Supporting Information

Visible light-Promoted Ring-Opening Functionalization of Unstrained Cycloalkanols via Inert C-C Bond Scission

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Table of Contents

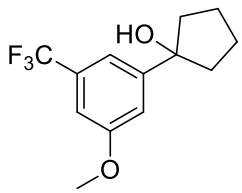
1. General experimental details

All reactions were maintained under a nitrogen atmosphere unless otherwise stated. Commercially available reagents were used without further purification. Infrared (FT-IR) spectra were recorded on a BRUKER VERTEX 70, ν_{max} in cm^{-1}. ^{1}H-NMR spectra were recorded on a BRUKER AVANCE III HD (400 MHz) spectrometer. Chemical shifts are reported in ppm from tetramethylsilane with the solvent resonance as internal standard ($CDCl_3$: δ 7.26). Data are reported as follows: chemical shift, multiplicity (s = singlet, d = doublet, t = triplet, q = quadruplet, br = broad, m = multiplet), coupling constants (Hz) and integration. ^{13}C-NMR spectra were recorded on a BRUKER AVANCE III HD (100 MHz) spectrometer with complete proton decoupling. Chemical shifts are reported in ppm from tetramethylsilane with the solvent resonance as the internal standard ($CDCl_3$: δ 77.16). ^{19}F-NMR spectra were recorded on a BRUKER AVANCE III HD (376 MHz) spectrometer. Mass spectra were measured with an Agilent Technologies 6120 Quadrupole LC/MS. High resolution mass spectrometry (HRMS) were measured with a GCT Premier^{TM} and BRUKER micrOTF-Q III. Melting points were measured using INESA WRR and values are uncorrected.

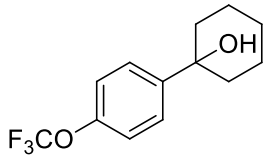
2. General procedure for the ring-opening bromination reactions

Cycloalkanol **1** (0.2 mmol, 1.0 equiv.), photocatalyst $[Ir(ppy)_2(dtbbpy)]PF_6$ (5.5 mg, 0.006 mmol, 3 mol %), PIDA (128.8 mg, 0.4 mmol, 2.0 equiv.), and NBS (53.4 mg, 0.3 mmol, 1.5 equiv.) were loaded in a reaction vial which was subjected to evacuation/ flushing with N_2 three times. $PhCF_3$/ H_2O (2 ml/ 0.1 ml) or CCl_4/ H_2O (2 ml/ 0.1 ml) was added to the mixture via syringe and the reaction was irradiated with 14 W blue LEDs. After the reaction completion, the reaction mixture was extracted with ethyl acetate (3 x 10 mL). The combined organic extracts were washed by brine, dried over Na_2SO_4, filtered, concentrated, and purified by flash column chromatography on silica gel (eluent: ethyl acetate/ petroleum ether) to give the desired product **2**.

3. Characterization of new starting materials

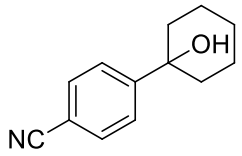


1h: white solid, m.p. 37-39 °C. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.33-7.31 (m, 1H), 7.24-7.22 (m, 1H), 7.01-6.99 (m, 1H), 3.85 (s, 3H), 2.05-1.82 (m, 8H), 1.75 (s, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 159.2, 149.5, 131.1 (q, J_{C-F} = 31.8 Hz), 123.6 (q, J_{C-F} = 270.9 Hz), 114.4, 113.8 (q, J_{C-F} = 3.9 Hz), 108.2 (q, J_{C-F} = 3.8 Hz), 82.7, 55.0, 41.8, 23.4; ^{19}F NMR (376 MHz, $CDCl_3$) δ -62.5 (s). FT-IR: ν (cm^{-1}) 3354, 2953, 2852, 2361, 1723, 1213. HRMS [ESI] calcd for $C_{13}H_{15}F_3O_2Na$ $[M+Na]^+$ 283.0916, found 283.0914.

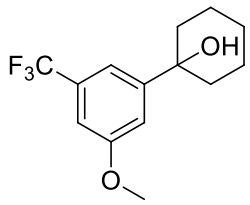


1p: white solid, m.p. 57-59 °C. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.56-7.49 (m, 2H), 7.21-7.15 (m, 2H), 1.85-1.60 (m, 10H), 1.35-1.22 (m, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 147.6, 147.4 (q, J_{C-F} = 16.4 Hz), 125.7, 120.1, 120.0 (q, J_{C-F} = 255.2 Hz), 72.4, 38.4, 24.9, 21.6; ^{19}F NMR (376 MHz, $CDCl_3$) δ -57.9 (s). FT-IR: ν (cm^{-1}) 3316, 2932, 2859, 1509, 1390,

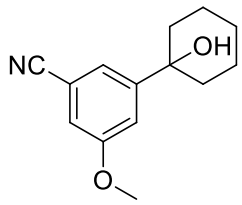
1251. HRMS [ESI] calcd for $C_{13}H_{15}F_3O_2Na$ $[M+Na]^+$ 283.0916, found 283.0921.



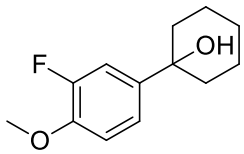
1q: white solid, m.p. 65-66 °C. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.62-7.54 (m, 5H), 2.23 (s, 1H), 1.80-1.60 (m, 9H), 1.33-1.21 (m, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 154.6, 131.5, 125.1, 118.5, 109.7, 72.8, 38.0, 24.8, 21.3. FT-IR: ν (cm^{-1}) 3338, 2936, 2864, 2230, 1607, 1264. HRMS [ESI] calcd for $C_{13}H_{15}NONa$ $[M+Na]^+$ 224.1046, found 224.1033.



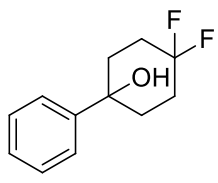
1s: yellow solid, m.p. 64-66 °C. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.35 (s, 1H), 7.28-7.25 (m, 1H), 7.01 (s, 1H), 3.86 (s, 3H), 1.87-1.59 (m, 10H), 1.38-1.25 (m, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 159.3, 151.9, 131.1 (q, $J_{C\text{-}F}$ = 31.7 Hz), 123.6 (q, $J_{C\text{-}F}$ = 270.9 Hz), 114.0 (q, $J_{C\text{-}F}$ = 0.9 Hz), 113.4 (d, $J_{C\text{-}F}$ = 3.9 Hz), 108.1 (q, $J_{C\text{-}F}$ = 3.8 Hz), 72.7, 55.0, 38.3, 24.8, 21.5; ^{19}F NMR (376 MHz, $CDCl_3$) δ -62.5 (s). FT-IR: ν (cm^{-1}) 3349, 3007, 2944, 2856, 1601, 1258. HRMS [ESI] calcd for $C_{14}H_{18}F_3O_2$ $[M+H]^+$ 275.1253, found 275.1257.



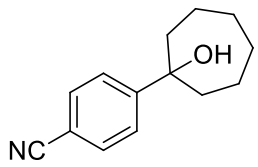
1t: yellow oil. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.36 (dd, J = 1.6, 1.6 Hz, 1H), 7.30 (dd, J = 2.4, 1.6 Hz, 1H), 6.98 (dd, J = 2.4, 1.2 Hz, 1H), 3.82 (s, 3H), 1.90 (s, 1H), 1.82-1.60 (m, 9H), 1.34-1.20 (m, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 159.2, 152.4, 120.8, 118.6, 115.8, 114.2, 112.3, 72.5, 55.1, 38.2, 24.8, 21.4. FT-IR: ν (cm^{-1}) 3448, 2929, 2853, 2231, 1590, 1260. HRMS [ESI] calcd for $C_{14}H_{17}NO_2Na$ $[M+Na]^+$ 254.1151, found 254.1156.



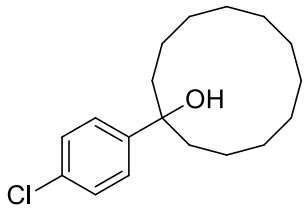
1u: yellow solid, m.p. 54-55 °C. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.23 (dd, J = 13.2, 2.4 Hz, 1H), 7.20-7.16 (m, 1H), 6.92 (dd, J = 8.8, 8.8 Hz, 1H), 3.87 (s, 3H), 1.80-1.58 (m, 10H), 1.32-1.20 (m, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 151.6 (d, $J_{C\text{-}F}$ = 243.2 Hz), 145.6 (d, $J_{C\text{-}F}$ = 10.8 Hz), 142.4 (d, $J_{C\text{-}F}$ = 4.9 Hz), 119.7 (d, $J_{C\text{-}F}$ = 3.5 Hz), 112.6 (d, $J_{C\text{-}F}$ = 6.9 Hz), 112.5 (d, $J_{C\text{-}F}$ = 14.2 Hz), 72.1, 55.8, 38.4, 24.9, 21.7; ^{19}F NMR (376 MHz, $CDCl_3$) δ -135.2 (s). FT-IR: ν (cm^{-1}) 3400, 3017, 2926, 2858, 1624, 1270. HRMS [ESI] calcd for $C_{13}H_{17}FO_2Na$ $[M+Na]^+$ 247.1105, found 247.1117.



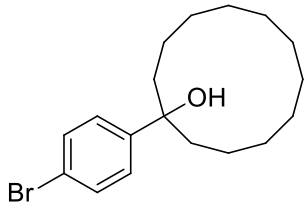
1ab: red solid, m.p. 50-51 °C. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.54-7.47 (m, 2H), 7.42-7.35 (m, 2H), 7.33-7.27 (m, 1H), 2.40-2.00 (m, 6H), 1.92-1.84 (m, 2H), 1.64 (s, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 146.9, 128.0, 126.9, 123.9, 123.1 (dd, $J_{C\text{-}F}$ = 241.3, 237.1 Hz), 71.4 (d, $J_{C\text{-}F}$ = 1.7 Hz), 34.9 (d, $J_{C\text{-}F}$ = 9.7 Hz), 29.4 (dd, $J_{C\text{-}F}$ = 25.0, 23.6 Hz); ^{19}F NMR (376 MHz, $CDCl_3$) δ -92.4 (d, J = -235.3 Hz), -104.2 (d, J = -235.3 Hz). FT-IR: ν (cm^{-1}) 3577, 3450, 3089, 2855, 1493, 1286. HRMS [ESI] calcd for $C_{12}H_{15}F_2O$ $[M+H]^+$ 213.1085, found 213.1089.



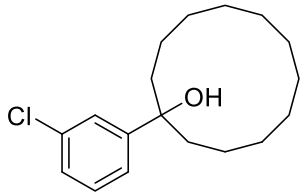
1ai: yellow solid, m.p. 57-59 °C. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.63-7.55 (m, 4H), 2.05-1.93 (m, 3H), 1.88-1.54 (m, 10H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 155.8, 131.5, 124.9, 118.5, 109.7, 76.3, 42.6, 28.3, 22.0. FT-IR: ν (cm^{-1}) 3458, 3342, 2920, 2226, 1459, 1245. HRMS [ESI] calcd for $C_{14}H_{17}NONa$ $[M+Na]^+$ 238.1202, found 238.1196.



1an: white solid, m.p. 141-143 °C. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.42-7.36 (m, 2H), 7.30-7.25 (m, 2H), 1.89-1.75 (m, 5H), 1.44-1.12 (m, 18H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 146.4, 132.0, 127.5, 126.3, 75.7, 34.9, 25.8, 25.5, 21.9, 21.6, 19.4. FT-IR: ν (cm^{-1}) 3268, 2926, 2848, 1487, 1397, 1252. HRMS [ESI] calcd for $C_{18}H_{27}ClONa$ $[M+Na]^+$ 317.1643, found 317.1651.

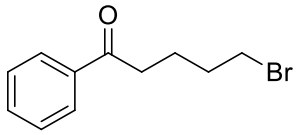


1ao: white solid, m.p. 145-146 °C. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.47-7.41 (m, 2H), 7.37-7.31 (m, 2H), 1.87-1.77 (m, 4H), 1.71 (s, 1H), 1.44-1.15 (m, 18H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 146.9, 130.5, 126.7, 120.2, 75.8, 34.9, 25.8, 25.5, 22.0, 21.6, 19.4. FT-IR: ν (cm^{-1}) 3270, 2926, 2848, 1485, 1394, 1252. HRMS [ESI] calcd for $C_{18}H_{27}BrONa$ $[M+Na]^+$ 361.1137, found 361.1130.

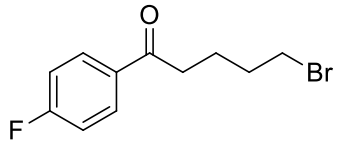


1ap: white solid, m.p. 138-139 °C. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.48 (dd, *J* = 1.6, 1.6 Hz, 1H), 7.37-7.33 (m, 1H), 7.29-7.20 (m, 2H), 1.95 (s, 1H), 1.88-1.78 (m, 4H), 1.46-1.16 (m, 18H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 150.5, 134.0, 129.2, 126.8, 125.7, 123.6, 76.3, 35.4, 26.2, 26.0, 22.5, 22.1, 19.8. FT-IR: ν (cm^{-1}) 3235, 2942, 2847, 1593, 1417, 1250. HRMS [ESI] calcd for $C_{18}H_{27}ClONa$ $[M+Na]^+$ 317.1643, found 317.1642.

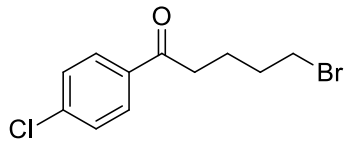
4. Characterization of products



2a: yellow solid, m.p. 53-55 °C. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.99-7.86 (m, 2H), 7.56-7.49 (m, 1H), 7.46-7.39 (m, 2H), 3.41 (t, *J* = 6.4 Hz, 2H), 2.97 (t, *J* = 6.8 Hz, 2H), 2.05-1.75 (m, 4H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 199.0, 136.3, 132.6, 128.1, 127.5, 36.9, 33.0, 31.7, 22.3. FT-IR: ν (cm^{-1}) 3653, 3335, 3060, 2866, 1674, 1343. HRMS [ESI] calcd for $C_{11}H_{13}BrONa$ $[M+Na]^+$ 263.0042, found 263.0048.

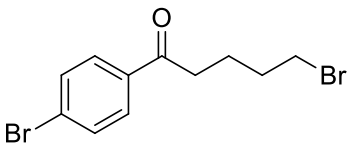


2b: yellow oil. ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.02-7.95 (m, 2H), 7.17-7.09 (m, 2H), 3.45 (t, *J* = 6.4 Hz, 2H), 2.99 (t, *J* = 6.8 Hz, 2H), 2.05-1.83 (m, 4H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 197.4, 165.3 (d, J_{C-F} = 253.2 Hz), 132.8 (d, J_{C-F} = 3.0 Hz), 130.2 (d, J_{C-F} = 9.2 Hz), 115.2 (d, J_{C-F} = 21.7 Hz), 36.9, 32.8, 31.7, 22.2; ^{19}F NMR (376 MHz, $CDCl_3$) δ -105.3 (s). FT-IR: ν (cm^{-1}) 3073, 2962, 2866, 1677, 1459, 1272. HRMS [ESI] calcd for $C_{11}H_{12}BrFONa$ $[M+Na]^+$ 280.9948, found 280.9955.

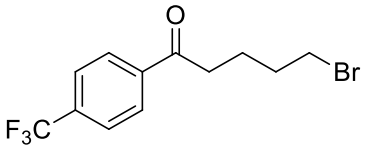


2c: yellow solid, m.p. 41-42 °C. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.94-7.85 (m, 2H), 7.48-7.39 (m, 2H), 3.45 (t, *J* = 6.4 Hz, 2H), 2.98 (t, *J* = 6.8 Hz, 2H), 2.02-1.84 (m, 4H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 197.8, 139.1, 134.6, 129.0, 128.5, 36.9, 32.8, 31.6, 22.2.

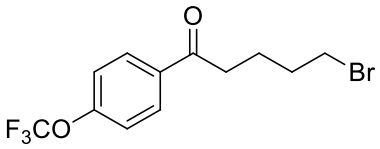
FT-IR: ν (cm^{-1}) 3036, 2933, 2851, 1934, 1676, 1255. HRMS [ESI] calcd for $C_{11}H_{12}BrClONa$ $[M+Na]^+$ 296.9652, found 296.9648.



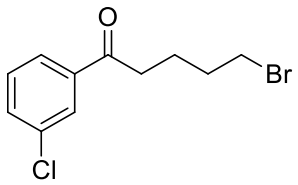
2d: yellow solid, m.p. 50-52 °C. ^1H NMR (400 MHz, $CDCl_3$) δ 7.85-7.78 (m, 2H), 7.64-7.56 (m, 2H), 3.45 (t, *J* = 6.4 Hz, 2H), 2.97 (t, *J* = 6.8 Hz, 2H), 2.00-1.82 (m, 4H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 198.0, 135.0, 131.5, 129.1, 127.8, 36.9, 32.8, 31.6, 22.2. FT-IR: ν (cm^{-1}) 2942, 2861, 2168, 1686, 1466, 1221. HRMS [ESI] calcd for $C_{11}H_{12}Br_2ONa$ $[M+Na]^+$ 340.9147, found 340.9157.



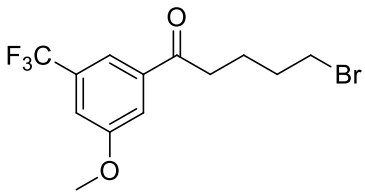
2e: yellow solid, m.p. 33-34 °C. ^1H NMR (400 MHz, $CDCl_3$) δ 8.05 (d, *J* = 8.0 Hz, 2H), 7.73 (d, *J* = 8.0 Hz, 2H), 3.46 (t, *J* = 6.4 Hz, 2H), 3.04 (t, *J* = 6.8 Hz, 2H), 2.02-1.86 (m, 4H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 198.5, 139.4 (q, J_{C-F} = 1.0 Hz), 134.4 (q, J_{C-F} = 32.5 Hz), 128.3, 125.7 (q, J_{C-F} = 3.8 Hz), 123.6 (q, J_{C-F} = 270.9 Hz), 37.8, 33.2, 32.0, 22.5; ^{19}F NMR (376 MHz, $CDCl_3$) δ -63.1 (s). FT-IR: ν (cm^{-1}) 2940, 2869, 1690, 1511, 1409, 1209. HRMS [ESI] calcd for $C_{12}H_{12}BrF_3ONa$ $[M+Na]^+$ 330.9916, found 330.9925.



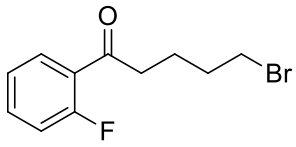
2f: yellow oil. ^1H NMR (400 MHz, $CDCl_3$) δ 8.04-7.98 (m, 2H), 7.29 (d, *J* = 8.0 Hz, 2H), 3.45 (t, *J* = 6.4 Hz, 2H), 3.00 (t, *J* = 6.8 Hz, 2H), 2.02-1.85 (m, 4H); ^{13}C NMR (100 MHz, CDCl3) δ 197.9, 152.6 (q, J_{C-F} = 1.7 Hz), 135.0, 130.0, 120.4 (q, J_{C-F} = 0.7 Hz), 120.3 (q, J_{C-F} = 257.2 Hz), 37.5, 33.2, 32.1, 22.6; ^{19}F NMR (376 MHz, $CDCl_3$) δ -57.6 (s). FT-IR: ν (cm^{-1}) 2940, 2871, 1687, 1505, 1413, 1207. HRMS [ESI] calcd for $C_{12}H_{12}BrF_3O_2Na$ $[M+Na]^+$ 346.9865, found 346.9858.



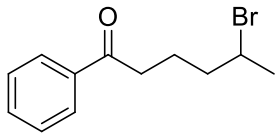
2g: yellow oil. ^1H NMR (400 MHz, $CDCl_3$) δ 7.92 (dd, *J* = 1.6, 1.6 Hz, 1H), 7.85-7.80 (m, 1H), 7.56-7.51 (m, 1H), 7.41 (dd, *J* = 6.8, 6.8 Hz, 1H), 3.45 (t, *J* = 6.4 Hz, 2H), 2.99 (t, *J* = 6.8 Hz, 2H), 2.04-1.78 (m, 4H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 197.7, 137.9, 134.5, 132.6, 129.5, 127.7, 125.6, 37.1, 32.7, 31.6, 22.1. FT-IR: ν (cm^{-1}) 3064, 2919, 2850, 1686, 1469, 1256. HRMS [ESI] calcd for $C_{11}H_{12}BrClONa$ $[M+Na]^+$ 296.9652 found 296.9656.



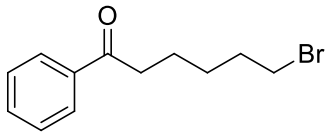
2h: white solid, m.p. 51-53 °C. ^1H NMR (400 MHz, $CDCl_3$) δ 7.77-7.74 (m, 1H), 7.65-7.63 (m, 1H), 7.33-7.31 (m, 1H), 3.90 (s, 3H), 3.46 (t, *J* = 6.4 Hz, 2H), 3.02 (t, *J* = 6.8 Hz, 2H), 2.01-1.87 (m, 4H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 198.0, 160.2, 138.8, 132.3 (q, J_{C-F} = 32.7 Hz), 123.5 (q, J_{C-F} = 271.1 Hz), 117.0 (q, J_{C-F} = 3.8 Hz), 116.0 (q, J_{C-F} = 0.5 Hz), 115.7 (q, J_{C-F} = 3.7 Hz), 55.9, 37.6, 33.2, 32.0, 22.5; ^{19}F NMR (376 MHz, $CDCl_3$) δ -62.8 (s). FT-IR: ν (cm^{-1}) 2954, 2873, 2360, 1684, 1408, 1243. HRMS [ESI] calcd for $C_{13}H_{14}BrF_3O_2Na$ $[M+Na]^+$ 361.0021, found 361.0020.



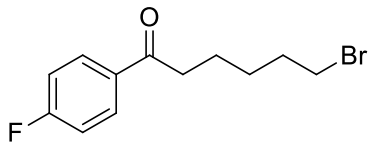
2i: yellow oil. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.86 (ddd, J = 7.6, 7.6, 1.6 Hz, 1H), 7.57-7.46 (m, 1H), 7.23 (ddd, J = 7.6, 7.6, 0.8 Hz, 1H), 7.17-7.10 (m, 1H), 3.44 (t, J = 6.4 Hz, 2H), 3.02 (td, J = 6.8, 3.2 Hz, 2H), 2.00-1.80 (m, 4H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 198.0 (d, J_{C-F} = 4.1 Hz), 161.9 (d, J_{C-F} = 252.6 Hz), 134.5 (d, J_{C-F} = 9.0 Hz), 130.6 (d, J_{C-F} = 2.7 Hz), 125.6 (d, J_{C-F} = 13.0 Hz), 124.5 (d, J_{C-F} = 3.3 Hz), 116.7 (d, J_{C-F} = 23.8 Hz), 42.5 (d, J_{C-F} = 7.3 Hz), 33.3, 32.2, 22.5 (d, J_{C-F} = 2.0 Hz); ^{19}F NMR (376 MHz, $CDCl_3$) δ -109.5 (s). FT-IR: ν (cm^{-1}) 2930, 2869, 1685, 1479, 1365, 1210. HRMS [ESI] calcd for $C_{11}H_{12}BrFONa$ $[M+Na]^+$ 280.9948, found 280.9958.



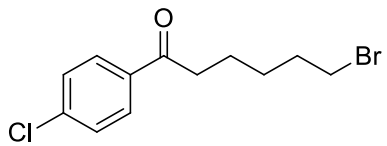
2j: yellow oil. ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.00-7.92 (m, 2H), 7.61-7.53 (m, 1H), 7.51-7.43 (m, 2H), 4.23-4.12 (m, 1H), 3.06-2.94 (m, 2H), 2.04-1.79 (m, 4H), 1.74 (d, J = 6.8 Hz, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 199.7, 136.8, 133.1, 128.6, 128.0, 51.2, 40.5, 37.6, 26.4, 22.4. FT-IR: ν (cm^{-1}) 2964, 2869, 2361, 1683, 1448, 1244. HRMS [ESI] calcd for $C_{12}H_{15}BrONa$ $[M+Na]^+$ 277.0198, found 277.0196.



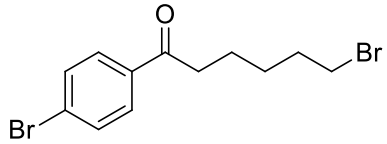
2k: yellow solid, m.p. 33-35 °C. ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.00-7.92 (m, 2H), 7.59 -7.52 (m, 1H), 7.49-7.43 (m, 2H), 3.43 (t, J = 6.8 Hz, 2H), 3.00 (t, J = 7.2 Hz, 2H), 2.01-1.87 (m, 2H), 1.83-1.72 (m, 2H), 1.60-1.48 (m, 2H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 199.5, 136.5, 132.5, 128.1, 127.5, 37.8, 33.2, 32.2, 27.4, 22.8. FT-IR: ν (cm^{-1}) 3057, 2946, 2861, 1969, 1678, 1263. HRMS [ESI] calcd for $C_{12}H_{15}BrONa$ $[M+Na]^+$ 277.0198, found 277.0204.



2l: yellow oil. ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.02-7.94 (m, 2H), 7.16-7.09 (m, 2H), 3.43 (t, J = 6.8 Hz, 2H), 2.96 (t, J = 7.2 Hz, 2H), 1.96-1.87 (m, 2H), 1.81-1.71 (m, 2H), 1.58-1.48 (m, 2H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 197.9, 165.2 (d, J_{C-F} = 253.0 Hz), 132.9 (d, J_{C-F} = 3.0 Hz), 130.1 (d, J_{C-F} = 9.2 Hz), 115.2 (d, J_{C-F} = 21.7 Hz), 37.7, 33.1, 32.1, 27.4, 22.8; ^{19}F NMR (376 MHz, $CDCl_3$) δ -105.4 (s). FT-IR: ν (cm^{-1}) 3053, 2936, 2864, 1917, 1723, 1262. HRMS [ESI] calcd for $C_{12}H_{15}BrFO$ $[M+H]^+$ 273.0285, found 273.0294.

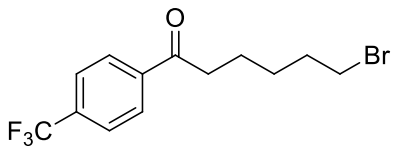


2m: yellow solid, m.p. 38-40 °C. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.92-7.86 (m, 2H), 7.45-7.40 (m, 2H), 3.42 (t, J = 6.8 Hz, 2H), 2.96 (t, J = 7.2 Hz, 2H), 1.96-1.86 (m, 2H), 1.81-1.71 (m, 2H), 1.58-1.48 (m, 2H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 198.2, 139.0, 134.8, 128.9, 128.4, 37.8, 33.1, 32.1, 27.3, 22.7. FT-IR: ν (cm^{-1}) 3092, 2962, 2838, 1937, 1681, 1268. HRMS [ESI] calcd for $C_{12}H_{15}BrClO$ $[M+H]^+$ 288.9989, found 288.9993.

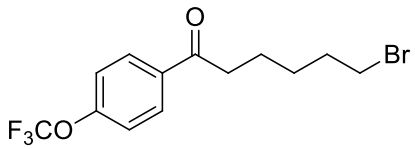


2n: yellow solid, m.p. 41-43 °C. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.85-7.76 (m, 2H), 7.64-7.56 (m, 2H), 3.42 (t, J = 6.8 Hz, 2H), 2.95 (t, J = 7.2 Hz, 2H), 1.96-1.86 (m, 2H), 1.81-1.70 (m, 2H), 1.57-1.46 (m, 2H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 198.4,

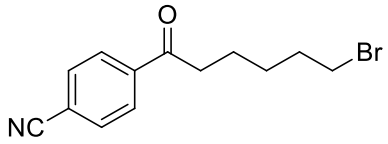
135.2, 131.4, 129.1, 127.7, 37.8, 33.1, 32.1, 27.3, 22.7. FT-IR: ν (cm^{-1}) 3090, 2959, 2861, 1937, 1681, 1269. HRMS [ESI] calcd for $C_{12}H_{15}Br_2O$ $[M+H]^+$ 332.9484, found 332.9498.



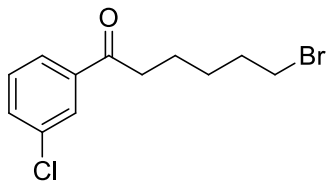
2o: yellow oil. ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.05 (d, *J* = 8.0 Hz, 2H), 7.73 (d, *J* = 8.0 Hz, 2H), 3.43 (t, *J* = 6.8 Hz, 2H), 3.02 (t, *J* = 7.2 Hz, 2H), 1.97-1.88 (m, 2H), 1.83-1.74 (m, 2H), 1.58-1.49 (m, 2H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 198.9, 139.5, 134.3 (q, J_{C-F} = 32.3 Hz), 128.3, 125.7 (q, J_{C-F} = 3.5 Hz), 123.6 (q, J_{C-F} = 271.4 Hz), 38.6, 33.5, 32.6, 27.8, 23.1; ^{19}F NMR (376 MHz, $CDCl_3$) δ -63.1 (s). FT-IR: ν (cm^{-1}) 2961, 2869, 2361, 1692, 1511, 1258. HRMS [ESI] calcd for $C_{13}H_{15}BrF_3O$ $[M+H]^+$ 323.0253, found 323.0245.



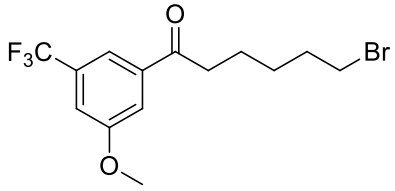
2p: yellow oil. ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.01 (d, *J* = 8.8 Hz, 2H), 7.29 (d, *J* = 8.4 Hz, 2H), 3.43 (t, *J* = 6.8 Hz, 2H), 2.98 (t, *J* = 7.2 Hz, 2H), 2.00-1.86 (m, 2H), 1.83-1.72 (m, 2H), 1.58-1.48 (m, 2H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 198.3, 152.6 (q, J_{C-F} = 1.6 Hz), 135.2, 130.0, 120.4, 120.3 (q, J_{C-F} = 257.2 Hz), 38.3, 33.6, 32.6, 27.8, 23.2; ^{19}F NMR (376 MHz, $CDCl_3$) δ -57.6 (s). FT-IR: ν (cm^{-1}) 2938, 2864, 1687, 1505, 1412, 1251. HRMS [ESI] calcd for $C_{13}H_{15}BrF_3O_2$ $[M+H]^+$ 339.0202, found 339.0197.



2q: yellow solid, m.p. 49-51 °C. ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.04 (d, *J* = 8.4 Hz, 2H), 7.77 (d, *J* = 8.4 Hz, 2H), 3.43 (t, *J* = 6.8 Hz, 2H), 3.01 (t, *J* = 7.2 Hz, 2H), 1.96-1.87 (m, 2H), 1.83-1.73 (m, 2H), 1.58-1.48 (m, 2H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 198.0, 139.4, 132.1, 127.9, 117.5, 115.8, 38.1, 33.0, 32.0, 27.2, 22.5. FT-IR: ν (cm^{-1}) 3093, 2952, 2849, 2232, 1687, 1216. HRMS [ESI] calcd for $C_{13}H_{14}BrNONa$ $[M+Na]^+$ 302.0151, found 302.0139.

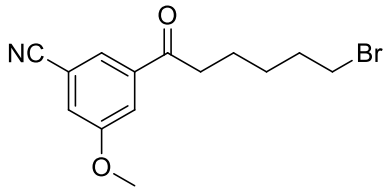


2r: yellow oil. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.93-7.90 (m, 1H), 7.84-7.80 (m, 1H), 7.55-7.51 (m, 1H), 7.41 (dd, *J* = 8.0, 8.0 Hz, 1H), 3.43 (t, *J* = 6.8 Hz, 2H), 2.97 (t, *J* = 7.2 Hz, 2H), 1.96-1.86 (m, 2H), 1.81-1.72 (m, 2H), 1.58-1.49 (m, 2H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 198.1, 138.0, 134.5, 132.5, 129.5, 127.7, 125.6, 37.9, 33.1, 32.1, 27.3, 22.6. FT-IR: ν (cm^{-1}) 3066, 2937, 2859, 1687, 1459, 1205. HRMS [ESI] calcd for $C_{12}H_{15}BrClO$ $[M+H]^+$ 288.9989, found 288.9981.

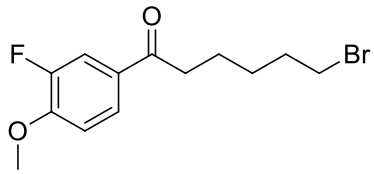


2s: yellow oil. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.75 (s, 1H), 7.64 (s, 1H), 7.31 (s, 1H), 3.90 (s, 3H), 3.43 (t, *J* = 6.8 Hz, 2H), 3.00 (t, *J* = 7.2 Hz, 2H), 1.97-1.88 (m, 2H), 1.83-1.73 (m, 2H), 1.58-1.49 (m, 2H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 198.4, 160.1, 138.9, 132.3 (q, J_{C-F} = 32.6 Hz), 123.5 (q, J_{C-F} = 271.0 Hz), 117.1 (q, J_{C-F} = 3.8 Hz), 116.0 (q, J_{C-F} = 0.4 Hz), 115.6 (q, J_{C-F} = 3.7 Hz), 55.9, 38.4, 33.5, 32.6, 27.8, 23.1; ^{19}F NMR (376 MHz, $CDCl_3$) δ

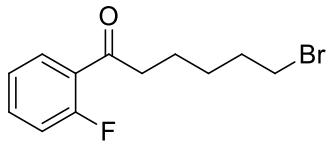
-62.8 (s). FT-IR: ν (cm^{-1}) 3069, 2963, 2852, 1684, 1407, 1266. HRMS [ESI] calcd for $C_{14}H_{16}BrF_3O_2Na$ $[M+Na]^+$ 375.0178, found 375.0171.



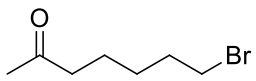
2t: yellow solid, m.p. 54-55 °C. ^1H NMR (400 MHz, $CDCl_3$) δ 7.78 (dd, *J* = 1.2, 1.2 Hz, 1H), 7.68 (dd, *J* = 2.4, 1.2 Hz, 1H), 7.32 (dd, *J* = 2.4, 1.2 Hz, 1H), 3.89 (s, 3H), 3.43 (t, *J* = 6.4 Hz, 2H), 2.97 (t, *J* = 7.2 Hz, 2H), 1.96-1.87 (m, 2H), 1.80-1.72 (m, 2H), 1.58-1.48 (m, 2H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 197.2, 159.6, 138.6, 123.5, 121.0, 117.4, 117.1, 113.3, 55.5, 38.0, 33.0, 32.0, 27.2, 22.5. FT-IR: ν (cm^{-1}) 3079, 2967, 2839, 2232, 1682, 1262. HRMS [ESI] calcd for $C_{14}H_{16}BrNO_2Na$ $[M+Na]^+$ 332.0257, found 332.0270.



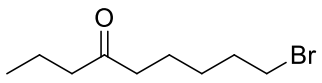
2u: yellow solid, m.p. 52-54 °C. ^1H NMR (400 MHz, $CDCl_3$) δ 7.76-7.71 (m, 1H), 7.69 (dd, *J* = 12.0, 2.0 Hz, 1H), 6.99 (dd, *J* = 8.4, 8.4 Hz, 1H), 3.95 (s, 3H), 3.42 (t, *J* = 6.8 Hz, 2H), 2.92 (t, *J* = 7.2 Hz, 2H), 1.95-1.85 (m, 2H), 1.80-1.70 (m, 2H), 1.57-1.46 (m, 2H); ^{13}C NMR (100MHz, $CDCl_3$) δ 197.7 (d, J_{C-F} = 1.7 Hz), 152.0 (d, J_{C-F} = 246.3 Hz), 151.8 (d, J_{C-F} = 10.8 Hz), 130.3 (d, J_{C-F} = 4.8 Hz), 125.3 (d, J_{C-F} = 3.4 Hz), 115.7 (d, J_{C-F} = 18.8 Hz), 112.3 (d, J_{C-F} = 1.8 Hz), 56.3, 37.9, 33.6, 32.6, 27.9, 23.4; ^{19}F NMR (376 MHz, $CDCl_3$) δ -134.3 (s). FT-IR: ν (cm^{-1}) 3077, 2963, 2854, 1676, 1465, 1218. HRMS [ESI] calcd for $C_{13}H_{16}BrFO_2Na$ $[M+Na]^+$ 325.0210, found 325.0204.



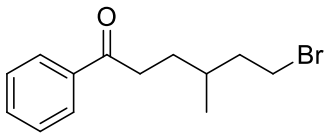
2v: yellow oil. ^1H NMR (400 MHz, $CDCl_3$) δ 7.85 (ddd, *J* = 7.6, 7.6, 2.0 Hz, 1H), 7.54-7.47 (m, 1H), 7.22 (ddd, *J* = 7.6, 7.6, 0.8 Hz, 1H), 7.13 (ddd, *J* = 11.2, 8.4, 0.8 Hz, 1H), 3.42 (t, *J* = 6.8 Hz, 2H), 3.00 (td, *J* = 7.2, 3.2 Hz, 2H), 1.96-1.86 (m, 2H), 1.80-1.70 (m, 2H), 1.57-1.47 (m, 2H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 198.0 (d, J_{C-F} = 4.2 Hz), 161.4 (d, J_{C-F} = 252.7 Hz), 133.9 (d, J_{C-F} = 9.0 Hz), 130.1 (d, J_{C-F} = 2.7 Hz), 125.3 (d, J_{C-F} = 13.1 Hz), 124.0 (d, J_{C-F} = 3.4 Hz), 116.2 (d, J_{C-F} = 23.8 Hz), 42.8 (d, J_{C-F} = 7.0 Hz), 33.1, 32.1, 27.3, 22.6 (d, J_{C-F} = 1.9 Hz); ^{19}F NMR (376 MHz, $CDCl_3$) δ -109.6 (s). FT-IR: ν (cm^{-1}) 3080, 2933, 2858, 1685, 1404, 1210. HRMS [ESI] calcd for $C_{12}H_{15}BrFO$ $[M+H]^+$ 273.0285, found 273.0298.



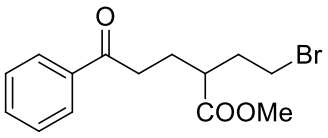
2w: yellow oil. ^1H NMR (400 MHz, $CDCl_3$) δ 3.40 (t, *J* = 6.8 Hz, 2H), 2.45 (t, *J* = 7.2 Hz, 2H), 2.14 (s, 3H), 1.92-1.81 (m, 2H), 1.65-1.55 (m, 2H), 1.48-1.38 (m, 2H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 208.7, 43.4, 33.6, 32.5, 30.0, 27.7, 22.8. FT-IR: ν (cm^{-1}) 2935, 2860, 1713, 1457, 1358, 1228. HRMS [ESI] calcd for $C_7H_{13}BrONa$ $[M+Na]^+$ 215.0042, found 215.0034.



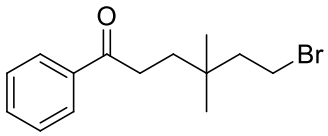
2x: yellow oil. ^1H NMR (400 MHz, $CDCl_3$) δ 3.40 (t, *J* = 6.8 Hz, 2H), 2.45-2.34 (m, 4H), 1.90-1.81 (m, 2H), 1.65-1.54 (m, 4H), 1.47-1.38 (m, 2H), 0.91 (t, *J* = 7.2 Hz, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 211.0, 44.8, 42.4, 33.6, 32.6, 27.8, 22.8, 17.3, 13.8. FT-IR: ν (cm^{-1}) 2961, 2873, 1710, 1458, 1373, 1251. HRMS [ESI] calcd for $C_9H_{18}BrO$ $[M+H]^+$ 221.0536, found 221.0523.



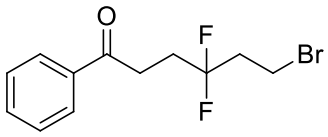
2y: yellow oil. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.98-7.94 (m, 2H), 7.59-7.54 (m, 1H), 7.50-7.44 (m, 2H), 3.54-3.39 (m, 2H), 3.07-2.92 (m, 2H), 1.98-1.88 (m, 1H), 1.87-1.70 (m, 3H), 1.62-1.56 (m, 1H), 0.97 (d, J = 6.4 Hz, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 200.2, 136.9, 133.0, 128.6, 128.0, 39.8, 36.1, 31.8, 31.4, 30.6, 18.8. FT-IR: ν (cm^{-1}) 2960, 2928, 2316, 1683, 1411, 1207. HRMS [ESI] calcd for $C_{13}H_{17}BrONa$ $[M+Na]^+$ 291.0355, found 291.0350.



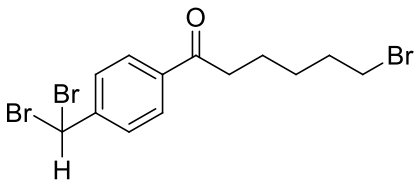
2z: yellow oil. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.97-7.92 (m, 2H), 7.59-7.54 (m, 1H), 7.49-7.43 (m, 2H), 3.70 (s, 3H), 3.52-3.35 (m, 2H), 3.09-2.94 (m, 2H), 2.79-2.70 (m, 1H), 2.35-2.25 (m, 1H), 2.12-1.96 (m, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 198.9, 175.1, 136.7, 133.2, 128.6, 128.0, 51.9, 43.2, 35.8, 35.1, 30.7, 25.9. FT-IR: ν (cm^{-1}) 3504, 3059, 2851, 1731, 1684, 1245. HRMS [ESI] calcd for $C_{14}H_{17}BrO_3Na$ $[M+Na]^+$ 335.0253, found 335.0265.



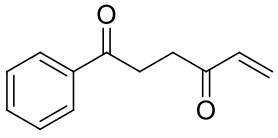
2aa: yellow solid, m.p. 47-48 °C. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.95 (d, J = 7.6 Hz, 2H), 7.55 (dd, J = 7.2, 7.2 Hz, 1H), 7.47 (dd, J = 7.6, 7.6 Hz, 2H), 3.44-3.35 (m, 2H), 2.97-2.89 (m, 2H), 1.94-1.86 (m, 2H), 1.70-1.64 (m, 2H), 0.96 (s, 6H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 199.8, 136.5, 132.6, 128.2, 127.6, 45.0, 35.1, 33.6, 32.9, 28.6, 26.2. FT-IR: ν (cm^{-1}) 3065, 2869, 2361, 1975, 1681, 1246. HRMS [ESI] calcd for $C_{14}H_{20}BrO$ $[M+H]^+$ 283.0692, found 283.0691.



2ab: yellow solid, m.p. 54-56 °C. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.98 (d, J = 7.2 Hz, 2H), 7.59 (dd, J = 7.2, 7.2 Hz, 1H), 7.48 (dd, J = 7.6, 7.6 Hz, 2H), 3.50 (t, J = 8.0 Hz, 2H), 3.23 (t, J = 7.2 Hz, 2H), 2.59-2.43 (m, 2H), 2.43-2.27 (m, 2H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 197.3, 135.9, 132.9, 128.2, 127.6, 122.9 (t, J_{C-F} = 240.6 Hz), 40.2 (t, J_{C-F} = 25.4 Hz), 30.5 (t, J_{C-F} = 3.8 Hz), 30.3 (t, J_{C-F} = 24.6 Hz), 22.8 (t, J_{C-F} = 6.0 Hz); ^{19}F NMR (376 MHz, $CDCl_3$) δ -100.1 (s). FT-IR: ν (cm^{-1}) 2982, 2851, 2361, 1679, 1423, 1215. HRMS [ESI] calcd for $C_{12}H_{13}BrF_2ONa$ $[M+Na]^+$ 313.0010, found 313.0006.

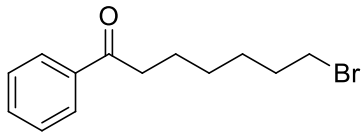


2ac: yellow oil. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.98-7.93 (m, 2H), 7.78-7.64 (m, 2H), 6.66 (s, 1H), 3.43 (t, J = 6.8 Hz, 2H), 2.99 (t, J = 7.2 Hz, 2H), 1.96-1.88 (m, 2H), 1.82-1.72 (m, 2H), 1.58-1.49 (m, 2H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 198.4, 145.6, 137.3, 128.0, 126.4, 39.2, 38.0, 33.1, 32.1, 27.3, 22.7. FT-IR: ν (cm^{-1}) 3029, 2869, 1951, 1678, 1465, 1262. HRMS [ESI] calcd for $C_{13}H_{15}Br_3ONa$ $[M+Na]^+$ 446.8565, found 446.8554.

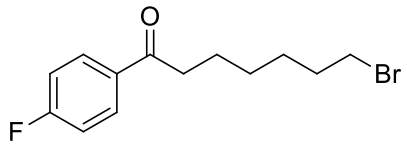


2ad: yellow oil. ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.02-7.96 (m, 2H), 7.59-7.53 (m, 1H), 7.49-7.43 (m, 2H), 6.44 (dd, J = 17.6, 10.4 Hz, 1H), 6.32 (dd, J = 17.6, 1.2 Hz, 1H), 5.89 (dd, J = 10.4, 1.2 Hz, 1H), 3.34 (t, J = 6.4 Hz, 2H), 3.07 (t, J = 6.4 Hz, 2H); ^{13}C NMR (100 MHz, $CDCl_3$)

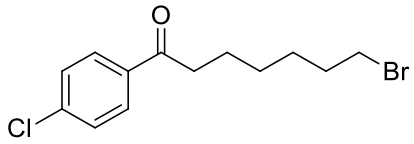
δ 199.2, 198.5, 136.7, 136.4, 133.2, 128.6, 128.5, 128.1, 33.3, 32.3. FT-IR: ν (cm^{-1}) 3060, 3026, 2855, 2911, 1678, 1328. HRMS [ESI] calcd for $C_{12}H_{13}O_2$ $[M+H]^+$ 189.0910, found 189.0920.



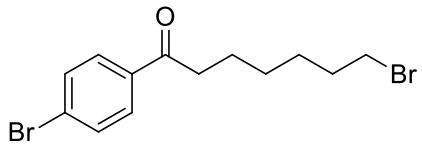
2ae: yellow solid, m.p. 36-38 °C. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.99-7.93 (m, 2H), 7.59-7.53 (m, 1H), 7.50-7.43 (m, 2H), 3.41 (t, *J* = 6.8 Hz, 2H), 2.98 (t, *J* = 7.2 Hz, 2H), 1.93-1.83 (m, 2H), 1.81-1.71 (m, 2H), 1.55-1.37 (m, 4H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 199.8, 136.5, 132.5, 128.1, 127.6, 37.9, 33.4, 32.1, 28.0, 27.5, 23.6. FT-IR: ν (cm-1) 3058, 2959, 2853, 1677, 1426, 1221. HRMS [ESI] calcd for $C_{13}H_{17}BrONa$ $[M+Na]^+$ 291.0355, found 291.0353.



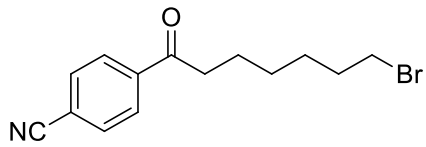
2af: white solid, m.p. 40-42 °C. ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.02-7.94 (m, 2H), 7.17-7.09 (m, 2H), 3.41 (t, *J* = 6.8 Hz, 2H), 2.95 (t, *J* = 7.2 Hz, 2H), 1.92-1.83 (m, 2H), 1.80-1.69 (m, 2H), 1.55-1.36 (m, 4H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 198.6, 165.7 (d, $J_{C\text{-}F}$ = 252.8 Hz), 133.4 (d, $J_{C\text{-}F}$ = 3.1 Hz), 130.6 (d, $J_{C\text{-}F}$ = 9.2 Hz), 115.7 (d, $J_{C\text{-}F}$ = 21.9 Hz), 38.3, 33.8, 32.6, 28.4, 28.0, 24.0; ^{19}F NMR (376 MHz, $CDCl_3$) δ -105.6 (s). FT-IR: ν (cm^{-1}) 3052, 2936, 2836, 1930, 1676, 1256. HRMS [ESI] calcd for $C_{13}H_{16}BrFONa$ $[M+Na]^+$ 309.0261, found 309.0266.



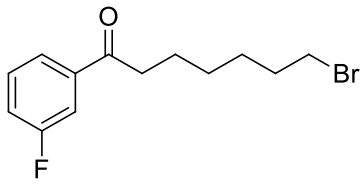
2ag: yellow solid, m.p. 47-48 °C. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.92-7.86 (m, 2H), 7.46-7.41 (m, 2H), 3.44-3.38 (t, *J* = 6.8 Hz, 2H), 2.94 (t, *J* = 7.2 Hz, 2H), 1.92-1.83 (m, 2H), 1.80-1.70 (m, 2H), 1.54-1.36 (m, 4H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 199.0, 139.4, 135.3, 129.5, 128.9, 38.3, 33.8, 32.5, 28.4, 28.0, 23.9. FT-IR: ν (cm^{-1}) 3091, 2932, 2852, 1952, 1675, 1285. HRMS [ESI] calcd for $C_{13}H_{16}BrClONa$ $[M+Na]^+$ 324.9965, found 324.9965.



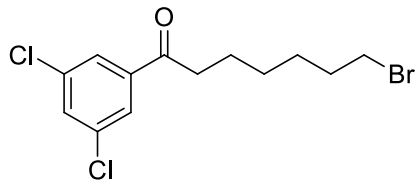
2ah: yellow solid, m.p. 49-50 °C. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.84-7.79 (m 2H), 7.62-7.57 (m, 2H), 3.41 (t, *J* = 6.8 Hz, 2H), 2.94 (t, *J* = 7.2 Hz, 2H), 1.92-1.82 (m, 2H), 1.79-1.69 (m, 2H), 1.53-1.35 (m, 4H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 199.2, 135.7, 131.9, 129.6, 128.1, 38.3, 33.8, 32.5, 28.4, 28.0, 23.9. FT-IR: ν (cm^{-1}) 3087, 2915, 2852, 1935, 1676, 1254. HRMS [ESI] calcd for $C_{13}H_{17}Br_2O$ $[M+H]^+$ 346.9641, found 346.9657.



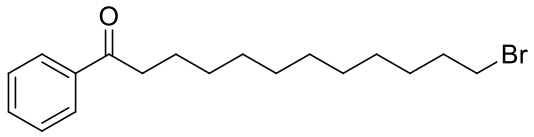
2ai: white solid, m.p. 55-57 °C. ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.06-8.00 (m, 2H), 7.79-7.74 (m, 2H), 3.41 (t, *J* = 6.8 Hz, 2H), 2.99 (t, *J* = 7.2 Hz, 2H), 1.92-1.82 (m, 2H), 1.81-1.71 (m, 2H), 1.55-1.36 (m, 4H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 198.2, 139.4, 132.0, 128.0, 117.5, 115.8, 38.2, 33.3, 32.0, 27.8, 27.4, 23.2. FT-IR: ν (cm^{-1}) 2941, 2852, 2361, 2230, 1684, 1249. HRMS [ESI] calcd for $C_{14}H_{16}BrNONa$ $[M+Na]^+$ 316.0307, found 316.0306.



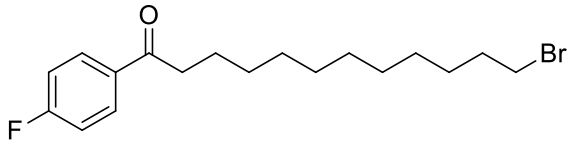
2aj: yellow solid, m.p. 28-29 °C. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.77-7.70 (m, 1H), 7.66-7.60 (m, 1H), 7.48-7.40 (m, 1H), 7.29-7.22 (m, 1H), 3.41 (t, J = 6.8 Hz, 2H), 2.95 (t, J = 7.2 Hz, 2H), 1.93-1.82 (m, 2H), 1.81-1.71 (m, 2H), 1.55-1.36 (m, 4H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 198.9, 162.9 (d, J_{C-F} = 246.3 Hz), 139.1 (d, J_{C-F} = 5.9 Hz), 130.2 (d, J_{C-F} = 7.6 Hz), 123.8 (d, J_{C-F} = 3.0 Hz), 120.0 (d, J_{C-F} = 21.4 Hz), 114.8 (d, J_{C-F} = 22.1 Hz), 38.5, 33.8, 32.5, 28.4, 28.0, 23.9; ^{19}F NMR (376 MHz, $CDCl_3$) δ -111.9 (s). FT-IR: ν (cm^{-1}) 2935, 2857, 2361, 1682, 1442, 1251. HRMS [ESI] calcd for $C_{13}H_{16}BrFONa$ $[M+Na]^+$ 309.0261, found 309.0261.



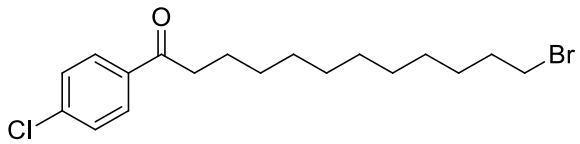
2ak: white solid, m.p. 50-52 °C. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.79 (d, J = 2.0 Hz, 2H), 7.54 (dd, J = 2.0, 2.0 Hz, 1H), 3.42 (t, J = 6.8 Hz, 2H), 2.93 (t, J = 7.2 Hz, 2H), 1.92-1.84 (m, 2H), 1.79-1.70 (m, 2H), 1.54-1.36 (m, 4H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 197.5, 139.3, 135.6, 132.6, 126.5, 38.5, 33.8, 32.5, 28.3, 27.9, 23.7. FT-IR: ν (cm^{-1}) 3078, 2960, 2853, 2360, 1787, 1337. HRMS [EI] calcd for $C_{13}H_{15}BrCl_2O$ $[M]^+$ 335.9683, found 335.9675.



2al: yellow solid, m.p. 32-33 °C. ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.00-7.91 (m, 2H), 7.58-7.52 (m, 1H), 7.49-7.42 (m, 2H), 3.40 (t, J = 6.8 Hz, 2H), 2.96 (t, J = 7.2 Hz, 2H), 1.89-1.79 (m, 2H), 1.78-1.68 (m, 2H), 1.48-1.18 (m, 14H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 200.1, 136.6, 132.4, 128.1, 127.6, 38.1, 33.6, 32.4, 29.0, 29.0, 29.0, 28.9, 28.9, 28.3, 27.7, 23.9. FT-IR: ν (cm^{-1}) 2921, 2850, 1686, 1578, 1406, 1264. HRMS [ESI] calcd for $C_{18}H_{27}BrONa$ $[M+Na]^+$ 361.1137, found 361.1146.

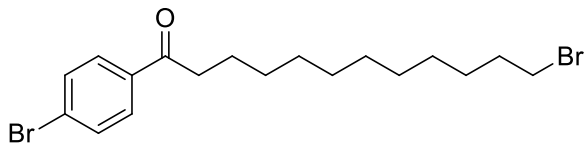


2am: yellow oil. ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.01-7.95 (m, 2H), 7.16-7.08 (m, 2H), 3.40 (t, J = 6.8 Hz, 2H), 2.93 (t, J = 7.2 Hz, 2H), 1.89-1.79 (m, 2H), 1.76-1.67 (m, 2H), 1.46-1.23 (m, 14H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 198.5, 165.1 (d, J_{C-F} = 252.8 Hz), 133.0 (d, J_{C-F} = 3.0 Hz), 130.2 (d, J_{C-F} = 9.2 Hz), 115.1 (d, J_{C-F} = 21.7 Hz), 38.1, 33.6, 32.3, 29.0, 29.0, 28.9, 28.9, 28.8, 28.3, 27.7, 23.8; ^{19}F NMR (376 MHz, $CDCl_3$) δ -105.8 (s). FT-IR: ν (cm^{-1}) 2925, 2853, 1686, 1506, 1409, 1263. HRMS [ESI] calcd for $C_{18}H_{26}BrFONa$ $[M+Na]^+$ 379.1043, found 379.1051.

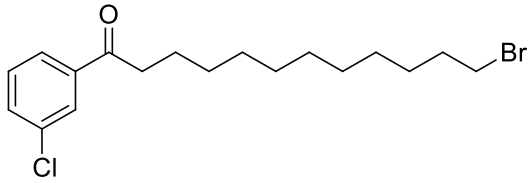


2an: white solid, m.p. 45-46 °C. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.92-7.86 (m, 2H), 7.45-7.40 (m, 2H), 3.40 (t, J = 6.8 Hz, 2H), 2.92 (t, J = 7.2 Hz, 2H), 1.89-1.79 (m, 2H), 1.77-1.67 (m, 2H), 1.46-1.22 (m, 14H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 199.3, 139.3, 135.4, 129.5, 128.9, 38.6, 34.1, 32.8, 29.5, 29.4, 29.4, 29.4, 29.3, 28.7, 28.2, 24.3. FT-IR: ν (cm^{-1}) 3002, 2849, 2362, 1804, 1687, 1275. HRMS [ESI]

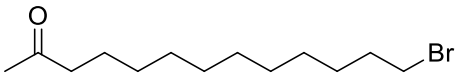
calcd for $C_{18}H_{27}BrClO$ $[M+H]^+$ 373.0928, found 373.0929.



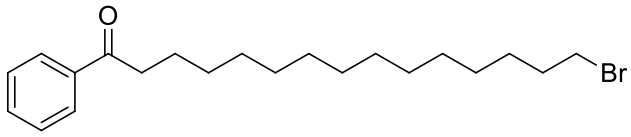
2ao: yellow solid, m.p. 57-58 °C. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.84-7.79 (m, 2H), 7.62-7.57 (m, 2H), 3.40 (t, *J* = 6.8 Hz, 2H), 2.92 (t, *J* = 7.2 Hz, 2H), 1.89-1.80 (m, 2H), 1.76-1.67 (m, 2H), 1.47-1.23 (m, 14H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 199.5, 135.8, 131.9, 129.6, 128.0, 38.6, 34.1, 32.8, 29.5, 29.4, 29.4, 29.4, 29.3, 28.7, 28.2, 24.3. FT-IR: ν (cm^{-1}) 2961, 2850, 2360, 1678, 1466, 1217. HRMS [ESI] calcd for $C_{18}H_{27}Br_2O$ $[M+H]^+$ 417.0423, found 417.0414.



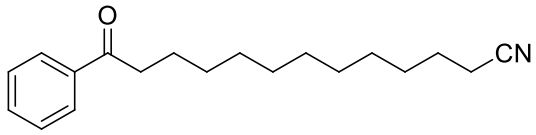
2ap: white solid, m.p. 51-53 °C. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.92 (dd, *J* = 1.6, 1.6 Hz, 1H), 7.85-7.80 (m, 1H), 7.52 (ddd, *J* = 8.0, 2.0, 0.8 Hz, 1H), 7.40 (dd, *J* = 8.0, 8.0 Hz, 1H), 3.40 (t, *J* = 6.8 Hz, 2H), 2.93 (t, *J* = 7.2 Hz, 2H), 1.90-1.80 (m, 2H), 1.78-1.67 (m, 2H), 1.47-1.21 (m, 14H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 199.2, 138.6, 134.9, 132.8, 129.9, 128.2, 126.1, 38.7, 34.1, 32.8, 29.5, 29.4 (three carbons overlap), 29.3, 28.8, 28.2, 24.2. FT-IR: ν (cm^{-1}) 2919, 2850, 2361, 1679, 1570, 1243. HRMS [ESI] calcd for $C_{18}H_{26}BrClONa$ $[M+Na]^+$ 395.0748, found 395.0742.



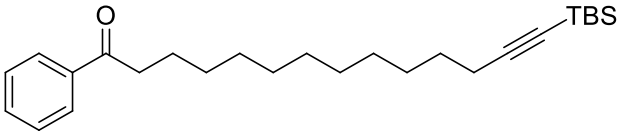
2aq: yellow oil. ^{1}H NMR (400 MHz, $CDCl_3$) δ 3.40 (t, *J* = 6.8 Hz, 2H), 2.41 (t, *J* = 7.2 Hz, 2H), 2.13 (s, 3H), 1.90-1.80 (m, 2H), 1.62-1.52 (m, 3H), 1.46-1.36 (m, 3H), 1.31-1.23 (m, 10H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 208.9, 43.3, 33.6, 32.3, 29.4, 29.2, 29.0, 29.0, 28.9, 28.7, 28.3, 27.7, 23.4. FT-IR: ν (cm^{-1}) 2924, 2853, 1716, 1494, 1359, 1226. HRMS [ESI] calcd for $C_{13}H_{25}BrONa$ $[M+Na]^+$ 299.0981, found 299.0973.



2ar: white solid, m.p. 67-68 °C. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.98-7.94 (m, 2H), 7.58-7.52 (m, 1H), 7.49-7.43 (m, 2H), 3.41 (t, *J* = 6.8 Hz, 2H), 2.96 (t, *J* = 7.2 Hz, 2H), 1.90-1.81 (m, 2H), 1.78-1.69 (m, 2H), 1.46-1.22 (m, 20H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 200.1, 136.6, 132.4, 128.1, 127.6, 38.2, 33.6, 32.4, 29.1, 29.1, 29.0, 29.0, 29.0, 29.0, 28.9, 28.3, 27.7, 23.9. FT-IR: ν (cm^{-1}) 2915, 2848, 1677, 1445, 1337, 1211. HRMS [ESI] calcd for $C_{21}H_{34}BrO$ $[M+H]^+$ 381.1788, found 381.1779.

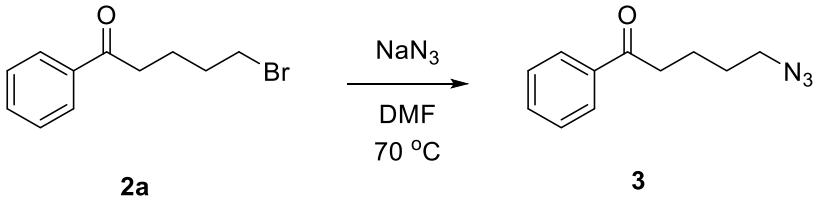


9: white solid, m.p. 40-42 °C. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.98-7.93 (m, 2H), 7.58-7.52 (m, 1H), 7.49-7.42 (m, 2H), 2.96 (t, *J* = 7.2 Hz, 2H), 2.33 (t, *J* = 7.2 Hz, 2H), 1.78-1.68 (m, 2H), 1.68-1.58 (m, 2H), 1.48-1.24 (m, 14H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 200.6, 137.1, 132.9, 128.5, 128.0, 119.9, 38.6, 29.4, 29.4, 29.4, 29.3, 29.3, 28.7, 28.7, 25.4, 24.3, 17.1. FT-IR: ν (cm^{-1}) 2935, 2852, 2342, 1686, 1449, 1248. HRMS [ESI] calcd for $C_{19}H_{27}NONa$ $[M+Na]^+$ 308.1985, found 308.1977.



10: yellow oil. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.98-7.94 (m, 2H), 7.58-7.52 (m, 1H), 7.49-7.43 (m, 2H), 2.96 (t, *J* = 7.2 Hz, 2H), 2.22 (t, *J* = 7.2 Hz, 2H), 1.77-1.69 (m, 2H), 1.55-1.46 (m, 2H), 1.43-1.24 (m, 14H), 0.93 (s, 9H), 0.08 (s, 6H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 200.6, 137.1, 132.8, 128.5, 128.0, 108.3, 82.3, 38.6, 29.5, 29.5, 29.4, 29.1, 28.7, 28.7, 26.1, 24.4, 19.8, 16.5, -4.4. FT-IR: ν (cm^{-1}) 2926, 2854, 2361, 1687, 1361, 1248. HRMS [ESI] calcd for $C_{26}H_{42}OSiNa$ $[M+Na]^+$ 421.2897, found 421.2889.

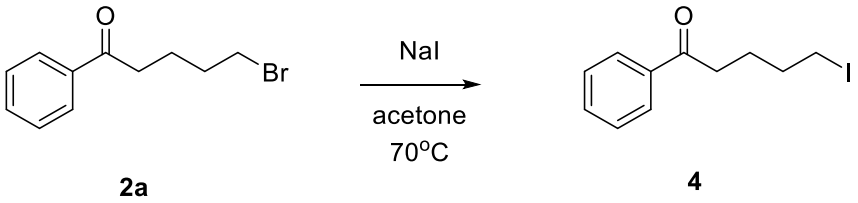
5. Transformation of products



2a **3**

Compound **2a** (48.2 mg, 0.2 mmol, 1.0 equiv.) and NaN_3 (64.0 mg, 0.4 mmol, 2.0 equiv.) were suspended in DMF (2.0 mL) and the reaction mixture was stirred at 70 °C for 2 h. After completion of the reaction, the reaction mixture was diluted with Et_2O and washed with water. The organic layer was separated and dried over anhydrous Na_2SO_4. The solvent was removed under reduced pressure and the residue was purified by flash column chromatography on silica gel (eluent: ethyl acetate/ petroleum ether) to afford the desired product **3** (35.4 mg, 87%).

3: yellow oil. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.99-7.93 (m, 2H), 7.59-7.54 (m, 1H), 7.49-7.43 (m, 2H), 3.33 (t, *J* = 6.8 Hz, 2H), 3.02 (t, *J* = 7.2 Hz, 2H), 1.88-1.79 (m, 2H), 1.74-1.64 (m, 2H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 199.6, 136.8, 133.1, 128.6, 128.0, 51.3, 37.8, 28.5, 21.3. FT-IR: ν (cm^{-1}) 3087, 2939, 2091, 1683, 1580, 1254. HRMS [ESI] calcd for $C_{11}H_{13}N_3ONa$ $[M+Na]^+$ 226.0951, found 226.0944.

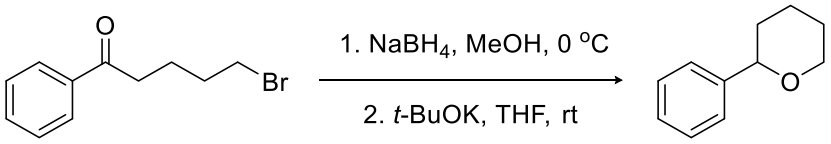


2a **4**

Compound **2a** (48.2 mg, 0.2 mmol, 1.0 equiv.) and NaI (149.9 mg, 1 mmol, 5.0 equiv.) were suspended in acetone (2.0 mL) and the reaction mixture was stirred at 70 °C for 13 h. After completion of the reaction, the solvent was removed under reduced pressure and the residue was purified by flash column chromatography on silica gel (eluent: ethyl acetate/ petroleum ether) to afford the desired product **4** (49.3 mg, 86%).

