Supporting Information

Manganese-Catalyzed Regiospecific sp^3 C-S Bond Formation through C-C Bond Cleavage of Cyclobutanols

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Table of Contents

1. General experimental details

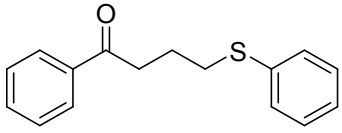
All reactions were maintained under a nitrogen atmosphere unless otherwise stated. Commercially available reagents were used without further purification. Infrared (FT-IR) spectra were recorded on a BRUKER VERTEX 70, ν_{max} in cm^{-1}. ^{1}H-NMR spectra were recorded on a BRUKER AVANCE III HD (400 MHz) spectrometer. Chemical shifts are reported in ppm from tetramethylsilane with the solvent resonance as internal standard ($CDCl_3$: δ 7.26). 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 77.16). ^{19}F-NMR spectra were recorded on a BRUKER AVANCE III HD (376 MHz) spectrometer. Mass spectra were measured with an Agelent 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.

Tertiary cyclobutanols were prepared by the addition of Grignard reagent to the corresponding cyclobutanones according to the reported procedures.[1]

2. General procedure for the synthesis of thioethers

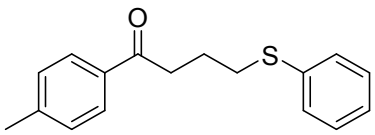
Cyclobutanol **1** (0.2 mmol, 1.0 equiv), $Mn(OAc)_3{\cdot}2H_2O$ (0.04 mmol, 0.2 equiv), Bipy (0.044 mmol, 0.22 equiv), ArSSAr (0.6 mmol, 3.0 equiv) and BI-OH (0.6 mmol, 3.0 equiv) were loaded in a flask which was subjected to evacuation/flushing with nitrogen three times. CH_3CN (1.5 mL) was added to the mixture via syringe and the mixture was then stirred at 25 °C for about 1 h. Subsequently, the reaction which was allowed for stirring at 70 °C until the starting material had been consumed as determined by TLC. The reaction mixture was extracted with EtOAc (3× 10 mL). The combined organic layers were washed by brine, dried over Na_2SO_4, filtered, concentrated, and purified by flash chromatography on silica gel (ethyl acetate/petroleum ether) to give the product **2**.

3. Characterization of products

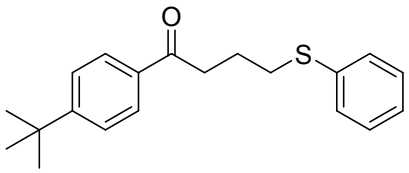


2a: yellow solid, m.p. 36-37 °C. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.96-7.92 (m, 2H), 7.58-7.53 (m, 1H), 7.48-7.42 (m, 2H), 7.37-7.33 (m, 2H), 7.30-7.25 (m, 2H), 7.19-7.14 (m, 1H), 3.14 (t, *J* = 7.2 Hz, 2H), 3.04 (t, *J* = 7.2 Hz, 2H), 2.13-2.06 (m, 2H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 199.0, 136.4, 135.7, 132.6, 128.8, 128.5, 128.1, 127.6, 125.5, 36.5, 32.6, 23.0. FT-IR: ν (cm^{-1}) 3050, 2954, 2917, 1676, 1595, 1470, 1448, 1368, 1191. HRMS [ESI] ~~calcd for $C_{16}H_{17}OS$ $[M+H]^+$ 257.1~~000, found 257.1001.

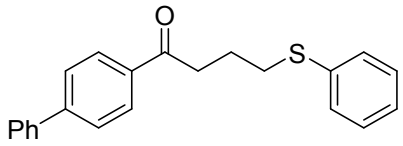
[1] (a) B. M. Casey, C. A. Eakin and R. A. Flowers, II, *Tetrahedron Lett.,* **2009**, *50*, 1264-1266; (b) H.-J. Xu, F.-F. Zhu, Y.-Y. Shen, X. Wan and Y.-S. Feng, *Tetrahedron,* **2012**, *68*, 4145-4151; (c) D. Rosa, A. Chtchemelinine and A. Orellana, *Synthesis,* **2012**, *12*, 1885-1891.



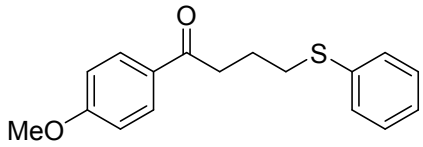
2b: yellow solid, m.p. 46-47 °C. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.84 (d, *J* = 8.4 Hz, 2H), 7.37-7.33 (m, 2H), 7.29-7.23 (m, 4H), 7.18-7.14 (m, 1H), 3.11 (t, *J* = 7.2 Hz, 2H), 3.03 (t, *J* = 7.2 Hz, 2H), 2.40 (s, 3H), 2.12-2.04 (m, 2H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 198.6, 143.4, 135.7, 133.9, 128.8, 128.7, 128.5, 127.7, 125.5, 36.4, 32.7, 23.1, 21.2. FT-IR: ν (cm^{-1}) 3061, 2918, 2850, 1670, 1605, 1478, 1307, 1230, 1180. HRMS [ESI] calcd for $C_{17}H_{19}OS$ $[M+H]^+$ 271.1157, found 217.1153.



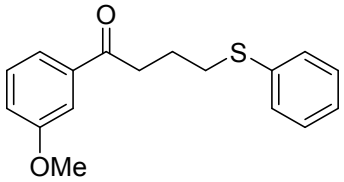
2c: yellow solid, m.p. 55-56 °C. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.89 (d, *J* = 8.4 Hz, 2H), 7.46 (d, *J* = 8.4 Hz, 2H), 7.37-7.33 (m, 2H), 7.27 (dd, *J* = 8.0, 7.2 Hz, 2H), 7.19-7.13 (m, 1H), 3.12 (t, *J* = 7.2 Hz, 2H), 3.03 (t, *J* = 7.2 Hz, 2H), 2.12-2.04 (m, 2H), 1.34 (s, 9H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 198.6, 156.3, 135.7, 133.8, 128.7, 128.5, 127.5, 125.5, 125.1, 36.4, 34.6, 32.7, 30.6, 23.1. FT-IR: ν (cm^{-1}) 3061, 2958, 2850, 1676, 1603, 1584, 1479, 1190, 1107. HRMS [ESI] calcd for $C_{20}H_{24}OSNa$ $[M+Na]^+$ 335.1446, found 335.1430.



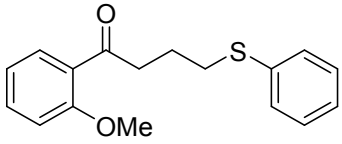
2d: white solid, m.p. 73-75 °C. ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.03-7.99 (m, 2H), 7.69-7.65 (m, 2H), 7.64-7.60 (m, 2H), 7.50-7.44 (m, 2H), 7.42-7.34 (m, 3H), 7.30-7.25 (m, 2H), 7.19-7.14 (m, 1H), 3.17 (t, *J* = 7.2 Hz, 2H), 3.06 (t, *J* = 7.2 Hz, 2H), 2.16-2.08 (m, 2H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 198.5, 145.3, 139.4, 135.7, 135.1, 128.8, 128.5, 128.5, 128.2, 127.8, 126.8, 126.8, 125.5, 36.5, 32.7, 23.0. FT-IR: ν (cm^{-1}) 3052, 2920, 2850, 1663, 1602, 1480, 1260, 1190. HRMS [ESI] calcd for $C_{22}H_{21}OS$ $[M+H]^+$ 333.1313, found 333.1316.



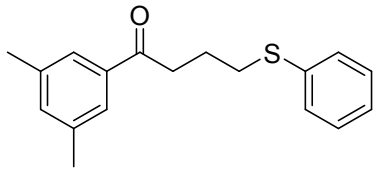
2e: yellow solid, m.p. 44-46 °C. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.95-7.90 (m, 2H), 7.37-7.33 (m, 2H), 7.30-7.25 (m, 2H), 7.19-7.14 (m, 1H), 6.94-6.90 (m, 2H), 3.87 (s, 3H), 3.09 (t, *J* = 7.2 Hz, 2H), 3.04 (t, *J* = 7.2 Hz, 2H), 2.12-2.04 (m, 2H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 197.5, 163.0, 135.7, 129.8, 129.5, 128.7, 128.4, 125.5, 113.2, 55.0, 36.1, 32.7, 23.2. FT-IR: ν (cm^{-1}) 2956, 2920, 2851, 1670, 1597, 1508, 1439, 1370, 1263. HRMS [ESI] calcd for $C_{17}H_{19}O_2S$ $[M+H]^+$ 287.1106, found 287.1097.



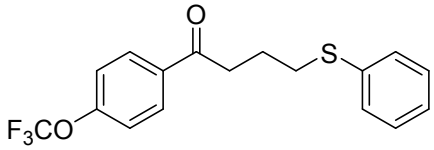
2f: yellow oil. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.54-7.50 (m, 1H), 7.47 (dd, *J* = 2.4, 1.6 Hz, 1H), 7.37-7.33 (m, 3H), 7.30-7.25 (m, 2H), 7.19-7.14 (m, 1H), 7.10 (ddd, *J* = 8.0, 2.8, 0.8 Hz, 1H), 3.84 (s, 3H), 3.12 (t, *J* = 7.2 Hz, 2H), 3.04 (t, *J* = 7.2 Hz, 2H), 2.13-2.05 (m, 2H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 199.2, 159.8, 138.2, 136.2, 129.6, 129.2, 128.9, 126.0, 120.7, 119.6, 112.2, 55.5, 37.1, 33.1, 23.5. FT-IR: ν (cm^{-1}) 3058, 2921, 2850, 1682, 1582, 1429, 1256, 1165. HRMS [ESI] calcd for $C_{17}H_{18}O_2SNa$ $[M+Na]^+$ 309.0925, found 309.0915.



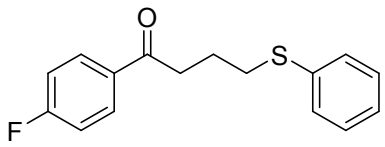
2g: yellow oil. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.67 (dd, J = 8.0, 2.0 Hz, 1H), 7.45 (ddd, J = 8.4, 7.2, 1.6 Hz, 1H), 7.35-7.31 (m, 2H), 7.29-7.23 (m, 2H), 7.18-7.12 (m, 1H), 6.99 (ddd, J = 7.6, 7.2, 0.8 Hz, 1H), 6.94 (d, J = 8.4 Hz, 1H), 3.87 (s, 3H), 3.13 (t, J = 7.2 Hz, 2H), 3.00 (t, J = 7.2 Hz, 2H), 2.08-2.01 (m, 2H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 201.8, 158.5, 136.6, 133.5, 130.3, 128.9, 128.8, 128.2, 125.8, 120.7, 111.5, 55.5, 42.5, 33.1, 23.9. FT-IR: ν (cm^{-1}) 3058, 2918, 2848, 1669, 1596, 1482, 1436, 1243. HRMS [ESI] calcd for $C_{17}H_{18}O_2SNa$ $[M+Na]^+$ 309.0925, found 309.0921.



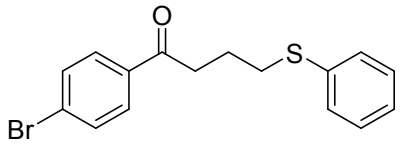
2h: yellow oil. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.54 (s, 2H), 7.37-7.34 (m, 2H), 7.30-7.25 (m, 2H), 7.20-7.14 (m, 2H), 3.11 (t, J = 7.2 Hz, 2H), 3.03 (t, J = 7.2 Hz, 2H), 2.36 (s, 6H), 2.12-2.04 (m, 2H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 199.4, 137.7, 136.5, 135.7, 134.2, 128.7, 128.5, 125.5, 125.4, 36.6, 32.7, 23.1, 20.8. FT-IR: ν (cm^{-1}) 3054, 2918, 2858, 1679, 1604, 1480, 1438, 1317, 1297. HRMS [ESI] calcd for $C_{18}H_{20}OSNa$ $[M+Na]^+$ 307.1133, found 307.1124.



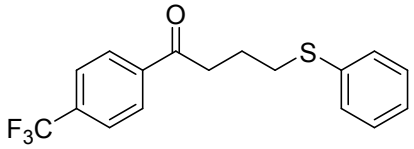
2i: yellow oil.^{1}H NMR (400 MHz, $CDCl_3$) δ 8.01-7.96 (m, 2H), 7.37-7.33 (m, 2H), 7.30-7.24 (m, 4H), 7.19-7.14 (m, 1H), 3.13 (t, J = 7.2 Hz, 2H), 3.04 (t, J = 7.2 Hz, 2H), 2.13-2.05 (m, 2H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 197.8, 152.6 (q, J_{C-F} = 1.7 Hz), 136.0, 135.0, 130.0, 129.3, 129.0, 126.1, 120.4 (q, J_{C-F} = 0.7 Hz), 120.3 (q, J_{C-F} = 257.1 Hz), 36.9, 33.1, 23.3; ^{19}F NMR (376 MHz, $CDCl_3$) δ -57.6 (s). FT-IR: ν (cm^{-1}) 3061, 2926, 2855, 1687, 1602, 1481, 1439, 1253, 1208, 1162. HRMS [ESI] calcd for $C_{17}H_{15}F_3O_2SNa$ $[M+Na]^+$ 363.0643, found 363.0645.



2j: yellow oil. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.91-7.85 (m, 2H), 7.29-7.25 (m, 2H), 7.22-7.17 (m, 2H), 7.11-7.06 (m, 1H), 7.06-7.00 (m, 2H), 3.03 (t, J = 7.2 Hz, 2H), 2.96 (t, J = 7.2 Hz, 2H), 2.05-1.96 (m, 2H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 197.3, 165.3 (d, J_{C-F} = 253.1 Hz), 135.6, 132.8 (d, J_{C-F} = 3.0 Hz), 130.2 (d, J_{C-F} = 9.2 Hz), 128.8, 128.5, 125.6, 115.2 (d, J_{C-F} = 21.7 Hz), 36.3, 32.6, 22.9; ^{19}F NMR (376 MHz, $CDCl_3$) δ -105.3 (s). FT-IR: ν (cm^{-1}) 3060, 2926, 2855, 1684, 1596, 1505, 1480, 1225, 1156. HRMS [ESI] calcd for $C_{16}H_{15}FOSNa$ $[M+Na]^+$ 297.0725, found 297.0734.

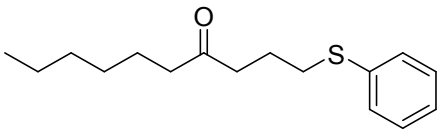


2k: yellow solid, m.p. 35-36 ^{o}C. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.81-7.77 (m, 2H), 7.61-7.56 (m, 2H), 7.37-7.32 (m, 2H), 7.30-7.24 (m, 2H), 7.20-7.14 (m, 1H), 3.10 (t, J = 7.2 Hz, 2H), 3.03 (t, J = 7.2 Hz, 2H), 2.12-2.04 (m, 2H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 197.9, 135.5, 135.0, 131.4, 129.1, 128.8, 128.5, 127.8, 125.6, 36.4, 32.6, 22.8. FT-IR: ν (cm^{-1}) 3054, 2918, 2849, 1676, 1583, 1479, 1315, 1194. HRMS [ESI] calcd for $C_{16}H_{15}BrOSNa$ $[M+Na]^+$ 356.9925, found 356.9921.

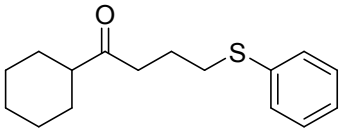


2l: yellow oil. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.96 (d, J = 8.0 Hz, 2H), 7.64 (d, J = 8.0 Hz, 2H), 7.30-7.26 (m, 2H),

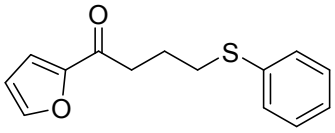
7.23-7.18 (m, 2H), 7.13-7.08 (m, 1H), 3.10 (t, J = 7.2 Hz, 2H), 2.98 (t, J = 7.2 Hz, 2H), 2.08-1.99 (m, 2H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 197.9, 138.9 (q, $J_{C\text{-}F}$ = 1.0 Hz), 135.4, 133.9 (q, $J_{C\text{-}F}$ = 32.5 Hz), 128.8, 128.5, 127.9, 125.7, 125.2 (q, $J_{C\text{-}F}$ = 3.6 Hz), 123.1 (q, $J_{C\text{-}F}$ = 271.0 Hz), 36.7, 32.5, 22.7; ^{19}F NMR (376 MHz, $CDCl_3$) δ -63.1 (s). FT-IR: ν (cm^{-1}) 3062, 2960, 2853, 1683, 1581, 1481, 1365, 1326. HRMS [ESI] calcd for $C_{17}H_{15}F_3OSNa$ $[M+Na]^+$ 347.0693, found 347.0695.



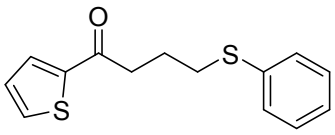
2m: yellow solid, m.p. 33-34 °C. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.28-7.24 (m, 2H), 7.23-7.18 (m, 2H), 7.12-7.07 (m, 1H), 2.87 (t, J = 7.2 Hz, 2H), 2.49 (t, J = 7.2 Hz, 2H), 2.30 (t, J = 7.2 Hz, 2H), 1.88-1.80 (m, 2H), 1.54-1.44 (m, 2H), 1.23-1.19 (m, 6H), 0.81 (t, J = 6.8 Hz, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 210.0, 135.7, 128.7, 128.4, 125.5, 42.5, 40.4, 32.5, 31.1, 28.4, 23.3, 22.5, 22.0, 13.6. FT-IR: ν (cm^{-1}) 3057, 2927, 2870, 1698, 1583, 1479, 1381, 1230. HRMS [ESI] calcd for $C_{16}H_{24}OSNa$ $[M+Na]^+$ 287.1446, found 287.1440.



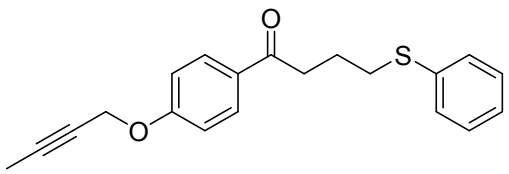
2n: yellow oil. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.28-7.24 (dd, J = 8.4, 1.2 Hz, 2H), 7.23-7.18 (m, 2H), 7.12-7.07 (m, 1H), 2.86 (t, J = 7.2 Hz, 2H), 2.53 (t, J = 7.2 Hz, 2H), 2.27-2.20 (m, 1H), 1.87-1.79 (m, 2H), 1.78-1.66 (m, 4H), 1.62-1.54 (m, 1H), 1.30-1.12 (m, 5H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 212.9, 135.8, 128.7, 128.4, 125.5, 50.4, 38.3, 32.6, 28.0, 25.4, 25.2, 22.4. FT-IR: ν (cm^{-1}) 3058, 2926, 2852, 1704, 1584, 1480, 1406, 1290. HRMS [ESI] calcd for $C_{16}H_{22}OSNa$ $[M+Na]^+$ 285.1289, found 285.1282.



2o: yellow oil. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.57 (d, J = 1.2 Hz, 1H), 7.37-7.33 (m, 2H), 7.30-7.25 (m, 2H), 7.19-7.15 (m, 2H), 6.52 (dd, J = 3.6, 1.6 Hz, 1H), 3.02 (t, J = 7.2 Hz, 2H), 3.00 (t, J = 7.2 Hz, 2H), 2.11-2.03 (m, 2H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 188.1, 152.2, 145.8, 135.6, 128.8, 128.4, 125.5, 116.5, 111.7, 36.4, 32.6, 22.9. FT-IR: ν (cm^{-1}) 3131, 2924, 2852, 1671, 1568, 1467, 1394, 1251. HRMS [ESI] calcd for $C_{14}H_{14}O_2SNa$ $[M+Na]^+$ 269.0612, found 269.0595.

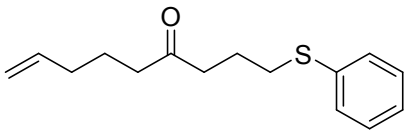


2p: yellow oil. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.62 (dd, J = 4.0, 1.2 Hz, 1H), 7.55 (dd, J = 4.8, 1.2 Hz, 1H), 7.30-7.26 (m, 2H), 7.23-7.18 (m, 2H), 7.12-7.07 (m, 1H), 7.04 (dd, J = 4.8, 4.0 Hz, 1H), 3.01 (t, J = 7.2 Hz, 2H), 2.96 (t, J = 7.2 Hz, 2H), 2.06-1.98 (m, 2H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 191.9, 143.7, 135.6, 133.1, 131.4, 128.8, 128.5, 127.6, 125.6, 37.2, 32.6, 23.3. FT-IR: ν (cm^{-1}) 3075, 2924, 2855, 1656, 1582, 1518, 1414, 1234. HRMS [ESI] calcd for $C_{14}H_{14}OS_2Na$ $[M+Na]^+$ 285.0384, found 285.0373.

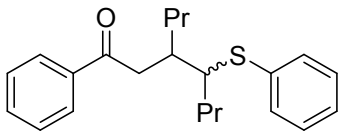


2q: yellow oil. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.95-7.91 (m, 2H), 7.37-7.33 (m, 2H), 7.29-7.26 (m, 2H), 7.19-7.14 (m, 1H), 7.01-6.97 (m, 2H),

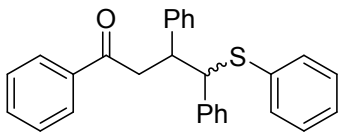
4.71 (q, *J* = 2.4 Hz, 2H), 3.09 (t, *J* = 7.2 Hz, 2H), 3.04 (t, *J* = 6.8 Hz, 2H), 2.12-2.05 (m, 2H), 1.87 (t, *J* = 2.4 Hz, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 197.5, 161.1, 135.7, 129.9, 129.7, 128.7, 128.4, 125.5, 114.1, 84.0, 72.8, 56.1, 36.2, 32.7, 23.1, 3.2. FT-IR: ν (cm^{-1}) 3058, 2921, 2853, 1674, 1599, 1508, 1480, 1439, 1309, 1223. HRMS [ESI] calcd for $C_{20}H_{21}O_2S$ $[M+H]^+$ 325.1262, found 325.1268.



2r: yellow oil. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.35-7.32 (m, 2H), 7.30-7.25 (m, 2H), 7.20-7.14 (m, 1H), 5.80-5.70 (m, 1H), 5.04-4.94 (m, 2H), 2.94 (t, *J* = 7.2 Hz, 2H), 2.56 (t, *J* = 7.2 Hz, 2H), 2.39 (t, *J* = 7.2 Hz, 2H), 2.04 (dd, *J* = 14.4, 7.2 Hz, 2H), 1.95-1.87 (m, 2H), 1.71-1.62 (m, 2H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 209.6, 137.5, 135.7, 128.8, 128.4, 125.5, 114.8, 41.5, 40.5, 32.6, 32.5, 22.5, 22.3. FT-IR: ν (cm^{-1}) 3075, 2919, 2850, 1710, 1640, 1584, 1481, 1439, 1371, 1302. HRMS [ESI] calcd for $C_{15}H_{21}OS$ $[M+H]^+$ 249.1313, found 249.1301.

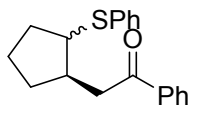


2s (*dr* = 1.2:1): yellow oil. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.95-7.88 (m, 4H, two isomers), 7.57-7.49 (m, 2H, two isomers), 7.46-7.34 (m, 6H, two isomers), 7.32-7.27 (m, 2H, two isomers), 7.25-7.07 (m, 6H, two isomers), 3.48 (dd, *J* = 16.8, 6.4 Hz, 1H, one isomer), 3.35-3.31 (m, 1H, one isomer), 3.29-3.25 (m, 1H, one isomer), 3.06 (dd, *J* = 16.8, 7.2 Hz, 1H, one isomer), 2.99 (dd, *J* =16.8 Hz, 5.6 Hz, 1H, one isomer), 2.79 (dd, *J* =16.4 Hz, 6.8 Hz, 1H, one isomer), 2.55-2.44 (m, 2H, two isomers), 1.72-1.37 (m, 16H, two isomers), 0.95-0.82 (m, 12H, two isomers); ^{13}C NMR (100 MHz, $CDCl_3$) δ 200.0 & 199.4 (two isomers), 136.8 & 136.7 (two isomers), 136.1 & 136.0 (two isomers), 132.5 & 132.4 (two isomers), 130.7 & 130.6 (two isomers), 128.4 & 128.3 (two isomers), 128.1 & 128.0 (two isomers), 127.6 & 127.6 (two isomers), 125.9 & 125.8 (two isomers), 52.7 & 52.4 (two isomers), 39.9 & 39.7 (two isomers), 37.2 & 37.1 (two isomers), 34.5 & 33.7 (two isomers), 33.6 & 32.2 (two isomers), 20.7 & 20.4 (two isomers), 20.3 & 20.1 (two isomers), 13.7 & 13.7 (two isomers), 13.5 & 13.4 (two isomers). FT-IR: ν (cm^{-1}) 3059, 2956, 2926, 2855, 1683, 1581, 1478, 1363, 1286. HRMS [ESI] calcd for $C_{22}H_{28}OSNa$ $[M+Na]^+$ 363.1759, found 363.1749.

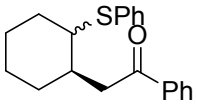


2t (*dr* = 1.3:1): yellow solid, m.p. 90-92 ^{o}C. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.95-7.91 (m, 2H, two isomers), 7.82-7.77 (m, 2H, two isomers), 7.58-7.49 (m, 2H, two isomers), 7.48-7.43 (m, 2H, two isomers), 7.42-7.32 (m, 2H, two isomers), 7.27-7.17 (m, 14H, two isomers), 7.15-7.05 (m, 16H, two isomers), 4.58 (d, *J* = 8.8 Hz, 1H, one isomer), 4.56 (d, *J* = 8.8 Hz, 1H, one isomer), 4.07 (ddd, *J* = 8.4, 8.4, 4.2 Hz, 1H, one isomer), 4.00 (ddd, *J* = 8.4, 8.4, 4.2 Hz, 1H, one isomer), 3.93 (dd, *J* = 17.2, 5.2 Hz, 1H, one isomer), 3.55 (dd, *J* = 17.2, 9.2 Hz, 1H, one isomer), 3.49 (dd, *J* = 16.8, 5.2 Hz, 1H, one isomer), 3.40 (dd, *J* = 17.2, 8.8 Hz, 1H, one isomer); ^{13}C NMR (100 MHz, $CDCl_3$) δ 197.9 &197.8 (two isomers), 140.7 & 140.5 (two isomers), 140.1, & 139.8 (two isomers), 136.6 & 136.5 (two isomers), 134.6 & 134.6 (two isomers), 132.5 & 132.5 (two isomers), 131.7 & 131.4 (two isomers), 128.3 & 128.2 (two isomers), 128.2 & 128.2 (two isomers), 128.1 & 128.1 (two isomers), 128.1 & 128.0 (two isomers), 127.7 &127.7 (two isomers), 127.6 & 127.5 (two isomers), 127.4 & 127.3 (two isomers),

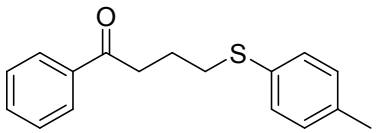
126.8 & 126.6 (two isomers), 126.5 & 126.4 (two isomers), 126.4 & 126.1 (two isomers), 59.1 & 58.8 (two isomers), 46.4 & 45.9 (two isomers), 42.5 & 42.1 (two isomers). FT-IR: ν (cm^{-1}) 3029, 2918, 2851, 1677, 1602, 1561, 1449, 1367. HRMS [ESI] calcd for $C_{28}H_{24}OSNa$ $[M+Na]^+$ 431.1446, found 431.1436.



