Electronic Supplementary Material (ESI) for Organic Chemistry Frontiers.

Supporting Information

Azidoheteroarylation of unactivated olefins through distal heteroaryl migration

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1. General experimental details

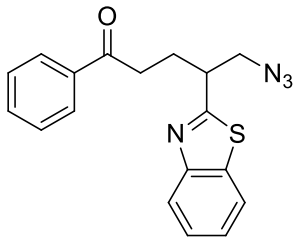
All reactions were maintained under a nitrogen atmosphere unless otherwise stated. Commercially available reagents were used without further purification. Infrared (FT-IR) spectra were recorded on a BRUKER VERTEX 70, ν_{max} in cm^{-1}. ^{1}H-NMR spectra were recorded on a BRUKER AVANCE III HD (400 MHz) spectrometer. Chemical shifts are reported in ppm from tetramethylsilane with the solvent resonance as internal standard ($CDCl_3$: δ 7.26，DMSO: δ 2.50). 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 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 76.6, DMSO: δ 39.5). ^{19}F-NMR spectra were recorded on a BRUKER AVANCE III HD (376 MHz) spectrometer. Mass spectra were measured with an Agilent Technologies 6120 Quadrupole LC/MS. High resolution mass spectrometry (HRMS) were measured with a GCT Premier^{TM} and BRUKER micrOTF-Q III. Melting points were measured using INESA WRR and values are uncorrected.

The starting materials (tertiary alcohols) were generally prepared by the addition of heteroaryl lithium reagent (HetArLi) to the precursor ketones.

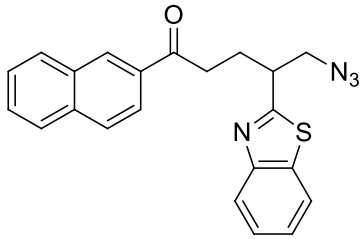
2. General procedure for heteroaryl migration

The aryl-substituted tertiary alcohol **1** (0.2 mmol, 1.0 equiv.) and PIDA (0.35 mmol, 1.75 equiv.) were loaded in a reaction vial which was subjected to evacuation/ flushing with nitrogen three times. CH_3CN (2.0 mL) and $TMSN_3$ (0.6 mmol, 3.0 equiv.) were then added to the mixture via syringe, and the mixture was stirred at 25 °C until the starting material had been consumed as determined by TLC. The mixture was extracted with ethyl acetate (3 × 10 mL). The combined organic extracts were washed by brine, dried over Na_2SO_4, filtered, concentrated, and purified by flash column chromatography on silica gel (ethyl acetate/ petroleum ether) to give the product **2**.

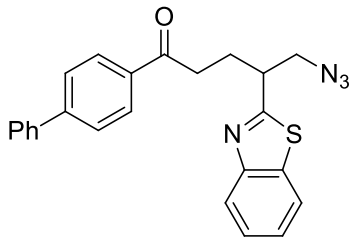
3. Characterization of products



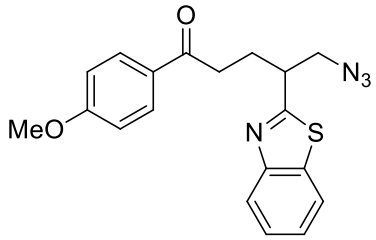
2a: yellow oil. ^{1}H NMR (400 MHz, DMSO) δ 8.08 (d, *J* = 8.0 Hz, 1H), 7.98 (d, *J* = 8.0 Hz, 1H), 7.94-7.88 (m, 2H), 7.63-7.57 (m, 1H), 7.53-7.45 (m, 3H), 7.45-7.40 (m, 1H), 3.93-3.83 (m, 2H), 3.63-3.55 (m, 1H), 3.22-3.03 (m, 2H) , 2.18 (q, *J* = 7.2 Hz, 2H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 198.3, 171.1, 152.5, 136.1, 134.4, 132.7, 128.1, 127.5, 125.7, 124.8, 122.5, 121.3, 54.9, 43.6, 35.1, 26.7. FT-IR: ν (cm^{-1}) 3062, 2929, 2866, 2098, 1682, 1597, 1512, 1448, 1352, 1242. HRMS [ESI] calcd for $C_{18}H_{16}N_4OS$ Na $[M+Na]^+$ 359.0937, found 359.0940.



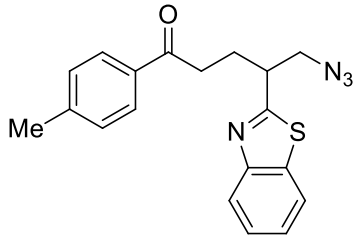
2b: yellow oil. ^{1}H NMR (400 MHz, DMSO) δ 8.61 (s, 1H), 8.12-8.04 (m, 2H), 8.01-7.92 (m, 4H), 7.69-7.57 (m, 2H), 7.53-7.47 (m, 1H), 7.46-7.41 (m, 1H), 3.96-3.85 (m, 2H), 3.68-3.58 (m, 1H), 3.33-3.20 (m, 2H), 2.29-2.19 (m, 2H); ^{13}C NMR (100 MHz, DMSO) δ 199.1, 172.3, 152.5, 135.0, 134.5, 133.7, 132.1, 129.7, 129.5, 128.6, 128.2, 127.6, 126.9, 126.2, 125.1, 123.5, 122.5, 122.2, 54.3, 43.3, 35.3, 26.9. FT-IR: ν (cm^{-1}) 3060, 2926, 2854, 2098, 1678, 1578, 1510, 1437, 1353, 1244. HRMS [ESI] calcd for $C_{22}H_{18}N_4OS$ Na $[M+Na]^+$ 409.1094, found 409.1090.



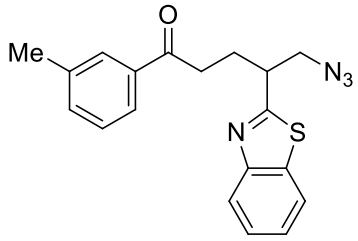
2c: yellow solid, m.p. 70-71 °C. ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.04 (d, *J* = 8.0 Hz, 1H), 8.00-7.92 (m, 2H), 7.89 (d, *J* = 8.0 Hz, 1H), 7.67-7.57 (m, 4H), 7.54-7.36 (m, 5H), 3.90 (dd, *J* = 12.0, 7.2 Hz, 1H), 3.79 (dd, *J* = 12.0, 6.0 Hz, 1H), 3.67-3.58 (m, 1H), 3.09 (t, *J* = 7.2 Hz, 2H), 2.48-2.31 (m, 2H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 198.0, 171.0, 152.5, 145.4, 139.3, 134.8, 134.4, 128.5, 128.1, 127.8, 126.8, 126.8, 125.7, 124.8, 122.6, 121.3, 55.0, 43.7, 35.1, 26.8. FT-IR: ν (cm^{-1}) 3061, 2924, 2855, 2089, 1682, 1604, 1515, 1437, 1372, 1283. HRMS [ESI] calcd for $C_{24}H_{21}N_4OS$ $[M+H]^+$ 413.1431, found 413.1424.



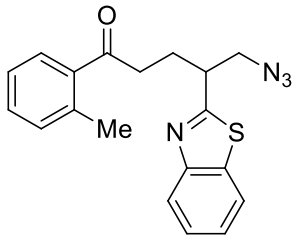
2d: yellow oil. 1H NMR (400 MHz, DMSO) δ 8.09 (d, *J* = 7.6 Hz, 1H), 7.98 (d, *J* = 8.0 Hz, 1H), 7.92-7.86 (m, 2H), 7.53-7.47 (m, 1H), 7.45-7.40 (m, 1H), 7.02-6.96 (m, 2H), 3.92-3.84 (m, 2H), 3.81 (s, 3H), 3.62-3.53 (m, 1H), 3.14-2.96 (m, 2H), 2.15 (q, *J* = 7.2 Hz, 2H); ^{13}C NMR (100 MHz, DMSO) δ 197.4, 172.3, 163.1, 152.5, 134.5, 130.1, 129.4, 126.2, 125.1, 122.5, 122.2, 113.8, 55.5, 54.3, 43.3, 34.8, 27.0. FT-IR: ν (cm^{-1}) 3062, 2929, 2841, 2098, 1673, 1598, 1510, 1438, 1356, 1256. HRMS [ESI] calcd for $C_{19}H_{18}N_4O_2SNa$ $[M+Na]^+$ 389.1043, found 389.1053.



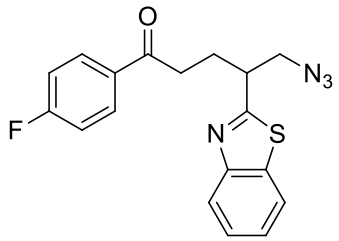
2e: yellow oil. ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.02 (d, *J* = 8.0 Hz, 1H), 7.88 (d, *J* = 8.0 Hz, 1H), 7.79 (d, *J* = 8.4 Hz, 2H), 7.52-7.46 (m, 1H), 7.42-7.37 (m, 1H), 7.21 (d, *J* = 8.4 Hz, 2H), 3.87 (dd, *J* = 12.4, 7.2 Hz, 1H), 3.76 (dd, *J* = 12.4, 5.6 Hz, 1H), 3.61-3.53 (m, 1H), 3.02 (t, *J* = 7.2 Hz, 2H), 2.42-2.28 (m, 2H), 2.38 (s, 3H); ^{13}C NMR (100 MHz, DMSO) δ 198.6, 172.3, 152.5, 143.5, 134.5, 134.0, 129.2, 127.9, 126.1, 125.1, 122.5, 122.2, 54.3, 43.3, 35.1, 26.8, 21.1. FT-IR: ν (cm^{-1}) 3061, 2925, 2858, 2099, 1679, 1606, 1512, 1408, 1351, 1241. HRMS [ESI] calcd for $C_{19}H_{18}N_4OSNa$ $[M+Na]^+$ 373.1094, found 373.1101.



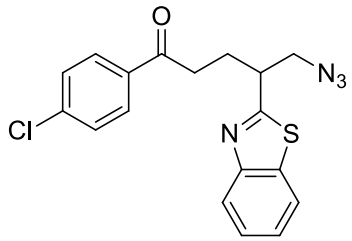
2f: yellow oil. ^{1}H NMR (400 MHz, DMSO) δ 8.11-8.07 (m, 1H), 7.99-7.96 (m, 1H), 7.73-7.68 (m, 2H), 7.50 (ddd, *J* = 8.0, 7.2, 1.2 Hz, 1H), 7.45-7.39 (m, 2H), 7.39-7.33 (m, 1H), 3.93-3.83 (m, 2H), 3.63-3.54 (m, 1H), 3.21-3.01 (m, 2H), 2.33 (s, 3H), 2.17 (dd, *J* = 14.4, 7.2 Hz, 2H); ^{13}C NMR (100 MHz, DMSO) δ 199.2, 172.3, 152.5, 138.0, 136.5, 134.5, 133.7, 128.5, 128.2, 126.2, 125.1, 125.0, 122.5, 122.2, 54.3, 43.2, 35.3, 26.8, 20.8. FT-IR: ν (cm^{-1}) 3062, 2925, 2864, 2098, 1734, 1681, 1512, 1437, 1311, 1243. HRMS [ESI] calcd for $C_{19}H_{18}N_4OSNa$ $[M+Na]^+$ 373.1094, found 373.1102.



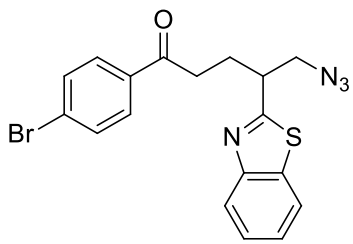
2g: yellow oil. ^{1}H NMR (400 MHz, DMSO) δ 8.11-8.07 (m, 1H), 7.99-7.95 (m, 1H), 7.70-7.66 (m, 1H), 7.50 (ddd, *J* = 8.4, 7.2, 1.2 Hz, 1H), 7.45-7.36 (m, 2H), 7.28-7.23 (m, 2H), 3.91-3.82 (m, 2H), 3.61-3.52 (m, 1H), 3.10-2.94 (m, 2H), 2.35 (s, 3H), 2.20-2.09 (m, 2H); ^{13}C NMR (100 MHz, DMSO) δ 203.2, 172.2, 152.5, 137.7, 136.8, 134.5, 131.5, 131.2, 128.4, 126.2, 125.8, 125.1, 122.5, 122.2, 54.2, 43.2, 38.2, 26.8, 20.6. FT-IR: ν (cm^{-1}) 3062, 2927, 2098, 1682, 1570, 1513, 1437, 1455, 1311, 1283. HRMS [ESI] calcd for $C_{19}H_{18}N_4OSNa$ $[M+Na]^+$ 373.1094, found 373.1102.



2h: yellow oil. ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.00 (d, *J* = 8.0 Hz, 1H), 7.94-7.85 (m, 3H), 7.52-7.46 (m, 1H), 7.42-7.36 (m, 1H), 7.12-7.05 (m, 2H), 3.86 (dd, *J* = 12.0, 7.2 Hz, 1H), 3.76 (dd, *J* = 12.0, 6.0 Hz, 1H), 3.58-3.50 (m, 1H), 3.02 (t, *J* = 7.2 Hz, 2H), 2.44-2.25 (m, 2H); ^{13}C NMR (100 MHz, DMSO) δ 197.7, 172.3, 165.0 (d, $J_{C\text{-}F}$ = 250.0 Hz), 152.5, 134.5, 133.2 (d, $J_{C\text{-}F}$ = 2.8 Hz), 130.8 (d, $J_{C\text{-}F}$ = 9.4 Hz), 126.2, 125.1, 122.5, 122.2, 115.6 (d, $J_{C\text{-}F}$ = 21.7 Hz), 54.2, 43.2, 35.2, 26.7; ^{19}F NMR (376 MHz, $CDCl_3$) δ -105.0 (s). FT-IR: ν (cm^{-1}) 3065, 2927, 2856, 2098, 1683, 1596, 1506, 1437, 1351, 1226. HRMS [ESI] calcd for $C_{18}H_{15}FN_4OSNa$ $[M+Na]^+$ 377.0843, found 377.0852.

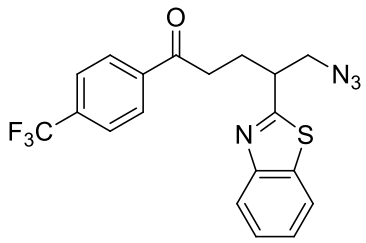


2i: yellow oil. ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.01 (d, *J* = 8.0 Hz, 1H), 7.88 (d, *J* = 7.6 Hz, 1H), 7.84-7.79 (m, 2H), 7.52-7.47 (m, 1H), 7.43-7.36 (m, 3H), 3.87 (dd, *J* = 12.4, 7.2 Hz, 1H), 3.76 (dd, *J* = 12.4, 6.0 Hz, 1H), 3.61-3.51 (m, 1H), 3.02 (t, *J* = 7.2 Hz, 2H), 2.43-2.26 (m, 2H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 197.1, 171.0, 152.2, 139.2, 134.4, 134.2, 129.0, 128.4, 125.8, 124.9, 122.5, 121.3, 55.0, 43.5, 35.0, 26.7. FT-IR: ν (cm^{-1}) 3063, 2927, 2099, 1683, 1571, 1511, 1488, 1437, 1350, 1278. HRMS [ESI] calcd for $C_{18}H_{15}ClN_4OSNa$ $[M+Na]^+$ 393.0547, found 393.0557.

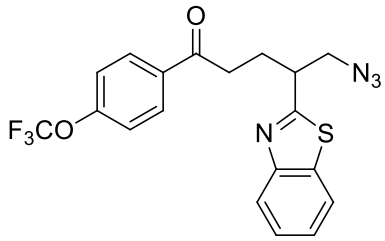


2j: yellow oil. ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.00 (d, *J* = 8.0 Hz, 1H), 7.88 (d, *J* = 8.0 Hz, 1H), 7.74 (d, *J* = 8.4 Hz, 2H), 7.55 (d, *J* = 8.8 Hz, 2H), 7.52-7.46 (m, 1H), 7.43-7.37 (m, 1H), 3.86 (dd, *J* = 12.0, 7.2 Hz, 1H), 3.75 (dd, *J* = 12.0, 6.0 Hz, 1H), 3.60-3.51 (m, 1H), 3.01 (t, *J* = 7.2 Hz, 2H), 2.43-2.25 (m, 2H); ^{13}C NMR

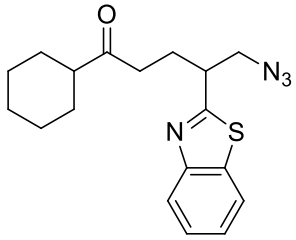
(100 MHz, $CDCl_3$) δ 197.3, 170.9, 152.3, 134.8, 134.2, 131.4, 129.1, 127.9, 125.8, 124.9, 122.5, 121.3, 55.0, 43.5, 35.0, 26.6. FT-IR: ν (cm^{-1}) 3060, 2927, 2362, 2098, 1683, 1584, 1437, 1397, 1269. HRMS [ESI] calcd for $C_{18}H_{15}BrN_4OSNa$ $[M+Na]^+$ 437.0042, found 437.0034.



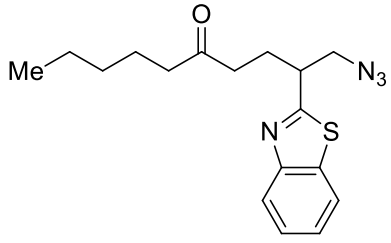
2k: yellow oil. ^1H NMR (400 MHz, $CDCl_3$) δ 8.02-7.96 (m, 3H), 7.88 (d, *J* = 8.0 Hz, 1H), 7.68 (d, *J* = 8.0 Hz, 2H), 7.52-7.46 (m, 1H), 7.43-7.37 (m, 1H), 3.87 (dd, *J* = 12.4, 7.2 Hz, 1H), 3.76 (dd, *J* = 12.4, 6.0 Hz, 1H), 3.60-3.51 (m, 1H), 3.07 (t, *J* = 7.2 Hz, 2H), 2.47-2.28 (m, 2H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 197.9, 171.1, 152.9, 139.2, 134.7, 134.5 (q, J_{C-F} = 32.4 Hz), 128.3, 126.3, 125.7 (q, J_{C-F} = 3.7 Hz), 125.3, 123.5 (q, J_{C-F} = 271 Hz), 123.0, 121.7, 55.5, 44.0, 35.9, 27.0; ^{19}F NMR (376 MHz, $CDCl_3$) δ -63.1 (s). FT-IR: ν (cm^{-1}) 3064, 2919, 2100, 1690, 1582, 1511, 1455, 1410, 1322, 1262. HRMS [ESI] calcd for $C_{19}H_{15}F_3N_4OSNa$ $[M+Na]^+$ 427.0811, found 427.0810.



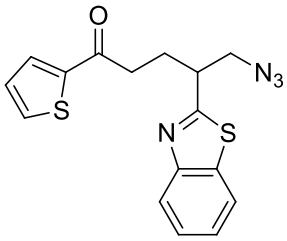
2l: yellow oil. ^1H NMR (400 MHz, DMSO) δ 8.11-8.07 (m, 1H), 8.07-8.02 (m, 2H), 7.99-7.94 (m, 1H), 7.52-7.41 (m, 4H), 3.93-3.82 (m, 2H), 3.62-3.54 (m, 1H), 3.23-3.06 (m, 2H), 2.18 (dd, *J* = 14.4, 7.2 Hz, 2H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 196.8, 170.9, 152.3, 152.2 (q, J_{C-F} = 1.5 Hz), 134.3, 134.2, 129.6, 125.8, 124.9, 122.5, 121.3, 119. 9, 119.8 (q, J_{C-F} = 257.3 Hz), 55.0, 43.5, 35.1, 26.6; ^{19}F NMR (376 MHz, $CDCl_3$) δ -51.9 (s). FT-IR: ν (cm^{-1}) 3068, 2926, 2854, 2100, 1687, 1602, 1507, 1438, 1352, 1254. HRMS [ESI] calcd for $C_{19}H_{15}F_3N_4O_2SNa$ $[M+Na]^+$443.0760, found 443.0764.



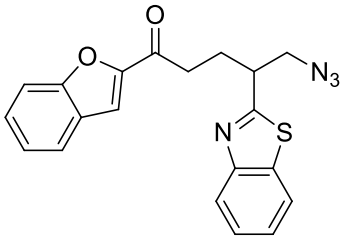
2m: yellow oil. ^1H NMR (400 MHz, DMSO) δ 8.09 (d, *J* = 7.6 Hz, 1H), 7.98 (d, *J* = 8.0 Hz, 1H), 7.51 (ddd, *J* = 8.0, 7.2, 1.2 Hz, 1H), 7.46-7.40 (m, 1H), 3.80 (d, *J* = 6.4 Hz, 2H), 3.49-3.40 (m, 1H), 2.62-2.44 (m, 2H), 2.35-2.24 (m, 1H), 2.05-1.91 (m, 2H), 1.74-1.60 (m, 4H), 1.59-1.52 (m, 1H), 1.24-1.05 (m, 5H); ^{13}C NMR (100 MHz, DMSO) δ 212.4, 172.2, 152.5, 134.4, 126.2, 125.1, 122.5, 122.2, 54.3, 49.5, 43.2, 36.9, 28.0, 27.8, 26.3, 25.4, 25.1, 25.0. FT-IR: ν (cm^{-1}) 3065, 2928, 2854, 2099, 1705, 1513, 1449, 1409, 1350, 1279. HRMS [ESI] calcd for $C_{18}H_{22}N_4OSNa$ $[M+Na]^+$ 365.1407, found 365.1409.



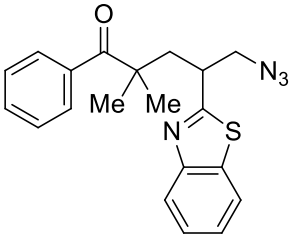
2n: yellow oil. ^1H NMR (400 MHz, DMSO) δ 8.09 (d, *J* = 8.0 Hz, 1H), 7.98 (d, *J* = 7.6 Hz, 1H), 7.51 (ddd, *J* = 8.4, 7.6, 1.2 Hz, 1H), 7.46-7.41 (m, 1H), 3.80 (d, *J* = 6.4 Hz, 2H), 3.50-3.41 (m, 1H), 2.50-2.39 (m, 2H), 2.34 (t, *J* = 7.2 Hz, 2H), 2.03-1.92 (m, 2H), 1.43-1.35 (m, 2H), 1.25-1.10 (m, 4H), 0.81 (t, *J* = 7.2 Hz, 3H); ^{13}C NMR (100 MHz, DMSO) δ 209.7, 172.2, 152.5, 134.4, 126.2, 125.1, 122.5, 122.2, 54.3, 43.2, 41.8, 38.8, 30.7, 26.3, 22.8, 21.9, 13.8. FT-IR: ν (cm^{-1}) 3064, 2928, 2859, 2362, 2099, 1711, 1512, 1438, 1277. HRMS [ESI] calcd for $C_{17}H_{22}N_4OSNa$ $[M+Na]^+$ 353.1407, found 353.1416.



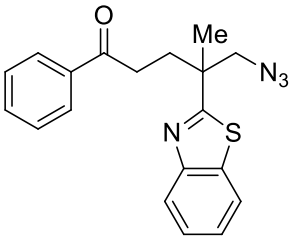
2o: yellow oil. ^{1}H NMR (400 MHz, DMSO) δ 8.09 (d, *J* = 7.6 Hz, 1H), 8.00-7.94 (m, 2H), 7.88 (dd, *J* = 3.6, 0.8 Hz, 1H), 7.53-7.47 (m, 1H), 7.45-7.39 (m, 1H), 7.20 (dd, *J* = 4.8, 4.0 Hz, 1H), 3.91-3.82 (m, 2H), 3.62-3.53 (m, 1H), 3.15-2.97 (m, 2H), 2.17 (dd, *J* = 14.4, 7.2 Hz, 2H); ^{13}C NMR (100 MHz, DMSO) δ 192.2, 172.1, 152.5, 143.4, 134.7, 134.5, 133.2, 128.7, 126.2, 125.1, 122.5, 122.2, 54.2, 43.2, 35.6, 26.9. FT-IR: ν (cm^{-1}) 3067, 2925, 2854, 2098, 1658, 1516, 1414, 1353, 1238. HRMS [ESI] calcd for $C_{16}H_{14}N_4OS_2Na$ $[M+Na]^+$ 365.0501, found 365.0507.



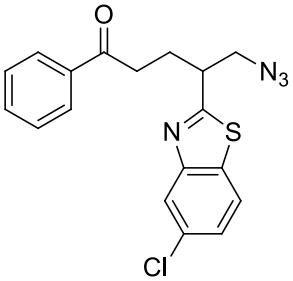
2p: yellow solid, m.p. 80-81 °C. ^{1}H NMR (400 MHz, DMSO) δ 8.22-8.15 (m, 2H), 7.64-7.58 (m, 2H), 7.58-7.54 (m, 1H), 7.50 (d, *J* = 8.0 Hz, 1H), 7.26-7.17 (m, 2H), 6.82 (s, 1H), 3.74 (d, *J* = 6.8 Hz, 2H), 3.35-3.25 (m, 3H), 3.22-3.07 (m, 2H); ^{13}C NMR (100 MHz, DMSO) δ 194.2, 166.1, 157.9, 154.1, 152.9, 136.3, 128.1, 127.9, 127.3, 125.0, 123.8, 123.1, 122.7, 120.7, 110.9, 104.2, 53.3, 38.3, 35.6, 24.4. FT-IR: ν (cm^{-1}) 3068, 2938, 2875, 2099, 1687, 1582, 1454, 1402, 1316, 1253. HRMS [ESI] calcd for $C_{20}H_{16}N_4O_2SNa$ $[M+Na]^+$ 399.0886, found 399.0868.



2q: yellow oil. ^{1}H NMR (400 MHz, DMSO) δ 8.06-8.02 (m, 1H), 7.91-7.87 (m, 1H), 7.63-7.58 (m, 2H), 7.50-7.44 (m, 2H), 7.43-7.35 (m, 3H), 3.72-3.62 (m, 2H), 3.53-3.45 (m, 1H), 2.54 (dd, *J* = 14.4, 8.8 Hz, 1H), 2.20 (dd, *J* = 14.4, 3.2 Hz, 1H), 1.25 (s, 3H), 1.20 (s, 3H); ^{13}C NMR (100 MHz, DMSO) δ 207.3, 172.9, 152.2, 138.0, 134.7, 131.0, 128.0, 127.6, 126.1, 125.1, 122.4, 122.1, 56.0, 47.0, 42.1, 41.0, 26.0, 26.0. FT-IR: ν (cm^{-1}) 3062, 2927, 2855, 2099, 1671, 1578, 1511, 1437, 1390, 1265. HMS [ESI] calcd for $C_{20}H_{20}N_4OSNa$ $[M+Na]^+$ 387.1250, found 387.1257.

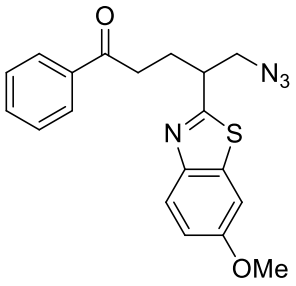


2r: yellow oil. ^{1}H NMR (400 MHz, DMSO) δ 8.09 (d, *J* = 7.6 Hz, 1H), 7.98 (d, *J* = 7.6 Hz, 1H), 7.93-7.88 (m, 2H), 7.62-7.57 (m, 1H), 7.52-7.40 (m, 4H), 3.95 (d, *J* = 12.4 Hz, 1H), 3.81 (d, *J* = 12.4 Hz, 1H), 3.14-3.04 (m, 1H), 3.00-2.90 (m, 1H), 2.30-2.11 (m, 1H), 2.18-2.08 (m, 1H), 1.54 (s, 3H); ^{13}C NMR (100 MHz, DMSO) δ 199.1, 176.4, 152.4, 136.4, 134.5, 133.1, 128.6, 127.9, 126.2, 125.1, 122.6, 122.1, 59.7, 45.1, 33.1, 33.1, 22.9. FT-IR: ν (cm^{-1}) 3062, 2926, 2854, 2101, 1683, 1597, 1506, 1448, 1366, 1293. HRMS [ESI] calcd for $C_{19}H_{18}N_4OSNa$ $[M+Na]^+$ 373.1094, found 373.1099.

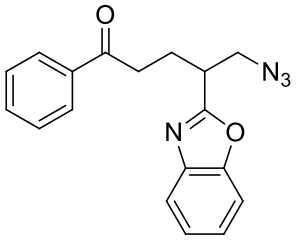


2s: yellow solid, m.p. 78-79 °C. ^{1}H NMR (400 MHz, DMSO) δ 8.15-8.10 (m, 1H), 8.06-8.02 (m, 1H), 7.92-7.88 (m, 2H), 7.63-7.57 (m, 1H), 7.51-7.44 (m, 3H), 3.93-3.82 (m, 2H), 3.64-3.56 (m, 1H), 3.21-3.03 (m, 2H), 2.17 (dd, *J* = 14.4, 7.2 Hz, 2H); ^{13}C NMR (100 MHz, DMSO) δ 199.0, 174.9, 153.4, 136.4, 133.3, 133.1, 131.0, 128.6, 127.8, 125.2, 123.7, 122.0, 54.1, 43.3, 35.2, 26.7. FT-IR: ν

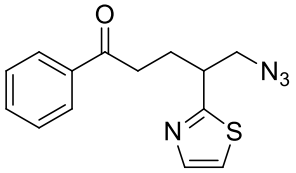
(cm^{-1}) 3050, 2931, 2098, 1682, 1585, 1497, 1435, 1347, 1259. HMS [ESI] calcd for $C_{18}H_{15}ClN_4OSNa$ $[M+Na]^+$ 393.0547, found 393.0543.



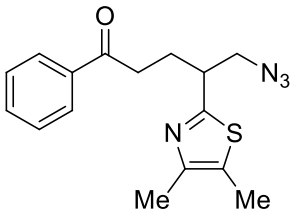
2t: yellow solid, m.p. 64-65 °C. ^{1}H NMR (400 MHz, DMSO) δ 8.03-7.99 (m, 2H), 7.95 (d, *J* = 8.8 Hz, 1H), 7.75 (d, *J* = 2.8 Hz, 1H), 7.74-7.68 (m, 1H), 7.62-7.56 (m, 2H), 7.19 (dd, *J* = 9.2, 2.8 Hz, 1H), 3.96-3.89 (m, 2H), 3.92 (s, 3H), 3.66-3.58 (m, 1H), 3.29-3.13 (m, 2H), 2.24 (dd, *J* = 14.4, 7.2 Hz, 2H); ^{13}C NMR (100 MHz, DMSO) δ 199.1, 169.4, 157.2, 146.9, 136.4, 135.9, 133.2, 128.7, 127.8, 123.0, 115.4, 104.8, 55.7, 54.3, 43.1, 35.3, 26.7. FT-IR: ν (cm^{-1}) 3056, 2955, 2921, 2087, 1686, 1602, 1518, 1469, 1372, 1280. HMS [ESI] calcd for $C_{19}H_{18}N_4O_2SNa$ $[M+Na]^+$ 389.1043, found 389.1051.