4: white solid, m.p. 69-70 °C. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.99-7.92 (m, 2H), 7.60-7.53 (m, 1H),

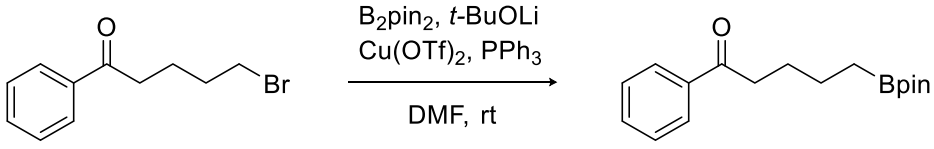
7.50-7.43 (m, 2H), 3.23 (t, *J* = 6.8 Hz, 2H), 3.00 (t, *J* = 7.2 Hz, 2H), 1.97-1.81 (m, 4H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 199.1, 136.3, 132.6, 128.2, 127.5, 36.8, 32.5, 24.6, 5.8. FT-IR: ν (cm^{-1}) 3056, 2927, 2851, 1673, 1403, 1209. HRMS [ESI] calcd for $C_{11}H_{13}IONa$ $[M+Na]^+$ 310.9903, found 310.9911.



2a **5**

Compound **2a** (48.2 mg, 0.2 mmol, 1.0 equiv.) was dissolved in MeOH (2.0 mL), then sodium borohydride (15.1 mg, 0.4 mmol, 2.0 equiv.) was added in one portion at 0 °C. The reaction mixture was stirred for 20 min. After completion, the reaction mixture was quenched with saturated aqueous ammonium chloride (5.0 mL) and the aqueous layer was extracted by DCM (3 x 5.0 mL). The combined organic layer was dried over anhydrous Na_2SO_4. The solvent was removed under reduced pressure and the residue was purified by flash column chromatography on silica gel (eluent: ethyl acetate/ petroleum ether) to afford the corresponding alcohol product (48.6 mg, quantitative yield). The alcohol (48.6 mg, 0.2 mmol, 1.0 equiv.) and potassium *tert*-butoxide (45.0 mg, 0.4 mmol, 2.0 equiv.) were suspended in THF (2.0 mL), and the reaction mixture was stirred at rt under N_2 for 11 h. The solvent was removed under reduced pressure and the residue was purified by flash column chromatography on silica gel (eluent: ethyl acetate/ petroleum ether) to afford the desired product **5** (26.4 mg, 82%).

5: yellow oil. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.37-7.22 (m, 5H), 4.35-4.29 (m, 1H), 4.17-4.11 (m, 1H), 3.66-3.58 (m, 1H), 2.01-1.90 (m, 1H), 1.88-1.79 (m, 1H), 1.76-1.58 (m, 4H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 142.8, 127.8, 126.8, 125.4, 79.7, 68.5, 33.5, 25.4, 23.5. FT-IR: ν (cm^{-1}) 3062, 2935, 2731, 1605, 1439, 1204. HRMS [ESI] calcd for $C_{11}H_{15}O$ $[M+H]^+$ 163.1117, found 163.1122.

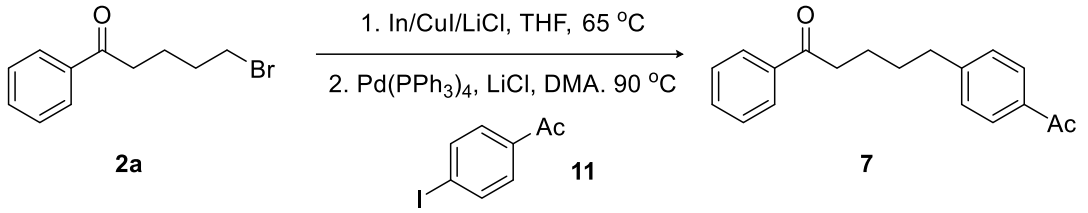


2a **6**

Compound **2a** (48.2 mg, 0.2 mmol, 1.0 equiv.), $Cu(OTf)_2$ (7.2 mg, 0.01 mmol, 0.1 equiv.), PPh_3 (6.8 mg, 0.026 mmol, 0.13 equiv.), *t*-BuOLi (32.0mg, 0.4 mmol, 2.0 equiv), and B_2pin_2 (75.0 mg, 0.3 mmol, 1.5 equiv.) were suspended in DMF (1.0 mL) and the reaction mixture was stirred at rt under N_2 for 10 h. After completion of the reaction, the reaction mixture was diluted with Et_2O and washed with water. The organic layer was separated and dried over anhydrous Na_2SO_4. The solvent was removed under reduced pressure and the residue was purified by flash column chromatography on silica gel (eluent: ethyl acetate/ petroleum ether) to afford the desired product **6** (20.0 mg, 35%).

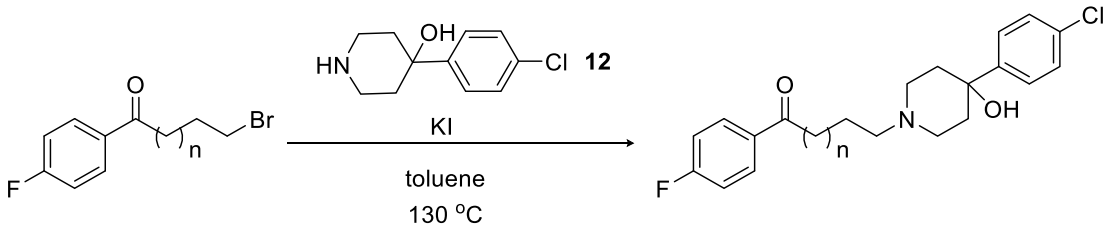
6: yellow oil. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.97-7.92 (m, 2H), 7.57-7.51 (m, 1H), 7.47-7.42 (m,

2H), 2.96 (t, *J* = 7.2 Hz, 2H), 1.79-1.70 (m, 2H), 1.56-1.47 (m, 2H), 1.23 (s, 12H), 0.84 (t, *J* = 8.0 Hz, 2H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 200.1, 136.6, 132.3, 128.0, 127.6, 82.5, 38.0, 26.5, 24.3, 23.4; ^{11}B NMR (128 MHz, $CDCl_3$) δ 34.1 (s). FT-IR: ν (cm^{-1}) 3061, 2977, 2866, 1685, 1408, 1214. HRMS [ESI] calcd for $C_{17}H_{25}BO_3Na$ $[M+Na]^+$ 311.1789, found 311.1799.



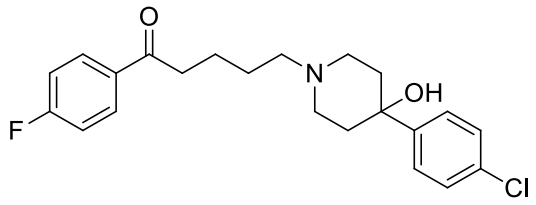
Compound **2a** (120.5 mg, 0.5 mmol, 1.7 equiv.), indium (57.1 mg, 0.5 mmol, 1.7 equiv.), CuI (95.2 mg, 0.5 mmol, 1.7 equiv), LiCl (21.2 mg, 0.5 mmol, 1.7 equiv.), and THF (1.5 mL) were loaded in a 5 mL reaction vial. The reaction was stirred vigorously at 65 °C for 15 h. After completion of the reaction, it was kept still for 10 min. Then the upper clear solution was separated from the bottom black precipitate by syringe. The residual black precipitate was washed with 3 mL THF and the THF layer was separated by syringe. The combined organic layers were concentrated to give the residue which was then dissolved in 1.5 mL DMA and transferred to another 5 mL reaction vial. Aryl halide **11** (73.8 mg, 0.3 mmol, 1.0 equiv.), LiCl (21.2 mg, 0.5 mmol, 1.7 equiv.), and $Pd(PPh_3)_4$ (28.9 mg, 0.025 mmol, 0.083 equiv.) was added to the vial sequentially. The reaction mixture was stirred at 90 °C for 27 h. After completion of the reaction, the reaction mixture was diluted with Et_2O and washed with water. The organic layer was separated and dried over anhydrous Na_2SO_4. The solvent was removed under reduced pressure and the residue was purified by flash column chromatography on silica gel (eluent: ethyl acetate/ petroleum ether) to afford the desired product **7** (53.8 mg, 64%).

7: yellow solid, m.p. 61-63 °C. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.97-7.91 (m, 2H), 7.90-7.85 (m, 2H), 7.58-7.52 (m, 1H), 7.48-7.42 (m, 2H), 7.30-7.25 (m, 2H), 2.99 (t, *J* = 6.8 Hz, 2H), 2.73 (t, *J* = 7.6 Hz, 2H), 2.57 (s, 3H), 1.84-1.68 (m, 4H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 200.0, 197.8, 148.1, 137.0, 135.0, 133.0, 128.6, 128.6, 128.5, 128.0, 38.3, 35.8, 30.7, 26.6, 23.8. FT-IR: ν (cm^{-1}) 2930, 2860, 2360, 1735, 1522, 1268. HRMS [ESI] calcd for $C_{19}H_{20}O_2Na$ $[M+Na]^+$ 303.1356, found 303.1346.

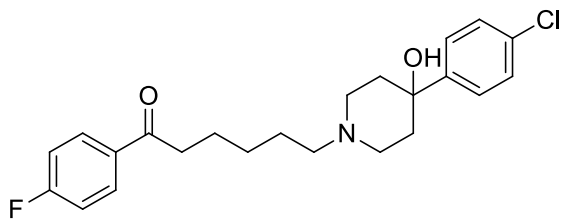


The alkyl bromide (0.2 mmol, 1.0 equiv.), compound **12** (84.7 mg, 0.4 mmol, 2.0 equiv.), and KI (1.0 mg, 0.006 mmol, 0.03 equiv.) were dissolved in anhydrous toluene (2.0 mL). The reaction mixture was stirred at 130 °C for 60 h. After completion of the reaction, the solvent was removed under reduced pressure and the residue was purified by flash column chromatography on silica gel

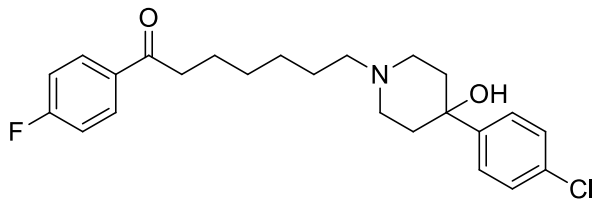
(eluent: ethyl acetate/ petroleum ether) to afford the desired product **8a** (n = 2, 63.8 mg, 82%), **8b** (n = 3, 64.8 mg, 81%), **8c** (n = 4, 70.9 mg, 85%), and **8d** (n = 9, 74.0 mg, 76%) respectively.



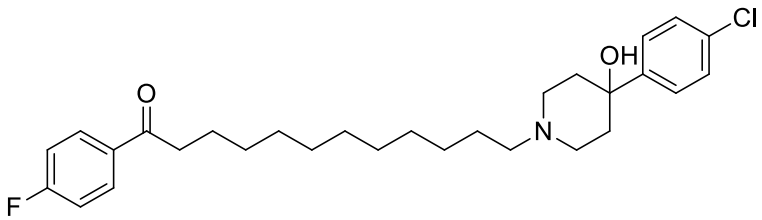
8a: yellow solid, m.p. 70-72 °C. ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.01-7.95 (m, 2H), 7.44-7.39 (m, 2H), 7.32-7.27 (m, 2H), 7.16-7.09 (m, 2H), 2.97 (t, J = 7.2 Hz, 2H), 2.85-2.77 (m, 2H), 2.48-2.37 (m, 4H), 2.14-2.04 (m, 2H), 1.81-1.68 (m, 4H), 1.66-1.56 (m, 2H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 198.5, 165.7 (d, $J_{C\text{-}F}$ = 252.9 Hz), 146.9, 133.4 (d, $J_{C\text{-}F}$ = 3.0 Hz), 132.7, 130.7 (d, $J_{C\text{-}F}$ = 9.2 Hz), 128.4, 126.1, 115.7 (d, $J_{C\text{-}F}$ = 21.7 Hz), 71.1, 58.4, 49.4, 38.4, 38.3, 26.6, 22.3; ^{19}F NMR (376 MHz, $CDCl_3$) δ -105.5 (s). FT-IR: ν (cm^{-1}) 3358, 3192, 2953, 2772, 1690, 1225. HRMS [ESI] calcd for $C_{22}H_{26}ClFNO_2$ $[M+H]^+$ 390.1631, found 390.1645.



8b: yellow solid, m.p. 111-113 °C. ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.01-7.95 (m, 2H), 7.47-7.41 (m, 2H), 7.33-7.28 (m, 2H), 7.16-7.09 (m, 2H), 2.95 (t, J = 7.2 Hz, 2H), 2.86-2.79 (m, 2H), 2.46-2.37 (m, 4H), 2.17-2.08 (m, 2H), 1.81-1.69 (m, 4H), 1.64-1.54 (m, 2H), 1.46-1.36 (m, 2H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 198.3, 165.2 (d, $J_{C\text{-}F}$ = 252.9 Hz), 146.5, 132.9 (d, $J_{C\text{-}F}$ = 3.0 Hz), 132.2, 130.2 (d, $J_{C\text{-}F}$ = 9.2 Hz), 127.9, 125.7, 115.2 (d, $J_{C\text{-}F}$ = 21.6 Hz), 70.5, 58.2, 49.0, 37.9, 37.9, 26.9, 26.4, 23.7; ^{19}F NMR (376 MHz, $CDCl_3$) δ -105.5 (s). FT-IR: ν (cm^{-1}) 3177, 2951, 2772, 1684, 1487, 1262. HRMS [ESI] calcd for $C_{23}H_{28}ClFNO_2$ $[M+H]^+$ 404.1787, found 404.1799.



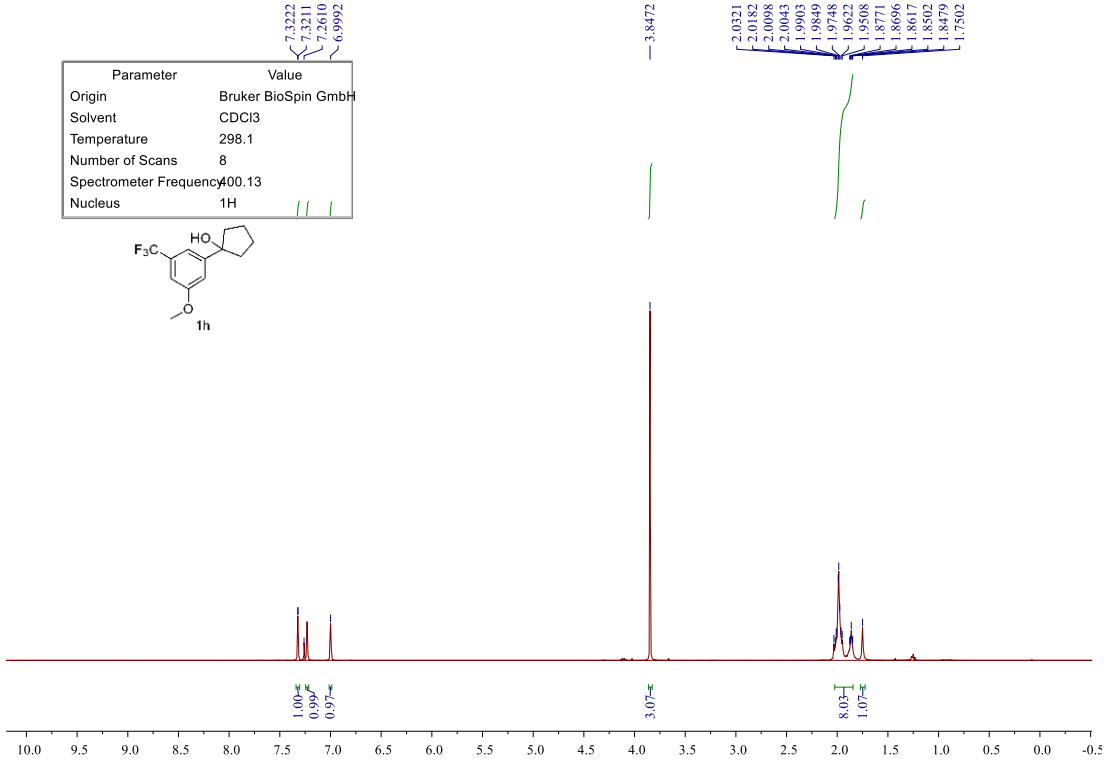
8c: yellow solid, m.p. 98-100 °C. ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.01-7.94 (m, 2H), 7.46-7.41 (m, 2H), 7.33-7.28 (m, 2H), 7.16-7.08 (m, 2H), 2.93 (t, J = 7.2 Hz, 2H), 2.85-2.78 (m, 2H), 2.46-2.36 (m, 4H), 2.17-2.07 (m, 2H), 1.79-1.68 (m, 4H), 1.59-1.50 (m, 2H), 1.45-1.33 (m, 4H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 198.8, 165.6 (d, $J_{C\text{-}F}$ = 252.8 Hz), 147.0, 133.4 (d, $J_{C\text{-}F}$ = 3.0 Hz), 132.7, 130.6 (d, $J_{C\text{-}F}$ = 9.2 Hz), 128.4, 126.1, 115.6 (d, $J_{C\text{-}F}$ = 21.7 Hz), 71.1, 58.8, 49.5, 38.5, 38.4, 29.3, 27.6, 26.9, 24.2; ^{19}F NMR (376 MHz, $CDCl_3$) δ -105.6 (s). FT-IR: ν (cm^{-1}) 2957, 2830, 2361, 1679, 1471, 1274. HRMS [ESI] calcd for $C_{24}H_{30}ClFNO_2$ $[M+H]^+$ 418.1944, found 418.1954.

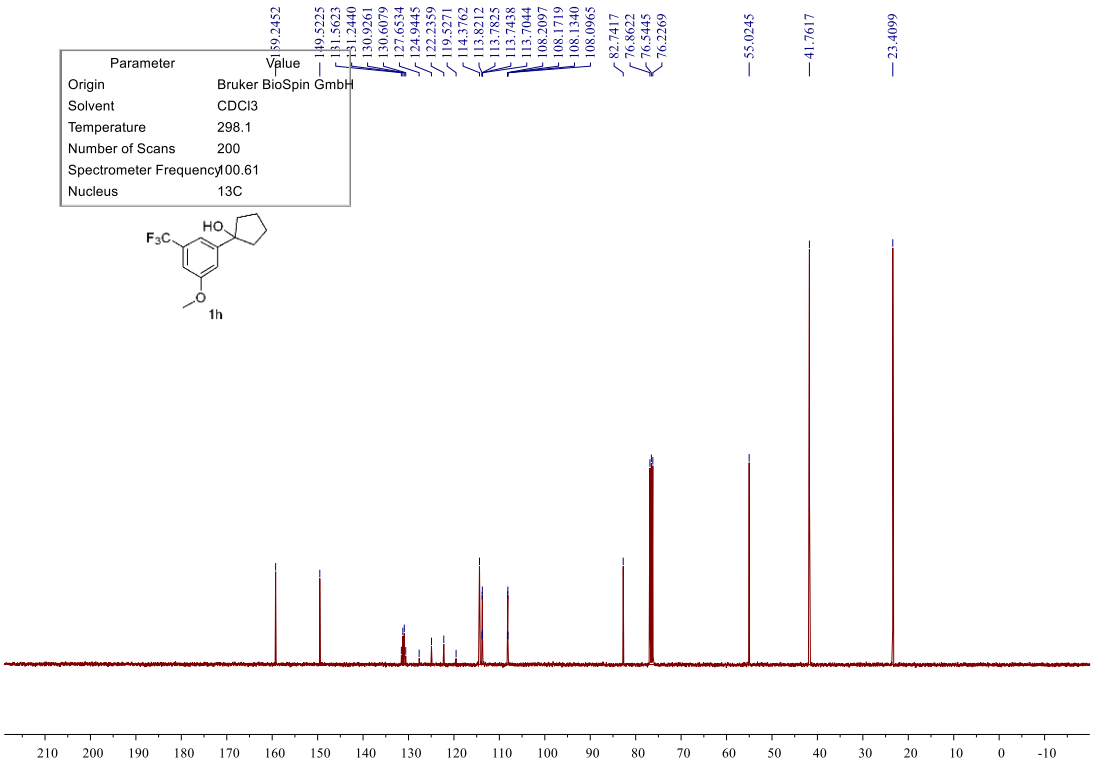


8d: yellow solid, m.p. 88-90 °C. ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.01-7.94 (m 2H), 7.46-7.41 (m, 2H), 7.34-7.27 (m, 2H), 7.15-7.08 (m, 2H), 2.92 (t,

J = 7.2 Hz, 2H), 2.85-2.77 (m, 2H), 2.44-2.34 (m, 4H), 2.16-2.07 (m, 2H), 1.76-1.66 (m, 4H), 1.56-1.46 (m, 2H), 1.40-1.22 (m, 14H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 199.0, 165.6 (d, J_{C-F} = 252.9 Hz), 147.1, 133.4 (d, J_{C-F} = 3.0 Hz), 132.6, 130.7 (d, J_{C-F} = 9.2 Hz), 128.3, 126.1, 115.6 (d, J_{C-F} = 21.7 Hz), 71.0, 59.0, 49.5, 38.5, 38.4, 29.6, 29.6, 29.5, 29.3, 27.7, 27.0, 24.3; ^{19}F NMR (376 MHz, $CDCl_3$) δ -105.7 (s). FT-IR: ν (cm^{-1}) 3132, 2959, 2774, 1685, 1405, 1209. HRMS [ESI] calcd for $C_{29}H_{40}ClFNO_2$ $[M+H]^+$ 488.2726, found 488.2734.

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

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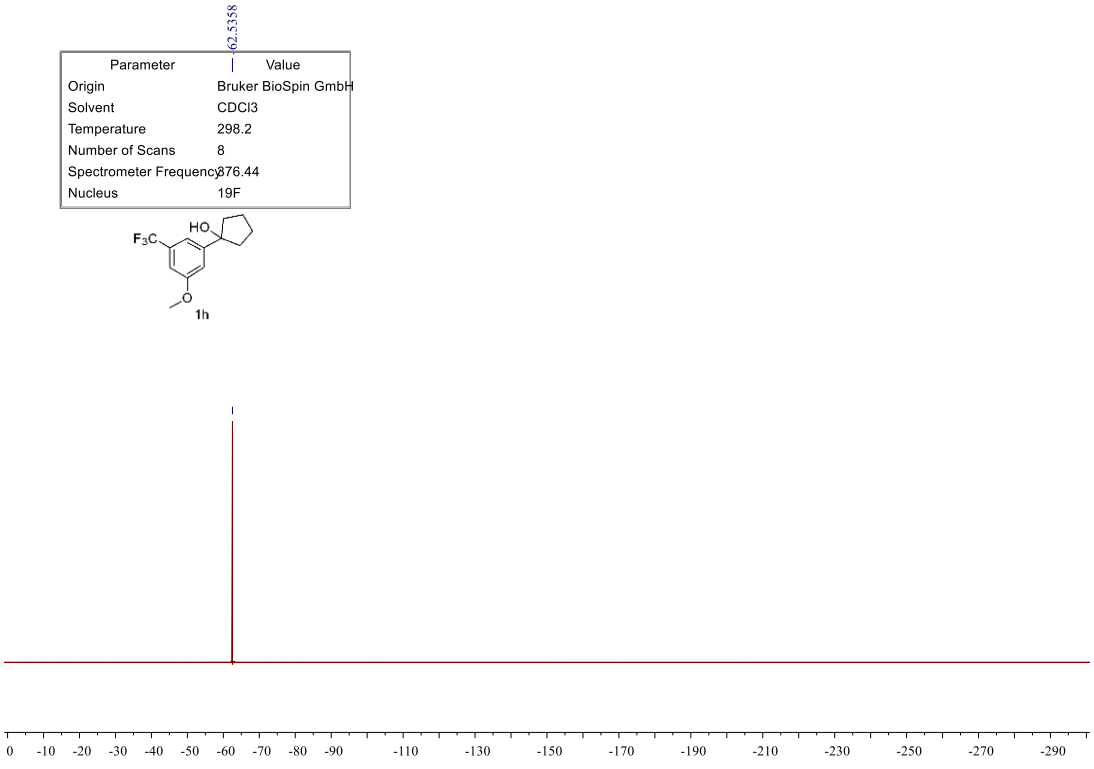
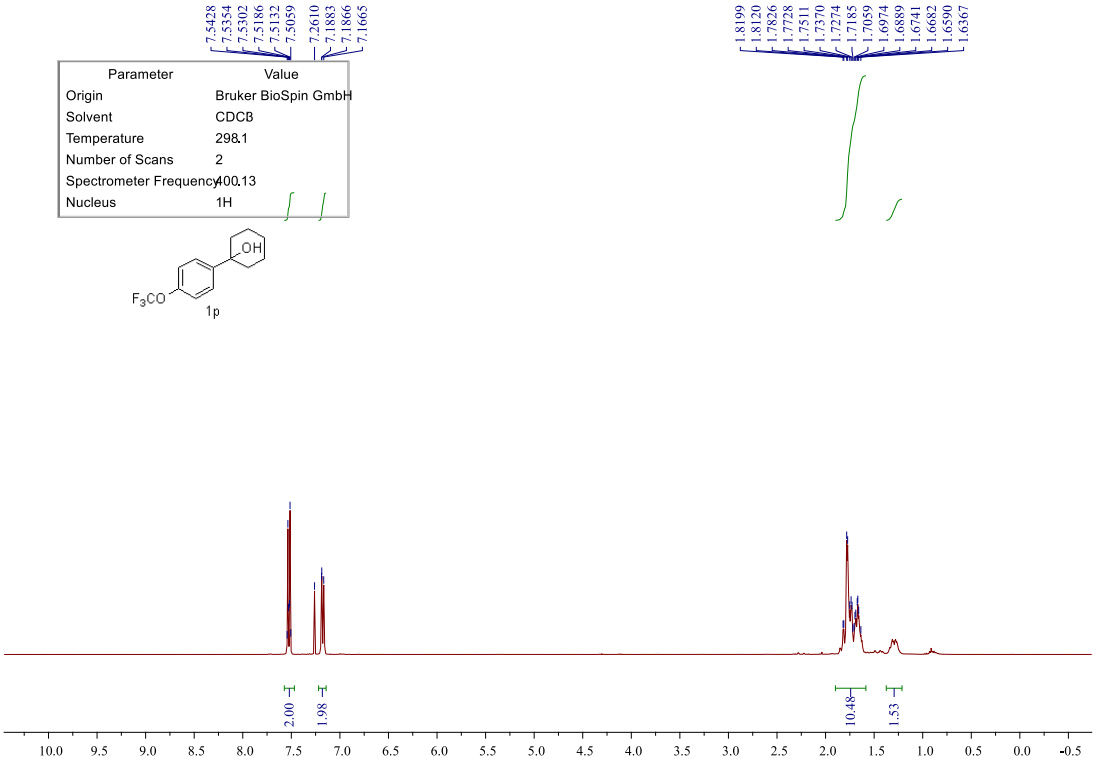
Origin Bruker BioSpin GmbH
Solvent CDCl3
Temperature 298.1
Number of Scans 200
Spectrometer Frequency 100.61
Nucleus 13C
HO
F3C
O
1h
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10


62.5358
Parameter Value
Origin Bruker BioSpin GmbH
Solvent CDCl3
Temperature 298.2
Number of Scans 8
Spectrometer Frequency 376.44
Nucleus 19F
HO
F3C
O
1h
0 -10 -20 -30 -40 -50 -60 -70 -80 -90 -110 -130 -150 -170 -190 -210 -230 -250 -270 -290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7.5132
7.5059
7.2610
7.1883
7.1866
7.1665
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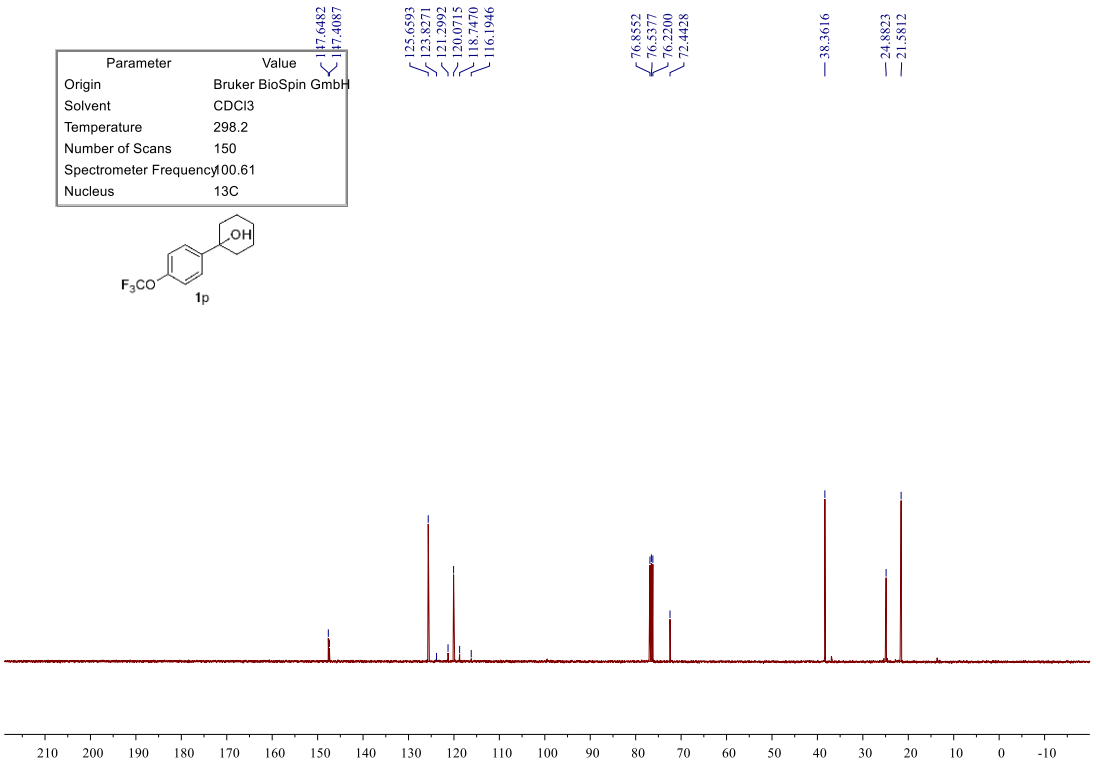
1.8120
1.7826
1.7728
1.7511
1.7370
1.7274
1.7185
1.7059
1.6974
1.6889
1.6741
1.6682
1.6590
1.6367
Parameter Value
Origin Bruker BioSpin GmbH
Solvent CDCB
Temperature 298.1
Number of Scans 2
Spectrometer Frequency 400.13
Nucleus 1H
OH
F3CO
1p
2.00
1.98
10.48
1.53
10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5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125.6593
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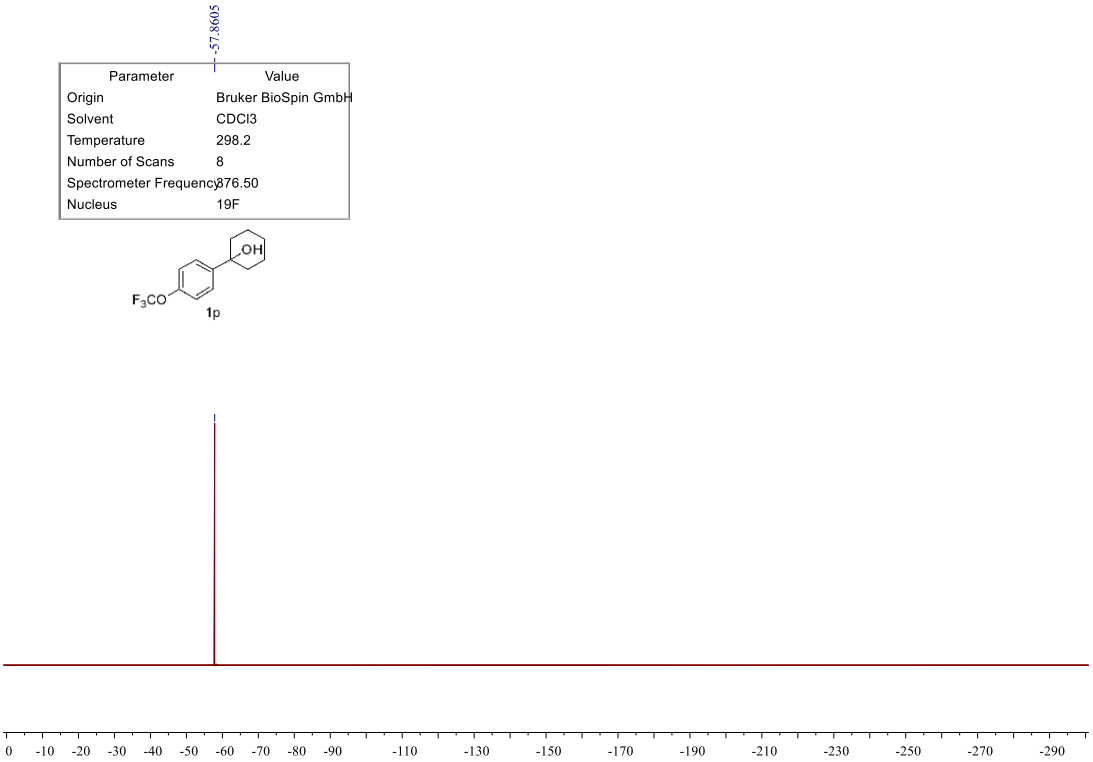
121.2992
120.0715
118.7470
116.1946
76.8552
76.5377
76.2200
72.4428
38.3616
24.8823
21.5812
Parameter Value
Origin Bruker BioSpin GmbH
Solvent CDCl3
Temperature 298.2
Number of Scans 150
Spectrometer Frequency 100.61
Nucleus 13C
OH
F3CO
1p
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10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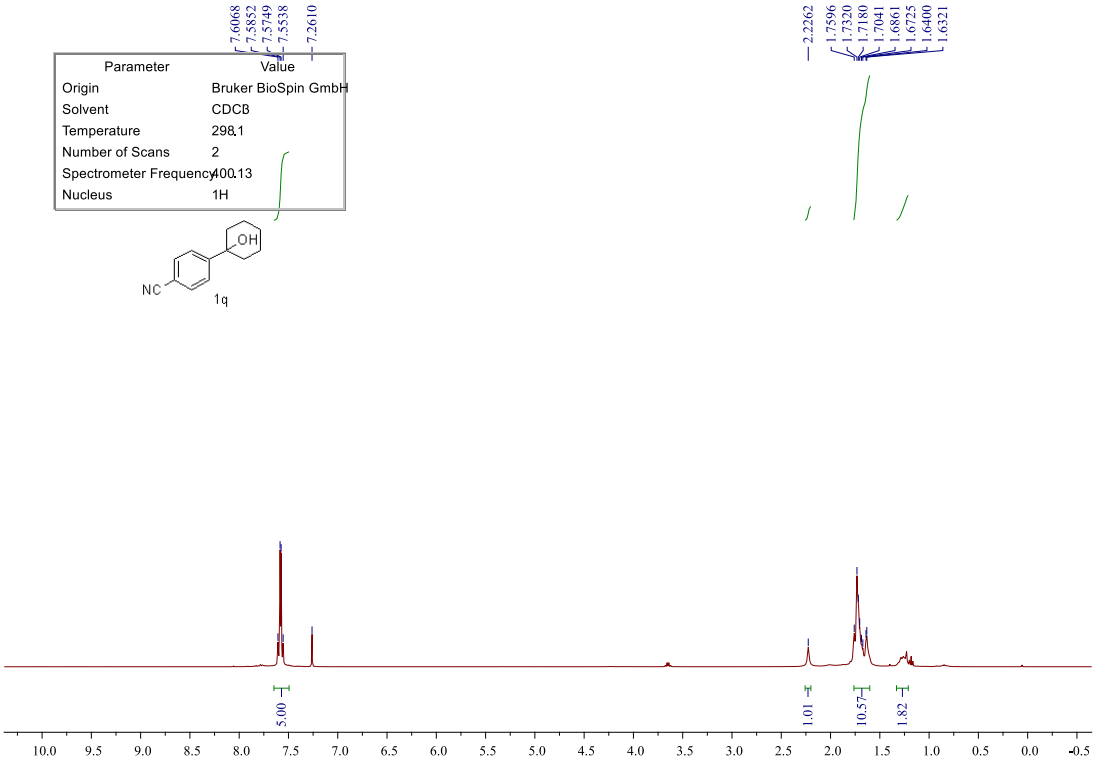
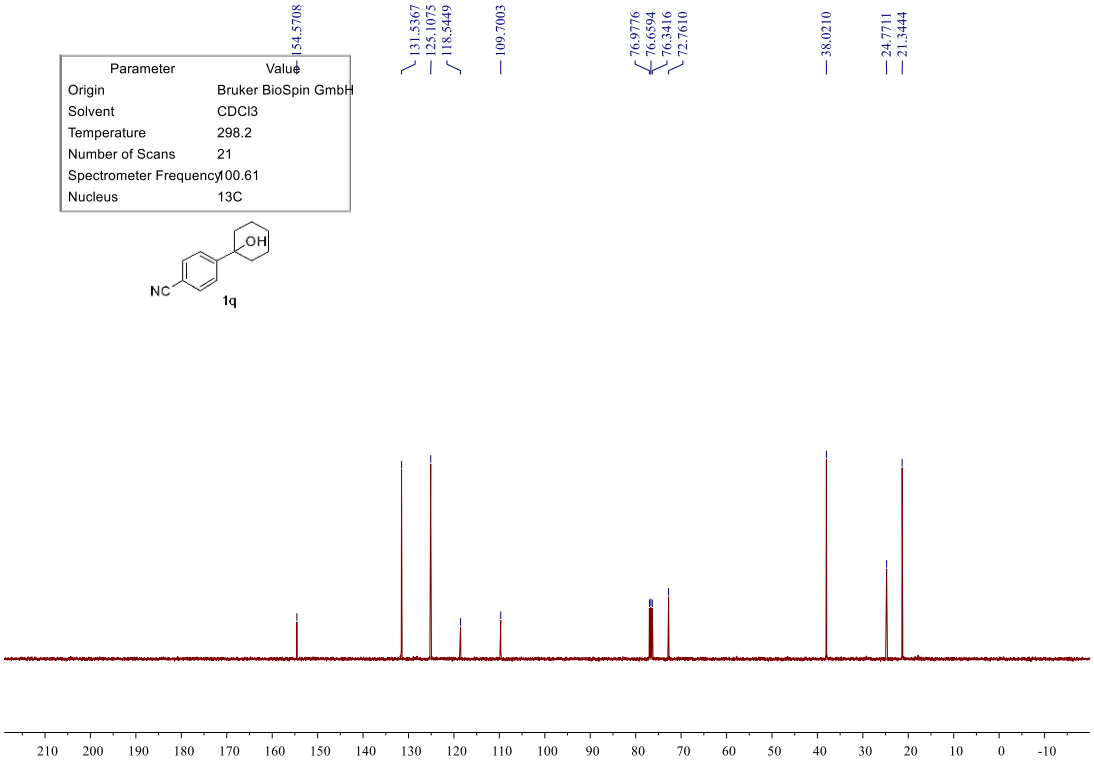
Parameter Value
Origin Bruker BioSpin GmbH
Solvent CDCl3
Temperature 298.2
Number of Scans 8
Spectrometer Frequency 376.50
Nucleus 19F
OH
F3CO
1p
0 -10 -20 -30 -40 -50 -60 -70 -80 -90 -110 -130 -150 -170 -190 -210 -230 -250 -270 -290


7.6068
7.5852
7.5749
7.5538
7.2610
Parameter Value
Origin Bruker BioSpin GmbH
Solvent CDCB
Temperature 298.1
Number of Scans 2
Spectrometer Frequency 400.13
Nucleus 1H
OH
NC
1q
2.2262
1.7596
1.7320
1.7180
1.7041
1.6861
1.6725
1.6400
1.6321
5.00
1.01
10.57
1.82
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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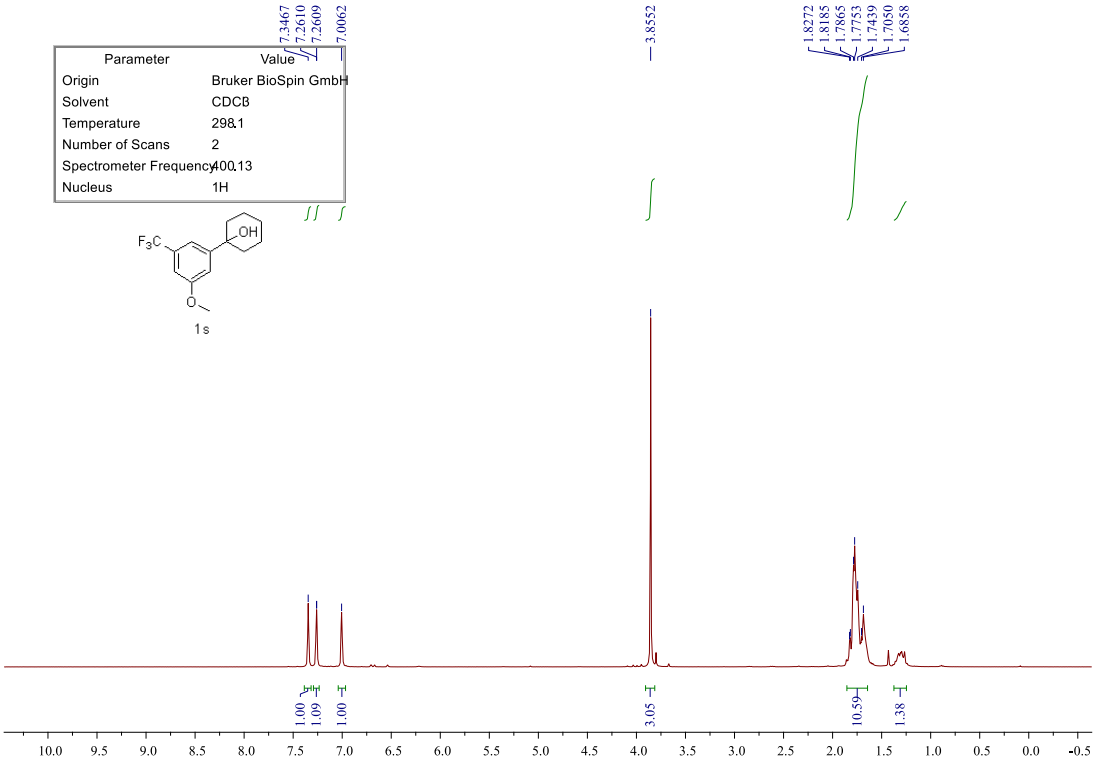
109.7003
76.9776
76.6594
76.3416
72.7610
38.0210
24.7711
21.3444
Parameter Value
Origin Bruker BioSpin GmbH
Solvent CDCl3
Temperature 298.2
Number of Scans 21
Spectrometer Frequency 100.61
Nucleus 13C
OH
NC
1q
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10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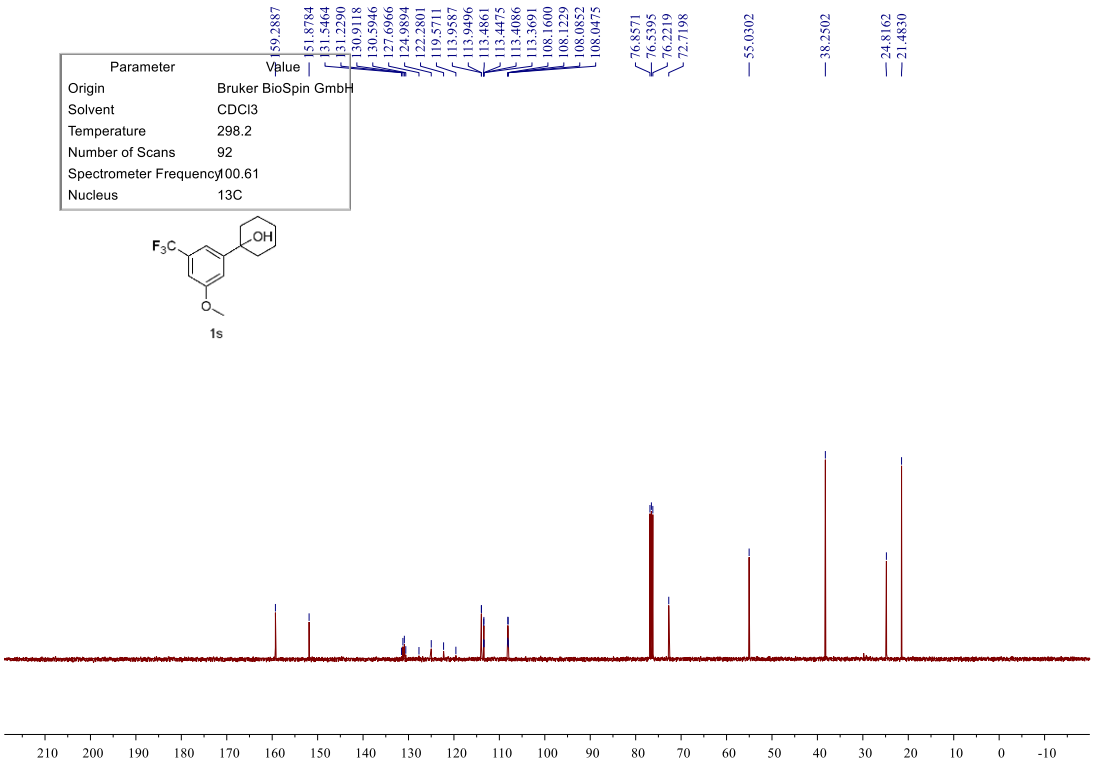
7.2609
7.0062
3.8552
1.8272
1.8185
1.7865
1.7753
1.7439
1.7050
1.6858
Parameter Value
Origin Bruker BioSpin GmbH
Solvent CDCl3
Temperature 298.1
Number of Scans 2
Spectrometer Frequency 400.13
Nucleus 1H
OH
F3C
O
1s
1.00
1.09
1.00
3.05
10.59
1.38
10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5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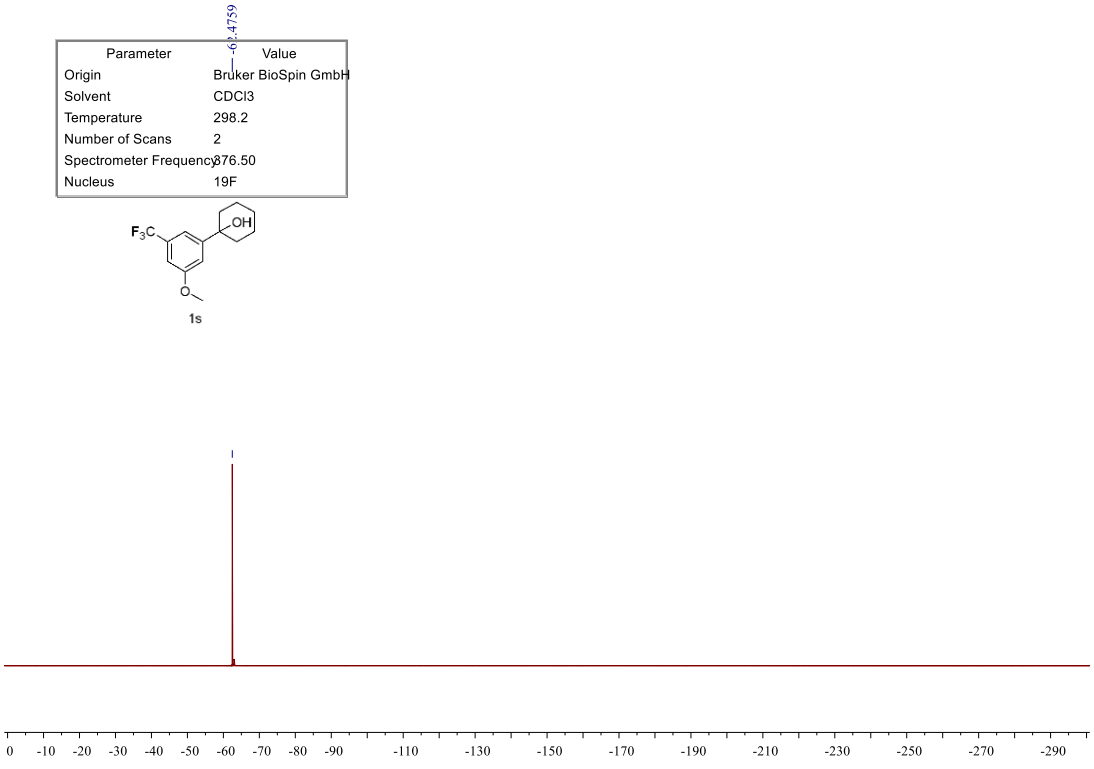
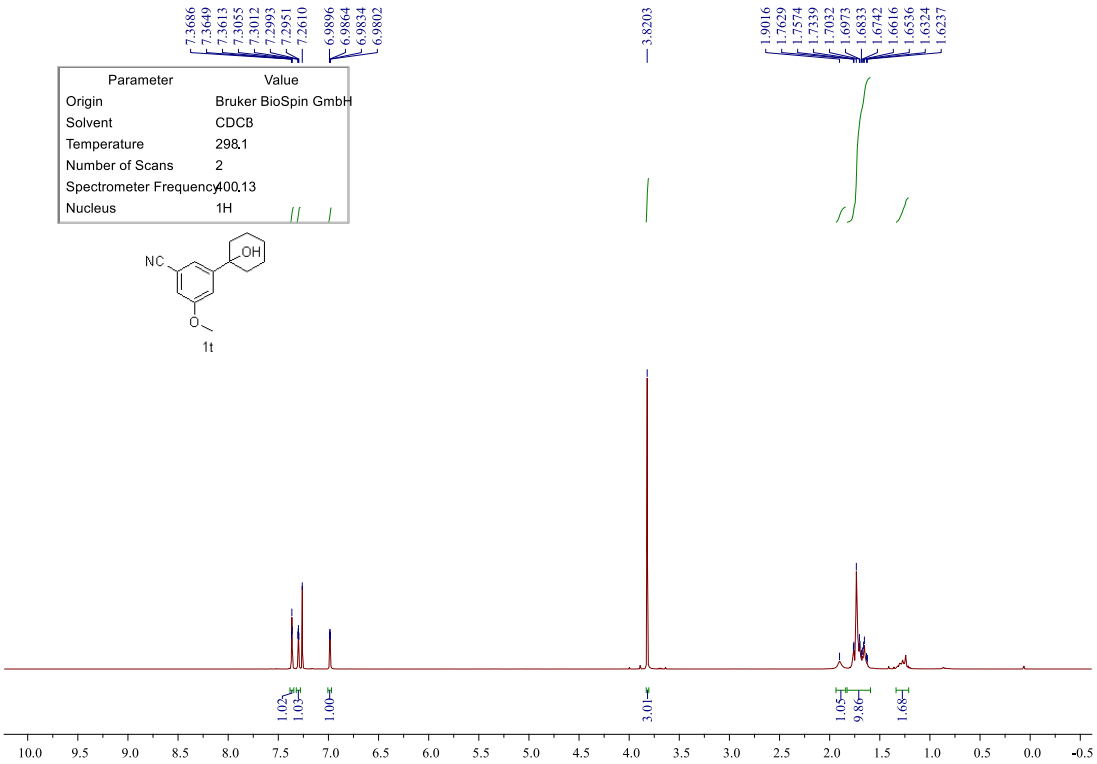
151.8784
131.5464
131.2290
130.9118
130.5946
127.6966
124.9894
122.2801
119.5711
113.9587
113.9496
113.4861
113.4475
113.4086
113.3691
108.1600
108.1229
108.0852
108.0475
76.8571
76.5395
76.2219
72.7198
55.0302
38.2502
24.8162
21.4830
Parameter Value
Origin Bruker BioSpin GmbH
Solvent CDCl3
Temperature 298.2
Number of Scans 92
Spectrometer Frequency 100.61
Nucleus 13C
F3C
OH
O
1s
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10


-62.4759
Parameter Value
Origin Bruker BioSpin GmbH
Solvent CDCl3
Temperature 298.2
Number of Scans 2
Spectrometer Frequency 376.50
Nucleus 19F
F3C
OH
O
1s
0 -10 -20 -30 -40 -50 -60 -70 -80 -90 -110 -130 -150 -170 -190 -210 -230 -250 -270 -290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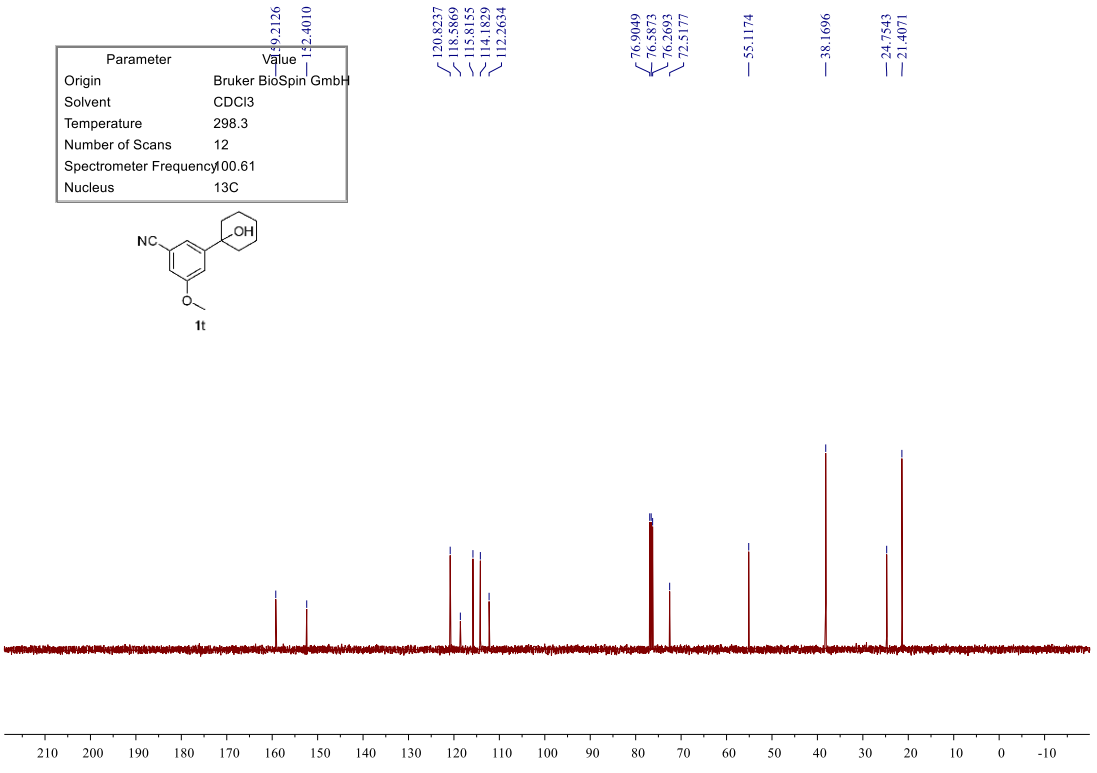
7.3613
7.3055
7.3012
7.2993
7.2951
7.2610
6.9896
6.9864
6.9834
6.9802
3.8203
1.9016
1.7629
1.7574
1.7339
1.7032
1.6973
1.6833
1.6742
1.6616
1.6536
1.6324
1.6237
Parameter Value
Origin Bruker BioSpin GmbH
Solvent CDCB
Temperature 298.1
Number of Scans 2
Spectrometer Frequency 400.13
Nucleus 1H
NC
OH
O
1t
1.02
1.03
1.00
3.01
1.05
9.86
1.68
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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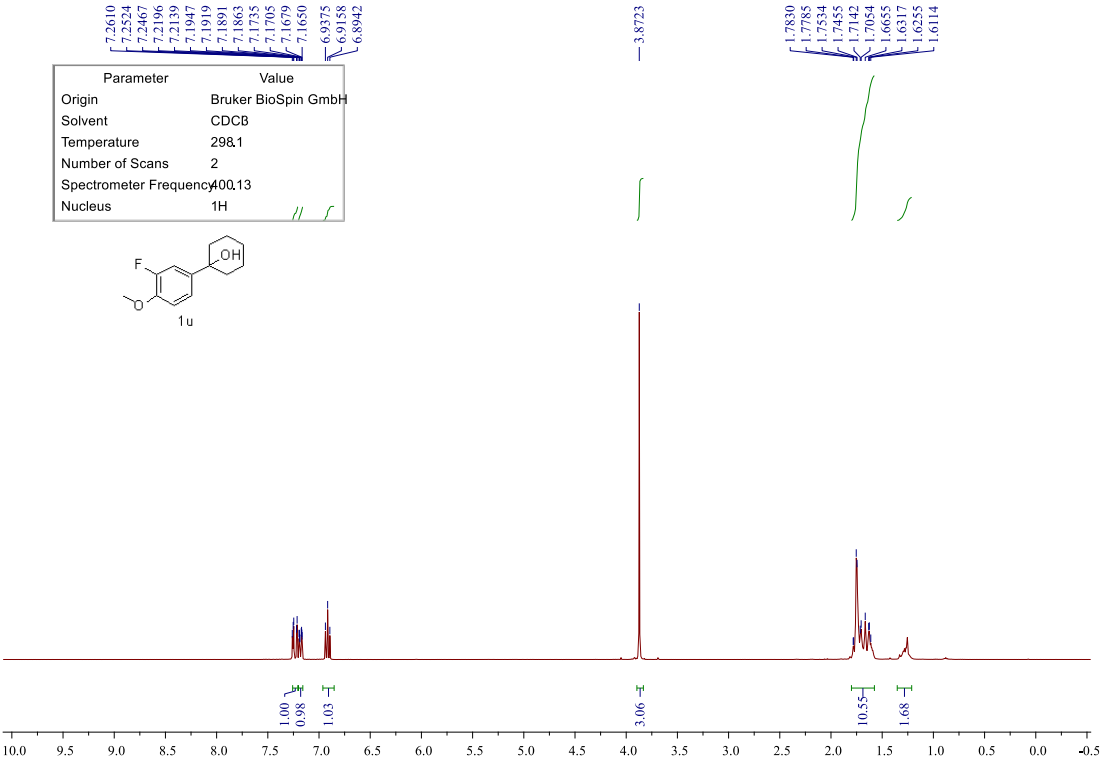
115.8155
114.1829
112.2634
76.9049
76.5873
76.2693
72.5177
55.1174
38.1696
24.7543
21.4071
Parameter Value
Origin Bruker BioSpin GmbH
Solvent CDCl3
Temperature 298.3
Number of Scans 12
Spectrometer Frequency 100.61
Nucleus 13C
NC
OH
O
1t
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10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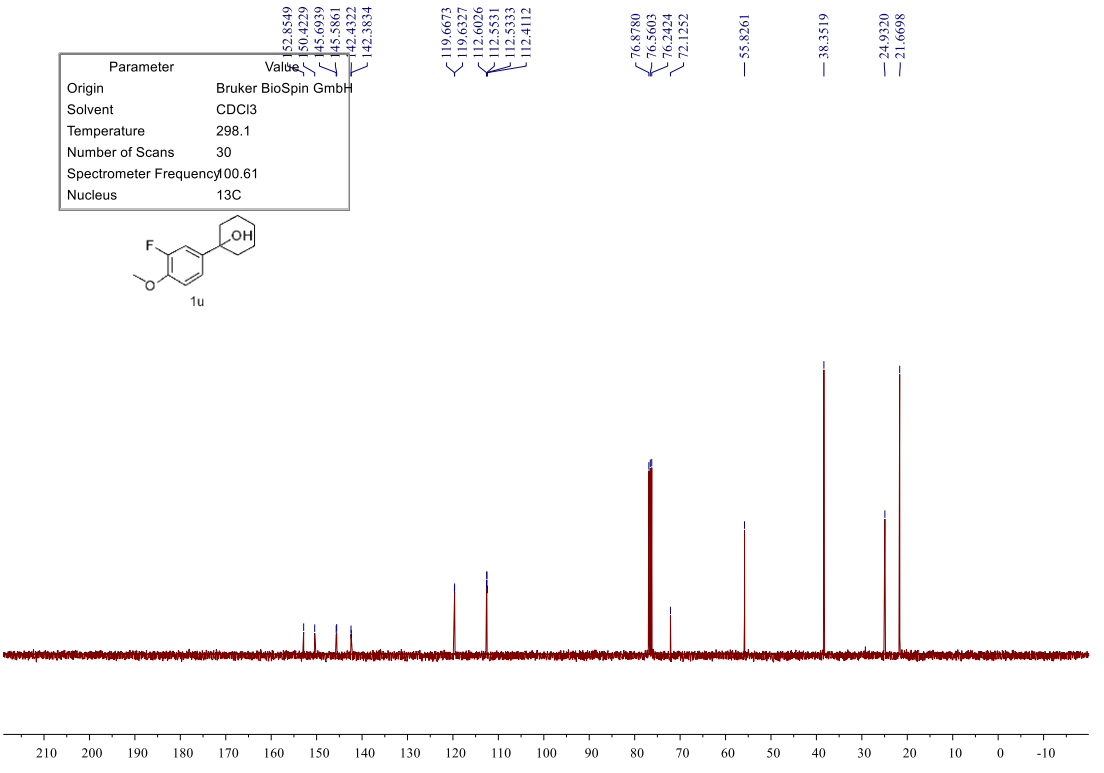
7.2467
7.2196
7.2139
7.1947
7.1919
7.1891
7.1863
7.1735
7.1705
7.1679
7.1650
6.9375
6.9158
6.8942
3.8723
1.7830
1.7785
1.7534
1.7455
1.7142
1.7054
1.6655
1.6317
1.6255
1.6114
Parameter Value
Origin Bruker BioSpin GmbH
Solvent CDCl3
Temperature 298.1
Number of Scans 2
Spectrometer Frequency 400.13
Nucleus 1H
F
OH
O
1u
1.00
0.98
1.03
3.06
10.55
1.68
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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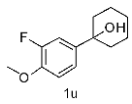
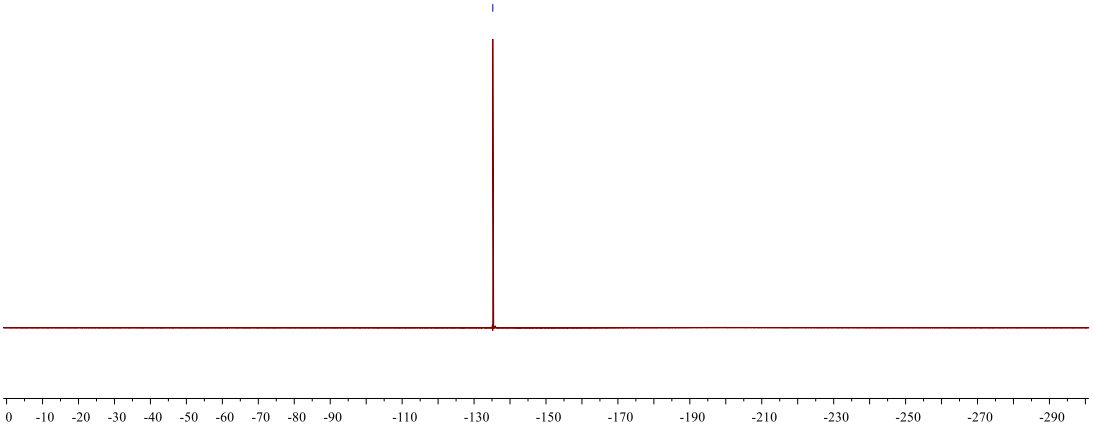
112.5333
112.4112
76.8780
76.5603
76.2424
72.1252
55.8261
38.3519
24.9320
21.6698
Parameter Value
Origin Bruker BioSpin GmbH
Solvent CDCl3
Temperature 298.1
Number of Scans 30
Spectrometer Frequency 100.61
Nucleus 13C
F
OH
O
1u
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10

Parameter	Value
Origin	Bruker BioSpin GmbH
Solvent	CDCl3
Temperature	298.2
Number of Scans	2
Spectrometer Frequency	376.44
Nucleus	19F



1u

-135.2104



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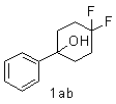
7.3850
7.3656
7.3178
7.3003
7.2815
7.2610

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



1ab

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2.2350
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2.2013
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2.1269
2.0950
2.0792
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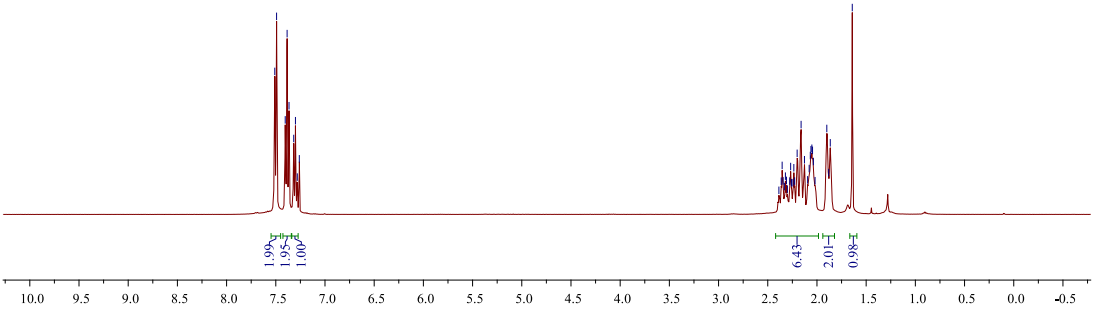
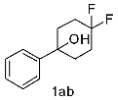
1.8647
1.6411



Parameter	Value
Origin	Bruker BioSpin GmbH
Solvent	CDCl3
Temperature	298.2
Number of Scans	45
Spectrometer Frequency	100.61
Nucleus	13C