2u (*dr* = 1.2:1): colorless oil. ^1H NMR (400 MHz, $CDCl_3$) δ 7.95-7.90 (m, 2H, two isomers), 7.90-7.85 (m, 2H, two isomers), 7.58-7.50 (m, 2H, two isomers), 7.47-7.38 (m, 6H, two isomers), 7.36-7.32 (m, 2H, two isomers), 7.30-7.26 (m, 2H, two isomers), 7.25-7.18 (m, 3H, two isomers), 7.14-7.08 (m, 1H, one isomer), 3.90 (dd, *J* = 10.8, 6.0 Hz, 1H, one isomer), 3.42 (dd, *J* = 16.0, 3.6 Hz, 1H, one isomer), 3.41 (dd, *J* = 17.2, 6.4 Hz, 1H, one isomer), 3.19 (dd, *J* = 15.6, 7.2 Hz, 1H, one isomer), 2.95 (dd, *J* = 17.2, 8.0 Hz, 1H, one isomer), 2.84 (dd, *J* = 16.0, 10.0 Hz, 1H, one isomer), 2.88-2.78 (m, 1H, one isomer), 2.42-2.31 (m, 1H, one isomer), 2.22-2.17 (m, 1H, one isomer), 2.13-2.07 (m, 2H, two isomers), 1.94-1.78 (m, 3H, two isomers), 1.74-1.63 (m, 4H, two isomers), 1.31-1.26 (m, 2H, two isomers); ^{13}C NMR (100 MHz, $CDCl_3$) δ 199.2 & 199.0 (two isomers), 136.6 & 136.5 (two isomers), 136.0 & 135.6 (two isomers), 132.5 & 132.4 (two isomers), 130.6 & 129.7 (two isomers), 128.4 & 128.4 (two isomers), 128.1 & 128.0 (two isomers), 127.7 & 127.6 (two isomers), 126.0 & 125.6 (two isomers), 51.8 & 51.2 (two isomers), 42.8 & 41.8 (two isomers), 39.5 & 39.1 (two isomers), 33.4 & 32.2 (two isomers), 31.1 & 29.6 (two isomers), 22.8 & 21.4 (two isomers). FT-IR: ν (cm^{-1}) 3017, 2926, 2855, 1681, 1598, 1452, 1276. HRMS [ESI] calcd for $C_{19}H_{20}OSNa$ $[M+Na]^+$ 319.1133, found 319.1146.

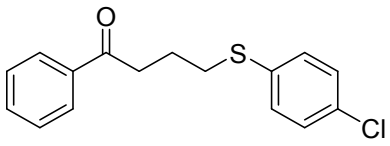


2v (*dr* = 1:1): yellow oil. ^1H NMR (400 MHz, $CDCl_3$) δ 7.99-7.94 (m, 2H, two isomers), 7.92-7.88 (m, 2H, two isomers), 7.58-7.50 (m, 2H, two isomers), 7.48-7.38 (m, 6H, two isomers), 7.35-7.16 (m, 7H, two isomers), 7.14-7.08 (m, 1H, one isomer), 3.81 (dd, *J* = 16.4, 3.2 Hz, 1H, one isomer), 3.65 (dd, *J* = 7.8, 3.6 Hz, 1H, one isomer), 3.37 (dd, *J* = 16.8, 6.0 Hz, 1H, one isomer), 2.95 (dd, *J* = 16.8, 6.8 Hz, 1H, one isomer), 2.89 (ddd, *J* = 11.2, 11.2, 4.0 Hz, 1H, one isomer), 2.80 (dd, *J* = 16.4, 6.4 Hz, 1H, one isomer), 2.62-2.53 (m, 1H, one isomer), 2.20-2.08 (m, 2H, two isomers), 1.97-1.60 (m, 7H, two isomers), 1.55-1.35 (m, 5H, two isomers), 1.34-1.05 (m, 3H, two isomers); ^{13}C NMR (100 MHz, $CDCl_3$) δ 199.4 & 199.3 (two isomers), 136.8 & 136.8 (two isomers), 135.6 & 134.4 (two isomers), 132.4 & 132.4 (two isomers), 131.9 & 130.8 (two isomers), 128.4 & 128.4 (two isomers), 128.1 & 128.0 (two isomers), 127.7 & 127.6 (two isomers), 126.4 & 125.9 (two isomers), 52.4 & 51.3 (two isomers), 43.5 & 38.5 (two isomers), 36.3 & 34.2 (two isomers), 32.7 & 30.8 (two isomers), 28.2 & 28.2 (two isomers), 26.1 & 25.0 (two isomers), 24.2 & 21.5 (two isomers). FT-IR: ν (cm^{-1}) 3058, 2925, 2853, 1682, 1581, 1447, 1403, 1249. HRMS [ESI] calcd for $C_{20}H_{22}OSNa$ $[M+Na]^+$ 333.1289, found 333.1278.

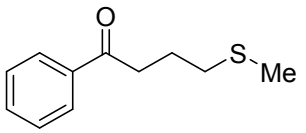


2w: yellow oil. ^1H NMR (400 MHz, $CDCl_3$) δ 7.96-7.92 (m, 2H), 7.58-7.53 (m, 1H), 7.47-7.42 (m, 2H), 7.28-7.25 (m, 2H), 7.09 (d, *J* = 8.0 Hz, 2H), 3.13 (t, *J* = 7.2 Hz, 2H), 3.00 (t, *J* = 7.2 Hz, 2H), 2.31 (s, 3H), 2.10-2.02 (m, 2H); ^{13}C NMR (100

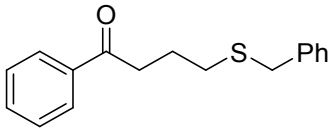
MHz, $CDCl_3$) δ 199.0, 136.4, 135.7, 132.6, 131.8, 129.7, 129.2, 128.1, 127.6, 36.5, 33.4, 23.0, 20.5. FT-IR: ν (cm^{-1}) 3058, 3022, 2922, 1683, 1597, 1492, 1448, 1223. HRMS [ESI] calcd for $C_{17}H_{18}OSNa$ $[M+Na]^+$ 293.0976, found 293.0981.



2x: yellow solid, m.p. 48-50 °C. ^1H NMR (400 MHz, $CDCl_3$) δ 7.89-7.85 (m, 2H), 7.52-7.47 (m, 1H), 7.39 (dd, *J* = 7.6, 7.6 Hz, 2H), 7.23-7.15 (m, 4H), 3.06 (t, *J* = 7.2 Hz, 2H), 2.95 (t, *J* = 7.2 Hz, 2H), 2.05-1.97 (m, 2H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 198.8, 136.3, 134.2, 132.7, 131.5, 130.1, 128.6, 128.2, 127.5, 36.4, 32.8, 22.8. FT-IR: ν (cm^{-1}) 3058, 2926, 2852, 1682, 1598, 1476, 1447, 1366. HRMS [ESI] calcd for $C_{16}H_{15}ClOSNa$ $[M+Na]^+$ 313.0430, found 313.0423.

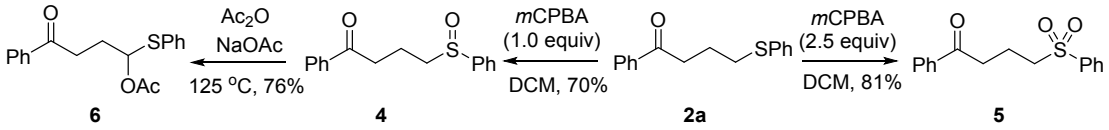


2y: yellow oil. ^1H NMR (400 MHz, $CDCl_3$) δ 7.98-7.96 (m, 2H), 7.59-7.54 (m, 1H), 7.48-7.44 (m, 2H), 3.12 (t, *J* = 7.2 Hz, 2H), 2.61 (t, *J* = 7.2 Hz, 2H), 2.11 (s, 3H), 2.10-2.02 (m, 2H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 199.2, 136.5, 132.6, 128.1, 127.6, 36.5, 33.2, 22.6, 14.8. FT-IR: ν (cm^{-1}) 3060, 2916, 2854, 1682, 1597, 1580, 1448, 1364, 1224. HRMS [ESI] calcd for $C_{11}H_{15}OS$ $[M+H]^+$ 195.0844, found 195.0843.



2z: yellow oil. ^1H NMR (400 MHz, $CDCl_3$) δ 7.96-7.94 (m, 2H), 7.59-7.54 (m, 1H), 7.49-7.43 (m, 2H), 7.33-7.28 (m, 4H), 7.25-7.20 (m, 1H), 3.72 (s, 2H), 3.07 (t, *J* = 7.2 Hz, 2H), 2.53 (t, *J* = 7.2 Hz, 2H), 2.06-1.98 (m, 2H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 199.1, 137.9, 136.4, 132.6, 128.4, 128.1, 128.0, 127.6, 126.5, 36.7, 35.6, 30.4, 22.8. FT-IR: ν (cm^{-1}) 3029, 2922, 2951, 1730, 1684, 1598, 1494, 1449, 1366, 1245. HRMS [ESI] calcd for $C_{17}H_{19}OS$ $[M+H]^+$ 271.1157, found 271.1168.

Preparation of the compound **4**, **5,** and **6**:

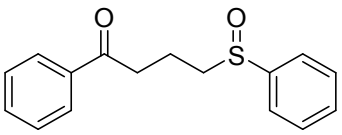


To a solution of **2a** (100 mg, 0.39 mmol) in DCM (10 mL) was added dropwise *m*CPBA (75wt%, 90 mg, 0.39 mmol) at 0°C. After the mixture was stirred for 1 h, aqueous sat. $NaHCO_3$ solution (10 mL) was slowly added. The mixture was extracted with DCM (10 mL×3). The combined organic layers were washed with brine (20 mL), dried and concentrated to give a crude residue, which was purified by flash chromatography on silica gel (EA/PE = 1:1) to afford the product **4** (74 mg, 70%).

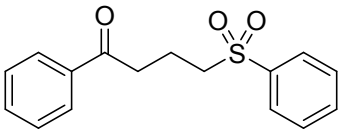
To a solution of **2a** (100 g, 0.39 mmol) in DCM (30 mL) was added dropwise *m*CPBA (75wt%, 225 mg, 0.98 mmol) at 0°C. After the mixture was stirred for 1 h, aqueous sat. $NaHCO_3$ solution (10 mL) was slowly added. The mixture was extracted with DCM (10 mL×3). The combined organic layers were washed with brine (20 mL), dried and concentrated to give a crude

residue, which was purified by flash chromatography on silica gel (EA/PE = 1:2) to afford the product **5** (91mg, 81%).

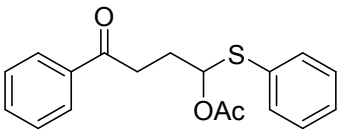
Ac_2O (1.0 mL) and NaOAc (90 mg, 1.1 mmol) was added to a flask, which was loaded with the compound **4** (30 mg, 0.11 mmol). The reaction mixture was heated to 125 °C and stirred for 12 h. After being cooled to room temperature, the reaction mixture was filtered and washed with DCM (5 mL×3). The solution was concentrated and the residue was purified by flash chromatography on silica gel (EA/PE = 1:6) to afford the product **6** (26 mg, 76%).



4: white solid, m.p. 75-77 °C. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.92 (d, *J* = 7.2 Hz, 2H), 7.62 (dd, *J* = 8.0, 1.6 Hz, 2H), 7.58-7.42 (m, 6H), 3.16 (ddd, *J* = 6.8, 6.8, 2.0 Hz, 2H), 3.01-2.84 (m, 2H), 2.29-2.17 (m, 1H), 2.17-2.05 (m, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 198.2, 143.2, 136.1, 132.8, 130.5, 128.8, 128.2, 127.5, 123.5, 55.7, 36.4, 16.5. FT-IR: ν (cm^{-1}) 3035, 2925, 2859, 1678, 1592, 1456, 1351, 1282. HRMS [ESI] calcd for $C_{16}H_{16}O_2SNa$ $[M+Na]^+$ 295.0769, found 295.0765.

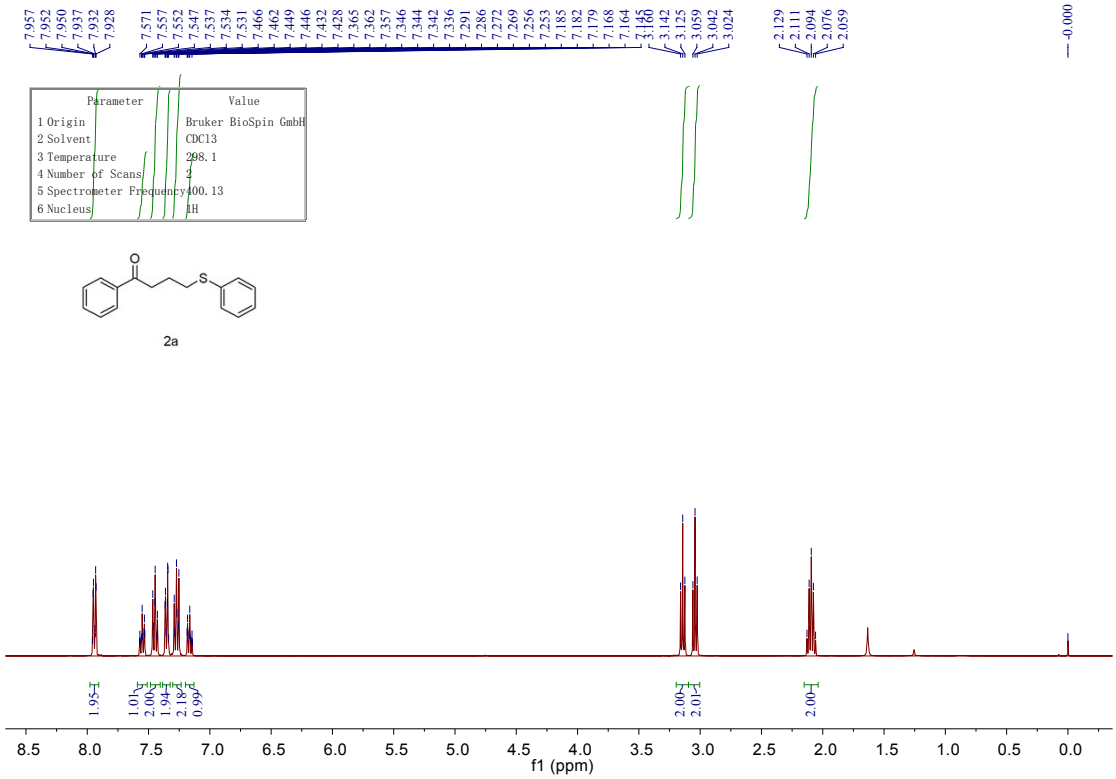


5: white solid, m.p. 83-85 °C. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.94-7.89 (m, 4H), 7.68-7.62 (m, 1H), 7.59-7.53 (m, 3H), 7.44 (dd, *J* = 8.0, 8.0 Hz, 2H), 3.25 (t, *J* = 7.2 Hz, 2H), 3.18 (t, *J* = 6.8 Hz, 2H), 2.21-2.12 (m, 2H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 197.9, 138.6, 135.9, 133.3, 132.9, 128.9, 128.2, 127.6, 127.5, 54.7, 35.8, 16.9. FT-IR: ν (cm^{-1}) 3026, 2928, 2842, 1670, 1587, 1452, 1350, 1280. HRMS [ESI] calcd for $C_{16}H_{16}O_3SNa$ $[M+Na]^+$ 311.0718, found 311.0729.



6: colorless oil. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.94 (d, *J* = 7.2 Hz, 2H), 7.57 (dd, *J* = 7.2, 7.2 Hz, 1H), 7.52-7.43 (m, 4H), 7.35-7.31 (m, 3H), 6.21 (t, *J* = 6.8 Hz, 1H), 3.16-3.10 (m, 2H), 2.28 (ddd, *J* = 14.8, 6.8, 2.4 Hz, 2H), 2.04 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 197.8, 169.2, 136.1, 133.4, 132.7, 130.7, 128.6, 128.2, 128.0, 127.5, 79.3, 34.1, 28.5, 20.6. FT-IR: ν (cm^{-1}) 3046, 2949, 2837, 1682, 1590, 1456, 1353, 1280.

4. ^{1}H, ^{13}C, and ^{19}F NMR spectra of products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Parameter Value
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3 Temperature 298.1
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6 Nucleus 1H
O
S
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1.01
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1.94
2.18
0.99
2.00
2.01
2.00
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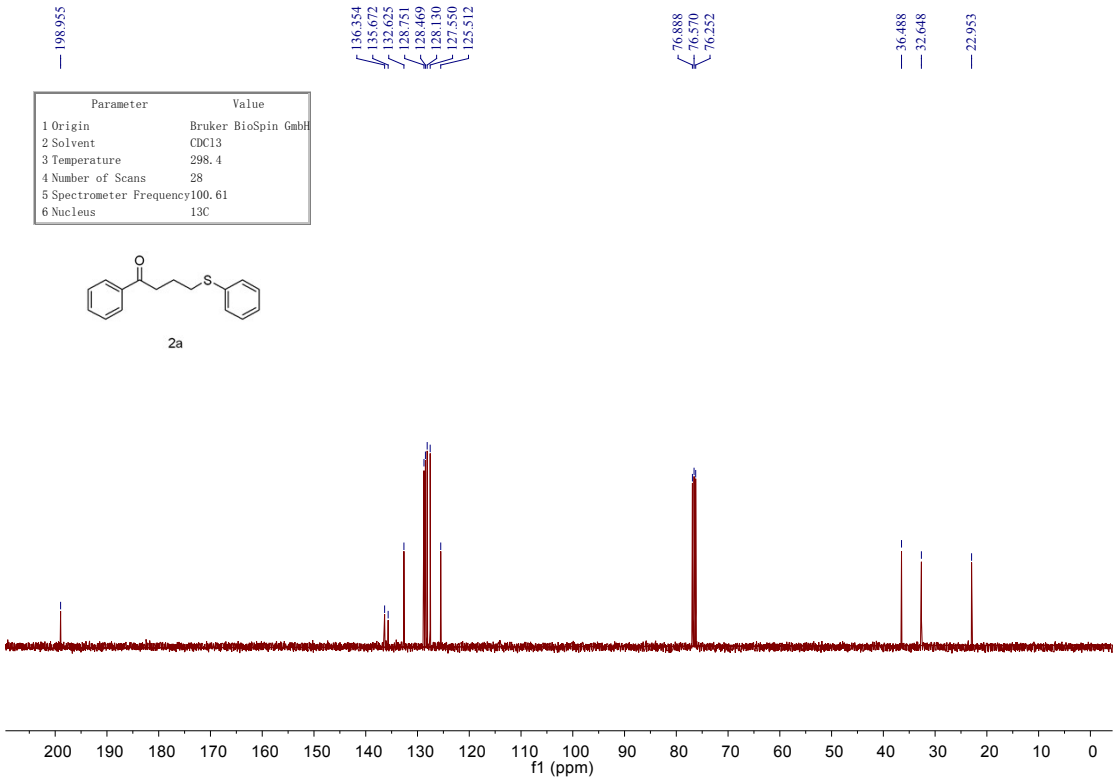
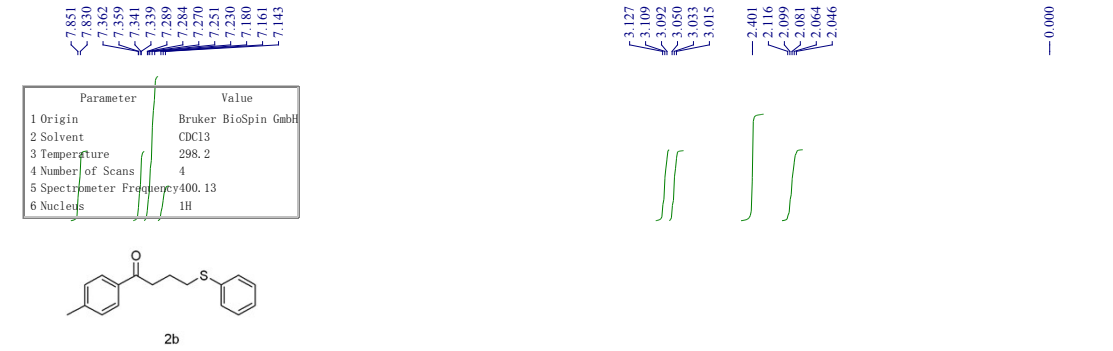
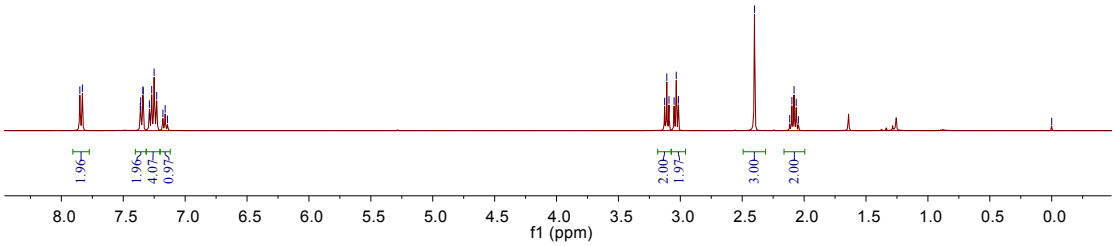
f1 (ppm)


198.955
136.354
135.672
132.625
128.751
128.469
128.130
127.550
125.512
76.888
76.570
76.252
36.488
32.648
22.953
Parameter Value
1 Origin Bruker BioSpin GmbH
2 Solvent CDCl3
3 Temperature 298.4
4 Number of Scans 28
5 Spectrometer Frequency 100.61
6 Nucleus 13C
O
S
2a
200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)

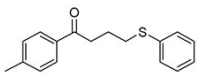


Parameter	Value
1 Origin	Bruker BioSpin GmbH
2 Solvent	CDCl3
3 Temperature	298.2
4 Number of Scans	4
5 Spectrometer Frequency	400.13
6 Nucleus	1H

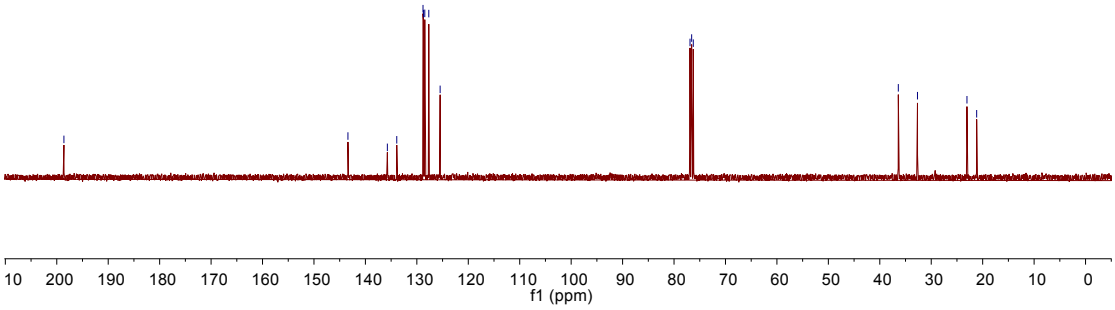
2b

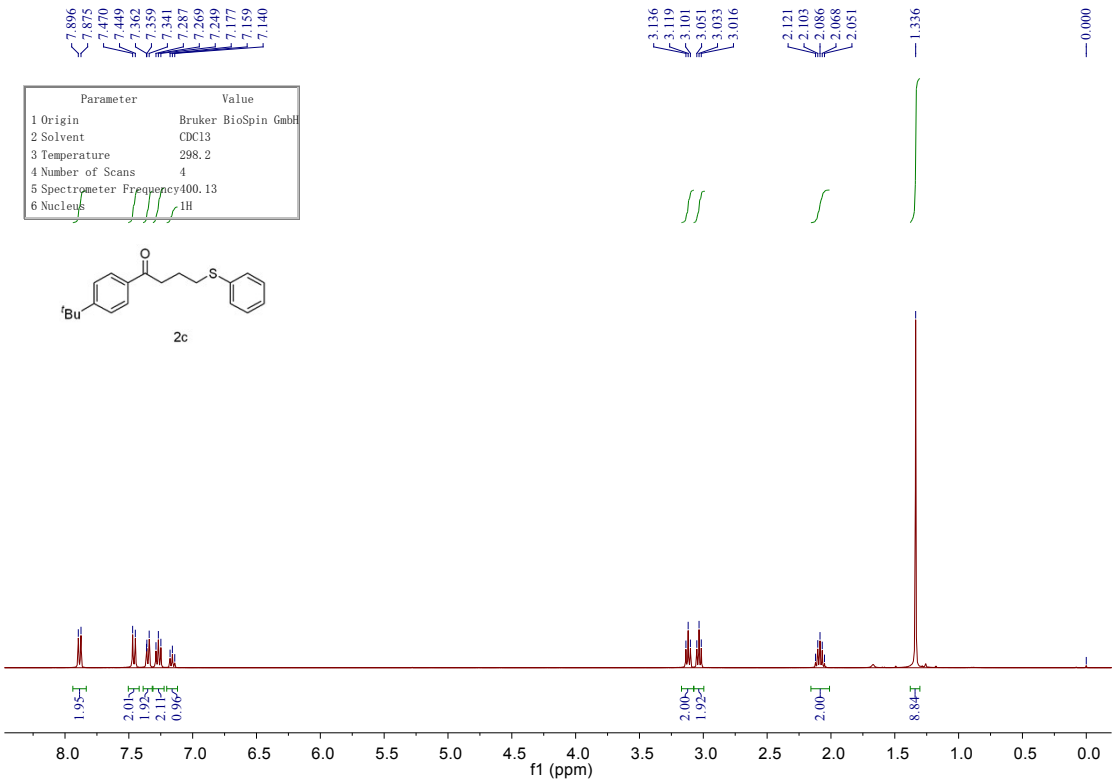


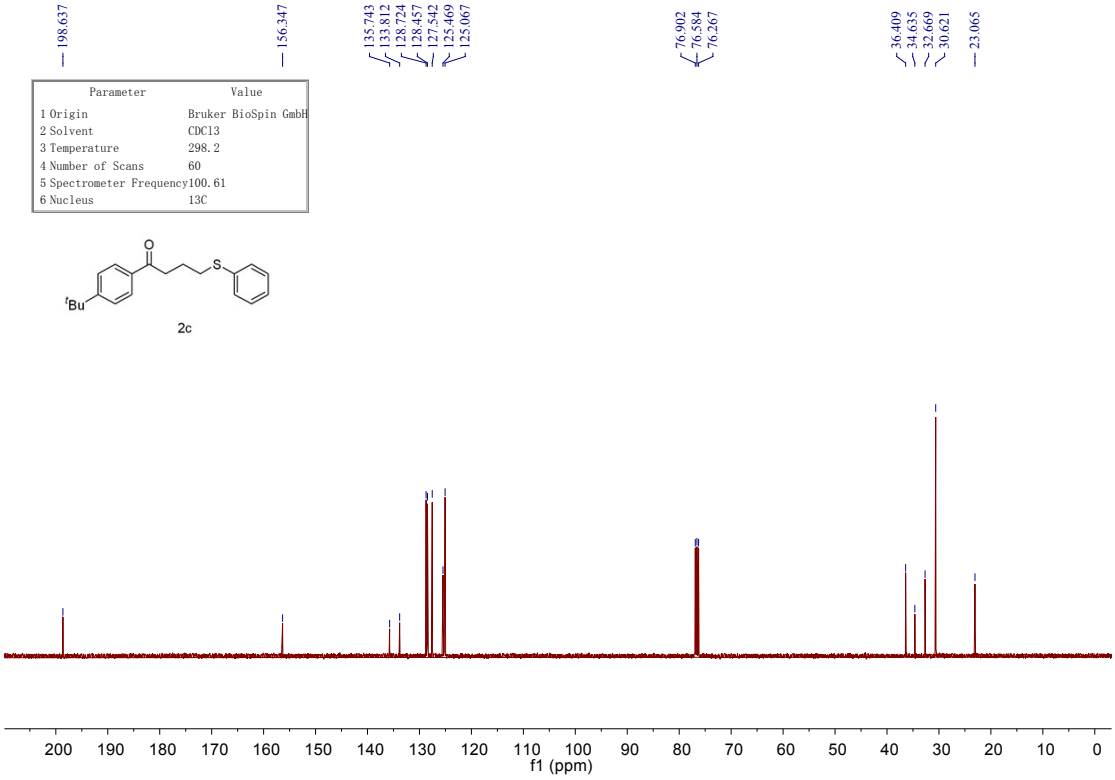
Parameter	Value
1 Origin	Bruker BioSpin GmbH
2 Solvent	CDCl3
3 Temperature	298.2
4 Number of Scans	44
5 Spectrometer Frequency	100.61
6 Nucleus	13C