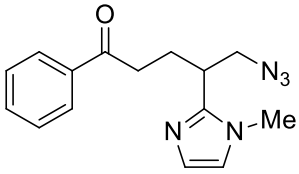
2u: yellow solid, m.p. 72-73 °C. ^{1}H NMR (400 MHz, DMSO) δ 7.94-7.88 (m, 2H), 7.74-7.66 (m, 2H), 7.64-7.58 (m, 1H), 7.53-7.45 (m, 2H), 7.41-7.33 (m, 2H), 3.95-3.83 (m, 2H), 3.49-3.41 (m, 1H), 3.21-3.12 (m, 2H), 3.25-3.01 (m, 2H); ^{13}C NMR (100 MHz, DMSO) δ 199.0, 166.5, 150.2, 140.6, 136.4, 133.1, 128.6, 127.8, 125.0, 124.4, 119.6, 110.7, 52.6, 38.7, 35.2, 24.4. FT-IR: ν (cm^{-1}) 3064, 2924, 2853, 2093, 1680, 1568, 1470, 1416, 1378, 1242. HRMS [ESI] calcd for $C_{18}H_{16}N_4O_2Na$ $[M+Na]^+$ 343.1165, found 343.1155.



2v: yellow oil. ^{1}H NMR (400 MHz, DMSO) δ 7.93-7.88 (m, 2H), 7.78 (d, *J* = 3.6 Hz, 1H), 7.66 (d, *J* = 3.2 Hz, 1H), 7.64-7.54 (m, 1H), 7.52-7.47 (m, 2H), 3.82-3.72 (m, 2H), 3.54-3.44 (m, 1H), 3.15-2.96 (m, 2H), 2.16-2.03 (m, 2H); ^{13}C NMR (100 MHz, DMSO) δ 199.1, 170.6, 142.3, 136.4, 133.1, 128.7, 127.8, 119.9, 54.6, 42.3, 35.2, 27.0. FT-IR: ν (cm^{-1}) 3086, 2927, 2856, 2098, 1682, 1597, 1498, 1448, 1266. HRMS [ESI] calcd for $C_{14}H_{14}N_4OSNa$ $[M+Na]^+$ 309.0781, found 309.0790.

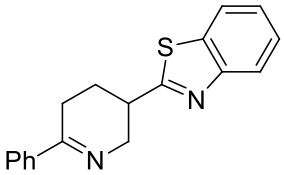


2w: yellow solid, m.p. 54-55 °C. ^{1}H NMR (400 MHz, DMSO) δ 7.93-7.88 (m, 2H), 7.64-7.59 (m, 1H), 7.53-7.47 (m, 2H), 3.74-3.64 (m, 2H), 3.32-3.25 (m, 1H), 3.13-2.96 (m, 2H), 2.29 (s, 3H), 2.20 (s, 3H), 2.09-1.94 (m, 2H); ^{13}C NMR (100 MHz, DMSO) δ 199.2, 165.7, 147.2, 136.4, 133.1, 128.7, 127.8, 125.6, 54.5, 42.2, 35.3, 27.0, 14.4, 10.8. FT-IR: ν (cm^{-1}) 3054, 2950, 2859, 2109, 1684, 1549, 1442, 1381, 1349, 1266. HRMS [ESI] calcd for $C_{16}H_{18}N_4OSNa$ $[M+Na]^+$ 337.1094, found 337.1101.

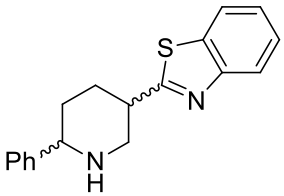


2x: yellow oil. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.89-7.84 (m, 2H), 7.58-7.53 (m, 1H), 7.47-7.41 (m, 2H), 7.07 (s, 1H), 6.82 (s, 1H), 3.88-3.78 (m, 1H), 3.65-3.57 (m, 1H), 3.62 (s, 3H), 3.37-3.31 (m, 1H), 3.12-3.03 (m, 1H), 2.85-2.76 (m, 1H), 2.37-2.28 (m, 1H), 2.27-2.20 (m, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 199.2, 147.1, 136.1, 132.8, 128.1, 127.5, 127.0, 120.4, 55.1, 35.3, 34.4, 32.1, 25.8. FT-IR: ν (cm^{-1}) 3062, 2930,

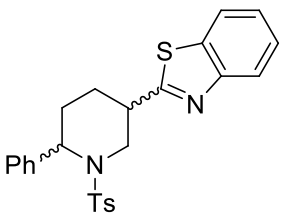
2365, 2098, 1681, 1597, 1490, 1448, 1278, 1222. HRMS [ESI] calcd for $C_{15}H_{17}N_5ONa$ $[M+Na]^+$ 306.1325, found 306.1332.



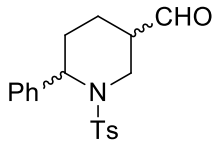
3: yellow solid, m.p. 116-117 °C. ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.01 (d, *J* = 8.0 Hz, 1H), 7.88 (d, *J* = 7.6 Hz, 1H), 7.85-7.79 (m, 2H), 7.51-7.45 (m, 1H), 7.44-7.34 (m, 4H), 4.52-4.43 (m, 1H), 4.12-4.01 (m, 1H), 3.51-3.41 (m, 1H), 3.03-2.92 (m, 1H), 2.86-2.73 (m, 1H), 2.53-2.42 (m, 1H), 2.29-2.17 (m, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 173.1, 165.0, 152.7, 138.8, 134.1, 129.5, 127.9, 125.6, 125.6, 124.4, 122.3, 121.2, 54.5, 37.8, 26.5, 25.6. FT-IR: ν (cm^{-1}) 3057, 2921, 2851, 2555, 1635, 1577, 1503, 1435, 1360, 1294. HRMS [ESI] calcd for $C_{18}H_{17}N_2S$ $[M+H]^+$ 293.1107, found 293.1117.



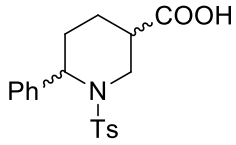
4 (*d.r.* = 1: 0.33): yellow solid, m.p. 120-121 °C. ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.08-8.02 (m, 1.33H, two isomers), 7.94-7.90 (m, 0.33H, one isomer), 7.90-7.85 (m, 1H, one isomer), 7.51-7.41 (m, 3.99H, two isomers), 7.41-7.34 (m, 3.99H, two isomers), 7.33-7.27 (m, 1.33H, two isomers), 3.80-3.70 (m, 1.33H, two isomers), 3.70-3.64 (m, 1H, one isomer), 3.64-3.58 (m, 0.33H, one isomer), 3.57-3.53 (m, 0.33H, one isomer), 3.45-3.34 (m, 1H, one isomer), 3.29 (dd, *J* = 12.0, 3.2 Hz, 0.33H, one isomer), 3.14 (dd, *J* = 11.2, 11.2 Hz, 1H, one isomer), 2.48-2.38 (m, 1H, one isomer), 2.36-2.28 (m, 0.33H, one isomer), 2.21-2.09 (m, 1.33H, two isomers), 2.07-1.82 (m, 2.66H, two isomers), 1.80-1.68 (m, 1.33H, two isomers); ^{13}C NMR (100 MHz, $CDCl_3$) δ (major isomer) 173.5, 152.7, 144.1, 134.0, 128.0, 126.9, 126.2, 125.5, 124.3, 122.3, 121.1, 61.0, 52.5, 41.8, 33.9, 31.8; (minor isomer) 174.0, 152.0, 144.5, 135.3, 128.0, 126.7, 126.3, 125.3, 124.1, 122.1, 120.9, 61.2, 49.7, 38.4, 30.0, 29.8. FT-IR: ν (cm^{-1}) 3059, 2920, 2852, 1953, 1638, 1514, 1491, 1438, 1312, 1237. HMS [ESI] calcd for $C_{18}H_{19}N_2S$ $[M+H]^+$ 295.1263, found 295.1271.



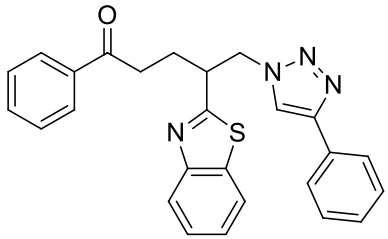
5 (*d.r.* = 1: 0.33): yellow solid. m.p. 116-117 °C. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.94-7.86 (m, 1.33H, two isomers), 7.85-7.77 (m, 2H, one isomer), 7.50-7.41 (m, 3.33H, two isomers), 7.41-7.26 (m, 8.67H, two isomers), 6.76-6.70 (m, 2H, one isomer), 5.43 (d, *J* = 3.6 Hz, 0.33H, one isomer), 5.05 (t, *J* = 4.4 Hz, 1H, one isomer), 4.36 (dd, *J* = 14.4, 3.6 Hz, 0.33H, one isomer), 4.14 (dd, *J* = 14.0, 4.0 Hz, 1H, one isomer), 3.90 (dd, *J* = 14.0, 4.0 H, 1H, one isomer), 3.37-3.31 (m, 1H, one isomer), 3.31-3.25 (m, 0.33H, one isomer), 3.16-3.06 (m, 0.33H, one isomer), 2.48-2.41 (m, 0.33H, one isomer), 2.44 (s, 1H, one isomer), 2.40-2.32 (m, 1 H, one isomer), 2.31-2.23 (m, 1H, one isomer), 2.18-2.10 (m, 1H, one isomer), 2.14 (s, 3H, one isomer), 2.08-1.97 (m, 1.33H, two isomers), 1.93-1.78 (m, 0.66H, one isomer); ^{13}C NMR (100 MHz, $CDCl_3$) δ (major isomer) 172.7, 152.9, 142.6, 138.9, 137.1, 135.2, 129.0, 128.6, 127.3, 127.2, 126.8, 125.9, 124.9, 122.9, 121.5, 57.3, 47.2, 38.6, 27.0, 23.7, 21.4; (minor isomer) 171.7, 152.9, 143.5, 138.2, 137.9, 134.3, 130.0, 128.9, 127.1, 127.1, 126.8, 126.1, 125.0, 122.8, 121.6, 54.5, 45.6, 40.2, 26.8, 26.5, 21.6. FT-IR: ν (cm^{-1}) 3057, 2924, 2857, 1737, 1598, 1494, 1446, 1438, 1339, 1242. HRMS [ESI] calcd for $C_{25}H_{25}N_2O_2S_2$ $[M+H]^+$ 449.1352, found 449.1349.



6 (*d.r.* = 1: 0.7): yellow oil. ^{1}H NMR (400 MHz, $CDCl_3$) δ 9.48 (s, 1H, one isomer), 9.45 (s, 0.7H, one isomer), 7.77-7.73 (m, 2H, one isomer), 7.67 -7.63 (m, 1.4H, one isomer), 7.34-7.21 (m, 11.9H, two isomers), 5.35 (d, *J* = 4.4 Hz, 1H, one isomer), 5.19 (t, *J* = 4.0 Hz, 0.7H, one isomer), 4.17 (d, *J* = 14.4 Hz, 0.7H, one isomer), 4.08 (dd, *J* = 14.4, 4.0 Hz, 1H, one isomer), 3.48 (dd, *J* = 14.4, 4.8 Hz, 0.7H, one isomer), 2.98 (dd, *J* = 14.4, 11.6 Hz, 1H, one isomer), 2.43 (s, 3H, one isomer), 2.42 (s, 2.1H, one isomer), 2.40-2.33 (m, 2H, one isomer), 2.27-2.22 (m, 0.7H, one isomer), 2.20-2.13 (m, 0.7H, one isomer), 2.04-1.98 (m, 0.7H, one isomer), 1.94-1.86 (m, 1.4H, one isomer), 1.84-1.76 (m, 1H, one isomer), 1.69-1.55 (m, 1H, one isomer), 1.48-1.36 (m, 1H, one isomer); ^{13}C NMR (100 MHz, $CDCl_3$) δ (major isomer) 201.5, 143.5, 138.0, 137.7, 129.9, 128.8, 127.2, 127.0, 126.7, 54.6, 47.1, 40.7, 26.4, 21.6, 19.8; (minor isomer) 202.3, 143.5, 138.2, 137.4, 129.6, 128.7, 127.2, 127.1, 126.9, 55.8, 45.7, 40.3, 25.8, 19.8, 17.7. FT-IR: ν (cm^{-1}) 3029, 2927, 2867, 2728, 1721, 1598, 1495, 1336, 1305, 1288. HMS [ESI] calcd for $C_{19}H_{21}NO_3SNa$ $[M+Na]^+$ 366.1134, found 366.1125.

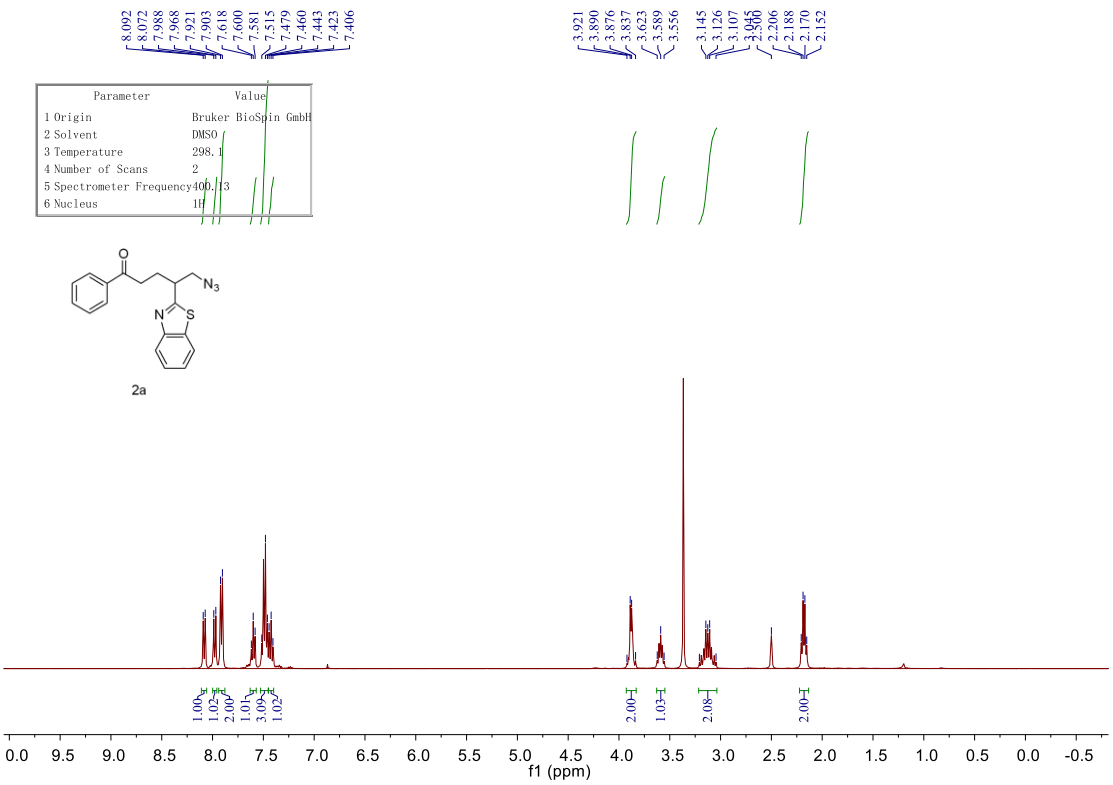


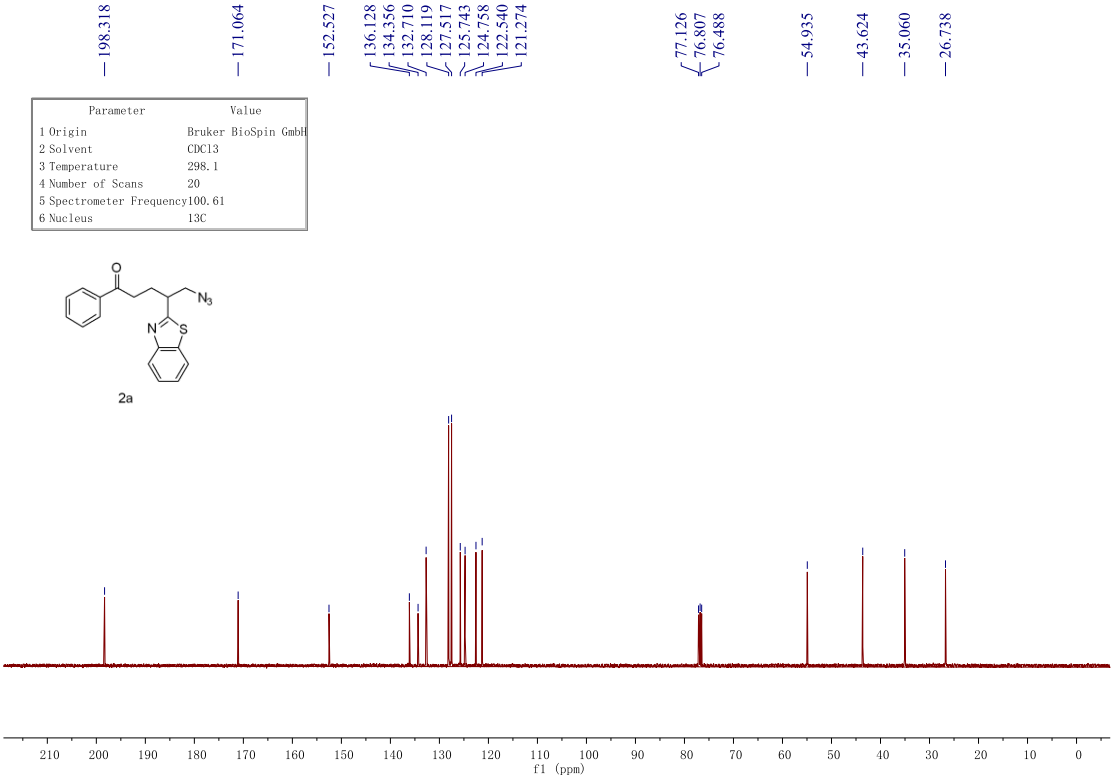
7 (*d. r.* = 1: 0.7): yellow oil. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.79-7.74 (m, 2H, one isomer), 7.65-7.60 (m, 1.4H, one isomer), 7.36-7.21 (m, 10.5H, two isomers), 7.21-7.15 (m, 1.4H, one isomer), 5.33 (d, *J* = 4.4 Hz, 1H, one isomer), 5.09 (t, *J* = 4.4 Hz, 0.7H, one isomer), 4.08 (dd, *J* = 14.4, 4.0 Hz, 1H, one isomer), 4.00 (dd, *J* = 14.0, 3.2 Hz, 0.7H, one isomer), 3.51 (dd, *J* = 14.0, 4.8 Hz, 0.7H, one isomer), 3.02 (dd, *J* = 14.8, 12.0 Hz, 1H, one isomer), 2.56-2.48 (m, 0.7H, one isomer), 2.44 (s, 3H, one isomer), 2.42-2.35 (m, 1.4H, one isomer), 2.33 (s, 2.1H, one isomer), 2.18-2.10 (m, 0.7H, one isomer), 2.08-2.00 (m, 0.7H, one isomer), 1.97-1.81 (m, 2 H, one isomer), 1.80-1.63 (m, 2H, one isomer),1.61-1.49 (m, 1H, one isomer); ^{13}C NMR (100 MHz, $CDCl_3$) δ (major isomer) 178.5, 143.5, 138.1, 137.6, 130.0, 128.8, 127.2, 127.0, 126.7, 54.3, 42.1, 39.8, 26.2, 22.2, 21.6; (minor isomer) 178.8, 143.1, 138.6, 137.4, 129.3, 128.6, 127.4, 127.1, 127.0, 56.5, 42.7, 38.7, 26.8, 21.5, 20.3. FT-IR: ν (cm^{-1}) 3368, 2957, 2922, 2853, 1735, 1572, 1489, 1464, 1399, 1289. HRMS [ESI] calcd for $C_{19}H_{22}NO_4S$ $[M+H]^+$ 360.1264, found 360.1261.

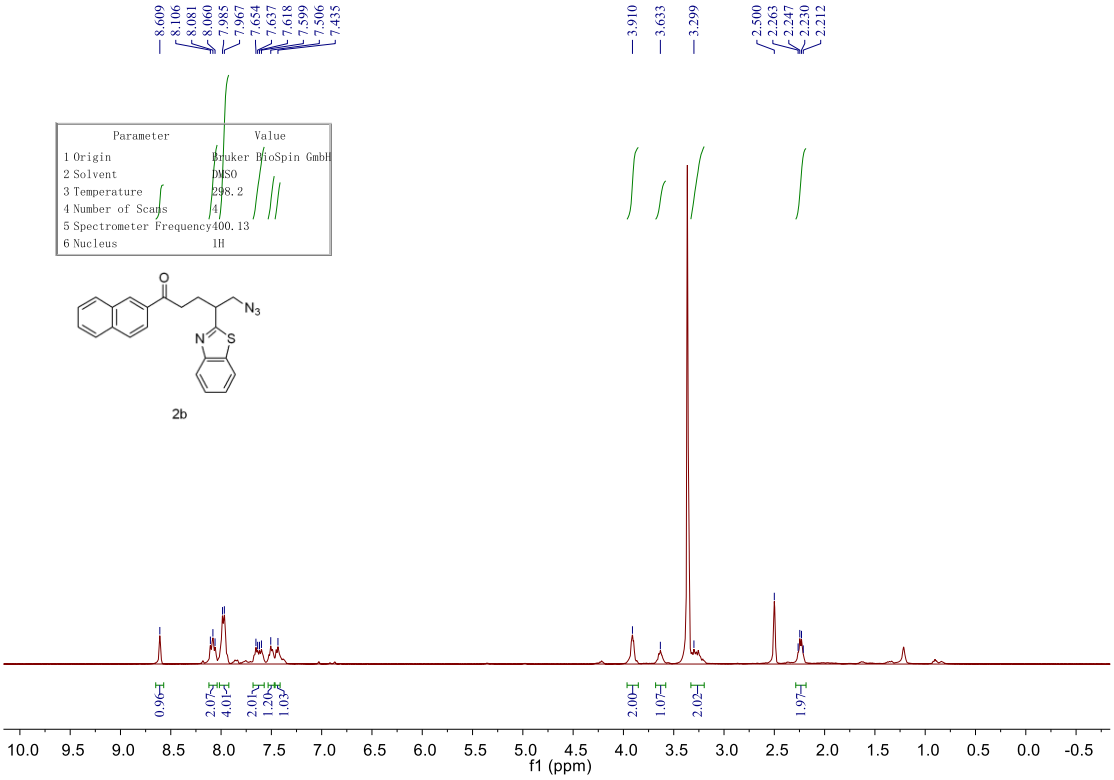


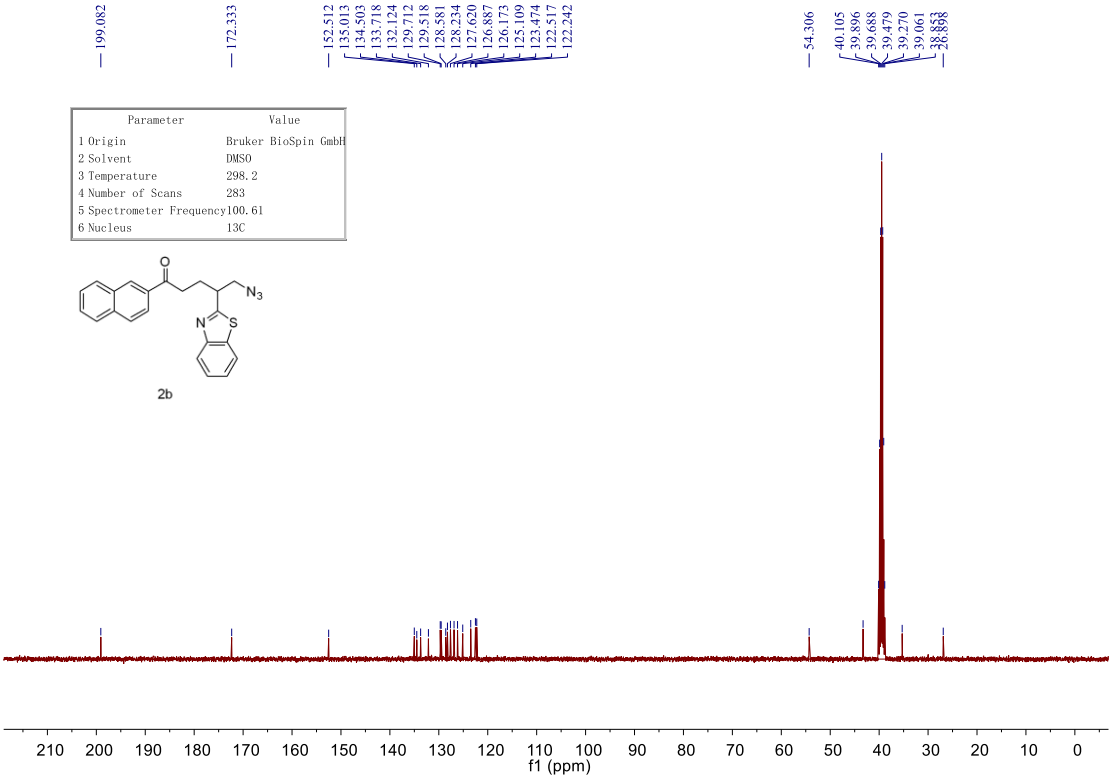
8: white solid, m.p. 172-173 °C. ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.01 (d, *J* = 8.0 Hz, 1H), 7.89-7.84 (m, 2H), 7.82 (d, *J* = 8.0 Hz, 1H), 7.73-7.69 (m, 2H), 7.68 (s, 1H), 7.54-7.46 (m, 2H), 7.42-7.33 (m, 5H), 7.31-7.26 (m, 1H), 5.01-4.87 (m, 2H), 4.08-3.98 (m, 1H), 3.15-3.02 (m, 2H), 2.48-2.28 (m, 2H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 198.2, 169.9, 152.6, 147.2, 136.0, 134.2, 132.8, 130.0, 128.3, 128.1, 127.6, 127.5, 125.9, 125.3, 124.9, 122.5, 121.4, 120.1, 53.4, 44.0, 34.8, 26.8. FT-IR: ν (cm^{-1}) 3064, 2923, 2852, 2361, 2341, 1681, 1408, 1318, 1223. HMS [ESI] calcd for $C_{26}H_{22}N_4OSNa$ $[M+Na]^+$ 461.1407, found 461.1392.

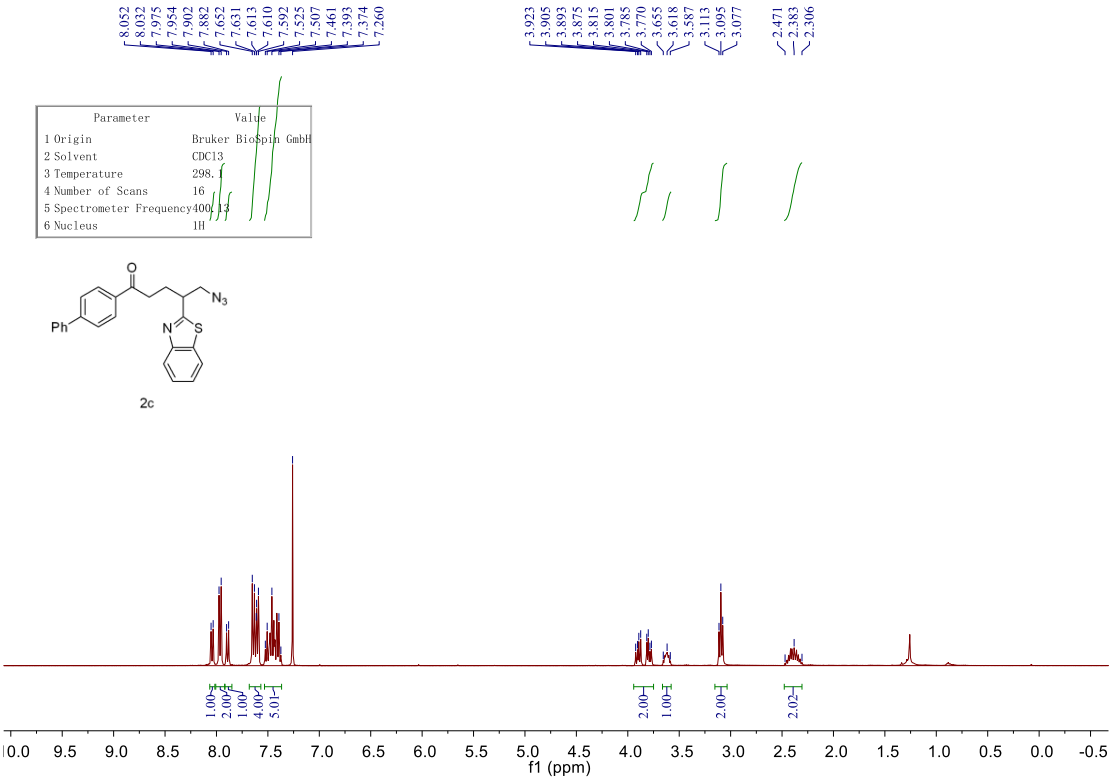
4. ^{1}H, ^{13}C, and ^{19}F NMR spectra






8.609
8.106
8.081
8.060
7.985
7.967
7.654
7.637
7.618
7.599
7.506
7.435
3.910
3.633
3.299
2.500
2.263
2.247
2.230
2.212
Parameter Value
1 Origin Bruker BioSpin GmbH
2 Solvent DMSO
3 Temperature 298.2
4 Number of Scans 4
5 Spectrometer Frequency 400.13
6 Nucleus 1H
O
N3
N
S
2b
0.96
2.07
4.01
2.01
1.26
1.03
2.00
1.07
2.02
1.97
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 -0.5
f1 (ppm)


199.082
172.333
152.512
135.013
134.503
133.718
132.124
129.712
129.518
128.581
128.234
127.620
126.887
126.173
125.109
123.474
122.517
122.242
54.306
40.105
39.896
39.688
39.479
39.270
39.061
38.853
26.898
Parameter Value
1 Origin Bruker BioSpin GmbH
2 Solvent DMSO
3 Temperature 298.2
4 Number of Scans 283
5 Spectrometer Frequency 100.61
6 Nucleus 13C
O
N3
N
S
2b
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)