1ab

146.9247
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126.9155
125.2411
123.8907
122.8703
122.8280
120.4570
76.8897
76.5719
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71.4083
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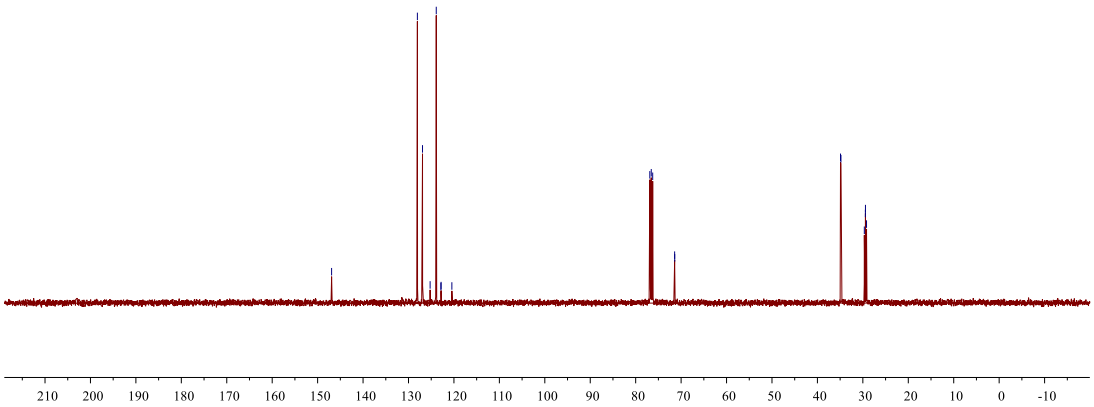
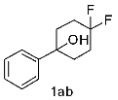
34.8214
29.6774
29.4417
29.4277
29.1918



Parameter	Value
Origin	Bruker BioSpin GmbH
Solvent	CDCl3
Temperature	298.2
Number of Scans	2
Spectrometer Frequency	376.50
Nucleus	19F



1ab

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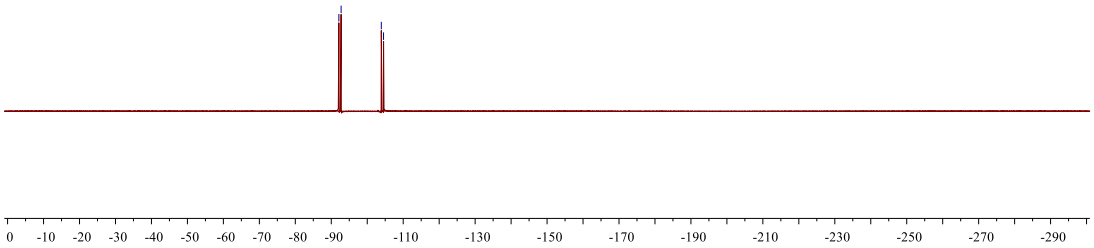
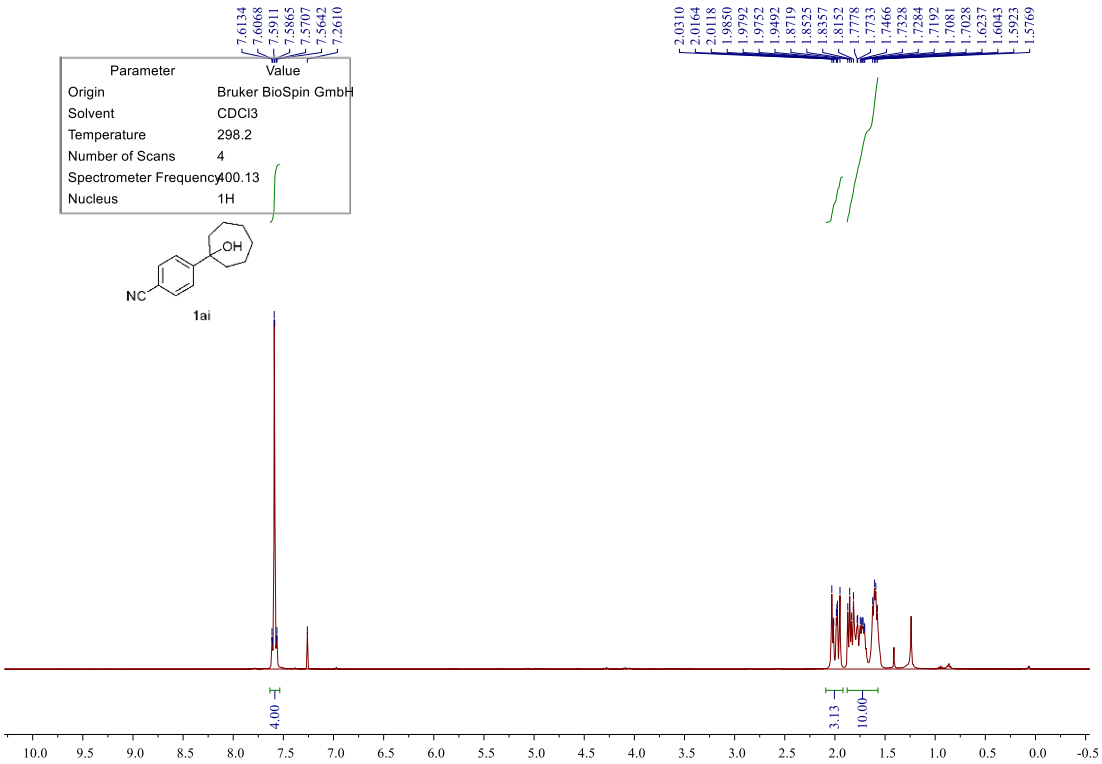
-104.5337

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7.5911
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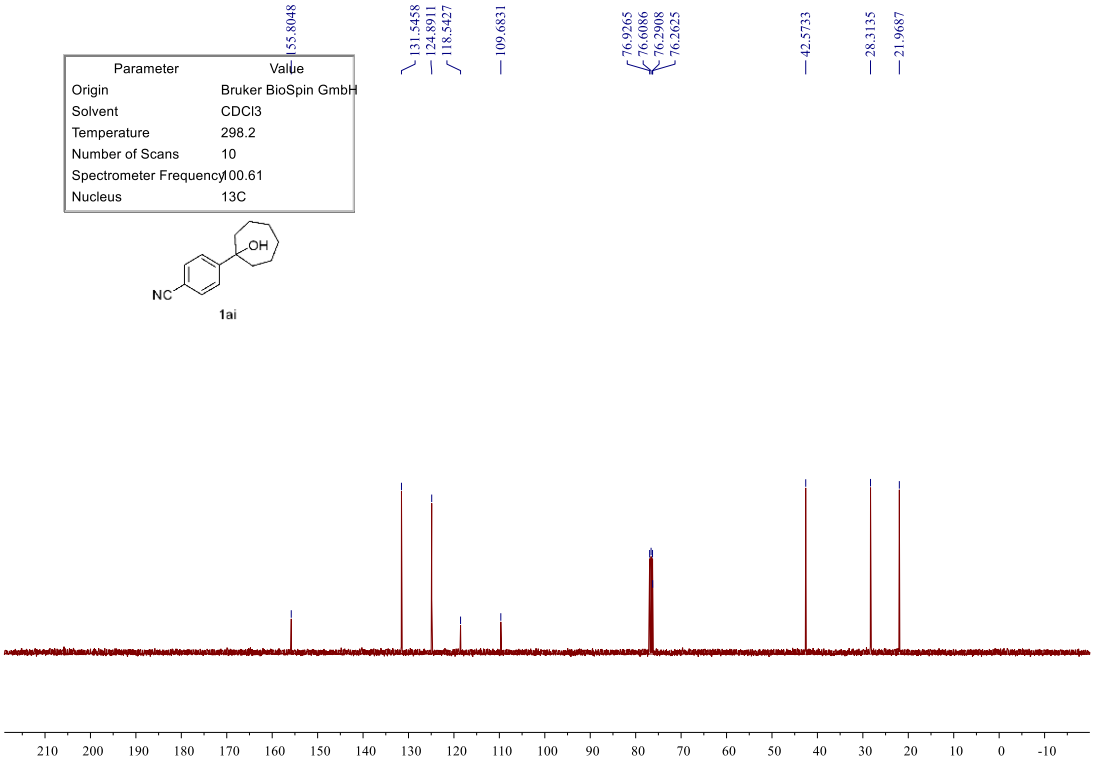
7.5707
7.5642
7.2610
2.0310
2.0164
2.0118
1.9850
1.9792
1.9752
1.9492
1.8719
1.8525
1.8357
1.8152
1.7778
1.7733
1.7466
1.7328
1.7284
1.7192
1.7081
1.7028
1.6237
1.6043
1.5923
1.5769
Parameter Value
Origin Bruker BioSpin GmbH
Solvent CDCl3
Temperature 298.2
Number of Scans 4
Spectrometer Frequency 400.13
Nucleus 1H
OH
NC
1ai
4.00
3.13
10.00
10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5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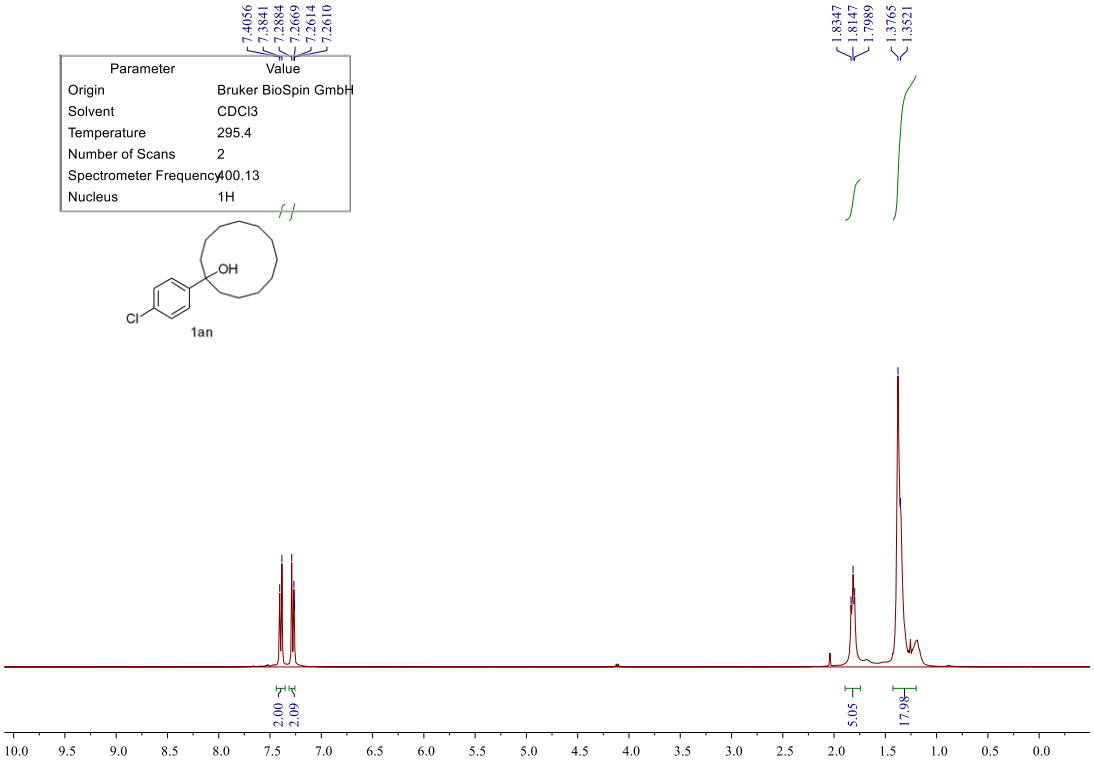
124.8911
118.5427
109.6831
76.9265
76.6086
76.2908
76.2625
42.5733
28.3135
21.9687
Parameter Value
Origin Bruker BioSpin GmbH
Solvent CDCl3
Temperature 298.2
Number of Scans 10
Spectrometer Frequency 100.61
Nucleus 13C
OH
NC
1ai
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10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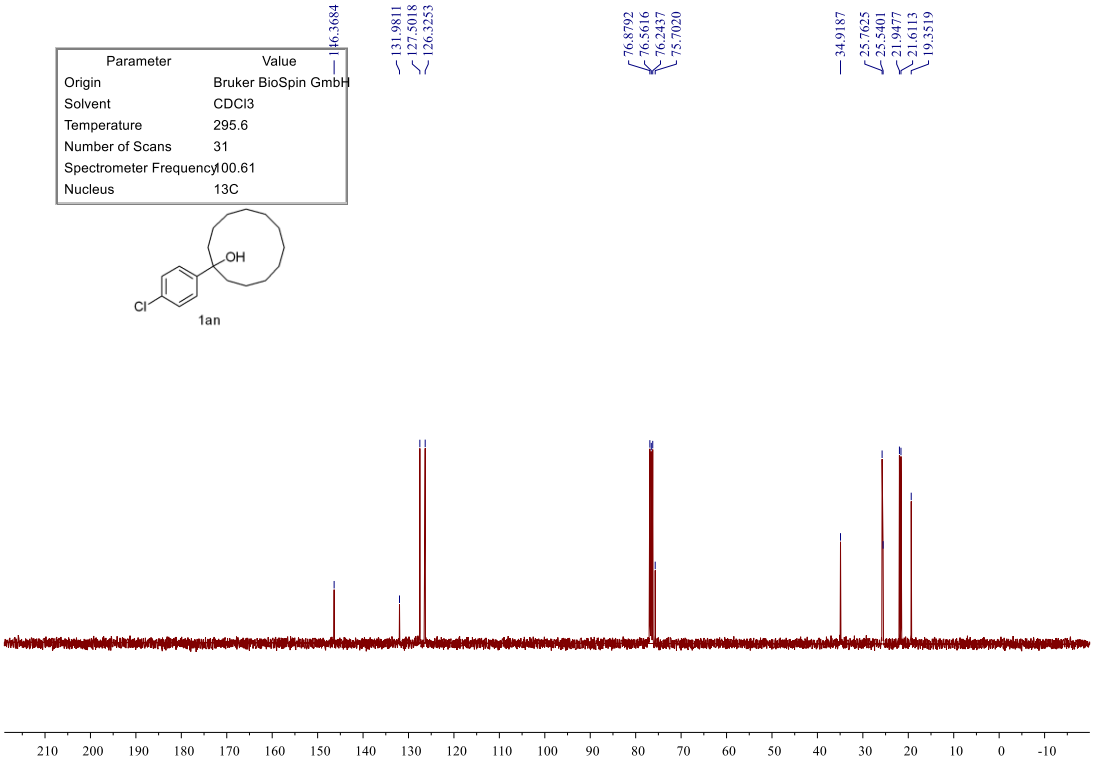
7.2669
7.2614
7.2610
1.8347
1.8147
1.7989
1.3765
1.3521
Parameter Value
Origin Bruker BioSpin GmbH
Solvent CDCl3
Temperature 295.4
Number of Scans 2
Spectrometer Frequency 400.13
Nucleus 1H
OH
Cl
1an
2.00
2.09
5.05
17.98
10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0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126.3253
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76.5616
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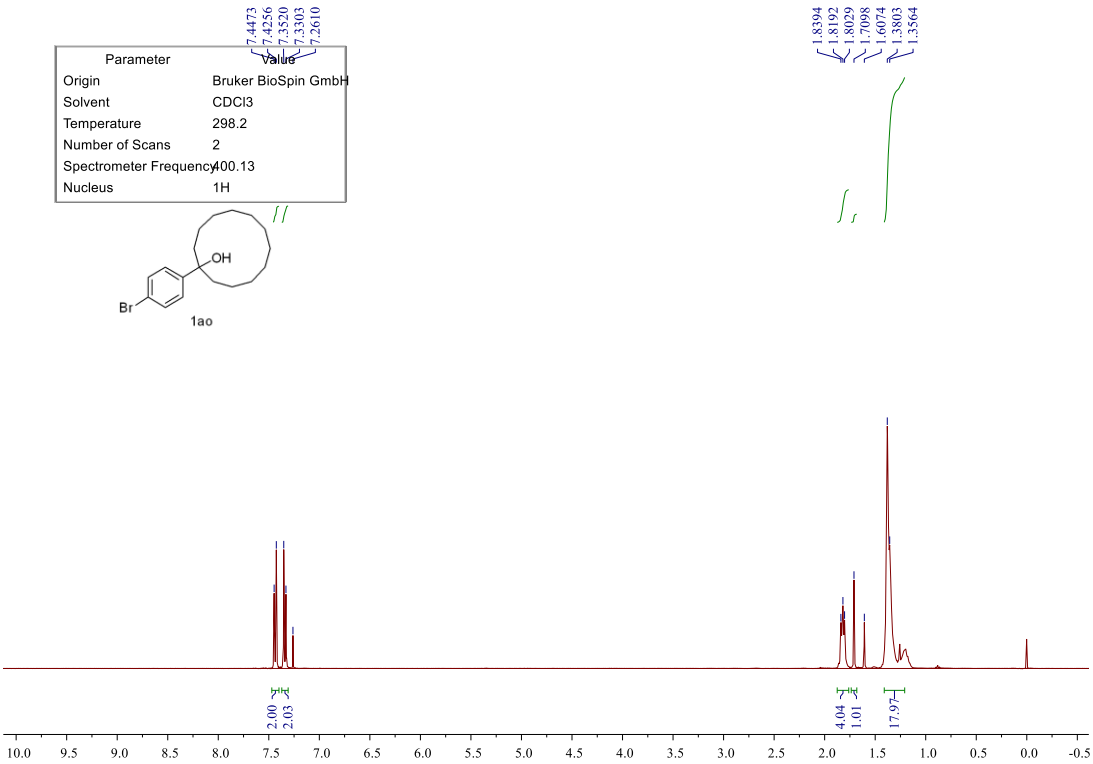
75.7020
34.9187
25.7625
25.5401
21.9477
21.6113
19.3519
Parameter Value
Origin Bruker BioSpin GmbH
Solvent CDCl3
Temperature 295.6
Number of Scans 31
Spectrometer Frequency 100.61
Nucleus 13C
OH
Cl
1an
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10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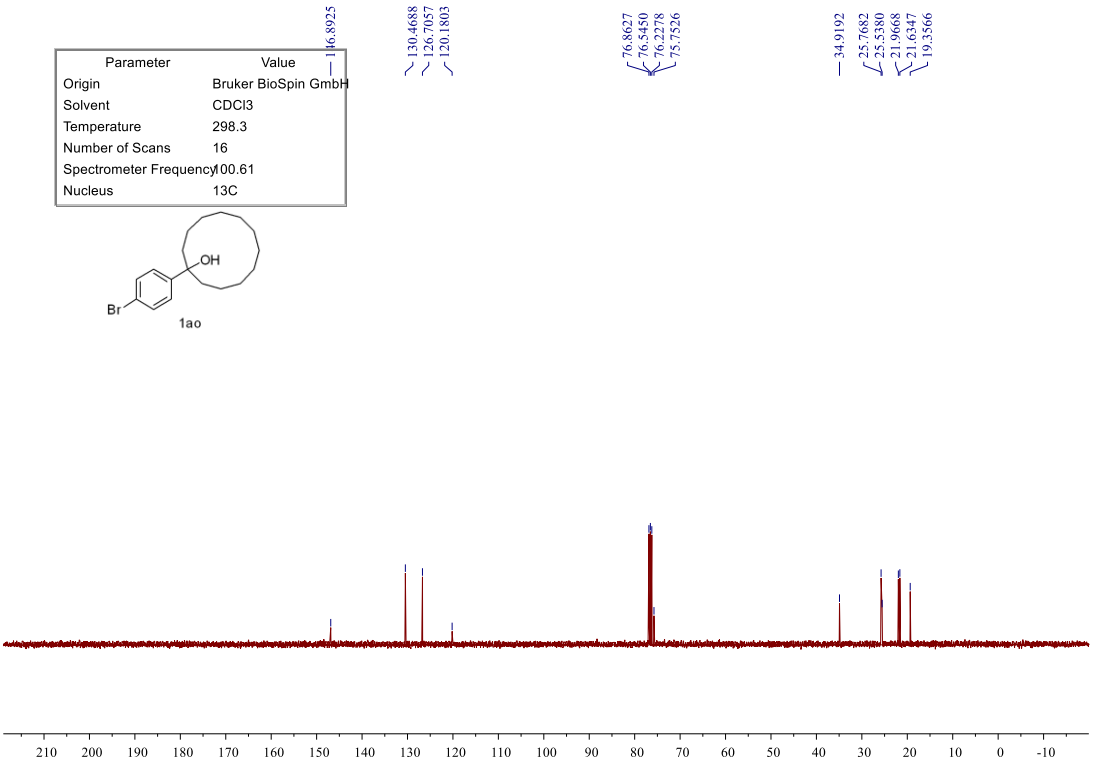
7.2610
1.8394
1.8192
1.8029
1.7098
1.6074
1.3803
1.3564
Parameter Value
Origin Bruker BioSpin GmbH
Solvent CDCl3
Temperature 298.2
Number of Scans 2
Spectrometer Frequency 400.13
Nucleus 1H
OH
Br
1ao
2.00
2.03
4.04
1.01
17.97
10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5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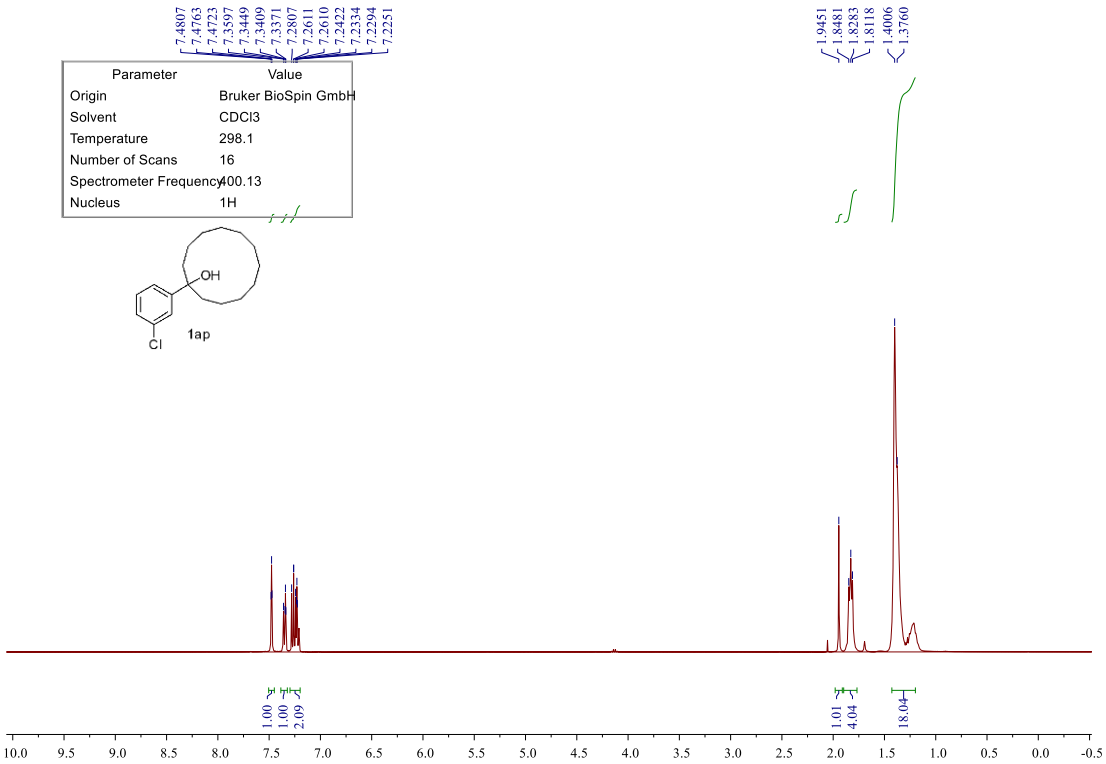
76.2278
75.7526
34.9192
25.7682
25.5380
21.9668
21.6347
19.3566
Parameter Value
Origin Bruker BioSpin GmbH
Solvent CDCl3
Temperature 298.3
Number of Scans 16
Spectrometer Frequency 100.61
Nucleus 13C
OH
Br
1ao
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10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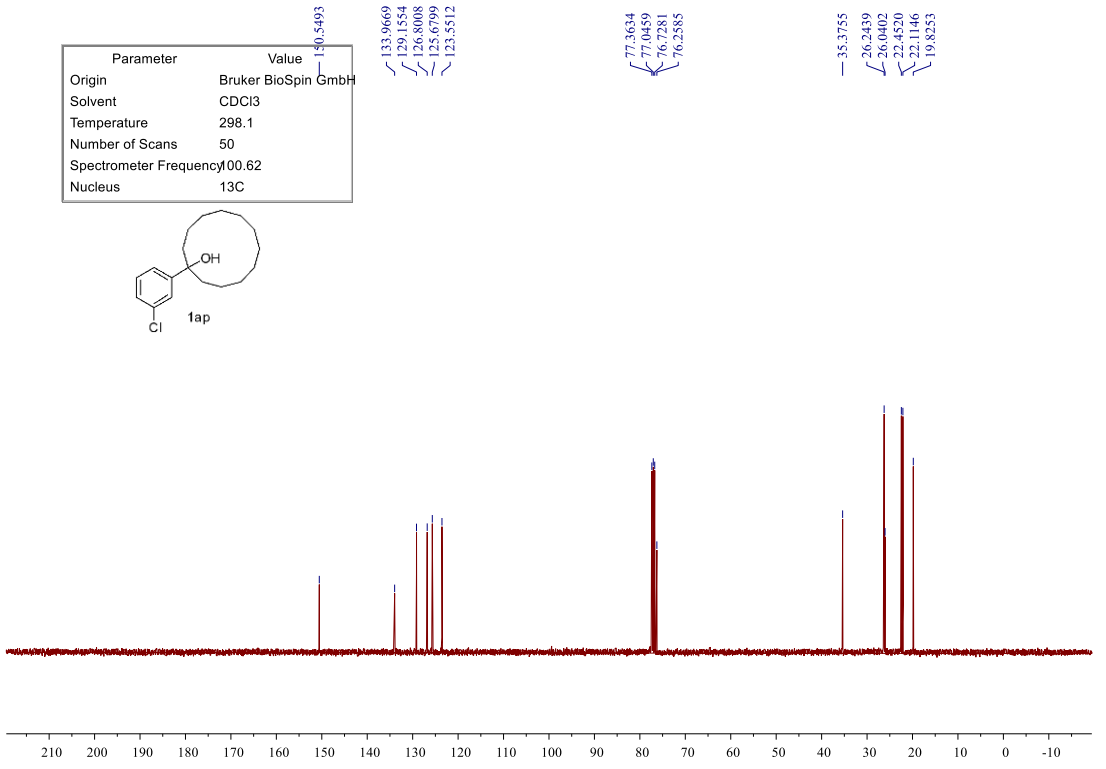
7.4723
7.3597
7.3449
7.3409
7.3371
7.2807
7.2611
7.2610
7.2422
7.2334
7.2294
7.2251
1.9451
1.8481
1.8283
1.8118
1.4006
1.3760
Parameter Value
Origin Bruker BioSpin GmbH
Solvent CDCl3
Temperature 298.1
Number of Scans 16
Spectrometer Frequency 400.13
Nucleus 1H
OH
Cl
1ap
1.00
1.00
2.09
1.01
4.04
18.04
10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5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129.1554
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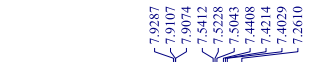
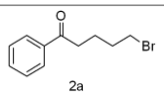
125.6799
123.5512
77.3634
77.0459
76.7281
76.2585
35.3755
26.2439
26.0402
22.4520
22.1146
19.8253
Parameter Value
Origin Bruker BioSpin GmbH
Solvent CDCl3
Temperature 298.1
Number of Scans 50
Spectrometer Frequency 100.62
Nucleus 13C
OH
Cl
1ap
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10



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



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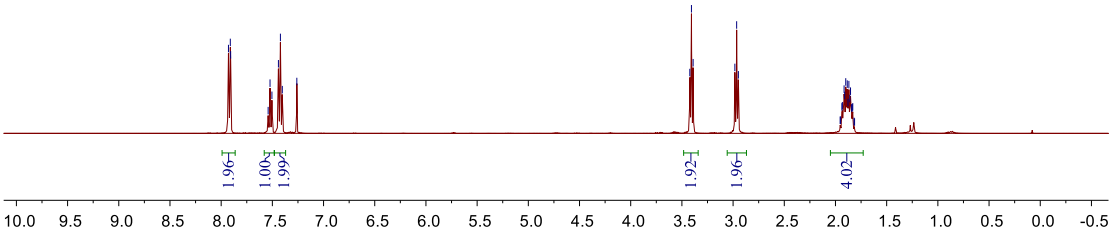
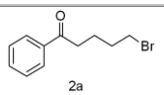


Parameter	Value
1 Origin	Bruker BioSpin GmbH
2 Solvent	CDCl3
3 Temperature	298.2
4 Number of Scans	19
5 Spectrometer Frequency	100.61
6 Nucleus	13C



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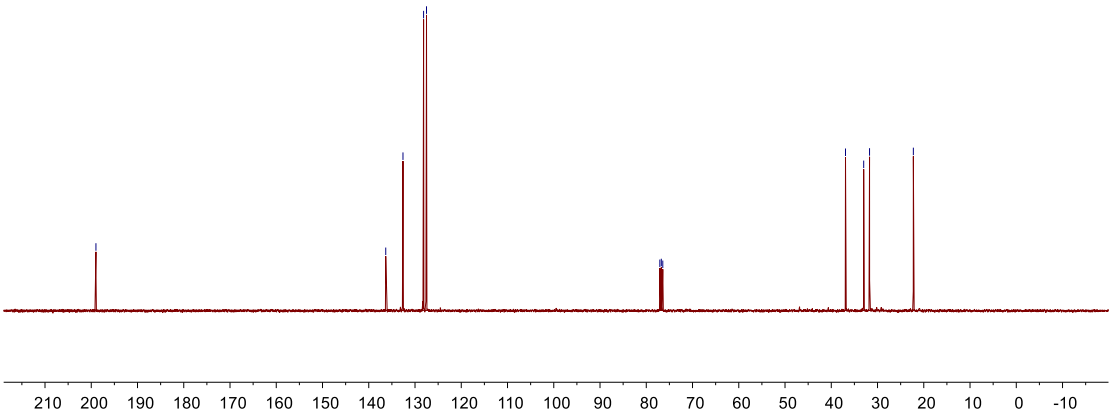

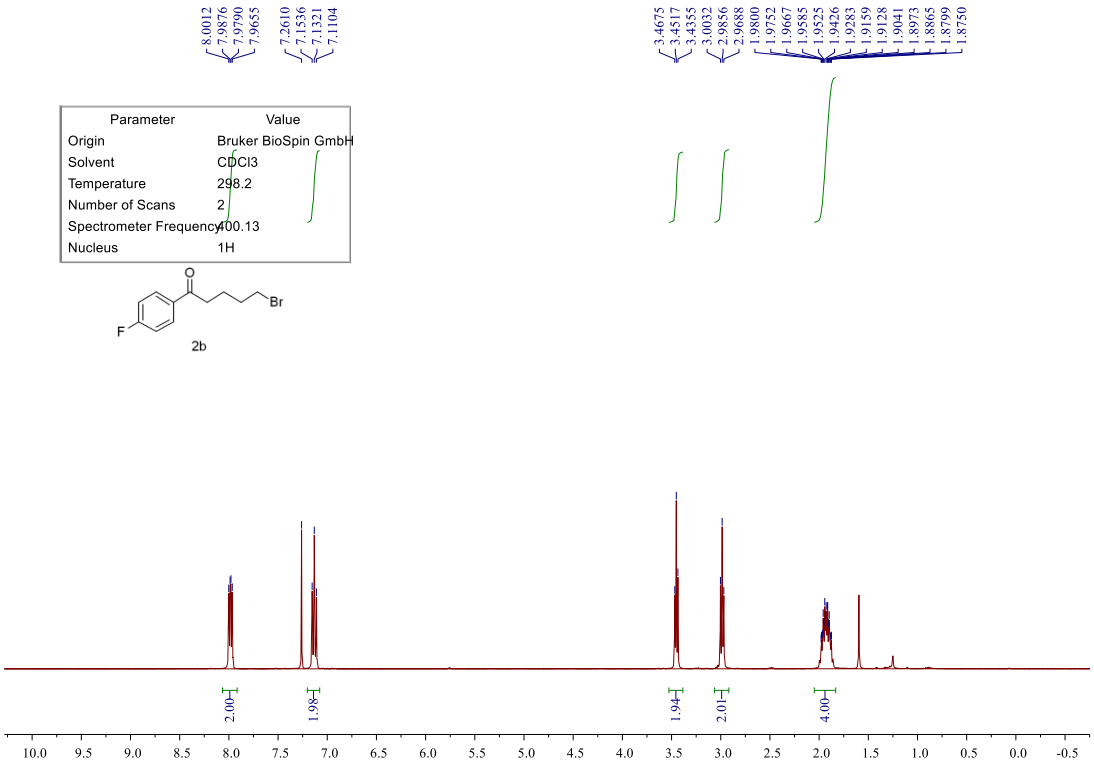
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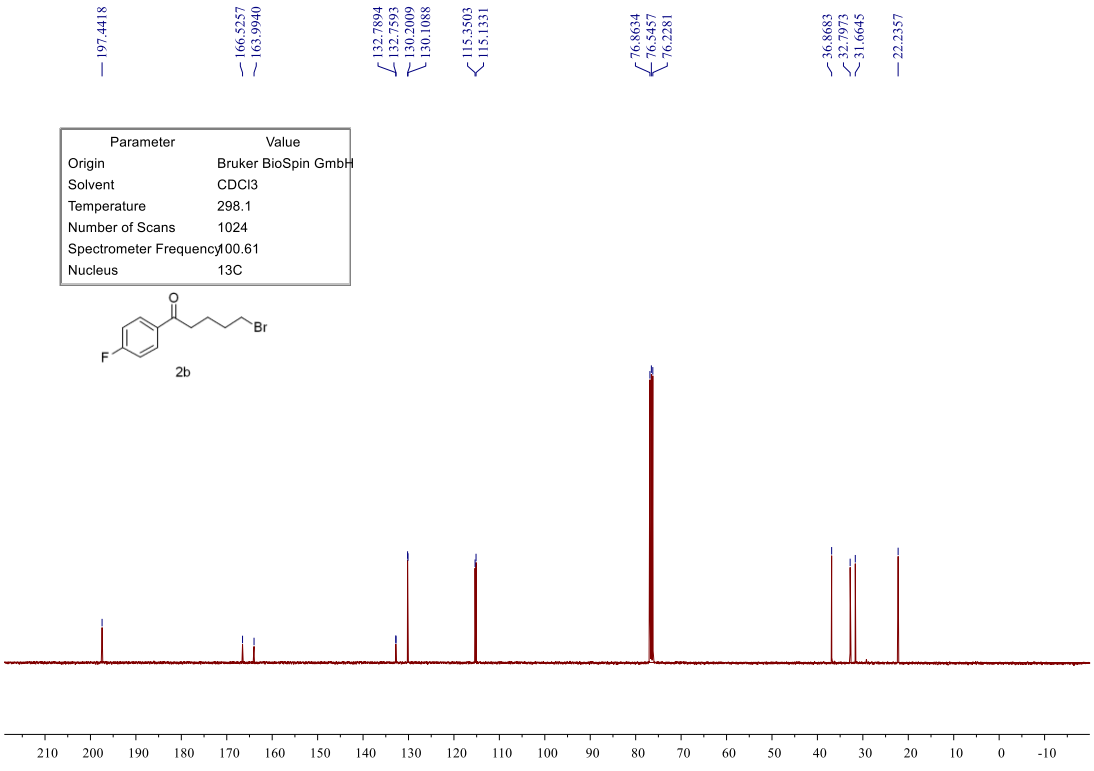
7.9655
7.2610
7.1536
7.1321
7.1104
3.4675
3.4517
3.4355
3.0032
2.9856
2.9688
1.9800
1.9752
1.9667
1.9585
1.9525
1.9426
1.9283
1.9159
1.9128
1.9041
1.8973
1.8865
1.8799
1.8750
Parameter Value
Origin Bruker BioSpin GmbH
Solvent CDCl3
Temperature 298.2
Number of Scans 2
Spectrometer Frequency 400.13
Nucleus 1H
O
Br
F
2b
2.00
1.98
1.94
2.01
4.00
10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5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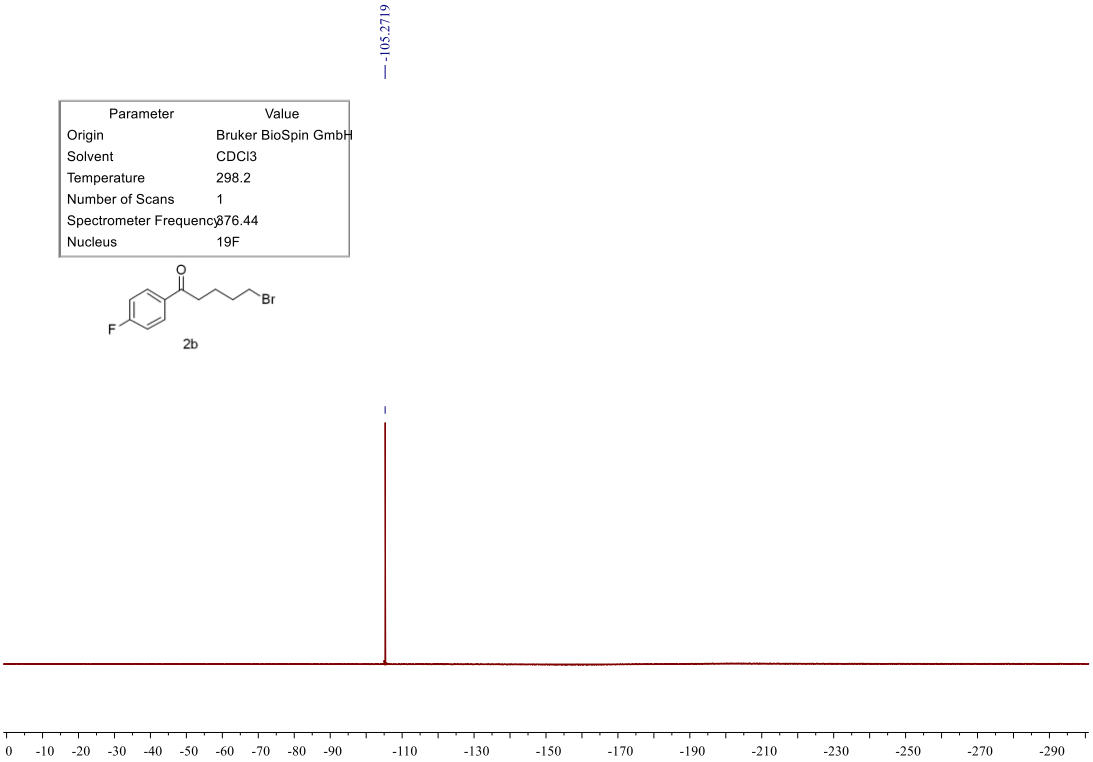
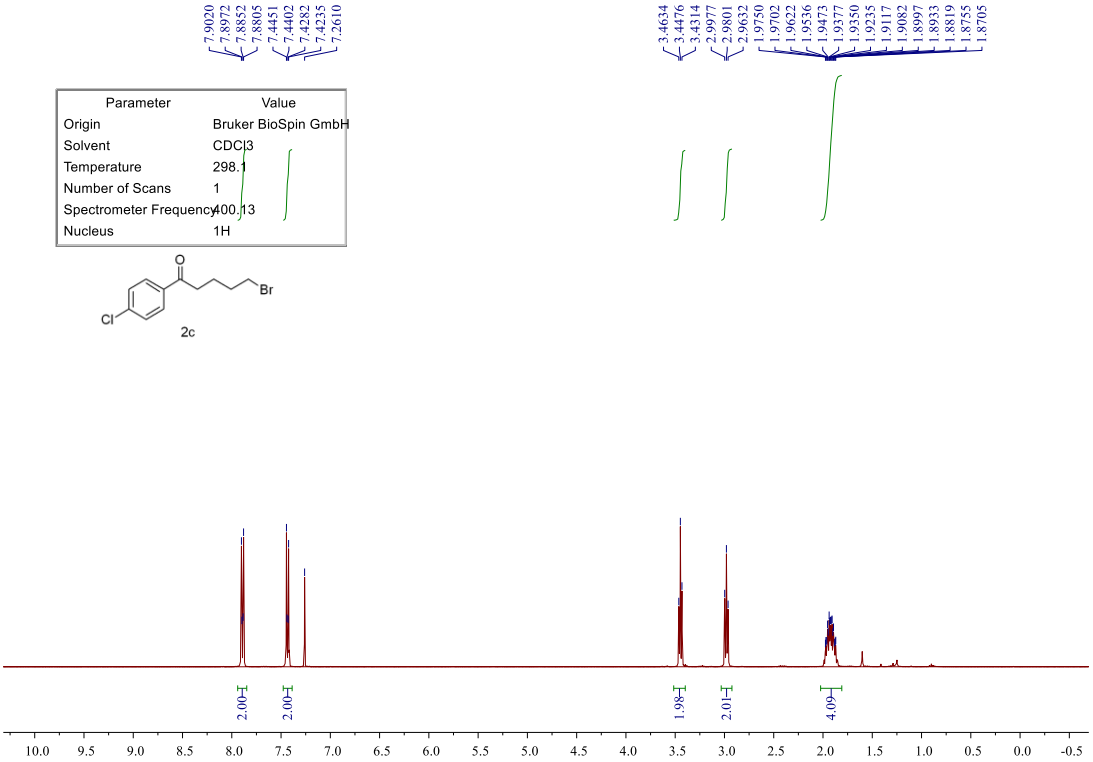
163.9940
132.7894
132.7593
130.2009
130.1088
115.3503
115.1331
76.8634
76.5457
76.2281
36.8683
32.7973
31.6645
22.2357
Parameter Value
Origin Bruker BioSpin GmbH
Solvent CDCl3
Temperature 298.1
Number of Scans 1024
Spectrometer Frequency 100.61
Nucleus 13C
O
Br
F
2b
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10


