Electronic Supplementary Material (ESI) for Organic Chemistry Frontiers.

Supporting Information

Regiospecific Synthesis of Distally Chlorinated Ketones via C-C Bond Cleavage of Cycloalkanols

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1. General experimental details

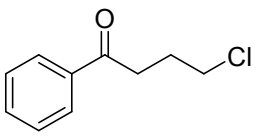
All reactions were maintained under a nitrogen atmosphere unless otherwise stated. Commercially available reagents were used without further purification. Infrared (FT-IR) spectra were recorded on a BRUKER VERTEX 70, ν_{max} in cm^{-1}. ^{1}H-NMR spectra were recorded on a BRUKER AVANCE III HD (400 MHz) spectrometer. Chemical shifts are reported in ppm from tetramethylsilane with the solvent resonance as internal standard ($CDCl_3$: δ 7.26). 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™ and BRUKER micrOTF-Q III. Melting points were measured using INESA WRR and values are uncorrected.

Tertiary cyclopropanols were prepared by the addition of Grignard reagent to the precursor esters according to the reported procedure.[1] Other tertiary cycloalkanols were prepared by the addition of Grignard reagent to the corresponding cycloketones according to the reported procedure.[2]

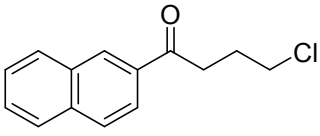
2. General procedure for the ring-opening chlorination

Cyclobutanol **5** (0.2 mmol, 1.0 equiv), $AgNO_3$ (0.04 mmol, 0.2 equiv), $K_2S_2O_8$ (0.24 mmol, 1.2 equiv), and NCS (0.3 mmol, 1.5 equiv) were loaded in a flask which was subjected to evacuation/flushing with nitrogen three times. A mixed solvent DCE/H_2O (0.5/0.5 mL, 0.2 M) was added to the mixture via syringe and the mixture was then stirred at 25 °C until the starting material had been consumed as determined by TLC. The mixture was extracted with CH_2Cl_2 (3× 10 mL). The combined organic extracts were washed by brine, dried over Na_2SO_4, filtered, concentrated, and purified by flash chromatography on silica gel (ethyl acetate/PE) to give the product **6**.

3. Characterization of products

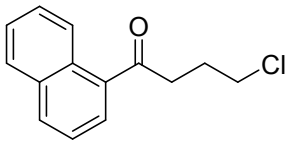


6a: colorless oil. ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.02-7.95 (m, 2H), 7.61-7.54 (m, 1H), 7.51-7.44 (m, 2H), 3.68 (t, *J* = 6.4 Hz, 2H), 3.18 (t, *J* = 6.8 Hz, 2H), 2.29-2.18 (m, 2H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 198.5, 136.3, 132.7, 128.2, 127.5, 44.2, 34.8, 26.3. FT-IR: ν (cm^{-1}) 3061, 2962, 1683, 1448, 1225. HRMS[ESI] calcd for $C_{10}H_{12}ClO$ $[M+H]^+$ 183.0577, found 183.0572. ESI $[M+H]^+$ 183.1.



6b: yellow oil. ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.50 (s, 1H), 8.04 (dd, *J* = 8.8, 1.6 Hz, 1H), 7.97 (d, *J* = 8.0 Hz, 1H), 7.90 (d, *J* = 8.8 Hz, 1H), 7.88 (d, *J* = 8.0 Hz, 1H), 7.65-7.52 (m, 2H), 3.73 (t, *J* = 6.4 Hz,

2H), 3.32 (t, J = 6.8 Hz, 2H), 2.36-2.24 (m, 2H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 198.4, 135.2, 133.6, 132.0, 129.3, 129.1, 128.1, 128.0, 127.3, 126.4, 123.3, 44.3, 34.9, 26.4. FT-IR: ν (cm^{-1}) 3054, 2954, 2931, 1682, 1626, 1373, 1220. HRMS[ESI] calcd for $C_{14}H_{14}ClO$ $[M+H]^+$ 233.0733, found 233.0723. ESI $[M+H]^+$ 233.1.



6c: yellow solid, m.p. 42-44 °C. ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.60 (d, J = 8.4 Hz, 1H), 8.00 (d, J = 8.0 Hz, 1H), 7.92 (dd, J = 7.2, 1.2 Hz, 1H), 7.89 (d, J = 8.0 Hz, 1H), 7.64 -7.48 (m, 3H), 3.72 (t, J = 6.0 Hz, 2H), 3.27 (t, J = 6.8 Hz, 2H), 2.36-2.25 (m, 2H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 203.2, 135.7, 134.0, 132.8, 130.1, 128.5, 128.0, 127.7, 126.5, 125.7, 124.4, 44.7, 38.7, 27.2. FT-IR: ν (cm^{-1}) 3049, 2960, 2920, 1678, 1574, 1460, 1232. HRMS[ESI] calcd for $C_{14}H_{14}ClO$ $[M+H]^+$ 233.0733, found 233.0725. ESI $[M+H]^+$ 233.1.

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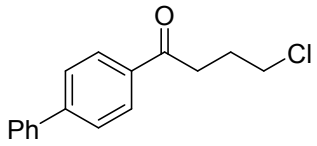
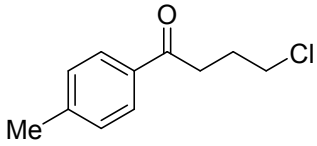
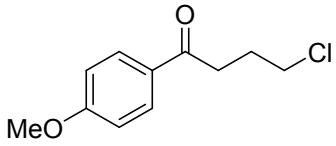


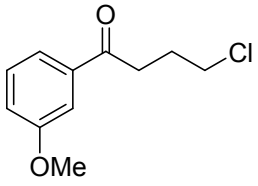
6d: white solid, m.p. 119-121 °C. ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.06 (d, J = 8.4 Hz, 2H), 7.70 (d, J = 8.4 Hz, 2H), 7.67-7.60 (m, 2H), 7.52 -7.45 (m, 2H), 7.44-7.38 (m, 1H), 3.71 (t, J = 6.4 Hz, 2H), 3.22 (t, J = 6.8 Hz, 2H), 2.33-2.20 (m, 2H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 198.1, 145.4, 139.4, 135.0, 128.5, 128.2, 127.8, 126.9, 126.8, 44.3, 34.9, 26.3. FT-IR: ν (cm^{-1}) 3058, 2956, 1678, 1603, 1323, 1268,1183. HRMS[ESI] calcd for $C_{16}H_{16}ClO$ $[M+H]^+$ 259.0890, found 259.0883. ESI $[M+H]^+$ 259.1.



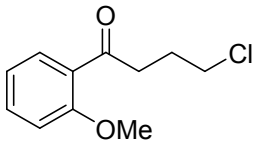
6e: yellow solid, m.p. 30-32 °C.^{1}H NMR (400 MHz, $CDCl_3$) δ 7.88 (d, J = 8.4 Hz, 2H), 7.26 (d, J = 8.0 Hz, 2H), 3.67 (t, J = 6.4 Hz, 2H), 3.15 (t, J = 6.8 Hz, 2H), 2.41 (s, 3H), 2.27-2.17 (m, 2H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 198.1, 143.5, 133.8, 128.8, 127.7, 44.3, 34.7, 26.4, 21.2. FT-IR: ν (cm^{-1}) 2955, 2920, 1673, 1604, 1453, 1409, 1368, 1318, 1308. HRMS[ESI] calcd for $C_{11}H_{14}ClO$ $[M+H]^+$ 197.0733, found 197.0733. ESI $[M+H]^+$ 197.1.



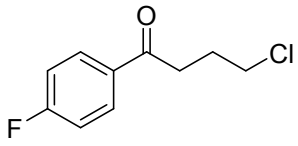
6f: yellow solid, m.p. 31-33 °C. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.98-7.93 (m, 2H), 6.96-6.91 (m, 2H), 3.87 (s, 3H), 3.67 (t, J = 6.4 Hz, 2H), 3.12 (t, J = 6.8 Hz, 2H), 2.26-2.16 (m, 2H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 197.0, 163.1, 129.8, 129.4, 113.3, 55.0, 44.3, 34.4, 26.5. FT-IR: ν (cm^{-1}) 2959, 2842, 1674, 1598, 1509, 1419, 1311, 1233. HRMS[ESI] calcd for $C_{11}H_{14}ClO_2$ $[M+H]^+$ 213.0682, found 213.0672. ESI $[M+H]^+$ 213.1.



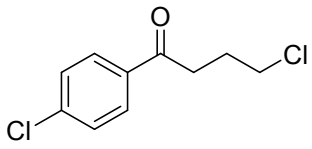
6g: colorless oil. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.56 (ddd, J = 7.6, 1.6, 0.8 Hz, 1H), 7.49 (dd, J = 2.4, 1.6 Hz, 1H), 7.37 (t, J = 8.0 Hz, 1H), 7.12 (ddd, J = 8.0, 2.8, 0.8 Hz, 1H), 3.85 (s, 3H), 3.67 (t, J = 6.4 Hz, 2H), 3.16 (t, J = 6.8 Hz, 2H), 2.29-2.16 (m, 2H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 198.3, 159.4, 137.6, 129.2, 120.2, 119.2, 111.8, 55.0, 44.2, 34.9, 26.3. FT-IR: ν (cm^{-1}) 3003, 2836, 1683, 1583, 1429, 1255. HRMS[ESI] calcd for $C_{11}H_{14}ClO_2$ $[M+H]^+$ 213.0682, found 213.0680. ESI $[M+H]^+$ 213.1.



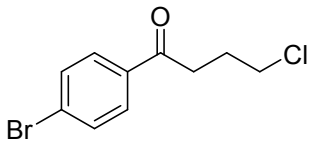
6h: colorless oil. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.70 (dd, J = 8.0, 2.0 Hz, 1H), 7.46 (ddd, J = 8.4, 7.2, 2.0 Hz, 1H), 7.05-6.93 (m, 2H), 3.91 (s, 3H), 3.64 (t, J = 6.8 Hz, 2H), 3.16 (t, J = 7.2 Hz, 2H), 2.24-2.13 (m, 2H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 200.8, 158.2, 133.1, 129.8, 127.6, 120.2, 111.1, 55.0, 44.4, 40.2, 26.7. FT-IR: ν (cm^{-1}) 3003, 2839, 1670, 1596, 1579, 1464, 1281, 1243. HRMS[ESI] calcd for $C_{11}H_{14}ClO_2$ $[M+H]^+$ 213.0682, found 213.0683. ESI $[M+H]^+$ 213.1.



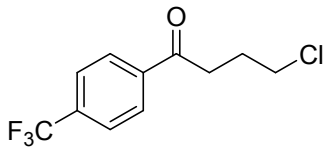
6i: colorless oil. ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.05-7.95 (m, 2H), 7.18-7.08 (m, 2H), 3.67 (t, J = 6.4 Hz, 2H), 3.15 (t, J = 6.8 Hz, 2H), 2.28-2.15 (m, 2H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 196.8, 165.3 (d, $J_{C\text{-}F}$ = 253.0 Hz), 132.7 (d, $J_{C\text{-}F}$ = 3.0 Hz), 130.2 (d, $J_{C\text{-}F}$ = 9.0 Hz), 115.3 (d, $J_{C\text{-}F}$ = 22.0 Hz), 44.1, 34.7, 26.2; ^{19}F NMR (376 MHz, $CDCl_3$) δ -105.0 (s). FT-IR: ν (cm^{-1}) 2965, 2927, 1684, 1596, 1506, 1409, 1225, 1156. HRMS[ESI] calcd for $C_{10}H_{11}ClFO$ $[M+H]^+$ 201.0482, found 201.0471. ESI $[M+H]^+$ 201.1.



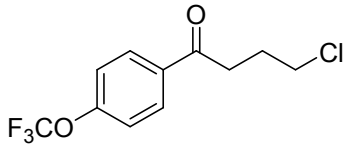
6j: colorless oil. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.97-7.87 (m, 2H), 7.51-7.40 (m, 2H), 3.67 (t, J = 6.4 Hz, 2H), 3.15 (t, J = 6.8 Hz, 2H), 2.29-2.17 (m, 2H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 197.2, 139.2, 134.6, 129.0, 128.5, 44.1, 34.8, 26.2. FT-IR: ν (cm^{-1}) 2922, 2850, 1685, 1589, 1401, 1200. HRMS[ESI] calcd for $C_{10}H_{11}Cl_2O$ $[M+H]^+$ 217.0187, found 217.0181. ESI $[M+H]^+$ 217.1.



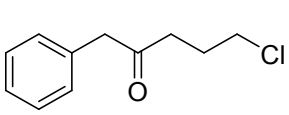
6k: yellow solid, m.p. 33-35 ^{o}C. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.90-7.79 (m, 2H), 7.68-7.56 (m, 2H), 3.67 (t, J = 6.4 Hz, 2H), 3.15 (t, J = 6.8 Hz, 2H), 2.30-2.16 (m, 2H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 197.9, 135.4, 132.2, 129.5, 128.3, 44.4, 35.2, 26.7. FT-IR: ν (cm^{-1}) 2960, 2923, 1683, 1585, 1397, 1273. HRMS[ESI] calcd for $C_{10}H_{11}BrClO$ $[M+H]^+$ 260.9682, found 260.9672. ESI $[M+H]^+$ 261.0.



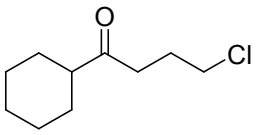
6l: colorless oil. ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.08 (d, J = 8.4 Hz, 2H), 7.74 (d, J = 8.4 Hz, 2H), 3.69 (t, J = 6.4 Hz, 2H), 3.21 (t, J = 6.8 Hz, 2H), 2.31-2.20 (m, 2H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 197.4, 138.9 (q, $J_{C\text{-}F}$ = 1.0 Hz), 134.1 (q, $J_{C\text{-}F}$ = 32.5 Hz), 127.9, 125.3 (q, $J_{C\text{-}F}$ = 3.7 Hz), 123.1 (q, $J_{C\text{-}F}$ = 271.1 Hz), 44.0, 35.1, 26.0; ^{19}F NMR (376 MHz, $CDCl_3$) δ -63.1 (s). FT-IR: ν (cm^{-1}) 2962, 2920, 2850, 1688, 1603, 1505, 1413, 1254, 1208, 1162. HRMS[ESI] calcd for $C_{11}H_{11}ClF_3O$ $[M+H]^+$ 251.0451, found 251.0444. ESI $[M+H]^+$ 251.1.



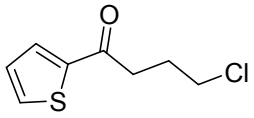
6m: colorless oil. ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.06-8.00 (m, 2H), 7.30 (d, J = 8.0 Hz, 2H), 3.68 (t, J = 6.4 Hz, 2H), 3.17 (t, J = 6.8 Hz, 2H), 2.29-2.18 (m, 2H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 196.9, 152.2 (q, $J_{C\text{-}F}$ = 2.0 Hz), 134.5, 129.6, 120.0 (q, $J_{C\text{-}F}$ = 1.0 Hz), 119.8 (q, $J_{C\text{-}F}$ = 257.0 Hz), 44.1, 34.8, 26.1; ^{19}F NMR (376 MHz, $CDCl_3$) δ -57.6 (s). FT-IR: ν (cm^{-1}) 2965, 2929, 1688, 1603, 1254, 1209, 1165. HRMS[ESI] calcd for $C_{11}H_{11}ClF_3O_2$ $[M+H]^+$ 267.0400, found 267.0389. ESI $[M+H]^+$ 267.0.



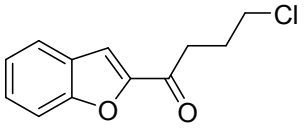
6n: colorless oil. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.37-7.31 (m, 2H), 7.30-7.24 (m, 1H), 7.24-7.18 (m, 2 H), 3.70 (s, 2H), 3.52 (t, J = 6.4 Hz, 2H), 2.65 (t, J = 6.8 Hz, 2H), 2.07-1.94 (m, 2H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 206.7, 133.5, 128.9, 128.3, 126.7, 49.8, 43.9, 38.1, 25.8. FT-IR: ν (cm^{-1}) 3028, 2962, 1711, 1454, 1435, 1365, 1247. HRMS[ESI] calcd for $C_{11}H_{14}ClO$ $[M+H]^+$ 197.0733, found 197.0731. ESI $[M+H]^+$ 197.1.



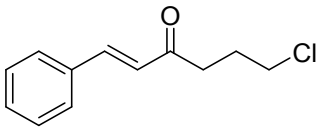
6o: colorless oil. ^{1}H NMR (400 MHz, $CDCl_3$) δ 3.56 (t, J = 6.4 Hz, 2H), 2.63 (t, J = 6.8 Hz, 2H), 2.37-2.28 (m, 1H), 2.05-1.97 (m, 2H), 1.87-1.73 (m, 4H), 1.69-1.61 (m, 1H), 1.38-1.17 (m, 5H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 212.5, 50.5, 44.2, 36.6, 28.0, 25.8, 25.3, 25.2. FT-IR: ν (cm^{-1}) 2929, 2854, 1705, 1448, 1375, 1309, 1144. HRMS[ESI] calcd for $C_{10}H_{18}ClO$ $[M+H]^+$ 189.1046, found 189.1039. ESI $[M+H]^+$ 189.1.



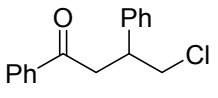
6p: yellow oil. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.75 (dd, J = 4.0, 1.2 Hz, 1H), 7.64 (dd, J = 4.8, 1.2 Hz, 1H), 7.14 (dd, J = 4.8, 4.0 Hz, 1H), 3.66 (t, J = 6.4 Hz, 2H), 3.12 (t, J = 6.8 Hz, 2H), 2.28-2.17 (m, 2H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 191.4, 143.6, 133.3, 131.5, 127.7, 44.1, 35.5, 26.5. FT-IR: ν (cm^{-1}) 3103, 2961, 2923, 1658, 1415, 1234. HRMS[ESI] calcd for $C_8H_{10}ClOS$ $[M+H]^+$ 189.0141, found 189.0143. ESI $[M+H]^+$ 189.0.



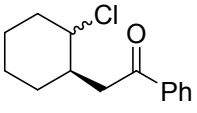
6q: yellow solid, m.p. 75-77 °C. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.72 (d, J = 8.0 Hz, 1H), 7.62-7.53 (m, 2H), 7.52-7.44 (m, 1H), 7.36-7.28 (m, 1H), 3.69 (t, J = 6.4 Hz, 2H), 3.18 (t, J = 6.8 Hz, 2H), 2.32-2.21 (m, 2H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 189.6, 155.2, 151.9, 127.9, 126.5, 123.5, 122.9, 112.4 112.0, 44.0, 35.2, 26.1. FT-IR: ν (cm^{-1}) 3110, 2957, 1667, 1590, 1330. HRMS[ESI] calcd for $C_{12}H_{12}ClO_2$ $[M+H]^+$ 223.0526, found 223.0523. ESI $[M+H]^+$ 223.0.



6r: colorless oil. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.59 (d, J = 16.4 Hz, 1H), 7.58-7.54 (m, 2H), 7.42-7.39 (m, 3H), 6.75 (d, J = 16.0 Hz, 1H), 3.65 (t, J = 6.4 Hz, 2H), 2.89 (t, J = 7.2 Hz, 2H), 2.20-2.13 (m, 2H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 198.5, 142.4, 133.9, 130.1, 128.5, 127.8, 125.6, 44.2, 36.9, 26.3. FT-IR: ν (cm^{-1}) 3061, 3027, 2956, 2925, 1773, 1660, 1455, 1209. HRMS [ESI] calcd for $C_{12}H_{14}ClO$ $[M+H]^+$ 209.0733, found 209.0740.

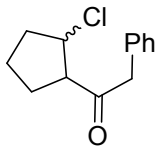


6s: yellow solid, m.p. 73-75 °C. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.99-7.89 (m, 2H), 7.59-7.52 (m, 1H), 7.49-7.40 (m, 2H), 7.36-7.21 (m, 5H), 3.90-3.75 (m, 3H), 3.68-3.57 (m, 1H), 3.44-3.35 (m, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 197.4, 140.8, 136.4, 132.8, 128.2, 128.2, 127.6, 127.3, 126.8, 48.6, 42.3, 41.1. FT-IR: ν (cm^{-1}) 2956, 2923, 1681, 1493, 1408, 1347, 1227. HRMS[ESI] calcd for $C_{16}H_{16}ClO$ $[M+H]^+$ 259.0890, found 259.0881. ESI $[M+H]^+$ 259.0.



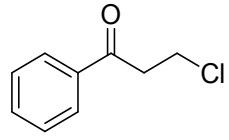
6t: *dr* = 1.2:1, colorless oil. ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.03-7.93 (m, 4H,

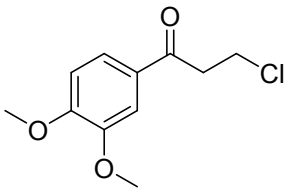
two isomers), 7.59-7.53 (m, 2H, two isomers), 7.50-7.43 (m, 4H, two isomers), 4.54-4.47 (m, 1H, one isomer), 3.77 (ddd, J = 11.2, 11.2, 4.0 Hz, 1H, one isomer), 3.63 (dd, J = 16.4, 2.8 Hz, 1H, one isomer), 3.20 (dd, J = 17.6, 6.8 Hz, 1H, one isomer), 2.88 (dd, J = 17.6, 6.0 Hz, 1H, one isomer), 2.75 (dd, J = 16.0, 9.6 Hz, 1H, one isomer), 2.52-2.42 (m, 1H, one isomer), 2.32-2.19 (m, 2H, two isomers), 2.10-2.02 (m, 1H, one isomer), 2.00-1.93 (m, 1H, one isomer), 1.93-1.62 (m, 6H, two isomers), 1.58-1.27 (m, 6H, two isomers), 1.15-1.01 (m, 1H, one isomer); ^{13}C NMR (100 MHz, $CDCl_3$) δ 198.9 & 198.7 (two isomers), 136.7 & 136.6 (two isomers), 132.6 & 132.5 (two isomers), 128.1 & 128.1 (two isomers), 127.7 & 127.6 (two isomers), 65.0 & 64.5 (two isomers), 42.6 & 42.3 (two isomers), 42.1 & 37.1 (two isomers), 37.4 & 33.8 (two isomers), 32.0 & 26.0 (two isomers), 26.2 & 24.7 (two isomers), 24.8 & 19.4 (two isomers). FT-IR: ν (cm^{-1}) 2927, 2857, 2361, 1677, 1448, 1217. HRMS[ESI] calcd for $C_{14}H_{18}ClO$ $[M+H]^+$ 237.1046, found 237.1039. ESI $[M+H]^+$ 237.1.



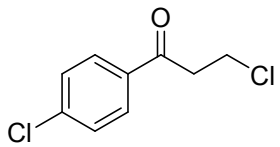
6u: dr = 1.2:1, colorless oil. ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.03-7.94 (m, 4H, two isomers), 7.60-7.53 (m, 2H, two isomers), 7.51-7.43 (m, 4H, two isomers), 4.67-4.63 (m, 1H, one isomer), 3.88 (dd, J = 15.2, 7.2 Hz, 1H, one isomer), 3.45-3.32 (m, 2H, two isomers), 3.10 (dd, J = 18.0, 6.0 Hz, 1H, one isomer), 2.83 (dd, J = 16.4, 9.6 Hz, 1H, one isomer), 2.70-2.61 (m, 1H, one isomer), 2.60-2.50 (m, 1H, one isomer), 2.29-2.09 (m, 4H, two isomers), 2.01-1.80 (m, 4H, two isomers), 1.78-1.64 (m, 2H, two isomers), 1.29-1.23 (m, 2H, two isomers); ^{13}C NMR (100 MHz, $CDCl_3$) δ 198.8 & 198.5 (two isomers), 136.5 & 136.4 (two isomers), 132.7 & 132.6 (two isomers), 128.2 & 128.1 (two isomers), 127.6 & 127.5 (two isomers), 67.2 & 63.8 (two isomers), 45.1 (one isomer), 41.5 (one isomer), 41.1 (one isomer), 39.7 (one isomer), 35.9 & 35.0 (two isomers), 29.2 & 27.8 (two isomers), 21.2 & 20.7 (two isomers). FT-IR: ν (cm^{-1}) 2959, 1925, 1684, 1597, 1448, 1208. HRMS[ESI] calcd for $C_{13}H_{16}ClO$ $[M+H]^+$ 223.0890, found 223.0894.

8a: colorless oil. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.99-7.94 (m, 2H), 7.62-7.57 (m, 1H), 7.49 (t, J = 7.6 Hz, 2H), 3.93 (t, J = 6.8 Hz, 2H), 3.47 (t, J = 6.8 Hz, 2H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 196.2, 135.9, 133.1, 128.3, 127.6, 40.8, 38.2. FT-IR: ν (cm^{-1}) 2977, 2601, 1654, 1475, 1383, 1035, 806. HRMS [ESI] calcd for $C_9H_{10}ClO$ $[M+H]^+$ 169.0420, found 169.0417. ESI $[M+H]^+$ 169.0.



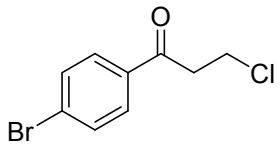


8b: white solid, m.p. 108-110 °C. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.58 (dd, J = 8.4, 1.6 Hz, 1H), 7.53 (d, J = 1.6 Hz, 1H), 6.90 (d, J = 8.4 Hz, 1H), 3H), 3.92 (t, J = 6.8 Hz, 2H), 3.42 (t, J = 6.8 Hz, 3.96 (s, 3H), 3.94 (s, 2H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 194.8, 153.2, 148.7, 129.2, 122.4, 109.6, 109.5, 55.6, 55.5, 40.3, 38.6. FT-IR: ν (cm^{-1}) 2995, 2923, 2845, 1649, 1584, 1240, 1148, 1018. HRMS [CI] calcd for $C_{11}H_{14}ClO_3$ $[M+H]^+$ 229.0632, found 229.0620. ESI $[M+H]^+$ 229.0.

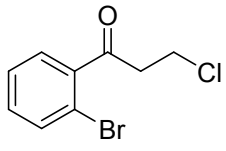


8c: white solid, m.p. 49-51 °C. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.90 (d, J = 8.4 Hz, 2H), 7.46 (d, J = 8.4 Hz, 2H), 3.91 (t, J = 6.8 Hz, 2H), 3.43 (t, J = 6.8 Hz, 2H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 195.0, 139.6, 134.2, 129.0,

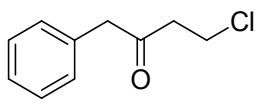
128.6, 40.7, 38.0. FT-IR: ν (cm^{-1}) 3357, 3090, 2969, 2915, 1684, 1400, 1202, 1091, 1013. HRMS [ESI] calcd for $C_9H_9Cl_2O$ $[M+H]^+$ 203.0030, found 203.0033. ESI $[M+H]^+$ 203.0.



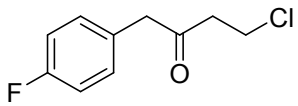
8d: white solid, m.p. 58-60 °C. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.82 (d, *J* = 8.4 Hz, 2H), 7.63 (d, *J* = 8.4 Hz, 2H), 3.91 (t, *J* = 6.8 Hz, 2H), 3.42 (t, *J* = 6.8 Hz, 2H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 195.2, 134.6, 131.6, 129.1, 128.4, 40.7, 38.0. FT-IR: ν (cm^{-1}) 3083, 2976, 2931, 2851, 1682, 1585, 1234, 1116, 1008. HRMS [ESI] calcd for C_9H_9BrClO $[M+H]^+$ 246.9525, found 246.9526. ESI $[M+H]^+$ 246.9.



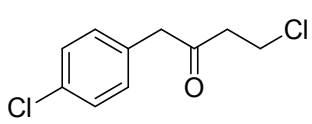
8e: yellow oil. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.65 (d, *J* = 8.0 Hz, 1H), 7.47 (dd, *J* = 7.6, 1.6 Hz, 1H), 7.42 (dd, *J* = 7.6, 7.2 Hz, 1H), 7.35 (ddd, *J* = 7.6, 7.2, 2.0 Hz, 1H), 3.91 (t, *J* = 6.8 Hz, 2H), 3.45 (t, *J* = 6.8 Hz, 2H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 200.0, 140.3, 133.3, 131.6, 128.4, 127.1, 118.3, 44.7, 38.0. FT-IR: ν (cm^{-1}) 3063, 2966, 2925, 2853, 1698, 1587, 1428, 1225, 1026. HRMS [ESI] calcd for C_9H_9BrClO $[M+Na]^+$ 246.9525, found 246.9526. ESI $[M+H]^+$ 246.9.



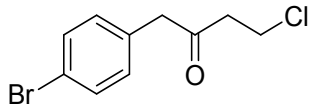
8f: colorless oil. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.34 (t, *J* = 7.2 Hz, 2H), 7.28 (d, *J* = 7.2 Hz, 1H), 7.20 (d, *J* = 7.2 Hz, 2H), 3.72 (s, 3H), 3.69 (t, *J* = 6.8 Hz, 2H), 2.90 (t, *J* = 6.8 Hz, 2H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 204.4, 133.0, 129.0, 128.4, 126.8, 50.0, 43.7, 37.8. FT-IR: ν (cm^{-1}) 3087, 3030, 2920, 1715, 1496, 1074. HRMS [ESI] calcd for $C_{10}H_{12}ClO$ $[M+H]^+$ 183.0577, found 183.0568. ESI $[M+H]^+$ 183.1.



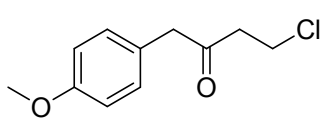
8g: colorless oil. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.16 (dd, *J* = 8.4, 5.6 Hz, 2H), 7.03 (dd, *J* = 8.8, 8.4 Hz, 2H), 3.71 (t, *J* = 6.8 Hz, 2H), 3.71 (t, *J* = 6.4 Hz, 2H), 2.91 (t, *J* = 6.8 Hz, 2H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 204.1, 161.6 (d, $J_{C\text{-}F}$ = 246.0 Hz), 130.5 (d, $J_{C\text{-}F}$ = 8.0 Hz), 128.6 (d, $J_{C\text{-}F}$ = 3.2 Hz), 115.2 (d, $J_{C\text{-}F}$ = 21.6 Hz), 49.0, 43.8, 37.7; ^{19}F NMR (376 MHz, $CDCl_3$) δ -115.3 (s). FT-IR: ν (cm^{-1}) 3072, 3044, 2970, 2901, 1717, 1509, 1359, 1220, 1076. HRMS [ESI] calcd for $C_{10}H_{11}ClFO$ $[M+H]^+$ 201.0482, found 201.0481. ESI $[M+H]^+$ 201.0.



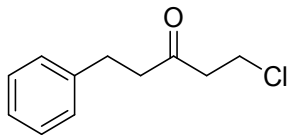
8h: yellow oil. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.33-7.29 (m, 2H), 7.13 (d, *J* = 8.4 Hz, 2H), 3.71 (t, *J* = 6.8 Hz, 4H), 2.91 (t, *J* = 6.8 Hz, 2H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 203.8, 132.8, 131.3, 130.3, 128.5, 49.1, 43.8, 37.7. FT-IR: ν (cm^{-1}) 2966, 2902, 1718, 1492, 1321, 1086, 1016. HRMS [ESI] calcd for $C_{10}H_{11}Cl_2O$ $[M+H]^+$ 217.0187, found 217.0178. ESI $[M+H]^+$ 217.0.



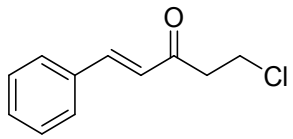
8i: yellow oil. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.48-7.45 (m, 2H), 7.07 (d, *J* = 8.4 Hz, 2H), 3.73-3.69 (m, 4H), 2.91 (t, *J* = 6.8 Hz, 2H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 203.7, 131.8, 131.5, 130.7, 120.9, 49.2, 43.9, 37.7. FT-IR: ν (cm^{-1}) 3324, 2973, 2881, 1380, 1046. HRMS [CI] calcd for $C_{10}H_{11}BrClO$ $[M+H]^+$ 260.9682, found 260.9670 ESI $[M+H]^+$ 260.8.



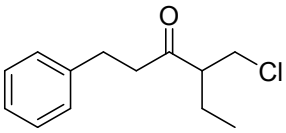
8j: colorless oil. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.14-7.09 (m, 2H), 6.90-6.85 (m, 2H), 3.80 (s, 3H), 3.69 (t, *J* = 6.8 Hz, 2H), 3.66 (s, 2H), 2.89 (t, *J* = 6.8 Hz, 2H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 204.9, 158.4, 13.0, 125.0, 113.8, 54.8, 49.2, 43.5, 37.8. FT-IR: ν (cm^{-1}) 2968, 2900, 1898, 1717, 1488, 1354, 1070, 1012. HRMS [ESI] calcd for $C_{11}H_{14}ClO_2$ $[M+H]^+$ 213.0682, found 213.0677. ESI $[M+H]^+$ 213.1.



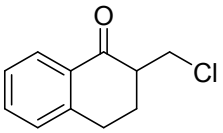
8k: colorless oil. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.28 (t, *J* = 7.2 Hz, 2H), 7.20-7.16 (m, 3H), 3.73 (t, *J* = 6.8 Hz, 2H), 2.92 (t, *J* = 7.6 Hz, 2H), 2.85 (t, *J* = 6.8 Hz, 2H), 2.78 (t, *J* = 7.6 Hz, 2H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 206.0, 140.2, 128.1, 127.8, 125.8, 44.7, 44.3, 37.8, 29.0. FT-IR: ν (cm^{-1}) 4062, 3027, 2926, 1714, 1370, 1091. HRMS [ESI] calcd for $C_{11}H_{14}ClO$ $[M+H]^+$ 197.0733, found 197.0733. ESI $[M+H]^+$ 197.0.



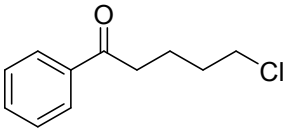
8l: colorless oil. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.60 (d, *J* = 16.0 Hz, 1H), 7.58-7.55 (m, 2H), 7.43-7.40 (m, 3H), 6.76 (d, *J* = 16.0 Hz, 1H), 3.86 (t, *J* = 6.8 Hz, 2H), 3.17 (t, *J* = 6.8 Hz, 2H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 196.1, 143.2, 133.7, 130.4, 128.6, 127.9, 125.3, 42.6, 38.2. FT-IR: ν (cm^{-1}) 3060, 3029, 2956, 2925, 2855, 1774, 1662, 1612, 1450, 1202, 1029. HRMS [ESI] calcd for $C_{11}H_{12}ClO$ $[M+H]^+$ 195.0577, found 195.0567. ESI $[M+H]^+$ 195.1.



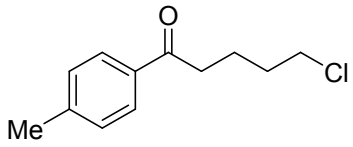
8m: yellow oil. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.31-7.25 (m, 2H), 7.22-7.16 (m, 3H), 3.70 (dd, *J* = 10.8, 8.4 Hz, 1H), 3.54 (dd, *J* = 10.8, 5.2 Hz, 1H), 2.94-2.89 (m, 2H), 2.85-2.78 (m, 3H), 1.74-1.60 (m, 1H), 1.55-1.47 (m, 1H), 0.85 (t, *J* = 7.6 Hz, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 209.9, 140.5, 128.0, 127.9, 125.7, 54.9, 44.6, 43.2, 28.8, 22.6, 10.7. FT-IR: ν (cm^{-1}) 3083, 2976, 2931, 2851, 1682, 1585, 1234, 1116, 1008. HRMS [ESI] calcd for $C_{13}H_{17}ClONa$ $[M+Na]^+$ 247.0866, found 247.0853.



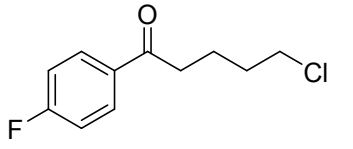
8n: colorless oil. ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.03 (dd, *J* = 8.0, 1.2 Hz, 1H), 7.49 (ddd, *J* = 7.6, 7.2, 1.2 Hz, 1H), 7.32 (dd, *J* = 8.0, 7.2 Hz, 1H), 7.26 (d, *J* = 7.6 Hz, 1H), 4.07 (dd, *J* = 11.2, 3.6 Hz, 1H), 3.85 (dd, *J* = 11.2, 7.2 Hz, 1H), 3.16-2.97 (m, 2H), 2.88-2.82 (m, 1H), 2.49-2.44 (m, 1H), 2.12-2.07 (m, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 196.2, 143.6, 133.2, 131.7, 128.4, 127.1, 126.3, 49.1, 43.9, 28.2, 26.4. FT-IR: ν (cm^{-1}) 3066, 2935, 2869, 2839, 1680, 1600, 1455, 1232. HRMS [ESI] calcd for $C_{11}H_{12}ClO$ $[M+H]^+$ 195.0577, found 195.0571. ESI $[M+H]^+$ 195.0.



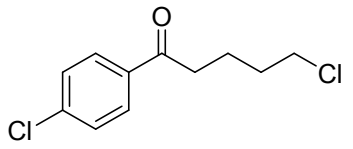
10a: yellow solid, m.p. 46-48 °C. ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.00-7.93 (m, 2H), 7.60-7.53 (m, 1H), 7.50-7.42 (m, 2H), 3.59 (t, *J* = 6.4 Hz, 2H), 3.02 (t, *J* = 6.8 Hz, 2H), 1.97-1.82 (m, 4H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 199.1, 136.4, 132.6, 128.2, 127.5, 44.2, 37.1, 31.6, 21.0. FT-IR: ν (cm^{-1}) 3061, 2951, 2868, 1673, 1595, 1447, 1291, 1238. HRMS[ESI] calcd for $C_{11}H_{14}ClO$ $[M+H]^+$ 197.0733, found 197.0724. ESI $[M+H]^+$ 197.1.



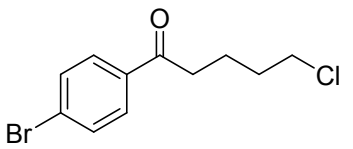
10b: yellow solid, m.p. 67-69 °C. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.85 (d, J = 8.0 Hz, 2H), 7.26 (d, J = 8.0 Hz, 2H), 3.58 (t, J = 6.4 Hz, 2H), 2.98 (t, J = 6.8 Hz, 2H), 2.41 (s, 3H), 1.94-1.80 (m, 4H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 199.3, 143.9, 134.4, 129.3, 128.1, 44.8, 37.4, 32.1, 21.7, 21.6. FT-IR: ν (cm^{-1}) 2923, 2867, 1671, 1605, 1407, 1374, 1287. HRMS[ESI] calcd for $C_{12}H_{16}ClO$ $[M+H]^+$ 211.0890, found 211.0886. ESI $[M+H]^+$ 211.0.



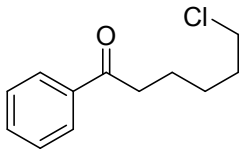
10c: colorless oil. ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.02-7.94 (m, 2H), 7.17-7.08 (m, 2H), 3.58 (t, J = 6.4 Hz, 2H), 2.99 (t, J = 6.8 Hz, 2H), 1.96- 1.81 (m, 4H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 197.5, 165.3 (d, $J_{C\text{-}F}$ = 253.1 Hz), 132.8 (d, $J_{C\text{-}F}$ = 3.1 Hz), 130.2 (d, $J_{C\text{-}F}$ = 9.3 Hz), 115.2 (d, $J_{C\text{-}F}$ = 21.8 Hz), 44.2, 37.0, 31.5, 21.0; ^{19}F NMR (376 MHz, $CDCl_3$) δ -105.3 (s). FT-IR: ν (cm^{-1}) 2957, 2872, 2361, 1684, 1597, 1506, 1360, 1226. HRMS[ESI] calcd for $C_{11}H_{13}ClFO$ $[M+H]^+$ 215.0639, found 215.0641. ESI $[M+H]^+$ 215.0.



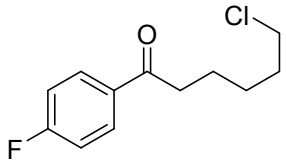
10d: colorless oil. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.89 (d, J = 8.4 Hz, 2H), 7.43 (d, J = 8.4 Hz, 2H), 3.58 (t, J = 6.0 Hz, 2H), 2.98 (t, J = 6.8 Hz, 2H), 1.93-1.82 (m, 4H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 197.9, 139.0, 134.6, 129.0, 128.5, 44.2, 37.1, 31.5, 20.9. FT-IR: ν (cm^{-1}) 2956, 2871, 1685, 1589, 1340, 1216. HRMS [ESI] calcd for $C_{11}H_{13}Cl_2O$ $[M+H]^+$ 231.0343, found 231.0335. ESI $[M+H]^+$ 231.1.



10e: colorless oil. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.84-7.79 (m, 2H), 7.63-7.58 (m, 2H), 3.58 (t, J = 6.4 Hz, 2H), 2.98 (t, J = 6.8 Hz, 2H), 1.94-1.83 (m, 4H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 198.5, 135.6, 132.0, 129.6, 128.3, 44.7, 37.5, 32.0, 21.4. FT-IR: ν (cm^{-1}) 2924, 2852, 1733, 1653, 1484, 1397, 1215. HRMS [ESI] calcd for $C_{11}H_{13}BrClO$ $[M+H]^+$ 274.9838, found 274.9833. ESI $[M+H]^+$ 275.0.

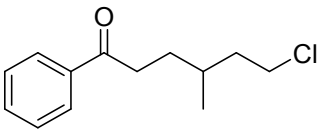


12a: colorless oil. ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.01-7.92 (m, 2H), 7.56 (t, J = 7.2 Hz, 1H), 7.46 (t, J = 8.0 Hz, 2H), 3.55 (t, J = 6.4 Hz, 2H), 2.99 (t, J = 6.8 Hz, 2H), 1.90-1.72 (m, 4H), 1.59-1.48 (m, 2H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 199.6, 136.5, 132.5, 128.1, 127.5, 44.4, 37.8, 32.0, 26.1, 23.0. FT-IR: ν (cm^{-1}) 2935, 2865, 2361, 1683, 1597, 1448, 1361, 1180. HRMS[ESI] calcd for $C_{12}H_{16}ClO$ $[M+H]^+$ 211.0890, found 211.0890. ESI $[M+H]^+$ 211.1.

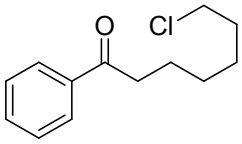


12b: colorless oil. ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.04-7.94 (m, 2H), 7.18-7.09 (m, 2H), 3.56 (t, J = 6.8 Hz, 2H), 2.96 (t, J = 7.2 Hz, 2H), 1.89-1.80 (m, 2H), 1.80-1.71 (m, 2H), 1.58-1.47 (m, 2H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 198.4, 165.7 (d, $J_{C\text{-}F}$ = 253.0 Hz), 133.4 (d, $J_{C\text{-}F}$ = 3.0 Hz), 130.6 (d, $J_{C\text{-}F}$ = 9.2 Hz), 115.7 (d, $J_{C\text{-}F}$ = 21.7 Hz), 44.8, 38.2, 32.5, 26.6, 23.4; ^{19}F NMR (376 MHz, $CDCl_3$) δ -105.5 (s). FT-IR: ν (cm^{-1}) 2931, 2865, 1685, 1597, 1506, 1228, 1156. HRMS [ESI] calcd for $C_{12}H_{15}ClFO$ $[M+H]^+$ 229.0795, found 229.0800. ESI $[M+H]^+$

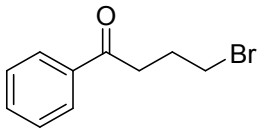
229.0.



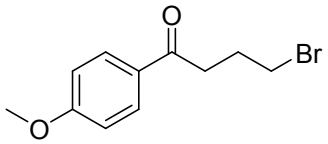
12c: yellow oil. ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.01-7.94 (m, 2H), 7.61-7.56 (m, 1H), 7.49 (dd, J = 10.2, 4.8 Hz, 2H), 3.68-3.54 (m, 2H), 3.10-2.93 (m, 2H), 1.92-1.76 (m, 3H), 1.73-1.55 (m, 2H), 1.00 (d, J = 6.4 Hz, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 199.8, 136.5, 132.5, 128.1, 127.5, 42.6, 39.1, 35.6, 30.2, 29.7, 18.5. FT-IR: ν (cm^{-1}) 3060, 2960, 2928, 2872, 1683, 1597, 1448, 1273, 1207, 1076. HRMS [ESI] calcd for $C_{13}H_{17}ClONa$ $[M+Na]^+$ 247.0866, found 247.0861.



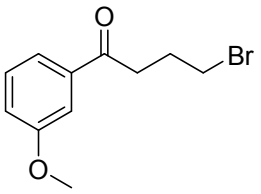
14: yellow solid, m.p. 42-44 °C. ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.01-7.90 (m, 2H), 7.59-7.52 (m, 1H), 7.50-7.42 (m, 2H), 3.54 (t, J = 6.4 Hz, 2H), 2.98 (t, J = 6.8 Hz, 2H), 1.84-1.71 (m, 4H), 1.54-1.36 (m, 4H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 199.8, 136.5, 132.5, 128.1, 127.6, 44.6, 37.9, 31.9, 28.1, 26.2, 23.6. FT-IR: ν (cm^{-1}) 2930, 2855, 2361, 1678, 1597, 1448, 1351. HRMS[ESI] calcd for $C_{13}H_{18}ClO$ $[M+H]^+$ 225.1046, found 225.1047. ESI $[M+H]^+$ 225.1.



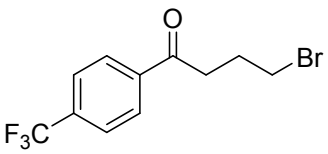
15a: colorless oil. ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.00-7.96 (m, 2H), 7.60-7.55 (m, 1H), 7.47 (t, J = 7.6 Hz, 2H), 3.55 (t, J = 6.4 Hz, 2H), 3.18 (t, J = 6.8 Hz, 2H), 2.35-2.27 (m, 2H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 198.3, 136.3, 132.8, 128.2, 127.5, 36.1, 33.2, 26.4. FT-IR: ν (cm^{-1}) 3060, 2962, 2917, 2849, 1682, 1597, 1448, 1221, 1022. HRMS [ESI] calcd for $C_{10}H_{12}BrO$ $[M+H]^+$ 227.0072, found 227.0066. ESI $[M+H]^+$ 227.0.



15b: colorless oil. ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.04-7.98 (m, 2H), 7.02-6.97 (m, 2H), 3.92 (s, 3H), 3.60 (t, J = 6.4 Hz, 2H), 3.18 (t, J = 6.8 Hz, 2H), 2.41-2.29 (m, 2H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 196.9, 163.1, 129.8, 129.4, 113.3, 55.0, 35.7, 33.3, 26.6. FT-IR: ν (cm^{-1}) 2961, 2933, 2840, 1674, 1599, 1507, 1260, 1027, 1027. HRMS [CI] calcd for $C_{11}H_{14}BrO_2$ $[M+H]^+$ 257.0177, found 257.0180. ESI $[M+H]^+$ 257.0.

