Supporting Information

Cyanotrifluoromethylthiolation of unactivated dialkyl-substituted alkynes via cyano migration: synthesis of trifluoromethylthiolated acrylonitrile

Meishan Ji,[†] Jiajia Yu,[†] and Chen Zhu*[,†,]

[†] Key Laboratory of Organic Synthesis of Jiangsu Province, College of Chemistry, Chemical Engineering and Materials Science, Soochow University, 199 Ren-Ai Road, Suzhou, Jiangsu 215123, China

Email: chzhu@suda.edu.cn

Table of Contents

1. General experimental details

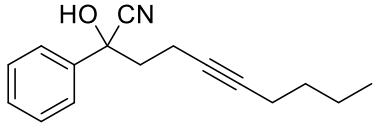
All reactions were maintained under a nitrogen atmosphere unless otherwise stated. Commercially available reagents were used without further purification. Infrared (FT-IR) spectra were recorded on a BRUKER VERTEX 70, ν_{max} in cm^{-1}. ^{1}H-NMR spectra were recorded on a BRUKER AVANCE III HD (400 MHz) 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.

The starting materials **1a**-**1y** (tertiary alcohols) were prepared by the addition of TMSCN to the precursor ketones, which were synthesized according to the reported procedures.[1] The precursor ketone of **3** was prepared based on the reported procedure.[2]

2. General procedure for the cyanotrifluoromethylthiolation of alkynes

Tertiary alcohol **1** (0.2 mmol, 1.0 equiv.), $AgSCF_3$ (63 mg, 0.3 mmol, 1.5 equiv.), and $K_2S_2O_8$ (162 mg, 0.6 mmol, 3.0 equiv.) were loaded in a reaction vial which was subjected to evacuation/ flushing with N_2 three times. DMSO (2 mL) was added to the mixture via syringe and the reaction was stirred at rt for a few hours until the starting material **1** was consumed monitored by TLC. After the reaction completion, water (15 mL) was added to the reaction. The resultant reaction mixture was extracted with ethyl acetate (3 x 15 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**.

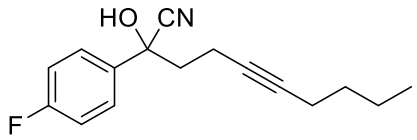
3. Characterization of starting materials



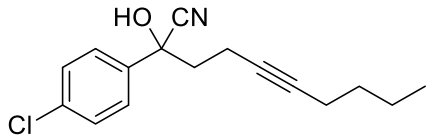
1a: yellow oil. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.57-7.53 (m, 2H), 7.44-7.35 (m, 3H), 2.59-2.47 (m, 1H), 2.42-2.32 (m, 1H), 2.26-2.11 (m, 4H), 1.51-1.33 (m, 4H), 0.91 (t, *J* = 7.2 Hz, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 139.5, 129.1, 128.8, 124.8,

[1] S. Chang, Y. Na, E. Choi and S. Kim, *Org. Lett.*, 2001, **3**, 2089.
[2] H. Y. Kim, J.-Y. Li and K. Oh, *J. Org. Chem.*, 2012, **77**, 11132.

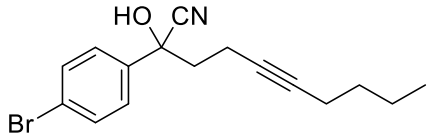
120.2, 83.1, 77.8, 74.5, 42.2, 30.8, 21.9, 18.3, 14.6, 13.5. FT-IR: ν (cm^{-1}) 3416, 2959, 2933, 2272, 2243, 1449, 1097. HRMS [ESI] calcd for $C_{16}H_{19}NONa$ $[M+Na]^+$ 264.1359, found 264.1360.



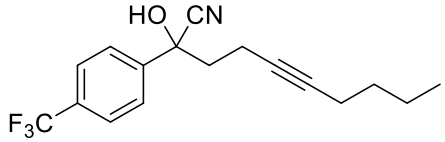
1b: yellow oil. ^1H NMR (400 MHz, $CDCl_3$) δ 7.54-7.48 (m, 2H), 7.12-7.05 (m, 2H), 4.30 (br, 1H), 2.56-2.43 (m, 1H), 2.40-2.30 (m, 1H), 2.22-2.06 (m, 4H), 1.48-1.32 (m, 4H), 0.90 (t, J = 7.2 Hz, 3H); ^{19}F NMR (376 MHz, $CDCl_3$) δ -112.4 (s); ^{13}C NMR (100 MHz, $CDCl_3$) δ 162.9 (d, J_{C-F} = 247.1 Hz), 135.3 (d, J_{C-F} = 3.1 Hz), 126.7 (d, J_{C-F} = 8.4 Hz), 120.1, 115.7 (d, J_{C-F} = 21.7 Hz), 83.2, 77.6, 73.9, 42.2, 30.7, 21.8, 18.2, 14.5, 13.5. FT-IR: ν (cm^{-1}) 3423, 2959, 2863, 2247, 1677, 1509, 1232. HRMS [ESI] calcd for $C_{16}H_{18}FNONa$ $[M+Na]^+$ 282.1265, found 282.1259.



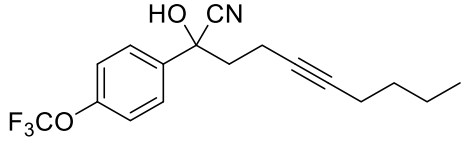
1c: yellow oil. ^1H NMR (400 MHz, $CDCl_3$) δ 7.47-7.42 (m, 2H), 7.39-7.34 (m, 2H), 4.38 (s, 1H), 2.52-2.40 (m, 1H), 2.38-2.28 (m, 1H), 2.20-2.03 (m, 4H), 1.50-1.31 (m, 4H), 0.89 (t, J = 7.2 Hz, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 137.9, 135.0, 128.9, 126.3, 119.9, 83.2, 77.5, 73.8, 42.1, 30.7, 21.8, 18.2, 14.4, 13.8. FT-IR: ν (cm^{-1}) 3082, 2930, 2850, 2244, 1674, 1098. HRMS [ESI] calcd for $C_{16}H_{18}ClNONa$ $[M+Na]^+$ 298.0969, found 298.0969.



1d: yellow oil. ^1H NMR (400 MHz, $CDCl_3$) δ 7.56-7.52 (m, 2H), 7.43-7.39 (m, 2H), 4.31 (s, 1H), 2.56-2.46 (m, 1H), 2.42-2.32 (m, 1H), 2.21-2.07 (m, 4H), 1.50-1.32 (m, 4H), 0.90 (t, J = 7.2 Hz, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 138.6, 131.9, 126.6, 123.2, 119.8, 83.5, 77.6, 74.0, 42.0, 30.7, 21.9, 18.3, 14.6, 13.5. FT-IR: ν (cm^{-1}) 3420, 2958, 2861, 2247, 1488, 1010. HRMS [ESI] calcd for $C_{16}H_{18}BrNONa$ $[M+Na]^+$ 342.0464, found 342.0467.

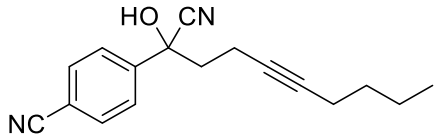


1e: yellow oil. ^1H NMR (400 MHz, $CDCl_3$) δ 7.68-7.64 (m, 4H), 4.61 (s, 1H), 2.54-2.44 (m, 1H), 3.43-2.32 (m, 1H), 2.23-2.08 (m, 4H), 1.49-1.32 (m, 4H), 0.89 (t, J = 7.2 Hz, 3H); ^{19}F NMR (376 MHz, $CDCl_3$) δ -62.8 (s); ^{13}C NMR (100 MHz, $CDCl_3$) δ 143.3, 131.3 (q, J_{C-F} = 32.5 Hz), 125.8 (q, J_{C-F} = 3.7 Hz), 125.4, 123.7 (q, J_{C-F} = 270.6 Hz), 119.8, 83.5, 77.4, 73.9, 42.1, 30.7, 21.8, 18.2, 14.4, 13.4. FT-IR: ν (cm^{-1}) 3421, 2934, 2864, 2247, 1621, 1413, 1016. HRMS [ESI] calcd for $C_{17}H_{18}F_3NONa$ $[M+Na]^+$ 332.1233, found 332.1239.

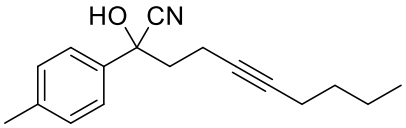


1f: yellow oil. ^1H NMR (400 MHz, $CDCl_3$) δ 7.59-7.55 (m, 2H), 7.26-7.23 (m, 2H), 4.47 (s, 1H), 2.55-2.45 (m, 1H), 2.42-2.33 (m, 1H), 2.22-2.09 (m, 4H), 1.49-1.32 (m, 4H), 0.90 (t, J = 7.2 Hz, 3H); ^{19}F NMR (376 MHz, $CDCl_3$) δ -58.0 (s); ^{13}C NMR (100 MHz, $CDCl_3$) δ 149.6 (q, J_{C-F} = 1.8 Hz), 138.1, 126.5, 121.1, 120.3 (q, J_{C-F} = 256.4 Hz), 119.9, 83.4, 77.5, 73.8, 42.2, 30.7, 21.9, 18.2, 14.5, 13.5. FT-IR: ν (cm^{-1}) 3422, 2960, 2934,

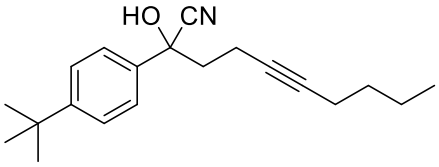
2864, 2248, 1509, 1089. HRMS [ESI] calcd for $C_{17}H_{18}F_3NO_2Na$ $[M+Na]^+$ 348.1182, found 348.1196.



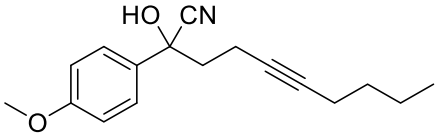
1g: yellow oil. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.78-7.66 (m, 4H), 4.64 (s, 1H), 2.62-2.50 (m, 1H), 2.48-2.38 (m, 1H), 2.24-2.08 (m, 4H), 1.50-1.32 (m, 4H), 0.90 (t, *J* = 7.2 Hz, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 144.6, 132.6, 125.8, 119.4, 118.0, 112.9, 84.0, 77.3, 74.0, 41.9, 30.7, 21.9, 18.2, 14.6, 13.5. FT-IR: ν (cm^{-1}) 3406, 2958, 2862, 2233, 1703, 1090. HRMS [ESI] calcd for $C_{17}H_{18}N_2ONa$ $[M+Na]^+$ 289.1311, found 289.1320.



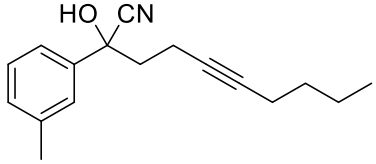
1h: yellow oil. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.42 (d, *J* = 8.0 Hz, 2H), 7.21 (d, *J* = 8.0 Hz, 2H), 2.55-2.43 (m, 1H), 2.37 (s, 3H), 2.37-2.28 (m, 1H), 2.25-2.10 (m, 4H), 1.50-1.33 (m, 4H), 0.90 (t, *J* = 7.2 Hz, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 139.0, 136.5, 129.4, 124.7, 120.3, 82.8, 77.9, 74.2, 42.1, 30.8, 21.9, 21.0, 18.3, 14.6, 13.5. FT-IR: ν (cm^{-1}) 3421, 2958, 2862, 2244, 1613, 1087. HRMS [ESI] calcd for $C_{17}H_{21}NONa$ $[M+Na]^+$ 278.1515, found 278.1525.



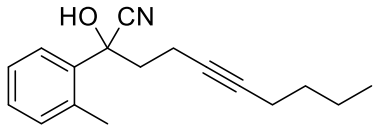
1i: yellow oil. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.50-7.41 (m, 4H), 4.01 (s, 1H), 2.56-2.44 (m, 1H), 2.40-2.31 (m, 1H), 2.29-2.10 (m, 4H), 1.51-1.35 (m, 4H), 1.33 (s, 9H), 0.91 (t, *J* = 7.2 Hz, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 152.2, 136.4, 125.7, 124.5, 120.3, 82.8, 77.9, 74.2, 42.1, 34.6, 31.2, 30.8, 21.9, 18.3, 14.6, 13.5. FT-IR: ν (cm^{-1}) 3424, 2960, 2871, 2365, 2248, 1364, 1088. HRMS [ESI] calcd for $C_{20}H_{27}NONa$ $[M+Na]^+$ 320.1985, found 320.1986.



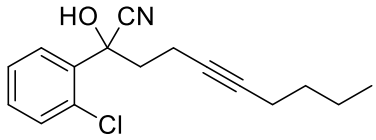
1j: yellow oil. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.44-7.40 (m, 2H), 6.90-6.86 (m, 2H), 4.17 (s, 1H), 3.78 (s, 3H), 2.48-2.37 (m, 1H), 2.33-2.24 (m, 1H), 2.24-2.06 (m, 4H), 1.48-1.31 (m, 4H), 0.89 (t, *J* = 7.2 Hz, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 159.9, 131.5, 126.1, 120.3, 114.0, 82.5, 77.8, 73.8, 55.2, 42.2, 30.7, 21.8, 18.2, 14.4, 13.5. FT-IR: ν (cm^{-1}) 3423, 2933, 2862, 2248, 2048, 1610, 1443, 1120. HRMS [ESI] calcd for $C_{17}H_{21}NO_2Na$ $[M+Na]^+$ 294.1465, found 294.1455.



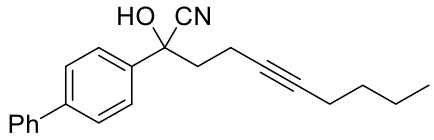
1k: yellow oil. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.37-7.32 (m, 2H), 7.31-7.27 (m, 1H), 7.18 (d, *J* = 7.2 Hz, 1H), 4.08 (s, 1H), 2.55-2.43 (m, 1H), 2.38 (s, 3H), 2.37-2.28 (m, 1H), 2.26-2.10 (m, 4H), 1.51-1.34 (m, 4H), 0.91 (t, *J* = 7.2 Hz, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 139.3, 138.6, 129.8, 128.6, 125.3, 121.8, 120.3, 82.8, 77.8, 74.2, 42.2, 30.8, 21.8, 21.4, 18.2, 14.5, 13.5. FT-IR: ν (cm^{-1}) 3422, 2958, 2862, 2244, 1445, 1083. HRMS [ESI] calcd for $C_{17}H_{21}NONa$ $[M+Na]^+$ 278.1515, found 278.1533.



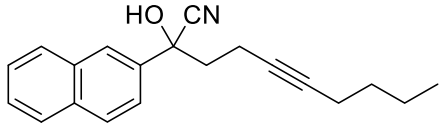
1l: yellow oil. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.60 (dd, *J* = 7.2, 1.6 Hz, 1H), 7.30-7.25 (m, 1H), 7.24-7.18 (m, 2H), 4.09 (s, 1H), 2.55 (s, 3H), 2.55-2.49 (m, 1H), 2.48-2.38 (m, 1H), 2.31-2.22 (m, 2H), 2.19-2.12 (m, 2H), 1.52-1.34 (m, 4H), 0.91 (t, *J* = 7.2 Hz, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 163.3, 135.0, 132.7, 128.9, 126.2, 125.5, 120.1, 83.1, 78.0, 73.9, 39.1, 30.8, 21.9, 20.7, 18.3, 14.5, 13.5. FT-IR: ν (cm^{-1}) 3411, 2958, 2861, 2241, 1456, 1180. HRMS [ESI] calcd for $C_{17}H_{21}NONa$ $[M+Na]^+$ 278.1515, found 278.1525.



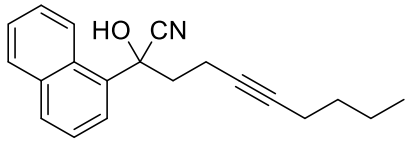
1m: yellow solid, m.p. 35-36 °C. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.78-7.73 (m, 1H), 7.43-7.39 (m, 1H), 7.37-7.29 (m, 2H), 4.62-4.56 (m, 1H), 2.62-2.38 (m, 3H), 2.30-2.22 (m, 1H), 2.20-2.10 (m, 2H), 1.52-1.34 (m, 4H), 0.91 (t, *J* = 7.2 Hz, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 135.5, 131.2, 130.9, 130.2, 127.2, 127.1, 119.0, 83.4(m), 78.1, 72.2 (m), 40.0, 30.7, 21.9, 18.3, 14.2, 13.5. FT-IR: ν (cm^{-1}) 3418, 2959, 2933, 2872, 2247, 1466, 1094. HRMS [ESI] calcd for $C_{16}H_{18}ClNONa$ $[M+Na]^+$ 298.0969, found 298.0975.



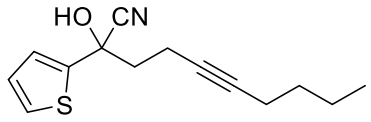
1n: yellow oil. ^{1}H NMR (400 MHz, $CDCl_3$) 7.70-7.63 (m, 4H), 7.61-7.56 (m, 2H), 7.48-7.44 (m, 2H), 7.41-7.37 (m, 1H), 4.17 (s, 1H), 2.59-2.53 (m, 1H), 2.46-2.36 (m, 1H), 2.32-2.20 (m, 2H), 2.19-2.13 (m, 2H), 1.53-1.44 (m, 2H), 1.43-1.36 (m, 2H), 0.93 (t, *J* = 7.2 Hz, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 141.9, 140.0, 138.3, 128.8, 127.7, 127.4, 127.0, 125.2, 120.2, 83.0, 77.8, 74.2, 42.1, 30.8, 21.9, 18.3, 14.6, 13.5. FT-IR: ν (cm^{-1}) 3423, 2958, 2931, 2872, 2250, 1487, 1075. HRMS [ESI] calcd for $C_{22}H_{23}NONa$ $[M+Na]^+$ 340.1672, found 340.1662.



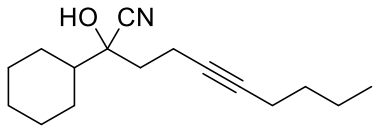
1o: yellow oil. ^{1}H NMR (400 MHz, $CDCl_3$) 8.05 (d, *J* = 1.2 Hz, 1H), 7.90-7.82 (m, 3H), 7.58 (dd, *J* = 8.8, 2.0 Hz 1H), 7.56-7.51 (m, 2H), 4.18 (s, 1H), 2.62-2.50 (m, 1H), 2.46-2.36 (m, 1H), 2.35-2.20 (m, 2H), 2.18-2.09 (m, 2H), 1.50-1.34 (m, 4H), 0.91 (t, *J* = 7.2 Hz, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 136.5, 133.3, 132.8, 128.9, 128.4, 127.6, 126.9, 126.8, 124.3, 122.1, 120.3, 83.2, 77.8, 74.6, 41.9, 30.8, 21.9, 18.3, 14.7, 13.5. FT-IR: ν (cm^{-1}) 2928, 2855, 2244, 1713, 1377, 1107. HRMS [ESI] calcd for $C_{20}H_{21}NONa$ $[M+Na]^+$ 314.1515, found 314.1517.



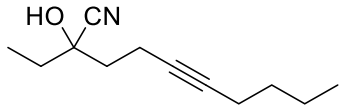
1p: yellow solid, m.p. 64-65 °C. ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.48 (d, *J* = 8.4 Hz, 1H), 7.92-7.82 (m, 3H), 7.60-7.50 (m, 2H), 7.44 (t, *J* = 7.8 Hz, 1H), 4.30 (s, 1H), 2.64-2.56 (m, 1H), 2.56-2.51 (m, 2H), 2.45-2.37 (m, 1H), 2.17-2.09 (m, 2H), 1.50-1.34 (m, 4H), 0.92 (t, *J* = 7.2 Hz, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 134.5, 133.3, 130.4, 129.3, 129.0, 126.5, 125.9, 124.7, 124.4, 124.1, 120.4, 82.9, 77.9, 74.7, 39.9, 30.7, 21.8, 18.3, 14.7, 13.5. FT-IR: ν (cm^{-1}) 3404, 2956, 2855, 2239, 1386, 1102. HRMS [ESI] calcd for $C_{20}H_{21}NONa$ $[M+Na]^+$ 314.1515, found 314.1523.



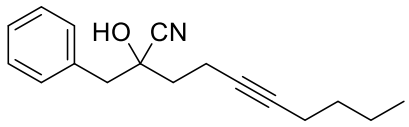
1q: yellow oil. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.36 (dd, *J* = 4.8, 1.2 Hz, 1H), 7.25 (dd, *J* = 3.6, 1.2 Hz, 1H), 7.02-7.00 (m, 1H), 4.16 (s, 1H), 2.65-2.54 (m, 1H), 2.48-2.40 (m, 1H), 2.40-2.24 (m, 2H), 2.19-2.12 (m, 2H), 1.51-1.34 (m, 4H), 0.91 (t, *J* = 7.2 Hz, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 143.4, 126.9, 126.7, 125.4, 119.4, 83.5, 77.5, 71.6, 42.1, 30.8, 21.9, 18.3, 14.7, 13.5. FT-IR: ν (cm^{-1}) 3419, 2958, 2862, 2361, 2249, 1649, 1082. HRMS [ESI] calcd for $C_{14}H_{17}NOSNa$ $[M+Na]^+$ 270.0932, found 270.0941.



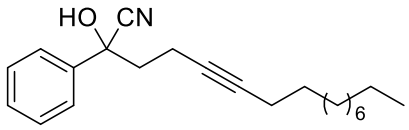
1r: yellow oil. ^{1}H NMR (400 MHz, $CDCl_3$) δ 3.76 (s, 1H), 2.59-2.41 (m, 2H), 2.17-2.10 (m, 2H), 2.01-1.90 (m, 2H), 1.90-1.78 (m, 4H), 1.72-1.64 (m, 1H), 1.62-1.53 (m, 1H), 1.50-1.40 (m, 2H), 1.40-1.32 (m, 2H), 1.28-1.10 (m, 5H), 0.89 (t, *J* = 7.2 Hz, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 120.3, 83.3, 78.3, 76.2, 46.3, 35.4, 30.7, 27.2, 26.5, 25.9, 25.8, 25.7, 21.8, 18.2, 14.3, 13.5. FT-IR: ν (cm^{-1}) 3449, 2931, 2857, 2238, 1694, 1507, 1105. HRMS [ESI] calcd for $C_{16}H_{25}NONa$ $[M+Na]^+$ 270.1828, found 270.1824.



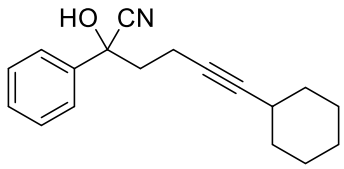
1s: yellow oil. ^{1}H NMR (400 MHz, $CDCl_3$) δ 3.88 (s, 1H), 2.59-2.48 (m, 1H), 2.48-2.38 (m, 1H), 2.17-2.09 (m, 2H), 1.98-1.86 (m, 2H), 1.84-1.73 (m, 2H), 1.49-1.40 (m, 2H), 1.40-1.31 (m, 2H), 1.09 (t, *J* = 7.6 Hz, 3H), 0.88 (t, *J* = 7.2 Hz, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 120.5, 83.2, 78.1, 73.2, 37.7, 33.7, 30.7, 21.8, 18.2, 14.2, 13.5, 8.1. FT-IR: ν (cm^{-1}) 3442, 2959, 2933, 2241, 1461, 1131. HRMS [ESI] calcd for $C_{12}H_{19}NONa$ $[M+Na]^+$ 216.1359, found 216.1360.



1t: yellow oil. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.41-7.31 (m, 5H), 3.62 (s, 1H), 3.09 (d, *J* = 14.0 Hz, 1H), 3.03 (d, *J* = 14.0 Hz, 1H), 2.65-2.45 (m, 2H), 2.20-2.12 (m, 2H), 2.04-1.94 (m, 2H), 1.52-1.44 (m, 2H), 1.43-1.35 (m, 2H), 0.92 (t, *J* = 7.2 Hz, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 133.3, 130.5, 128.7, 127.8, 120.1, 83.2, 78.0, 72.6, 46.6, 38.1, 30.8, 21.9, 18.3, 14.3, 13.5. FT-IR: ν (cm^{-1}) 3362, 2960, 2931, 2245, 1680, 1092. HRMS [ESI] calcd for $C_{17}H_{21}NONa$ $[M+Na]^+$ 278.1515, found 278.1522.

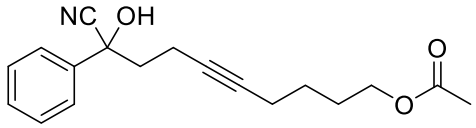


1u: yellow oil. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.56-7.51 (m, 2H), 7.43-7.34 (m, 3H), 4.19 (s, 1H), 2.52-2.42 (m, 1H), 2.38-2.28 (m, 1H), 2.25-2.08 (m, 4H), 1.52-1.42 (m, 2H), 1.41-1.25 (m, 14H), 0.89 (t, *J* = 6.8 Hz, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 139.4, 129.0, 128.7, 124.7, 120.2, 82.8, 77.8, 74.2, 42.2, 31.8, 29.5, 29.4, 29.2, 29.0, 28.8, 28.7, 22.6, 18.6, 14.5, 14.0. FT-IR: ν (cm^{-1}) 3422, 2925, 2854, 2364, 2245, 1603, 1450, 1070. HRMS [ESI] calcd for $C_{22}H_{32}NO$ $[M+H]^+$ 326.2478, found 326.2450.

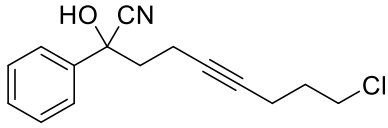


1v: yellow oil. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.56-7.51 (m, 2H), 7.44-7.34 (m, 3H), 4.27 (s, 1H), 2.56-2.46 (m, 1H), 2.42-2.27 (m, 2H), 2.25-2.09 (m, 2H), 1.82-1.73 (m, 2H), 1.72-1.64 (m, 2H), 1.57-1.46 (m, 1H), 1.44-1.34 (m, 2H), 1.32-1.22 (m, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 139.4, 129.0, 128.7, 124.7, 120.2,

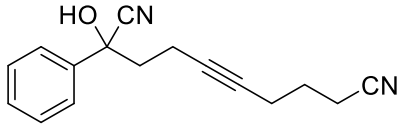
87.3, 77.7, 74.3, 42.2, 32.7, 29.0, 25.7, 24.8, 14.5. FT-IR: ν (cm^{-1}) 3422, 2930, 2854, 2246, 1448, 1096. HRMS [ESI] calcd for $C_{18}H_{21}NONa$ $[M+Na]^+$ 290.1515, found 290.1525.



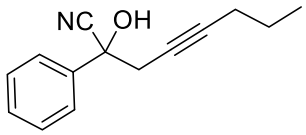
1w: yellow oil. ^1H NMR (400 MHz, $CDCl_3$) δ 7.59-7.52 (m, 2H), 7.49-7.35 (m, 3H), 4.06 (t, *J* = 6.4 Hz, 2H), 4.02 (s, 1H), 2.62-2.46 (m, 1H), 2.42-2.32 (m, 1H), 2.28-2.12 (m, 4H), 2.03 (s, 3H), 1.74-1.66 (m, 2H), 1.58-1.49 (m, 2H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 171.3, 139.5, 129.2, 128.8, 124.8, 120.3, 80.1, 78.5, 74.3, 64.0, 42.2, 27.7, 25.1, 21.0, 18.3, 14.6. FT-IR: ν (cm^{-1}) 3415, 2938, 2867, 2232, 1712, 1239. HRMS [ESI] calcd for $C_{18}H_{21}NO_3Na$ $[M+Na]^+$ 322.1414, found 322.1409.



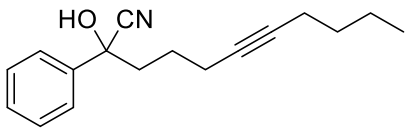
1x: yellow oil. ^1H NMR (400 MHz, $CDCl_3$) δ 7.56-7.48 (m, 2H), 7.45-7.34 (m, 3H), 3.97-3.90 (m, 1H), 3.61 (t, *J* = 6.4 Hz, 2H), 2.50-2.38 (m, 1H), 2.37-2.26 (m, 3H), 2.25-2.10 (m, 2H), 1.94-1.86 (m, 2H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 139.2, 129.1, 128.8, 124.7, 120.2, 80.3, 78.9, 73.9, 43.6, 42.2, 31.3, 16.0, 14.3. FT-IR: ν (cm^{-1}) 3416, 2961, 2846, 2241, 1449, 1096. HRMS [ESI] calcd for $C_{15}H_{16}ClNONa$ $[M+Na]^+$ 284.0813, found 384.0822.



1y: yellow oil. ^1H NMR (400 MHz, $CDCl_3$) δ 7.56-7.49 (m, 2H), 7.44-7.34 (m, 3H), 4.35-3.84 (m, 1H), 2.42 (t, *J* = 7.2 Hz, 2H), 2.39-2.30 (m, 2H), 2.30-2.22 (m, 2H), 2.22-2.10 (m, 2H), 1.82-1.70 (m, 2H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 139.3, 129.1, 128.7, 124.7, 120.3, 119.2, 79.9, 78.9, 73.5, 42.2, 24.4, 17.7, 15.9, 14.2. FT-IR: ν (cm^{-1}) 3404, 2940, 2846, 2360, 2250, 1707, 1449, 1099. HRMS [ESI] calcd for $C_{16}H_{16}N_2ONa$ $[M+Na]^+$ 275.1155, found 275.1156.

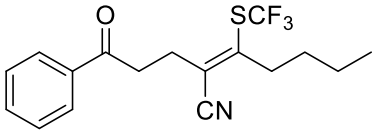


3: red oil. ^1H NMR (400 MHz, $CDCl_3$) δ 7.59-7.58 (m, 2H), 7.41-7.40 (m, 3H), 3.83 (s, 1H), 2.94-2.83 (m, 2H), 2.20-2.16 (m, 2H), 1.58-1.49 (m, 2H), 0.97 (t, *J* = 7.2 Hz, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 138.1, 129.2, 128.6, 124.9, 120.1, 86.5, 73.0, 72.4, 35.5, 21.9, 20.6, 13.3. FT-IR: ν (cm^{-1}) 3402, 2962, 2933, 2873, 2239, 1430, 1063. HRMS [ESI] calcd for $C_{14}H_{15}NONa$ $[M+Na]^+$ 236.1046, found 236.1033

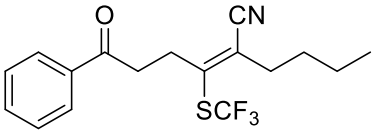


5: yellow oil. ^1H NMR (400 MHz, $CDCl_3$) δ 7.57-7.50 (m, 2H), 7.43-7.33 (m, 3H), 3.59 (s, 1H), 2.20-2.03 (m, 6H), 1.75-1.62 (m, 1H), 1.58-1.48 (m, 1H), 1.46-1.32 (m, 4H), 0.97 (t, *J* = 7.2 Hz, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 139.8, 129.0, 128.8, 124.8, 120.7, 81.4, 78.7, 74.4, 42.5, 31.0, 23.7, 21.8, 18.3, 13.5. FT-IR: ν (cm^{-1}) 3419, 2957, 2932, 2871, 2247, 1450, 1099. HRMS [ESI] calcd for $C_{17}H_{21}NONa$ $[M+Na]^+$ 278.1515, found 278.1523.

4. Characterization of products

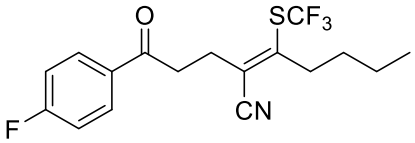


2a

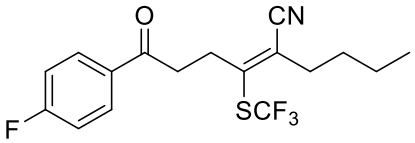


2a'

Yellow oil (**2a**: **2a'** = 3.0:1). ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.99-7.94 (m, 2H, major/ minor), 7.62-7.56 (m, 1H, major/ minor), 7.51-7.45 (m, 2H, major/ minor), 3.35 (t, *J* = 7.2 Hz, 2H, minor), 3.29 (t, *J* = 7.2 Hz, 2H, major), 3.21 (t, *J* = 7.2 Hz, 2H, minor), 2.99 (t, *J* = 7.2 Hz, 2H, major), 2.78 (t, *J* = 7.6 Hz, 2H, major), 2.58 (t, *J* = 7.6 Hz, 2H, minor), 1.68-1.55 (m, 2H, major/ minor), 1.41-1.31 (m, 2H, major/ minor), 0.95 (t, *J* = 7.2 Hz, 3H, minor), 0.94 (t, *J* = 7.2 Hz, 3H, major); ^{19}F NMR (376 MHz, $CDCl_3$) δ -38.0 (s, major), -38.2 (s, minor); ^{13}C NMR (100 MHz, $CDCl_3$) δ (major) 197.2, 147.9 (q, J_{C-F} = 1.4 Hz), 136.2, 133.5, 128.7, 128.5 (q, J_{C-F} = 308.6 Hz), 128.0, 121.4 (q, J_{C-F} = 1.9 Hz), 116.3, 37.8 (q, J_{C-F} = 0.9 Hz), 35.9, 30.3, 27.1, 21.9, 13.7; (minor) 197.2, 144.0 (q, J_{C-F} = 1.3 Hz), 136.2, 133.4, 128.7, 128.0, 125.6 (q, J_{C-F} = 1.9 Hz), 116.3, 36.4, 32.8, 32.6 (q, J_{C-F} = 1.0 Hz), 30.0, 21.9, 13.7. FT-IR: ν (cm^{-1}) 2961, 2865, 2215, 1687, 1449, 1101. HRMS [ESI] calcd for $C_{17}H_{19}F_3NOS$ $[M+H]^+$ 342.1134, found 342.1130.

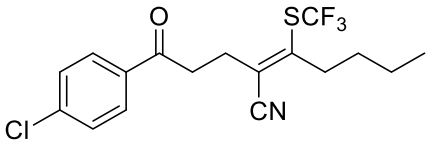


2b

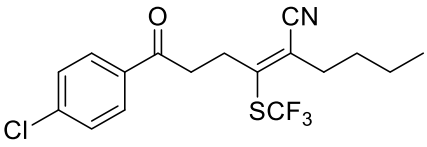


2b'

Yellow oil (**2b**: **2b'** = 3.0:1). ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.01-7.96 (m, 2H, major/ minor), 7.18-7.11 (m, 2H, major/ minor), 3.33-3.28 (m, 2H, minor), 3.25 (t, *J* = 7.4 Hz, 2H, major), 3.20 (t, *J* = 7.2 Hz, 2H, minor), 2.97 (t, *J* = 7.2 Hz, 2H, major), 2.78 (t, *J* = 7.6 Hz, 2H, major), 2.58 (t, *J* = 7.6 Hz, 2H, minor), 1.66-1.53 (m, 2H, major/ minor), 1.39-1.30 (m, 2H, major/ minor), 0.94 (t, *J* = 7.6 Hz, 3H, minor), 0.93 (t, *J* = 7.6 Hz, 3H, major); ^{19}F NMR (376 MHz, $CDCl_3$) δ -38.0 (s, major), -38.2 (s, minor), -104.3 (s, major), -104.5 (s, minor); ^{13}C NMR (100 MHz, $CDCl_3$) δ (major) 195.6, 166.0 (d, J_{C-F} = 254.0 Hz), 148.0 (q, J_{C-F} = 1.4 Hz), 128.5 (q, J_{C-F} = 308.6 Hz), 121.3 (q, J_{C-F} = 1.8 Hz), 116.2, 115.9 (d, J_{C-F} = 21.8 Hz), 132.6 (d, J_{C-F} = 3.1 Hz), 130.7 (d, J_{C-F} = 9.3 Hz), 37.8 (q, J_{C-F} = 0.8 Hz), 35.8, 30.3, 27.1, 21.9, 13.6; (minor) 195.5, 165.9 (d, J_{C-F} = 253.8 Hz), 143.8 (q, J_{C-F} = 1.4 Hz), 132.6 (d, J_{C-F} = 3.1 Hz), 130.7 (d, J_{C-F} = 9.3 Hz), 128.4 (q, J_{C-F} = 308.9 Hz), 125.7 (q, J_{C-F} = 1.6 Hz), 116.3, 115.8 (d, J_{C-F} = 21.8 Hz), 36.3, 32.8, 32.5 (q, J_{C-F} = 1.0 Hz), 29.9, 21.9, 13.6. FT-IR: ν (cm-1) 2963, 2933, 2875, 2216, 1687, 1100. HRMS [ESI] calcd for $C_{17}H_{18}F_4NOS$ $[M+H]^+$ 360.1040, found 360.1046.