8.052
8.032
7.975
7.954
7.902
7.882
7.652
7.631
7.613
7.610
7.592
7.525
7.507
7.461
7.393
7.374
7.260
3.923
3.905
3.893
3.875
3.815
3.801
3.785
3.770
3.655
3.618
3.587
3.113
3.095
3.077
2.471
2.383
2.306
Parameter Value
1 Origin Bruker BioSpin GmbH
2 Solvent CDCl3
3 Temperature 298.1
4 Number of Scans 16
5 Spectrometer Frequency 400.13
6 Nucleus 1H
O
N3
Ph
N
S
2c
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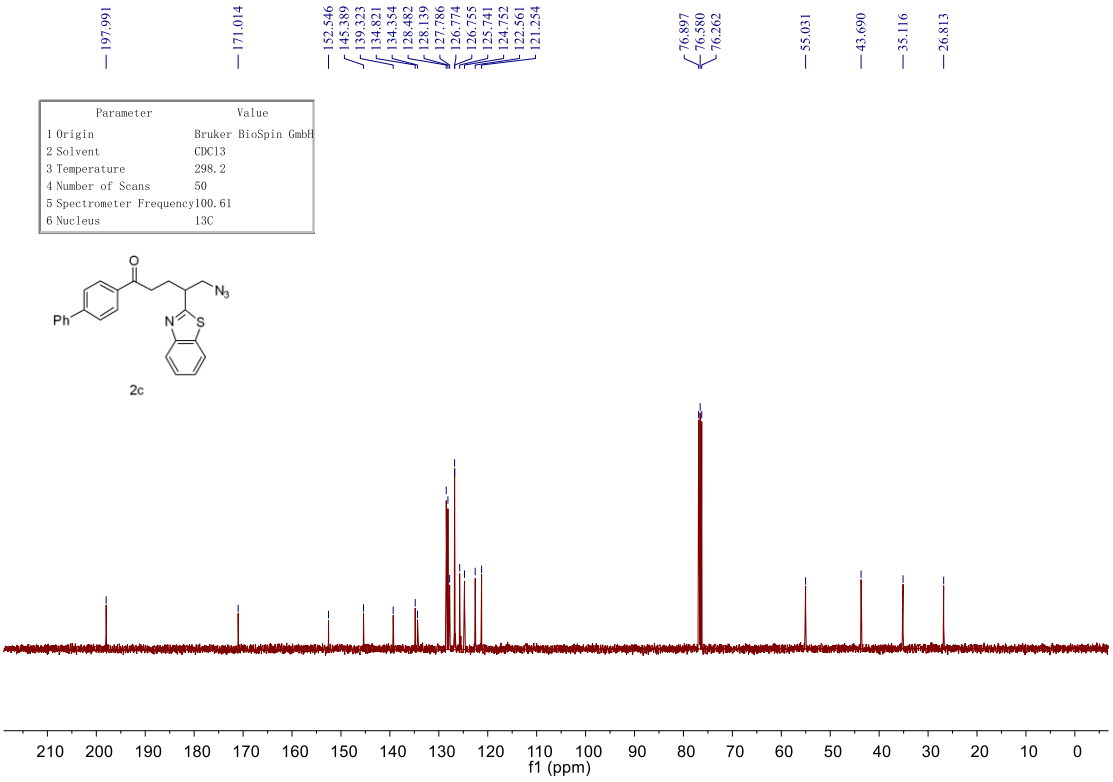
2.00
1.00
4.00
5.01
2.00
1.00
2.00
2.02
f1 (ppm)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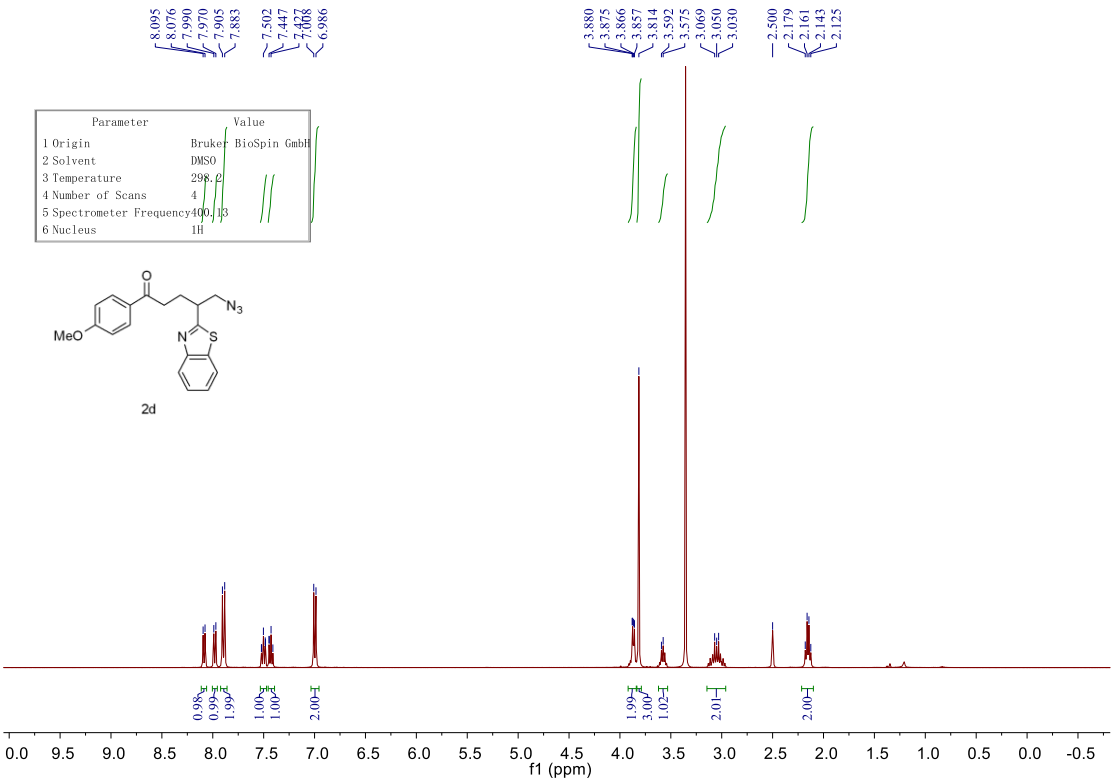
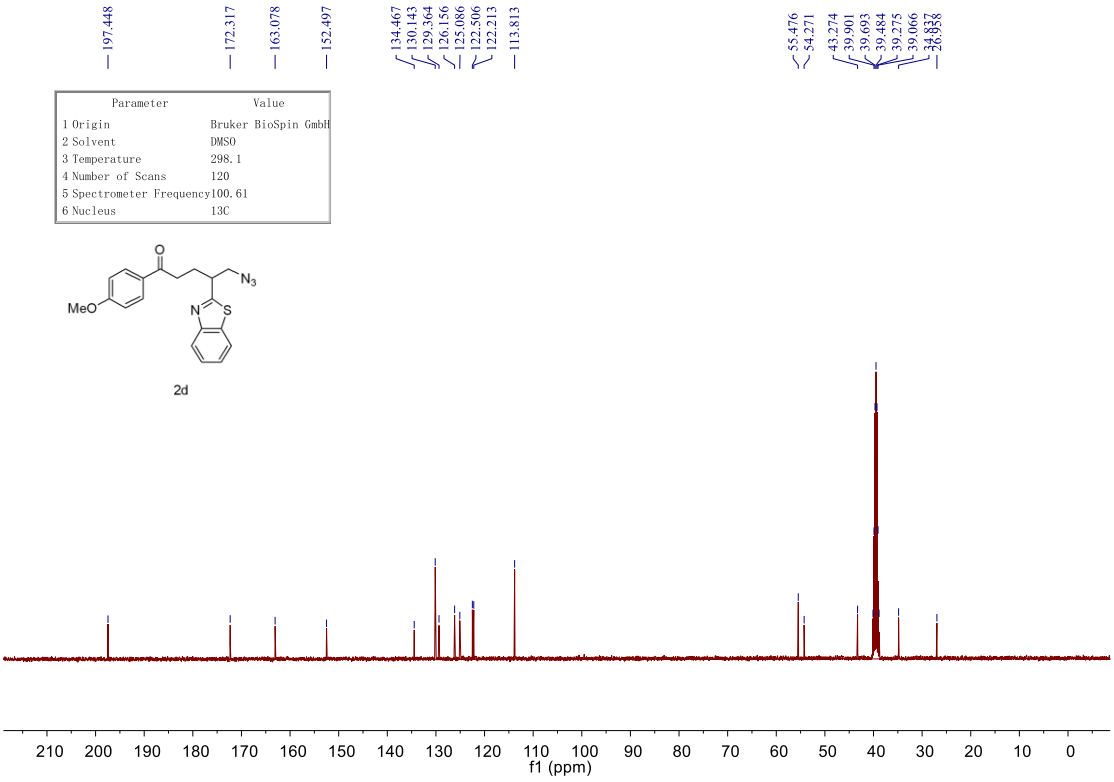
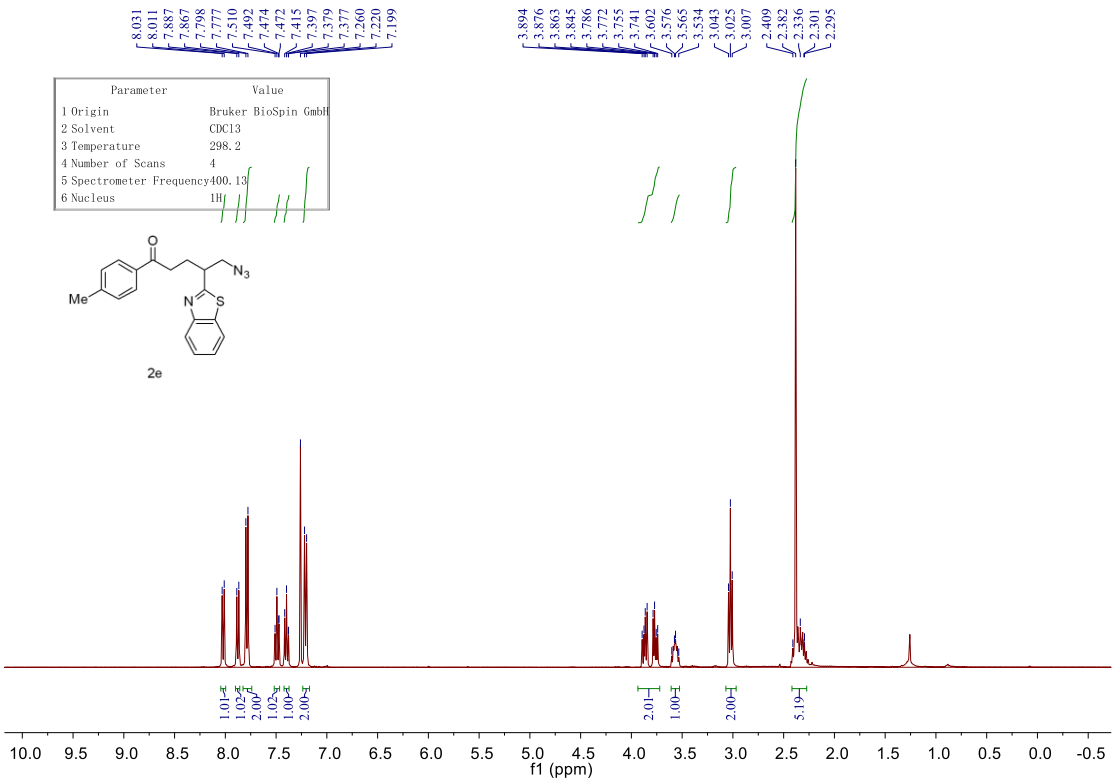
171.014
152.546
145.389
139.323
134.821
134.354
128.482
128.139
127.786
126.774
126.755
125.741
124.752
122.561
121.254
76.897
76.580
76.262
55.031
43.690
35.116
26.813
Parameter Value
1 Origin Bruker BioSpin GmbH
2 Solvent CDCl3
3 Temperature 298.2
4 Number of Scans 50
5 Spectrometer Frequency 100.61
6 Nucleus 13C
O
N3
Ph
N
S
2c
f1 (ppm)


8.095
8.076
7.990
7.970
7.905
7.883
7.502
7.447
6.986
3.880
3.875
3.866
3.857
3.814
3.592
3.575
3.069
3.050
3.030
2.500
2.179
2.161
2.143
2.125
Parameter Value
1 Origin Bruker BioSpin GmbH
2 Solvent DMSO
3 Temperature 298.2
4 Number of Scans 4
5 Spectrometer Frequency 400.13
6 Nucleus 1H
MeO
N3
N
S
O
2d
0.98
0.99
1.99
1.00
1.00
2.00
1.99
3.00
1.02
2.01
2.00
f1 (ppm)


197.448
172.317
163.078
152.497
134.467
130.143
129.364
126.156
125.086
122.506
122.213
113.813
55.476
54.271
43.274
39.901
39.693
39.484
39.275
39.066
Parameter Value
1 Origin Bruker BioSpin GmbH
2 Solvent DMSO
3 Temperature 298.1
4 Number of Scans 120
5 Spectrometer Frequency 100.61
6 Nucleus 13C
MeO
N3
N
S
O
2d
f1 (ppm)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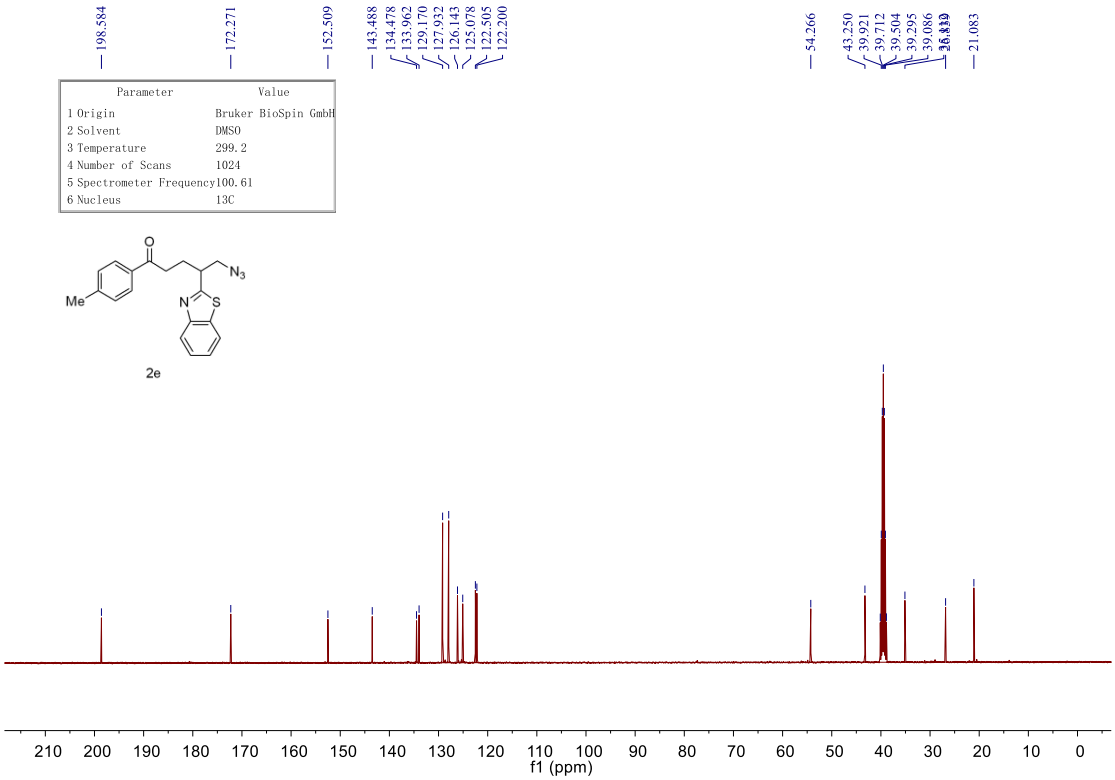
7.887
7.867
7.798
7.777
7.510
7.492
7.474
7.472
7.415
7.397
7.379
7.377
7.260
7.220
7.199
3.894
3.876
3.863
3.845
3.786
3.772
3.755
3.741
3.602
3.576
3.565
3.534
3.043
3.025
3.007
2.409
2.382
2.336
2.301
2.295
Parameter Value
1 Origin Bruker BioSpin GmbH
2 Solvent CDCl3
3 Temperature 298.2
4 Number of Scans 4
5 Spectrometer Frequency 400.13
6 Nucleus 1H
O
N3
Me
N
S
2e
1.01
1.02
2.00
1.02
1.00
2.00
2.01
1.00
2.00
5.19
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 -0.5
f1 (ppm)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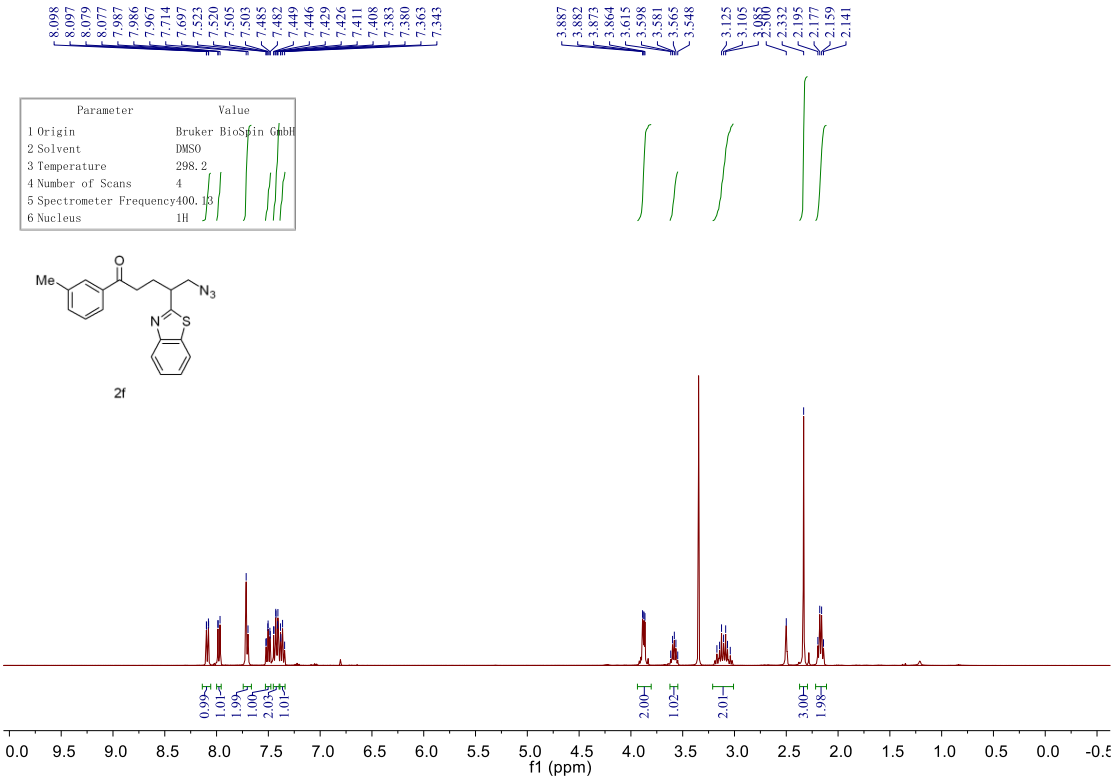
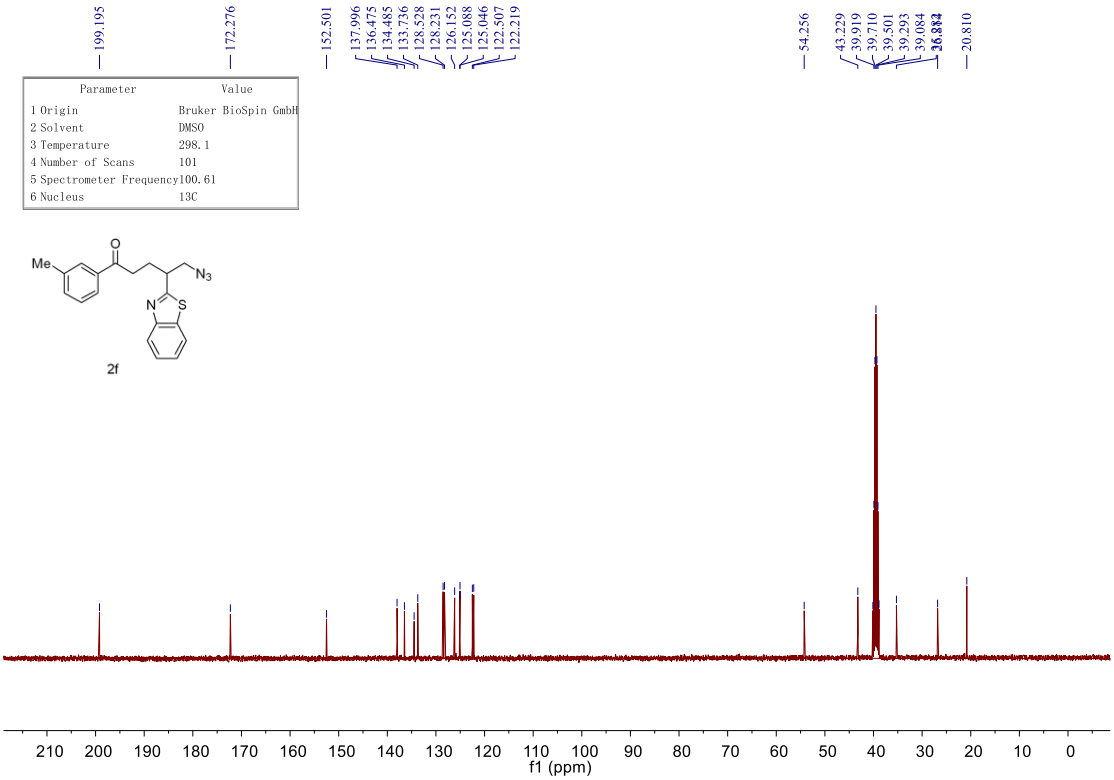
172.271
152.509
143.488
134.478
133.962
129.170
127.932
126.143
125.078
122.505
122.200
54.266
43.250
39.921
39.712
39.504
39.295
39.086
21.083
Parameter Value
1 Origin Bruker BioSpin GmbH
2 Solvent DMSO
3 Temperature 299.2
4 Number of Scans 1024
5 Spectrometer Frequency 100.61
6 Nucleus 13C
O
N3
Me
N
S
2e
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)


8.098
8.097
8.079
8.077
7.987
7.986
7.967
7.714
7.697
7.523
7.520
7.505
7.503
7.485
7.482
7.449
7.446
7.429
7.426
7.411
7.408
7.383
7.380
7.363
7.343
3.887
3.882
3.873
3.864
3.615
3.598
3.581
3.565
3.548
3.125
3.105
3.085
3.066
2.332
2.195
2.177
2.159
2.141
Parameter Value
1 Origin Bruker BioSpin GmbH
2 Solvent DMSO
3 Temperature 298.2
4 Number of Scans 4
5 Spectrometer Frequency 400.13
6 Nucleus 1H
Me
O
N3
N
S
2f
0.99
1.01
1.90
1.00
2.05
1.01
2.00
1.02
2.01
3.00
1.98
f1 (ppm)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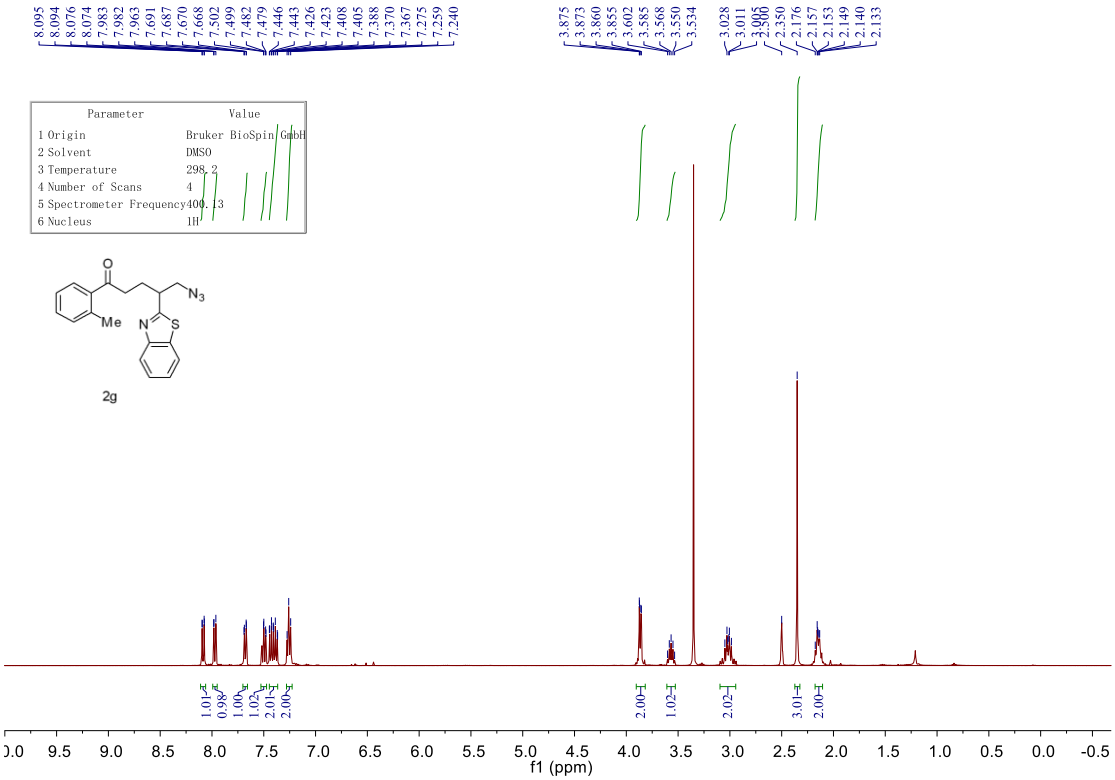
134.485
133.736
128.528
128.231
126.152
125.088
125.046
122.507
122.219
54.256
43.229
39.919
39.710
39.501
39.293
39.084
20.810
Parameter Value
1 Origin Bruker BioSpin GmbH
2 Solvent DMSO
3 Temperature 298.1
4 Number of Scans 101
5 Spectrometer Frequency 100.61
6 Nucleus 13C
Me
O
N3
N
S
2f
f1 (ppm)


8.095
8.094
8.076
8.074
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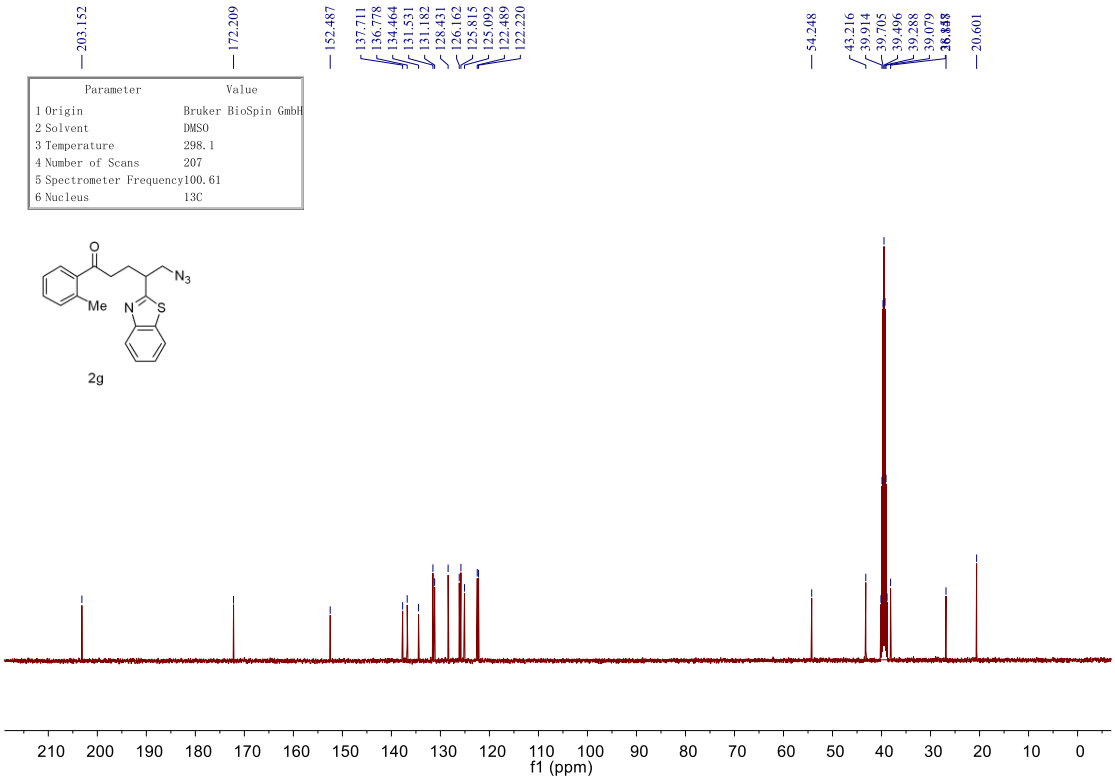
7.982
7.963
7.691
7.687
7.670
7.668
7.502
7.499
7.482
7.479
7.446
7.443
7.426
7.423
7.408
7.405
7.388
7.370
7.367
7.275
7.259
7.240
3.875
3.873
3.860
3.855
3.602
3.585
3.568
3.550
3.534
3.028
3.011
3.005
3.000
2.350
2.176
2.157
2.153
2.149
2.140
2.133
Parameter Value
1 Origin Bruker BioSpin GmbH
2 Solvent DMSO
3 Temperature 298.2
4 Number of Scans 4
5 Spectrometer Frequency 400.13
6 Nucleus 1H
O
N3
Me
N
S
2g
1.01
0.98
1.00
1.02
2.01
2.00
2.00
1.02
2.02
3.01
2.00
f1 (ppm)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131.182
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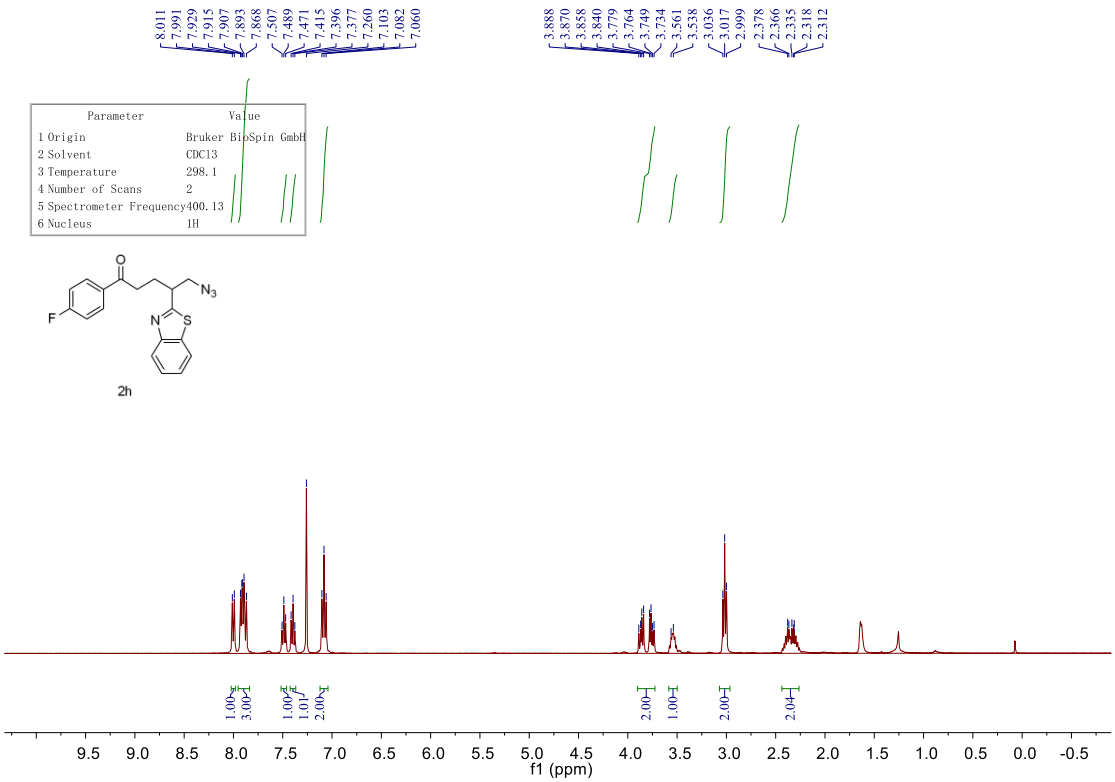
126.162
125.815
125.092
122.489
122.220
54.248
43.216
39.914
39.705
39.496
39.288
39.079
20.601
Parameter Value
1 Origin Bruker BioSpin GmbH
2 Solvent DMSO
3 Temperature 298.1
4 Number of Scans 207
5 Spectrometer Frequency 100.61
6 Nucleus 13C
O
N3
Me
N
S
2g
f1 (ppm)