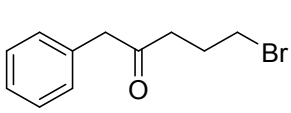


15c: yellow oil. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.57 (d, J = 7.6 Hz, 1H), 7.50 (dd, J = 2.4, 1.6 Hz, 1H), 7.38 (t, J = 8.0 Hz, 1H), 7.15-7.09 (m, 1H), 3.86 (s, 3H), 3.55 (t, J = 6.4 Hz, 2H), 3.17 (t, J = 6.8 Hz, 2H), 2.35-2.27 (m, 2H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 198.2, 159.4, 137.6, 129.2, 120.2, 119.2, 111.8, 55.0, 36.2, 33.1, 26.5. FT-IR: ν (cm^{-1}) 3072, 3044, 2970, 2901, 1717, 1509, 1359, 1220, 1076. HRMS [ESI] calcd for $C_{11}H_{13}BrO_2Na$ $[M+Na]^+$ 278.9997, found 278.9997.



15d: yellow oil. ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.08-7.99 (m, 2H), 7.30 (d, J = 8.4 Hz, 2H), 3.55 (t, J = 6.4 Hz, 2H), 3.18 (t, J = 6.8 Hz, 2H), 2.37-2.36 (m, 2H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 197.3, 138.8 (q, $J_{C\text{-}F}$ = 1.0 Hz), 134.1 (q, $J_{C\text{-}F}$ = 32.6 Hz), 127.9, 125.3 (q, $J_{C\text{-}F}$ = 3.7 Hz), 123.1 (q, $J_{C\text{-}F}$ = 271 Hz), 36.4, 32.9, 26.1; ^{19}F NMR (376 MHz, $CDCl_3$) δ -57.6 (s). FT-IR: ν (cm^{-1}) 2918, 1692, 1512, 1410, 1322, 1219. HRMS[ESI] calcd

for $C_{11}H_{11}BrF_3O$ $[M+H]^+$ 294.9945, found 294.9934. ESI $[M+H]^+$ 295.0.



15e: yellow oil. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.38-7.30 (m, 2H), 7.30-7.25 (m, 1H), 7.24-7.17 (m, 2H), 3.70 (s, 2H), 3.39 (t, J = 6.4 Hz, 2H), 2.65 (t, J = 6.8 Hz, 2H), 2.14-2.04 (m, 2H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 206.6, 133.5, 128.9, 128.3, 126.7, 49.8, 39.3, 32.8, 25.9. FT-IR: ν (cm^{-1}) 3028, 2918, 2850, 2361, 1711, 1496, 1454, 1365, 1247. HRMS[ESI] calcd for $C_{11}H_{14}BrO$ $[M+H]^+$ 241.0228, found 241.0223. ESI $[M+H]^+$ 241.0.

4. Computational studies

Computational Methods

The B3LYP density functional method [3] with the 6-31+G(d,p) basis set [4] was employed to optimize geometries of all stationary points. Frequencies were analytically computed at the same level of theory to confirm whether the structures are minima (no imaginary frequency) or transition states and to obtain the thermodynamic energy corrections. Intrinsic reaction coordinate (IRC) computations were carried out to confirm that transition states connect appropriate reactants and products. Larger basis set, 6-311++G(d,p), was utilized for single-point energy calculations on stationary points. The Gibbs free energy was determined by adding the single-point energy calculated at the larger basis set and the gas-phase thermal correction to the Gibbs free energy obtained from the vibrational frequency calculations. The Gaussian 09 suite of programs [5] was used for all the calculations.

Cartesian Coordinates and Energies

1a

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.370876	-0.751810	-0.727024
2	6	0	-1.431341	0.346197	0.000029
3	6	0	-2.371019	-0.751711	0.727086
4	1	0	-3.191883	-0.284757	-1.258540
5	1	0	-1.816176	-1.511317	-1.268587
6	1	0	-1.816436	-1.511140	1.268873
7	1	0	-3.192138	-0.284586	1.258364
8	6	0	0.054573	0.114086	0.000037
9	6	0	0.895309	1.238107	0.000030
10	6	0	0.640156	-1.163204	-0.000017
11	6	0	2.282556	1.088924	0.000034
12	1	0	0.441494	2.223141	0.000054
13	6	0	2.028468	-1.311565	-0.000029
14	1	0	0.022980	-2.057473	-0.000065
15	6	0	2.856430	-0.185850	0.000010
16	1	0	2.916811	1.970924	0.000052
17	1	0	2.461630	-2.307751	-0.000064
18	1	0	3.936287	-0.301564	0.000002
19	8	0	-1.908514	1.540685	-0.000128

Zero-point correction= 0.153034 (Hartree/Particle)

Thermal correction to Energy= 0.161576

Thermal correction to Enthalpy= 0.162520

Thermal correction to Gibbs Free Energy= 0.118867

Sum of electronic and zero-point Energies= -423.395560

Sum of electronic and thermal Energies= -423.387017

Sum of electronic and thermal Enthalpies= -423.386073

Sum of electronic and thermal Free Energies= -423.429726

B3LYP/6-311++G(d,p)//B3LYP/6-31+G(d,p) E = -423.63203548

TS_1

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.380058	-0.779336	-0.610692
2	6	0	-1.425004	0.363114	-0.122946

3	6	0	-2.379217	-0.734899	0.843984
4	1	0	-3.242007	-0.377653	-1.133783
5	1	0	-1.887892	-1.611175	-1.107316
6	1	0	-1.758463	-1.410129	1.421690
7	1	0	-3.147220	-0.182951	1.371328
8	6	0	0.056026	0.117545	-0.059920
9	6	0	0.898660	1.237439	0.029518
10	6	0	0.638232	-1.160920	-0.098490
11	6	0	2.283977	1.083066	0.079034
12	1	0	0.445558	2.222458	0.056225
13	6	0	2.024905	-1.314353	-0.046674
14	1	0	0.019873	-2.051283	-0.167474
15	6	0	2.854212	-0.193031	0.041844
16	1	0	2.919898	1.961226	0.146850
17	1	0	2.456095	-2.310904	-0.077325
18	1	0	3.932922	-0.313113	0.080635
19	8	0	-1.896146	1.545223	-0.115596

Zero-point correction= 0.152322 (Hartree/Particle)

Thermal correction to Energy= 0.160461

Thermal correction to Enthalpy= 0.161405

Thermal correction to Gibbs Free Energy= 0.118459

Sum of electronic and zero-point Energies= -423.395875

Sum of electronic and thermal Energies= -423.387736

Sum of electronic and thermal Enthalpies= -423.386792

Sum of electronic and thermal Free Energies= -423.429738

B3LYP/6-311++G(d,p)//B3LYP/6-31+G(d,p) E = -423.63190348

1b

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.403541	-0.460186	-0.481700
2	6	0	-1.330429	0.622080	-0.225540
3	6	0	-2.730779	-1.179339	0.785149
4	1	0	-3.275305	0.082747	-0.859701
5	1	0	-2.063685	-1.155471	-1.256471
6	1	0	-2.251042	-2.116537	1.045513
7	1	0	-3.336798	-0.689990	1.540127
8	6	0	0.111151	0.223383	-0.113181
9	6	0	1.057486	1.229328	0.149402
10	6	0	0.551615	-1.100690	-0.272875
11	6	0	2.411136	0.917919	0.252698

12	1	0	0.705318	2.248422	0.269260
13	6	0	1.908533	-1.412549	-0.168799
14	1	0	-0.156484	-1.896514	-0.477001
15	6	0	2.840081	-0.404825	0.093891
16	1	0	3.133176	1.703182	0.456669
17	1	0	2.237421	-2.440023	-0.293252
18	1	0	3.895666	-0.648369	0.173788
19	8	0	-1.672472	1.787728	-0.089150

Zero-point correction= 0.151889 (Hartree/Particle)

Thermal correction to Energy= 0.161301

Thermal correction to Enthalpy= 0.162245

Thermal correction to Gibbs Free Energy= 0.116102

Sum of electronic and zero-point Energies= -423.416443

Sum of electronic and thermal Energies= -423.407031

Sum of electronic and thermal Enthalpies= -423.406087

Sum of electronic and thermal Free Energies= -423.452230

B3LYP/6-311++G(d,p)//B3LYP/6-31+G(d,p) E = -423.653053908

2a

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	3.082993	-0.650297	0.000044
2	6	0	2.019072	-0.367276	1.078464
3	6	0	1.100928	0.398068	-0.000052
4	6	0	2.019078	-0.367403	-1.078422
5	1	0	3.879039	0.096634	0.000005
6	1	0	3.529155	-1.648027	0.000108
7	1	0	2.285449	0.252287	1.936455
8	1	0	1.498744	-1.268366	1.411764
9	1	0	2.285480	0.252057	-1.936481
10	1	0	1.498790	-1.268547	-1.411640
11	6	0	-0.397607	0.136003	-0.000026
12	6	0	-1.294273	1.213051	-0.000013
13	6	0	-0.916752	-1.168239	-0.000014
14	6	0	-2.673888	0.992373	0.000010
15	1	0	-0.897128	2.222417	-0.000020
16	6	0	-2.295290	-1.391547	0.000011
17	1	0	-0.246865	-2.024501	-0.000022
18	6	0	-3.180350	-0.309805	0.000022
19	1	0	-3.353423	1.840176	0.000018
20	1	0	-2.676576	-2.408861	0.000021

21	1	0	-4.252954	-0.481088	0.000040
22	8	0	1.458353	1.690781	-0.000050

Zero-point correction= 0.181529 (Hartree/Particle)

Thermal correction to Energy= 0.190471

Thermal correction to Enthalpy= 0.191415

Thermal correction to Gibbs Free Energy= 0.146481

Sum of electronic and zero-point Energies= -462.671447

Sum of electronic and thermal Energies= -462.662506

Sum of electronic and thermal Enthalpies= -462.661561

Sum of electronic and thermal Free Energies= -462.706496

B3LYP/6-311++G(d,p)//B3LYP/6-31+G(d,p) E = -462.942848793

TS_2

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.541196	-1.117352	0.447522
2	6	0	-2.111680	-0.527923	-0.914988
3	6	0	-1.141521	0.549470	-0.330574
4	6	0	-1.985618	0.052732	1.249546
5	1	0	-3.616874	-1.275794	0.567825
6	1	0	-2.026648	-2.052920	0.683661
7	1	0	-2.926049	0.002604	-1.412504
8	1	0	-1.655136	-1.230551	-1.618524
9	1	0	-2.671926	0.863826	1.479461
10	1	0	-1.228125	-0.111436	2.012922
11	6	0	0.329508	0.191310	-0.174234
12	6	0	1.247429	1.221092	0.083564
13	6	0	0.804294	-1.125033	-0.275613
14	6	0	2.605619	0.941511	0.234438
15	1	0	0.877060	2.238550	0.150296
16	6	0	2.165411	-1.405638	-0.124199
17	1	0	0.121150	-1.943794	-0.478540
18	6	0	3.070777	-0.373906	0.132619
19	1	0	3.303511	1.751512	0.427521
20	1	0	2.515858	-2.430316	-0.210715
21	1	0	4.128672	-0.591420	0.248218
22	8	0	-1.434954	1.792771	-0.477264

Zero-point correction= 0.181033 (Hartree/Particle)

Thermal correction to Energy= 0.190264

Thermal correction to Enthalpy= 0.191208

Thermal correction to Gibbs Free Energy= 0.145466

Sum of electronic and zero-point Energies= -462.669818

Sum of electronic and thermal Energies= -462.660587

Sum of electronic and thermal Enthalpies= -462.659643

Sum of electronic and thermal Free Energies= -462.705384

B3LYP/6-311++G(d,p)//B3LYP/6-31+G(d,p) E = -462.941546179

2b

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.522027	-1.095217	0.324253
2	6	0	-1.959962	-0.337520	-0.924966
3	6	0	-0.899372	0.692143	-0.564915
4	6	0	-3.237854	-0.219892	1.295768
5	1	0	-3.208791	-1.859869	-0.067151
6	1	0	-1.705246	-1.628691	0.822426
7	1	0	-2.772636	0.205663	-1.414306
8	1	0	-1.566820	-1.073210	-1.635665
9	1	0	-4.178734	0.246996	1.020464
10	1	0	-2.779565	0.084426	2.230395
11	6	0	0.502992	0.246738	-0.256686
12	6	0	1.411129	1.204967	0.227000
13	6	0	0.943961	-1.074792	-0.438621
14	6	0	2.724786	0.850342	0.524582
15	1	0	1.060812	2.223113	0.360022
16	6	0	2.262228	-1.429650	-0.143759
17	1	0	0.268329	-1.834285	-0.817088
18	6	0	3.154052	-0.469026	0.339296
19	1	0	3.415990	1.599375	0.899924
20	1	0	2.591722	-2.453760	-0.292515
21	1	0	4.178948	-0.745869	0.569472
22	8	0	-1.197951	1.878444	-0.495960

Zero-point correction= 0.180035 (Hartree/Particle)

Thermal correction to Energy= 0.190968

Thermal correction to Enthalpy= 0.191912

Thermal correction to Gibbs Free Energy= 0.141153

Sum of electronic and zero-point Energies= -462.703406

Sum of electronic and thermal Energies= -462.692473

Sum of electronic and thermal Enthalpies= -462.691529

Sum of electronic and thermal Free Energies= -462.742288

B3LYP/6-311++G(d,p)//B3LYP/6-31+G(d,p) E = -462.9751937

3a

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.602434	-0.115031	-1.232308
2	6	0	3.043111	-0.249522	-0.730566
3	6	0	0.813948	0.468472	-0.015801
4	6	0	1.596315	-0.146611	1.250136
5	6	0	2.870226	-0.816596	0.689403
6	1	0	3.741255	-0.639744	1.327911
7	1	0	2.721084	-1.902257	0.637029
8	1	0	1.825169	0.665642	1.945680
9	1	0	0.924246	-0.837303	1.764569
10	1	0	3.515049	0.737878	-0.689262
11	1	0	3.658204	-0.887664	-1.373654
12	1	0	1.188103	-1.095167	-1.493933
13	1	0	1.489432	0.537311	-2.103560
14	6	0	-0.685267	0.153561	-0.012072
15	6	0	-1.626087	1.189548	0.033307
16	6	0	-1.148011	-1.170787	-0.060268
17	6	0	-2.996137	0.909734	0.029717
18	1	0	-1.275256	2.214994	0.076423
19	6	0	-2.515303	-1.452988	-0.062044
20	1	0	-0.439886	-1.995395	-0.091265
21	6	0	-3.446689	-0.411098	-0.018212
22	1	0	-3.710728	1.727504	0.064069
23	1	0	-2.852491	-2.485254	-0.096821
24	1	0	-4.510908	-0.628423	-0.021095
25	8	0	1.084436	1.804473	0.103269

Zero-point correction= 0.212236 (Hartree/Particle)

Thermal correction to Energy= 0.222549

Thermal correction to Enthalpy= 0.223494

Thermal correction to Gibbs Free Energy= 0.175000

Sum of electronic and zero-point Energies= -501.982395

Sum of electronic and thermal Energies= -501.972082

Sum of electronic and thermal Enthalpies= -501.971137

Sum of electronic and thermal Free Energies= -502.019631

B3LYP/6-311++G(d,p)//B3LYP/6-31+G(d,p) E = -502.291887952

TS_3

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.608630	-0.006581	1.436546
2	6	0	-2.783888	-0.792827	0.912839
3	6	0	-0.762170	0.582811	-0.335362
4	6	0	-1.696827	-0.275423	-1.213340
5	6	0	-3.066340	-0.327578	-0.531079
6	1	0	-3.503530	0.676250	-0.518337
7	1	0	-3.764957	-0.995511	-1.045996
8	1	0	-1.742233	0.195110	-2.201755
9	1	0	-1.306099	-1.288501	-1.347721
10	1	0	-3.662926	-0.646523	1.554223
11	1	0	-2.550930	-1.864415	0.912175
12	1	0	-0.788797	-0.537252	1.913468
13	1	0	-1.815163	0.965949	1.874119
14	6	0	0.694926	0.179547	-0.178347
15	6	0	1.640259	1.187576	0.069057
16	6	0	1.139257	-1.149780	-0.267580
17	6	0	2.992289	0.877015	0.218042
18	1	0	1.292680	2.213005	0.134901
19	6	0	2.492333	-1.461896	-0.115884
20	1	0	0.434901	-1.955593	-0.448882
21	6	0	3.424616	-0.449671	0.126910
22	1	0	3.709999	1.671595	0.402411
23	1	0	2.817008	-2.496178	-0.187757
24	1	0	4.477054	-0.692550	0.242114
25	8	0	-1.048993	1.821932	-0.251722

Zero-point correction= 0.210282 (Hartree/Particle)
Thermal correction to Energy= 0.220551
Thermal correction to Enthalpy= 0.221495
Thermal correction to Gibbs Free Energy= 0.173156
Sum of electronic and zero-point Energies= -501.973925
Sum of electronic and thermal Energies= -501.963656
Sum of electronic and thermal Enthalpies= -501.962712
Sum of electronic and thermal Free Energies= -502.011052

B3LYP/6-311++G(d,p)//B3LYP/6-31+G(d,p) E = -502.282278531

3b

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z

1	6	0	-3.044034	0.697002	1.509888
2	6	0	-3.581572	-0.385398	0.634307
3	6	0	-0.465028	0.315770	-0.594558
4	6	0	-1.413556	-0.879473	-0.677887
5	6	0	-2.905139	-0.516822	-0.745418
6	1	0	-3.017762	0.418176	-1.304119
7	1	0	-3.431259	-1.294770	-1.310763
8	1	0	-1.118597	-1.432873	-1.582051
9	1	0	-1.223882	-1.559974	0.160556
10	1	0	-4.661426	-0.218574	0.459634
11	1	0	-3.528353	-1.350142	1.161293
12	1	0	-3.173262	0.649251	2.586873
13	1	0	-2.664568	1.618275	1.080531
14	6	0	0.972747	0.078766	-0.223324
15	6	0	1.822661	1.193671	-0.120429
16	6	0	1.501976	-1.202053	0.006751
17	6	0	3.166331	1.032924	0.209620
18	1	0	1.404641	2.177635	-0.304730
19	6	0	2.850717	-1.363713	0.331049
20	1	0	0.871435	-2.081170	-0.069873
21	6	0	3.684383	-0.247519	0.435257
22	1	0	3.811909	1.902688	0.289933
23	1	0	3.248696	-2.359441	0.503272
24	1	0	4.732537	-0.373936	0.691107
25	8	0	-0.848379	1.445740	-0.869151

Zero-point correction= 0.208424 (Hartree/Particle)

Thermal correction to Energy= 0.220420

Thermal correction to Enthalpy= 0.221364

Thermal correction to Gibbs Free Energy= 0.168311

Sum of electronic and zero-point Energies= -501.992854

Sum of electronic and thermal Energies= -501.980858

Sum of electronic and thermal Enthalpies= -501.979914

Sum of electronic and thermal Free Energies= -502.032967

B3LYP/6-311++G(d,p)//B3LYP/6-31+G(d,p) E = -502.300190395

4a

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.737327	-0.062726	1.265607
2	6	0	-3.352119	-0.677591	0.000642
3	6	0	-2.737387	-0.064938	-1.265420

4	6	0	-1.212364	-0.200138	-1.279692
5	6	0	-0.515282	0.412605	-0.000505
6	6	0	-1.212298	-0.197755	1.280013
7	1	0	-3.141815	-0.555847	-2.159664
8	1	0	-3.178349	-1.764238	0.001588
9	1	0	-4.439200	-0.534761	0.000557
10	1	0	-3.011497	0.996319	1.330074
11	1	0	-3.141606	-0.552175	2.160720
12	1	0	-0.923742	-1.256960	-1.318958
13	1	0	-0.776855	0.285691	-2.158648
14	1	0	-0.923529	-1.254465	1.321093
15	1	0	-0.776722	0.289729	2.158009
16	1	0	-3.011442	0.994031	-1.331643
17	6	0	0.994315	0.119382	-0.000159
18	6	0	1.913171	1.177055	-0.000607
19	6	0	1.489482	-1.194245	0.000516
20	6	0	3.288880	0.929735	-0.000354
21	1	0	1.538773	2.194941	-0.001135
22	6	0	2.863669	-1.444638	0.000772
23	1	0	0.804467	-2.038042	0.000849
24	6	0	3.770538	-0.381415	0.000345
25	1	0	3.984225	1.764698	-0.000706
26	1	0	3.224091	-2.469607	0.001306
27	1	0	4.839587	-0.573756	0.000539
28	8	0	-0.798257	1.747808	-0.001366

Zero-point correction= 0.240621 (Hartree/Particle)

Thermal correction to Energy= 0.251378

Thermal correction to Enthalpy= 0.252323

Thermal correction to Gibbs Free Energy= 0.203493

Sum of electronic and zero-point Energies= -541.277086

Sum of electronic and thermal Energies= -541.266329

Sum of electronic and thermal Enthalpies= -541.265384

Sum of electronic and thermal Free Energies= -541.314214

B3LYP/6-311++G(d,p)//B3LYP/6-31+G(d,p) E = -541.621921257

TS_4

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.660605	-0.623219	1.257276
2	6	0	3.354448	0.488820	0.452673
3	6	0	2.813914	0.609850	-0.980117

4	6	0	1.307012	0.888610	-1.025005
5	6	0	0.452587	-0.307343	-0.551039
6	6	0	1.183142	-0.419484	1.398630
7	1	0	3.340668	1.420181	-1.498460
8	1	0	3.223121	1.448007	0.975633
9	1	0	4.433254	0.295053	0.424816
10	1	0	2.849334	-1.598668	0.795413
11	1	0	3.095152	-0.665038	2.270966
12	1	0	1.077595	1.794847	-0.455336
13	1	0	0.991119	1.083559	-2.059516
14	1	0	0.844205	0.548105	1.767551
15	1	0	0.587925	-1.260033	1.744878
16	1	0	3.018507	-0.313984	-1.532366
17	6	0	-1.012819	-0.056162	-0.235094
18	6	0	-1.902941	-1.138988	-0.324586
19	6	0	-1.521210	1.202273	0.126265
20	6	0	-3.261649	-0.969860	-0.059700
21	1	0	-1.506200	-2.106435	-0.613856
22	6	0	-2.882438	1.372585	0.391663
23	1	0	-0.863064	2.061514	0.204843
24	6	0	-3.757608	0.287452	0.300796
25	1	0	-3.935893	-1.818154	-0.138961
26	1	0	-3.257611	2.353913	0.668253
27	1	0	-4.815895	0.420639	0.506352
28	8	0	0.789940	-1.458839	-0.946348

Zero-point correction= 0.239029 (Hartree/Particle)

Thermal correction to Energy= 0.250299

Thermal correction to Enthalpy= 0.251243

Thermal correction to Gibbs Free Energy= 0.201105

Sum of electronic and zero-point Energies= -541.265732

Sum of electronic and thermal Energies= -541.254461

Sum of electronic and thermal Enthalpies= -541.253517

Sum of electronic and thermal Free Energies= -541.303655

B3LYP/6-311++G(d,p)//B3LYP/6-31+G(d,p) E = -541.609947569

4b

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	3.048429	-1.128904	0.672959
2	6	0	3.470958	0.332319	0.394416

3	6	0	2.657853	1.087019	-0.674115
4	6	0	1.166488	1.291433	-0.365088
5	6	0	0.257090	0.147288	-0.810081
6	6	0	1.849743	-1.282236	1.548447
7	1	0	3.117448	2.074616	-0.802970
8	1	0	3.446707	0.895724	1.339077
9	1	0	4.519118	0.332323	0.069081
10	1	0	2.890091	-1.655159	-0.275682
11	1	0	3.907361	-1.631217	1.156650
12	1	0	1.015589	1.493701	0.701015
13	1	0	0.797997	2.184873	-0.892382
14	1	0	1.747403	-0.680044	2.448240
15	1	0	1.149638	-2.099434	1.410161
16	1	0	2.746828	0.569118	-1.635322
17	6	0	-1.163968	0.112362	-0.317967
18	6	0	-1.983951	-0.949424	-0.737053
19	6	0	-1.708089	1.099644	0.519944
20	6	0	-3.312001	-1.026468	-0.323910
21	1	0	-1.555293	-1.703447	-1.388763
22	6	0	-3.041257	1.025773	0.929549
23	1	0	-1.101195	1.933660	0.855315
24	6	0	-3.844859	-0.037605	0.510983
25	1	0	-3.934003	-1.854135	-0.652394
26	1	0	-3.450703	1.797377	1.575007
27	1	0	-4.880915	-0.095598	0.832395
28	8	0	0.650664	-0.698696	-1.603492

Zero-point correction= 0.236869 (Hartree/Particle)

Thermal correction to Energy= 0.250153

Thermal correction to Enthalpy= 0.251097

Thermal correction to Gibbs Free Energy= 0.195000

Sum of electronic and zero-point Energies= -541.279379

Sum of electronic and thermal Energies= -541.266094

Sum of electronic and thermal Enthalpies= -541.265150

Sum of electronic and thermal Free Energies= -541.321247

B3LYP/6-311++G(d,p)//B3LYP/6-31+G(d,p) E = -541.622204558

5. References

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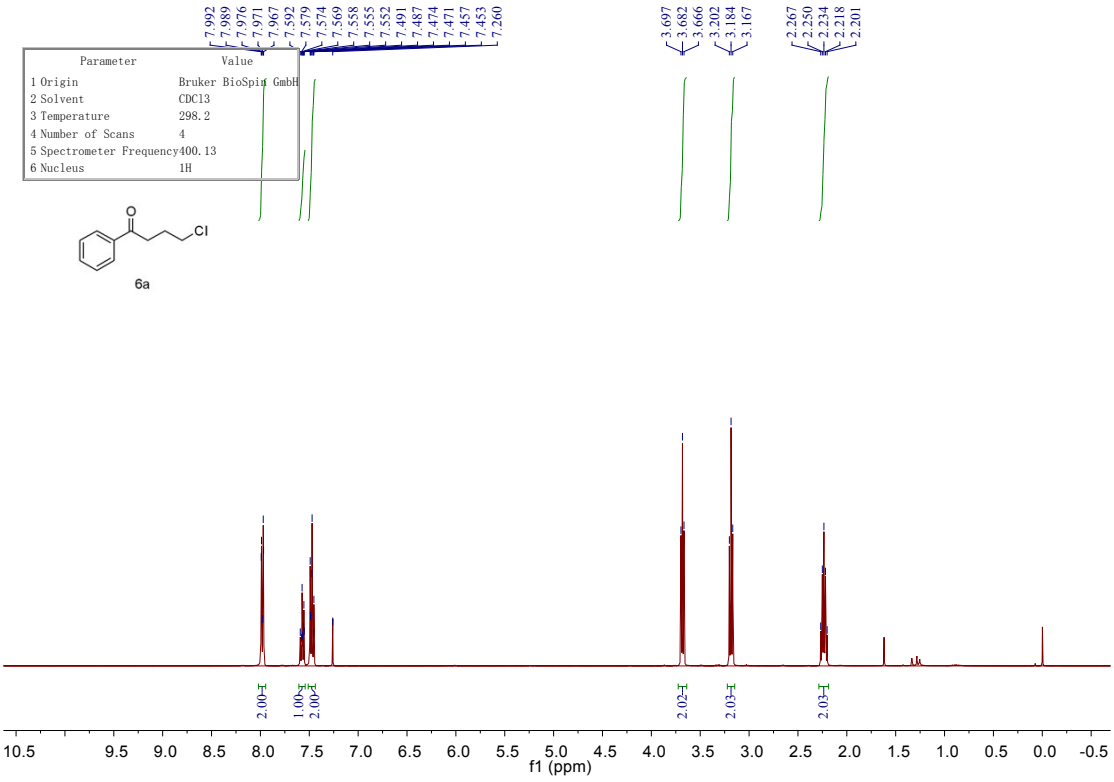
4. Hariharan, P. C.; Pople, J. A. *Theor. Chim. Acta* **1973**, *28*, 213-222.
5. Frisch, M. J.; Trucks, G. W.; Schlegel, H. B.; Scuseria, G. E.; Robb, M. A.; Cheeseman, J. R.; Scalmani, G.; Barone, V.; Mennucci, B.; Petersson, G. A.; Nakatsuji, H.; Caricato, M.; Li, X.; Hratchian, H. P.; Izmaylov, A. F.; Bloino, J.; Zheng, G.; Sonnenberg, J. L.; Hada, M.; Ehara, M.; Toyota, K.; Fukuda, R.; Hasegawa, J.; Ishida, M.; Nakajima, T.; Honda, Y.; Kitao, O.; Nakai, H.; Vreven, T.; Montgomery, J. A. Jr.; Peralta, J. E.; Ogliaro, F.; Bearpark, M.; Heyd, J. J.; Brothers, E.; Kudin, K. N.; Staroverov, V. N.; Keith, T.; Kobayashi, R.; Normand, J.; Raghavachari, K.; Rendell, A.; Burant, J. C.; Iyengar, S. S.; Tomasi, J.; Cossi, M.; Rega, N.; Millam, J. M.; Klene, M.; Knox, J. E.; Cross, J. B.; Bakken, V.; Adamo, C.; Jaramillo, J.; Gomperts, R.; Stratmann, R. E.; Yazyev, O.; Austin, A. J.; Cammi, R.; Pomelli, C.; Ochterski, J. W.; Martin, R. L.; Morokuma, K.; Zakrzewski, V. G.; Voth, G. A.; Salvador, P.; Dannenberg, J. J.; Dapprich, S.; Daniels, A. D.; Farkas, O.; Foresman, J. B.; Ortiz, J. V.; Cioslowski, J.; Fox, D. J. Gaussian 09, Revision C.01, Gaussian, Inc., Wallingford CT, 2010.

6. ^{1}H, ^{13}C, and ^{19}F NMR spectra of products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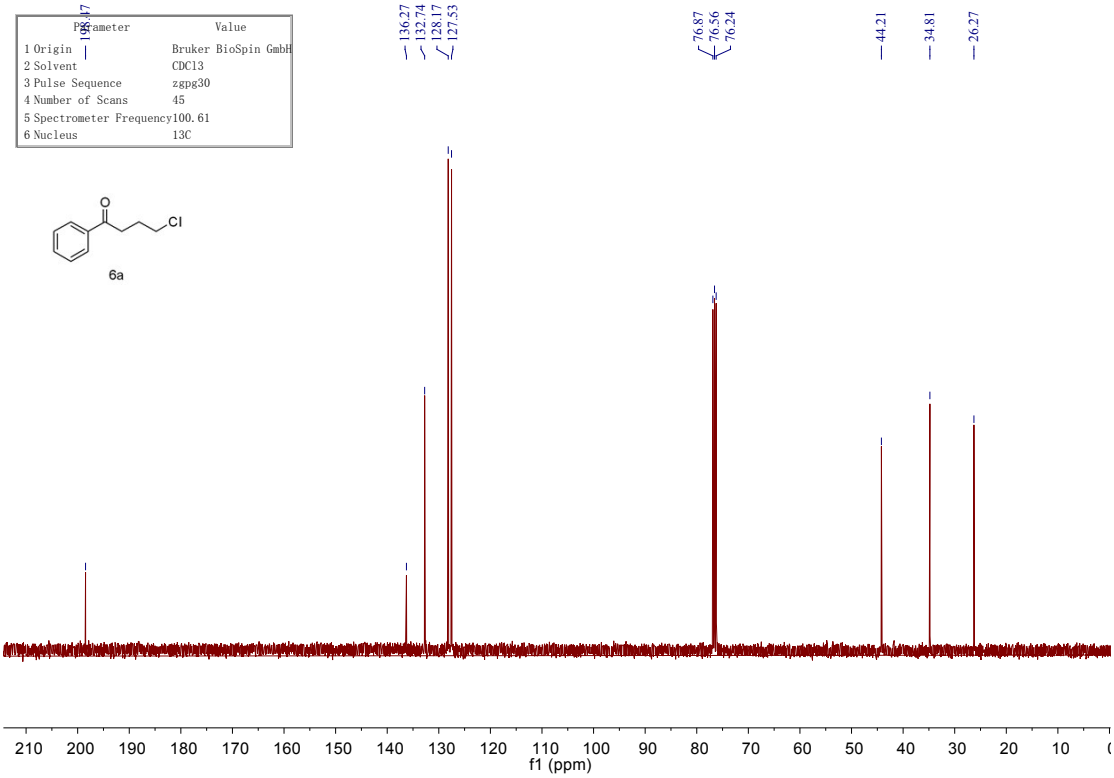
7.579
7.574
7.569
7.558
7.555
7.552
7.491
7.487
7.474
7.471
7.457
7.453
7.260
3.697
3.682
3.666
3.202
3.184
3.167
2.267
2.250
2.234
2.218
2.201
Parameter Value
1 Origin Bruker BioSpin GmbH
2 Solvent CDCl3
3 Temperature 298.2
4 Number of Scans 4
5 Spectrometer Frequency 400.13
6 Nucleus 1H
O
Cl
6a
2.00
1.00
2.00
2.02
2.03
2.03
10.5 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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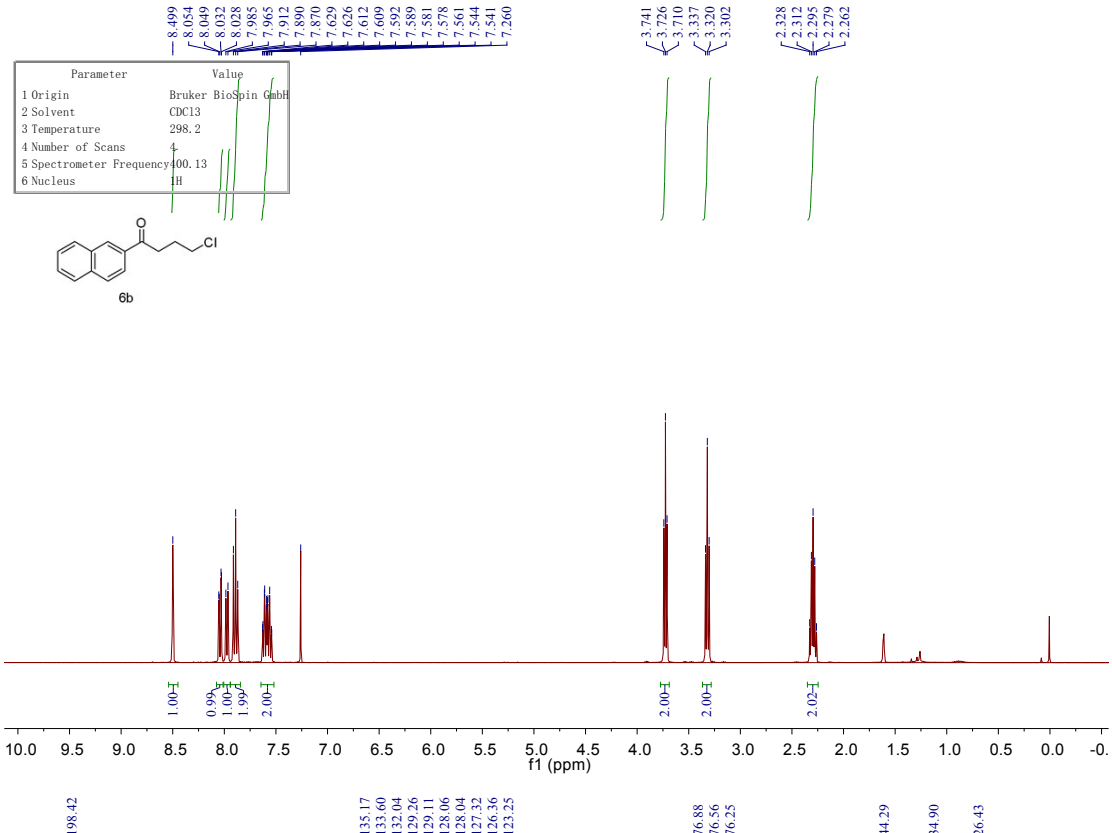
136.27
132.74
128.17
127.53
76.87
76.56
76.24
44.21
34.81
26.27
Parameter Value
1 Origin Bruker BioSpin GmbH
2 Solvent CDCl3
3 Pulse Sequence zgpg30
4 Number of Scans 45
5 Spectrometer Frequency 100.61
6 Nucleus 13C
O
Cl
6a
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10
f1 (ppm)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8.054
8.049
8.032
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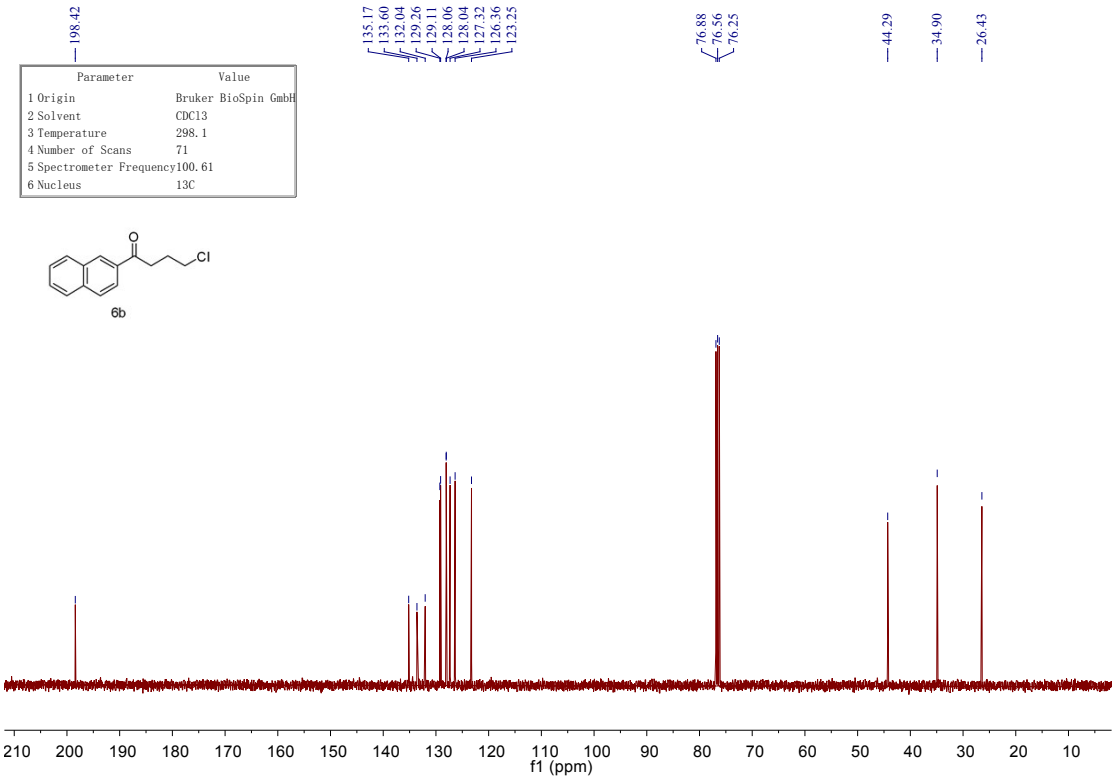
7.985
7.965
7.912
7.890
7.870
7.629
7.626
7.612
7.609
7.592
7.589
7.581
7.578
7.561
7.544
7.541
7.260
3.741
3.726
3.710
3.337
3.320
3.302
2.328
2.312
2.295
2.279
2.262
Parameter Value
1 Origin Bruker BioSpin GmbH
2 Solvent CDCl3
3 Temperature 298.2
4 Number of Scans 4
5 Spectrometer Frequency 400.13
6 Nucleus 1H
O
Cl
6b
1.00
0.93
1.00
1.99
2.00
2.00
2.00
2.02
10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.
f1 (ppm)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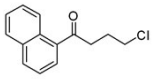
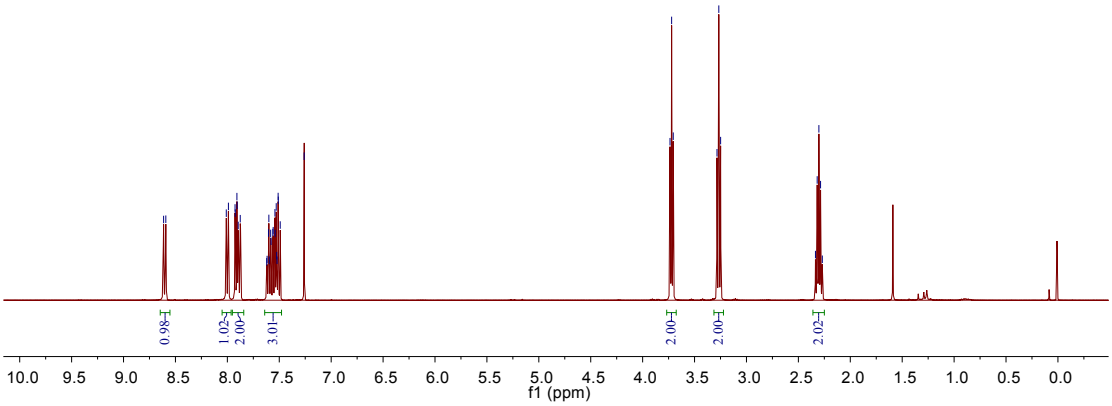
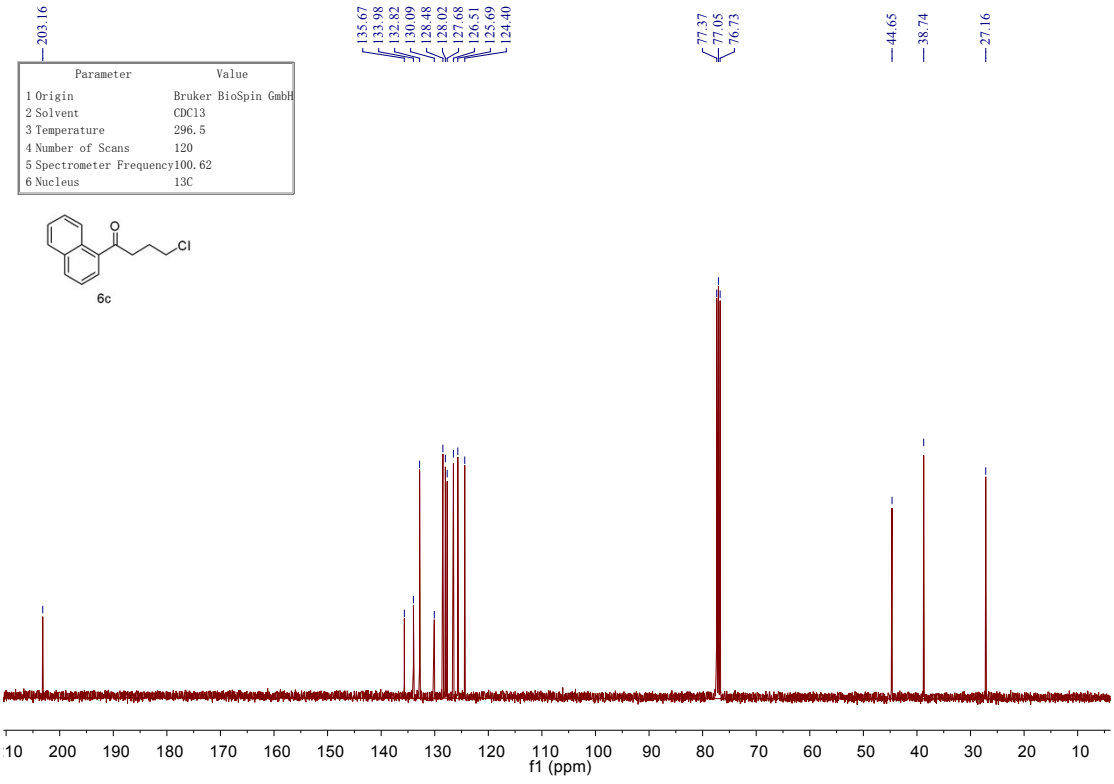
133.60
132.04
129.26
129.11
128.06
128.04
127.32
126.36
123.25
76.88
76.56
76.25
44.29
34.90
26.43
Parameter Value
1 Origin Bruker BioSpin GmbH
2 Solvent CDCl3
3 Temperature 298.1
4 Number of Scans 71
5 Spectrometer Frequency 100.61
6 Nucleus 13C
O
Cl
6b
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10
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



6c





Parameter	Value
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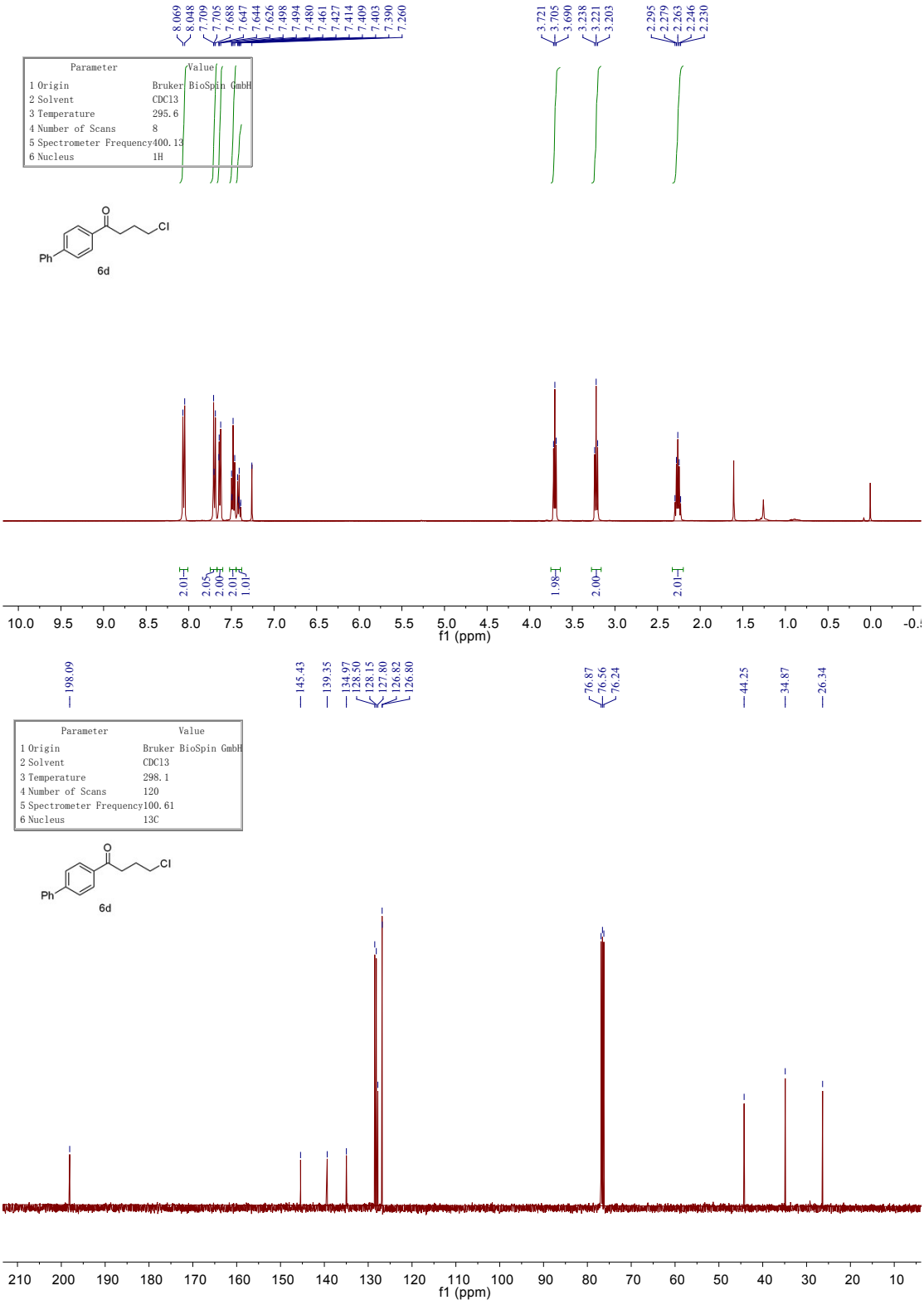
2 Solvent	CDCl3
3 Temperature	296.5
4 Number of Scans	120
5 Spectrometer Frequency	100.62
6 Nucleus	13C