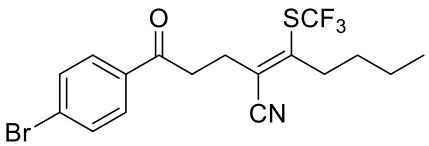


2c

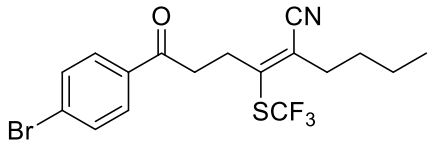


2c'

White solid (**2c**: **2c'** = 3.0:1), m.p. 34-35 °C. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.92-7.87 (m, 2H, major/ minor), 7.47-7.42 (m, 2H, major/ minor), 3.32-3.28 (m, 2H, minor), 3.27-3.23 (m, 2H, major), 3.19 (t, *J* = 7.2 Hz, 2H, minor), 2.97 (t, *J* = 7.2 Hz, 2H, major), 2.78 (t, *J* = 7.6 Hz, 2H, major), 2.57 (t, *J* = 7.6 Hz, 2H, minor), 1.68-1.52 (m, 2H, major/ minor), 1.40-1.30 (m, 2H, major/ minor), 0.94 (t, *J* = 7.2 Hz, 3H, minor), 0.93 (t, *J* = 7.2 Hz, 3H, major); ^{19}F NMR (376 MHz, $CDCl_3$) δ -38.0 (s, major), -38.2 (s, minor); ^{13}C NMR (100 MHz, $CDCl_3$) δ (major) 196.0, 148.0 (q, $J_{C\text{-}F}$ = 1.5 Hz), 140.0, 134.5, 129.4, 129.0, 128.5 (q, $J_{C\text{-}F}$ = 308.5 Hz), 121.2 (q, $J_{C\text{-}F}$ = 1.8 Hz), 116.2, 37.8 (q, $J_{C\text{-}F}$ = 0.9 Hz), 35.9, 30.3, 27.0, 21.9, 13.6; (minor) 196.0, 143.7 (q, $J_{C\text{-}F}$ = 1.4 Hz), 139.9, 134.5, 129.4, 129.0, 128.4 (q, $J_{C\text{-}F}$ = 309.0 Hz), 125.8 (q, $J_{C\text{-}F}$ = 1.7 Hz), 116.3, 36.3, 32.8, 32.4 (q, $J_{C\text{-}F}$ = 0.9 Hz), 29.9, 21.9, 13.6. FT-IR: ν (cm^{-1}) 2960, 2931, 2876, 2215, 1684, 1103. HRMS [ESI] calcd for $C_{17}H_{18}ClF_3NOS$ $[M+H]^+$ 376.0744, found 376.0741.

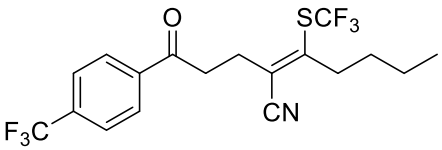


2d

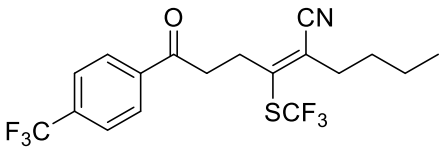


2d'

Yellow solid (**2d**: **2d'** = 3.0:1), m.p. 42-43 °C. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.85-7.79 (m, 2H, major/ minor), 7.65-7.59 (m, 2H, major/ minor), 3.32-3.27 (m, 2H, minor), 3.26-3.23 (m, 2H, major), 3.19 (t, *J* = 7.2 Hz, 2H, minor), 2.97 (t, *J* = 7.2 Hz, 2H, major), 2.78 (t, *J* = 7.6 Hz, 2H, major), 2.58 (t, *J* = 7.6 Hz, 2H, minor), 1.68-1.53 (m, 2H, major/ minor), 1.40-1.31 (m, 2H, major/ minor), 0.94 (t, *J* = 7.2 Hz, 3H, minor), 0.93 (t, *J* = 7.2 Hz, 3H, major); ^{19}F NMR (376 MHz, $CDCl_3$) δ -38.0 (s, major), -38.2 (s, minor); ^{13}C NMR (100 MHz, $CDCl_3$) δ (major) 196.2, 148.1 (q, $J_{C\text{-}F}$ = 1.5 Hz), 134.9, 132.1, 129.5, 128.8, 128.5 (q, $J_{C\text{-}F}$ = 308.7 Hz), 121.2 (q, $J_{C\text{-}F}$ = 1.8 Hz), 116.2, 37.9 (q, $J_{C\text{-}F}$ = 0.9 Hz), 35.9, 30.3, 27.0, 21.9, 13.6; (minor) 196.1, 143.7 (q, $J_{C\text{-}F}$ = 1.3 Hz), 134.9, 132.0, 129.5, 128.7, 128.4 (q, $J_{C\text{-}F}$ = 308.9 Hz), 125.8 (q, $J_{C\text{-}F}$ = 1.7 Hz), 116.3, 36.3, 32.8, 32.4 (q, $J_{C\text{-}F}$ = 0.7 Hz), 29.9, 21.9, 13.6. FT-IR: ν (cm^{-1}) 2959, 2931, 2215, 1683, 1102. HRMS [ESI] calcd for $C_{17}H_{18}BrF_3NOS$ $[M+H]^+$ 420.0239, found 420.0214.



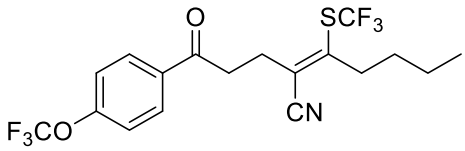
2e



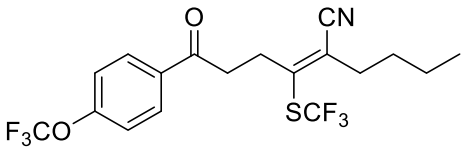
2e'

Yellow oil (**2e**: **2e'** = 3.0:1). ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.06 (d, *J* = 8.0 Hz, 2H, major/ minor), 7.75 (d, *J* = 8.4 Hz, 2H, major/ minor), 3.39-3.34 (m, 2H, minor), 3.31 (t, *J* = 7.2 Hz, 2H, major), 3.22 (t, *J* = 7.2 Hz, 2H, minor), 3.00 (t, *J* = 7.2 Hz, 2H, major), 2.79 (t, *J* = 7.2 Hz, 2H, major), 2.59 (t, *J* = 7.6 Hz, 2H, minor), 1.68-1.55 (m, 2H, major/ minor), 1.41-1.31 (m, 2H, major/ minor), 0.95 (t, *J* = 7.2 Hz, 3H, minor), 0.94 (t, *J* = 7.2 Hz, 3H, major); ^{19}F NMR (376 MHz, $CDCl_3$) δ

-38.0 (s, major), -38.2 (s, minor), -63.2 (s, minor), -63.2 (s, major); ^{13}C NMR (100 MHz, $CDCl_3$) δ (major) 196.3, 148.2 (q, J_{C-F} = 1.2 Hz), 138.8 (q, J_{C-F} = 0.9 Hz), 134.8 (q, J_{C-F} = 32.6 Hz), 128.3, 128.5 (q, J_{C-F} = 308.6 Hz), 125.8 (q, J_{C-F} = 3.6 Hz), 123.5 (q, J_{C-F} = 271.1 Hz), 121.1 (q, J_{C-F} = 1.7 Hz), 116.2, 37.9 (q, J_{C-F} = 0.9 Hz), 36.2, 30.3, 26.9, 21.9, 13.6; (minor) 196.2, 143.5 (q, J_{C-F} = 1.3 Hz), 138.8 (q, J_{C-F} = 1.0 Hz), 134.7 (q, J_{C-F} = 32.5 Hz), 128.3, 128.4 (q, J_{C-F} = 308.9 Hz), 126.0 (q, J_{C-F} = 1.7 Hz), 123.5 (q, J_{C-F} = 271.0 Hz), 116.3, 36.6, 32.8, 32.3 (q, J_{C-F} = 0.9 Hz), 30.0, 21.9, 13.6. FT-IR: ν (cm^{-1}) 2964, 2935, 2876, 2216, 1694, 1442, 1100. HRMS [ESI] calcd for $C_{18}H_{18}F_6NOS$ $[M+H]^+$ 410.1008, found 410.1003.

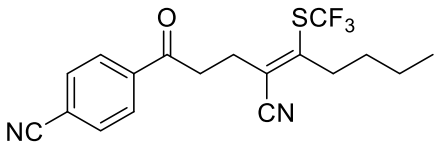


2f

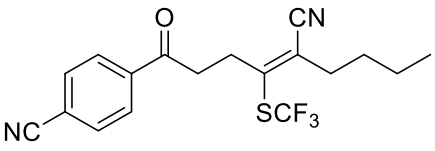


2f'

Yellow solid (**2f**: **2f'** = 3.0:1), m.p. 34-35 °C. ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.04-7.99 (m, 2H, major/ minor), 7.30 (d, *J* = 8.0 Hz, 2H, major/ minor), 3.33 (t, *J* = 7.6 Hz, 2H, minor), 3.27 (t, *J* = 7.2 Hz, 2H, major), 3.21 (t, *J* = 7.2 Hz, 2H, minor), 2.98 (t, *J* = 7.2 Hz, 2H, major), 2.78 (t, *J* = 7.6 Hz, 2H, major), 2.58 (t, *J* = 7.6 Hz, 2H, minor), 1.68-1.55 (m, 2H, major/ minor), 1.41-1.30 (m, 2H, major/ minor), 0.94 (t, *J* = 7.2 Hz, 3H, minor), 0.93 (t, *J* = 7.2 Hz, 3H, major); ^{19}F NMR (376 MHz, $CDCl_3$) δ -38.1 (s, major), -38.2 (s, minor), -57.7 (s, major/ minor); ^{13}C NMR (100 MHz, $CDCl_3$) δ (major) 195.7, 152.9 (q, J_{C-F} = 1.6 Hz), 148.1 (q, J_{C-F} = 1.4 Hz), 134.4, 130.1, 128.5 (q, J_{C-F} = 309.2 Hz), 121.2 (q, J_{C-F} = 1.8 Hz), 120.5, 120.2 (q, J_{C-F} = 257.5 Hz), 116.2, 37.9 (q, J_{C-F} = 0.7 Hz), 35.9, 30.3, 27.0, 21.9, 13.6; (minor) 195.6, 152.8 (q, J_{C-F} = 1.8 Hz), 143.7 (q, J_{C-F} = 1.3 Hz), 134.4, 130.1, 128.5 (q, J_{C-F} = 309.2 Hz), 125.9 (q, J_{C-F} = 1.6 Hz), 120.5, 120.2 (q, J_{C-F} = 257.5 Hz), 116.3, 36.4, 32.8, 32.4 (q, J_{C-F} = 0.7 Hz), 29.9, 21.9, 13.6. FT-IR: ν (cm^{-1}) 2963, 2934, 2866, 2216, 1691, 1255, 1135. HRMS [ESI] calcd for $C_{18}H_{18}F_6NO_2S$ $[M+H]^+$ 426.0957, found 426.0959.



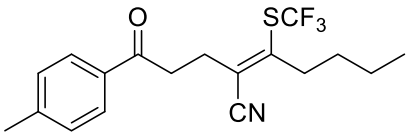
2g



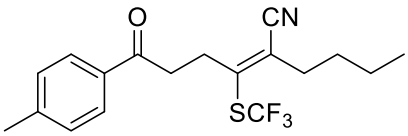
2g'

Yellow oil (**2g**: **2g'** = 2.1:1). ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.05 (d, *J* = 8.4 Hz, 2H, major/ minor), 7.79 (d, *J* = 8.4 Hz, 2H, major/ minor), 3.36-3.33 (m, 2H, minor), 3.20 (t, *J* = 7.2 Hz, 2H, major), 3.21 (t, *J* = 7.2 Hz, 2H, minor), 2.99 (t, *J* = 7.2 Hz, 2H, major), 2.78 (t, *J* = 7.2 Hz, 2H, major), 2.58 (t, *J* = 7.6 Hz, 2H, minor), 1.67-1.53 (m, 2H, major/ minor), 1.42-1.30 (m, 2H, major/ minor), 0.94 (t, *J* = 7.2 Hz, 3H, minor), 0.93 (t, *J* = 7.2 Hz, 3H, major); ^{19}F NMR (376 MHz, $CDCl_3$) δ -38.0 (s, major), -38.1 (s, minor); ^{13}C NMR (100 MHz, $CDCl_3$) δ (major) 195.9, 148.4 (q, J_{C-F} = 1.4 Hz), 139.0, 132.6, 128.4, 128.4 (q, J_{C-F} = 308.7 Hz), 120.9 (q, J_{C-F} = 1.8 Hz), 117.7, 116.8, 116.1, 37.9 (q, J_{C-F} = 0.6 Hz), 36.3, 30.3, 26.8, 21.9, 13.6; (minor) 195.8, 143.3 (q, J_{C-F} = 1.4 Hz), 139.0, 132.6, 128.4, 128.3 (q, J_{C-F} = 309.1 Hz), 126.1 (q, J_{C-F} = 1.7 Hz), 117.7, 116.7, 116.2, 36.7, 32.8, 32.2 (q, J_{C-F} = 0.6 Hz), 29.9, 21.9, 13.6. FT-IR: ν (cm^{-1}) 2968, 2902, 2228, 2215, 1695, 1106.

HRMS [ESI] calcd for $C_{18}H_{18}F_3N_2OS$ $[M+H]^+$ 367.1086, found 367.1077.

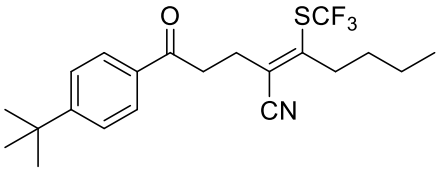


2h

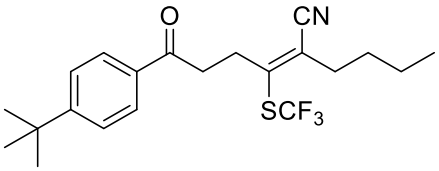


2h'

Yellow oil (**2h**: **2h'** = 3.1:1). ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.86 (d, *J* = 8.0 Hz, 2H, major/ minor), 7.27 (d, *J* = 7.2 Hz, 2H, major/ minor), 3.34-3.30 (m, 2H, minor), 3.26 (t, *J* = 7.2 Hz, 2H, major), 3.20 (t, *J* = 7.2 Hz, 2H, minor), 2.97 (t, *J* = 7.2 Hz, 2H, major), 2.78 (t, *J* = 7.2 Hz, 2H, major), 2.58 (t, *J* = 7.6 Hz, 2H, minor), 2.41 (s, 3H, major/ minor), 1.68-1.55 (m, 2H, major/ minor), 1.40-1.31 (m, 2H, major/ minor), 0.94 (t, *J* = 7.6 Hz, 3H, minor), 0.93 (t, *J* = 7.6 Hz, 3H, major); ^{19}F NMR (376 MHz, $CDCl_3$) δ -38.1 (s, major), -38.3 (s, minor); ^{13}C NMR (100 MHz, $CDCl_3$) δ (major) 196.8, 147.8 (q, $J_{C\text{-}F}$ = 1.4 Hz), 144.4, 133.7, 129.4, 128.5 (q, $J_{C\text{-}F}$ = 308.5 Hz), 128.1, 121.5 (q, $J_{C\text{-}F}$ = 1.8 Hz), 116.3, 37.8 (q, $J_{C\text{-}F}$ = 0.8 Hz), 35.8, 30.3, 27.2, 21.9, 21.6, 13.6; (minor) 196.7, 144.2, 144.1 (q, $J_{C\text{-}F}$ = 1.4 Hz), 133.8, 129.3, 128.1 (q, $J_{C\text{-}F}$ = 308.7 Hz), 128.1, 125.5 (q, $J_{C\text{-}F}$ = 1.7 Hz), 116.3, 36.3, 32.8, 32.6 (q, $J_{C\text{-}F}$ = 0.8 Hz), 29.9, 21.9, 21.6, 13.6. FT-IR: ν (cm^{-1}) 2961, 2932, 2865, 2216, 1683, 1102. HRMS [ESI] calcd for $C_{18}H_{21}F_3NOS$ $[M+H]^+$ 356.1290, found 356.1296.

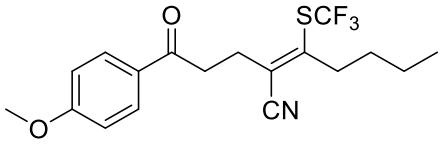


2i

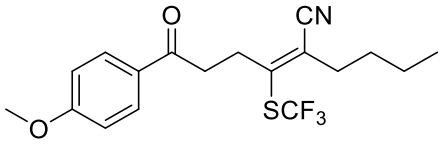


2i'

Yellow oil (**2i**: **2i'** = 3.2:1). ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.90 (d, *J* = 8.4 Hz, 2H, major/ minor), 7.49 (d, *J* = 8.4 Hz, 2H, major/ minor), 3.35-3.30 (m, 2H, minor), 3.27 (t, 2H, *J* = 7.2 Hz, major), 3.20 (t, 2H, *J* = 7.2 Hz, minor), 2.98 (t, *J* = 7.2 Hz, 2H, major), 2.78 (t, *J* = 7.6 Hz, 2H, major), 2.58 (t, *J* = 7.6 Hz, 2H, minor), 1.68-1.54 (m, 2H, major/ minor), 1.42-1.36 (m, 2H, major/ minor), 1.34 (s, 9H, major/ minor), 0.95 (t, *J* = 7.2 Hz, 3H, minor), 0.94 (t, *J* = 7.2 Hz, 3H, major); ^{19}F NMR (376 MHz, $CDCl_3$) δ -38.1 (s, major), -38.3 (s, minor); ^{13}C NMR (100 MHz, $CDCl_3$) δ (major) 196.9, 157.3, 147.8 (q, $J_{C\text{-}F}$ = 1.4 Hz), 133.6, 128.5 (q, $J_{C\text{-}F}$ = 308.6 Hz), 128.0, 125.6, 121.6 (q, $J_{C\text{-}F}$ = 1.8 Hz), 116.3, 37.8 (q, $J_{C\text{-}F}$ = 0.8 Hz), 35.8, 35.1, 31.0, 30.3, 27.2, 21.9, 13.6; (minor) 196.8, 157.2, 144.1 (q, $J_{C\text{-}F}$ = 1.4 Hz), 133.7, 128.0, 128.4 (q, $J_{C\text{-}F}$ = 308.8 Hz), 125.6, 125.5 (q, $J_{C\text{-}F}$ = 1.8 Hz), 116.3, 36.3, 32.8, 32.6 (q, $J_{C\text{-}F}$ = 0.9 Hz), 31.0, 29.9, 27.2, 21.9, 13.6. FT-IR: ν (cm^{-1}) 2963, 2873, 2215, 1683, 1364, 1102. HRMS [ESI] calcd for $C_{21}H_{27}F_3NOS$ $[M+H]^+$ 398.1760, found 398.1769.

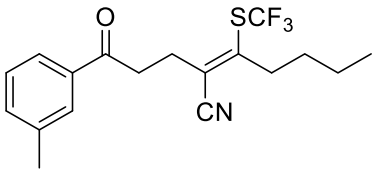


2j

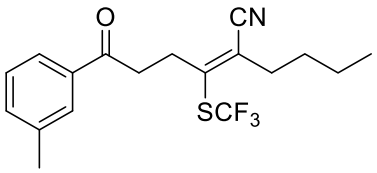


2j'

Yellow oil (**2j**: **2j'** = 3.2:1). ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.94 (d, *J* = 9.2 Hz, 2H, major/ minor), 6.94 (d, *J* = 8.8 Hz, 2H, major/ minor), 3.87 (s, 3H, major/ minor), 3.31-3.26 (m, 2H, minor), 3.23 (t, 2H, *J* = 7.2 Hz, major), 3.21-3.17 (m, 2H, minor), 2.96 (t, *J* = 7.2 Hz, 2H, major), 2.77 (t, *J* = 7.6 Hz, 2H, major), 2.57 (t, *J* = 7.6 Hz, 2H, minor), 1.67-1.54 (m, 2H, major/ minor), 1.40-1.30 (m, 2H, major/ minor), 0.94 (t, *J* = 7.2 Hz, 3H, minor), 0.93 (t, *J* = 7.2 Hz, 3H, major); ^{19}F NMR (376 MHz, $CDCl_3$) δ -38.1 (s, major), -38.3 (s, minor); ^{13}C NMR (100 MHz, $CDCl_3$) δ (major) 195.7, 163.8, 147.8 (q, J_{C-F} = 1.4 Hz), 130.3, 129.3, 128.5 (q, J_{C-F} = 308.5 Hz), 121.6 (q, J_{C-F} = 1.8 Hz), 116.3, 113.8, 55.5, 37.8 (q, J_{C-F} = 0.9 Hz), 35.5, 30.3, 27.3, 21.9, 13.6; (minor) 195.6, 163.7, 144.2 (q, J_{C-F} = 1.5 Hz), 130.3, 129.3, 128.4 (q, J_{C-F} = 308.7 Hz), 125.5 (q, J_{C-F} = 1.7 Hz), 116.3, 113.8, 55.5, 36.1, 32.8, 29.9, 21.9, 13.6. FT-IR: ν (cm^{-1}) 2961, 2934, 2875, 2215, 1677, 1442, 1100. HRMS [ESI] calcd for $C_{18}H_{21}F_3NO_2S$ $[M+H]^+$ 372.1240, found 372.1250.

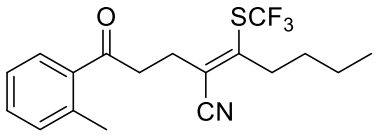


2k

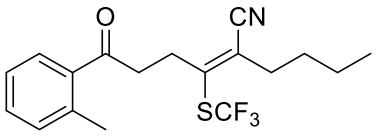


2k'

Yellow oil (**2k**: **2k'** = 3.2:1). ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.79-7.73 (m, 2H, major/ minor), 7.42-7.33 (m, 2H, major/ minor), 3.35-3.30 (m, 2H, minor), 3.27 (t, *J* = 7.2 Hz, 2H, major), 3.20 (t, *J* = 7.2 Hz, 2H, minor), 2.97 (t, *J* = 7.2 Hz, 2H, major), 2.78 (t, *J* = 7.6 Hz, 2H, major), 2.58 (t, *J* = 7.6 Hz, 2H, minor), 2.42 (s, 3H, major/ minor), 1.68-1.54 (m, 2H, major/ minor), 1.41-1.31 (m, 2H, major/ minor), 0.95 (t, *J* = 7.2 Hz, 3H, minor), 0.94 (t, *J* = 7.2 Hz, 3H, major); ^{19}F NMR (376 MHz, $CDCl_3$) δ -38.1 (s, major), -38.3 (s, minor); ^{13}C NMR (100 MHz, $CDCl_3$) δ (major) 197.4, 147.8 (q, J_{C-F} = 1.4 Hz), 138.5, 136.2, 134.3, 128.6, 128.5, 128.5 (q, J_{C-F} = 308.6 Hz), 125.2, 121.5 (q, J_{C-F} = 1.7 Hz), 116.3, 37.8 (q, J_{C-F} = 0.9 Hz), 35.9, 30.3, 27.2, 21.9, 21.3, 13.6; (minor) 197.3, 144.1 (q, J_{C-F} = 1.4 Hz), 138.5, 136.3, 134.2, 128.5, 128.5, 128.4 (q, J_{C-F} = 308.7 Hz), 125.6 (q, J_{C-F} = 1.7 Hz), 125.2, 116.3, 36.4, 32.8, 32.6 (q, J_{C-F} = 0.9 Hz), 29.9, 21.9, 21.3, 13.6. FT-IR: ν (cm^{-1}) 2961, 2932, 2865, 2216, 1686, 1440, 1102. HRMS [ESI] calcd for $C_{18}H_{21}F_3NOS$ $[M+H]^+$ 356.1290, found 356.1291.



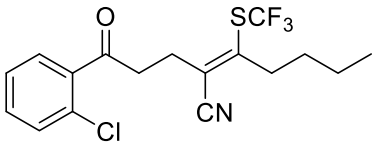
2l



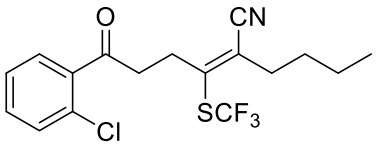
2l'

Yellow oil (**2l**: **2l'** = 4.4:1). ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.70-7.66 (m, 1H, major/ minor), 7.43-7.36 (m, 1H, major/ minor), 7.31-7.24 (m, 2H, major/ minor), 3.29-3.25 (m, 2H, minor), 3.22 (t, *J* = 7.2 Hz, 2H, major), 3.20-3.17 (m, 2H, minor), 2.96 (t, *J* = 7.2 Hz, 2H, major), 2.78 (t, *J* = 7.6 Hz, 2H, major), 2.58 (t, *J* = 7.6 Hz, 2H, minor), 2.51 (s, 3H, major/ minor), 1.68-1.54 (m, 2H, major/ minor), 1.42-1.32 (m, 2H, major/ minor), 0.94 (t, *J* = 7.6 Hz, 3H, major/ minor); ^{19}F NMR (376 MHz, $CDCl_3$) δ -38.0 (s, major), -38.2 (s, minor); ^{13}C NMR (100 MHz, $CDCl_3$) δ (major) 200.7, 147.8 (q, J_{C-F} = 1.4 Hz), 138.5, 136.7, 132.2, 131.8, 128.6, 128.6 (q, J_{C-F} = 308.6 Hz), 125.8,

121.6 (q, J_{C-F} = 1.7 Hz), 116.3, 38.5, 37.8 (q, J_{C-F} = 0.8 Hz), 30.3, 27.3, 21.9, 21.4, 13.6; (minor) 200.7, 144.2 (q, J_{C-F} = 1.4 Hz), 138.5, 136.8, 132.2, 131.7, 128.5, 128.4 (q, J_{C-F} = 308.9 Hz), 125.8, 125.4 (q, J_{C-F} = 1.7 Hz), 116.3, 39.0, 32.7, 30.0, 21.9, 21.4, 13.6. FT-IR: ν (cm^{-1}) 2962, 2932, 2875, 2215, 1686, 1487, 1100. HRMS [ESI] calcd for $C_{18}H_{21}F_3NOS$ $[M+H]^+$ 356.1290, found 356.1297.

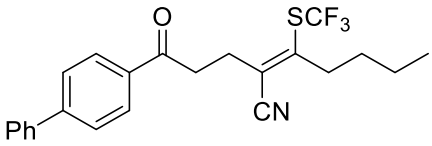


2m

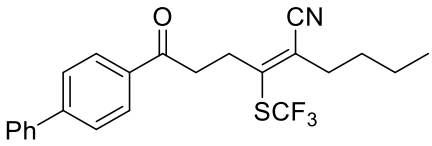


2m'

Yellow oil (**2m**: **2m'** = 6.1:1). ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.53-7.48 (m, 1H, major/ minor), 7.45-7.38 (m, 2H, major/ minor), 7.37-7.31 (m, 1H, major/ minor), 3.32 (t, *J* = 7.2 Hz, 2H, minor), 3.27 (t, *J* = 7.2 Hz, 2H, major), 3.20 (t, *J* = 7.2 Hz, 2H, minor), 2.98 (t, *J* = 7.2 Hz, 2H, major), 2.78 (t, *J* = 7.6 Hz, 2H, major), 2.57 (t, *J* = 7.6 Hz, 2H, minor), 1.68-1.54 (m, 2H, major/ minor), 1.41-1.321 (m, 2H, major/ minor), 0.94 (t, *J* = 7.2 Hz, 3H, major/ minor); ^{19}F NMR (376 MHz, $CDCl_3$) δ -38.0 (s, major), -38.2 (s, minor); ^{13}C NMR (100 MHz, $CDCl_3$) δ (major) 200.2, 148.1 (q, J_{C-F} = 1.4 Hz), 138.3, 132.2, 131.0, 130.7, 129.1, 128.5 (q, J_{C-F} = 308.6 Hz), 127.1, 121.1 (q, J_{C-F} = 1.7 Hz), 116.2, 40.2, 37.9 (q, J_{C-F} = 0.8 Hz), 30.3, 27.2, 21.9, 13.7; (minor) 200.2, 143.6 (q, J_{C-F} = 1.3 Hz), 138.5, 132.1, 131.0, 130.6, 129.1, 128.4 (q, J_{C-F} = 309.0 Hz), 127.1, 125.8 (q, J_{C-F} = 1.7 Hz), 116.2, 40.6, 32.8, 32.6 (q, J_{C-F} = 1.1 Hz), 29.9, 21.9, 13.7. FT-IR: ν (cm^{-1}) 2961, 2932, 2875, 2215, 1700, 1433, 1100. HRMS [ESI] calcd for $C_{17}H_{18}ClF_3NOS$ $[M+H]^+$ 376.0744, found 376.0741.

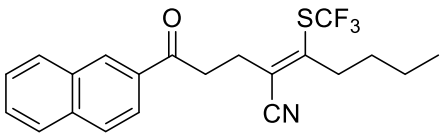


2n

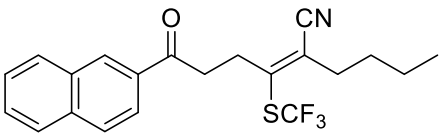


2n'

Yellow oil (**2n**: **2n'** = 3.2:1). ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.04 (d, *J* = 8.4 Hz, 2H, major/ minor), 7.71 (d, *J* = 8.4 Hz, 2H, major/ minor), 7.63 (d, *J* = 7.6 Hz, 2H, major/ minor), 7.50-7.46 (m, 2H, major/ minor), 7.41 (t, *J* = 7.2 Hz, 1H, major/ minor), 3.41-3.36 (m, 2H, minor), 3.33 (t, *J* = 7.2 Hz, 2H, major), 3.24 (t, *J* = 7.2 Hz, 2H, minor), 3.02 (t, *J* = 7.2 Hz, 2H, major), 2.80 (t, *J* = 7.6 Hz, 2H, major), 2.60 (t, *J* = 7.6 Hz, 2H, minor), 1.70-1.55 (m, 2H, major/ minor), 1.42-1.32 (m, 2H, major/ minor), 0.96 (t, *J* = 7.2 Hz, 3H, minor), 0.95 (t, *J* = 7.2 Hz, 3H, major); ^{19}F NMR (376 MHz, $CDCl_3$) δ -38.0 (s, major), -38.2 (s, minor); ^{13}C NMR (100 MHz, $CDCl_3$) δ (major) 196.8, 147.9 (q, J_{C-F} = 1.5 Hz), 146.2, 139.7, 134.9, 128.9, 128.6, 128.5 (q, J_{C-F} = 308.5 Hz), 128.3, 127.3, 127.2, 121.5 (q, J_{C-F} = 1.8 Hz), 116.3, 37.8 (q, J_{C-F} = 0.7 Hz), 35.9, 30.3, 27.2, 21.9, 13.7; (minor) 196.7, 146.1, 144.0 (q, J_{C-F} = 1.4 Hz), 139.7, 134.9, 128.9, 128.6, 128.4 (q, J_{C-F} = 308.9 Hz), 128.3, 127.3, 127.2, 125.7 (q, J_{C-F} = 1.8 Hz), 116.3, 36.4, 32.8, 32.6 (q, J_{C-F} = 0.7 Hz), 30.0, 21.9, 13.7. FT-IR: ν (cm^{-1}) 2967, 2928, 2216, 1678, 1404, 1076. HRMS [ESI] calcd for $C_{23}H_{23}F_3NOS$ $[M+H]^+$ 418.1447, found 418.1457.

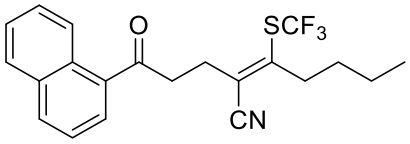


2o

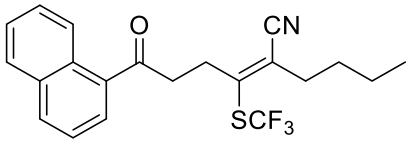


2o'

Yellow solid (**2o**: **2o'** = 3.0:1), m.p. 49-50 °C. ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.49 (s, 1H, major/ minor), 8.04-8.01 (m, 1H, major/ minor), 7.98 (d, *J* = 8.0 Hz, 1H, major/ minor), 7.93-7.87 (m, 2H, major/ minor), 7.65-7.54 (m, 2H, major/ minor), 3.48 (t, *J* = 7.2 Hz, 2H, minor), 3.43 (t, *J* = 7.2 Hz, 2H, major), 3.28 (t, *J* = 7.2 Hz, 2H, minor), 3.05 (t, *J* = 7.2 Hz, 2H, major), 2.80 (t, *J* = 7.6 Hz, 2H, major), 2.60 (t, *J* = 7.6 Hz, 2H, minor), 1.69-1.55 (m, 2H, major/ minor), 1.45-1.31 (m, 2H, major/ minor), 0.96 (t, *J* = 7.2 Hz, 3H, minor), 0.94 (t, *J* = 7.2 Hz, 3H, major); ^{19}F NMR (376 MHz, $CDCl_3$) δ -38.0 (s, major), -38.2 (s, minor); ^{13}C NMR (100 MHz, $CDCl_3$) δ (major) 197.2, 148.0 (q, $J_{C\text{-}F}$ = 1.4 Hz), 135.8, 133.5, 132.5, 129.8, 129.6, 128.7, 128.6, 128.6 (q, $J_{C\text{-}F}$ = 308.6 Hz), 127.8, 126.9, 123.6, 121.5 (q, $J_{C\text{-}F}$ = 1.8 Hz), 116.4, 37.9 (q, $J_{C\text{-}F}$ = 0.8 Hz), 36.0, 30.3, 27.3, 21.9, 13.7; (minor) 197.1, 144.1 (q, $J_{C\text{-}F}$ = 1.3 Hz), 135.7, 133.6, 132.5, 129.8, 129.6, 128.7, 128.6, 127.8, 126.9, 125.7 (q, $J_{C\text{-}F}$ = 1.5 Hz), 123.6, 116.4, 36.5, 32.8, 32.8 (q, $J_{C\text{-}F}$ = 0.8 Hz), 30.0, 21.9, 13.7. FT-IR: ν (cm^{-1}) 2967, 2931, 2881, 2210, 1678, 1106. HRMS [ESI] calcd for $C_{21}H_{21}F_3NOS$ $[M+H]^+$ 392.1290, found 392.1299.

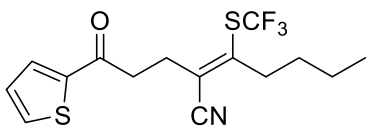


2p

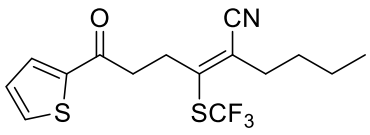


2p'

Yellow oil (**2p**: **2p'** = 4.7:1). ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.64 (d, *J* = 8.4 Hz, 1H, major/ minor), 8.02 (d, *J* = 8.0 Hz, 1H, major/ minor), 7.94-7.91 (m, 1H, major/ minor), 7.89 (d, *J* = 8.4 Hz, 1H, major/ minor), 7.64-7.59 (m, 1H, major/ minor), 7.58-7.49 (m, 2H, major/ minor), 3.46-3.42 (m, 2H, minor), 3.39 (t, *J* = 7.2 Hz, 2H, major), 3.29 (t, *J* = 7.2 Hz, 2H, minor), 3.06 (t, *J* = 7.2 Hz, 2H, major), 2.80 (t, *J* = 7.6 Hz, 2H, major), 2.58 (t, *J* = 7.6 Hz, 2H, minor), 1.68-1.54 (m, 2H, major/ minor), 1.43-1.32 (m, 2H, major/ minor), 0.95 (t, *J* = 7.2 Hz, 3H, minor), 0.94 (t, *J* = 7.2 Hz, 3H, major); ^{19}F NMR (376 MHz, $CDCl_3$) δ -38.0 (s, major), -38.2 (s, minor); ^{13}C NMR (100 MHz, $CDCl_3$) δ (major) 201.0, 148.0 (q, $J_{C\text{-}F}$ = 1.4 Hz), 134.7, 134.0, 133.3, 130.0, 128.6 (q, $J_{C\text{-}F}$ = 308.6 Hz), 128.5, 128.2, 128.0, 126.6, 125.6, 124.3, 121.5 (q, $J_{C\text{-}F}$ = 1.8 Hz), 116.3, 39.0, 37.9 (q, $J_{C\text{-}F}$ = 0.7 Hz), 30.3, 27.5, 21.9, 13.7; (minor) 201.0, 144.0 (q, $J_{C\text{-}F}$ = 1.4 Hz), 134.8, 134.0, 133.2, 130.1, 128.4, 128.2, 127.9, 126.6, 125.7, 124.3, 116.3, 39.5, 37.8, 33.0 (q, $J_{C\text{-}F}$ = 0.7 Hz), 30.0, 21.9, 13.7. FT-IR: ν (cm^{-1}) 3052, 2961, 2932, 2874, 2215, 1681, 1097. HRMS [ESI] calcd for $C_{21}H_{21}F_3NOS$ $[M+H]^+$ 392.1290, found 392.1296.