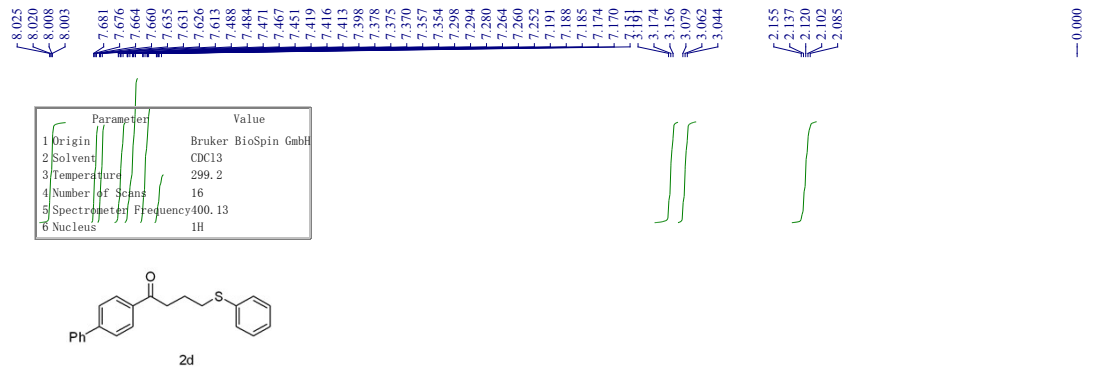


2b



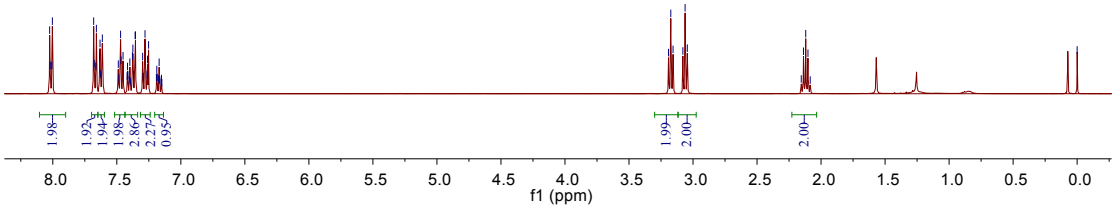

7.896
7.875
7.470
7.449
7.362
7.359
7.341
7.287
7.269
7.249
7.177
7.159
7.140
3.136
3.119
3.101
3.051
3.033
3.016
2.121
2.103
2.086
2.068
2.051
1.336
0.000
Parameter Value
1 Origin Bruker BioSpin GmbH
2 Solvent CDCl3
3 Temperature 298.2
4 Number of Scans 4
5 Spectrometer Frequency 400.13
6 Nucleus 1H
tBu
2c
1.95
2.01
1.92
2.11
0.96
2.00
1.92
2.00
8.84
f1 (ppm)

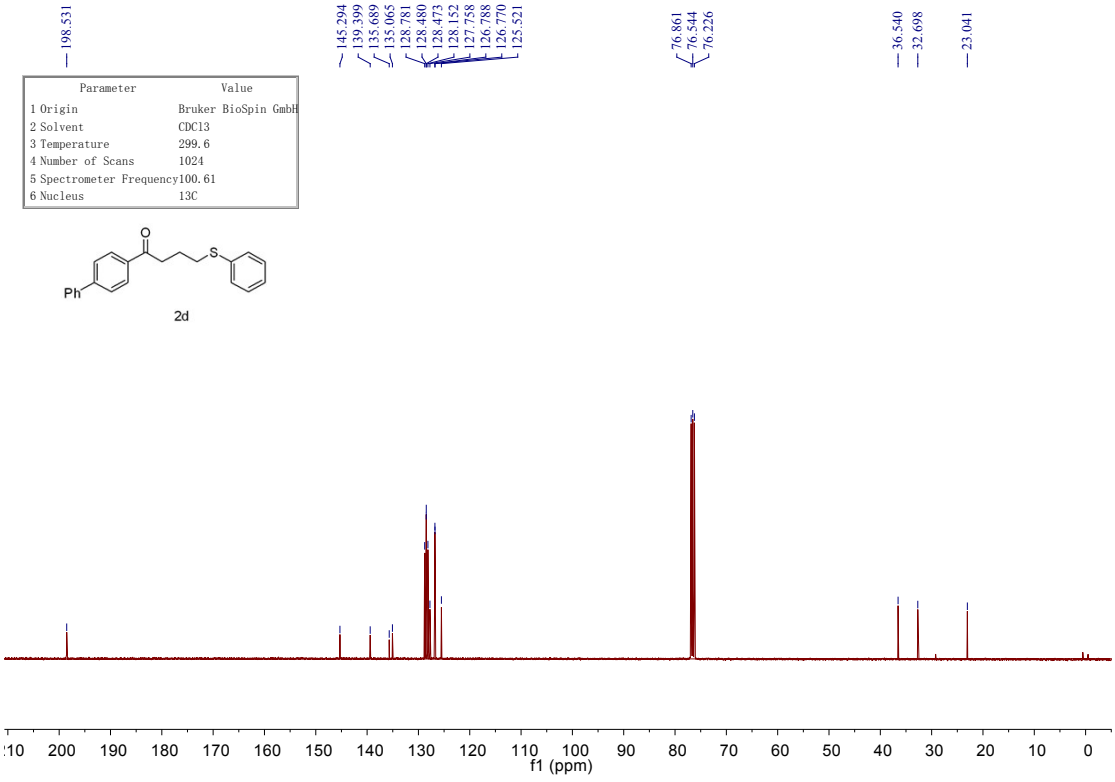

198.637
156.347
135.743
133.812
128.724
128.457
127.542
125.469
125.067
76.902
76.584
76.267
36.409
34.635
32.669
30.621
23.065
Parameter Value
1 Origin Bruker BioSpin GmbH
2 Solvent CDCl3
3 Temperature 298.2
4 Number of Scans 60
5 Spectrometer Frequency 100.61
6 Nucleus 13C
tBu
2c
f1 (ppm)



Parameter	Value
1 Origin	Bruker BioSpin GmbH
2 Solvent	CDCl3
3 Temperature	299.2
4 Number of Scans	16
5 Spectrometer Frequency	400.13
6 Nucleus	1H

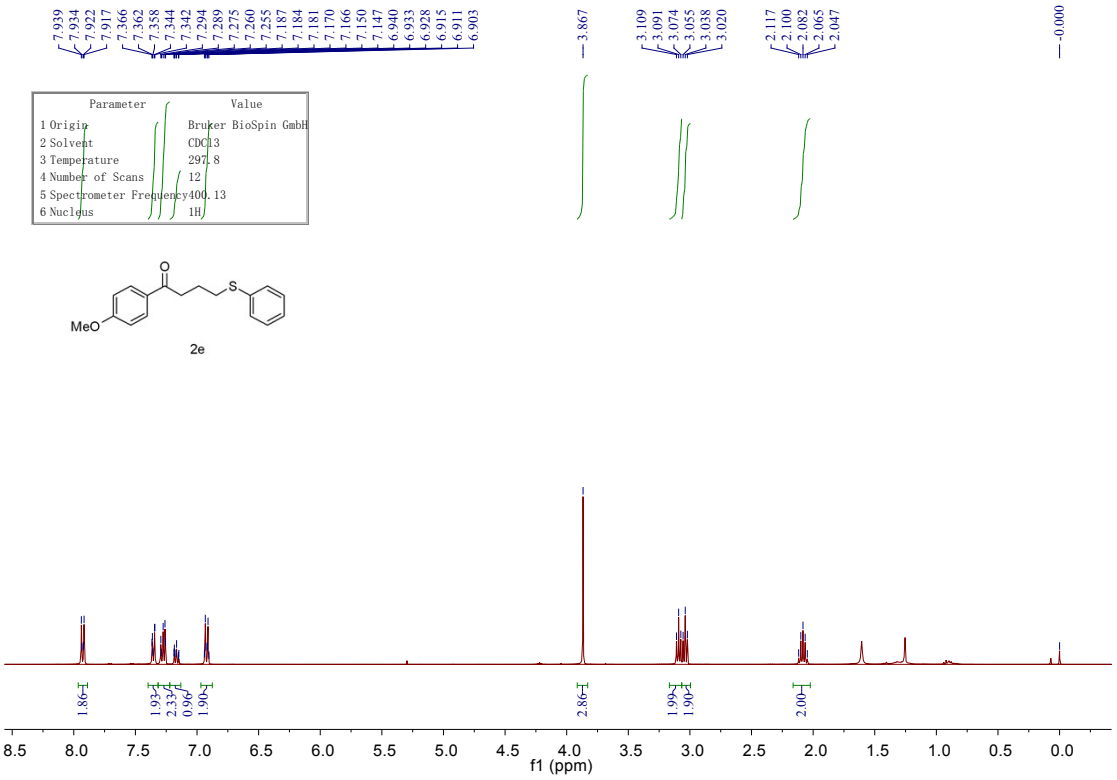
2d

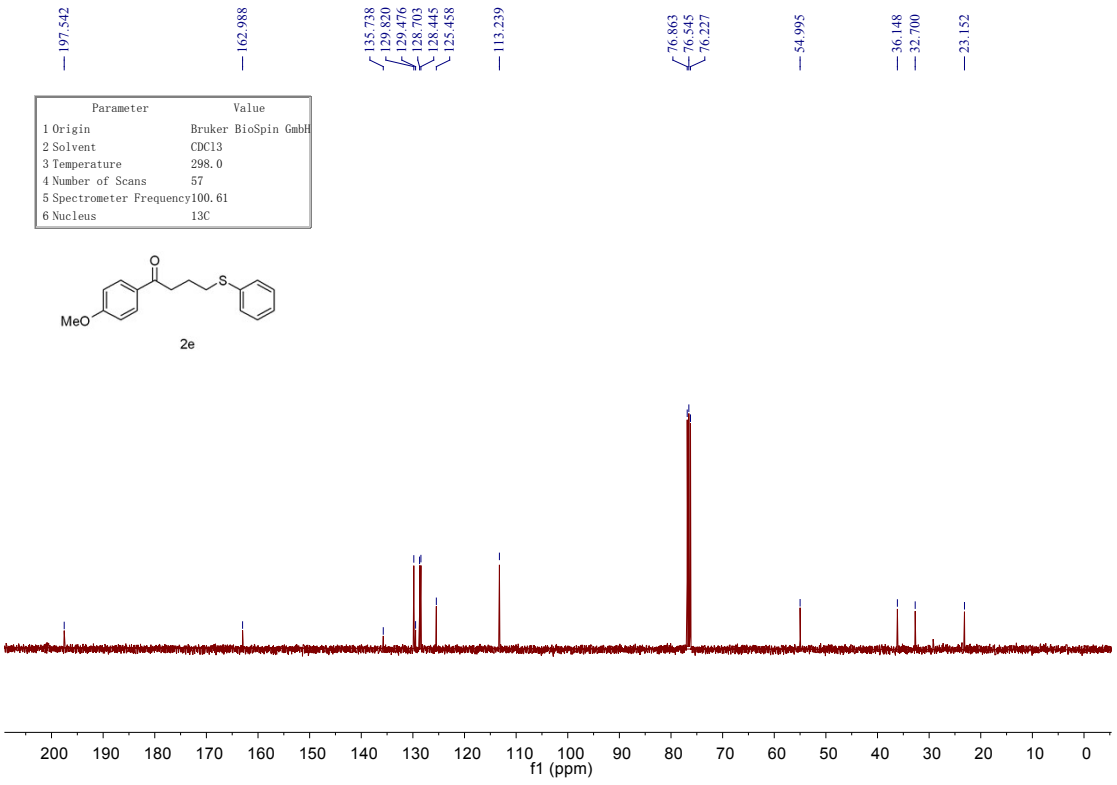


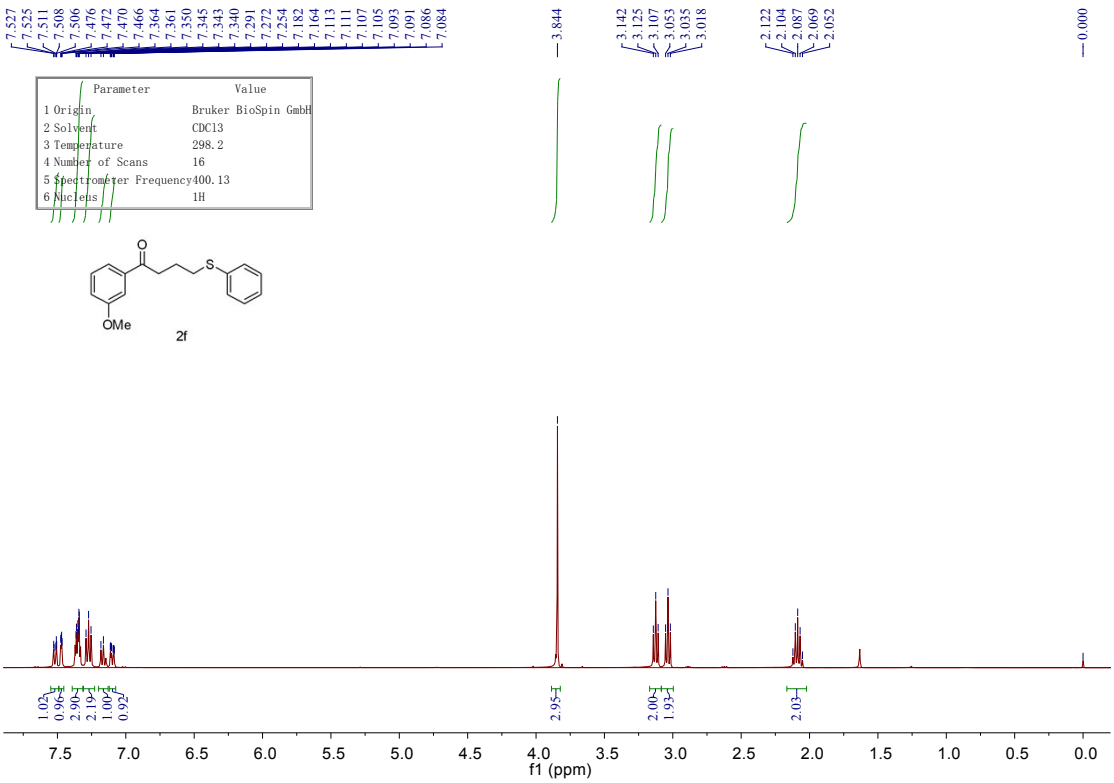


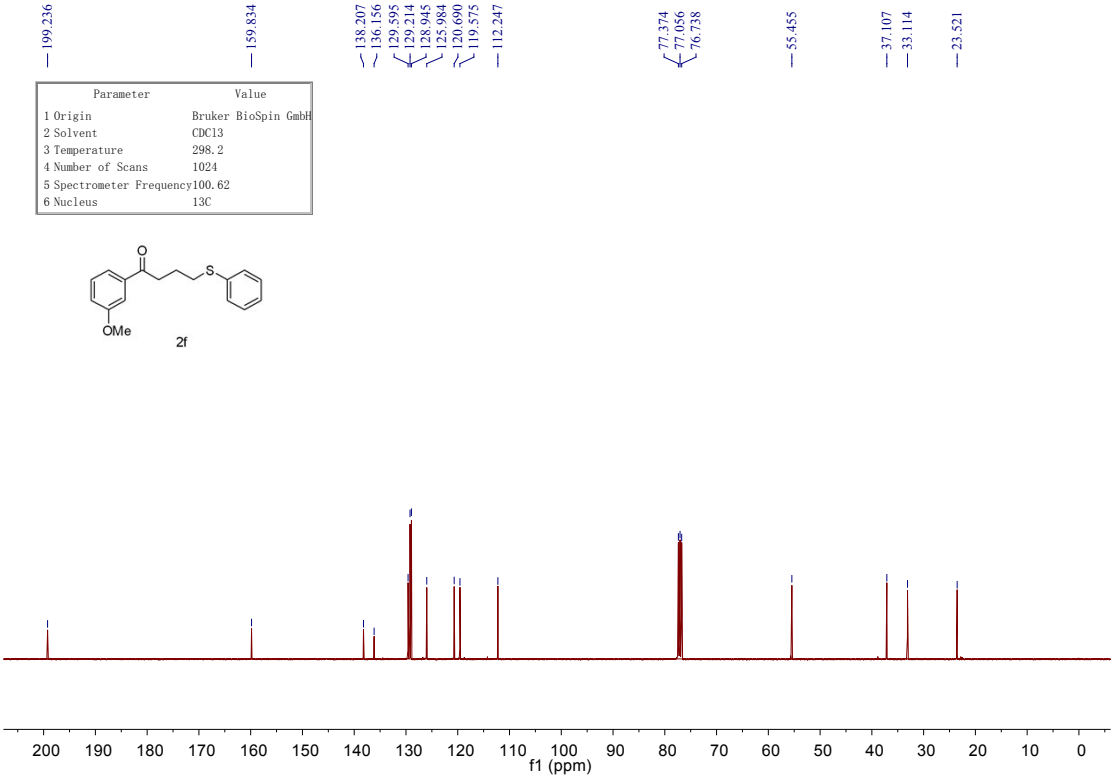
Parameter	Value
1 Origin	Bruker BioSpin GmbH
2 Solvent	CDCl3
3 Temperature	299.6
4 Number of Scans	1024
5 Spectrometer Frequency	100.61
6 Nucleus	13C

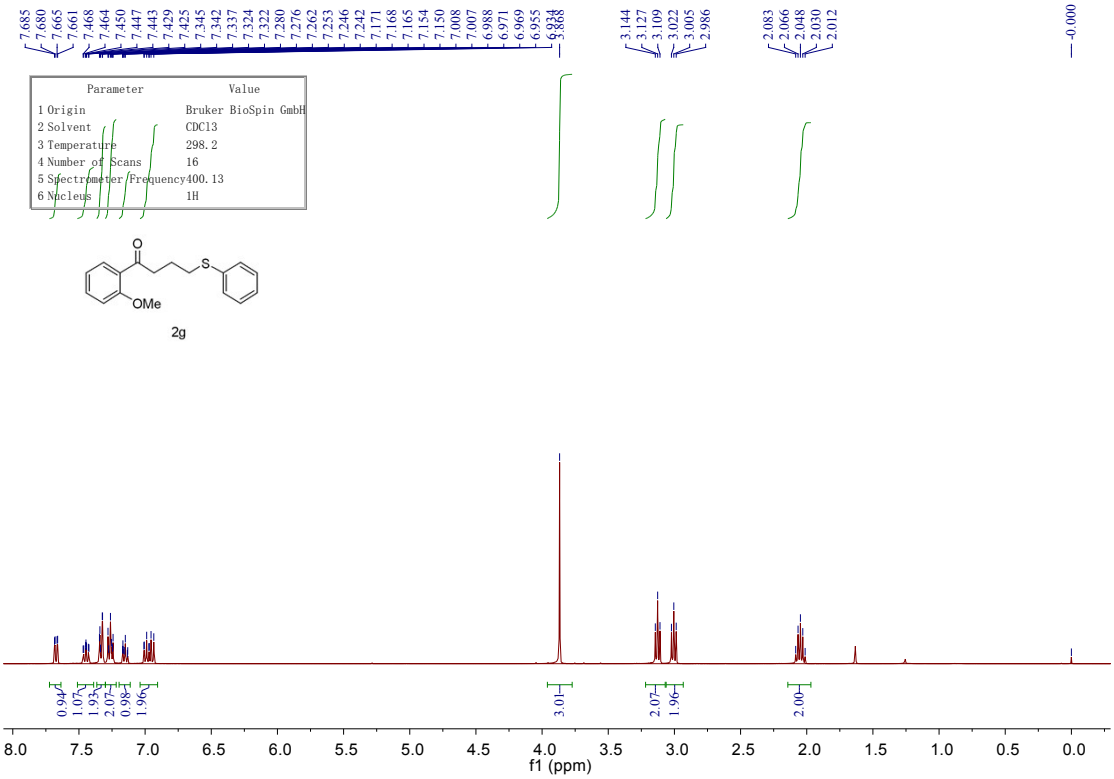
2d

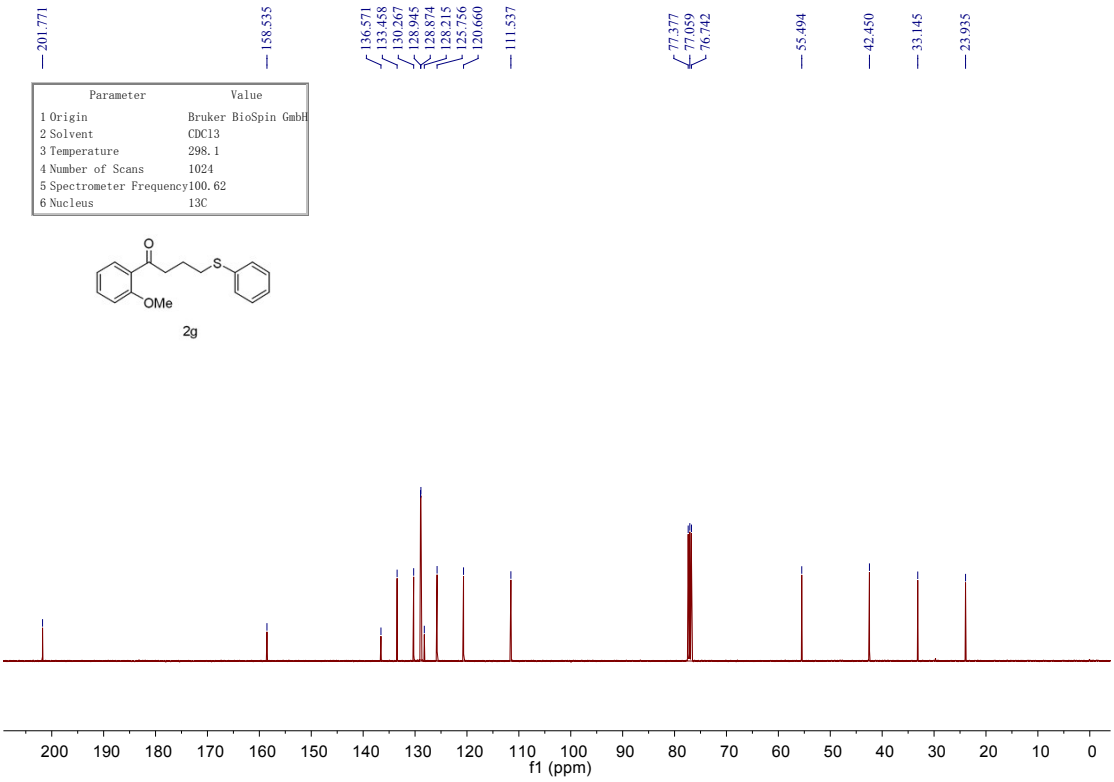

7.939
7.934
7.922
7.917
7.366
7.362
7.358
7.344
7.342
7.294
7.289
7.275
7.260
7.255
7.187
7.184
7.181
7.170
7.166
7.150
7.147
6.940
6.933
6.928
6.915
6.911
6.903
3.867
3.109
3.091
3.074
3.055
3.038
3.020
2.117
2.100
2.082
2.065
2.047
-0.000
Parameter Value
1 Origin Bruker BioSpin GmbH
2 Solvent CDCl3
3 Temperature 297.8
4 Number of Scans 12
5 Spectrometer Frequency 400.13
6 Nucleus 1H
O
S
MeO
2e
1.86
1.93
2.34
0.96
1.90
2.86
1.99
1.90
2.00
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)

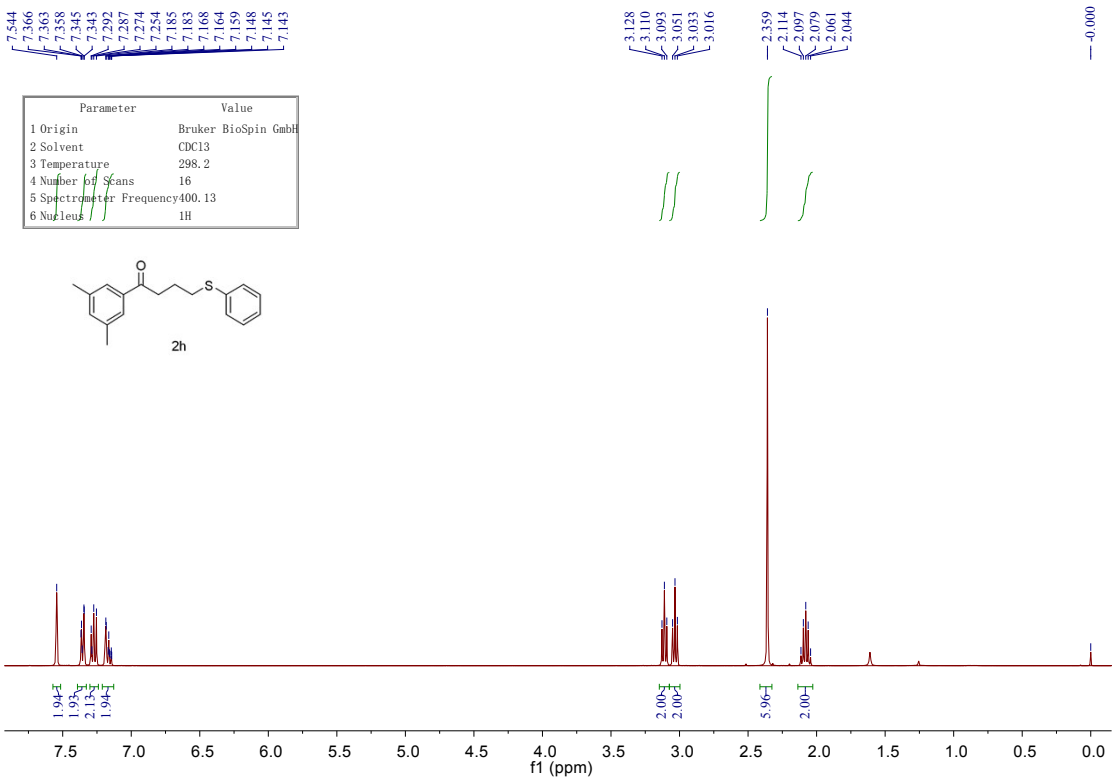

197.542
162.988
135.738
129.820
129.476
128.703
128.445
125.458
113.239
76.863
76.545
76.227
54.995
36.148
32.700
23.152
Parameter Value
1 Origin Bruker BioSpin GmbH
2 Solvent CDCl3
3 Temperature 298.0
4 Number of Scans 57
5 Spectrometer Frequency 100.61
6 Nucleus 13C
O
S
MeO
2e
200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)