8.011
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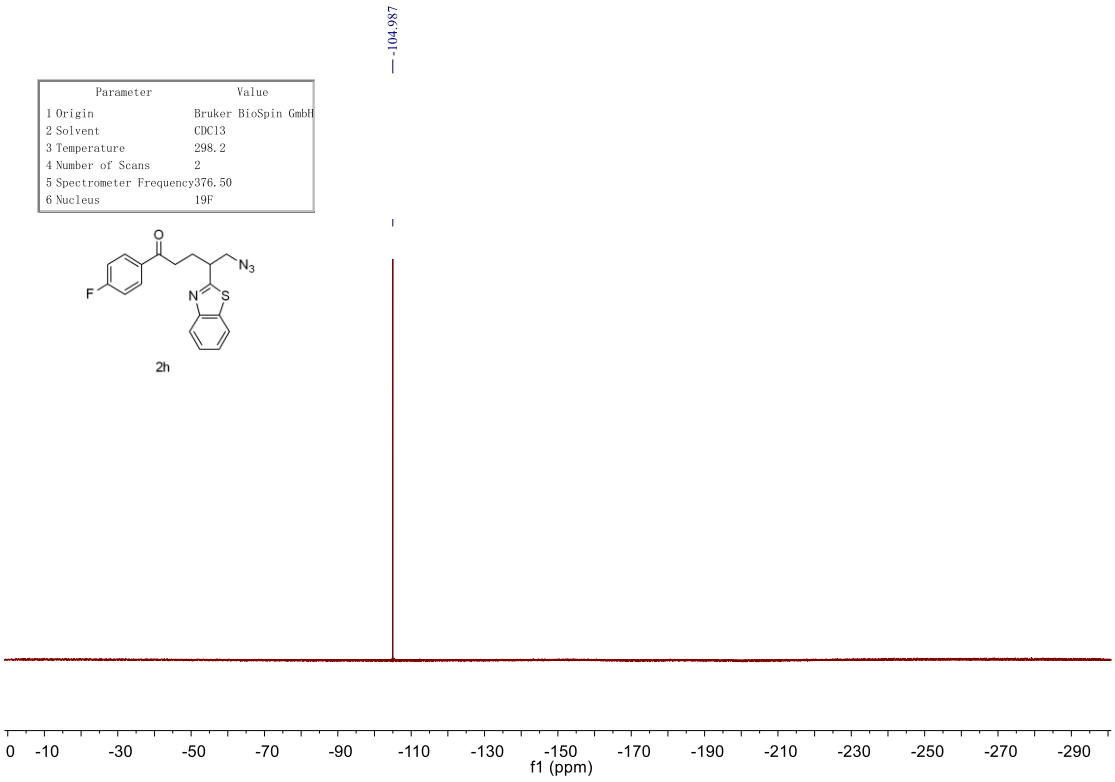
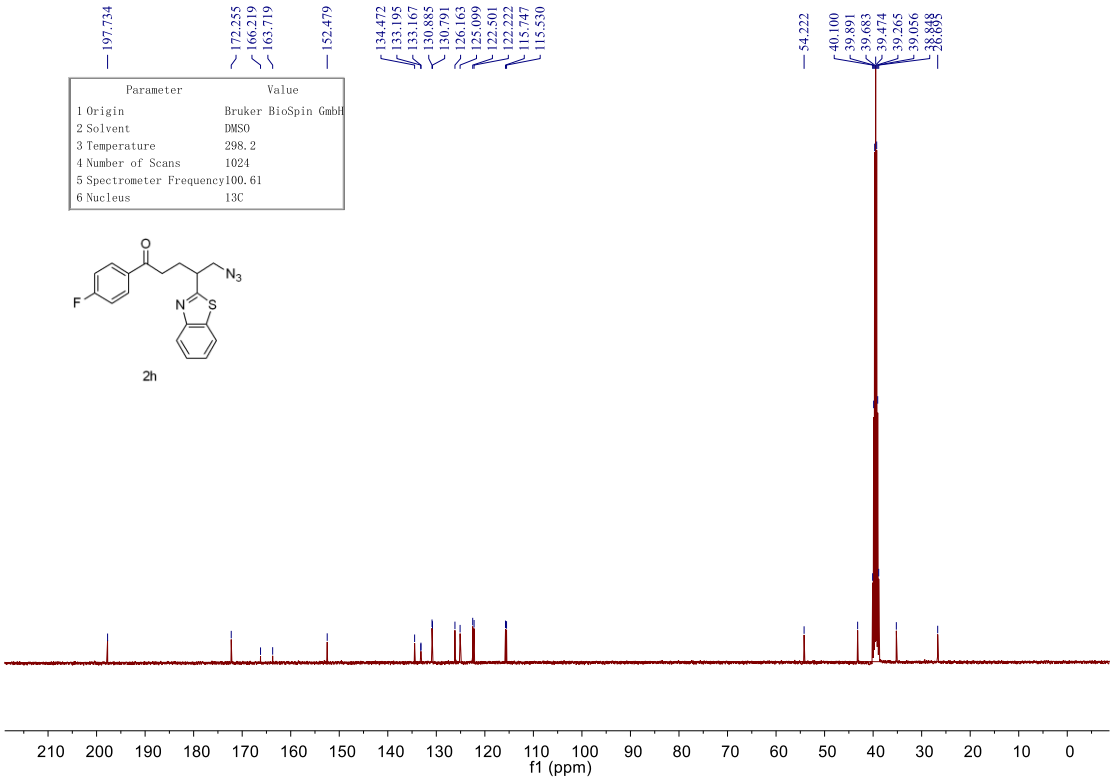
7.929
7.915
7.907
7.893
7.868
7.507
7.489
7.471
7.415
7.396
7.377
7.260
7.103
7.082
7.060
3.888
3.870
3.858
3.840
3.779
3.764
3.749
3.734
3.561
3.538
3.036
3.017
2.999
2.378
2.366
2.335
2.318
2.312
Parameter Value
1 Origin Bruker BioSpin GmbH
2 Solvent CDCl3
3 Temperature 298.1
4 Number of Scans 2
5 Spectrometer Frequency 400.13
6 Nucleus 1H
O
N3
F
N
S
2h
1.00
3.00
1.00
1.01
2.00
2.00
1.00
2.00
2.04
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 -0.5
f1 (ppm)


-104.987
Parameter Value
1 Origin Bruker BioSpin GmbH
2 Solvent CDCl3
3 Temperature 298.2
4 Number of Scans 2
5 Spectrometer Frequency 376.50
6 Nucleus 19F
O
N3
F
N
S
2h
0 -10 -30 -50 -70 -90 -110 -130 -150 -170 -190 -210 -230 -250 -270 -290
f1 (ppm)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134.472
133.195
133.167
130.885
130.791
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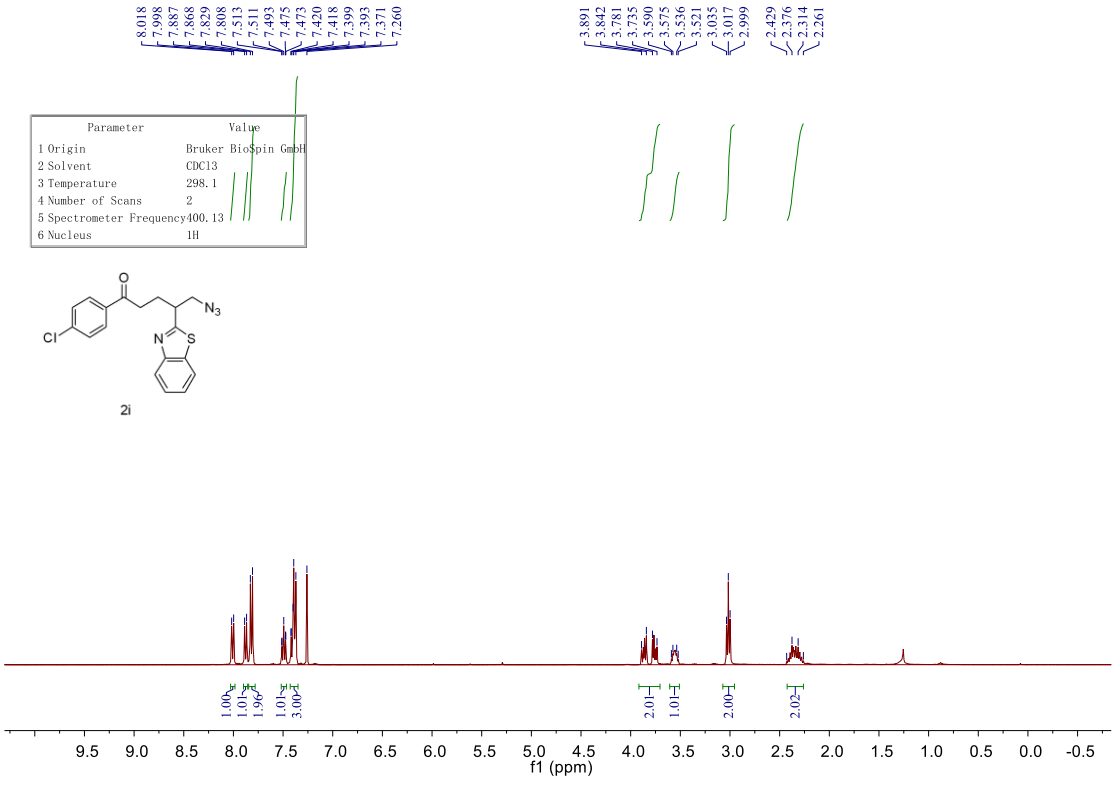
125.099
122.501
122.222
115.747
115.530
54.222
40.100
39.891
39.683
39.474
39.265
39.056
38.848
38.639
Parameter Value
1 Origin Bruker BioSpin GmbH
2 Solvent DMSO
3 Temperature 298.2
4 Number of Scans 1024
5 Spectrometer Frequency 100.61
6 Nucleus 13C
O
N3
F
N
S
2h
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)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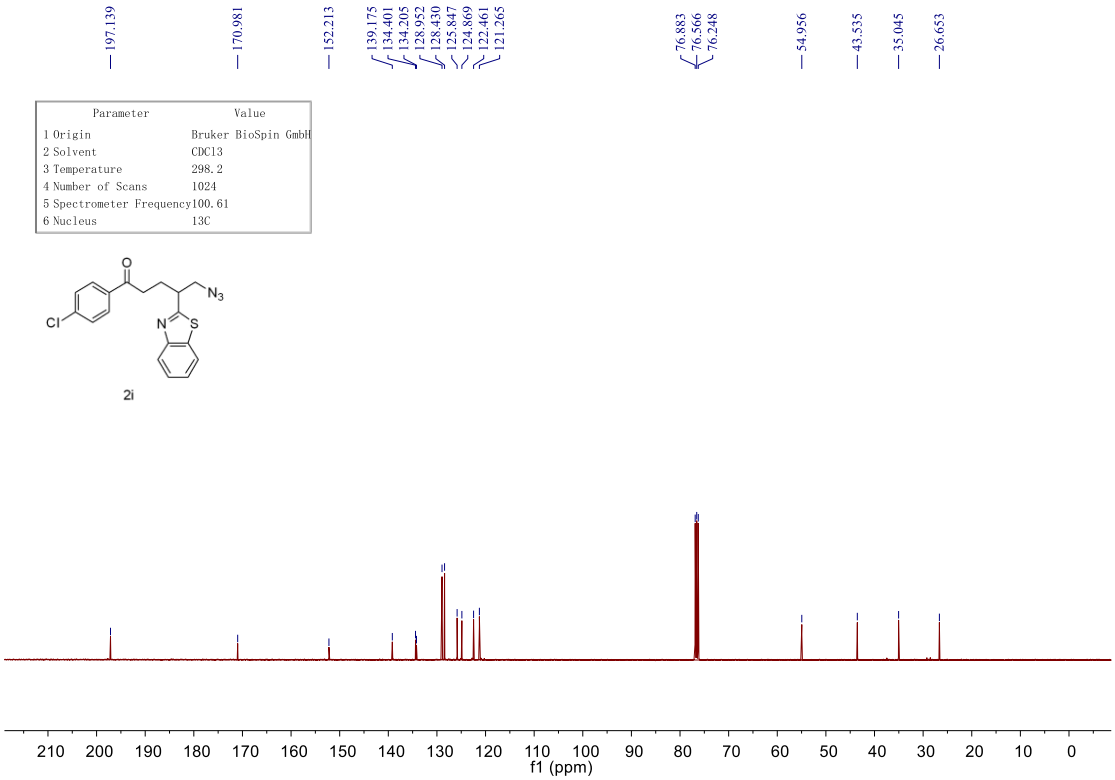
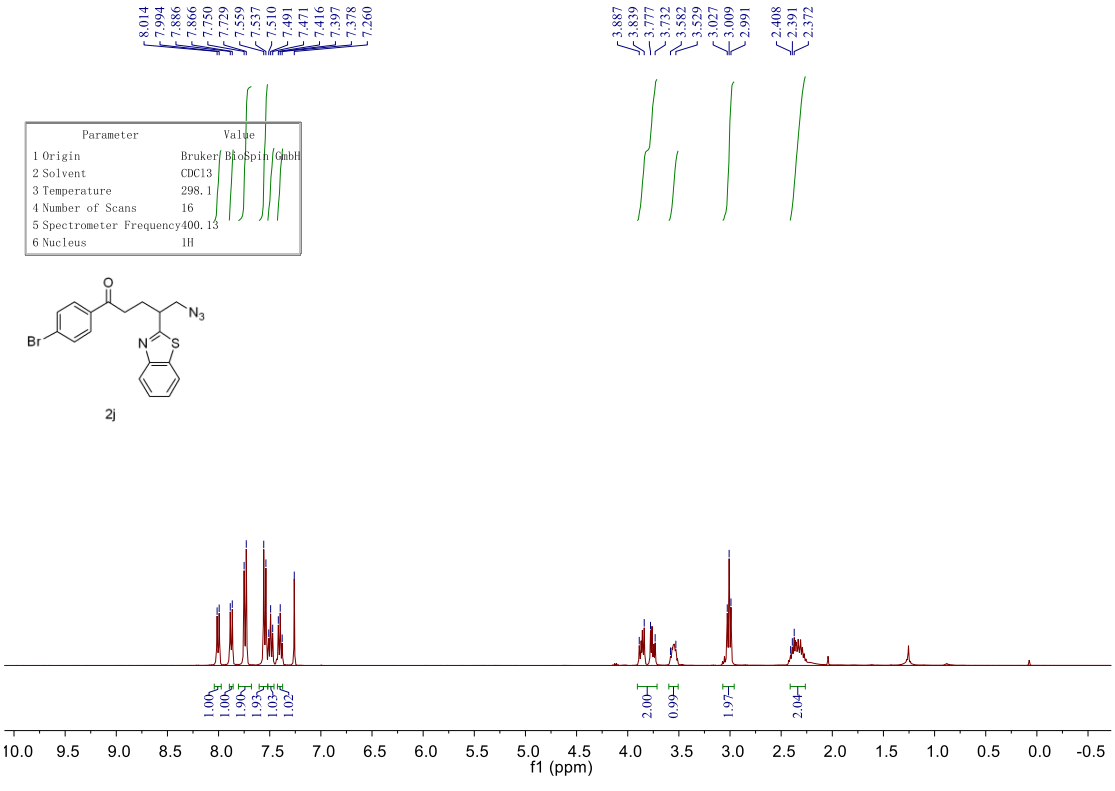
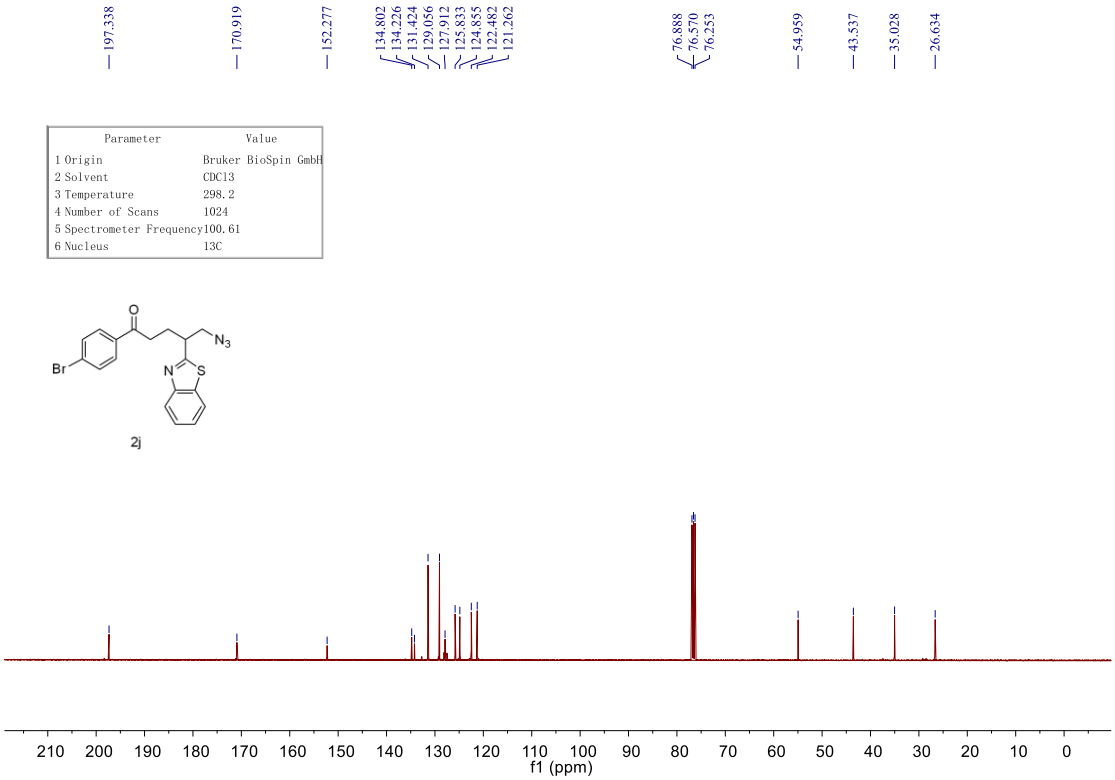
7.829
7.808
7.513
7.511
7.493
7.475
7.473
7.420
7.418
7.399
7.393
7.371
7.260
3.891
3.842
3.781
3.735
3.590
3.575
3.536
3.521
3.035
3.017
2.999
2.429
2.376
2.314
2.261
Parameter Value
1 Origin Bruker BioSpin GmbH
2 Solvent CDCl3
3 Temperature 298.1
4 Number of Scans 2
5 Spectrometer Frequency 400.13
6 Nucleus 1H
O
N3
Cl
N
S
2i
1.00
1.01
1.96
1.01
3.00
2.01
1.01
2.00
2.02
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 -0.5
f1 (ppm)


197.139
170.981
152.213
139.175
134.401
134.205
128.952
128.430
125.847
124.869
122.461
121.265
76.883
76.566
76.248
54.956
43.535
35.045
26.653
Parameter Value
1 Origin Bruker BioSpin GmbH
2 Solvent CDCl3
3 Temperature 298.2
4 Number of Scans 1024
5 Spectrometer Frequency 100.61
6 Nucleus 13C
O
N3
Cl
N
S
2i
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)


8.014
7.994
7.886
7.866
7.750
7.729
7.559
7.537
7.510
7.491
7.471
7.416
7.397
7.378
7.260
3.887
3.839
3.777
3.732
3.582
3.529
3.027
3.009
2.991
2.408
2.391
2.372
Parameter Value
1 Origin Bruker BioSpin GmbH
2 Solvent CDCl3
3 Temperature 298.1
4 Number of Scans 16
5 Spectrometer Frequency 400.13
6 Nucleus 1H
O
N3
Br
N
S
2j
1.00
1.00
1.90
1.93
1.03
1.02
2.00
0.99
1.97
2.04
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 -0.5
f1 (ppm)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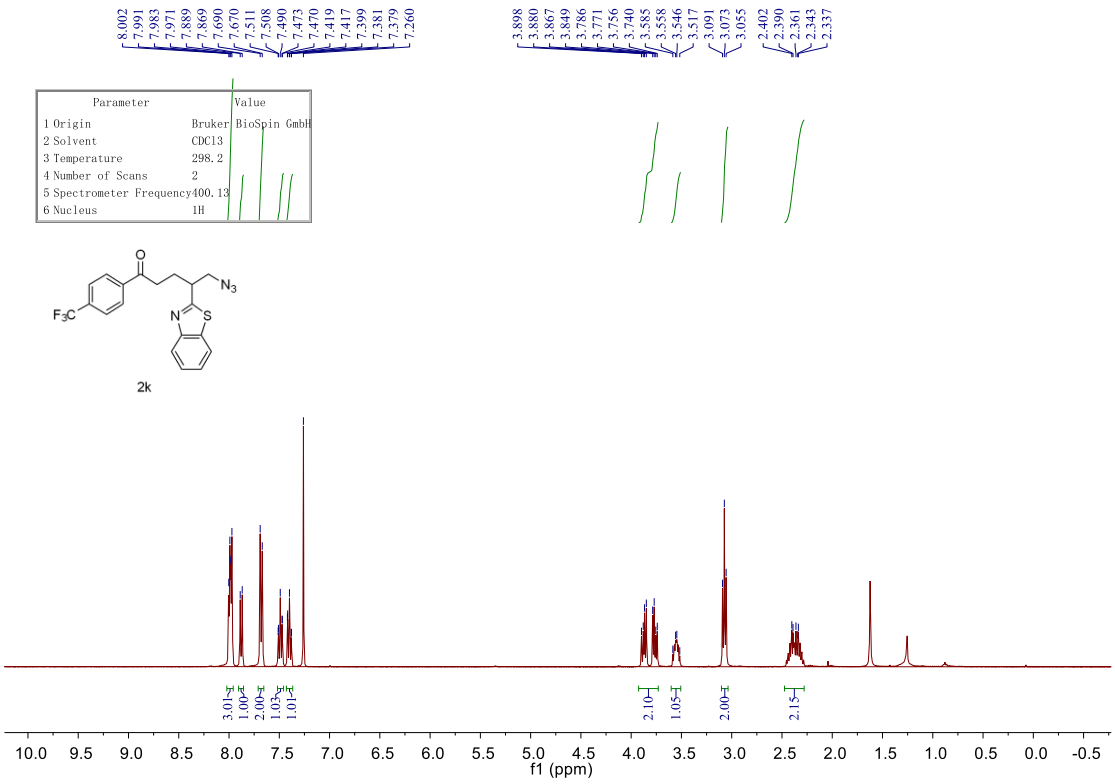
170.919
152.277
134.802
134.226
131.424
129.056
127.912
125.833
124.855
122.482
121.262
76.888
76.570
76.253
54.959
43.537
35.028
26.634
Parameter Value
1 Origin Bruker BioSpin GmbH
2 Solvent CDCl3
3 Temperature 298.2
4 Number of Scans 1024
5 Spectrometer Frequency 100.61
6 Nucleus 13C
O
N3
Br
N
S
2j
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)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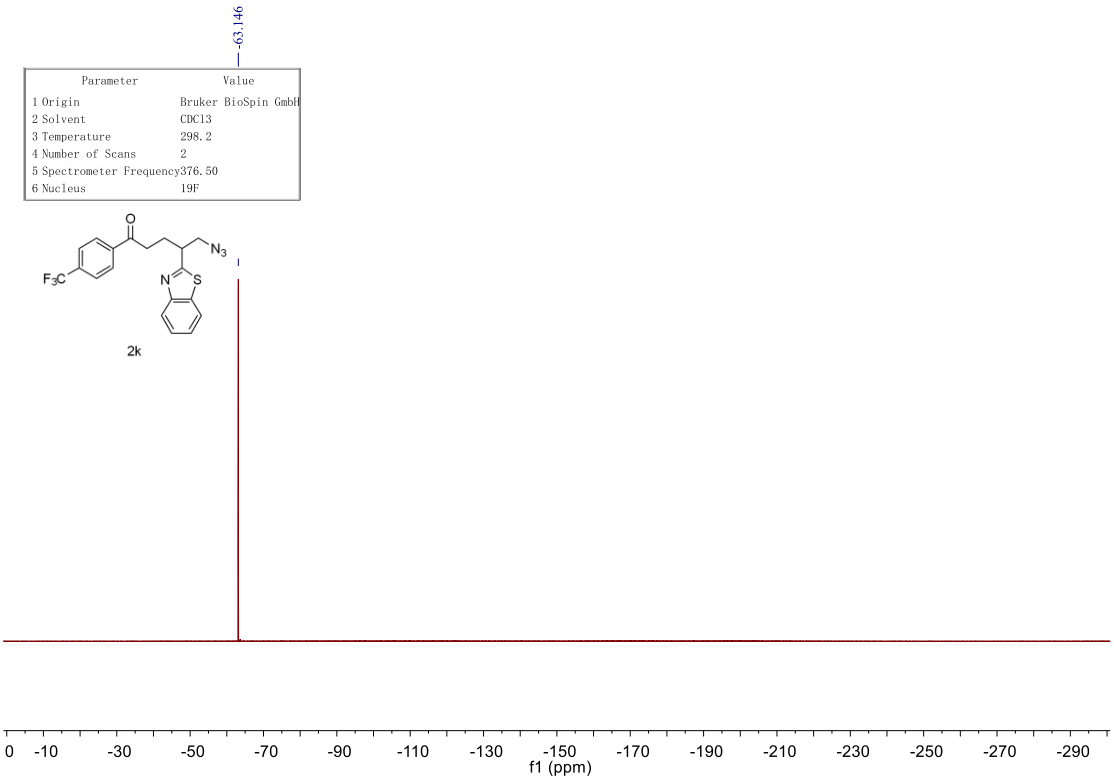
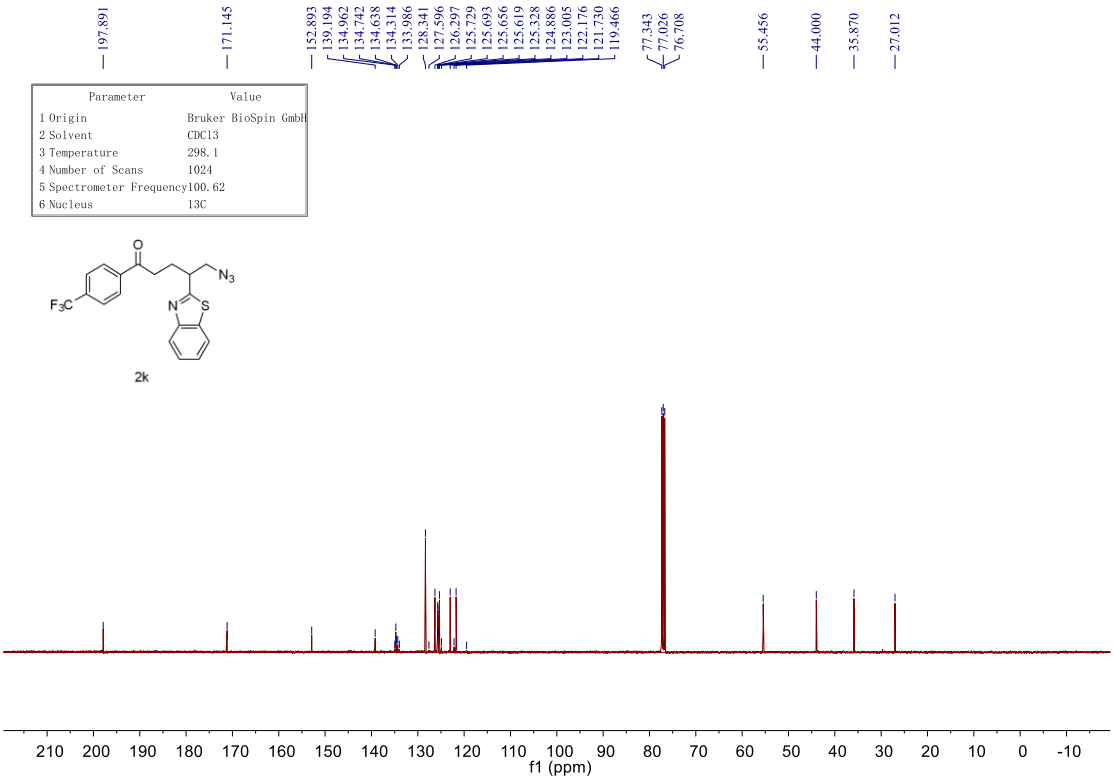
7.991
7.983
7.971
7.889
7.869
7.690
7.670
7.511
7.508
7.490
7.473
7.470
7.419
7.417
7.399
7.381
7.379
7.260
3.898
3.880
3.867
3.849
3.786
3.771
3.756
3.740
3.585
3.558
3.546
3.517
3.091
3.073
3.055
2.402
2.390
2.361
2.343
2.337
Parameter Value
1 Origin Bruker BioSpin GmbH
2 Solvent CDCl3
3 Temperature 298.2
4 Number of Scans 2
5 Spectrometer Frequency 400.13
6 Nucleus 1H
O
N3
F3C
N
S
2k
3.01
1.00
2.00
1.03
1.01
2.10
1.05
2.00
2.15
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 -0.5
f1 (ppm)