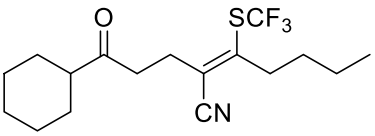
2q



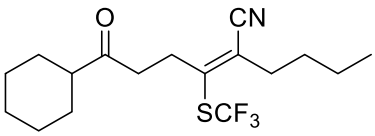
2q'

Yellow oil (**2q**: **2q'** = 2.5:1). ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.77-7.73 (m, 1H, major/ minor),

7.68-7.65 (m, 1H, major/ minor), 7.17-7.13 (m, 1H, major/ minor), 3.30-3.26 (m, 2H, minor), 3.24-3.21 (m, 2H, major), 3.20-3.18 (m, 2H, minor), 2.98 (t, J = 7.6 Hz, 2H, major), 2.77 (t, J = 7.6 Hz, 2H, major), 2.57 (t, J = 7.6 Hz, 2H, minor), 1.66-1.52 (m, 2H, major/ minor), 1.40-1.28 (m, 2H, major/ minor), 0.97-0.91 (m, 3H, major/ minor); ^{19}F NMR (376 MHz, $CDCl_3$) δ -38.0 (s, major), -38.2 (s, minor); ^{13}C NMR (100 MHz, $CDCl_3$) δ (major) 190.1, 148.2 (q, $J_{C\text{-}F}$ = 1.3 Hz), 143.3, 134.2, 132.2, 128.5 (q, $J_{C\text{-}F}$ = 308.5 Hz), 128.2, 121.1 (q, $J_{C\text{-}F}$ = 1.8 Hz), 116.2, 37.8 (d, $J_{C\text{-}F}$ = 0.9 Hz), 36.4, 30.3, 27.3, 21.9, 13.6; (minor) 190.0, 143.6 (q, $J_{C\text{-}F}$ = 1.4 Hz), 143.3, 134.1, 132.1, 128.4 (q, $J_{C\text{-}F}$ = 308.8 Hz), 128.2, 125.9 (q, $J_{C\text{-}F}$ = 1.8 Hz), 116.2, 36.9, 32.8, 32.8 (q, $J_{C\text{-}F}$ = 0.9 Hz), 29.9, 21.9, 13.6. FT-IR: ν (cm^{-1}) 2961, 2874, 2216, 1665, 1415, 1101. HRMS [ESI] calcd for $C_{15}H_{17}F_3NOS_2$ $[M+H]^+$ 348.0698, found 348.0699.

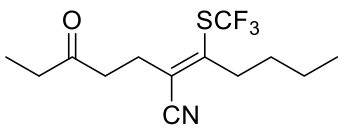


2r

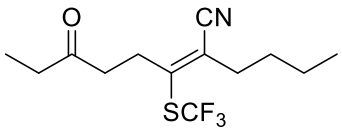


2r'

Yellow oil (**2r**: **2r'** = 5.8:1). ^{1}H NMR (400 MHz, $CDCl_3$) δ 3.00 (t, J = 7.2 Hz, 2H, minor), 2.82-2.71 (m, 6H, major & 2H, minor, overlap), 2.54 (t, J = 7.6 Hz, 2H, minor), 2.40-2.31 (m, 1H, major/ minor), 1.88-1.74 (m, 4H, major/ minor), 1.71-1.51 (m, 3H, major/ minor), 1.40-1.15 (m, 7H, major/ minor), 0.94 (t, J = 7.6 Hz, 3H, major/ minor); ^{19}F NMR (376 MHz, $CDCl_3$) δ -38.1 (s, major), -38.3 (s, minor); ^{13}C NMR (100 MHz, $CDCl_3$) δ (major) 211.2, 147.6 (q, $J_{C\text{-}F}$ = 1.4 Hz), 128.5 (q, $J_{C\text{-}F}$ = 308.5 Hz), 121.5 (q, $J_{C\text{-}F}$ = 1.7 Hz), 116.2, 50.7, 37.8 (q, $J_{C\text{-}F}$ = 1.1 Hz), 37.6, 32.7, 30.3, 28.4, 26.7, 25.7, 25.5, 21.8, 13.6; (minor) 211.0, 144.3 (q, $J_{C\text{-}F}$ = 1.4 Hz), 125.1 (q, $J_{C\text{-}F}$ = 1.7 Hz), 116.3, 50.7, 38.1, 32.6, 32.2 (q, $J_{C\text{-}F}$ = 1.1 Hz), 29.9, 28.7, 25.7, 25.6, 21.9, 13.6. FT-IR: ν (cm^{-1}) 2931, 2857, 2215, 1710, 1450, 1102. HRMS [ESI] calcd for $C_{17}H_{25}F_3NOS$ $[M+H]^+$ 348.1603, found 348.1604.

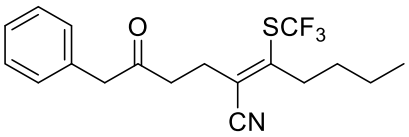


2s

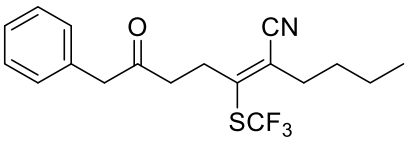


2s'

Yellow oil (**2s**: **2s'** = 5.2:1). ^{1}H NMR (400 MHz, $CDCl_3$) δ 3.05-3.00 (m, 2H, minor), 2.84-2.68 (m, 6H, major & 1H, minor, overlap), 2.65-2.51 (m, 3H, minor), 2.50-2.42 (m, 2H, major/ minor), 1.66-1.51 (m, 2H, major/ minor), 1.40-1.29 (m, 2H, major/ minor), 1.07 (t, J = 7.6 Hz, 3H, major/ minor), 0.93 (t, J = 7.6 Hz, 3H, major/ minor); ^{19}F NMR (376 MHz, $CDCl_3$) δ -38.1 (s, major), -38.3 (s, minor); ^{13}C NMR (100 MHz, $CDCl_3$) δ (major) 208.5, 147.7 (q, $J_{C\text{-}F}$ = 1.4 Hz), 128.5 (q, $J_{C\text{-}F}$ = 308.5 Hz), 121.4 (q, $J_{C\text{-}F}$ = 1.8 Hz), 116.2, 39.2, 37.8 (q, $J_{C\text{-}F}$ = 0.6 Hz), 36.0, 30.3, 26.7, 21.9, 13.6, 7.7; (minor) 208.3, 144.0 (q, $J_{C\text{-}F}$ = 1.3 Hz), 128.4 (q, $J_{C\text{-}F}$ = 308.5 Hz), 125.3 (q, $J_{C\text{-}F}$ = 1.6 Hz), 116.3, 39.8, 35.8, 32.7, 32.2 (q, $J_{C\text{-}F}$ = 1.1 Hz), 29.9, 21.9, 13.6, 7.7. FT-IR: ν (cm^{-1}) 2963, 2937, 2877, 2215, 1718, 1100. HRMS [ESI] calcd for $C_{13}H_{19}F_3NOS$ $[M+H]^+$ 294.1134, found 294.1144.

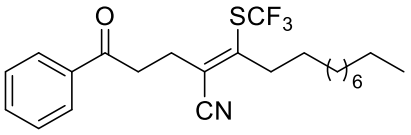


2t

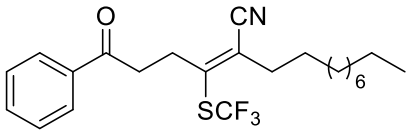


2t'

Yellow oil (**2t**: **2t'** = 5.4:1). ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.38-7.32 (m, 2H, major/ minor), 7.31-7.28 (m, 1H, major/ minor), 7.23-7.18 (m, 2H, major/ minor), 3.72 (s, 2H, major/ minor), 3.00 (t, *J* = 7.6 Hz, 2H, minor), 2.80 (t, *J* = 7.6 Hz, 2H, minor), 2.78-2.70 (m, 6H, major), 2.52 (t, *J* = 7.6 Hz, 2H, minor), 1.64-1.50 (m, 2H, major/ minor), 1.38-1.29 (m, 2H, major/ minor), 0.93 (t, *J* = 7.6 Hz, 3H, major/ minor); ^{19}F NMR (376 MHz, $CDCl_3$) δ -38.1 (s, major), -38.4 (s, minor); ^{13}C NMR (100 MHz, $CDCl_3$) δ (major) 205.5, 147.8 (q, $J_{C\text{-}F}$ = 1.3 Hz), 133.5, 129.3, 128.9, 128.5 (q, $J_{C\text{-}F}$ = 308.6 Hz), 127.3, 121.2 (q, $J_{C\text{-}F}$ = 1.8 Hz), 116.1, 50.1, 38.9, 37.8 (q, $J_{C\text{-}F}$ = 1.2 Hz), 30.3, 26.7, 21.9, 13.7; (minor) 205.3, 143.6 (q, $J_{C\text{-}F}$ = 1.9 Hz), 133.6, 129.4, 128.8, 127.2, 125.6 (q, $J_{C\text{-}F}$ = 1.8 Hz), 116.2, 50.0, 39.3, 32.7, 32.1 (q, $J_{C\text{-}F}$ = 0.9 Hz), 29.9, 21.9, 13.7. FT-IR: ν (cm^{-1}) 2961, 2933, 2875, 2216, 1717, 1131, 1100. HRMS [ESI] calcd for $C_{18}H_{21}F_3NOS$ $[M+H]^+$ 356.1290, found 356.1299.

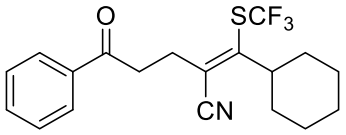


2u

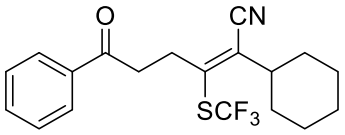


2u'

Yellow oil (**2u**: **2u'** = 3.1:1). ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.98-7.94 (m, 2H, major/ minor), 7.62-7.56 (m, 1H, major/ minor), 7.48 (t, *J* = 7.6 Hz, 2H, major/ minor), 3.37-3.32 (m, 2H, minor), 3.29 (t, *J* = 7.2 Hz, 2H, major), 3.24-3.18 (m, 2H, minor), 2.99 (t, *J* = 7.2 Hz, 2H, major), 2.78 (t, *J* = 7.6 Hz, 2H, major), 2.57 (t, *J* = 7.6 Hz, 2H, minor), 1.70-1.20 (m, 16H, major/ minor), 0.92-0.85 (m, 3H, major/ minor); ^{19}F NMR (376 MHz, $CDCl_3$) δ -38.1 (s, major), -38.2 (s, minor); ^{13}C NMR (100 MHz, $CDCl_3$) δ (major) 197.2, 148.0 (q, $J_{C\text{-}F}$ = 1.4 Hz), 136.2, 133.5, 128.7, 128.0, 128.5 (q, $J_{C\text{-}F}$ = 308.5 Hz), 121.5 (q, $J_{C\text{-}F}$ = 1.7 Hz), 116.3, 38.1 (q, $J_{C\text{-}F}$ = 0.8 Hz), 35.9, 31.8, 29.5, 29.4, 29.3, 29.2, 28.7, 28.2, 27.1, 22.6, 14.1; (minor) 197.1, 144.0 (q, $J_{C\text{-}F}$ = 1.3 Hz), 136.2, 133.4, 128.7, 128.0, 128.4 (q, $J_{C\text{-}F}$ = 308.8 Hz), 125.7 (q, $J_{C\text{-}F}$ = 1.8 Hz), 116.3, 36.4, 33.0, 32.6, 29.5, 29.4, 29.3, 29.2, 28.7, 27.9, 27.1, 22.6, 14.1. FT-IR: ν (cm^{-1}) 2926, 2855, 2215, 1687, 1449, 1104. HRMS [ESI] calcd for $C_{23}H_{31}F_3NOS$ $[M+H]^+$ 426.2073, found 426.2068.



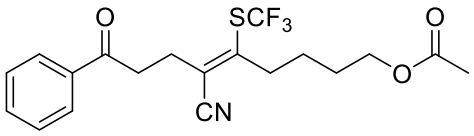
2v



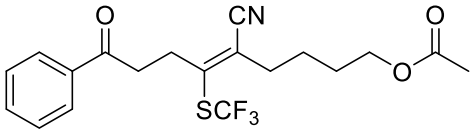
2v'

Yellow oil (**2v**: **2v'** = 8.2:1). ^{1}H NMR (400 MHz, $CDCl_3$) δ (major) 7.99-7.94 (m, 2H), 7.61-7.56 (m, 1H), 7.51-7.45 (m, 2H), 3.33-3.27 (m, 2H), 3.12-3.08 (m, 2H), 1.86-1.79 (m, 2H), 1.75-1.68 (m, 1H), 1.67-1.61 (m, 2H), 1.60-1.48 (m, 2H), 1.43-1.32 (m, 2H), 1.29-1.14 (m, 2H); ^{19}F NMR (376 MHz, $CDCl_3$) δ -37.4 (s, major), -38.3 (s, minor); ^{13}C NMR (100 MHz, $CDCl_3$) δ (major) 197.1, 150.8 (q, $J_{C\text{-}F}$ = 1.0 Hz), 136.2, 133.4, 128.7, 128.6 (q, $J_{C\text{-}F}$ = 308.8 Hz), 128.0, 125.3 (q,

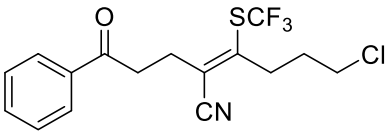
$J_{C\text{-}F}$ = 1.1 Hz), 116.2, 41.4, 35.9, 30.5, 27.9 (q, $J_{C\text{-}F}$ = 0.7 Hz), 25.6, 25.2; (minor) 197.2, 142.2 (q, $J_{C\text{-}F}$ = 1.3 Hz), 136.3, 133.4, 131.4 (q, $J_{C\text{-}F}$ = 1.7 Hz), 128.7, 128.5 (q, $J_{C\text{-}F}$ = 308.9 Hz), 128.0, 115.4, 47.8, 36.5, 32.6 (q, $J_{C\text{-}F}$ = 0.5 Hz), 30.9, 25.5, 25.1. FT-IR: ν (cm^{-1}) 2933, 2856, 2215, 1687, 1449. 1091. HRMS [ESI] calcd for $C_{19}H_{21}F_3NOS$ $[M+H]^+$ 368.1290, found 368.1293.



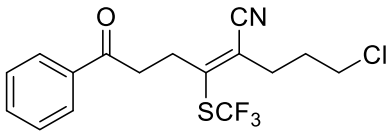
2w: yellow oil. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.98-7.94 (m, 2H), 7.59 (dd, *J* = 7.6, 7.6 Hz, 1H), 7.48 (dd, *J* = 7.6, 7.6 Hz, 2H), 4.08 (t, *J* = 6.0 Hz, 2H), 3.30 (t, *J* = 7.2 Hz, 2H), 2.99 (t, *J* = 7.2 Hz, 2H), 2.82 (t, *J* = 7.2 Hz, 2H), 2.04 (s, 3H), 1.78-1.60 (m, 4H); ^{19}F NMR (376 MHz, $CDCl_3$) δ -38.0 (s); ^{13}C NMR (100 MHz, $CDCl_3$) δ 197.2, 171.0, 147.1 (q, $J_{C\text{-}F}$ = 1.4 Hz), 136.1, 133.6, 128.7, 128.5 (q, $J_{C\text{-}F}$ = 308.6 Hz), 128.0, 122.2 (q, $J_{C\text{-}F}$ = 1.8 Hz), 116.2, 63.7, 37.6 (q, $J_{C\text{-}F}$ = 0.9 Hz), 35.8, 27.6, 27.2, 24.7, 20.9. FT-IR: ν (cm^{-1}) 2918, 2850, 2248, 2215, 1737, 1686, 1099. HRMS [ESI] calcd for $C_{19}H_{20}F_3NO_3SNa$ $[M+Na]^+$ 422.1008, found 422.0993.



2w': yellow oil. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.99-7.95 (m, 2H), 7.62-7.56 (m, 1H), 7.52-7.46 (m, 2H), 4.13-4.06 (m, 2H), 3.39-3.33 (m, 2H), 3.22 (t, *J* = 7.2 Hz, 2H), 2.65-2.59 (m, 2H), 2.06 (s, 3H), 1.73-1.65 (m, 4H); ^{19}F NMR (376 MHz, $CDCl_3$) δ -38.2 (s); ^{13}C NMR (100 MHz, $CDCl_3$) δ 197.1, 171.1, 144.7 (q, $J_{C\text{-}F}$ = 1.4 Hz), 136.2, 133.5, 128.7, 128.4 (q, $J_{C\text{-}F}$ = 309.0 Hz), 128.0, 125.1 (q, $J_{C\text{-}F}$ = 1.7 Hz), 116.1, 63.6, 36.3, 32.7 (q, $J_{C\text{-}F}$ = 0.8 Hz), 32.6, 27.7, 24.4, 20.9. FT-IR: ν (cm^{-1}) 2934, 2870, 2216, 1736, 1686, 1103. HRMS [ESI] calcd for $C_{19}H_{20}F_3NO_3SNa$ $[M+Na]^+$ 422.1008, found 422.0996.

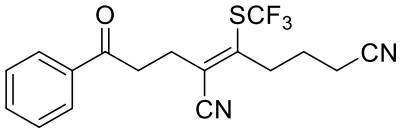


2x



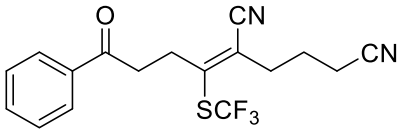
2x'

Yellow oil (**2x**: **2x'** = 3.0:1). ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.99-7.92 (m, 2H, major/ minor), 7.62-7.56 (m, 1H, major/ minor), 7.51-7.45 (m, 2H, major/ minor), 3.60-3.54 (m, 2H, major/ minor), 3.37 (t, *J* = 7.2 Hz, 2H, minor), 3.31 (t, *J* = 7.2 Hz, 2H, major), 3.22 (t, *J* = 7.2 Hz, 2H, minor), 3.01 (t, *J* = 7.2 Hz, 2H, major), 2.96 (t, *J* = 7.2 Hz, 2H, major), 2.79 (t, *J* = 7.2 Hz, 2H, minor), 2.18-2.04 (m, 2H, major/ minor); ^{19}F NMR (376 MHz, $CDCl_3$) δ -38.0 (s, major), -38.1 (s, minor); ^{13}C NMR (100 MHz, $CDCl_3$) δ (major) 197.2, 145.8 (q, $J_{C\text{-}F}$ = 1.4 Hz), 136.1, 133.6, 128.7, 128.0, 128.4 (q, $J_{C\text{-}F}$ = 308.9 Hz), 123.2 (q, $J_{C\text{-}F}$ = 1.7 Hz), 115.9, 43.3, 35.7, 35.5 (q, $J_{C\text{-}F}$ = 0.9 Hz), 30.7, 27.3; (minor) 197.1, 145.6 (q, $J_{C\text{-}F}$ = 1.4 Hz), 136.1, 133.5, 128.7, 128.0, 128.3 (q, $J_{C\text{-}F}$ = 309.0 Hz), 123.9 (q, $J_{C\text{-}F}$ = 1.6 Hz), 116.0, 43.2, 36.7, 32.6 (q, $J_{C\text{-}F}$ = 0.7 Hz), 30.3, 30.2. FT-IR: ν (cm^{-1}) 2920, 2851, 2244, 1672, 1104. HRMS [ESI] calcd for $C_{16}H_{16}ClF_3NOS$ $[M+H]^+$ 362.0588, found 362.0591.

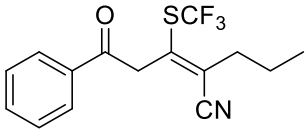


2y: yellow solid, m.p. 37-38 °C. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.98-7.93 (m, 2H), 7.63-7.57 (m, 1H), 7.49 (dd, *J* = 7.6,

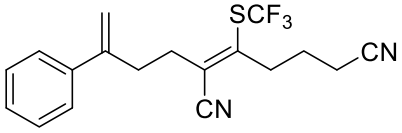
7.6 Hz, 2H), 3.34 (t, *J* = 7.2 Hz, 2H), 3.02 (t, *J* = 7.2 Hz, 2H), 2.94 (t, *J* = 7.2 Hz, 2H), 2.41 (t, *J* = 7.2 Hz, 2H), 2.11-2.01 (m, 2H); ^{19}F NMR (376 MHz, $CDCl_3$) δ -38.0 (s); ^{13}C NMR (100 MHz, $CDCl_3$) δ 197.3, 144.8 (q, J_{C-F} = 1.5 Hz), 136.0, 133.7, 128.8, 128.4 (q, J_{C-F} = 308.9 Hz), 128.0, 124.0 (q, J_{C-F} = 1.8 Hz), 118.5, 115.8, 36.8 (q, J_{C-F} = 0.9 Hz), 35.5, 27.3, 23.8, 16.3. FT-IR: ν (cm^{-1}) 2961, 2875, 2248, 2215, 1686, 1457, 1101. HRMS [ESI] calcd for $C_{17}H_{16}F_3N_2OS$ $[M+H]^+$ 353.0930, found 353.0937.



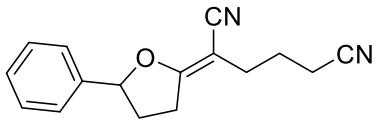
2y': yellow solid, m.p. 37-38 °C. ^{1}H NMR (400 MHz, $CDCl_3$) ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.98-7.94 (m, 2H), 7.63-7.57 (m, 1H), 7.49 (t, *J* = 7.6 Hz, 2H), 3.39 (t, *J* = 7.2 Hz, 2H), 3.24 (t, *J* = 7.2 Hz, 2H), 2.79 (t, *J* = 7.6 Hz, 2H), 2.46 (t, *J* = 7.2 Hz, 2H), 2.05-1.95 (m, 2H); ^{19}F NMR (376 MHz, $CDCl_3$) δ -38.1 (s); ^{13}C NMR (100 MHz, $CDCl_3$) δ 197.2, 146.6 (q, J_{C-F} = 1.4 Hz), 136.1, 133.6, 128.8, 128.3 (q, J_{C-F} = 309.0 Hz), 128.0, 123.2 (q, J_{C-F} = 1.6 Hz), 118.4, 115.8, 36.0, 32.8 (q, J_{C-F} = 0.4 Hz), 31.6, 23.6, 16.3. FT-IR: ν (cm^{-1}) 2971, 2902, 2250, 2216, 1680, 1094. HRMS [ESI] calcd for $C_{17}H_{16}F_3N_2OS$ $[M+H]^+$ 353.0930, found 353.0936.



4: yellow oil. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.98-7.95 (m, 2H), 7.65-7.61 (m, 1H), 7.51 (dd, *J* = 7.6, 7.6 Hz, 2H), 4.53 (s, 2H), 2.68 (t, *J* = 7.6 Hz, 2H), 1.76-1.66 (m, 2H), 1.04 (t, *J* = 7.6 Hz, 3H); ^{19}F NMR (376 MHz, $CDCl_3$) δ -38.8 (s); ^{13}C NMR (100 MHz, $CDCl_3$) δ 193.3, 137.7 (q, J_{C-F} = 1.8 Hz), 135.7, 134.0, 129.9 (q, J_{C-F} = 1.5 Hz), 128.9, 128.8 (q, J_{C-F} = 308.5 Hz), 128.1, 116.2, 47.5, 34.9, 21.3, 13.2. FT-IR: ν (cm^{-1}) 2966, 2935, 2877, 2219, 1688, 1450, 1104. HRMS [ESI] calcd for $C_{15}H_{14}F_3NOSNa$ $[M+Na]^+$ 336.0640, found 336.0649

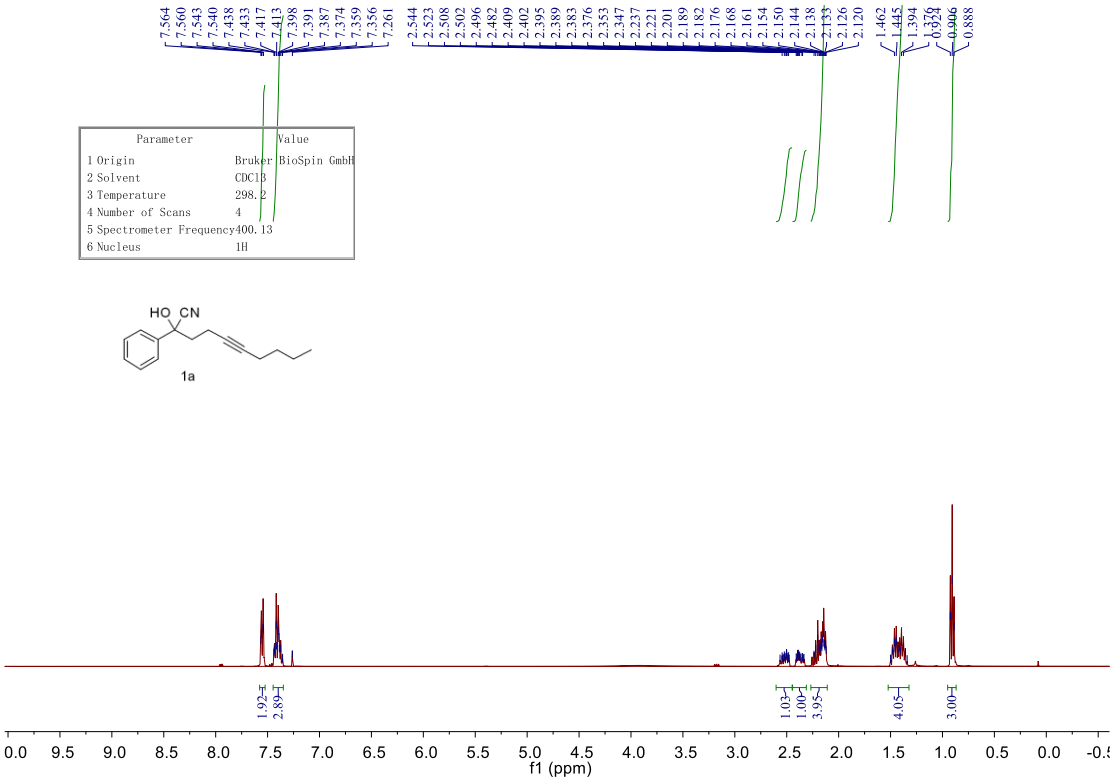


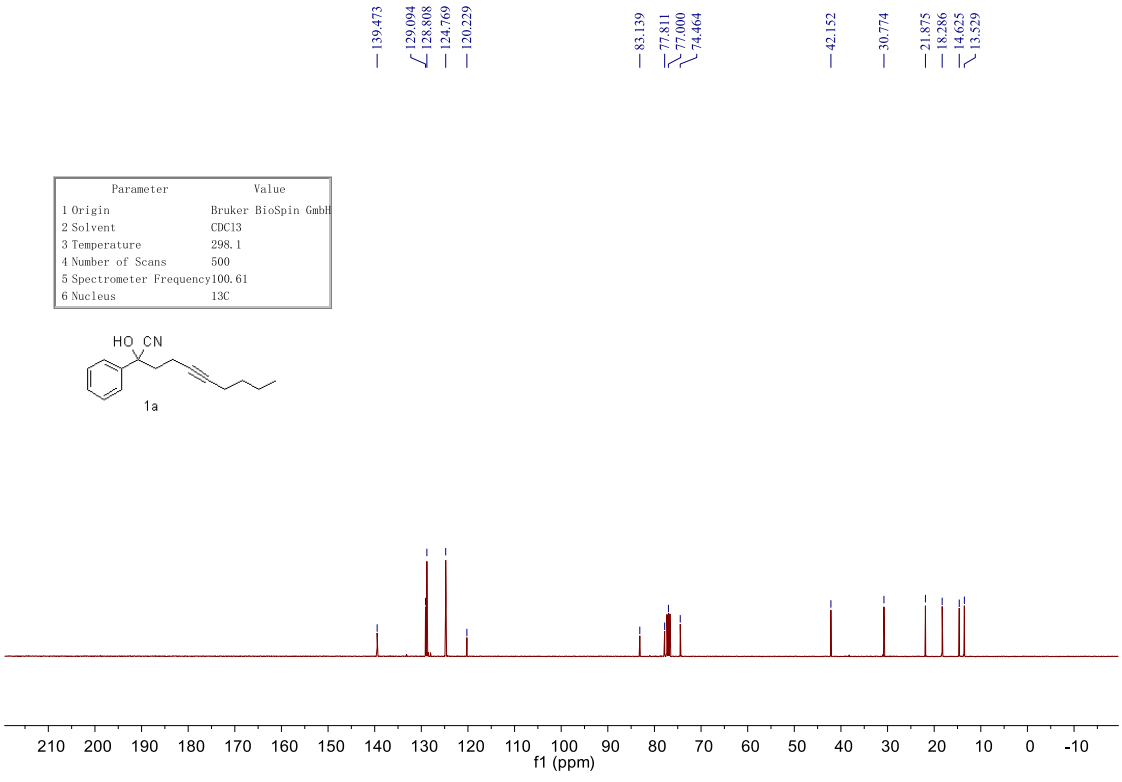
6: yellow oil. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.39-7.35 (m, 4H), 7.34-7.31 (m, 1H), 5.37 (d, *J* = 1.2 Hz, 1H), 5.14 (d, *J* = 1.2 Hz, 1H), 2.88-2.81 (m, 4H), 2.73 (t, *J* = 7.2 Hz, 2H), 2.39 (t, *J* = 7.2 Hz, 2H), 1.98-1.89 (m, 2H); ^{19}F NMR (376 MHz, $CDCl_3$) δ -38.0 (s); ^{13}C NMR (100 MHz, $CDCl_3$) δ 145.5, 144.3 (q, J_{C-F} = 1.6 Hz), 139.4, 128.6, 128.1, 126.0, 124.7 (q, J_{C-F} = 1.6 Hz), 118.4, 116.0, 114.6, 36.8 (q, J_{C-F} = 1.0 Hz), 33.1, 31.9, 24.0, 16.5. FT-IR: ν (cm^{-1}) 2997, 2260, 2248, 1682, 1448, 1108. HRMS [ESI] calcd for $C_{18}H_{17}F_3N_2SNa$ $[M+Na]^+$ 373.0957, found 373.0969.

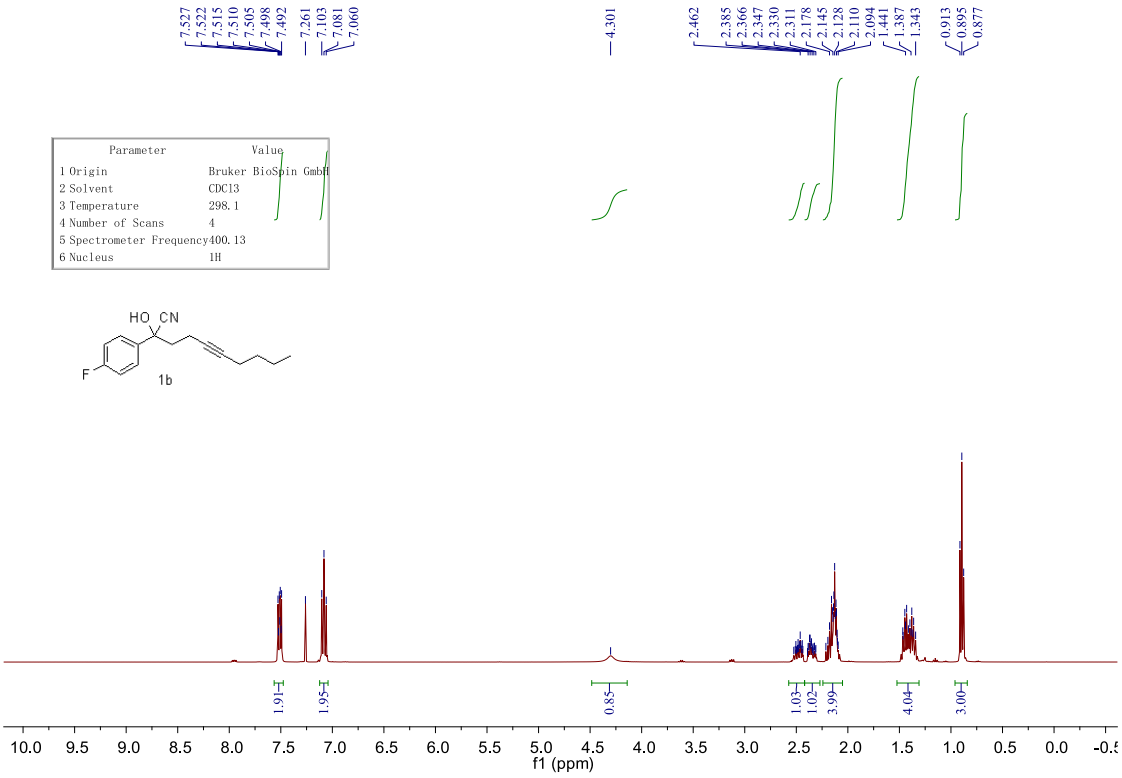


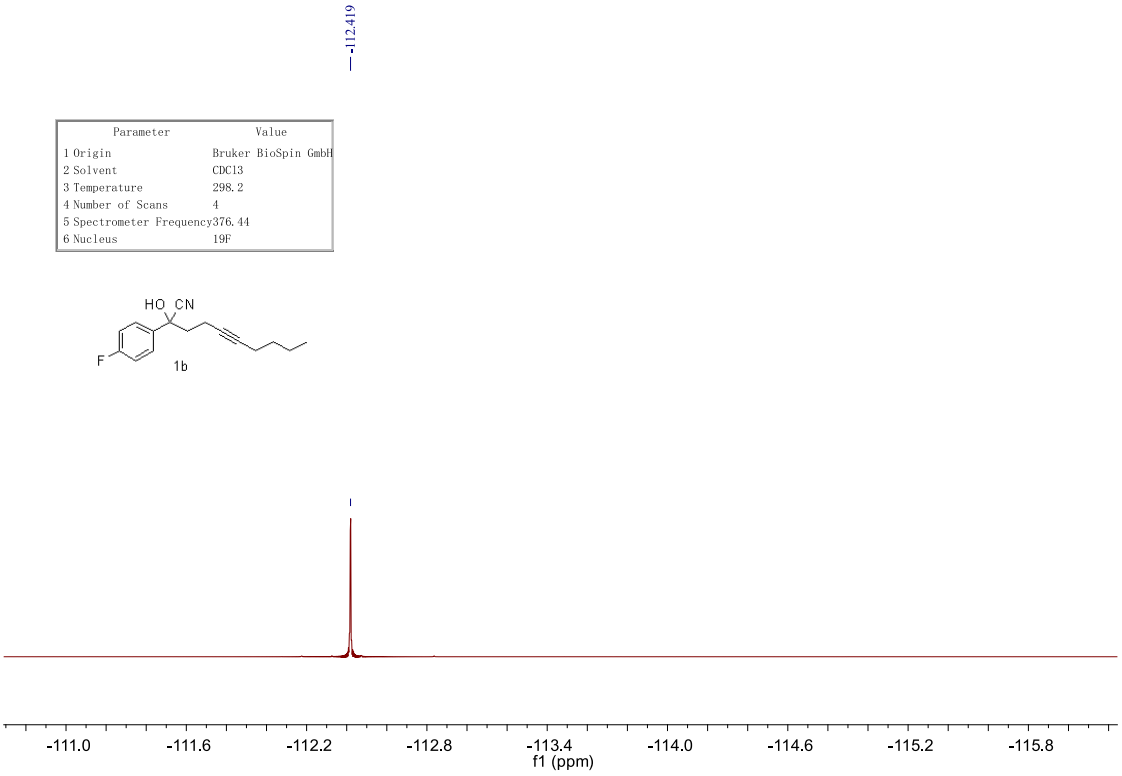
7: yellow oil. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.43-7.33 (m, 3H), 7.31-7.27 (m, 2H), 5.51 (dd, *J* = 8.0, 6.0 Hz, 1H), 3.14-3.05 (m, 1H), 3.03-2.92 (m, 1H), 2.62-2.52 (m, 1H), 2.45-2.36 (m, 4H), 2.17-2.06 (m, 1H), 1.95-1.86 (m, 2H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 172.3, 138.9, 128.8, 128.7, 125.5, 120.0, 119.2, 87.0, 80.6, 32.4, 30.9, 25.4, 24.1, 16.4. FT-IR: ν (cm^{-1}) 2960, 2932, 2874, 2216, 1756, 1505, 1099. HRMS [ESI] calcd for $C_{16}H_{16}N_2ONa$ $[M+Na]^+$ 275.1155, found 275.1165.

