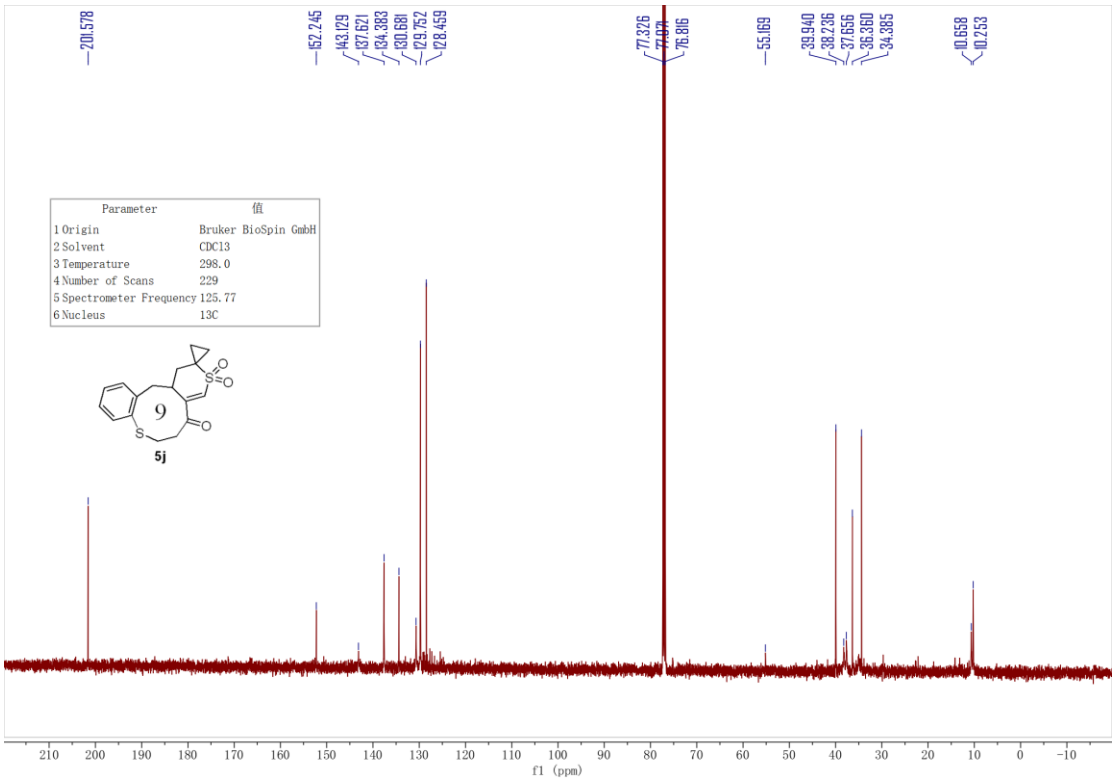
7.557
7.333
7.330
7.314
7.296
7.260
7.244
7.241
7.225
7.223
7.203
7.189
7.170
6.589
3.344
3.340
3.248
3.233
3.206
3.175
3.153
3.127
2.663
2.648
2.635
2.614
2.286
2.256
1.669
1.652
1.644
1.628
1.613
1.439
1.424
1.411
1.399
1.383
1.095
1.078
1.072
1.057
1.042
0.976
0.960
0.945
0.940
0.923
Parameter 值
1 Origin Bruker BioSpin GmbH
2 Solvent CDCl3
3 Temperature 298.0
4 Number of Scans 2
5 Spectrometer Frequency 400.13
6 Nucleus 1H
5j
0.97
1.02
2.06
1.00
1.06
5.09
2.00
1.01
1.06
1.05
1.00
1.03
f1 (ppm)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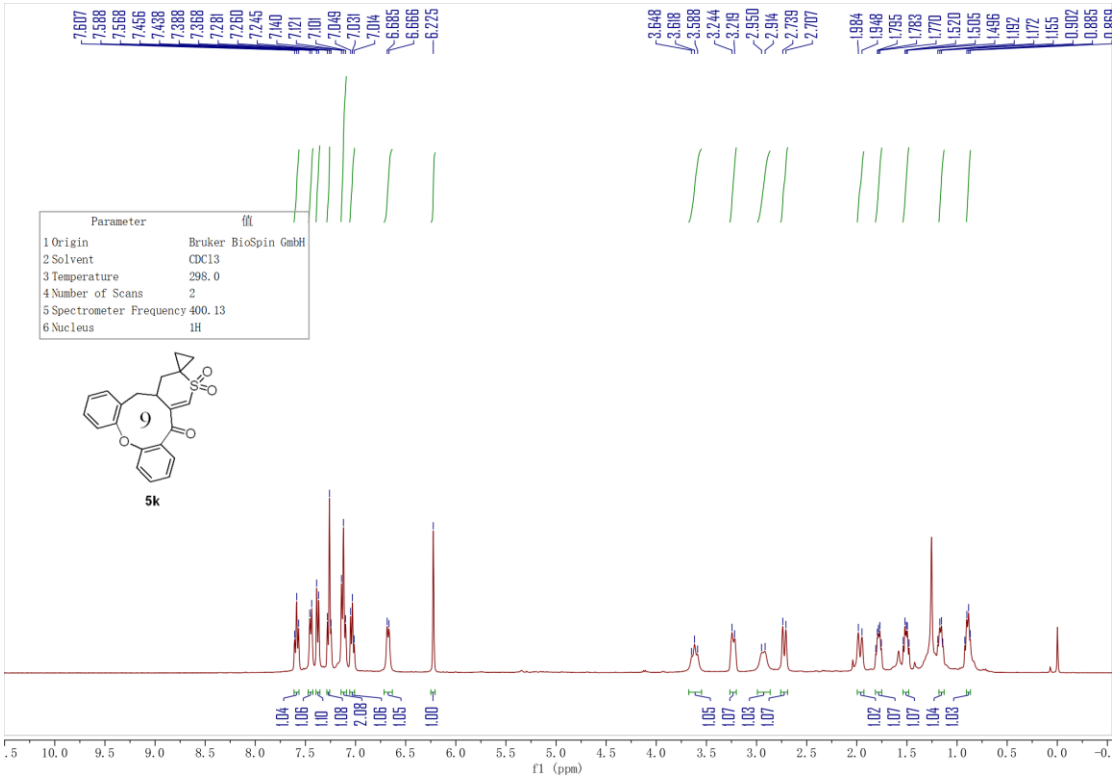
134.383
130.681
129.752
128.459
77.326
77.071
76.816
55.169
39.940
38.236
37.656
36.360
34.385
10.658
10.253
Parameter 值
1 Origin Bruker BioSpin GmbH