-63.146
Parameter Value
1 Origin Bruker BioSpin GmbH
2 Solvent CDCl3
3 Temperature 298.2
4 Number of Scans 2
5 Spectrometer Frequency 376.50
6 Nucleus 19F
O
N3
F3C
N
S
2k
0 -10 -30 -50 -70 -90 -110 -130 -150 -170 -190 -210 -230 -250 -270 -290
f1 (ppm)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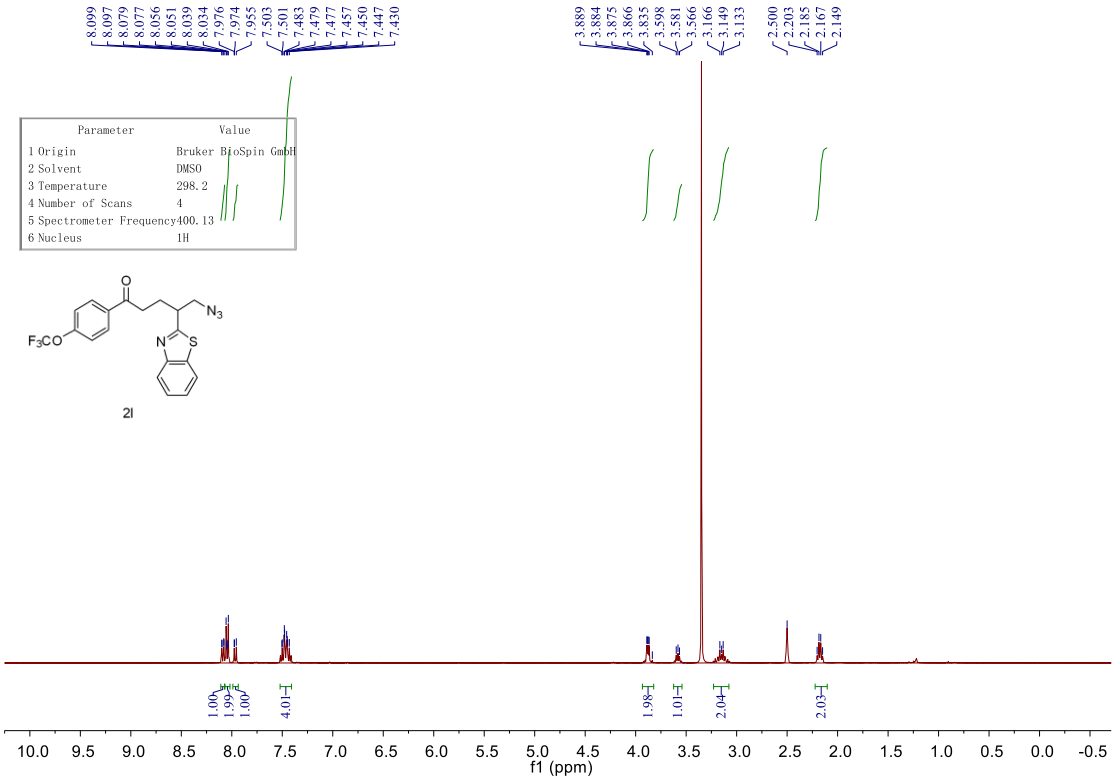
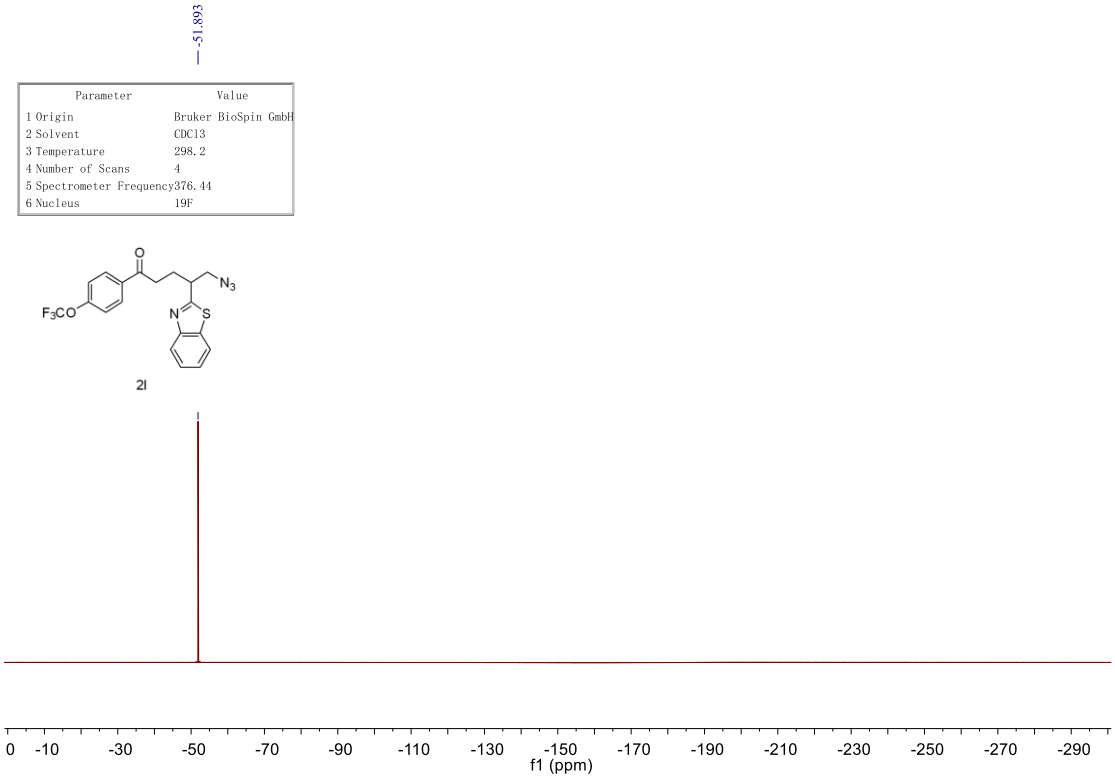
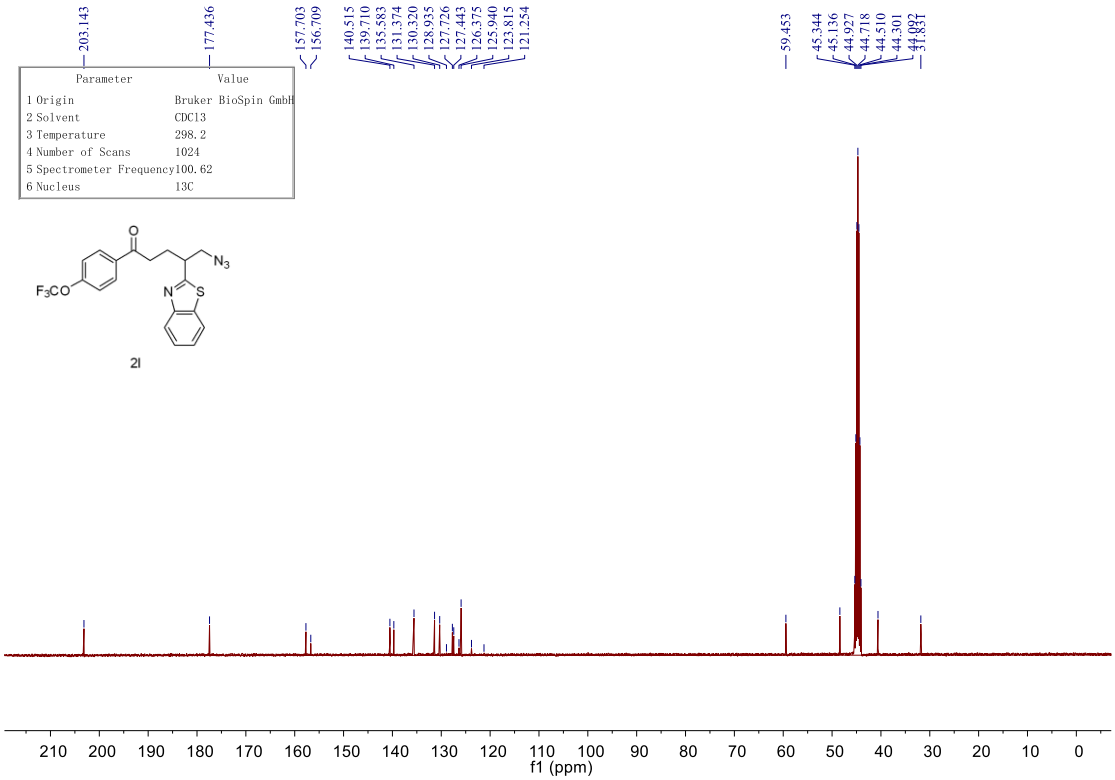
171.145
152.893
139.194
134.962
134.742
134.638
134.314
133.986
128.341
127.596
126.297
125.729
125.693
125.656
125.619
125.328
124.886
123.005
122.176
121.730
119.466
77.343
77.026
76.708
55.456
44.000
35.870
27.012
Parameter Value
1 Origin Bruker BioSpin GmbH
2 Solvent CDCl3
3 Temperature 298.1
4 Number of Scans 1024
5 Spectrometer Frequency 100.62
6 Nucleus 13C
O
N3
F3C
N
S
2k
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)


8.099
8.097
8.079
8.077
8.056
8.051
8.039
8.034
7.976
7.974
7.955
7.503
7.501
7.483
7.479
7.477
7.457
7.450
7.447
7.430
3.889
3.884
3.875
3.866
3.835
3.598
3.581
3.566
3.166
3.149
3.133
2.500
2.203
2.185
2.167
2.149
Parameter Value
1 Origin Bruker BioSpin GmbH
2 Solvent DMSO
3 Temperature 298.2
4 Number of Scans 4
5 Spectrometer Frequency 400.13
6 Nucleus 1H
O
N3
F3CO
N
S
2l
1.00
1.99
1.00
4.01
1.98
1.01
2.04
2.03
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 -0.5
f1 (ppm)


-51.893
Parameter Value
1 Origin Bruker BioSpin GmbH
2 Solvent CDCl3
3 Temperature 298.2
4 Number of Scans 4
5 Spectrometer Frequency 376.44
6 Nucleus 19F
O
N3
F3CO
N
S
2l
0 -10 -30 -50 -70 -90 -110 -130 -150 -170 -190 -210 -230 -250 -270 -290
f1 (ppm)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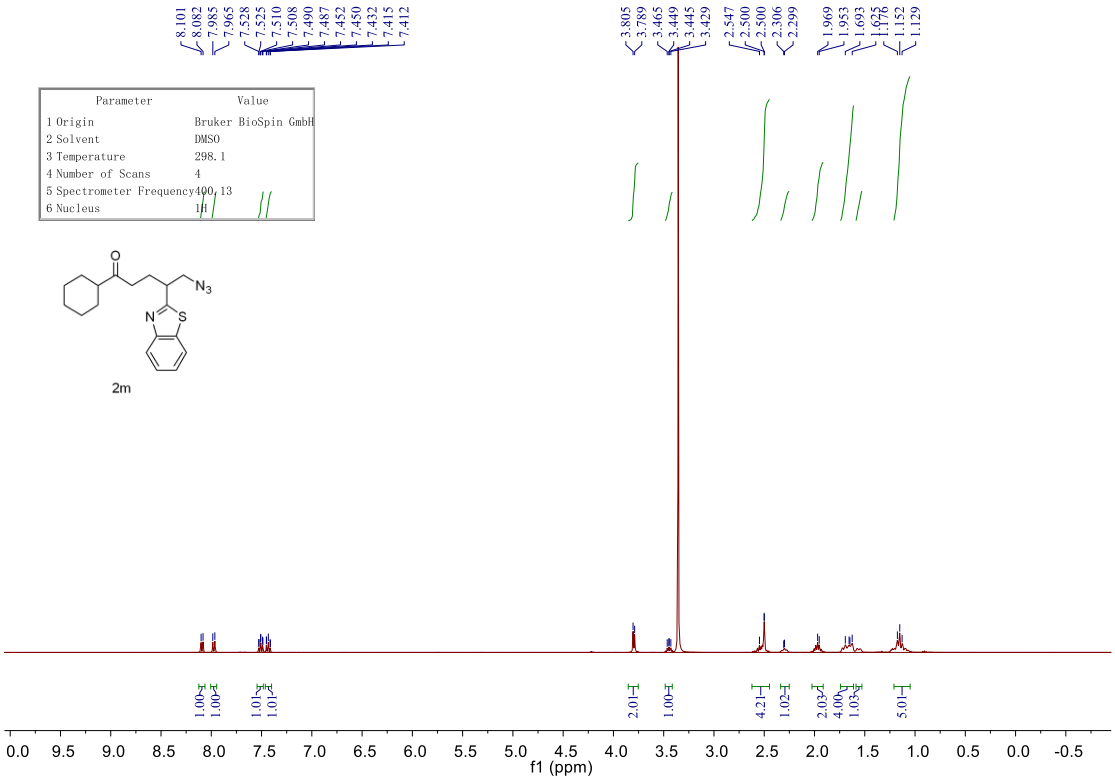
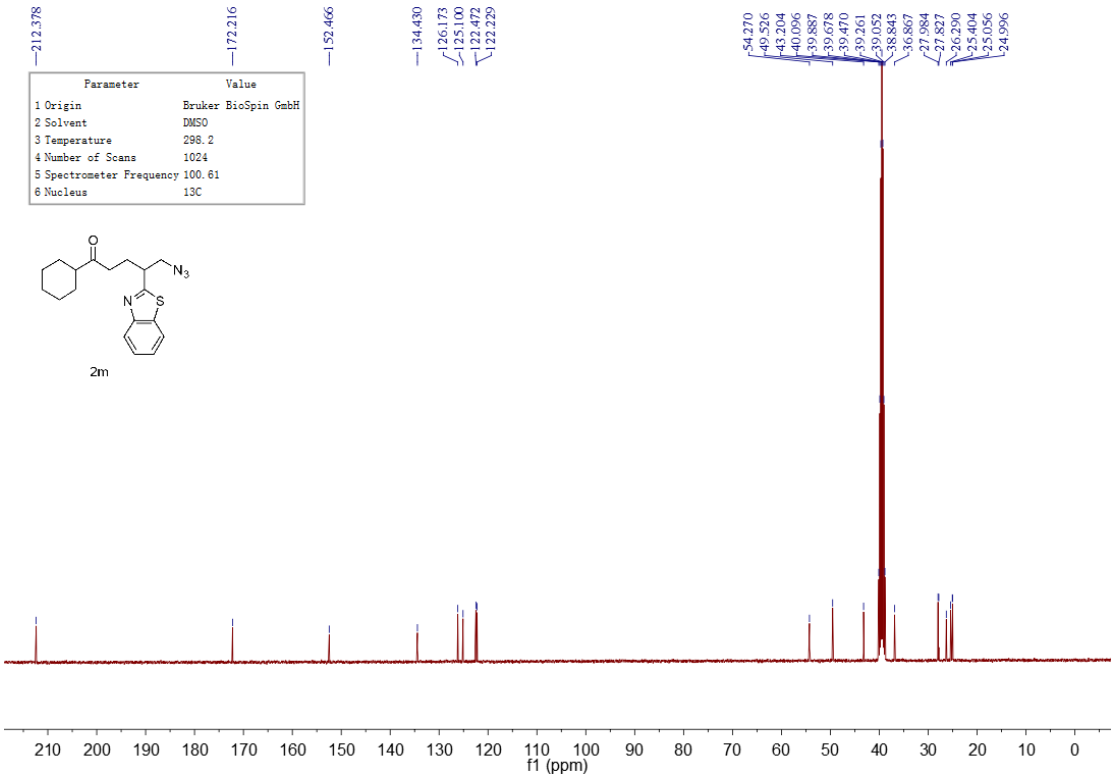
157.703
156.709
140.515
139.710
135.583
131.374
130.320
128.935
127.726
127.443
126.375
125.940
123.815
121.254
59.453
45.344
45.136
44.927
44.718
44.510
44.301
44.092
41.831
Parameter Value
1 Origin Bruker BioSpin GmbH
2 Solvent CDCl3
3 Temperature 298.2
4 Number of Scans 1024
5 Spectrometer Frequency 100.62
6 Nucleus 13C
O
N3
F3CO
N
S
2l
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)


8.101
8.082
7.985
7.965
7.528
7.525
7.510
7.508
7.490
7.487
7.452
7.450
7.432
7.415
7.412
3.805
3.789
3.465
3.449
3.445
3.429
2.547
2.500
2.500
2.306
2.299
1.969
1.953
1.693
1.625
1.176
1.152
1.129
Parameter Value
1 Origin Bruker BioSpin GmbH
2 Solvent DMSO
3 Temperature 298.1
4 Number of Scans 4
5 Spectrometer Frequency 400.13
6 Nucleus 1H
O
N3
N
S
2m
1.00
1.00
1.01
1.01
2.01
1.00
4.21
1.02
2.03
4.00
1.03
5.01
0.0 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 -0.5
f1 (ppm)


212.378
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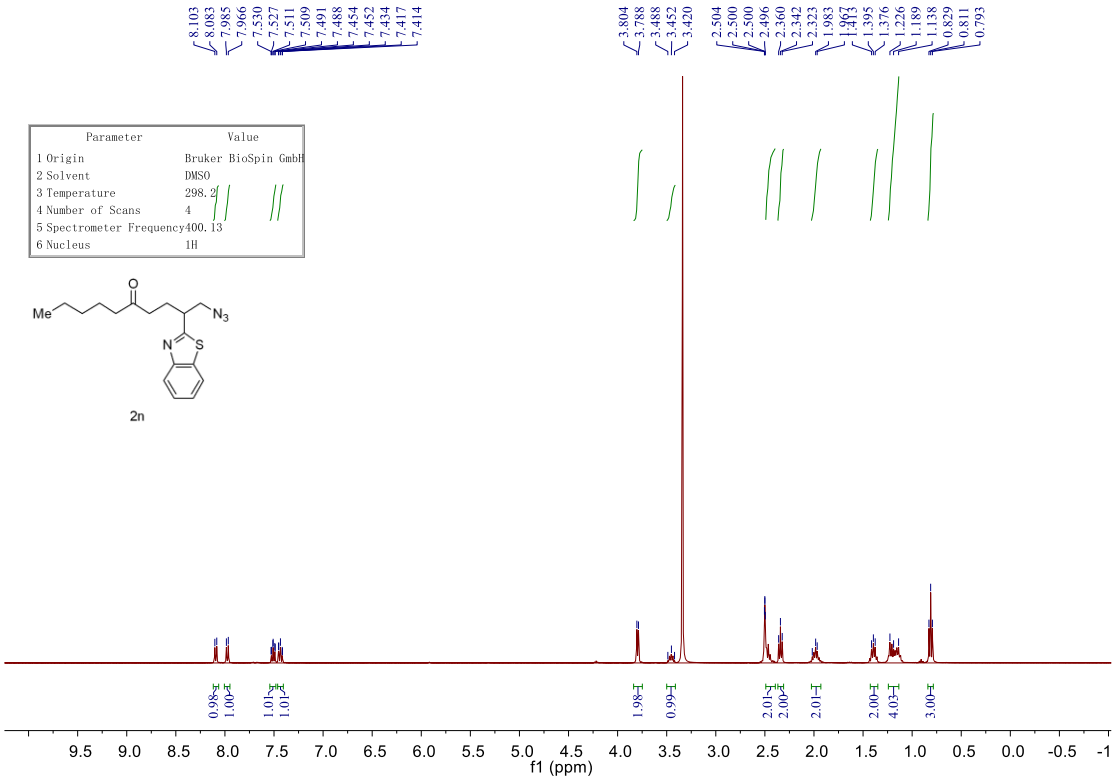
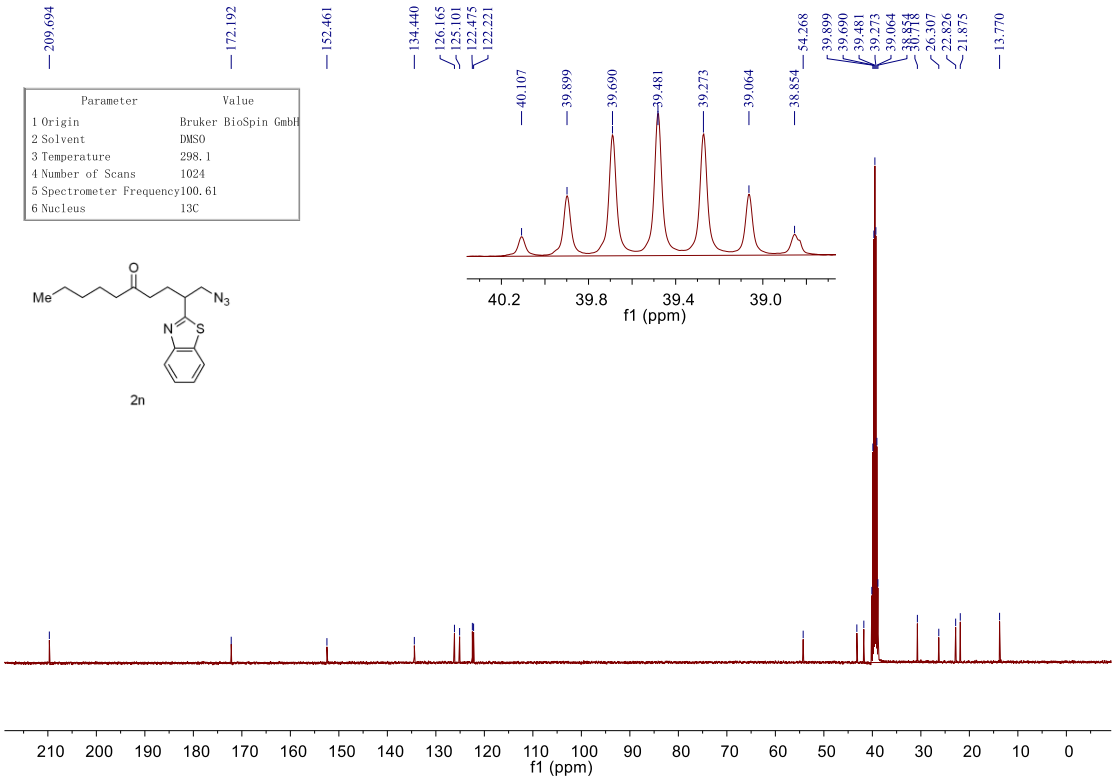
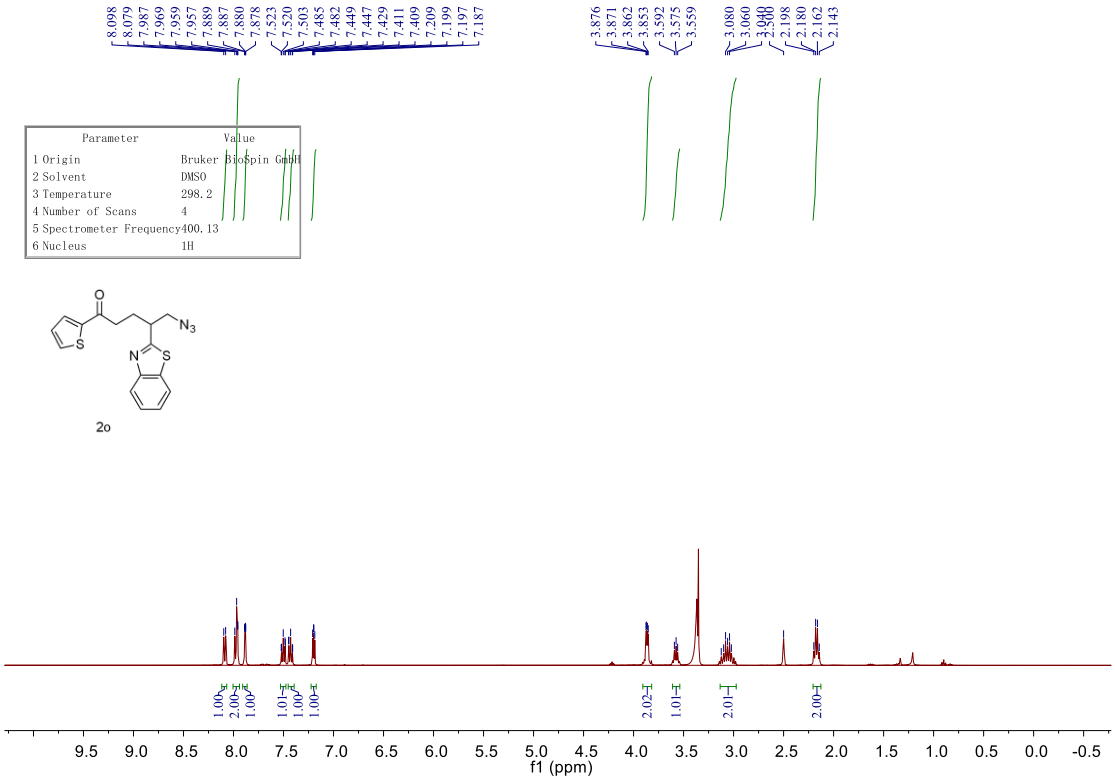
152.466
134.430
126.173
125.100
122.472
122.229
54.270
49.526
43.204
40.096
39.887
39.678
39.470
39.261
39.052
38.843
36.867
27.984
27.827
26.290
25.404
25.056
24.996
Parameter Value
1 Origin Bruker BioSpin GmbH
2 Solvent DMSO
3 Temperature 298.2
4 Number of Scans 1024
5 Spectrometer Frequency 100.61
6 Nucleus 13C
O
N3
N
S
2m
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)


8.103
8.083
7.985
7.966
7.530
7.527
7.511
7.509
7.491
7.488
7.454
7.452
7.434
7.417
7.414
3.804
3.788
3.488
3.452
3.420
2.504
2.500
2.500
2.496
2.360
2.342
2.323
1.983
1.967
1.947
1.395
1.376
1.226
1.189
1.138
0.829
0.811
0.793
Parameter Value
1 Origin Bruker BioSpin GmbH
2 Solvent DMSO
3 Temperature 298.2
4 Number of Scans 4
5 Spectrometer Frequency 400.13
6 Nucleus 1H
Me
O
N3
N
S
2n
0.98
1.00
1.01
1.01
1.98
0.99
2.01
2.00
2.01
2.00
4.03
3.00
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 -0.5 -1
f1 (ppm)


209.694
172.192
152.461
134.440
126.165
125.101
122.475
122.221
54.268
39.899
39.690
39.481
39.273
39.064
38.854
30.718
26.307
22.826
21.875
13.770
40.107
39.899
39.690
39.481
39.273
39.064
38.854
Parameter Value
1 Origin Bruker BioSpin GmbH
2 Solvent DMSO
3 Temperature 298.1
4 Number of Scans 1024
5 Spectrometer Frequency 100.61
6 Nucleus 13C
Me
N3
O
N
S
2n
40.2
39.8
39.4
39.0
f1 (ppm)
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)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8.079
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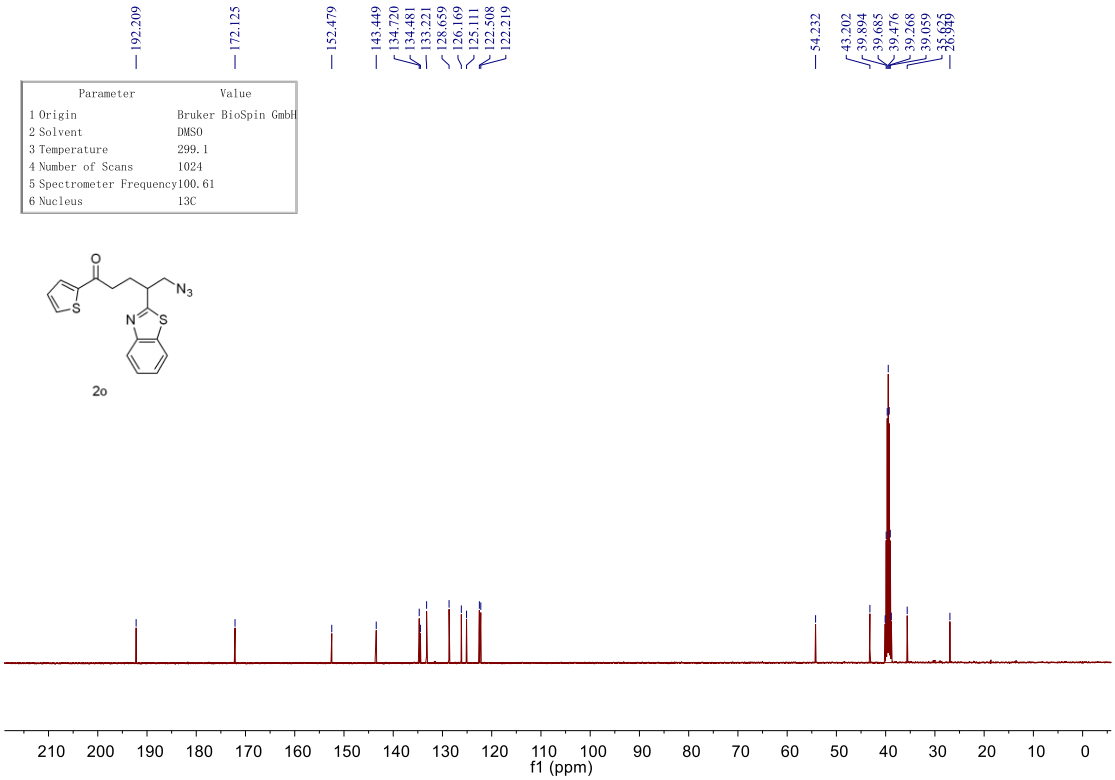
7.969
7.959
7.957
7.889
7.887
7.880
7.878
7.523
7.520
7.503
7.485
7.482
7.449
7.447
7.429
7.411
7.409
7.209
7.199
7.197
7.187
3.876
3.871
3.862
3.853
3.592
3.575
3.559
3.080
3.060
2.198
2.180
2.162
2.143
Parameter Value
1 Origin Bruker BioSpin GmbH
2 Solvent DMSO
3 Temperature 298.2
4 Number of Scans 4
5 Spectrometer Frequency 400.13
6 Nucleus 1H
O
N3
S
N
S
2o
1.00
2.00
1.00
1.01
1.00
1.00
2.02
1.01
2.01
2.00
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 -0.5
f1 (ppm)


192.209
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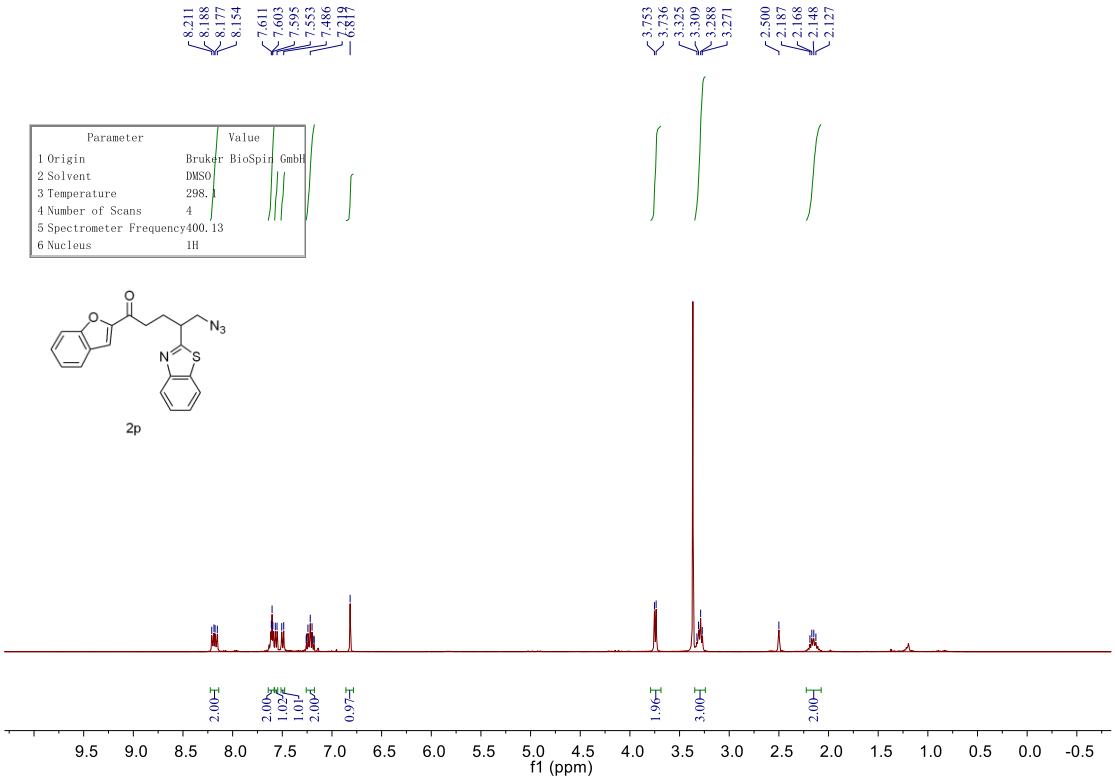
152.479
143.449
134.720
134.481
133.221
128.659
126.169
125.111
122.508
122.219
54.232
43.202
39.894
39.685
39.476
39.268
39.059
Parameter Value
1 Origin Bruker BioSpin GmbH
2 Solvent DMSO
3 Temperature 299.1
4 Number of Scans 1024
5 Spectrometer Frequency 100.61
6 Nucleus 13C
2o
f1 (ppm)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8.177
8.154
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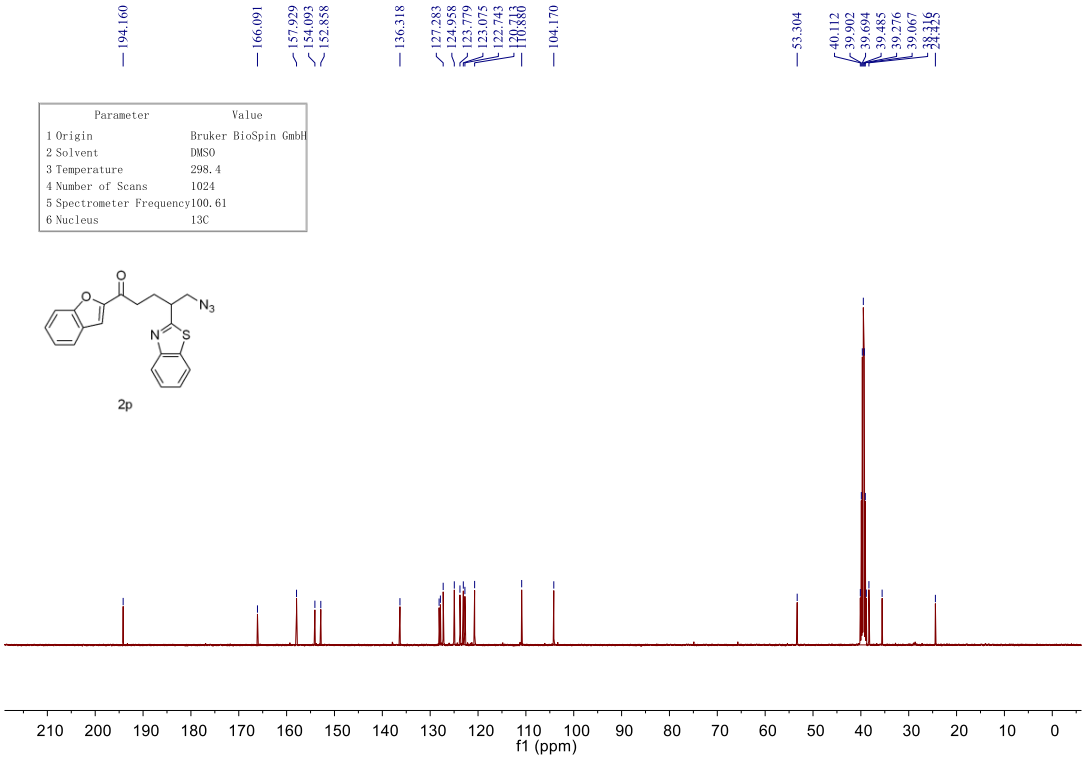
7.603
7.595
7.553
7.486
7.819
6.817
3.753
3.736
3.325
3.309
3.288
3.271
2.500
2.187
2.168
2.148
2.127
Parameter Value
1 Origin Bruker BioSpin GmbH
2 Solvent DMSO
3 Temperature 298.1
4 Number of Scans 4
5 Spectrometer Frequency 400.13
6 Nucleus 1H
2p
2.00
2.00
1.02
1.01
2.00
0.97
1.96
3.00
2.00
f1 (ppm)