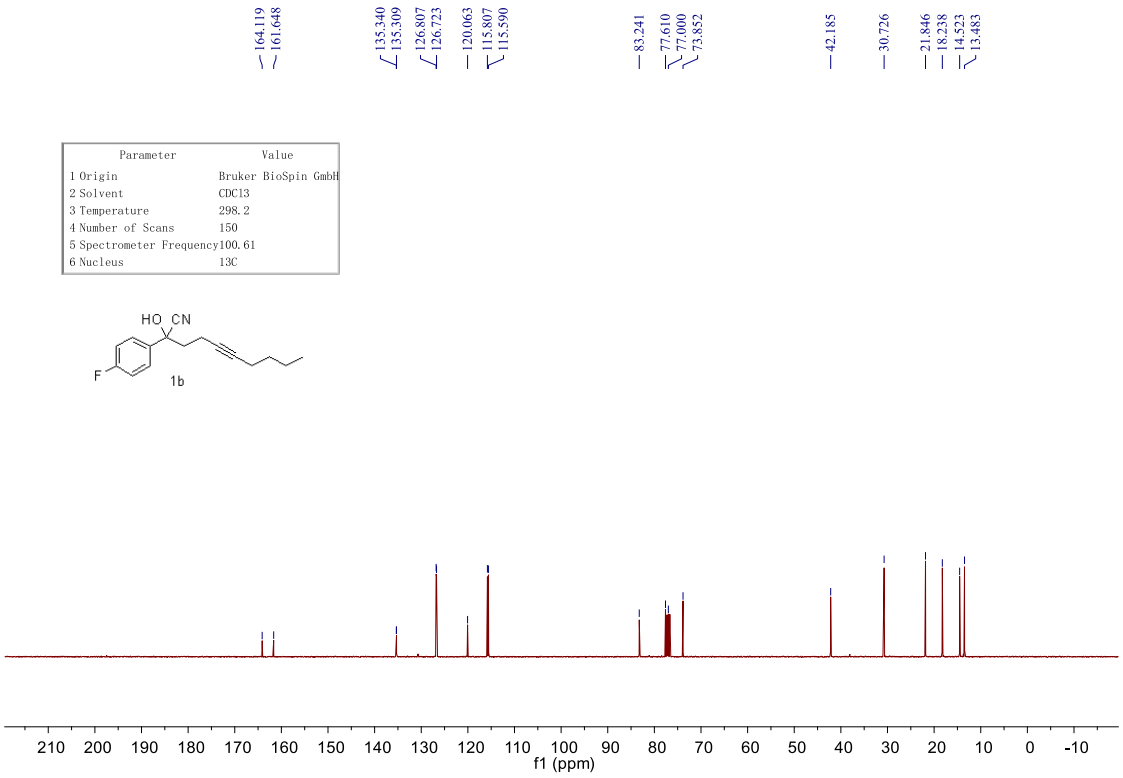
5. ^{1}H, ^{13}C, and ^{19}F NMR spectra

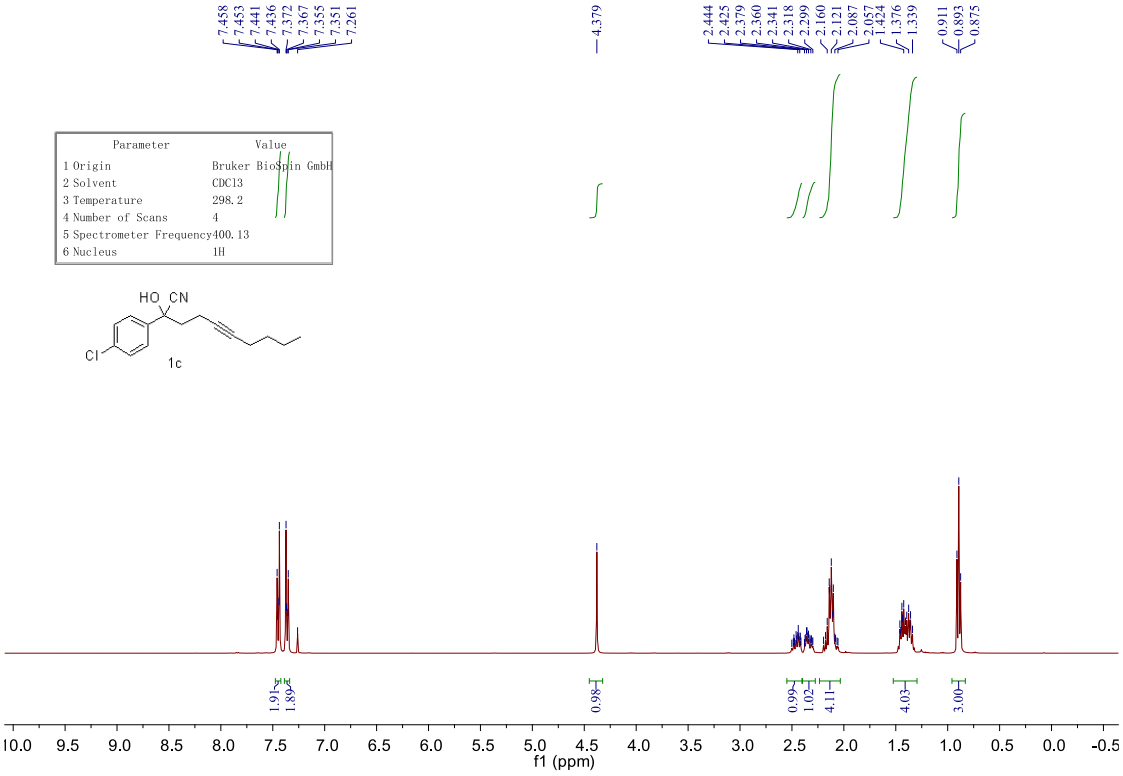


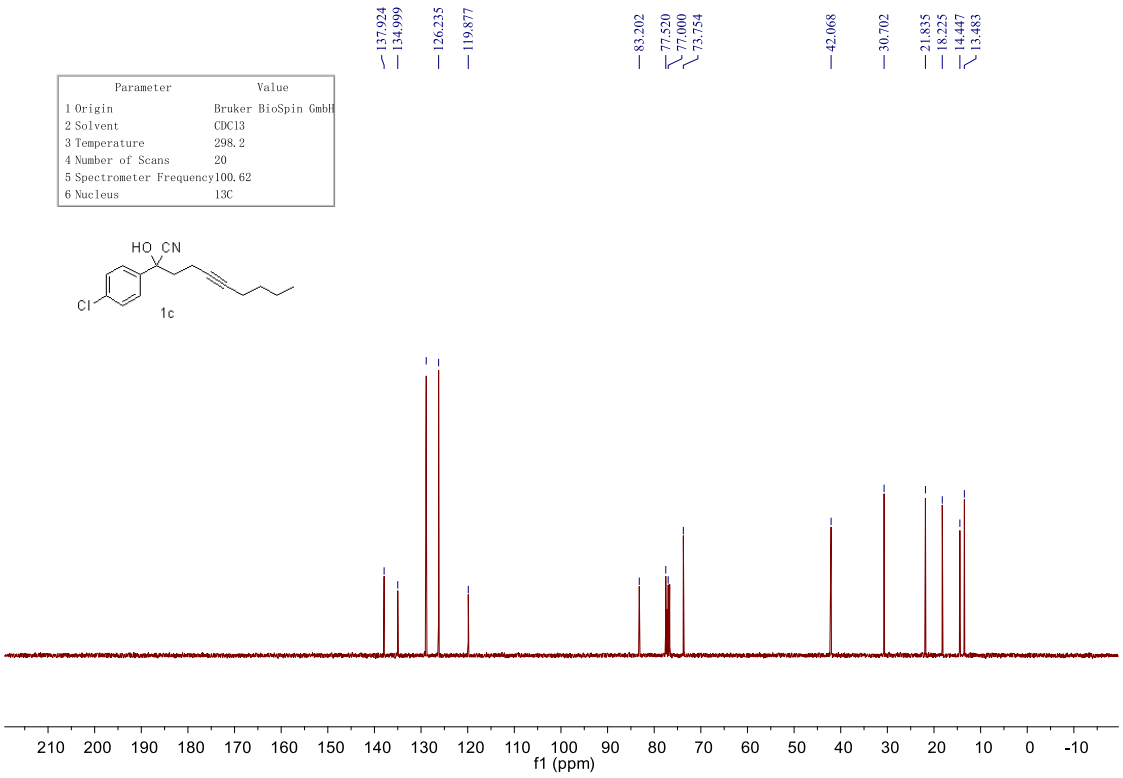


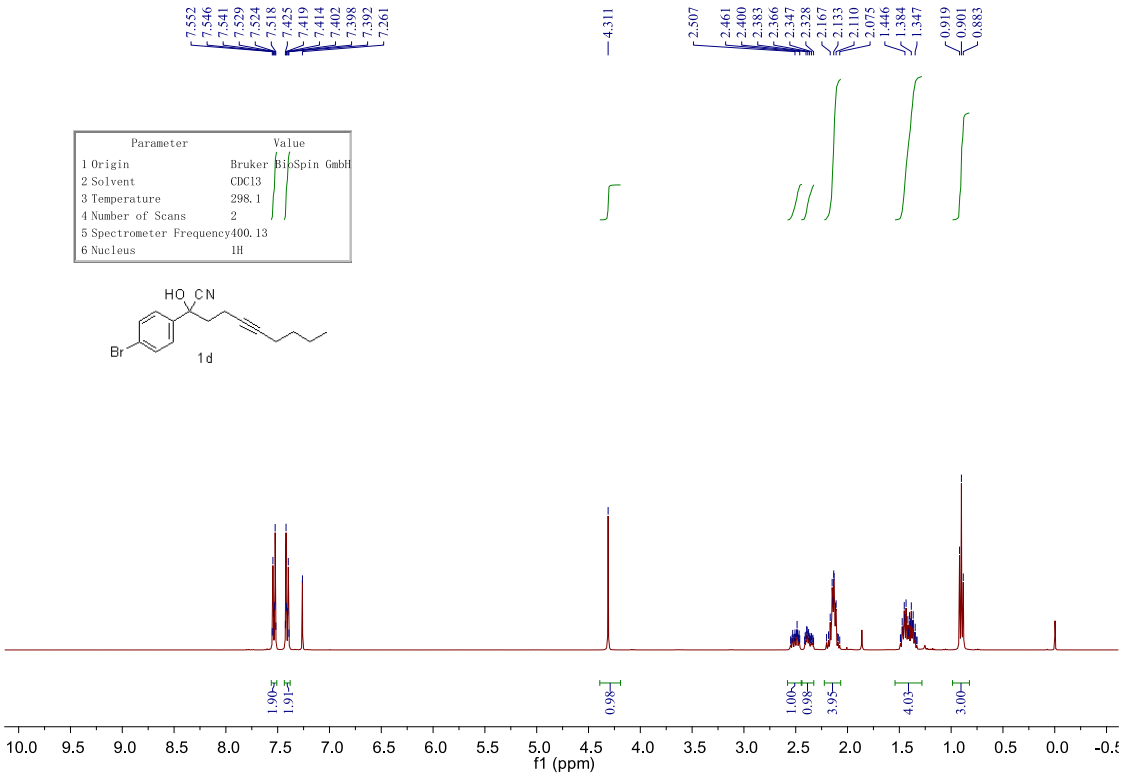

7.527
7.522
7.515
7.510
7.505
7.498
7.492
7.261
7.103
7.081
7.060
4.301
2.462
2.385
2.366
2.347
2.330
2.311
2.178
2.145
2.128
2.110
2.094
1.441
1.387
1.343
0.913
0.895
0.877
Parameter Value
1 Origin Bruker BioSpin GmbH
2 Solvent CDCl3
3 Temperature 298.1
4 Number of Scans 4
5 Spectrometer Frequency 400.13
6 Nucleus 1H
HO CN
F
1b
1.91
1.95
0.85
1.03
1.02
3.99
4.04
3.00
f1 (ppm)

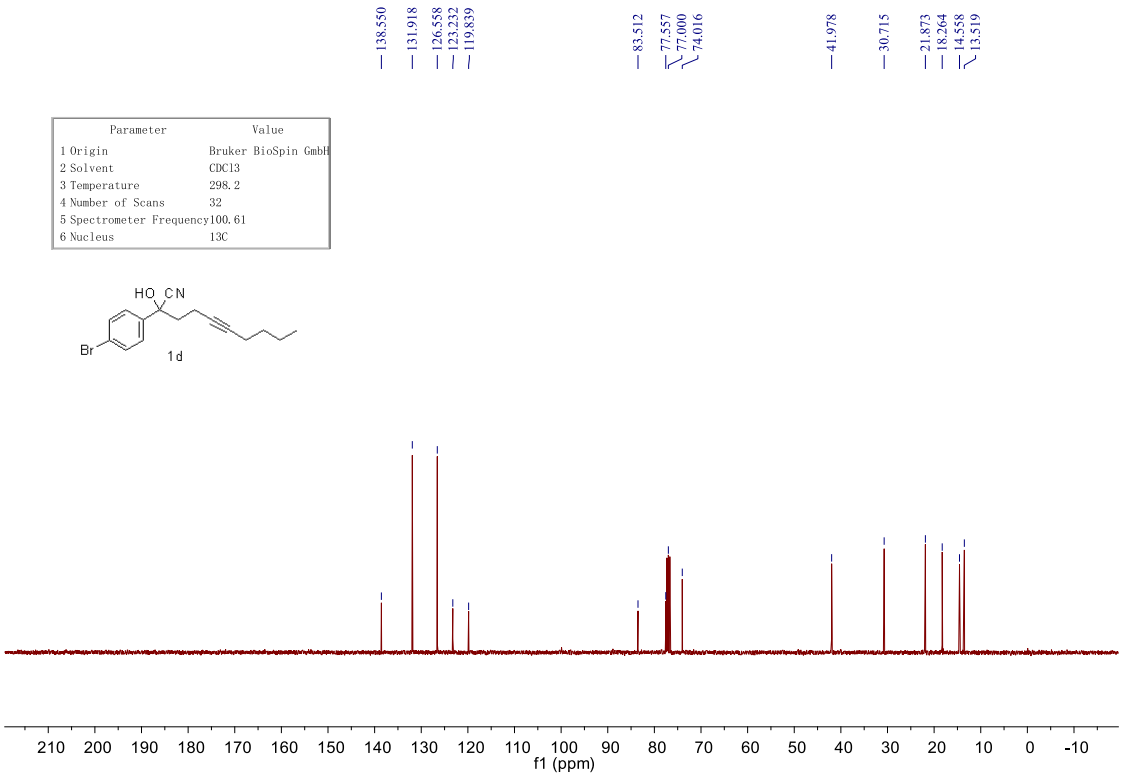

-112.419
Parameter Value
1 Origin Bruker BioSpin GmbH
2 Solvent CDCl3
3 Temperature 298.2
4 Number of Scans 4
5 Spectrometer Frequency 376.44
6 Nucleus 19F
HO CN
F
1b
f1 (ppm)

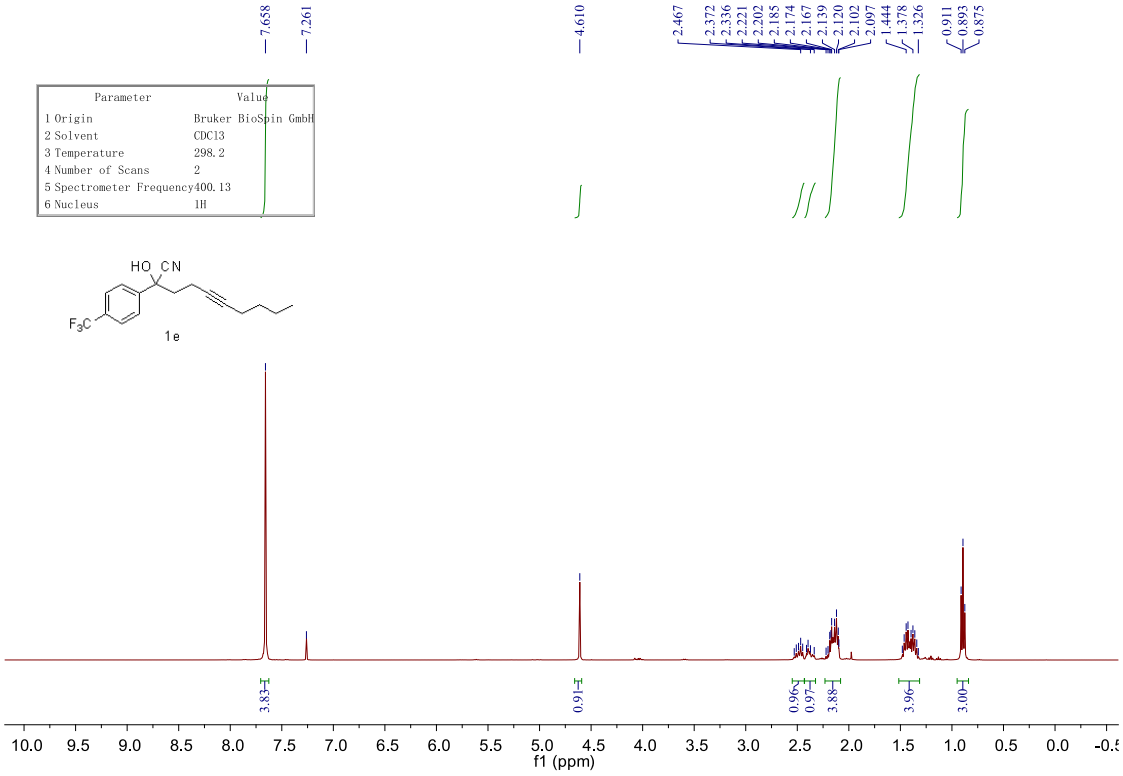

164.119
161.648
135.340
135.309
126.807
126.723
120.063
115.807
115.590
83.241
77.610
77.000
73.852
42.185
30.726
21.846
18.238
14.523
13.483
Parameter Value
1 Origin Bruker BioSpin GmbH
2 Solvent CDCl3
3 Temperature 298.2
4 Number of Scans 150
5 Spectrometer Frequency 100.61
6 Nucleus 13C
HO CN
F
1b
f1 (ppm)

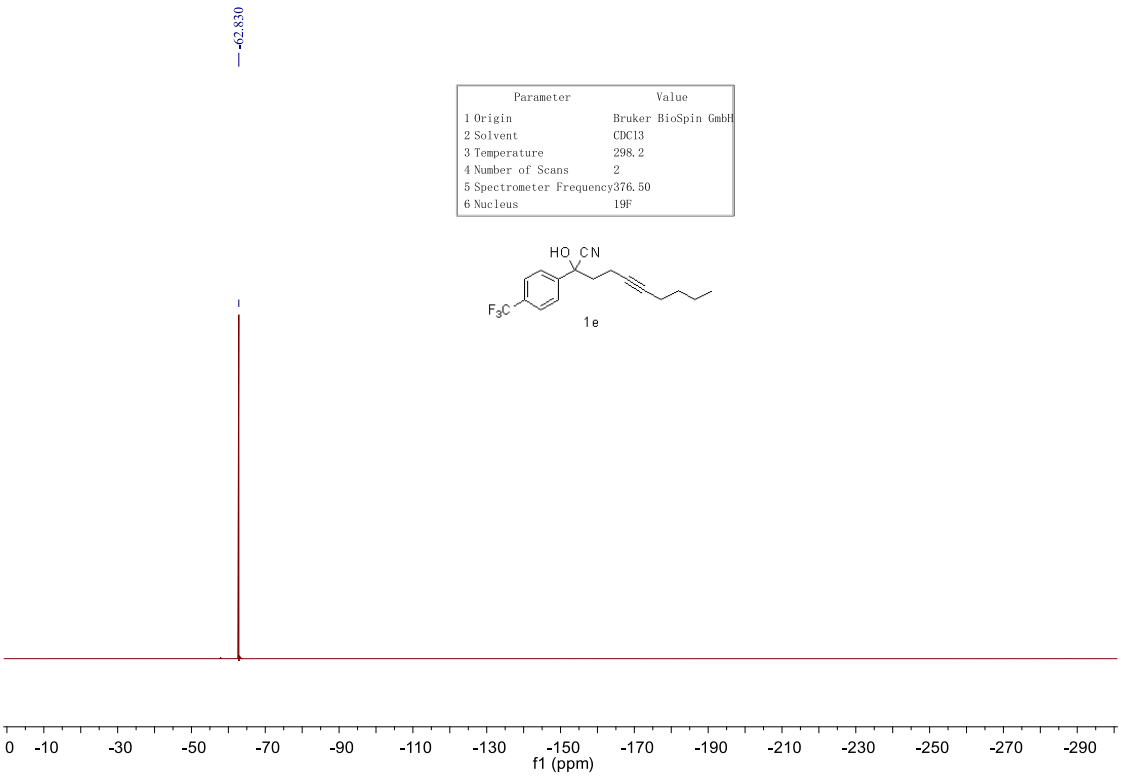

7.458
7.453
7.441
7.436
7.372
7.367
7.355
7.351
7.261
4.379
2.444
2.425
2.379
2.360
2.341
2.318
2.299
2.160
2.121
2.087
2.057
1.424
1.376
1.339
0.911
0.893
0.875
Parameter Value
1 Origin Bruker BioSpin GmbH
2 Solvent CDCl3
3 Temperature 298.2
4 Number of Scans 4
5 Spectrometer Frequency 400.13
6 Nucleus 1H
HO CN
Cl
1c
1.91
1.89
0.98
0.99
1.02
4.11
4.03
3.00
f1 (ppm)

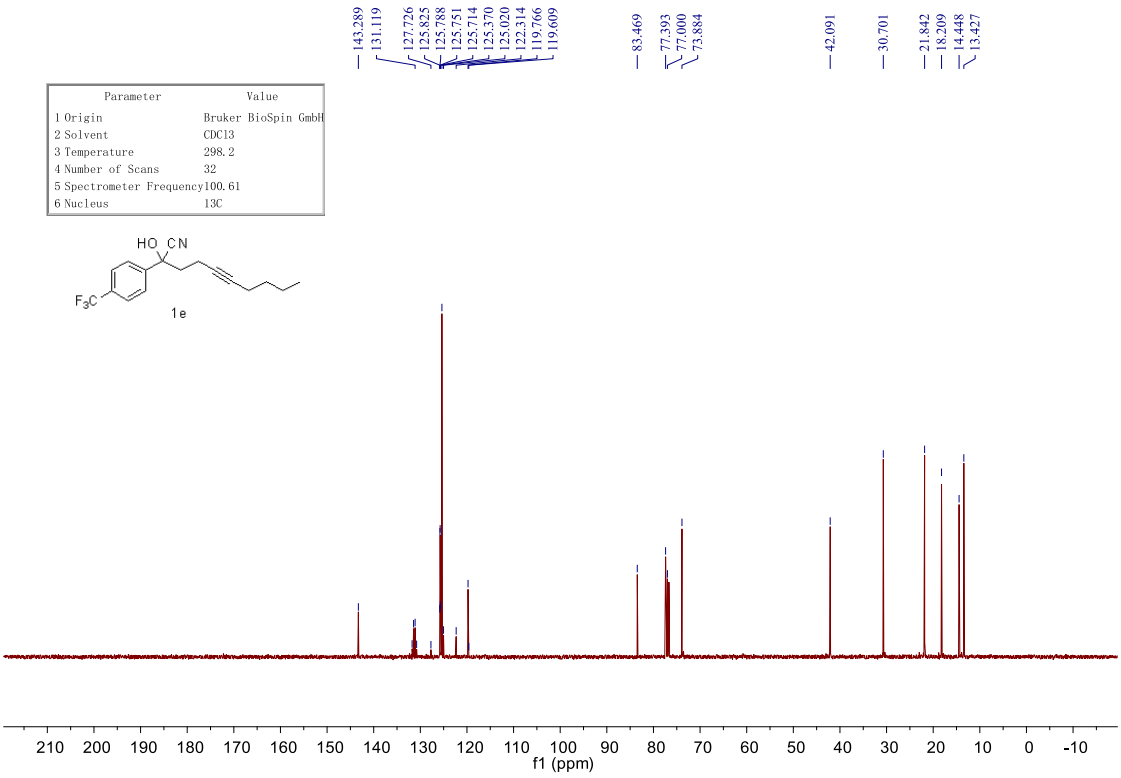

137.924
134.999
126.235
119.877
83.202
77.520
77.000
73.754
42.068
30.702
21.835
18.225
14.447
13.483
Parameter Value
1 Origin Bruker BioSpin GmbH
2 Solvent CDCl3
3 Temperature 298.2
4 Number of Scans 20
5 Spectrometer Frequency 100.62
6 Nucleus 13C
HO CN
Cl
1c
f1 (ppm)

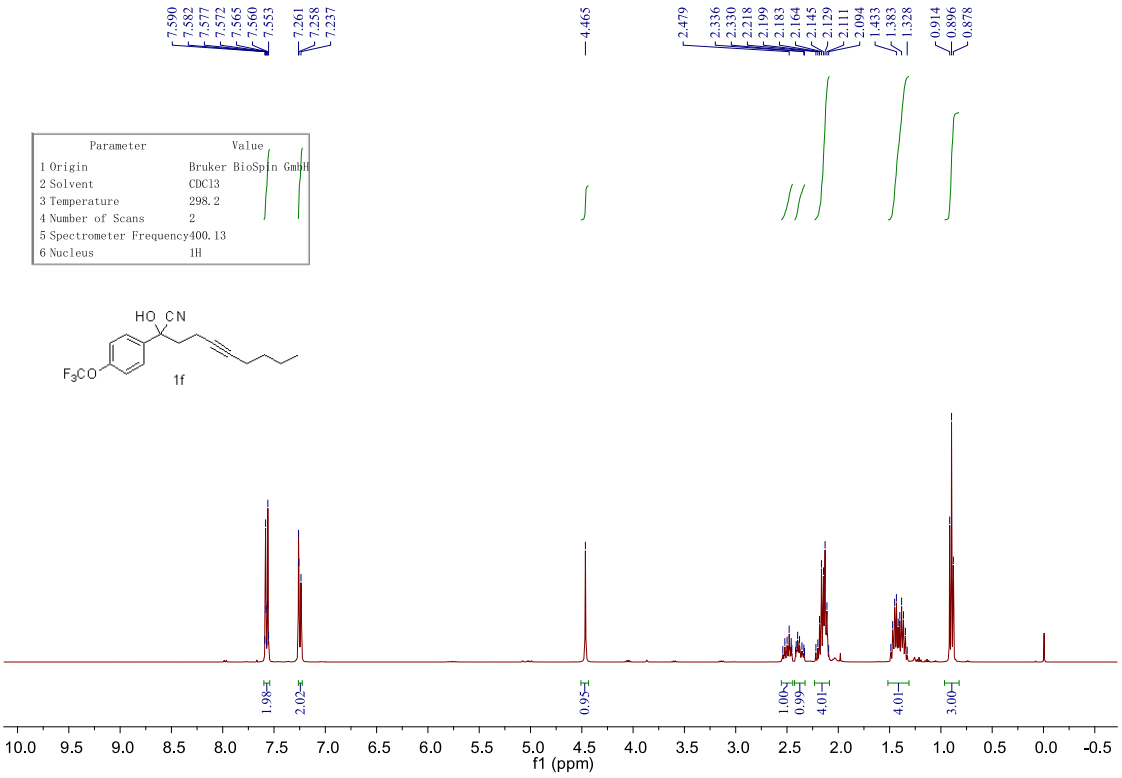

7.552
7.546
7.541
7.529
7.524
7.518
7.425
7.419
7.414
7.402
7.398
7.392
7.261
4.311
2.507
2.461
2.400
2.383
2.366
2.347
2.328
2.167
2.133
2.110
2.075
1.446
1.384
1.347
0.919
0.901
0.883
Parameter Value
1 Origin Bruker BioSpin GmbH
2 Solvent CDCl3
3 Temperature 298.1
4 Number of Scans 2
5 Spectrometer Frequency 400.13
6 Nucleus 1H
HO CN
Br
1d
1.90
1.91
0.98
1.00
0.98
3.95
4.03
3.00
f1 (ppm)

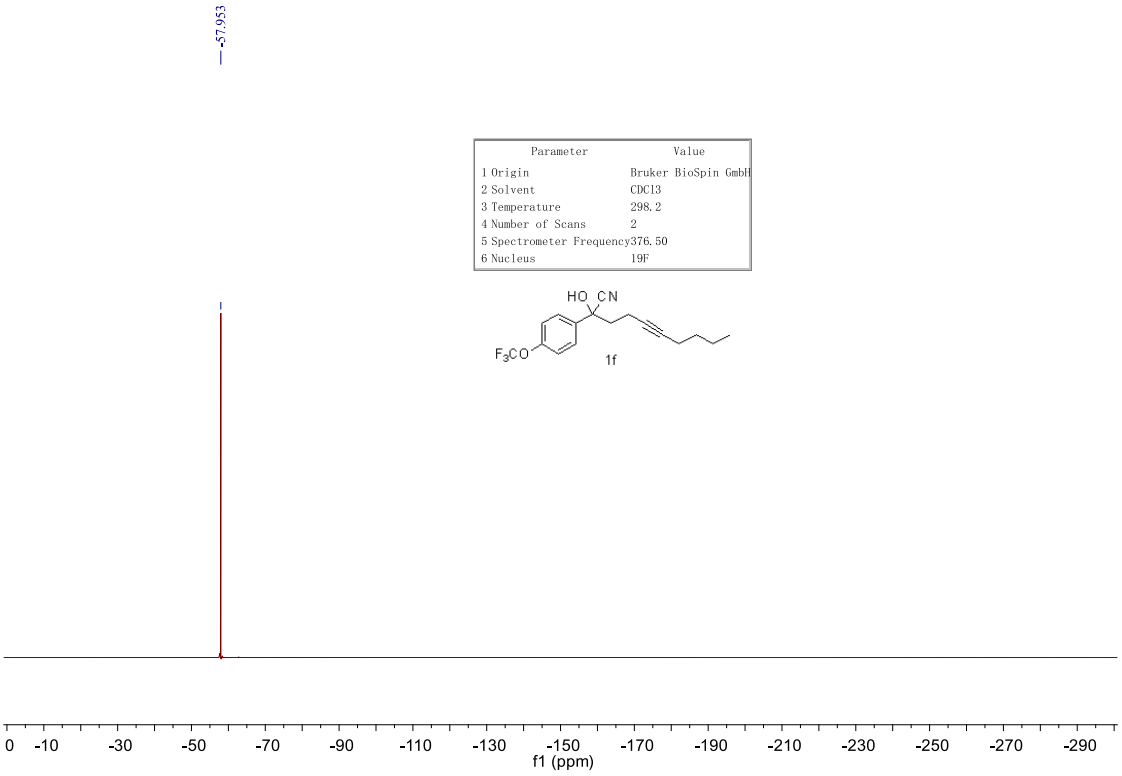

138.550
131.918
126.558
123.232
119.839
83.512
77.557
77.000
74.016
41.978
30.715
21.873
18.264
14.558
13.519
Parameter Value
1 Origin Bruker BioSpin GmbH
2 Solvent CDCl3
3 Temperature 298.2
4 Number of Scans 32
5 Spectrometer Frequency 100.61
6 Nucleus 13C
HO CN
Br
1d
f1 (ppm)

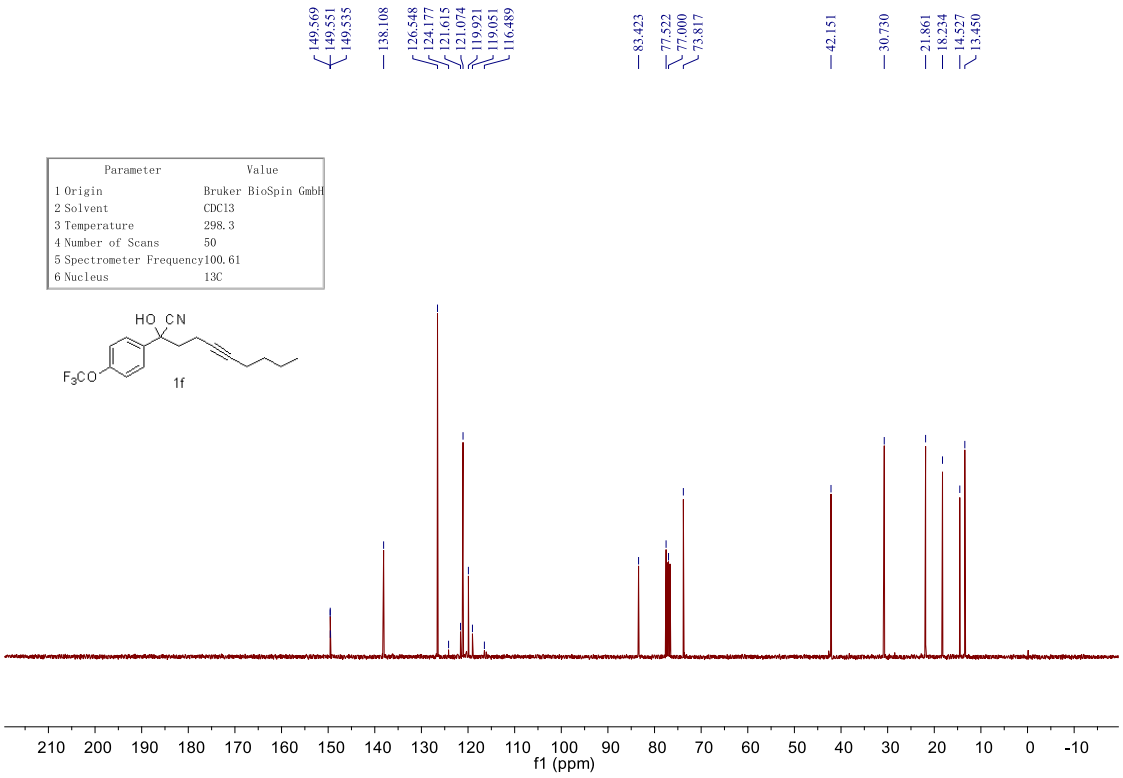

7.658
7.261
4.610
2.467
2.372
2.336
2.221
2.202
2.185
2.174
2.167
2.139
2.120
2.102
2.097
1.444
1.378
1.326
0.911
0.893
0.875
Parameter Value
1 Origin Bruker BioSpin GmbH
2 Solvent CDCl3
3 Temperature 298.2
4 Number of Scans 2
5 Spectrometer Frequency 400.13
6 Nucleus 1H
HO CN
F3C
1e
3.83
0.91
0.96
0.97
3.88
3.96
3.00
f1 (ppm)

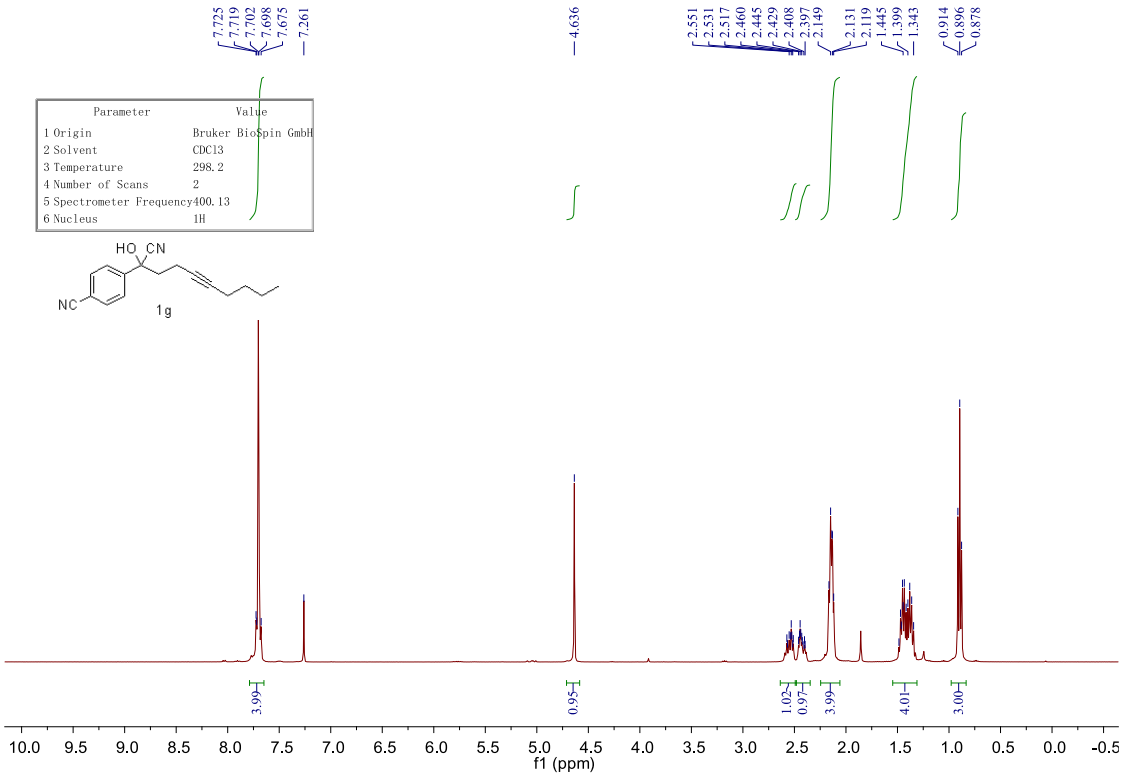

-62.830
Parameter Value
1 Origin Bruker BioSpin GmbH
2 Solvent CDCl3
3 Temperature 298.2
4 Number of Scans 2
5 Spectrometer Frequency 376.50
6 Nucleus 19F
HO CN
F3C
1e
0 -10 -30 -50 -70 -90 -110 -130 -150 -170 -190 -210 -230 -250 -270 -290
f1 (ppm)