2 Solvent CDCl3
3 Temperature 298.0
4 Number of Scans 229
5 Spectrometer Frequency 125.77
6 Nucleus 13C
5j
f1 (ppm)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7.588
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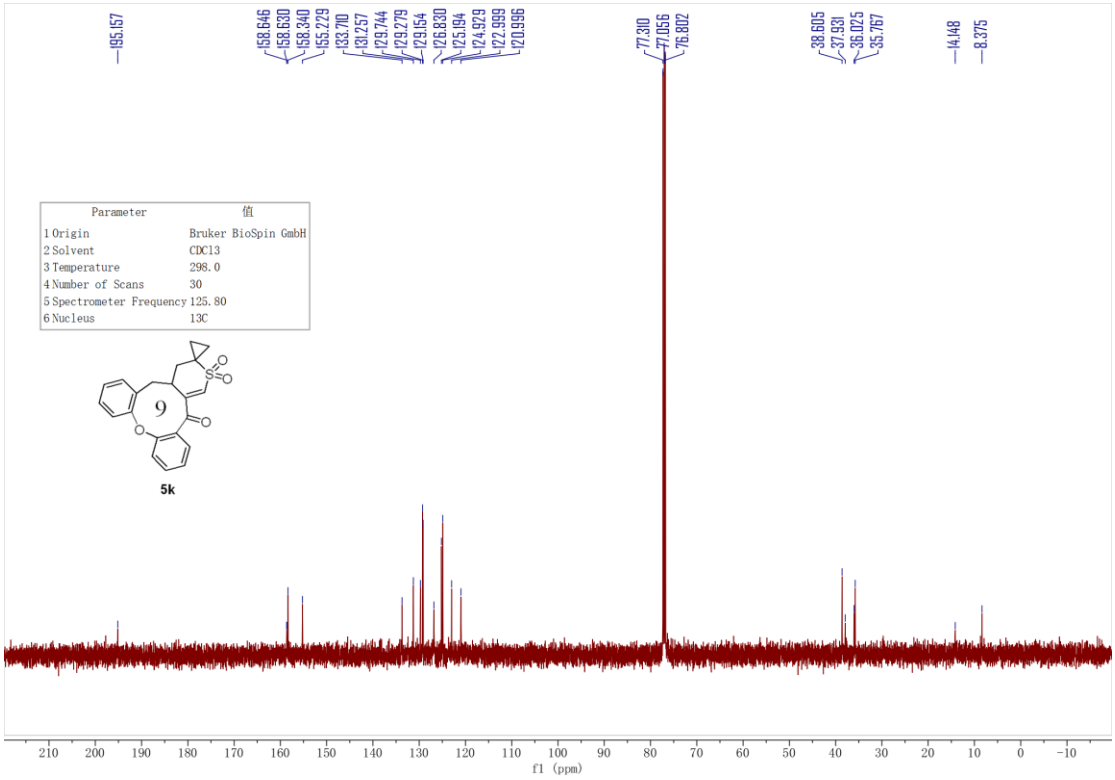
7.438
7.388
7.368
7.281
7.260
7.245
7.140
7.121
7.101
7.049
7.031
7.014
6.685
6.666
6.275
3.648
3.618
3.588
3.244
3.219
2.950
2.934
2.739
2.707
1.984
1.948
1.795
1.783
1.770
1.520
1.505
1.496
1.192
1.172
1.155
0.902
0.885
Parameter 值
1 Origin Bruker BioSpin GmbH
2 Solvent CDCl3
3 Temperature 298.0
4 Number of Scans 2
5 Spectrometer Frequency 400.13
6 Nucleus 1H
5k
1.04
1.06
1.10
1.08
2.08
1.06
1.05
1.00
1.05
1.07
1.03
1.07
1.02
1.07
1.07
1.04
1.03
f1 (ppm)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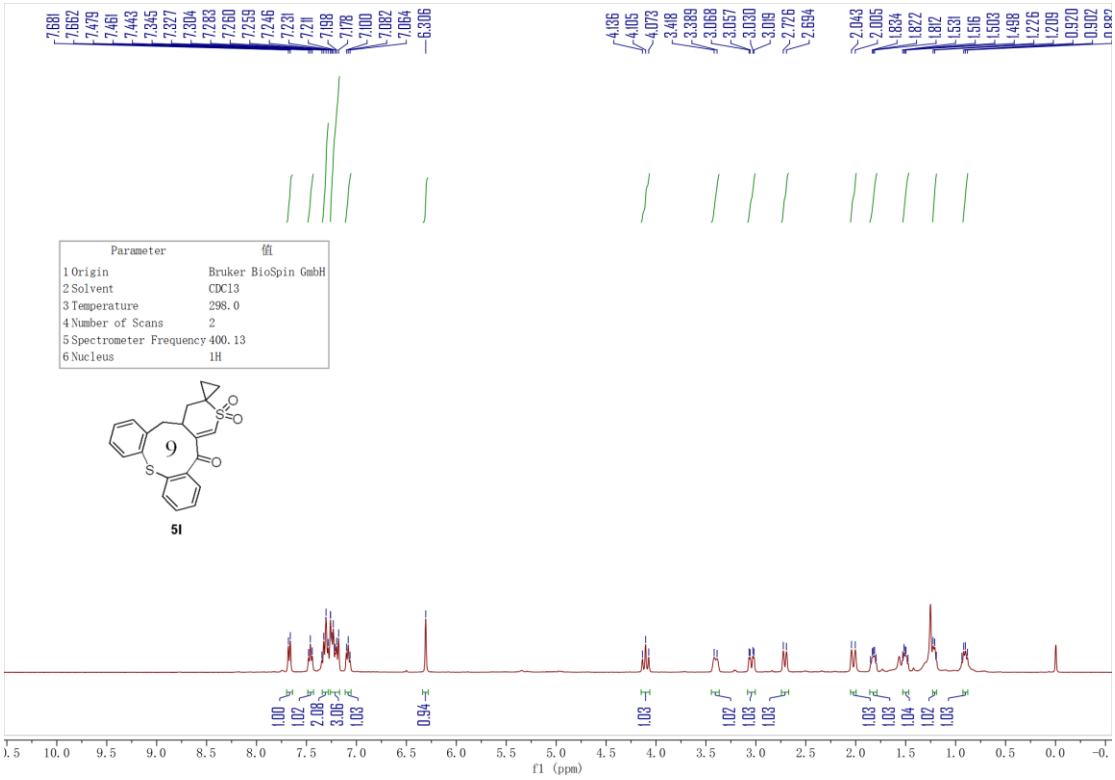