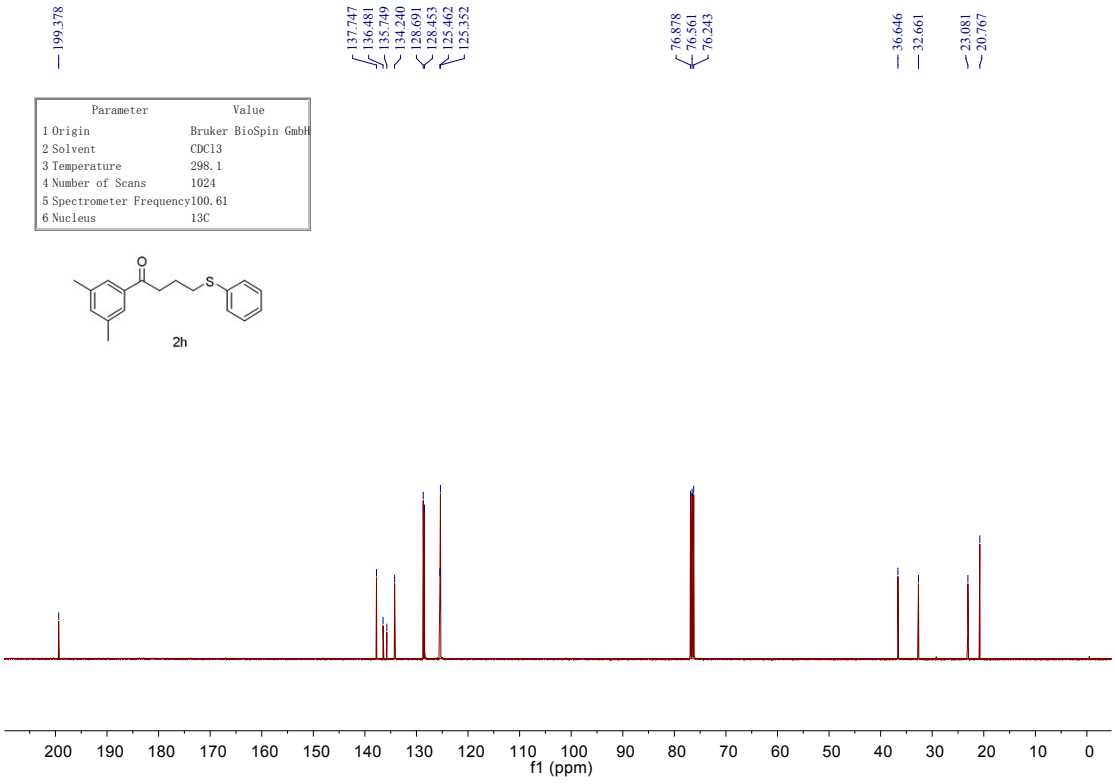

7.527
7.525
7.511
7.508
7.506
7.476
7.472
7.470
7.466
7.364
7.361
7.350
7.345
7.343
7.340
7.291
7.272
7.254
7.182
7.164
7.113
7.111
7.107
7.105
7.093
7.091
7.086
7.084
3.844
3.142
3.125
3.107
3.053
3.035
3.018
2.122
2.104
2.087
2.069
2.052
0.000
Parameter Value
1 Origin Bruker BioSpin GmbH
2 Solvent CDCl3
3 Temperature 298.2
4 Number of Scans 16
5 Spectrometer Frequency 400.13
6 Nucleus 1H
O
S
OMe
2f
1.02
0.96
2.90
2.19
1.00
0.92
2.95
2.00
1.93
2.03
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)

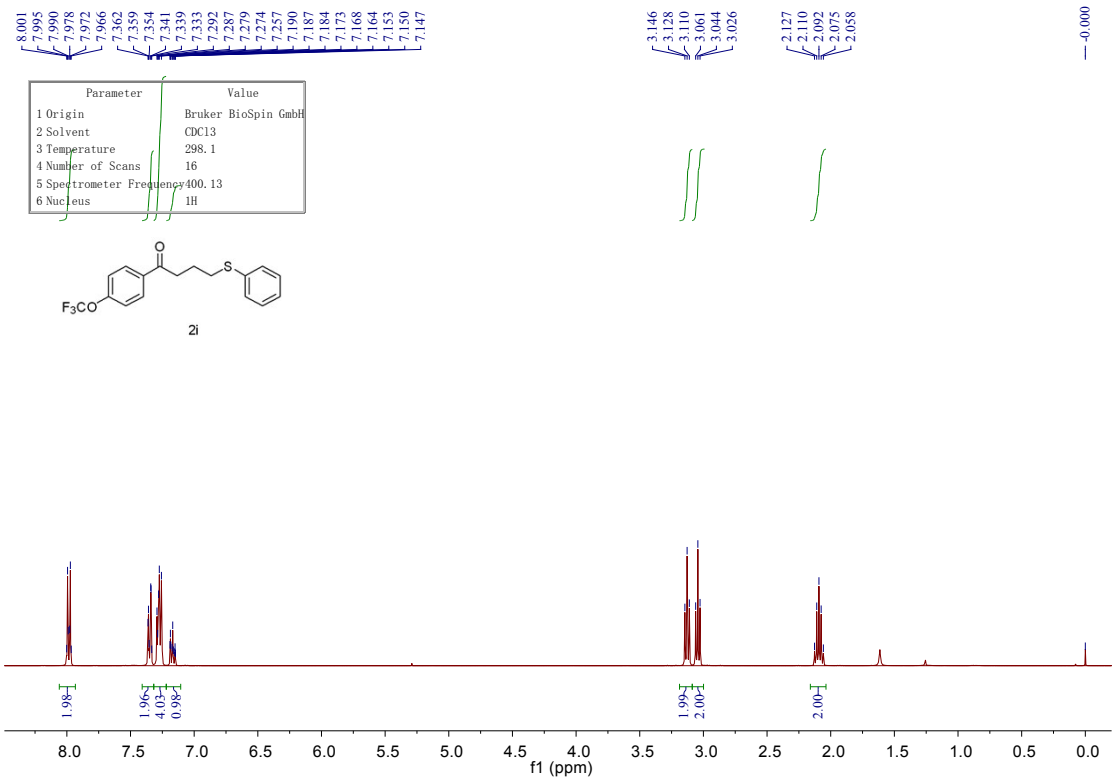

199.236
159.834
138.207
136.156
129.595
129.214
128.945
125.984
120.690
119.575
112.247
77.374
77.056
76.738
55.455
37.107
33.114
23.521
Parameter Value
1 Origin Bruker BioSpin GmbH
2 Solvent CDCl3
3 Temperature 298.2
4 Number of Scans 1024
5 Spectrometer Frequency 100.62
6 Nucleus 13C
O
S
OMe
2f
200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)

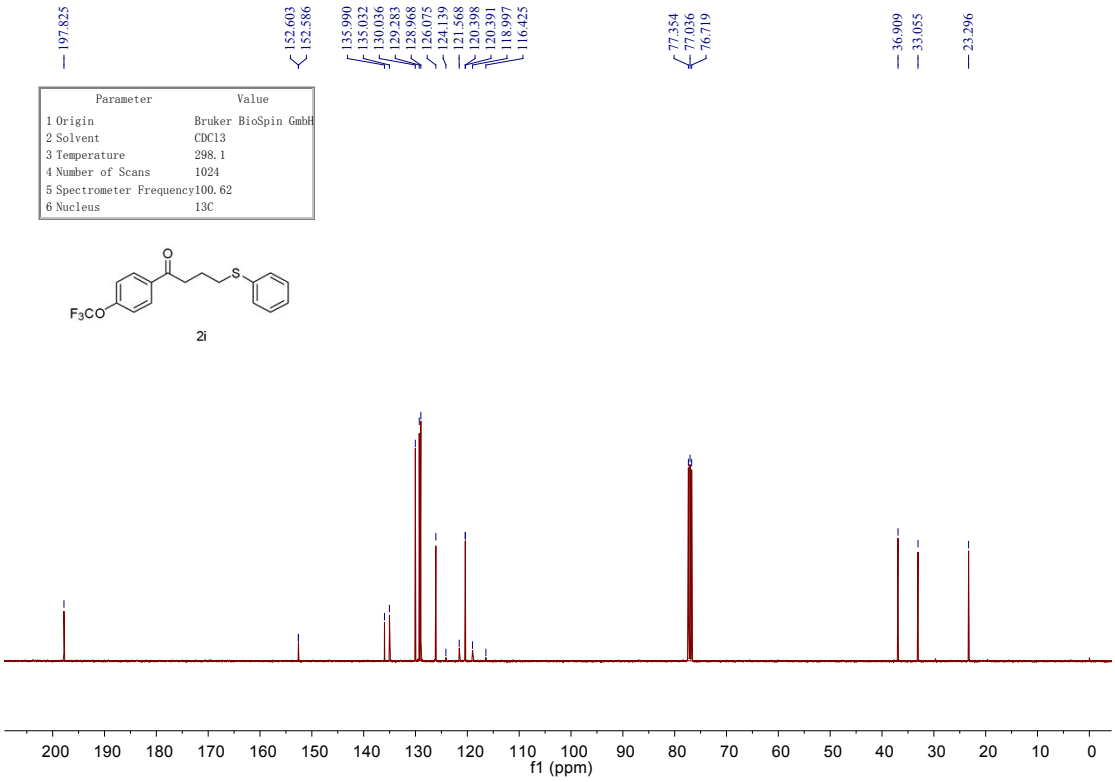

7.685
7.680
7.665
7.661
7.468
7.464
7.450
7.447
7.443
7.429
7.425
7.345
7.342
7.337
7.324
7.322
7.280
7.276
7.262
7.253
7.246
7.242
7.171
7.168
7.165
7.154
7.150
7.008
7.007
6.988
6.971
6.969
6.955
3.868
3.144
3.127
3.109
3.022
3.005
2.986
2.083
2.066
2.048
2.030
2.012
-0.000
Parameter Value
1 Origin Bruker BioSpin GmbH
2 Solvent CDCl3
3 Temperature 298.2
4 Number of Scans 16
5 Spectrometer Frequency 400.13
6 Nucleus 1H
O
S
OMe
2g
0.94
1.07
1.93
2.07
0.98
1.96
3.01
2.07
1.96
2.00
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)


201.771
158.535
136.571
133.458
130.267
128.945
128.874
128.215
125.756
120.660
111.537
77.377
77.059
76.742
55.494
42.450
33.145
23.935
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
S
OMe
2g
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)


7.544
7.366
7.363
7.358
7.345
7.343
7.292
7.287
7.274
7.254
7.185
7.183
7.168
7.164
7.159
7.148
7.145
7.143
3.128
3.110
3.093
3.051
3.033
3.016
2.359
2.114
2.097
2.079
2.061
2.044
-0.000
Parameter Value
1 Origin Bruker BioSpin GmbH
2 Solvent CDC13
3 Temperature 298.2
4 Number of Scans 16
5 Spectrometer Frequency 400.13
6 Nucleus 1H
O
S
2h
1.94
1.93
2.15
1.94
2.00
2.00
5.96
2.00
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)

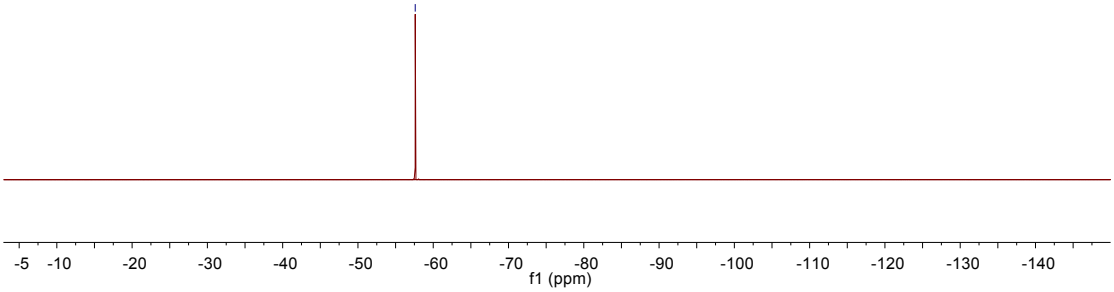

199.378
137.747
136.481
135.749
134.240
128.691
128.453
125.462
125.352
76.878
76.561
76.243
36.646
32.661
23.081
20.767
Parameter Value
1 Origin Bruker BioSpin GmbH
2 Solvent CDC13
3 Temperature 298.1
4 Number of Scans 1024
5 Spectrometer Frequency 100.61
6 Nucleus 13C
O
S
2h
200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)


8.001
7.995
7.990
7.978
7.972
7.966
7.362
7.359
7.354
7.341
7.339
7.333
7.292
7.287
7.279
7.274
7.257
7.190
7.187
7.184
7.173
7.168
7.164
7.153
7.150
7.147
3.146
3.128
3.110
3.061
3.044
3.026
2.127
2.110
2.092
2.075
2.058
-0.000
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
S
F3CO
2i
1.98
1.96
4.03
0.98
1.99
2.00
2.00
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)


197.825
152.603
152.586
135.990
135.032
130.036
129.283
128.968
126.075
124.139
121.568
120.398
120.391
118.997
116.425
77.354
77.036
76.719
36.909
33.055
23.296
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
S
F3CO
2i
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

Parameter	Value
1 Origin	Bruker BioSpin GmbH
2 Solvent	CDCl3
3 Temperature	298.1
4 Number of Scans	16
5 Spectrometer Frequency	376.44
6 Nucleus	19F

-57.609



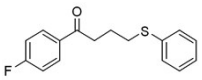
7.901 7.888 7.879 7.866 7.282 7.279 7.261 7.259 7.214 7.209 7.195 7.177 7.108 7.089 7.071 7.063 7.056 7.051 7.034 7.017 7.012 7.005

3.052 3.034 3.017 2.978 2.961 2.944

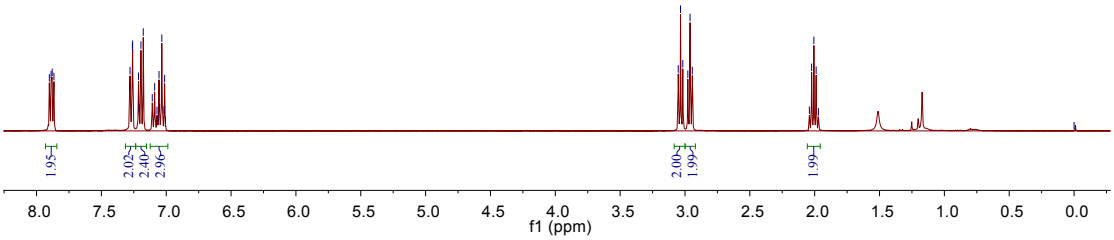
2.041 2.024 2.006 1.989 1.971

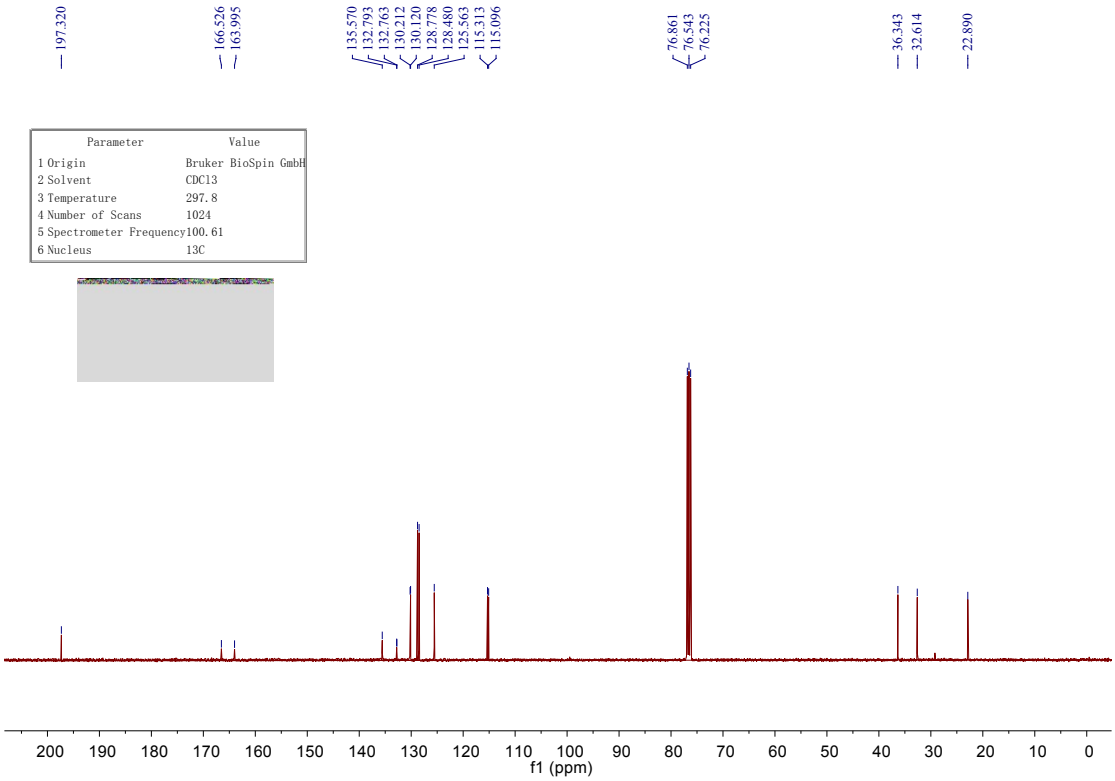
-0.000

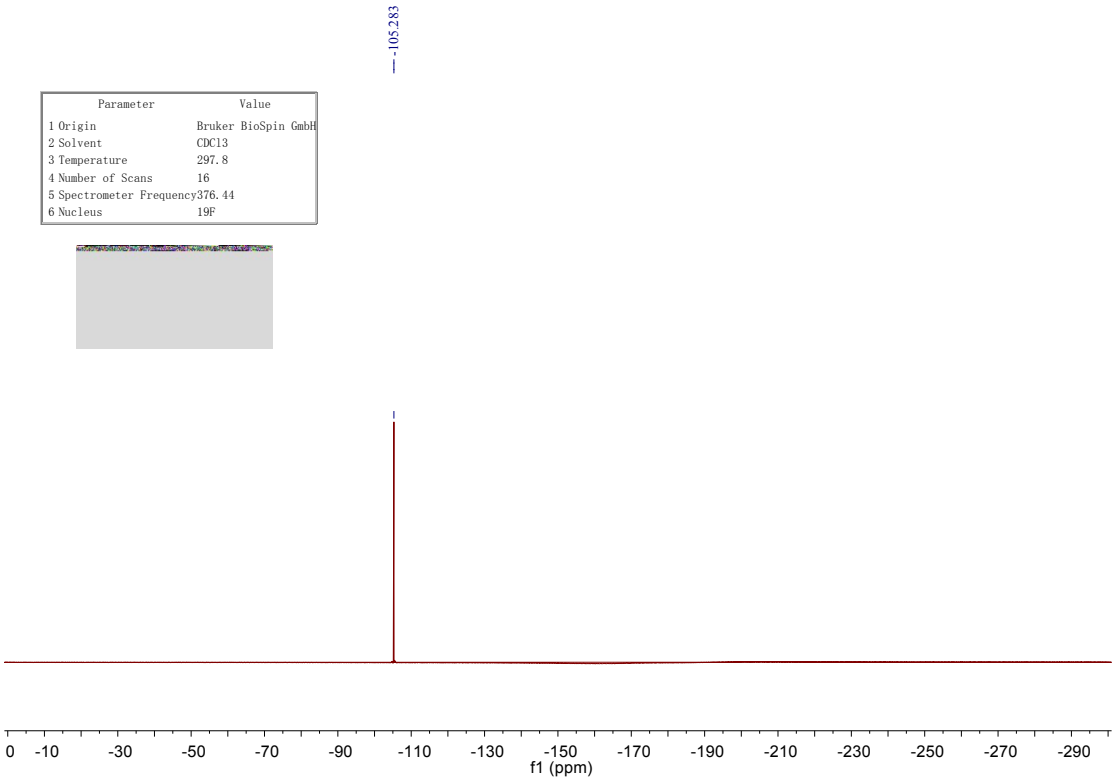
Parameter	Value
1 Origin	Bruker BioSpin GmbH
2 Solvent	CDCl3
3 Temperature	297.8
4 Number of Scans	2
5 Spectrometer Frequency	400.13
6 Nucleus	1H

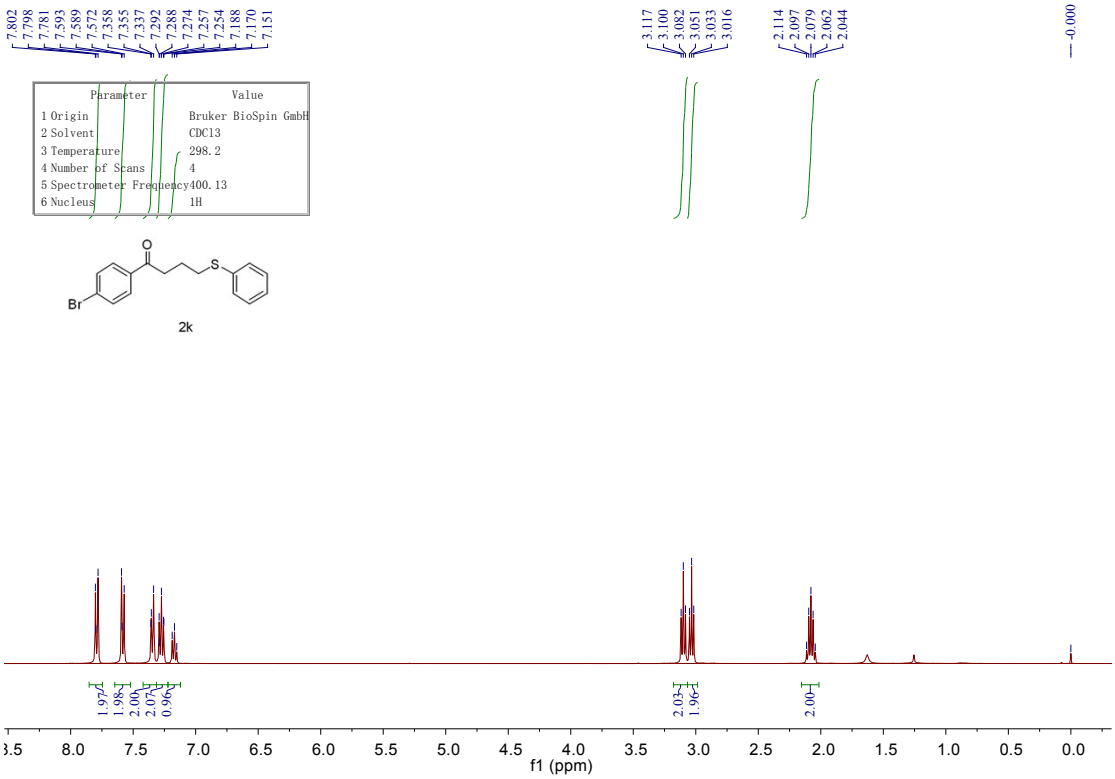


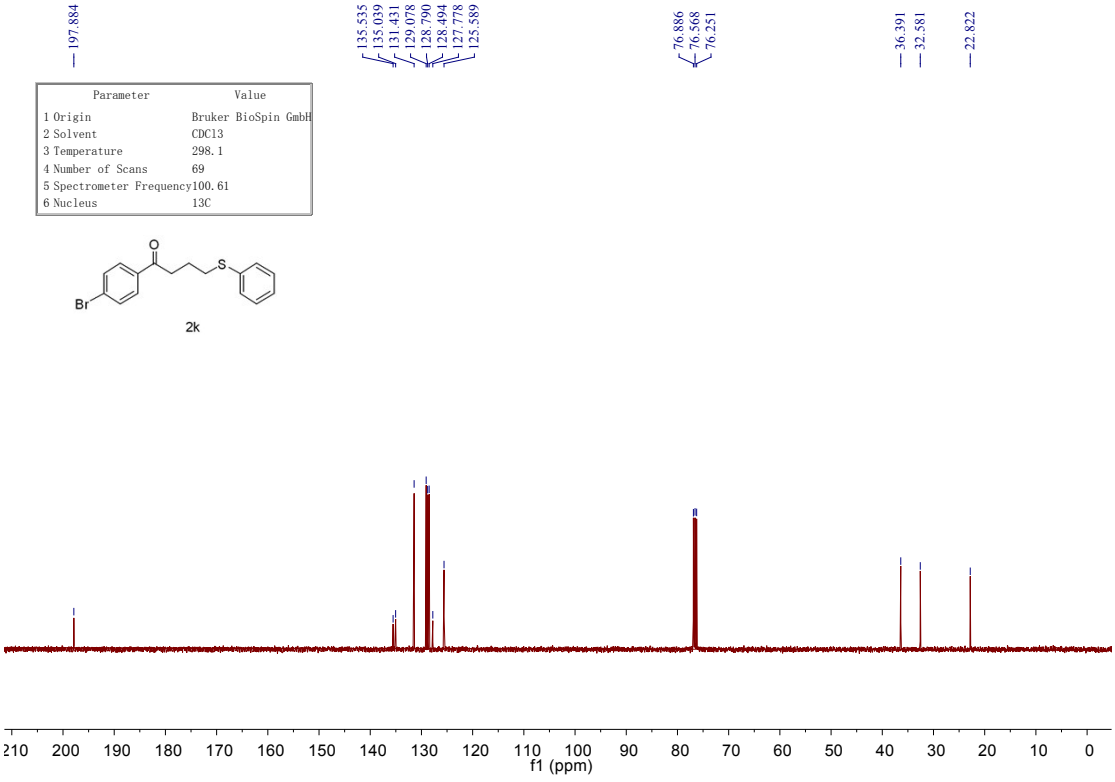
2j

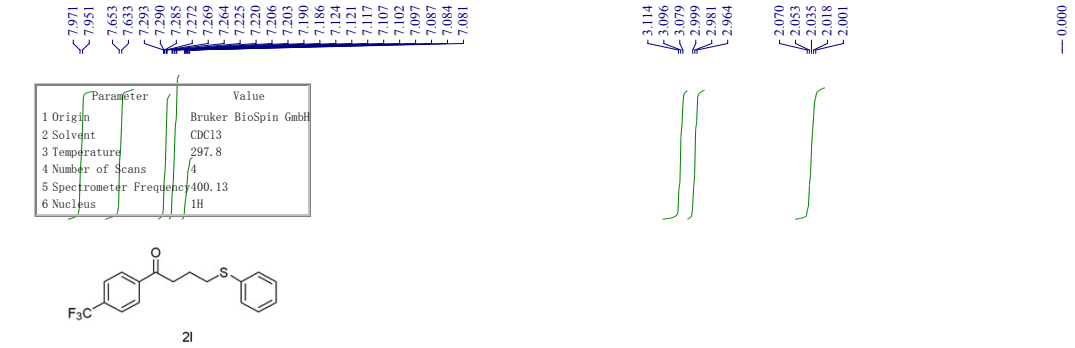



197.320
166.526
163.995
135.570
132.793
132.763
130.212
130.120
128.778
128.480
125.563
115.313
115.096
76.861
76.543
76.225
36.343
32.614
22.890
Parameter Value
1 Origin Bruker BioSpin GmbH
2 Solvent CDCl3
3 Temperature 297.8
4 Number of Scans 1024
5 Spectrometer Frequency 100.61
6 Nucleus 13C
200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)


-105.283
Parameter Value
1 Origin Bruker BioSpin GmbH
2 Solvent CDCl3
3 Temperature 297.8
4 Number of Scans 16
5 Spectrometer Frequency 376.44
6 Nucleus 19F
0 -10 -30 -50 -70 -90 -110 -130 -150 -170 -190 -210 -230 -250 -270 -290
f1 (ppm)


7.802
7.798
7.781
7.593
7.589
7.572
7.358
7.355
7.337
7.292
7.288
7.274
7.257
7.254
7.188
7.170
7.151
3.117
3.100
3.082
3.051
3.033
3.016
2.114
2.097
2.079
2.062
2.044
0.000
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
S
Br
2k
1.97
1.98
2.00
2.07
0.96
2.03
1.96
2.00
f1 (ppm)


197.884
135.535
135.039
131.431
129.078
128.790
128.494
127.778
125.589
76.886
76.568
76.251
36.391
32.581
22.822
Parameter Value
1 Origin Bruker BioSpin GmbH
2 Solvent CDCl3
3 Temperature 298.1
4 Number of Scans 69
5 Spectrometer Frequency 100.61
6 Nucleus 13C
O
S
Br
2k
f1 (ppm)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7.951
7.653
7.633
7.293
7.290
7.285
7.272
7.269
7.264
7.225
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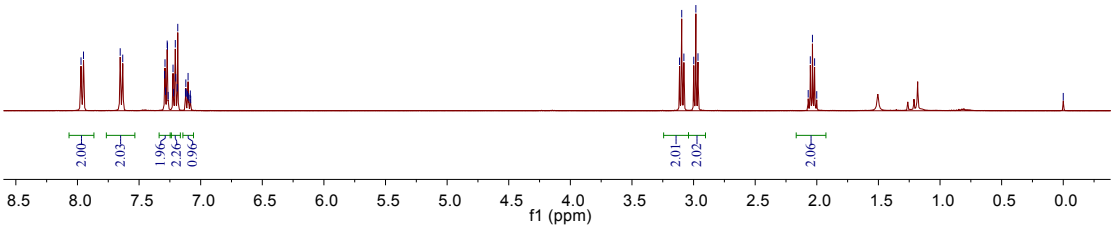
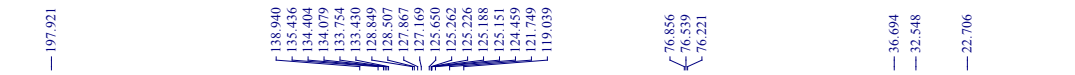
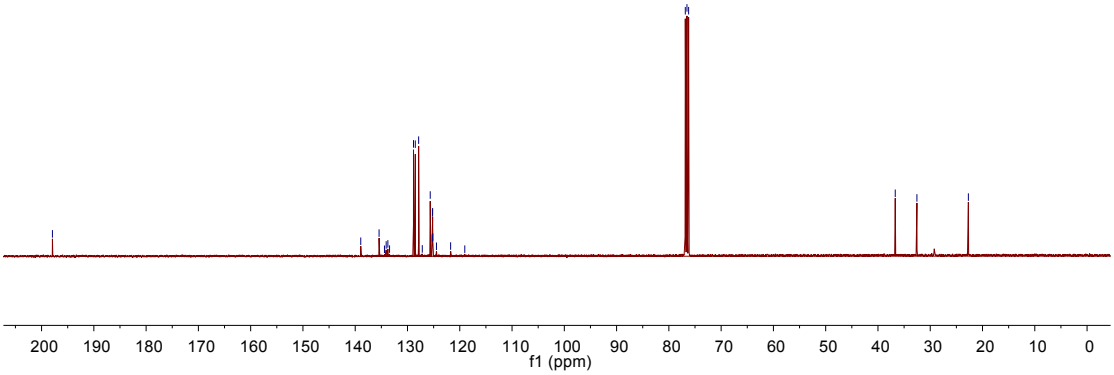
7.206
7.203
7.190
7.186
7.124
7.121
7.117
7.107
7.102
7.097
7.087
7.084
7.081
3.114
3.096
3.079
2.999
2.981
2.964
2.070
2.053
2.035
2.018
2.001
0.000
Parameter Value
1 Origin Bruker BioSpin GmbH
2 Solvent CDCl3
3 Temperature 297.8
4 Number of Scans 4
5 Spectrometer Frequency 400.13
6 Nucleus 1H
O
S
F3C