-105.2719
Parameter Value
Origin Bruker BioSpin GmbH
Solvent CDCl3
Temperature 298.2
Number of Scans 1
Spectrometer Frequency 376.44
Nucleus 19F
O
Br
F
2b
0 -10 -20 -30 -40 -50 -60 -70 -80 -90 -110 -130 -150 -170 -190 -210 -230 -250 -270 -290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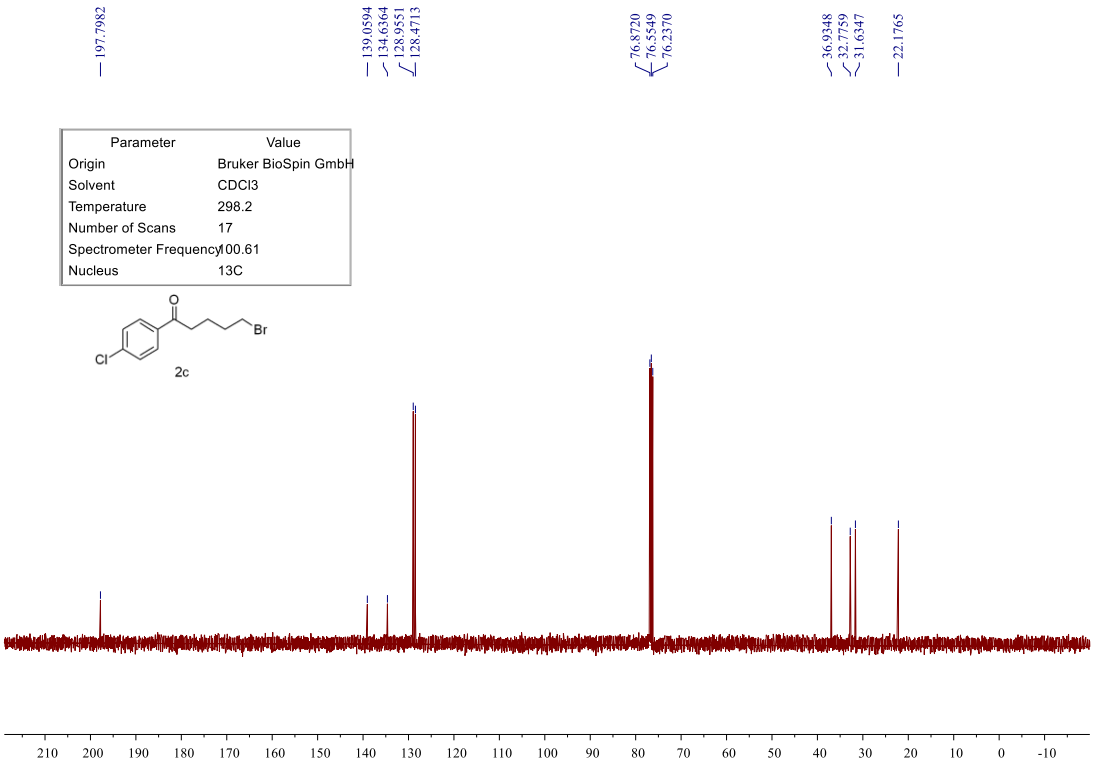
7.8852
7.8805
7.4451
7.4402
7.4282
7.4235
7.2610
3.4634
3.4476
3.4314
2.9977
2.9801
2.9632
1.9750
1.9702
1.9622
1.9536
1.9473
1.9377
1.9350
1.9235
1.9117
1.9082
1.8997
1.8933
1.8819
1.8755
1.8705
Parameter Value
Origin Bruker BioSpin GmbH
Solvent CDCl3
Temperature 298.1
Number of Scans 1
Spectrometer Frequency 400.13
Nucleus 1H
O
Br
Cl
2c
2.00
2.00
1.98
2.01
4.09
10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5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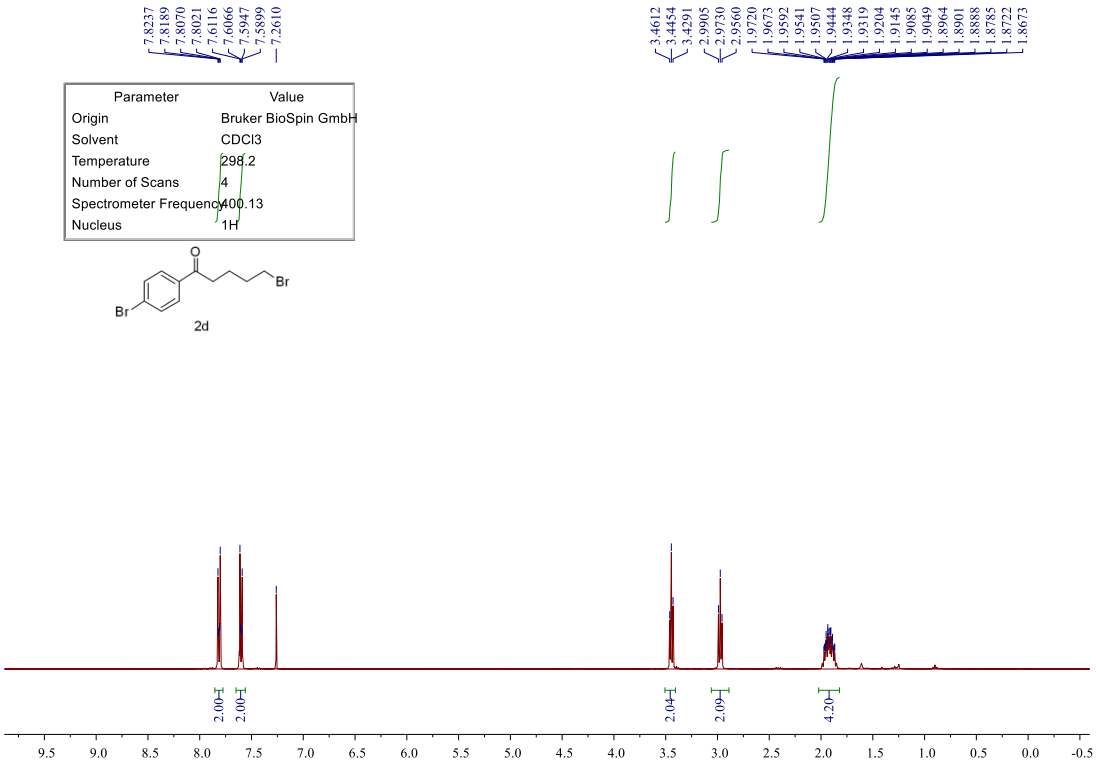
134.6364
128.9551
128.4713
76.8720
76.5549
76.2370
36.9348
32.7759
31.6347
22.1765
Parameter Value
Origin Bruker BioSpin GmbH
Solvent CDCl3
Temperature 298.2
Number of Scans 17
Spectrometer Frequency 100.61
Nucleus 13C
O
Br
Cl
2c
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10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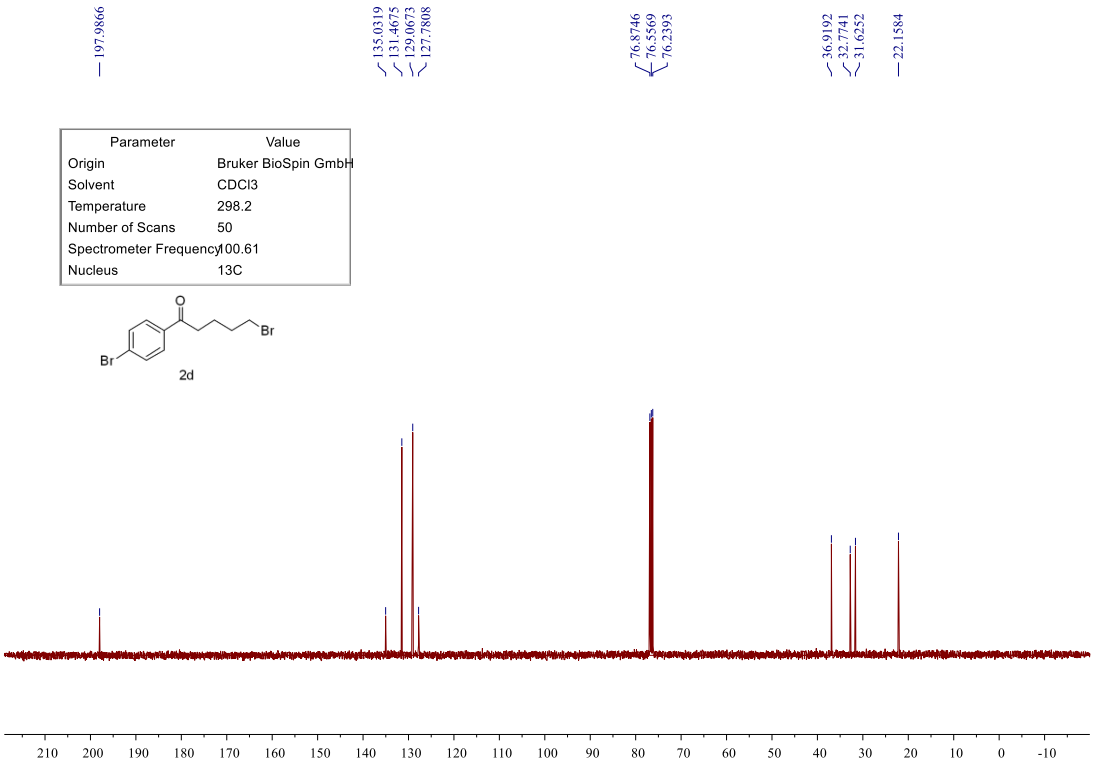
7.8070
7.8021
7.6116
7.6066
7.5947
7.5899
7.2610
3.4612
3.4454
3.4291
2.9905
2.9730
2.9560
1.9720
1.9673
1.9592
1.9541
1.9507
1.9444
1.9348
1.9319
1.9204
1.9145
1.9085
1.9049
1.8964
1.8901
1.8888
1.8785
1.8722
1.8673
Parameter Value
Origin Bruker BioSpin GmbH
Solvent CDCl3
Temperature 298.2
Number of Scans 4
Spectrometer Frequency 400.13
Nucleus 1H
O
Br
Br
2d
2.00
2.00
2.04
2.09
4.20
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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131.4675
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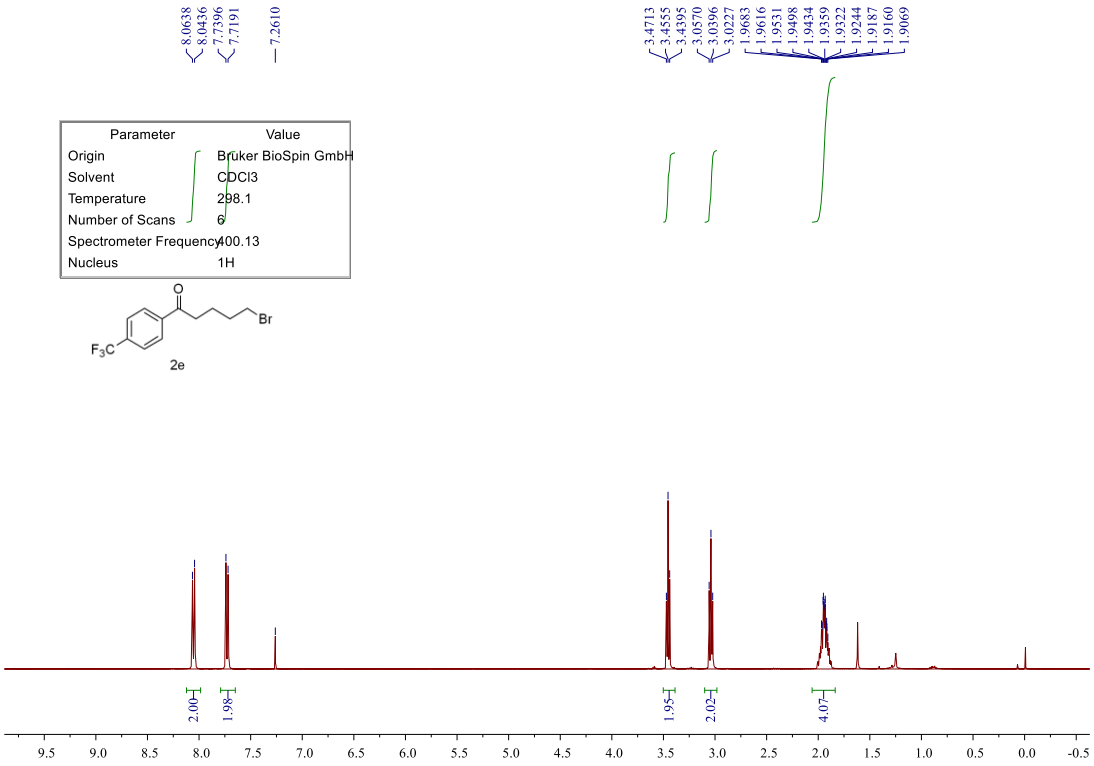
127.7808
76.8746
76.5569
76.2393
36.9192
32.7741
31.6252
22.1584
Parameter Value
Origin Bruker BioSpin GmbH
Solvent CDCl3
Temperature 298.2
Number of Scans 50
Spectrometer Frequency 100.61
Nucleus 13C
O
Br
Br
2d
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10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7.7191
7.2610
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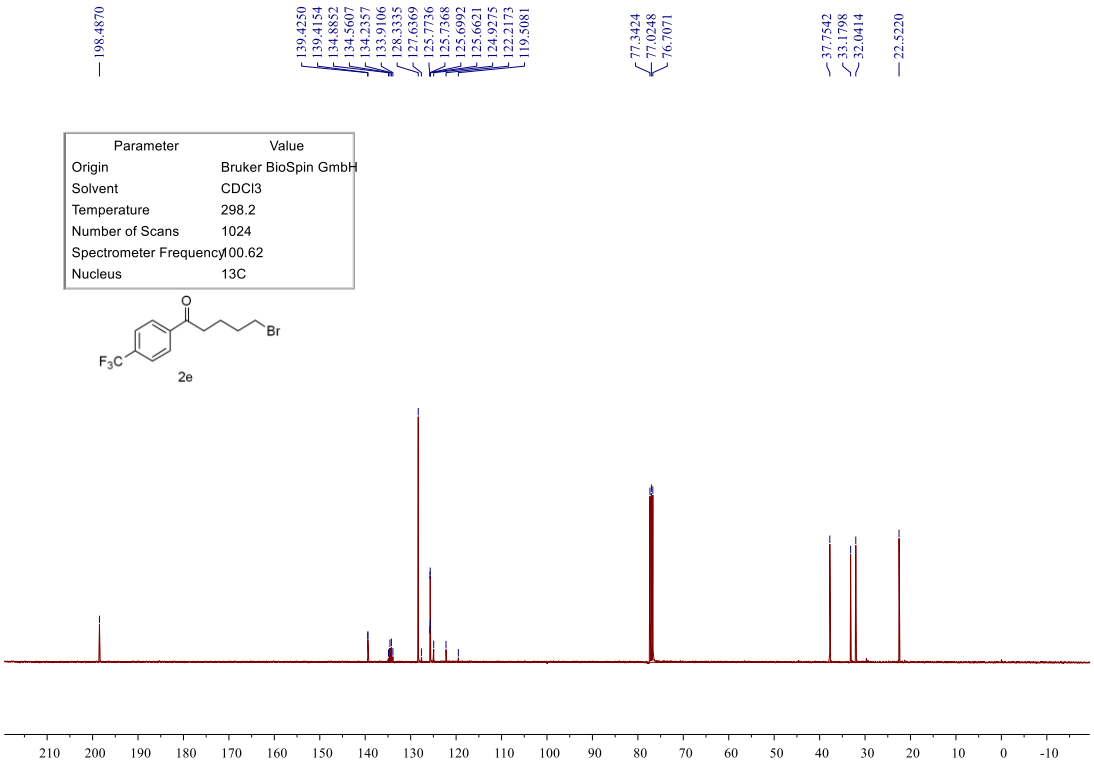
3.4555
3.4395
3.0570
3.0396
3.0227
1.9683
1.9616
1.9531
1.9498
1.9434
1.9359
1.9322
1.9244
1.9187
1.9160
1.9069
Parameter Value
Origin Bruker BioSpin GmbH
Solvent CDCl3
Temperature 298.1
Number of Scans 6
Spectrometer Frequency 400.13
Nucleus 1H
O
Br
F3C
2e
2.00
1.98
1.95
2.02
4.07
9.5 9.0 8.5 8.0 7.5 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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134.5607
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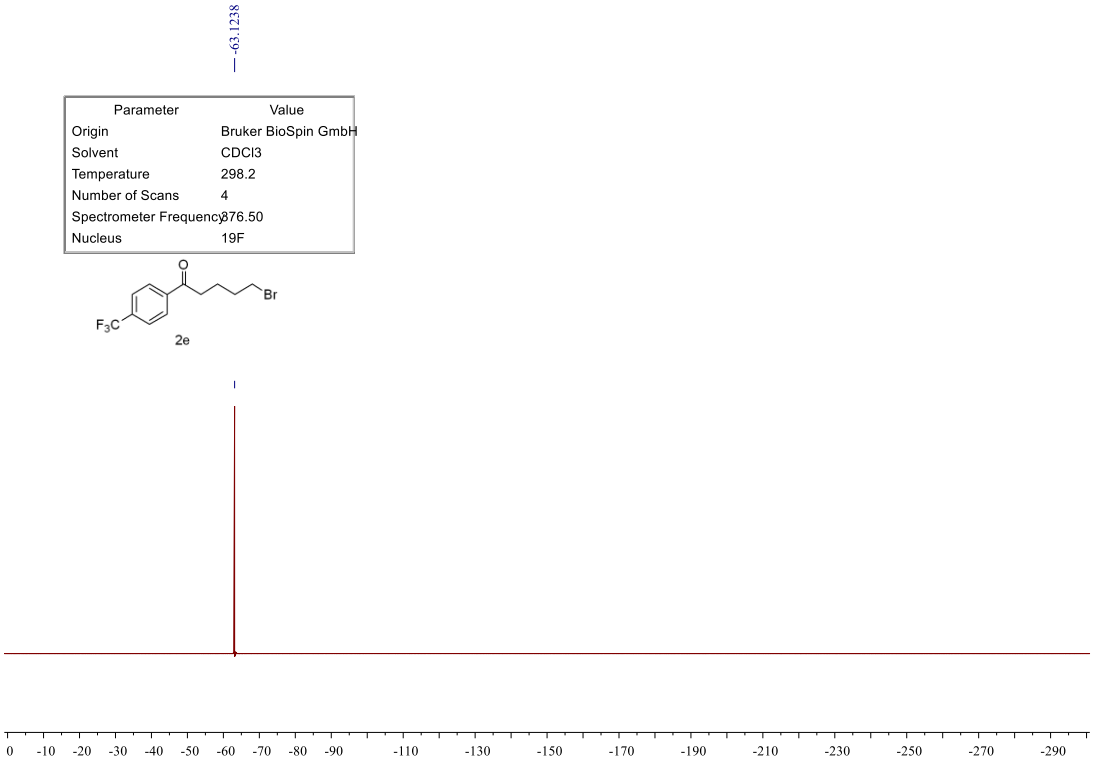
127.6369
125.7736
125.7368
125.6992
125.6621
124.9275
122.2173
119.5081
77.3424
77.0248
76.7071
37.7542
33.1798
32.0414
22.5220
Parameter Value
Origin Bruker BioSpin GmbH
Solvent CDCl3
Temperature 298.2
Number of Scans 1024
Spectrometer Frequency 100.62
Nucleus 13C
O
Br
F3C
2e
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10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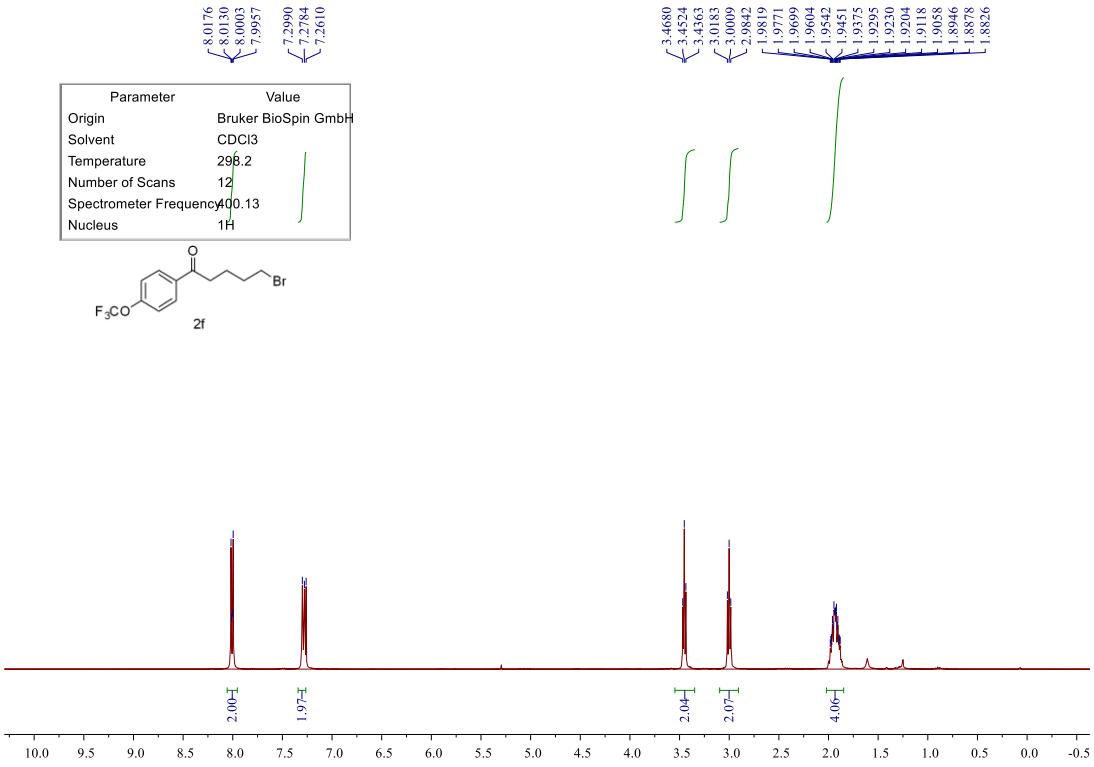
Parameter Value
Origin Bruker BioSpin GmbH
Solvent CDCl3
Temperature 298.2
Number of Scans 4
Spectrometer Frequency 376.50
Nucleus 19F
O
Br
F3C
2e
0 -10 -20 -30 -40 -50 -60 -70 -80 -90 -110 -130 -150 -170 -190 -210 -230 -250 -270 -290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7.2784
7.2610
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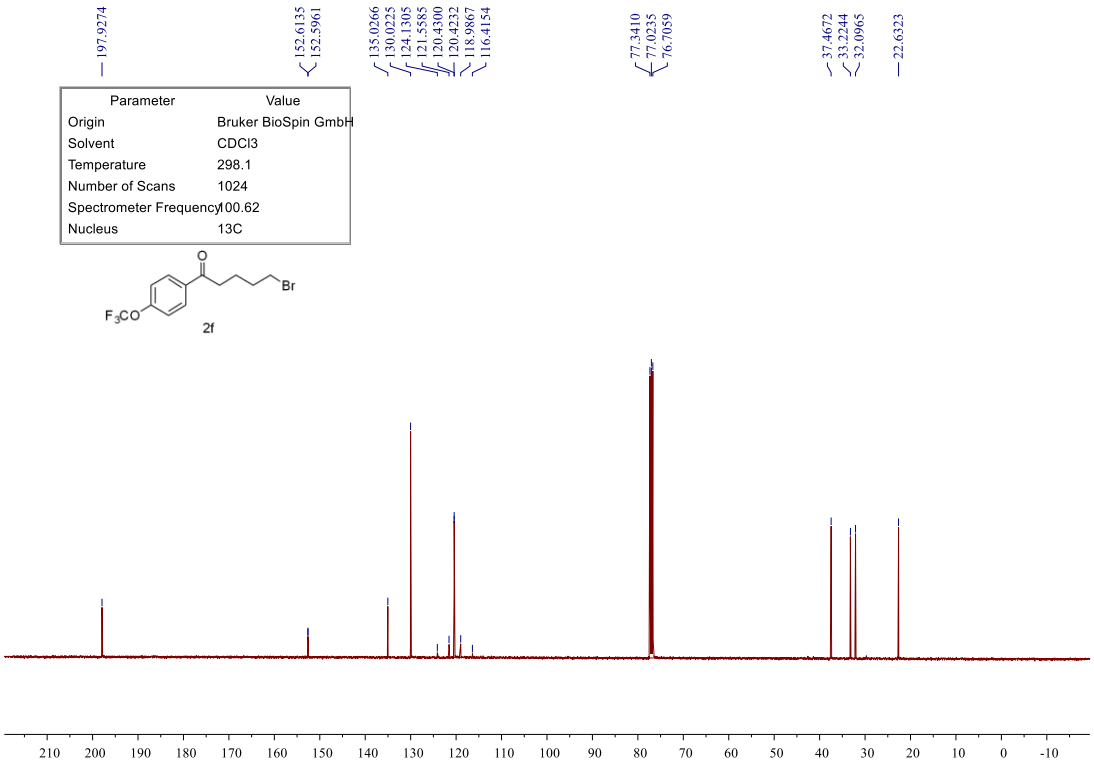
3.4524
3.4363
3.0183
3.0009
2.9842
1.9819
1.9771
1.9699
1.9604
1.9542
1.9451
1.9375
1.9295
1.9230
1.9204
1.9118
1.9058
1.8946
1.8878
1.8826
Parameter Value
Origin Bruker BioSpin GmbH
Solvent CDCl3
Temperature 298.2
Number of Scans 12
Spectrometer Frequency 400.13
Nucleus 1H
O
Br
F3CO
2f
2.00
1.97
2.04
2.07
4.06
10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5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152.5961
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121.5585
120.4300
120.4232
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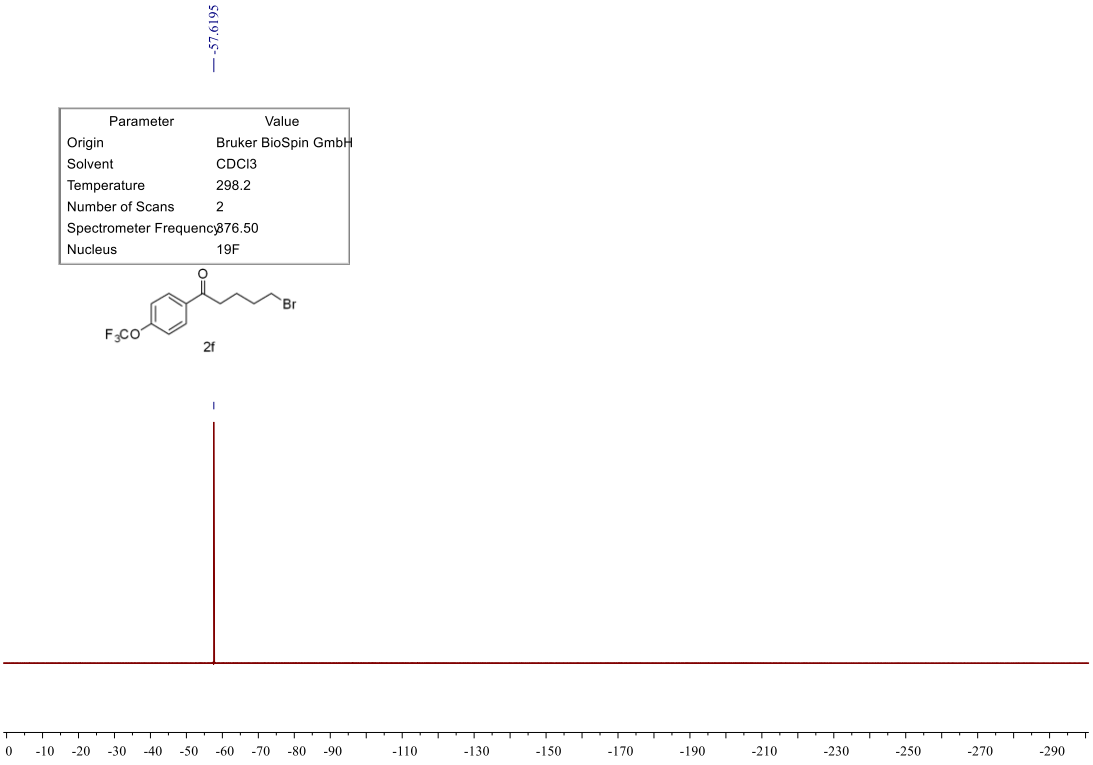
116.4154
77.3410
77.0235
76.7059
37.4672
33.2244
32.0965
22.6323
Parameter Value
Origin Bruker BioSpin GmbH
Solvent CDCl3
Temperature 298.1
Number of Scans 1024
Spectrometer Frequency 100.62
Nucleus 13C
O
Br
F3CO
2f
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10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Parameter Value
Origin Bruker BioSpin GmbH
Solvent CDCl3
Temperature 298.2
Number of Scans 2
Spectrometer Frequency 376.50
Nucleus 19F
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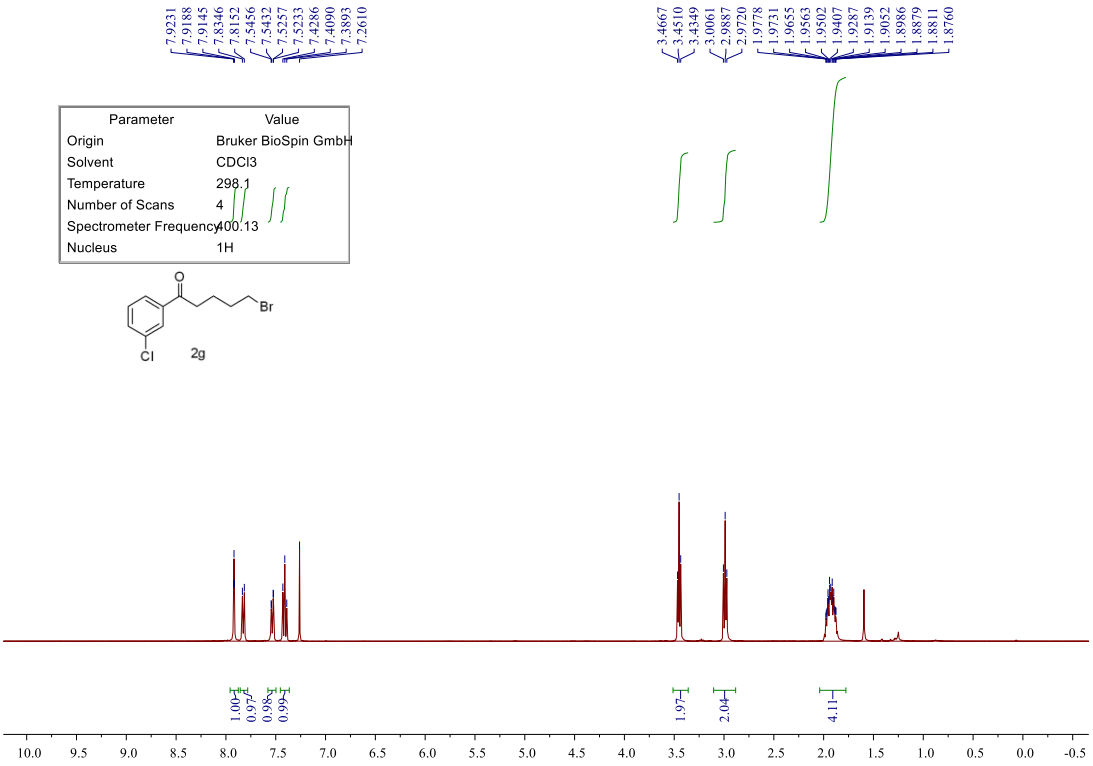
Br
F3CO
2f
0 -10 -20 -30 -40 -50 -60 -70 -80 -90 -110 -130 -150 -170 -190 -210 -230 -250 -270 -290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7.8152
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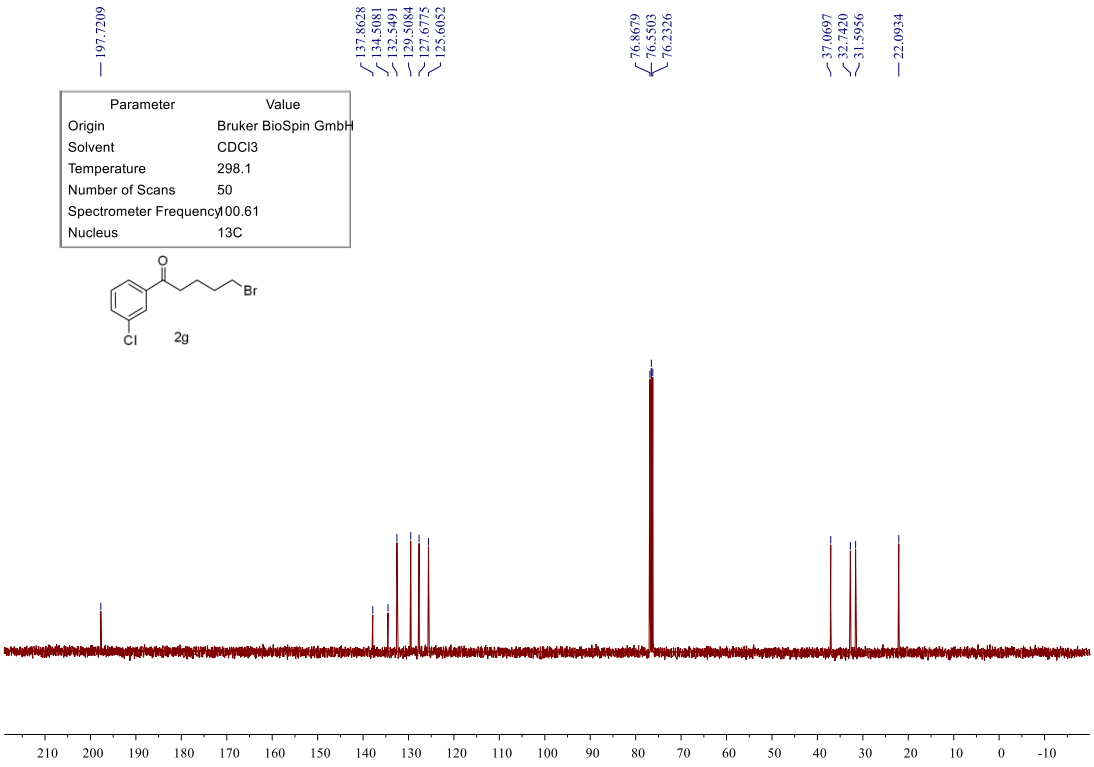
7.5233
7.4286
7.4090
7.3893
7.2610
3.4667
3.4510
3.4349
3.0061
2.9887
2.9720
1.9778
1.9731
1.9655
1.9563
1.9502
1.9407
1.9287
1.9139
1.9052
1.8986
1.8879
1.8811
1.8760
Parameter Value
Origin Bruker BioSpin GmbH
Solvent CDCl3
Temperature 298.1
Number of Scans 4
Spectrometer Frequency 400.13
Nucleus 1H
O
Br
Cl
2g
1.00
0.97
0.98
0.99
1.97
2.04
4.11
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 -0.5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127.6775
125.6052
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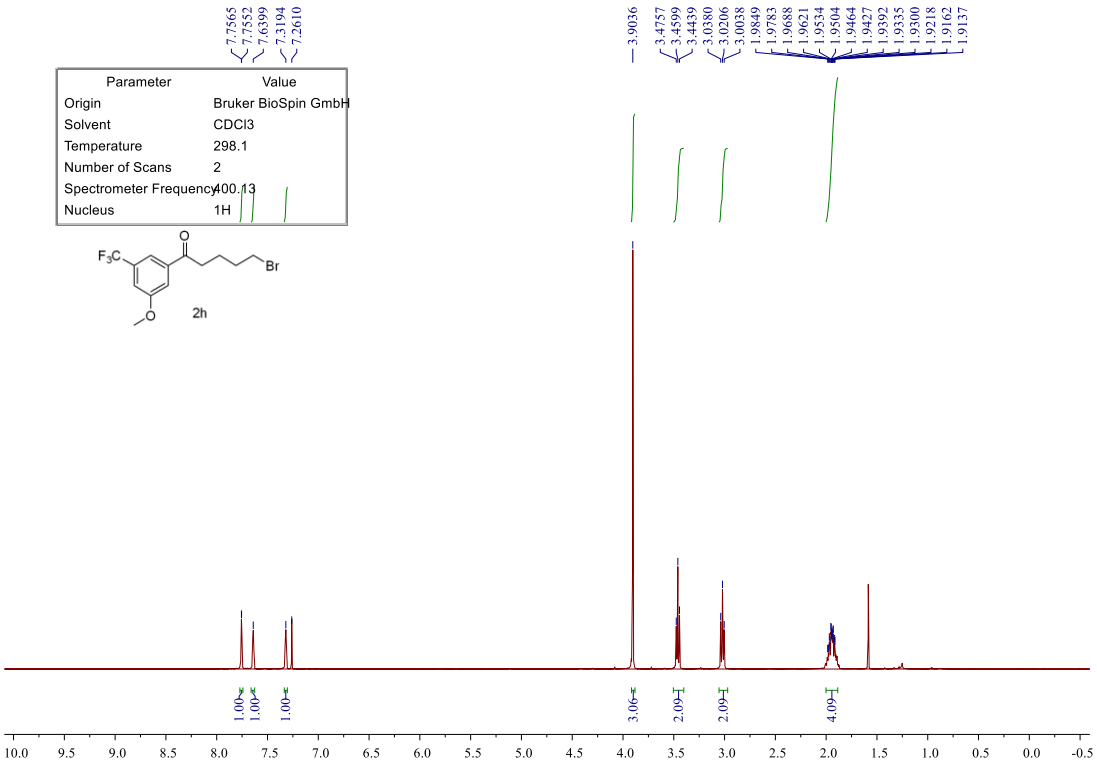
76.5503
76.2326
37.0697
32.7420
31.5956
22.0934
Parameter Value
Origin Bruker BioSpin GmbH
Solvent CDCl3
Temperature 298.1
Number of Scans 50
Spectrometer Frequency 100.61
Nucleus 13C
O
Br
Cl
2g
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10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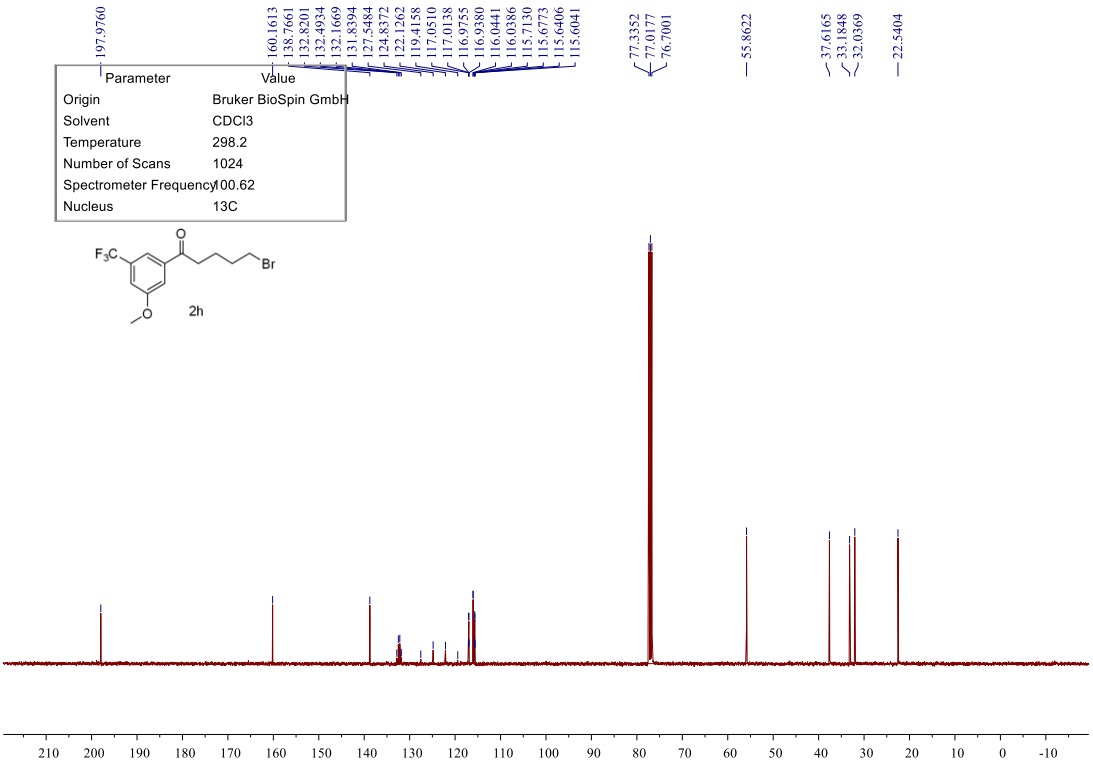
1.9534
1.9504
1.9464
1.9427
1.9392
1.9335
1.9300
1.9218
1.9162
1.9137
Parameter Value
Origin Bruker BioSpin GmbH
Solvent CDCl3
Temperature 298.1
Number of Scans 2
Spectrometer Frequency 400.13
Nucleus 1H
F3C
O
Br
O
2h
1.00
1.00
1.00
3.06
2.09
2.09
4.09
10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5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117.0138
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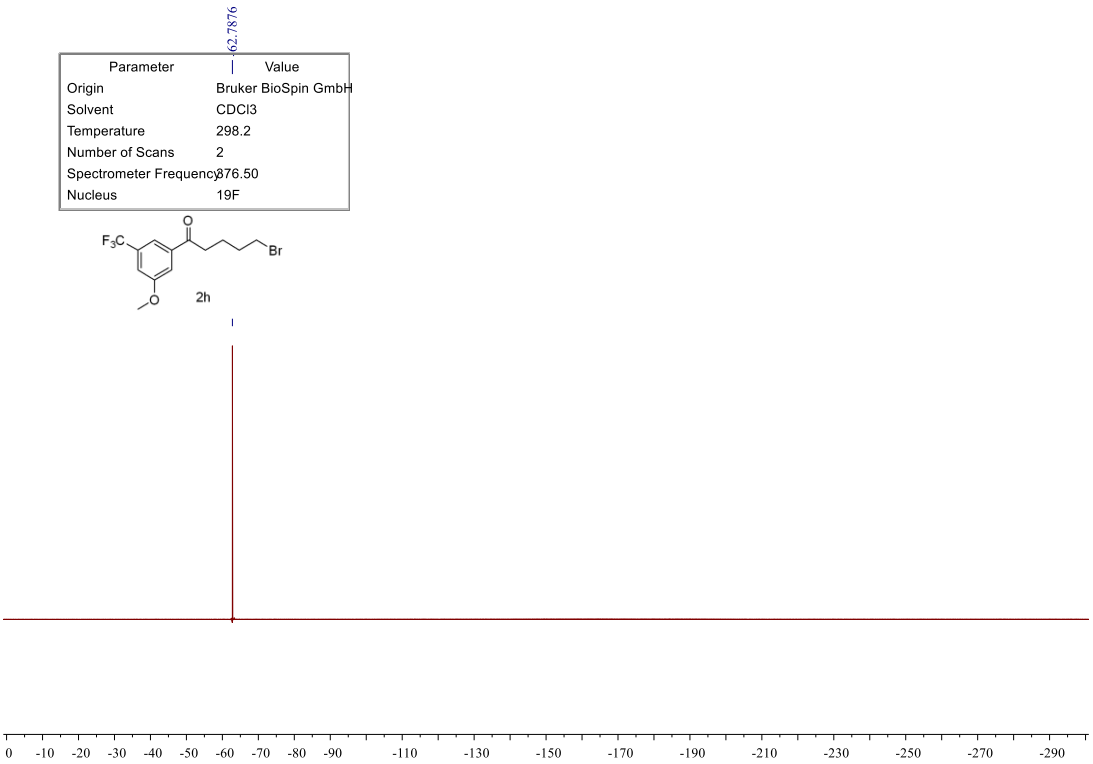
116.9380
116.0441
116.0386
115.7130
115.6773
115.6406
115.6041
77.3352
77.0177
76.7001
55.8622
37.6165
33.1848
32.0369
22.5404
Parameter Value
Origin Bruker BioSpin GmbH
Solvent CDCl3
Temperature 298.2
Number of Scans 1024
Spectrometer Frequency 100.62
Nucleus 13C
F3C
O
Br
O
2h
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10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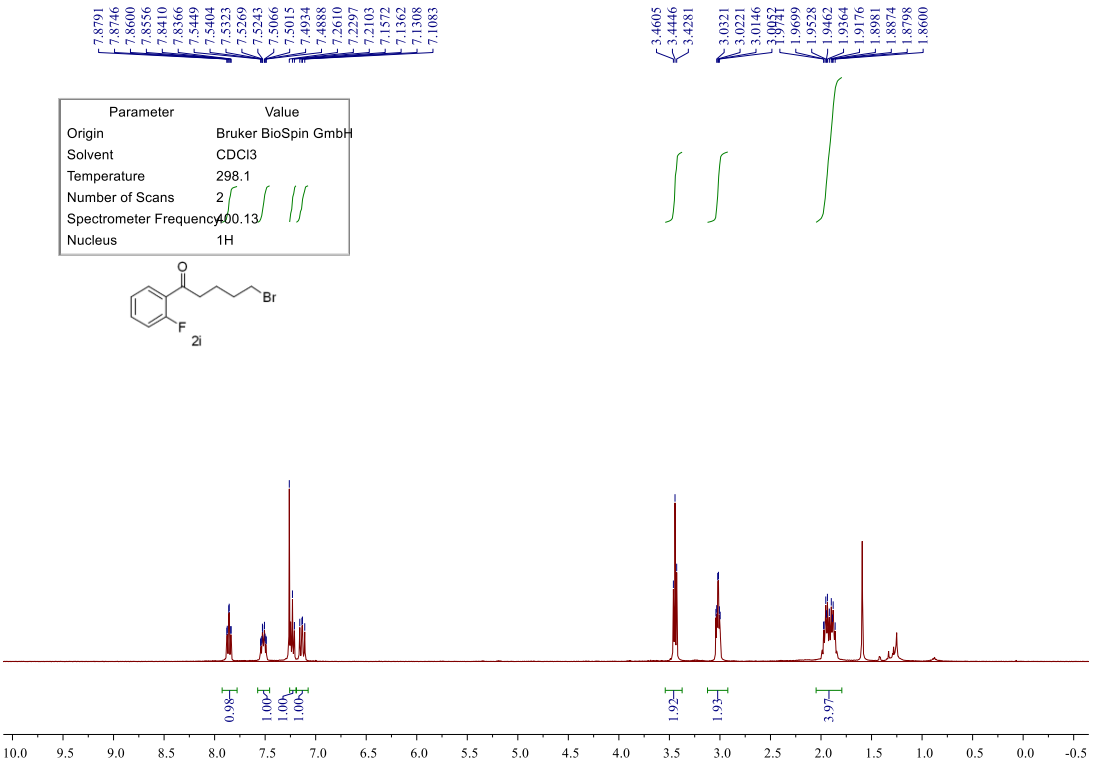
Parameter Value
Origin Bruker BioSpin GmbH
Solvent CDCl3
Temperature 298.2
Number of Scans 2
Spectrometer Frequency 376.50
Nucleus 19F
F3C
O
Br
O
2h
0 -10 -20 -30 -40 -50 -60 -70 -80 -90 -110 -130 -150 -170 -190 -210 -230 -250 -270 -290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7.8746
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7.8556
7.8410
7.8366
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7.5269
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7.5066
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7.2297
7.2103
7.1572
7.1362
7.1308
7.1083
3.4605
3.4446
3.4281
3.0321
3.0221
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3.0052
1.9741
1.9699
1.9528
1.9462
1.9364
1.9176
1.8981
1.8874
1.8798
1.8600
Parameter Value
Origin Bruker BioSpin GmbH
Solvent CDCl3
Temperature 298.1
Number of Scans 2
Spectrometer Frequency 400.13
Nucleus 1H
O
Br
F
2i
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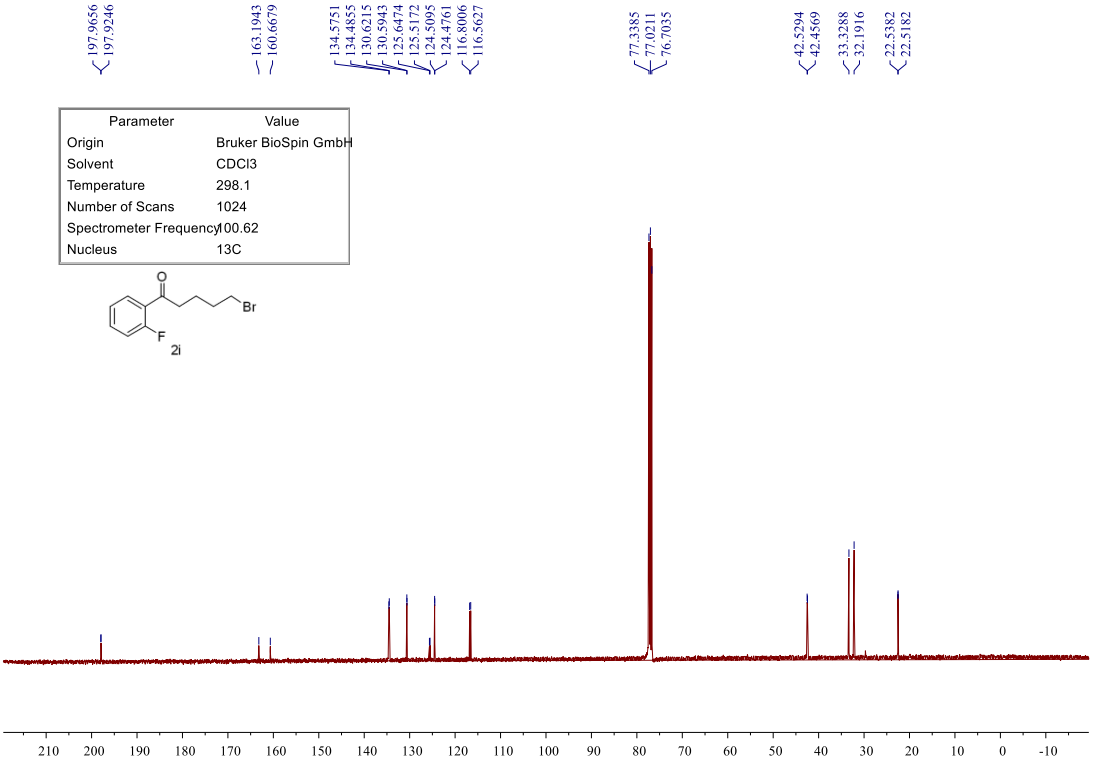
1.00
1.00
1.00
1.92
1.93
3.97
10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5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77.3385
77.0211
76.7035
42.5294
42.4569
33.3288
32.1916
22.5382
22.5182
Parameter Value
Origin Bruker BioSpin GmbH
Solvent CDCl3
Temperature 298.1
Number of Scans 1024
Spectrometer Frequency 100.62
Nucleus 13C
O
Br
F
2i
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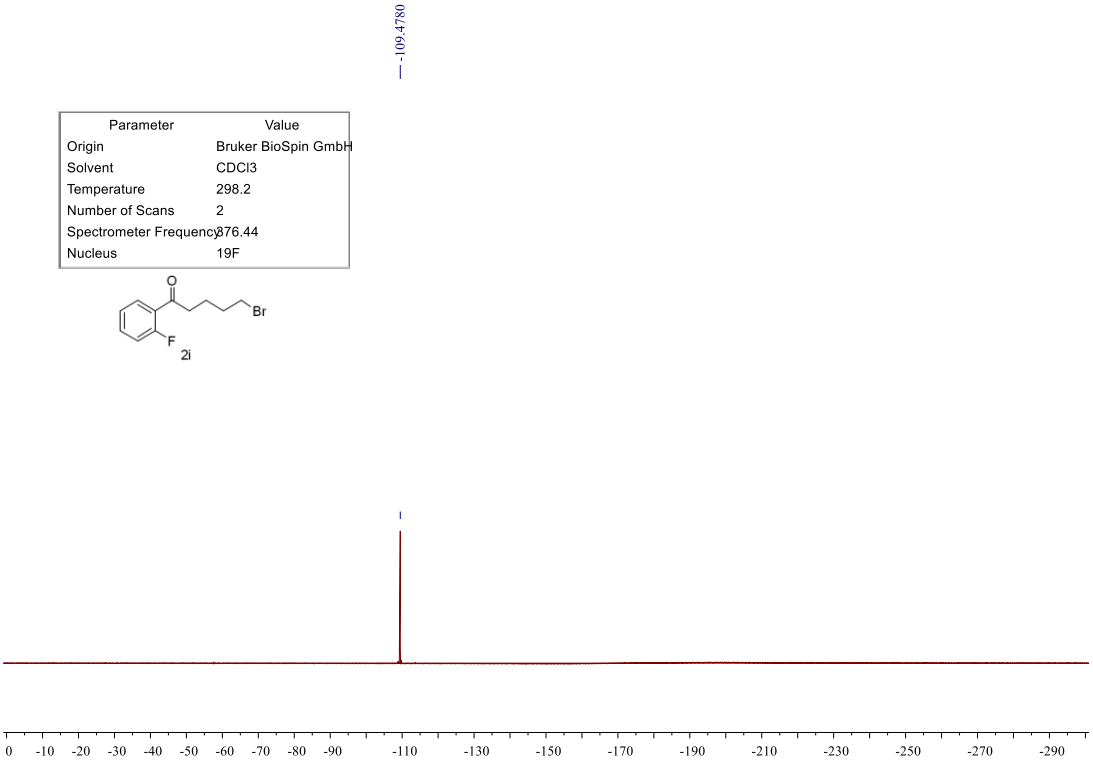
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Origin Bruker BioSpin GmbH
Solvent CDCl3
Temperature 298.2
Number of Scans 2
Spectrometer Frequency 376.44
Nucleus 19F
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Br
F
2i
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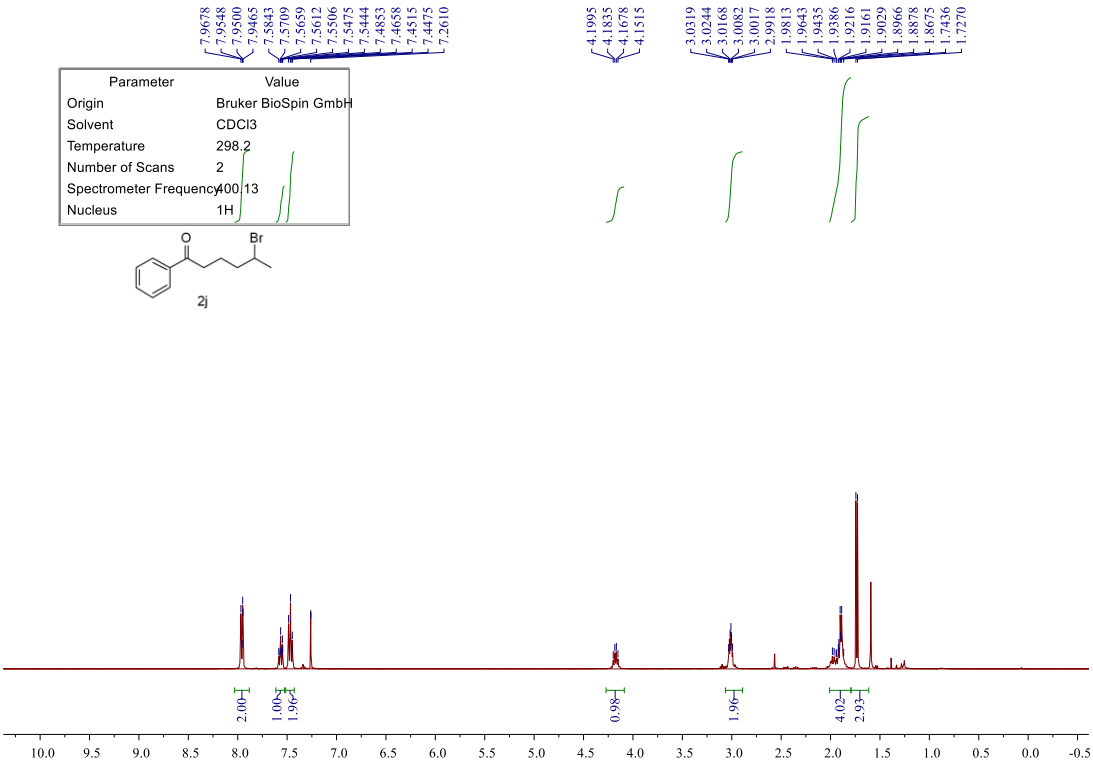
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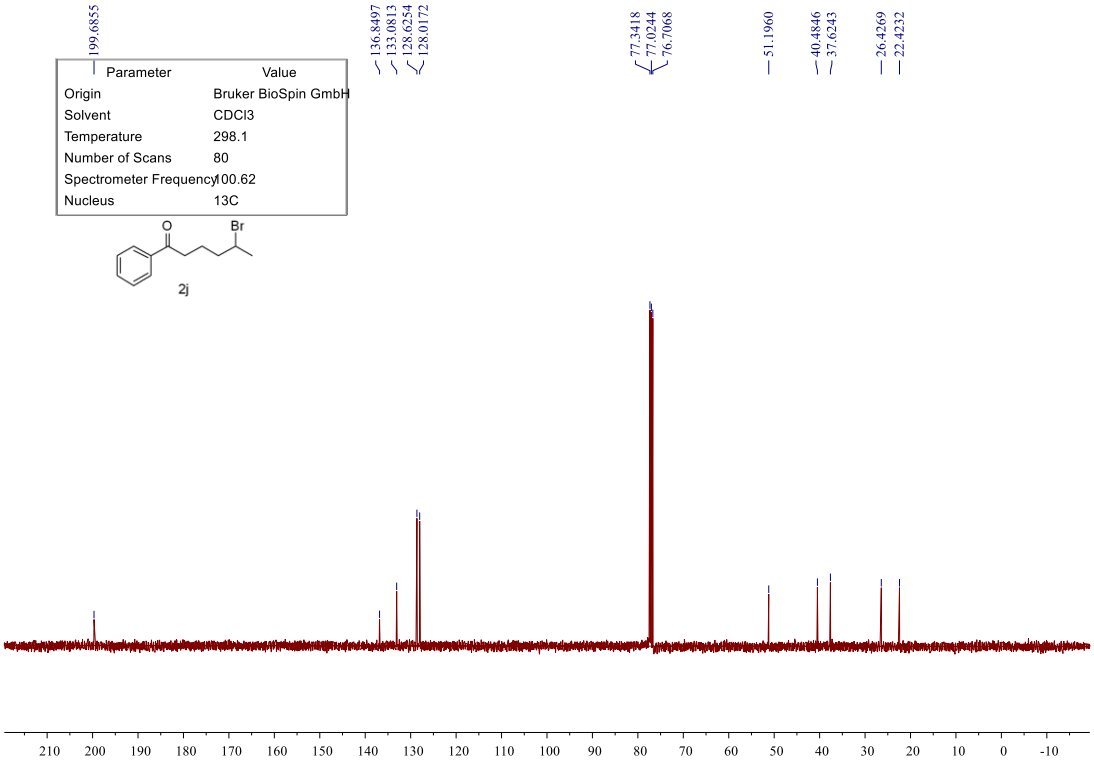
4.1995 4.1835 4.1678 4.1515
3.0319 3.0244 3.0168 3.0082 3.0017 2.9918 1.9813 1.9643 1.9435 1.9386 1.9216 1.9161 1.9029 1.8966 1.8878 1.8675 1.7436 1.7270
Parameter Value
Origin Bruker BioSpin GmbH
Solvent CDCl3
Temperature 298.2
Number of Scans 2
Spectrometer Frequency 400.13
Nucleus 1H
O
Br
2j
2.00 1.00 1.96 0.98 1.96 4.02 2.93
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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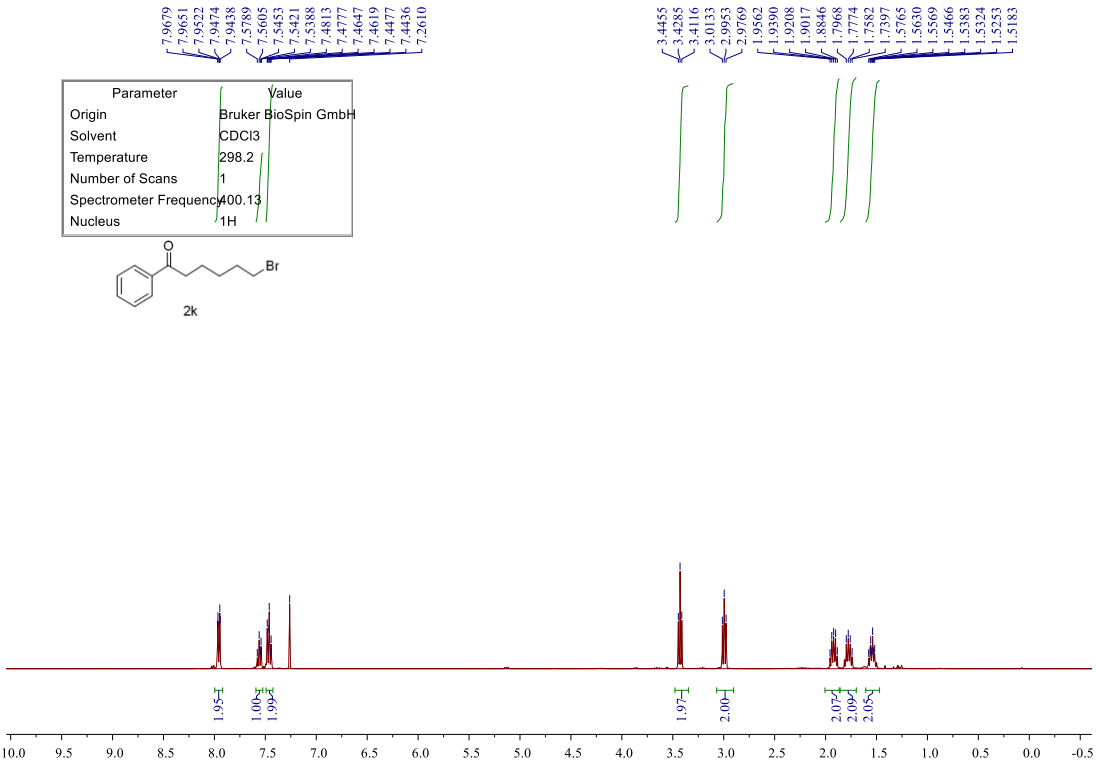
37.6243
26.4269
22.4232
Parameter Value
Origin Bruker BioSpin GmbH
Solvent CDCl3
Temperature 298.1
Number of Scans 80
Spectrometer Frequency 100.62
Nucleus 13C
O
Br
2j
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10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7.4477
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3.4116
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2.9769
1.9562
1.9390
1.9208
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1.7582
1.7397
1.5765
1.5630
1.5569
1.5466
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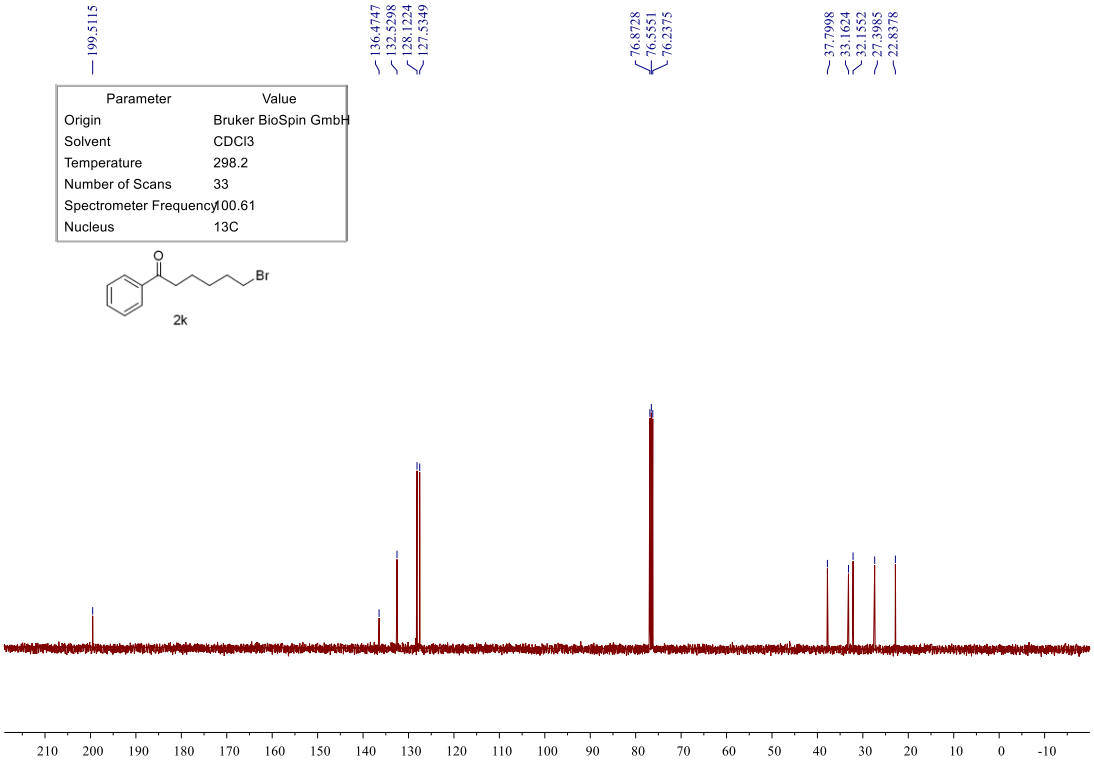
1.5324
1.5253
1.5183
Parameter Value
Origin Bruker BioSpin GmbH
Solvent CDCl3
Temperature 298.2
Number of Scans 1
Spectrometer Frequency 400.13
Nucleus 1H
O
Br
2k
1.95
1.00
1.99
1.97
2.00
2.07
2.09
2.05
10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5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32.1552
27.3985
22.8378
Parameter Value
Origin Bruker BioSpin GmbH
Solvent CDCl3
Temperature 298.2
Number of Scans 33
Spectrometer Frequency 100.61
Nucleus 13C
O
Br
2k
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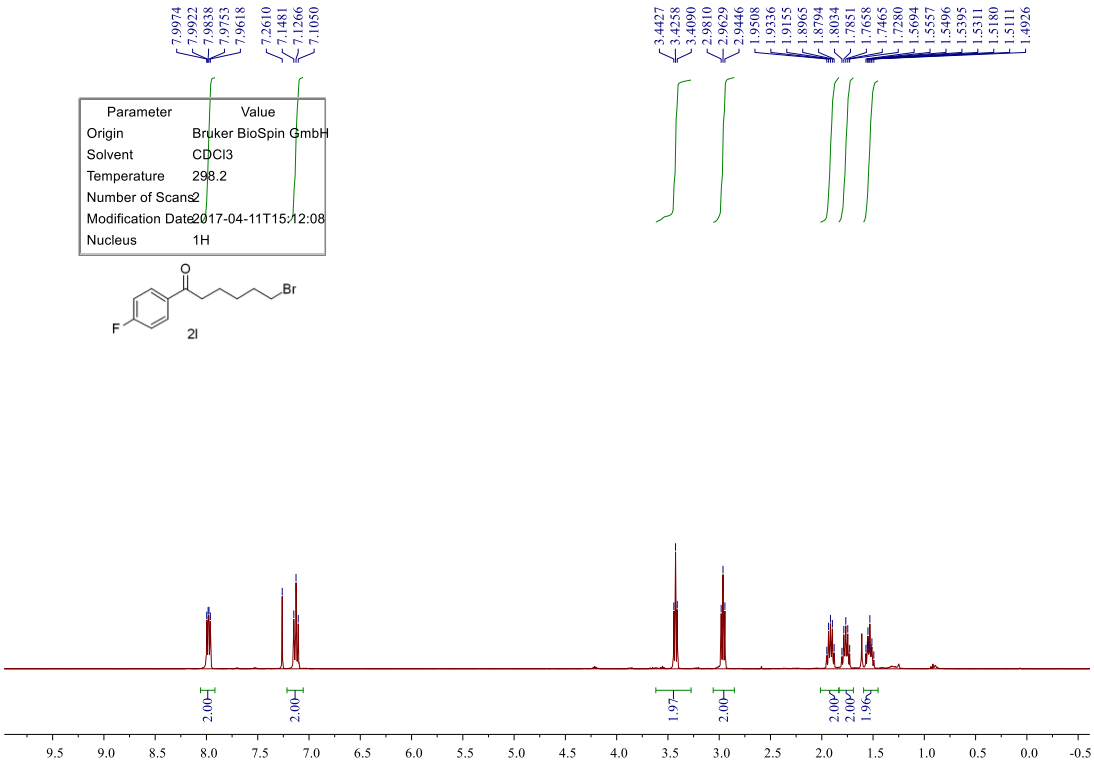
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3.4258
3.4090
2.9810
2.9629
2.9446
1.9508
1.9336
1.9155
1.8965
1.8794
1.8034
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1.7465
1.7280
1.5694
1.5557
1.5496
1.5395
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1.5111
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Parameter Value
Origin Bruker BioSpin GmbH
Solvent CDCl3
Temperature 298.2
Number of Scans 2
Modification Date 2017-04-11T15:12:08
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O
Br
F
2l
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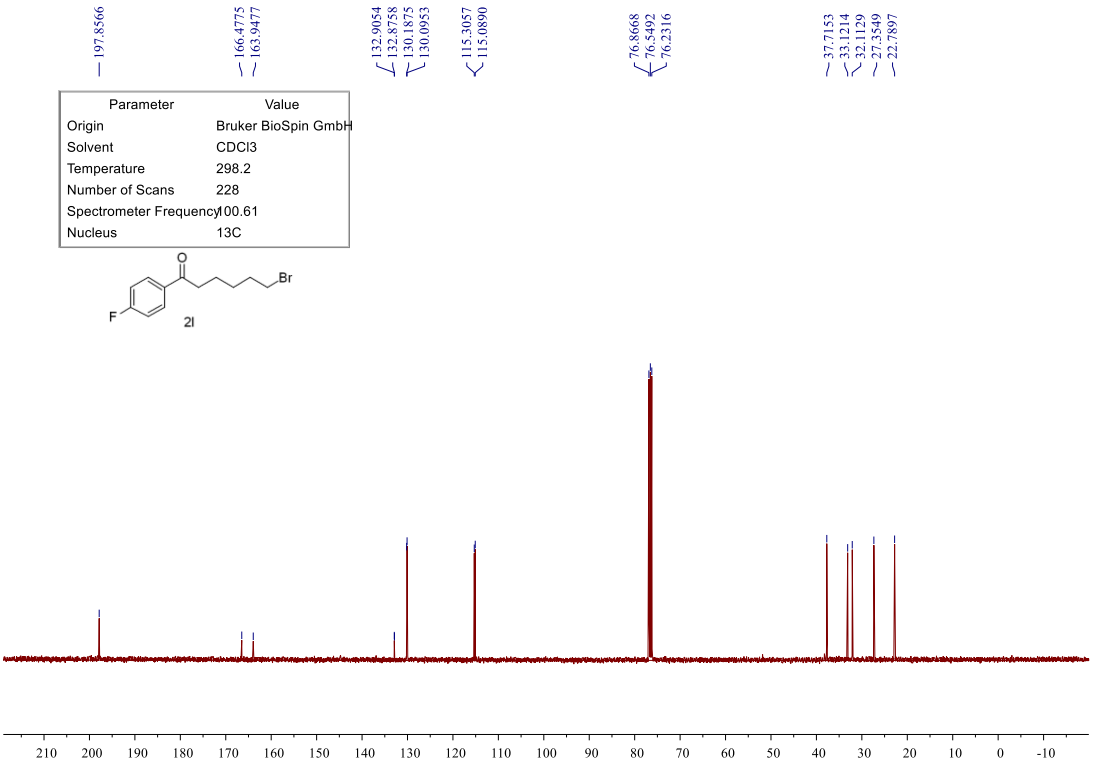
9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5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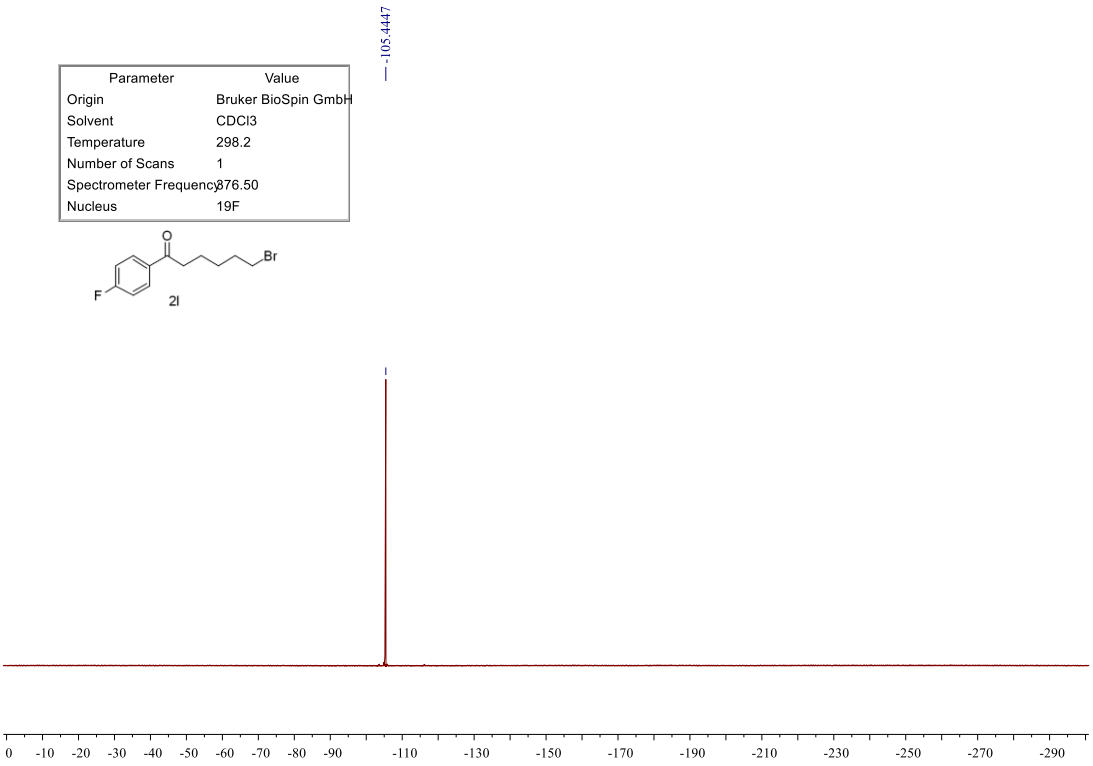
76.2316
37.7153
33.1214
32.1129
27.3549
22.7897
Parameter Value
Origin Bruker BioSpin GmbH
Solvent CDCl3
Temperature 298.2
Number of Scans 228
Spectrometer Frequency 100.61
Nucleus 13C
O
Br
F
2l
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10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Parameter Value
Origin Bruker BioSpin GmbH
Solvent CDCl3
Temperature 298.2
Number of Scans 1
Spectrometer Frequency 376.50
Nucleus 19F
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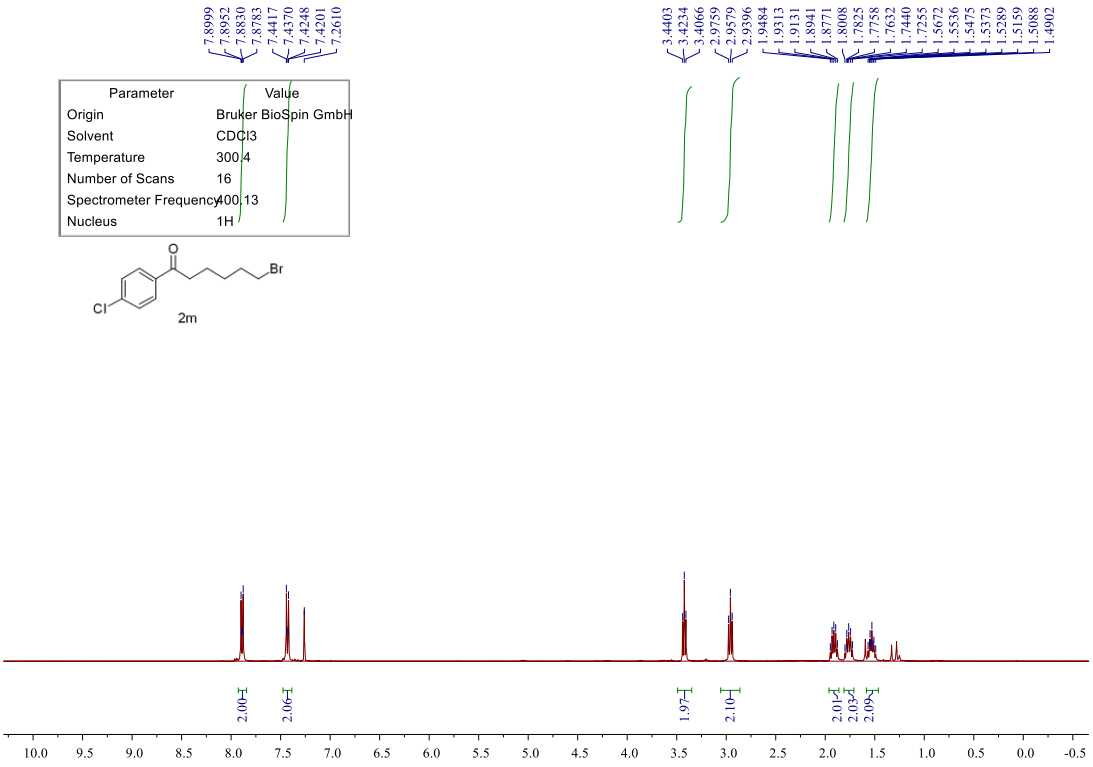
Br
F
2l
0 -10 -20 -30 -40 -50 -60 -70 -80 -90 -110 -130 -150 -170 -190 -210 -230 -250 -270 -290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3.4066
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2.9579
2.9396
1.9484
1.9313
1.9131
1.8941
1.8771
1.8008
1.7825
1.7758
1.7632
1.7440
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1.5536
1.5475
1.5373
1.5289
1.5159
1.5088
1.4902
Parameter Value
Origin Bruker BioSpin GmbH
Solvent CDCl3
Temperature 300.4
Number of Scans 16
Spectrometer Frequency 400.13
Nucleus 1H
O
Br
Cl
2m
2.00
2.06
1.97
2.10
2.01
2.03
2.09
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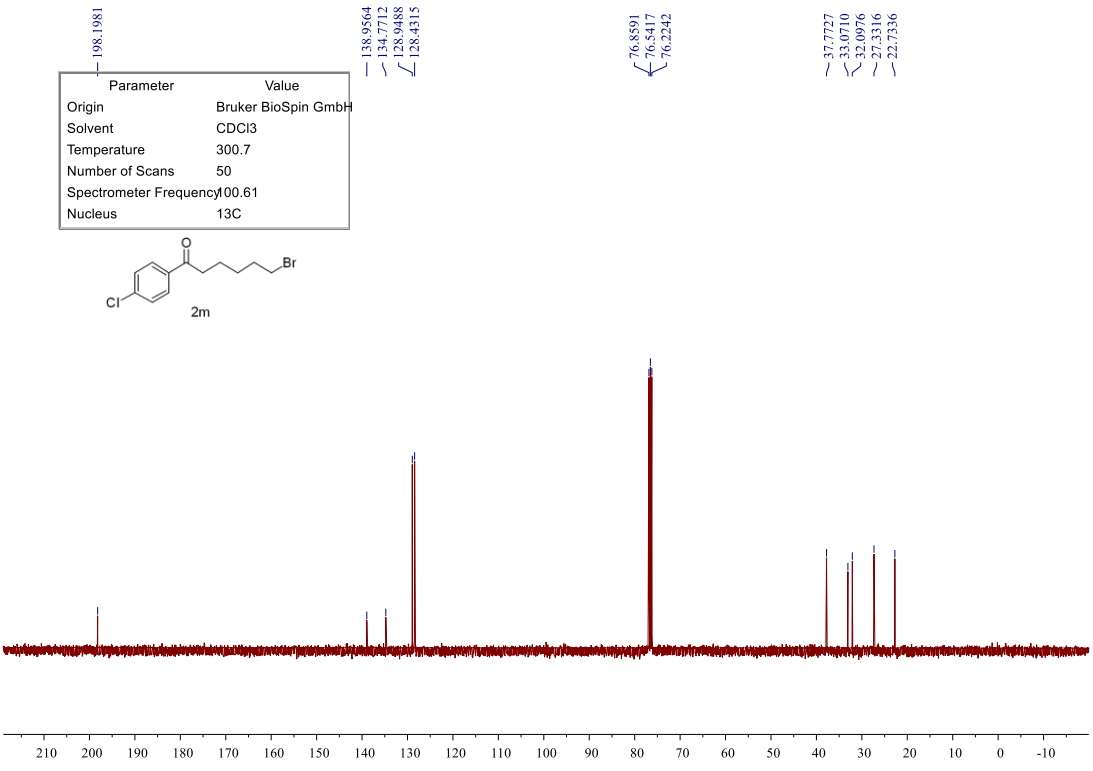
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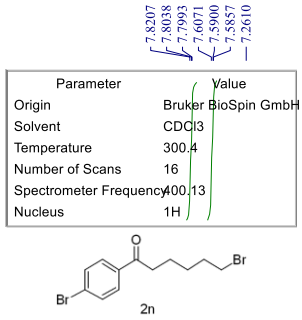
27.3316
22.7336
Parameter Value
Origin Bruker BioSpin GmbH
Solvent CDCl3
Temperature 300.7
Number of Scans 50
Spectrometer Frequency 100.61
Nucleus 13C
O
Br
Cl
2m
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10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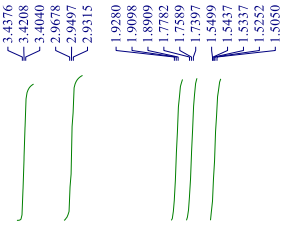
Parameter Value
Origin Bruker BioSpin GmbH
Solvent CDCl3
Temperature 300.4
Number of Scans 16
Spectrometer Frequency 400.13
Nucleus 1H
O
Br
Br
2n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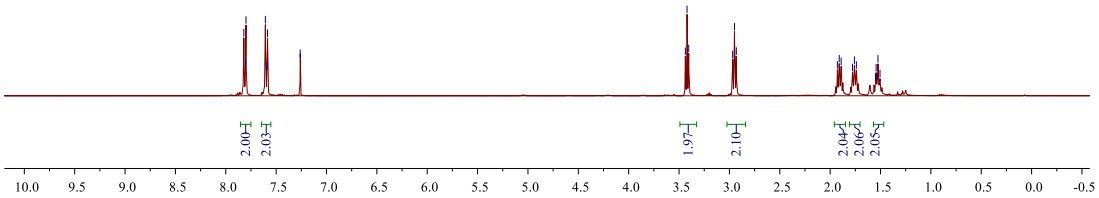
1.5252
1.5050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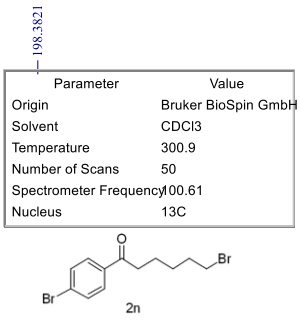
2.03
1.97
2.10
2.04
2.06
2.05
10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5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Origin Bruker BioSpin GmbH
Solvent CDCl3
Temperature 300.9
Number of Scans 50
Spectrometer Frequency 100.61
Nucleus 13C
O
Br
Br
2n