194.160
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157.929
154.093
152.858
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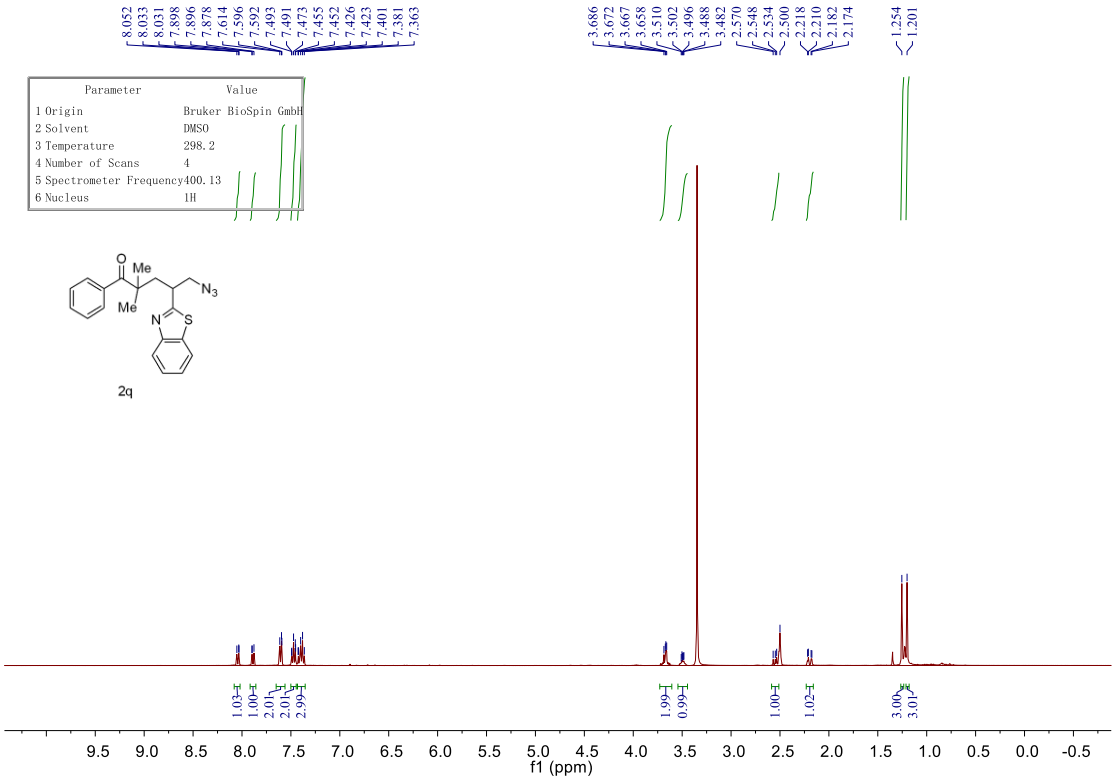
127.283
124.958
123.779
123.075
122.743
120.713
110.880
104.170
53.304
40.112
39.902
39.694
39.485
39.276
39.067
38.316
24.425
Parameter Value
1 Origin Bruker BioSpin GmbH
2 Solvent DMSO
3 Temperature 298.4
4 Number of Scans 1024
5 Spectrometer Frequency 100.61
6 Nucleus 13C
O
O
N3
N
S
2p
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)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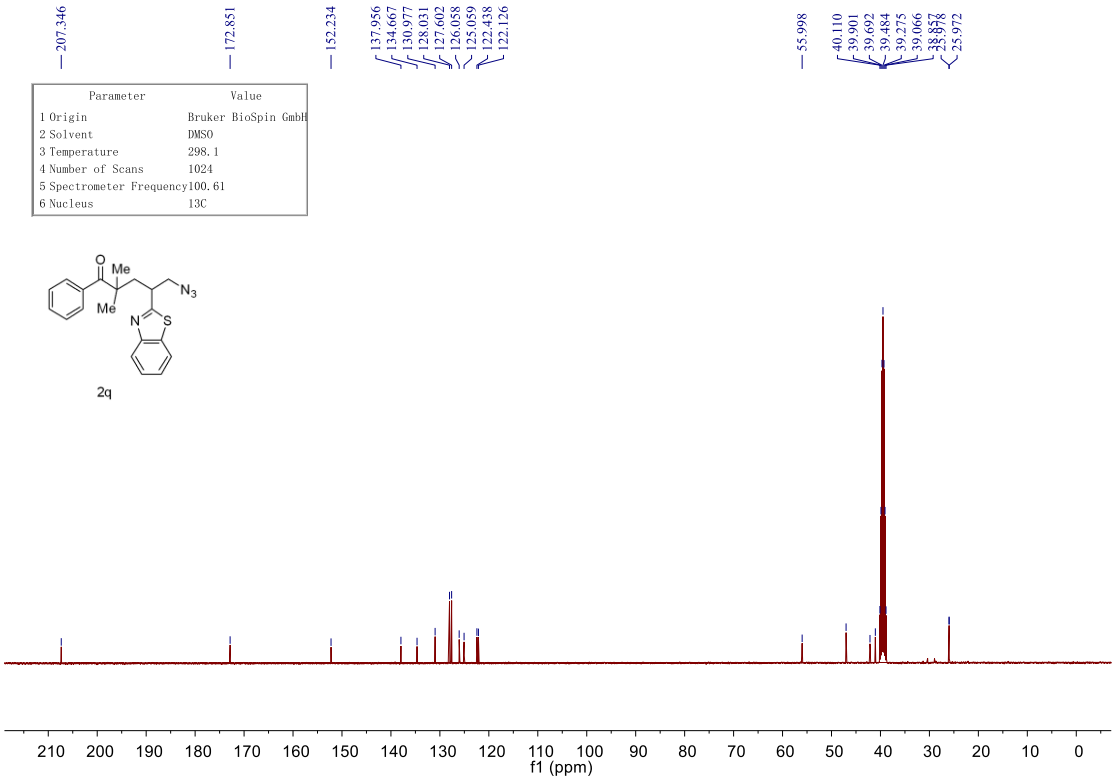
7.878
7.614
7.596
7.592
7.493
7.491
7.473
7.455
7.452
7.426
7.423
7.401
7.381
7.363
3.686
3.672
3.667
3.658
3.510
3.502
3.496
3.488
3.482
2.570
2.548
2.534
2.500
2.218
2.210
2.182
2.174
1.254
1.201
Parameter Value
1 Origin Bruker BioSpin GmbH
2 Solvent DMSO
3 Temperature 298.2
4 Number of Scans 4
5 Spectrometer Frequency 400.13
6 Nucleus 1H
O
Me
Me
N3
N
S
2q
1.03
1.00
2.01
2.01
2.99
1.99
0.99
1.00
1.02
3.00
3.01
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 -0.5
f1 (ppm)


207.346
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134.667
130.977
128.031
127.602
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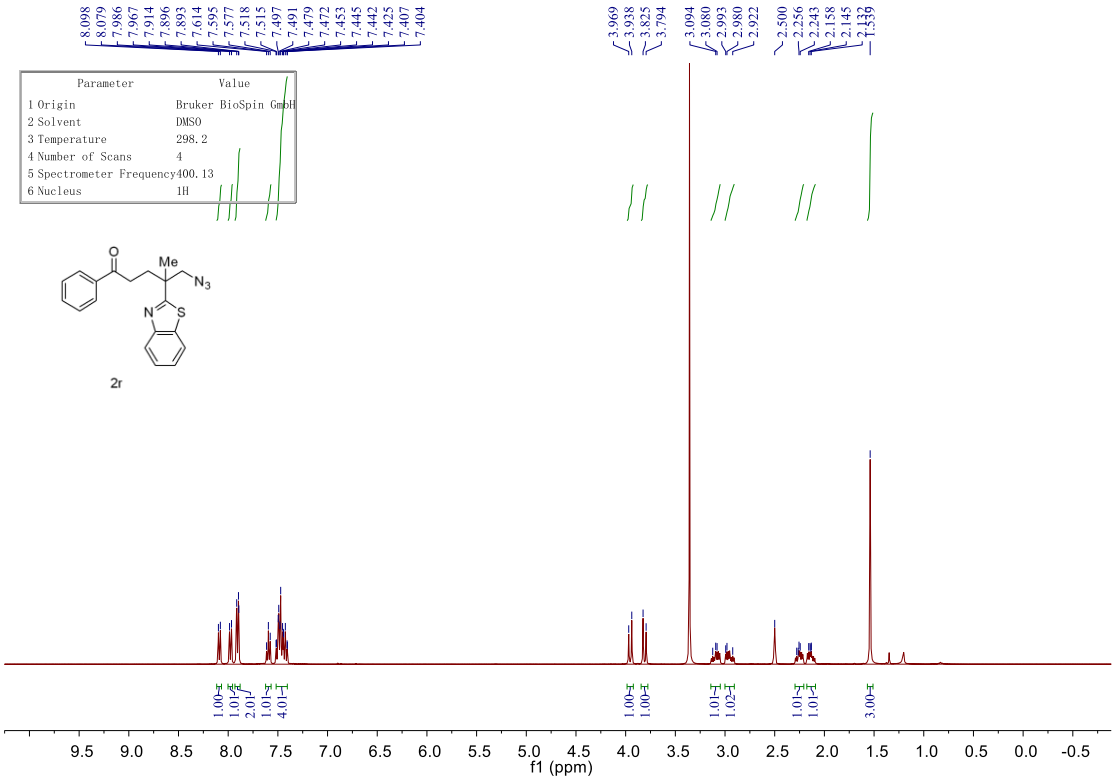
125.059
122.438
122.126
55.998
40.110
39.901
39.692
39.484
39.275
39.066
38.857
25.978
25.972
Parameter Value
1 Origin Bruker BioSpin GmbH
2 Solvent DMSO
3 Temperature 298.1
4 Number of Scans 1024
5 Spectrometer Frequency 100.61
6 Nucleus 13C
Me
Me
N3
N
S
2q
f1 (ppm)