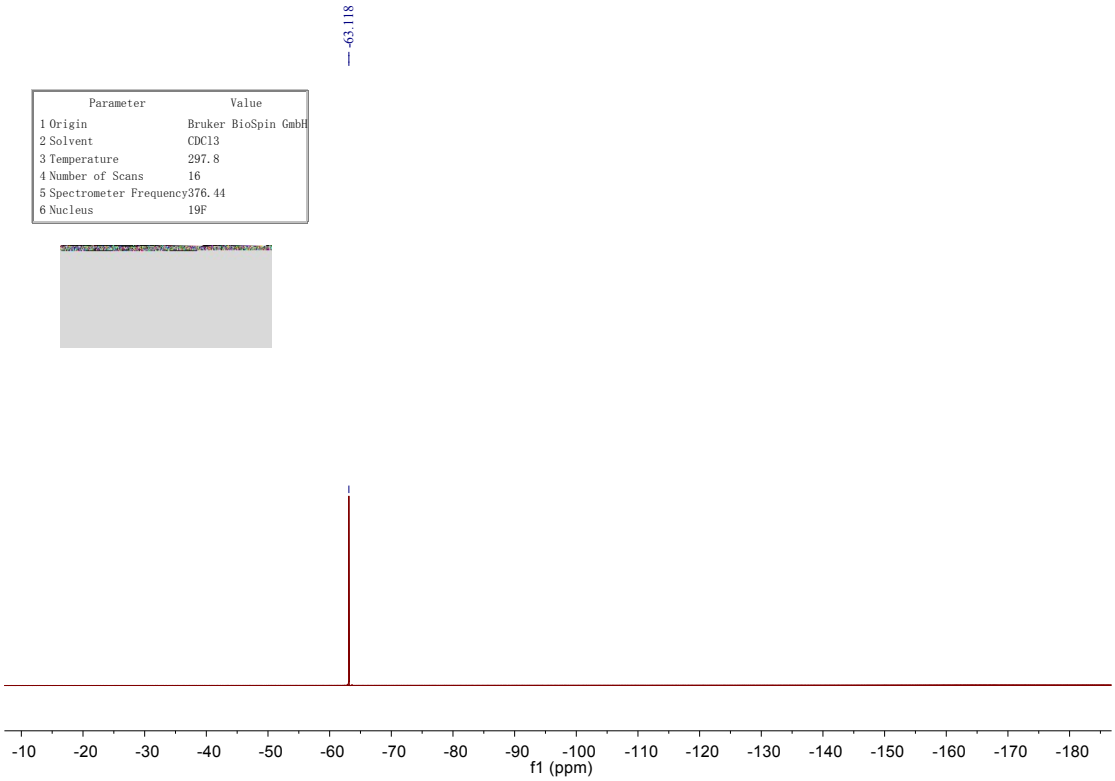
2l

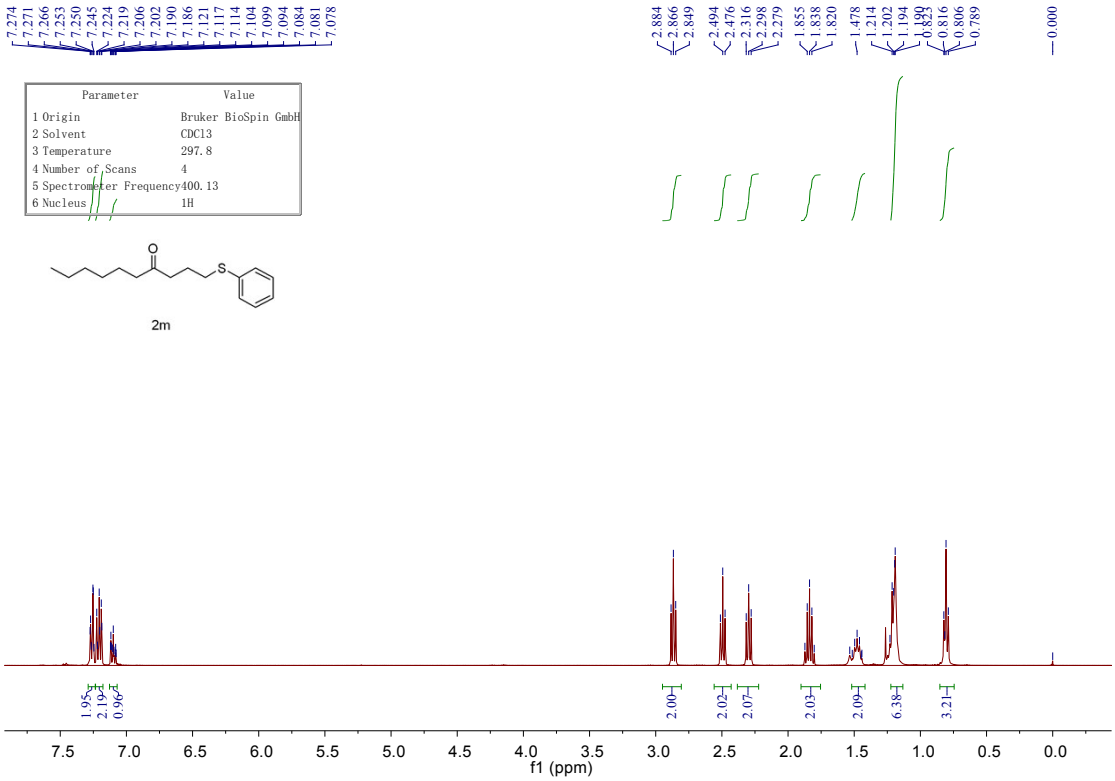

2.00
2.03
1.96
2.26
0.96
2.01
2.02
2.06
8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)

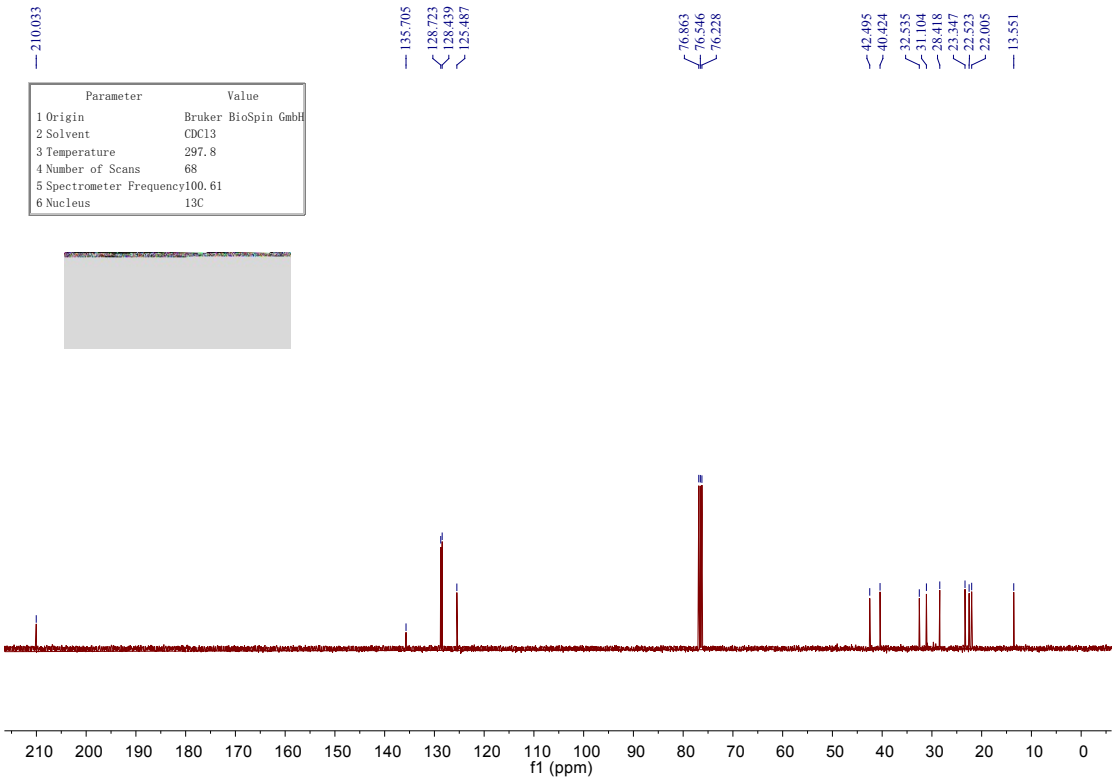

197.921
138.940
135.436
134.404
134.079
133.754
133.430
128.849
128.507
127.867
127.169
125.650
125.262
125.226
125.188
125.151
124.459
121.749
119.039
76.856
76.539
76.221
36.694
32.548
22.706
Parameter Value
1 Origin Bruker BioSpin GmbH
2 Solvent CDCl3
3 Temperature 297.8
4 Number of Scans 1024
5 Spectrometer Frequency 100.61
6 Nucleus 13C
O
S
F3C

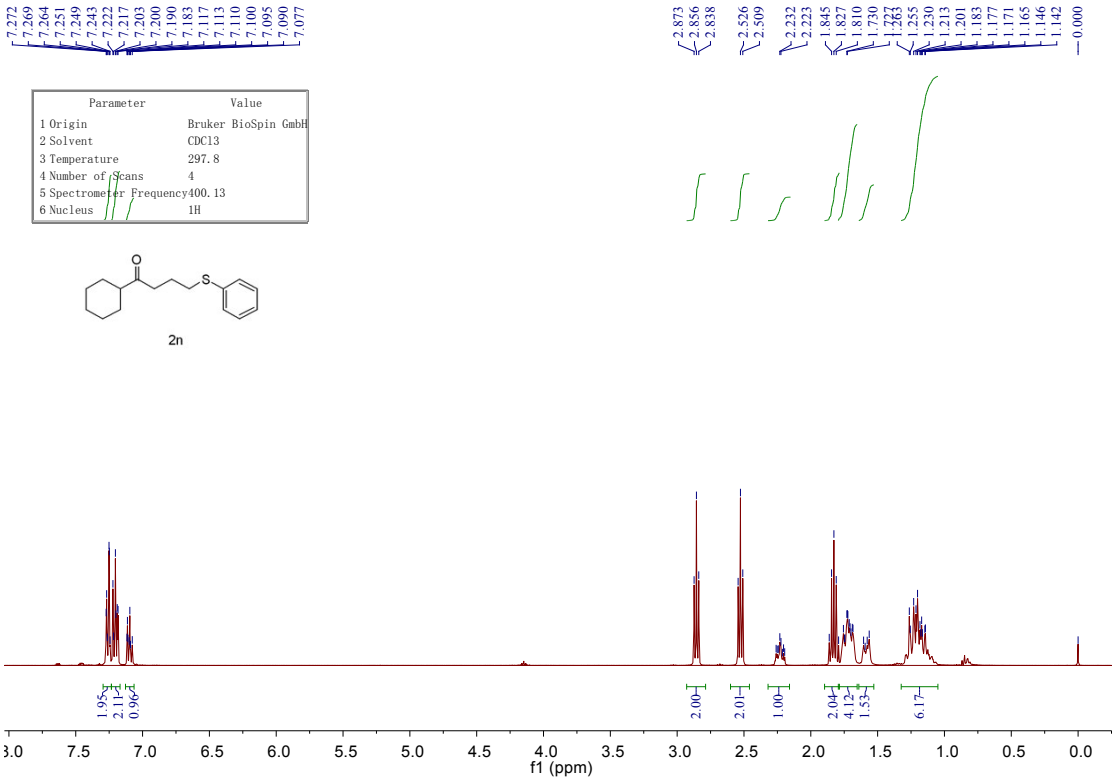
2l

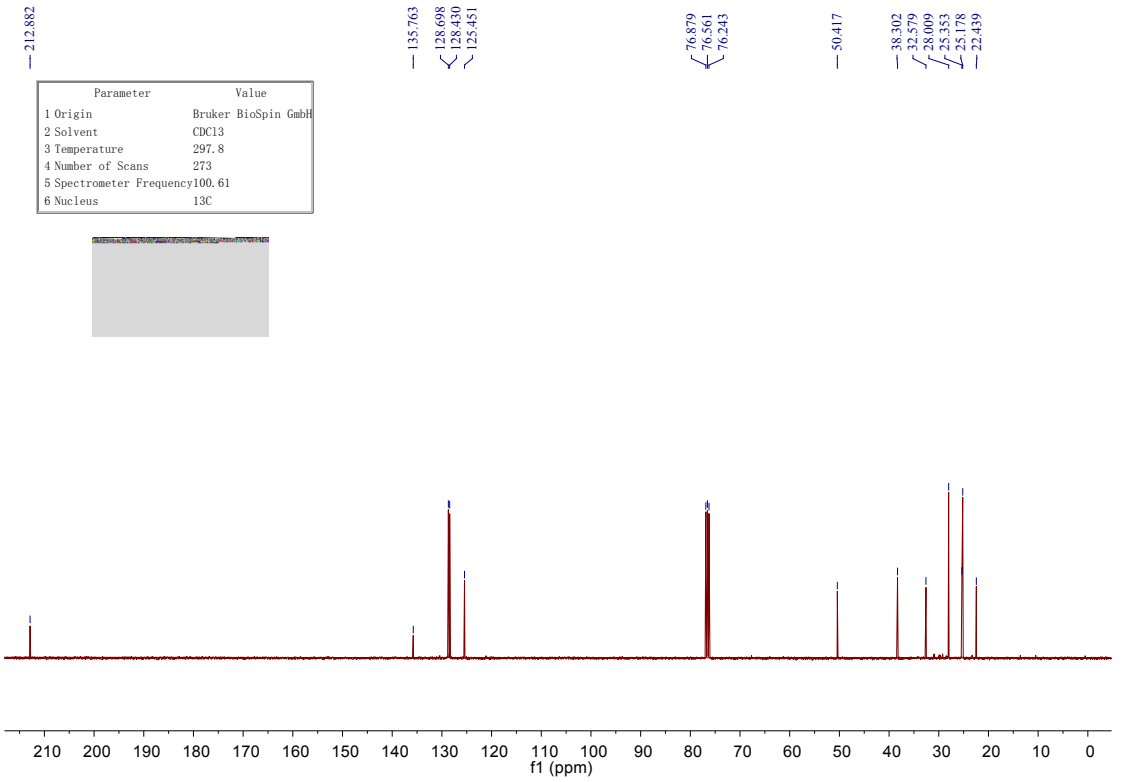

200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)

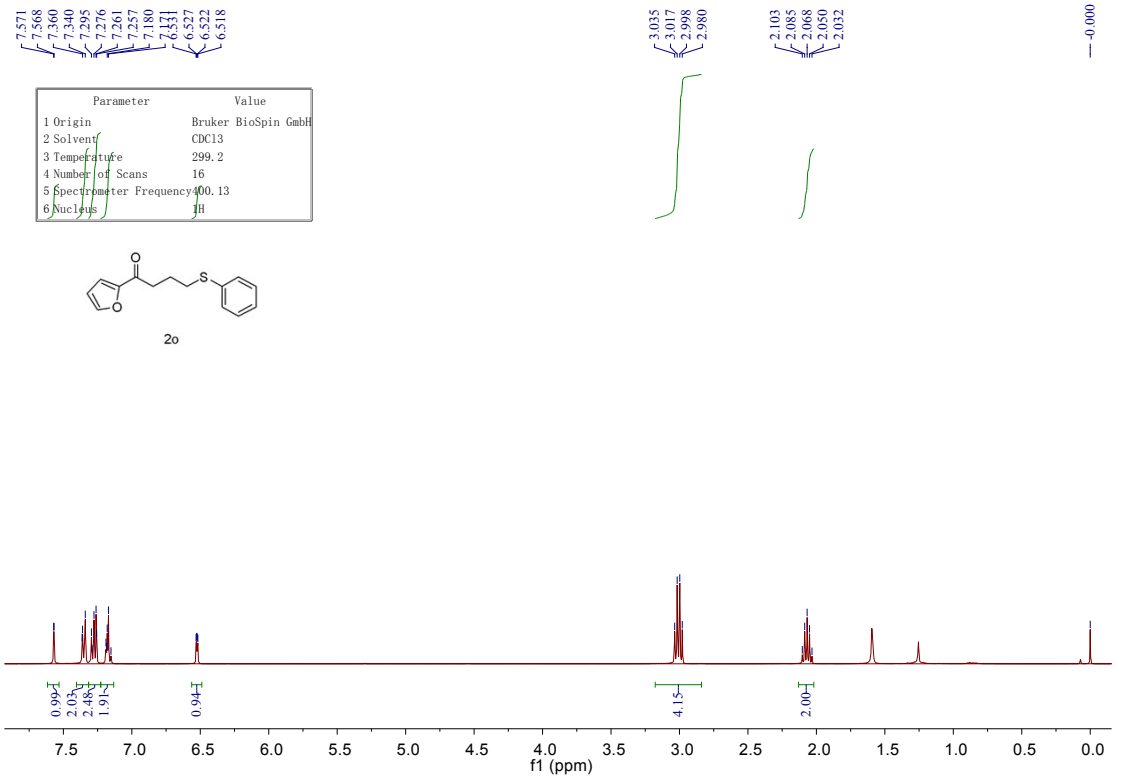

-63.118
Parameter Value
1 Origin Bruker BioSpin GmbH
2 Solvent CDCl3
3 Temperature 297.8
4 Number of Scans 16
5 Spectrometer Frequency 376.44
6 Nucleus 19F
-10 -20 -30 -40 -50 -60 -70 -80 -90 -100 -110 -120 -130 -140 -150 -160 -170 -180
f1 (ppm)


7.274 7.271 7.266 7.253 7.250 7.245 7.224 7.219 7.206 7.202 7.190 7.186 7.121 7.117 7.114 7.104 7.099 7.094 7.084 7.081 7.078
2.884 2.866 2.849 2.494 2.476 2.316 2.298 2.279 1.855 1.838 1.820 1.478 1.214 1.202 1.194 0.823 0.816 0.806 0.789 0.000
Parameter Value
1 Origin Bruker BioSpin GmbH
2 Solvent CDCl3
3 Temperature 297.8
4 Number of Scans 4
5 Spectrometer Frequency 400.13
6 Nucleus 1H
O
S
2m
1.95 2.19 0.96 2.00 2.02 2.07 2.03 2.09 6.38 3.21
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)

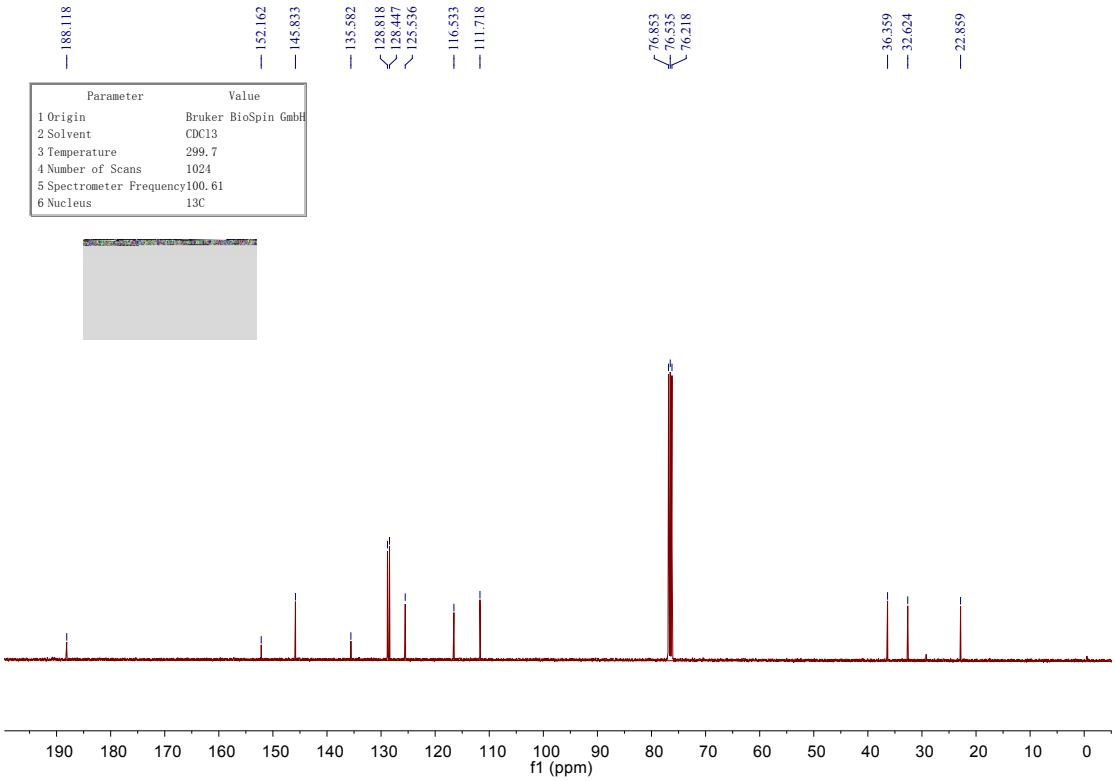

210.033
135.705
128.723
128.439
125.487
76.863
76.546
76.228
42.495
40.424
32.535
31.104
28.418
23.347
22.523
22.005
13.551
Parameter Value
1 Origin Bruker BioSpin GmbH
2 Solvent CDCl3
3 Temperature 297.8
4 Number of Scans 68
5 Spectrometer Frequency 100.61
6 Nucleus 13C
f1 (ppm)

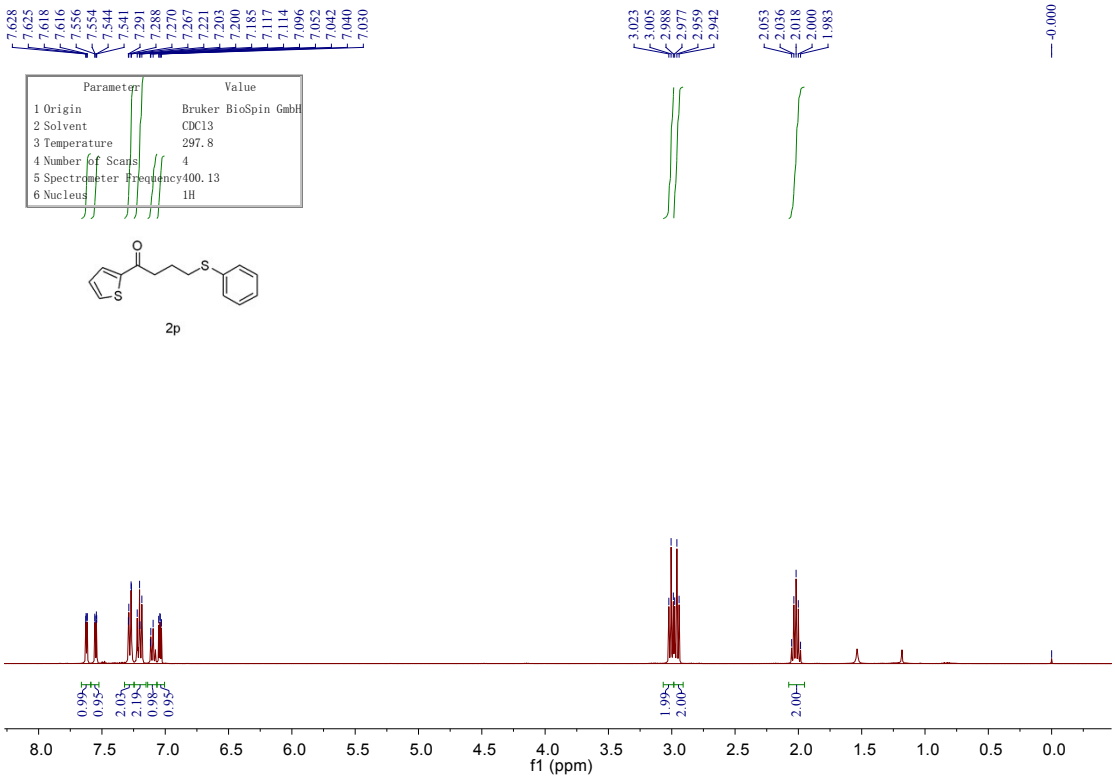

7.272
7.269
7.264
7.251
7.249
7.243
7.222
7.217
7.203
7.200
7.190
7.183
7.117
7.113
7.110
7.100
7.095
7.090
7.077
2.873
2.856
2.838
2.526
2.509
2.232
2.223
1.845
1.827
1.810
1.730
1.255
1.230
1.213
1.201
1.183
1.177
1.171
1.165
1.146
1.142
0.000
Parameter Value
1 Origin Bruker BioSpin GmbH
2 Solvent CDCl3
3 Temperature 297.8
4 Number of Scans 4
5 Spectrometer Frequency 400.13
6 Nucleus 1H
O
S
2n
1.95
2.11
0.96
2.00
2.01
1.00
2.04
4.12
1.53
6.17
f1 (ppm)

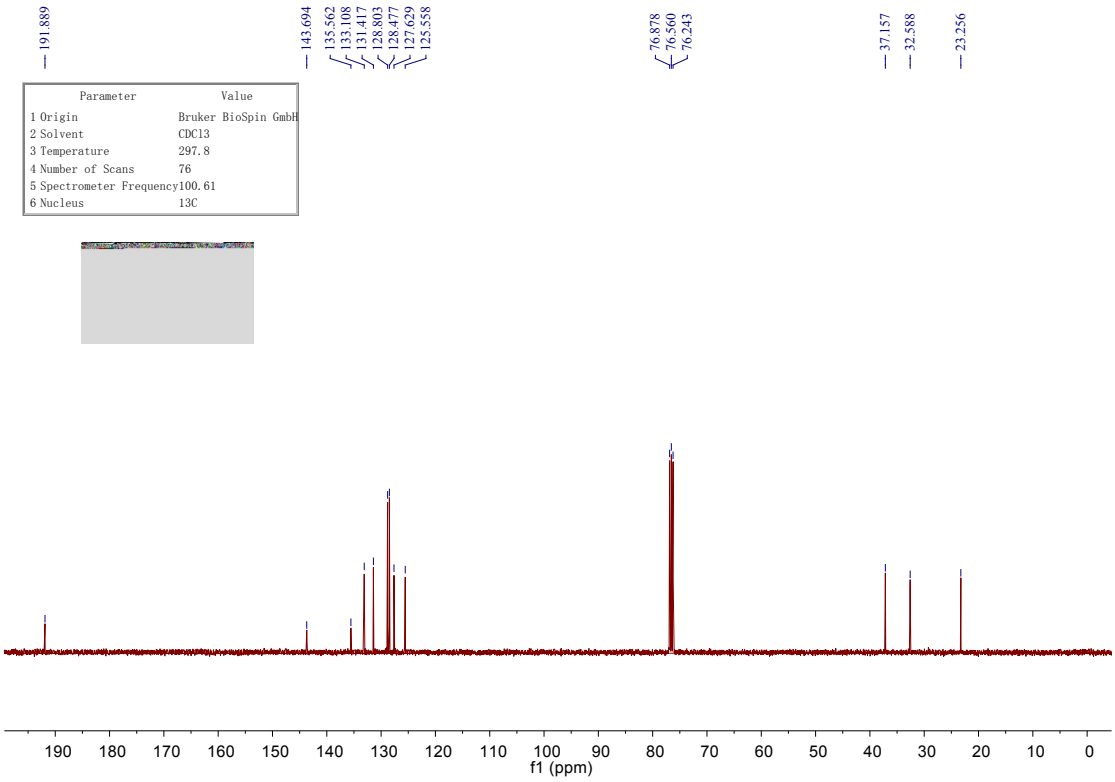

212.882
135.763
128.698
128.430
125.451
76.879
76.561
76.243
50.417
38.302
32.579
28.009
25.353
25.178
22.439
Parameter Value
1 Origin Bruker BioSpin GmbH
2 Solvent CDCl3
3 Temperature 297.8
4 Number of Scans 273
5 Spectrometer Frequency 100.61
6 Nucleus 13C
f1 (ppm)