6c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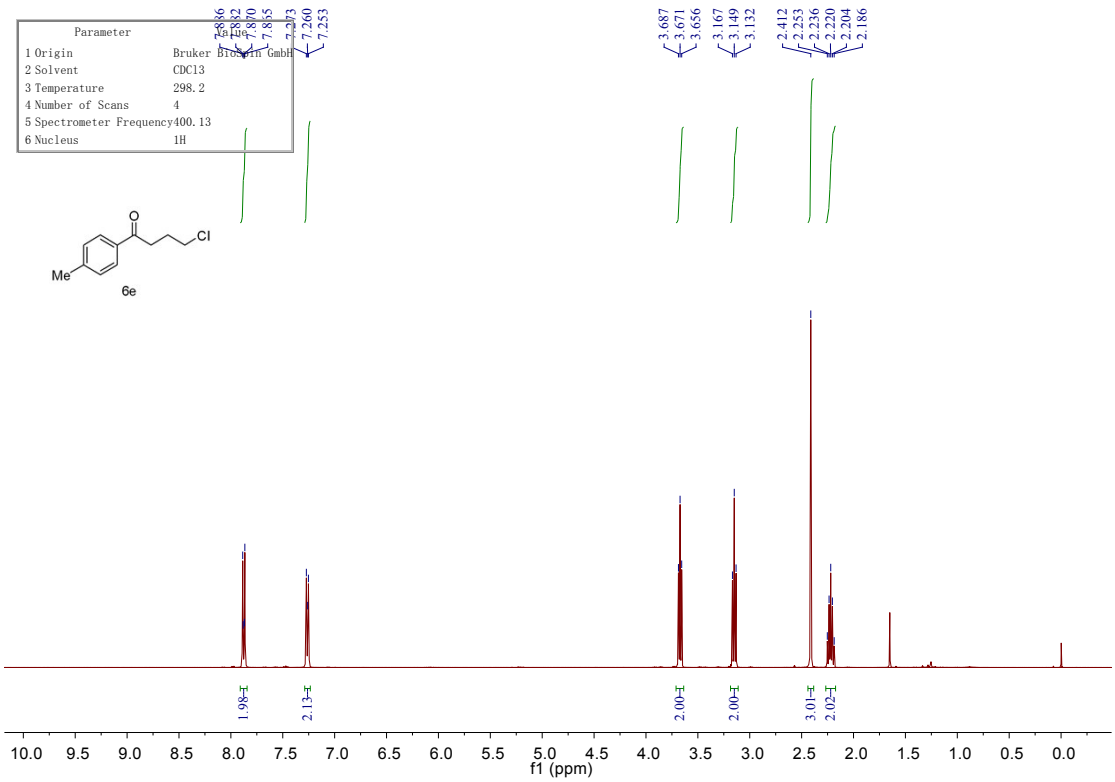
7.709
7.705
7.688
7.647
7.644
7.626
7.498
7.494
7.480
7.461
7.427
7.414
7.409
7.403
7.390
7.260
3.721
3.705
3.690
3.238
3.221
3.203
2.295
2.279
2.263
2.246
2.230
Parameter Value
1 Origin Bruker BioSpin GmbH
2 Solvent CDCl3
3 Temperature 295.6
4 Number of Scans 8
5 Spectrometer Frequency 400.13
6 Nucleus 1H
O
Cl
Ph
6d
2.01
2.05
2.00
2.01
1.01
1.98
2.00
2.01
10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)
198.09
145.43
139.35
134.97
128.50
128.15
127.80
126.82
126.80
76.87
76.56
76.24
44.25
34.87
26.34
Parameter Value
1 Origin Bruker BioSpin GmbH
2 Solvent CDCl3
3 Temperature 298.1
4 Number of Scans 120
5 Spectrometer Frequency 100.61
6 Nucleus 13C
O
Cl
Ph
6d
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10
f1 (ppm)


Parameter
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
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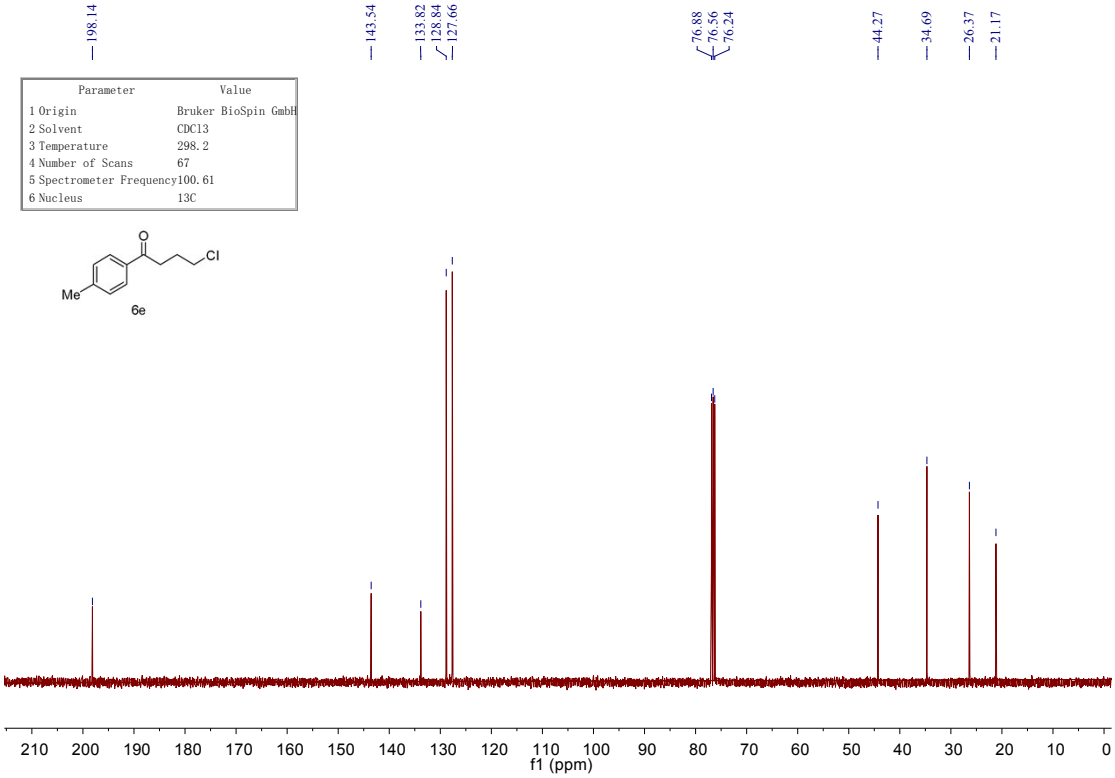
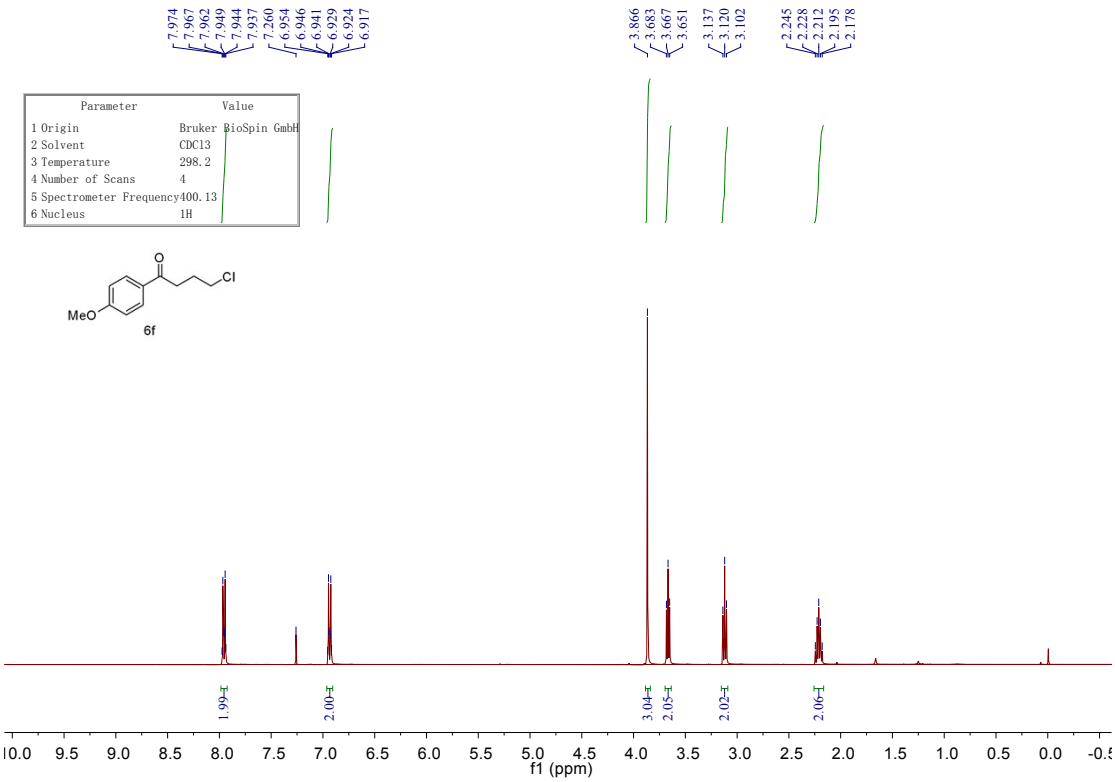
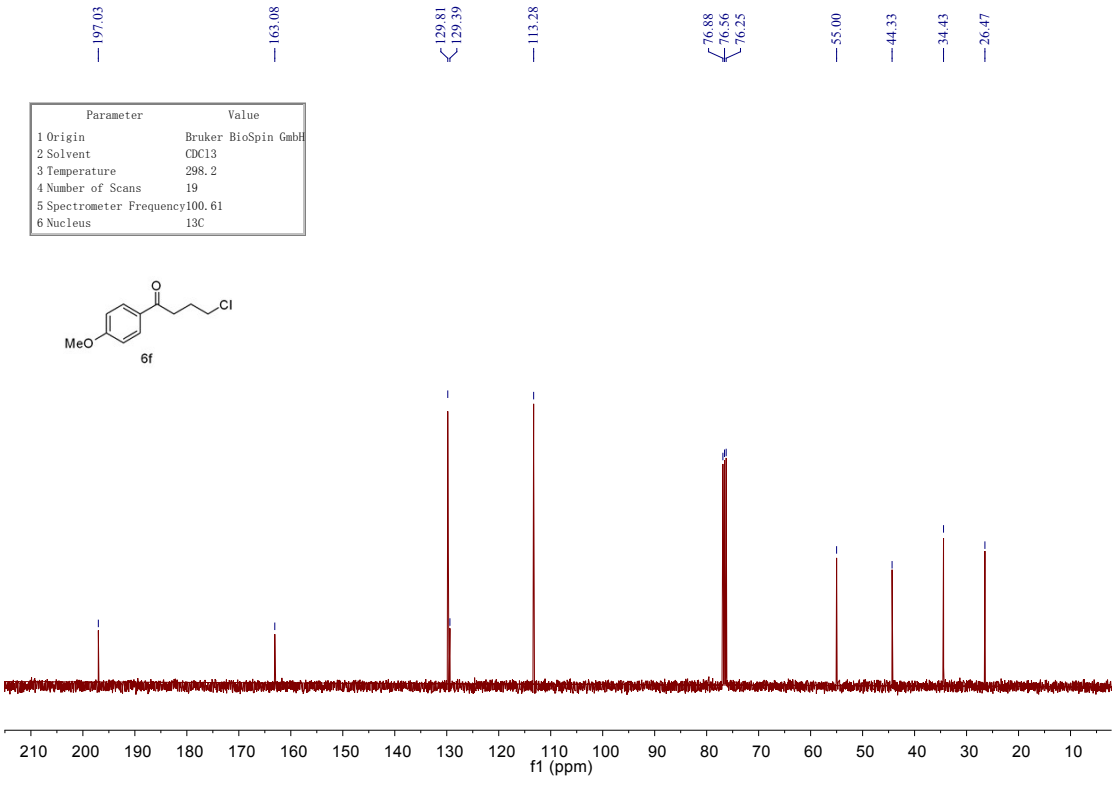
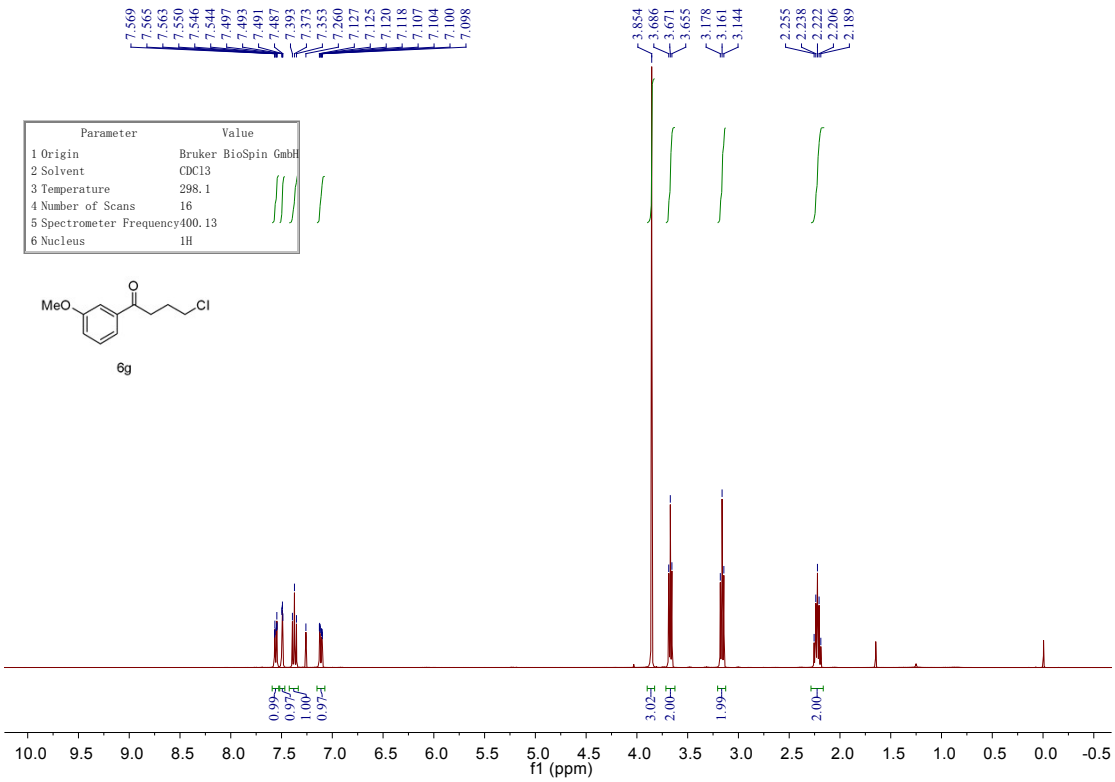
7.882
7.870
7.865
7.273
7.260
7.253
3.687
3.671
3.656
3.167
3.149
3.132
2.412
2.253
2.236
2.220
2.204
2.186
Cl
Me
6e
1.98
2.13
2.00
2.00
3.01
2.02
f1 (ppm)


198.14
143.54
133.82
128.84
127.66
76.88
76.56
76.24
44.27
34.69
26.37
21.17
Parameter Value
1 Origin Bruker BioSpin GmbH
2 Solvent CDCl3
3 Temperature 298.2
4 Number of Scans 67
5 Spectrometer Frequency 100.61
6 Nucleus 13C
Cl
Me
6e
f1 (ppm)


7.974
7.967
7.962
7.949
7.944
7.937
7.260
6.954
6.946
6.941
6.929
6.924
6.917
3.866
3.683
3.667
3.651
3.137
3.120
3.102
2.245
2.228
2.212
2.195
2.178
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
Cl
MeO
6f
1.99
2.00
3.04
2.05
2.02
2.06
f1 (ppm)


197.03
163.08
129.81
129.39
113.28
76.88
76.56
76.25
55.00
44.33
34.43
26.47
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
O
Cl
MeO
6f
f1 (ppm)


7.569
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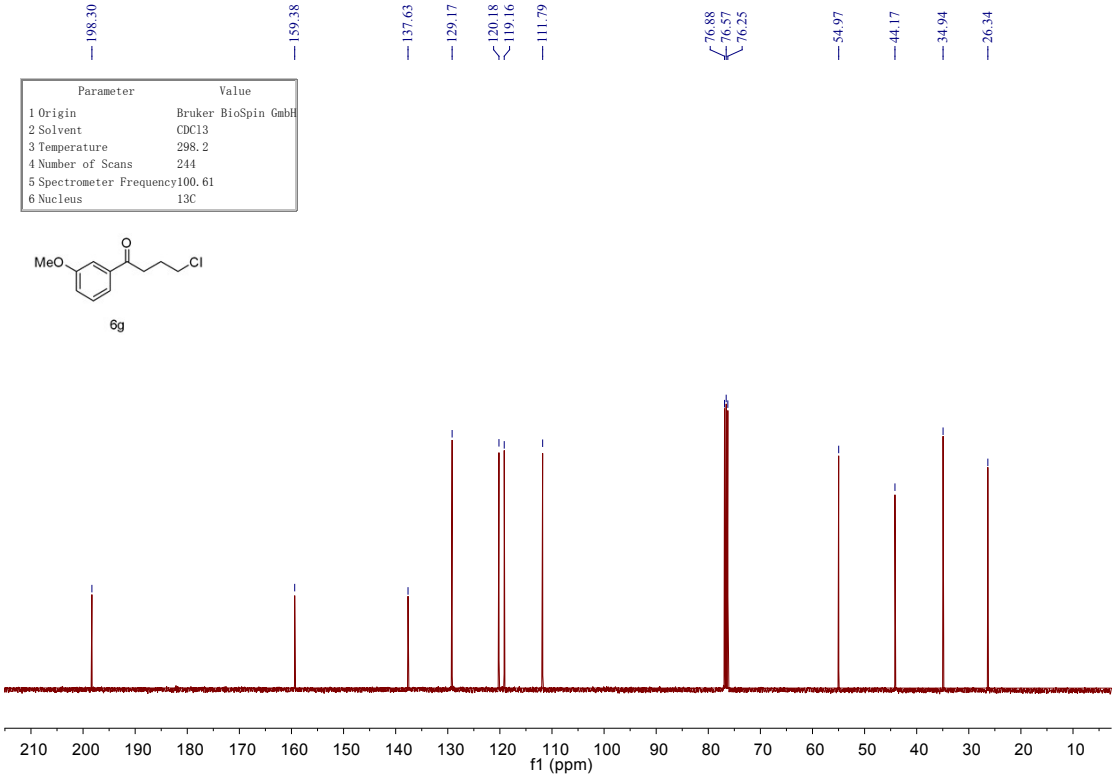
7.563
7.550
7.546
7.544
7.497
7.493
7.491
7.487
7.393
7.373
7.353
7.260
7.127
7.125
7.120
7.118
7.107
7.104
7.100
7.098
3.854
3.686
3.671
3.655
3.178
3.161
3.144
2.255
2.238
2.222
2.206
2.189
Parameter Value
1 Origin Bruker BioSpin GmbH
2 Solvent CDCl3
3 Temperature 298.1
4 Number of Scans 16
5 Spectrometer Frequency 400.13
6 Nucleus 1H
MeO
Cl
O
6g
0.99
0.97
1.00
0.97
3.02
2.00
1.99
2.00
f1 (ppm)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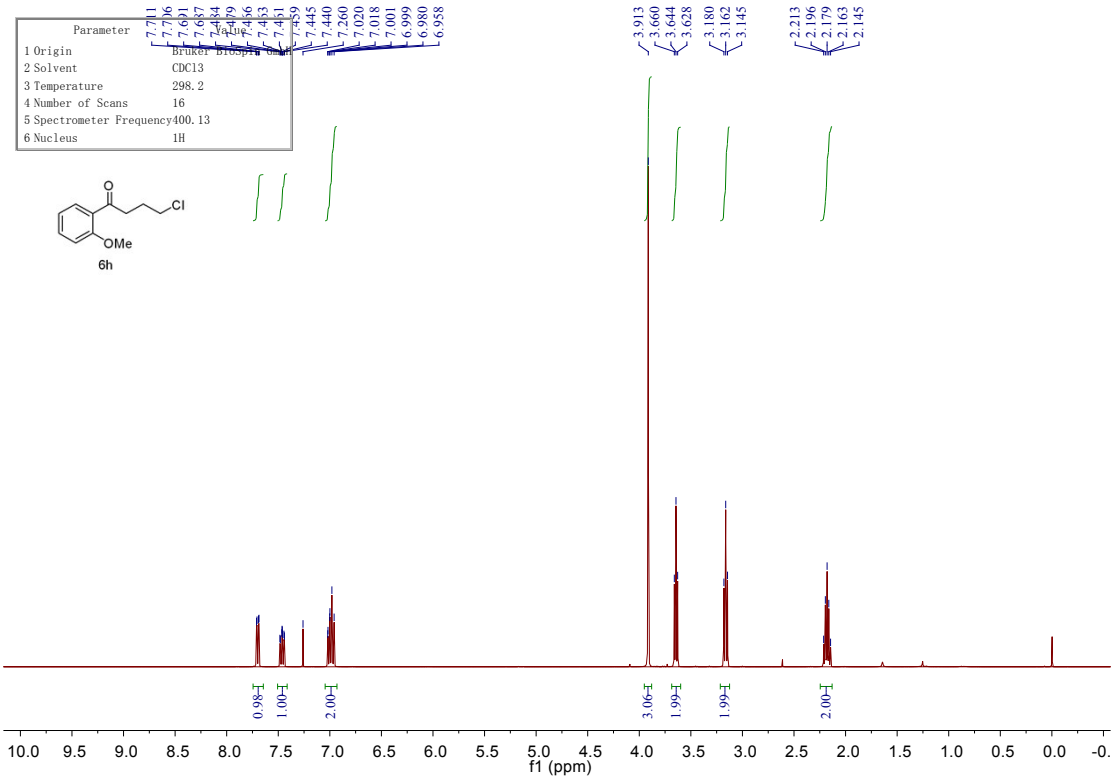
159.38
137.63
129.17
120.18
119.16
111.79
76.88
76.57
76.25
54.97
44.17
34.94
26.34
Parameter Value
1 Origin Bruker BioSpin GmbH
2 Solvent CDCl3
3 Temperature 298.2
4 Number of Scans 244
5 Spectrometer Frequency 100.61
6 Nucleus 13C
MeO
Cl
O
6g
f1 (ppm)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1 Origin Bruker BioSpin GmbH
2 Solvent CDCl3
3 Temperature 298.2
4 Number of Scans 16
5 Spectrometer Frequency 400.13
6 Nucleus 1H
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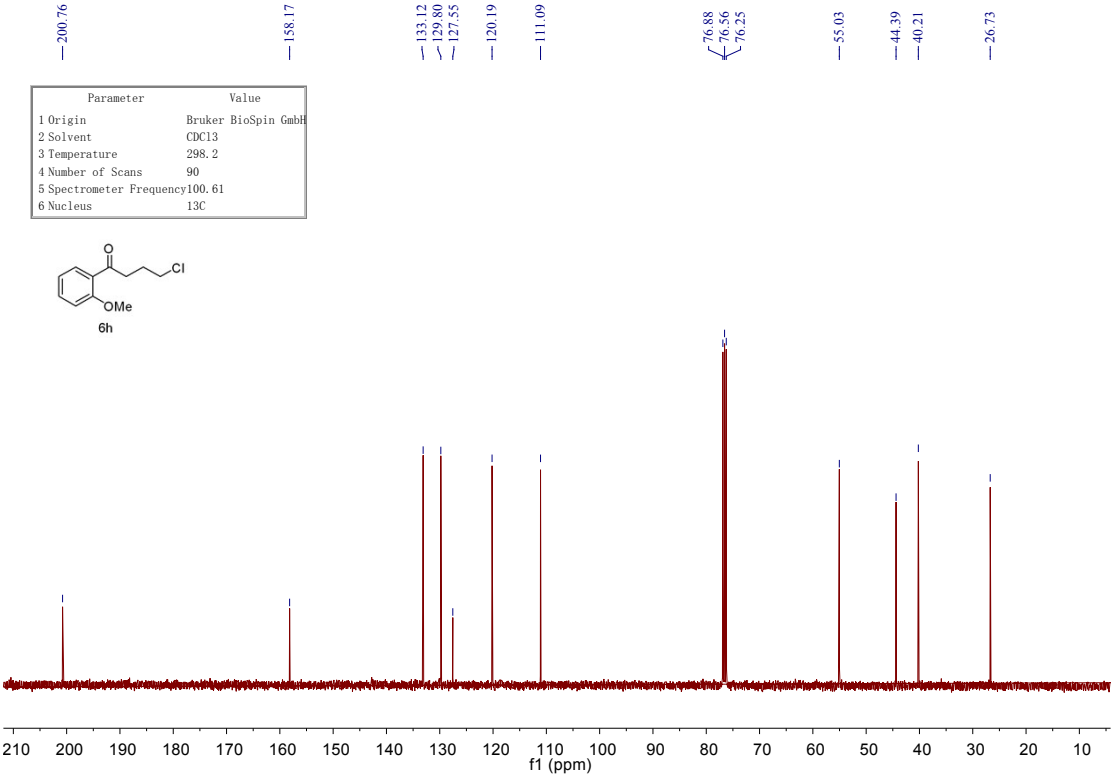
7.706
7.691
7.687
7.484
7.479
7.456
7.453
7.451
7.439
7.445
7.440
7.260
7.020
7.018
7.001
6.999
6.980
6.958
3.913
3.660
3.644
3.628
3.180
3.162
3.145
2.213
2.196
2.179
2.163
2.145
Cl
OMe
6h
0.98
1.00
2.00
3.06
1.99
1.99
2.00
f1 (ppm)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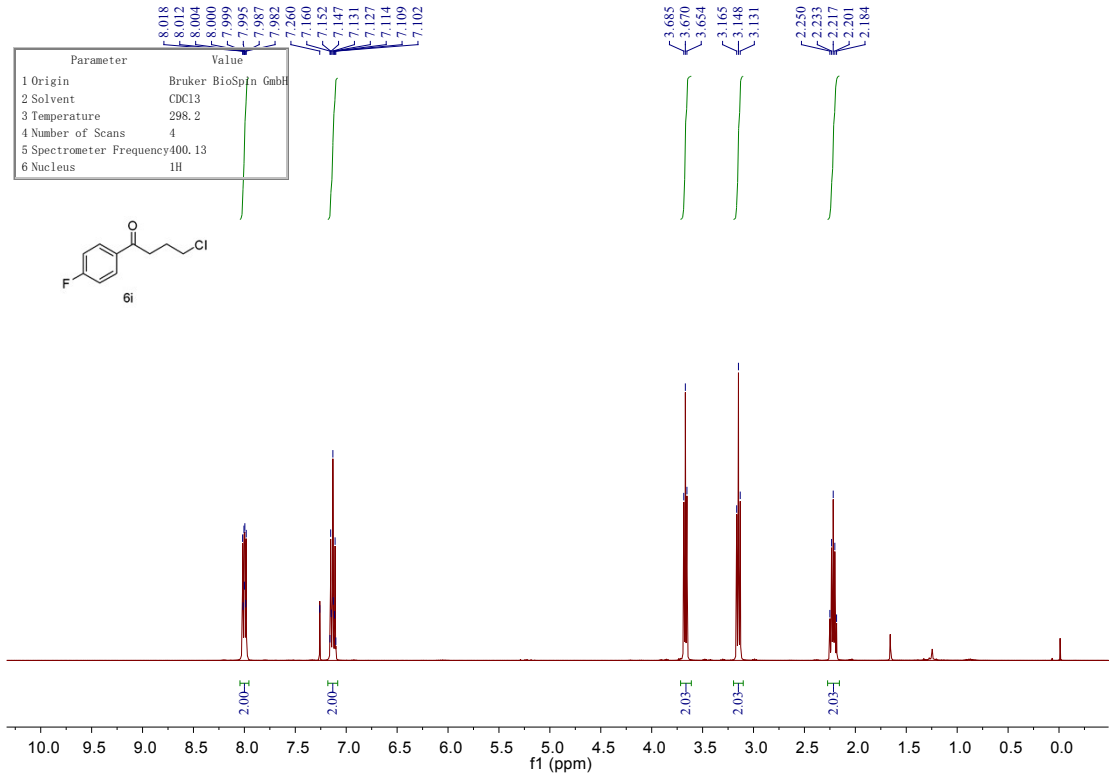
133.12
129.80
127.55
120.19
111.09
76.88
76.56
76.25
55.03
44.39
40.21
26.73
Parameter Value
1 Origin Bruker BioSpin GmbH
2 Solvent CDCl3
3 Temperature 298.2
4 Number of Scans 90
5 Spectrometer Frequency 100.61
6 Nucleus 13C
Cl
OMe
6h
f1 (ppm)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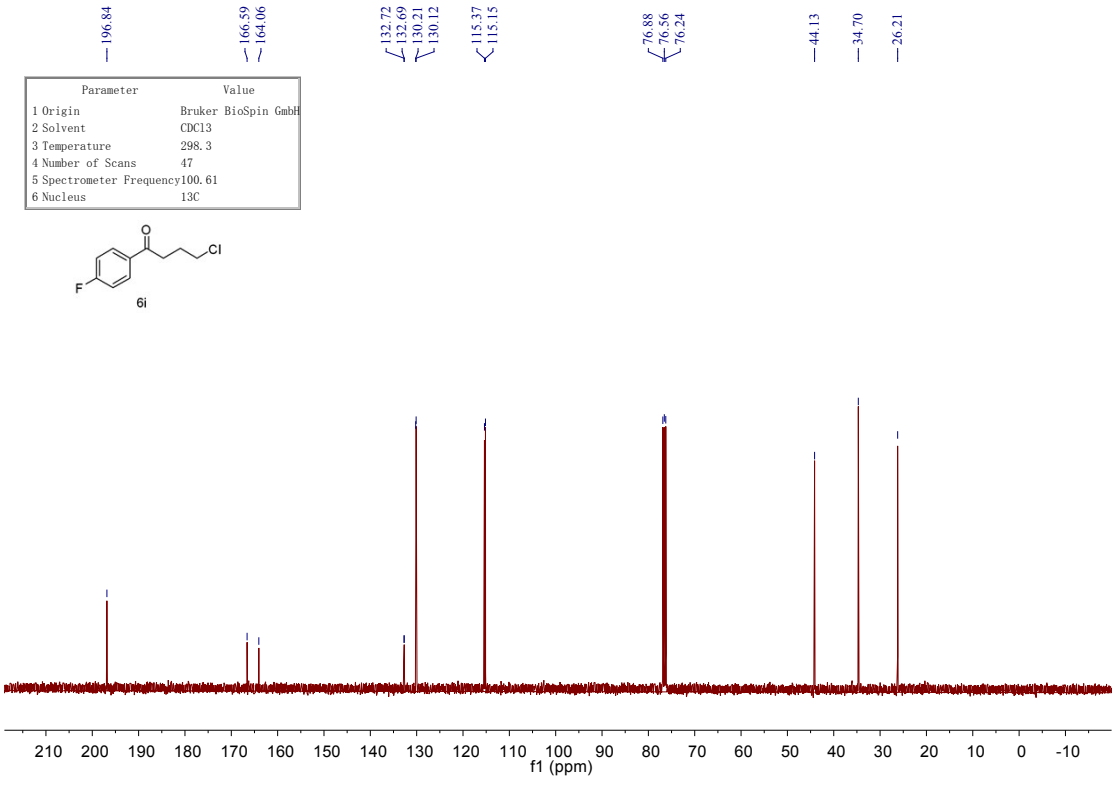
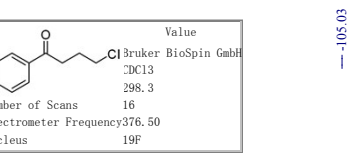
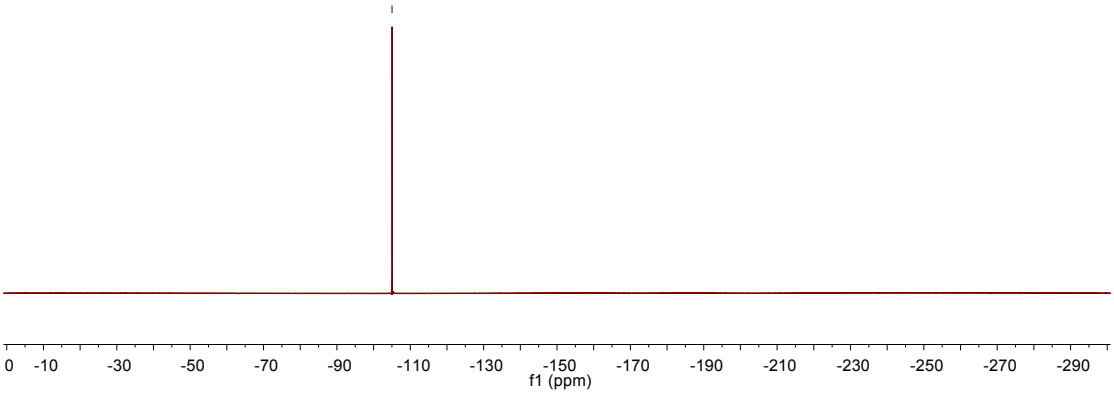
8.000
7.999
7.995
7.987
7.982
7.260
7.160
7.152
7.147
7.131
7.127
7.114
7.109
7.102
3.685
3.670
3.654
3.165
3.148
3.131
2.250
2.233
2.217
2.201
2.184
Parameter Value
1 Origin Bruker BioSpin GmbH
2 Solvent CDCl3
3 Temperature 298.2
4 Number of Scans 4
5 Spectrometer Frequency 400.13
6 Nucleus 1H
O
Cl
F
6i
2.00
2.00
2.03
2.03
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
f1 (ppm)


196.84
166.59
164.06
132.72
132.69
130.21
130.12
115.37
115.15
76.88
76.56
76.24
44.13
34.70
26.21
Parameter Value
1 Origin Bruker BioSpin GmbH
2 Solvent CDCl3
3 Temperature 298.3
4 Number of Scans 47
5 Spectrometer Frequency 100.61
6 Nucleus 13C
O
Cl
F
6i
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)

	Value
1	Bruker BioSpin GmbH
2	CDCl3
3	298.3
4 Number of Scans	16
5 Spectrometer Frequency	376.50
6 Nucleus	19F



-105.03

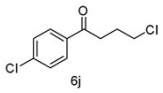


7.930 7.924 7.919 7.907 7.902 7.897 7.457 7.451 7.446 7.434 7.429 7.423 7.260

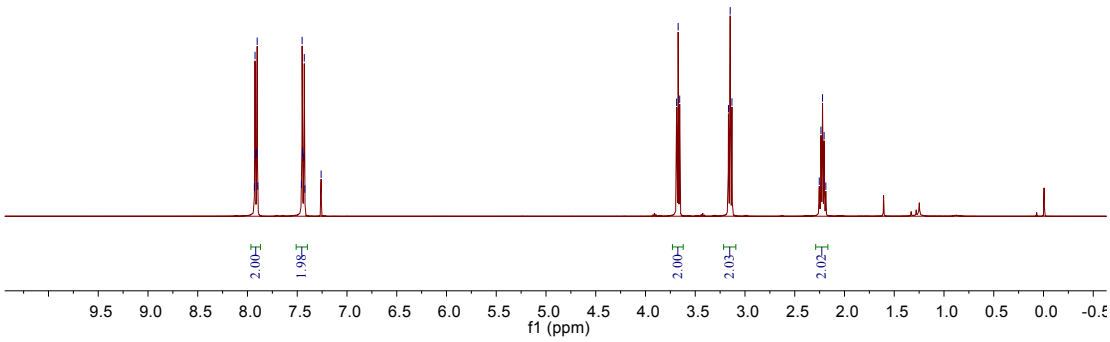
3.687 3.672 3.656 3.166 3.149 3.131

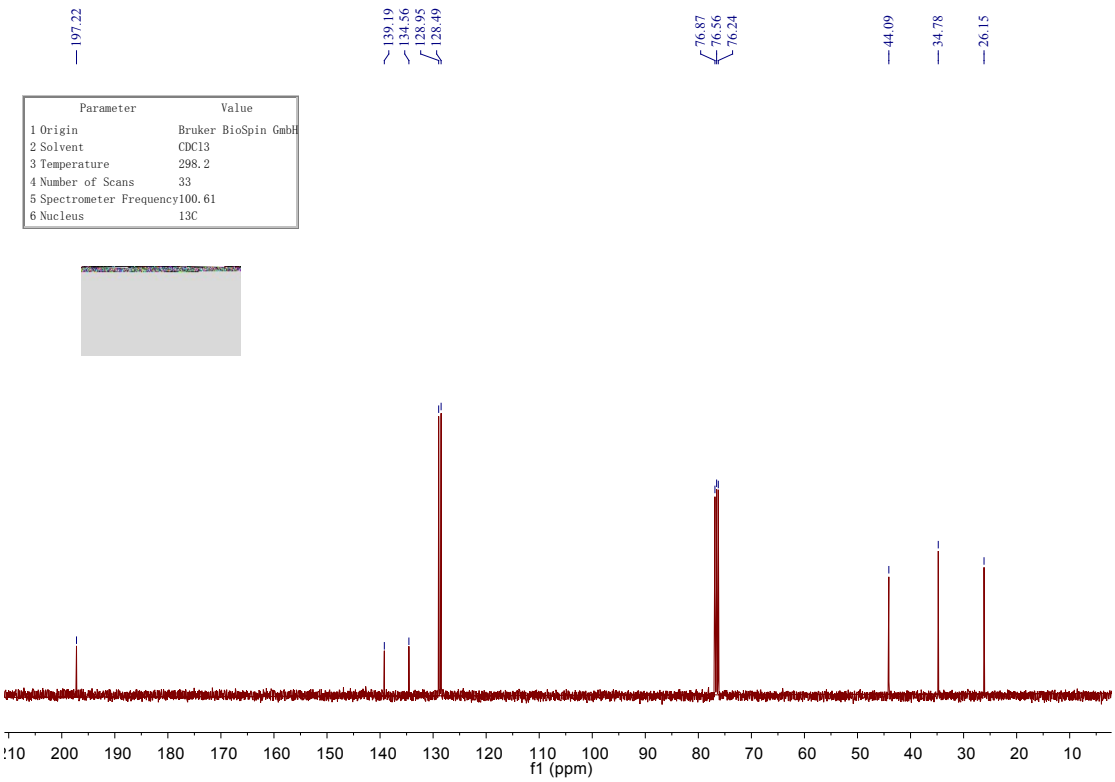
2.254 2.237 2.221 2.205 2.188

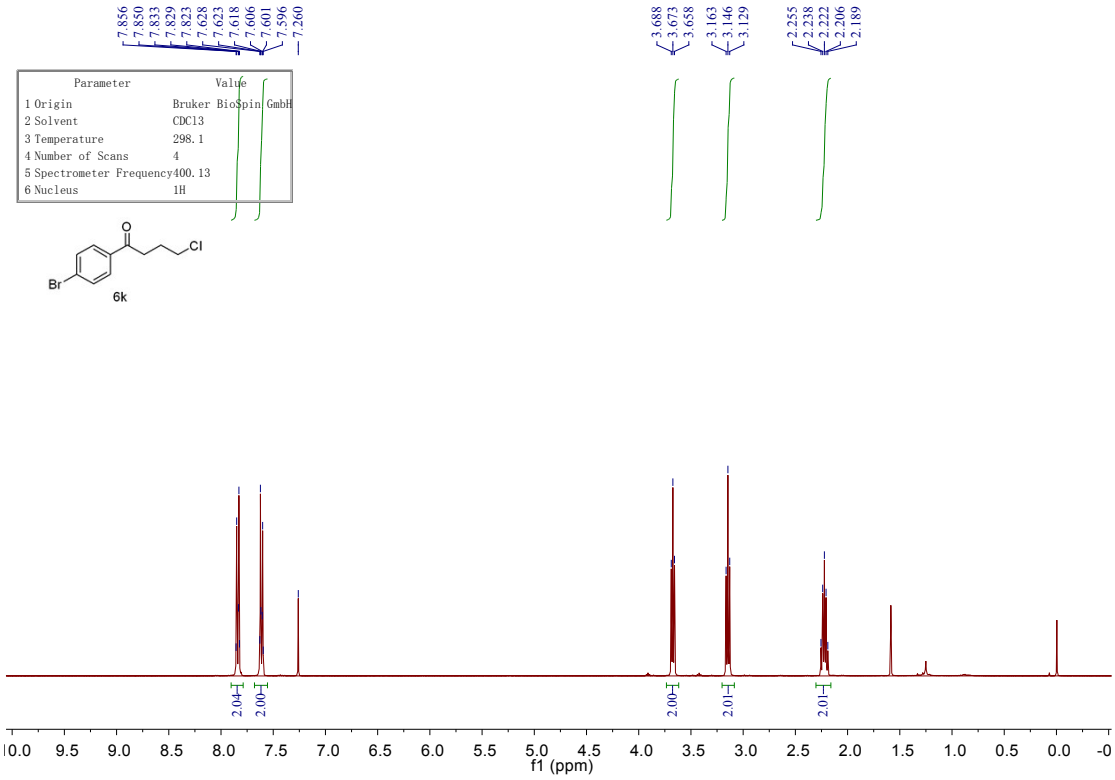
Parameter	Value
1 Origin	Bruker BioSpin GmbH
2 Solvent	CDCl3
3 Temperature	298.1
4 Number of Scans	8
5 Spectrometer Frequency	400.13
6 Nucleus	1H