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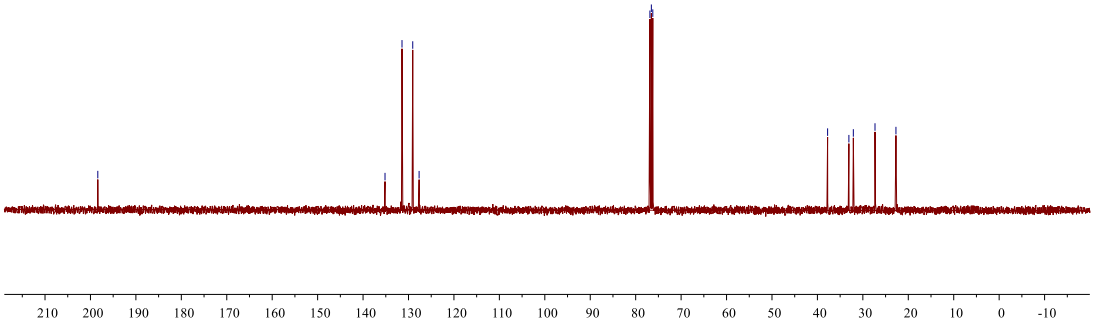
33.0730
32.0945
27.3250
22.7159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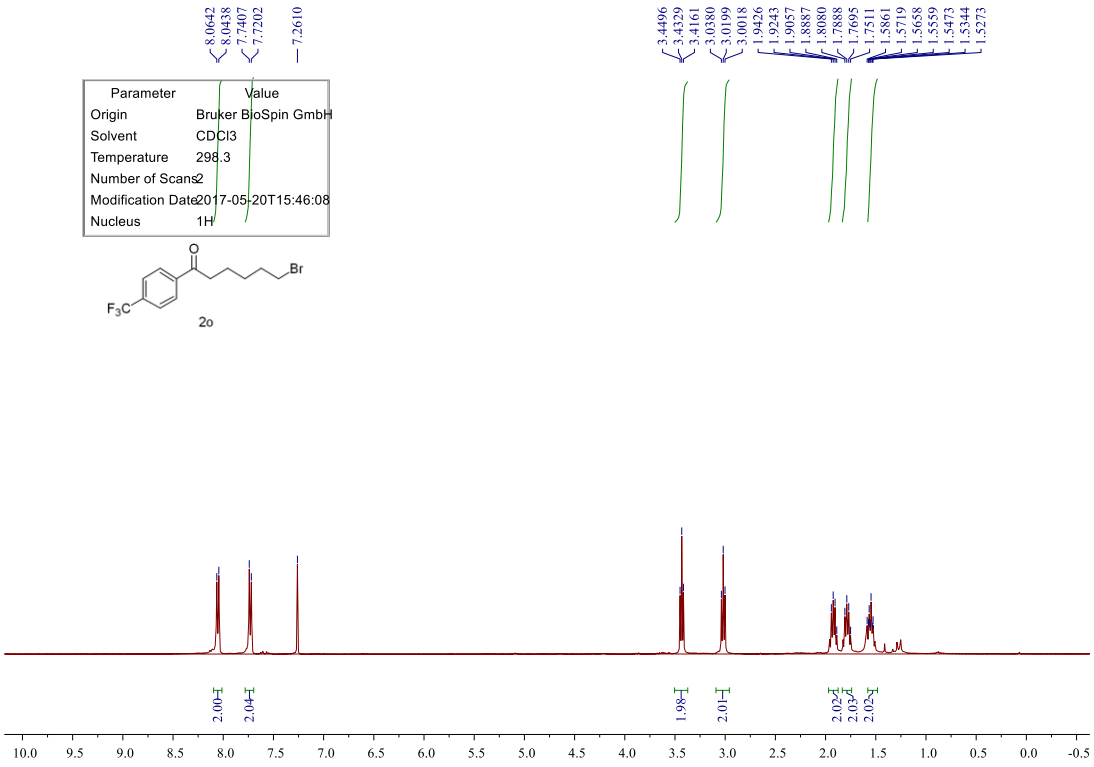
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1.5861
1.5719
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1.5559
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Parameter Value
Origin Bruker BioSpin GmbH
Solvent CDCl3
Temperature 298.3
Number of Scans 2
Modification Date 2017-05-20T15:46:08
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Br
F3C
2o
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2.02
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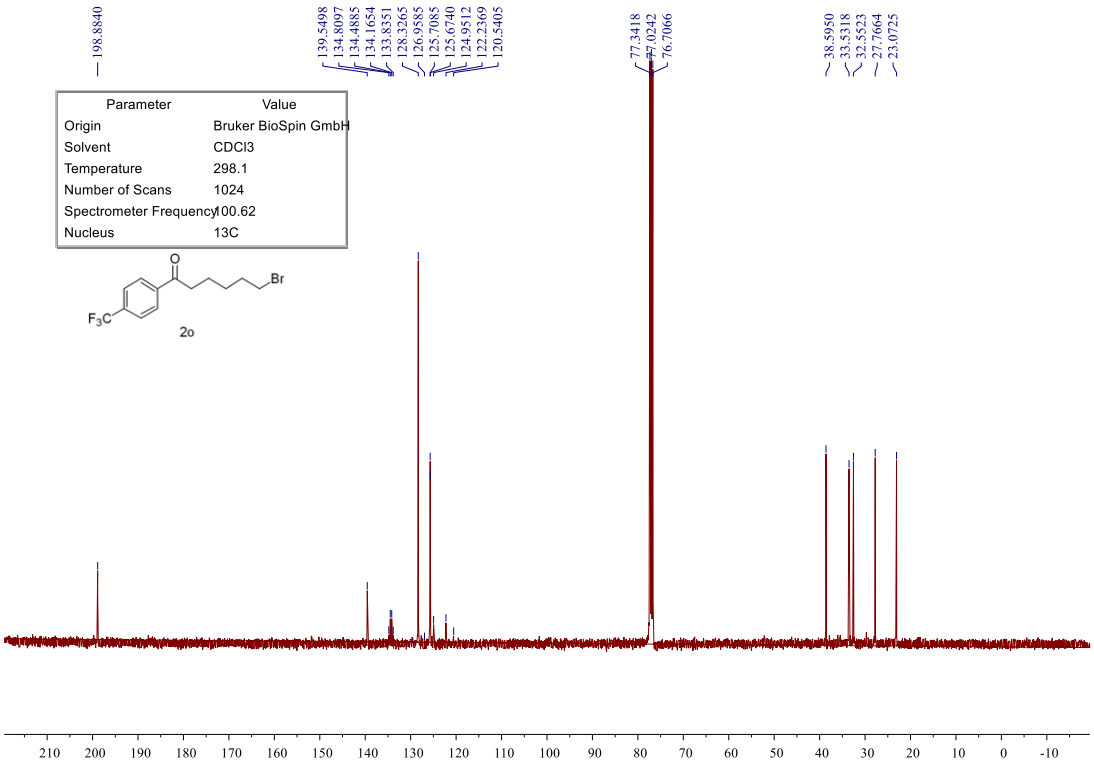
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122.2369
120.5405
77.3418
77.0242
76.7066
38.5950
33.5318
32.5523
27.7664
23.0725
Parameter Value
Origin Bruker BioSpin GmbH
Solvent CDCl3
Temperature 298.1
Number of Scans 1024
Spectrometer Frequency 100.62
Nucleus 13C
O
Br
F3C
2o
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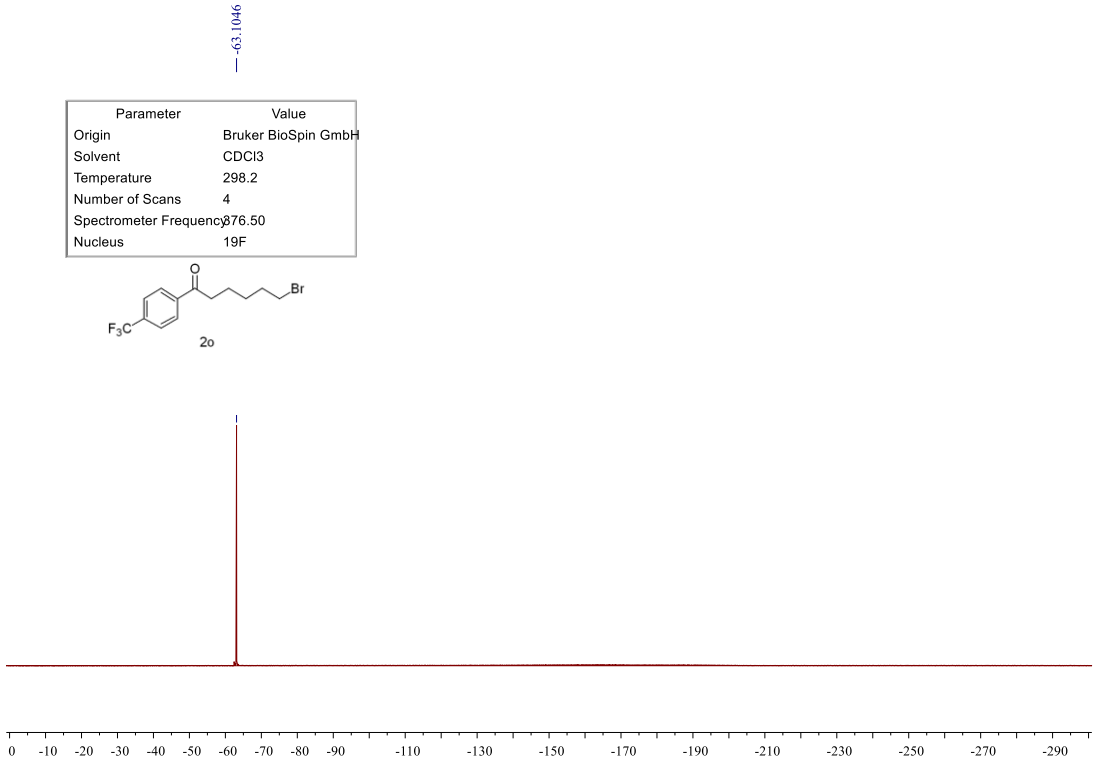
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Origin Bruker BioSpin GmbH
Solvent CDCl3
Temperature 298.2
Number of Scans 4
Spectrometer Frequency 376.50
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F3C
2o
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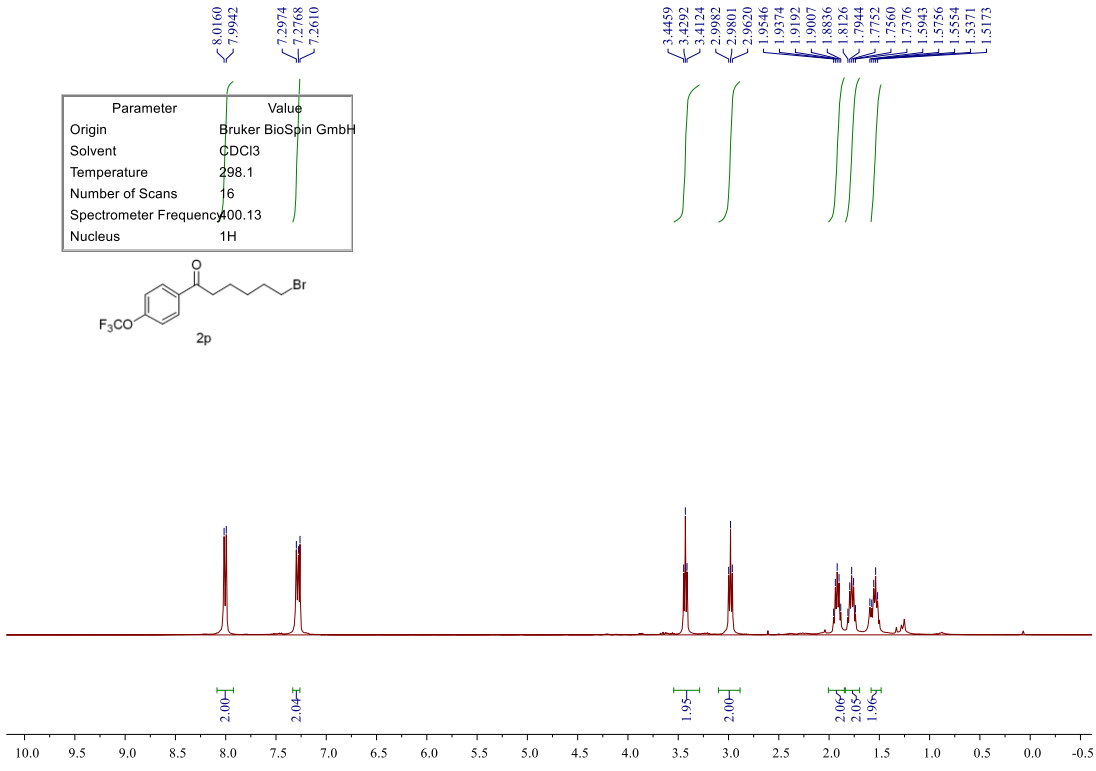
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2.9620
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1.9374
1.9192
1.9007
1.8836
1.8126
1.7944
1.7752
1.7560
1.7376
1.5943
1.5756
1.5554
1.5371
1.5173
Parameter Value
Origin Bruker BioSpin GmbH
Solvent CDCl3
Temperature 298.1
Number of Scans 16
Spectrometer Frequency 400.13
Nucleus 1H
O
Br
F3CO
2p
2.00
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1.95
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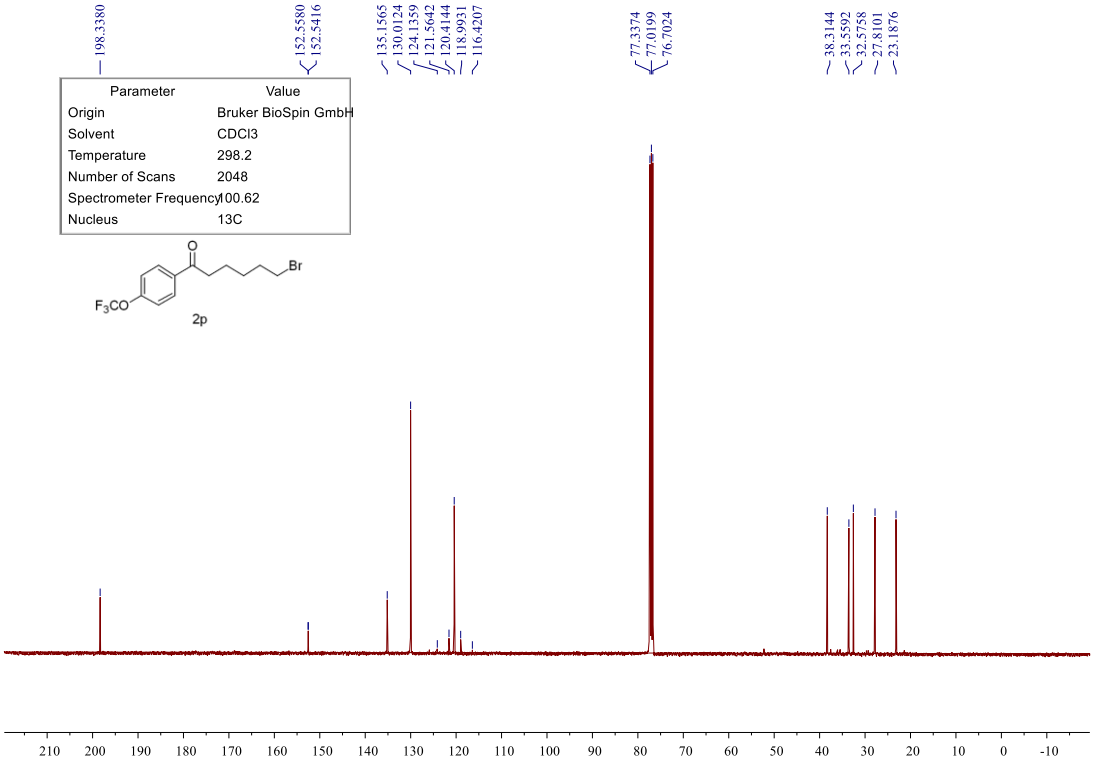
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77.0199
76.7024
38.3144
33.5592
32.5758
27.8101
23.1876
Parameter Value
Origin Bruker BioSpin GmbH
Solvent CDCl3
Temperature 298.2
Number of Scans 2048
Spectrometer Frequency 100.62
Nucleus 13C
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Br
F3CO
2p
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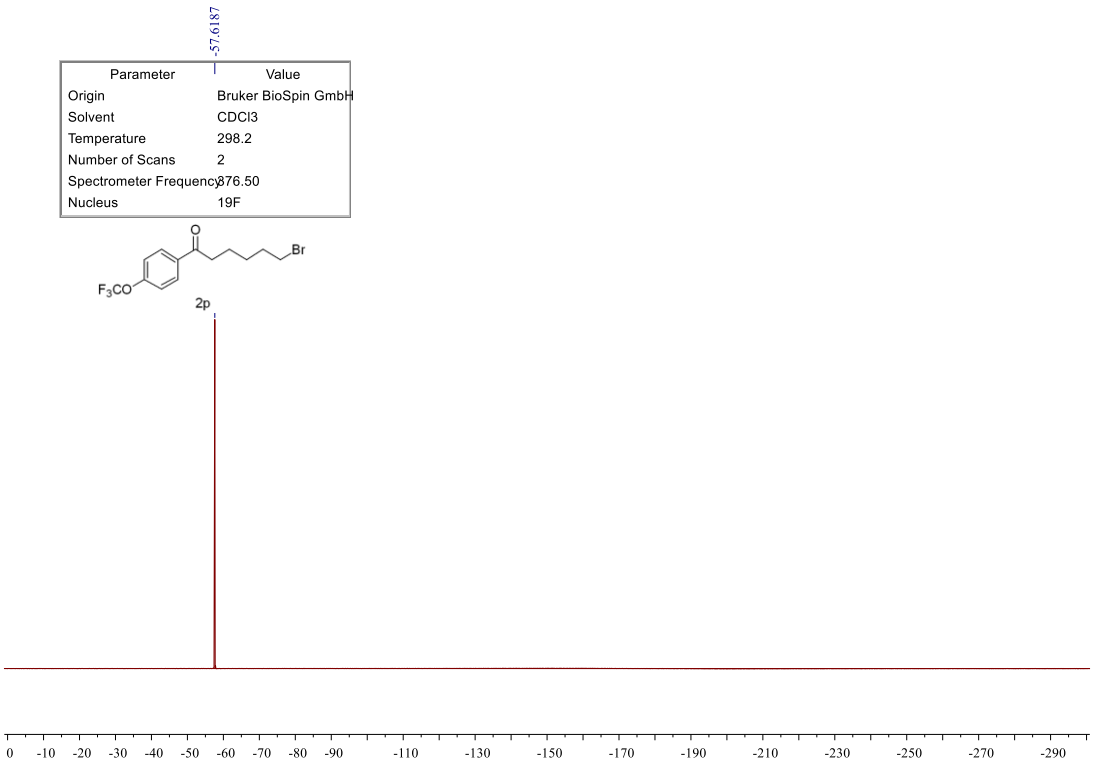
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Parameter Value
Origin Bruker BioSpin GmbH
Solvent CDCl3
Temperature 298.2
Number of Scans 2
Spectrometer Frequency 376.50
Nucleus 19F
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Br
F3CO
2p
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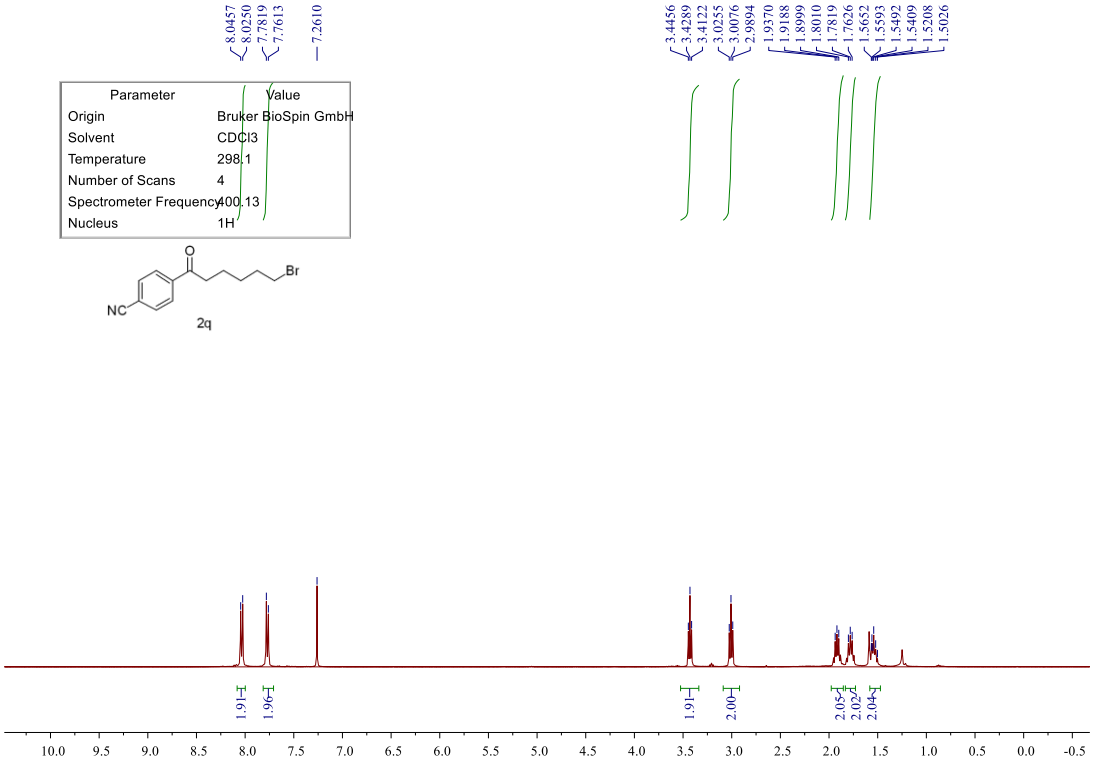
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1.5492
1.5409
1.5208
1.5026
Parameter Value
Origin Bruker BioSpin GmbH
Solvent CDCl3
Temperature 298.1
Number of Scans 4
Spectrometer Frequency 400.13
Nucleus 1H
O
Br
NC
2q
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1.96
1.91
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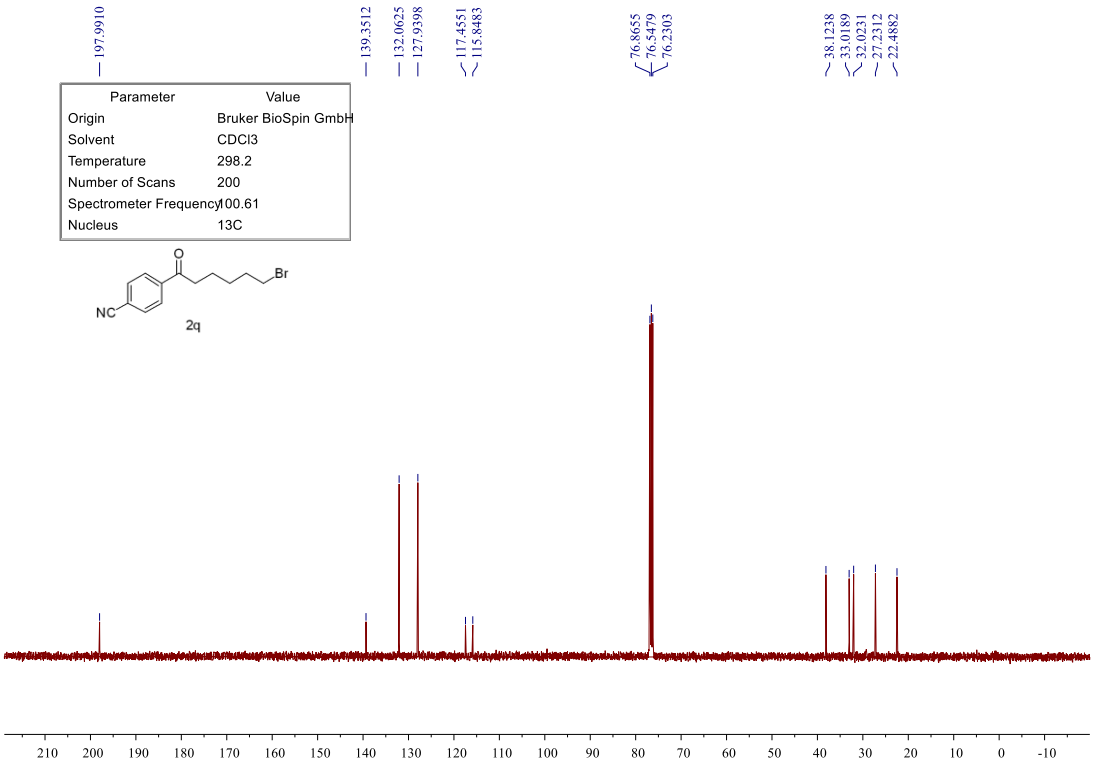
2.04
10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5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76.8655
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76.2303
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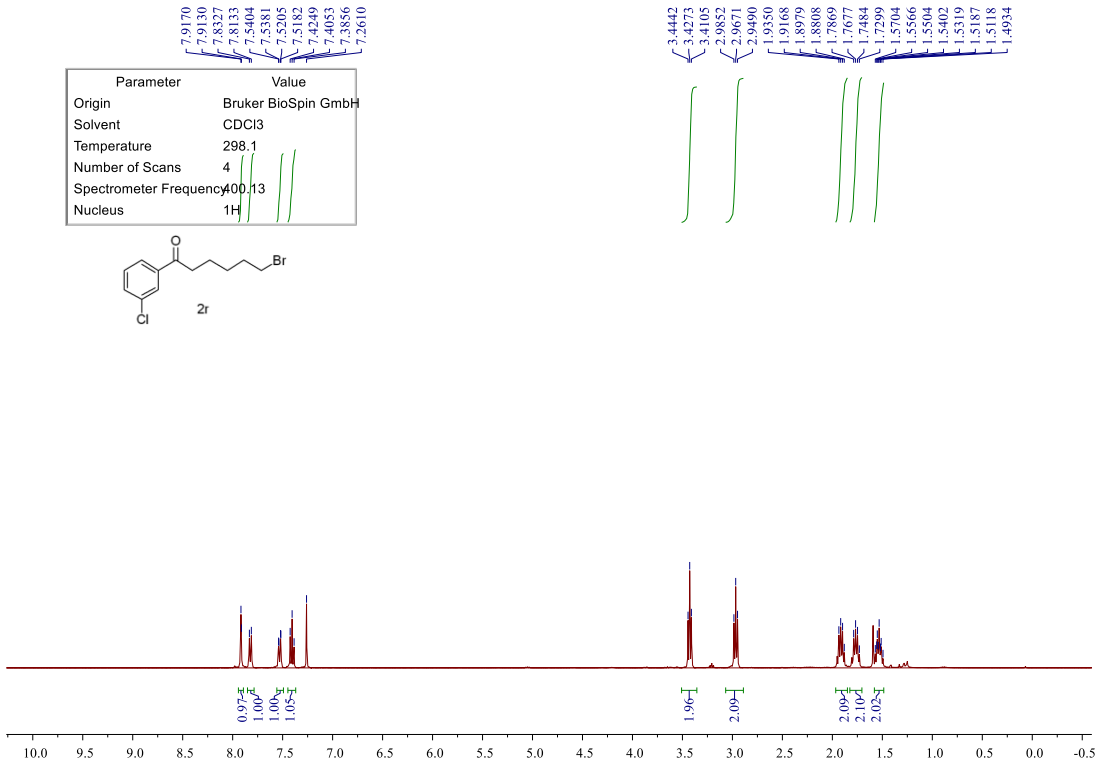
33.0189
32.0231
27.2312
22.4882
Parameter Value
Origin Bruker BioSpin GmbH
Solvent CDCl3
Temperature 298.2
Number of Scans 200
Spectrometer Frequency 100.61
Nucleus 13C
O
Br
NC
2q
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10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7.5205
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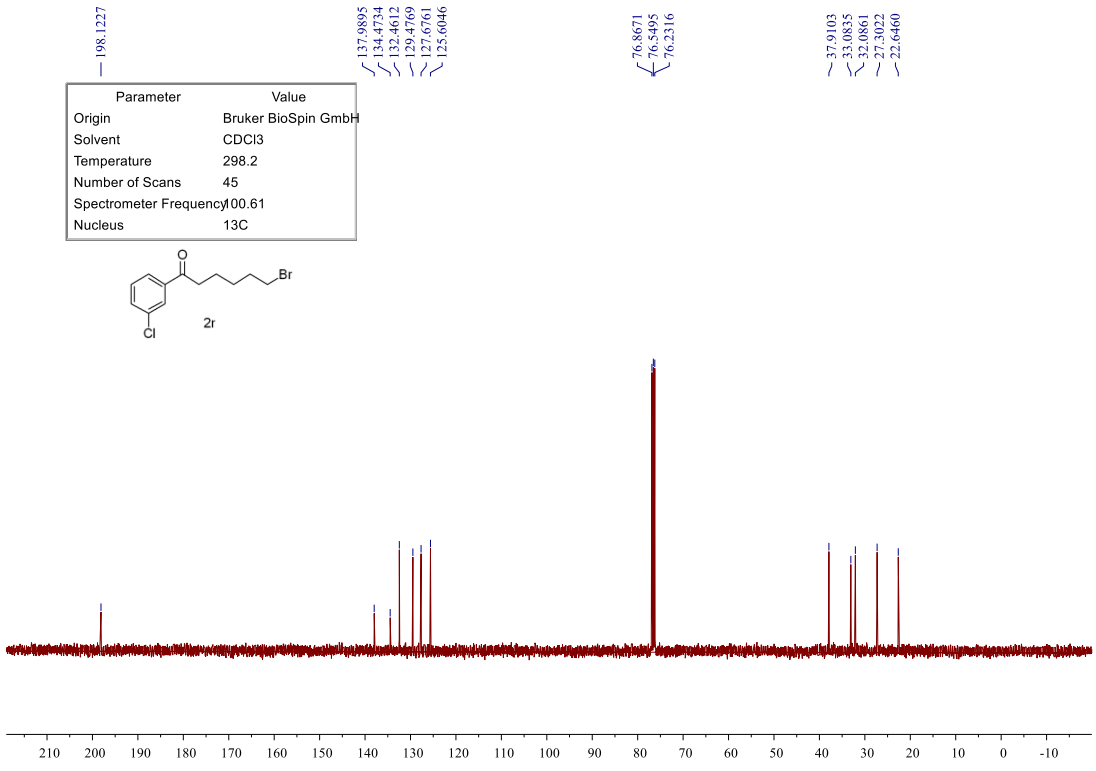
7.4053
7.3856
7.2610
3.4442
3.4273
3.4105
2.9852
2.9671
2.9490
1.9350
1.9168
1.8979
1.8808
1.7869
1.7677
1.7484
1.7299
1.5704
1.5566
1.5504
1.5402
1.5319
1.5187
1.5118
1.4934
Parameter Value
Origin Bruker BioSpin GmbH
Solvent CDCl3
Temperature 298.1
Number of Scans 4
Spectrometer Frequency 400.13
Nucleus 1H
O
Br
Cl
2r
0.97
1.00
1.00
1.05
1.96
2.09
2.09
2.10
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 -0.5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125.6046
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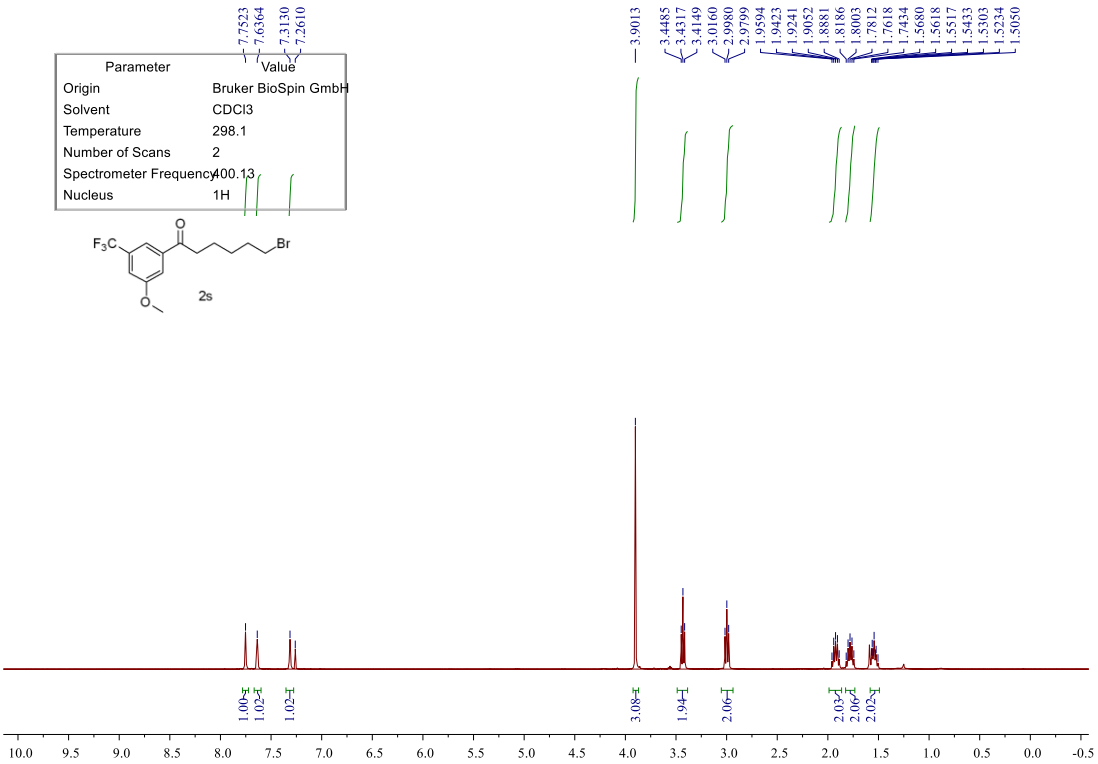
37.9103
33.0835
32.0861
27.3022
22.6460
Parameter Value
Origin Bruker BioSpin GmbH
Solvent CDCl3
Temperature 298.2
Number of Scans 45
Spectrometer Frequency 100.61
Nucleus 13C
O
Br
Cl
2r
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10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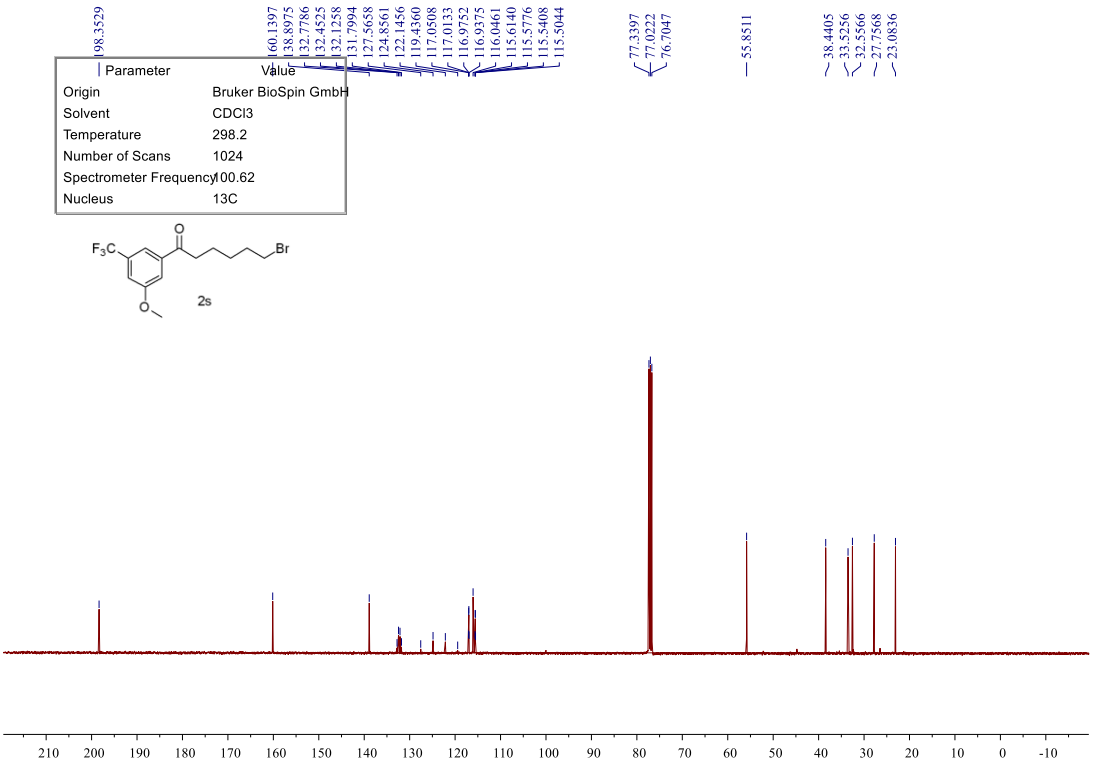
Parameter Value
Origin Bruker BioSpin GmbH
Solvent CDCl3
Temperature 298.1
Number of Scans 2
Spectrometer Frequency 400.13
Nucleus 1H
F3C
O
Br
O
2s
3.9013
3.4485
3.4317
3.4149
3.0160
2.9980
2.9799
1.9594
1.9423
1.9241
1.9052
1.8881
1.8186
1.8003
1.7812
1.7618
1.7434
1.5680
1.5618
1.5517
1.5433
1.5303
1.5234
1.5050
1.00
1.02
1.02
3.08
1.94
2.06
2.03
2.06
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 -0.5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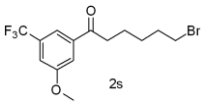
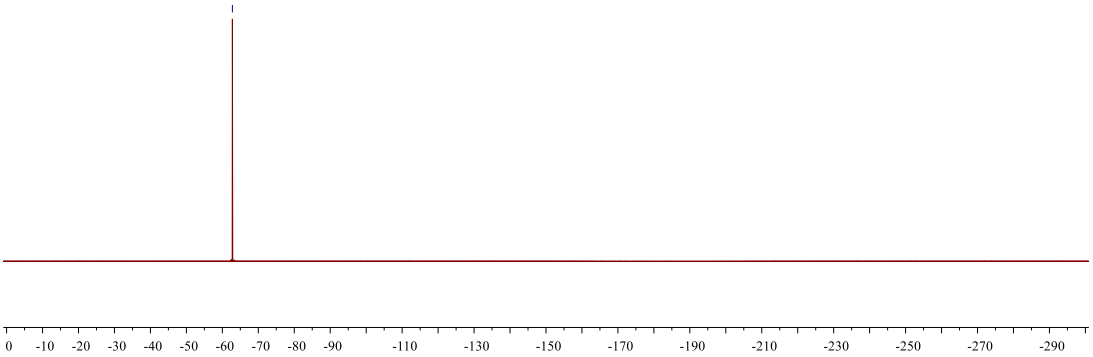
117.0508
117.0133
116.9752
116.9375
116.0461
115.6140
115.5776
115.5408
115.5044
77.3397
77.0222
76.7047
55.8511
38.4405
33.5256
32.5566
27.7568
23.0836
Parameter Value
Origin Bruker BioSpin GmbH
Solvent CDCl3
Temperature 298.2
Number of Scans 1024
Spectrometer Frequency 100.62
Nucleus 13C
F3C
O
Br
O
2s
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10

-62.7905

Parameter	Value
Origin	Bruker BioSpin GmbH
Solvent	CDCl3
Temperature	298.2
Number of Scans	2
Spectrometer Frequency	376.44
Nucleus	19F



2s



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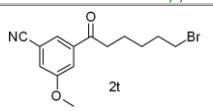
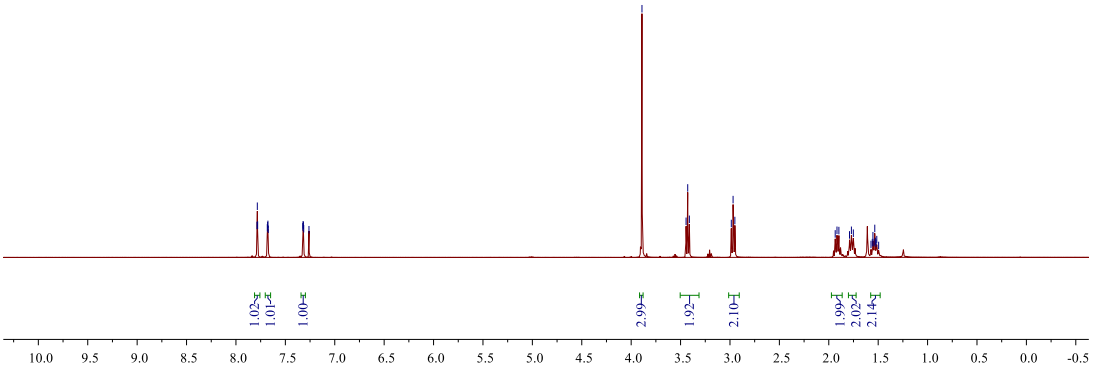
7.6765
7.6729
7.3237
7.3205
7.3173
7.3142
7.2610

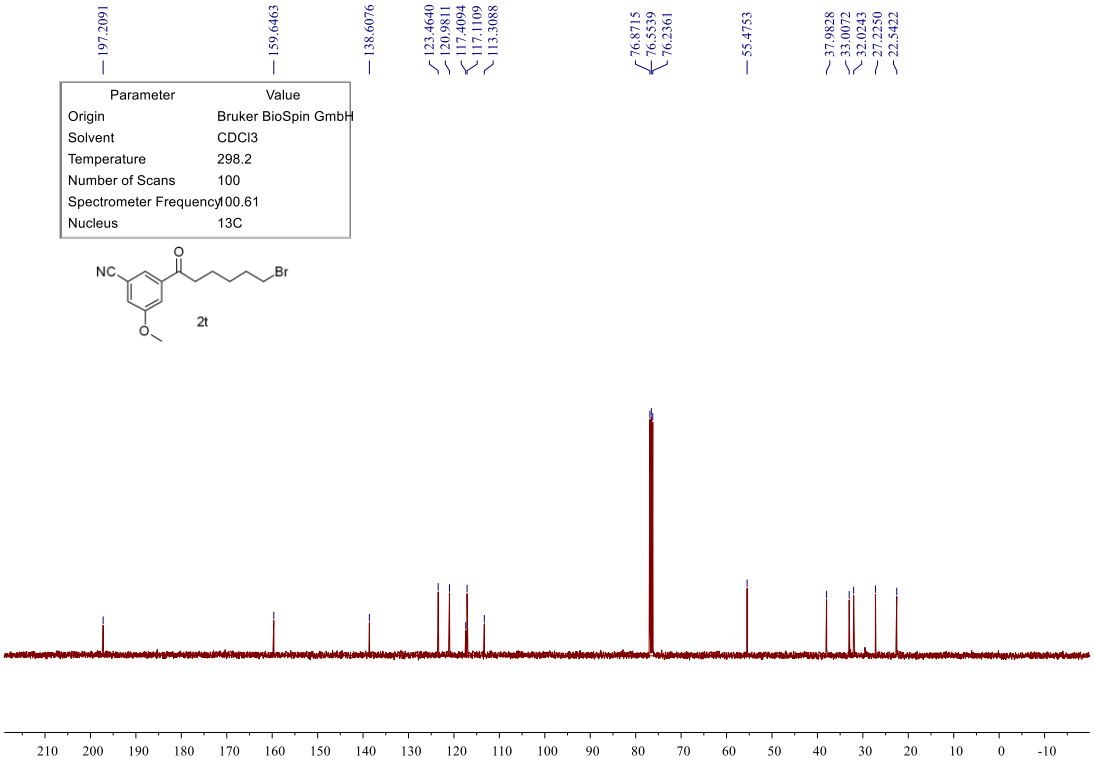
3.8907
3.4444
3.4277
3.4109
2.9865
2.9686
2.9504
1.9350
1.9169
1.8977
1.7901
1.7710
1.7515
1.5729
1.5594
1.5531
1.5430
1.5345
1.5288
1.5215
1.5141
1.4952

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



2t

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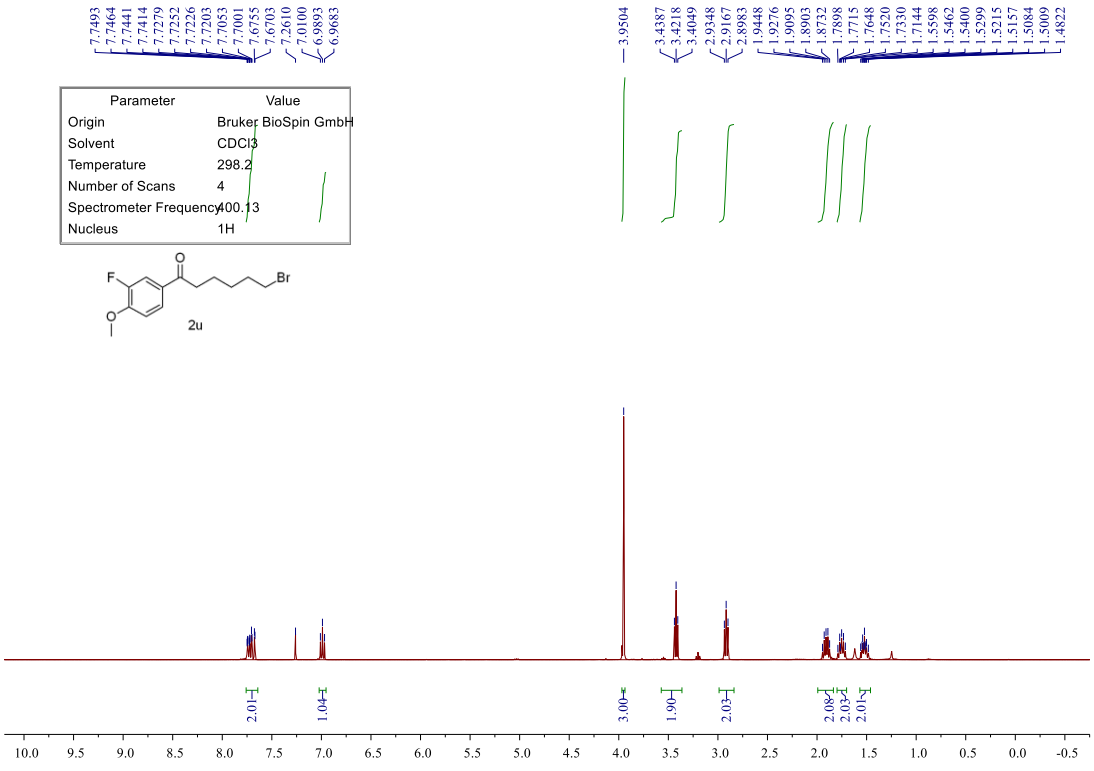
117.4094
117.1109
113.3088
76.8715
76.5539
76.2361
55.4753
37.9828
33.0072
32.0243
27.2250
22.5422
Parameter Value
Origin Bruker BioSpin GmbH
Solvent CDCl3
Temperature 298.2
Number of Scans 100
Spectrometer Frequency 100.61
Nucleus 13C
NC
O
Br
O
2t
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10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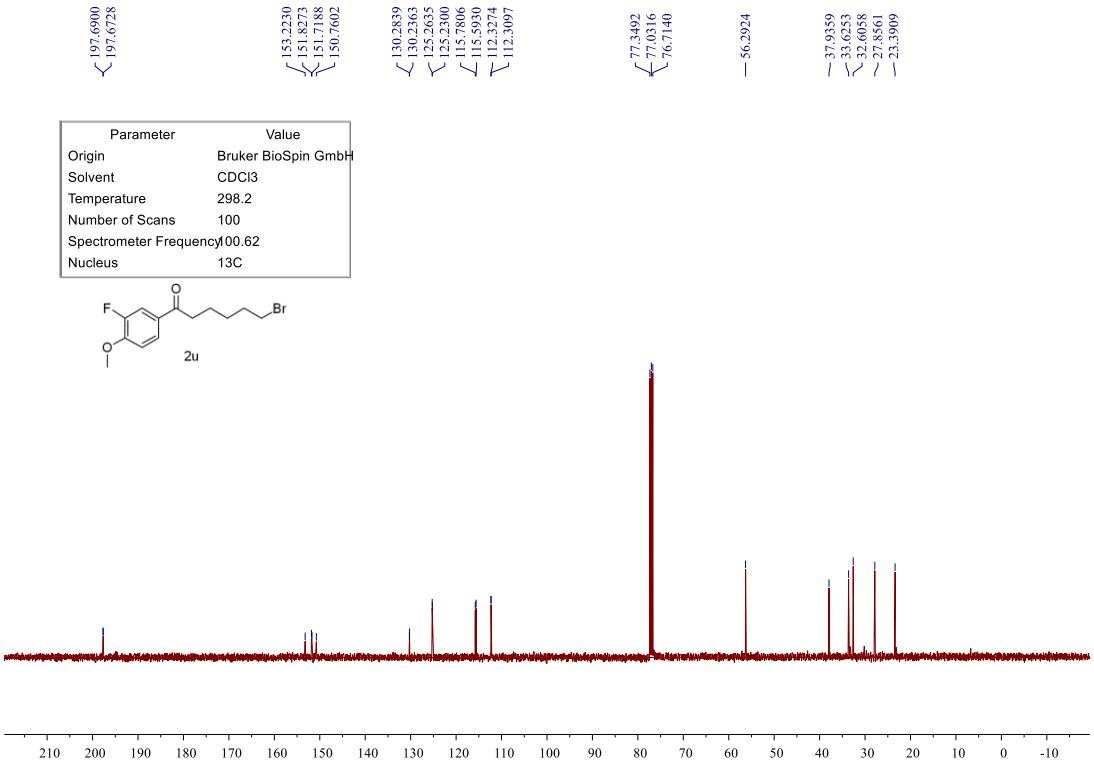
7.7001
7.6755
7.6703
7.2610
7.0100
6.9893
6.9683
3.9504
3.4387
3.4218
3.4049
2.9348
2.9167
2.8983
1.9448
1.9276
1.9095
1.8903
1.8732
1.7898
1.7715
1.7648
1.7520
1.7330
1.7144
1.5598
1.5462
1.5400
1.5299
1.5215
1.5157
1.5084
1.5009
1.4822
Parameter Value
Origin Bruker BioSpin GmbH
Solvent CDCl3
Temperature 298.2
Number of Scans 4
Spectrometer Frequency 400.13
Nucleus 1H
F
O
Br
O
2u
2.01
1.04
3.00
1.90
2.03
2.08
2.03
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 -0.5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125.2635
125.2300
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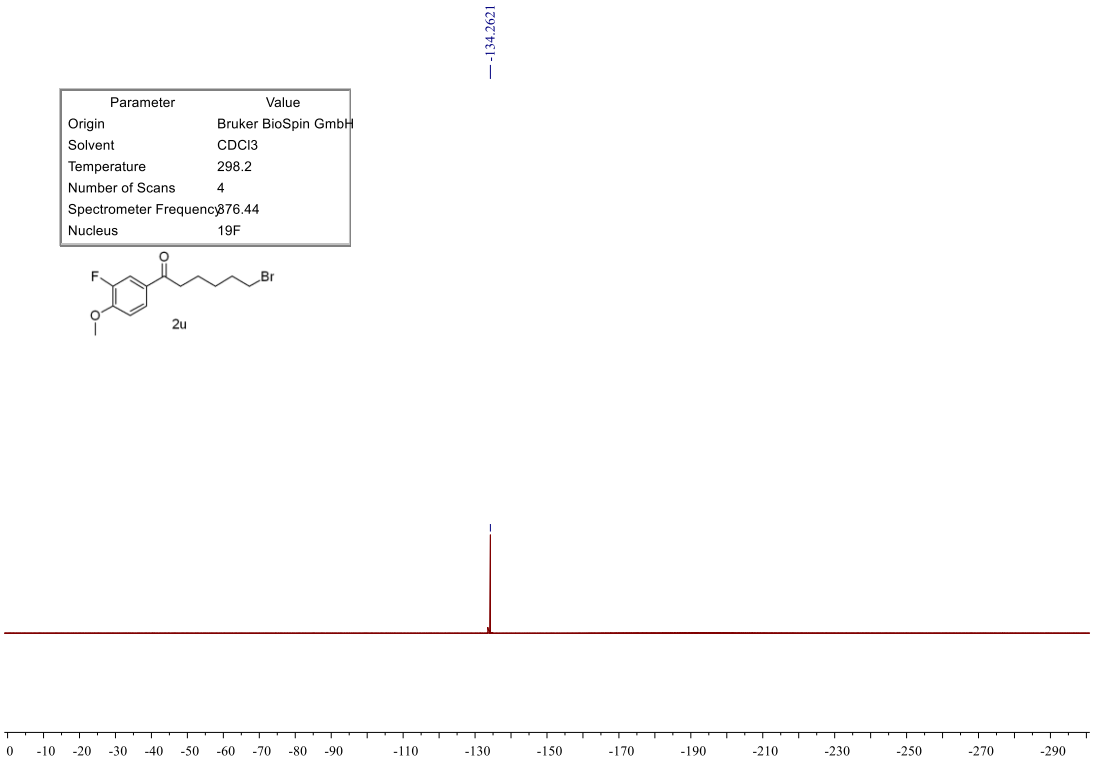
115.5930
112.3274
112.3097
77.3492
77.0316
76.7140
56.2924
37.9359
33.6253
32.6058
27.8561
23.3909
Parameter Value
Origin Bruker BioSpin GmbH
Solvent CDCl3
Temperature 298.2
Number of Scans 100
Spectrometer Frequency 100.62
Nucleus 13C
F
O
O
Br
2u
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10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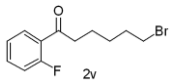
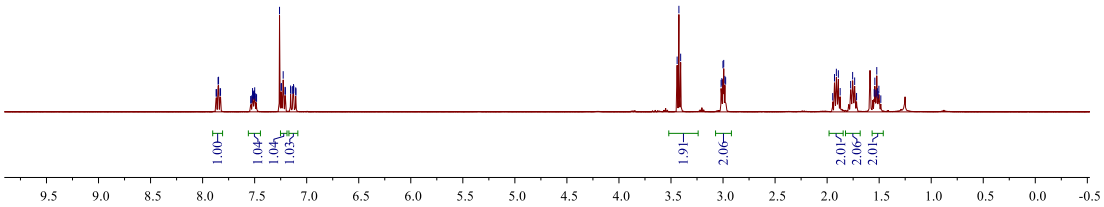
Parameter Value
Origin Bruker BioSpin GmbH
Solvent CDCl3
Temperature 298.2
Number of Scans 4
Spectrometer Frequency 376.44
Nucleus 19F
F
O
O
Br
2u
0 -10 -20 -30 -40 -50 -60 -70 -80 -90 -110 -130 -150 -170 -190 -210 -230 -250 -270 -290

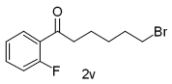
Parameter	Value
Origin	Bruker BioSpin GmbH
Solvent	CDCl3
Temperature	298.2
Number of Scans	2
Spectrometer Frequency	400.13
Nucleus	1H



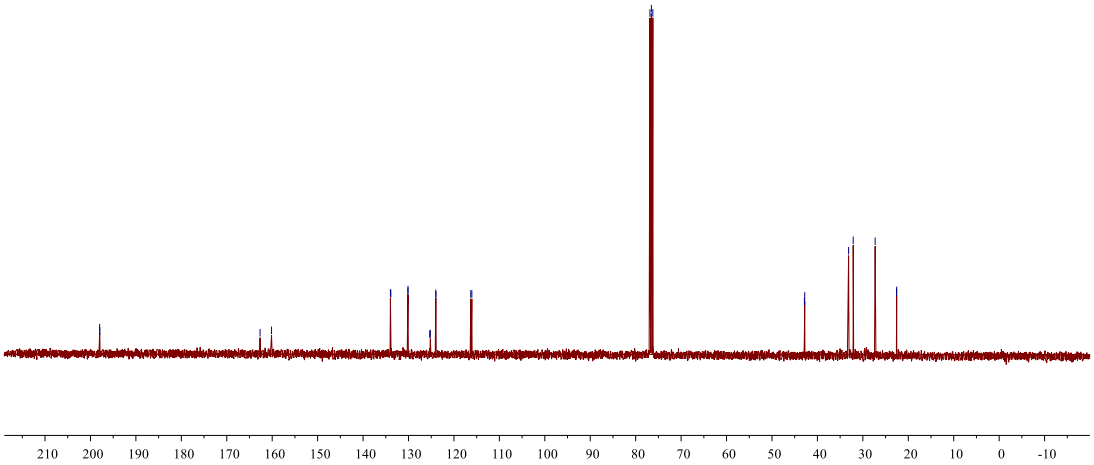
2v



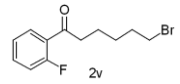
Parameter	Value
Origin	Bruker BioSpin GmbH
Solvent	CDCl3
Temperature	298.3
Number of Scans	120
Spectrometer Frequency	100.61
Nucleus	13C



2v

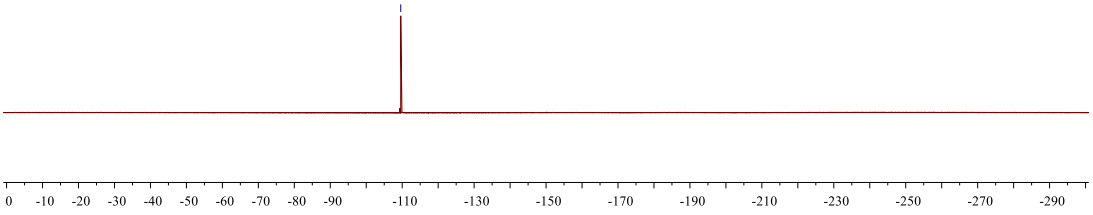


Parameter	Value
Origin	Bruker BioSpin GmbH
Solvent	CDCl3
Temperature	298.2
Number of Scans	4
Spectrometer Frequency	376.50
Nucleus	19F

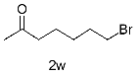


2v

-109.5933



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



2w

7.2610

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1.8457
1.8287
1.6358
1.6176
1.6102
1.5980
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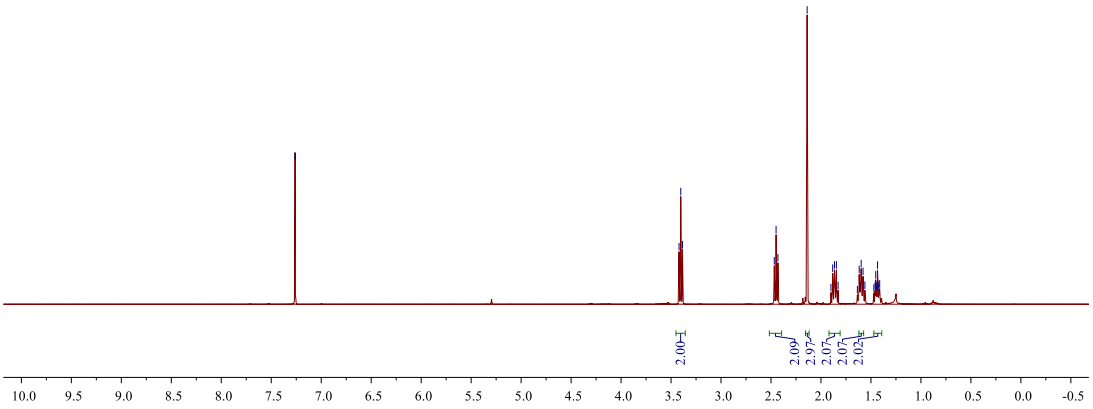
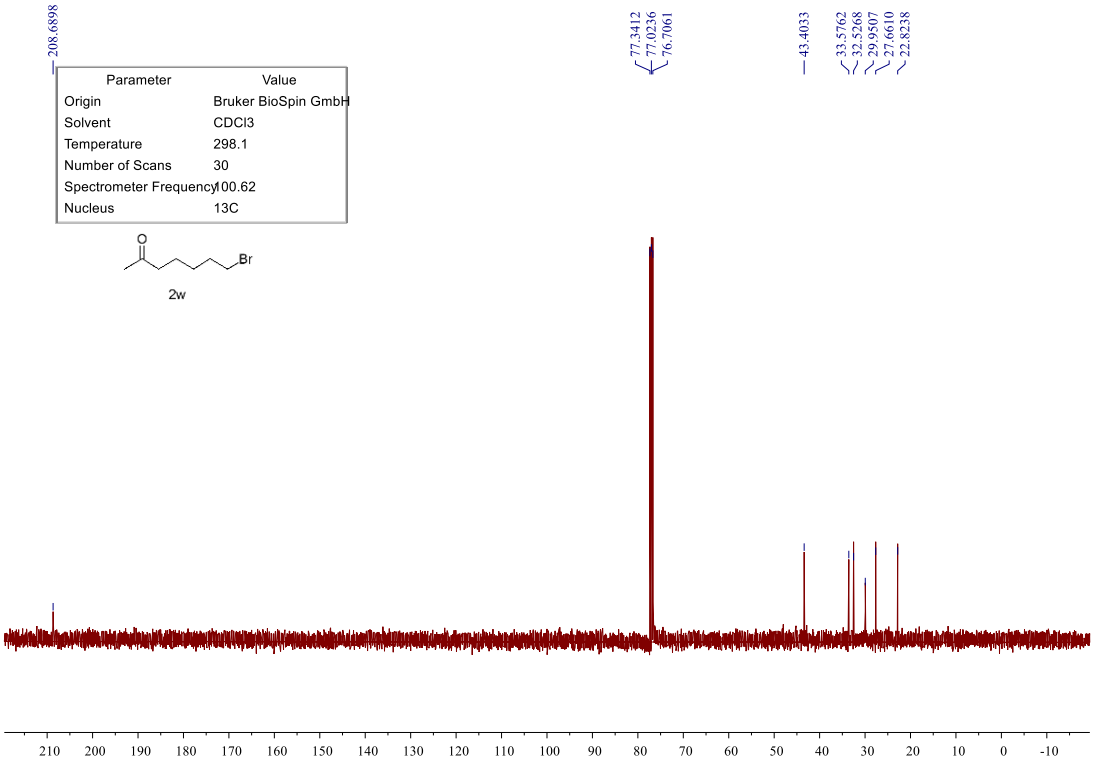
1.4212
1.4123

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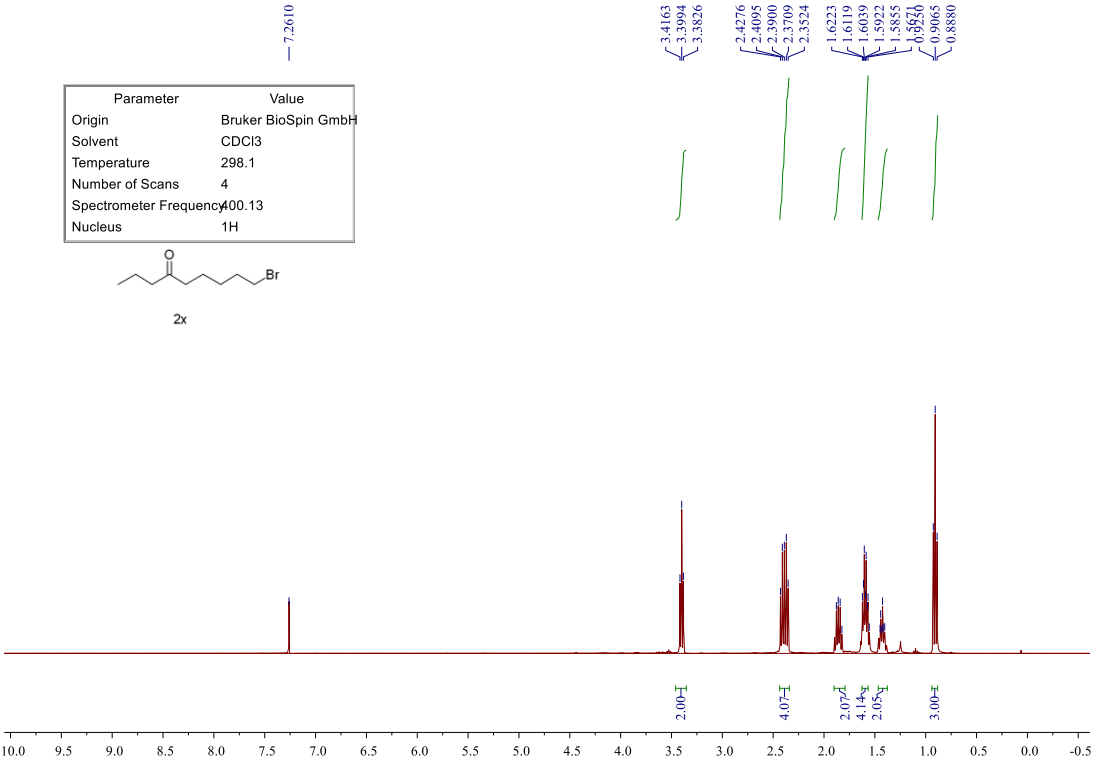
27.6610
22.8238
Parameter Value
Origin Bruker BioSpin GmbH
Solvent CDCl3
Temperature 298.1
Number of Scans 30
Spectrometer Frequency 100.62
Nucleus 13C
O
Br
2w
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10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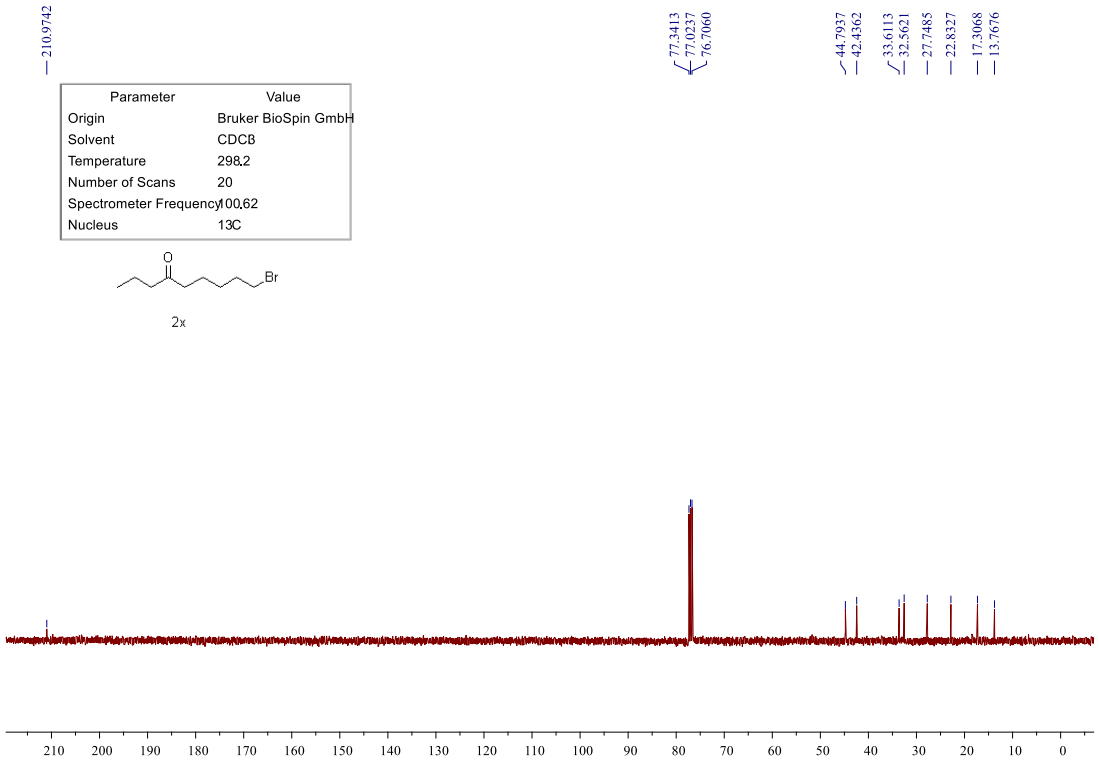
2.3900
2.3709
2.3524
1.6223
1.6119
1.6039
1.5922
1.5855
1.5671
0.9250
0.9065
0.8880
Parameter Value
Origin Bruker BioSpin GmbH
Solvent CDCl3
Temperature 298.1
Number of Scans 4
Spectrometer Frequency 400.13
Nucleus 1H
O
Br
2x
2.00
4.07
2.07
4.14
2.05
3.00
10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5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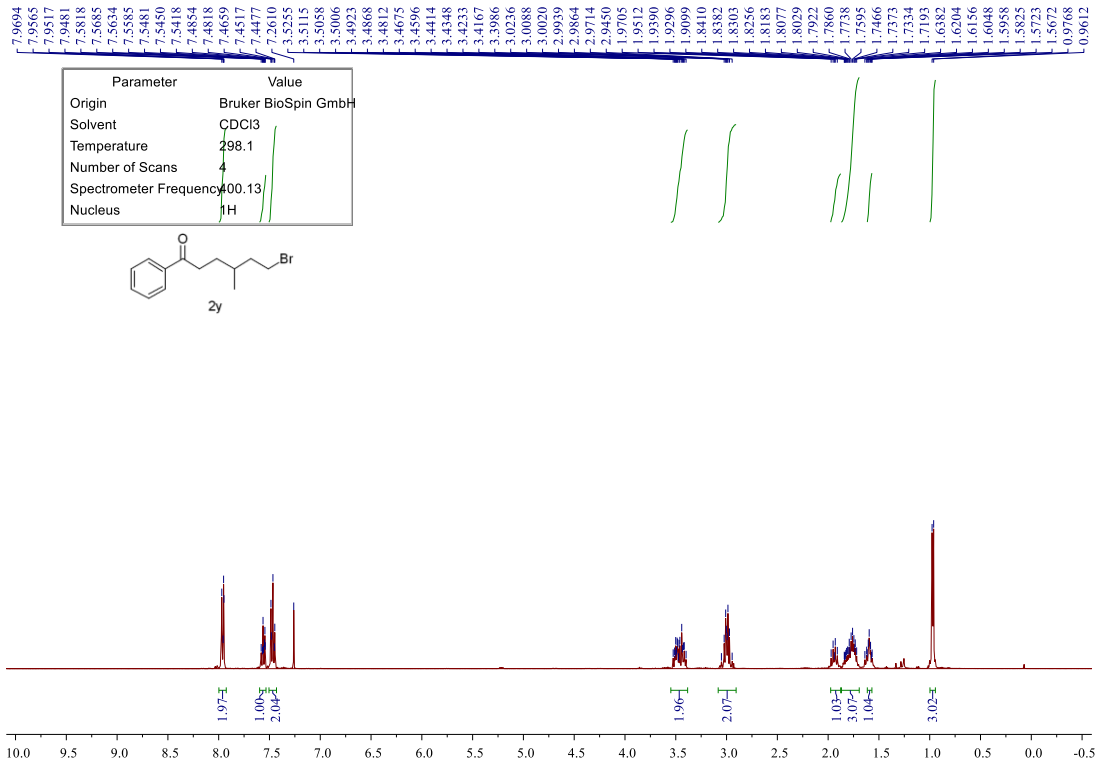
27.7485
22.8327
17.3068
13.7676
Parameter Value
Origin Bruker BioSpin GmbH
Solvent CDCB
Temperature 298.2
Number of Scans 20
Spectrometer Frequency 100.62
Nucleus 13C
O
Br
2x
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0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7.4818
7.4659
7.4517
7.4477
7.2610
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1.6048
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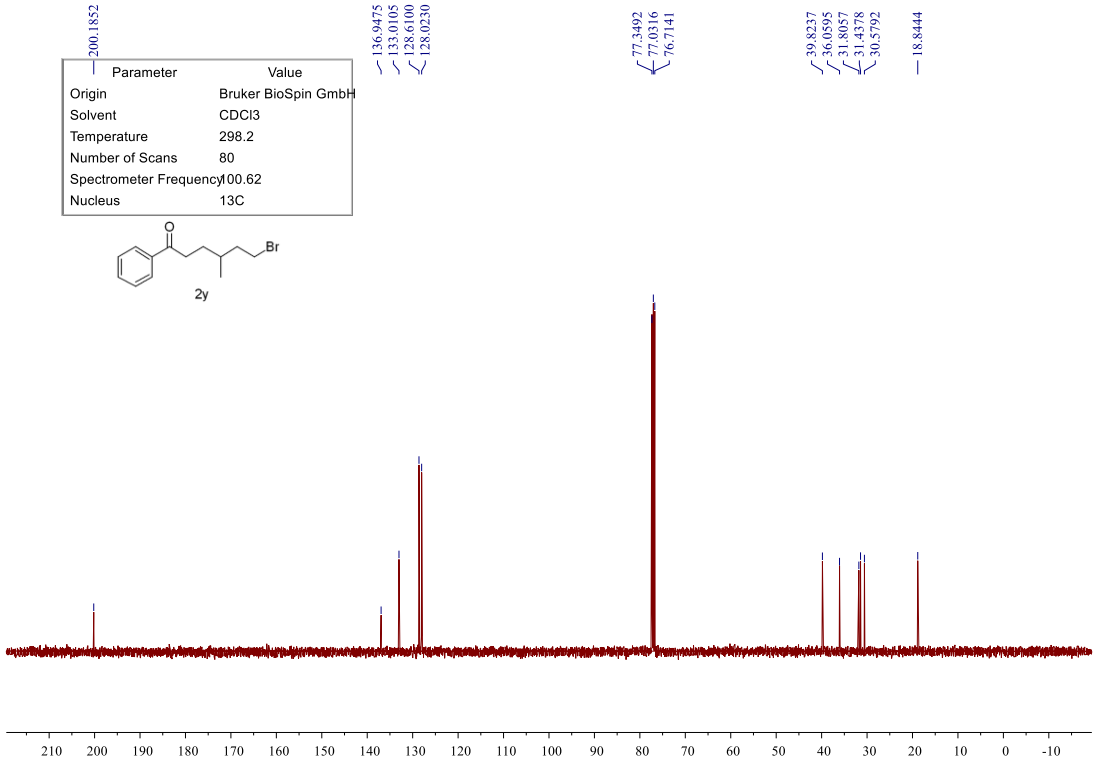
1.5825
1.5723
1.5672
0.9768
0.9612
Parameter Value
Origin Bruker BioSpin GmbH
Solvent CDCl3
Temperature 298.1
Number of Scans 4
Spectrometer Frequency 400.13
Nucleus 1H
O
Br
2y
1.97
1.00
2.04
1.96
2.07
1.03
3.07
1.04
3.02
10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5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39.8237
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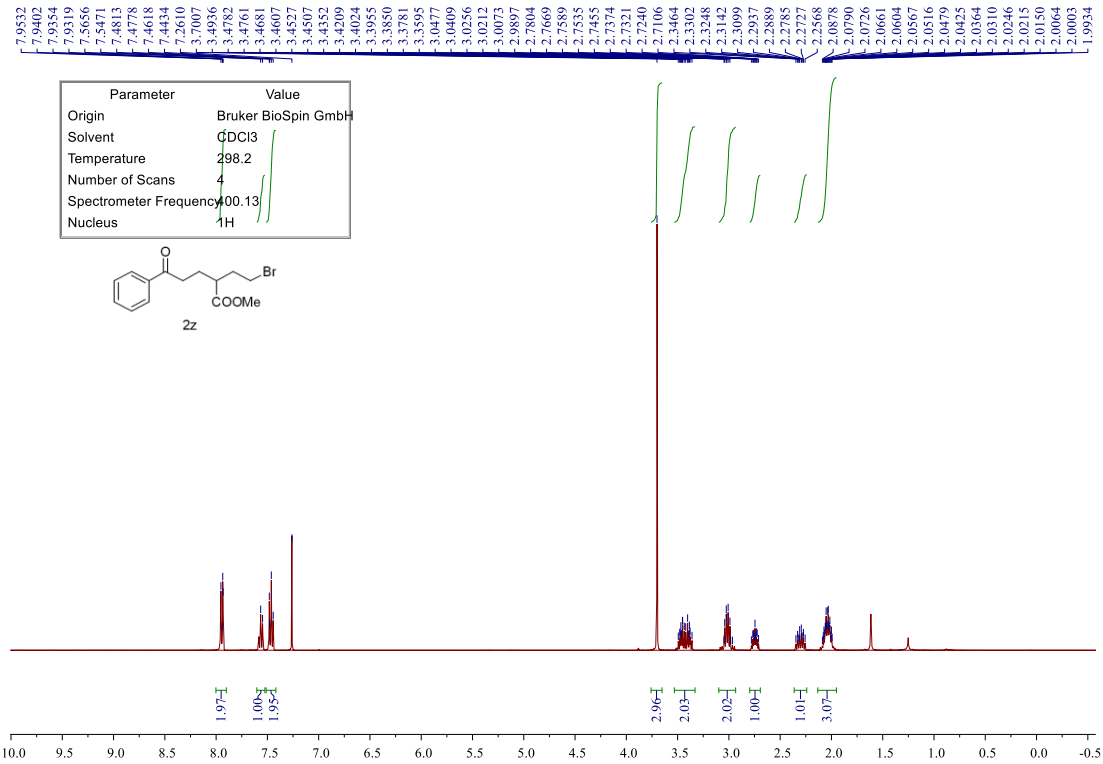
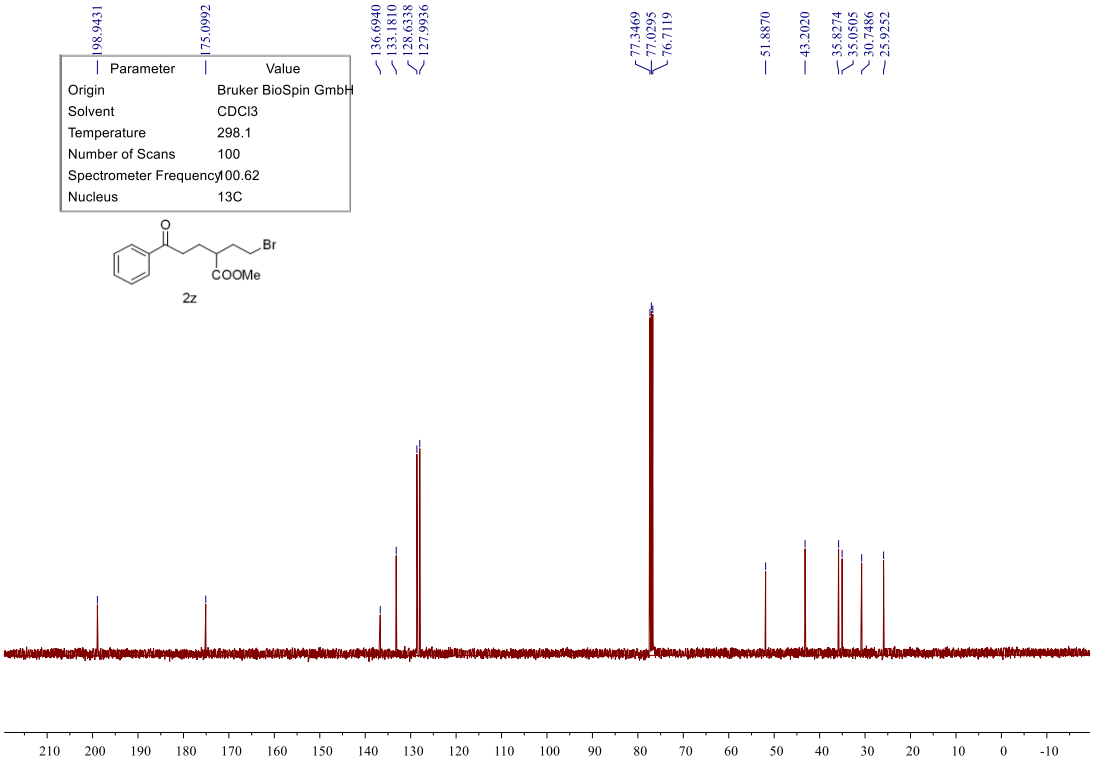
31.8057
31.4378
30.5792
18.8444
Parameter Value
Origin Bruker BioSpin GmbH
Solvent CDCl3
Temperature 298.2
Number of Scans 80
Spectrometer Frequency 100.62
Nucleus 13C
O
Br
2y