8.098
8.079
7.986
7.967
7.914
7.896
7.893
7.614
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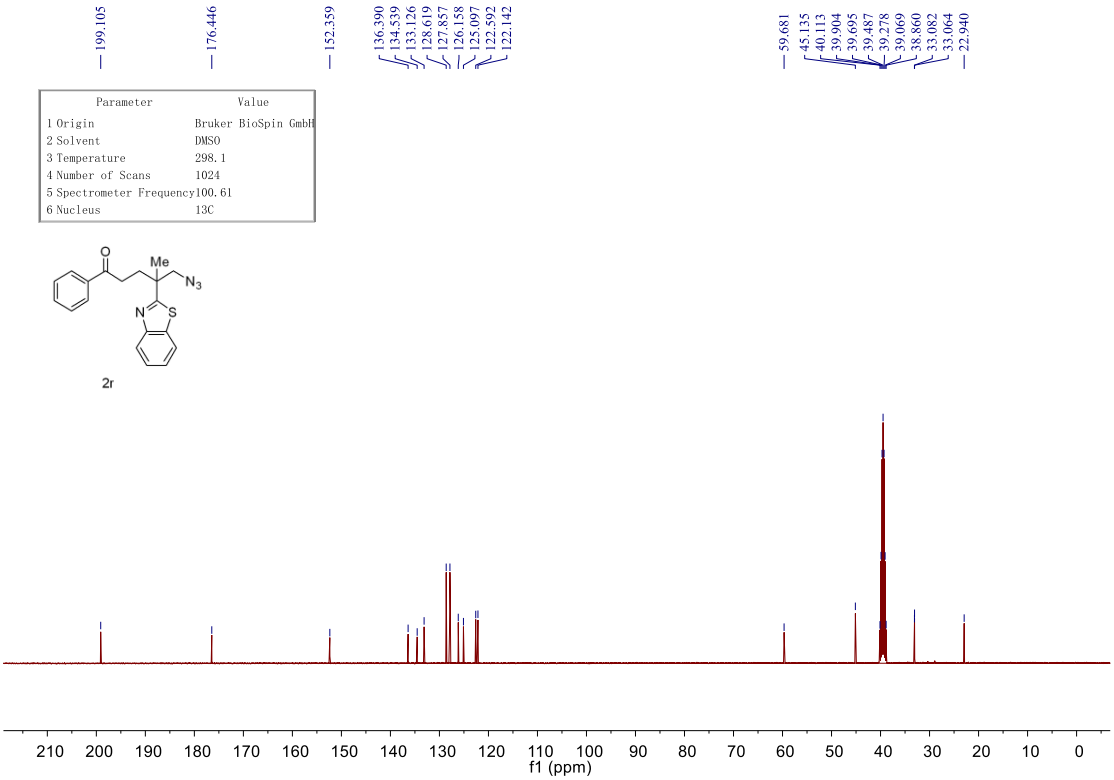
7.577
7.518
7.515
7.497
7.491
7.479
7.472
7.453
7.445
7.442
7.425
7.407
7.404
3.969
3.938
3.825
3.794
3.094
3.080
2.993
2.980
2.922
2.500
2.256
2.243
2.158
2.145
1.539
Parameter Value
1 Origin Bruker BioSpin GmbH
2 Solvent DMSO
3 Temperature 298.2
4 Number of Scans 4
5 Spectrometer Frequency 400.13
6 Nucleus 1H
Me
N3
N
S
2r
1.00
1.01
2.01
1.01
4.01
1.00
1.00
1.01
1.02
1.01
1.01
3.00
f1 (ppm)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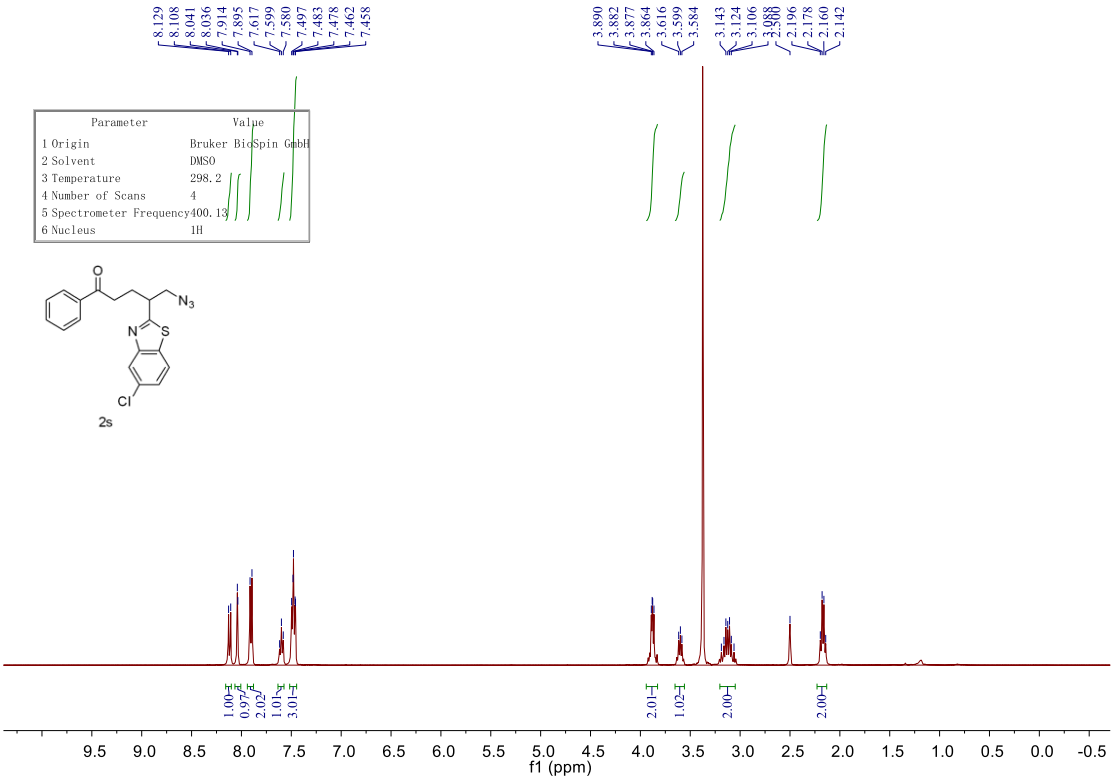
152.359
136.390
134.539
133.126
128.619
127.857
126.158
125.097
122.592
122.142
59.681
45.135
40.113
39.904
39.695
39.487
39.278
39.069
38.860
33.082
33.064
22.940
Parameter Value
1 Origin Bruker BioSpin GmbH
2 Solvent DMSO
3 Temperature 298.1
4 Number of Scans 1024
5 Spectrometer Frequency 100.61
6 Nucleus 13C
O
Me
N3
N
S
2r
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)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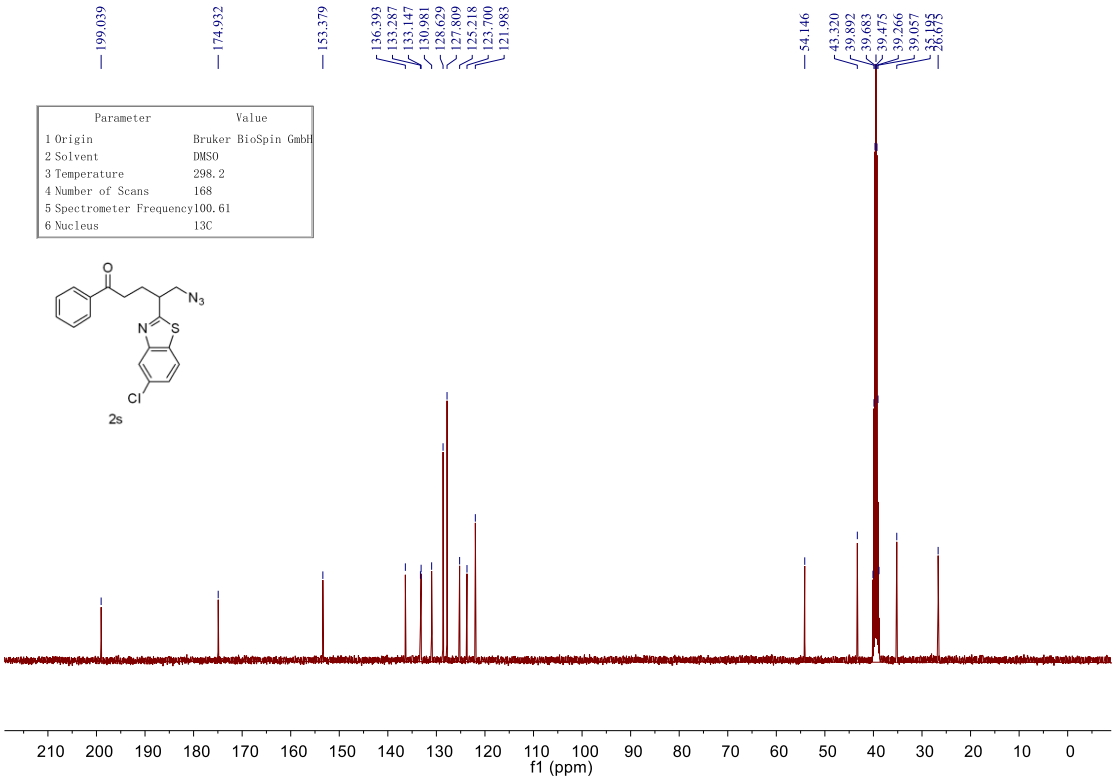
8.108
8.041
8.036
7.914
7.895
7.617
7.599
7.580
7.497
7.483
7.478
7.462
7.458
3.890
3.882
3.877
3.864
3.616
3.599
3.584
3.143
3.124
3.106
3.088
2.500
2.196
2.178
2.160
2.142
Parameter Value
1 Origin Bruker BioSpin GmbH
2 Solvent DMSO
3 Temperature 298.2
4 Number of Scans 4
5 Spectrometer Frequency 400.13
6 Nucleus 1H
O
N3
N
S
Cl
2s
1.00
0.97
2.02
1.01
3.01
2.01
1.02
2.00
2.00
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 -0.5
f1 (ppm)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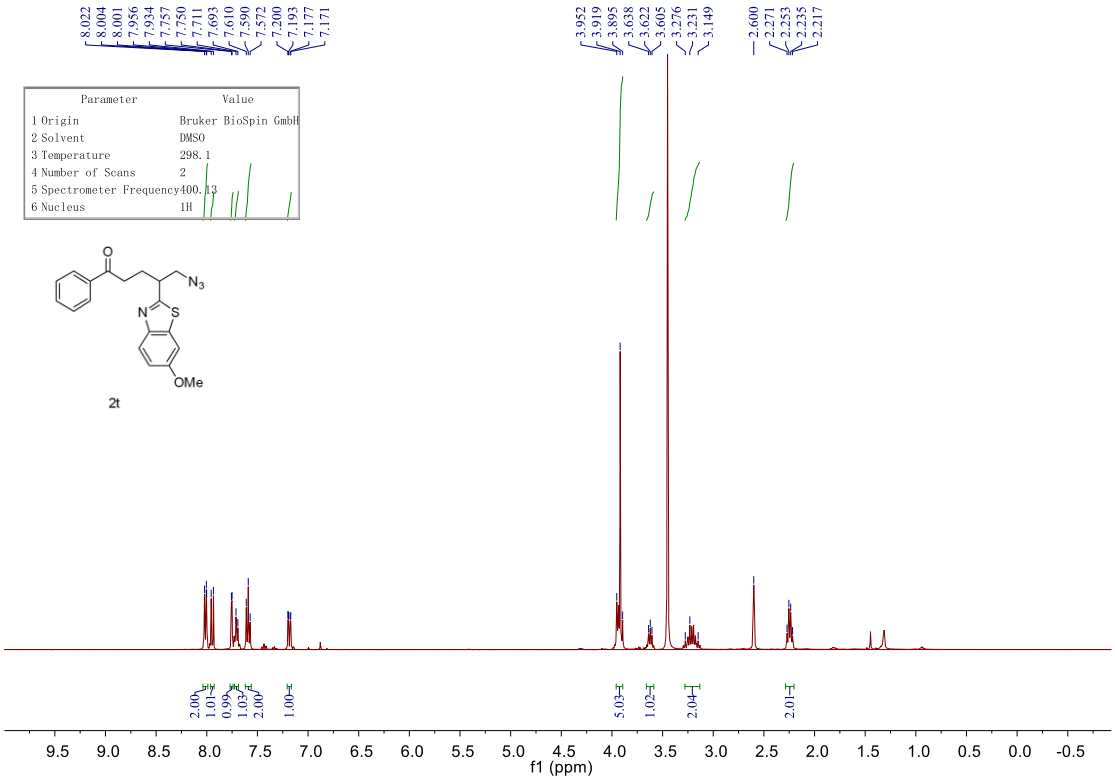
174.932
153.379
136.393
133.287
133.147
130.981
128.629
127.809
125.218
123.700
121.983
54.146
43.320
39.892
39.683
39.475
39.266
39.057
35.195
26.675
Parameter Value
1 Origin Bruker BioSpin GmbH
2 Solvent DMSO
3 Temperature 298.2
4 Number of Scans 168
5 Spectrometer Frequency 100.61
6 Nucleus 13C
O
N3
N
S
Cl
2s
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)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8.004
8.001
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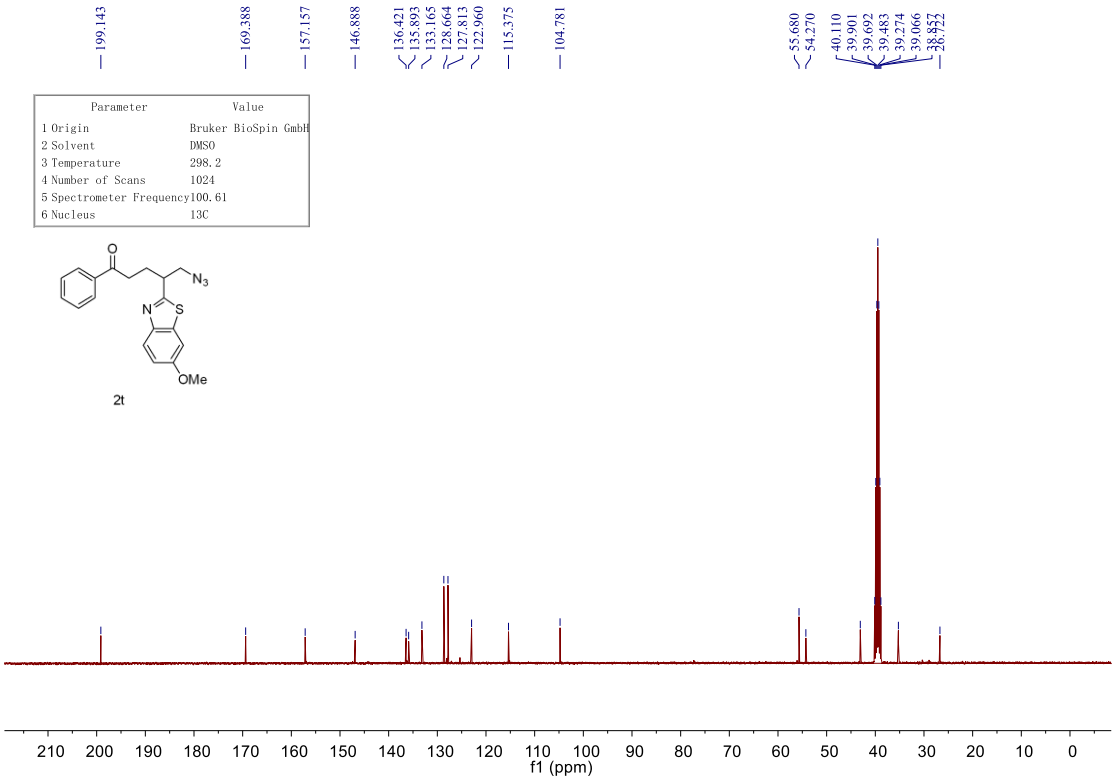
7.934
7.757
7.750
7.711
7.693
7.610
7.590
7.572
7.200
7.193
7.177
7.171
3.952
3.919
3.895
3.638
3.622
3.605
3.276
3.231
3.149
2.600
2.271
2.253
2.235
2.217
Parameter Value
1 Origin Bruker BioSpin GmbH
2 Solvent DMSO
3 Temperature 298.1
4 Number of Scans 2
5 Spectrometer Frequency 400.13
6 Nucleus 1H
O
N3
N
S
OMe
2t
2.00
1.01
0.99
1.03
2.00
1.00
5.03
1.02
2.04
2.01
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 -0.5
f1 (ppm)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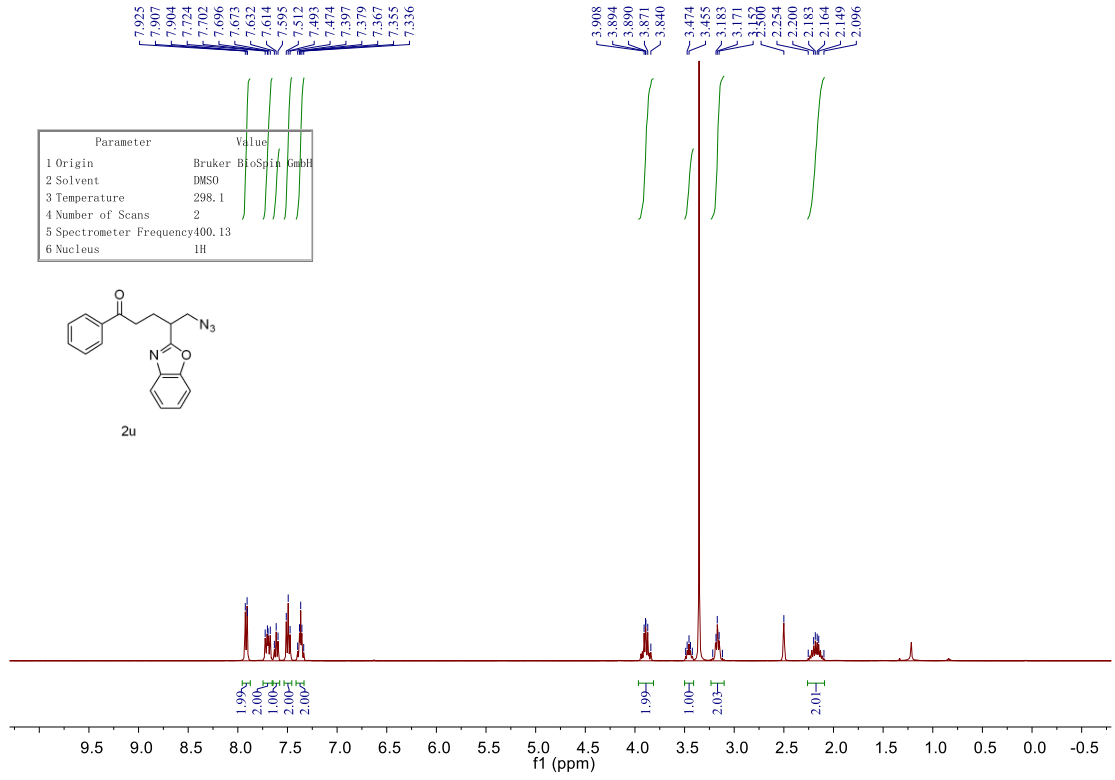
169.388
157.157
146.888
136.421
135.893
133.165
128.664
127.813
122.960
115.375
104.781
55.680
54.270
40.110
39.901
39.692
39.483
39.274
39.066
38.857
26.722
Parameter Value
1 Origin Bruker BioSpin GmbH
2 Solvent DMSO
3 Temperature 298.2
4 Number of Scans 1024
5 Spectrometer Frequency 100.61
6 Nucleus 13C
O
N3
N
S
OMe
2t
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)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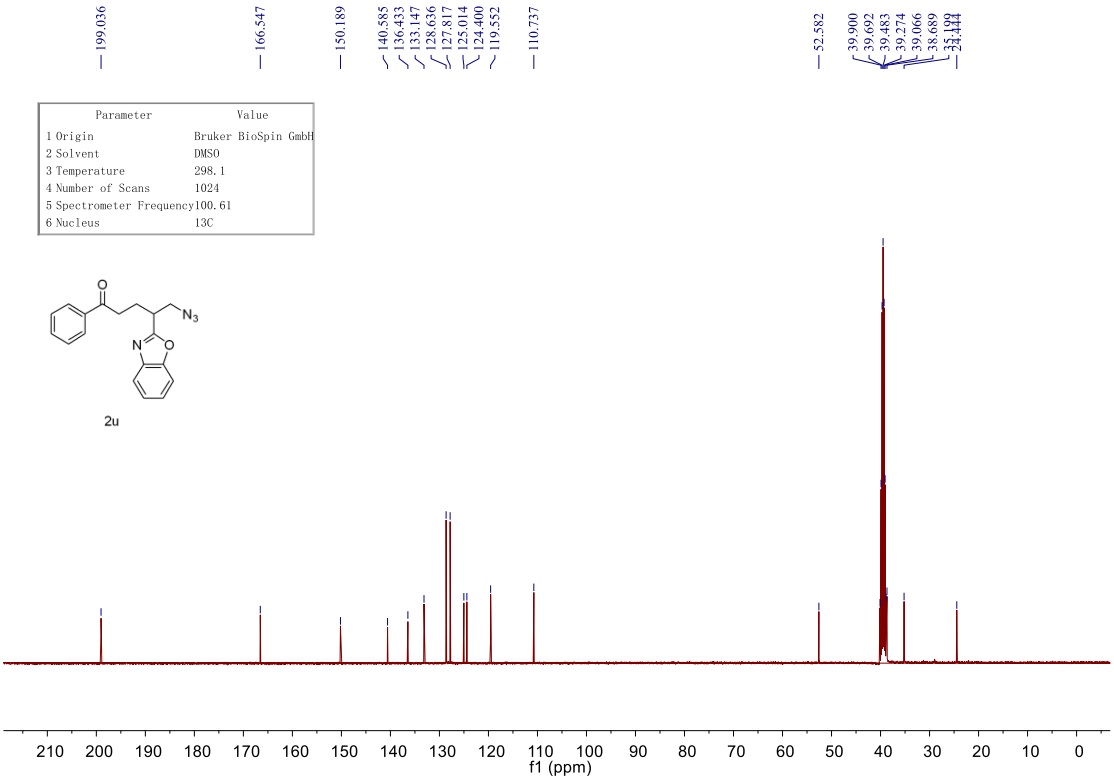
7.907
7.904
7.724
7.702
7.696
7.673
7.632
7.614
7.595
7.512
7.493
7.474
7.397
7.379
7.367
7.355
7.336
3.908
3.894
3.890
3.871
3.840
3.474
3.455
3.183
3.171
3.152
2.506
2.254
2.200
2.183
2.164
2.149
2.096
Parameter Value
1 Origin Bruker BioSpin GmbH
2 Solvent DMSO
3 Temperature 298.1
4 Number of Scans 2
5 Spectrometer Frequency 400.13
6 Nucleus 1H
O
N3
N
O
2u
1.99
2.00
1.00
2.00
2.00
1.99
1.00
2.03
2.01
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 -0.5
f1 (ppm)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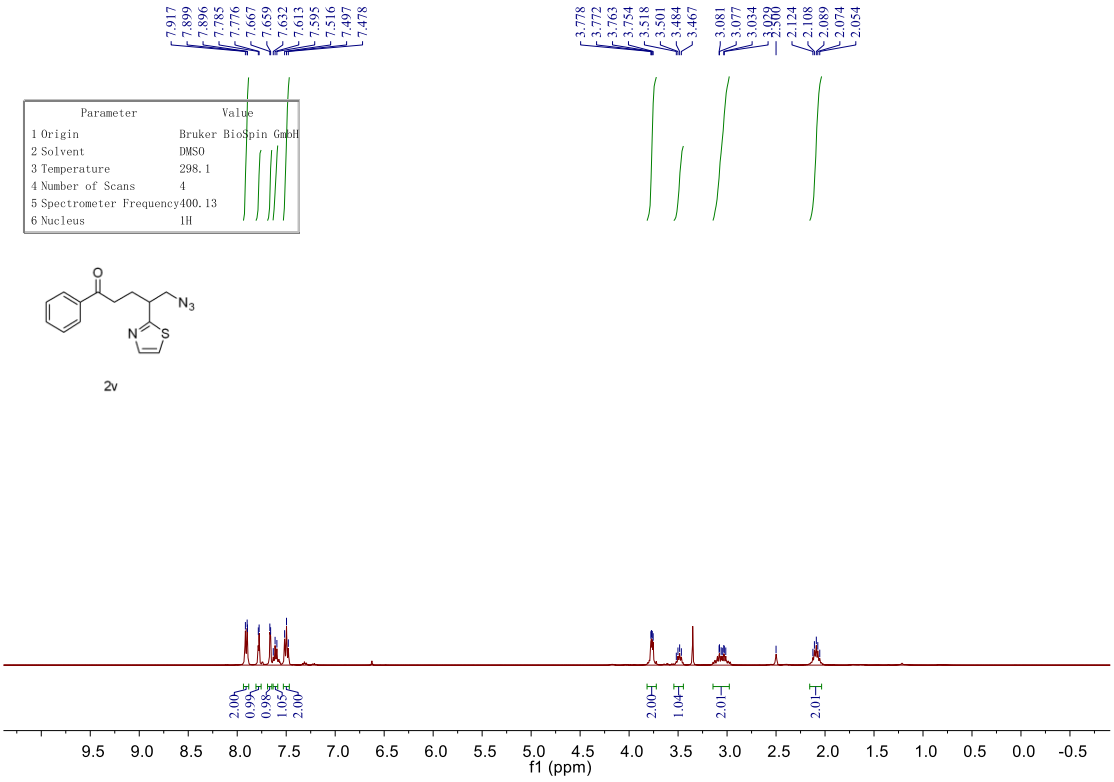
150.189
140.585
136.433
133.147
128.636
127.817
125.014
124.400
119.552
110.737
52.582
39.900
39.692
39.483
39.274
39.066
38.689
35.199
24.444
Parameter Value
1 Origin Bruker BioSpin GmbH
2 Solvent DMSO
3 Temperature 298.1
4 Number of Scans 1024
5 Spectrometer Frequency 100.61
6 Nucleus 13C
O
N3
N
O
2u
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)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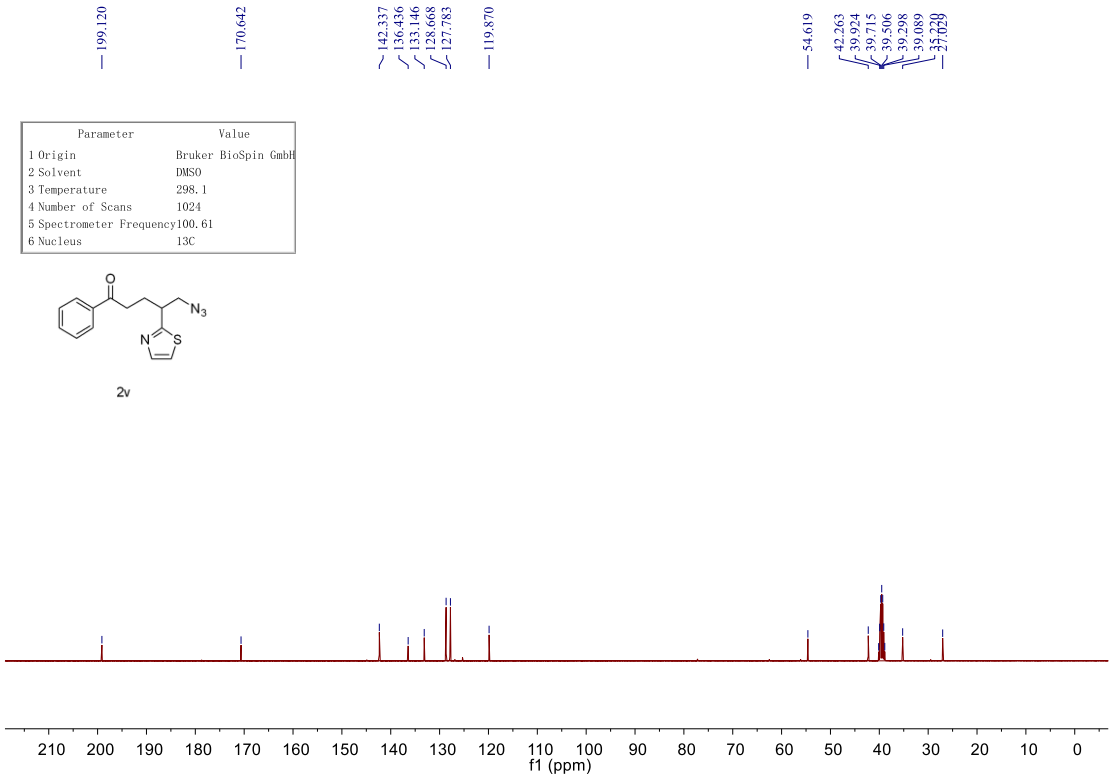
7.899
7.896
7.785
7.776
7.667
7.659
7.632
7.613
7.595
7.516
7.497
7.478
3.778
3.772
3.763
3.754
3.518
3.501
3.484
3.467
3.081
3.077
3.034
3.029
2.500
2.124
2.108
2.089
2.074
2.054
Parameter Value
1 Origin Bruker BioSpin GmbH
2 Solvent DMSO
3 Temperature 298.1
4 Number of Scans 4
5 Spectrometer Frequency 400.13
6 Nucleus 1H
O
N3
N
S
2v
2.00
0.99
0.98
1.05
2.00
2.00
1.04
2.01
2.01
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 -0.5
f1 (ppm)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142.337
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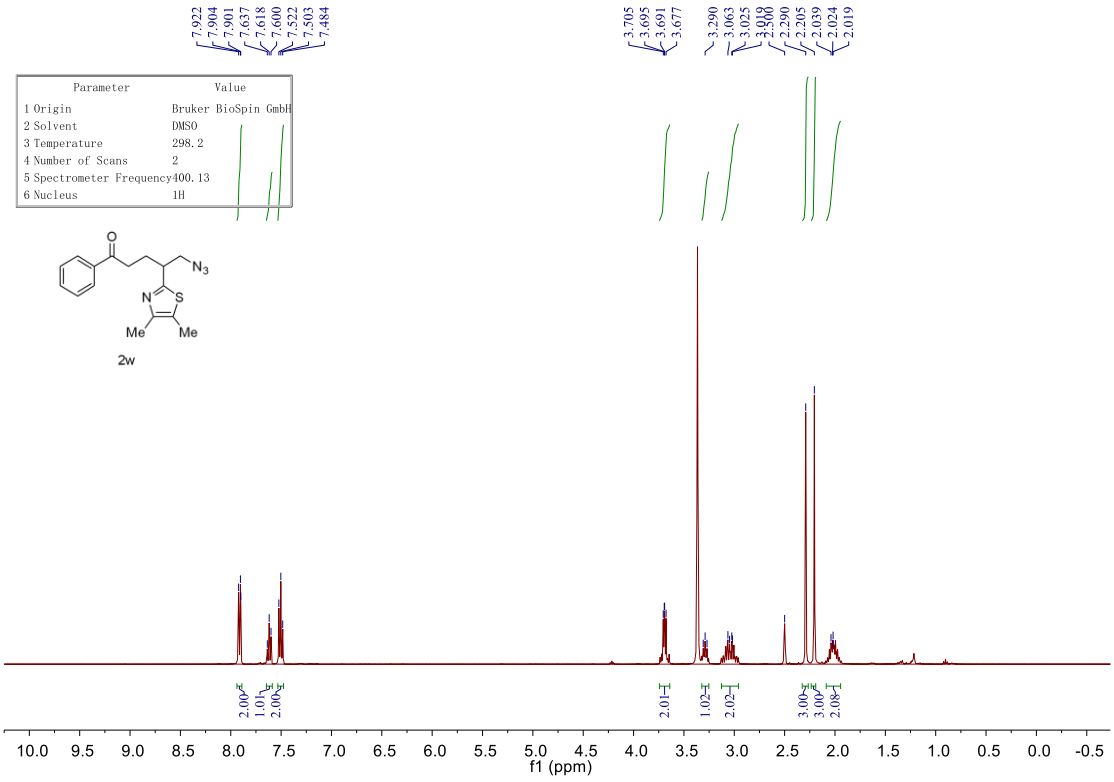
133.146
128.668
127.783
119.870
54.619
42.263
39.924
39.715
39.506
39.298
39.089
35.220
27.029
Parameter Value
1 Origin Bruker BioSpin GmbH
2 Solvent DMSO
3 Temperature 298.1
4 Number of Scans 1024
5 Spectrometer Frequency 100.61
6 Nucleus 13C
O
N3
N
S
2v
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)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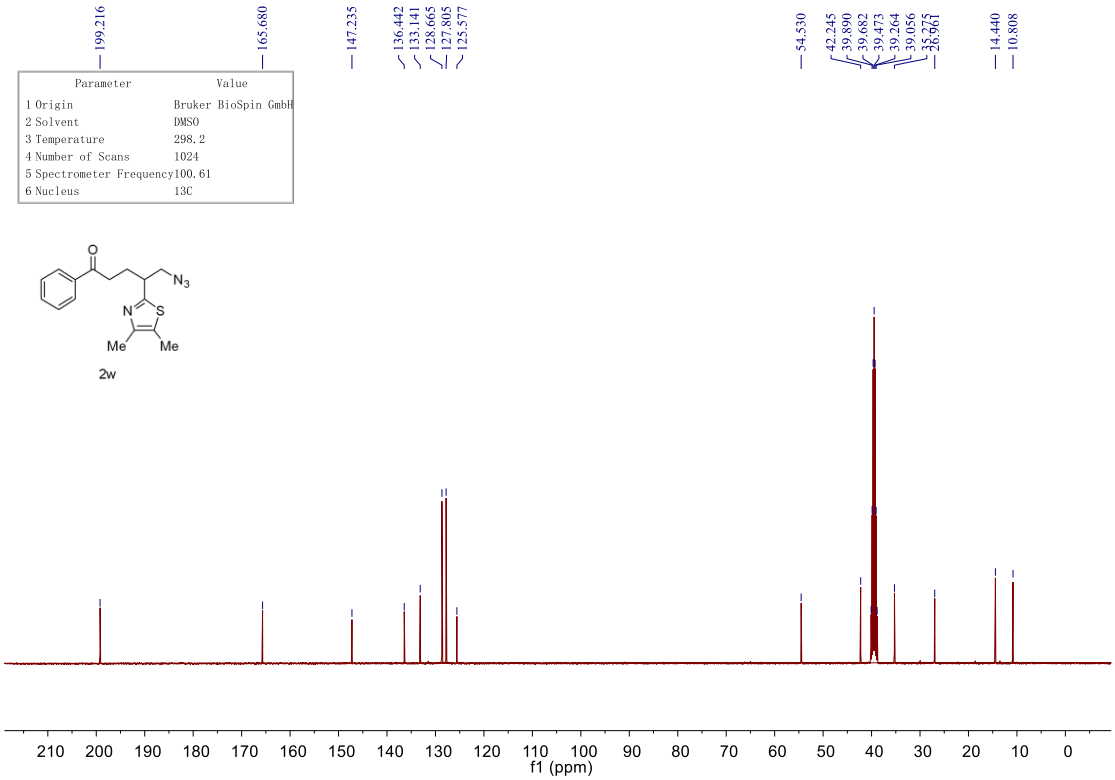
7.904
7.901
7.637
7.618
7.600
7.522
7.503
7.484
3.705
3.695
3.691
3.677
3.290
3.063
3.025
3.008
3.000
2.290
2.205
2.039
2.024
2.019
Parameter Value
1 Origin Bruker BioSpin GmbH
2 Solvent DMSO
3 Temperature 298.2
4 Number of Scans 2
5 Spectrometer Frequency 400.13
6 Nucleus 1H
O
N3
N
S
Me
Me
2w
2.00
1.01
2.00
2.01
1.02
2.02
3.00
3.00
2.08
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 -0.5
f1 (ppm)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136.442
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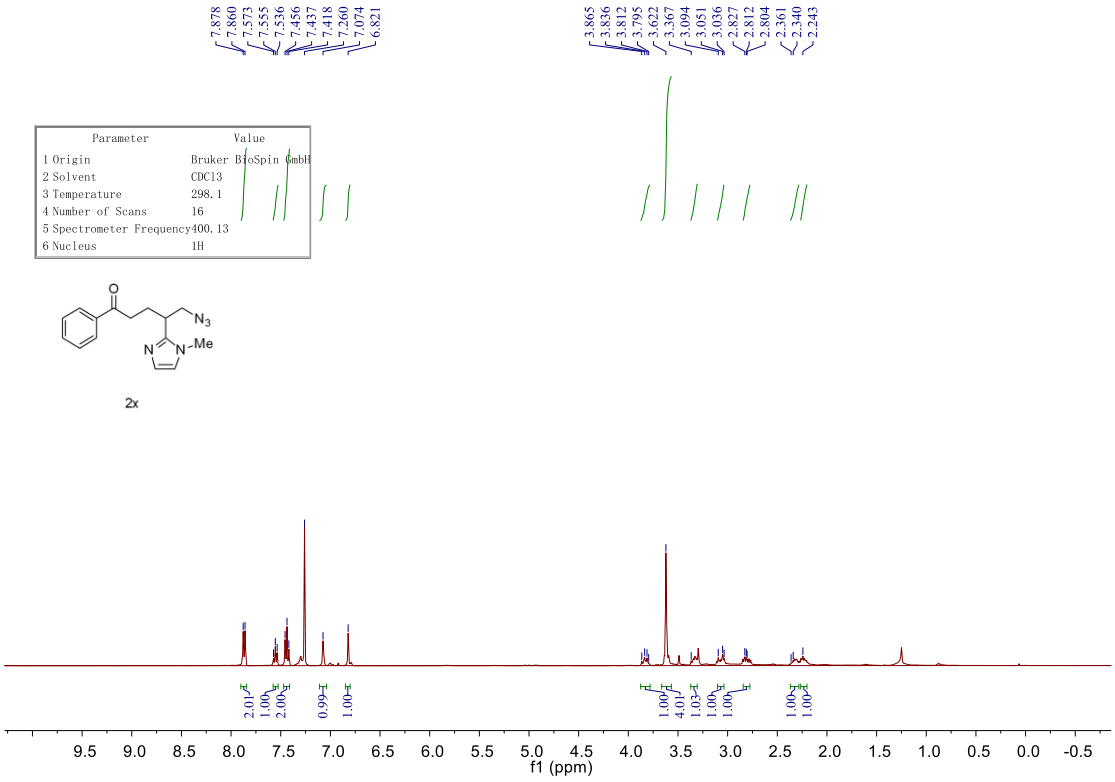
128.665
127.805
125.577
54.530
42.245
39.890
39.682
39.473
39.264
39.056
38.975
38.961
14.440
10.808
Parameter Value
1 Origin Bruker BioSpin GmbH
2 Solvent DMSO
3 Temperature 298.2
4 Number of Scans 1024
5 Spectrometer Frequency 100.61
6 Nucleus 13C
O
N3
N
S
Me
Me
2w
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)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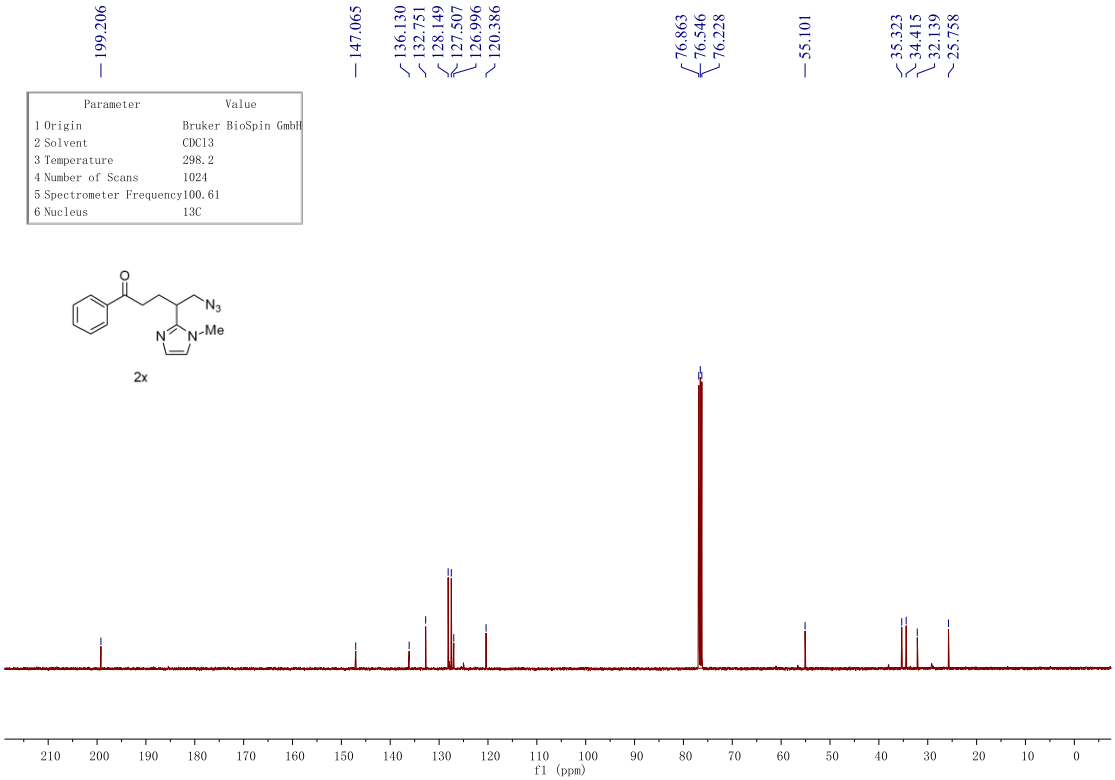
7.536
7.456
7.437
7.418
7.260
7.074
6.821
3.865
3.836
3.812
3.795
3.622
3.367
3.094
3.051
3.036
2.827
2.812
2.804
2.361
2.340
2.243
Parameter Value
1 Origin Bruker BioSpin GmbH
2 Solvent CDCl3
3 Temperature 298.1
4 Number of Scans 16
5 Spectrometer Frequency 400.13
6 Nucleus 1H
O
N3
N
N
Me
2x
2.01
1.00
2.00
0.99
1.00
1.00
4.01
1.03
1.00
1.00
1.00
1.00
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 -0.5
f1 (ppm)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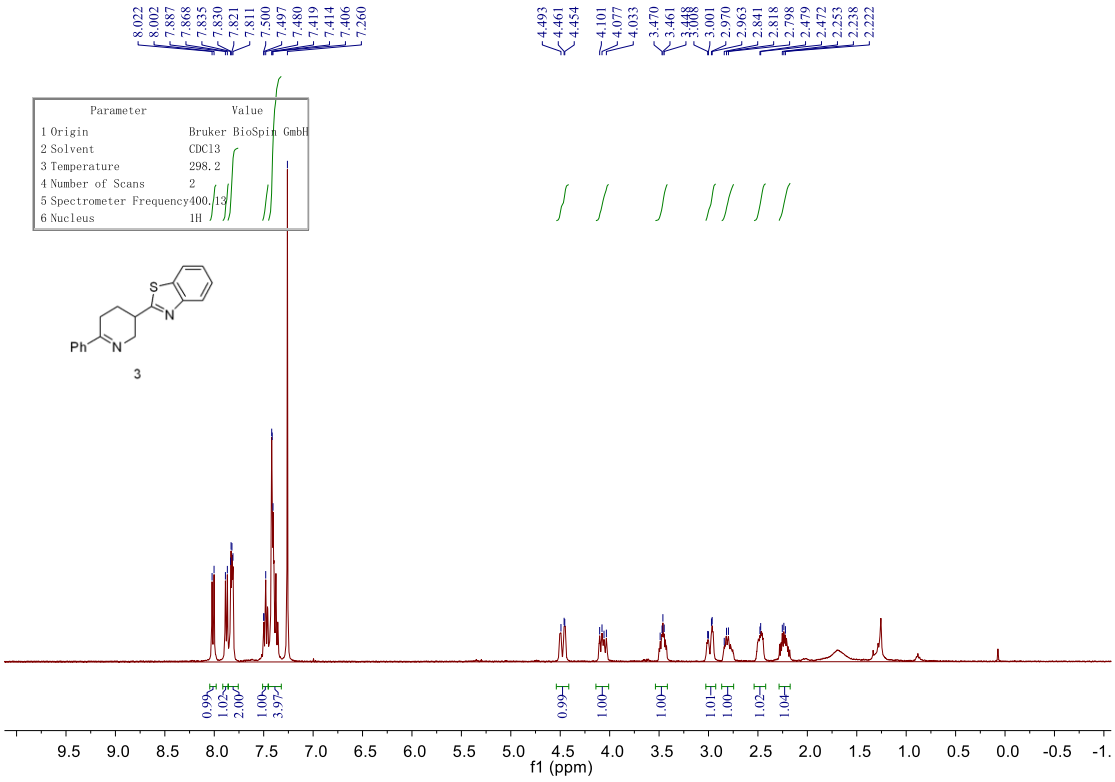
127.507
126.996
120.386
76.863
76.546
76.228
55.101
35.323
34.415
32.139
25.758
Parameter Value
1 Origin Bruker BioSpin GmbH
2 Solvent CDCl3
3 Temperature 298.2
4 Number of Scans 1024
5 Spectrometer Frequency 100.61
6 Nucleus 13C
O
N3
N
N
Me
2x
f1 (ppm)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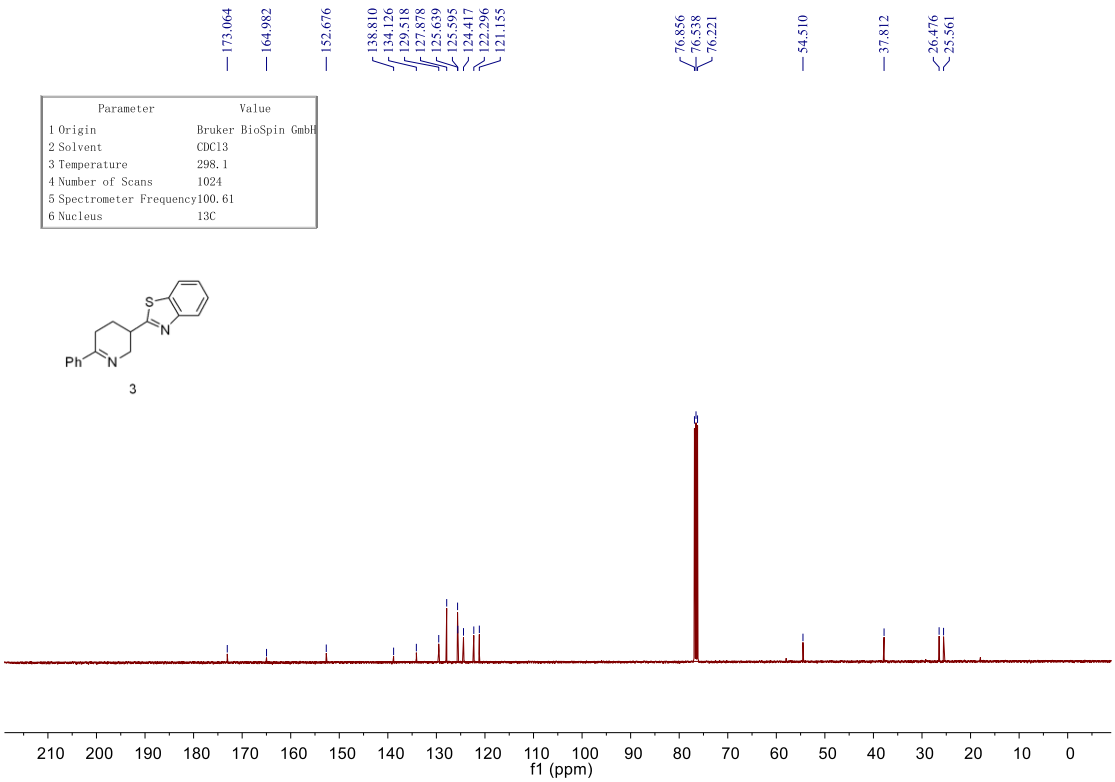
7.830
7.821
7.811
7.500
7.497
7.480
7.419
7.414
7.406
7.260
4.493
4.461
4.454
4.101
4.077
4.033
3.470
3.461
3.448
3.008
3.001
2.970
2.963
2.841
2.818
2.798
2.479
2.472
2.253
2.238
2.222
Parameter Value
1 Origin Bruker BioSpin GmbH
2 Solvent CDCl3
3 Temperature 298.2
4 Number of Scans 2
5 Spectrometer Frequency 400.13
6 Nucleus 1H
S
N
Ph
N
3
0.99
1.02
2.00
1.00
3.97
0.99
1.00
1.00
1.01
1.00
1.02
1.04
f1 (ppm)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164.982
152.676
138.810
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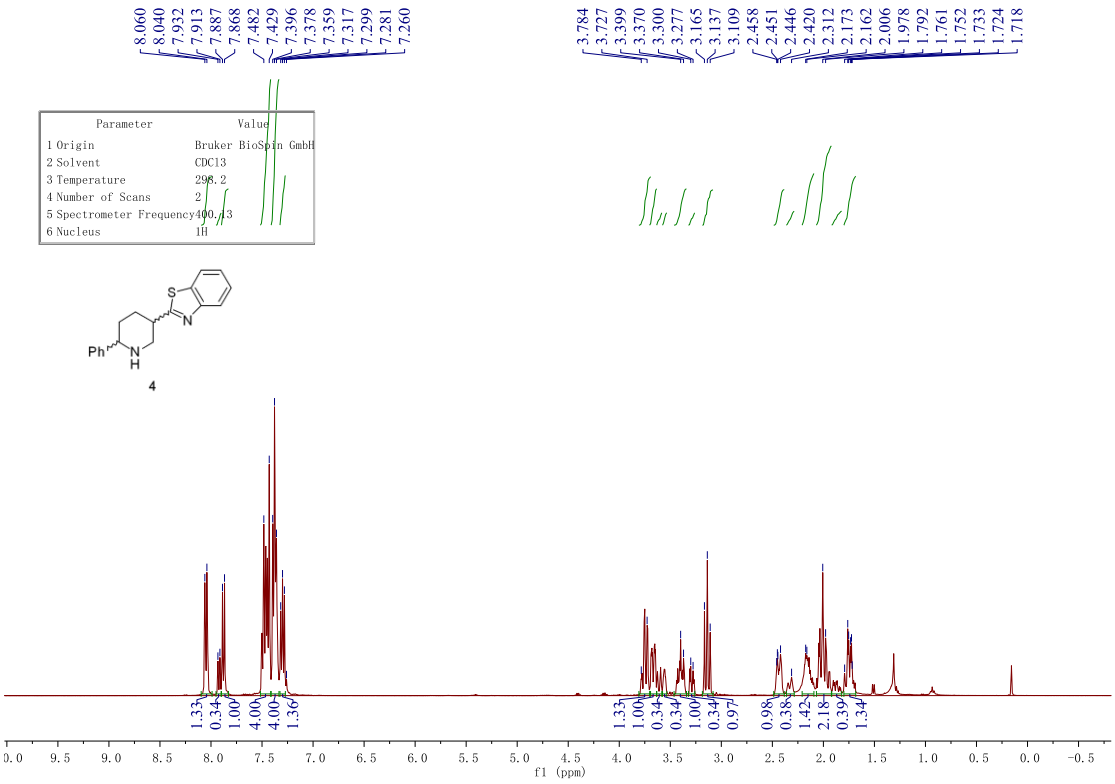
129.518
127.878
125.639
125.595
124.417
122.296
121.155
76.856
76.538
76.221
54.510
37.812
26.476
25.561
Parameter Value
1 Origin Bruker BioSpin GmbH
2 Solvent CDCl3
3 Temperature 298.1
4 Number of Scans 1024
5 Spectrometer Frequency 100.61
6 Nucleus 13C
S
N
Ph
N
3
f1 (ppm)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7.429
7.396
7.378
7.359
7.317
7.299
7.281
7.260
3.784
3.727
3.399
3.370
3.300
3.277
3.165
3.137
3.109
2.458
2.451
2.446
2.420
2.312
2.173
2.162
2.006
1.978
1.792
1.761
1.752
1.733
1.724
1.718
Parameter Value
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
S
N
Ph
N
H
4
1.33
0.34
1.00
4.00
4.00
1.36
1.33
1.00
0.34
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1.00
0.34
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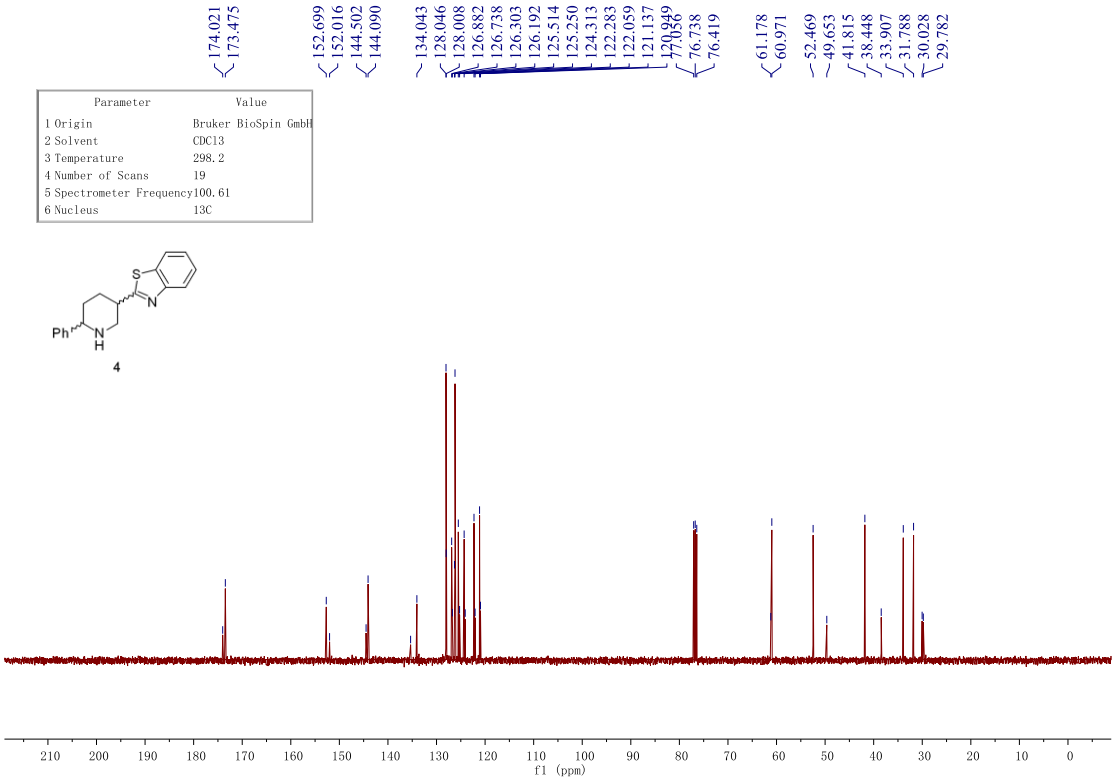
0.98
0.38
1.42
2.18
0.39
1.34
f1 (ppm)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152.699
152.016
144.502
144.090
134.043
128.046
128.008
126.882
126.738
126.303
126.192
125.514
125.250
124.313
122.283
122.059
121.137
120.949
77.056
76.738
76.419
61.178
60.971
52.469
49.653
41.815
38.448
33.907
31.788
30.028
29.782
Parameter Value
1 Origin Bruker BioSpin GmbH
2 Solvent CDCl3
3 Temperature 298.2
4 Number of Scans 19
5 Spectrometer Frequency 100.61
6 Nucleus 13C
Ph
N
H
S
N
4
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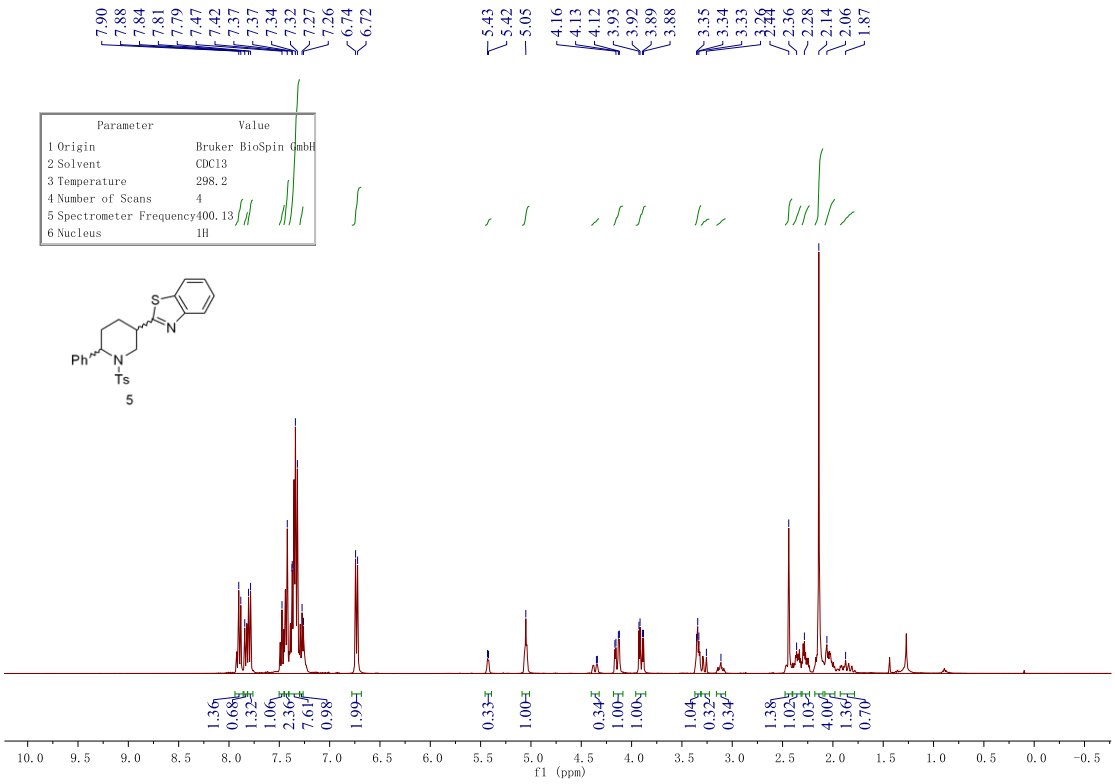
f1 (ppm)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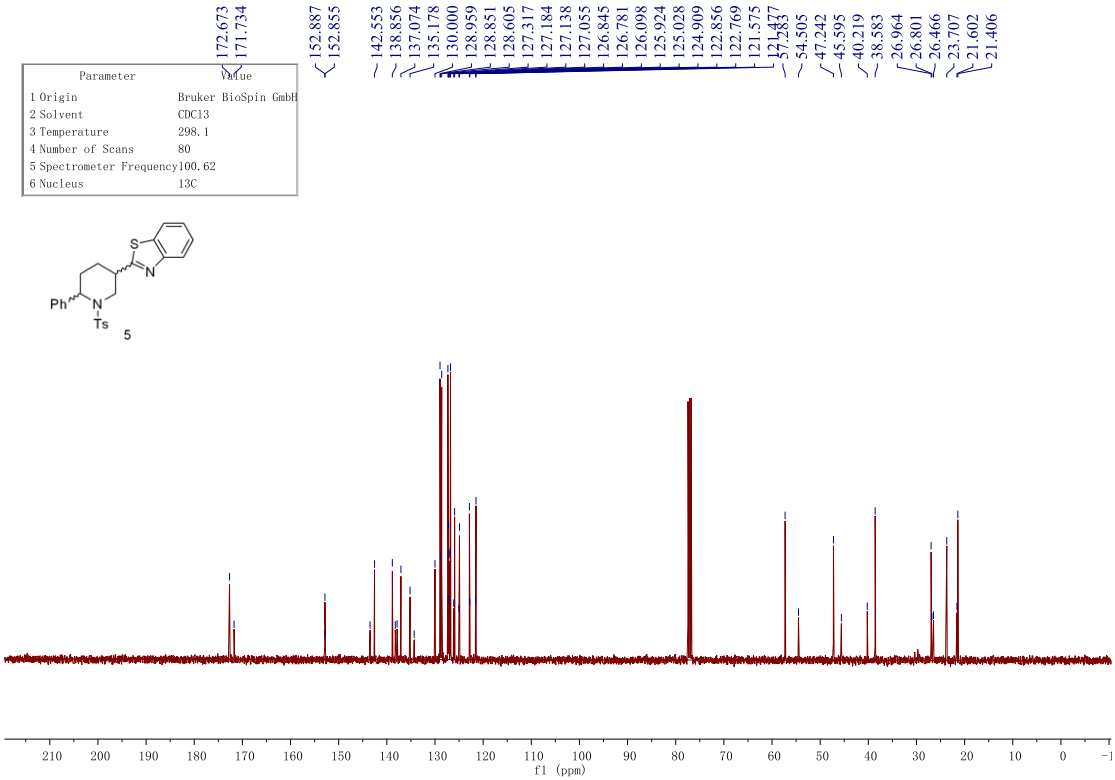
7.37
7.37
7.34
7.32
7.27
7.26
6.74
6.72
5.43
5.42
5.05
4.16
4.13
4.12
3.93
3.92
3.89
3.88
3.35
3.34
3.33
2.44
2.36
2.28
2.14
2.06
1.87
Parameter Value
1 Origin Bruker BioSpin GmbH
2 Solvent CDCl3
3 Temperature 298.2
4 Number of Scans 4
5 Spectrometer Frequency 400.13
6 Nucleus 1H
Ph
N
Ts
S
N
5
1.36
0.68
1.32
1.06
2.36
7.61
0.98
1.99
0.33
1.00
0.34
1.00
1.00
1.04
0.32
0.34
1.38
1.02
1.03
4.00
1.36
0.70
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 -0.5
f1 (ppm)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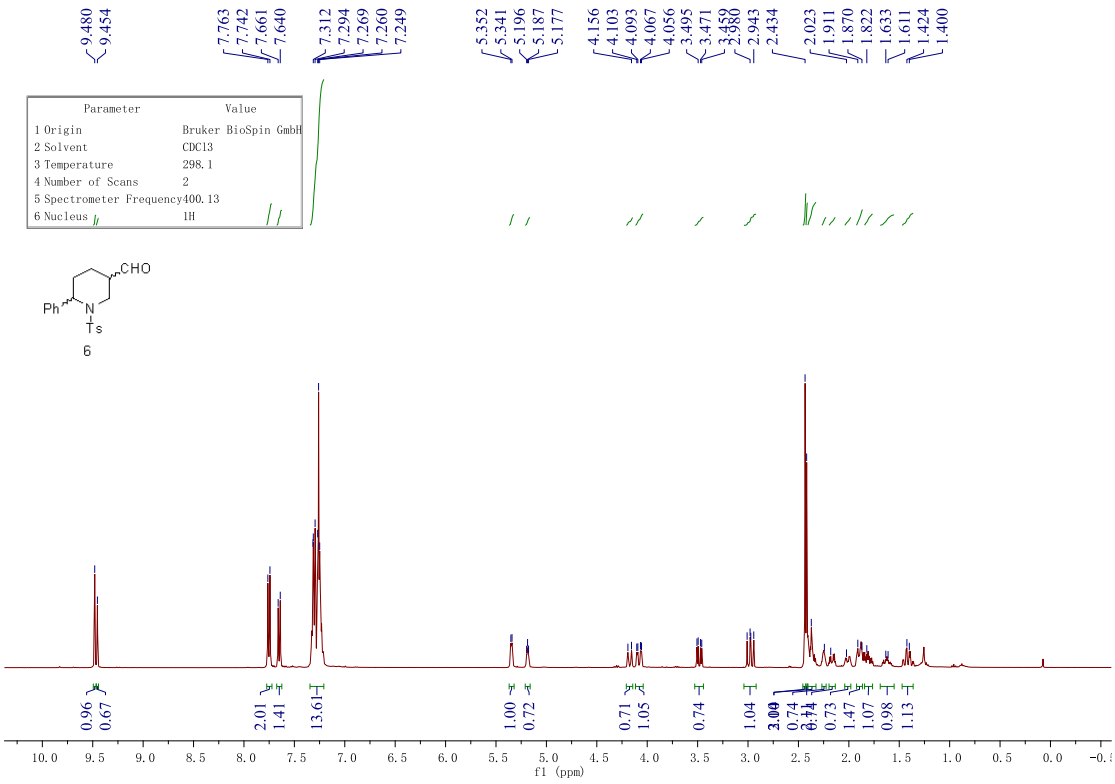
127.184
127.138
127.055
126.845
126.781
126.098
125.924
125.028
124.909
122.856
122.769
121.575
121.477
57.283
54.505
47.242
45.595
40.219
38.583
26.964
26.801
26.466
23.707
21.602
21.406
Parameter Value
1 Origin Bruker BioSpin GmbH
2 Solvent CDCl3
3 Temperature 298.1
4 Number of Scans 80
5 Spectrometer Frequency 100.62
6 Nucleus 13C
S
N
Ph
N
Ts
5
f1 (ppm)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7.294
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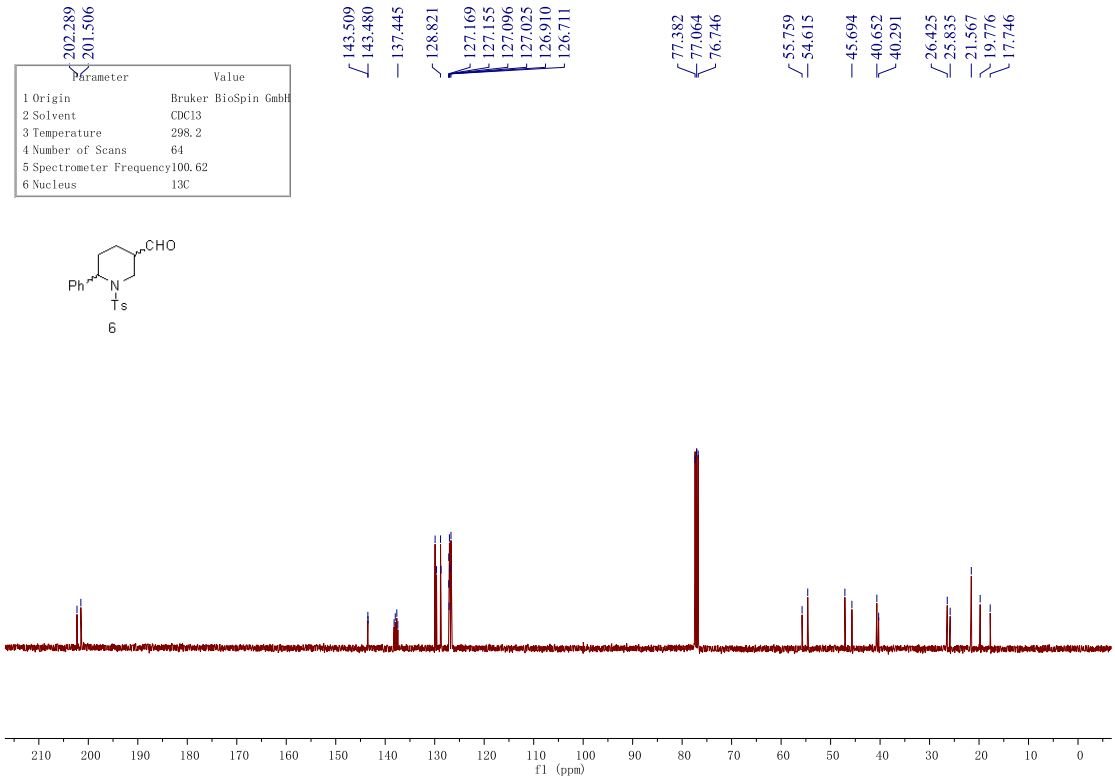
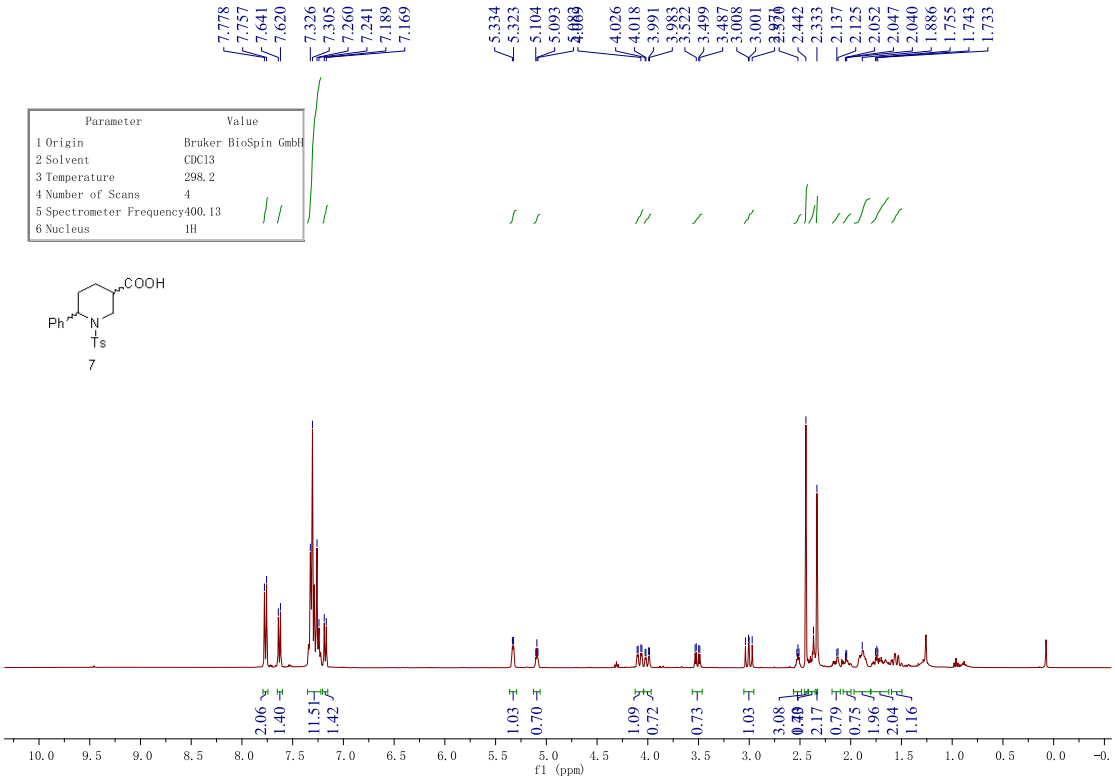
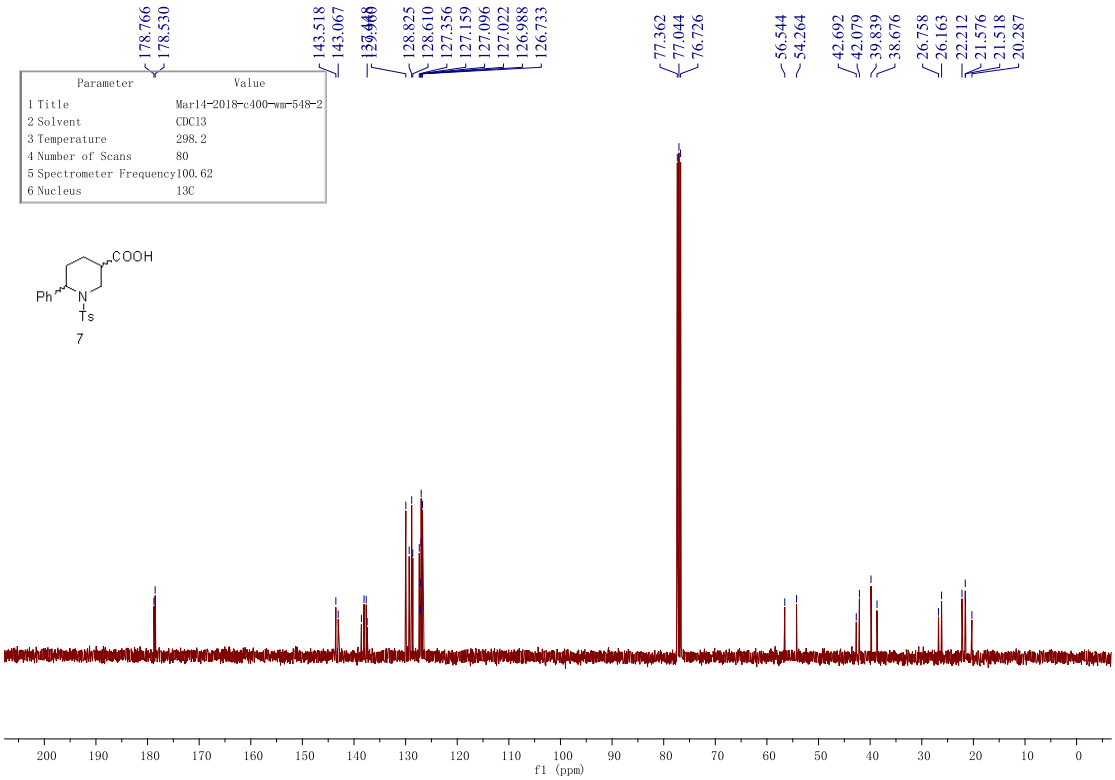
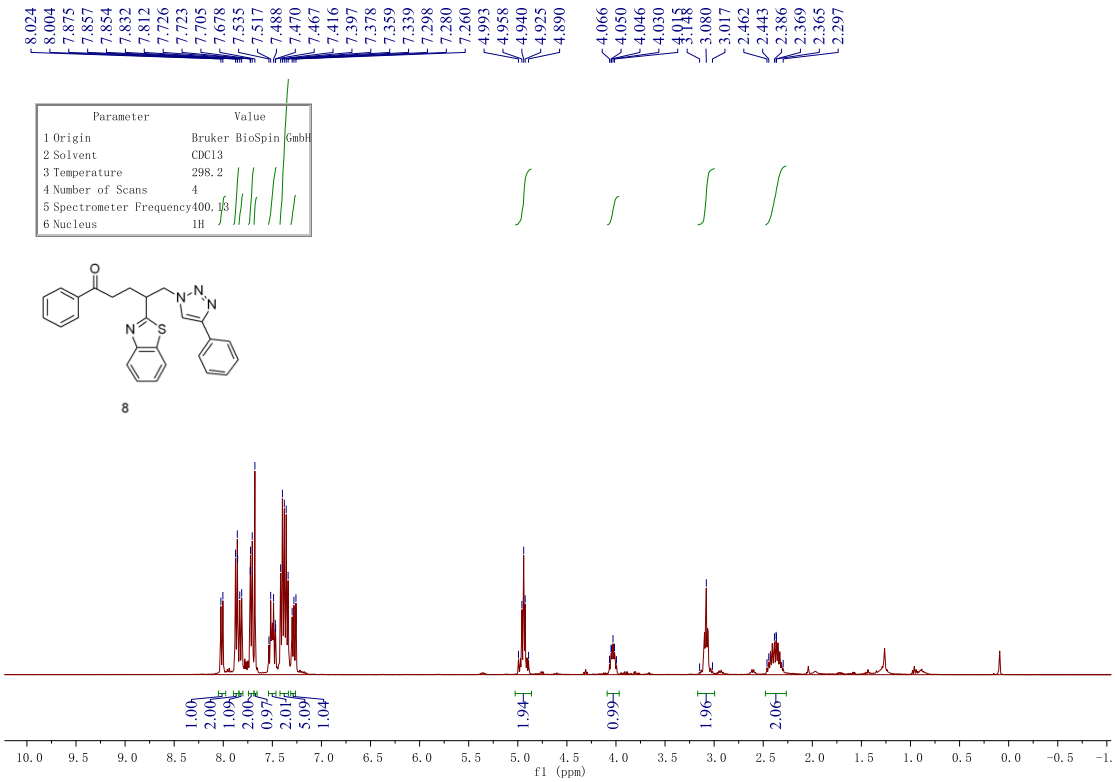
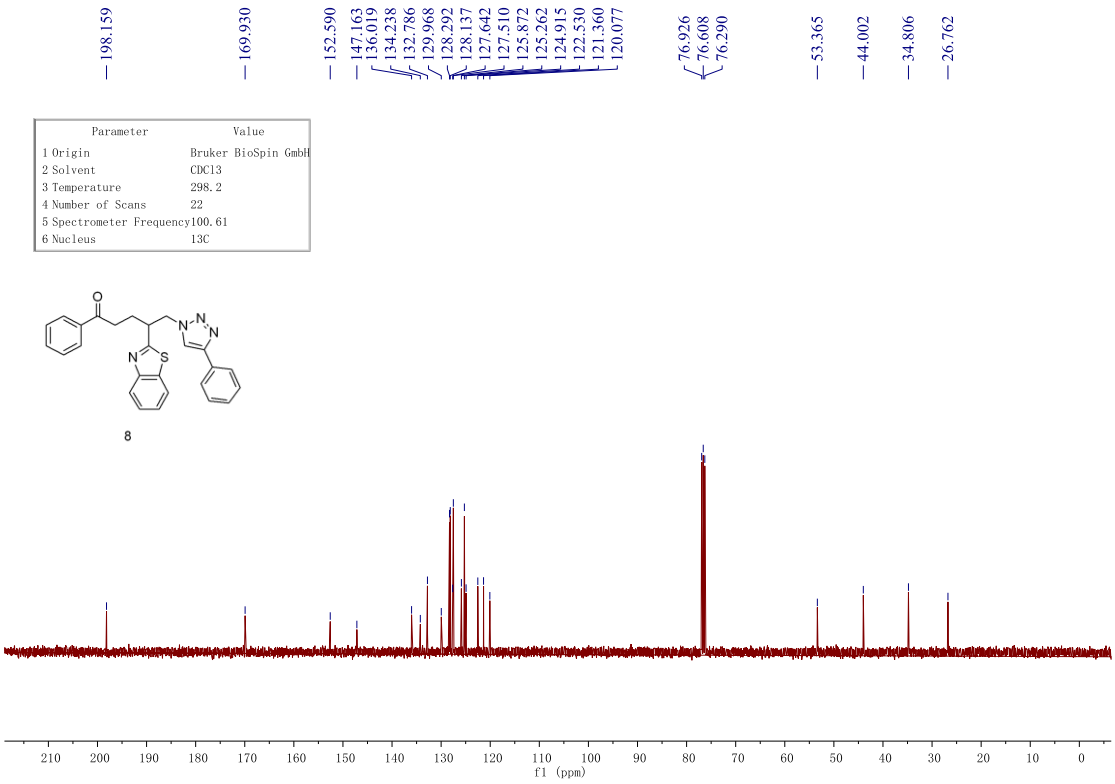
7.260
7.249
5.352
5.341
5.196
5.187
5.177
4.156
4.103
4.093
4.067
4.056
3.495
3.471
3.459
2.980
2.943
2.434
2.023
1.911
1.870
1.822
1.633
1.611
1.424
1.400
Parameter Value
1 Origin Bruker BioSpin GmbH
2 Solvent CDCl3
3 Temperature 298.1
4 Number of Scans 2
5 Spectrometer Frequency 400.13
6 Nucleus 1H
CHO
Ph
N
Ts
6
0.96
0.67
2.01
1.41
13.61
1.00
0.72
0.71
1.05
0.74
1.04
0.74
0.71
0.73
1.47
1.07
0.98
1.13
f1 (ppm)