158.630
158.340
155.229
133.710
131.257
129.744
129.279
129.154
126.830
125.194
124.929
122.999
120.996
77.310
77.056
76.802
38.605
37.931
36.025
35.767
14.148
8.375
Parameter 值
1 Origin Bruker BioSpin GmbH
2 Solvent CDCl3
3 Temperature 298.0
4 Number of Scans 30
5 Spectrometer Frequency 125.80
6 Nucleus 13C
5k
f1 (ppm)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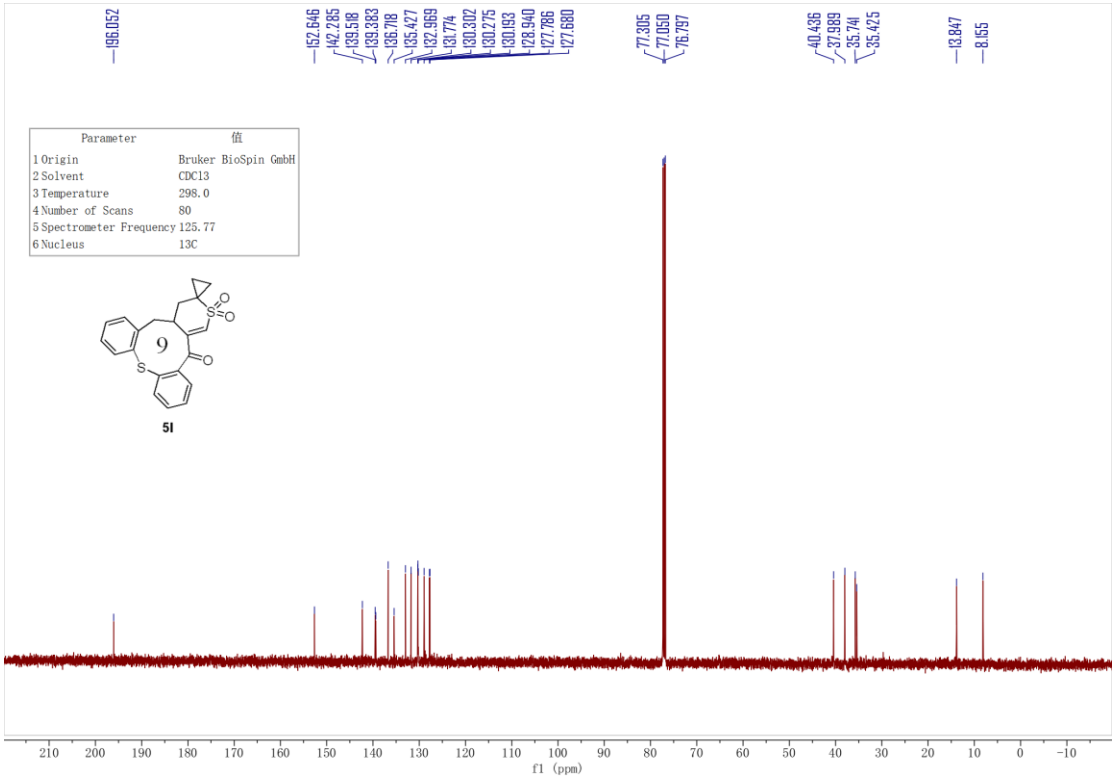
7.345
7.327
7.304
7.283
7.260
7.259
7.246
7.231
7.211
7.198
7.178
7.100
7.082
7.064
6.306
4.136
4.105
4.073
3.418
3.389
3.068
3.057
3.030
3.019
2.726
2.694
2.043
2.005
1.834
1.822
1.812
1.531
1.516
1.503
1.498
1.276
1.209
0.970
0.902
Parameter 值
1 Origin Bruker BioSpin GmbH
2 Solvent CDCl3
3 Temperature 298.0
4 Number of Scans 2
5 Spectrometer Frequency 400.13