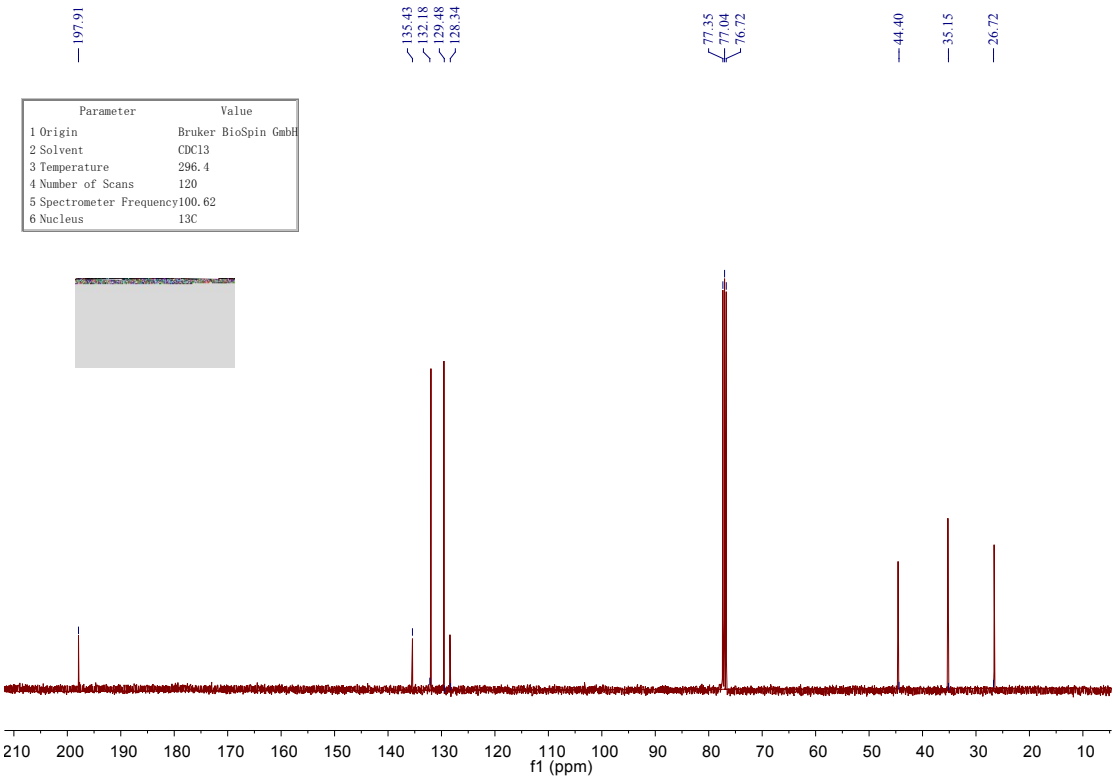


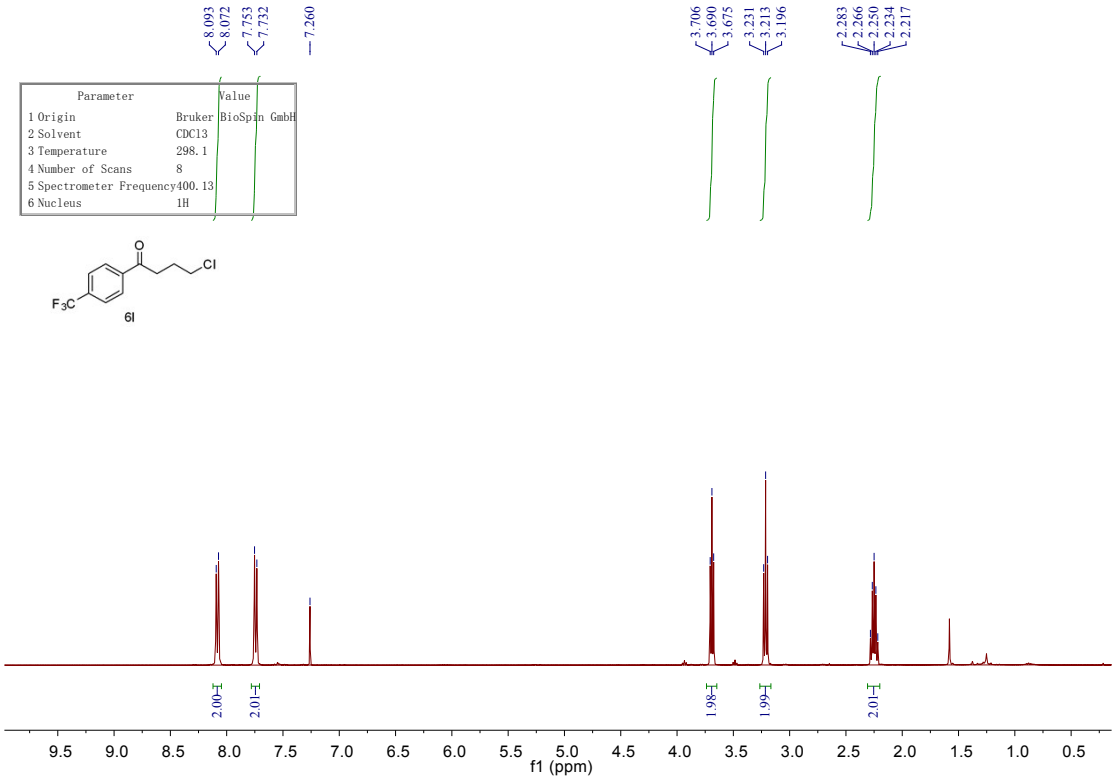
6j

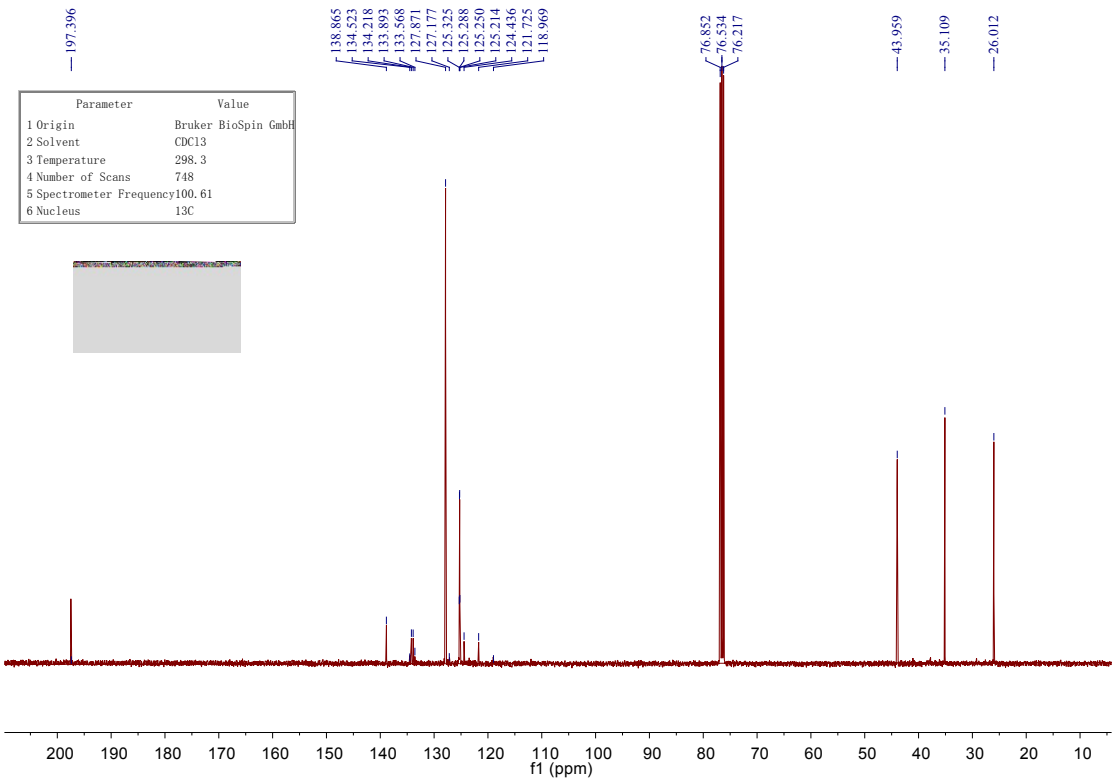


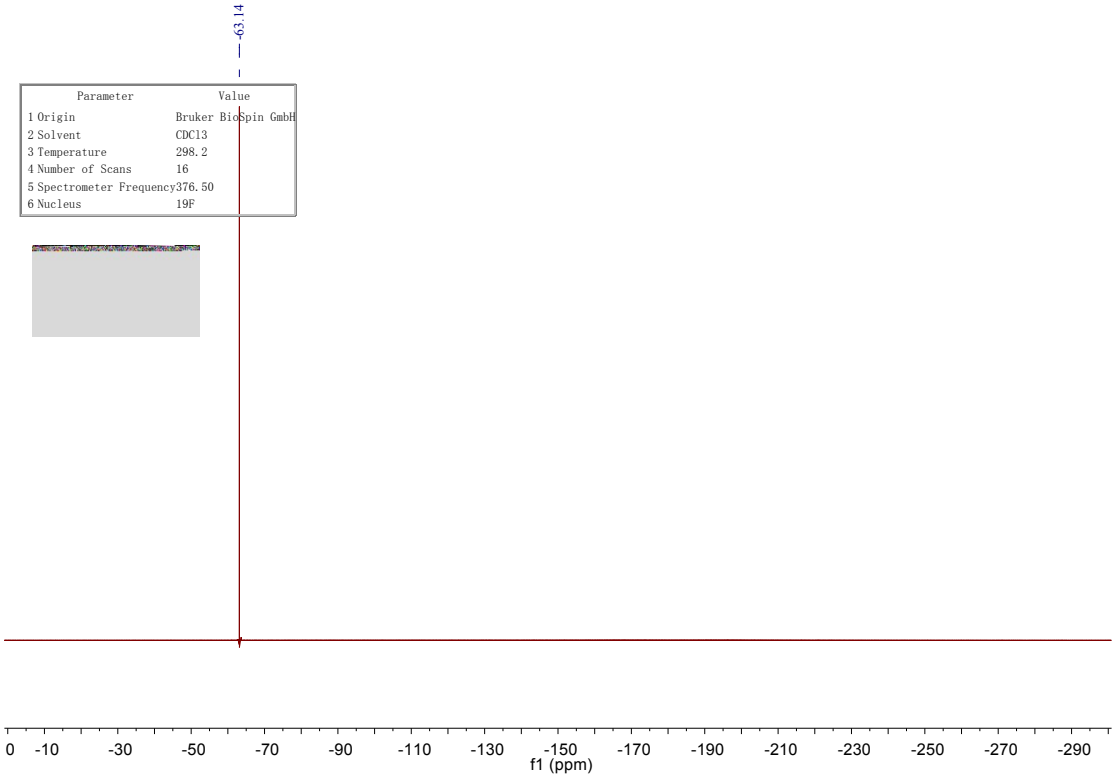

197.22
139.19
134.56
128.95
128.49
76.87
76.56
76.24
44.09
34.78
26.15
Parameter Value
1 Origin Bruker BioSpin GmbH
2 Solvent CDCl3
3 Temperature 298.2
4 Number of Scans 33
5 Spectrometer Frequency 100.61
6 Nucleus 13C
f1 (ppm)

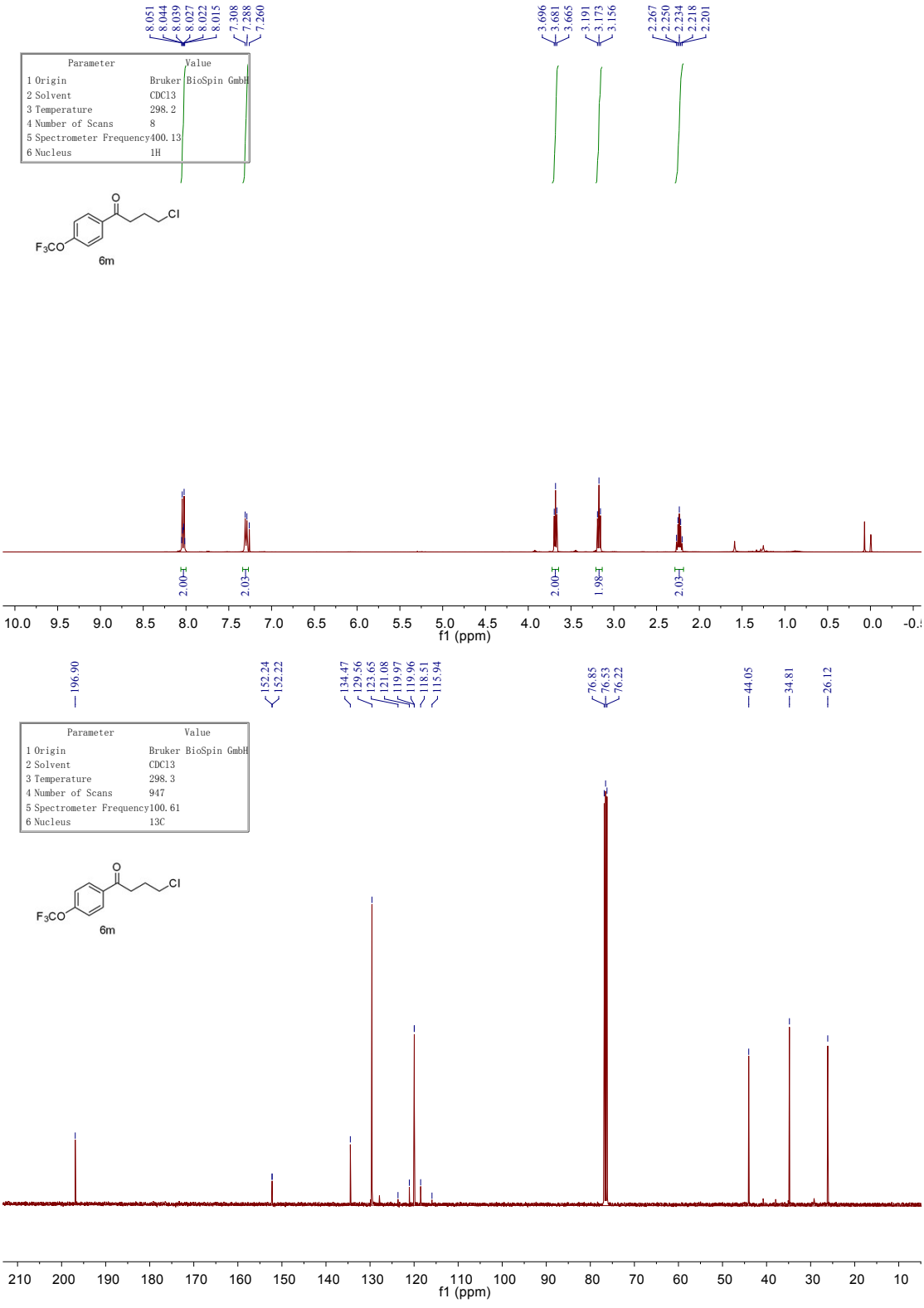

7.856
7.850
7.833
7.829
7.823
7.628
7.623
7.618
7.606
7.601
7.596
7.260
3.688
3.673
3.658
3.163
3.146
3.129
2.255
2.238
2.222
2.206
2.189
Parameter Value
1 Origin Bruker BioSpin GmbH
2 Solvent CDCl3
3 Temperature 298.1
4 Number of Scans 4
5 Spectrometer Frequency 400.13
6 Nucleus 1H
O
Cl
Br
6k
2.04
2.00
2.00
2.01
2.01
f1 (ppm)


197.91
135.43
132.18
129.48
128.34
77.35
77.04
76.72
44.40
35.15
26.72
Parameter Value
1 Origin Bruker BioSpin GmbH
2 Solvent CDCl3
3 Temperature 296.4
4 Number of Scans 120
5 Spectrometer Frequency 100.62
6 Nucleus 13C
f1 (ppm)


8.093
8.072
7.753
7.732
7.260
3.706
3.690
3.675
3.231
3.213
3.196
2.283
2.266
2.250
2.234
2.217
Parameter Value
1 Origin Bruker BioSpin GmbH
2 Solvent CDCl3
3 Temperature 298.1
4 Number of Scans 8
5 Spectrometer Frequency 400.13
6 Nucleus 1H
O
Cl
F3C
6l
2.00
2.01
1.98
1.99
2.01
f1 (ppm)

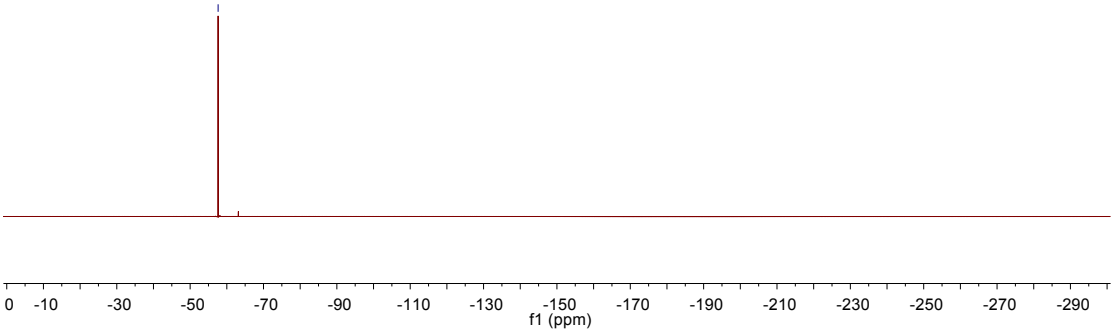

197.396
138.865
134.523
134.218
133.893
133.568
127.871
127.177
125.325
125.288
125.250
125.214
124.436
121.725
118.969
76.852
76.534
76.217
43.959
35.109
26.012
Parameter Value
1 Origin Bruker BioSpin GmbH
2 Solvent CDCl3
3 Temperature 298.3
4 Number of Scans 748
5 Spectrometer Frequency 100.61
6 Nucleus 13C
200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10
f1 (ppm)


-63.14
Parameter Value
1 Origin Bruker BioSpin GmbH
2 Solvent CDCl3
3 Temperature 298.2
4 Number of Scans 16
5 Spectrometer Frequency 376.50
6 Nucleus 19F
0 -10 -30 -50 -70 -90 -110 -130 -150 -170 -190 -210 -230 -250 -270 -290
f1 (ppm)


8.051
8.044
8.039
8.027
8.022
8.015
7.308
7.288
7.260
3.696
3.681
3.665
3.191
3.173
3.156
2.267
2.250
2.234
2.218
2.201
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
Cl
F3CO
6m
2.00
2.03
2.00
1.98
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
f1 (ppm)
196.90
152.24
152.22
134.47
129.56
123.65
121.08
119.97
119.96
118.51
115.94
76.85
76.53
76.22
44.05
34.81
26.12
Parameter Value
1 Origin Bruker BioSpin GmbH
2 Solvent CDCl3
3 Temperature 298.3
4 Number of Scans 947
5 Spectrometer Frequency 100.61
6 Nucleus 13C
O
Cl
F3CO
6m
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10
f1 (ppm)

-57.63

Parameter	Value
1 Origin	Bruker BioSpin GmbH
2 Solvent	CDCl3
3 Temperature	298.2
4 Number of Scans	16
5 Spectrometer Frequency	376.44
6 Nucleus	19F



7.357 7.354 7.350 7.341 7.337 7.333 7.321 7.318 7.292 7.289 7.285 7.276 7.271 7.264 7.255 7.218 7.214 7.197

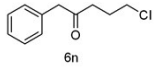
3.703 3.539 3.523 3.513 3.508

2.665 2.648 2.631

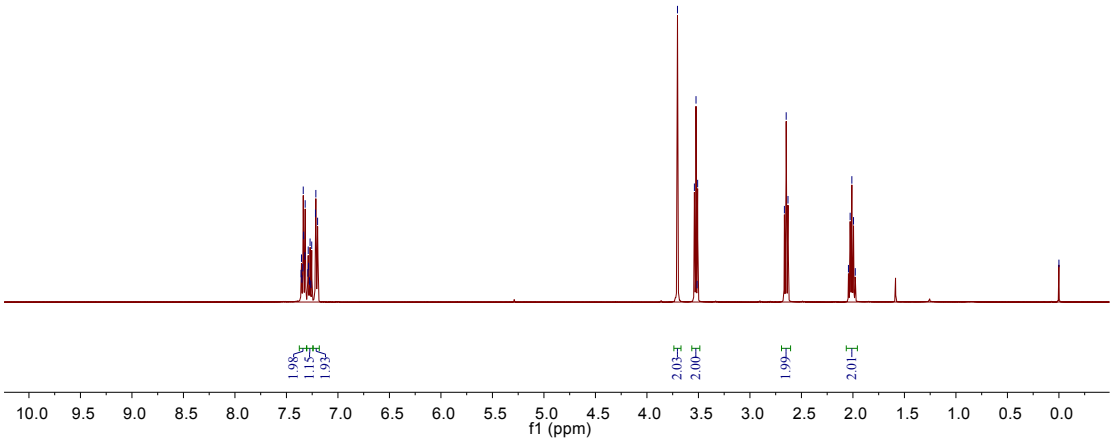
2.043 2.027 2.010 1.994 1.977

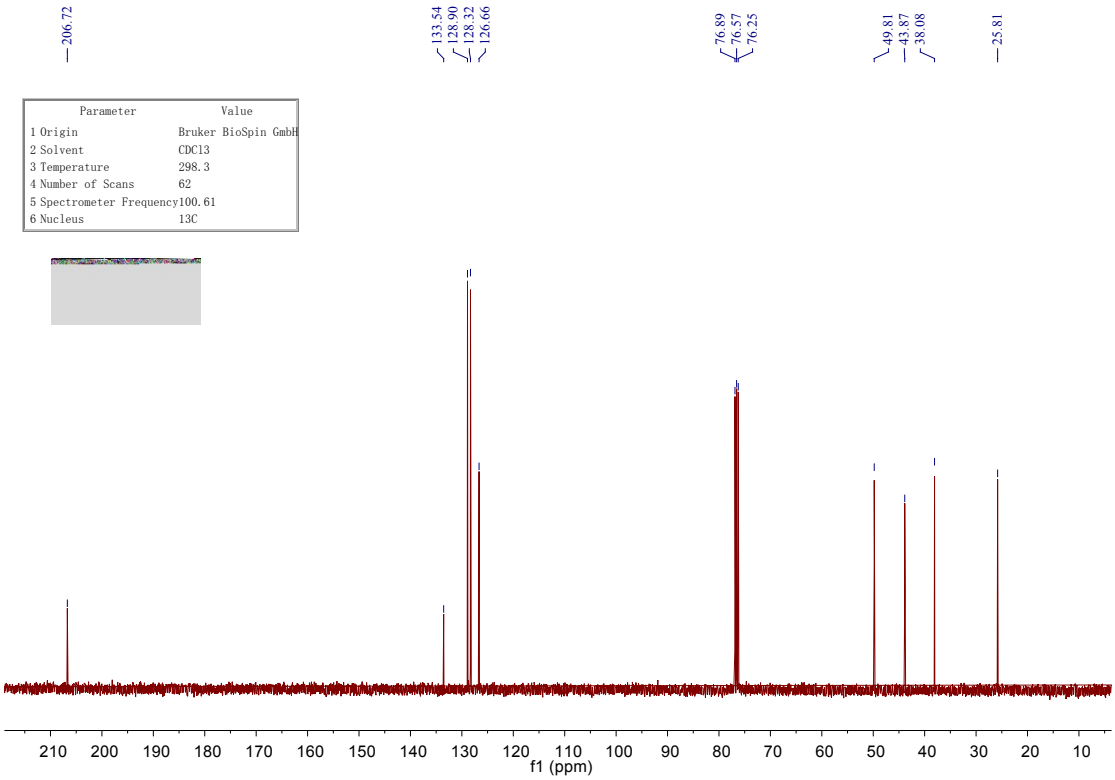
-0.000

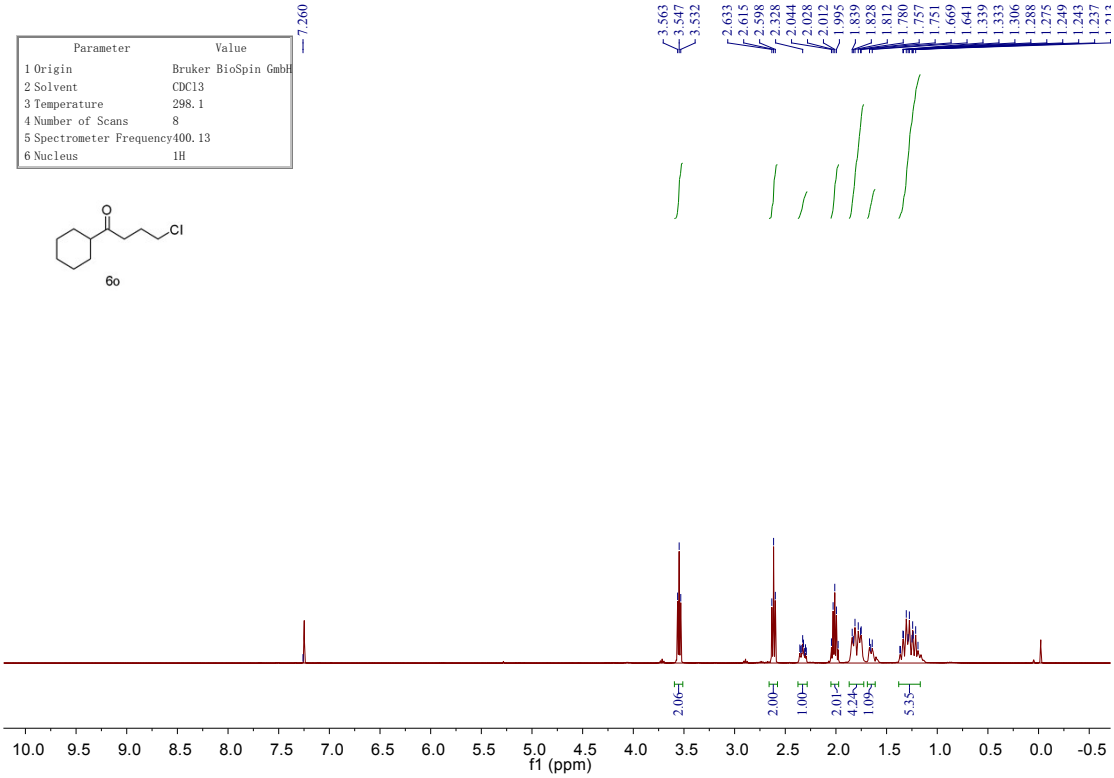
Parameter	Value
1 Origin	Bruker BioSpin GmbH
2 Solvent	CDCl3
3 Temperature	298.2
4 Number of Scans	8
5 Spectrometer Frequency	400.13
6 Nucleus	1H

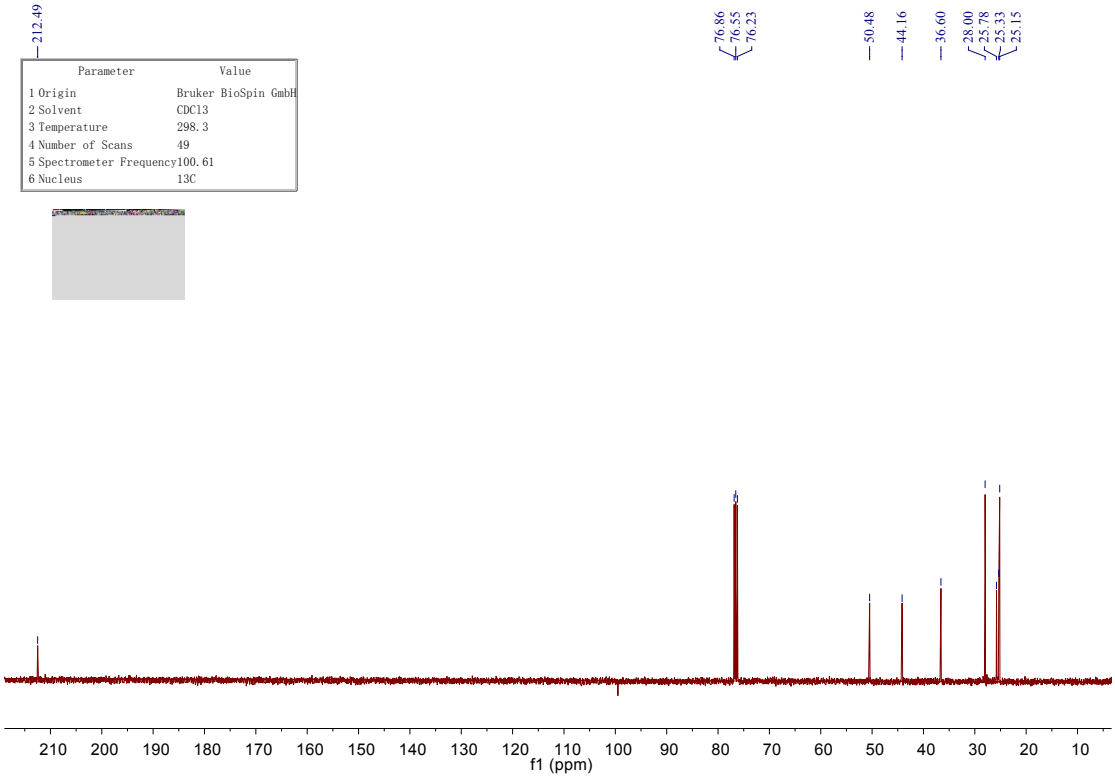


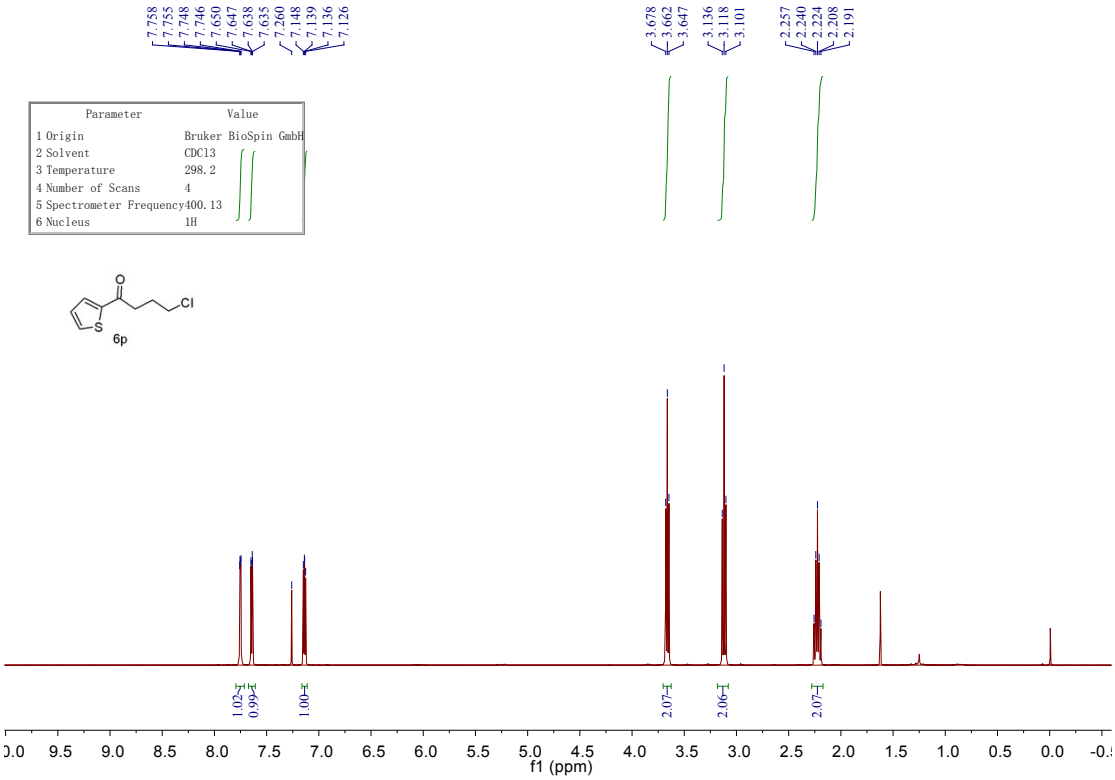
6n

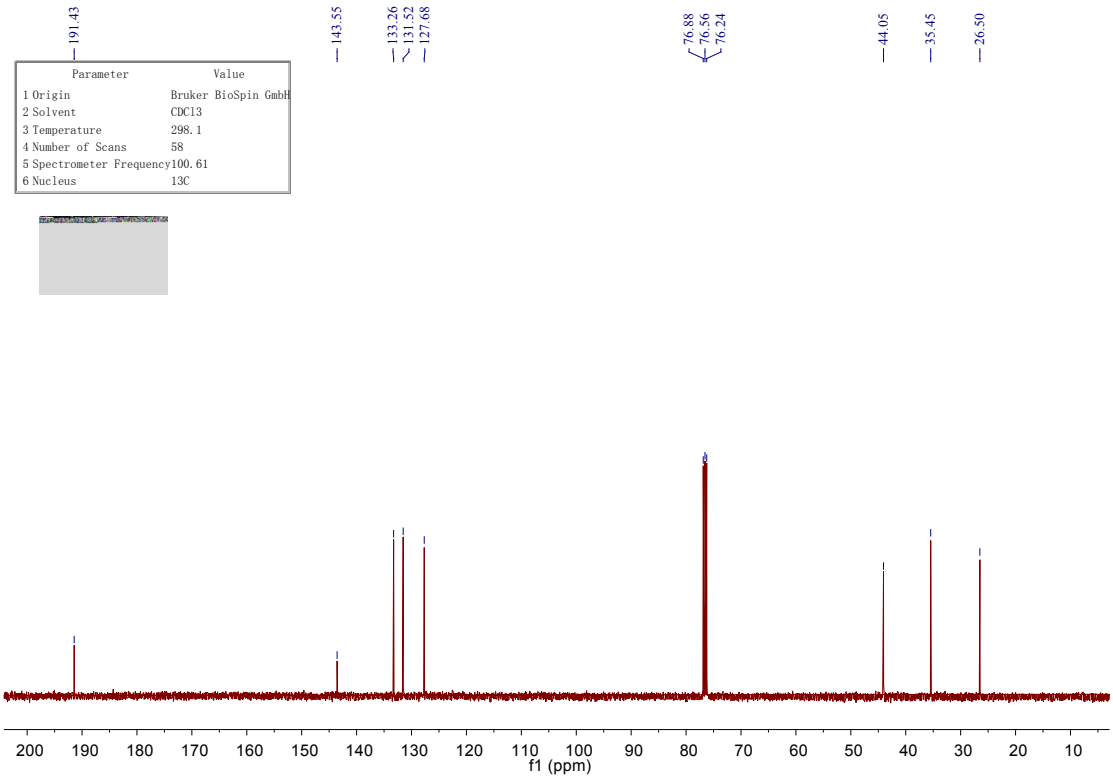


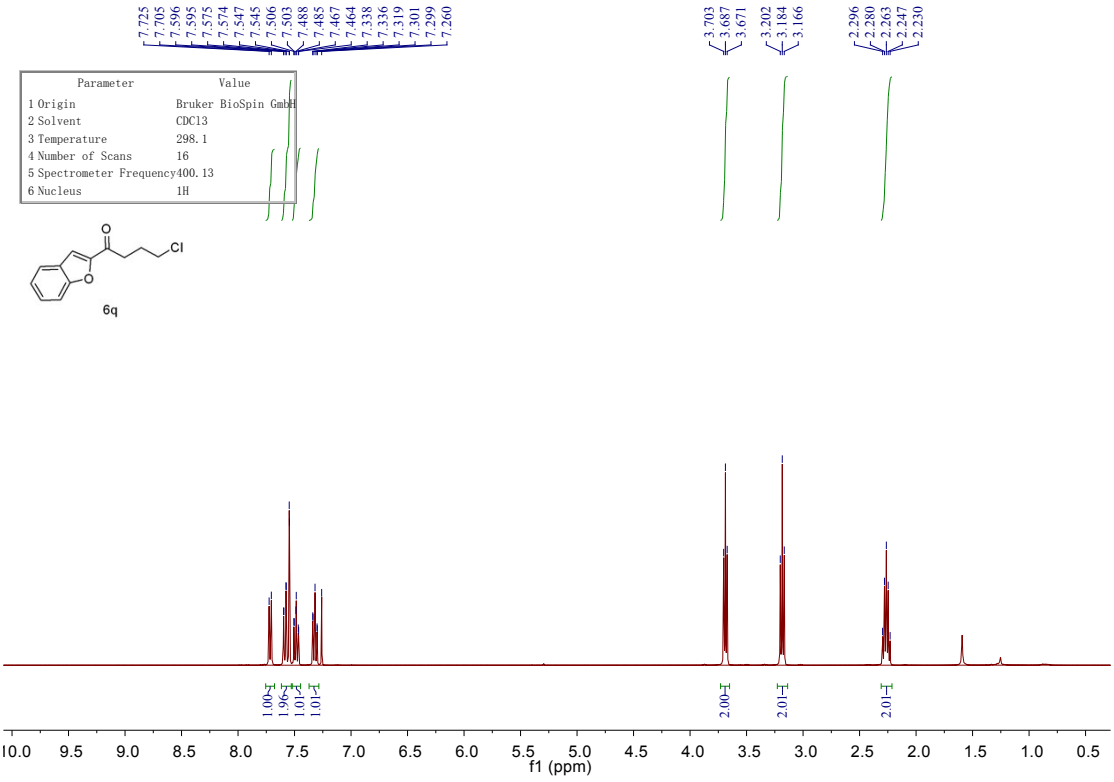

206.72
133.54
128.90
128.32
126.66
76.89
76.57
76.25
49.81
43.87
38.08
25.81
Parameter Value
1 Origin Bruker BioSpin GmbH
2 Solvent CDCl3
3 Temperature 298.3
4 Number of Scans 62
5 Spectrometer Frequency 100.61
6 Nucleus 13C
f1 (ppm)

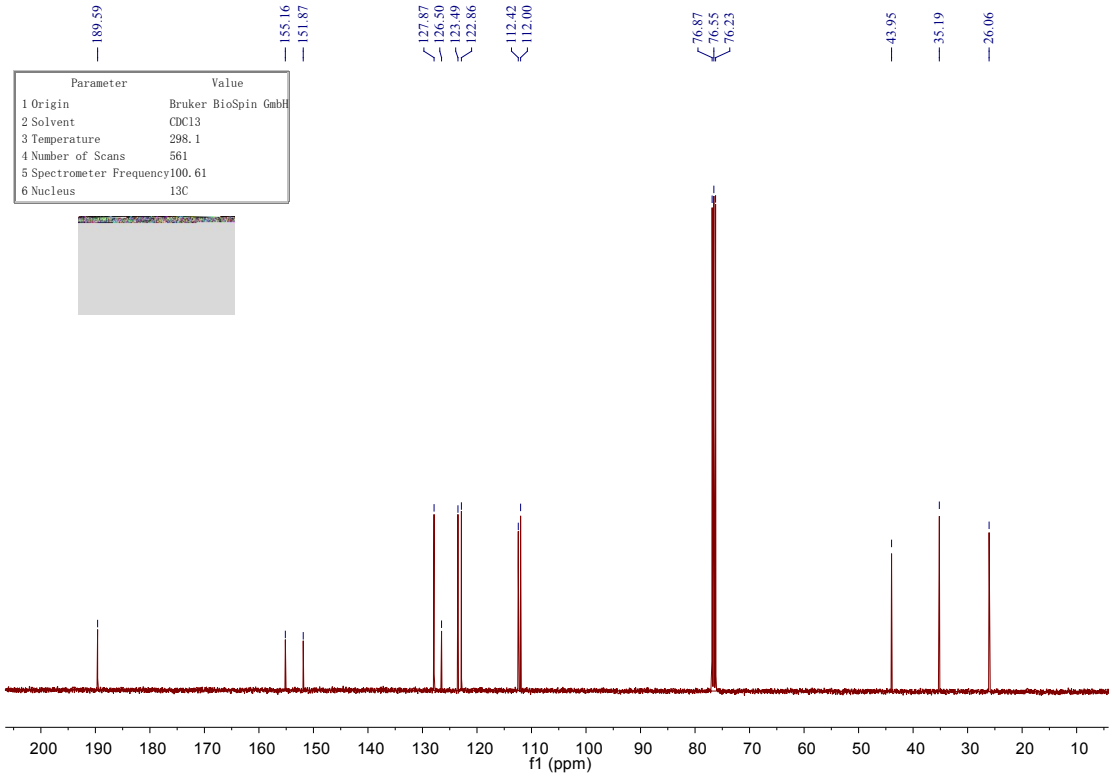

7.260
3.563
3.547
3.532
2.633
2.615
2.598
2.328
2.044
2.028
2.012
1.995
1.839
1.828
1.812
1.780
1.757
1.751
1.669
1.641
1.339
1.333
1.306
1.288
1.275
1.249
1.243
1.237
Parameter Value
1 Origin Bruker BioSpin GmbH
2 Solvent CDCl3
3 Temperature 298.1
4 Number of Scans 8
5 Spectrometer Frequency 400.13
6 Nucleus 1H
O
Cl
6o
2.06
2.00
1.00
2.01
4.24
1.09
5.35
f1 (ppm)


212.49
76.86
76.55
76.23
50.48
44.16
36.60
28.00
25.78
25.33
25.15
Parameter Value
1 Origin Bruker BioSpin GmbH
2 Solvent CDCl3
3 Temperature 298.3
4 Number of Scans 49
5 Spectrometer Frequency 100.61
6 Nucleus 13C
f1 (ppm)

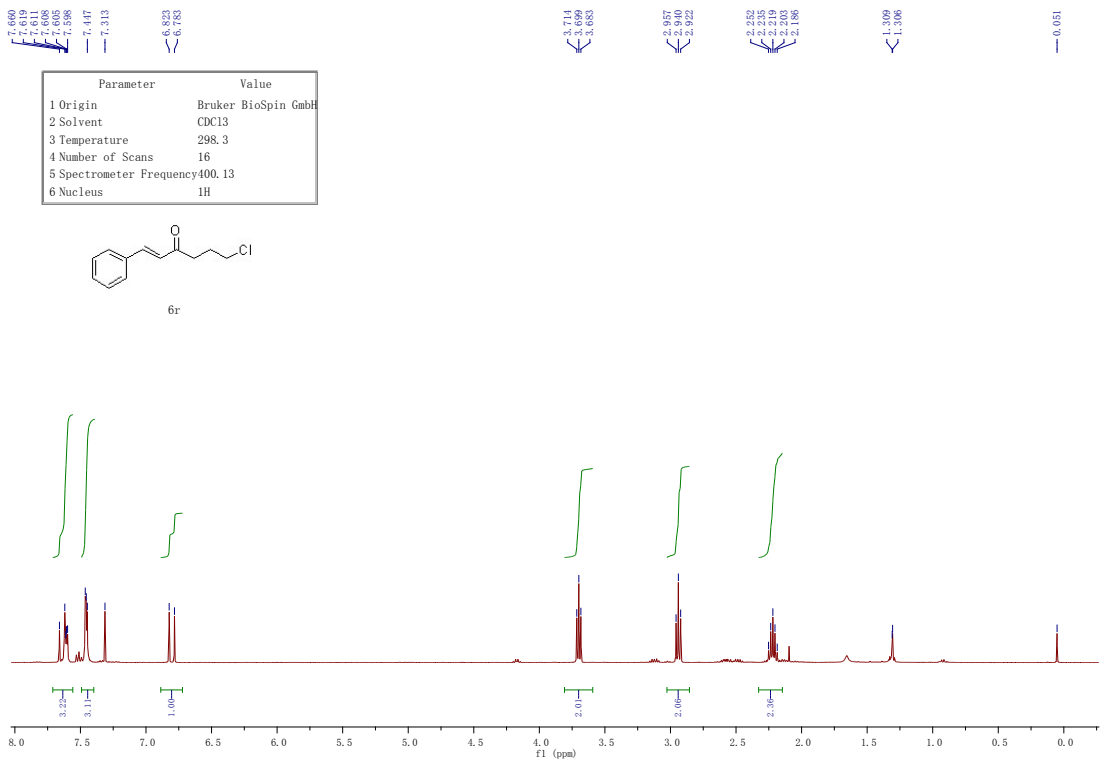

7.758
7.755
7.748
7.746
7.650
7.647
7.638
7.635
7.260
7.148
7.139
7.136
7.126
3.678
3.662
3.647
3.136
3.118
3.101
2.257
2.240
2.224
2.208
2.191
Parameter Value
1 Origin Bruker BioSpin GmbH
2 Solvent CDCl3
3 Temperature 298.2
4 Number of Scans 4
5 Spectrometer Frequency 400.13
6 Nucleus 1H
O
Cl
S
6p
1.02
0.99
1.00
2.07
2.06
2.07
f1 (ppm)


191.43
143.55
133.26
131.52
127.68
76.88
76.56
76.24
44.05
35.45
26.50
Parameter Value
1 Origin Bruker BioSpin GmbH
2 Solvent CDCl3
3 Temperature 298.1
4 Number of Scans 58
5 Spectrometer Frequency 100.61
6 Nucleus 13C
f1 (ppm)


7.725
7.705
7.596
7.595
7.575
7.574
7.547
7.545
7.506
7.503
7.488
7.485
7.467
7.464
7.338
7.336
7.319
7.301
7.299
7.260
3.703
3.687
3.671
3.202
3.184
3.166
2.296
2.280
2.263
2.247
2.230
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
Cl
O
6q
1.00
1.96
1.01
1.01
2.00
2.01
2.01
f1 (ppm)



Parameter	Value
1 Origin	Bruker BioSpin GmbH
2 Solvent	CDCl3
3 Temperature	298.1
4 Number of Scans	561
5 Spectrometer Frequency	100.61
6 Nucleus	13C

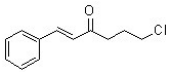


Parameter	Value
1 Origin	Bruker BioSpin GmbH
2 Solvent	CDCl3
3 Temperature	298.3
4 Number of Scans	16
5 Spectrometer Frequency	400.13
6 Nucleus	1H

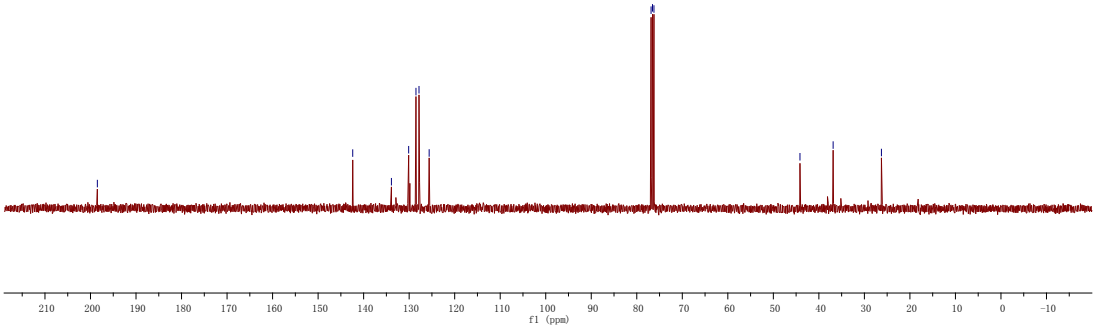
6r

198.493
142.396
133.897
130.109
128.504
127.837
126.606
76.861
76.543
76.225
44.152
36.866
26.258

Parameter	Value
1 Origin	Bruker BioSpin GmbH
2 Solvent	CDCl3
3 Temperature	298.8
4 Number of Scans	50
5 Spectrometer Frequency	100.61
6 Nucleus	13C

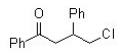


6r

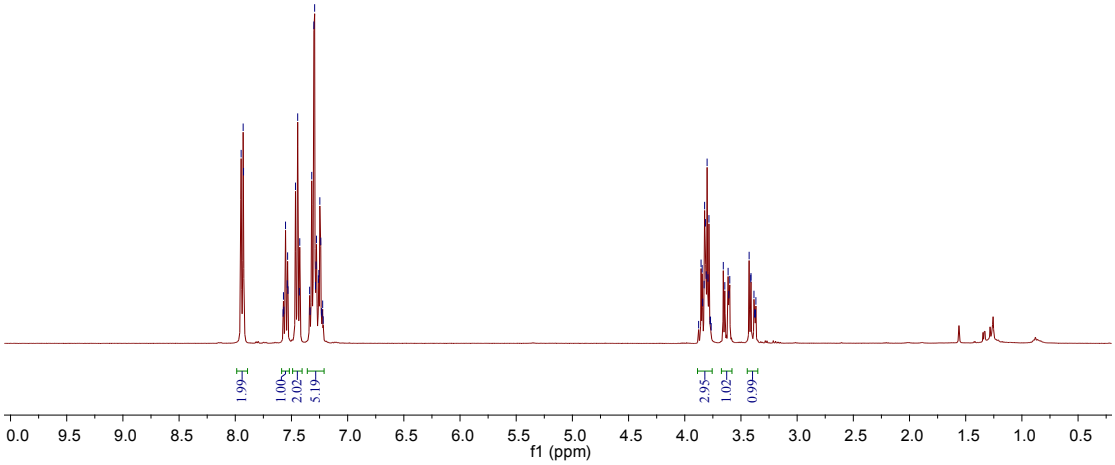


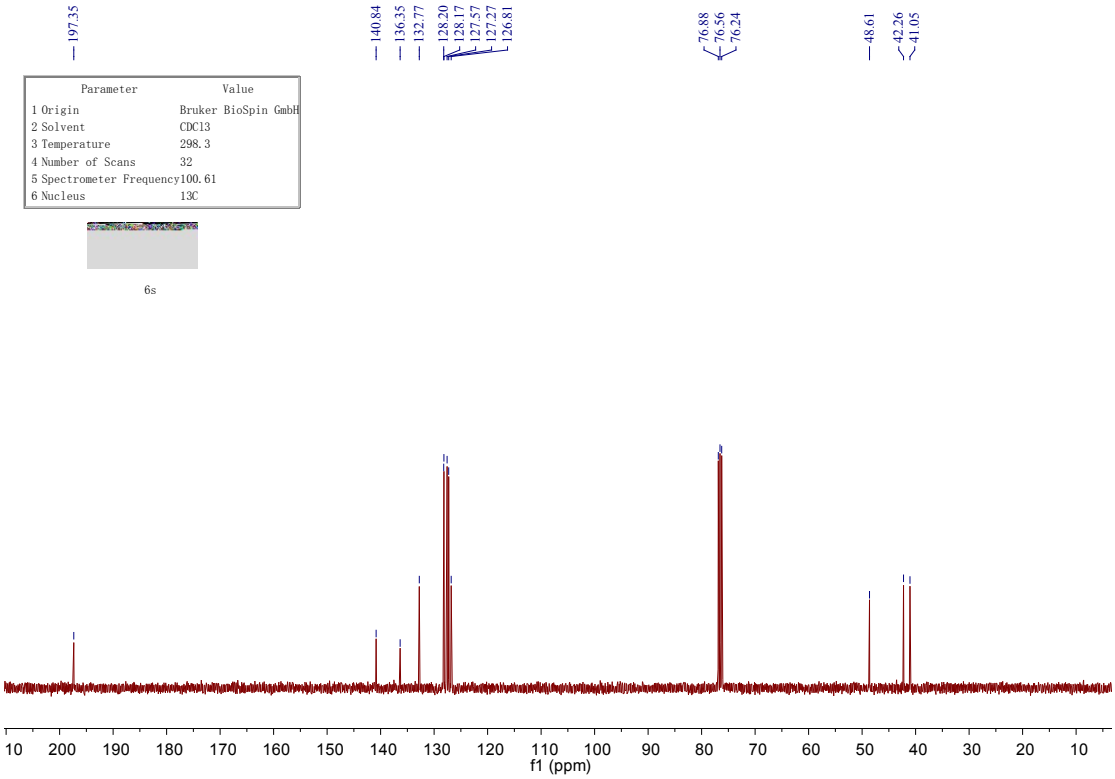
7.948
7.930
7.446
7.334
7.320
7.301
7.294
7.286
7.281
7.278
7.260
7.256
7.247
7.239
7.232
7.228
7.222
7.218
3.823
3.816
3.809
3.801
3.794
3.785
3.774
3.771
3.765
3.657
3.644
3.614
3.608
3.600
3.427
3.413
3.411
3.384
3.378
3.375
3.370
3.367