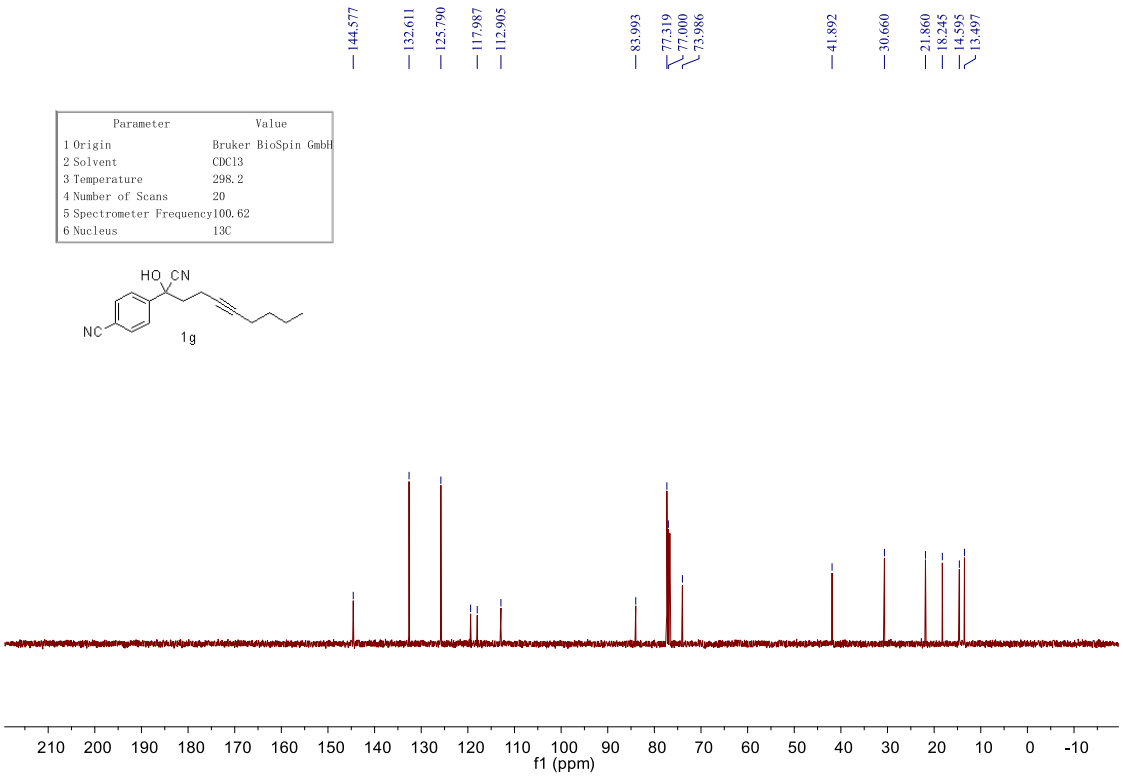

143.289
131.119
127.726
125.825
125.788
125.751
125.714
125.370
125.020
122.314
119.766
119.609
83.469
77.393
77.000
73.884
42.091
30.701
21.842
18.209
14.448
13.427
Parameter Value
1 Origin Bruker BioSpin GmbH
2 Solvent CDCl3
3 Temperature 298.2
4 Number of Scans 32
5 Spectrometer Frequency 100.61
6 Nucleus 13C
HO CN
F3C
1e
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)

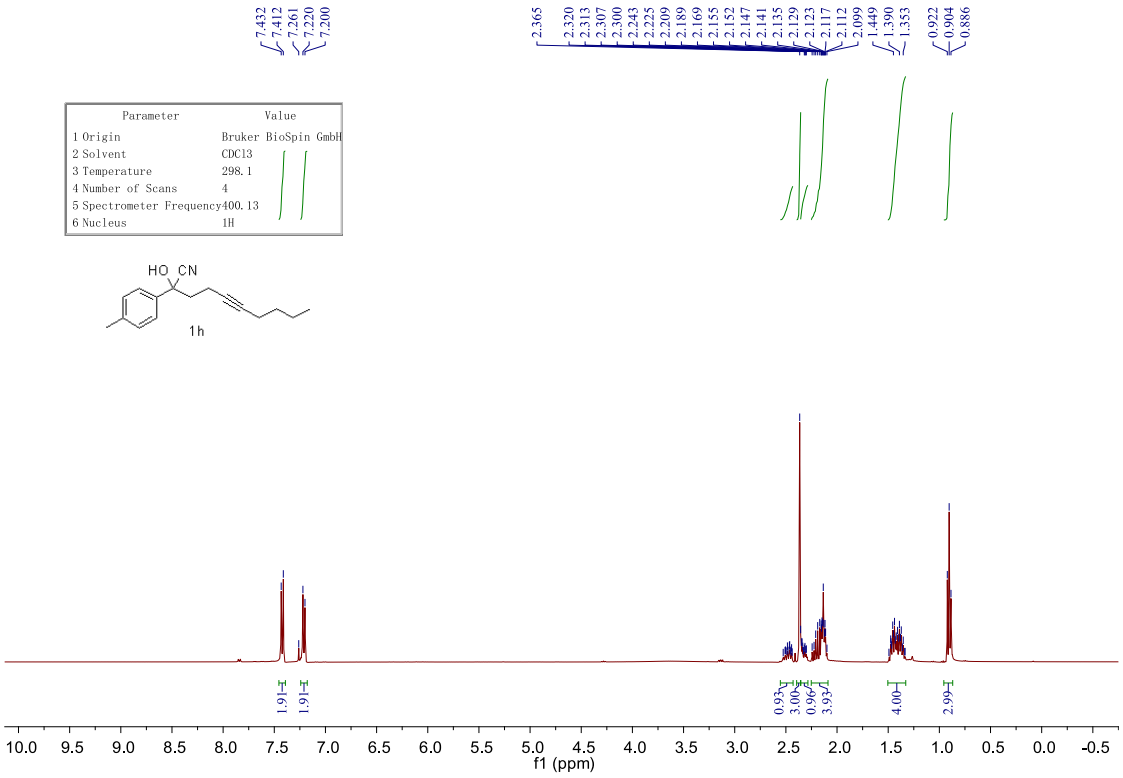

7.590
7.582
7.577
7.572
7.565
7.560
7.553
7.261
7.258
7.237
4.465
2.479
2.336
2.330
2.218
2.199
2.183
2.164
2.145
2.129
2.111
2.094
1.433
1.383
1.328
0.914
0.896
0.878
Parameter Value
1 Origin Bruker BioSpin GmbH
2 Solvent CDCl3
3 Temperature 298.2
4 Number of Scans 2
5 Spectrometer Frequency 400.13
6 Nucleus 1H
HO CN
F3CO
1f
1.98
2.02
0.95
1.00
0.99
4.01
4.01
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
f1 (ppm)

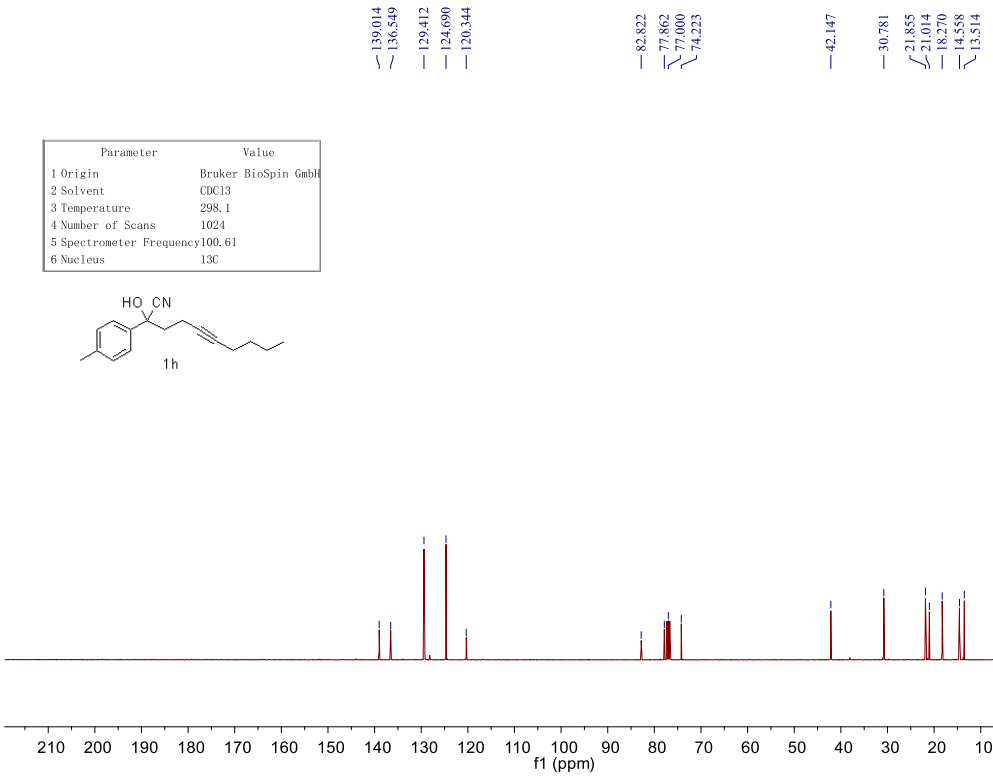

-57.953
Parameter Value
1 Origin Bruker BioSpin GmbH
2 Solvent CDCl3
3 Temperature 298.2
4 Number of Scans 2
5 Spectrometer Frequency 376.50
6 Nucleus 19F
HO CN
F3CO
1f
0 -10 -30 -50 -70 -90 -110 -130 -150 -170 -190 -210 -230 -250 -270 -290
f1 (ppm)

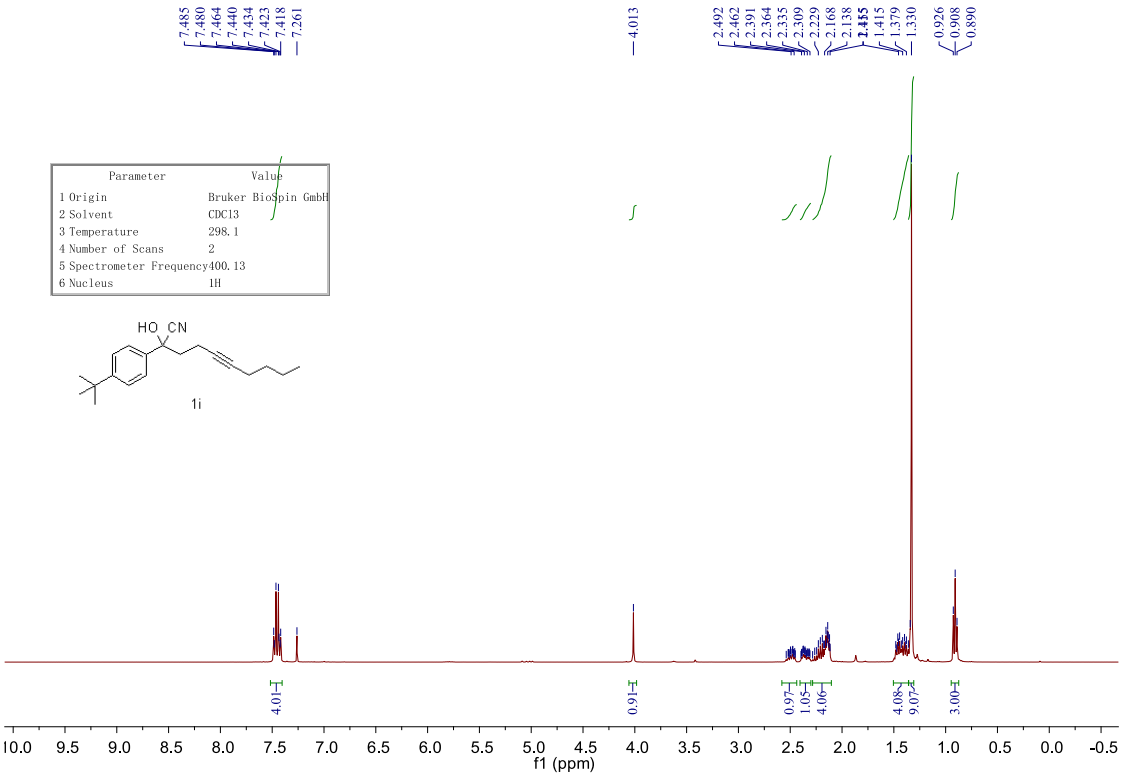

149.569
149.551
149.535
138.108
126.548
124.177
121.615
121.074
119.921
119.051
116.489
83.423
77.522
77.000
73.817
42.151
30.730
21.861
18.234
14.527
13.450
Parameter Value
1 Origin Bruker BioSpin GmbH
2 Solvent CDCl3
3 Temperature 298.3
4 Number of Scans 50
5 Spectrometer Frequency 100.61
6 Nucleus 13C
HO CN
F3CO
1f
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)

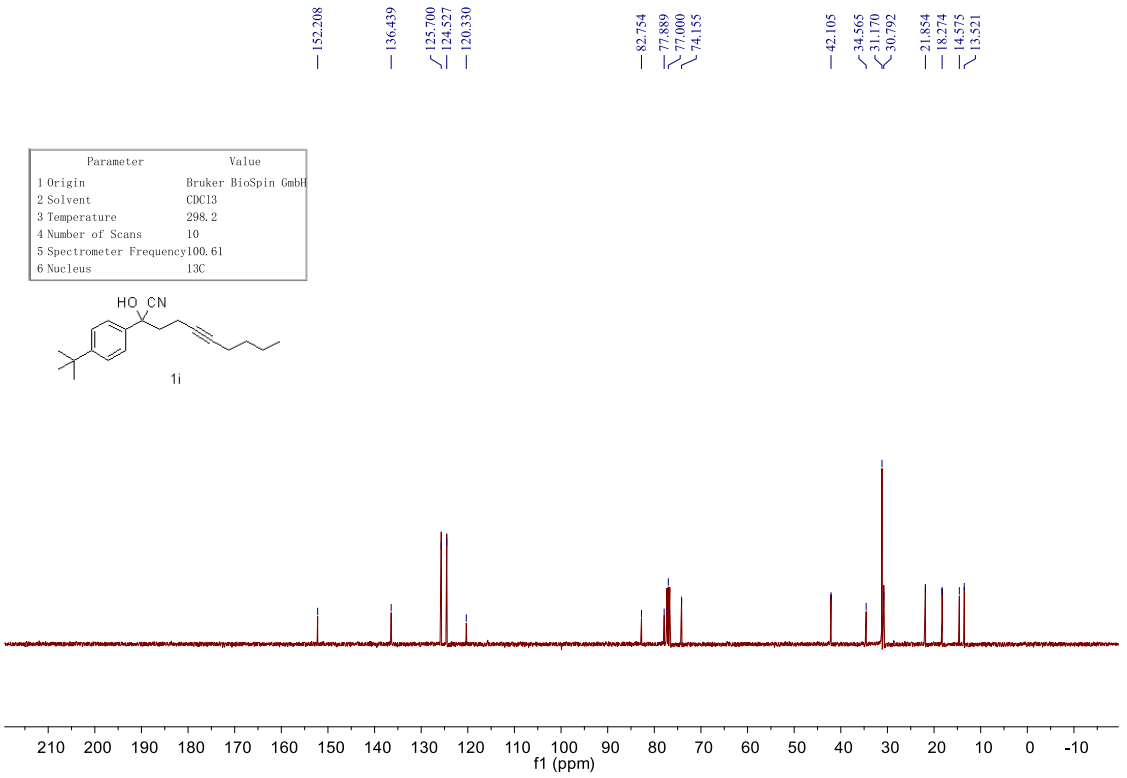

7.725
7.719
7.702
7.698
7.675
7.261
4.636
2.551
2.531
2.517
2.460
2.445
2.429
2.408
2.397
2.149
2.131
2.119
1.445
1.399
1.343
0.914
0.896
0.878
Parameter Value
1 Origin Bruker BioSpin GmbH
2 Solvent CDCl3
3 Temperature 298.2
4 Number of Scans 2
5 Spectrometer Frequency 400.13
6 Nucleus 1H
HO CN
NC
1g
3.99
0.95
1.02
0.97
3.99
4.01
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
f1 (ppm)

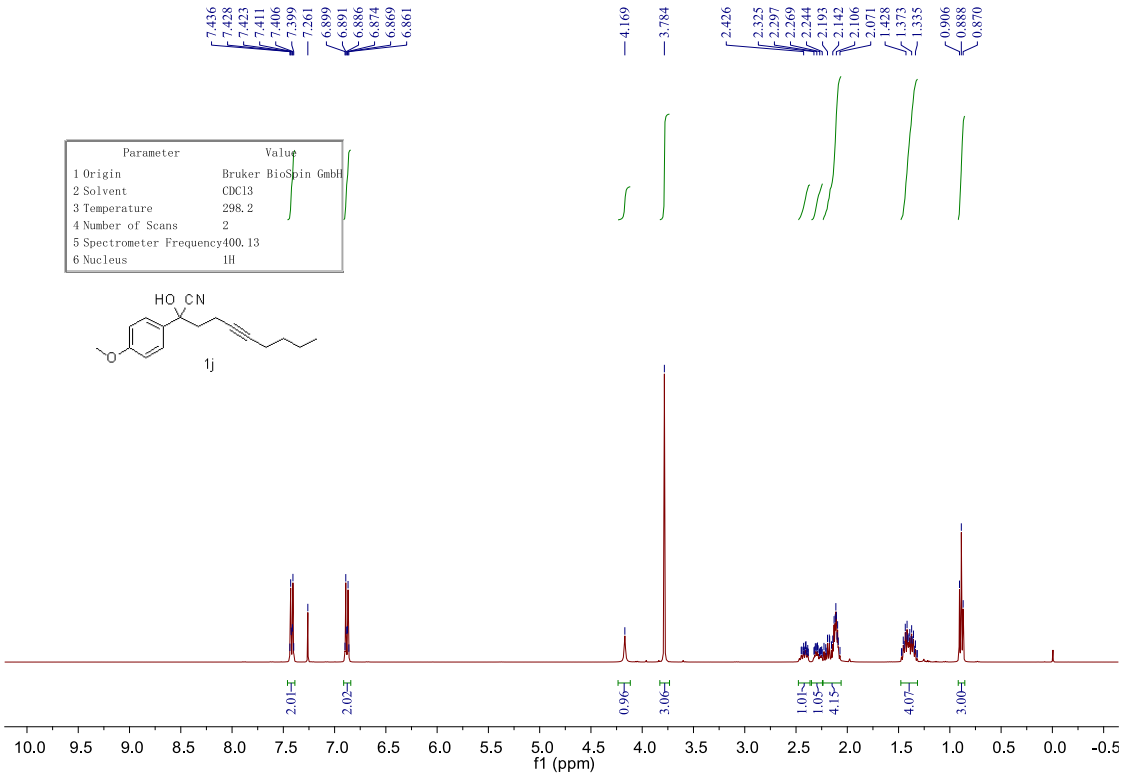

144.577
132.611
125.790
117.987
112.905
83.993
77.319
77.000
73.986
41.892
30.660
21.860
18.245
14.595
13.497
Parameter Value
1 Origin Bruker BioSpin GmbH
2 Solvent CDCl3
3 Temperature 298.2
4 Number of Scans 20
5 Spectrometer Frequency 100.62
6 Nucleus 13C
HO CN
NC
1g
f1 (ppm)

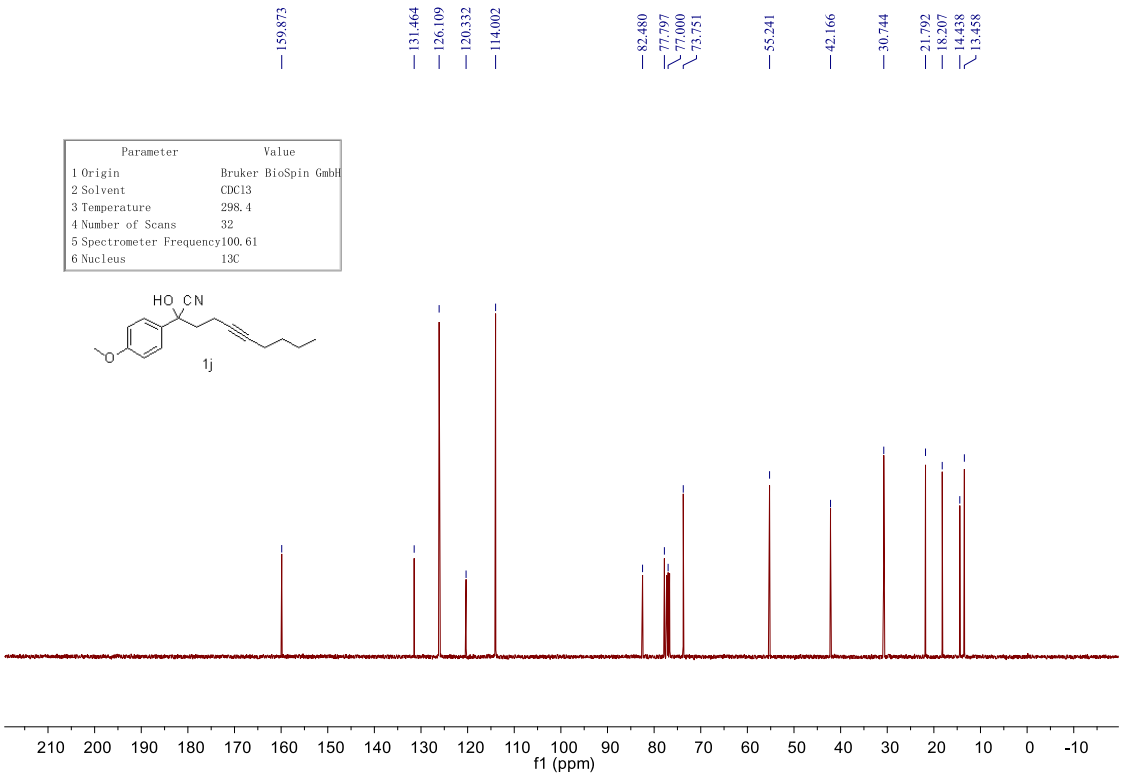

7.432
7.412
7.261
7.220
7.200
2.365
2.320
2.313
2.307
2.300
2.243
2.225
2.209
2.189
2.169
2.155
2.152
2.147
2.141
2.135
2.129
2.123
2.117
2.112
2.099
1.449
1.390
1.353
0.922
0.904
0.886
Parameter Value
1 Origin Bruker BioSpin GmbH
2 Solvent CDCl3
3 Temperature 298.1
4 Number of Scans 4
5 Spectrometer Frequency 400.13
6 Nucleus 1H
HO CN
1h
1.91
1.91
0.93
3.00
0.96
3.93
4.00
2.99
f1 (ppm)

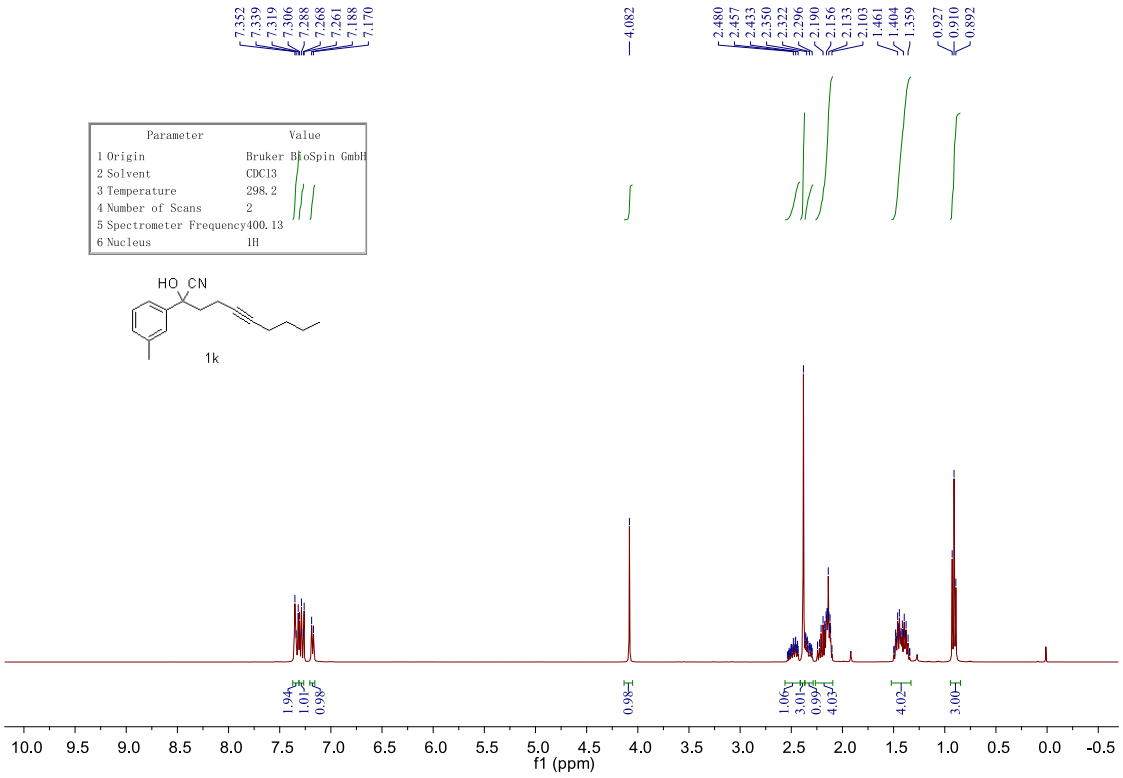

139.014
136.549
129.412
124.690
120.344
82.822
77.862
77.000
74.223
42.147
30.781
21.855
21.014
18.270
14.558
13.514
Parameter Value
1 Origin Bruker BioSpin GmbH
2 Solvent CDCl3
3 Temperature 298.1
4 Number of Scans 1024
5 Spectrometer Frequency 100.61
6 Nucleus 13C
HO CN
1h
f1 (ppm)

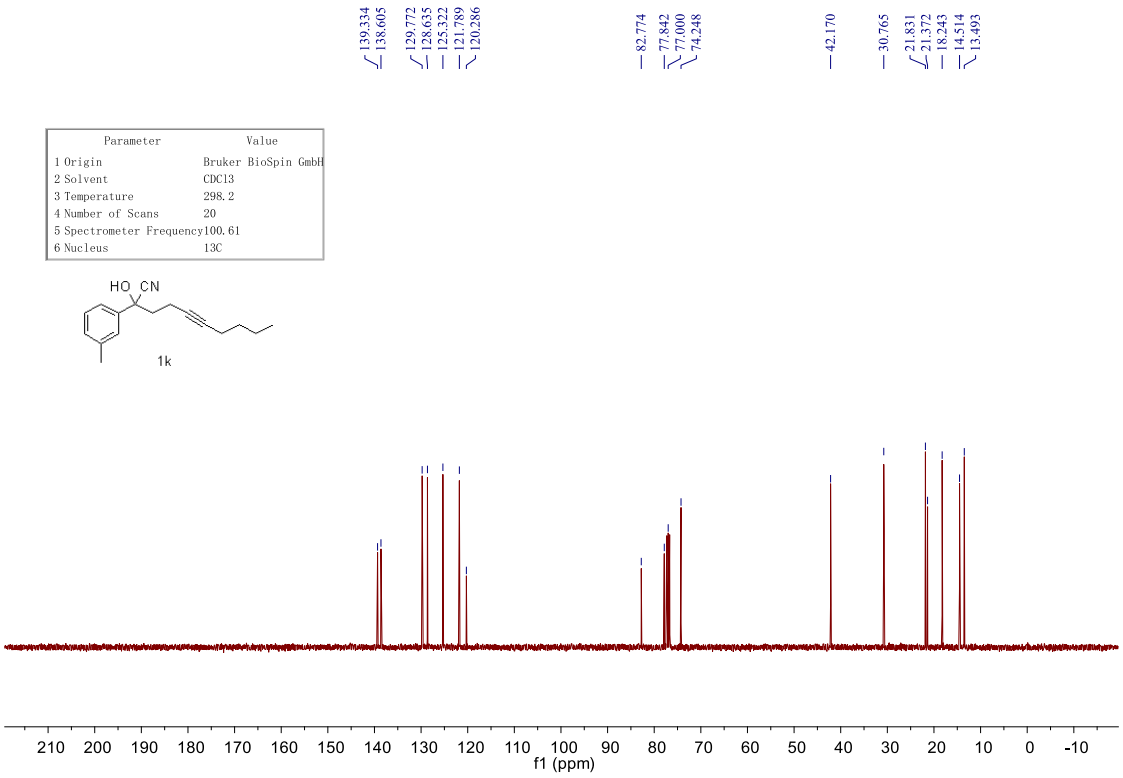

7.485
7.480
7.464
7.440
7.434
7.423
7.418
7.261
4.013
2.492
2.462
2.391
2.364
2.335
2.309
2.229
2.168
2.138
1.415
1.379
1.330
0.926
0.908
0.890
Parameter Value
1 Origin Bruker BioSpin GmbH
2 Solvent CDCl3
3 Temperature 298.1
4 Number of Scans 2
5 Spectrometer Frequency 400.13
6 Nucleus 1H
HO CN
1i
4.01
0.91
0.97
1.05
4.06
4.08
9.07
3.00
f1 (ppm)

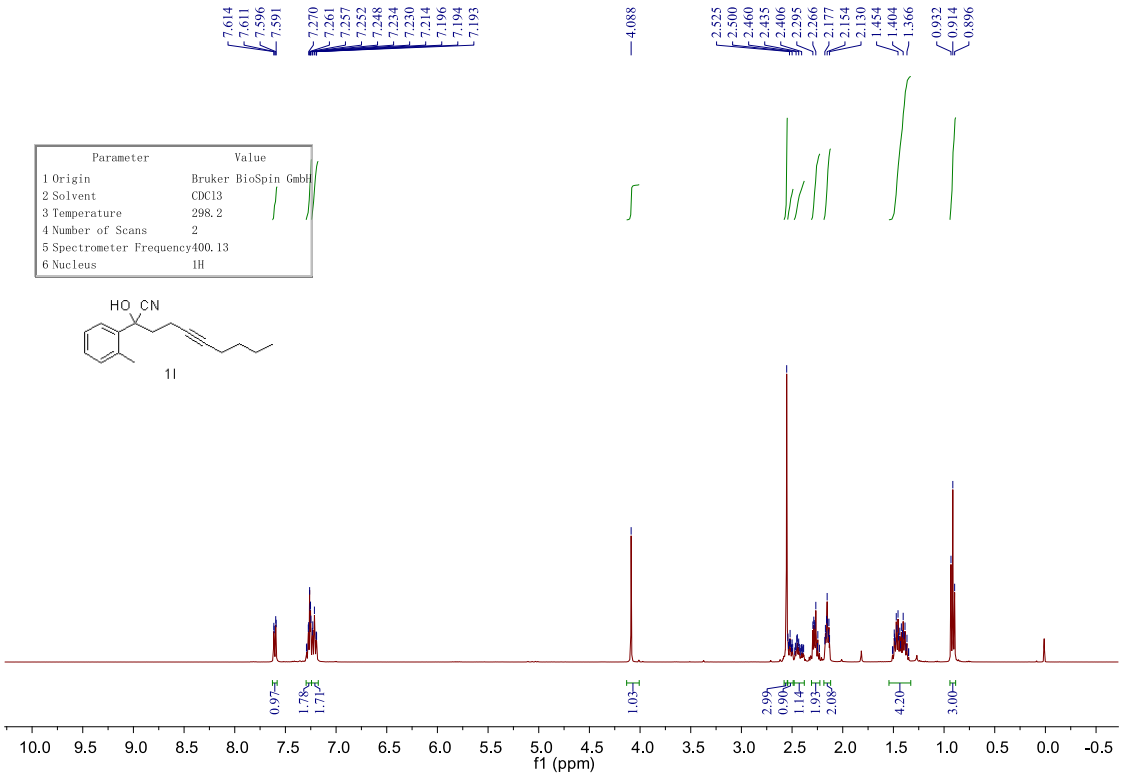

152.208
136.439
125.700
124.527
120.330
82.754
77.889
77.000
74.155
42.105
34.565
31.170
30.792
21.854
18.274
14.575
13.521
Parameter Value
1 Origin Bruker BioSpin GmbH
2 Solvent CDCl3
3 Temperature 298.2
4 Number of Scans 10
5 Spectrometer Frequency 100.61
6 Nucleus 13C
HO CN
1i
f1 (ppm)

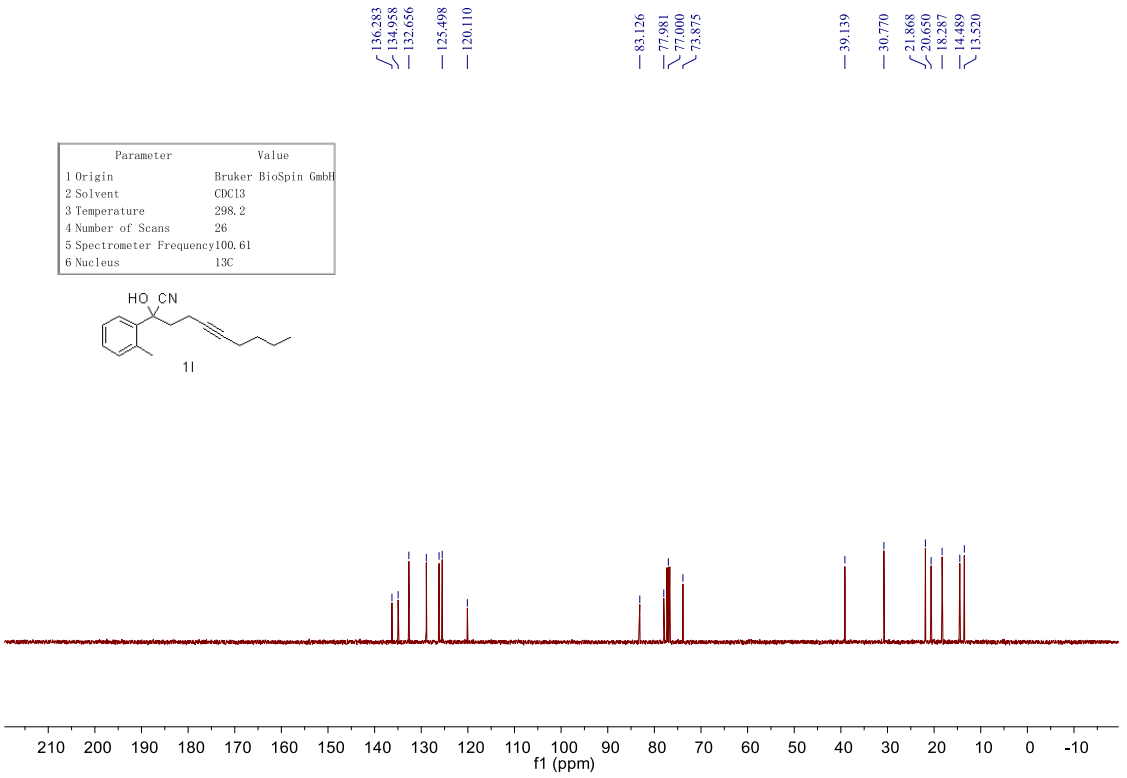

7.436
7.428
7.423
7.411
7.406
7.399
7.261
6.899
6.891
6.886
6.874
6.869
6.861
4.169
3.784
2.426
2.325
2.297
2.269
2.244
2.193
2.142
2.106
2.071
1.428
1.373
1.335
0.906
0.888
0.870
Parameter Value
1 Origin Bruker BioSpin GmbH
2 Solvent CDCl3
3 Temperature 298.2
4 Number of Scans 2
5 Spectrometer Frequency 400.13
6 Nucleus 1H
HO CN
O
1j
2.01
2.02
0.96
3.06
1.01
1.05
4.15
4.07
3.00
f1 (ppm)