6 Nucleus 1H
5l
1.00
1.02
2.08
3.06
1.03
0.94
1.03
1.02
1.03
1.03
1.03
1.03
1.04
1.02
1.03
f1 (ppm)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136.718
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132.969
131.774
130.302
130.275
130.193
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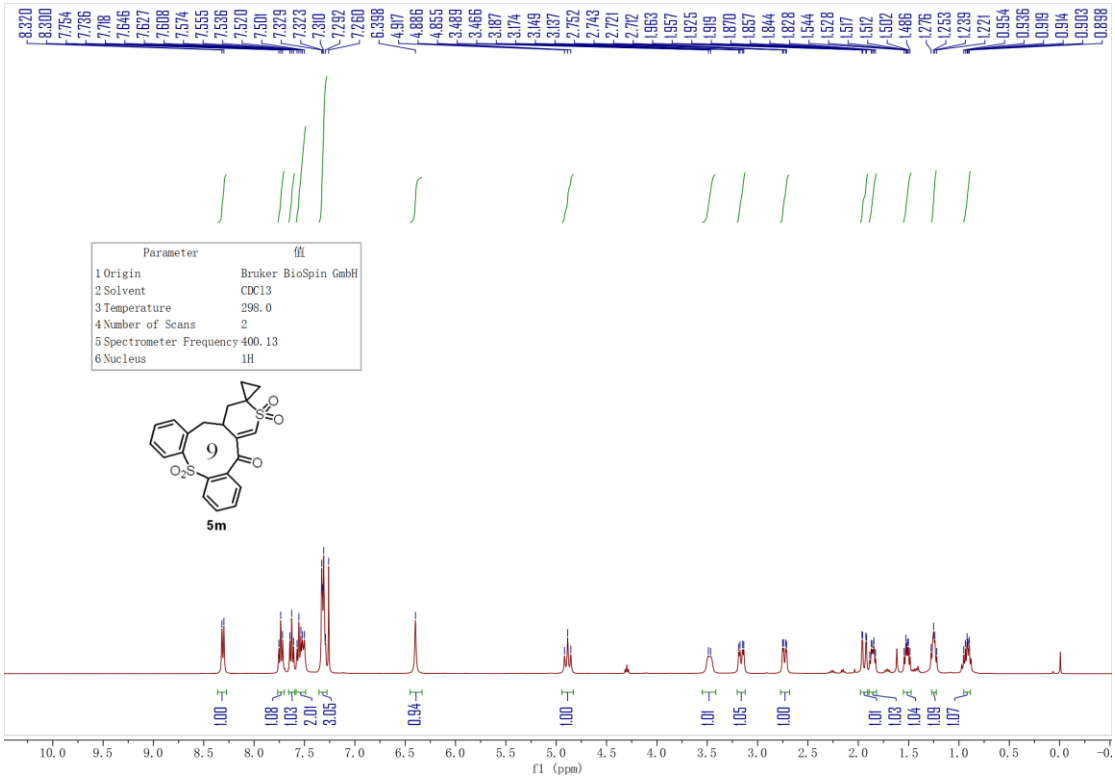
127.786
127.680
77.305
77.050
76.797
40.436
37.988
35.744
35.425
13.847
8.155
Parameter 值
1 Origin Bruker BioSpin GmbH
2 Solvent CDCl3
3 Temperature 298.0
4 Number of Scans 80
5 Spectrometer Frequency 125.77
6 Nucleus 13C
5l
f1 (ppm)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7.608
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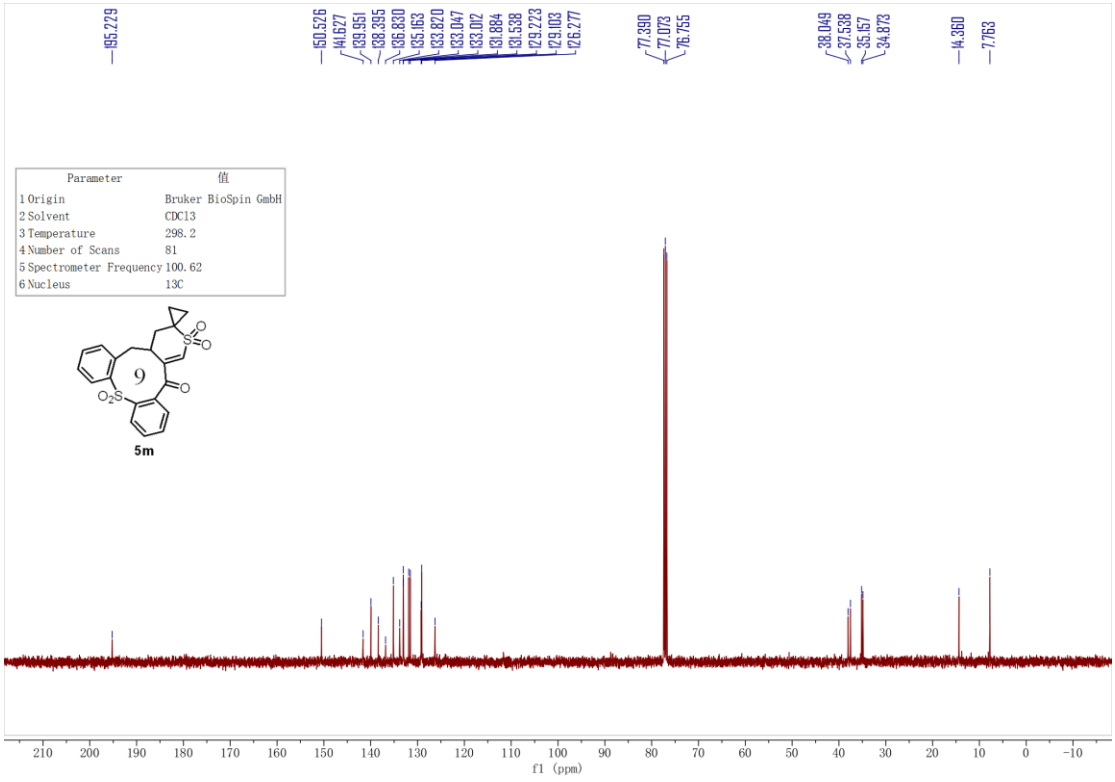
7.555
7.536
7.520
7.501
7.329
7.323
7.310
7.292
7.260