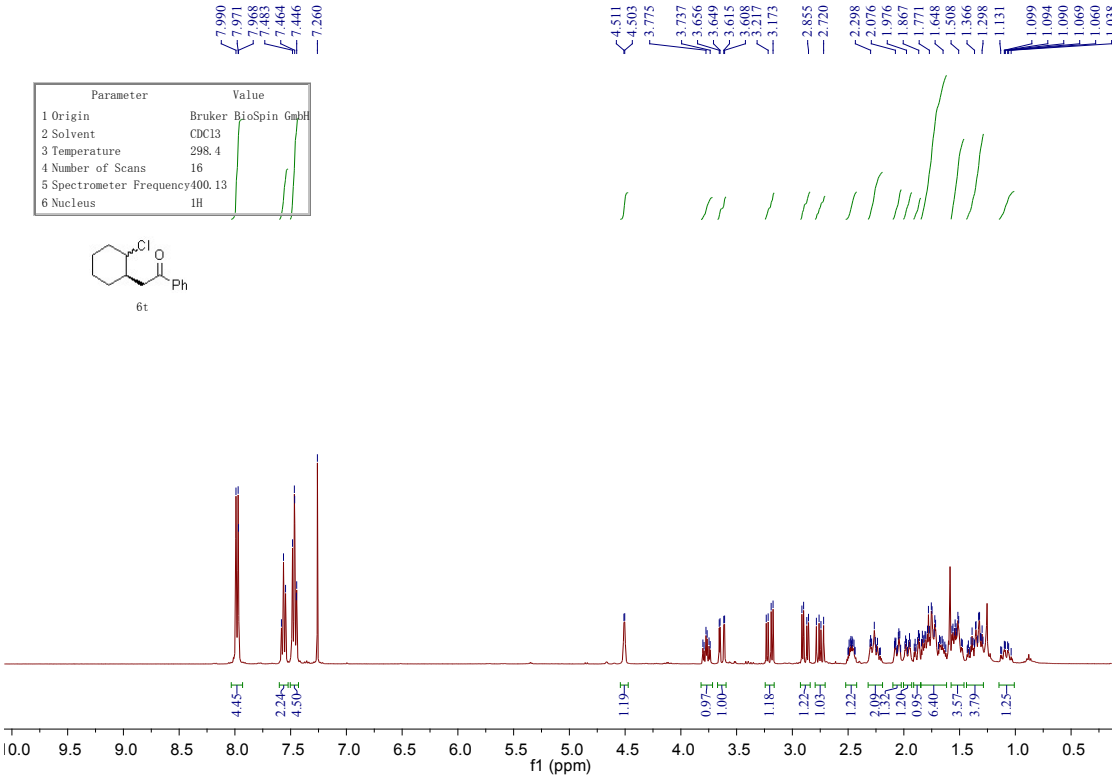
Parameter	Value
1 Origin	Bruker BioSpin GmbH
2 Solvent	CDCl3
3 Temperature	298.8
4 Number of Scans	4
5 Spectrometer Frequency	400.13
6 Nucleus	1H

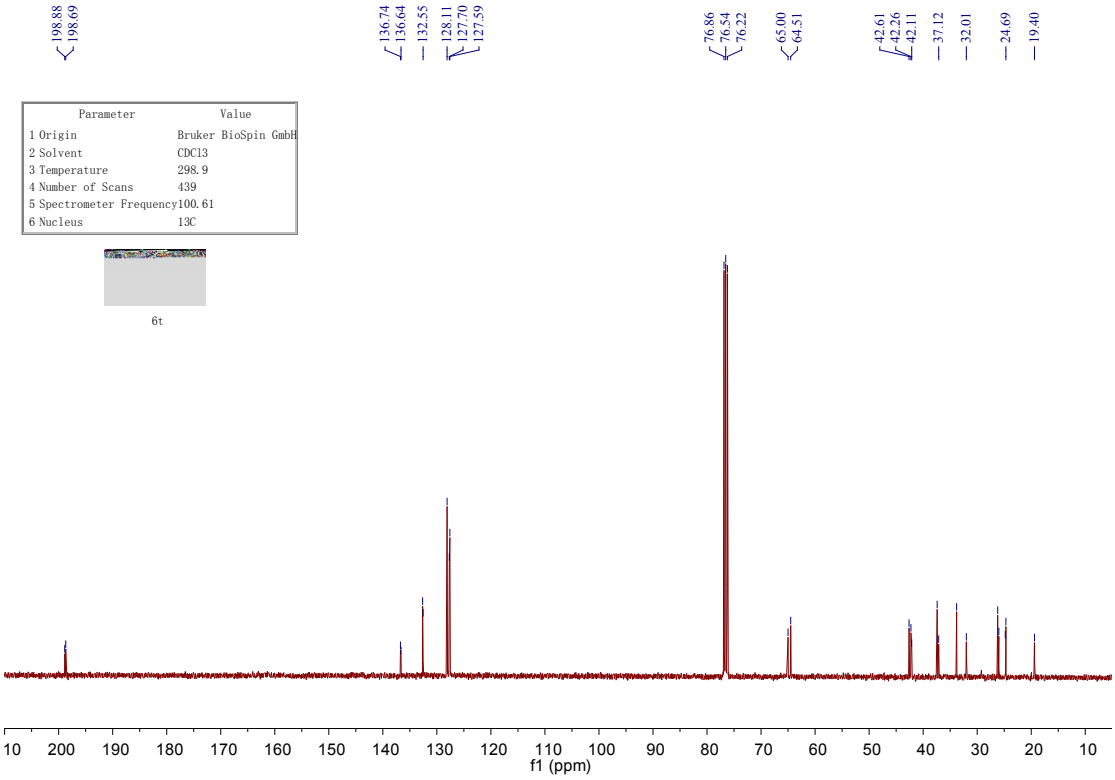


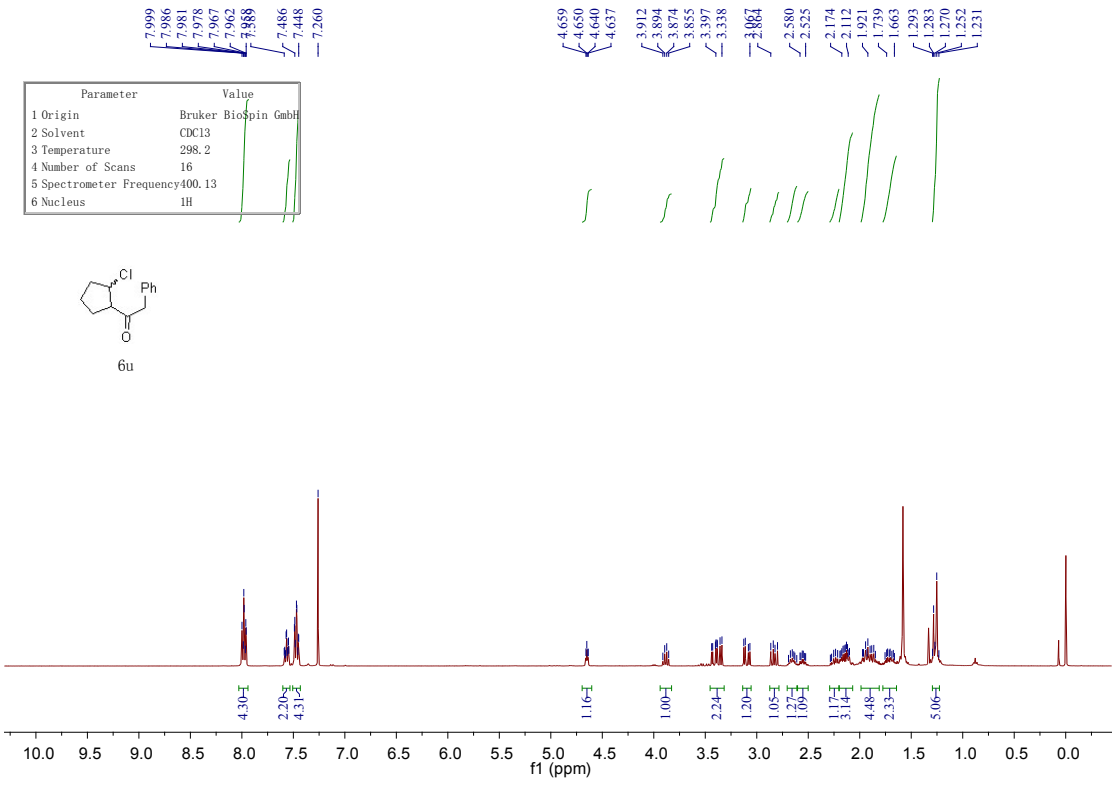
6s

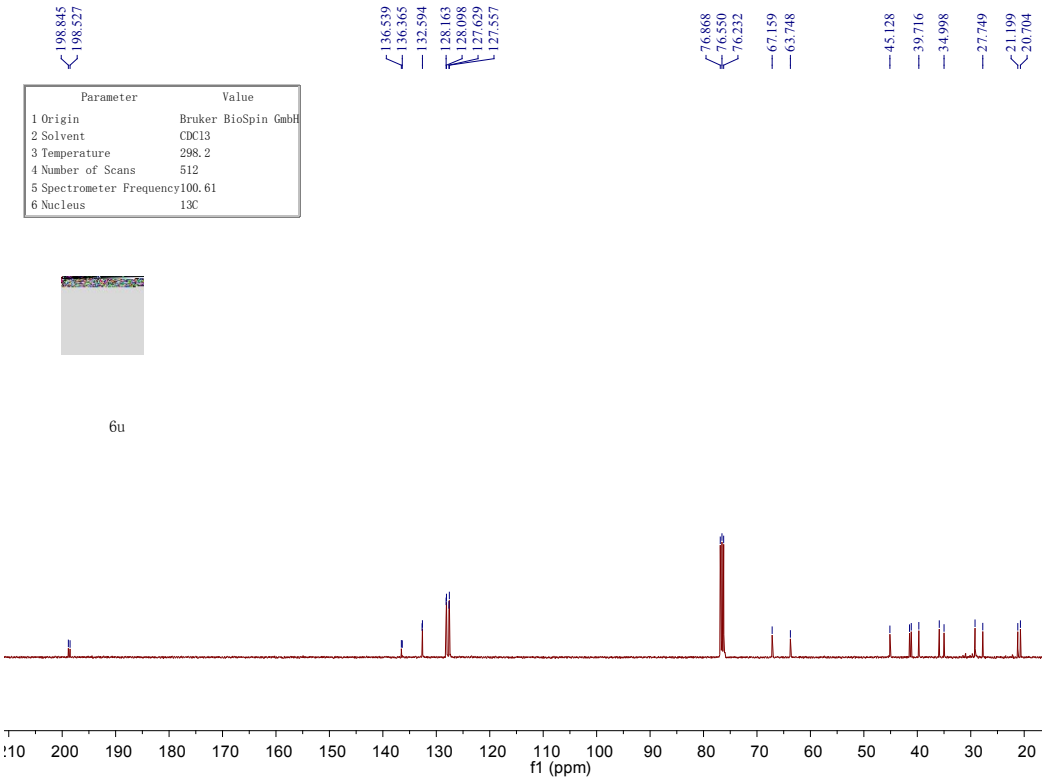



197.35
140.84
136.35
132.77
128.20
128.17
127.57
127.27
126.81
76.88
76.56
76.24
48.61
42.26
41.05
Parameter Value
1 Origin Bruker BioSpin GmbH
2 Solvent CDCl3
3 Temperature 298.3
4 Number of Scans 32
5 Spectrometer Frequency 100.61
6 Nucleus 13C
6s
f1 (ppm)

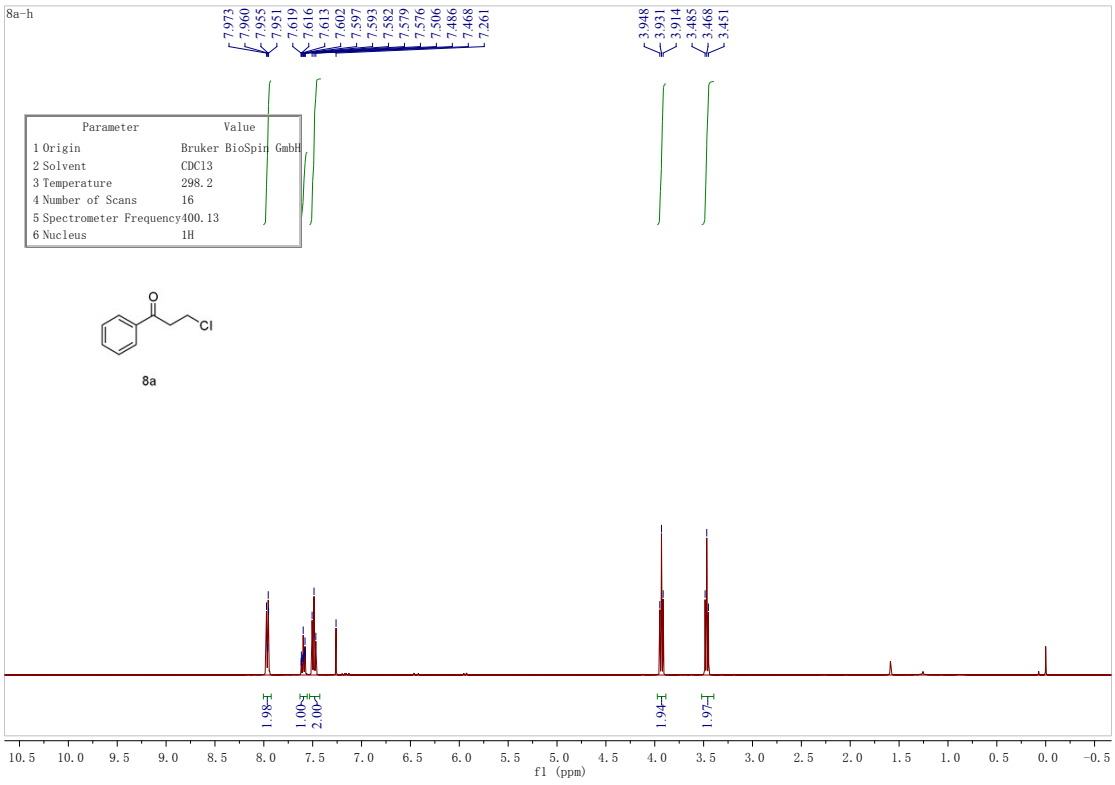

7.990
7.971
7.968
7.483
7.464
7.446
7.260
4.511
4.503
3.775
3.737
3.656
3.649
3.615
3.608
3.217
3.173
2.855
2.720
2.298
2.076
1.976
1.867
1.771
1.648
1.508
1.366
1.298
1.131
1.099
1.094
1.090
1.069
1.060
Parameter Value
1 Origin Bruker BioSpin GmbH
2 Solvent CDCl3
3 Temperature 298.4
4 Number of Scans 16
5 Spectrometer Frequency 400.13
6 Nucleus 1H
Cl
O
Ph
6t
4.45
2.24
4.50
1.19
0.97
1.00
1.18
1.22
1.03
1.22
2.02
1.32
1.20
0.95
6.40
3.57
3.79
1.25
f1 (ppm)


198.88
198.69
136.74
136.64
132.55
128.11
127.70
127.59
76.86
76.54
76.22
65.00
64.51
42.61
42.26
42.11
37.12
32.01
24.69
19.40
Parameter Value
1 Origin Bruker BioSpin GmbH
2 Solvent CDCl3
3 Temperature 298.9
4 Number of Scans 439
5 Spectrometer Frequency 100.61
6 Nucleus 13C
6t
f1 (ppm)


7.999
7.986
7.981
7.978
7.967
7.962
7.486
7.448
7.260
4.659
4.650
4.640
4.637
3.912
3.894
3.874
3.855
3.397
3.338
2.580
2.525
2.174
2.112
1.921
1.739
1.663
1.293
1.283
1.270
1.252
1.231
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
Cl
Ph
O
6u
4.30
2.20
4.31
1.16
1.00
2.24
1.20
1.05
1.27
1.09
1.17
3.14
4.48
2.33
5.06
f1 (ppm)


198.845
198.527
136.539
136.365
132.594
128.163
128.098
127.629
127.557
76.868
76.550
76.232
67.159
63.748
45.128
39.716
34.998
27.749
21.199
20.704
Parameter Value
1 Origin Bruker BioSpin GmbH
2 Solvent CDCl3
3 Temperature 298.2
4 Number of Scans 512
5 Spectrometer Frequency 100.61
6 Nucleus 13C
f1 (ppm)

6u

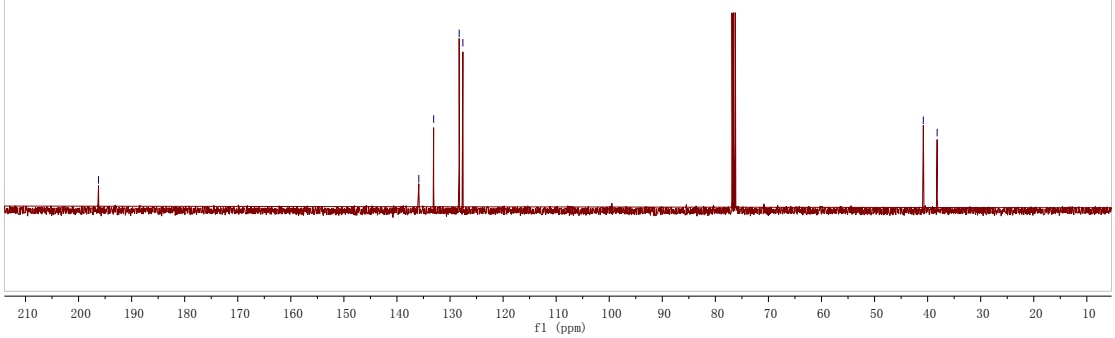

8a-h
7.973
7.960
7.955
7.951
7.619
7.616
7.613
7.602
7.597
7.593
7.582
7.579
7.576
7.506
7.486
7.468
7.261
3.948
3.931
3.914
3.485
3.468
3.451
Parameter Value
1 Origin Bruker BioSpin GmbH
2 Solvent CDCl3
3 Temperature 298.2
4 Number of Scans 16
5 Spectrometer Frequency 400.13
6 Nucleus 1H
O
Cl
1.98
1.00
2.00
1.94
1.97
f1 (ppm)

8a

8a-c

196.2
135.9
133.1
128.3
127.6
40.8
38.2

Parameter	Value
1 Origin	Bruker BioSpin GmbH
2 Solvent	CDCl3
3 Temperature	298.1
4 Number of Scans	55
5 Spectrometer Frequency	100.61
6 Nucleus	13C



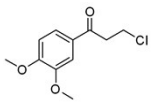
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10

f1 (ppm)

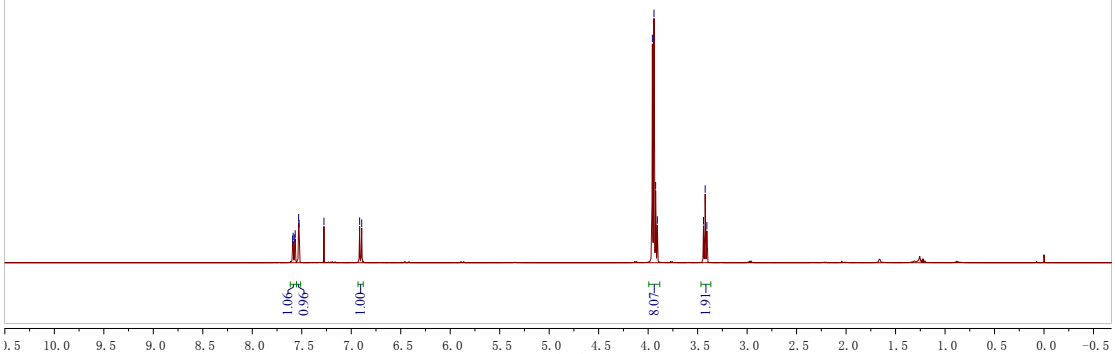
8b-h

7.592
7.587
7.571
7.566
7.532
7.527
7.276
6.915
6.894
3.957
3.941
3.924
3.907
3.441
3.424
3.407

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



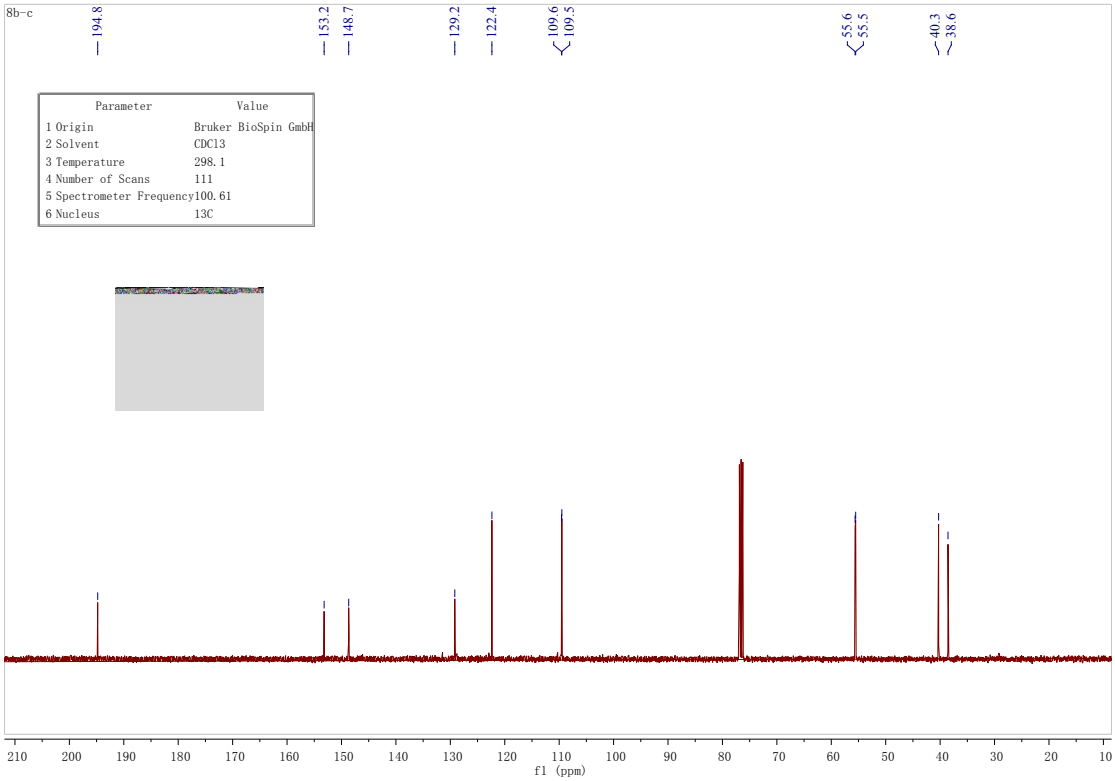
8b

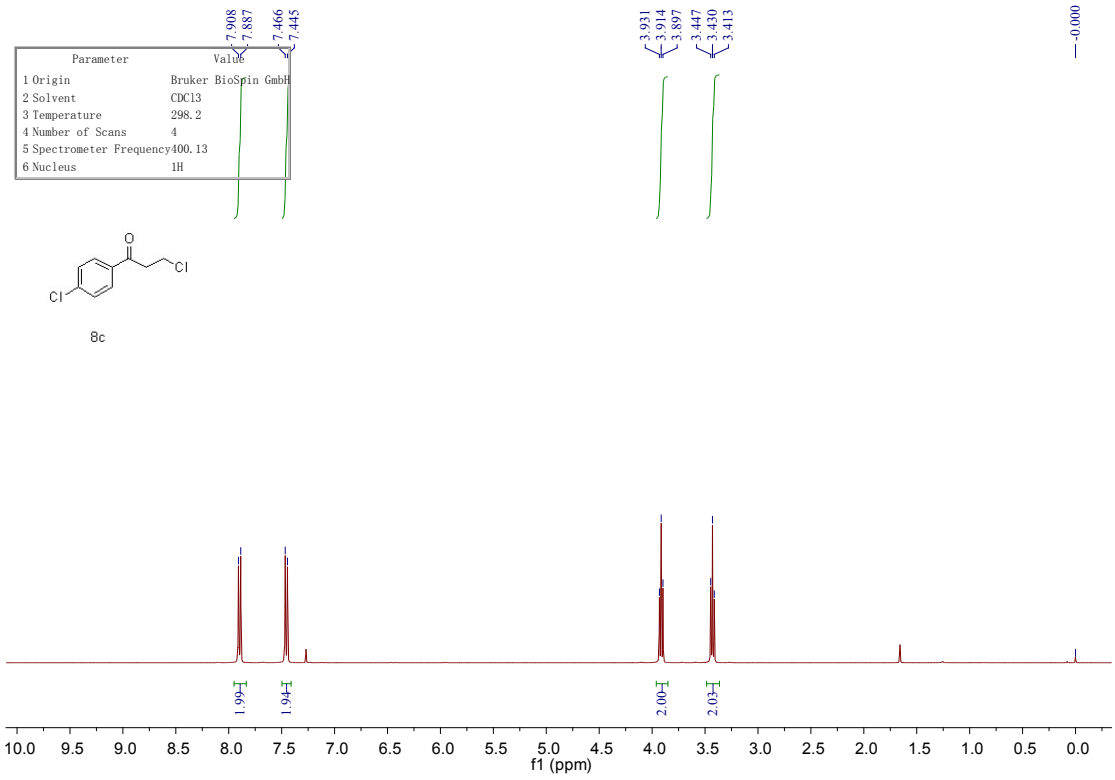


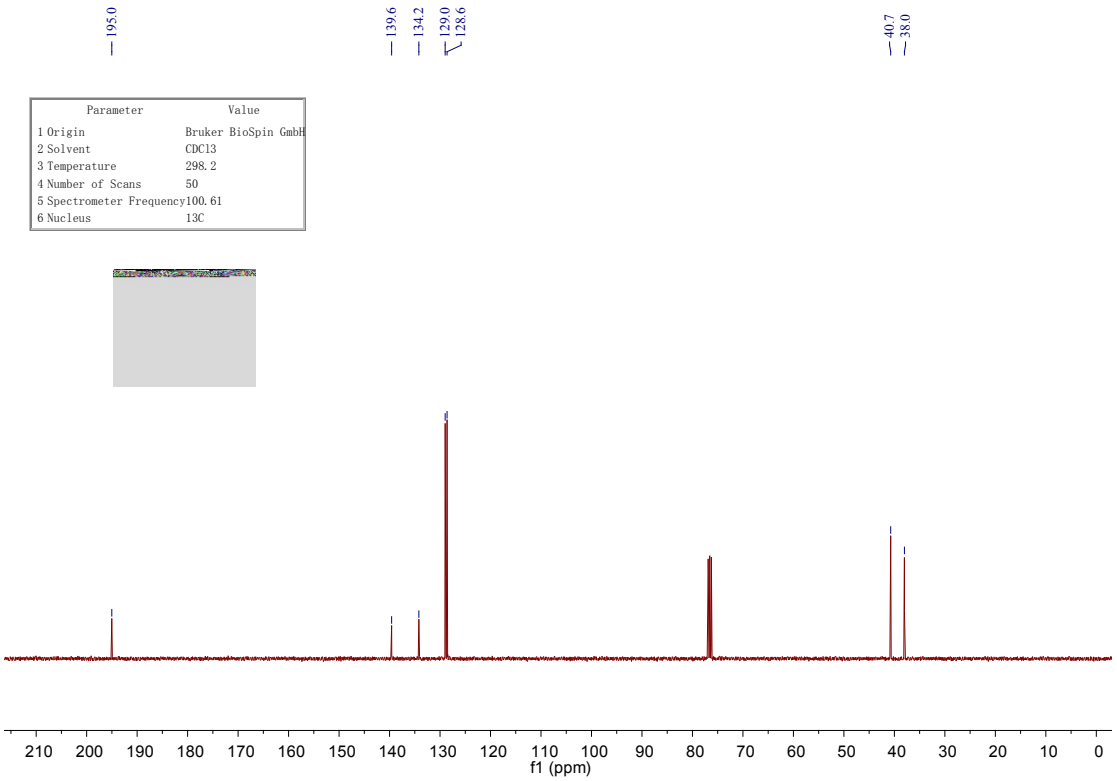
1.06
0.96
1.00
8.07
1.91

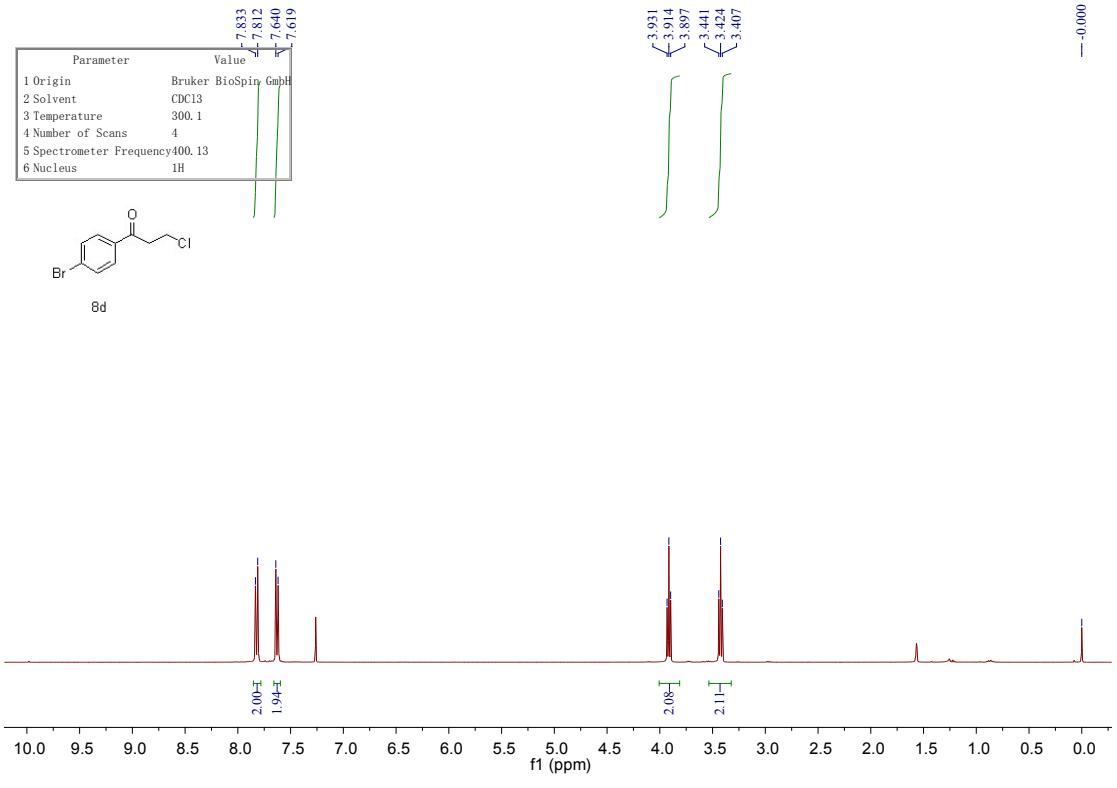
10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5

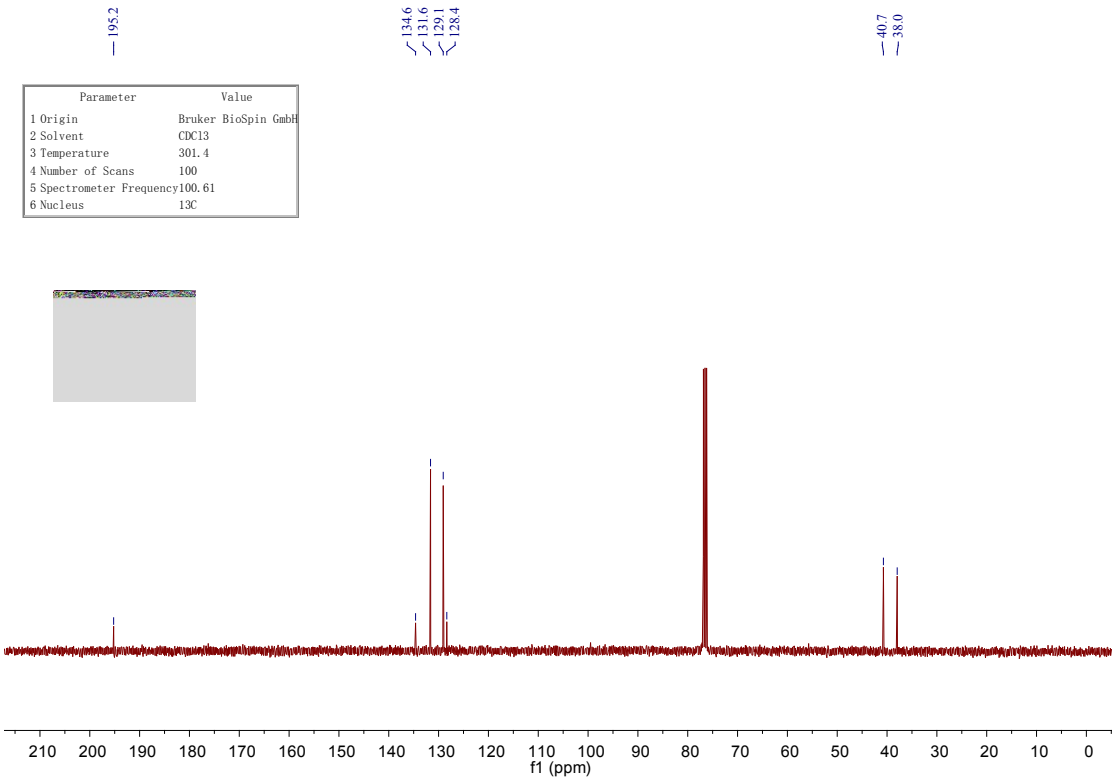
f1 (ppm)

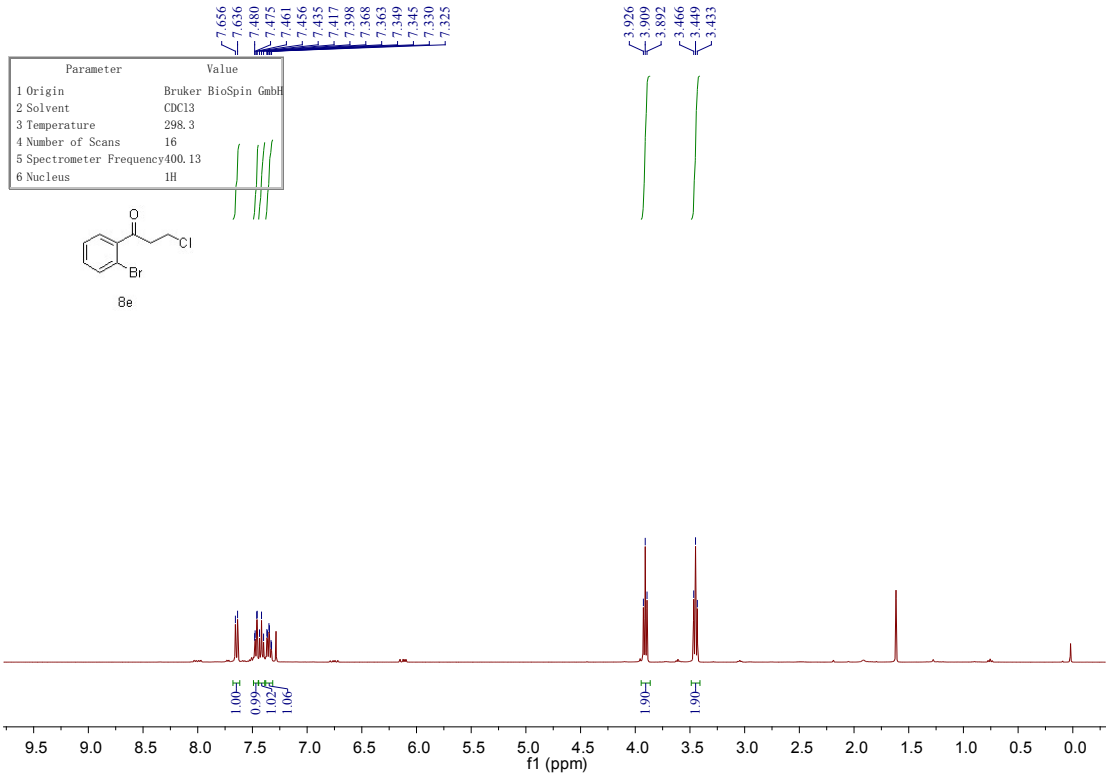

8b-c
194.8
153.2
148.7
129.2
122.4
109.6
109.5
55.6
55.5
40.3
38.6
Parameter Value
1 Origin Bruker BioSpin GmbH
2 Solvent CDCl3
3 Temperature 298.1
4 Number of Scans 111
5 Spectrometer Frequency 100.61
6 Nucleus 13C
f1 (ppm)

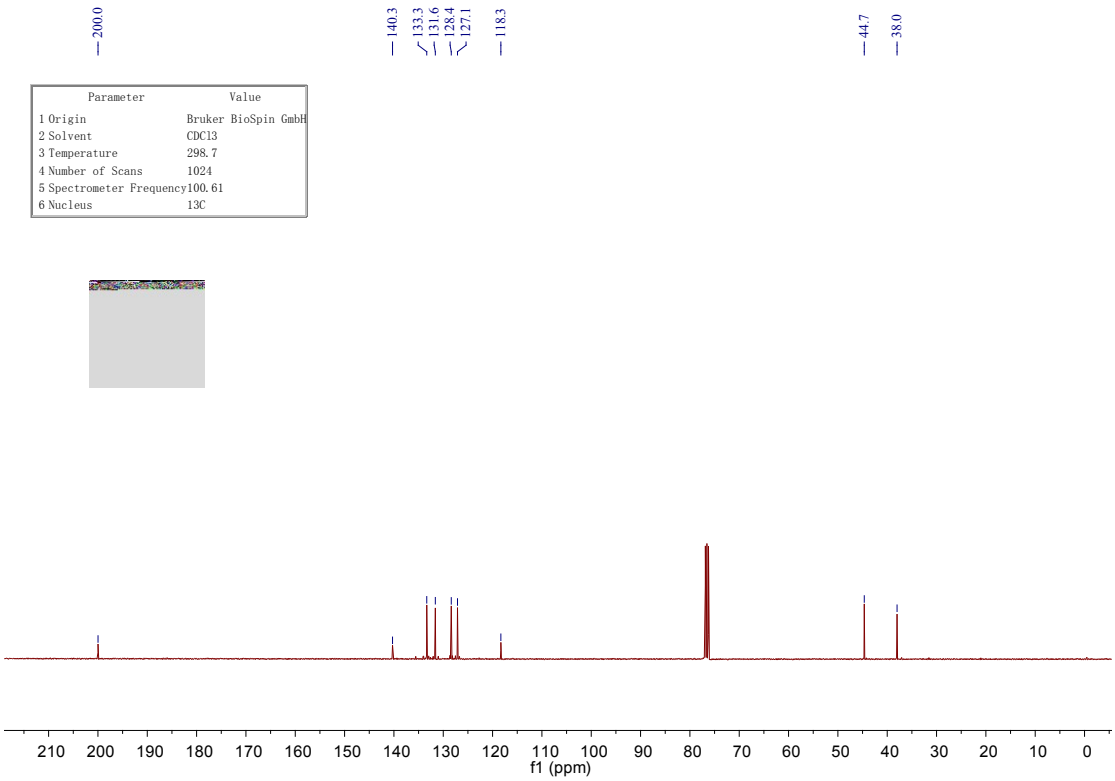

7.908
7.887
7.466
7.445
3.931
3.914
3.897
3.447
3.430
3.413
-0.000
Parameter Value
1 Origin Bruker BioSpin GmbH
2 Solvent CDCl3
3 Temperature 298.2
4 Number of Scans 4
5 Spectrometer Frequency 400.13
6 Nucleus 1H
O
Cl
Cl
8c
1.99
1.94
2.00
2.03
f1 (ppm)

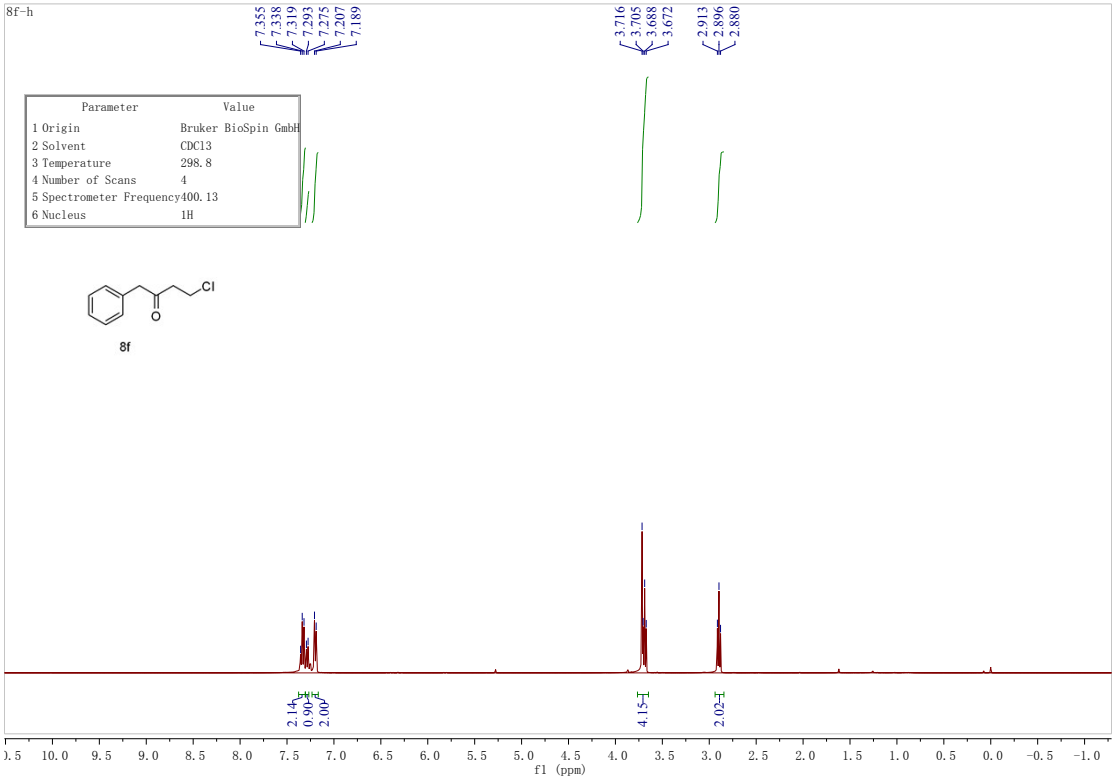

195.0
139.6
134.2
129.0
128.6
40.7
38.0
Parameter Value
1 Origin Bruker BioSpin GmbH
2 Solvent CDCl3
3 Temperature 298.2
4 Number of Scans 50
5 Spectrometer Frequency 100.61
6 Nucleus 13C
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)

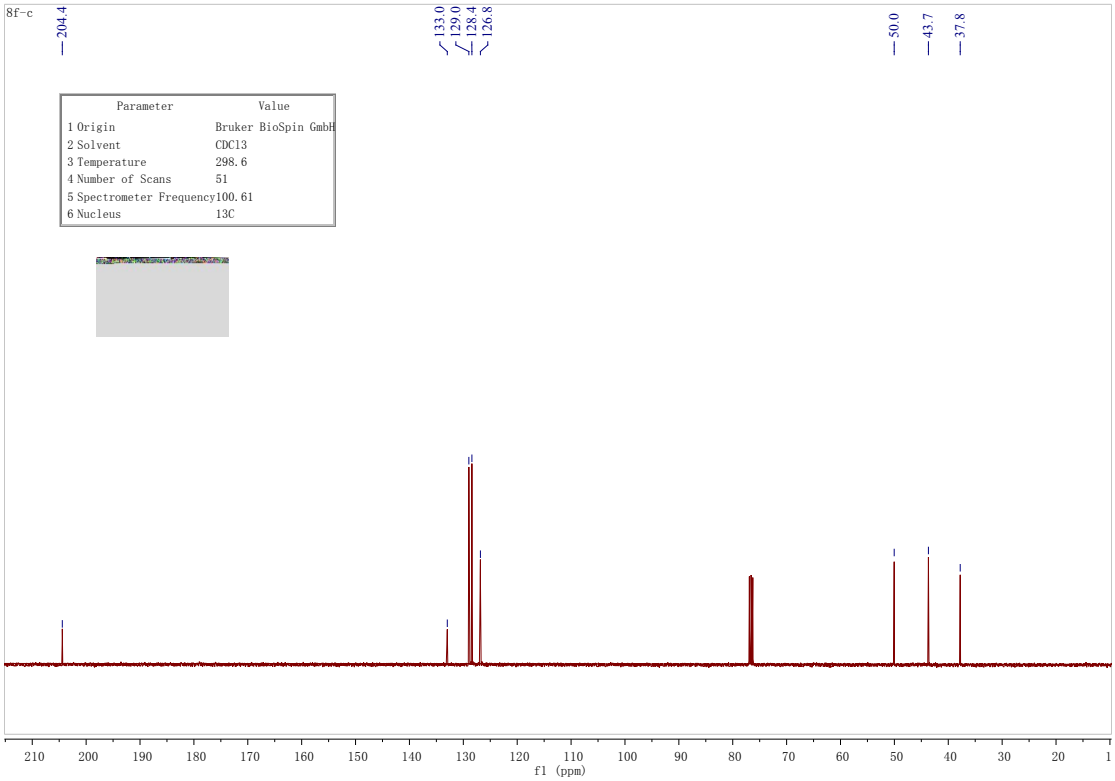

7.833
7.812
7.640
7.619
3.931
3.914
3.897
3.441
3.424
3.407
-0.000
Parameter Value
1 Origin Bruker BioSpin GmbH
2 Solvent CDCl3
3 Temperature 300.1
4 Number of Scans 4
5 Spectrometer Frequency 400.13
6 Nucleus 1H
O
Cl
Br
8d
2.00
1.94
2.08
2.11
10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)