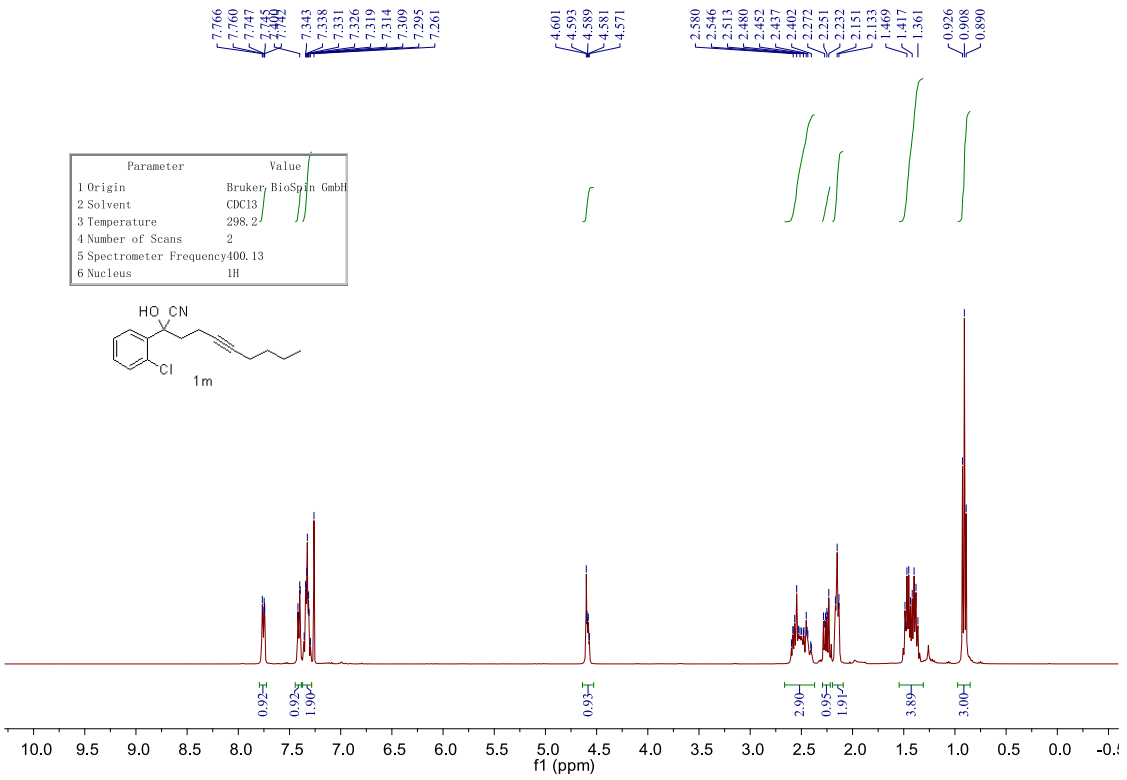

159.873
131.464
126.109
120.332
114.002
82.480
77.797
77.000
73.751
55.241
42.166
30.744
21.792
18.207
14.438
13.458
Parameter Value
1 Origin Bruker BioSpin GmbH
2 Solvent CDCl3
3 Temperature 298.4
4 Number of Scans 32
5 Spectrometer Frequency 100.61
6 Nucleus 13C
HO CN
O
1j
f1 (ppm)

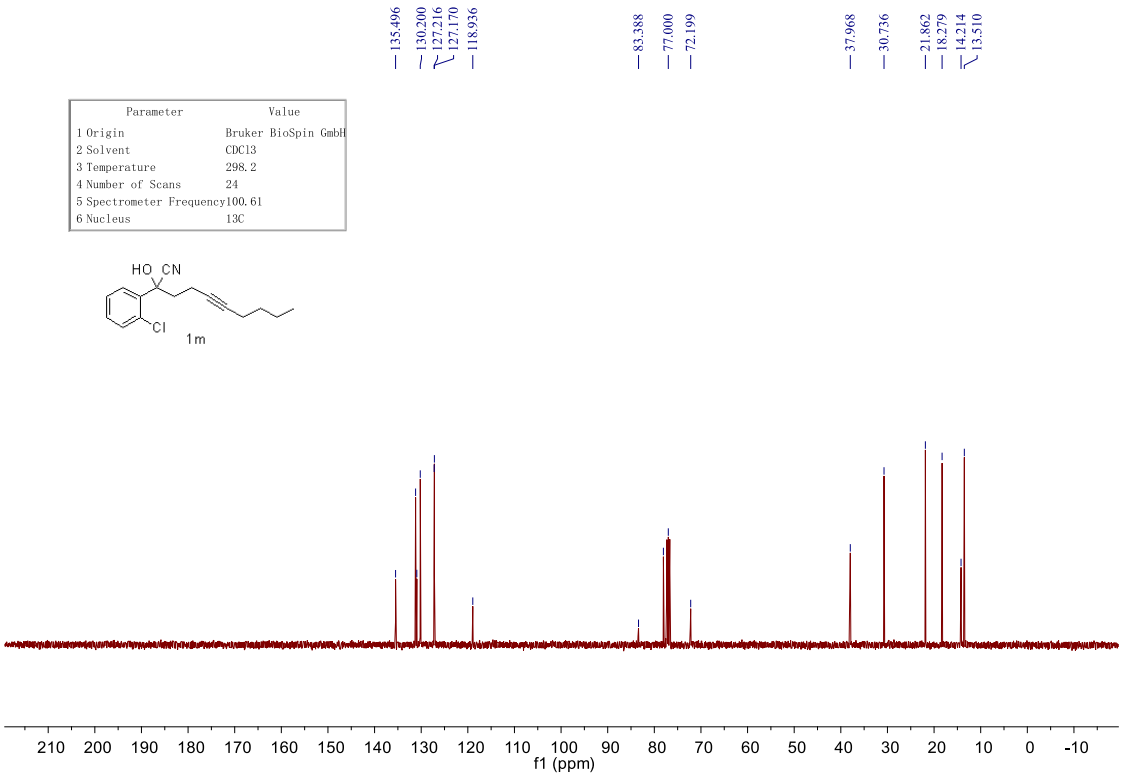

7.352
7.339
7.319
7.306
7.288
7.268
7.261
7.188
7.170
4.082
2.480
2.457
2.433
2.350
2.322
2.296
2.190
2.156
2.133
2.103
1.461
1.404
1.359
0.927
0.910
0.892
Parameter Value
1 Origin Bruker BioSpin GmbH
2 Solvent CDCl3
3 Temperature 298.2
4 Number of Scans 2
5 Spectrometer Frequency 400.13
6 Nucleus 1H
HO CN
1k
1.94
1.01
0.98
0.98
1.06
3.01
0.99
4.03
4.02
3.00
f1 (ppm)

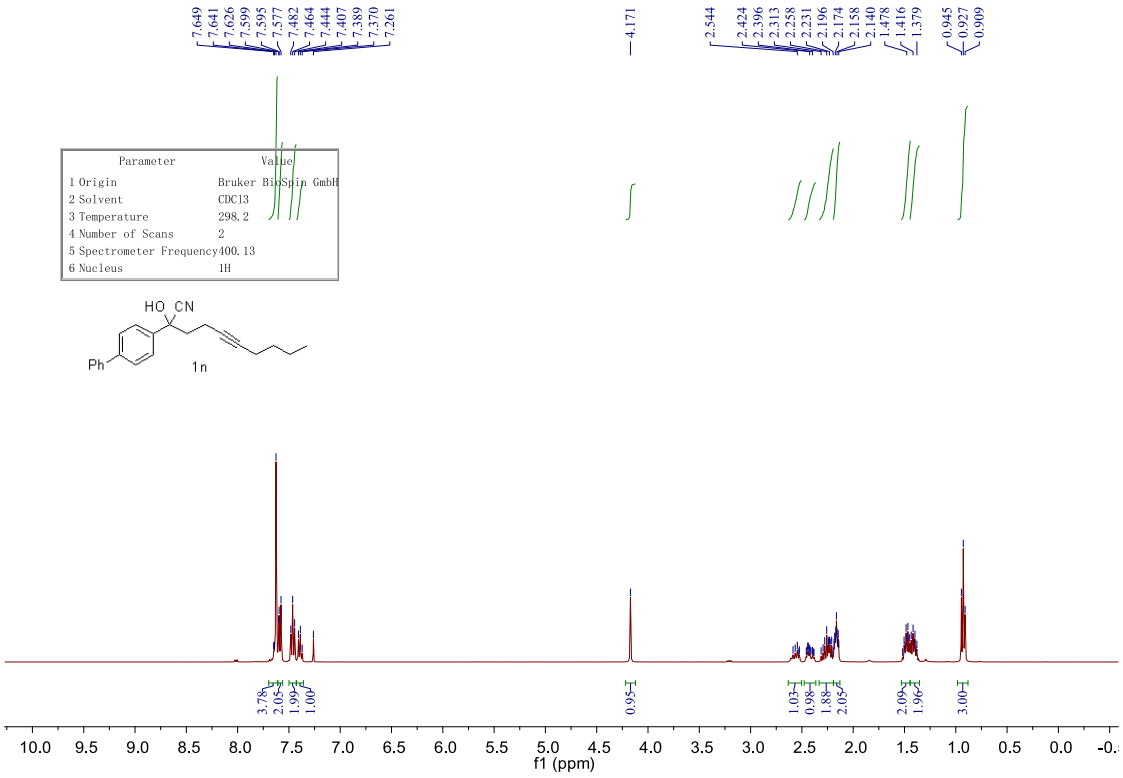

139.334
138.605
129.772
128.635
125.322
121.789
120.286
82.774
77.842
77.000
74.248
42.170
30.765
21.831
21.372
18.243
14.514
13.493
Parameter Value
1 Origin Bruker BioSpin GmbH
2 Solvent CDCl3
3 Temperature 298.2
4 Number of Scans 20
5 Spectrometer Frequency 100.61
6 Nucleus 13C
HO CN
1k
f1 (ppm)

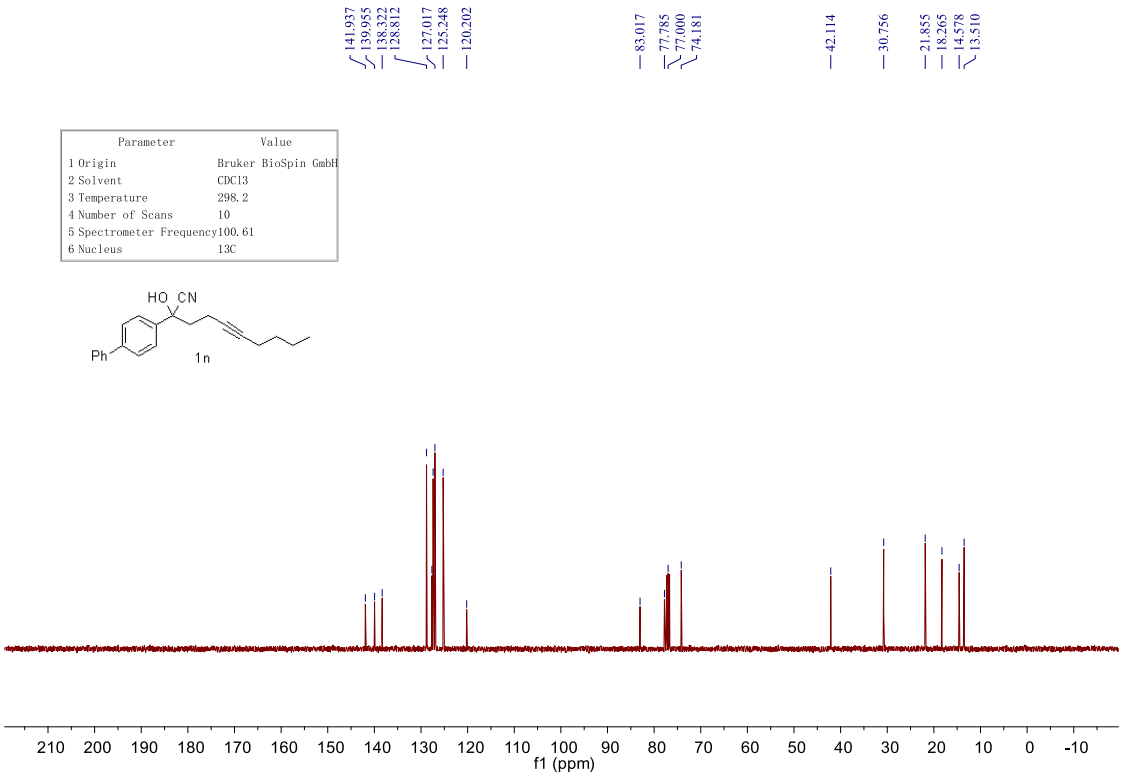

7.614
7.611
7.596
7.591
7.270
7.261
7.257
7.252
7.248
7.234
7.230
7.214
7.196
7.194
7.193
4.088
2.525
2.500
2.460
2.435
2.406
2.295
2.266
2.177
2.154
2.130
1.454
1.404
1.366
0.932
0.914
0.896
Parameter Value
1 Origin Bruker BioSpin GmbH
2 Solvent CDCl3
3 Temperature 298.2
4 Number of Scans 2
5 Spectrometer Frequency 400.13
6 Nucleus 1H
HO CN
1l
0.97
1.78
1.71
1.03
2.99
0.90
1.14
1.93
2.08
4.20
3.00
f1 (ppm)

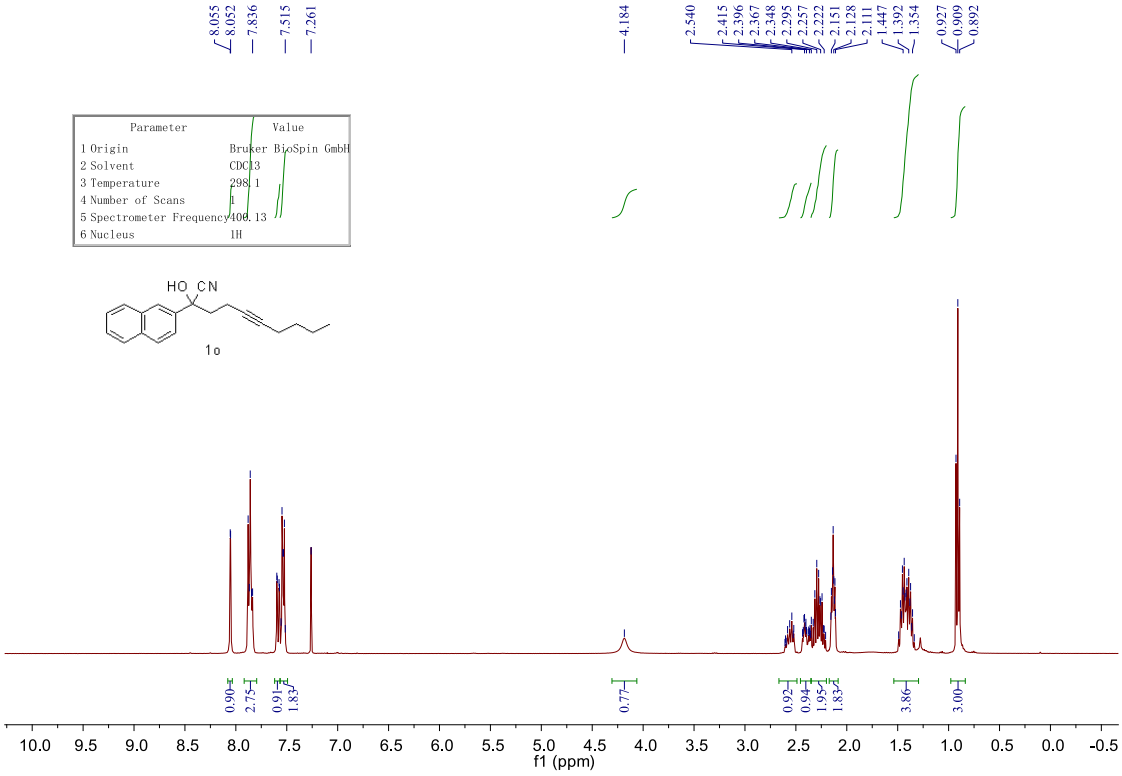

136.283
134.958
132.656
125.498
120.110
83.126
77.981
77.000
73.875
39.139
30.770
21.868
20.650
18.287
14.489
13.520
Parameter Value
1 Origin Bruker BioSpin GmbH
2 Solvent CDCl3
3 Temperature 298.2
4 Number of Scans 26
5 Spectrometer Frequency 100.61
6 Nucleus 13C
HO CN
1l
f1 (ppm)

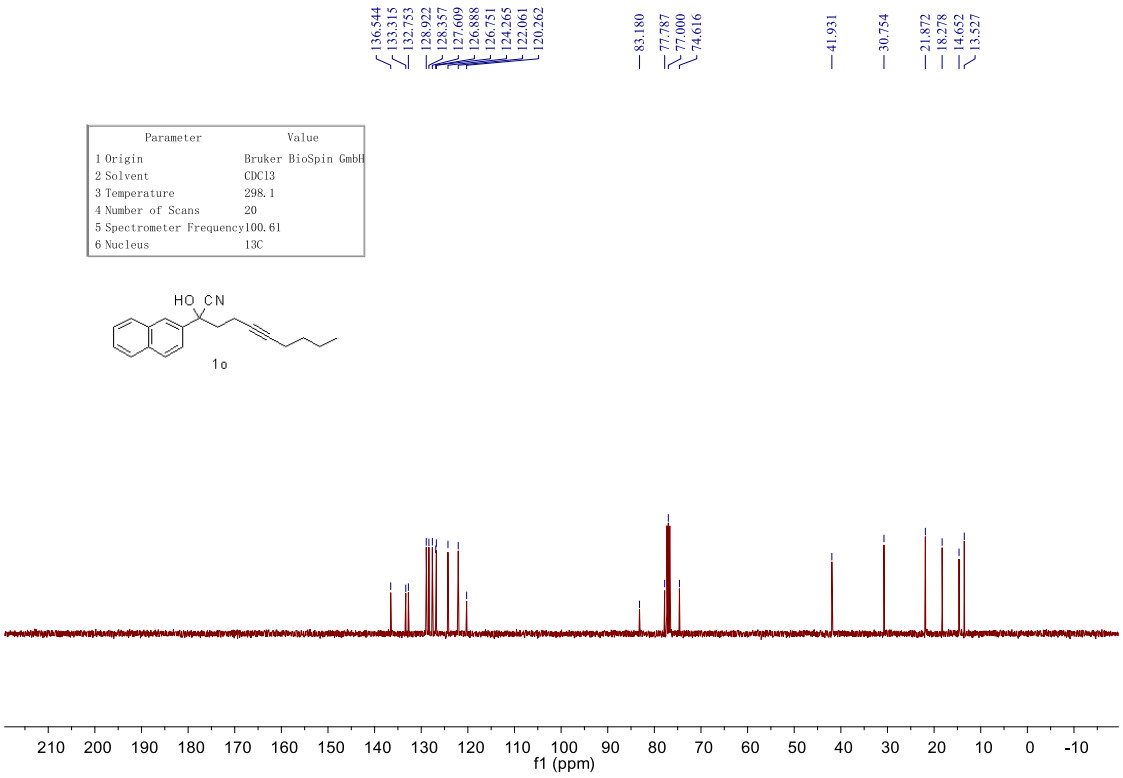

7.766
7.760
7.747
7.745
7.343
7.338
7.331
7.326
7.319
7.314
7.309
7.295
7.261
4.601
4.593
4.589
4.581
4.571
2.580
2.546
2.513
2.480
2.452
2.437
2.402
2.272
2.251
2.232
2.151
2.133
1.469
1.417
1.361
0.926
0.908
0.890
Parameter Value
1 Origin Bruker BioSpin GmbH
2 Solvent CDCl3
3 Temperature 298.2
4 Number of Scans 2
5 Spectrometer Frequency 400.13
6 Nucleus 1H
HO CN
Cl
1m
0.92
0.92
1.90
0.93
2.90
0.95
1.91
3.89
3.00
f1 (ppm)

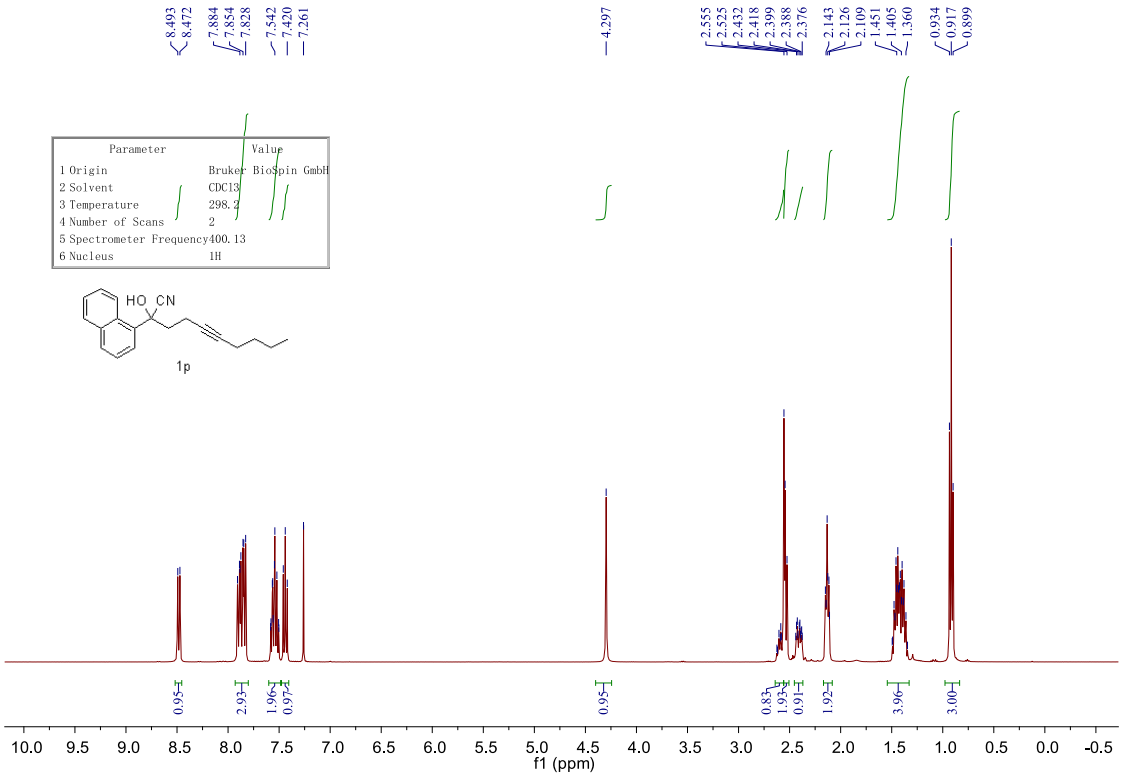

135.496
130.200
127.216
127.170
118.936
83.388
77.000
72.199
37.968
30.736
21.862
18.279
14.214
13.510
Parameter Value
1 Origin Bruker BioSpin GmbH
2 Solvent CDCl3
3 Temperature 298.2
4 Number of Scans 24
5 Spectrometer Frequency 100.61
6 Nucleus 13C
HO CN
Cl
1m
f1 (ppm)


7.649
7.641
7.626
7.599
7.595
7.577
7.482
7.464
7.444
7.407
7.389
7.370
7.261
4.171
2.544
2.424
2.396
2.313
2.258
2.231
2.196
2.174
2.158
2.140
1.478
1.416
1.379
0.945
0.927
0.909
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
HO CN
Ph
1n
3.78
2.05
1.99
1.00
0.95
1.03
0.98
1.88
2.05
2.09
1.96
3.00
f1 (ppm)

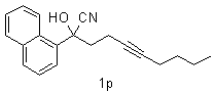

141.937
139.955
138.322
128.812
127.017
125.248
120.202
83.017
77.785
77.000
74.181
42.114
30.756
21.855
18.265
14.578
13.510
Parameter Value
1 Origin Bruker BioSpin GmbH
2 Solvent CDCl3
3 Temperature 298.2
4 Number of Scans 10
5 Spectrometer Frequency 100.61
6 Nucleus 13C
HO CN
Ph
1n
f1 (ppm)


8.055
8.052
7.836
7.515
7.261
4.184
2.540
2.415
2.396
2.367
2.348
2.295
2.257
2.222
2.151
2.128
2.111
1.447
1.392
1.354
0.927
0.909
0.892
Parameter Value
1 Origin Bruker BioSpin GmbH
2 Solvent CDCl3
3 Temperature 298.1
4 Number of Scans 1
5 Spectrometer Frequency 400.13
6 Nucleus 1H
HO CN
1o
0.90
2.75
0.91
1.83
0.77
0.92
0.94
1.95
1.83
3.86
3.00
f1 (ppm)

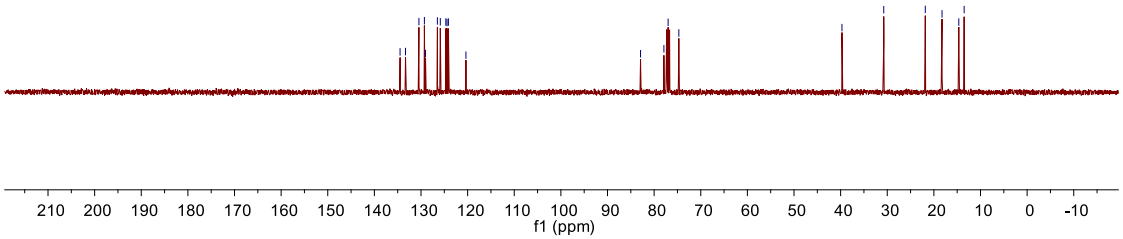

136.544
133.315
132.753
128.922
128.357
127.609
126.888
126.751
124.265
122.061
120.262
83.180
77.787
77.000
74.616
41.931
30.754
21.872
18.278
14.652
13.527
Parameter Value
1 Origin Bruker BioSpin GmbH
2 Solvent CDCl3
3 Temperature 298.1
4 Number of Scans 20
5 Spectrometer Frequency 100.61
6 Nucleus 13C
HO CN
1o
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)


8.493
8.472
7.884
7.854
7.828
7.542
7.420
7.261
4.297
2.555
2.525
2.432
2.418
2.399
2.388
2.376
2.143
2.126
2.109
1.451
1.405
1.360
0.934
0.917
0.899
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
HO CN
1p
0.95
2.93
1.96
0.97
0.95
0.83
1.93
0.91
1.92
3.96
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
f1 (ppm)

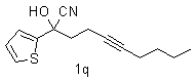
Parameter	Value
1 Origin	Bruker BioSpin GmbH
2 Solvent	CDCl3
3 Temperature	298.3
4 Number of Scans	6
5 Spectrometer Frequency	100.61
6 Nucleus	13C



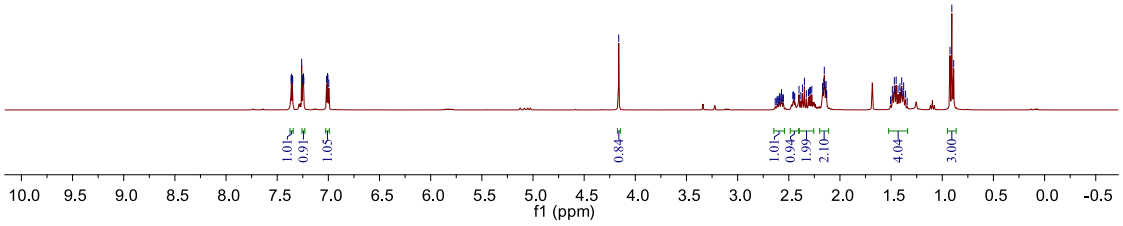
1p

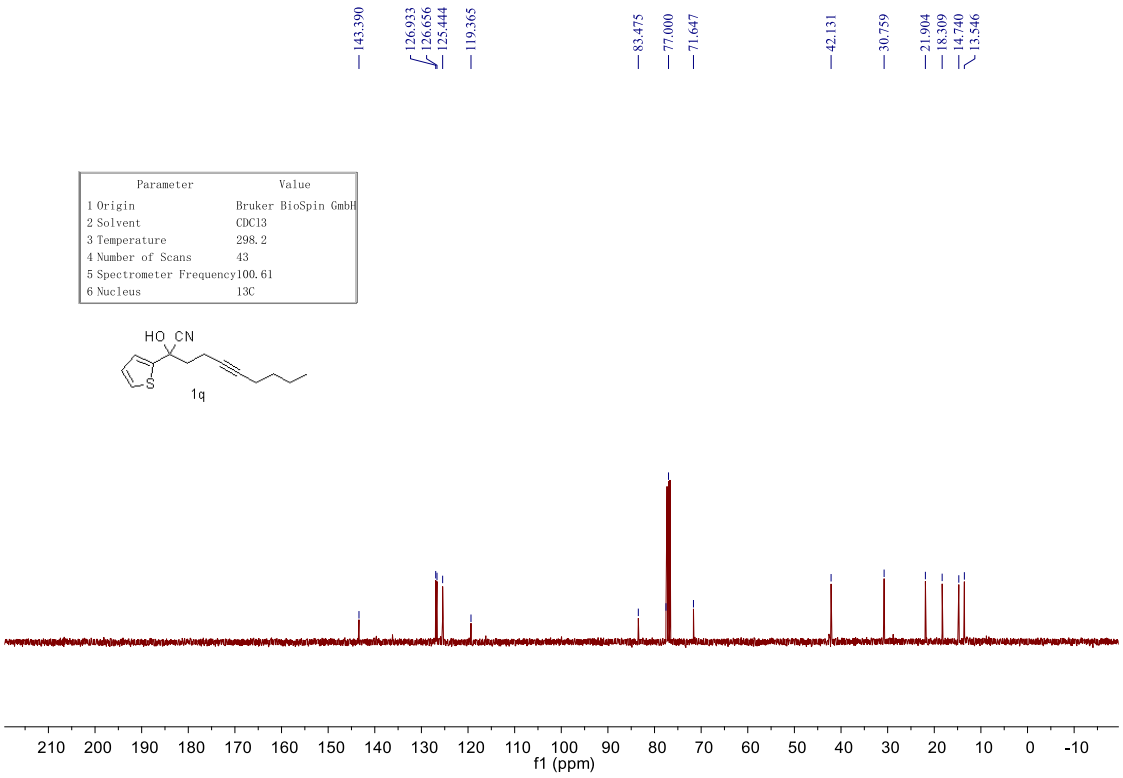


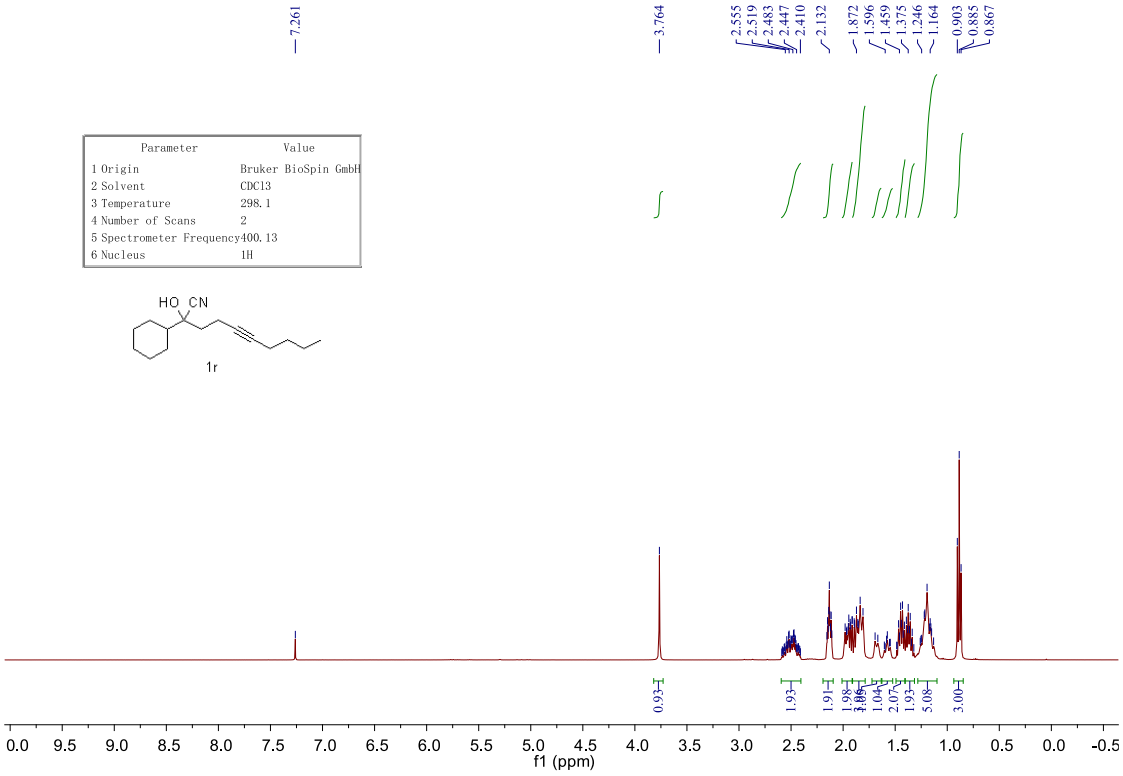
Parameter	Value
1 Origin	Bruker BioSpin GmbH
2 Solvent	CDCl3
3 Temperature	298.2
4 Number of Scans	4
5 Spectrometer Frequency	400.13
6 Nucleus	1H