6.398
4.917
4.886
4.855
3.489
3.466
3.187
3.174
3.149
3.137
2.752
2.743
2.721
2.712
1.963
1.957
1.925
1.919
1.870
1.857
1.844
1.828
1.544
1.528
1.517
1.512
1.502
1.486
1.276
1.253
1.239
1.221
0.954
0.936
0.919
0.914
0.903
0.898
Parameter 值
1 Origin Bruker BioSpin GmbH
2 Solvent CDCl3
3 Temperature 298.0
4 Number of Scans 2
5 Spectrometer Frequency 400.13
6 Nucleus 1H
5m
1.00
1.08
1.03
2.01
3.05
0.94
1.00
1.01
1.05
1.00
1.01
1.03
1.04
1.09
1.07
f1 (ppm)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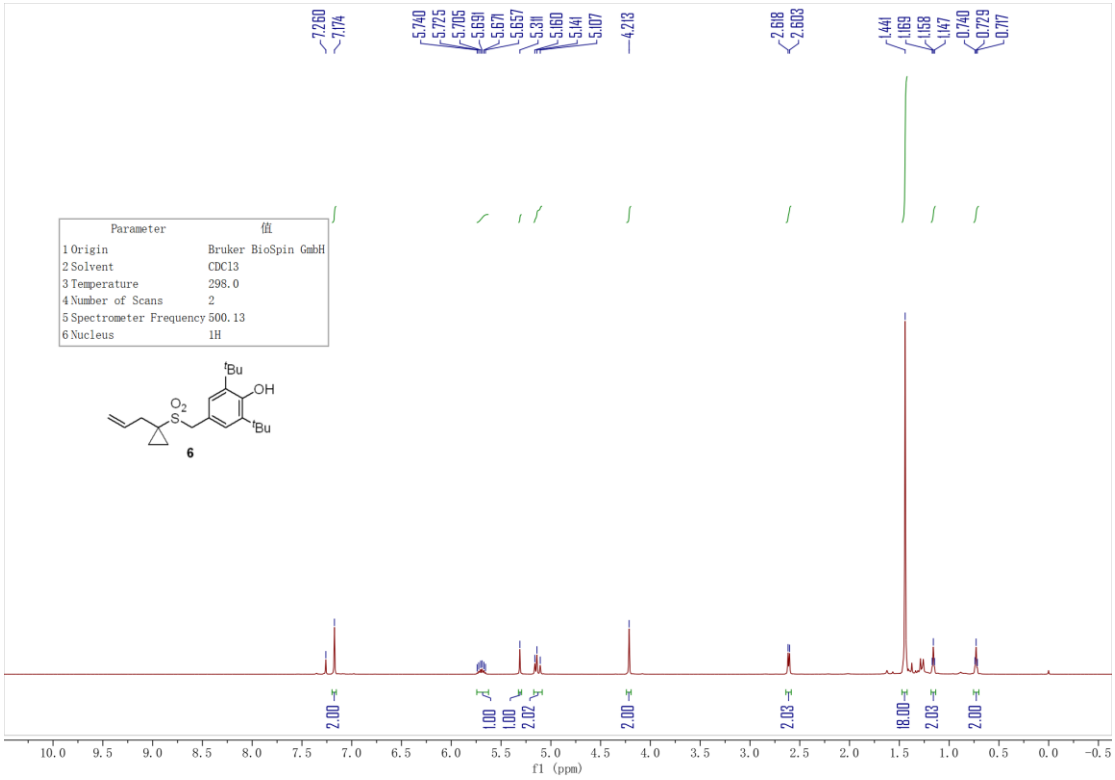
129.223
129.103
126.277
77.390
77.073
76.755
38.049
37.538
35.157
34.873
14.360
7.763
Parameter 值
1 Origin Bruker BioSpin GmbH
2 Solvent CDCl3
3 Temperature 298.2
4 Number of Scans 81
5 Spectrometer Frequency 100.62
6 Nucleus 13C
5m