202.289
201.506
143.509
143.480
137.445
128.821
127.169
127.155
127.096
127.025
126.910
126.711
77.382
77.064
76.746
55.759
54.615
45.694
40.652
40.291
26.425
25.835
21.567
19.776
17.746
Parameter Value
1 Origin Bruker BioSpin GmbH
2 Solvent CDCl3
3 Temperature 298.2
4 Number of Scans 64
5 Spectrometer Frequency 100.62
6 Nucleus 13C
CHO
Ph
N
Ts
6
f1 (ppm)


7.778
7.757
7.641
7.620
7.326
7.305
7.260
7.241
7.189
7.169
5.334
5.323
5.104
5.093
4.026
4.018
3.991
3.983
3.522
3.499
3.487
3.008
3.001
2.442
2.333
2.137
2.125
2.052
2.047
2.040
1.886
1.755
1.743
1.733
Parameter Value
1 Origin Bruker BioSpin GmbH
2 Solvent CDCl3
3 Temperature 298.2
4 Number of Scans 4
5 Spectrometer Frequency 400.13
6 Nucleus 1H
COOH
Ph
N
Ts
7
2.06
1.40
11.51
1.42
1.03
0.70
1.09
0.72
0.73
1.03
3.08
2.17
0.79
0.75
1.96
2.04
1.16
f1 (ppm)


178.766
178.530
143.518
143.067
128.825
128.610
127.356
127.159
127.096
127.022
126.988
126.733
77.362
77.044
76.726
56.544
54.264
42.692
42.079
39.839
38.676
26.758
26.163
22.212
21.576
21.518
20.287
Parameter Value
1 Title Mar14-2018-c400-wwm-548-2
2 Solvent CDCl3
3 Temperature 298.2
4 Number of Scans 80
5 Spectrometer Frequency 100.62
6 Nucleus 13C
COOH
Ph
N
Ts
7
f1 (ppm)


8.024
8.004
7.875
7.857
7.854
7.832
7.812
7.726
7.723
7.705
7.678
7.535
7.517
7.488
7.470
7.467
7.416
7.397
7.378
7.359
7.339
7.298
7.280
7.260
4.993
4.958
4.940
4.925
4.890
4.066
4.050
4.046
4.030
4.015
4.008
3.148
3.080
3.017
2.462
2.443
2.386
2.369
2.365
2.297
Parameter Value
1 Origin Bruker BioSpin GmbH
2 Solvent CDCl3
3 Temperature 298.2
4 Number of Scans 4
5 Spectrometer Frequency 400.13
6 Nucleus 1H
O
N
N
N
S
8
1.00
2.00
1.09
2.00
0.97
2.01
5.09
1.04
1.94
0.99
1.96
2.06
f1 (ppm)


198.159
169.930
152.590
147.163
136.019
134.238
132.786
129.968
128.292
128.137
127.642
127.510
125.872
125.262
124.915
122.530
121.360
120.077
76.926
76.608
76.290
53.365
44.002
34.806
26.762
Parameter Value
1 Origin Bruker BioSpin GmbH
2 Solvent CDCl3
3 Temperature 298.2
4 Number of Scans 22
5 Spectrometer Frequency 100.61
6 Nucleus 13C
O
N
N
N
N
S
8
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)