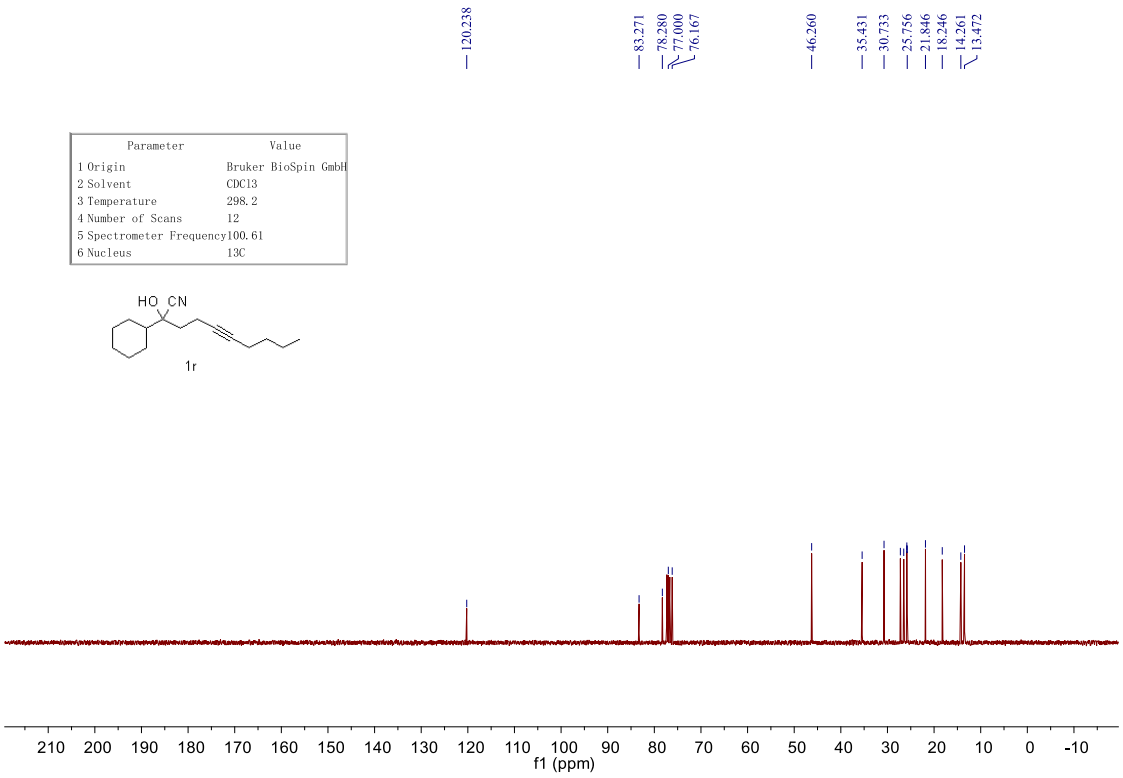


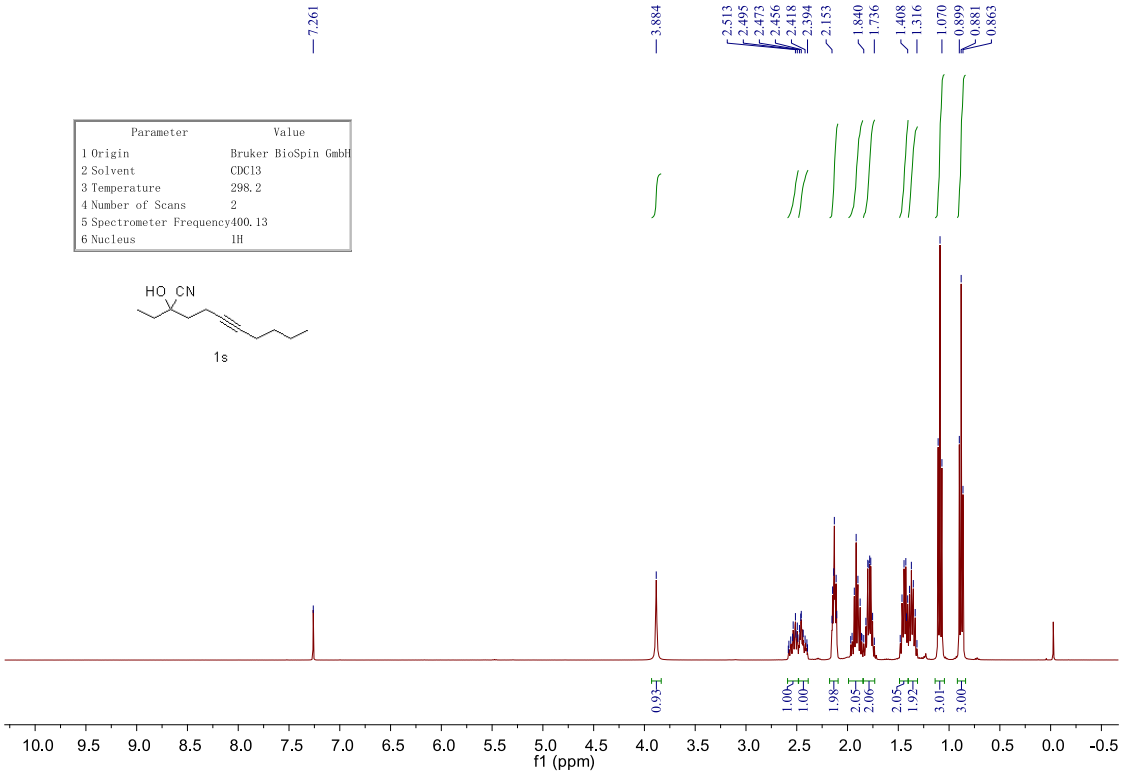
1q

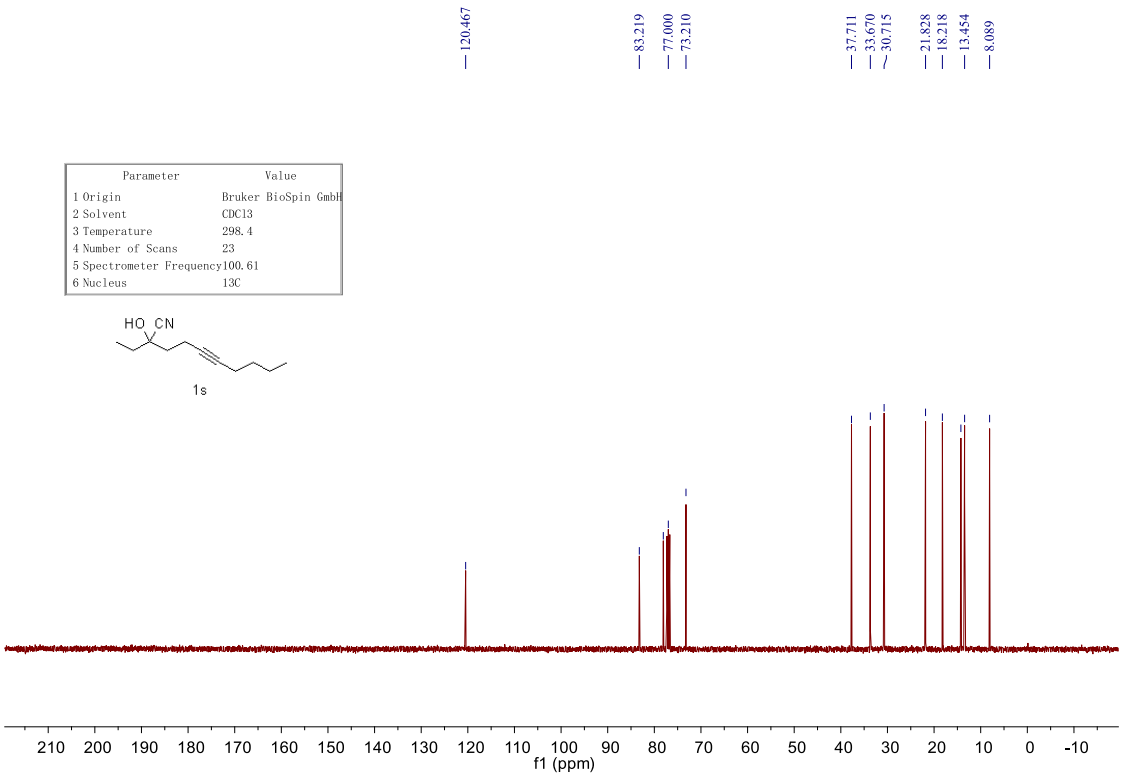


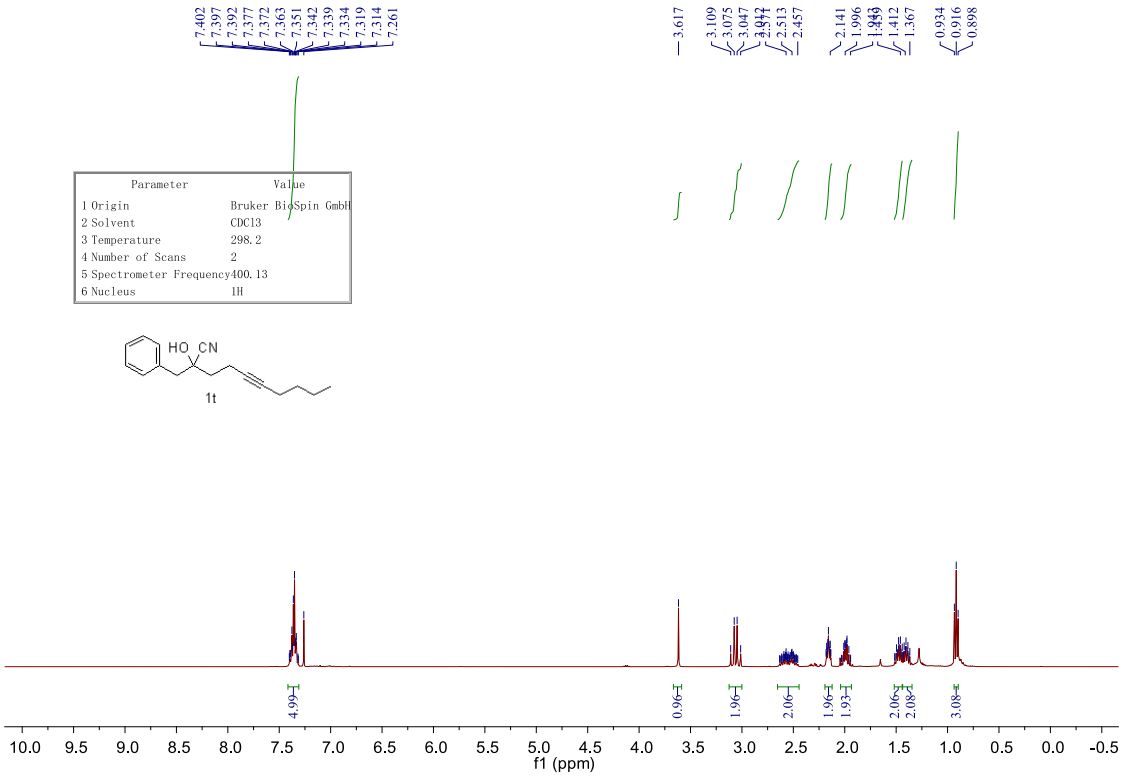

143.390
126.933
126.656
125.444
119.365
83.475
77.000
71.647
42.131
30.759
21.904
18.309
14.740
13.546
Parameter Value
1 Origin Bruker BioSpin GmbH
2 Solvent CDCl3
3 Temperature 298.2
4 Number of Scans 43
5 Spectrometer Frequency 100.61
6 Nucleus 13C
HO CN
S
1q
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)

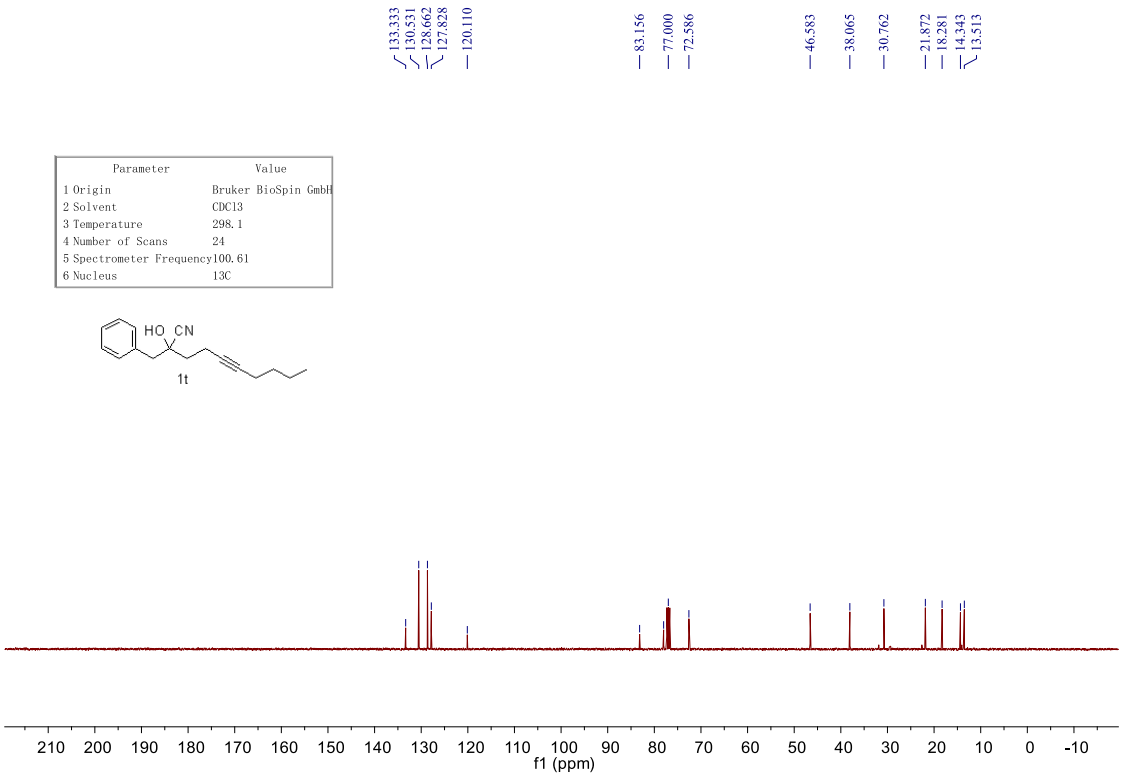

7.261
3.764
2.555
2.519
2.483
2.447
2.410
2.132
1.872
1.596
1.459
1.375
1.246
1.164
0.903
0.885
0.867
Parameter Value
1 Origin Bruker BioSpin GmbH
2 Solvent CDCl3
3 Temperature 298.1
4 Number of Scans 2
5 Spectrometer Frequency 400.13
6 Nucleus 1H
HO CN
1r
0.93
1.93
1.91
1.98
1.04
2.07
1.93
5.08
3.00
0.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5
f1 (ppm)

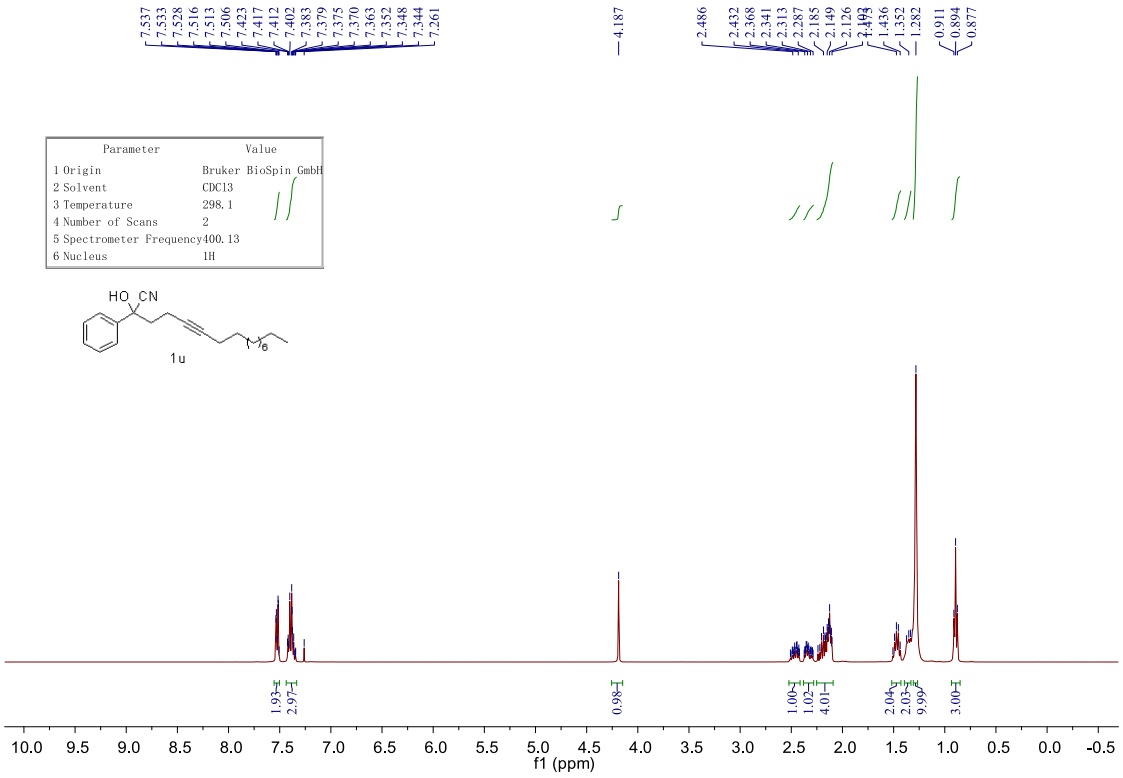

120.238
83.271
78.280
77.000
76.167
46.260
35.431
30.733
25.756
21.846
18.246
14.261
13.472
Parameter Value
1 Origin Bruker BioSpin GmbH
2 Solvent CDCl3
3 Temperature 298.2
4 Number of Scans 12
5 Spectrometer Frequency 100.61
6 Nucleus 13C
HO CN
1r
f1 (ppm)

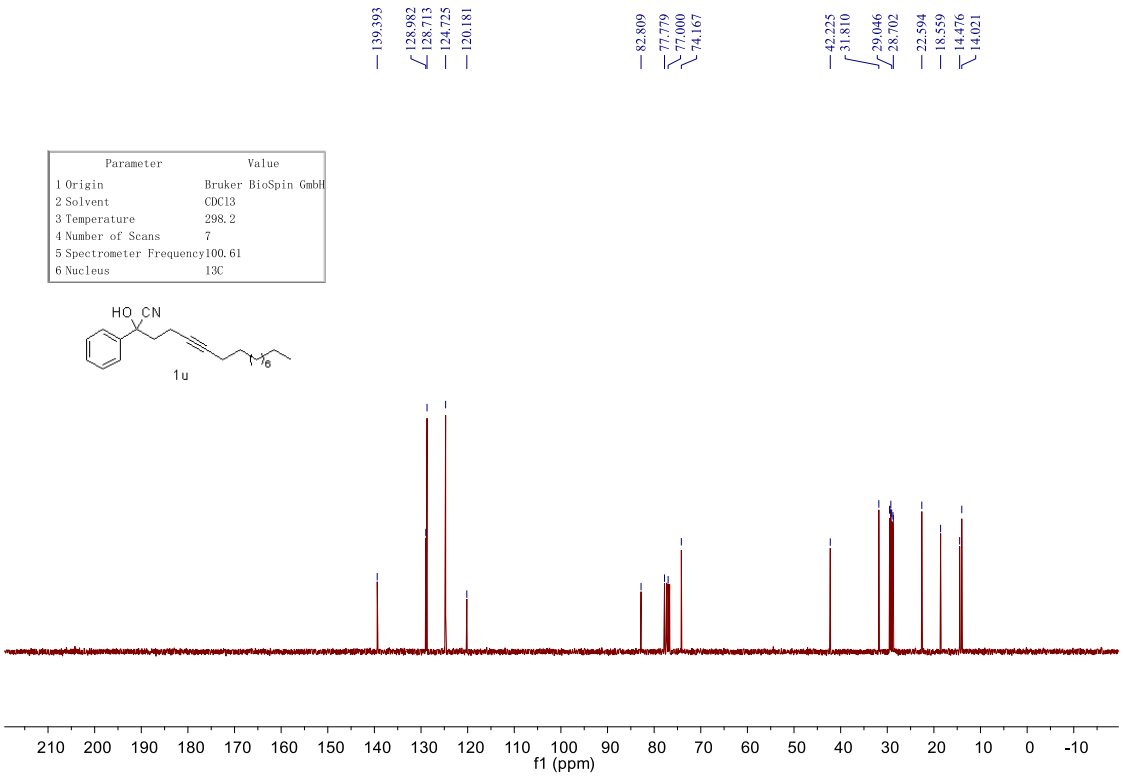

7.261
3.884
2.513
2.495
2.473
2.456
2.418
2.394
2.153
1.840
1.736
1.408
1.316
1.070
0.899
0.881
0.863
Parameter Value
1 Origin Bruker BioSpin GmbH
2 Solvent CDCl3
3 Temperature 298.2
4 Number of Scans 2
5 Spectrometer Frequency 400.13
6 Nucleus 1H
HO CN
1s
0.93
1.00
1.00
1.98
2.05
2.06
2.05
1.92
3.01
3.00
f1 (ppm)

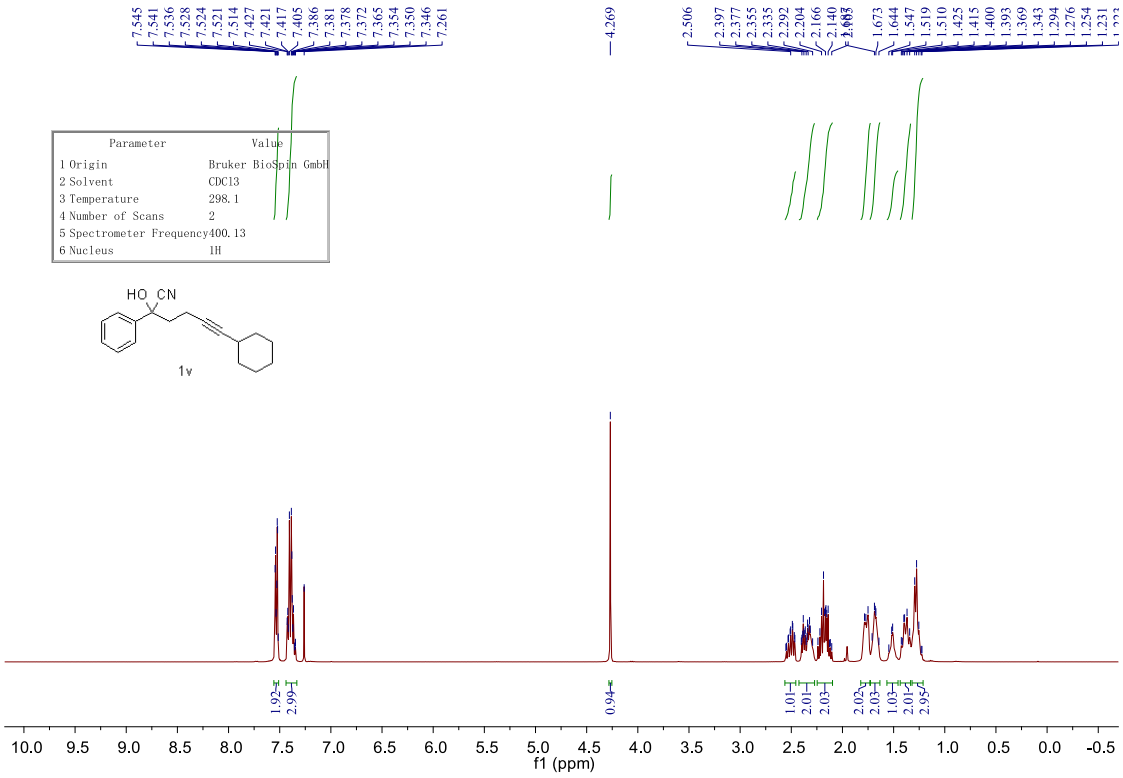

120.467
83.219
77.000
73.210
37.711
33.670
30.715
21.828
18.218
13.454
8.089
Parameter Value
1 Origin Bruker BioSpin GmbH
2 Solvent CDCl3
3 Temperature 298.4
4 Number of Scans 23
5 Spectrometer Frequency 100.61
6 Nucleus 13C
HO CN
1s
f1 (ppm)

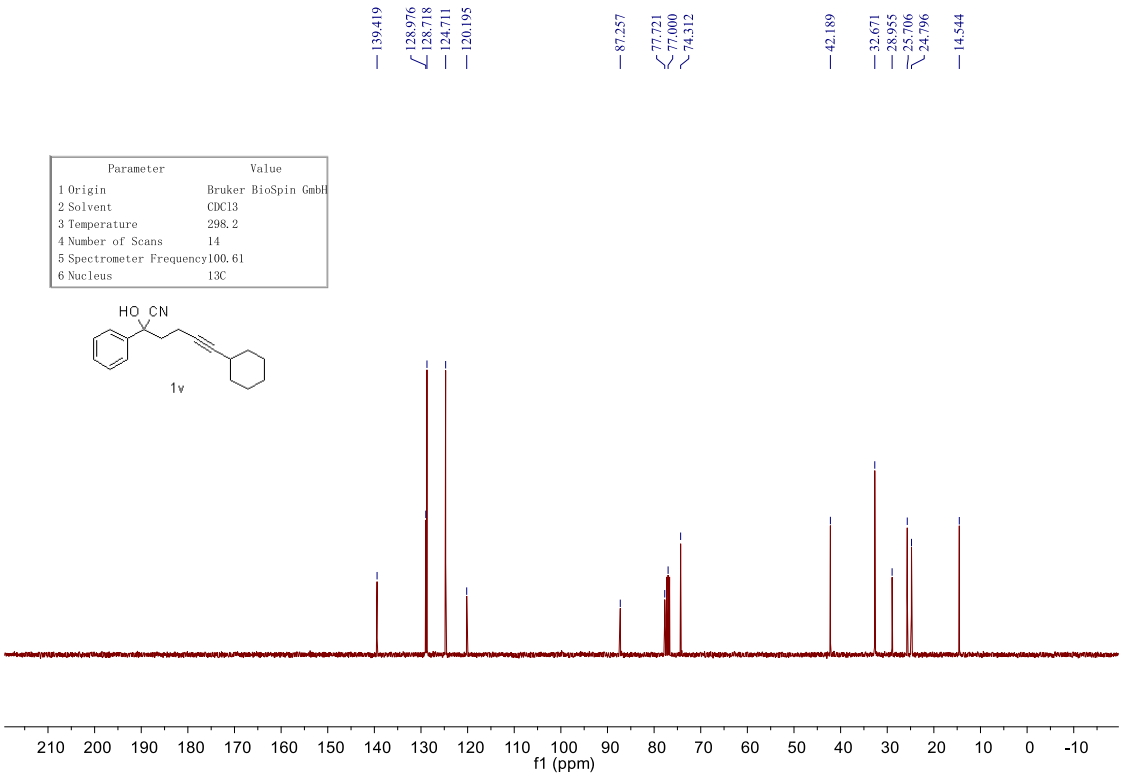

7.402
7.397
7.392
7.377
7.372
7.363
7.351
7.342
7.339
7.334
7.319
7.314
7.261
3.617
3.109
3.075
3.047
2.513
2.457
2.141
1.996
1.412
1.367
0.934
0.916
0.898
Parameter Value
1 Origin Bruker BioSpin GmbH
2 Solvent CDCl3
3 Temperature 298.2
4 Number of Scans 2
5 Spectrometer Frequency 400.13
6 Nucleus 1H
HO CN
1t
4.99
0.96
1.96
2.06
1.96
1.93
2.06
2.08
3.08
f1 (ppm)

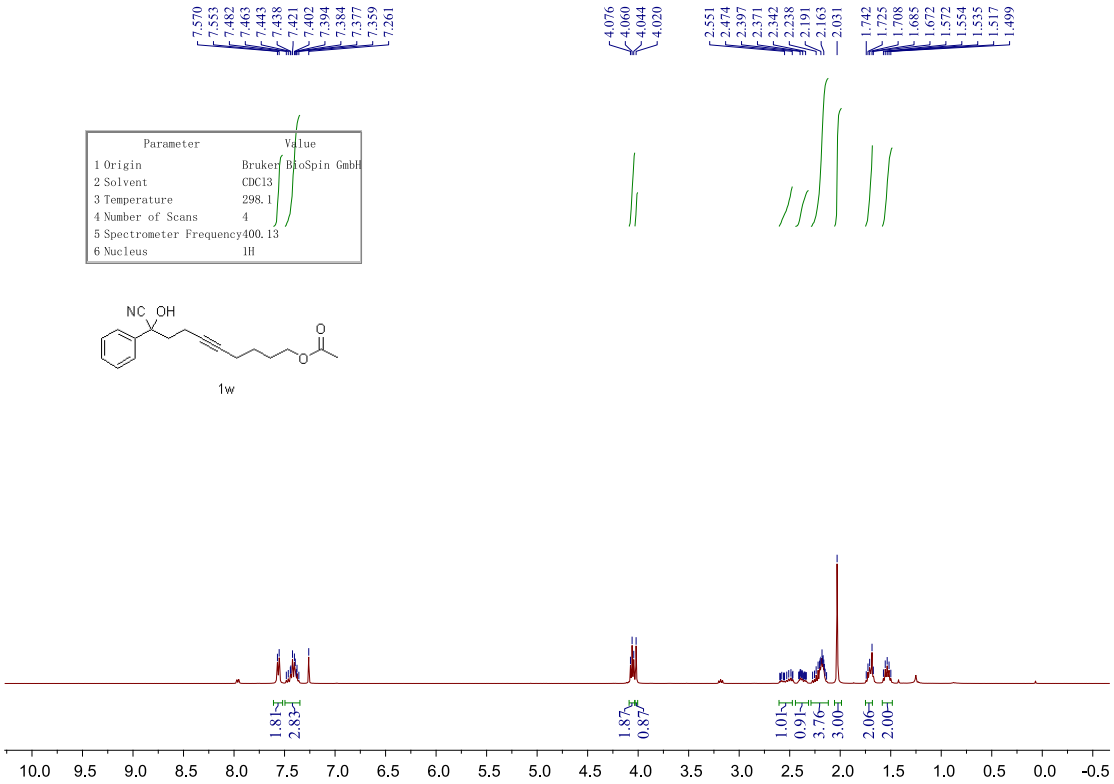

133.333
130.531
128.662
127.828
120.110
83.156
77.000
72.586
46.583
38.065
30.762
21.872
18.281
14.343
13.513
Parameter Value
1 Origin Bruker BioSpin GmbH
2 Solvent CDCl3
3 Temperature 298.1
4 Number of Scans 24
5 Spectrometer Frequency 100.61
6 Nucleus 13C
HO CN
1t
f1 (ppm)

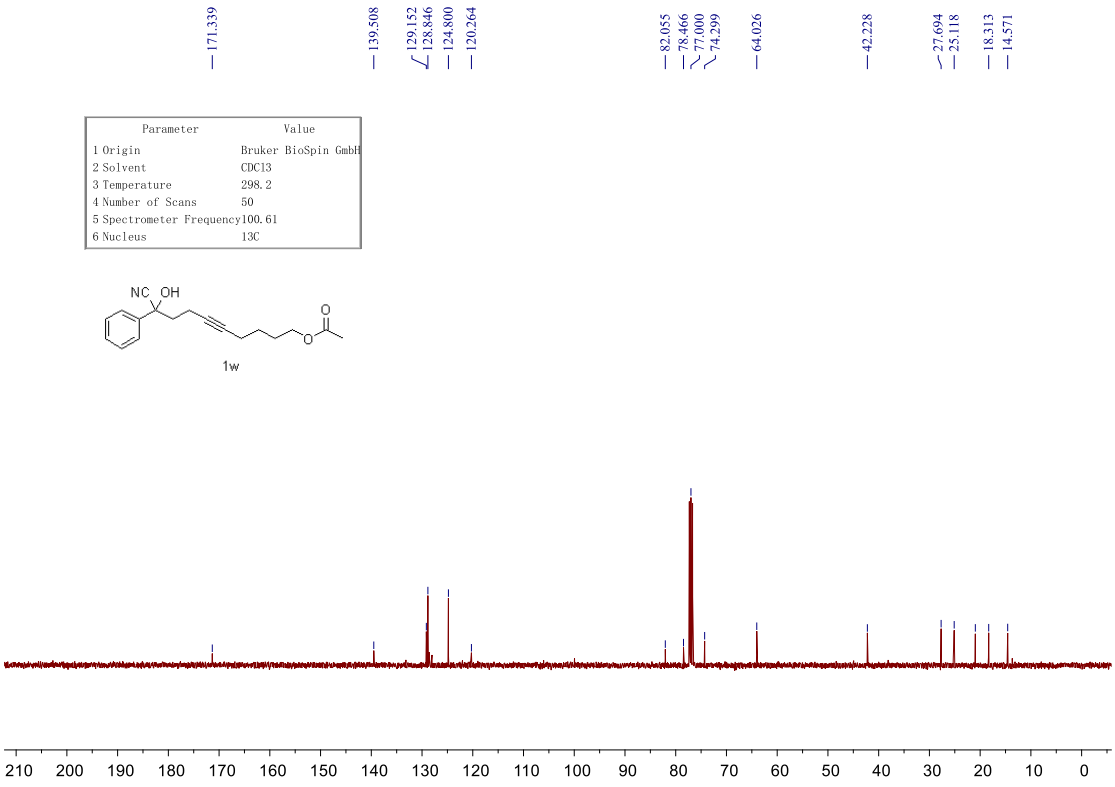

7.537
7.533
7.528
7.516
7.513
7.506
7.423
7.417
7.412
7.402
7.383
7.379
7.375
7.370
7.363
7.352
7.348
7.344
7.261
4.187
2.486
2.432
2.368
2.341
2.313
2.287
2.185
2.149
2.126
1.436
1.352
1.282
0.911
0.894
0.877
Parameter Value
1 Origin Bruker BioSpin GmbH
2 Solvent CDCl3
3 Temperature 298.1
4 Number of Scans 2
5 Spectrometer Frequency 400.13
6 Nucleus 1H
HO CN
1u
1.93
2.97
0.98
1.00
1.02
4.01
2.04
2.03
9.99
3.00
f1 (ppm)

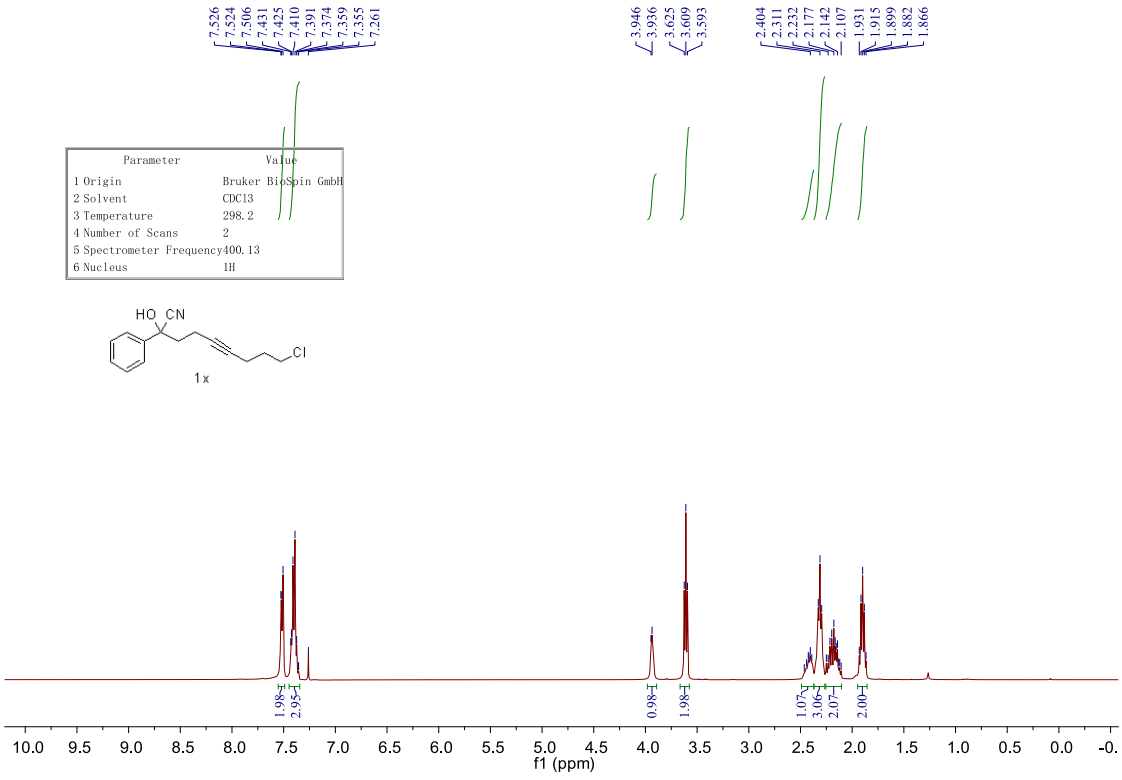

139.393
128.982
128.713
124.725
120.181
82.809
77.779
77.000
74.167
42.225
31.810
29.046
28.702
22.594
18.559
14.476
14.021
Parameter Value
1 Origin Bruker BioSpin GmbH
2 Solvent CDCl3
3 Temperature 298.2
4 Number of Scans 7
5 Spectrometer Frequency 100.61
6 Nucleus 13C
HO CN
1u
f1 (ppm)

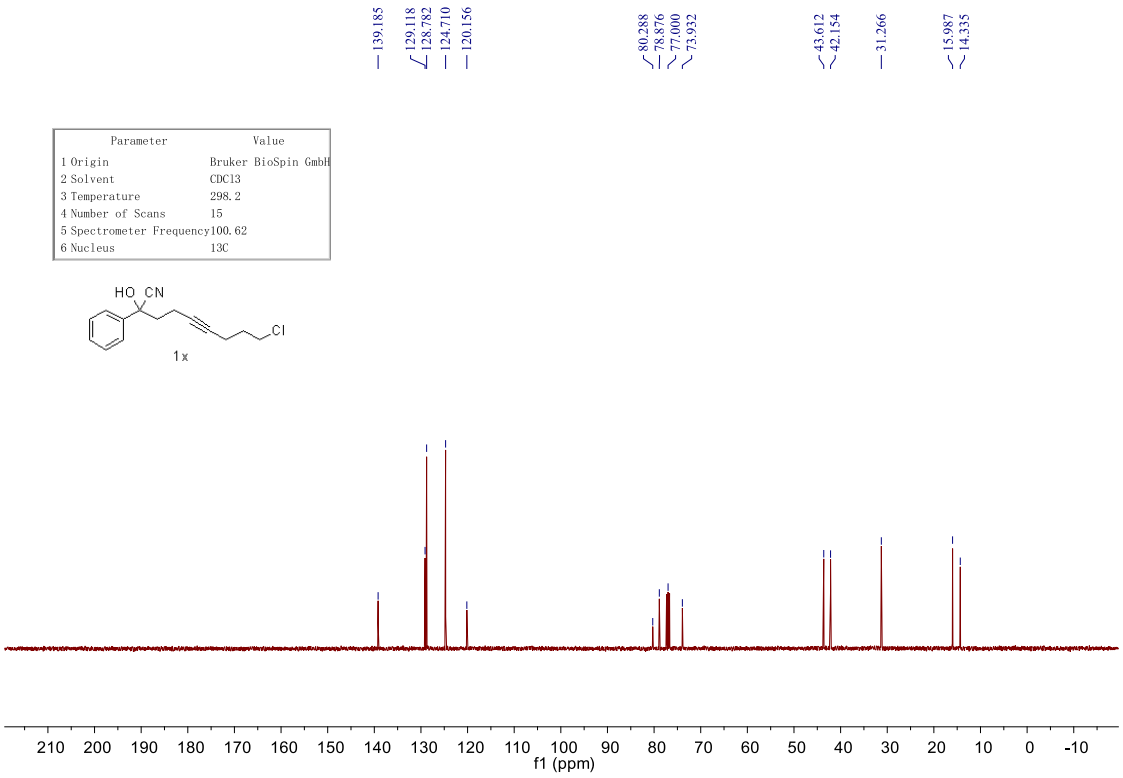

7.545
7.541
7.536
7.528
7.524
7.521
7.514
7.427
7.421
7.417
7.405
7.386
7.381
7.378
7.372
7.365
7.354
7.350
7.346
7.261
4.269
2.506
2.397
2.377
2.355
2.335
2.292
2.204
2.166
2.140
1.673
1.644
1.547
1.519
1.510
1.425
1.415
1.400
1.393
1.369
1.343
1.294
1.276
1.254
1.231
Parameter Value
1 Origin Bruker BioSpin GmbH
2 Solvent CDCl3
3 Temperature 298.1
4 Number of Scans 2
5 Spectrometer Frequency 400.13
6 Nucleus 1H
HO CN
1v
1.92
2.99
0.94
1.01
2.01
2.03
2.02
2.03
1.03
2.01
2.95
f1 (ppm)