f1 (ppm)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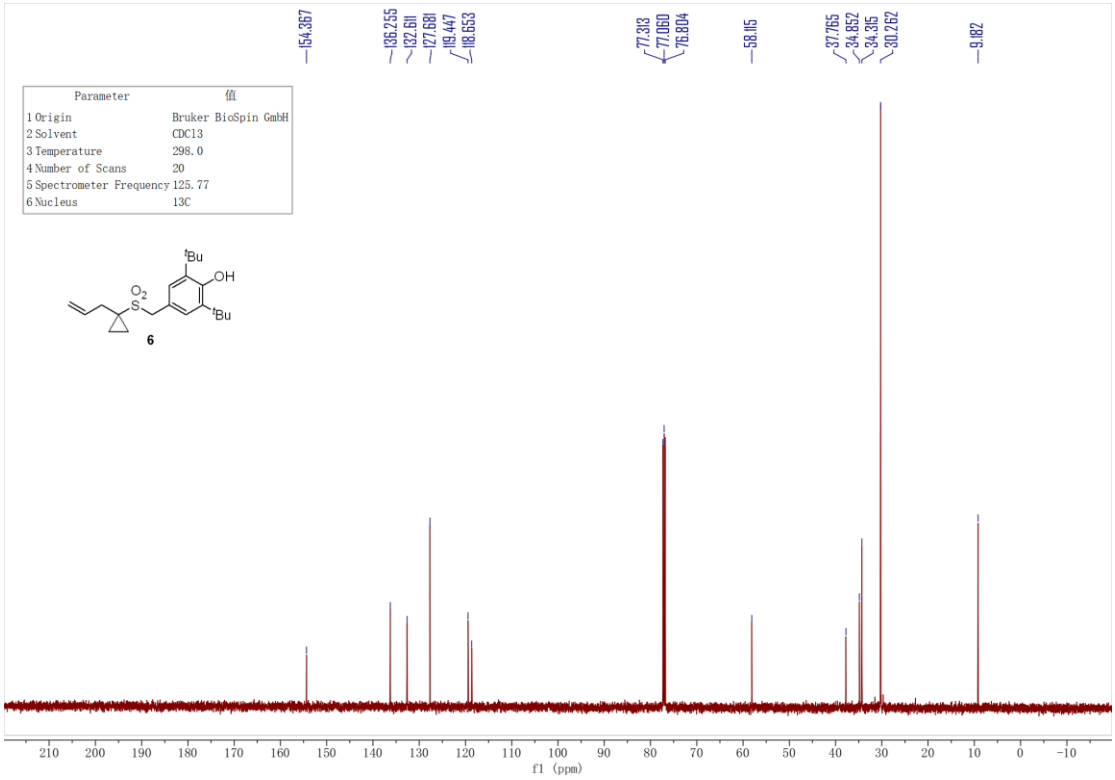
5.740
5.725
5.705
5.691
5.671
5.657
5.311
5.160
5.141
5.107
4.213
2.618
2.603
1.441
1.169
1.158
1.147
0.740
0.729
0.717
Parameter 值
1 Origin Bruker BioSpin GmbH
2 Solvent CDCl3
3 Temperature 298.0
4 Number of Scans 2
5 Spectrometer Frequency 500.13
6 Nucleus 1H
6
f1 (ppm)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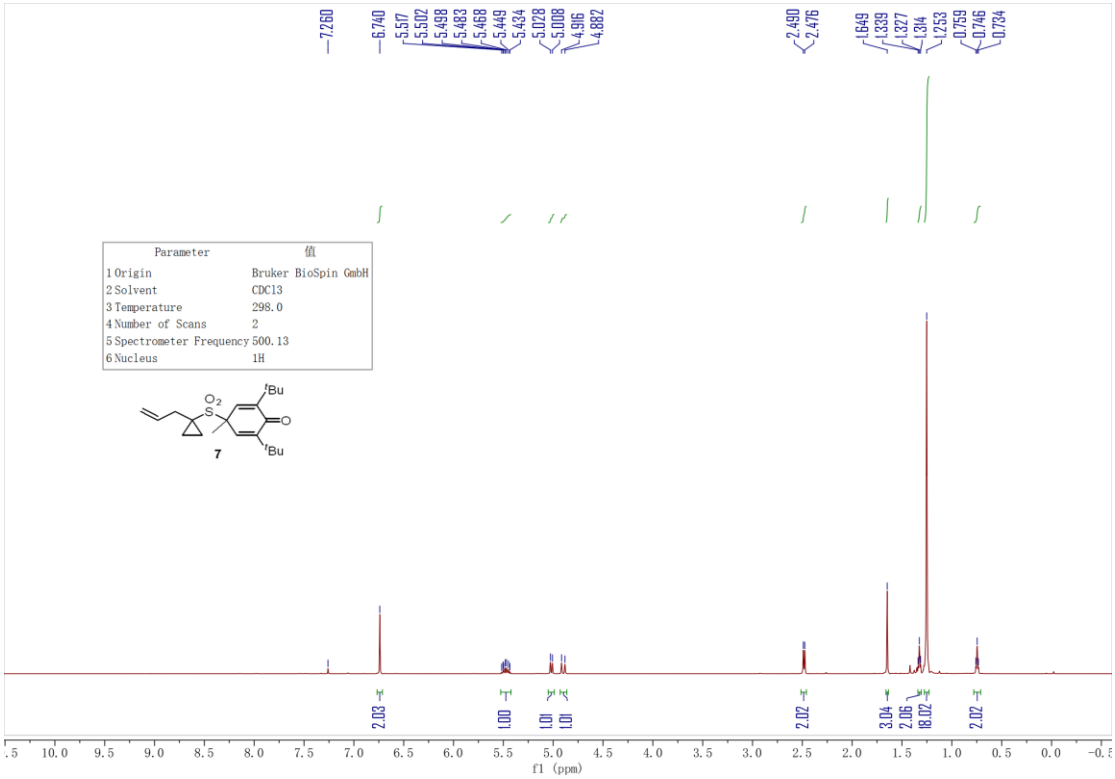
132.611
127.688
119.447
118.653
77.313
77.060
76.804
58.115
37.765
34.852
34.345
30.262
9.182
Parameter 值
1 Origin Bruker BioSpin GmbH
2 Solvent CDCl3
3 Temperature 298.0
4 Number of Scans 20
5 Spectrometer Frequency 125.77
6 Nucleus 13C
tBu
OH
O2
S
tBu
6
f1 (ppm)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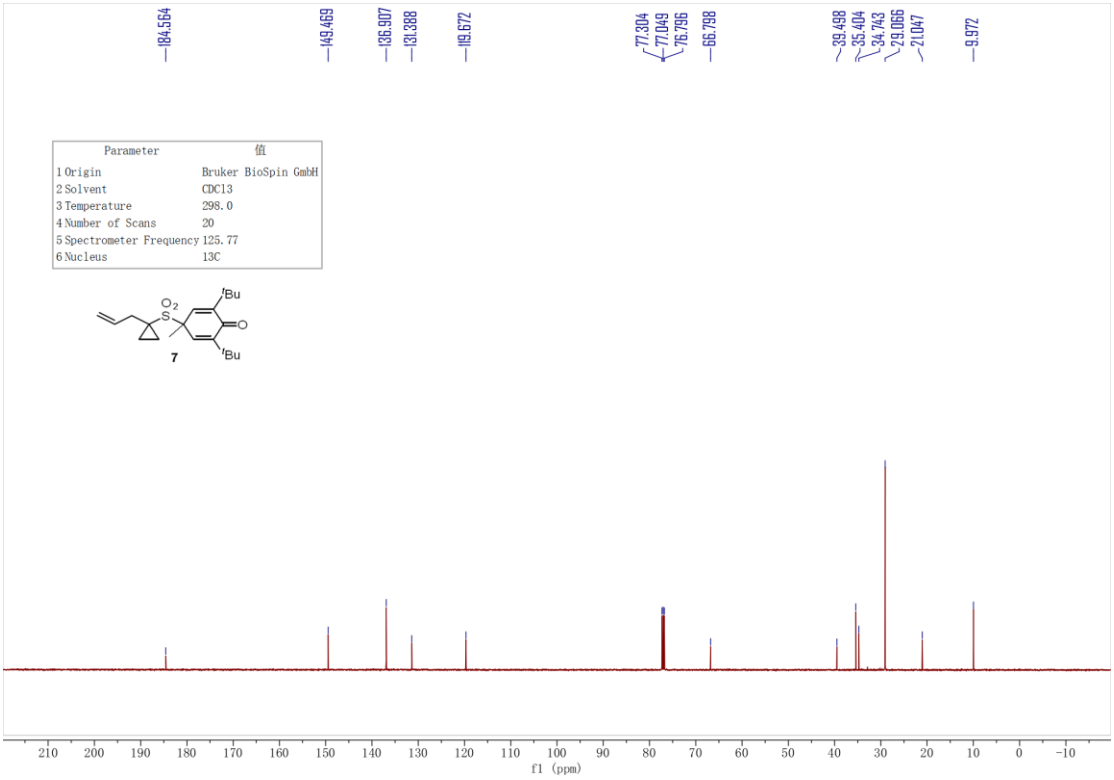