Parameter Value
Origin Bruker BioSpin GmbH
Solvent CDCl3
Temperature 298.2
Number of Scans 4
Spectrometer Frequency 400.13
Nucleus 1H
O
Br
COOMe
2z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35.0505
30.7486
25.9252
Parameter Value
Origin Bruker BioSpin GmbH
Solvent CDCl3
Temperature 298.1
Number of Scans 100
Spectrometer Frequency 100.62
Nucleus 13C
O
Br
COOMe
2z
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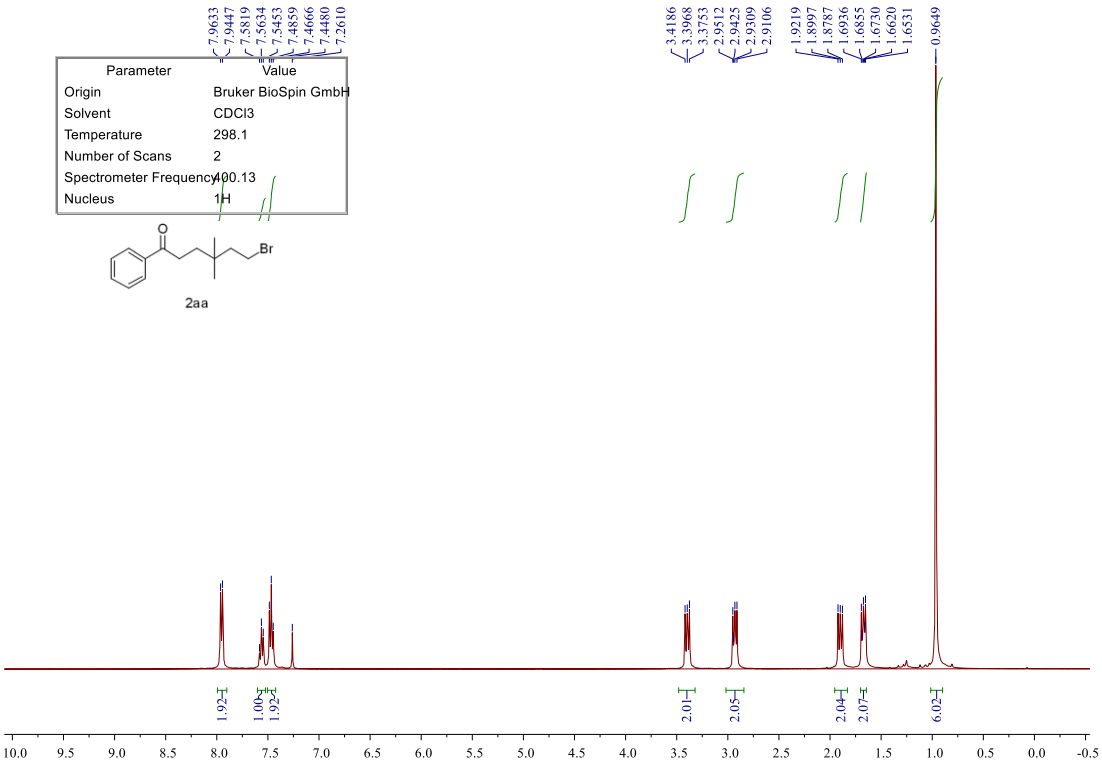
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7.2610
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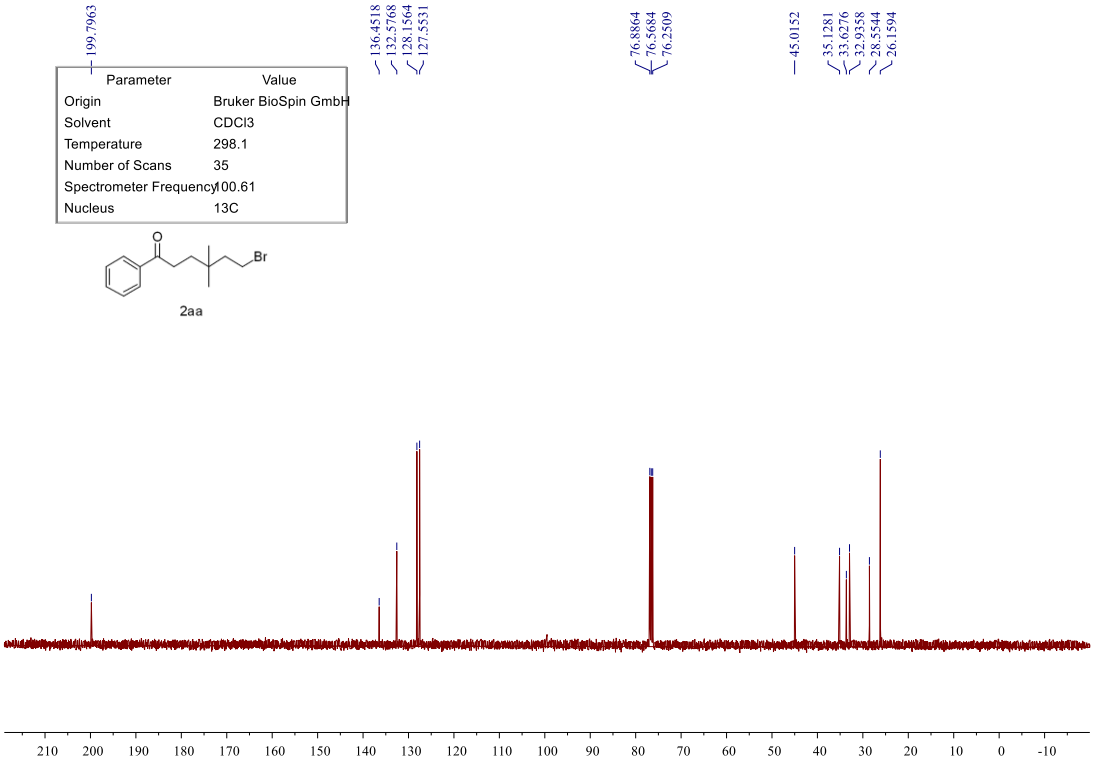
3.3968
3.3753
2.9512
2.9425
2.9309
2.9106
1.9219
1.8997
1.8787
1.6936
1.6855
1.6730
1.6620
1.6531
0.9649
Parameter Value
Origin Bruker BioSpin GmbH
Solvent CDCl3
Temperature 298.1
Number of Scans 2
Spectrometer Frequency 400.13
Nucleus 1H
O
Br
2aa
1.92
1.00
1.92
2.01
2.05
2.04
2.07
6.02
10.0 9.5 9.0 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 -0.5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32.9358
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Parameter Value
Origin Bruker BioSpin GmbH
Solvent CDCl3
Temperature 298.1
Number of Scans 35
Spectrometer Frequency 100.61
Nucleus 13C
O
Br
2aa
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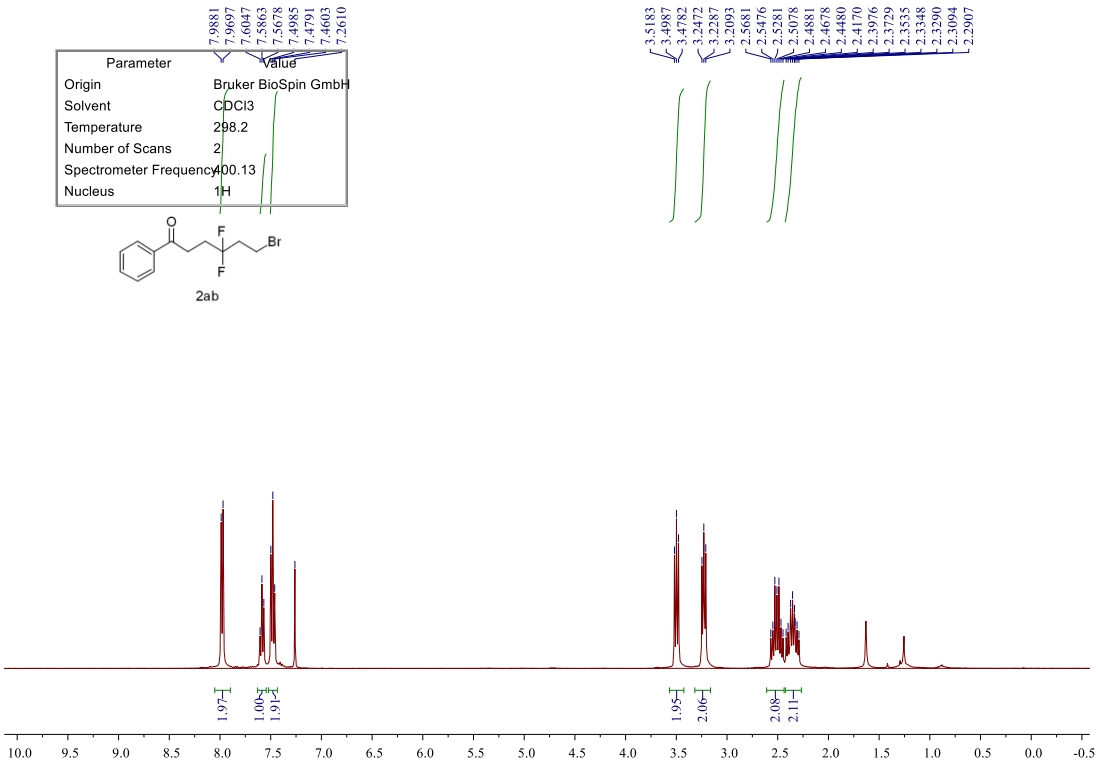
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3.4782
3.2472
3.2287
3.2093
2.5681
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2.5281
2.5078
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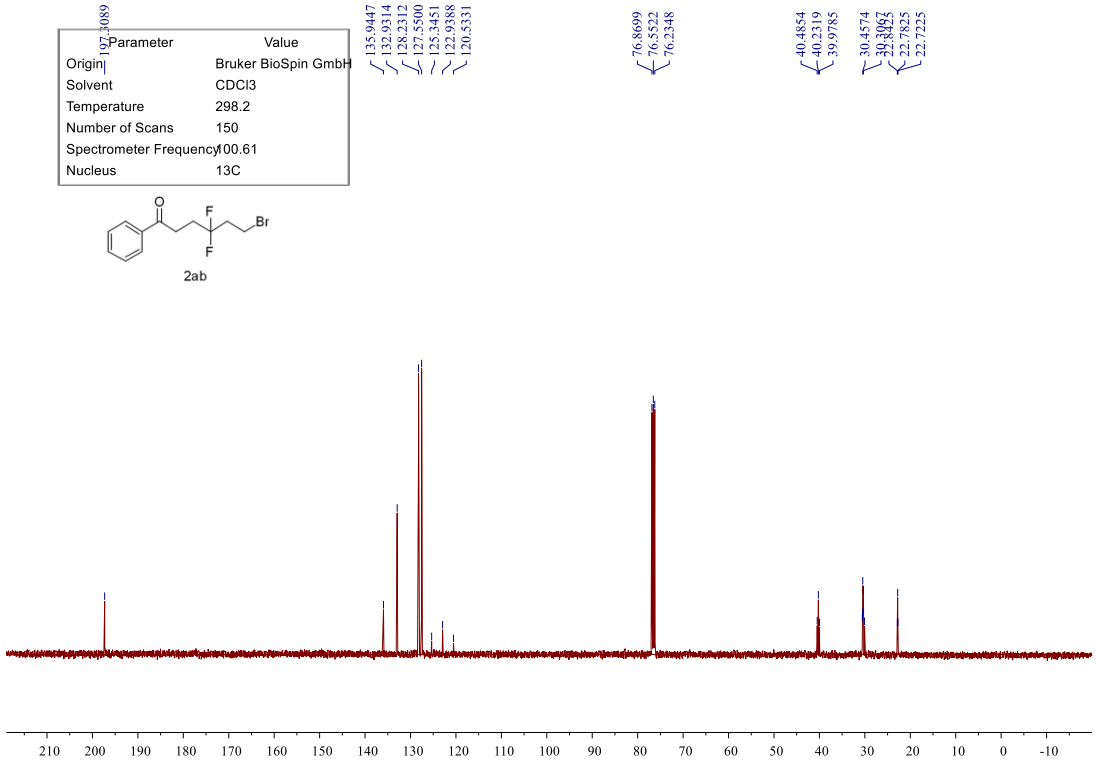
2.4678
2.4480
2.4170
2.3976
2.3729
2.3535
2.3348
2.3290
2.3094
2.2907
Parameter Value
Origin Bruker BioSpin GmbH
Solvent CDCl3
Temperature 298.2
Number of Scans 2
Spectrometer Frequency 400.13
Nucleus 1H
O
F
F
Br
2ab
1.97
1.00
1.91
1.95
2.06
2.08
2.11
10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5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39.9785
30.4574
30.3097
22.7825
22.7225
Parameter Value
Origin Bruker BioSpin GmbH
Solvent CDCl3
Temperature 298.2
Number of Scans 150
Spectrometer Frequency 100.61
Nucleus 13C
O
F
F
Br
2ab
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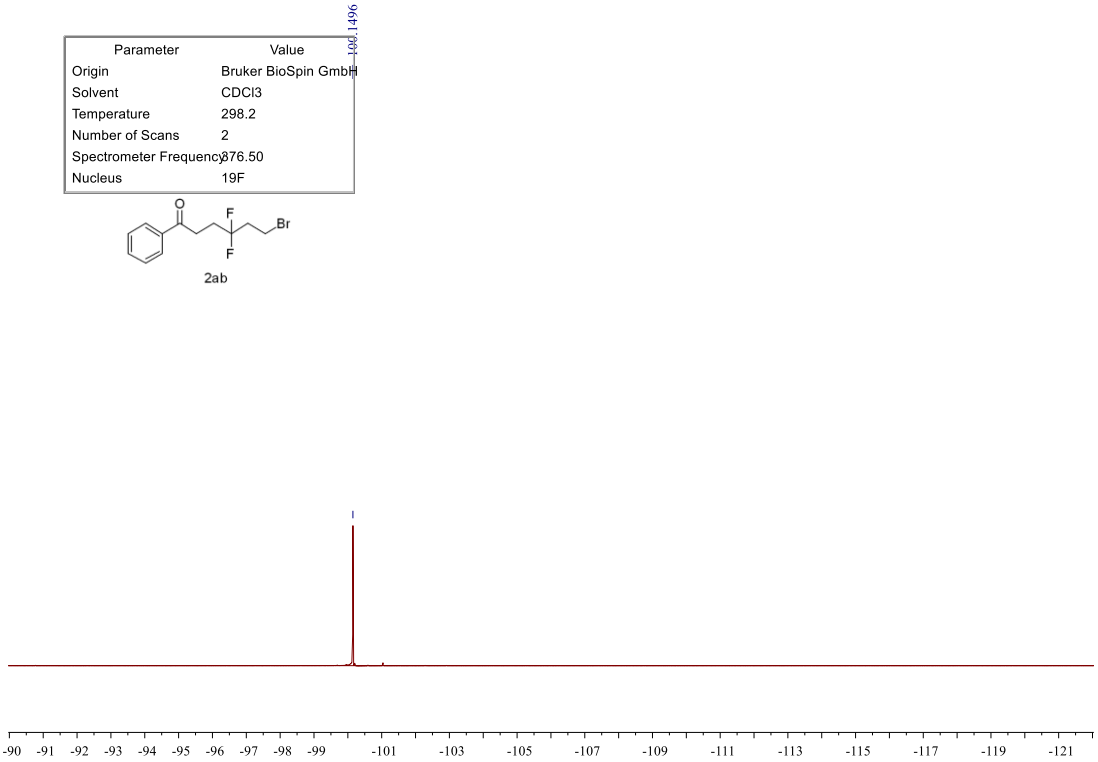
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Solvent CDCl3
Temperature 298.2
Number of Scans 2
Spectrometer Frequency 376.50
Nucleus 19F
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F
F
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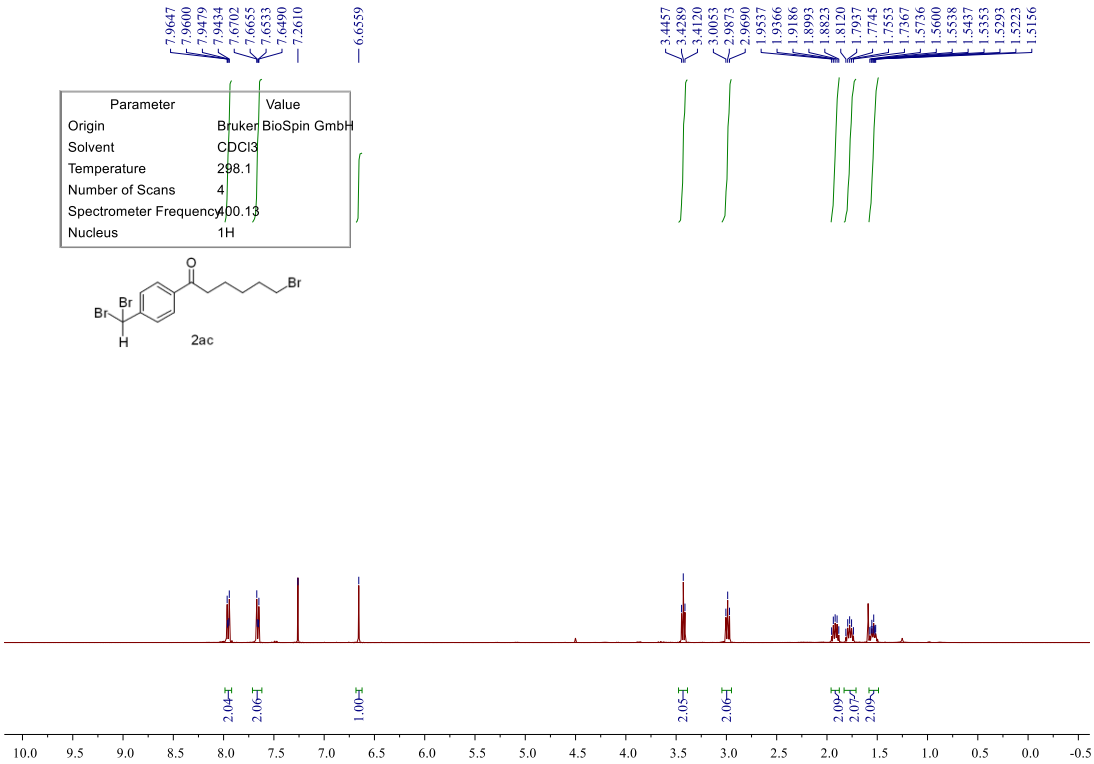
-90 -91 -92 -93 -94 -95 -96 -97 -98 -99 -101 -103 -105 -107 -109 -111 -113 -115 -117 -119 -121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3.4289
3.4120
3.0053
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1.9537
1.9366
1.9186
1.8993
1.8823
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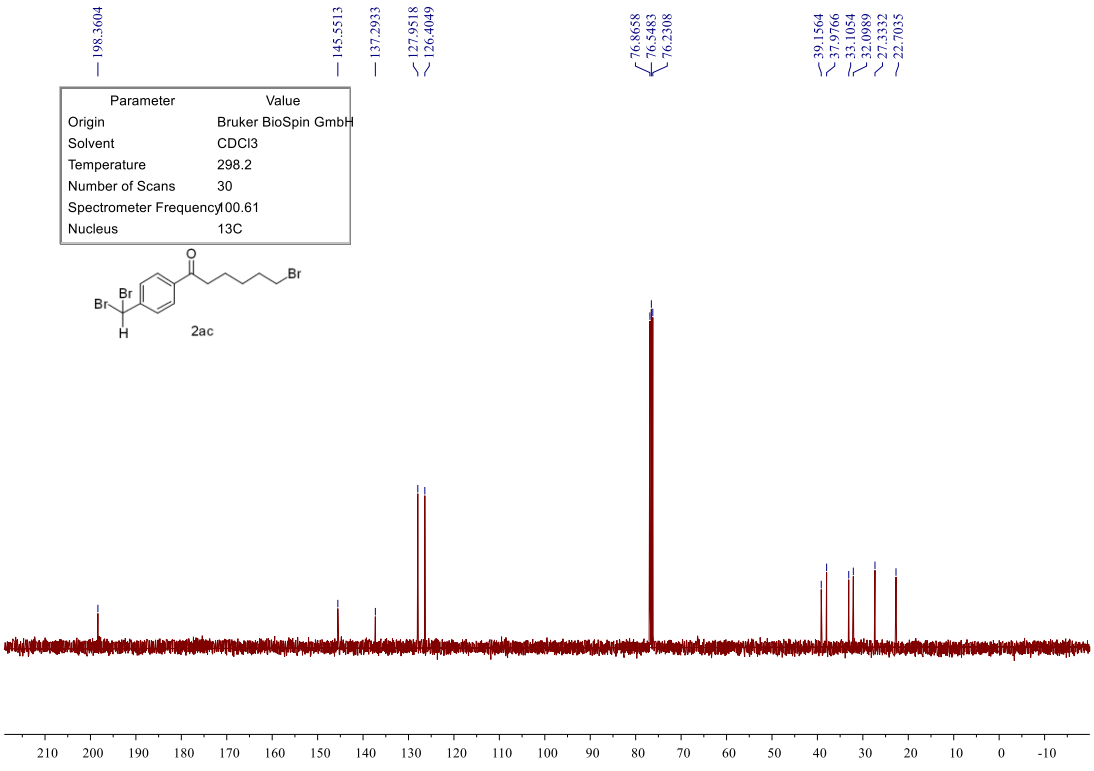
1.7937
1.7745
1.7553
1.7367
1.5736
1.5600
1.5538
1.5437
1.5353
1.5293
1.5223
1.5156
Parameter Value
Origin Bruker BioSpin GmbH
Solvent CDCl3
Temperature 298.1
Number of Scans 4
Spectrometer Frequency 400.13
Nucleus 1H
O
Br
Br
Br
H
2ac
2.04
2.06
1.00
2.05
2.06
2.09
2.07
2.09
10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5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32.0989
27.3332
22.7035
Parameter Value
Origin Bruker BioSpin GmbH
Solvent CDCl3
Temperature 298.2
Number of Scans 30
Spectrometer Frequency 100.61
Nucleus 13C
O
Br
Br
Br
H
2ac
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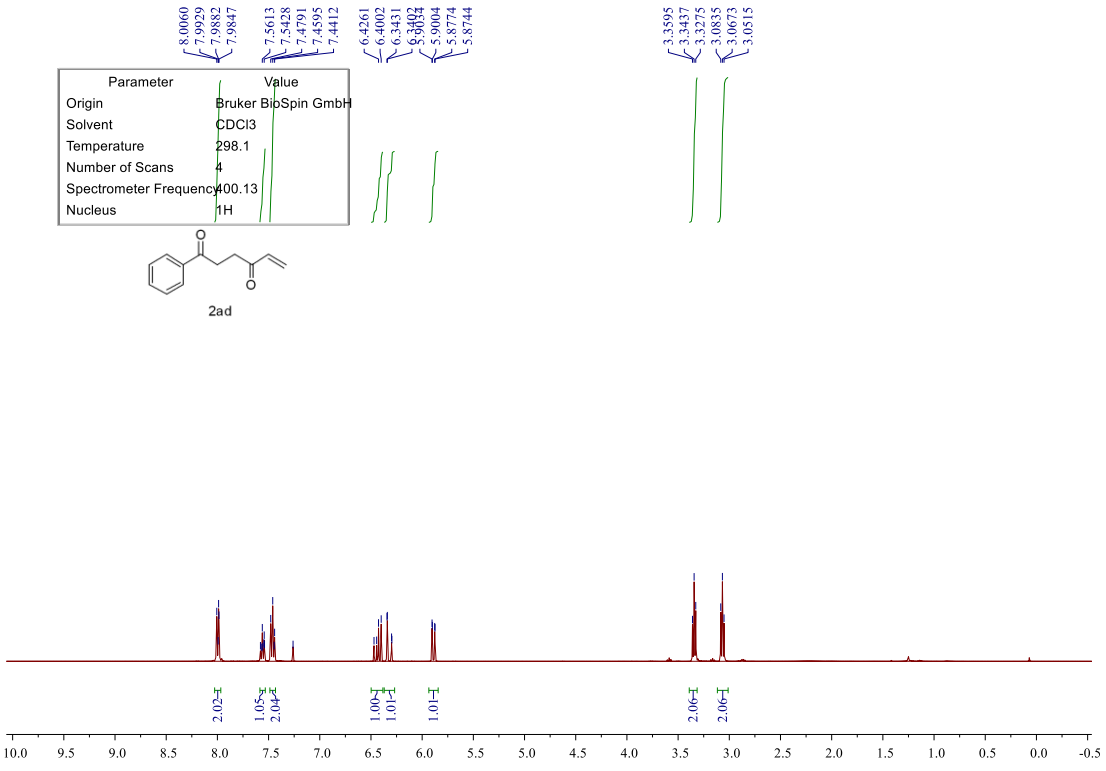
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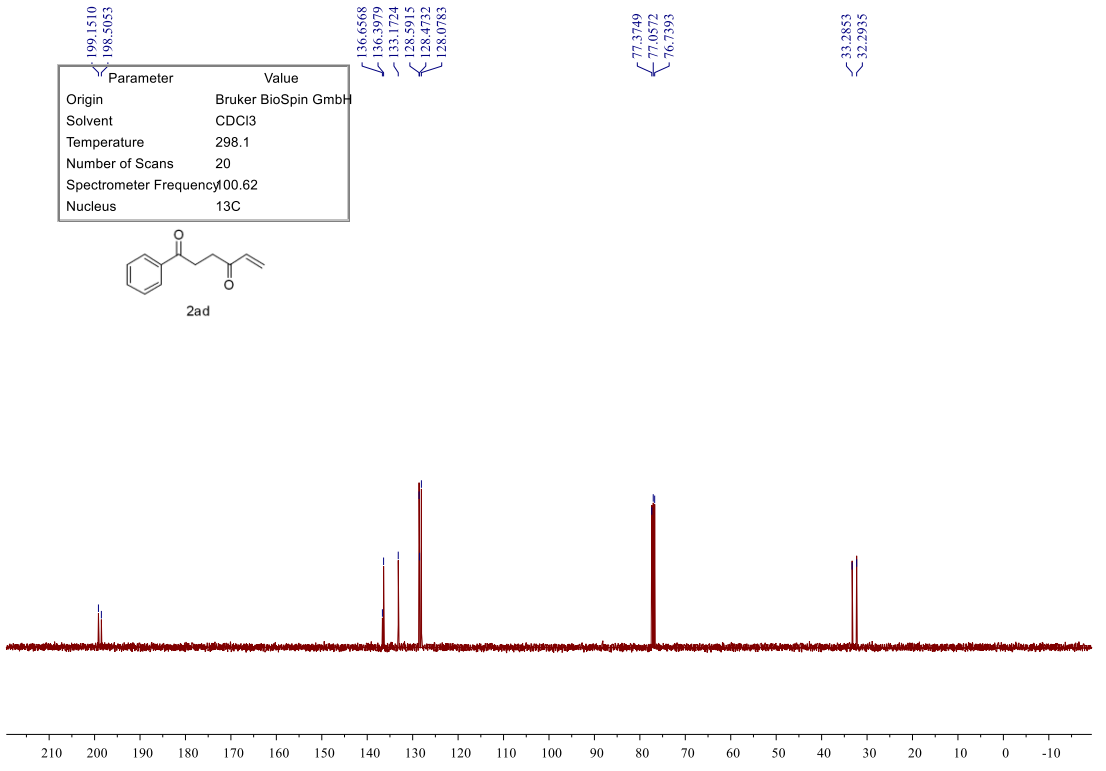
5.9034
5.9004
5.8774
5.8744
3.3595
3.3437
3.3275
3.0835
3.0673
3.0515
Parameter Value
Origin Bruker BioSpin GmbH
Solvent CDCl3
Temperature 298.1
Number of Scans 4
Spectrometer Frequency 400.13
Nucleus 1H
2ad
2.02
1.05
2.04
1.00
1.01
1.01
2.06
2.06
10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5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136.3979
133.1724
128.5915
128.4732
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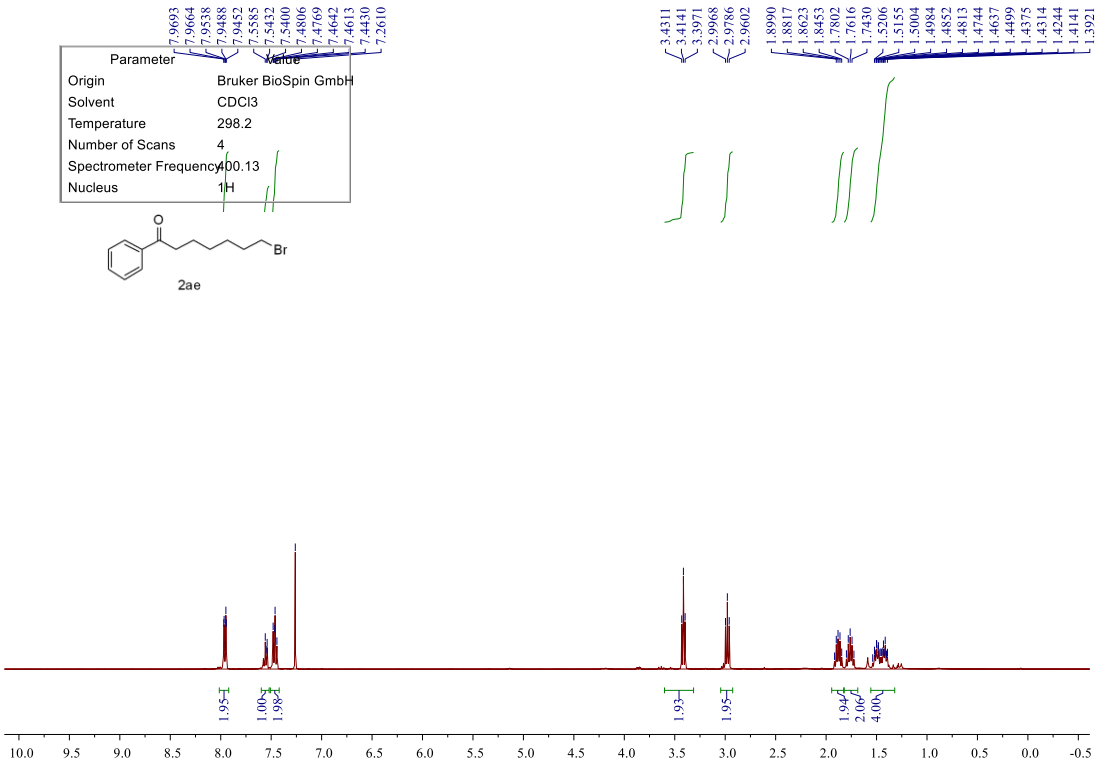
77.3749
77.0572
76.7393
33.2853
32.2935
Parameter Value
Origin Bruker BioSpin GmbH
Solvent CDCl3
Temperature 298.1
Number of Scans 20
Spectrometer Frequency 100.62
Nucleus 13C
2ad
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10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7.5400
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7.4769
7.4642
7.4613
7.4430
7.2610
Parameter Value
Origin Bruker BioSpin GmbH
Solvent CDCl3
Temperature 298.2
Number of Scans 4
Spectrometer Frequency 400.13
Nucleus 1H
O
Br
2ae
3.4311
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3.3971
2.9968
2.9786
2.9602
1.8990
1.8817
1.8623
1.8453
1.7802
1.7616
1.7430
1.5206
1.5155
1.5004
1.4984
1.4852
1.4813
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1.4637
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1.4375
1.4314
1.4244
1.4141
1.3921
1.95
1.00
1.98
1.93
1.95
1.94
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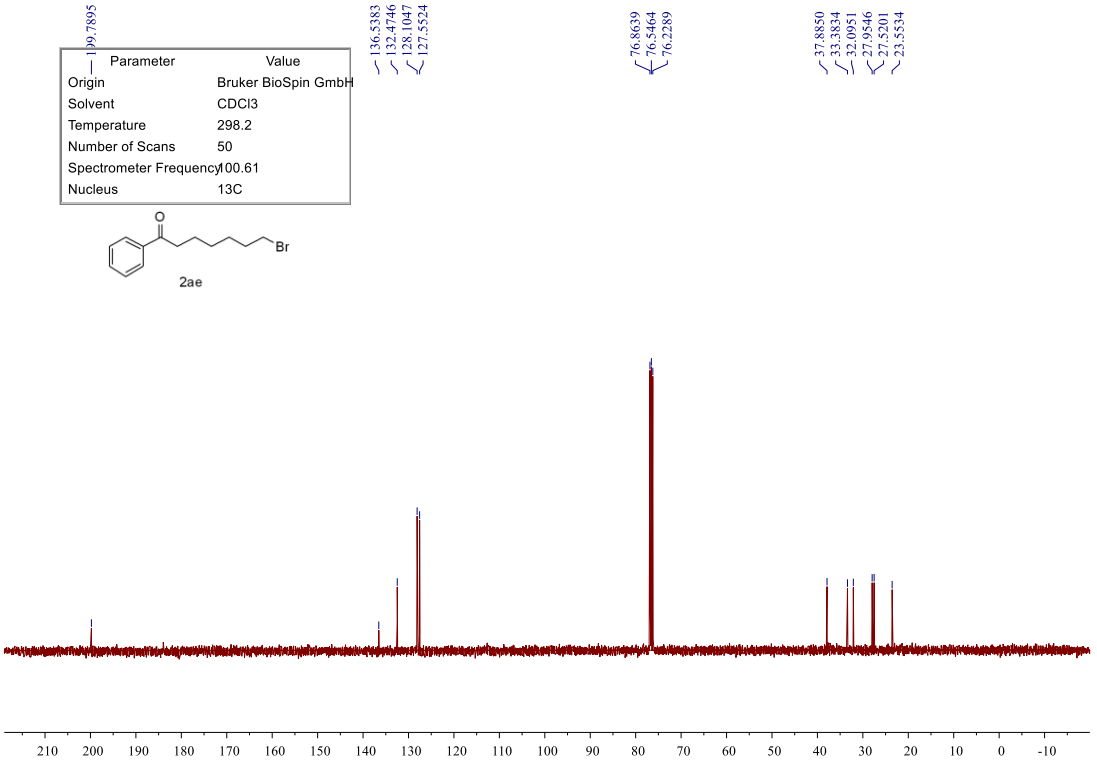
4.00
10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5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27.9546
27.5201
23.5534
Parameter Value
Origin Bruker BioSpin GmbH
Solvent CDCl3
Temperature 298.2
Number of Scans 50
Spectrometer Frequency 100.61
Nucleus 13C
O
Br
2ae
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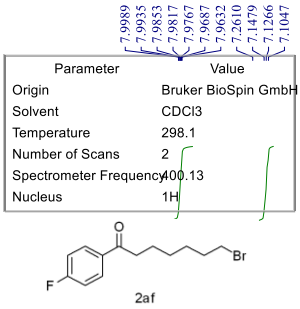
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7.9632
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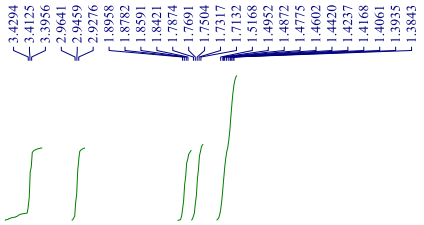
7.1479
7.1266
7.1047
Parameter Value
Origin Bruker BioSpin GmbH
Solvent CDCl3
Temperature 298.1
Number of Scans 2
Spectrometer Frequency 400.13
Nucleus 1H
O
Br
F
2af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1.7691
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1.5168
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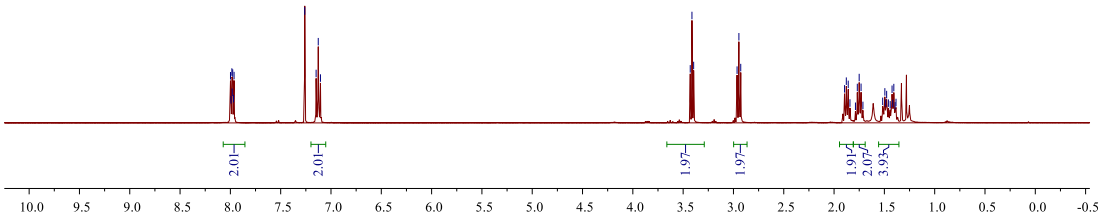
1.3935
1.3843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3.93
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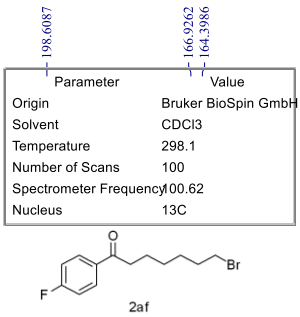
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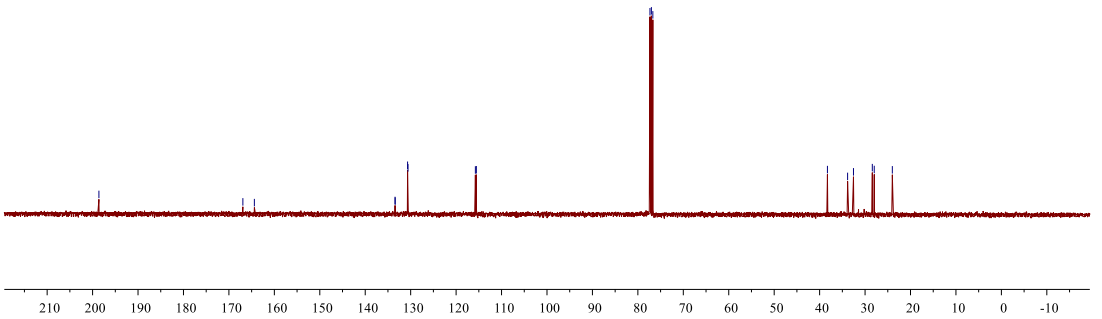
76.7052
38.2813
33.8412
32.5503
28.4054
27.9782
23.9987
Parameter Value
Origin Bruker BioSpin GmbH
Solvent CDCl3
Temperature 298.1
Number of Scans 100
Spectrometer Frequency 100.62
Nucleus 13C
O
Br
F
2af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Parameter	Value
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Solvent	CDCl3
Temperature	298.2
Number of Scans	2
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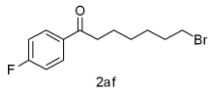
Nucleus	19F



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Parameter	Value
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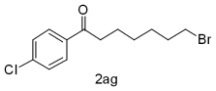
Solvent	CDCl3
Temperature	298.2
Number of Scans	4
Spectrometer Frequency	400.13
Nucleus	1H



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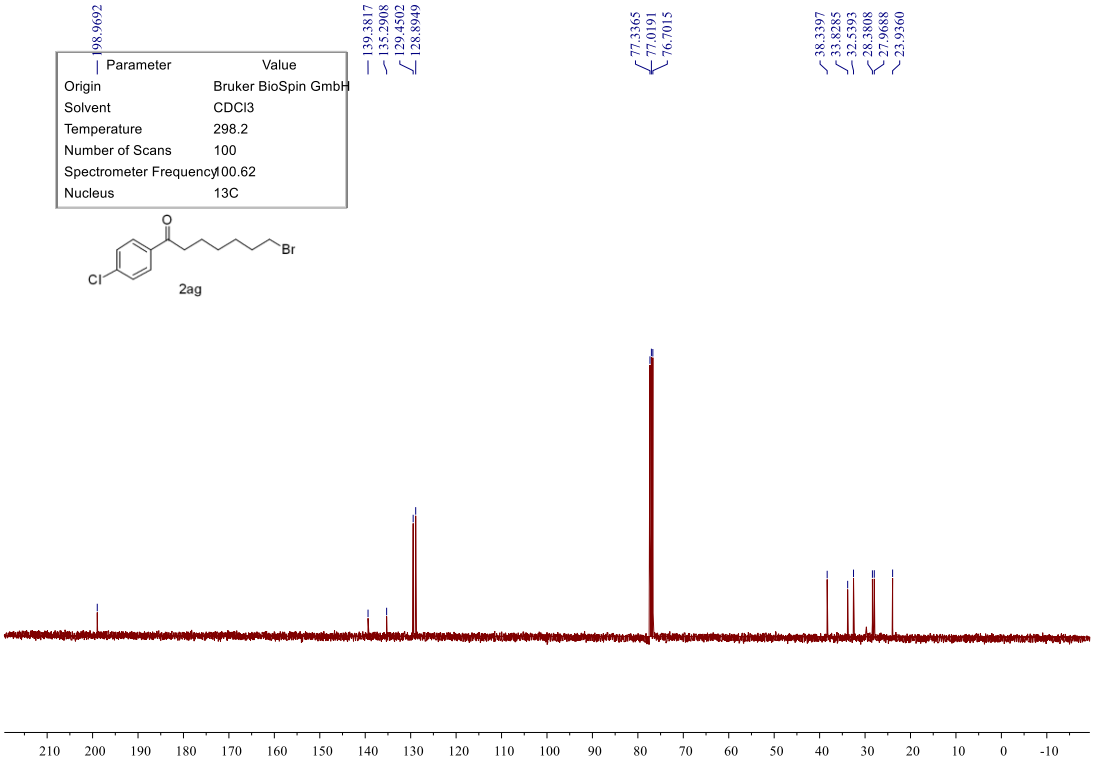
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28.3808
27.9688
23.9360
Parameter Value
Origin Bruker BioSpin GmbH
Solvent CDCl3
Temperature 298.2
Number of Scans 100
Spectrometer Frequency 100.62
Nucleus 13C
O
Br
Cl
2ag
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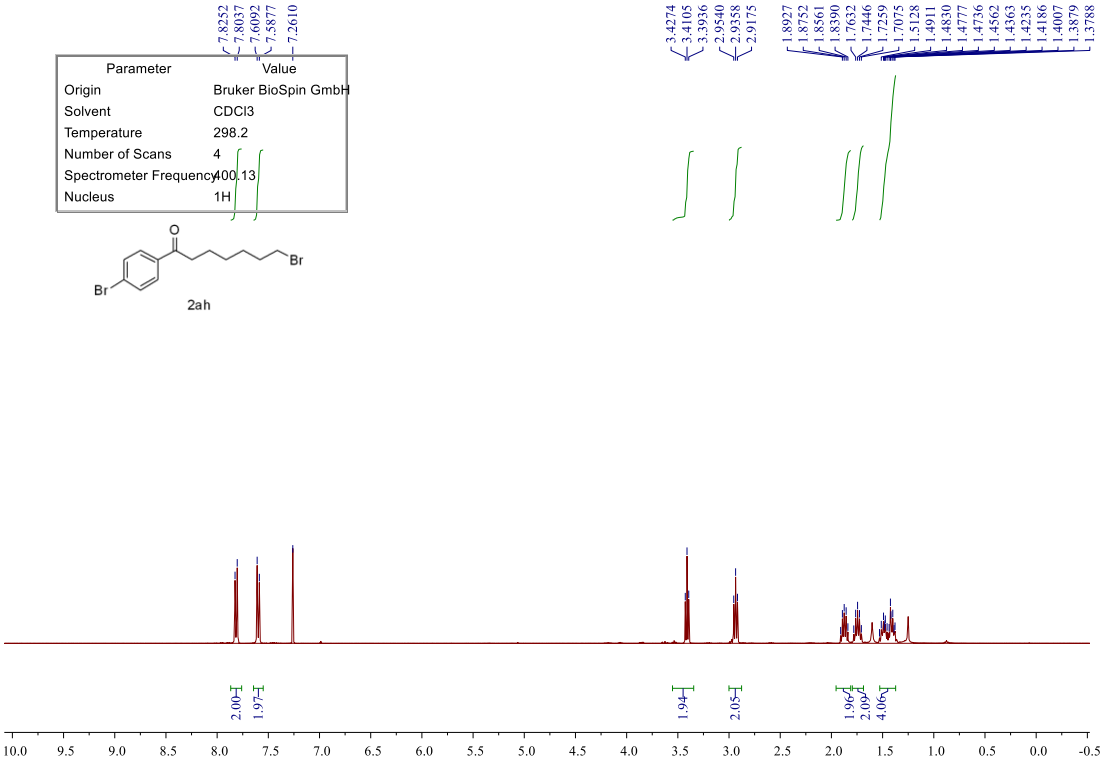
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1.7446
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1.4007
1.3879
1.3788
Parameter Value
Origin Bruker BioSpin GmbH
Solvent CDCl3
Temperature 298.2
Number of Scans 4
Spectrometer Frequency 400.13
Nucleus 1H
O
Br
Br
2ah
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1.94
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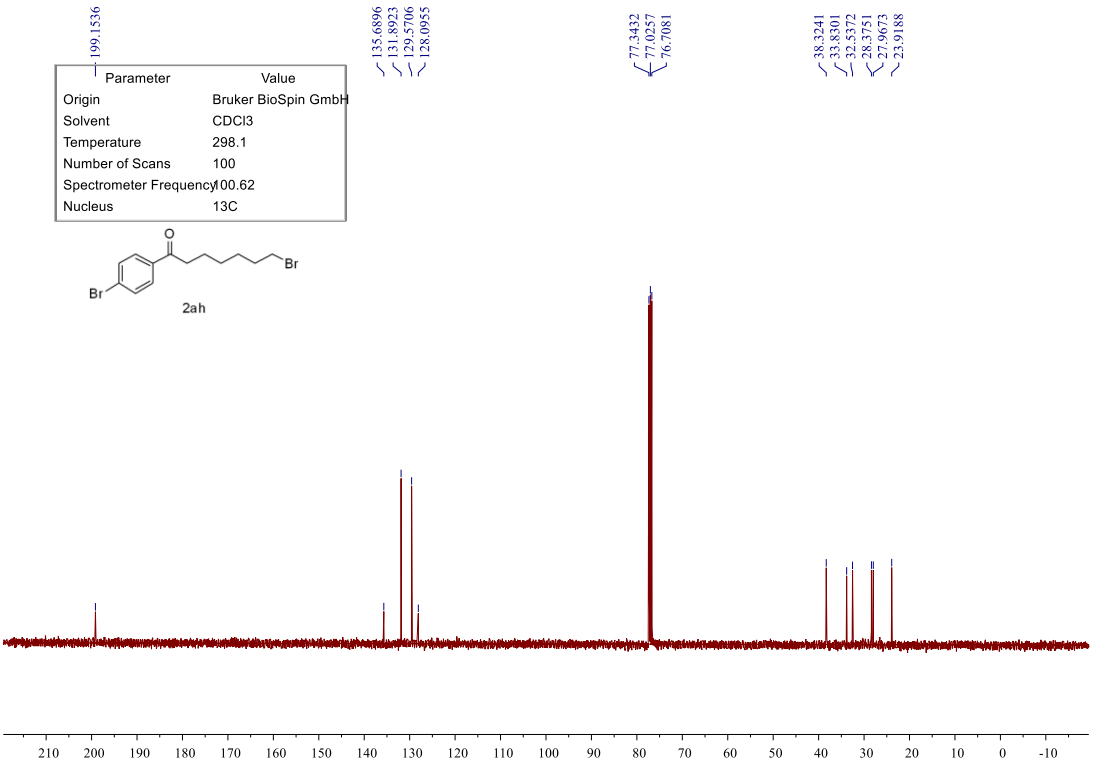
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32.5372
28.3751
27.9673
23.9188
Parameter Value
Origin Bruker BioSpin GmbH
Solvent CDCl3
Temperature 298.1
Number of Scans 100
Spectrometer Frequency 100.62
Nucleus 13C
O
Br
Br
2ah
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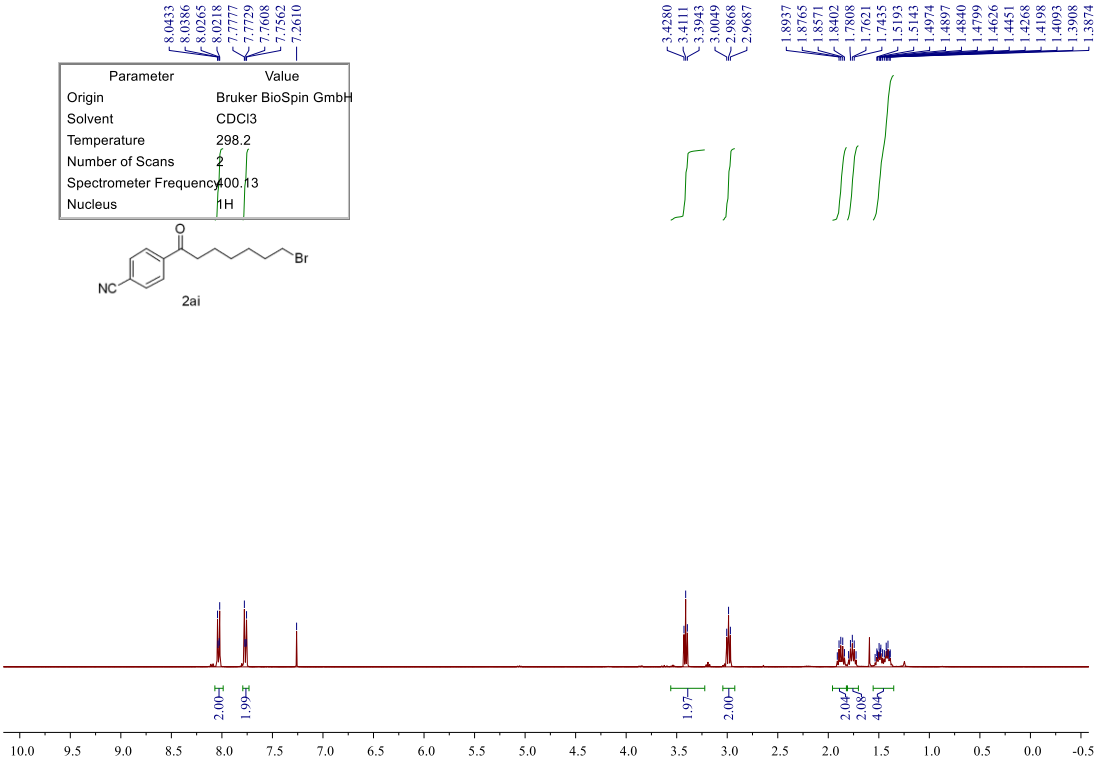
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Parameter Value
Origin Bruker BioSpin GmbH
Solvent CDCl3
Temperature 298.2
Number of Scans 2
Spectrometer Frequency 400.13
Nucleus 1H
O
Br
NC
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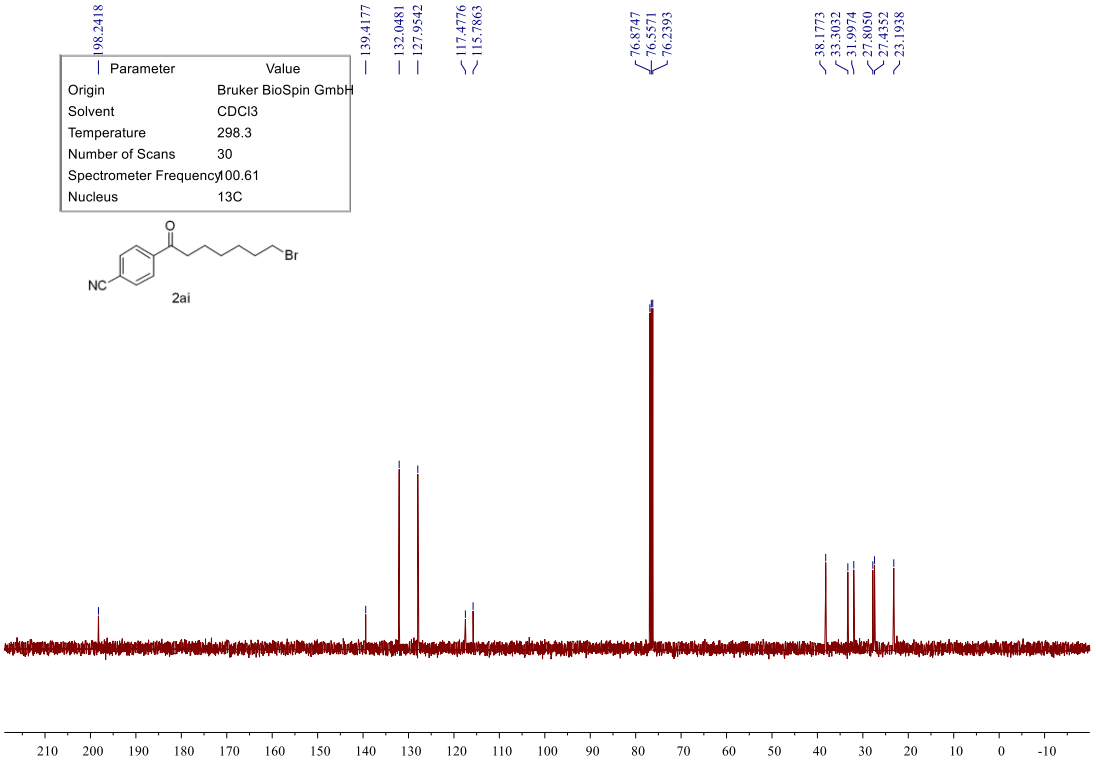
1.97
2.00
2.04
2.08
4.04
10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5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33.3032
31.9974
27.8050
27.4352
23.1938
Parameter Value
Origin Bruker BioSpin GmbH
Solvent CDCl3
Temperature 298.3
Number of Scans 30
Spectrometer Frequency 100.61
Nucleus 13C
O
Br
NC
2ai
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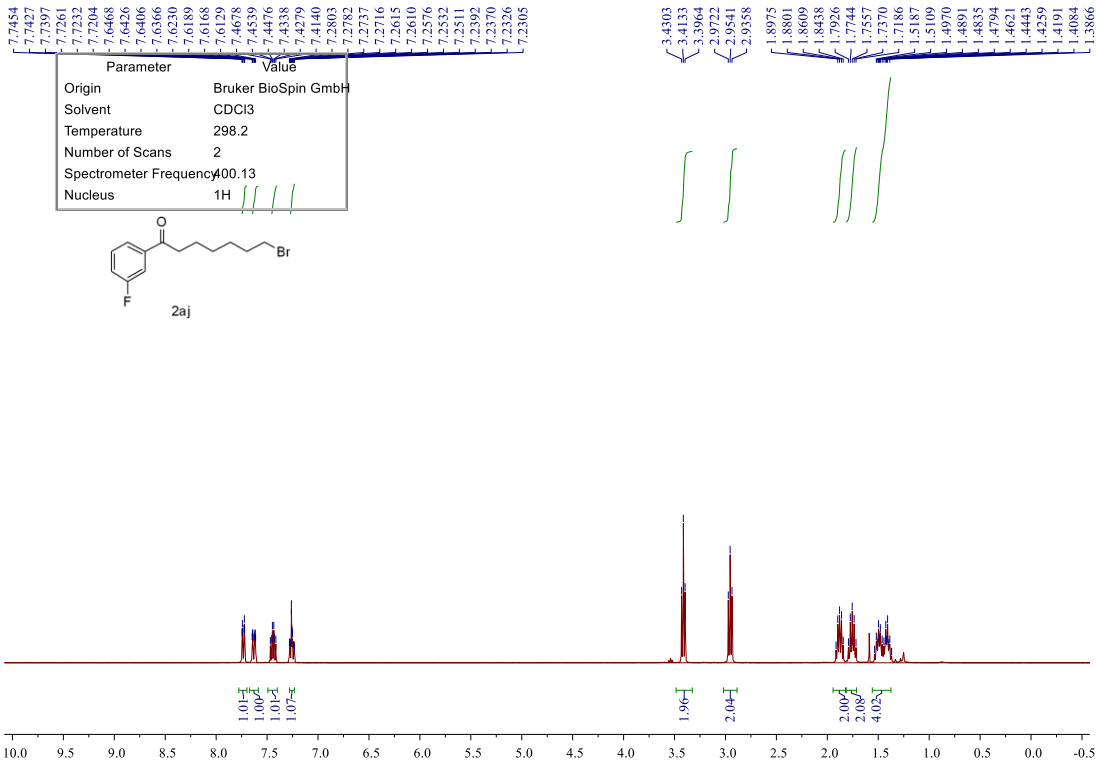
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7.4476
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7.4140
7.2803
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7.2737
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7.2615
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7.2576
7.2532
7.2511
7.2392
7.2370
7.2326
7.2305
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3.4133
3.3964
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2.9541
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1.8801
1.8609
1.8438
1.7926
1.7744
1.7557
1.7370
1.7186
1.5187
1.5109
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1.4443
1.4259
1.4191
1.4084
1.3866
Parameter Value
Origin Bruker BioSpin GmbH
Solvent CDCl3
Temperature 298.2
Number of Scans 2
Spectrometer Frequency 400.13
Nucleus 1H
O
Br
F
2aj
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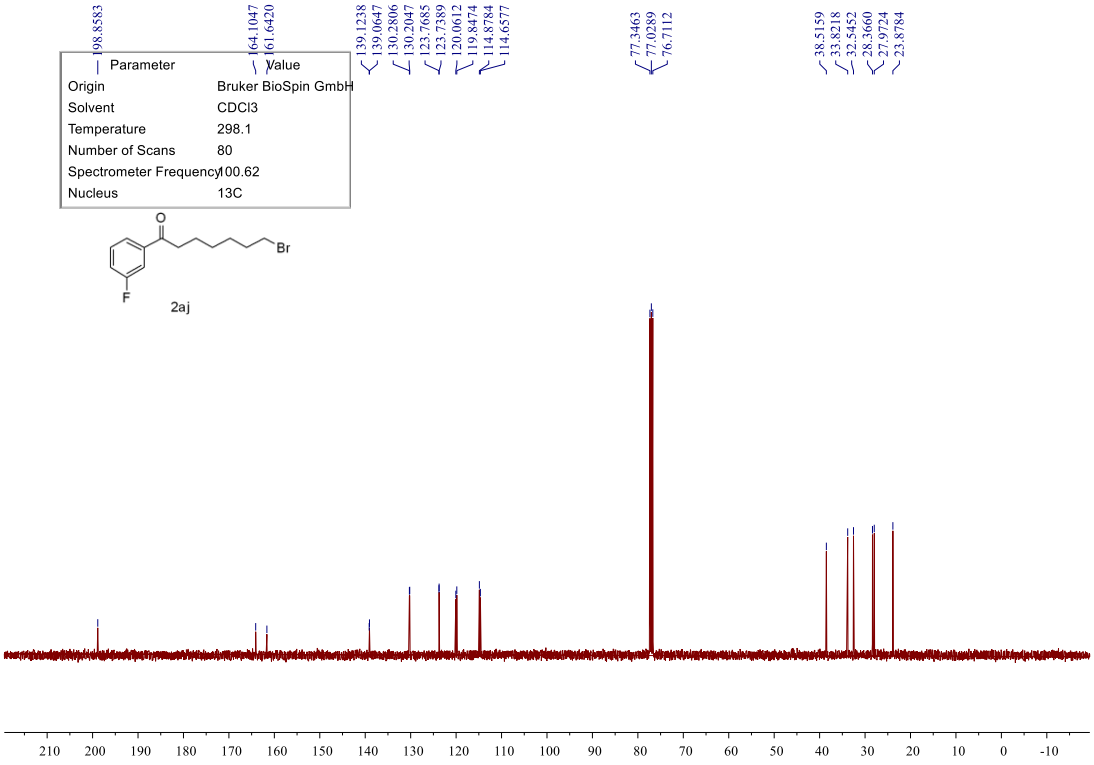
1.00
1.01
1.07
1.96
2.04
2.00
2.08
4.02
10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5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114.6577
77.3463
77.0289
76.7112
38.5159
33.8218
32.5452
28.3660
27.9724
23.8784
Parameter Value
Origin Bruker BioSpin GmbH
Solvent CDCl3
Temperature 298.1
Number of Scans 80
Spectrometer Frequency 100.62
Nucleus 13C
O
Br
F
2aj
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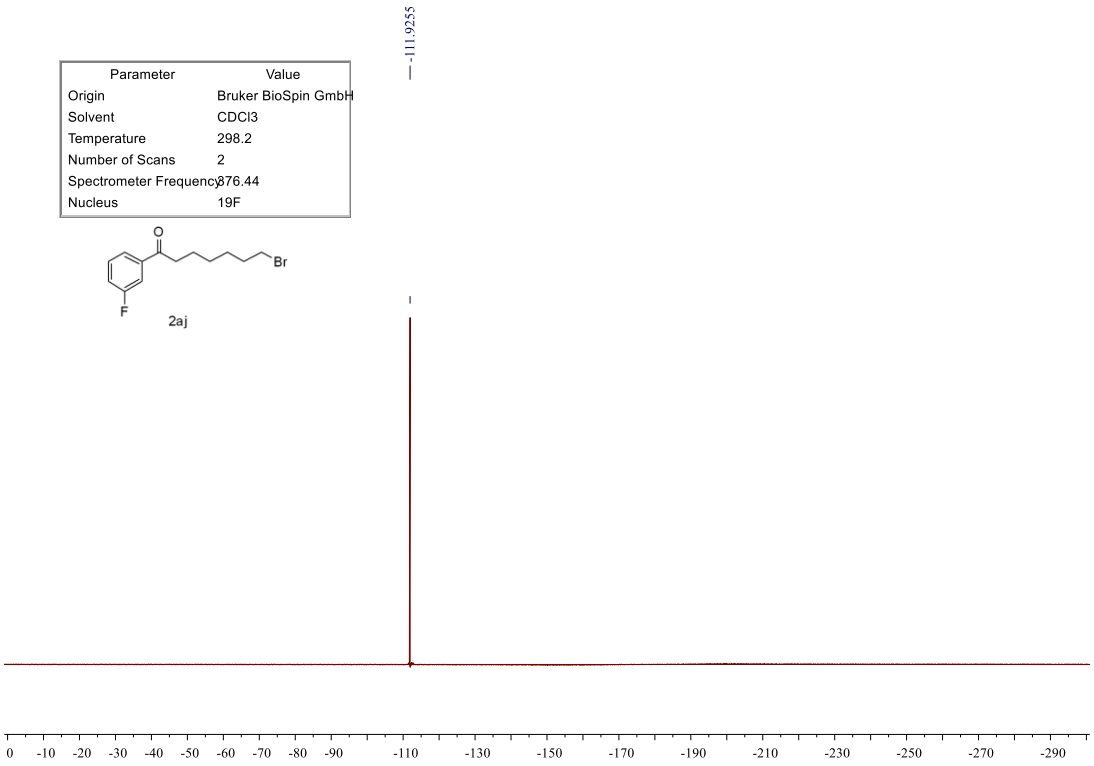
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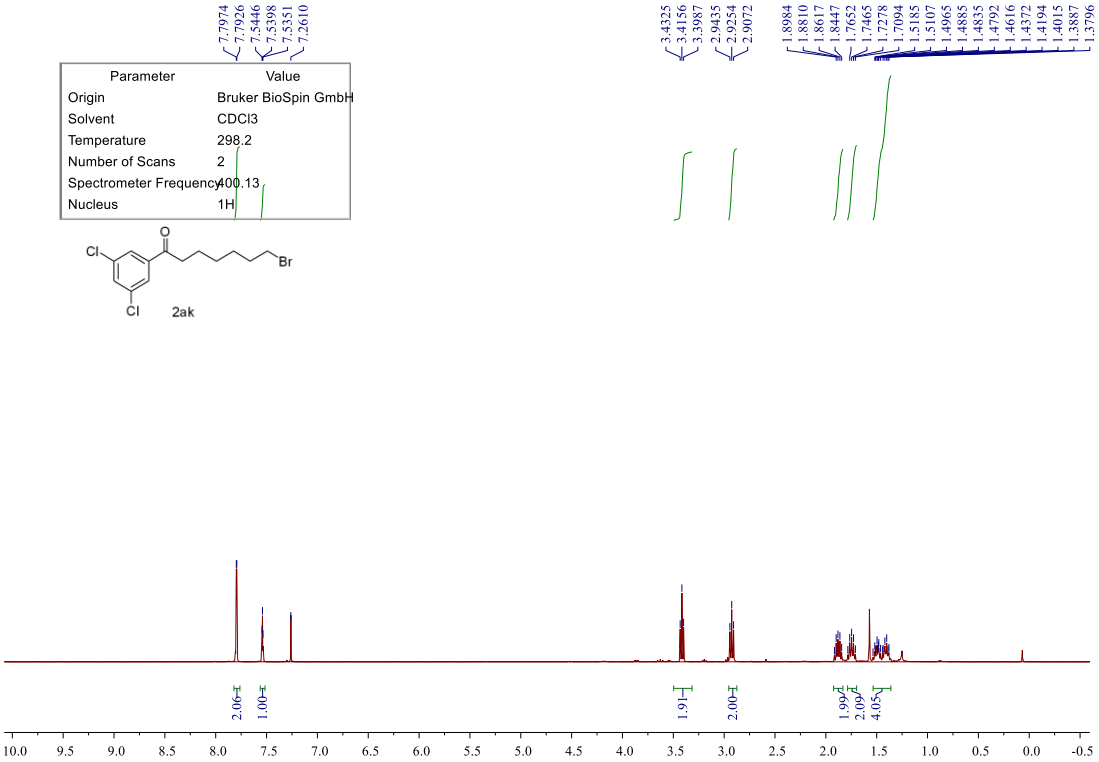
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1.7465
1.7278
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1.5107
1.4965
1.4885
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1.4792
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1.4372
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1.4015
1.3887
1.3796
Parameter Value
Origin Bruker BioSpin GmbH
Solvent CDCl3
Temperature 298.2
Number of Scans 2
Spectrometer Frequency 400.13
Nucleus 1H
Cl
O
Br
Cl
2ak
2.06
1.00
1.91
2.00
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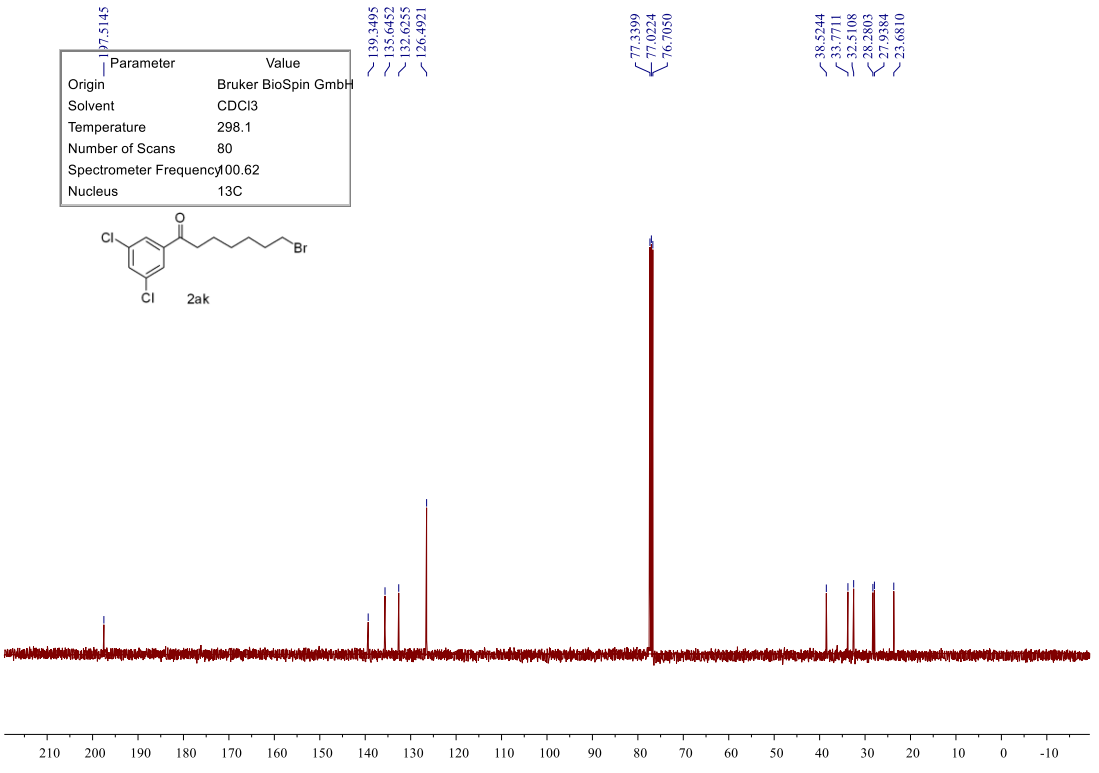
2.09
4.05
10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5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Parameter Value
Origin Bruker BioSpin GmbH
Solvent CDCl3
Temperature 298.1
Number of Scans 80
Spectrometer Frequency 100.62
Nucleus 13C
Cl
O
Br
Cl
2ak
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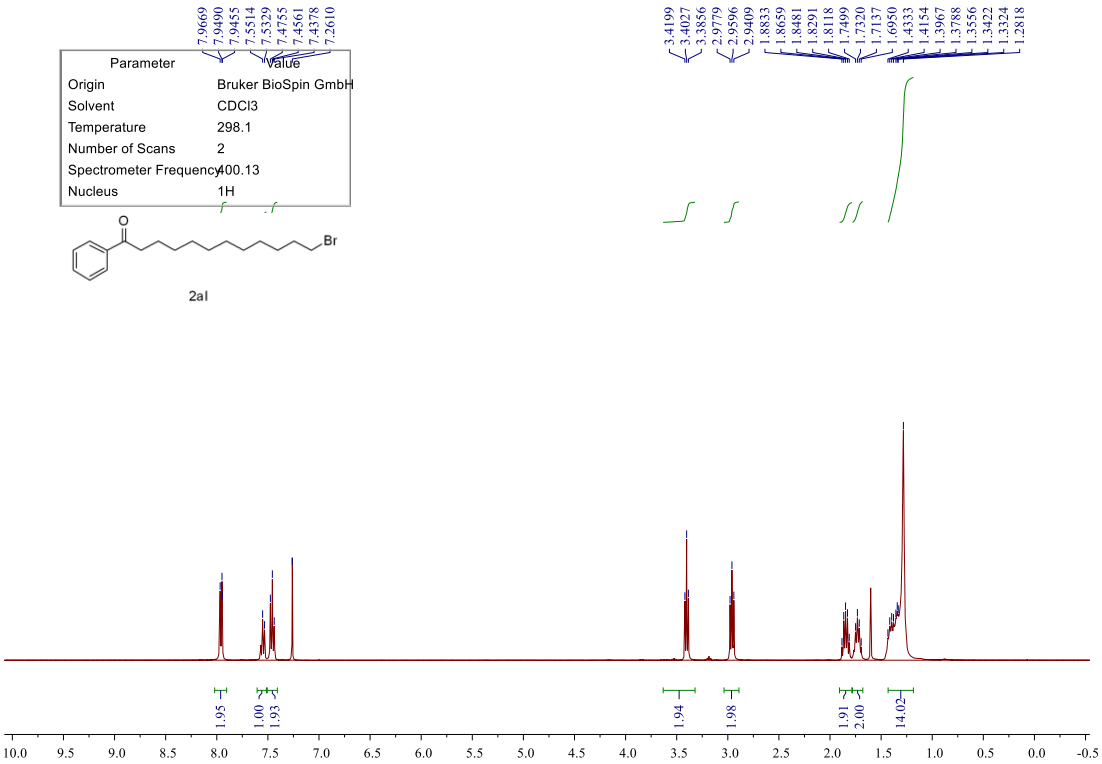
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Parameter Value
Origin Bruker BioSpin GmbH
Solvent CDCl3
Temperature 298.1
Number of Scans 2
Spectrometer Frequency 400.13
Nucleus 1H
O
Br
2aI
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3.3856
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2.9409
1.8833
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1.8481
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1.8118
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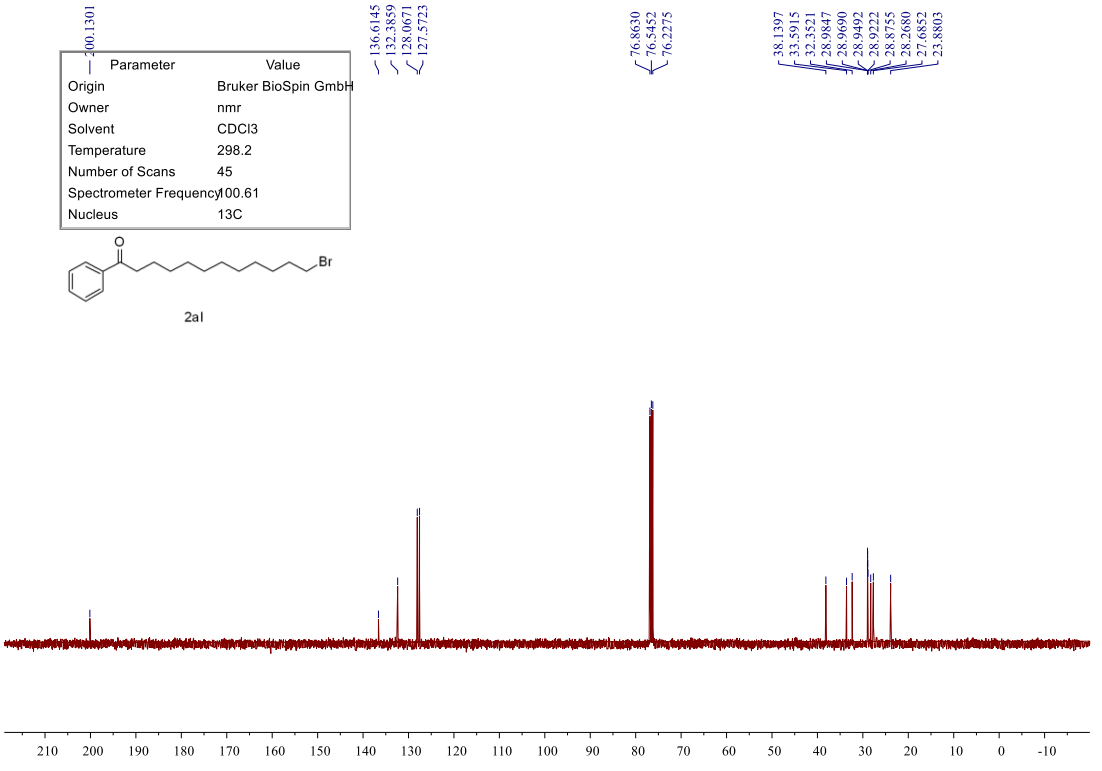
1.6950
1.4333
1.4154
1.3967
1.3788
1.3556
1.3422
1.3324
1.2818
1.95
1.00
1.93
1.94
1.98
1.91
2.00
14.02
10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5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Owner nmr
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Temperature 298.2
Number of Scans 45
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O
Br
2aI
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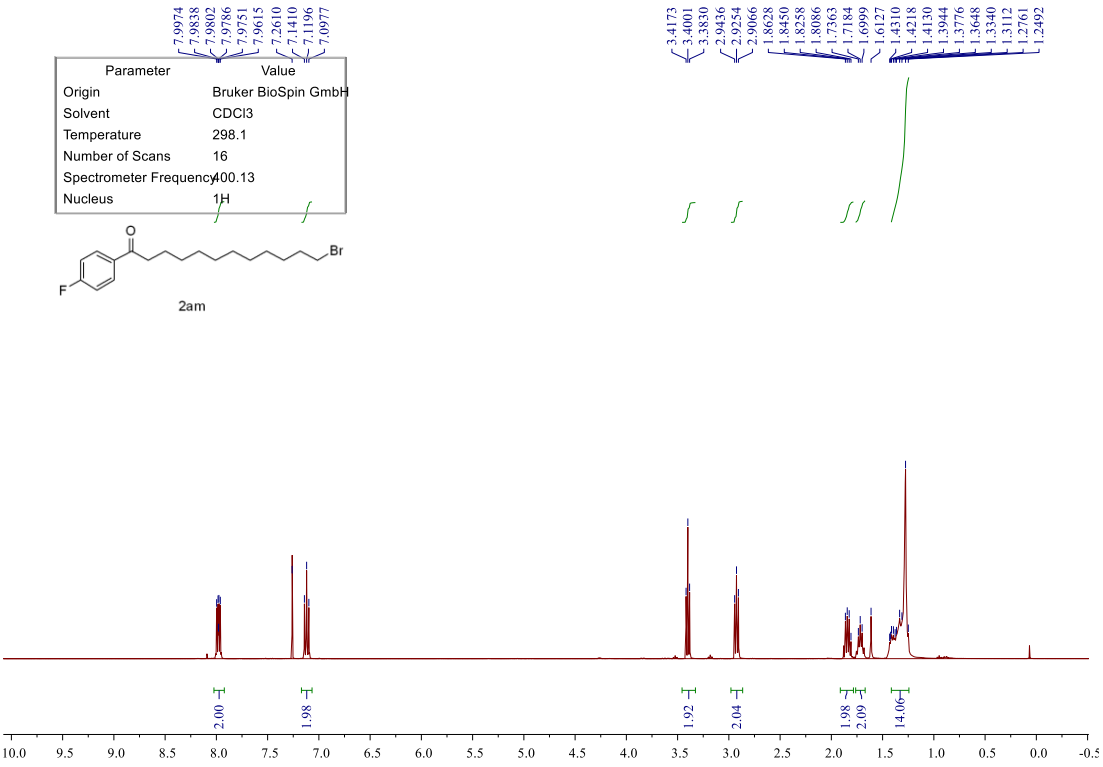
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Parameter Value
Origin Bruker BioSpin GmbH
Solvent CDCl3
Temperature 298.1
Number of Scans 16
Spectrometer Frequency 400.13
Nucleus 1H
O
Br
F
2am
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3.4001
3.3830
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2.9254
2.9066
1.8628
1.8450
1.8258
1.8086
1.7363
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1.6999
1.6127
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1.4218
1.4130
1.3944
1.3776
1.3648
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1.3112
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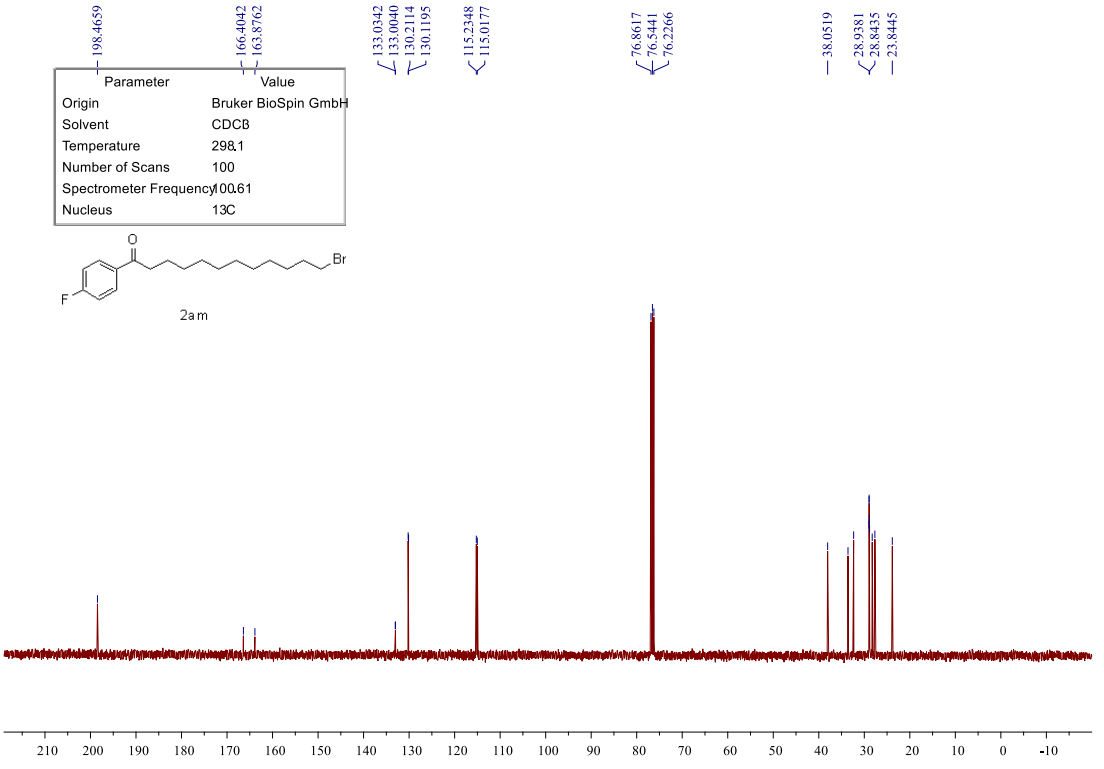
1.2492
2.00
1.98
1.92
2.04
1.98
2.09
14.06
10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5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76.2266
38.0519
28.9381
28.8435
23.8445
Parameter Value
Origin Bruker BioSpin GmbH
Solvent CDCl3
Temperature 298.1
Number of Scans 100
Spectrometer Frequency 100.61
Nucleus 13C
O
Br
F
2am
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10