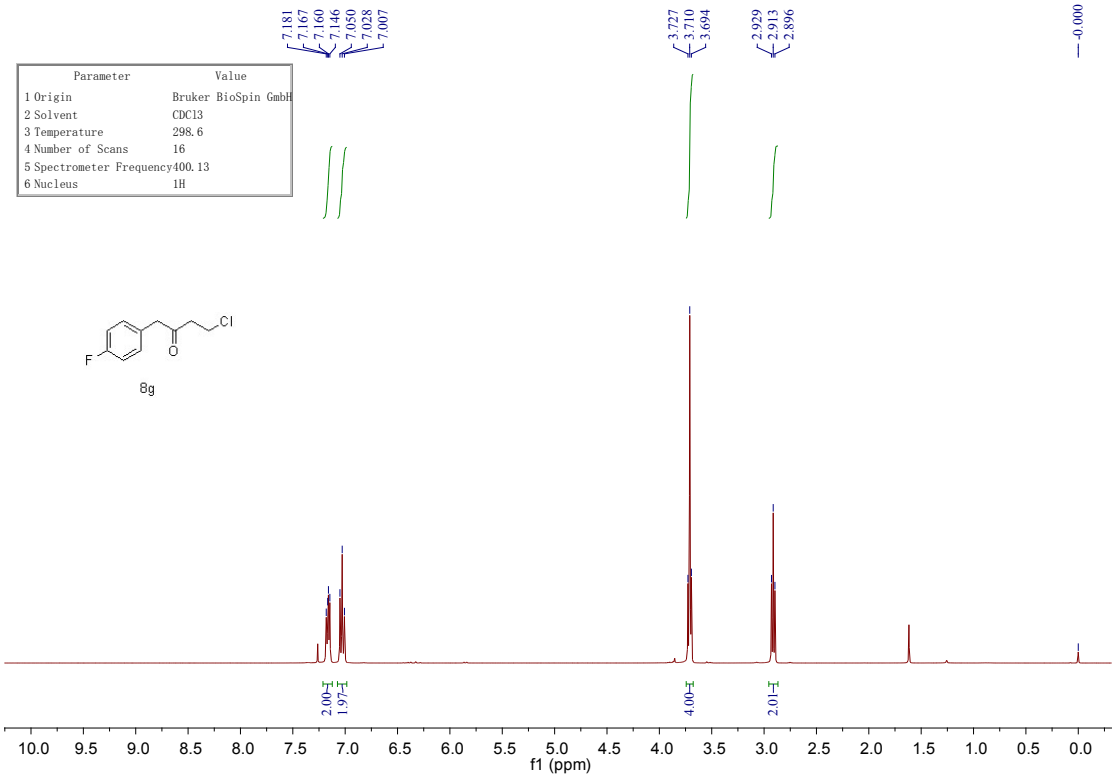

195.2
134.6
131.6
129.1
128.4
40.7
38.0
Parameter Value
1 Origin Bruker BioSpin GmbH
2 Solvent CDCl3
3 Temperature 301.4
4 Number of Scans 100
5 Spectrometer Frequency 100.61
6 Nucleus 13C
f1 (ppm)

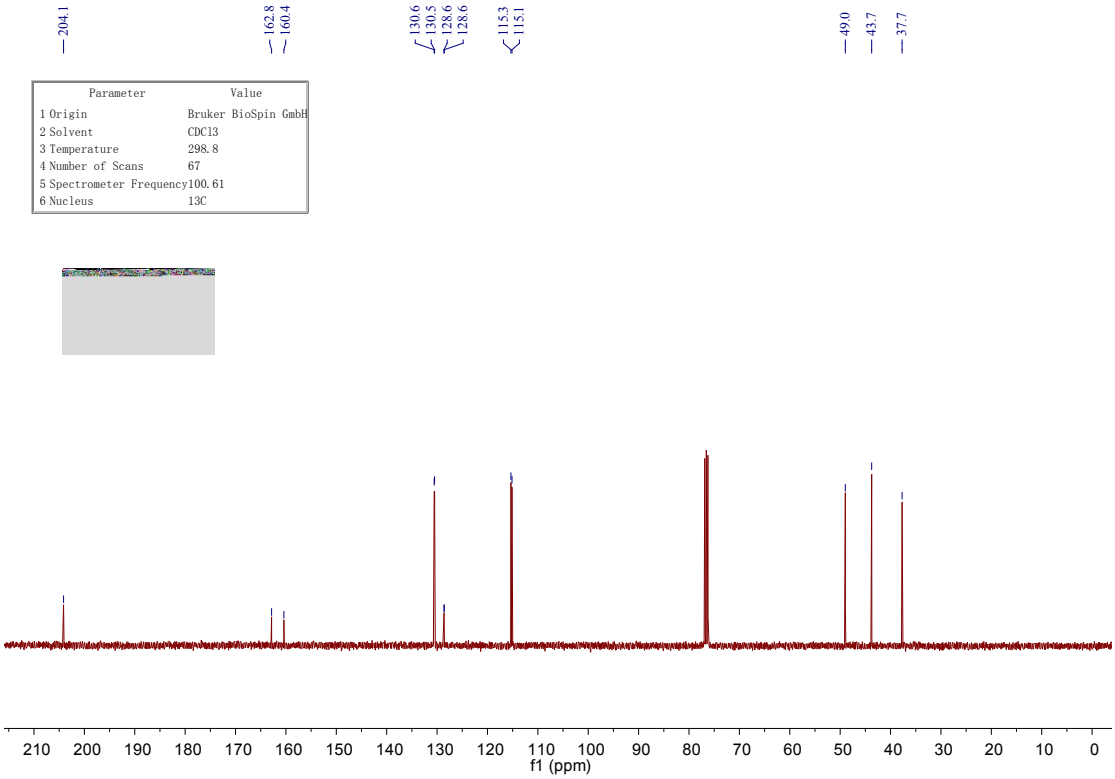

7.656
7.636
7.480
7.475
7.461
7.456
7.435
7.417
7.398
7.368
7.363
7.349
7.345
7.330
7.325
3.926
3.909
3.892
3.466
3.449
3.433
Parameter Value
1 Origin Bruker BioSpin GmbH
2 Solvent CDCl3
3 Temperature 298.3
4 Number of Scans 16
5 Spectrometer Frequency 400.13
6 Nucleus 1H
O
Cl
Br
8e
1.00
0.99
1.02
1.06
1.90
1.90
f1 (ppm)

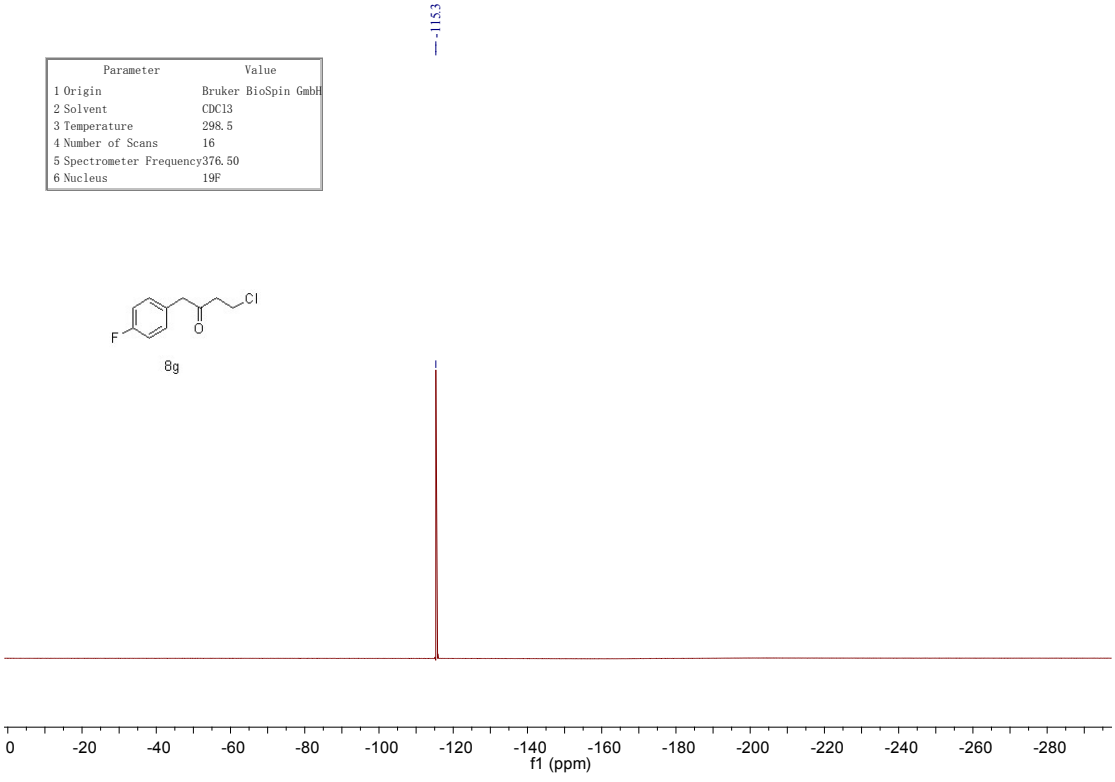

200.0
140.3
133.3
131.6
128.4
127.1
118.3
44.7
38.0
Parameter Value
1 Origin Bruker BioSpin GmbH
2 Solvent CDCl3
3 Temperature 298.7
4 Number of Scans 1024
5 Spectrometer Frequency 100.61
6 Nucleus 13C
f1 (ppm)

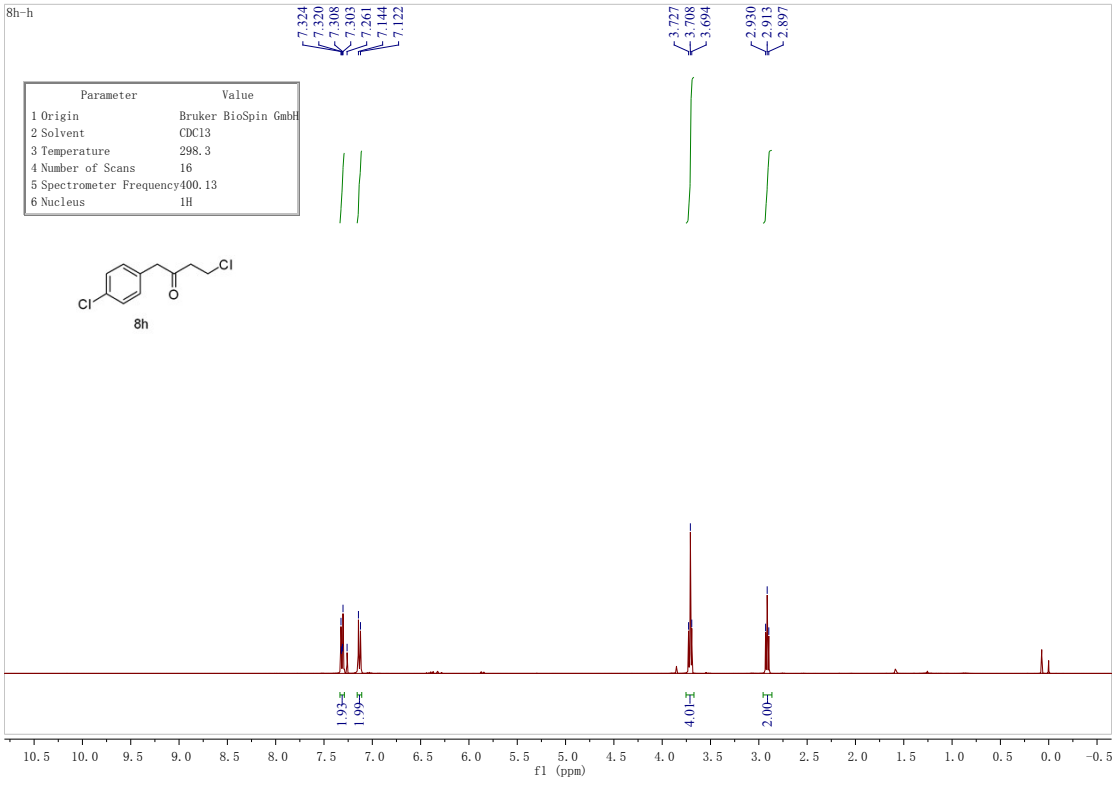

8f-h
7.355
7.338
7.319
7.293
7.275
7.207
7.189
3.716
3.705
3.688
3.672
2.913
2.896
2.880
Parameter Value
1 Origin Bruker BioSpin GmbH
2 Solvent CDCl3
3 Temperature 298.8
4 Number of Scans 4
5 Spectrometer Frequency 400.13
6 Nucleus 1H
Cl
O
8f
2.14
0.90
2.00
4.15
2.02
f1 (ppm)

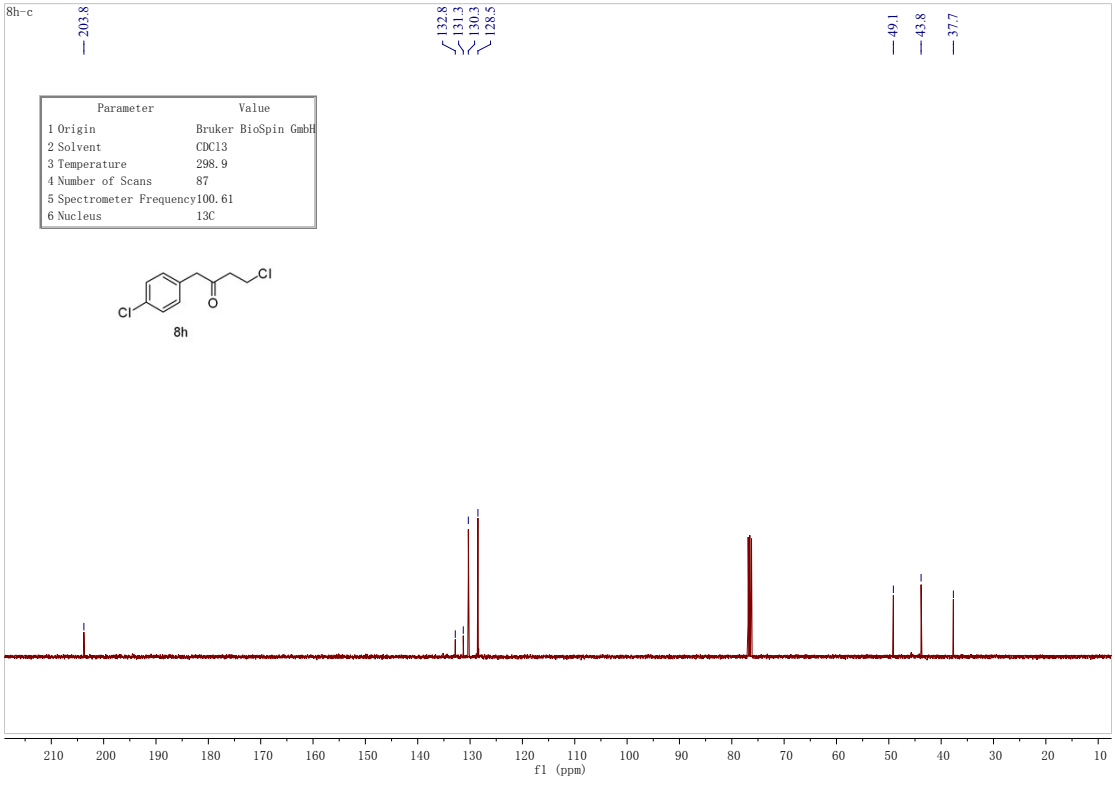

8f-c
204.4
133.0
129.0
128.4
126.8
50.0
43.7
37.8
Parameter Value
1 Origin Bruker BioSpin GmbH
2 Solvent CDCl3
3 Temperature 298.6
4 Number of Scans 51
5 Spectrometer Frequency 100.61
6 Nucleus 13C
f1 (ppm)


7.181
7.167
7.160
7.146
7.059
7.028
7.007
3.727
3.710
3.694
2.929
2.913
2.896
-0.000
Parameter Value
1 Origin Bruker BioSpin GmbH
2 Solvent CDCl3
3 Temperature 298.6
4 Number of Scans 16
5 Spectrometer Frequency 400.13
6 Nucleus 1H
Cl
O
F
8g
2.00
1.97
4.00
2.01
f1 (ppm)

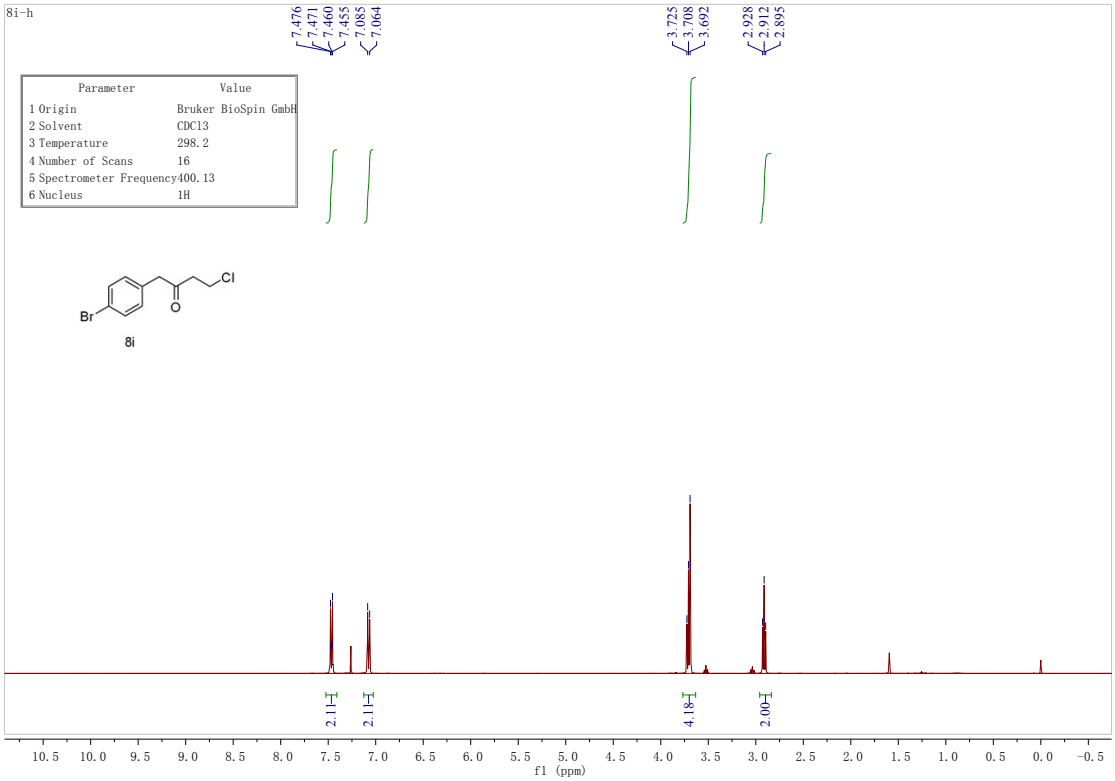

204.1
162.8
160.4
130.6
130.5
128.6
128.6
115.3
115.1
49.0
43.7
37.7
Parameter Value
1 Origin Bruker BioSpin GmbH
2 Solvent CDCl3
3 Temperature 298.8
4 Number of Scans 67
5 Spectrometer Frequency 100.61
6 Nucleus 13C
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)


-115.3
Parameter Value
1 Origin Bruker BioSpin GmbH
2 Solvent CDCl3
3 Temperature 298.5
4 Number of Scans 16
5 Spectrometer Frequency 376.50
6 Nucleus 19F
F
O
Cl
8g
0 -20 -40 -60 -80 -100 -120 -140 -160 -180 -200 -220 -240 -260 -280
f1 (ppm)


8h-h
7.324
7.320
7.308
7.303
7.261
7.144
7.122
3.727
3.708
3.694
2.930
2.913
2.897
Parameter Value
1 Origin Bruker BioSpin GmbH
2 Solvent CDCl3
3 Temperature 298.3
4 Number of Scans 16
5 Spectrometer Frequency 400.13
6 Nucleus 1H
Cl
O
Cl
8h
1.93
1.99
4.01
2.00
10.5 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)


8h-c
203.8
132.8
131.3
130.3
128.5
49.1
43.8
37.7
Parameter Value
1 Origin Bruker BioSpin GmbH
2 Solvent CDCl3
3 Temperature 298.9
4 Number of Scans 87
5 Spectrometer Frequency 100.61
6 Nucleus 13C
Cl
O
Cl
8h
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10
f1 (ppm)

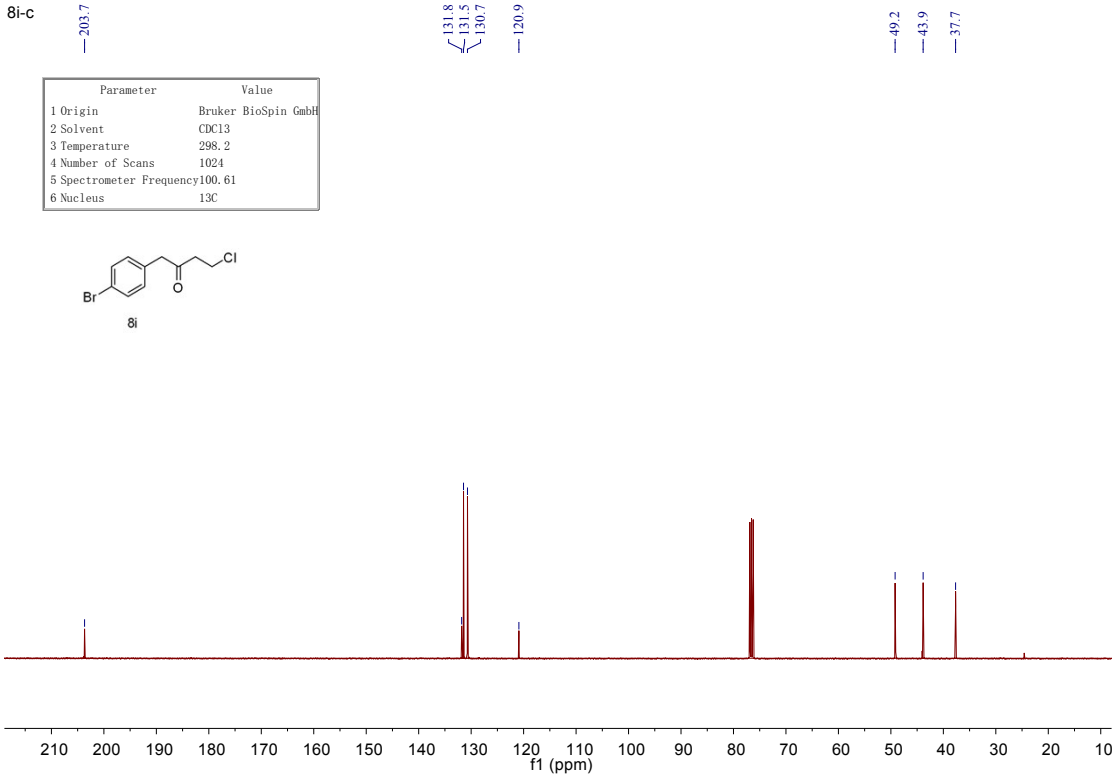
8i-h



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

8i

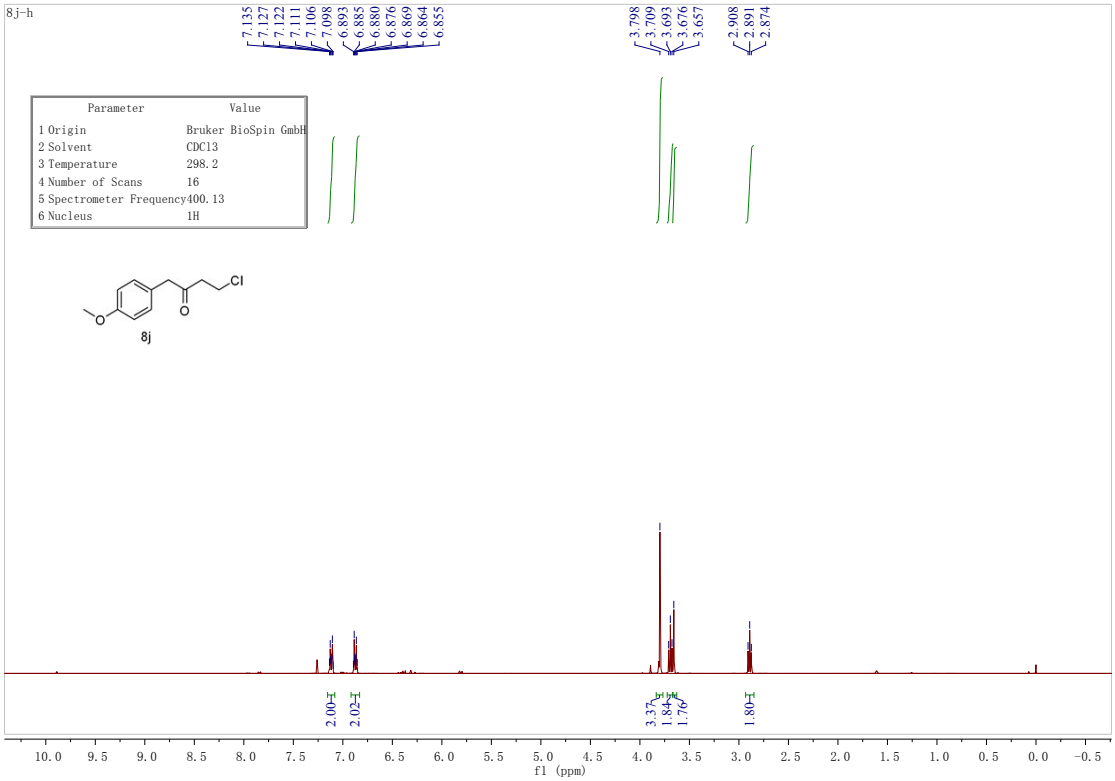
8i-c



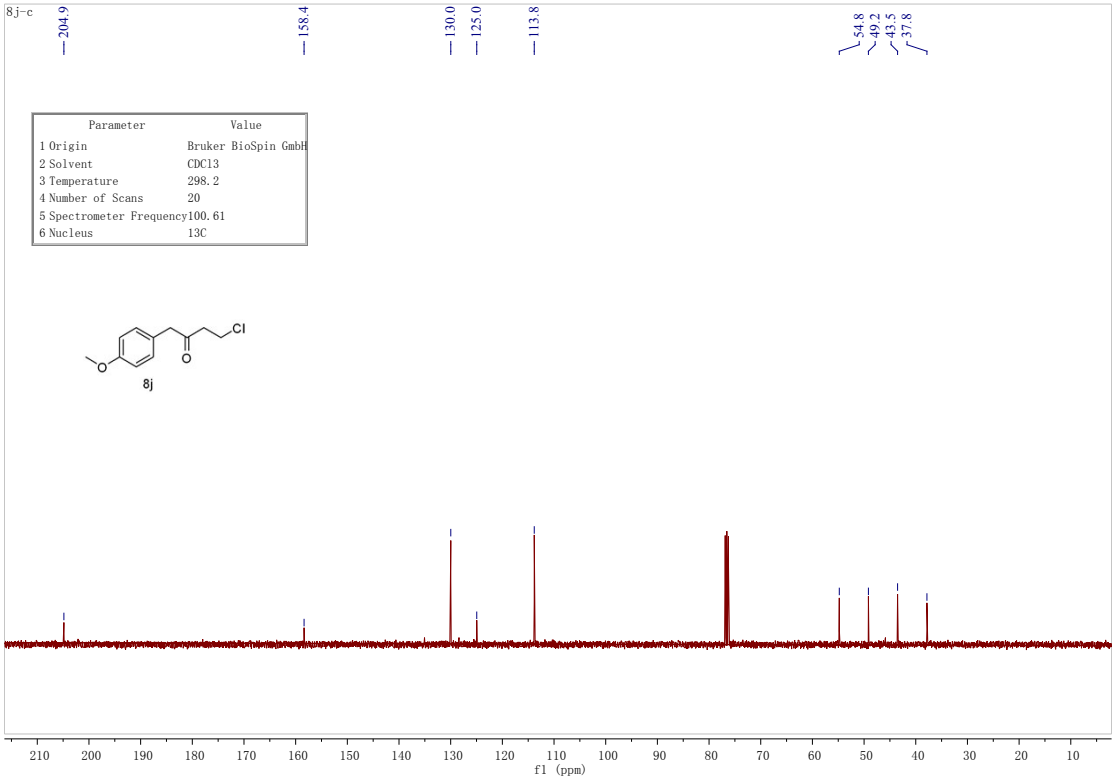
Parameter	Value
1 Origin	Bruker BioSpin GmbH
2 Solvent	CDCl3
3 Temperature	298.2
4 Number of Scans	1024
5 Spectrometer Frequency	100.61
6 Nucleus	13C

8i

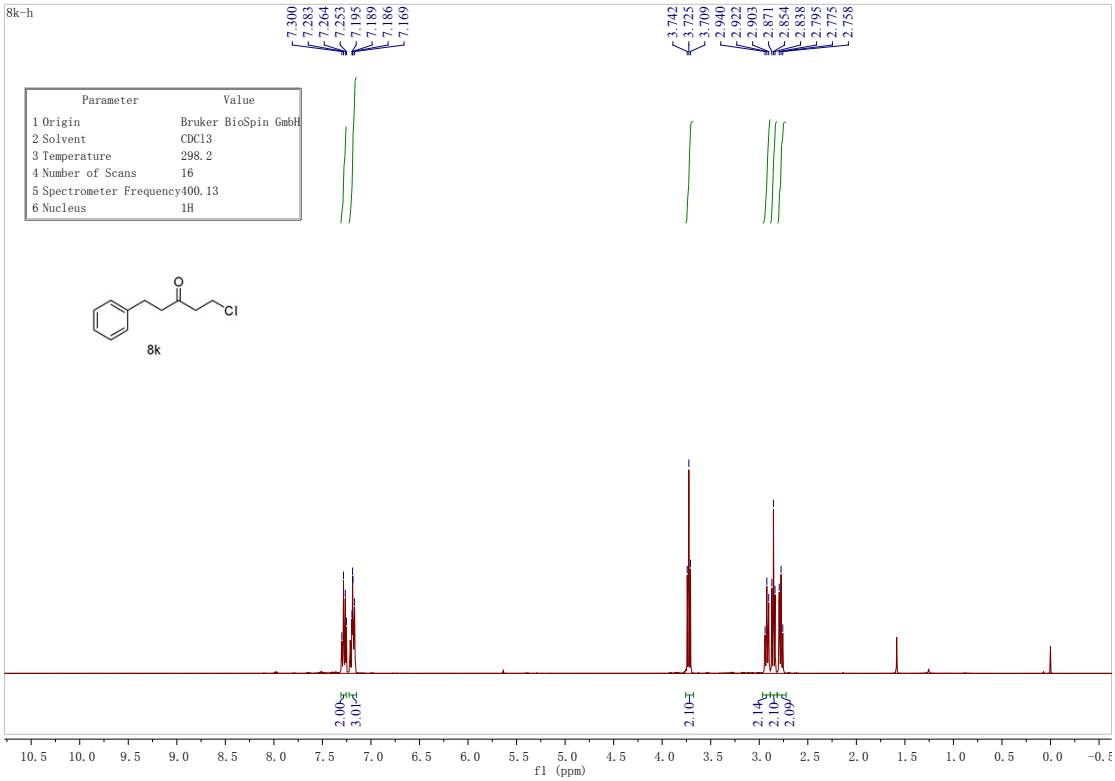
8j-h


7.135
7.127
7.122
7.111
7.106
7.098
6.893
6.885
6.880
6.876
6.869
6.864
6.855
3.798
3.709
3.693
3.676
3.657
2.908
2.891
2.874
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
Cl
O
O
8j
2.00
2.02
3.37
1.84
1.76
1.80
f1 (ppm)

8j-c


204.9
158.4
130.0
125.0
113.8
54.8
49.2
43.5
37.8
Parameter Value
1 Origin Bruker BioSpin GmbH
2 Solvent CDCl3
3 Temperature 298.2
4 Number of Scans 20
5 Spectrometer Frequency 100.61
6 Nucleus 13C
Cl
O
O
8j
f1 (ppm)

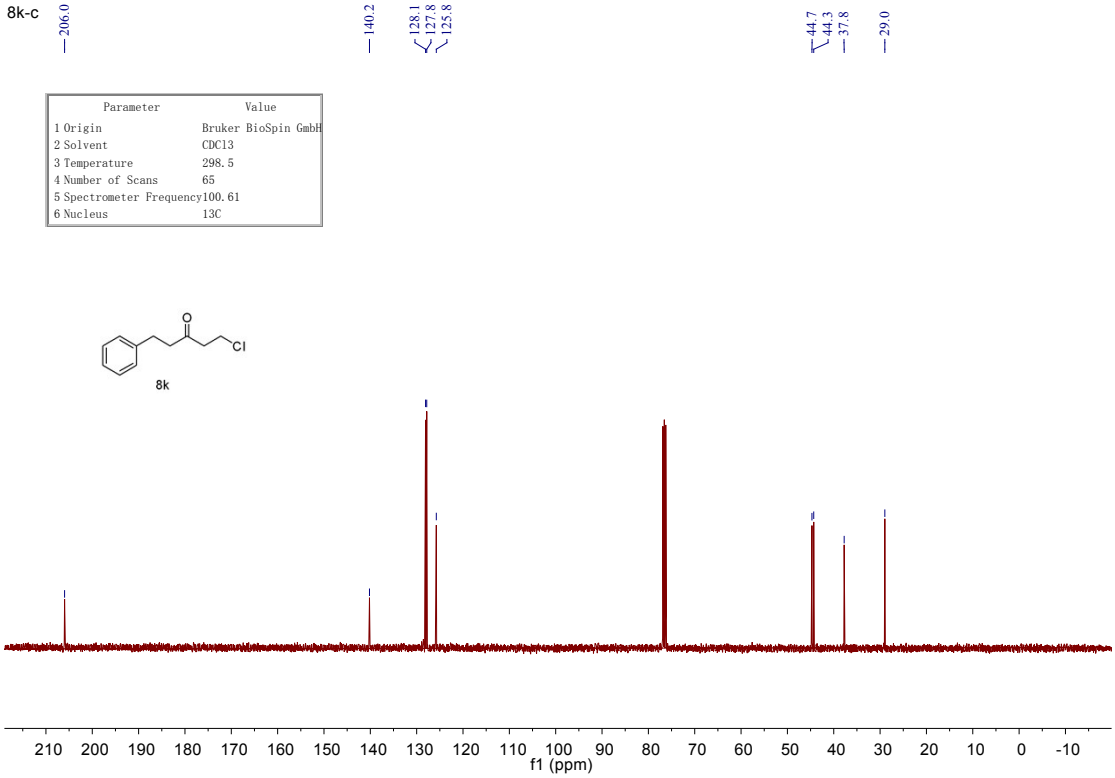
8k-h



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

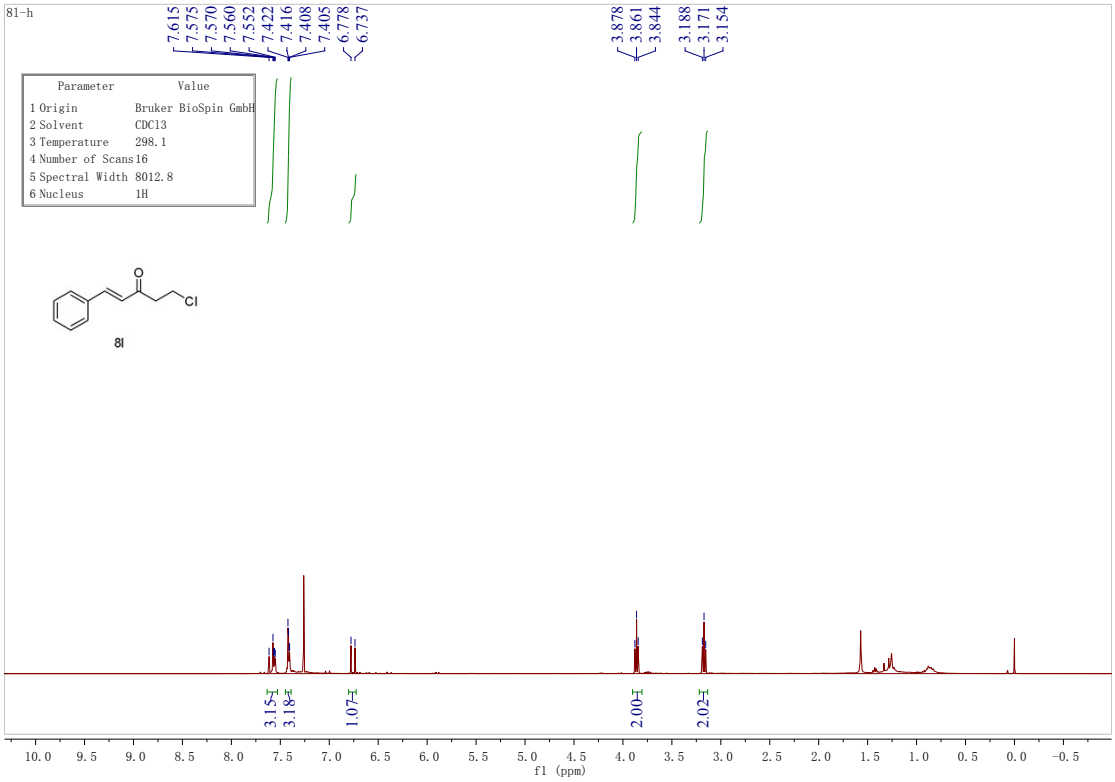
8k

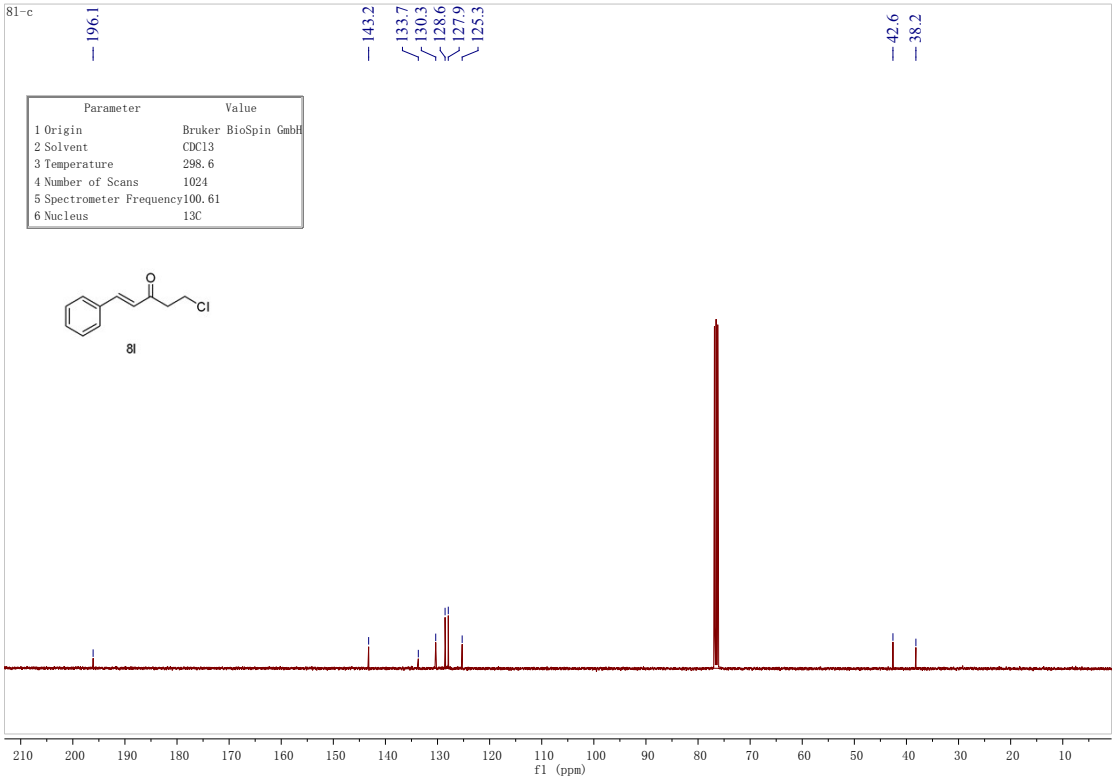
8k-c

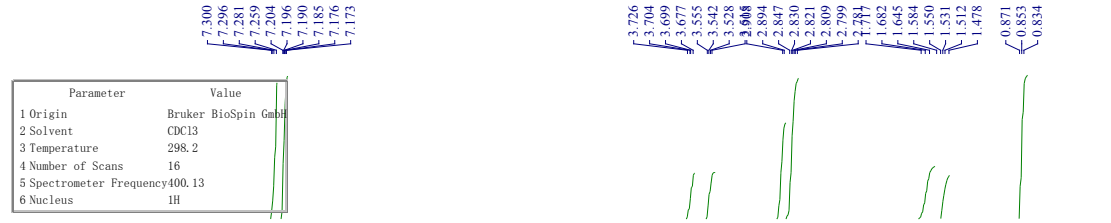


Parameter	Value
1 Origin	Bruker BioSpin GmbH
2 Solvent	CDCl3
3 Temperature	298.5
4 Number of Scans	65
5 Spectrometer Frequency	100.61
6 Nucleus	13C

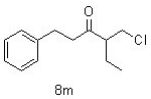
8k


81-h
7.615
7.575
7.570
7.560
7.552
7.422
7.416
7.408
7.405
6.778
6.737
3.878
3.861
3.844
3.188
3.171
3.154
Parameter Value
1 Origin Bruker BioSpin GmbH
2 Solvent CDCl3
3 Temperature 298.1
4 Number of Scans 16
5 Spectral Width 8012.8
6 Nucleus 1H
O
Cl
8l
3.15
3.18
1.07
2.00
2.02
f1 (ppm)

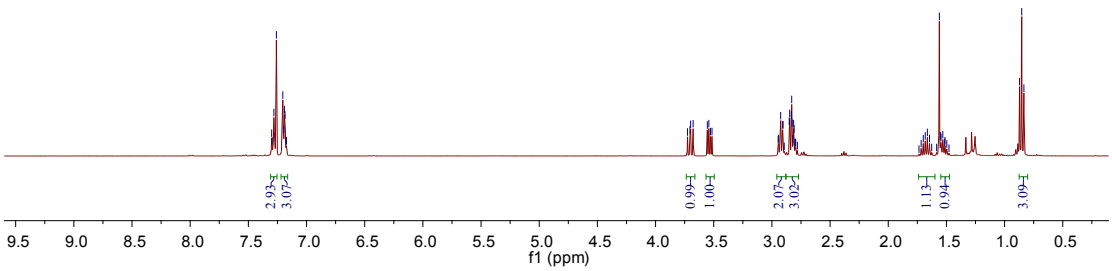

81-c
196.1
143.2
133.7
130.3
128.6
127.9
125.3
42.6
38.2
Parameter Value
1 Origin Bruker BioSpin GmbH
2 Solvent CDCl3
3 Temperature 298.6
4 Number of Scans 1024
5 Spectrometer Frequency 100.61
6 Nucleus 13C
O
Cl
8l
f1 (ppm)

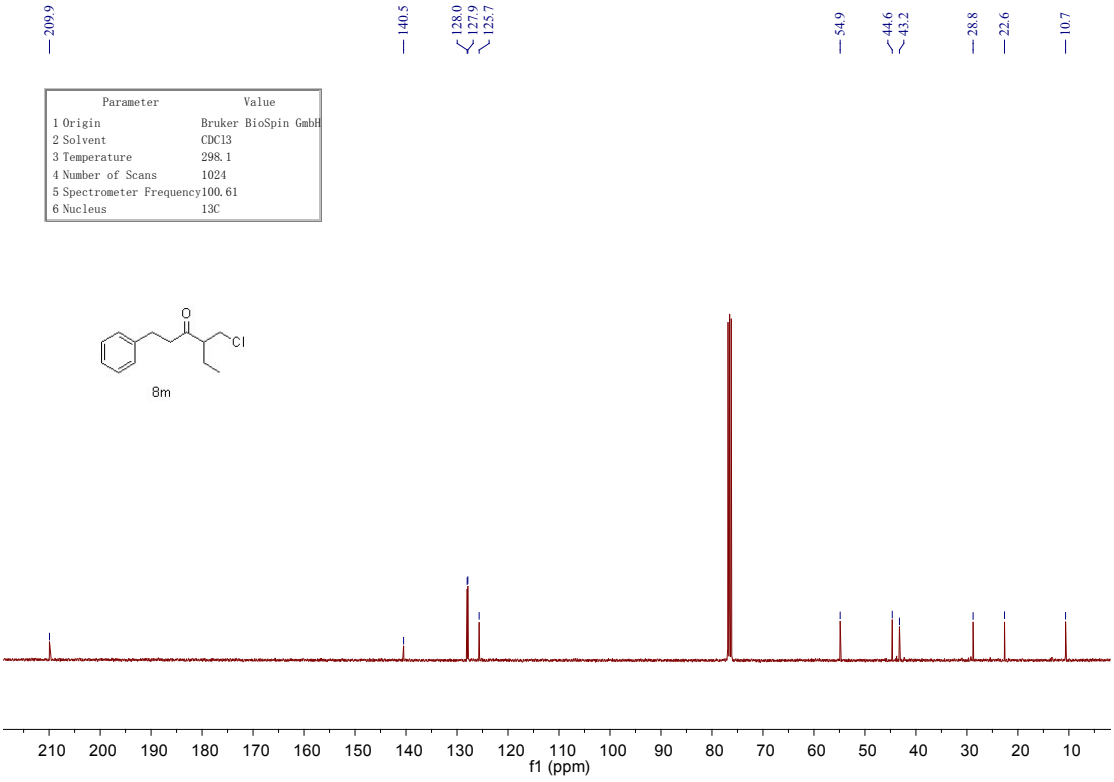


Parameter	Value
1 Origin	Bruker BioSpin GmbH
2 Solvent	CDCl3
3 Temperature	298.2
4 Number of Scans	16
5 Spectrometer Frequency	400.13
6 Nucleus	1H