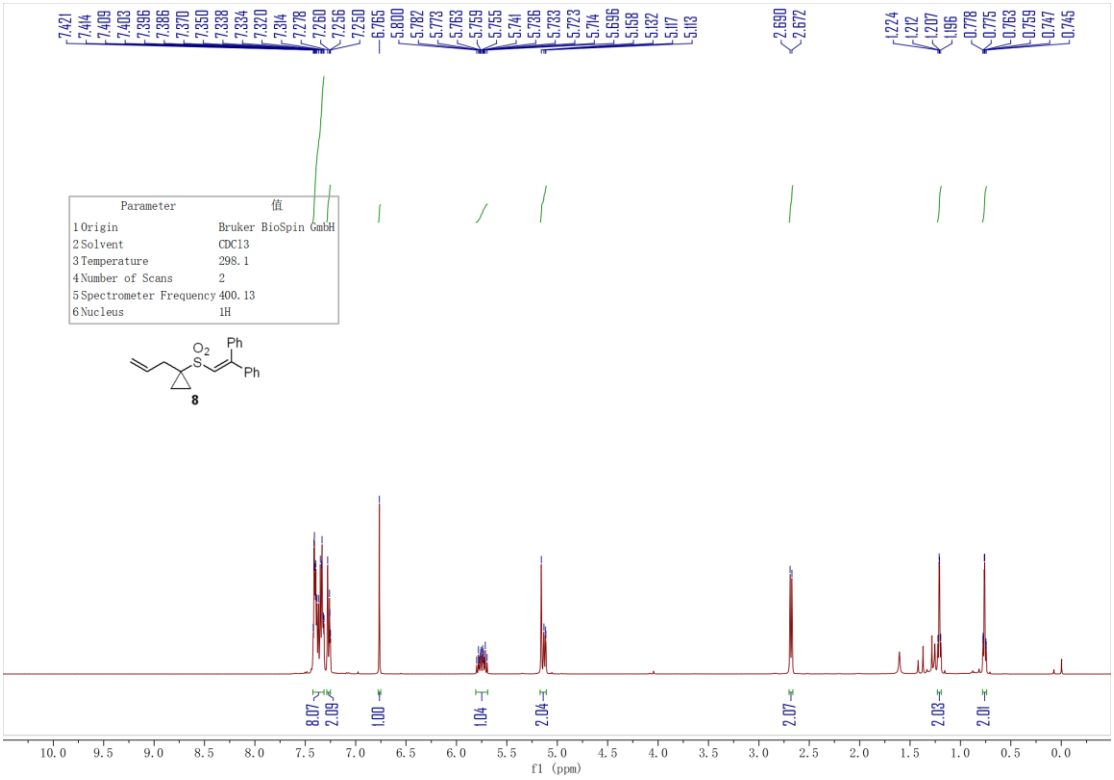
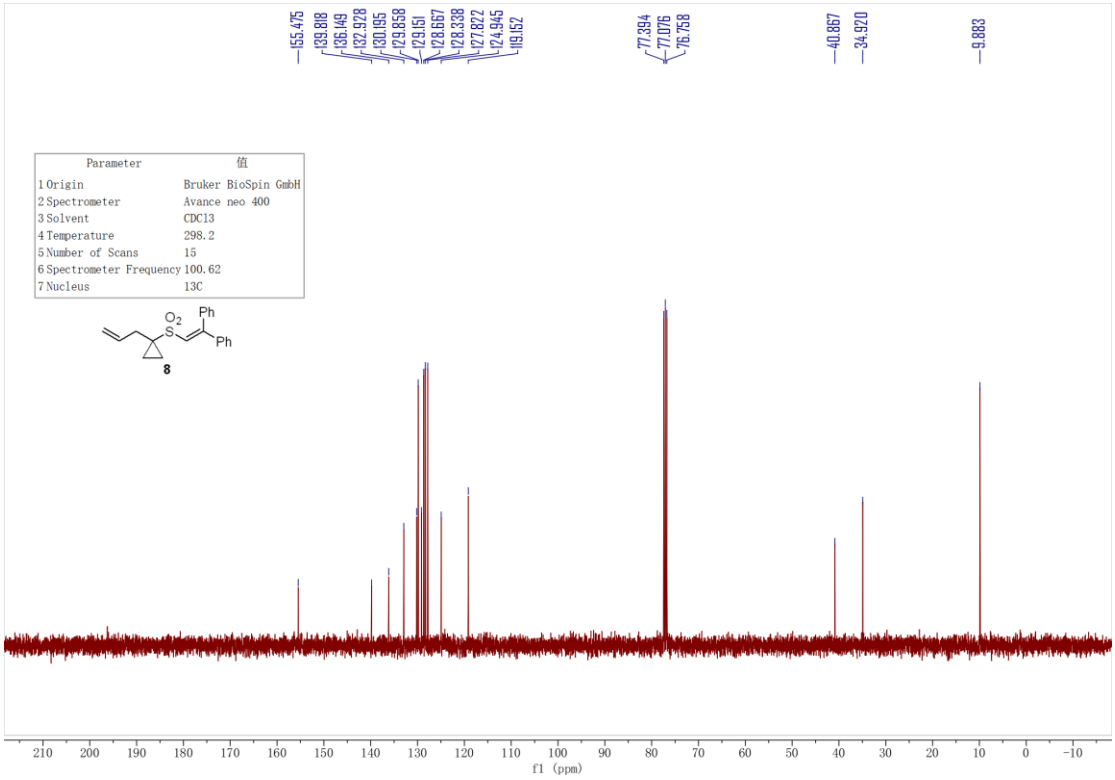
5.498
5.483
5.468
5.449
5.434
5.028
5.008
4.916
4.882
2.490
2.476
1.649
1.339
1.327
1.314
1.253
0.759
0.746
0.734
Parameter 值
1 Origin Bruker BioSpin GmbH
2 Solvent CDCl3
3 Temperature 298.0
4 Number of Scans 2
5 Spectrometer Frequency 500.13
6 Nucleus 1H
O2
S
tBu
O
tBu
7
2.03
1.00
1.01
1.01
2.02
3.04
2.06
18.02
2.02
f1 (ppm)


184.564
149.469
136.907
131.388
119.672
77.304
77.049
76.796
66.798
39.498
35.404
34.743
29.066
21.047
9.972
Parameter 值
1 Origin Bruker BioSpin GmbH
2 Solvent CDCl3
3 Temperature 298.0
4 Number of Scans 20
5 Spectrometer Frequency 125.77
6 Nucleus 13C
tBu
O2
S
O
tBu
7
f1 (ppm)


7.421
7.414
7.409
7.403
7.396
7.386
7.370
7.350
7.338
7.334
7.320
7.314
7.278
7.260
7.256
7.250
6.765
5.800
5.782
5.773
5.763
5.759
5.755
5.744
5.736
5.733
5.723
5.714
5.696
5.158
5.132
5.117
5.113
2.690
2.672
1.224
1.212
1.207
1.196
0.778
0.775
0.763
0.759
0.747
0.745
Parameter 值
1 Origin Bruker BioSpin GmbH
2 Solvent CDCl3
3 Temperature 298.1
4 Number of Scans 2
5 Spectrometer Frequency 400.13
6 Nucleus 1H
O2
S
Ph
Ph
8
8.07
2.09
1.00
1.04
2.04
2.07
2.03
2.01
f1 (ppm)


155.475
139.818
136.149
132.978
130.195
129.858
129.151
128.667
128.338
127.822
124.945
119.152
77.394
77.076
76.758
40.867
34.920
9.883
Parameter 值
1 Origin Bruker BioSpin GmbH
2 Spectrometer Avance neo 400
3 Solvent CDCl3
4 Temperature 298.2
5 Number of Scans 15
6 Spectrometer Frequency 100.62
7 Nucleus 13C
O2
S
Ph
Ph
8
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 −10
f1 (ppm)