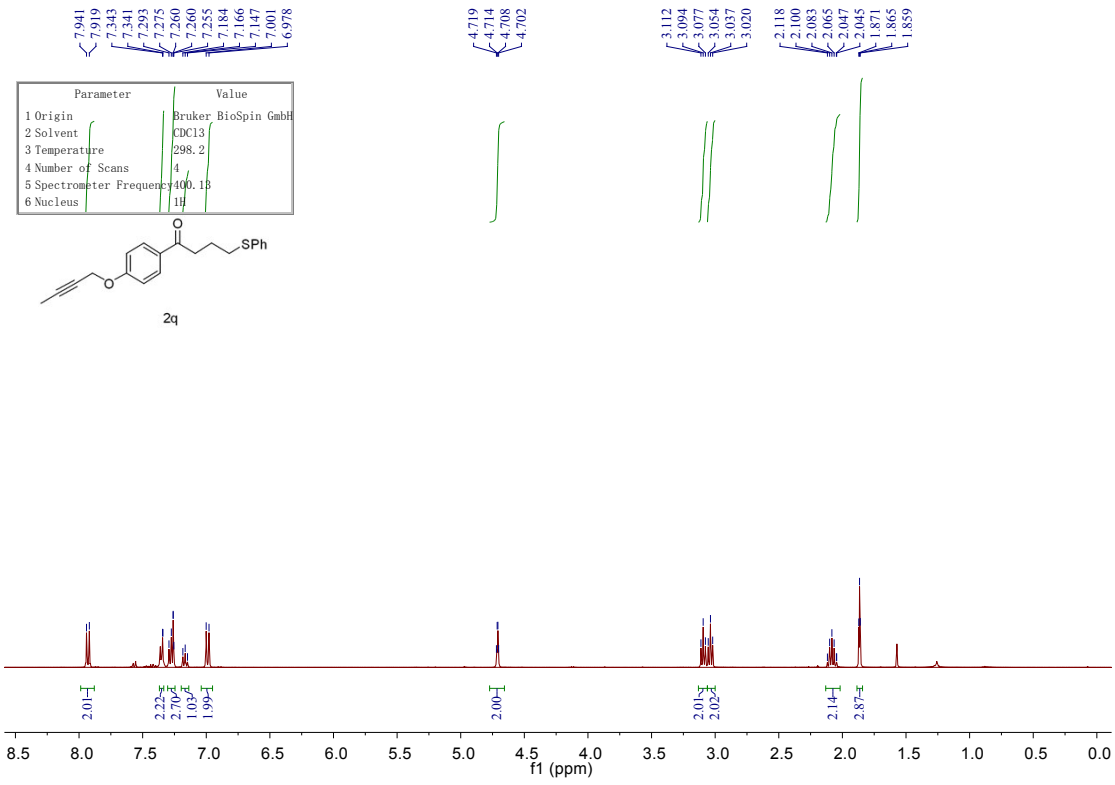

7.571
7.568
7.360
7.340
7.295
7.276
7.261
7.257
7.180
7.171
6.531
6.527
6.522
6.518
3.035
3.017
2.998
2.980
2.103
2.085
2.068
2.050
2.032
-0.000
Parameter Value
1 Origin Bruker BioSpin GmbH
2 Solvent CDCl3
3 Temperature 299.2
4 Number of Scans 16
5 Spectrometer Frequency 400.13
6 Nucleus 1H
O
S
O
0.99
2.03
2.48
1.91
0.94
4.15
2.00
f1 (ppm)

2o


188.118
152.162
145.833
135.582
128.818
128.447
125.536
116.533
111.718
76.853
76.535
76.218
36.359
32.624
22.859
Parameter Value
1 Origin Bruker BioSpin GmbH
2 Solvent CDCl3
3 Temperature 299.7
4 Number of Scans 1024
5 Spectrometer Frequency 100.61
6 Nucleus 13C
f1 (ppm)


7.628
7.625
7.618
7.616
7.556
7.554
7.544
7.541
7.291
7.288
7.270
7.267
7.221
7.203
7.200
7.185
7.117
7.114
7.096
7.052
7.042
7.040
7.030
3.023
3.005
2.988
2.977
2.959
2.942
2.053
2.036
2.018
2.000
1.983
0.000
Parameter Value
1 Origin Bruker BioSpin GmbH
2 Solvent CDCl3
3 Temperature 297.8
4 Number of Scans 4
5 Spectrometer Frequency 400.13
6 Nucleus 1H
O
S
S
2p
0.99
0.95
2.03
2.19
0.98
0.95
1.99
2.00
2.00
f1 (ppm)


191.889
143.694
135.562
133.108
131.417
128.803
128.477
127.629
125.558
76.878
76.560
76.243
37.157
32.588
23.256
Parameter Value
1 Origin Bruker BioSpin GmbH
2 Solvent CDCl3
3 Temperature 297.8
4 Number of Scans 76
5 Spectrometer Frequency 100.61
6 Nucleus 13C
f1 (ppm)


7.941
7.919
7.343
7.341
7.293
7.275
7.260
7.260
7.255
7.184
7.166
7.147
7.001
6.978
4.719
4.714
4.708
4.702
3.112
3.094
3.077
3.054
3.037
3.020
2.118
2.100
2.083
2.065
2.047
2.045
1.871
1.865
1.859
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
SPh
O
2q
2.01
2.22
2.70
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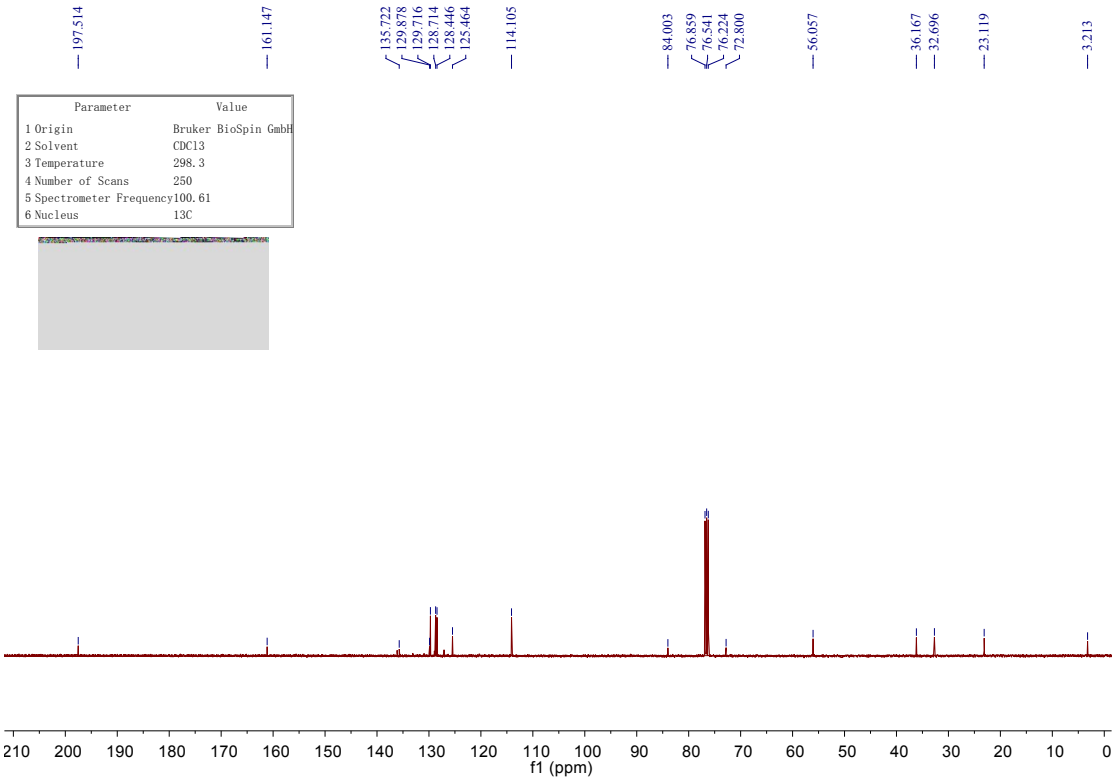
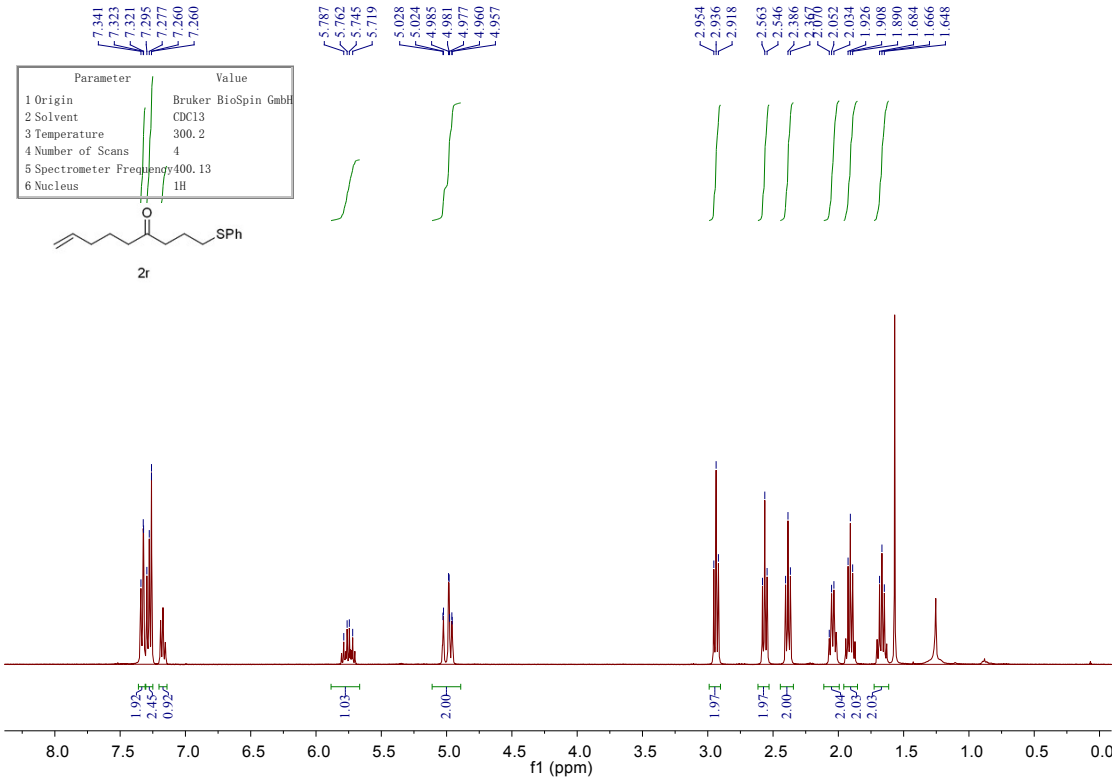
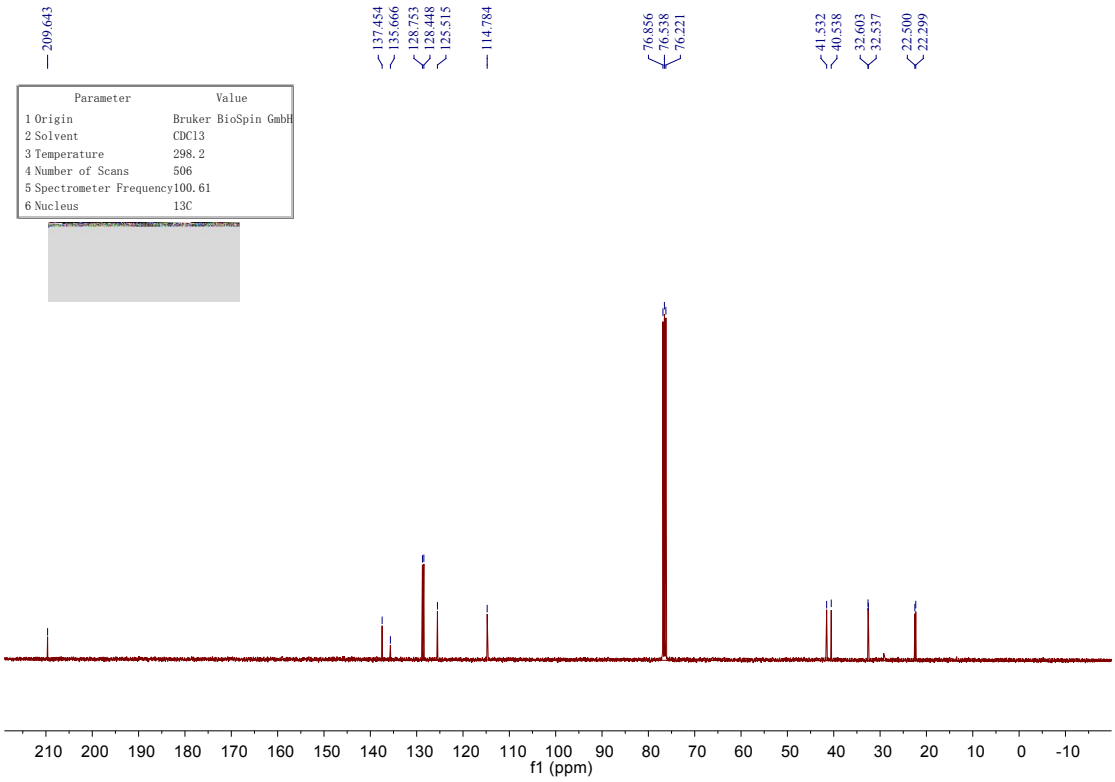
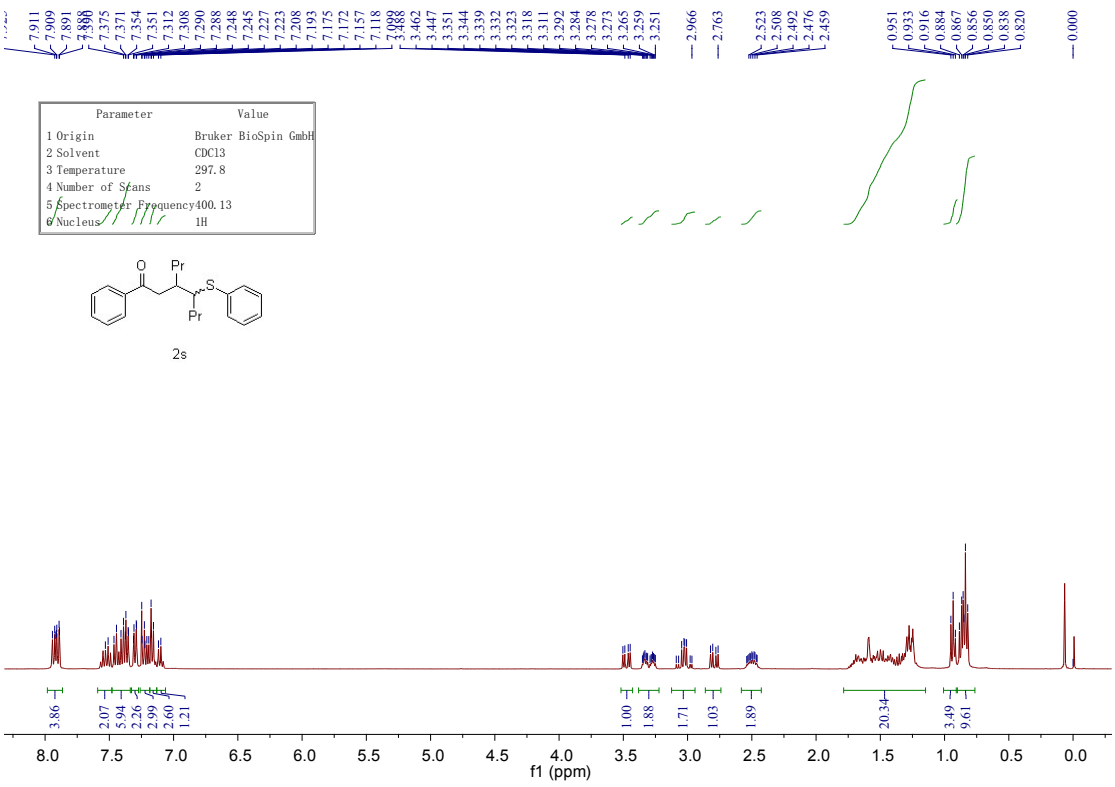
2.01
2.02
2.14
2.87
f1 (ppm)


197.514
161.147
135.722
129.878
129.716
128.714
128.446
125.464
114.105
84.003
76.859
76.541
76.224
72.800
56.057
36.167
32.696
23.119
3.213
Parameter Value
1 Origin Bruker BioSpin GmbH
2 Solvent CDCl3
3 Temperature 298.3
4 Number of Scans 250
5 Spectrometer Frequency 100.61
6 Nucleus 13C
f1 (ppm)


7.341
7.323
7.321
7.295
7.277
7.260
7.260
5.787
5.762
5.745
5.719
5.028
5.024
4.985
4.981
4.977
4.960
4.957
2.954
2.936
2.918
2.563
2.546
2.386
2.367
2.070
2.052
2.034
1.926
1.908
1.890
1.684
1.666
1.648
Parameter Value
1 Origin Bruker BioSpin GmbH
2 Solvent CDCl3
3 Temperature 300.2
4 Number of Scans 4
5 Spectrometer Frequency 400.13
6 Nucleus 1H
O
SPh
2r
1.92
2.45
0.92
1.03
2.00
1.97
1.97
2.00
2.04
2.03
2.03
f1 (ppm)


209.643
137.454
135.666
128.753
128.448
125.515
114.784
76.856
76.538
76.221
41.532
40.538
32.603
32.537
22.500
22.299
Parameter Value
1 Origin Bruker BioSpin GmbH
2 Solvent CDCl3
3 Temperature 298.2
4 Number of Scans 506
5 Spectrometer Frequency 100.61
6 Nucleus 13C
f1 (ppm)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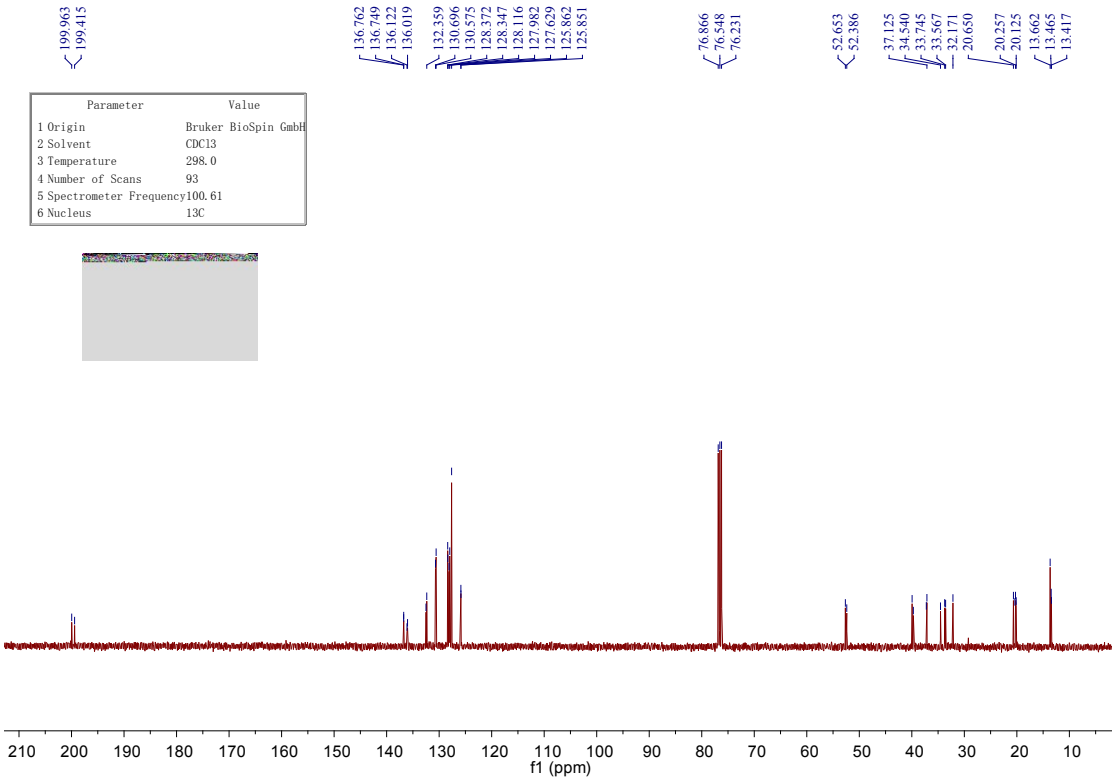
7.354
7.351
7.312
7.308
7.290
7.288
7.248
7.245
7.227
7.223
7.208
7.193
7.175
7.172
7.157
7.118
3.462
3.447
3.351
3.344
3.339
3.332
3.323
3.318
3.311
3.292
3.284
3.278
3.273
3.265
3.259
3.251
2.966
2.763
2.523
2.508
2.492
2.476
2.459
0.951
0.933
0.916
0.884
0.867
0.856
0.850
0.838
0.820
0.000
Parameter Value
1 Origin Bruker BioSpin GmbH
2 Solvent CDCl3
3 Temperature 297.8
4 Number of Scans 2
5 Spectrometer Frequency 400.13
6 Nucleus 1H
O
Pr
S
Pr
3.86
2.07
5.94
2.26
2.99
2.60
1.21
1.00
1.88
1.71
1.03
1.89
20.34
3.49
9.61
f1 (ppm)