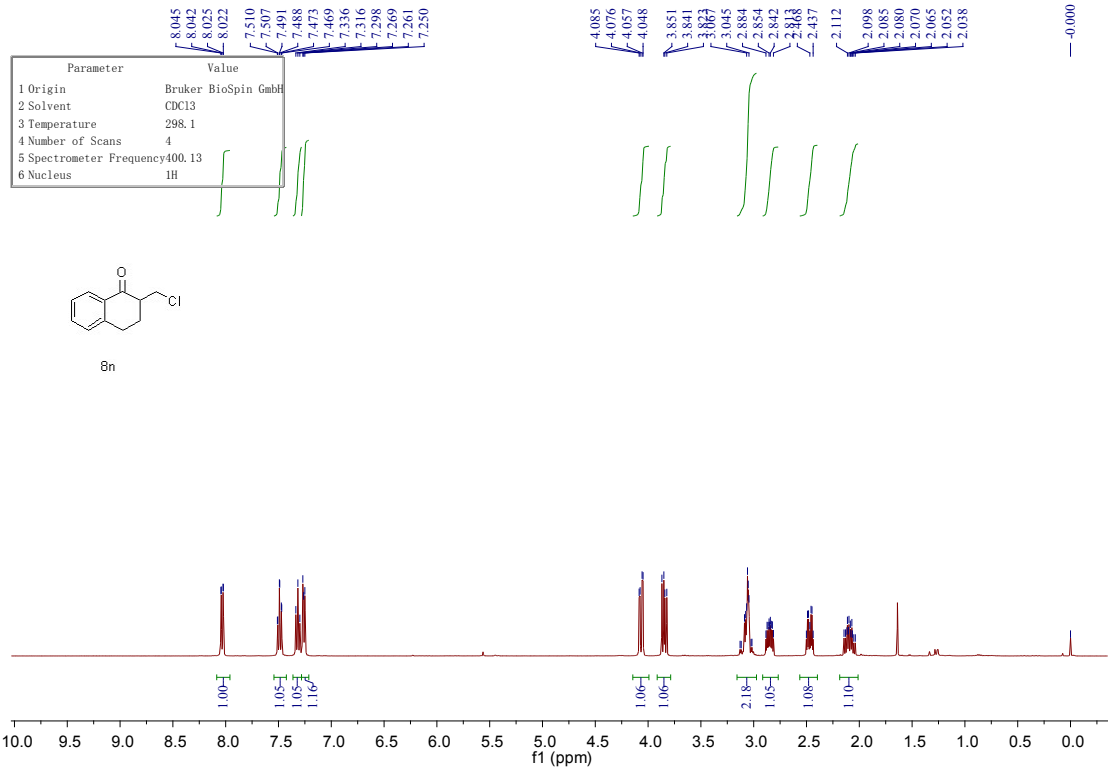
8m

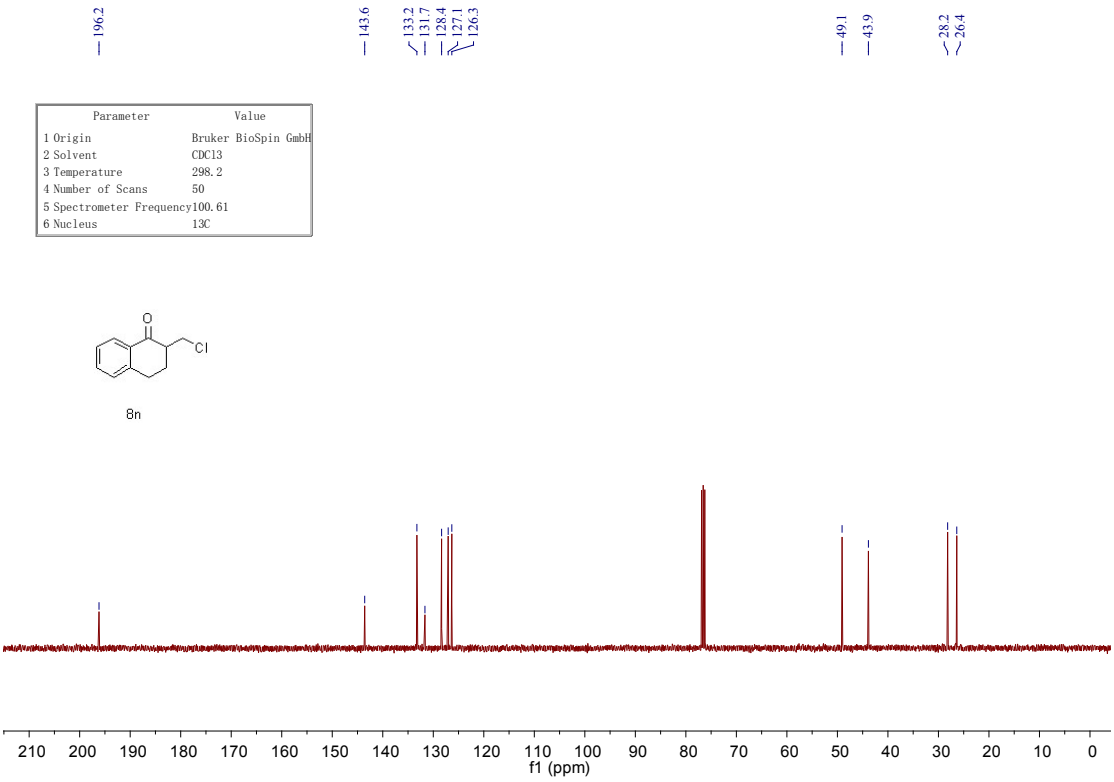


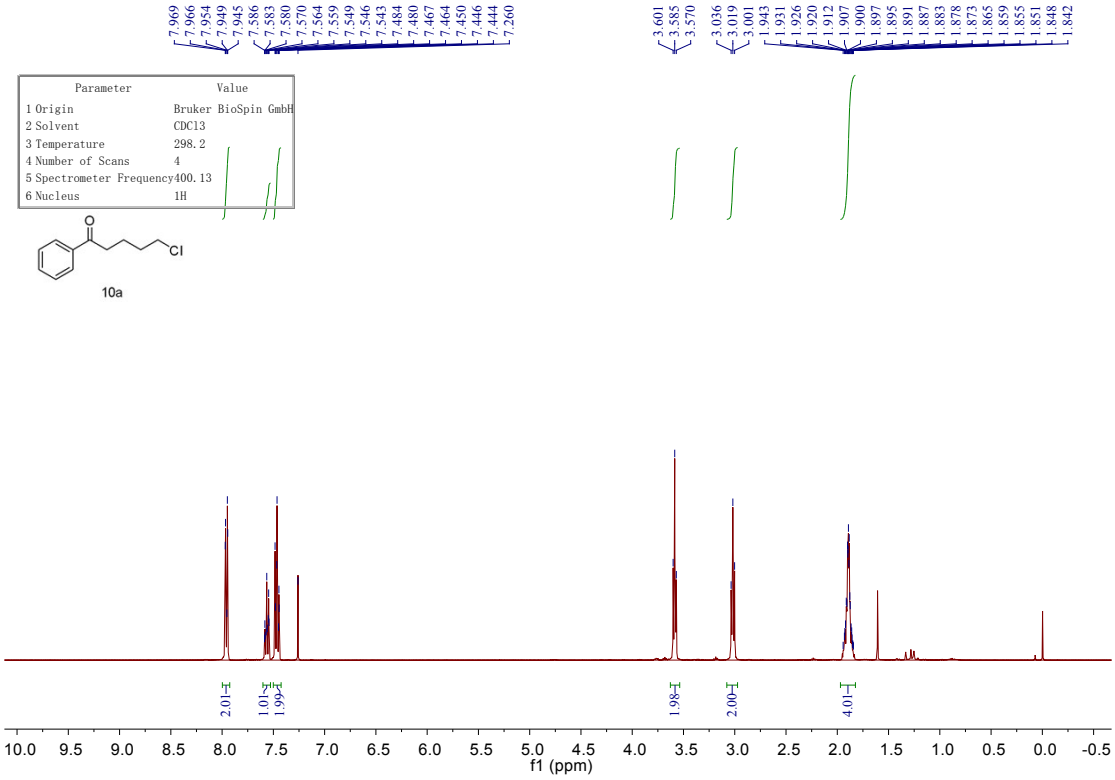


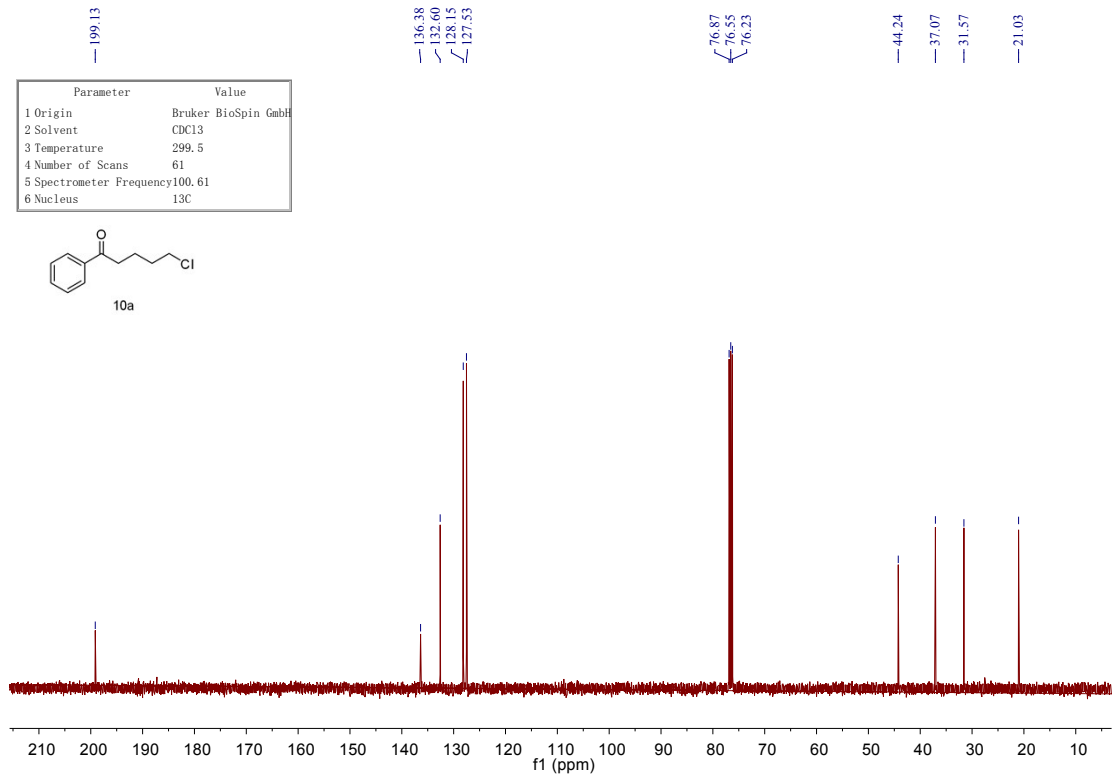
Parameter	Value
1 Origin	Bruker BioSpin GmbH
2 Solvent	CDCl3
3 Temperature	298.1
4 Number of Scans	1024
5 Spectrometer Frequency	100.61
6 Nucleus	13C

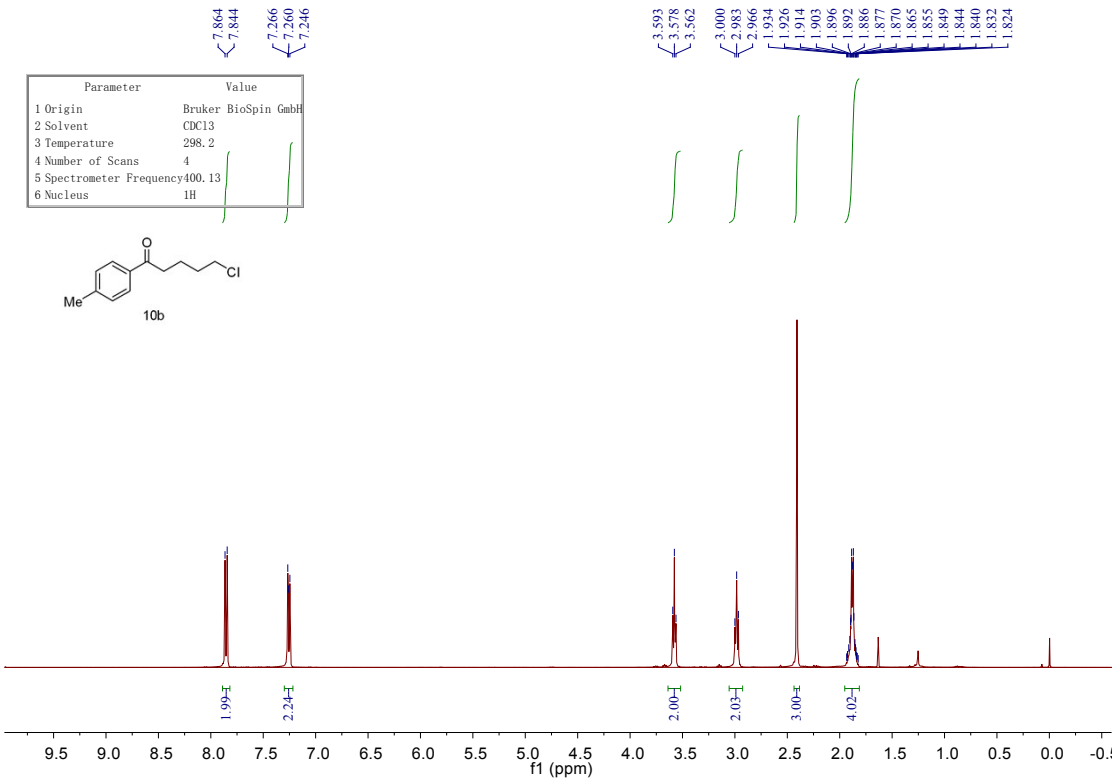
8m

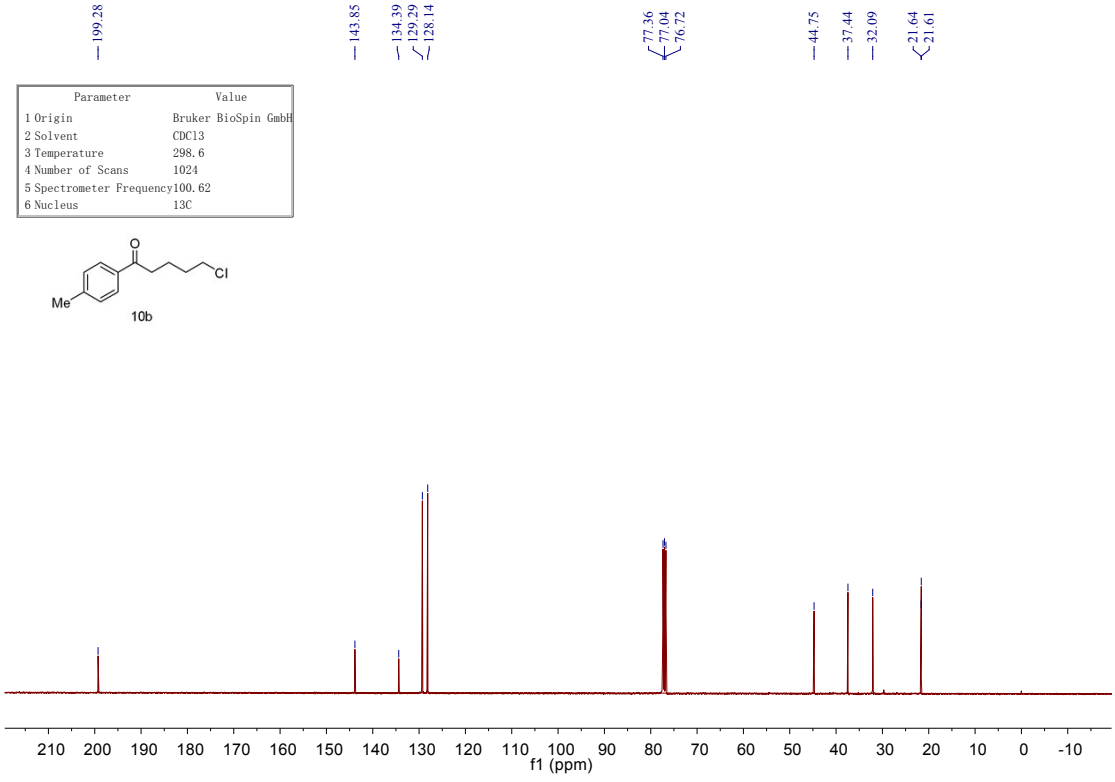

8.045
8.042
8.025
8.022
7.510
7.507
7.491
7.488
7.473
7.469
7.336
7.316
7.298
7.269
7.261
7.250
4.085
4.076
4.057
4.048
3.851
3.841
3.045
2.884
2.854
2.842
2.437
2.112
2.098
2.085
2.080
2.070
2.065
2.052
2.038
0.000
Parameter Value
1 Origin Bruker BioSpin GmbH
2 Solvent CDCl3
3 Temperature 298.1
4 Number of Scans 4
5 Spectrometer Frequency 400.13
6 Nucleus 1H
O
Cl
8n
1.00
1.05
1.05
1.16
1.06
1.06
2.18
1.05
1.08
1.10
10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)

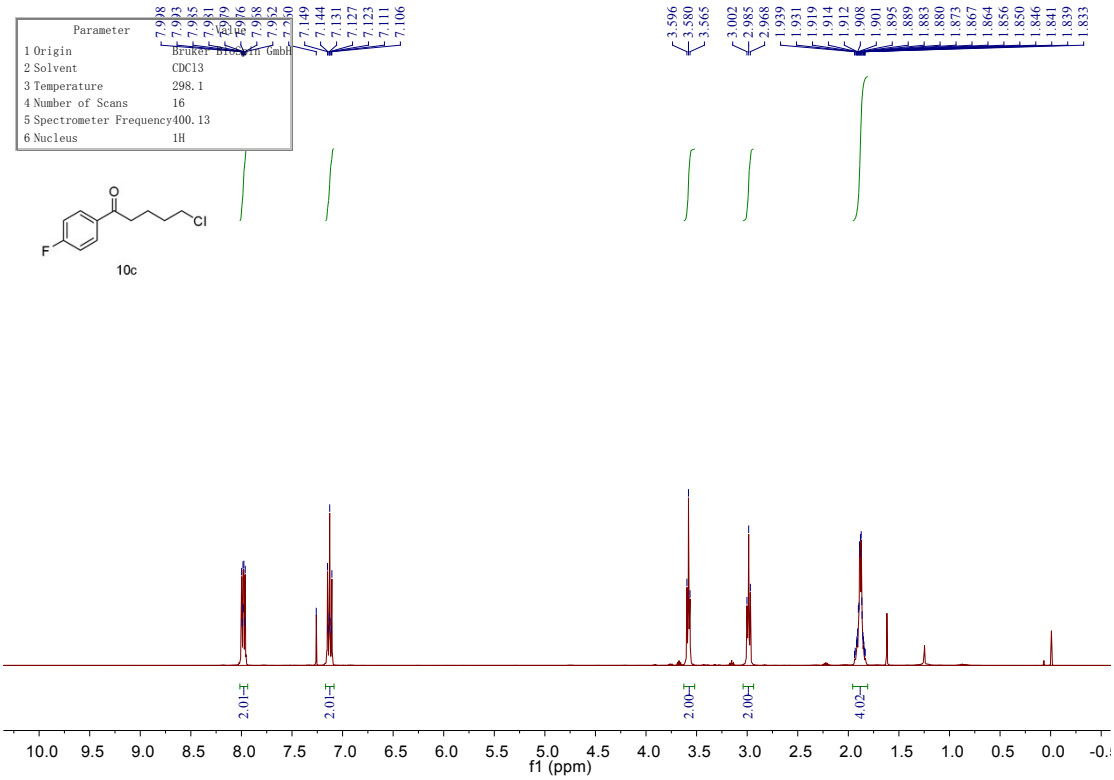

196.2
143.6
133.2
131.7
128.4
127.1
126.3
49.1
43.9
28.2
26.4
Parameter Value
1 Origin Bruker BioSpin GmbH
2 Solvent CDCl3
3 Temperature 298.2
4 Number of Scans 50
5 Spectrometer Frequency 100.61
6 Nucleus 13C
O
Cl
8n
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)

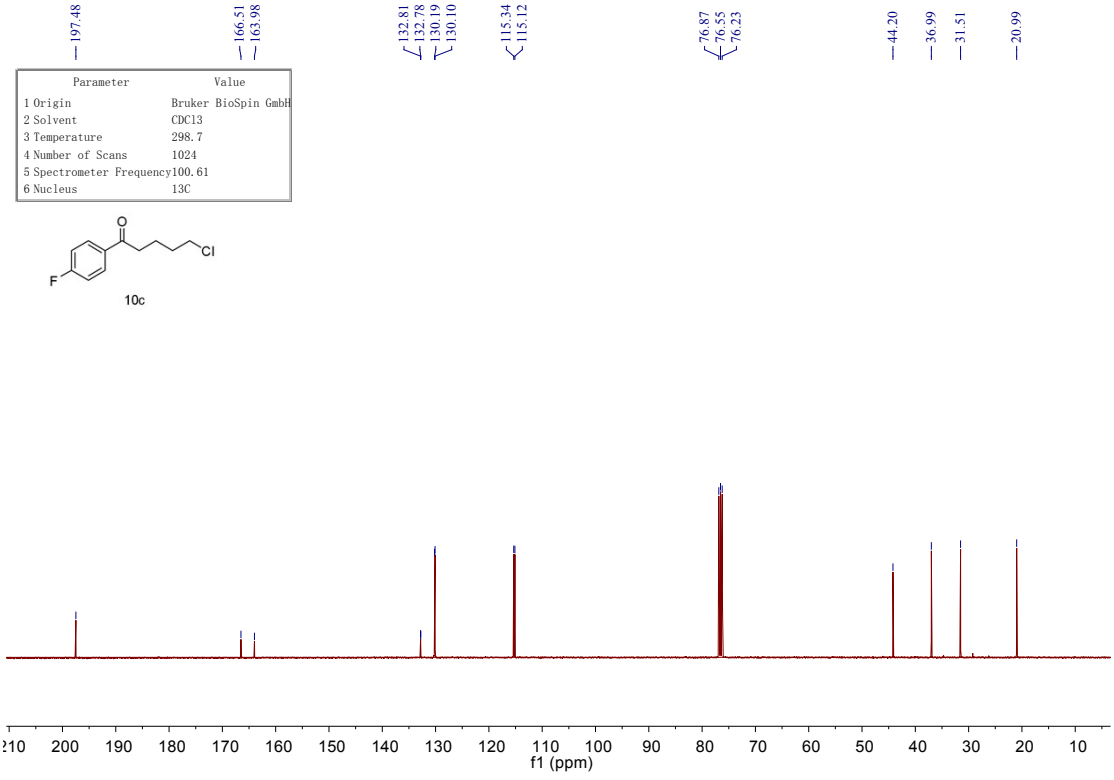

7.969
7.966
7.954
7.949
7.945
7.586
7.583
7.580
7.570
7.564
7.559
7.549
7.546
7.543
7.484
7.480
7.467
7.464
7.450
7.446
7.444
7.260
3.601
3.585
3.570
3.036
3.019
3.001
1.943
1.931
1.926
1.920
1.912
1.907
1.900
1.897
1.895
1.891
1.887
1.883
1.878
1.873
1.865
1.859
1.855
1.851
1.848
1.842
Parameter Value
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
Cl
10a
2.01
1.01
1.99
1.98
2.00
4.01
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)


199.13
136.38
132.60
128.15
127.53
76.87
76.55
76.23
44.24
37.07
31.57
21.03
Parameter Value
1 Origin Bruker BioSpin GmbH
2 Solvent CDCl3
3 Temperature 299.5
4 Number of Scans 61
5 Spectrometer Frequency 100.61
6 Nucleus 13C
O
Cl
10a
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10
f1 (ppm)

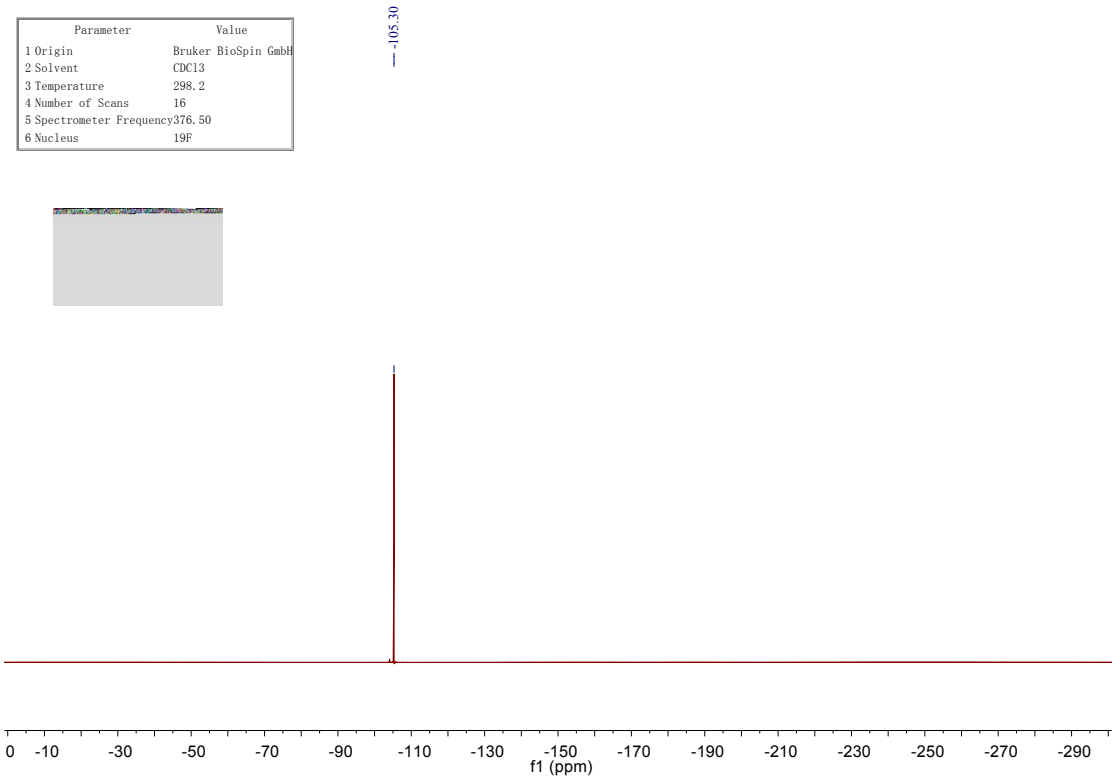

7.864
7.844
7.266
7.260
7.246
3.593
3.578
3.562
3.000
2.983
2.966
1.934
1.926
1.914
1.903
1.896
1.892
1.886
1.877
1.870
1.865
1.855
1.849
1.844
1.840
1.832
1.824
Parameter Value
1 Origin Bruker BioSpin GmbH
2 Solvent CDCl3
3 Temperature 298.2
4 Number of Scans 4
5 Spectrometer Frequency 400.13
6 Nucleus 1H
O
Cl
Me
10b
1.99
2.24
2.00
2.03
3.00
4.02
f1 (ppm)


199.28
143.85
134.39
129.29
128.14
77.36
77.04
76.72
44.75
37.44
32.09
21.64
21.61
Parameter Value
1 Origin Bruker BioSpin GmbH
2 Solvent CDCl3
3 Temperature 298.6
4 Number of Scans 1024
5 Spectrometer Frequency 100.62
6 Nucleus 13C
O
Cl
Me
10b
f1 (ppm)


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
7.908 7.903 7.985 7.981 7.979 7.976 7.968 7.962 7.250 7.149 7.144 7.131 7.127 7.123 7.111 7.106
3.596 3.580 3.565 3.002 2.985 2.968 1.939 1.931 1.919 1.914 1.912 1.908 1.901 1.895 1.889 1.883 1.880 1.873 1.867 1.864 1.856 1.850 1.846 1.841 1.839 1.833
O
Cl
F
10c
2.01 2.01 2.00 2.00 4.02
10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)

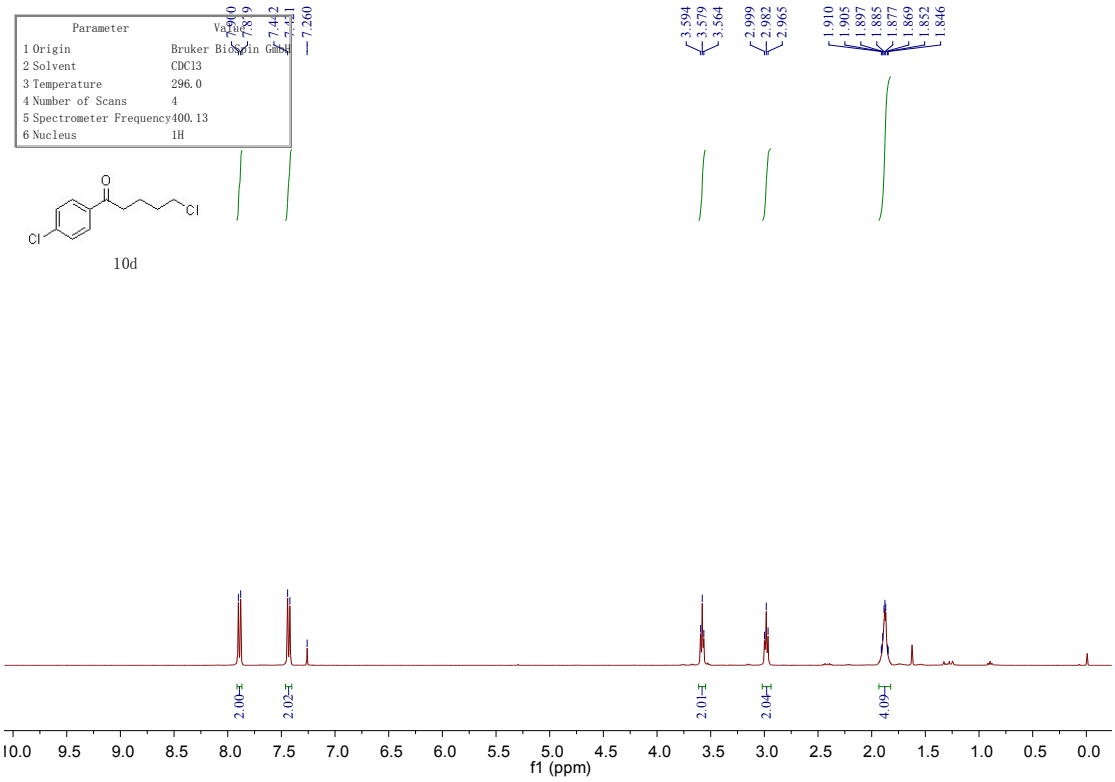

197.48 166.51 163.98 132.81 132.78 130.19 130.10 115.34 115.12 76.87 76.55 76.23 44.20 36.99 31.51 20.99
Parameter Value
1 Origin Bruker BioSpin GmbH
2 Solvent CDCl3
3 Temperature 298.7
4 Number of Scans 1024
5 Spectrometer Frequency 100.61
6 Nucleus 13C
O
Cl
F
10c
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10
f1 (ppm)

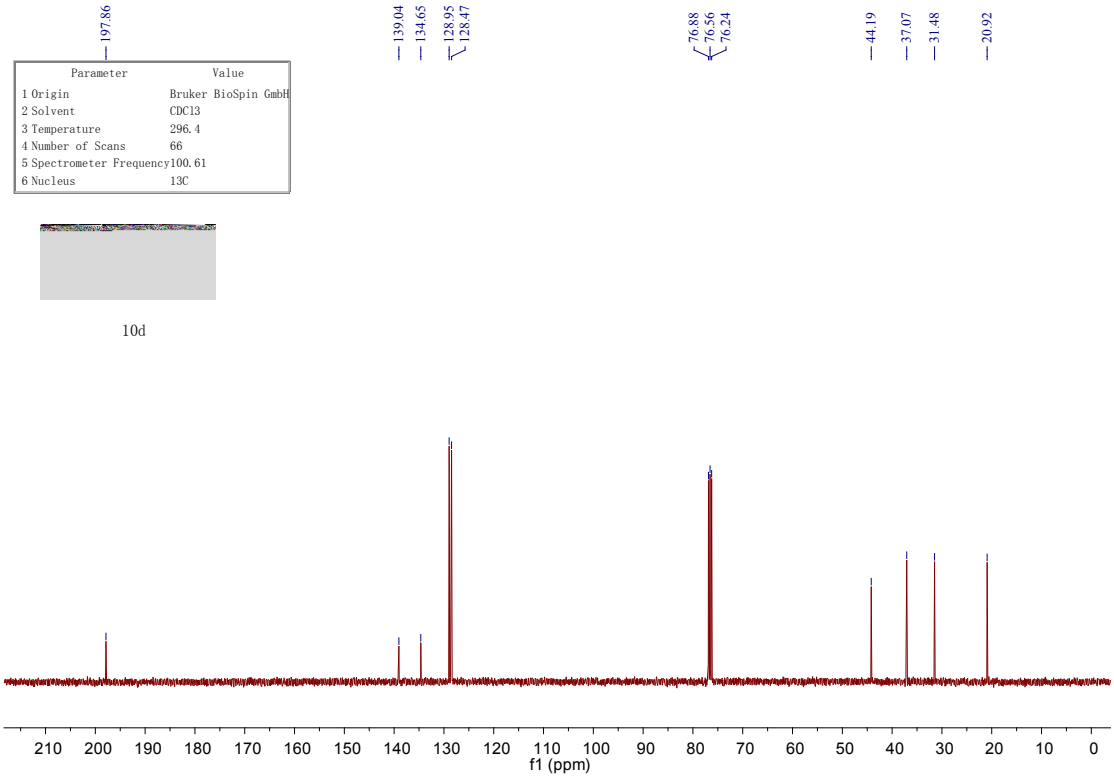
Parameter	Value
1 Origin	Bruker BioSpin GmbH
2 Solvent	CDCl3
3 Temperature	298.2
4 Number of Scans	16
5 Spectrometer Frequency	376.50
6 Nucleus	19F



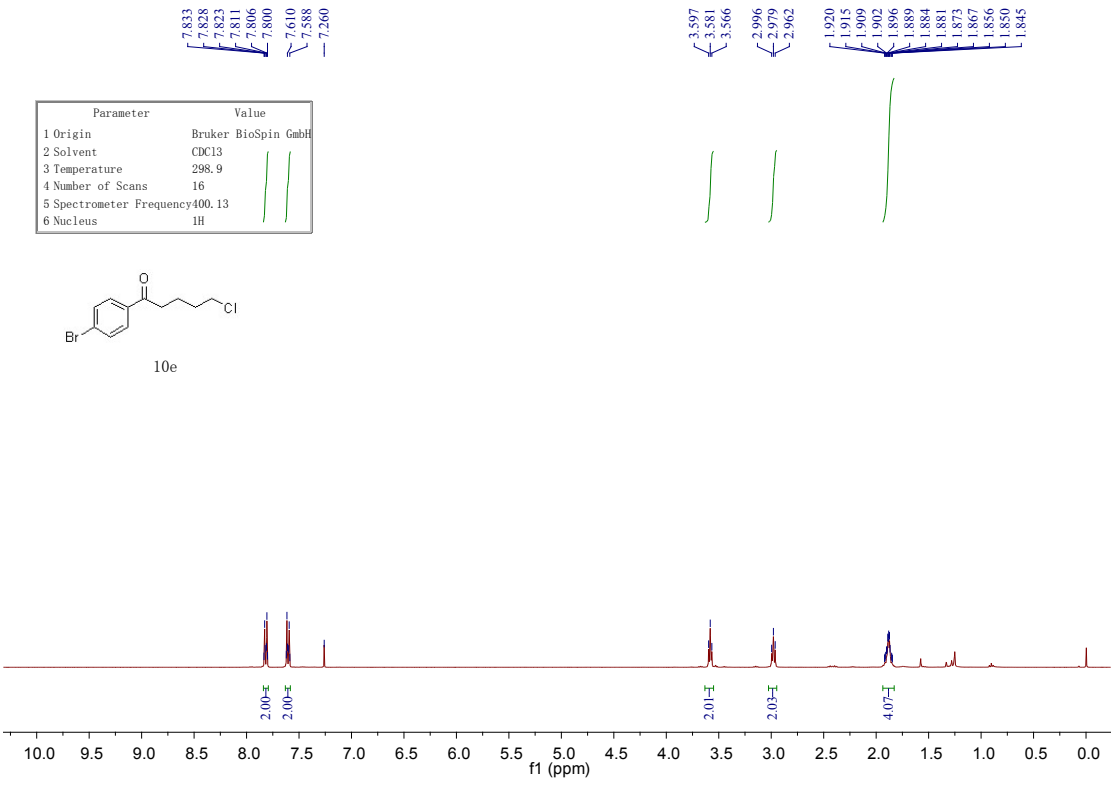
Parameter	Value
1 Origin	Bruker BioSpin GmbH
2 Solvent	CDCl3
3 Temperature	296.0
4 Number of Scans	4
5 Spectrometer Frequency	400.13
6 Nucleus	1H

10d



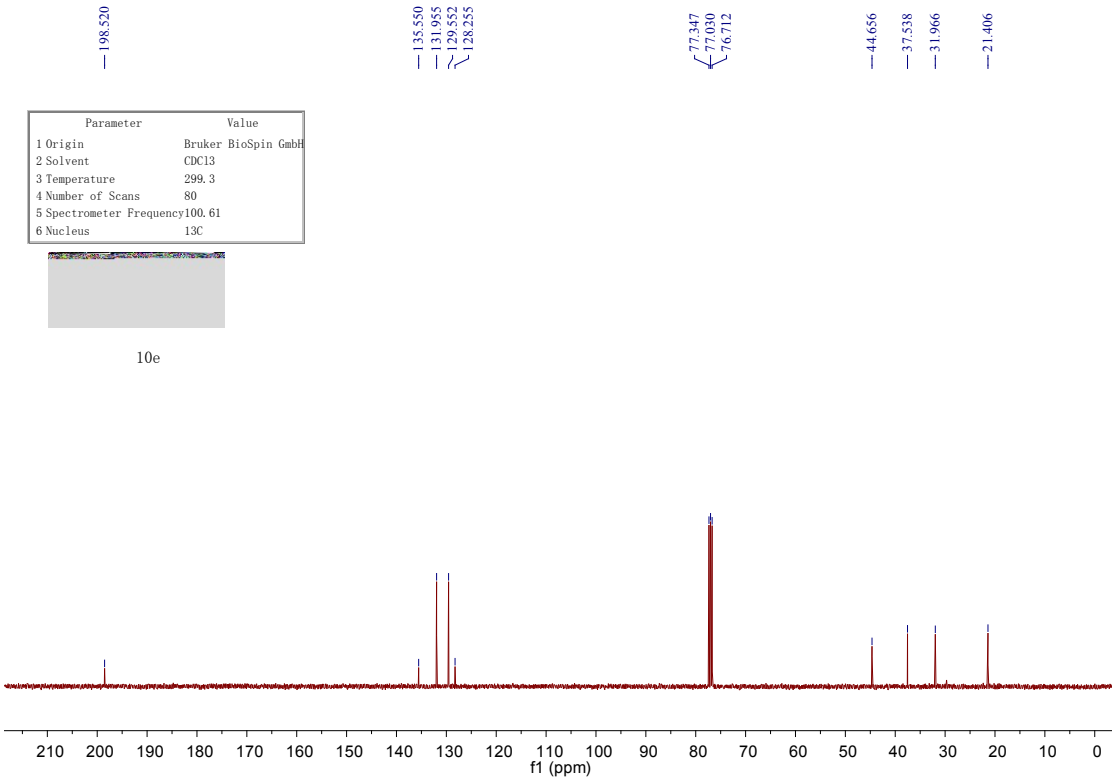

197.86
139.04
134.65
128.95
128.47
76.88
76.56
76.24
44.19
37.07
31.48
20.92
Parameter Value
1 Origin Bruker BioSpin GmbH
2 Solvent CDCl3
3 Temperature 296.4
4 Number of Scans 66
5 Spectrometer Frequency 100.61
6 Nucleus 13C
f1 (ppm)

10d

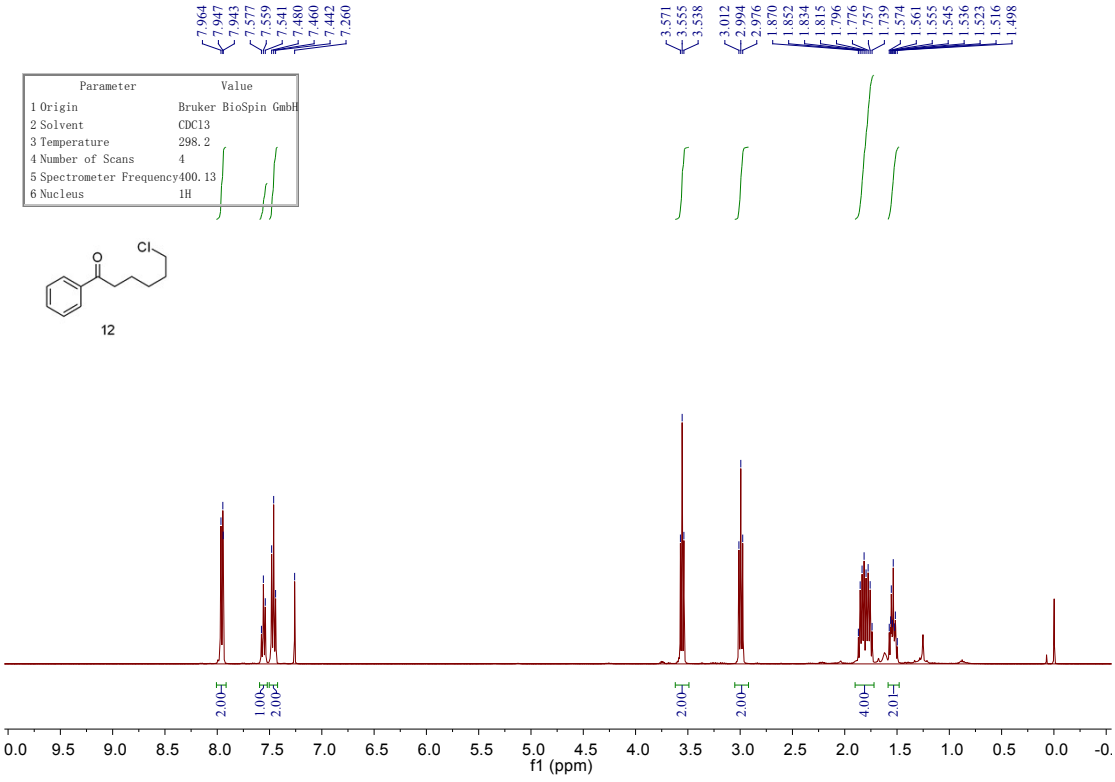

7.833
7.828
7.823
7.811
7.806
7.800
7.610
7.588
7.260
3.597
3.581
3.566
2.996
2.979
2.962
1.920
1.915
1.909
1.902
1.896
1.889
1.884
1.881
1.873
1.867
1.856
1.850
1.845
Parameter Value
1 Origin Bruker BioSpin GmbH
2 Solvent CDCl3
3 Temperature 298.9
4 Number of Scans 16
5 Spectrometer Frequency 400.13
6 Nucleus 1H
2.00
2.00
2.01
2.03
4.07
f1 (ppm)

O
Cl
Br

10e

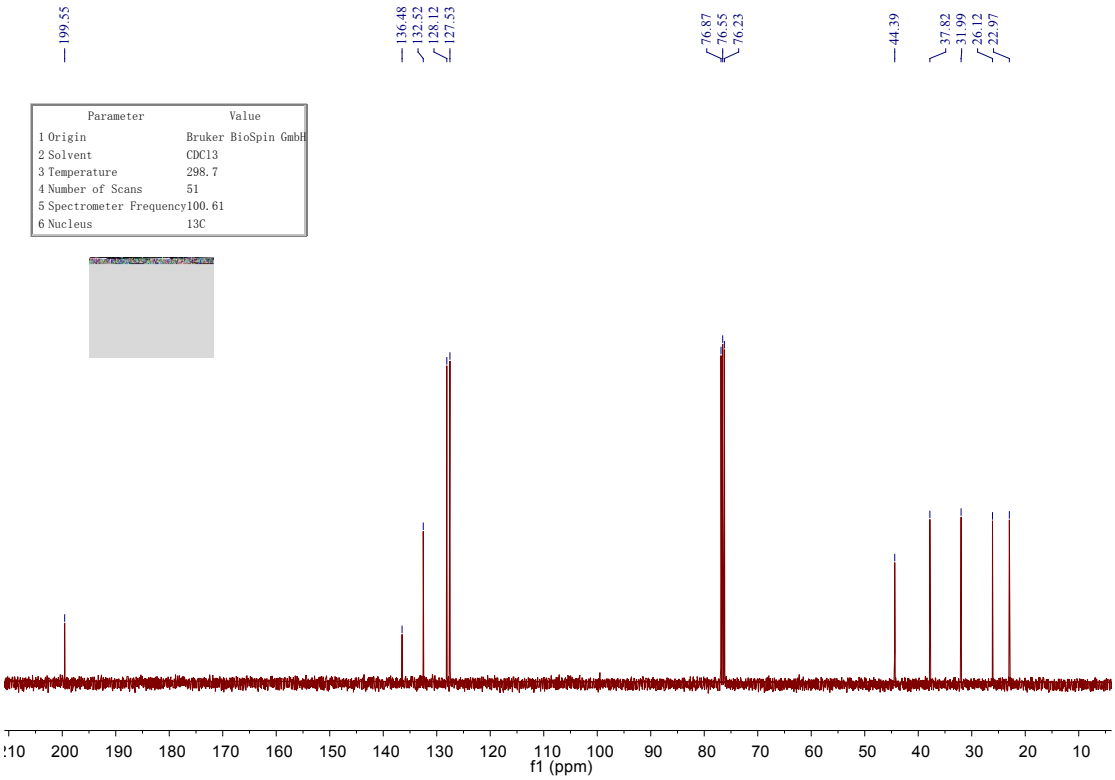

198.520
135.550
131.955
129.552
128.255
77.347
77.030
76.712
44.656
37.538
31.966
21.406
Parameter Value
1 Origin Bruker BioSpin GmbH
2 Solvent CDCl3
3 Temperature 299.3
4 Number of Scans 80
5 Spectrometer Frequency 100.61
6 Nucleus 13C
f1 (ppm)

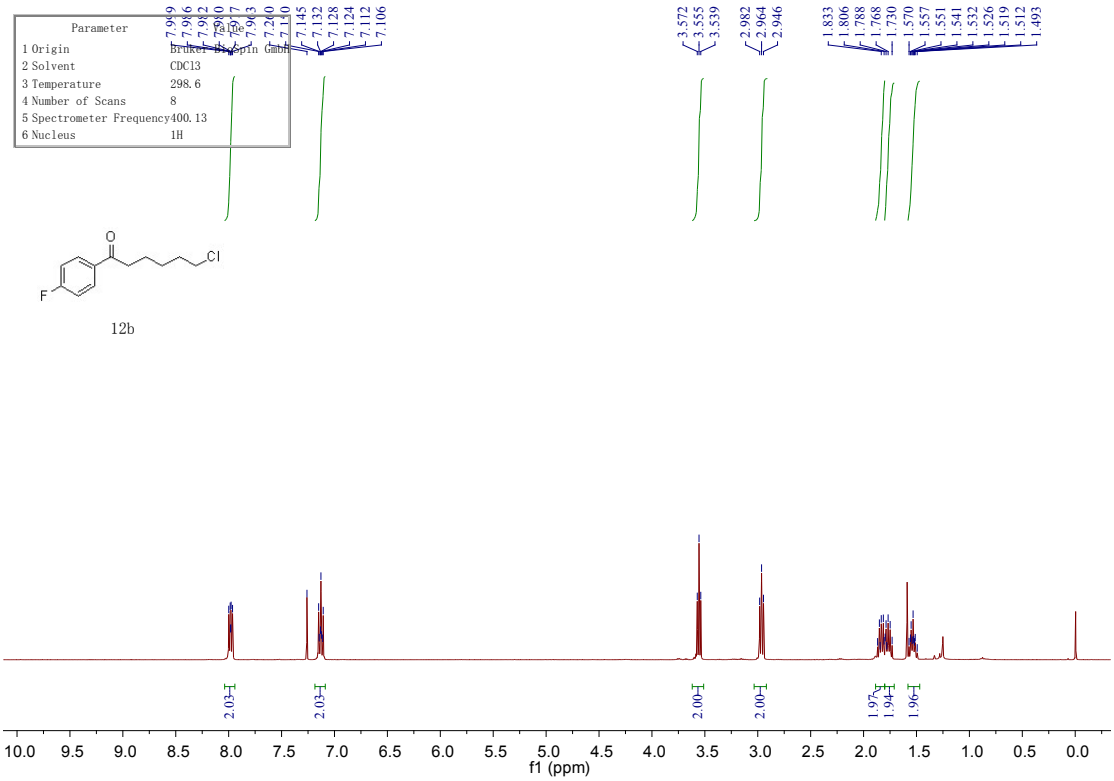
10e


7.964
7.947
7.943
7.577
7.559
7.541
7.480
7.460
7.442
7.260
3.571
3.555
3.538
3.012
2.994
2.976
1.870
1.852
1.834
1.815
1.796
1.776
1.757
1.739
1.574
1.561
1.555
1.545
1.536
1.523
1.516
1.498
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
2.00
1.00
2.00
2.00
2.00
4.00
2.01
f1 (ppm)