Parameter	Value
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Solvent	CDCl3
Temperature	298.2
Number of Scans	16
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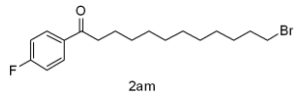
Nucleus	19F



2am

Parameter	Value
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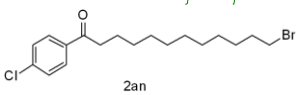
Solvent	CDCl3
Temperature	298.2
Number of Scans	4
Spectrometer Frequency	400.13
Nucleus	1H



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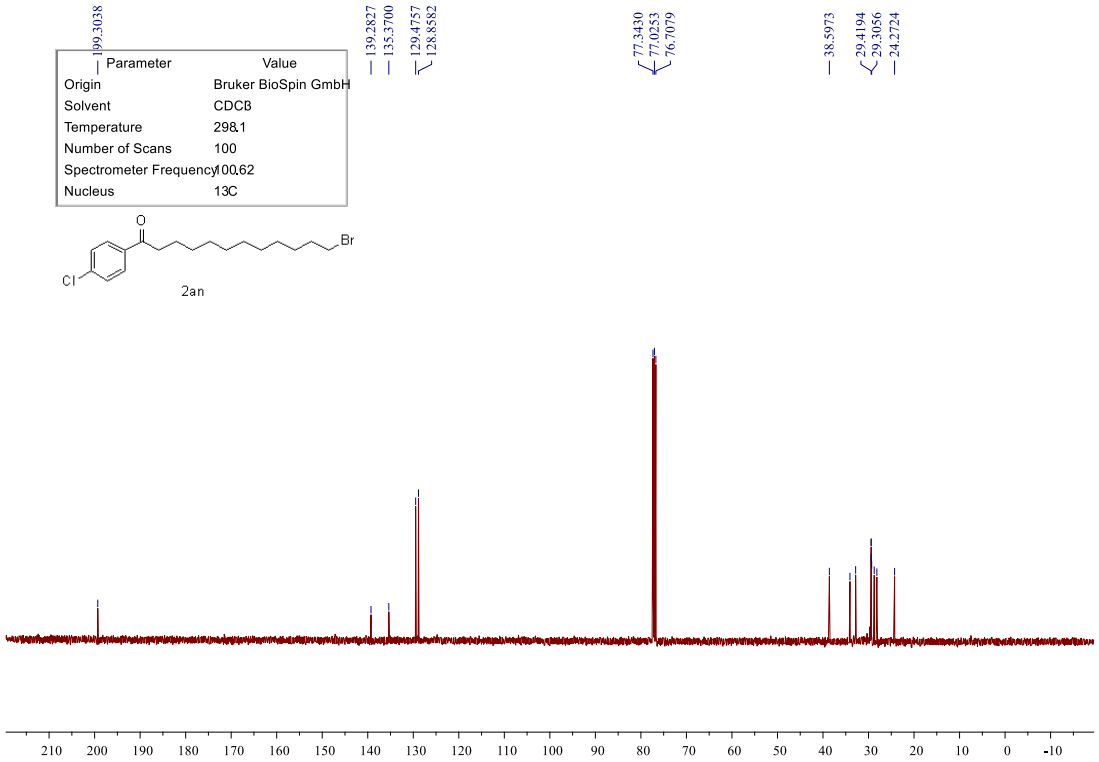
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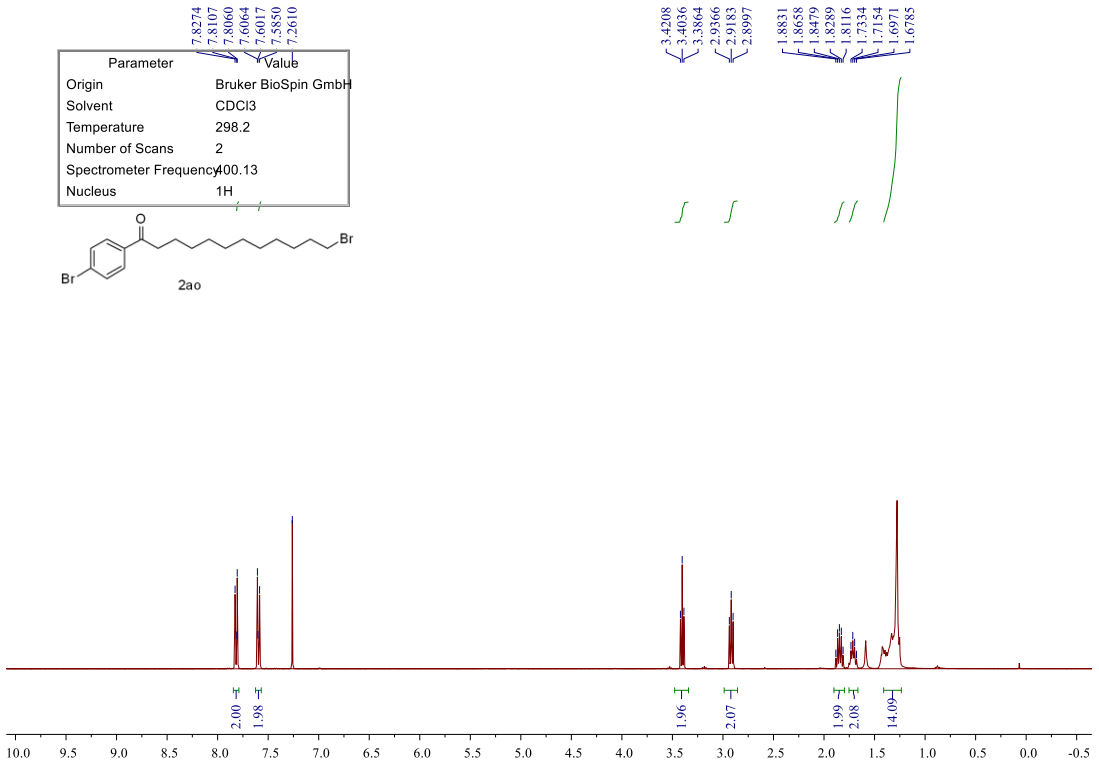
29.3056
24.2724
Parameter Value
Origin Bruker BioSpin GmbH
Solvent CDCl3
Temperature 298.1
Number of Scans 100
Spectrometer Frequency 100.62
Nucleus 13C
O
Br
Cl
2an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1.7334
1.7154
1.6971
1.6785
Parameter Value
Origin Bruker BioSpin GmbH
Solvent CDCl3
Temperature 298.2
Number of Scans 2
Spectrometer Frequency 400.13
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O
Br
Br
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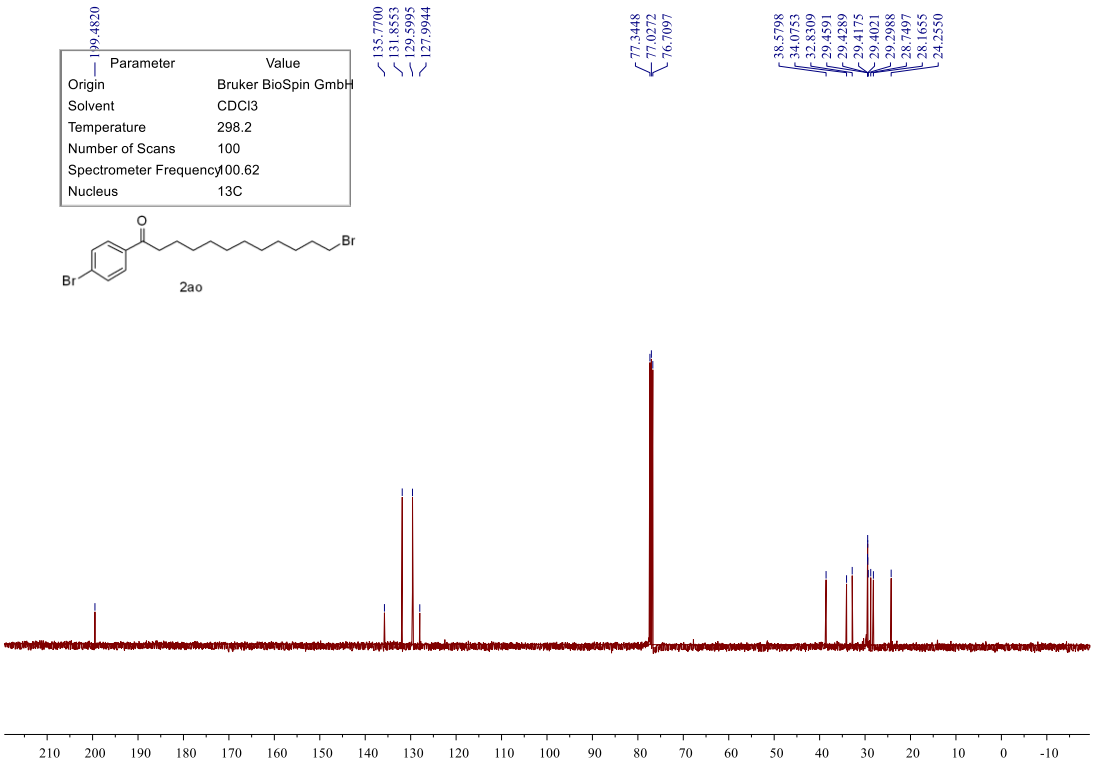
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29.4289
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29.4021
29.2988
28.7497
28.1655
24.2550
Parameter Value
Origin Bruker BioSpin GmbH
Solvent CDCl3
Temperature 298.2
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Spectrometer Frequency 100.62
Nucleus 13C
O
Br
Br
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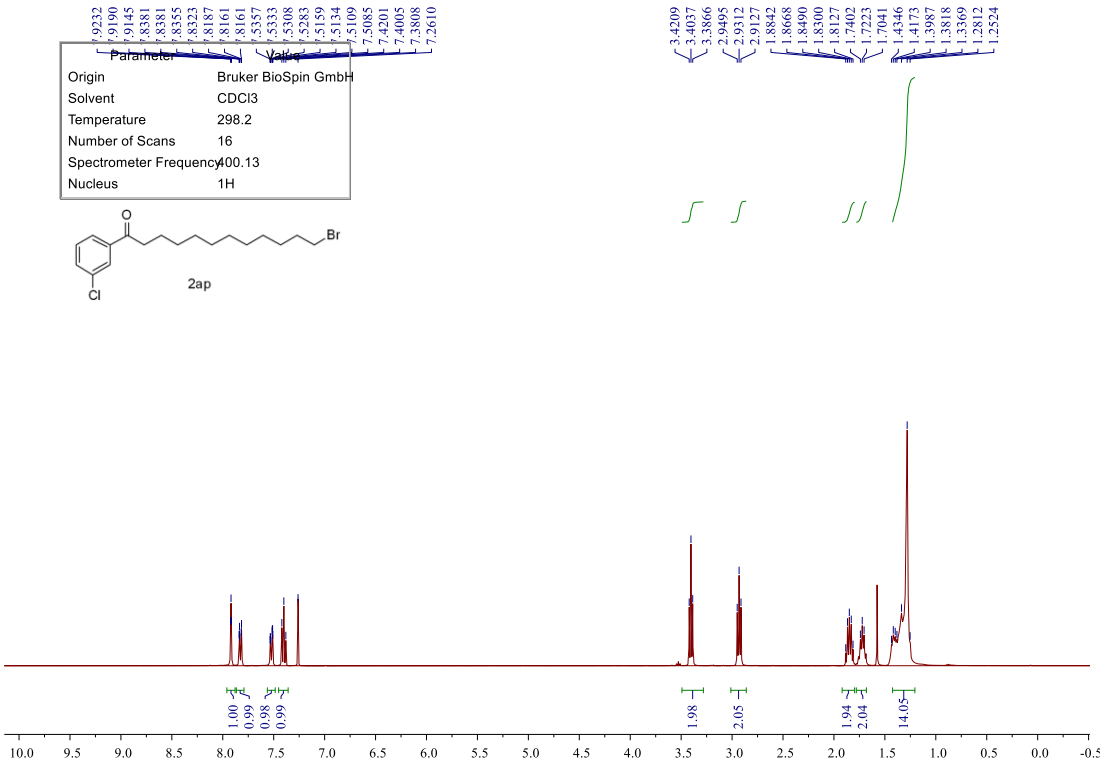
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1.3818
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1.2812
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Parameter Value
Origin Bruker BioSpin GmbH
Solvent CDCl3
Temperature 298.2
Number of Scans 16
Spectrometer Frequency 400.13
Nucleus 1H
O
Br
Cl
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0.98
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2.04
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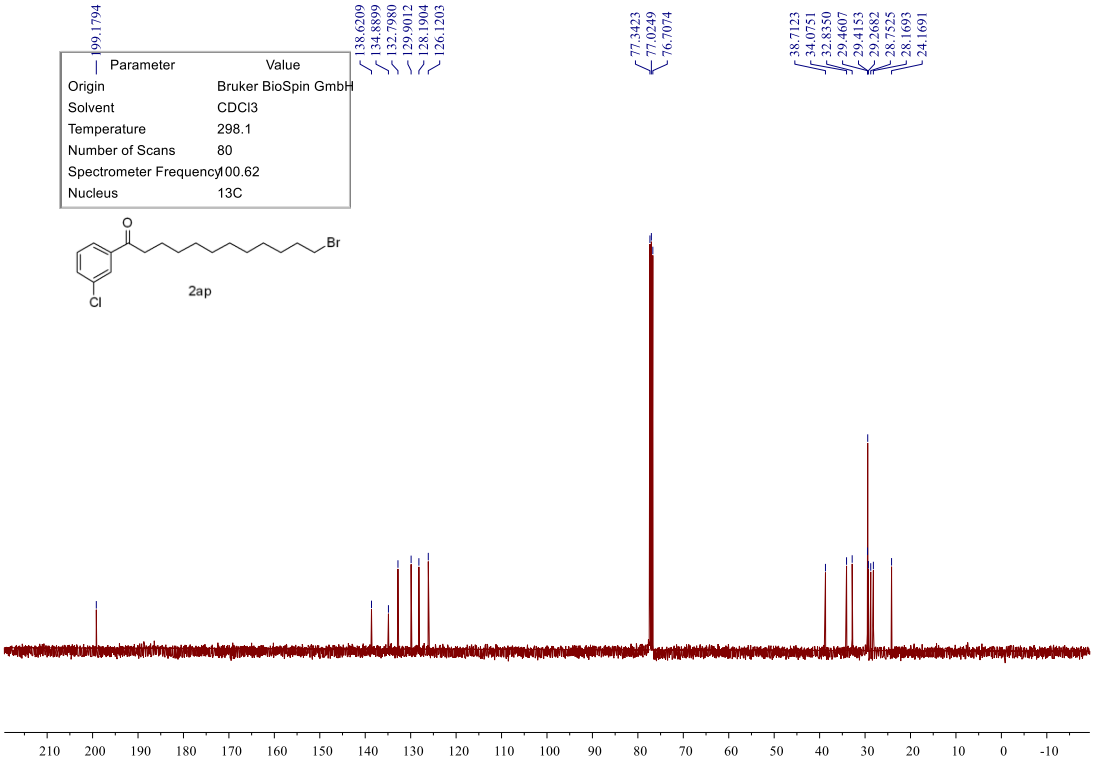
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29.4607
29.4153
29.2682
28.7525
28.1693
24.1691
Parameter Value
Origin Bruker BioSpin GmbH
Solvent CDCl3
Temperature 298.1
Number of Scans 80
Spectrometer Frequency 100.62
Nucleus 13C
O
Br
Cl
2ap
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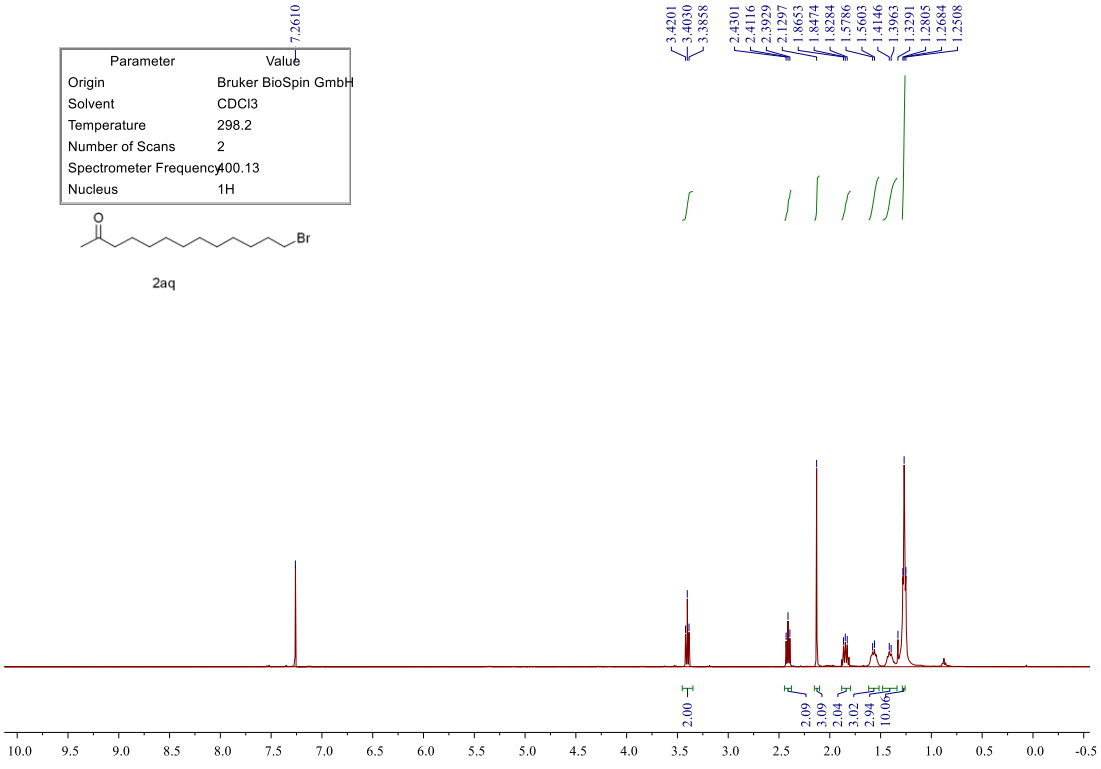
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1.5603
1.4146
1.3963
1.3291
1.2805
1.2684
1.2508
Parameter Value
Origin Bruker BioSpin GmbH
Solvent CDCl3
Temperature 298.2
Number of Scans 2
Spectrometer Frequency 400.13
Nucleus 1H
O
Br
2aq
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2.04
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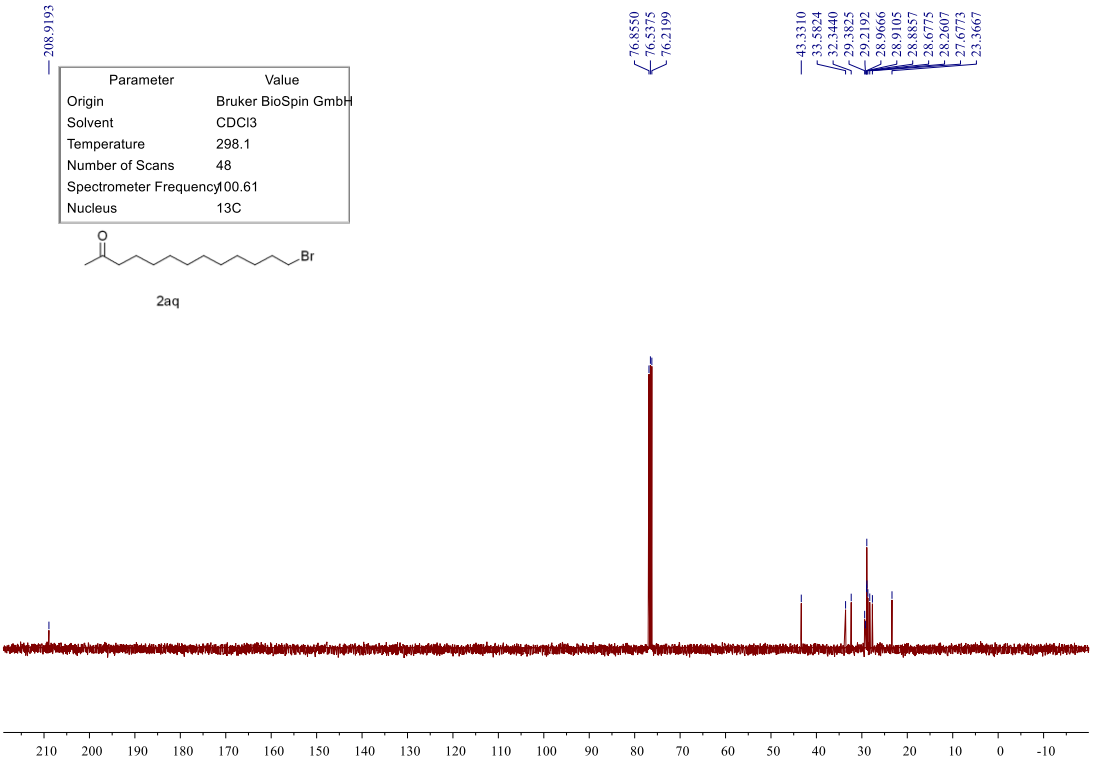
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Parameter Value
Origin Bruker BioSpin GmbH
Solvent CDCl3
Temperature 298.1
Number of Scans 48
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Br
2aq
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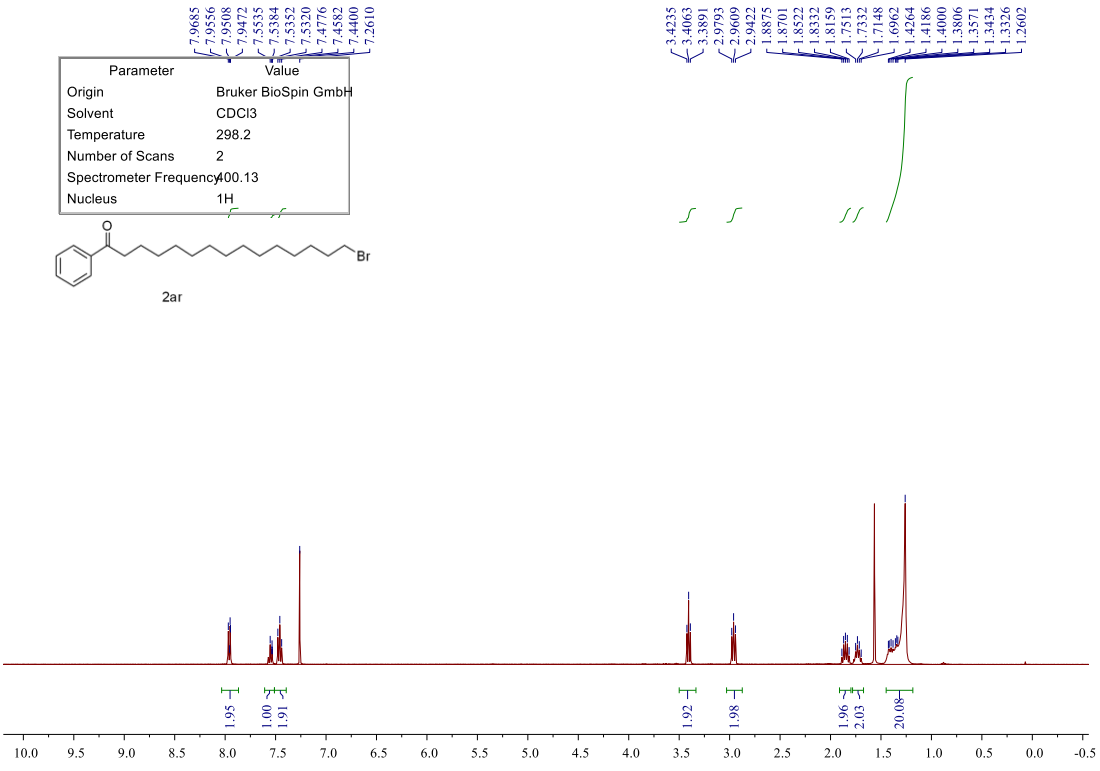
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Parameter Value
Origin Bruker BioSpin GmbH
Solvent CDCl3
Temperature 298.2
Number of Scans 2
Spectrometer Frequency 400.13
Nucleus 1H
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Br
2ar
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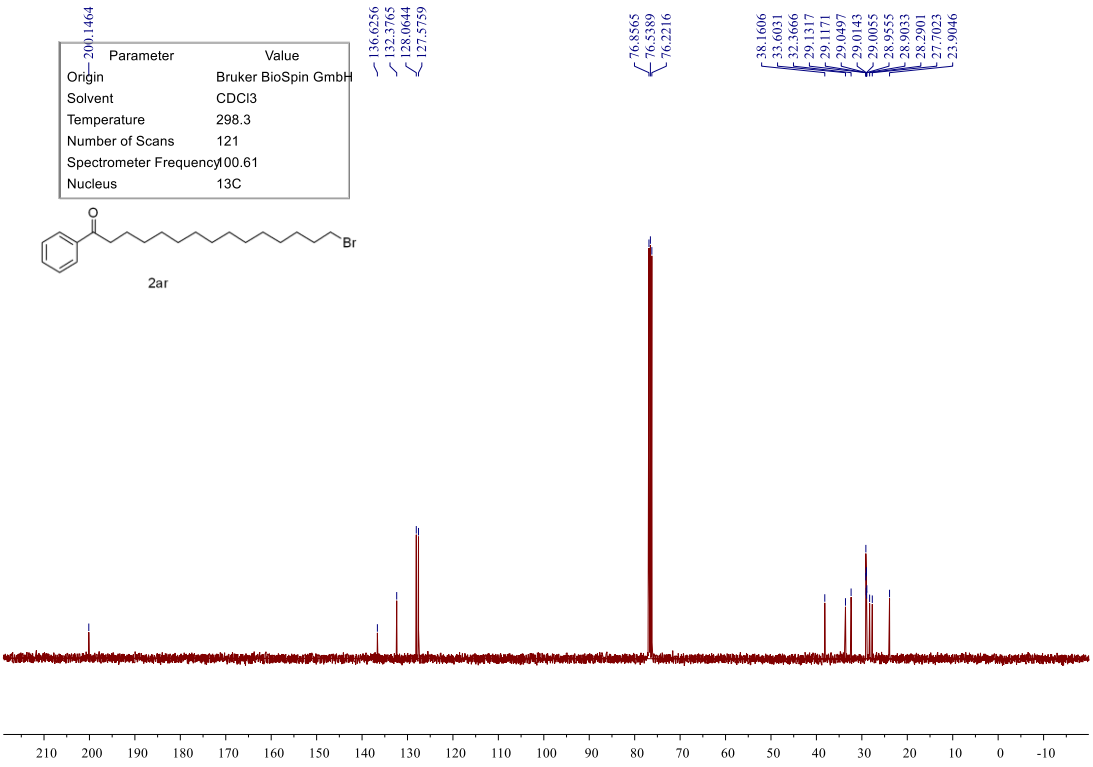
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Parameter Value
Origin Bruker BioSpin GmbH
Solvent CDCl3
Temperature 298.3
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Br
2ar
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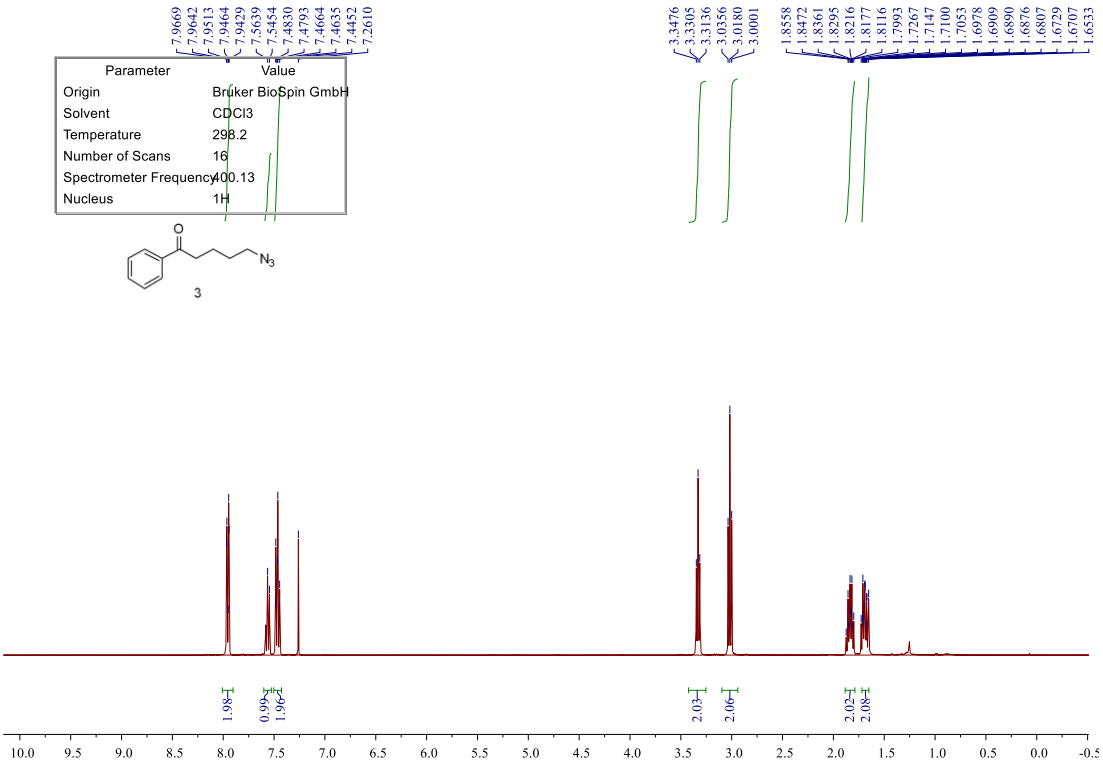
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Parameter Value
Origin Bruker BioSpin GmbH
Solvent CDCl3
Temperature 298.2
Number of Scans 16
Spectrometer Frequency 400.13
Nucleus 1H
O
N3
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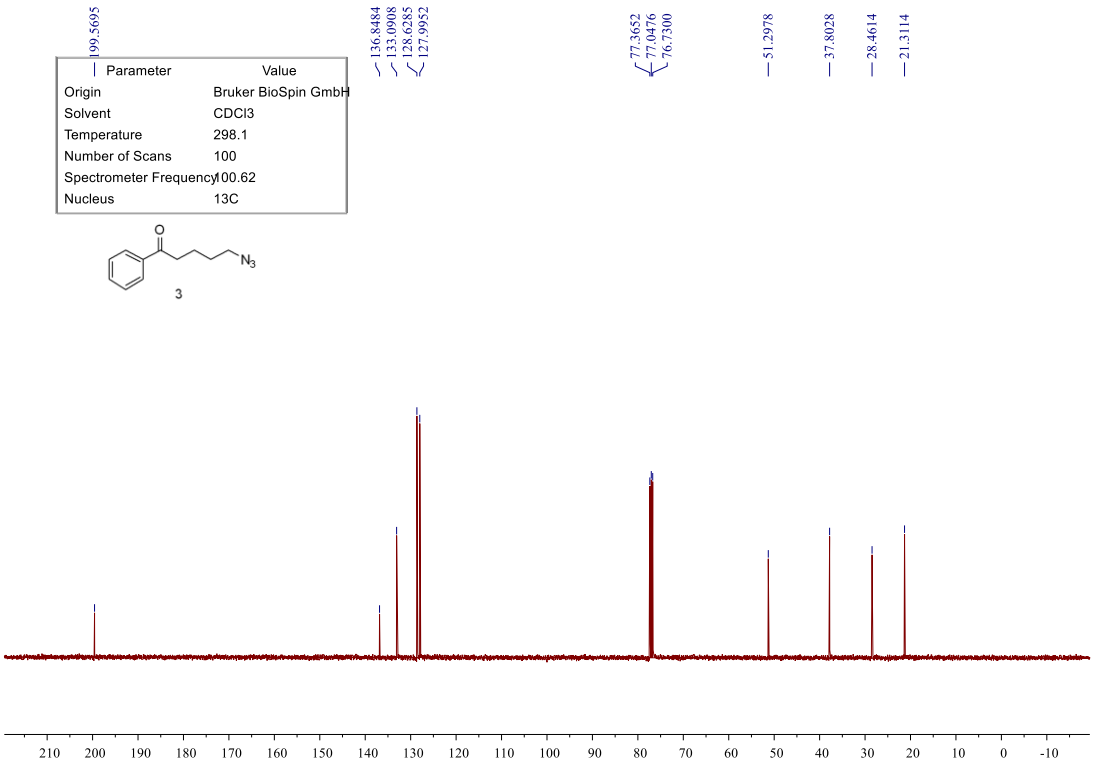
1.96
2.03
2.06
2.02
2.08
10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5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28.4614
21.3114
Parameter Value
Origin Bruker BioSpin GmbH
Solvent CDCl3
Temperature 298.1
Number of Scans 100
Spectrometer Frequency 100.62
Nucleus 13C
O
N3
3
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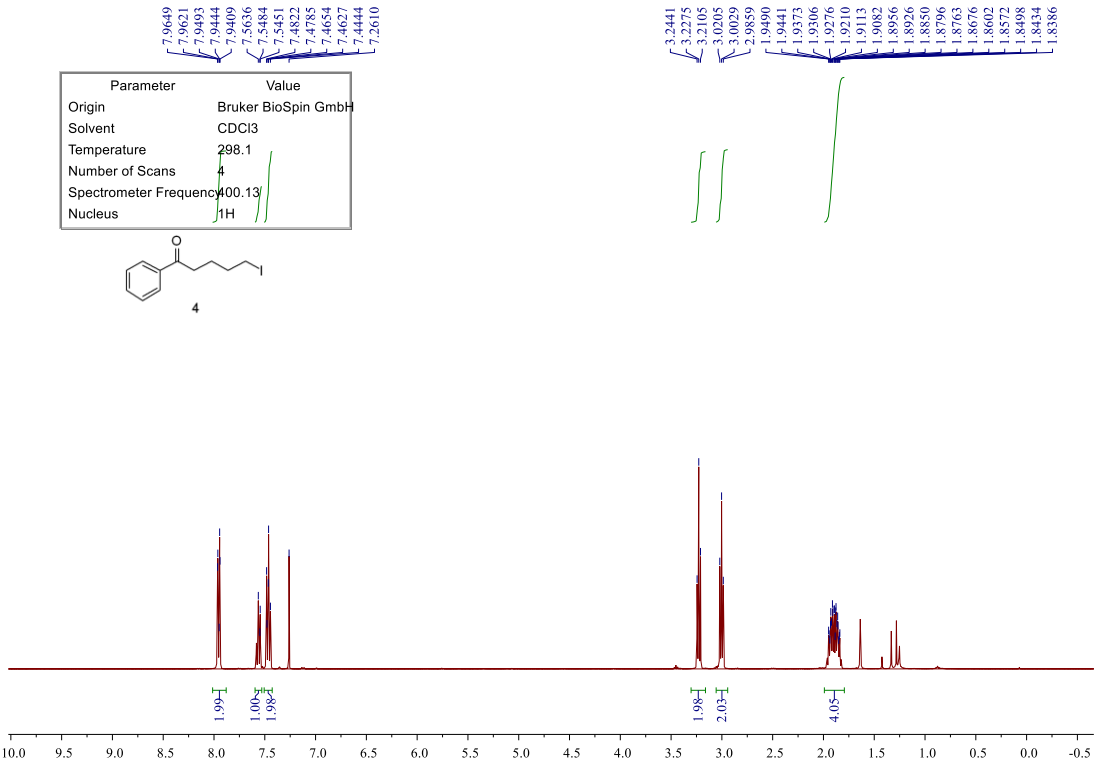
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3.2441
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3.2105
3.0205
3.0029
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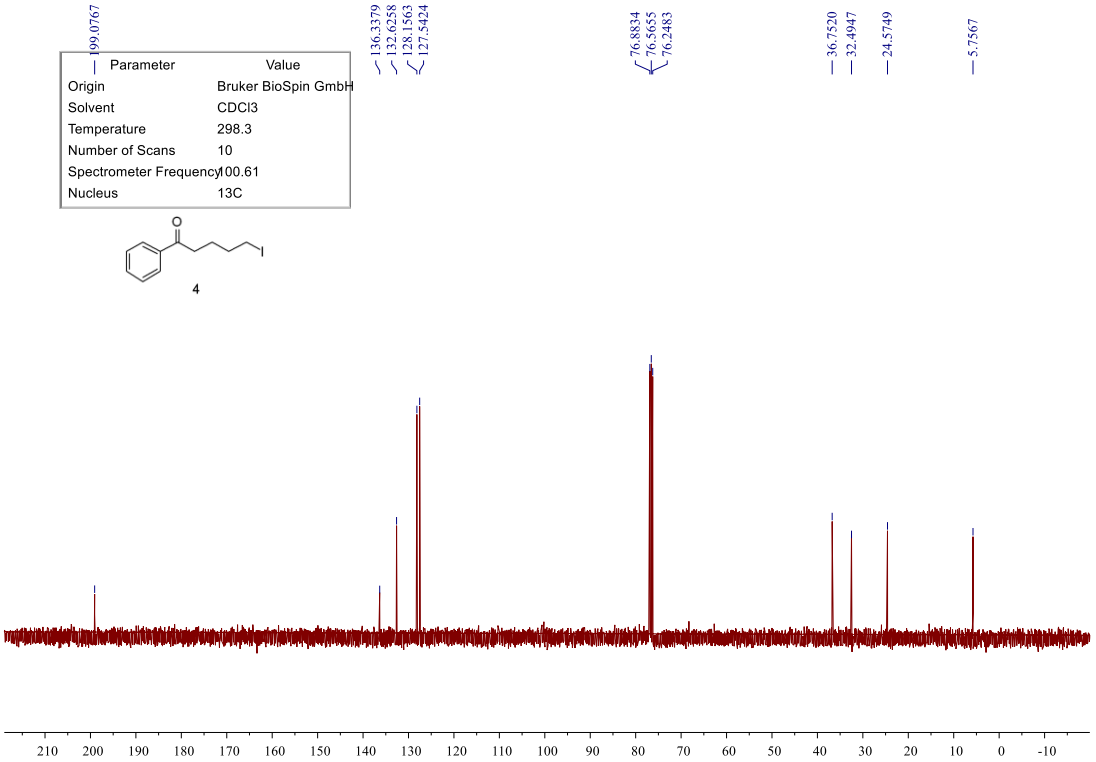
1.9306
1.9276
1.9210
1.9113
1.9082
1.8956
1.8926
1.8850
1.8796
1.8763
1.8676
1.8602
1.8572
1.8498
1.8434
1.8386
Parameter Value
Origin Bruker BioSpin GmbH
Solvent CDCl3
Temperature 298.1
Number of Scans 4
Spectrometer Frequency 400.13
Nucleus 1H
O
I
4
1.99
1.00
1.98
1.98
2.03
4.05
10.0 9.5 9.0 8.5 8.0 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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24.5749
5.7567
Parameter Value
Origin Bruker BioSpin GmbH
Solvent CDCl3
Temperature 298.3
Number of Scans 10
Spectrometer Frequency 100.61
Nucleus 13C
O
I
4
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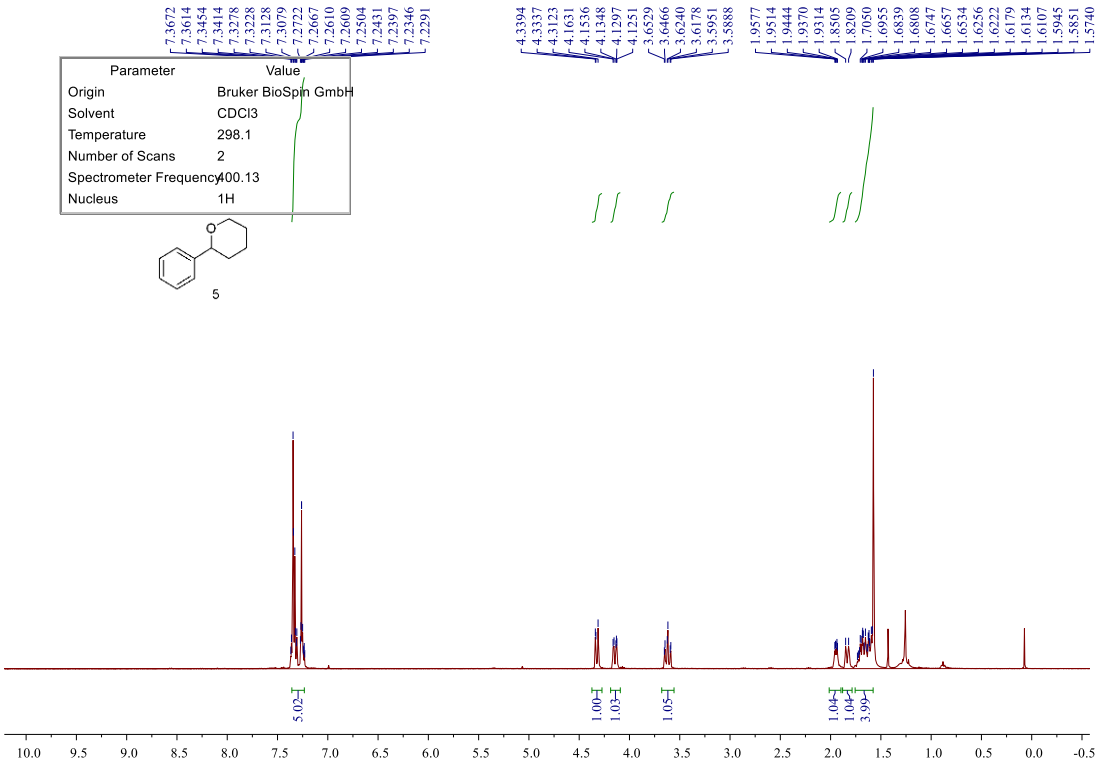
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7.2609
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7.2431
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7.2346
7.2291
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4.3123
4.1631
4.1536
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4.1297
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3.6178
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1.9514
1.9444
1.9370
1.9314
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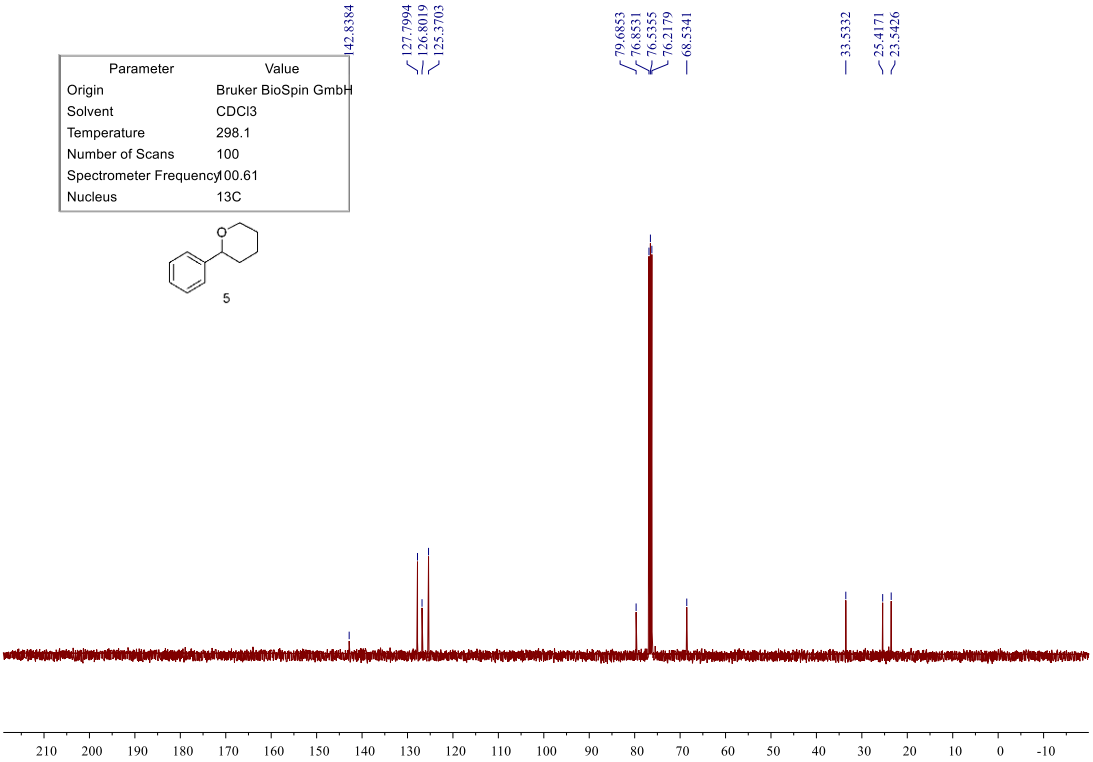
1.8209
1.7050
1.6955
1.6839
1.6808
1.6747
1.6657
1.6534
1.6256
1.6222
1.6179
1.6134
1.6107
1.5945
1.5851
1.5740
Parameter Value
Origin Bruker BioSpin GmbH
Solvent CDCl3
Temperature 298.1
Number of Scans 2
Spectrometer Frequency 400.13
Nucleus 1H
O
5
5.02
1.00
1.03
1.05
1.04
1.04
3.99
10.0 9.5 9.0 8.5 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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76.5355
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23.5426
Parameter Value
Origin Bruker BioSpin GmbH
Solvent CDCl3
Temperature 298.1
Number of Scans 100
Spectrometer Frequency 100.61
Nucleus 13C
5
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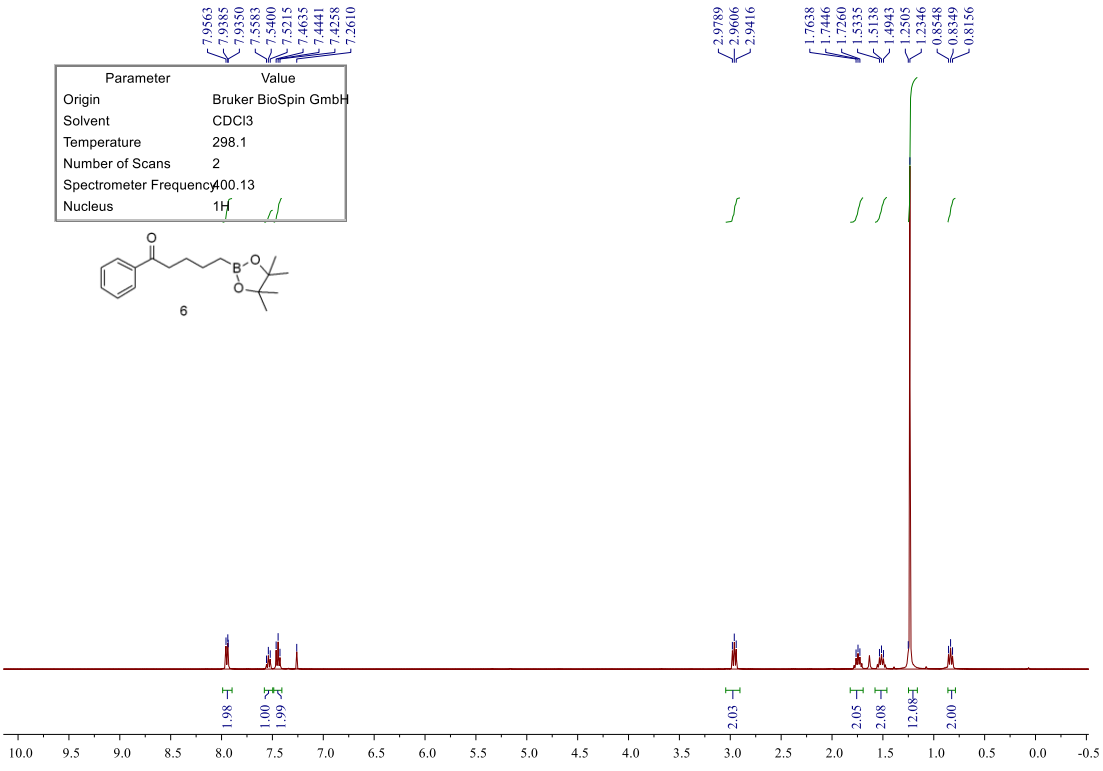
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2.9606
2.9416
1.7638
1.7446
1.7260
1.5335
1.5138
1.4943
1.2505
1.2346
0.8548
0.8349
0.8156
Parameter Value
Origin Bruker BioSpin GmbH
Solvent CDCl3
Temperature 298.1
Number of Scans 2
Spectrometer Frequency 400.13
Nucleus 1H
6
1.98
1.00
1.99
2.03
2.05
2.08
12.08
2.00
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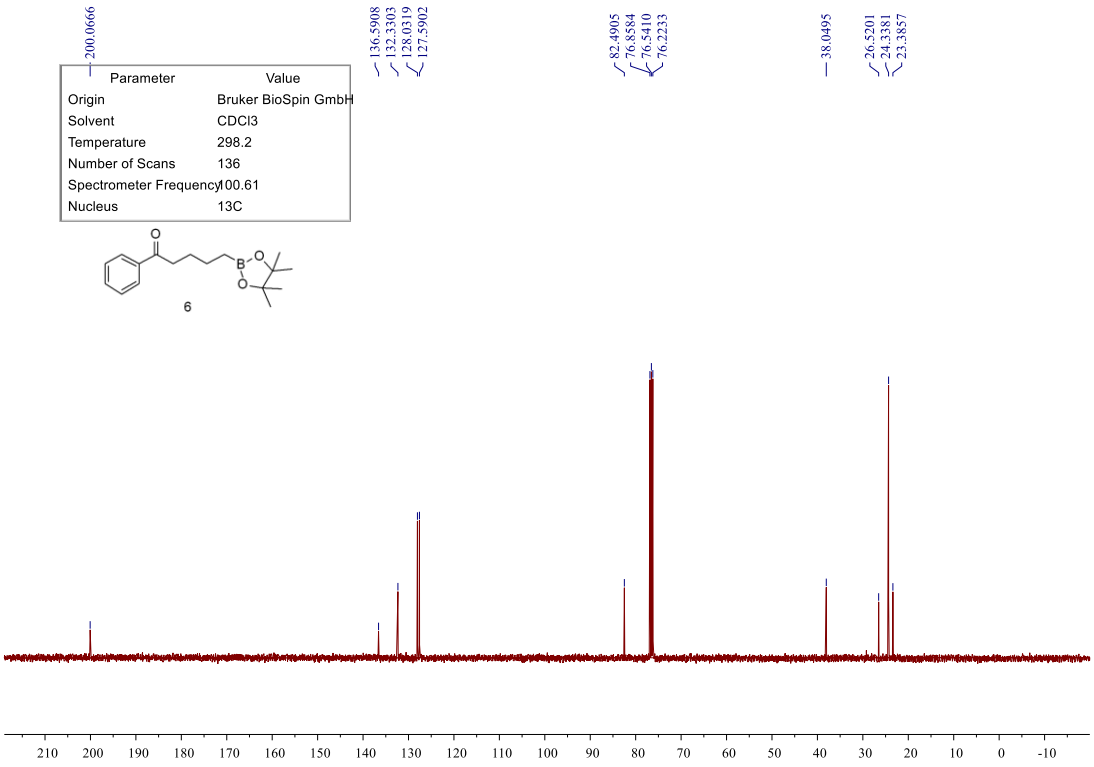
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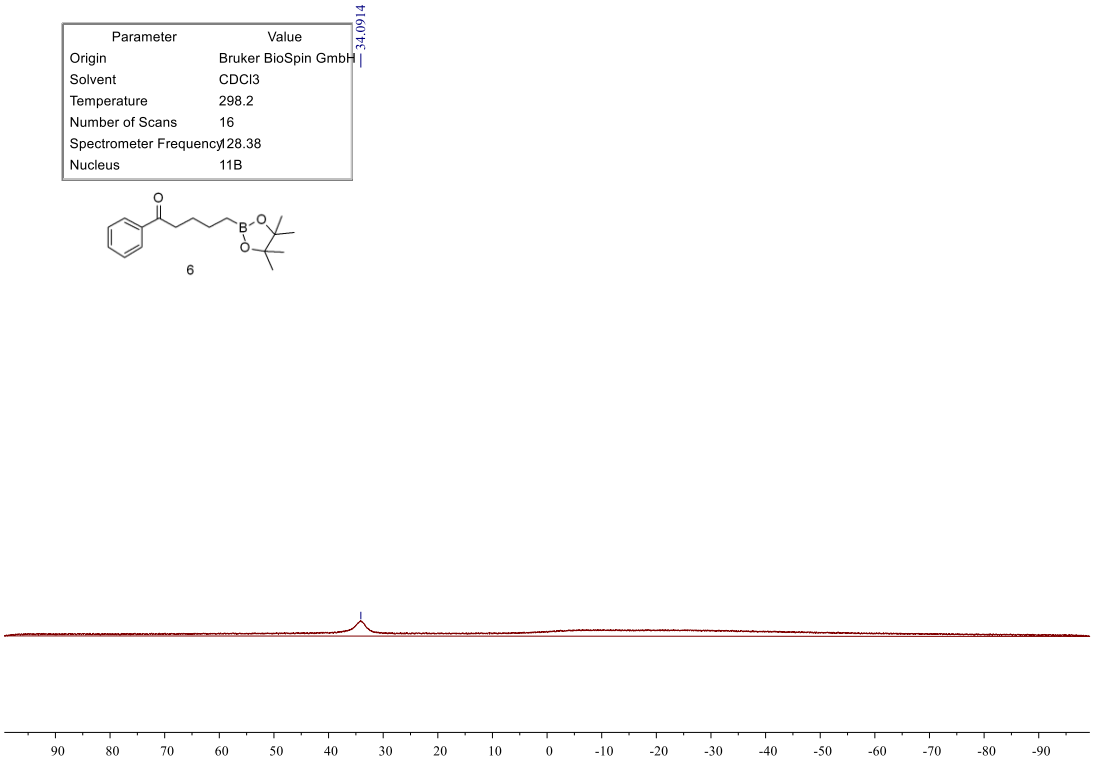
26.5201
24.3381
23.3857
Parameter Value
Origin Bruker BioSpin GmbH
Solvent CDCl3
Temperature 298.2
Number of Scans 136
Spectrometer Frequency 100.61
Nucleus 13C
O
B
O
O
6
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10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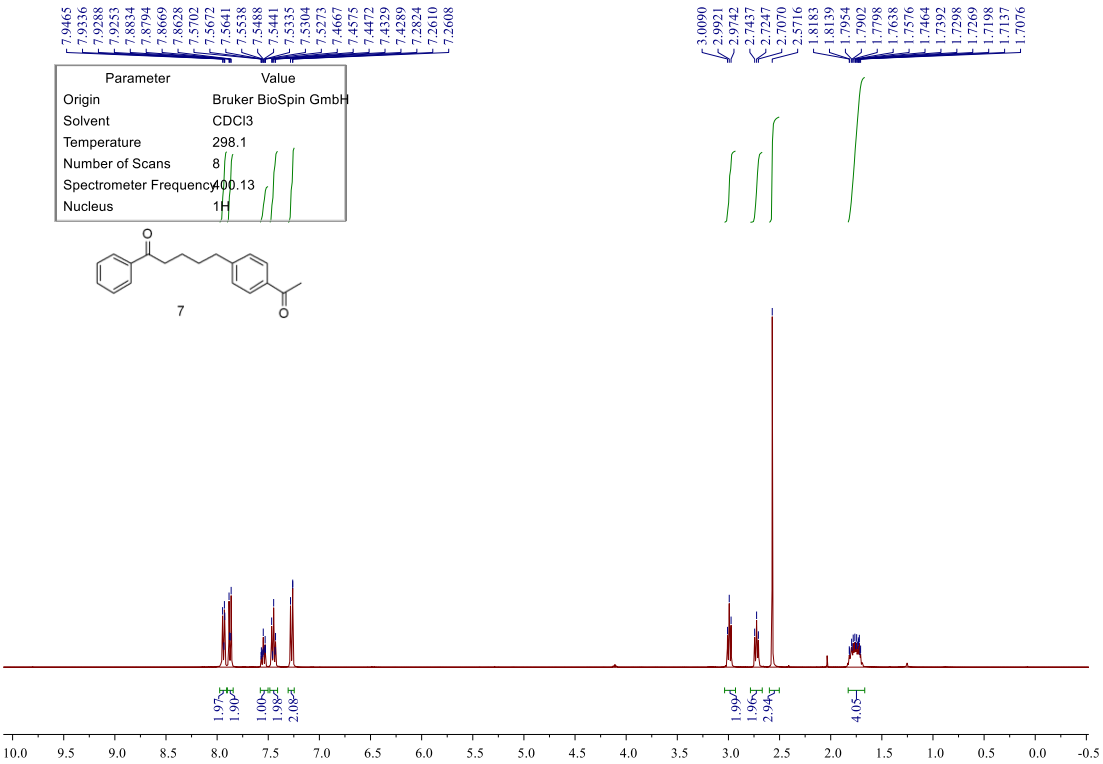
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7.5538
7.5488
7.5441
7.5335
7.5304
7.5273
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7.4575
7.4472
7.4329
7.4289
7.2824
7.2610
7.2608
3.0090
2.9921
2.9742
2.7437
2.7247
2.7070
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1.8139
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1.7576
1.7464
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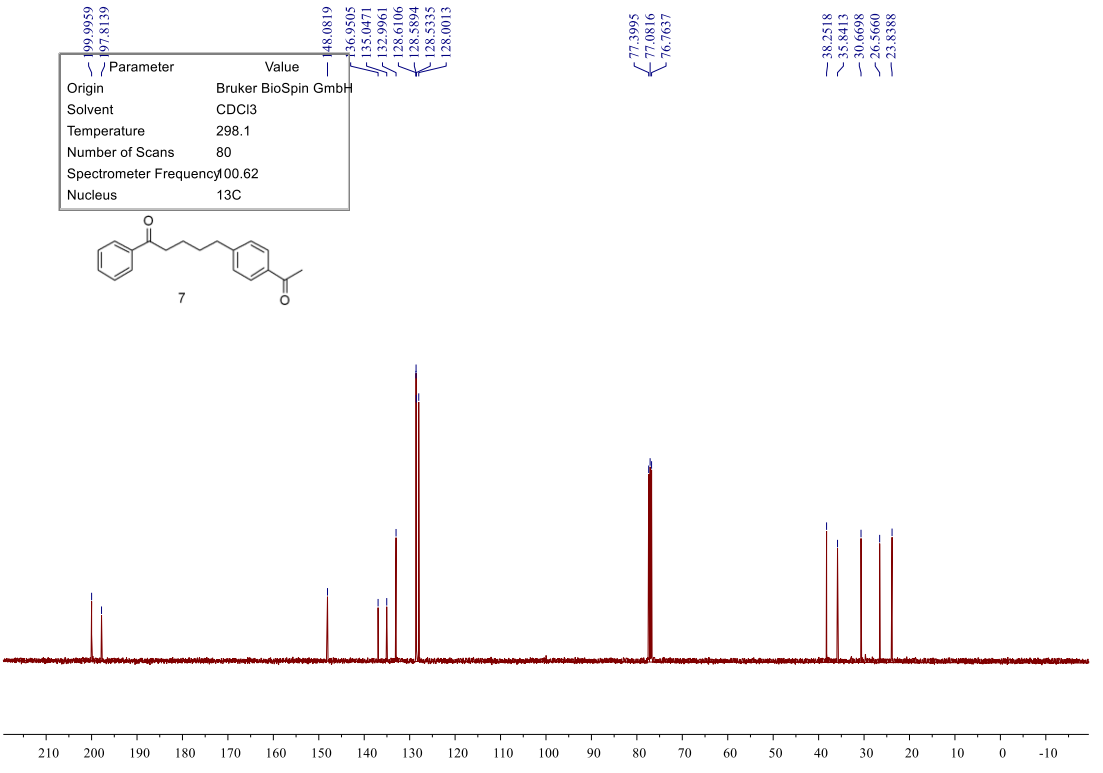
1.7298
1.7269
1.7198
1.7137
1.7076
Parameter Value
Origin Bruker BioSpin GmbH
Solvent CDCl3
Temperature 298.1
Number of Scans 8
Spectrometer Frequency 400.13
Nucleus 1H
O
O
7
1.97
1.90
1.00
1.98
2.08
1.99
1.96
2.94
4.05
10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5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77.0816
76.7637
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35.8413
30.6698
26.5660
23.8388
Parameter Value
Origin Bruker BioSpin GmbH
Solvent CDCl3
Temperature 298.1
Number of Scans 80
Spectrometer Frequency 100.62
Nucleus 13C
O
O
7
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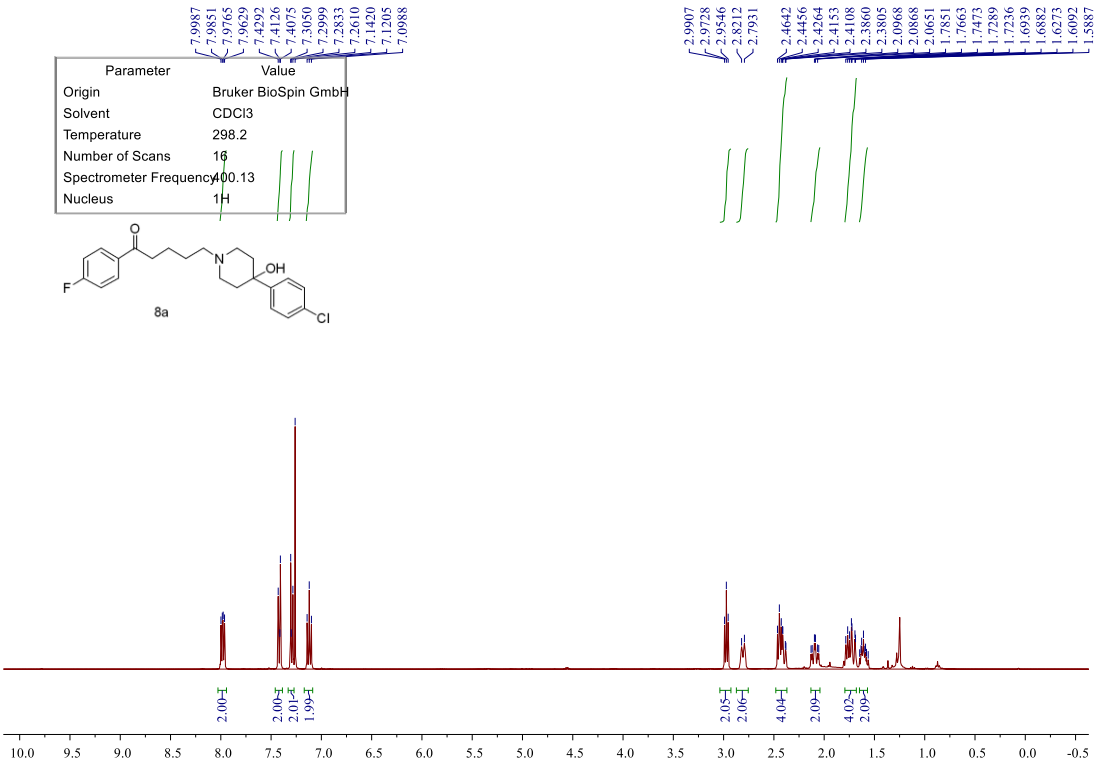
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2.4153
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2.3860
2.3805
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2.0868
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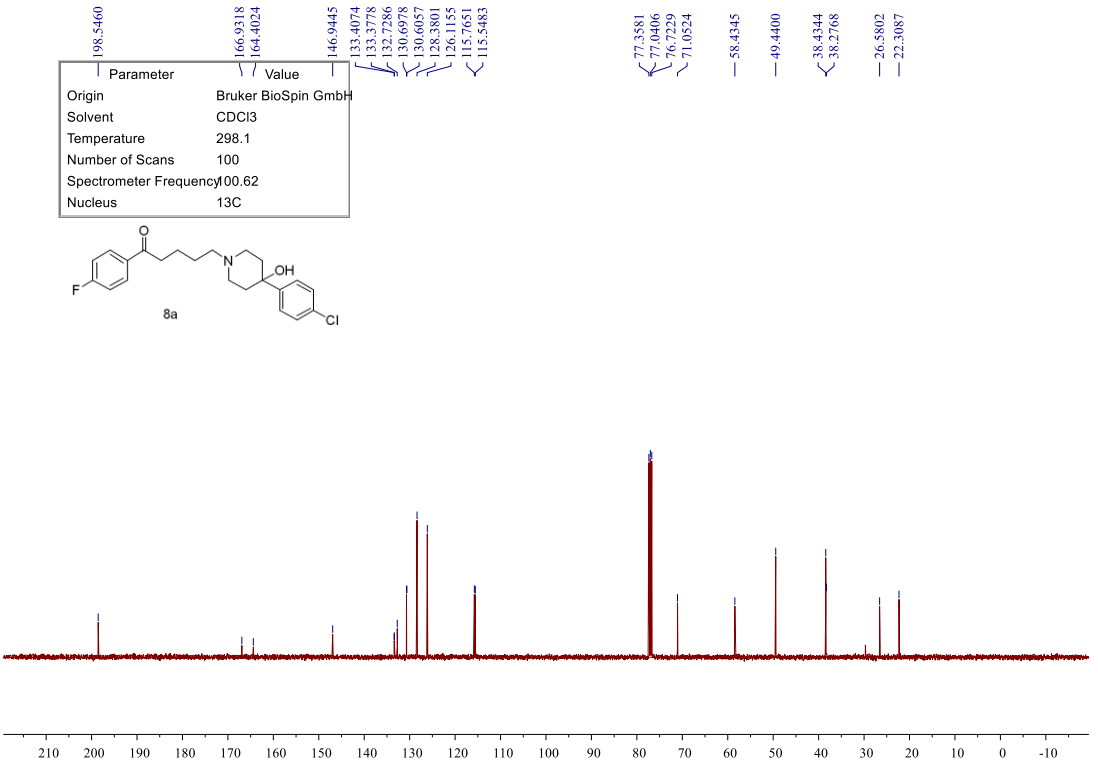
1.7851
1.7663
1.7473
1.7289
1.7236
1.6939
1.6882
1.6273
1.6092
1.5887
Parameter Value
Origin Bruker BioSpin GmbH
Solvent CDCl3
Temperature 298.2
Number of Scans 16
Spectrometer Frequency 400.13
Nucleus 1H
O
N
OH
F
Cl
8a
2.00
2.00
2.01
1.99
2.05
2.06
4.04
2.09
4.02
2.09
10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5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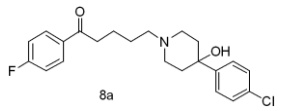
115.7651
115.5483
77.3581
77.0406
76.7229
71.0524
58.4345
49.4400
38.4344
38.2768
26.5802
22.3087
Parameter Value
Origin Bruker BioSpin GmbH
Solvent CDCl3
Temperature 298.1
Number of Scans 100
Spectrometer Frequency 100.62
Nucleus 13C
O
N
OH
F
Cl
8a
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10