2s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199.415
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136.749
136.122
136.019
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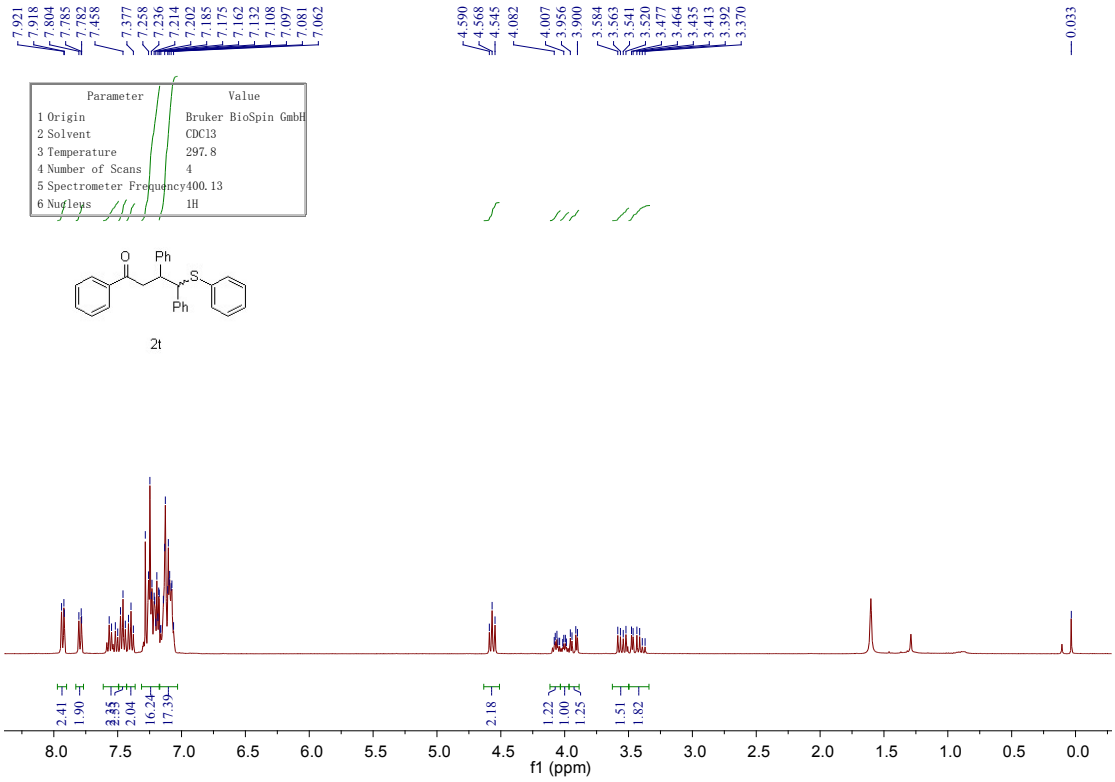
130.696
130.575
128.372
128.347
128.116
127.982
127.629
125.862
125.851
76.866
76.548
76.231
52.653
52.386
37.125
34.540
33.745
33.567
32.171
20.650
20.257
20.125
13.662
13.465
13.417
Parameter Value
1 Origin Bruker BioSpin GmbH
2 Solvent CDCl3
3 Temperature 298.0
4 Number of Scans 93
5 Spectrometer Frequency 100.61
6 Nucleus 13C
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10
f1 (ppm)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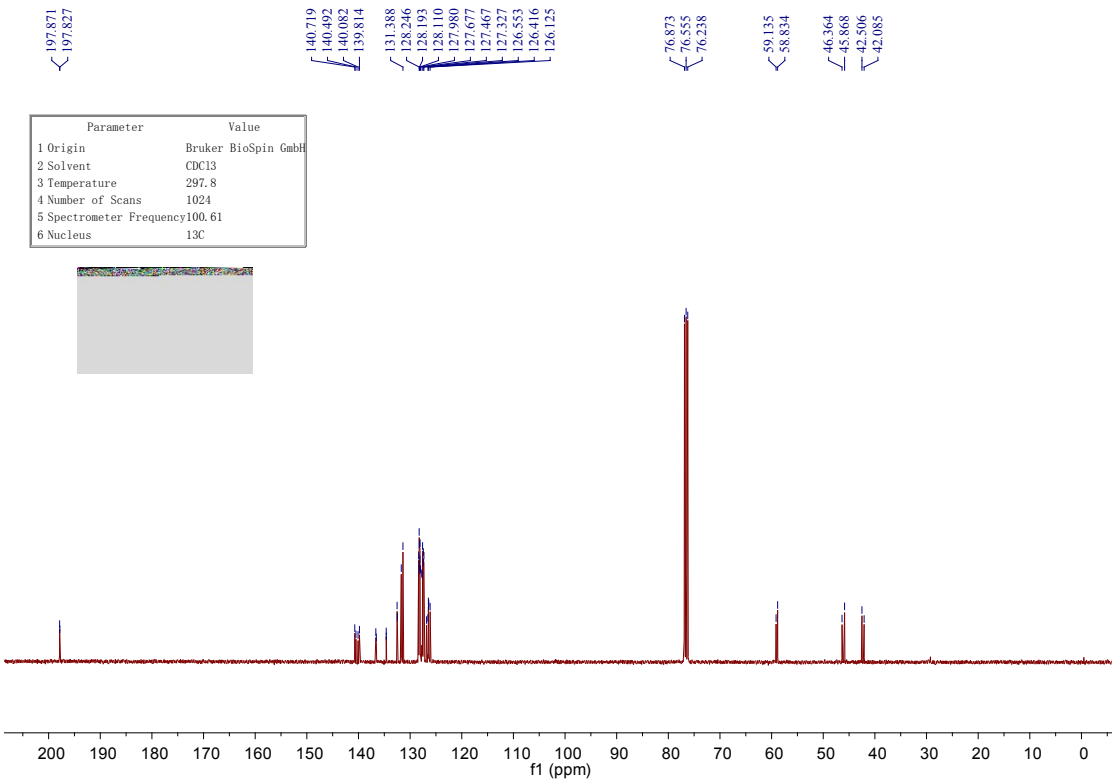
7.918
7.804
7.785
7.782
7.458
7.377
7.258
7.236
7.214
7.202
7.185
7.175
7.162
7.132
7.108
7.097
7.081
7.062
4.590
4.568
4.545
4.082
4.007
3.956
3.900
3.584
3.563
3.541
3.520
3.477
3.464
3.435
3.413
3.392
3.370
0.033
Parameter Value
1 Origin Bruker BioSpin GmbH
2 Solvent CDCl3
3 Temperature 297.8
4 Number of Scans 4
5 Spectrometer Frequency 400.13
6 Nucleus 1H
O
Ph
S
Ph
2t
2.41
1.90
3.35
3.35
2.04
16.24
17.39
2.18
1.22
1.00
1.25
1.51
1.82
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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140.082
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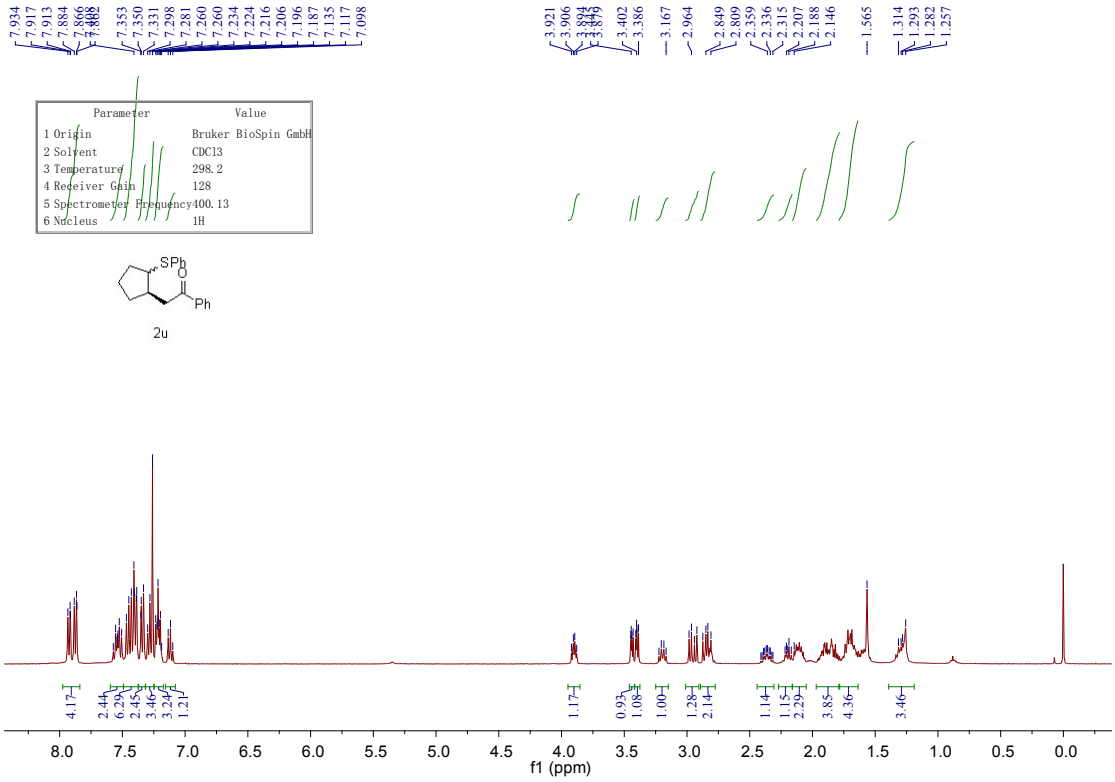
128.193
128.110
127.980
127.677
127.467
127.327
126.553
126.416
126.125
76.873
76.555
76.238
59.135
58.834
46.364
45.868
42.506
42.085
Parameter Value
1 Origin Bruker BioSpin GmbH
2 Solvent CDCl3
3 Temperature 297.8
4 Number of Scans 1024
5 Spectrometer Frequency 100.61
6 Nucleus 13C
f1 (ppm)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7.913
7.884
7.866
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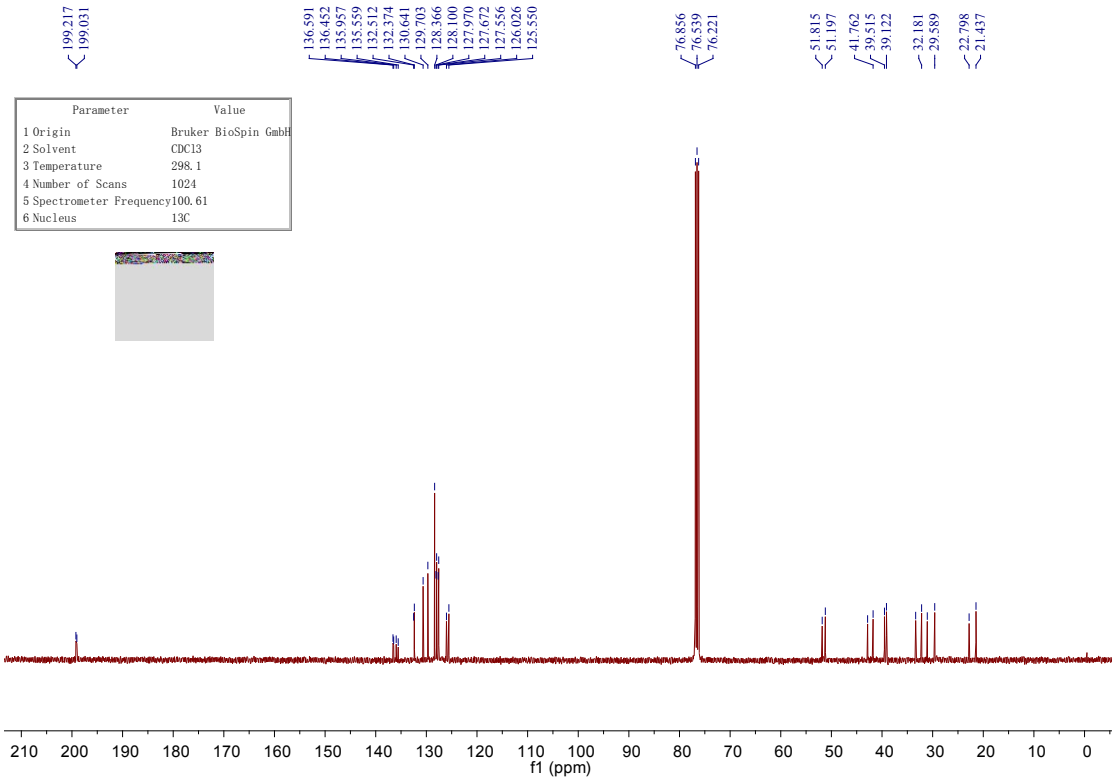
7.350
7.331
7.298
7.281
7.260
7.234
7.224
7.216
7.206
7.196
7.187
7.135
7.117
7.098
3.921
3.906
3.402
3.386
3.167
2.964
2.849
2.809
2.359
2.336
2.315
2.207
2.188
2.146
1.565
1.314
1.293
1.282
1.257
Parameter Value
1 Origin Bruker BioSpin GmbH
2 Solvent CDCl3
3 Temperature 298.2
4 Receiver Gain 128
5 Spectrometer Frequency 400.13
6 Nucleus 1H
SPh
O
Ph
4.17
2.44
6.29
2.45
3.46
3.24
1.21
1.17
0.93
1.08
1.00
1.28
2.14
1.14
1.15
2.29
3.85
4.36
3.46
f1 (ppm)

2u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136.452
135.957
135.559
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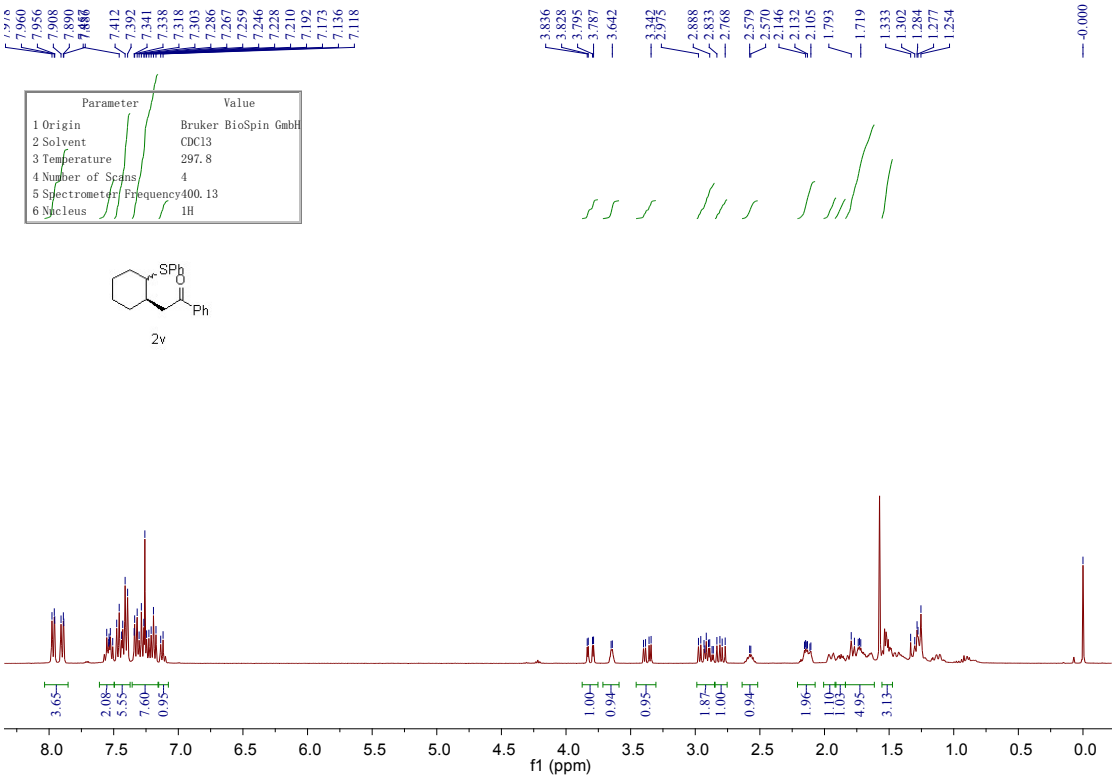
132.374
130.641
129.703
128.366
128.100
127.970
127.672
127.556
126.026
125.550
76.856
76.539
76.221
51.815
51.197
41.762
39.515
39.122
32.181
29.589
22.798
21.437
Parameter Value
1 Origin Bruker BioSpin GmbH
2 Solvent CDCl3
3 Temperature 298.1
4 Number of Scans 1024
5 Spectrometer Frequency 100.61
6 Nucleus 13C
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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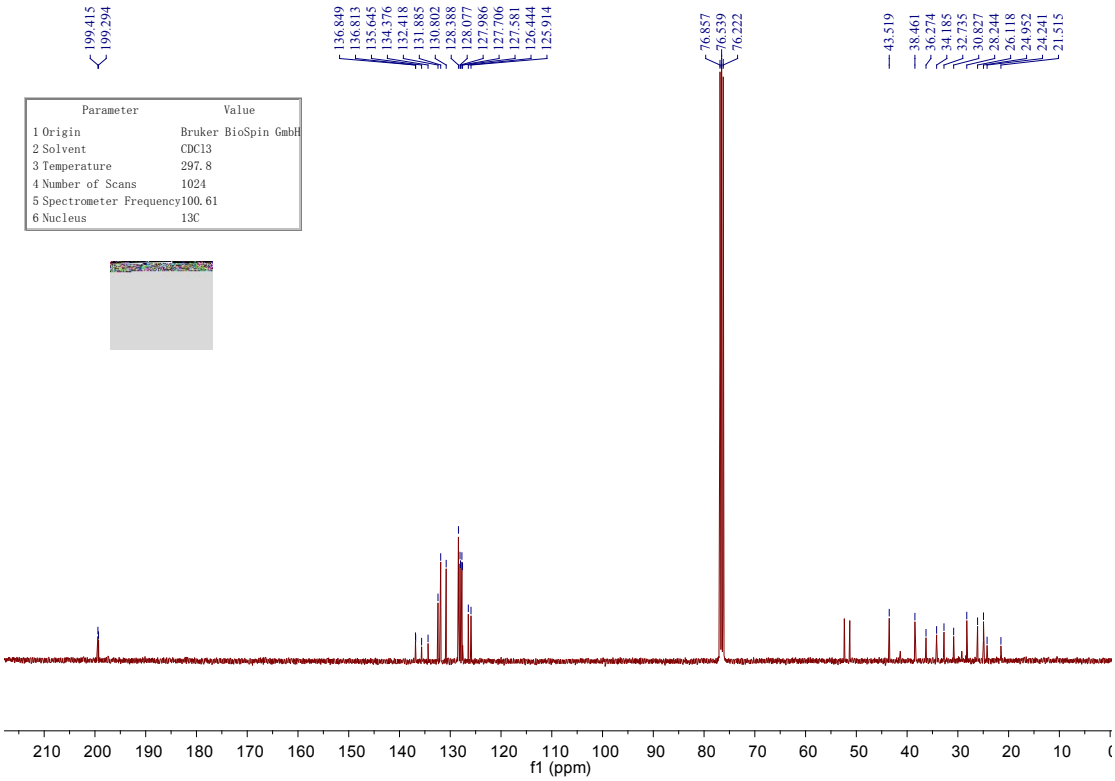
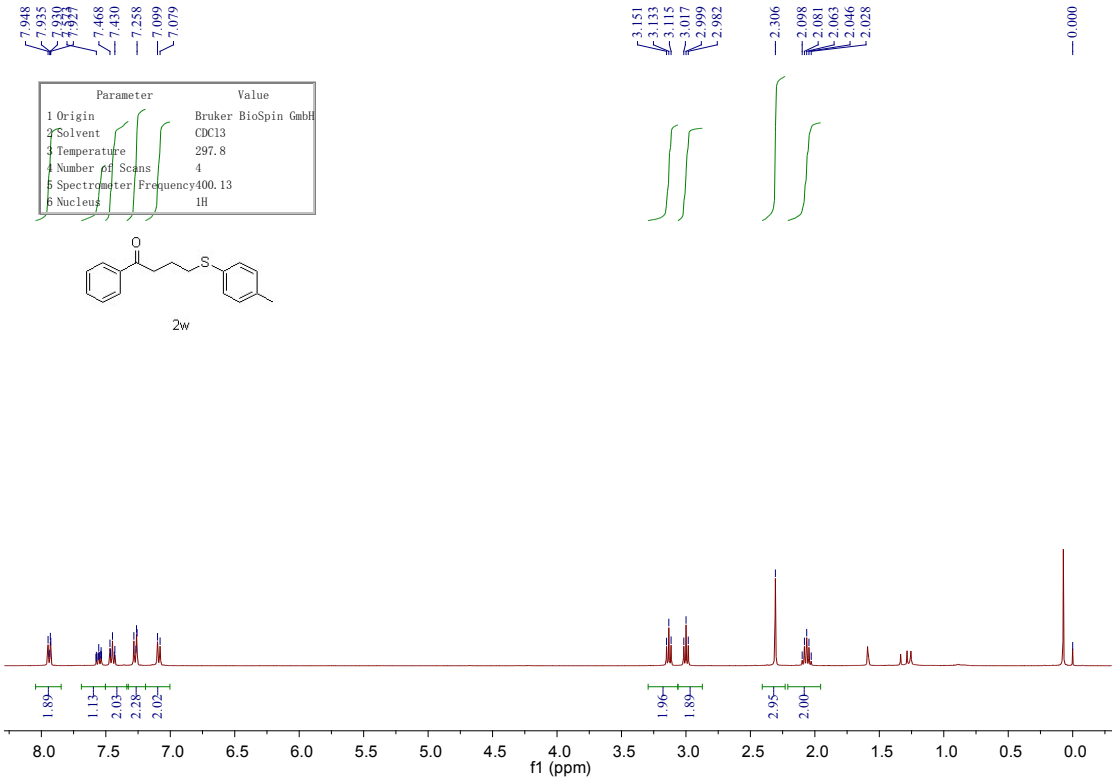
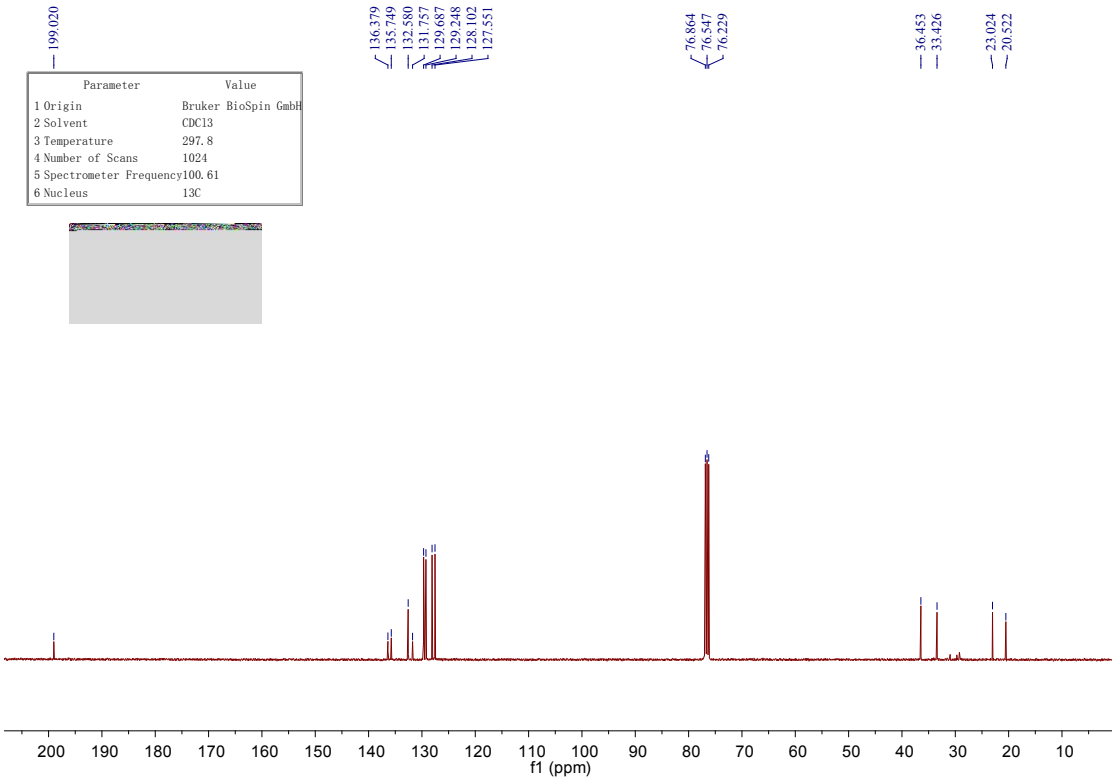
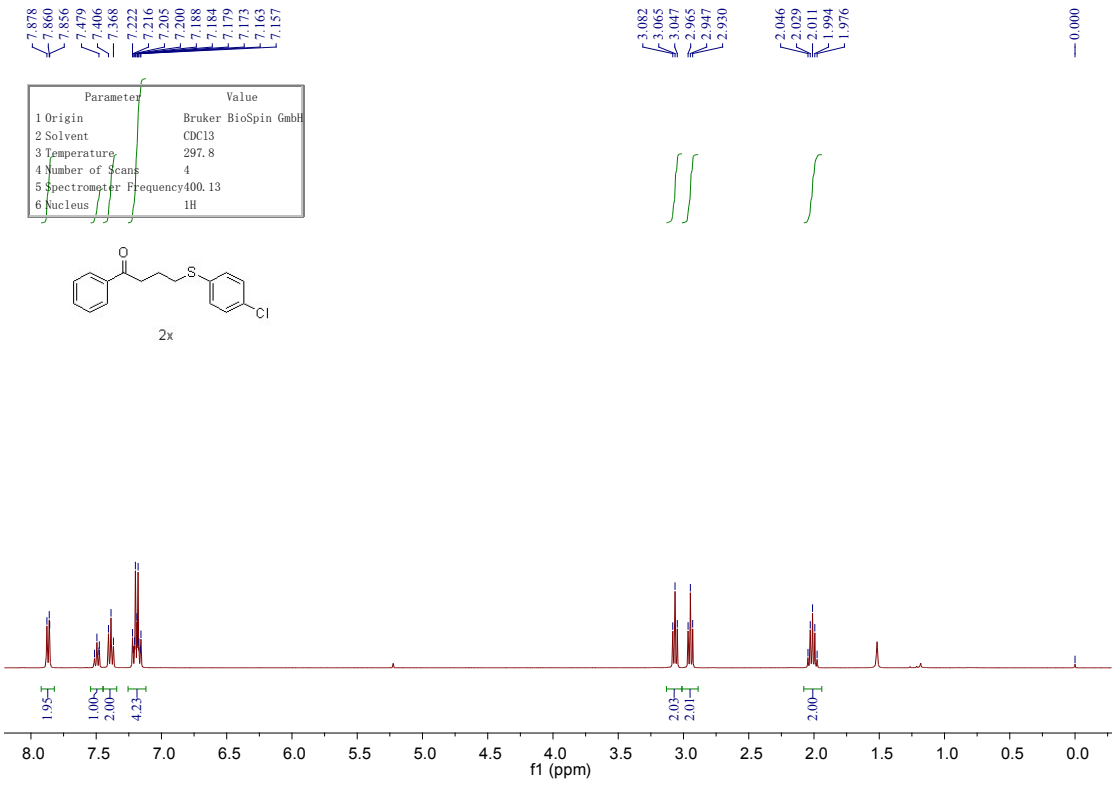
7.286
7.267
7.259
7.246
7.228
7.210
7.192
7.173
7.136
7.118
3.836
3.828
3.795
3.787
3.642
3.342
2.975
2.888
2.833
2.768
2.579
2.570
2.146
2.132
2.105
1.793
1.719
1.333
1.302
1.284
1.277
1.254
-0.000
Parameter Value
1 Origin Bruker BioSpin GmbH
2 Solvent CDCl3
3 Temperature 297.8
4 Number of Scans 4
5 Spectrometer Frequency 400.13
6 Nucleus 1H
SPh
O
Ph
2v
3.65
2.08
5.55
7.60
0.95
1.00
0.94
0.95
1.87
1.00
0.94
1.96
1.10
1.05
4.95
3.13
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)


199.415
199.294
136.849
136.813
135.645
134.376
132.418
131.885
130.802
128.388
128.077
127.986
127.706
127.581
126.444
125.914
76.857
76.539
76.222
43.519
38.461
36.274
34.185
32.735
30.827
28.244
26.118
24.952
24.241
21.515
Parameter Value
1 Origin Bruker BioSpin GmbH
2 Solvent CDCl3
3 Temperature 297.8
4 Number of Scans 1024
5 Spectrometer Frequency 100.61
6 Nucleus 13C
f1 (ppm)


7.948
7.935
7.930
7.927
7.468
7.430
7.258
7.099
7.079
3.151
3.133
3.115
3.017
2.999
2.982
2.306
2.098
2.081
2.063
2.046
2.028
0.000
Parameter Value
1 Origin Bruker BioSpin GmbH
2 Solvent CDCl3
3 Temperature 297.8
4 Number of Scans 4
5 Spectrometer Frequency 400.13
6 Nucleus 1H
O
S
2w
1.89
1.13
2.03
2.28
2.02
1.96
1.89
2.95
2.00
f1 (ppm)


199.020
136.379
135.749
132.580
131.757
129.687
129.248
128.102
127.551
76.864
76.547
76.229
36.453
33.426
23.024
20.522
Parameter Value
1 Origin Bruker BioSpin GmbH
2 Solvent CDCl3
3 Temperature 297.8
4 Number of Scans 1024
5 Spectrometer Frequency 100.61
6 Nucleus 13C
200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10
f1 (ppm)


7.878
7.860
7.856
7.479
7.406
7.368
7.222
7.216
7.205
7.200
7.188
7.184
7.179
7.173
7.163
7.157
3.082
3.065
3.047
2.965
2.947
2.930
2.046
2.029
2.011
1.994
1.976
0.000
Parameter Value
1 Origin Bruker BioSpin GmbH
2 Solvent CDCl3
3 Temperature 297.8
4 Number of Scans 4
5 Spectrometer Frequency 400.13
6 Nucleus 1H
O
S
Cl
2x
1.95
1.00
2.00
4.23
2.03
2.01
2.00
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)

198.768

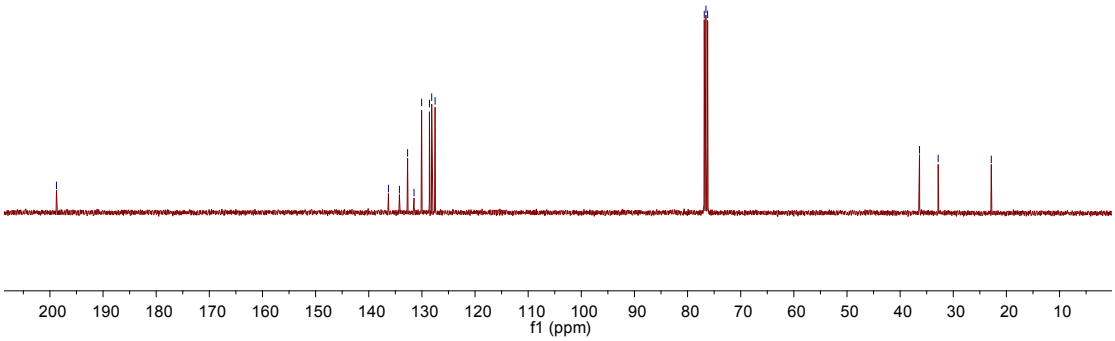
136.293
134.229
132.690
131.478
130.053
128.580
128.151
127.517

76.861
76.543
76.226

36.351
32.843

22.844

Parameter	Value
1 Origin	Bruker BioSpin GmbH
2 Solvent	CDCl3
3 Temperature	297.8
4 Number of Scans	125
5 Spectrometer Frequency	100.61
6 Nucleus	13C



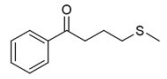
7.983
7.965
7.962
7.580
7.562
7.543
7.483
7.463
7.445
7.260