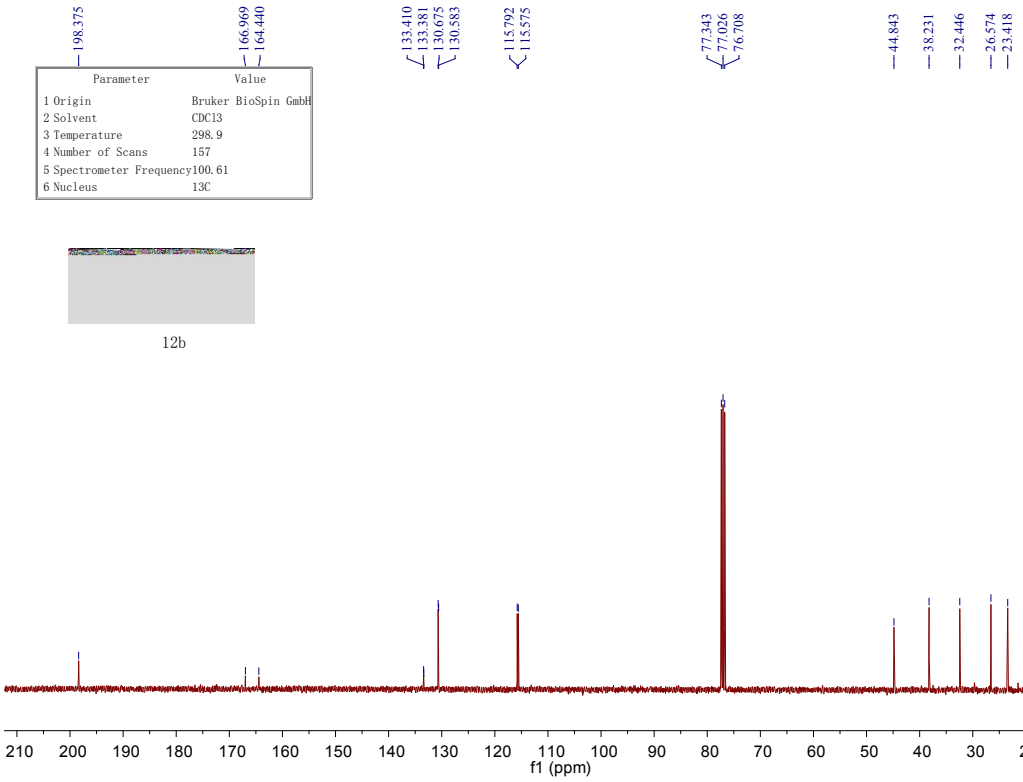
O
Cl

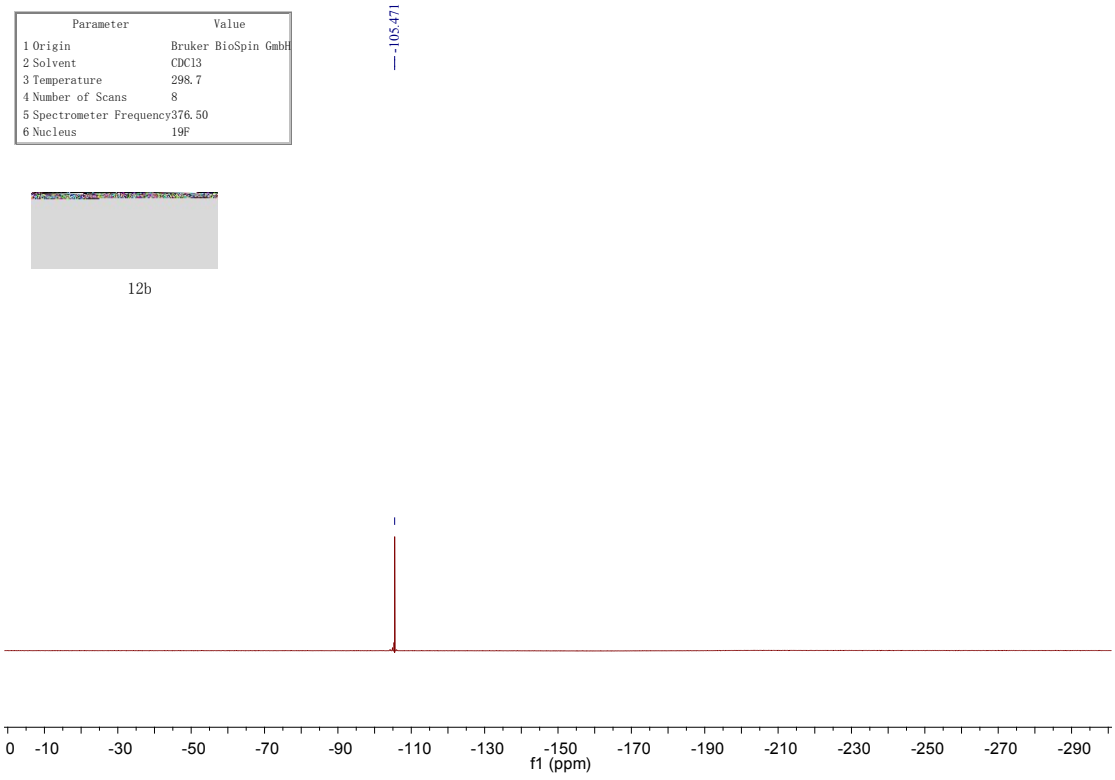
12

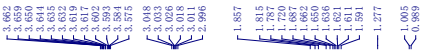

199.55
136.48
132.52
128.12
127.53
76.87
76.55
76.23
44.39
37.82
31.99
26.12
22.97
Parameter Value
1 Origin Bruker BioSpin GmbH
2 Solvent CDCl3
3 Temperature 298.7
4 Number of Scans 51
5 Spectrometer Frequency 100.61
6 Nucleus 13C
f1 (ppm)


7.949
7.946
7.942
7.940
7.937
7.943
7.240
7.110
7.145
7.132
7.128
7.124
7.112
7.106
3.572
3.555
3.539
2.982
2.964
2.946
1.833
1.806
1.788
1.768
1.730
1.570
1.557
1.551
1.541
1.532
1.526
1.519
1.512
1.493
Parameter
1 Origin Bruker BioSpin GmbH
2 Solvent CDCl3
3 Temperature 298.6
4 Number of Scans 8
5 Spectrometer Frequency 400.13
6 Nucleus 1H
O
Cl
F
2.03
2.03
2.00
2.00
1.97
1.94
1.96
f1 (ppm)

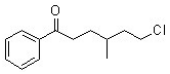
12b


198.375
166.969
164.440
133.410
133.381
130.675
130.583
115.792
115.575
77.343
77.026
76.708
44.843
38.231
32.446
26.574
23.418
Parameter Value
1 Origin Bruker BioSpin GmbH
2 Solvent CDCl3
3 Temperature 298.9
4 Number of Scans 157
5 Spectrometer Frequency 100.61
6 Nucleus 13C
12b
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10
f1 (ppm)

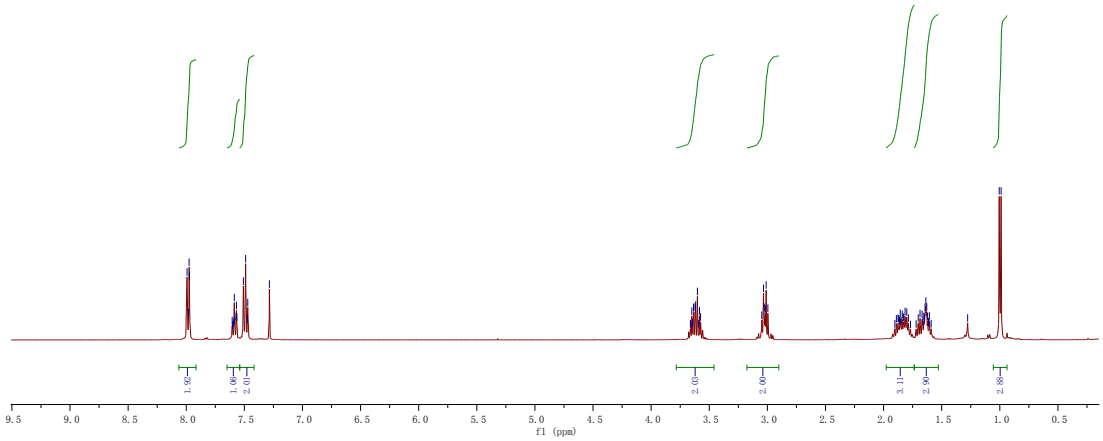

-105.471
Parameter Value
1 Origin Bruker BioSpin GmbH
2 Solvent CDCl3
3 Temperature 298.7
4 Number of Scans 8
5 Spectrometer Frequency 376.50
6 Nucleus 19F
12b
0 -10 -30 -50 -70 -90 -110 -130 -150 -170 -190 -210 -230 -250 -270 -290
f1 (ppm)



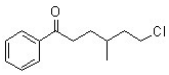
Parameter	Value
1 Origin	Bruker BioSpin GmbH
2 Solvent	CDCl3
3 Temperature	298.1
4 Number of Scans	16
5 Spectrometer Frequency	400.13
6 Nucleus	1H



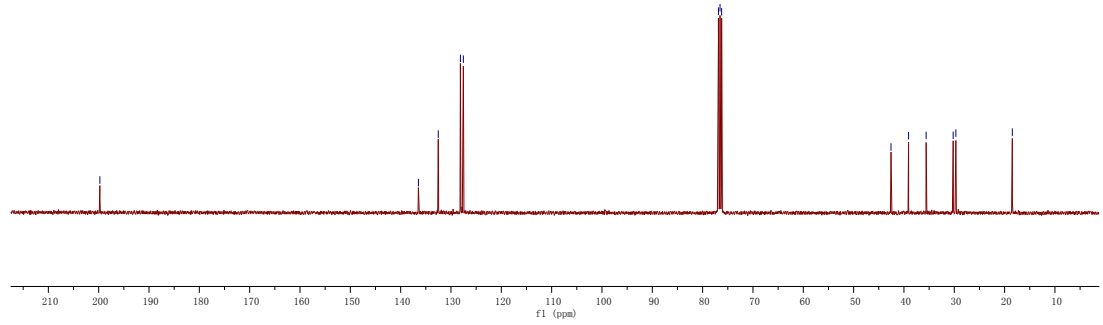
12c

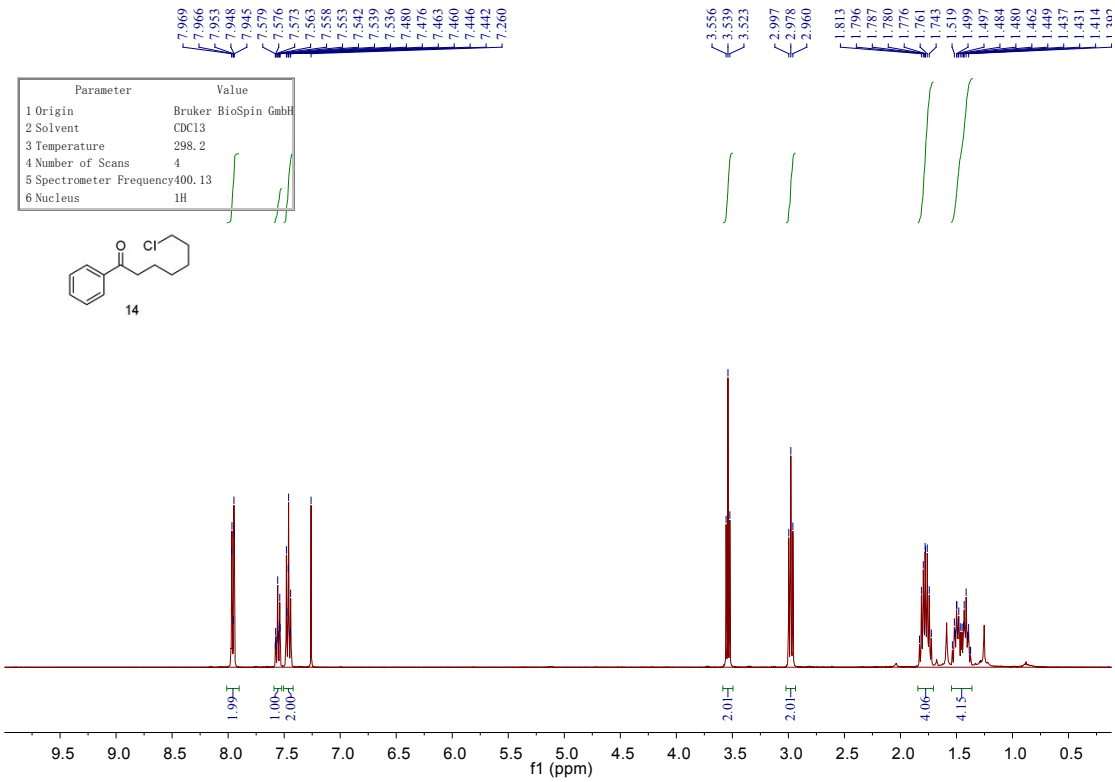


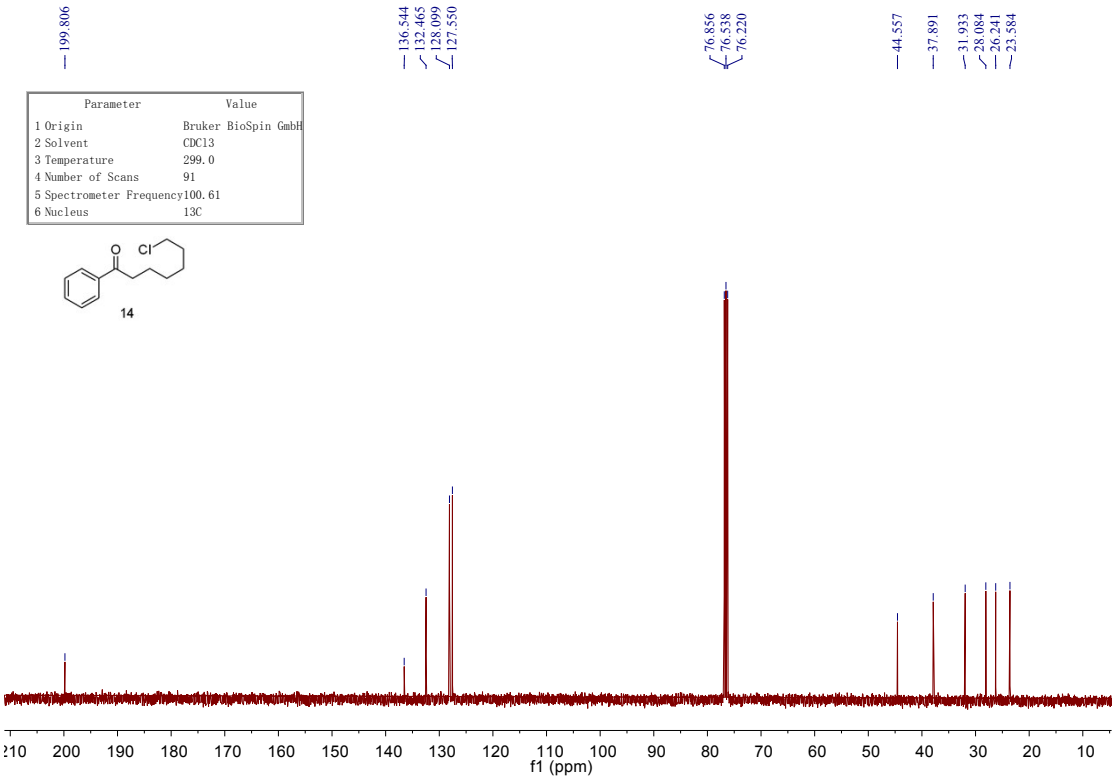
Parameter	Value
1 Origin	Bruker BioSpin GmbH
2 Solvent	CDCl3
3 Temperature	298.2
4 Number of Scans	400
5 Spectrometer Frequency	100.61
6 Nucleus	13C

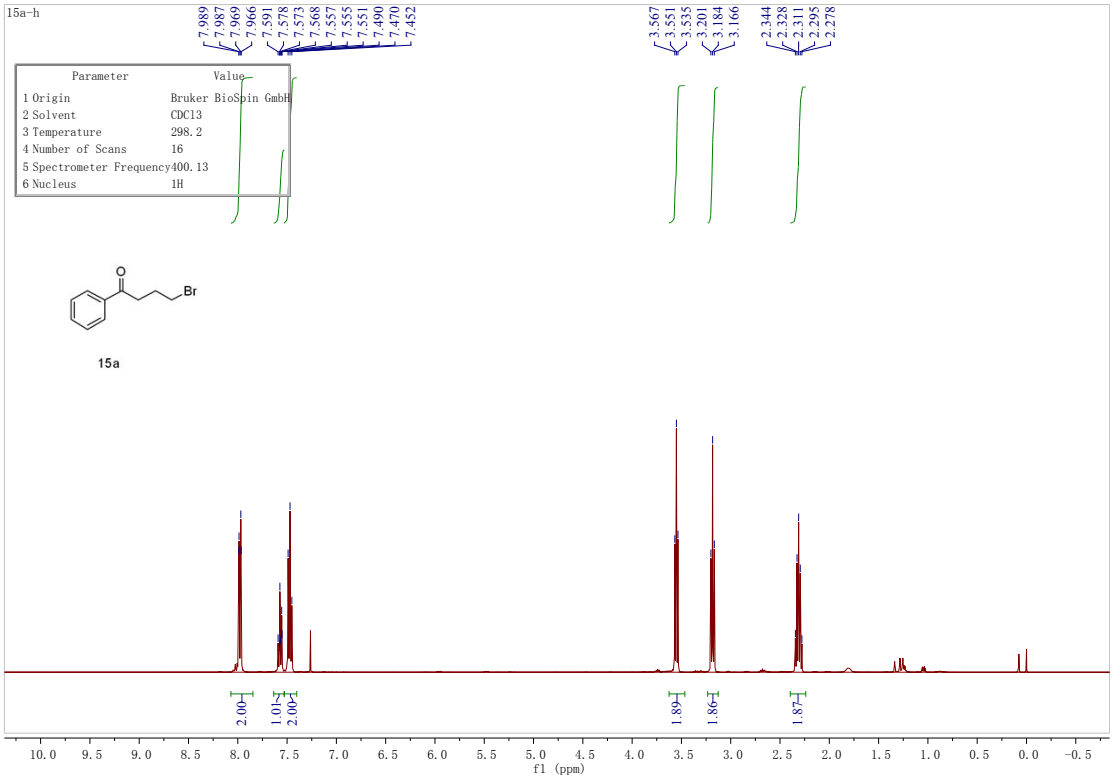


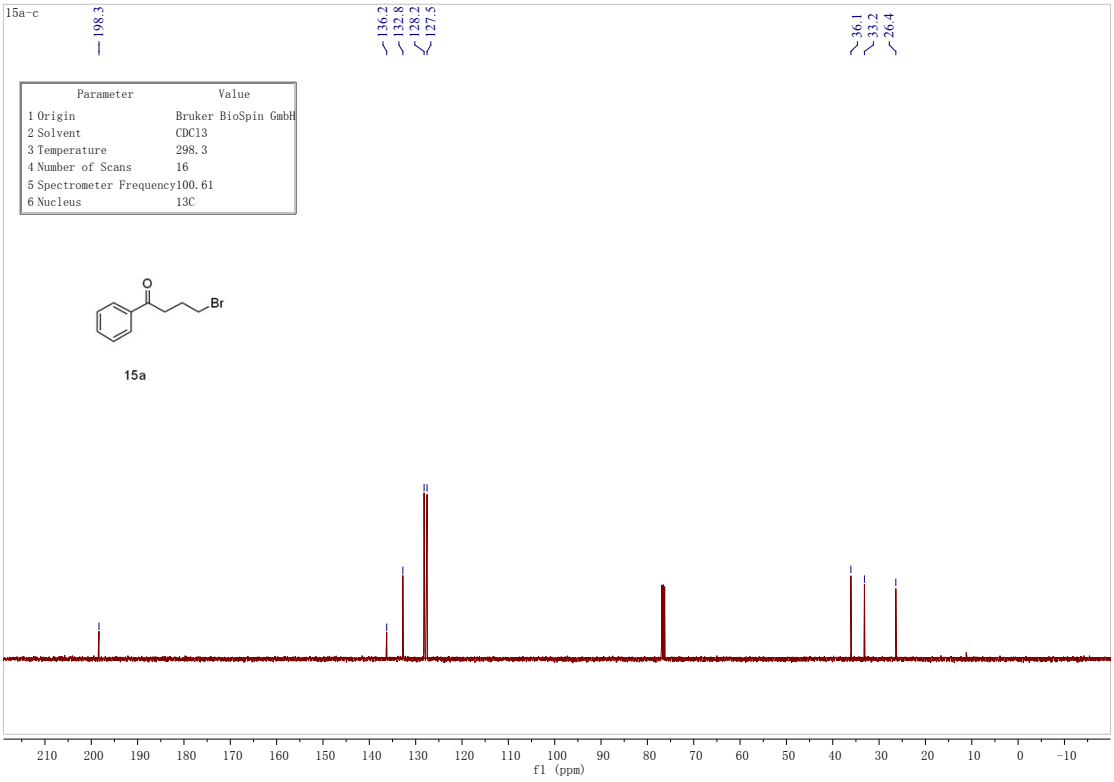
12c



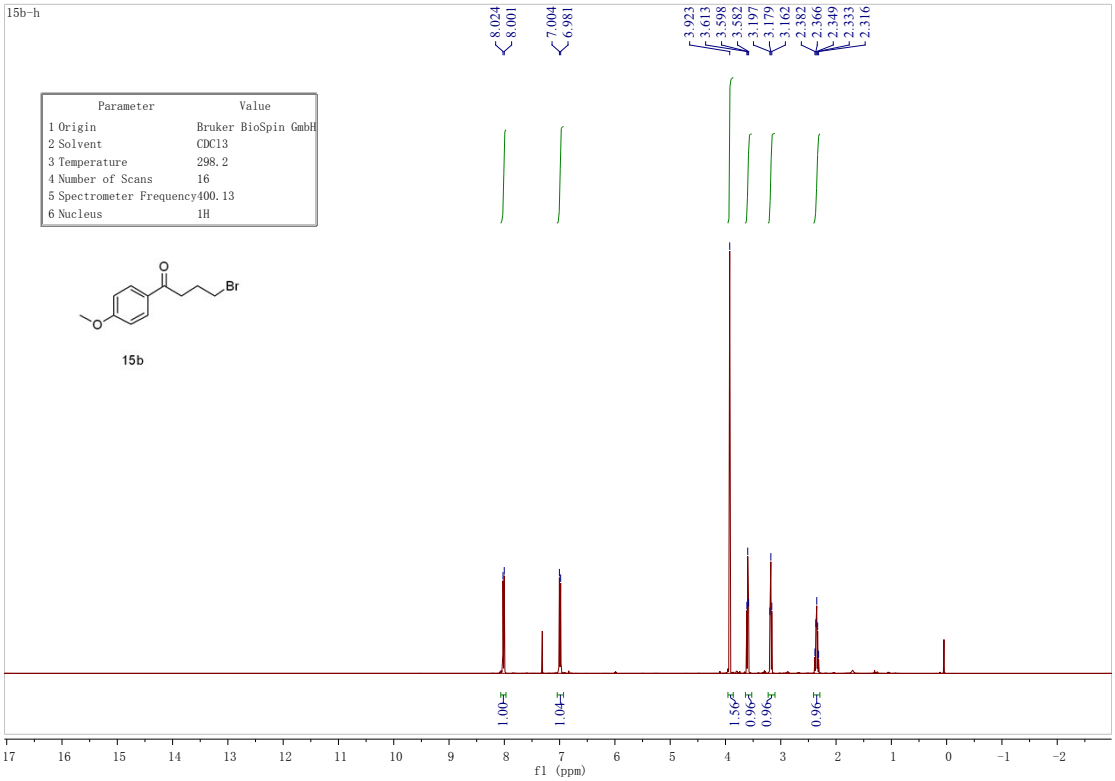

7.969
7.966
7.953
7.948
7.945
7.579
7.576
7.573
7.563
7.558
7.553
7.542
7.539
7.536
7.480
7.476
7.463
7.460
7.446
7.442
7.260
3.556
3.539
3.523
2.997
2.978
2.960
1.813
1.796
1.787
1.780
1.776
1.761
1.743
1.519
1.499
1.497
1.484
1.480
1.462
1.449
1.437
1.431
1.414
Parameter Value
1 Origin Bruker BioSpin GmbH
2 Solvent CDCl3
3 Temperature 298.2
4 Number of Scans 4
5 Spectrometer Frequency 400.13
6 Nucleus 1H
O
Cl
14
1.99
1.00
2.00
2.01
2.01
4.06
4.15
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
f1 (ppm)


199.806
136.544
132.465
128.099
127.550
76.856
76.538
76.220
44.557
37.891
31.933
28.084
26.241
23.584
Parameter Value
1 Origin Bruker BioSpin GmbH
2 Solvent CDCl3
3 Temperature 299.0
4 Number of Scans 91
5 Spectrometer Frequency 100.61
6 Nucleus 13C
O
Cl
14
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10
f1 (ppm)


15a-h
7.989
7.987
7.969
7.966
7.591
7.578
7.573
7.568
7.557
7.555
7.551
7.490
7.470
7.452
3.567
3.551
3.535
3.201
3.184
3.166
2.344
2.328
2.311
2.295
2.278
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
Br
15a
2.00
1.01
2.00
1.89
1.86
1.87
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)


15a-c
198.3
136.2
132.8
128.2
127.5
36.1
33.2
26.4
Parameter Value
1 Origin Bruker BioSpin GmbH
2 Solvent CDCl3
3 Temperature 298.3
4 Number of Scans 16
5 Spectrometer Frequency 100.61
6 Nucleus 13C
O
Br
15a
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)

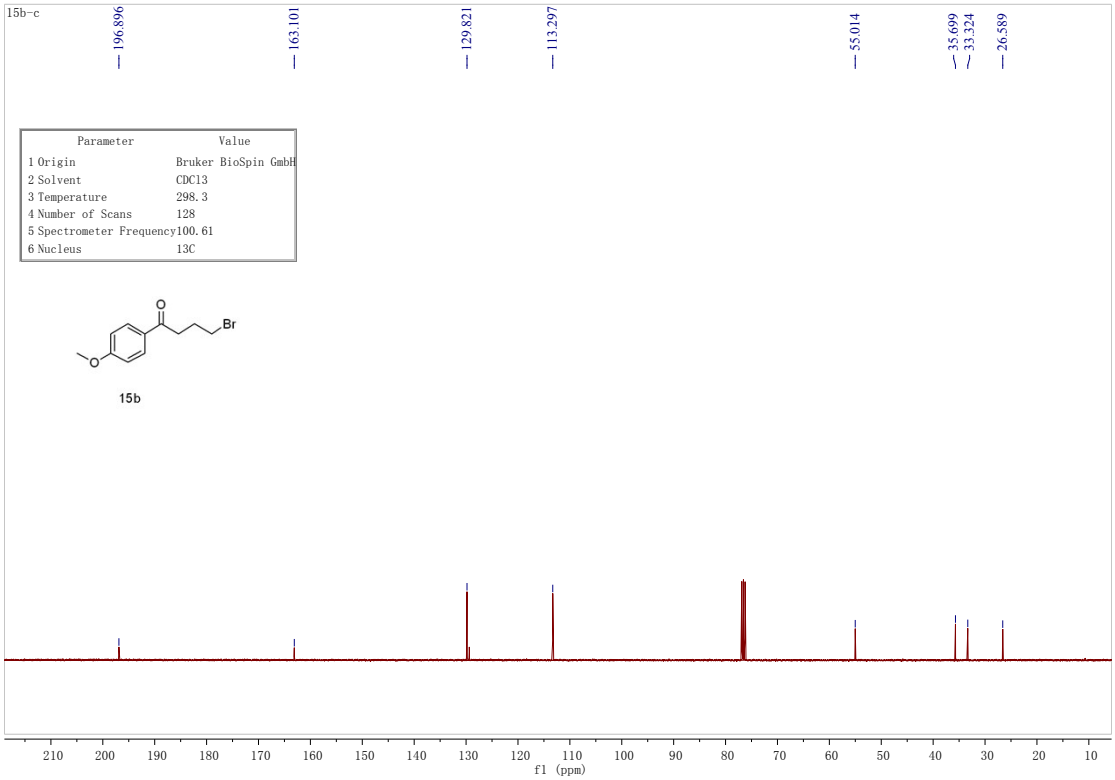
15b-h



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

15b

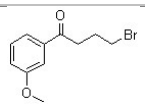
15b-c



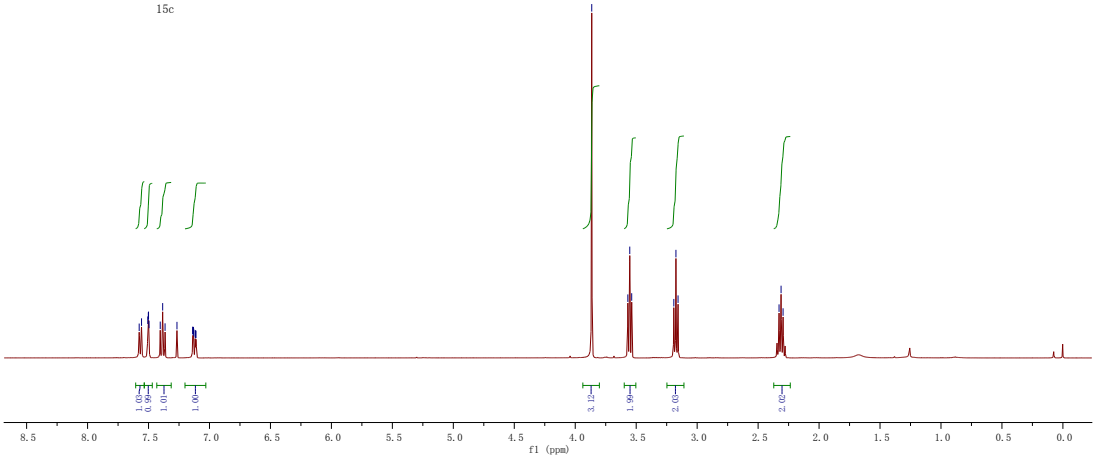
Parameter	Value
1 Origin	Bruker BioSpin GmbH
2 Solvent	CDCl3
3 Temperature	298.3
4 Number of Scans	128
5 Spectrometer Frequency	100.61
6 Nucleus	13C

15b

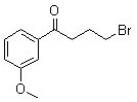
Parameter	Value
1 Origin	Bruker BioSpin GmbH
2 Solvent	CDCl3
3 Temperature	298.1
4 Number of Scans	16
5 Spectrometer Frequency	400.13
6 Nucleus	1H



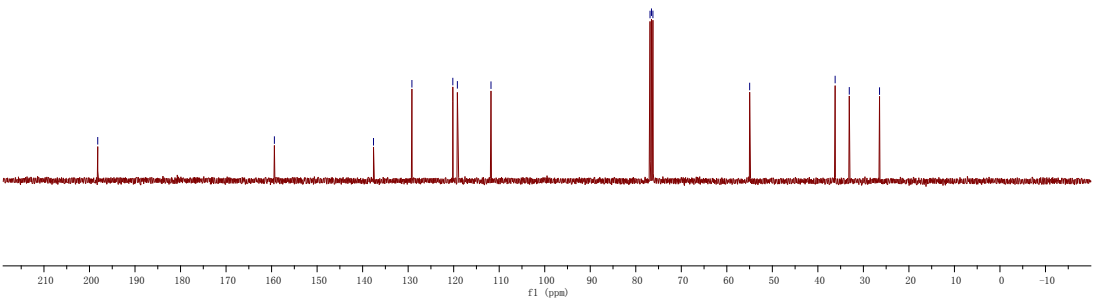
15c

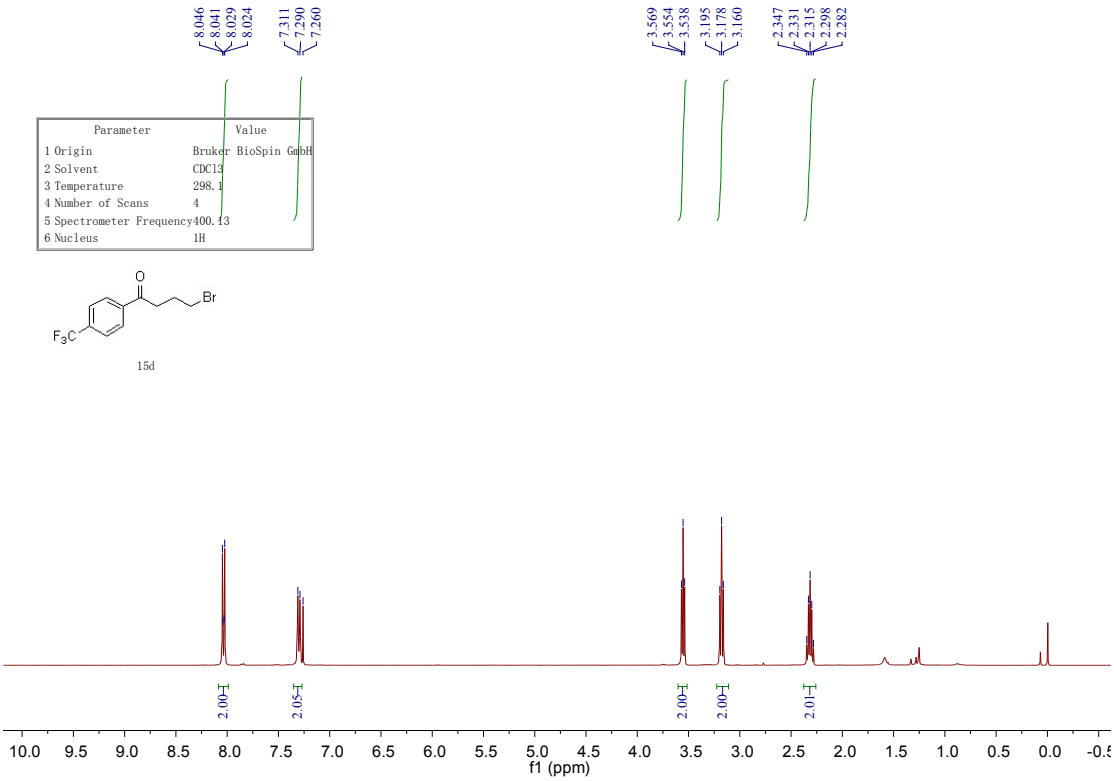


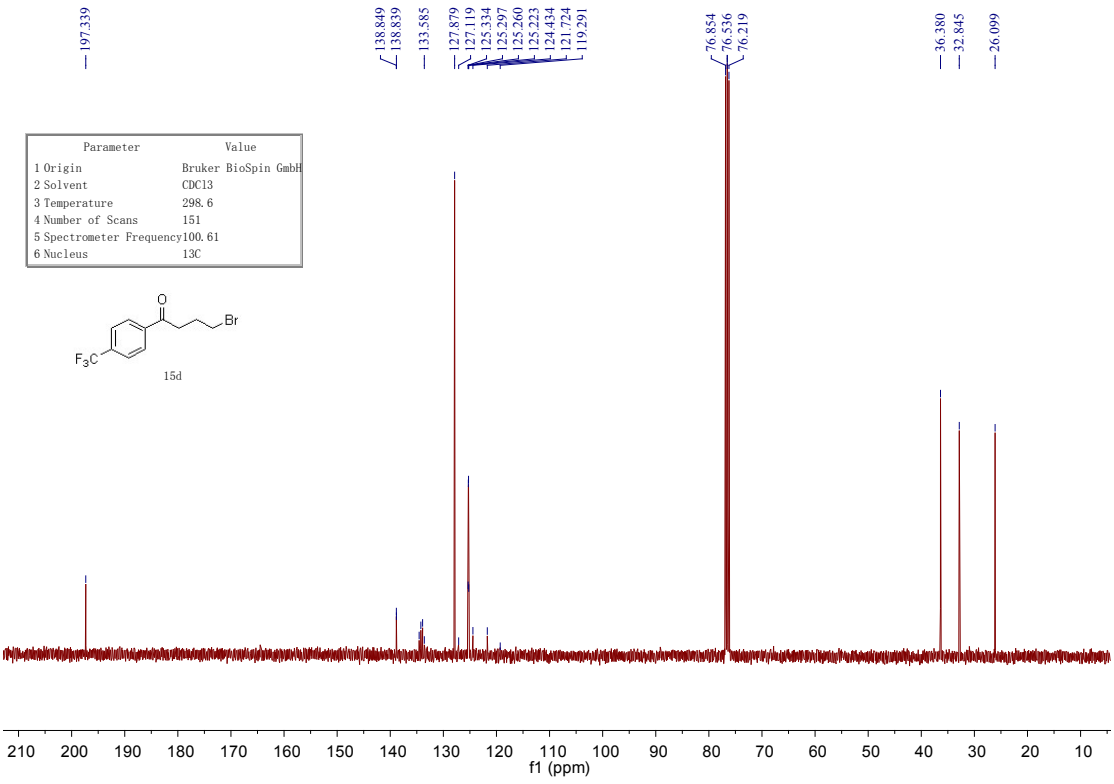
Parameter	Value
1 Origin	Bruker BioSpin GmbH
2 Solvent	CDCl3
3 Temperature	298.4
4 Number of Scans	65
5 Spectrometer Frequency	100.61
6 Nucleus	13C

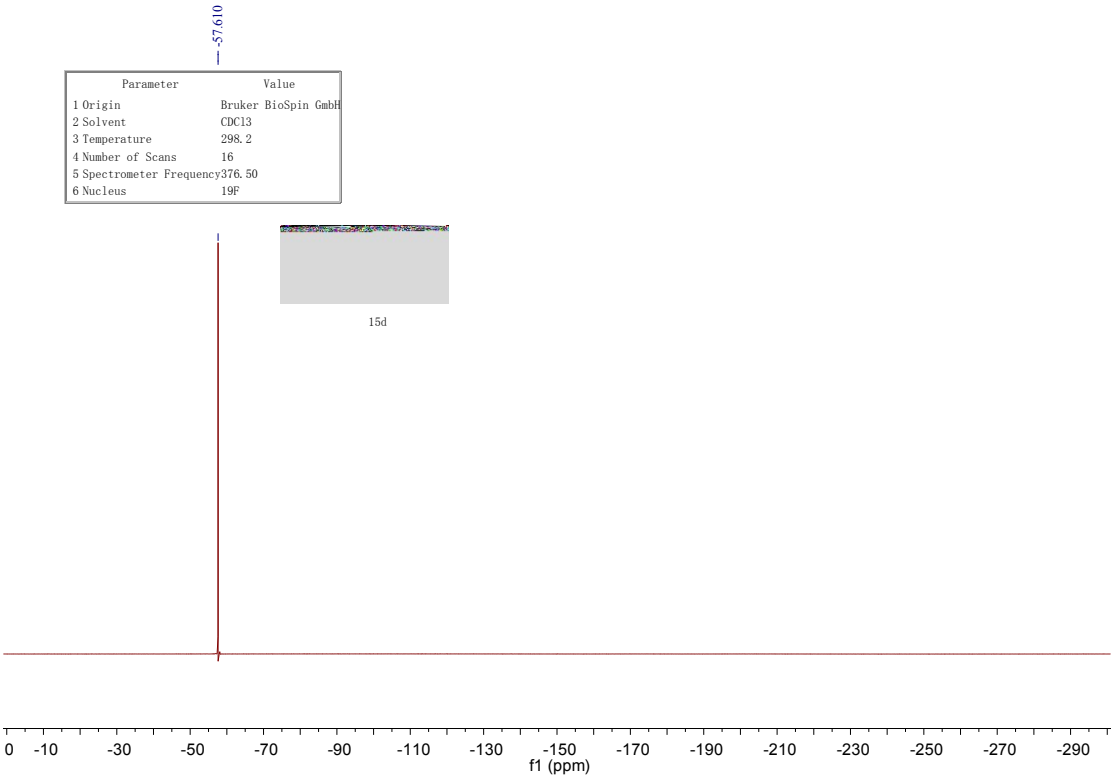


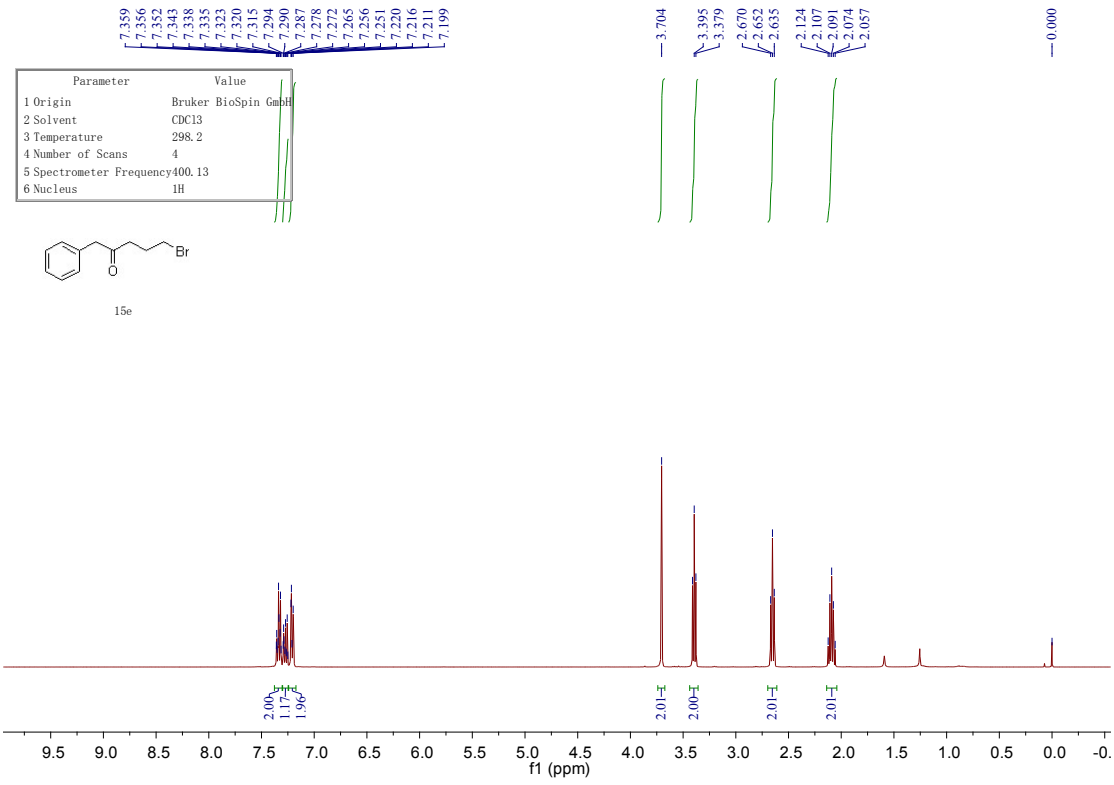
15c

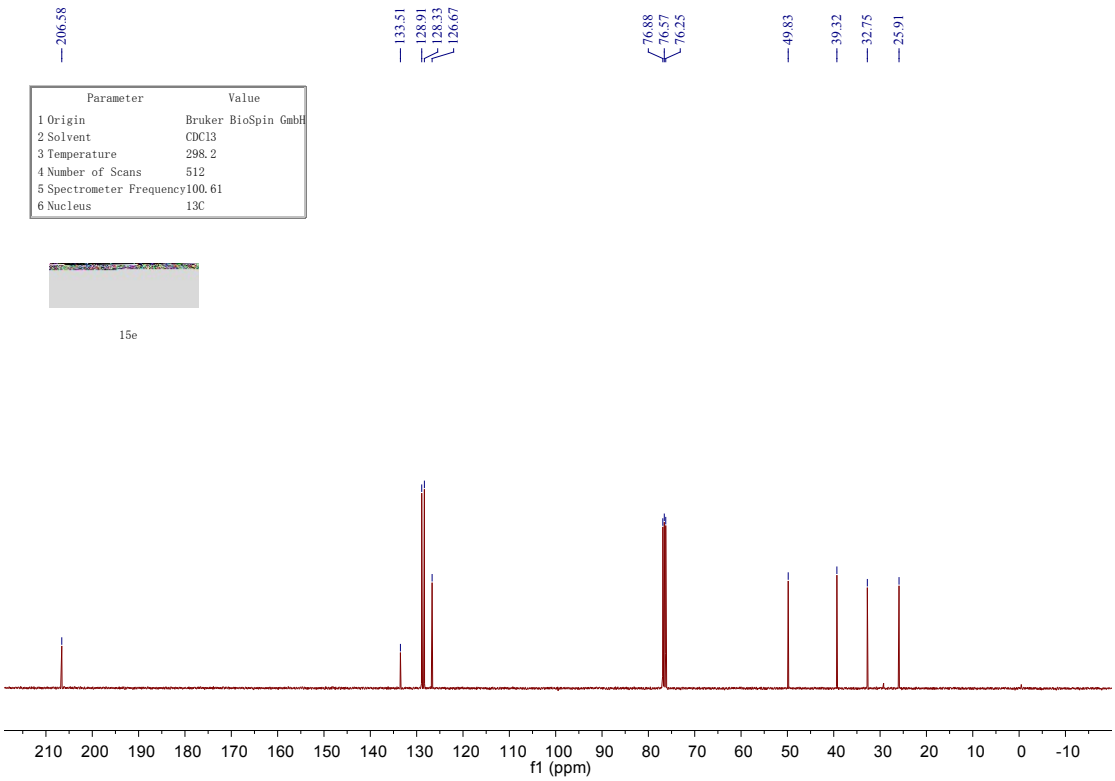



8.046
8.041
8.029
8.024
7.311
7.290
7.260
3.569
3.554
3.538
3.195
3.178
3.160
2.347
2.331
2.315
2.298
2.282
Parameter Value
1 Origin Bruker BioSpin GmbH
2 Solvent CDCl3
3 Temperature 298.1
4 Number of Scans 4
5 Spectrometer Frequency 400.13
6 Nucleus 1H
O
Br
F3C
15d
2.00
2.05
2.00
2.00
2.01
10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)


197.339
138.849
138.839
133.585
127.879
127.119
125.334
125.297
125.260
125.223
124.434
121.724
119.291
76.854
76.536
76.219
36.380
32.845
26.099
Parameter Value
1 Origin Bruker BioSpin GmbH
2 Solvent CDCl3
3 Temperature 298.6
4 Number of Scans 151
5 Spectrometer Frequency 100.61
6 Nucleus 13C
O
Br
F3C
15d
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10
f1 (ppm)


-57.610
Parameter Value
1 Origin Bruker BioSpin GmbH
2 Solvent CDCl3
3 Temperature 298.2
4 Number of Scans 16
5 Spectrometer Frequency 376.50
6 Nucleus 19F
15d
0 -10 -30 -50 -70 -90 -110 -130 -150 -170 -190 -210 -230 -250 -270 -290
f1 (ppm)


7.359 7.356 7.352 7.343 7.338 7.335 7.323 7.320 7.315 7.294 7.290 7.287 7.278 7.272 7.265 7.256 7.251 7.220 7.216 7.211 7.199
3.704 3.395 3.379 2.670 2.652 2.635 2.124 2.107 2.091 2.074 2.057
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
Br
O
15e
2.00 1.17 1.96 2.01 2.00 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.
f1 (ppm)


206.58
133.51
128.91
128.33
126.67
76.88
76.57
76.25
49.83
39.32
32.75
25.91
Parameter Value
1 Origin Bruker BioSpin GmbH
2 Solvent CDCl3
3 Temperature 298.2
4 Number of Scans 512
5 Spectrometer Frequency 100.61
6 Nucleus 13C
15e
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)