Parameter	Value
Origin	Bruker BioSpin GmbH
Solvent	CDCl3
Temperature	298.2
Number of Scans	2
Spectrometer Frequency	376.50
Nucleus	19F



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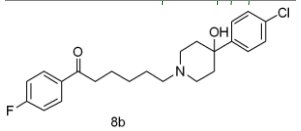
Parameter	Value
Origin	Bruker BioSpin GmbH
Solvent	CDCl3
Temperature	298.1
Number of Scans	2
Spectrometer Frequency	400.13
Nucleus	1H



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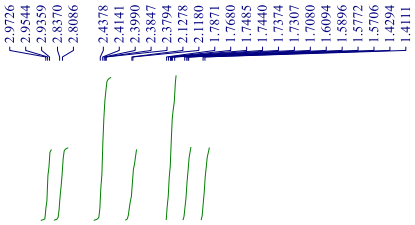

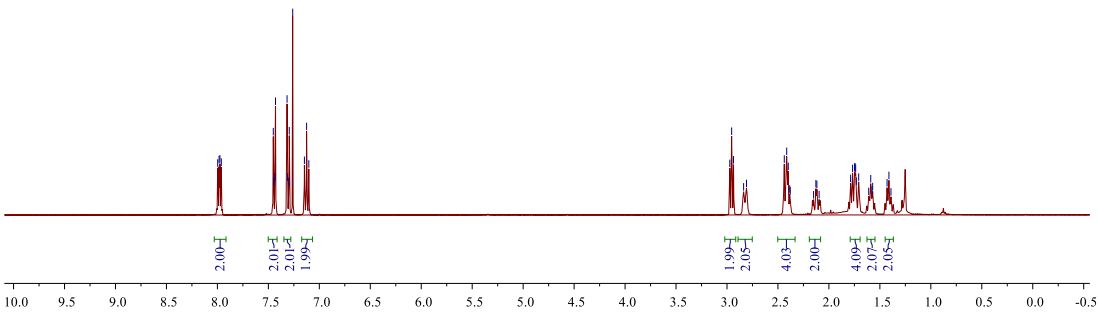

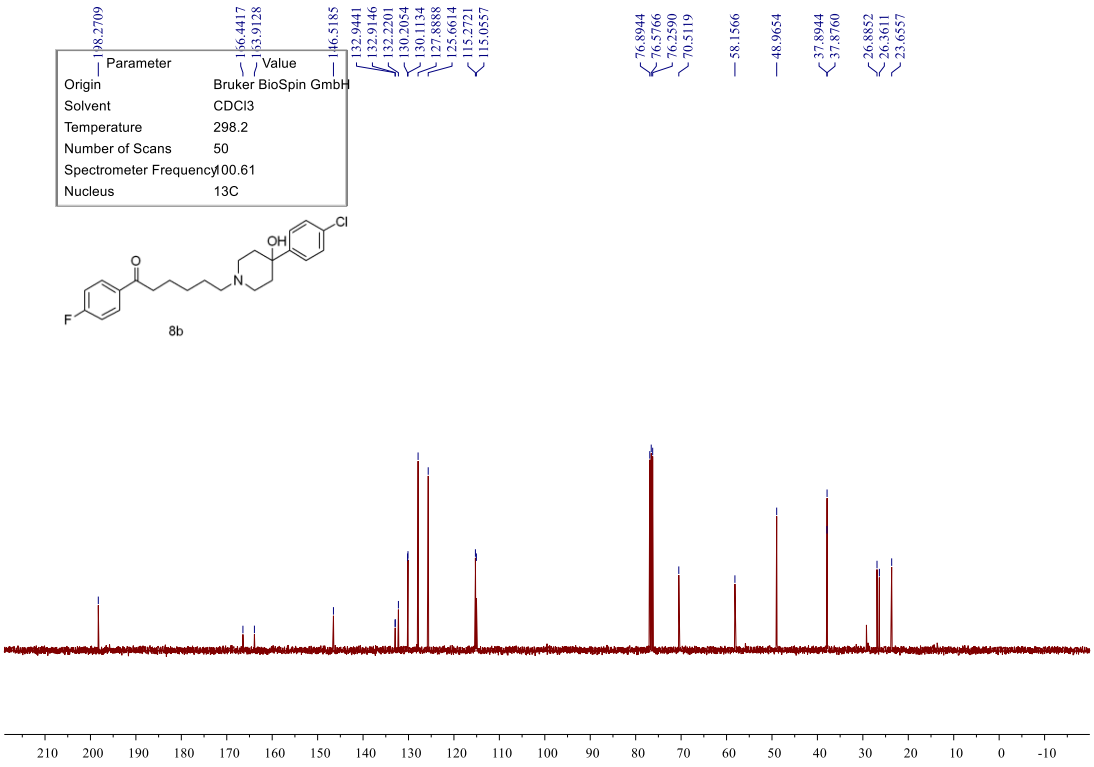
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115.2721
115.0557
76.8944
76.5766
76.2590
70.5119
58.1566
48.9654
37.8944
37.8760
26.8852
26.3611
23.6557
Parameter Value
Origin Bruker BioSpin GmbH
Solvent CDCl3
Temperature 298.2
Number of Scans 50
Spectrometer Frequency 100.61
Nucleus 13C
OH
Cl
O
N
F
8b
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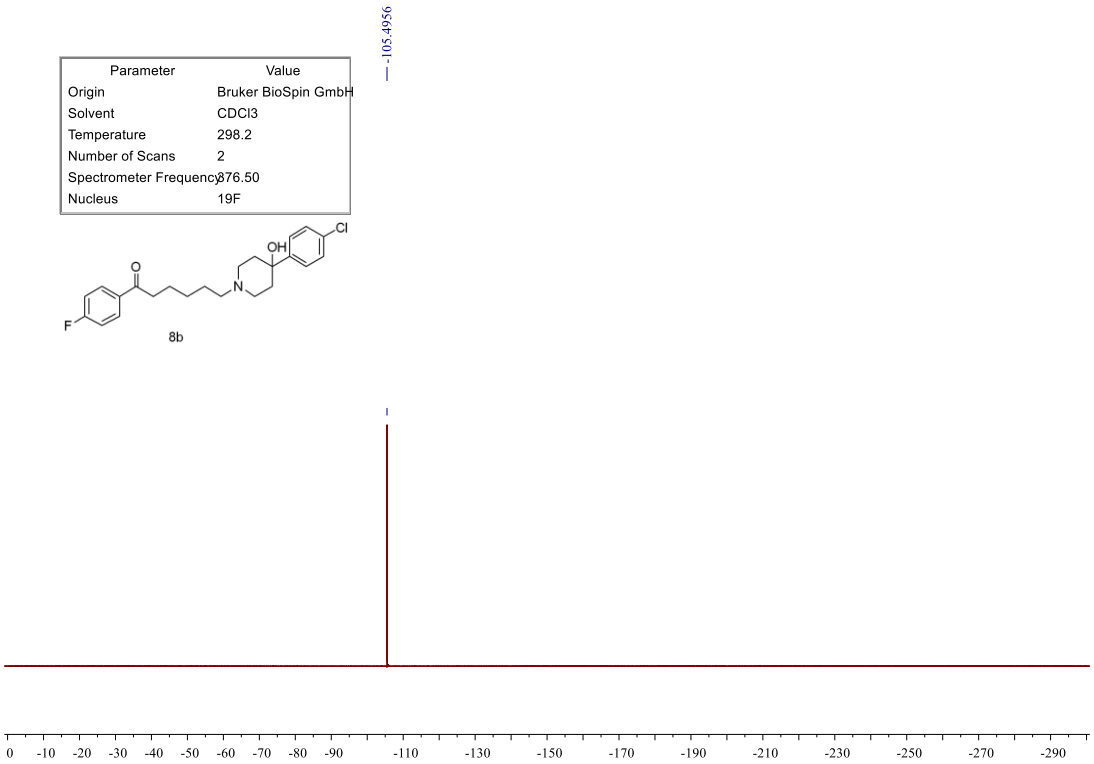
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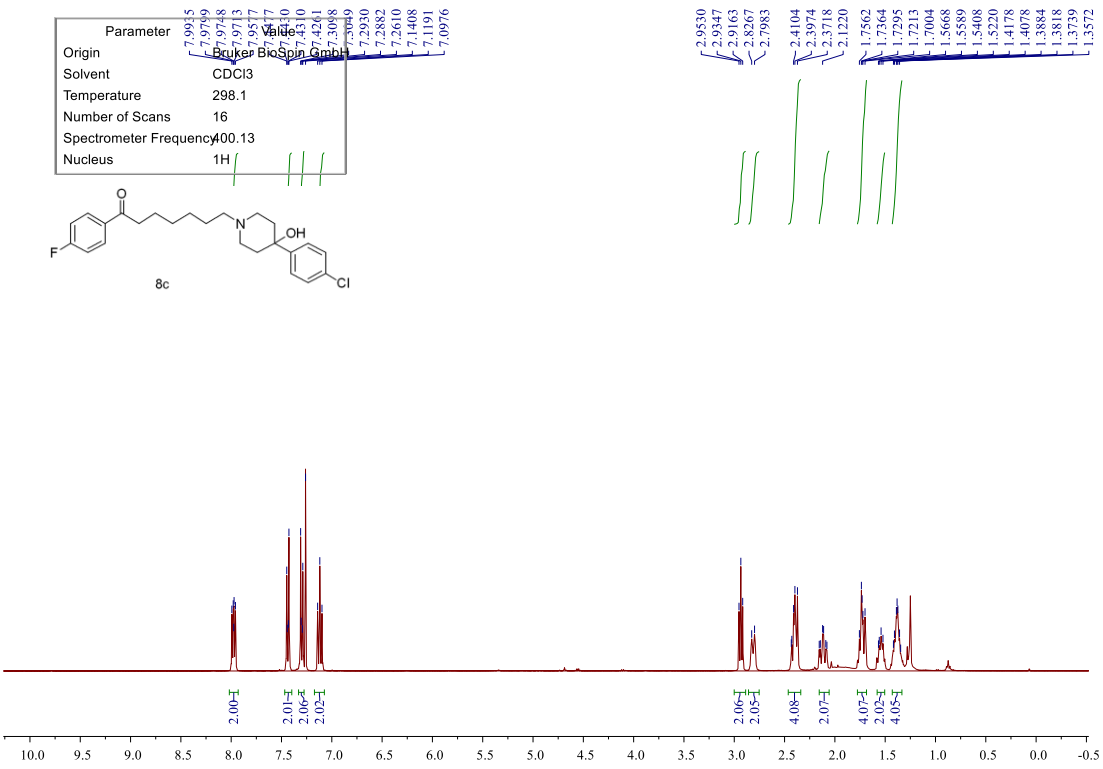
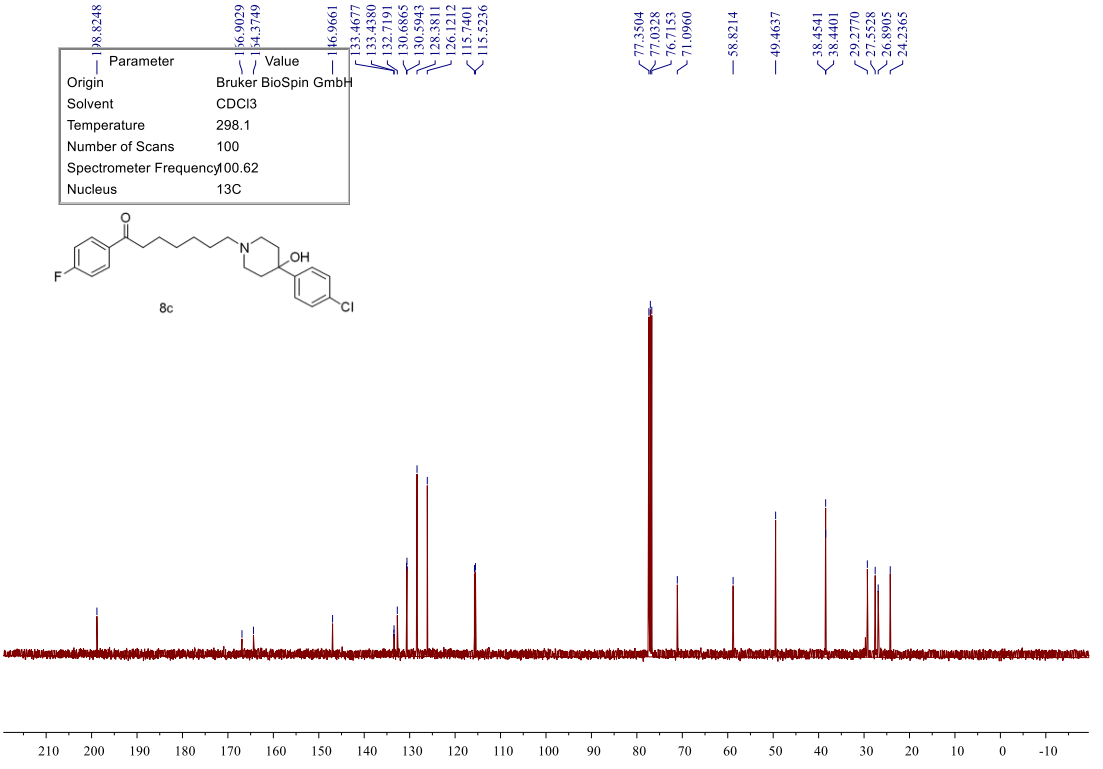
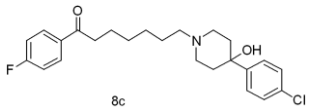
Parameter Value
Origin Bruker BioSpin GmbH
Solvent CDCl3
Temperature 298.2
Number of Scans 2
Spectrometer Frequency 376.50
Nucleus 19F
OH
Cl
O
N
F
8b
0 -10 -20 -30 -40 -50 -60 -70 -80 -90 -110 -130 -150 -170 -190 -210 -230 -250 -270 -290


Parameter Value
Origin Bruker BioSpin GmbH
Solvent CDCl3
Temperature 298.1
Number of Scans 16
Spectrometer Frequency 400.13
Nucleus 1H
8c


Parameter Value
Origin Bruker BioSpin GmbH
Solvent CDCl3
Temperature 298.1
Number of Scans 100
Spectrometer Frequency 100.62
Nucleus 13C
8c

Parameter	Value
Origin	Bruker BioSpin GmbH
Solvent	CDCl3
Temperature	298.2
Number of Scans	8
Spectrometer Frequency	376.50
Nucleus	19F



8c

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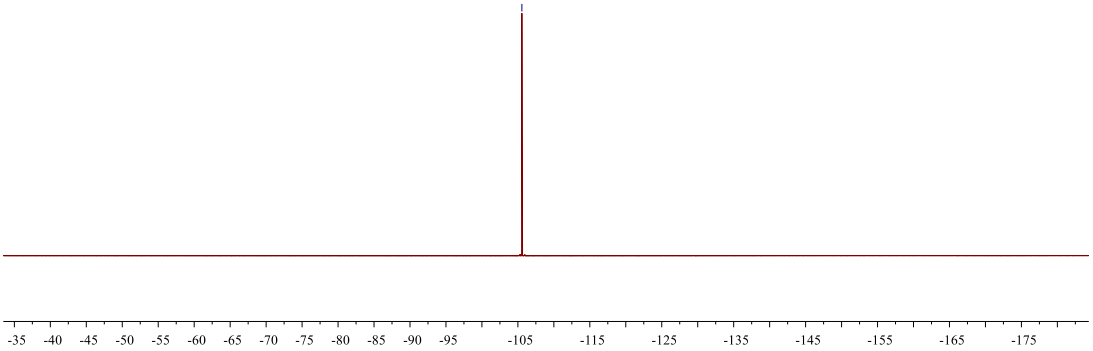

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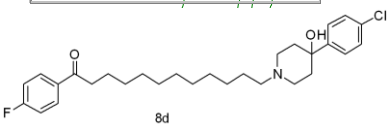
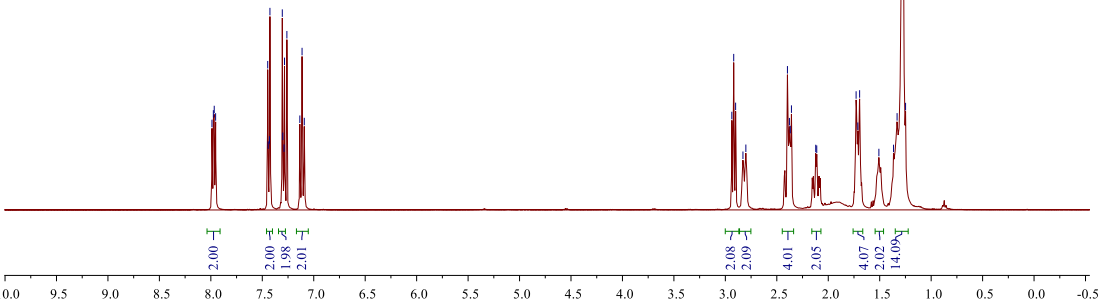
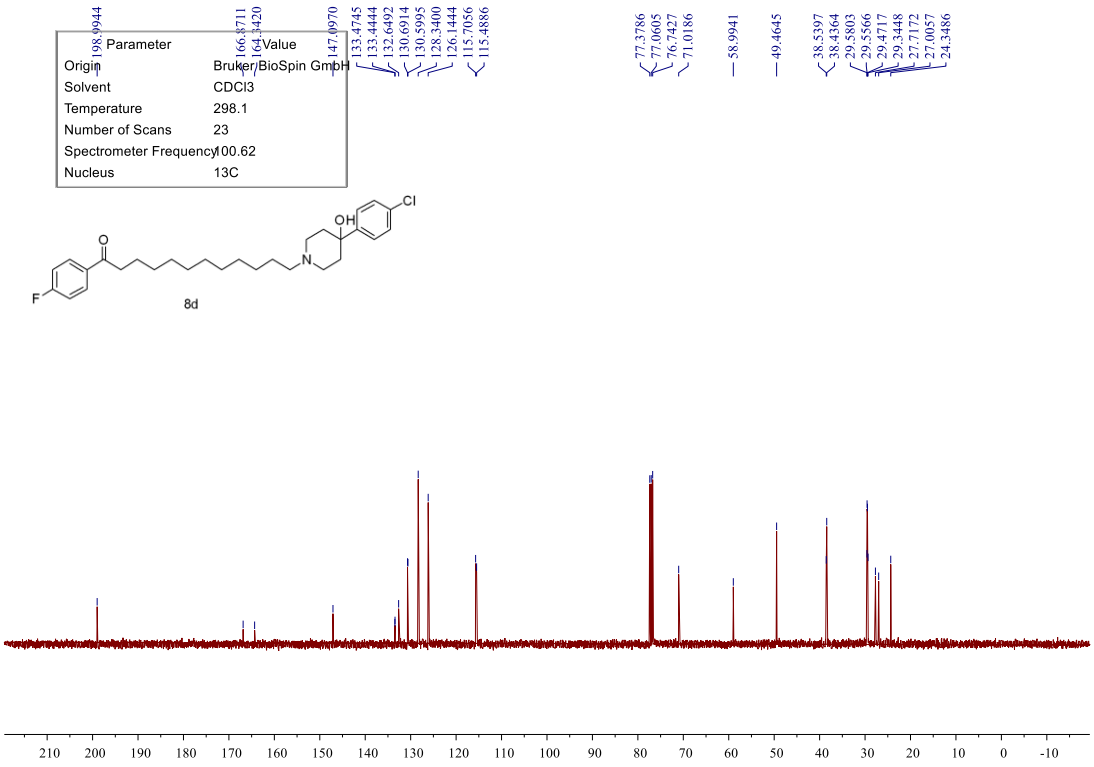
2.9372 2.9188 2.9002 2.8291 2.8007 2.3966 2.3773 2.3691 1.7127 1.6952 1.5080 1.3657 1.3312 1.2778 1.2486

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



8d

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38.4364
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29.4717
29.3448
27.7172
27.0057
24.3486
Parameter Value
Origin Bruker/BioSpin GmbH
Solvent CDCl3
Temperature 298.1
Number of Scans 23
Spectrometer Frequency 100.62
Nucleus 13C
Cl
OH
O
N
F
8d
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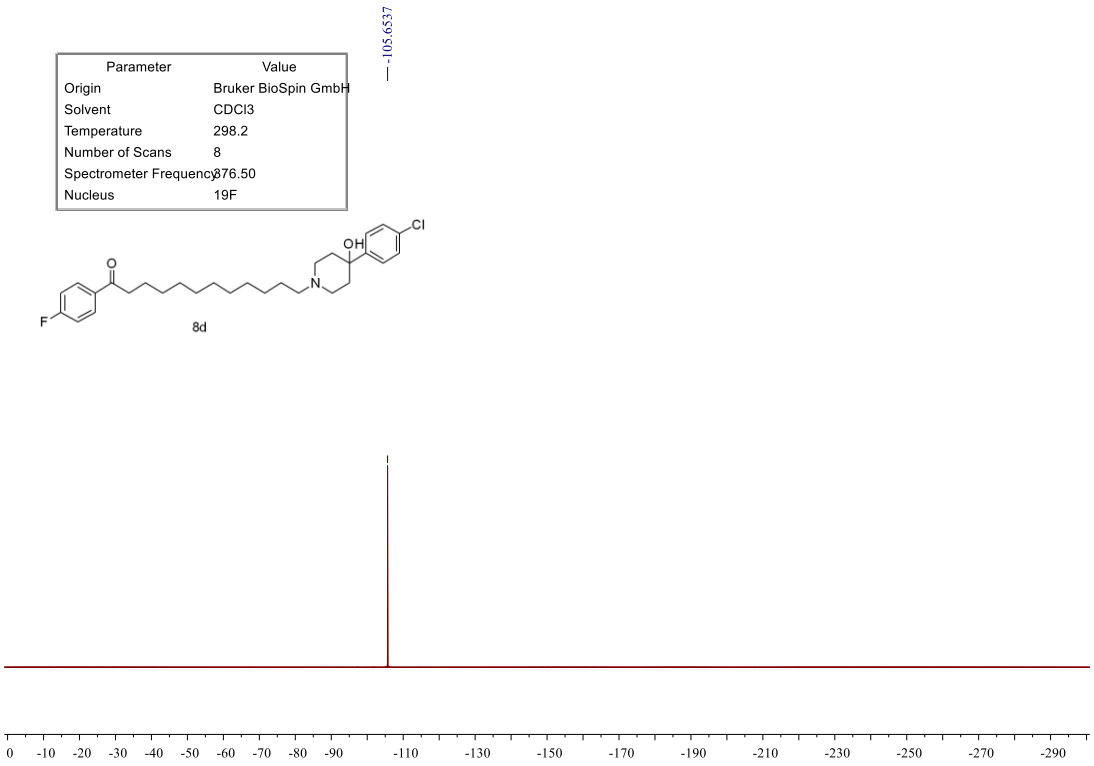
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Parameter Value
Origin Bruker BioSpin GmbH
Solvent CDCl3
Temperature 298.2
Number of Scans 8
Spectrometer Frequency 376.50
Nucleus 19F
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F
8d
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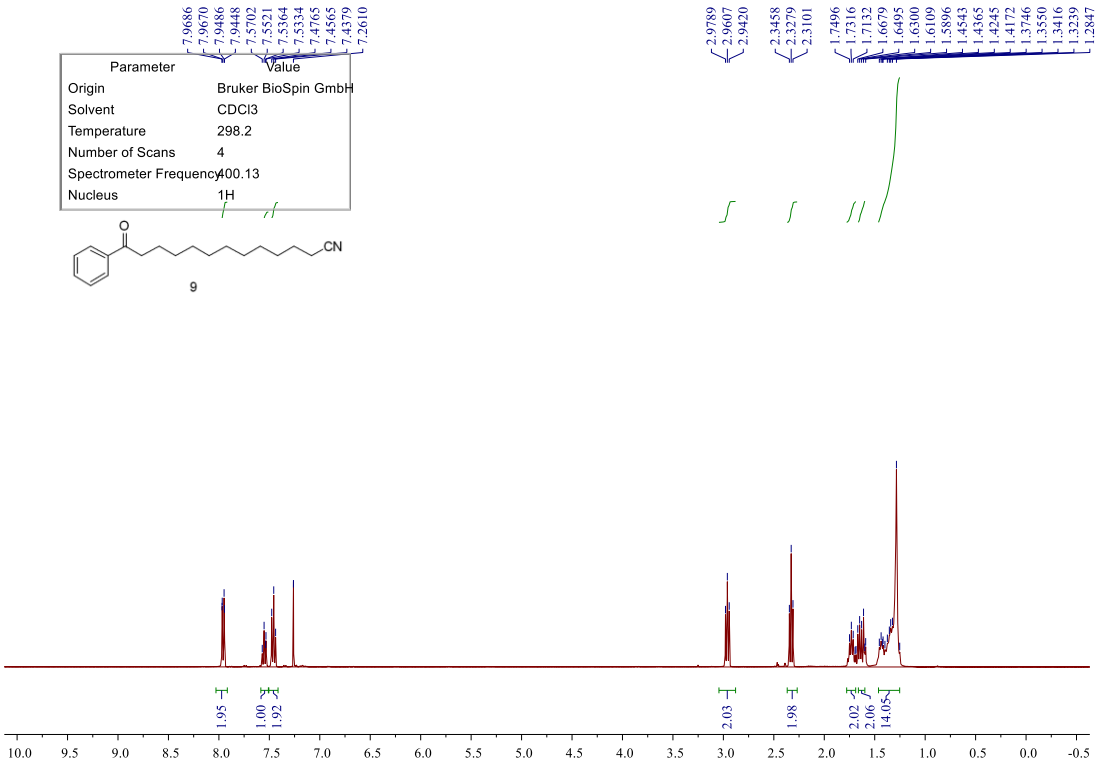
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1.4172
1.3746
1.3550
1.3416
1.3239
1.2847
Parameter Value
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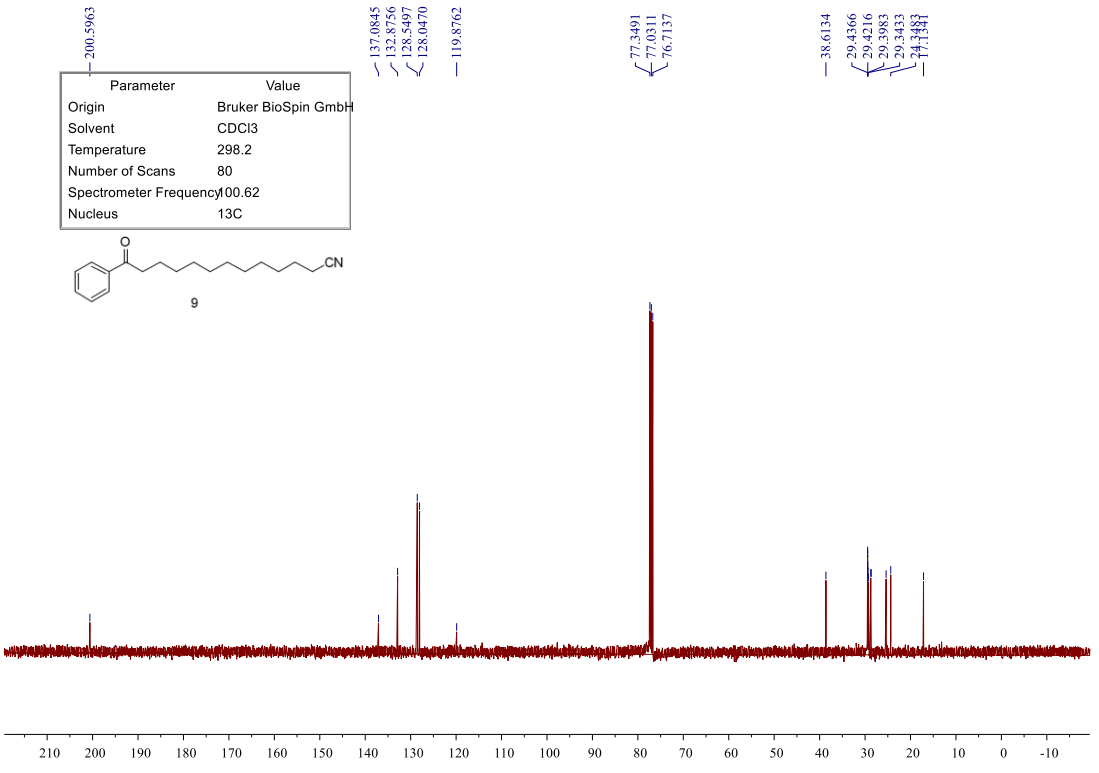
Solvent CDCl3
Temperature 298.2
Number of Scans 4
Spectrometer Frequency 400.13
Nucleus 1H
O
CN
9
1.95
1.00
1.92
2.03
1.98
2.02
2.06
14.05
10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5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29.3433
24.3483
24.1341
Parameter Value
Origin Bruker BioSpin GmbH
Solvent CDCl3
Temperature 298.2
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Spectrometer Frequency 100.62
Nucleus 13C
O
CN
9
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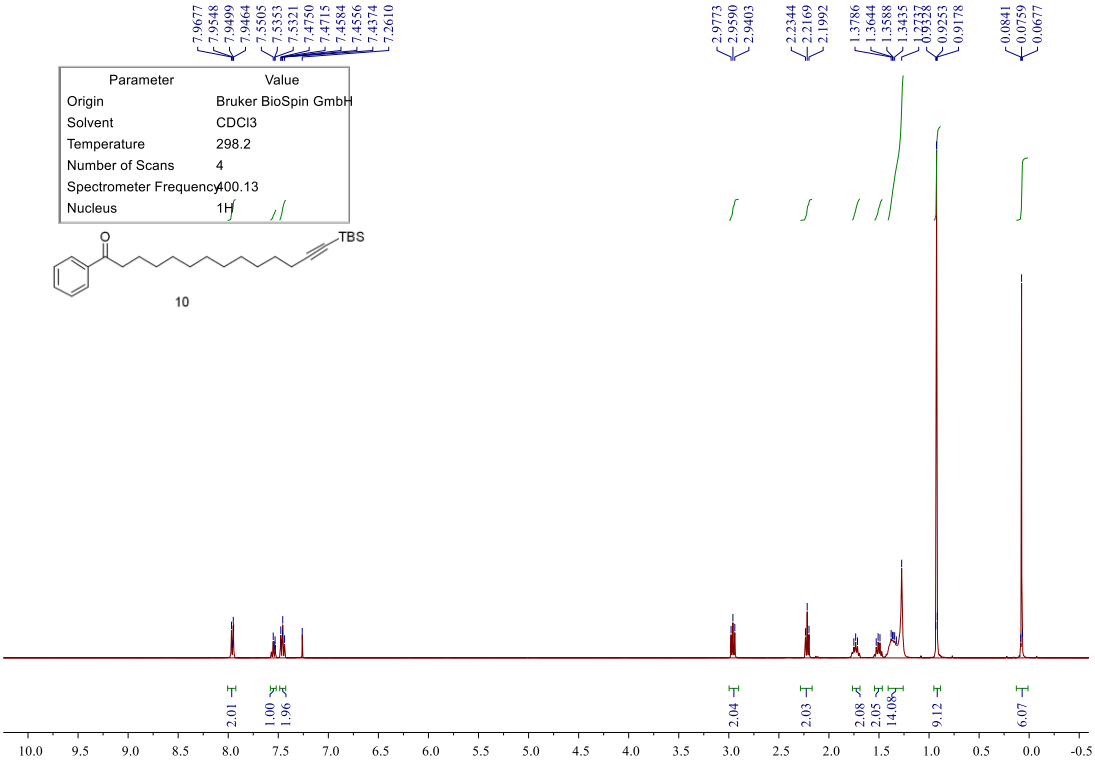
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2.2169
2.1992
1.3786
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1.3435
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0.9178
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0.0759
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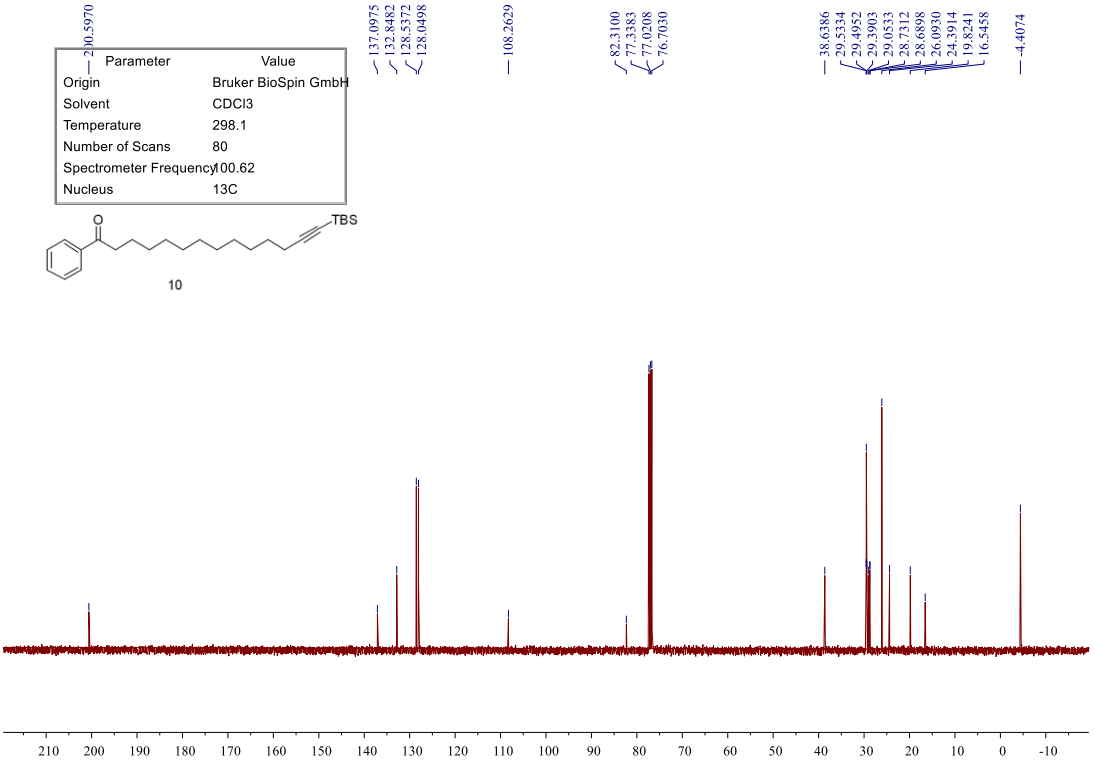
Parameter Value
Origin Bruker BioSpin GmbH
Solvent CDCl3
Temperature 298.2
Number of Scans 4
Spectrometer Frequency 400.13
Nucleus 1H
O
TBS
10
2.01
1.00
1.96
2.04
2.03
2.08
2.05
14.08
9.12
6.07
10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5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29.4952
29.3903
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24.3914
19.8241
16.5458
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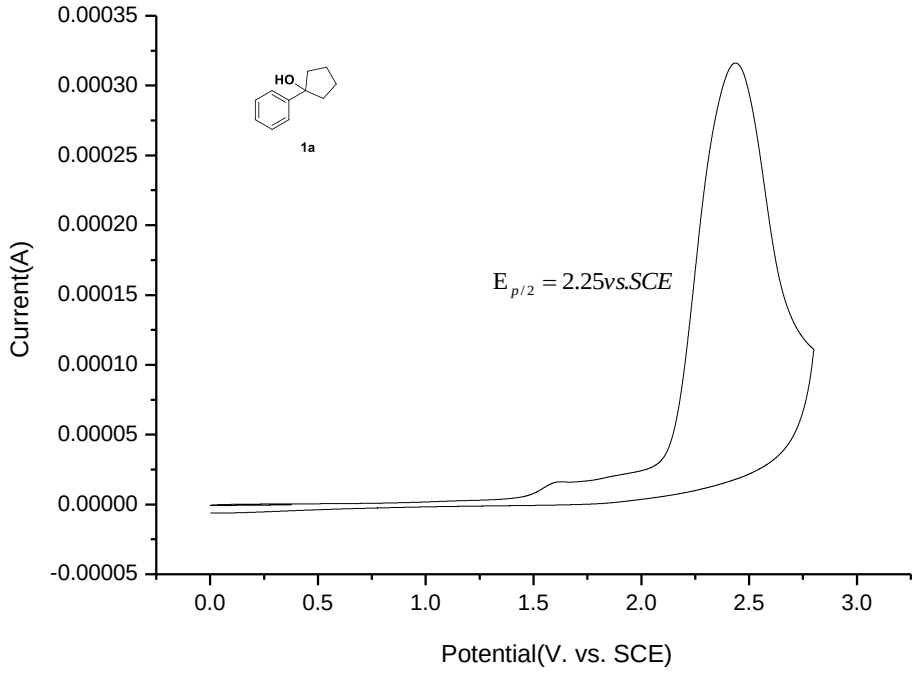
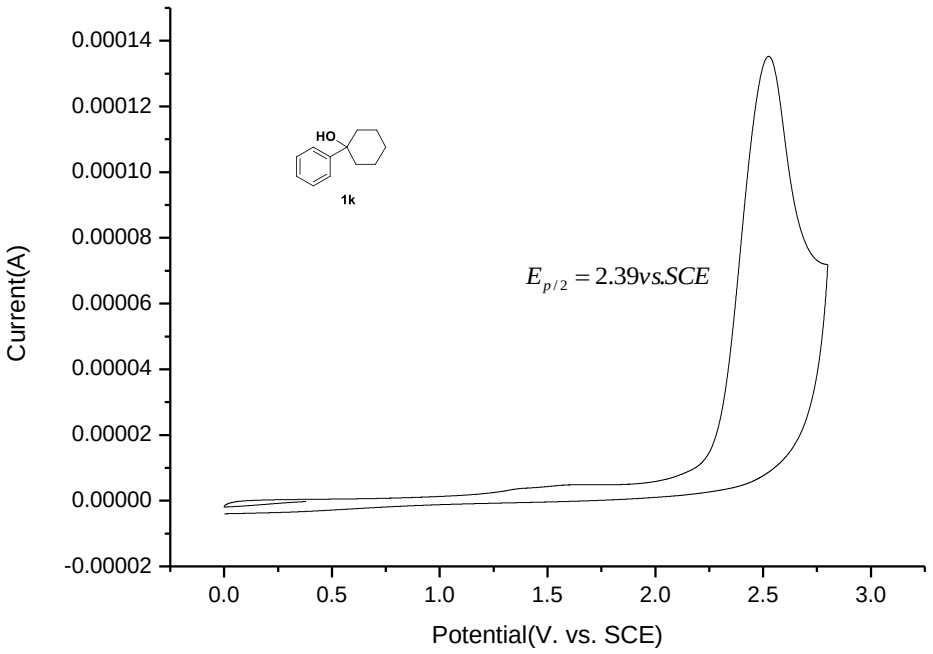
Parameter Value
Origin Bruker BioSpin GmbH
Solvent CDCl3
Temperature 298.1
Number of Scans 80
Spectrometer Frequency 100.62
Nucleus 13C
O
TBS
10
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10

7. Cyclic voltammograms of 1a and 1k

All voltammograms were taken at room temperature using a saturated calomel (SCE) reference electrode, a mesh platinum (Pt) counter electrode, and a glassy carbon working electrode. The conditions of the experiments were the following: an acetonitrile solution of 100 mM tetrabutylammonium hexafluorophosphate (NBu_4PF_6) and 1 mM aryl alcohol, a scan rate of 0.1 V/s, and a positive initial scan direction. The reported potentials were averages over segments, and were taken at half-height of the cathodic peaks ($E_{p/2}$) of **1a**, since all oxidations were nonreversible. To convert the potentials from SCE to Fc/Fc+ reference, 380 mV were subtracted from the measured values. The positive peaks on the return sweep of most substrates were thought to signify an ECE-type mechanism.

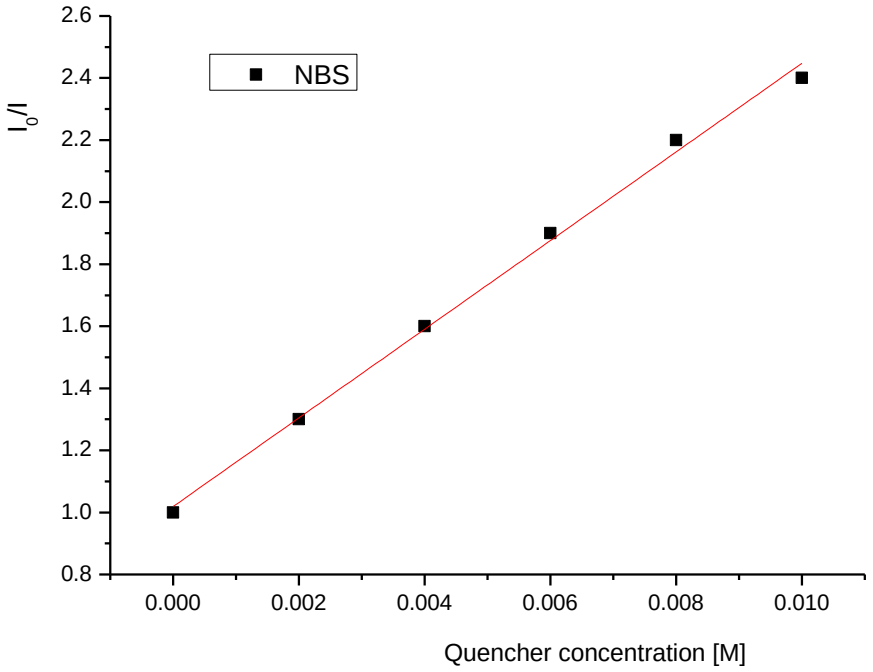


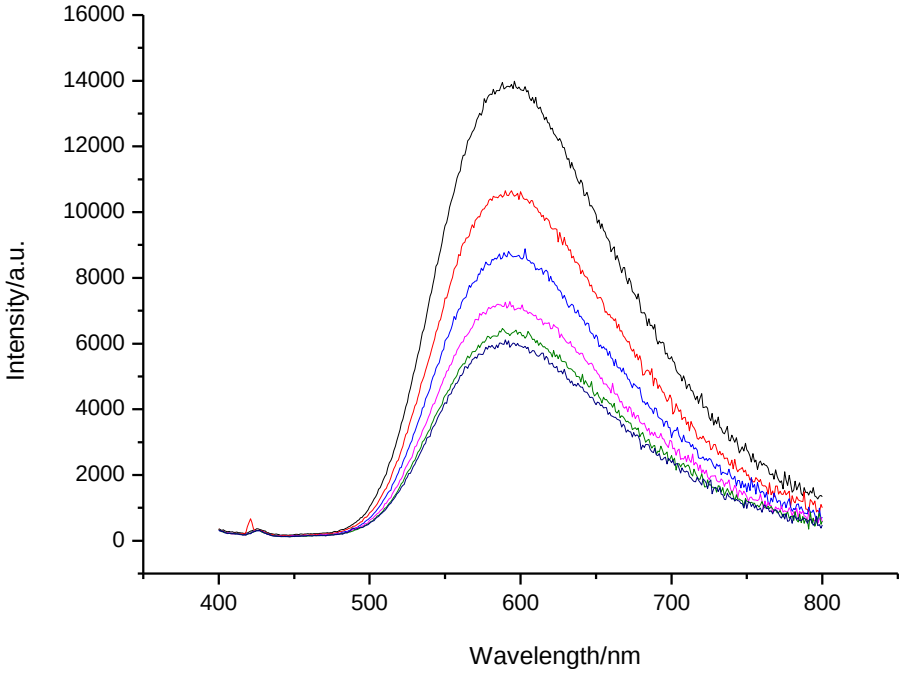
All voltammograms were taken at room temperature using a saturated calomel (SCE) reference electrode, a mesh platinum (Pt) counter electrode, and a glassy carbon working electrode. The conditions of the experiments were the following: an acetonitrile solution of 100 mM tetrabutylammonium hexafluorophosphate (NBu_4PF_6) and 1 mM aryl alcohol, a scan rate of 0.1 V/s, and a positive initial scan direction. The reported potentials were averages over segments, and were taken at half-height of the cathodic peaks ($E_{p/2}$) of **1k**, since all oxidations were nonreversible. To convert the potentials from SCE to Fc/Fc+ reference, 380 mV were subtracted from the measured values. The positive peaks on the return sweep of most substrates were thought to signify an ECE-type mechanism.



8. Emission quenching experiments (Stern–Volmer studies)

Emission intensities were recorded using a FLS980 (Edinburgh Instrument, UK) luminescence spectrophotometer. All $[Ir(ppy)_2(dtbbpy)]PF_6$ solutions were excited at 380 nm and the emission intensity was collected at 588 nm. In a typical experiment, to a $2 \cdot 10^{-5}$ M solution of $[Ir(ppy)_2(dtbbpy)]PF_6$ in CH_3CN was added the appropriate amount of NBS in a screw-top quartz cuvette. After degassing the sample with a stream of N_2 for 10 minutes, the emission of the sample was collected.




16000
14000
12000
10000
8000
6000
4000
2000
0
Intensity/a.u.
400
500
600
700
800
Wavelength/nm