3.141
3.123
3.105

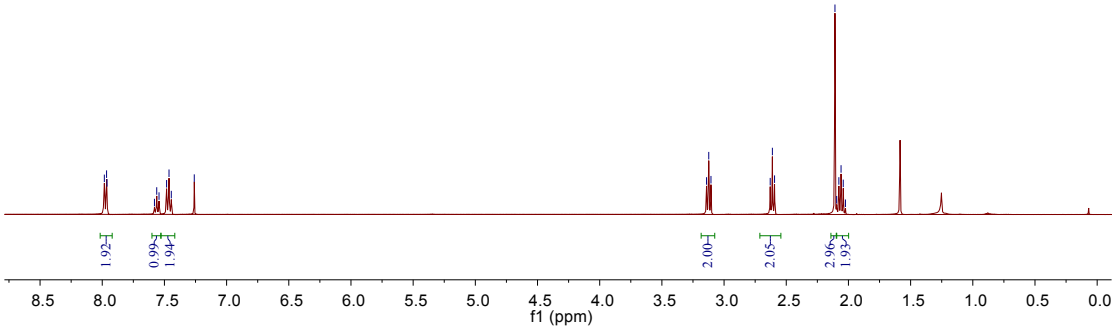
2.629
2.611
2.594

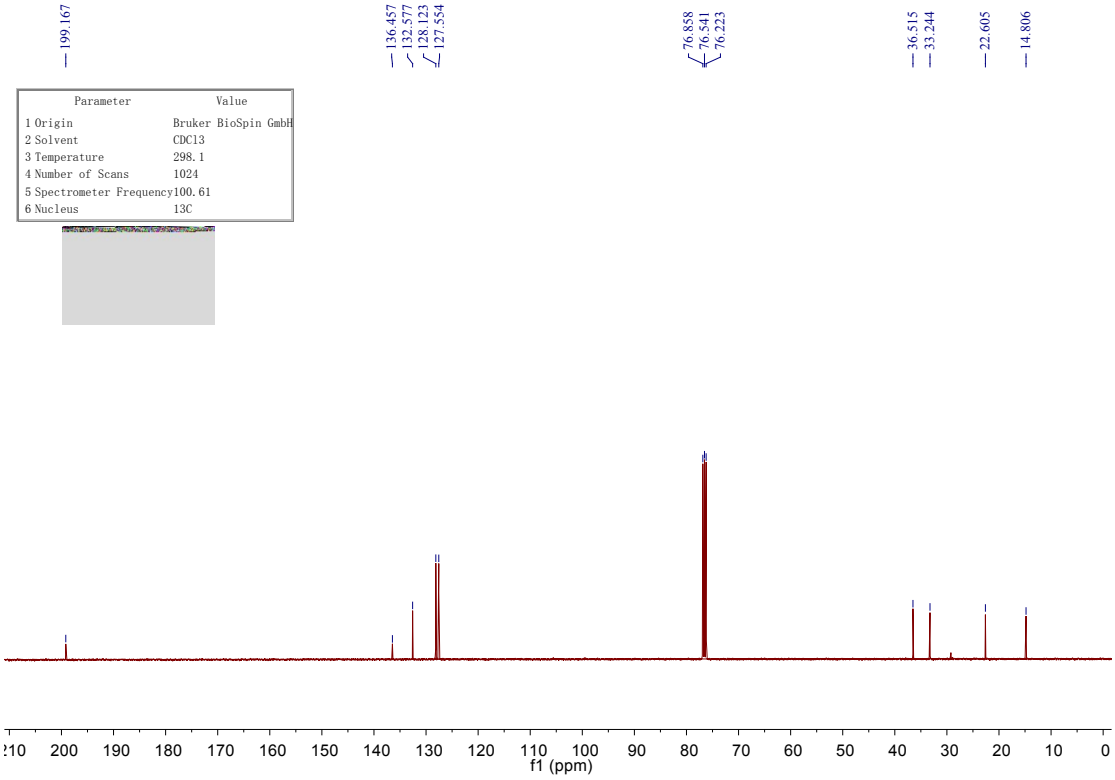
2.108
2.095
2.077
2.059
2.042
2.024

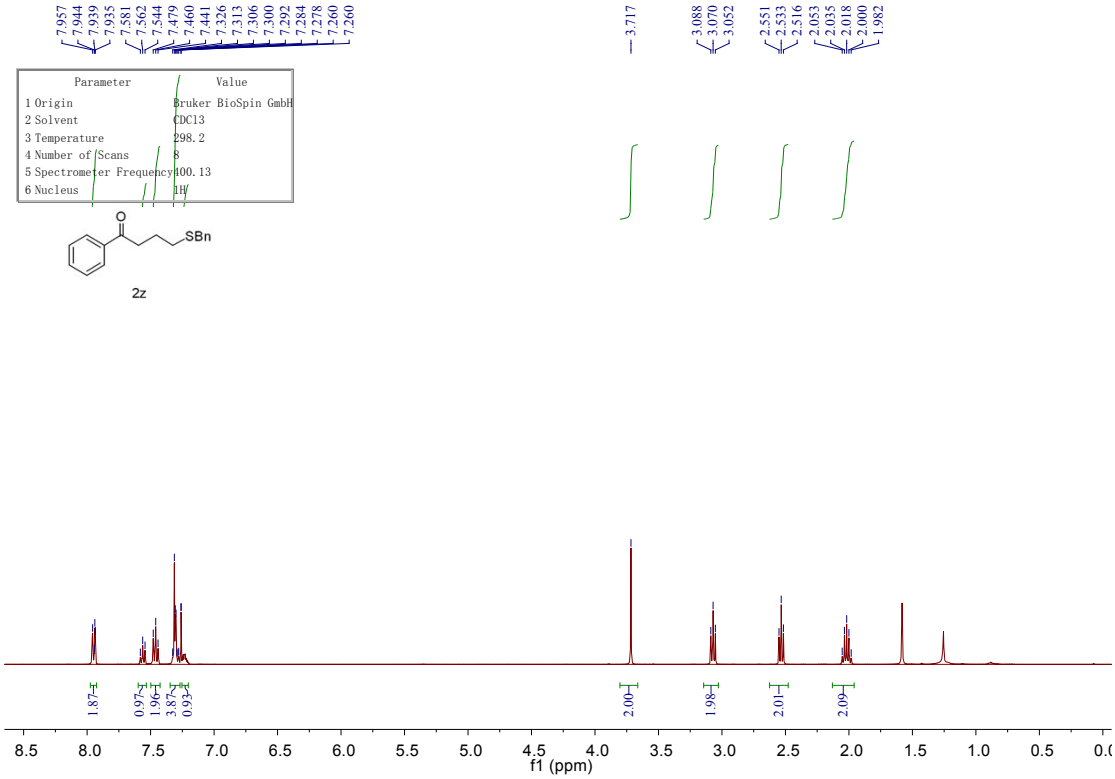
Parameter	Value
1 Origin	Bruker BioSpin GmbH
2 Solvent	CDCl3
3 Temperature	300.2
4 Number of Scans	4
5 Spectrometer Frequency	400.13
6 Nucleus	1H

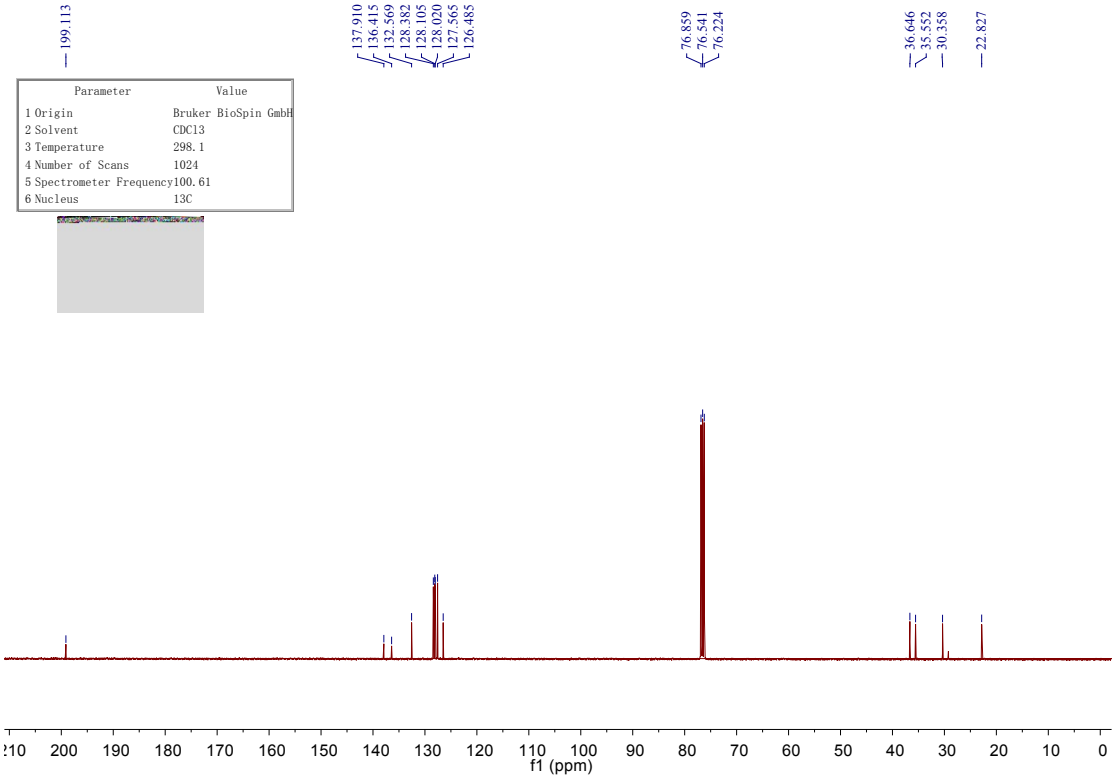


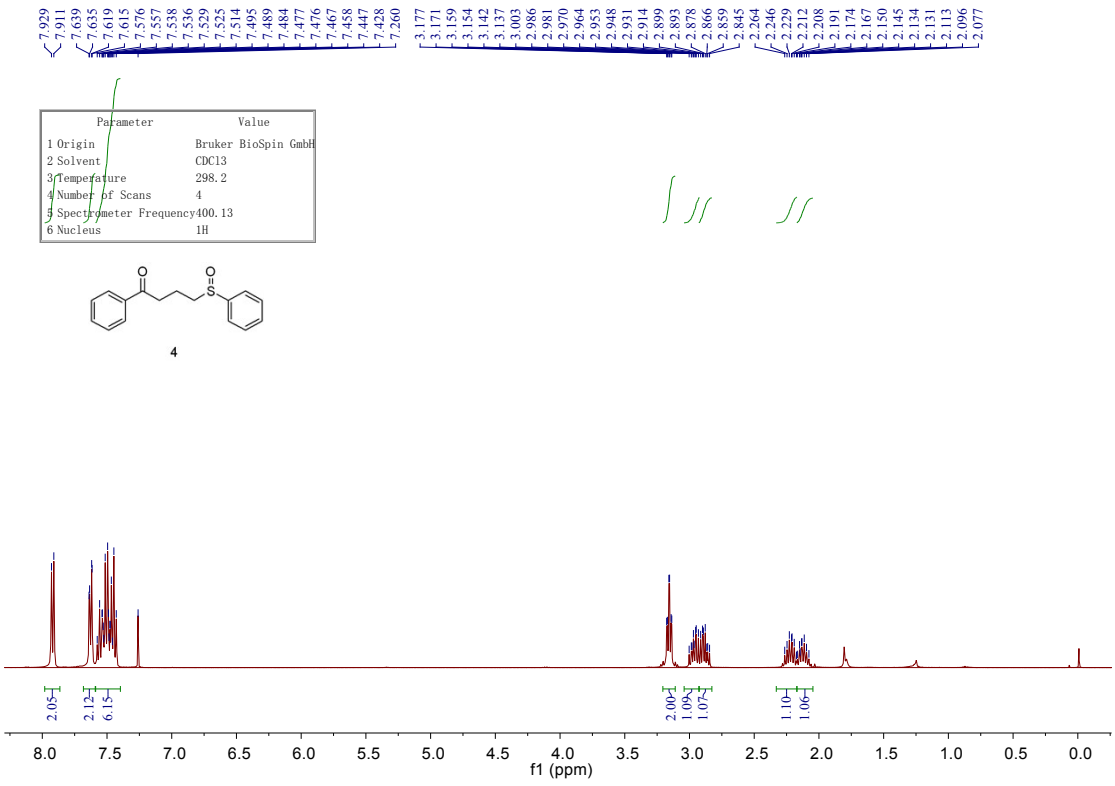
2y

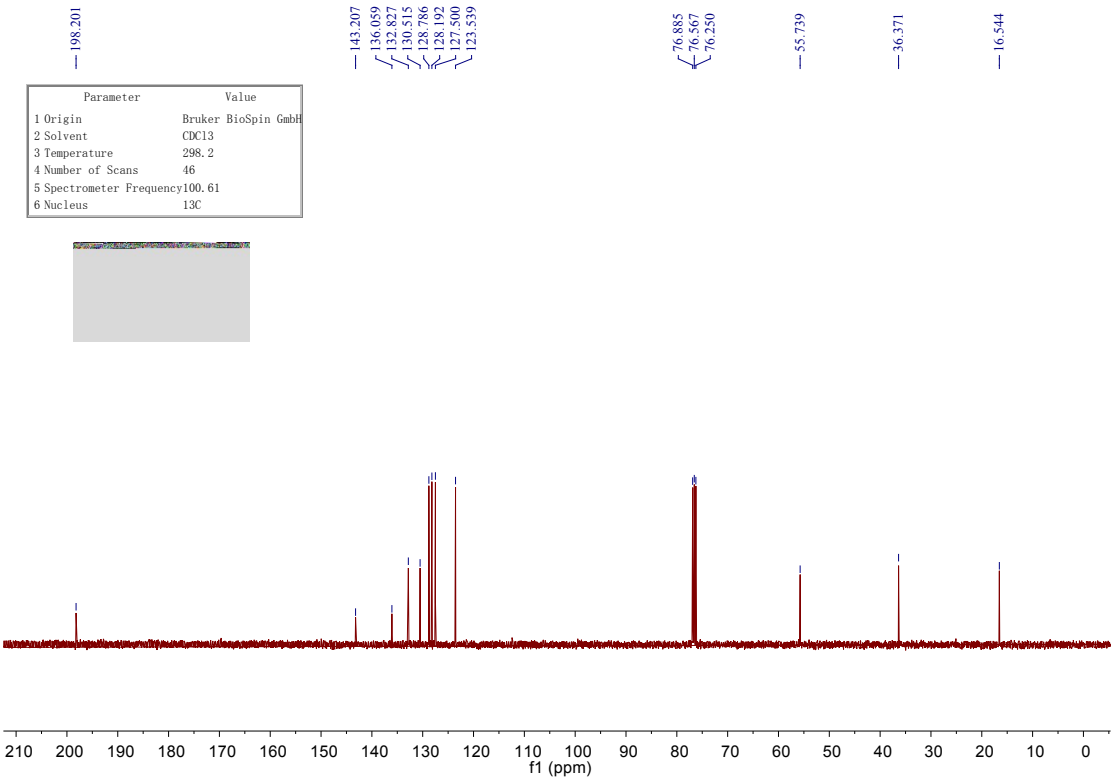


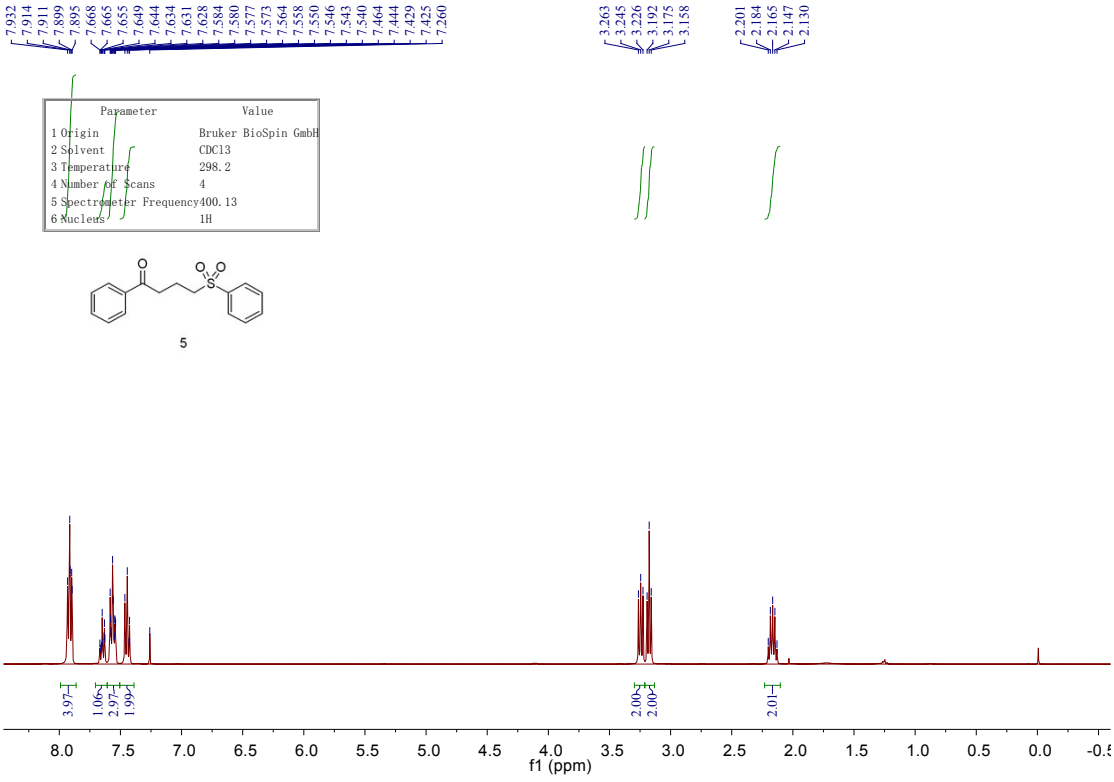

199.167
136.457
132.577
128.123
127.554
76.858
76.541
76.223
36.515
33.244
22.605
14.806
Parameter Value
1 Origin Bruker BioSpin GmbH
2 Solvent CDCl3
3 Temperature 298.1
4 Number of Scans 1024
5 Spectrometer Frequency 100.61
6 Nucleus 13C
f1 (ppm)

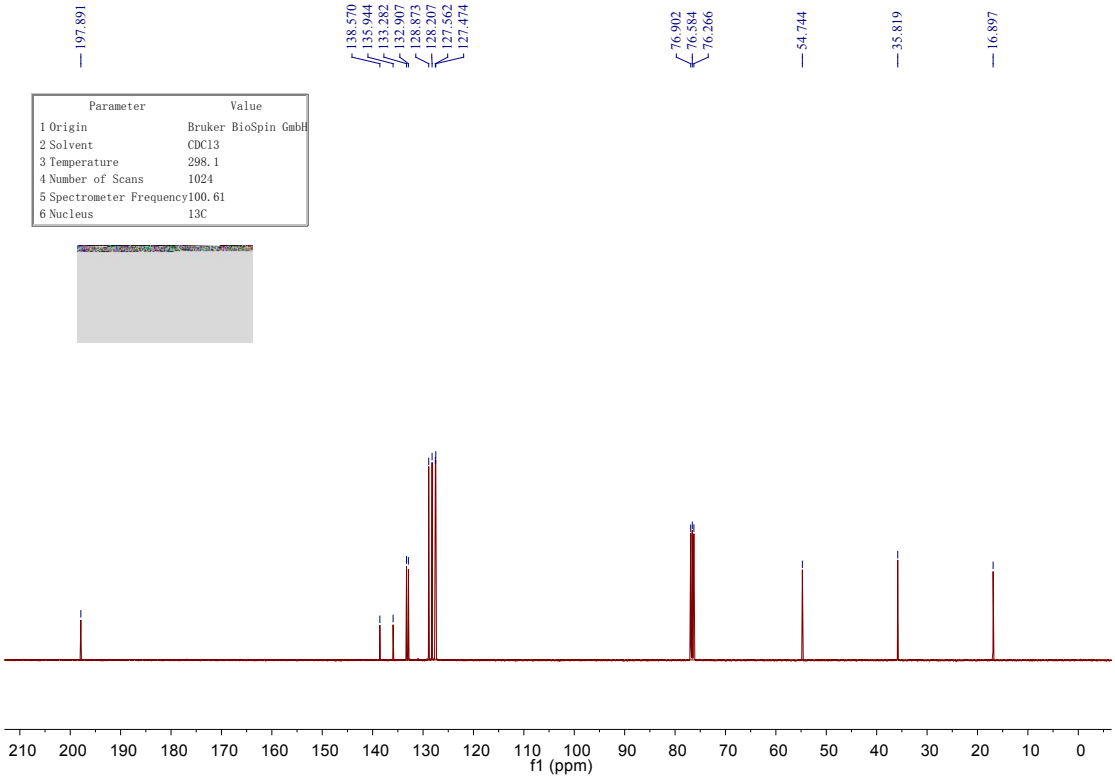

7.957
7.944
7.939
7.935
7.581
7.562
7.544
7.479
7.460
7.441
7.326
7.313
7.306
7.300
7.292
7.284
7.278
7.260
7.260
3.717
3.088
3.070
3.052
2.551
2.533
2.516
2.053
2.035
2.018
2.000
1.982
Parameter Value
1 Origin Bruker BioSpin GmbH
2 Solvent CDCl3
3 Temperature 298.2
4 Number of Scans 8
5 Spectrometer Frequency 400.13
6 Nucleus 1H
O
SBn
2z
1.87
0.97
1.96
3.87
0.93
2.00
1.98
2.01
2.09
f1 (ppm)

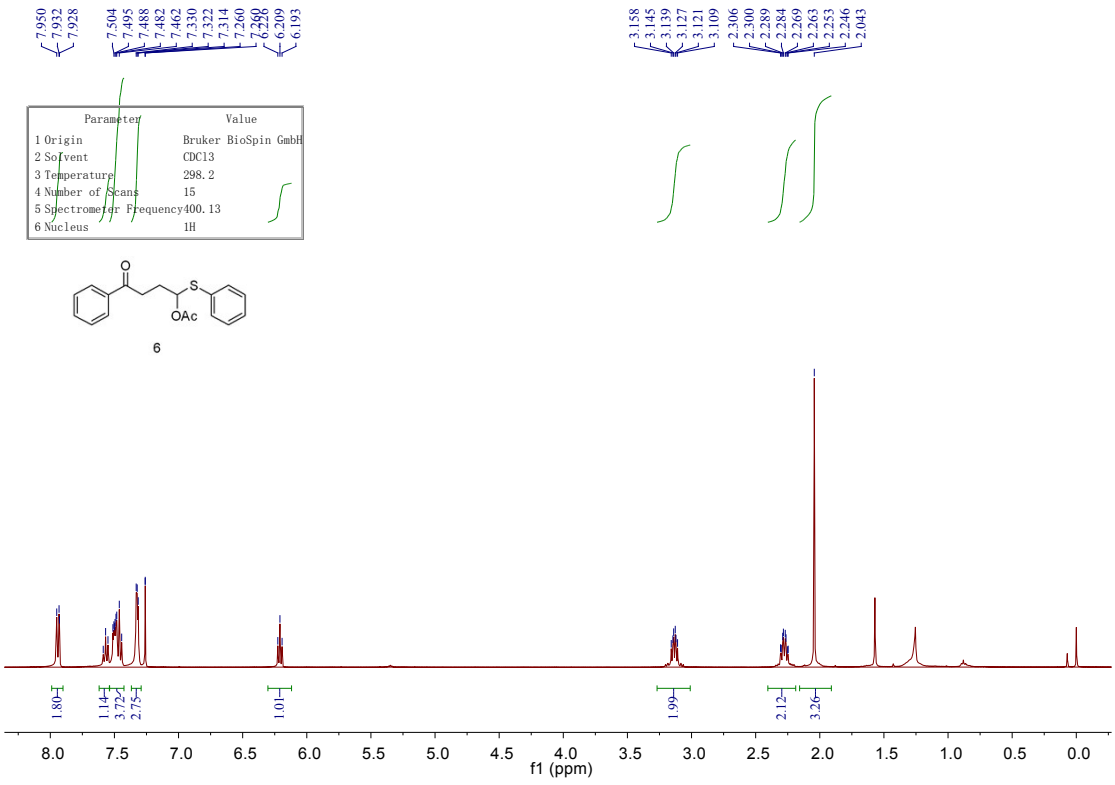

199.113
137.910
136.415
132.569
128.382
128.105
128.020
127.565
126.485
76.859
76.541
76.224
36.646
35.552
30.358
22.827
Parameter Value
1 Origin Bruker BioSpin GmbH
2 Solvent CDCl3
3 Temperature 298.1
4 Number of Scans 1024
5 Spectrometer Frequency 100.61
6 Nucleus 13C
f1 (ppm)

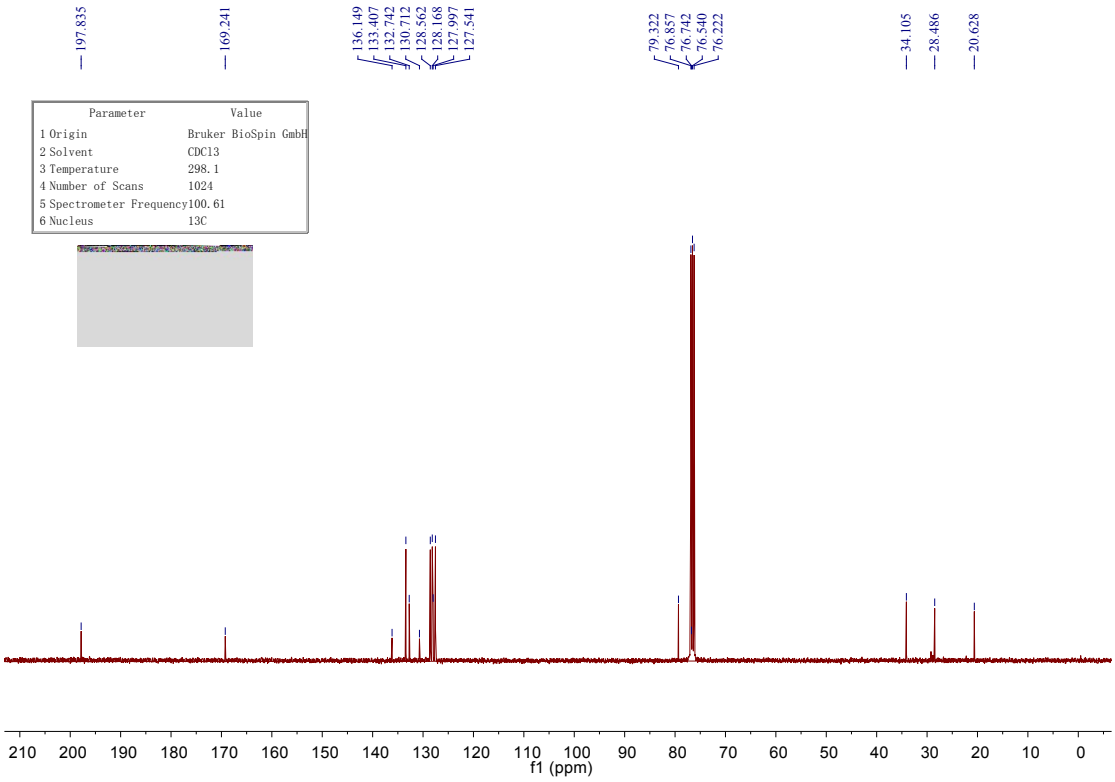

7.929
7.911
7.639
7.635
7.619
7.615
7.576
7.557
7.538
7.536
7.529
7.525
7.514
7.495
7.489
7.484
7.477
7.476
7.467
7.458
7.447
7.428
7.260
3.177
3.171
3.159
3.154
3.142
3.137
3.003
2.986
2.981
2.970
2.964
2.953
2.948
2.931
2.914
2.899
2.893
2.878
2.866
2.859
2.845
2.264
2.246
2.229
2.212
2.208
2.191
2.174
2.167
2.150
2.145
2.134
2.131
2.113
2.096
2.077
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
O
S=O
4
2.05
2.12
6.15
2.00
1.09
1.07
1.10
1.06
f1 (ppm)


198.201
143.207
136.059
132.827
130.515
128.786
128.192
127.500
123.539
76.885
76.567
76.250
55.739
36.371
16.544
Parameter Value
1 Origin Bruker BioSpin GmbH
2 Solvent CDCl3
3 Temperature 298.2
4 Number of Scans 46
5 Spectrometer Frequency 100.61
6 Nucleus 13C
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)


7.932
7.914
7.911
7.899
7.895
7.668
7.665
7.655
7.649
7.644
7.634
7.631
7.628
7.584
7.580
7.577
7.573
7.564
7.558
7.550
7.546
7.543
7.540
7.464
7.444
7.429
7.425
7.260
3.263
3.245
3.226
3.192
3.175
3.158
2.201
2.184
2.165
2.147
2.130
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
O
O
S
5
3.97
1.06
2.97
1.99
2.00
2.00
2.01
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)


197.891
138.570
135.944
133.282
132.907
128.873
128.207
127.562
127.474
76.902
76.584
76.266
54.744
35.819
16.897
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
f1 (ppm)


7.950
7.932
7.928
7.504
7.495
7.488
7.482
7.462
7.330
7.322
7.314
7.260
6.209
6.193
3.158
3.145
3.139
3.127
3.121
3.109
2.306
2.300
2.289
2.284
2.269
2.263
2.253
2.246
2.043
Parameter Value
1 Origin Bruker BioSpin GmbH
2 Solvent CDCl3
3 Temperature 298.2
4 Number of Scans 15
5 Spectrometer Frequency 400.13
6 Nucleus 1H
O
S
OAc
6
1.80
1.14
3.72
2.75
1.01
1.99
2.12
3.26
f1 (ppm)


197.835
169.241
136.149
133.407
132.742
130.712
128.562
128.168
127.997
127.541
79.322
76.857
76.742
76.540
76.222
34.105
28.486
20.628
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
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)