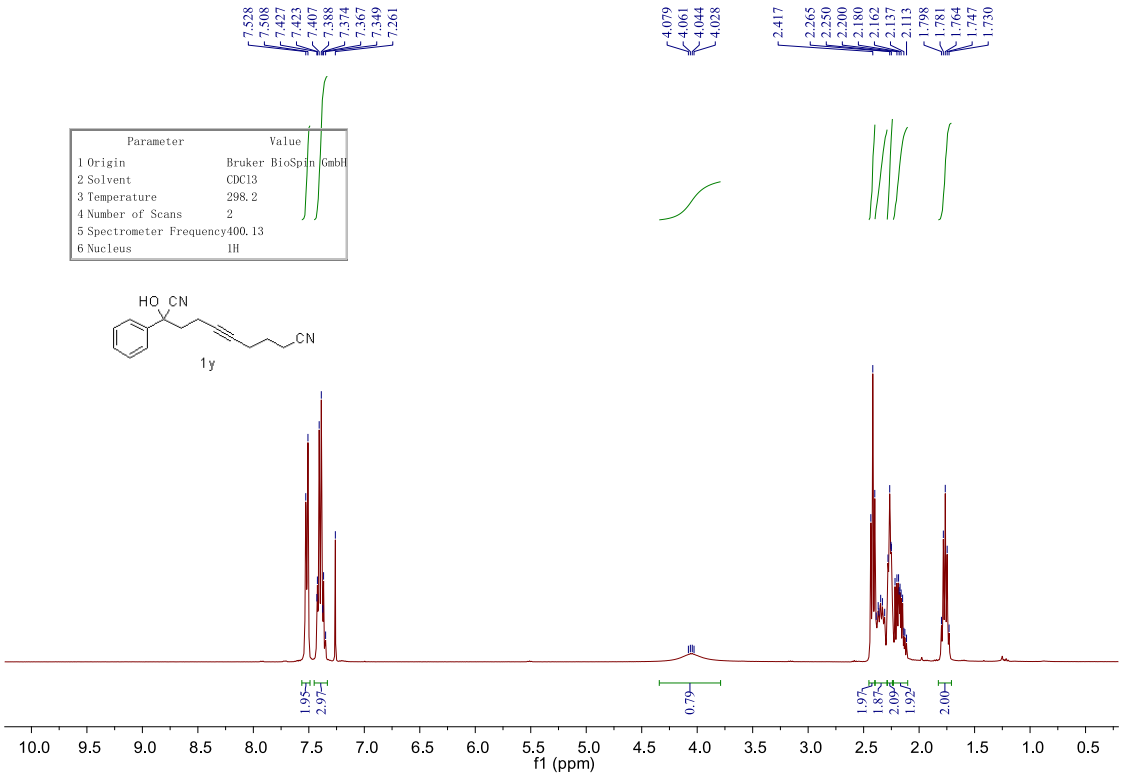

139.419
128.976
128.718
124.711
120.195
87.257
77.721
77.000
74.312
42.189
32.671
28.955
25.706
24.796
14.544
Parameter Value
1 Origin Bruker BioSpin GmbH
2 Solvent CDCl3
3 Temperature 298.2
4 Number of Scans 14
5 Spectrometer Frequency 100.61
6 Nucleus 13C
HO CN
1v
f1 (ppm)

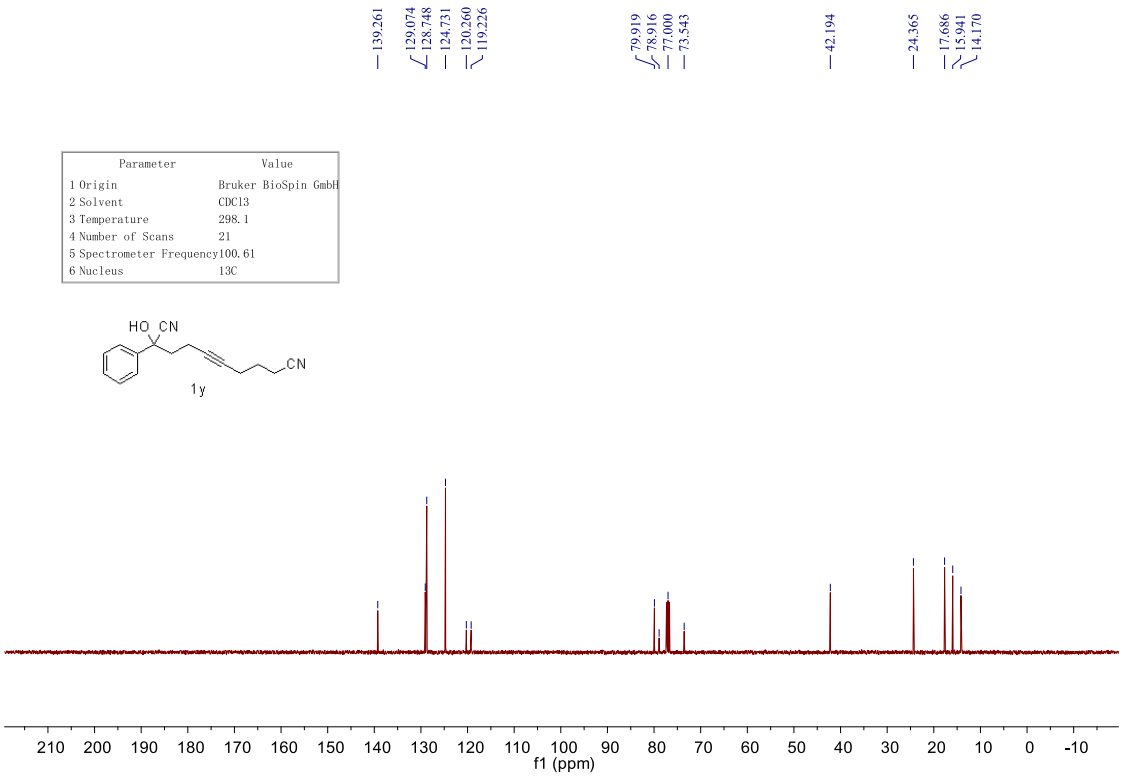

7.570
7.553
7.482
7.463
7.443
7.438
7.421
7.402
7.394
7.384
7.377
7.359
7.261
4.076
4.060
4.044
4.020
2.551
2.474
2.397
2.371
2.342
2.238
2.191
2.163
2.031
1.742
1.725
1.708
1.685
1.672
1.572
1.554
1.535
1.517
1.499
Parameter Value
1 Origin Bruker BioSpin GmbH
2 Solvent CDCl3
3 Temperature 298.1
4 Number of Scans 4
5 Spectrometer Frequency 400.13
6 Nucleus 1H
NC OH
O
O
1w
1.81
2.83
1.87
0.87
1.01
0.91
3.76
3.00
2.06
2.00

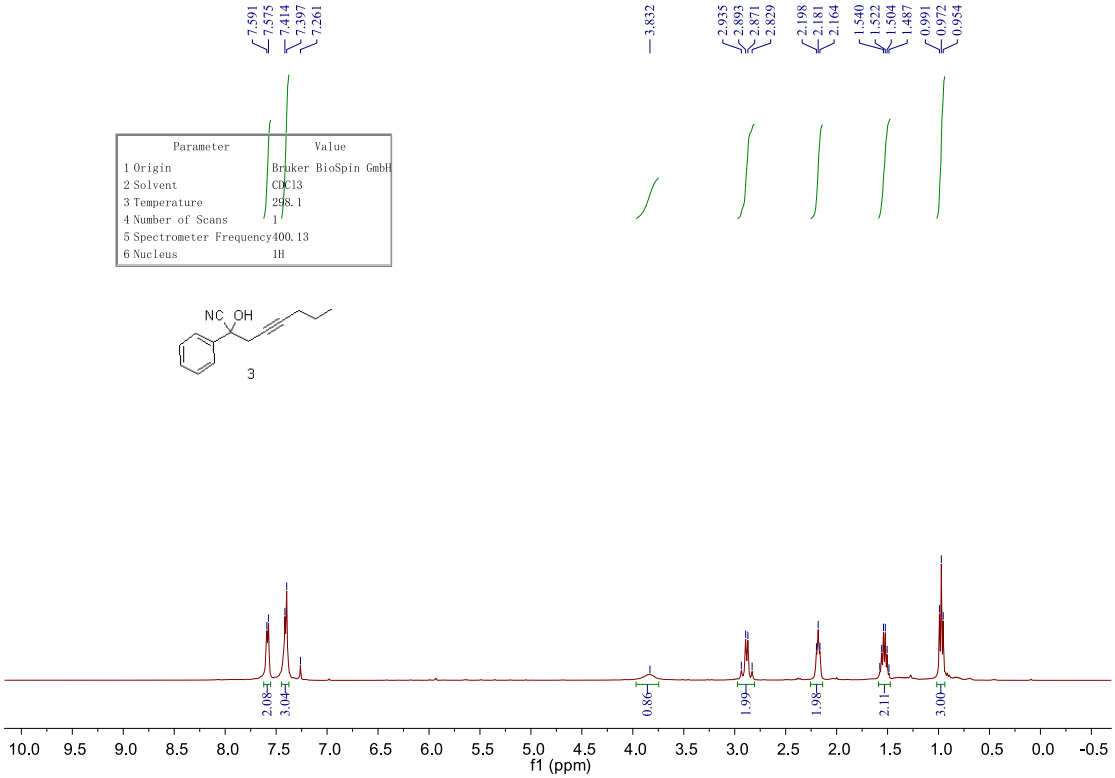

171.339
139.508
129.152
128.846
124.800
120.264
82.055
78.466
77.000
74.299
64.026
42.228
27.694
25.118
18.313
14.571
Parameter Value
1 Origin Bruker BioSpin GmbH
2 Solvent CDCl3
3 Temperature 298.2
4 Number of Scans 50
5 Spectrometer Frequency 100.61
6 Nucleus 13C
NC OH
O
O
1w
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0

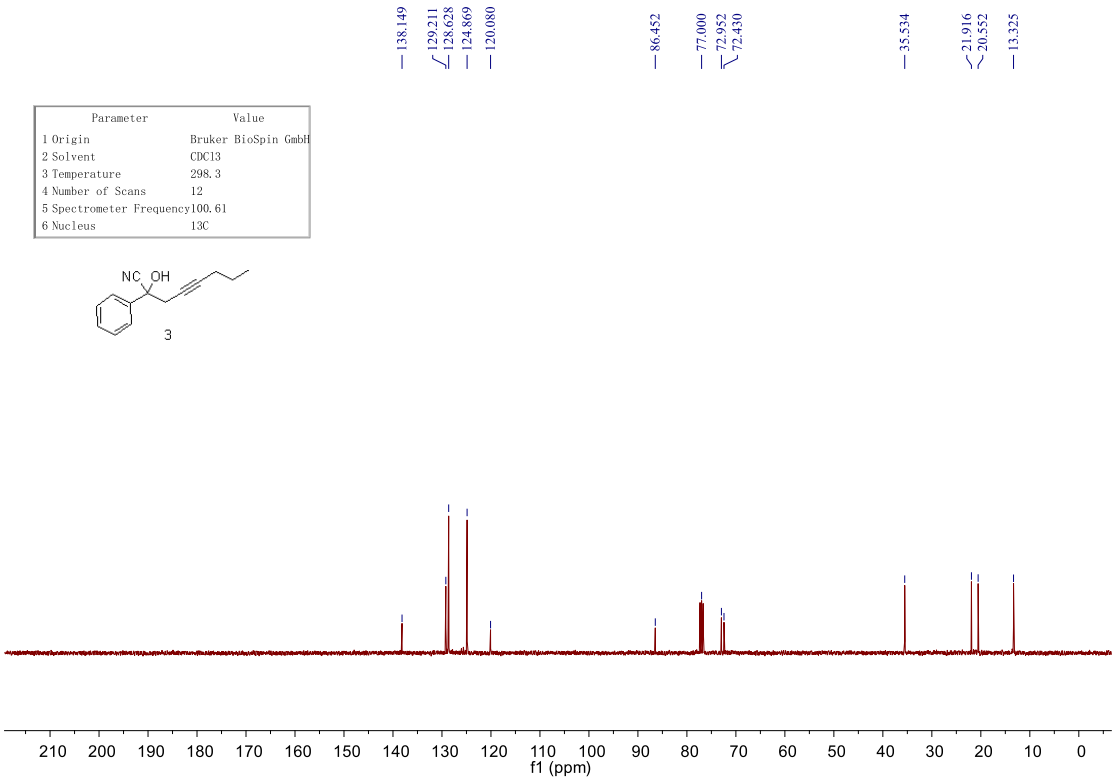

7.526
7.524
7.506
7.431
7.425
7.410
7.391
7.374
7.359
7.355
7.261
3.946
3.936
3.625
3.609
3.593
2.404
2.311
2.232
2.177
2.142
2.107
1.931
1.915
1.899
1.882
1.866
Parameter Value
1 Origin Bruker BioSpin GmbH
2 Solvent CDCl3
3 Temperature 298.2
4 Number of Scans 2
5 Spectrometer Frequency 400.13
6 Nucleus 1H
HO CN
Cl
1x
1.98
2.95
0.98
1.98
1.07
3.06
2.07
2.00
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.
f1 (ppm)

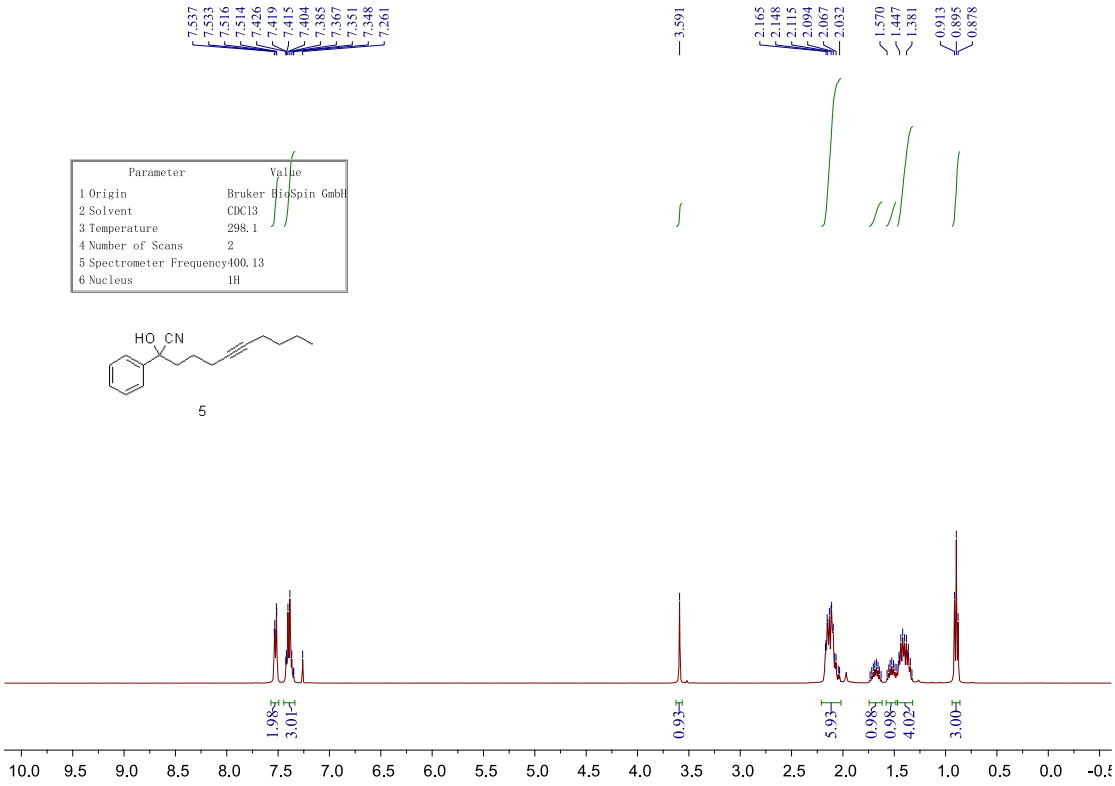

139.185
129.118
128.782
124.710
120.156
80.288
78.876
77.000
73.932
43.612
42.154
31.266
15.987
14.335
Parameter Value
1 Origin Bruker BioSpin GmbH
2 Solvent CDCl3
3 Temperature 298.2
4 Number of Scans 15
5 Spectrometer Frequency 100.62
6 Nucleus 13C
HO CN
Cl
1x
f1 (ppm)

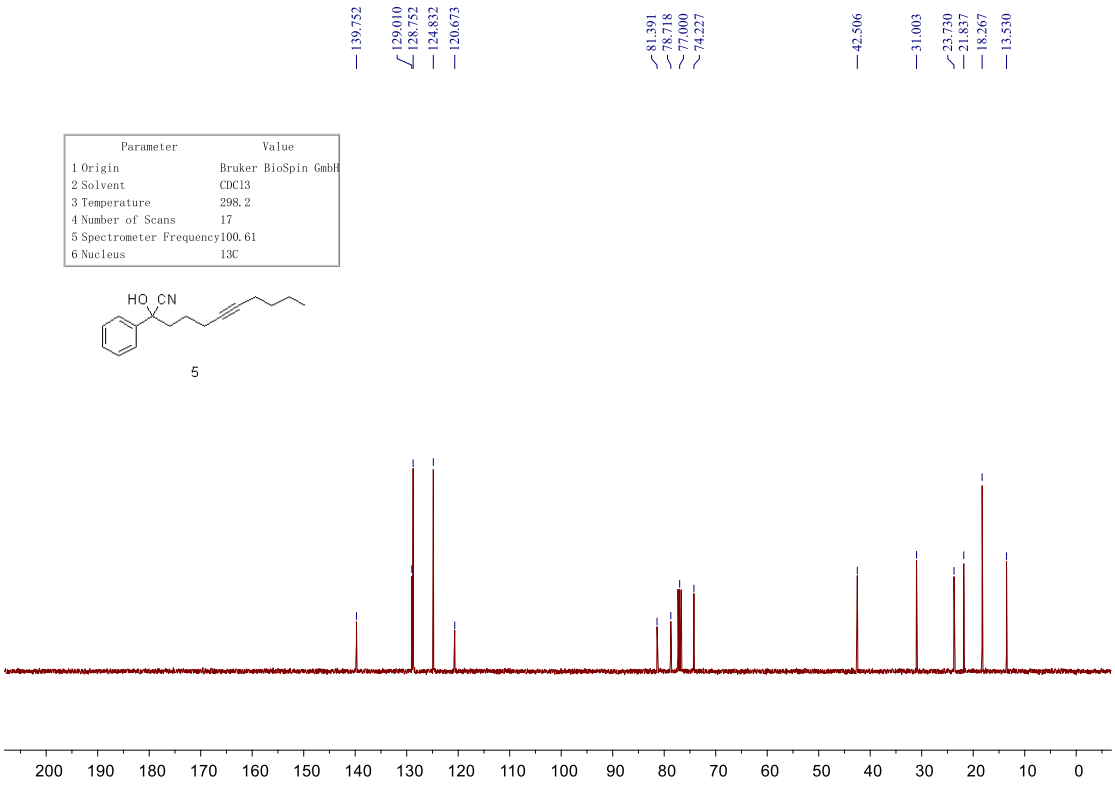

7.528
7.508
7.427
7.423
7.407
7.388
7.374
7.367
7.349
7.261
4.079
4.061
4.044
4.028
2.417
2.265
2.250
2.200
2.180
2.162
2.137
2.113
1.798
1.781
1.764
1.747
1.730
Parameter Value
1 Origin Bruker BioSpin GmbH
2 Solvent CDCl3
3 Temperature 298.2
4 Number of Scans 2
5 Spectrometer Frequency 400.13
6 Nucleus 1H
HO CN
CN
1y
1.95
2.97
0.79
1.97
1.87
2.09
1.92
2.00
f1 (ppm)

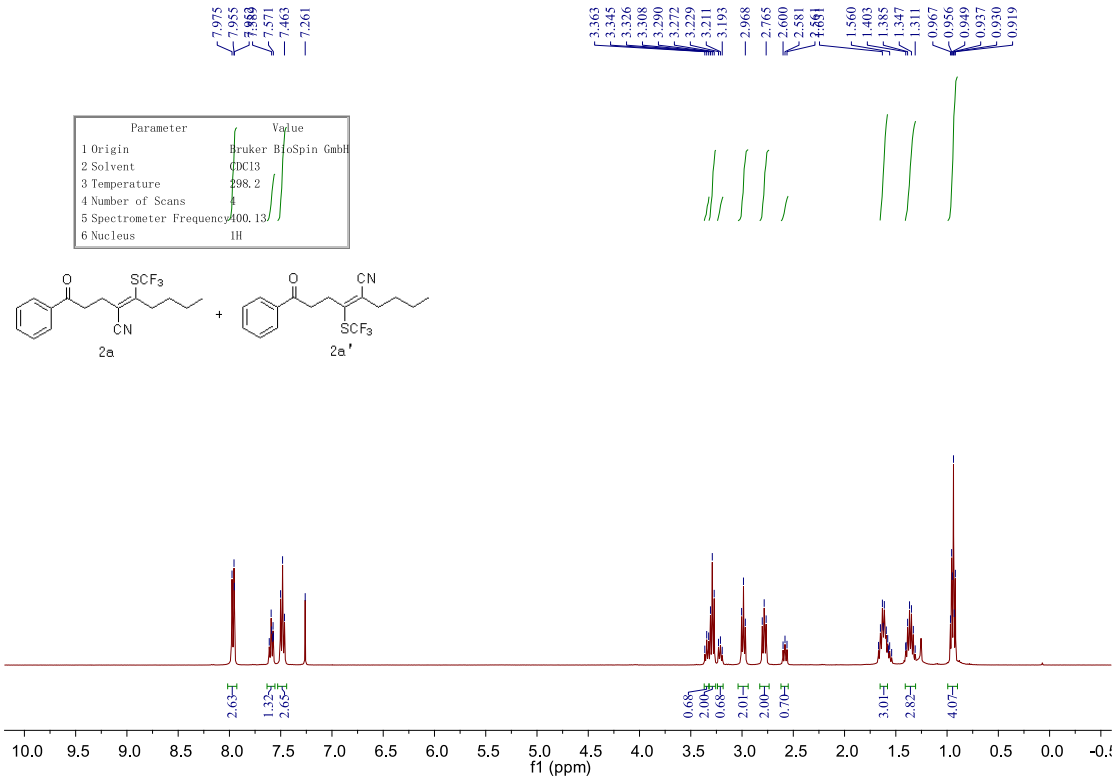

139.261
129.074
128.748
124.731
120.260
119.226
79.919
78.916
77.000
73.543
42.194
24.365
17.686
15.941
14.170
Parameter Value
1 Origin Bruker BioSpin GmbH
2 Solvent CDCl3
3 Temperature 298.1
4 Number of Scans 21
5 Spectrometer Frequency 100.61
6 Nucleus 13C
HO CN
CN
1y
f1 (ppm)

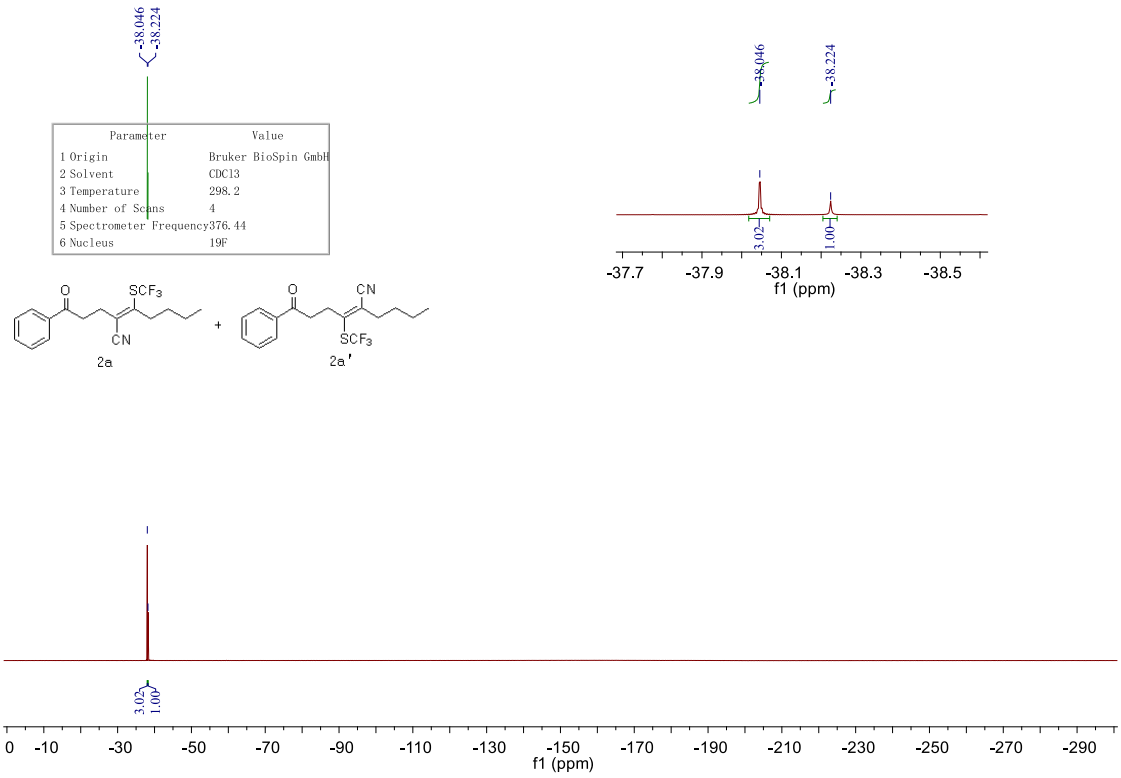

7.591
7.575
7.414
7.397
7.261
3.832
2.935
2.893
2.871
2.829
2.198
2.181
2.164
1.540
1.522
1.504
1.487
0.991
0.972
0.954
Parameter Value
1 Origin Bruker BioSpin GmbH
2 Solvent CDCl3
3 Temperature 298.1
4 Number of Scans 1
5 Spectrometer Frequency 400.13
6 Nucleus 1H
NC OH
3
2.08
3.04
0.86
1.99
1.98
2.11
3.00
f1 (ppm)

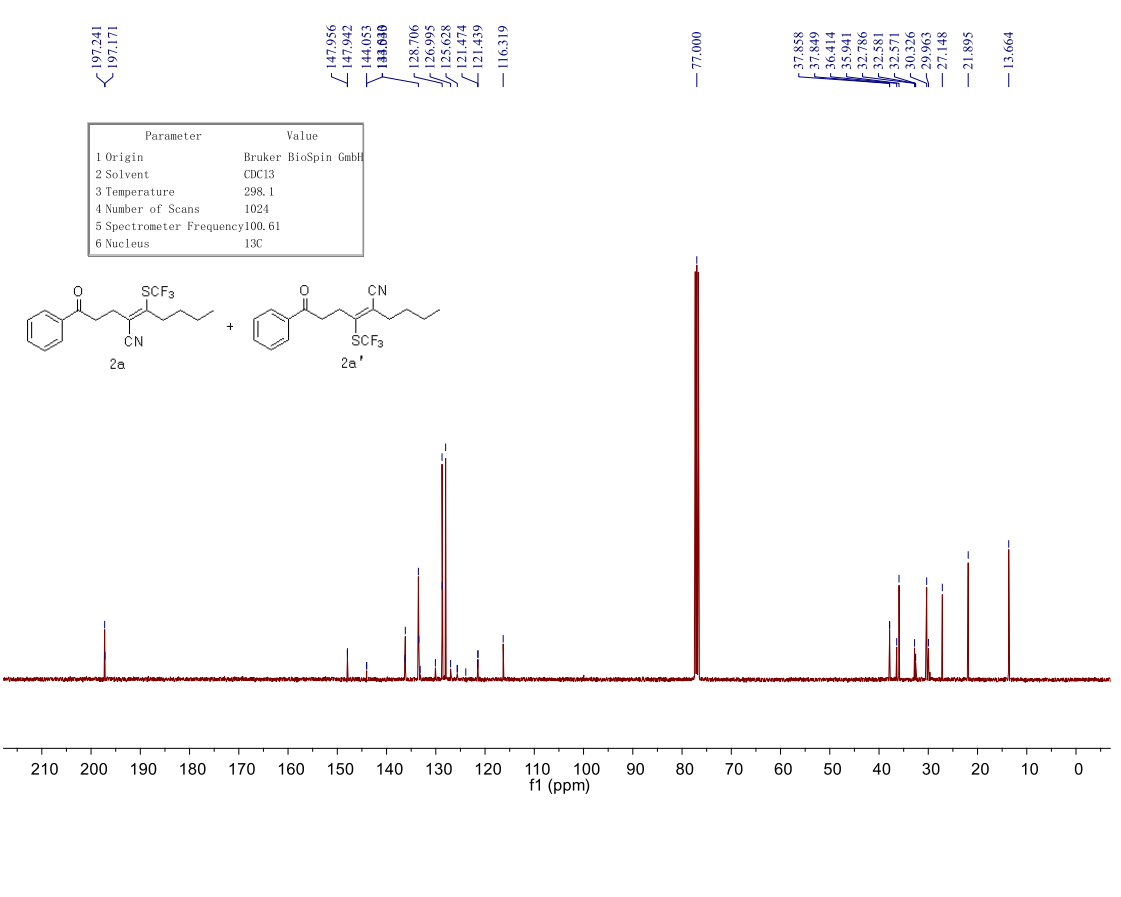

138.149
129.211
128.628
124.869
120.080
86.452
77.000
72.952
72.430
35.534
21.916
20.552
13.325
Parameter Value
1 Origin Bruker BioSpin GmbH
2 Solvent CDCl3
3 Temperature 298.3
4 Number of Scans 12
5 Spectrometer Frequency 100.61
6 Nucleus 13C
NC OH
3
f1 (ppm)


7.537
7.533
7.516
7.514
7.426
7.419
7.415
7.404
7.385
7.367
7.351
7.348
7.261
3.591
2.165
2.148
2.115
2.094
2.067
2.032
1.570
1.447
1.381
0.913
0.895
0.878
Parameter Value
1 Origin Bruker BioSpin GmbH
2 Solvent CDCl3
3 Temperature 298.1
4 Number of Scans 2
5 Spectrometer Frequency 400.13
6 Nucleus 1H
HO CN
5
1.98
3.01
0.93
5.93
0.98
0.98
4.02
3.00

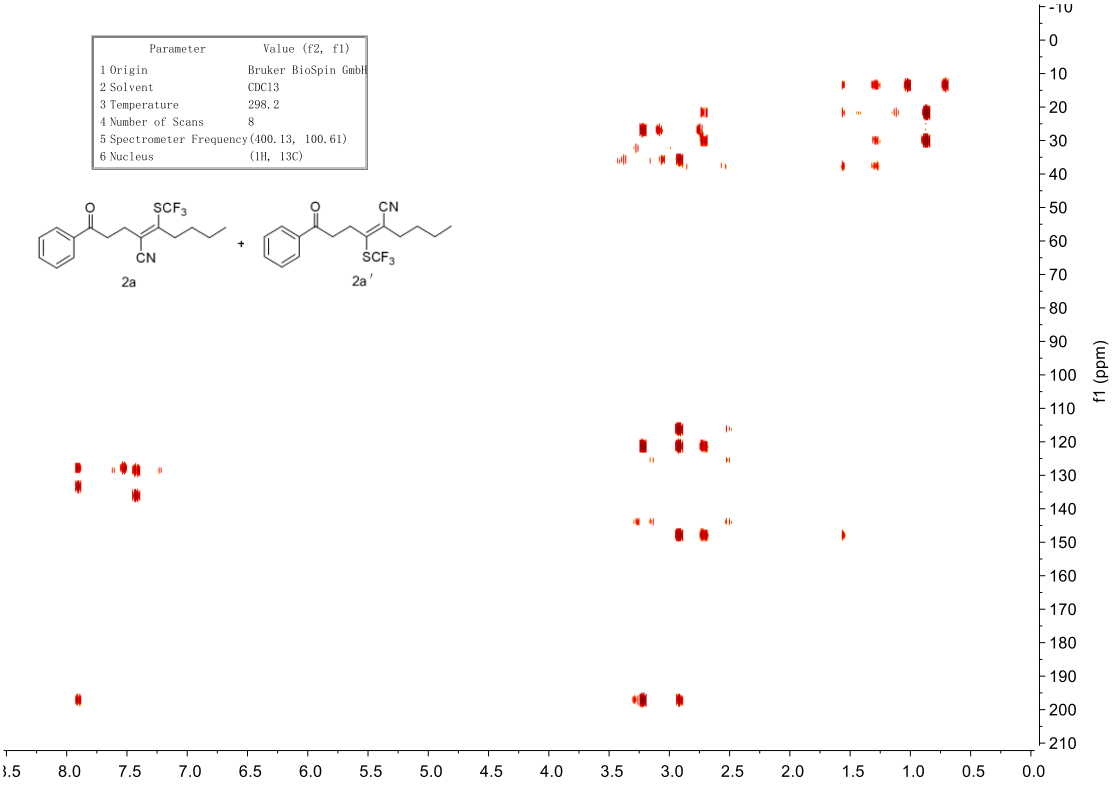

139.752
129.010
128.752
124.832
120.673
81.391
78.718
77.000
74.227
42.506
31.003
23.730
21.837
18.267
13.530
Parameter Value
1 Origin Bruker BioSpin GmbH
2 Solvent CDCl3
3 Temperature 298.2
4 Number of Scans 17
5 Spectrometer Frequency 100.61
6 Nucleus 13C
HO CN
5
200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0

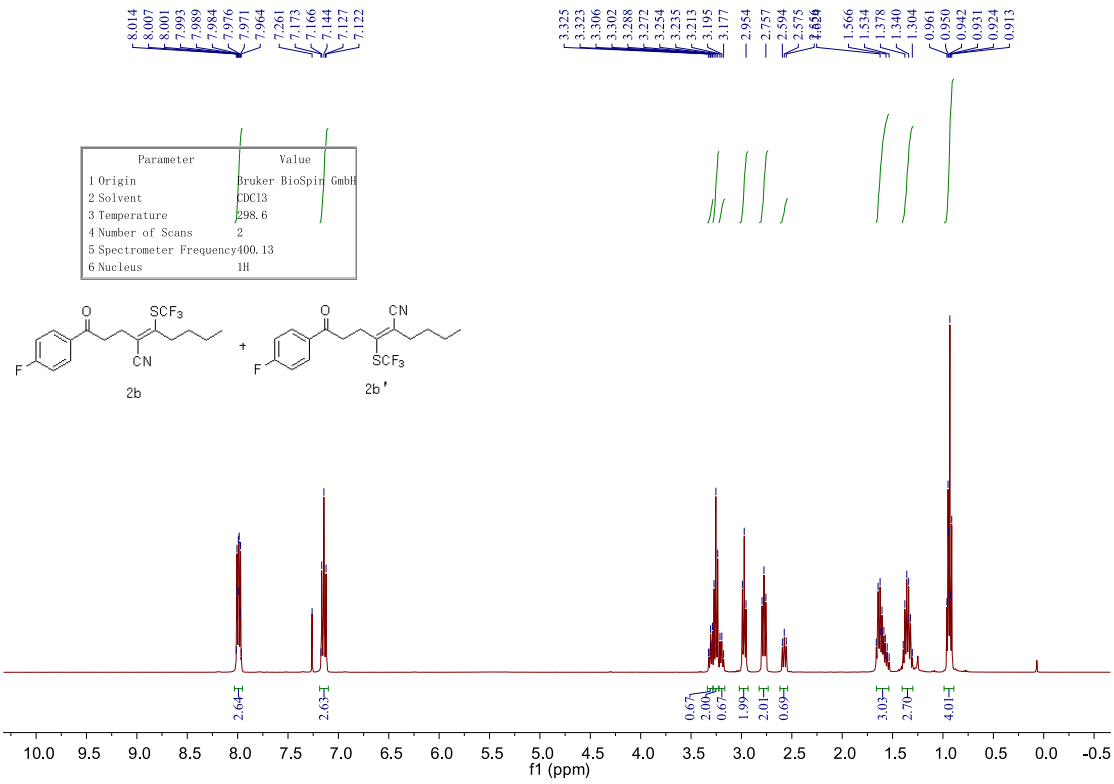

7.975
7.955
7.571
7.463
7.261
3.363
3.345
3.326
3.308
3.290
3.272
3.229
3.211
3.193
2.968
2.765
2.600
2.581
1.560
1.403
1.385
1.347
1.311
0.967
0.956
0.949
0.937
0.930
0.919
Parameter Value
1 Origin Bruker BioSpin GmbH
2 Solvent CDCl3
3 Temperature 298.2
4 Number of Scans 4
5 Spectrometer Frequency 400.13
6 Nucleus 1H
O SCF3 CN
2a
+
O CN SCF3
2a'
2.63 1.32 2.65 0.68 2.00 0.68 2.01 2.00 0.70 3.01 2.82 4.07
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
f1 (ppm)

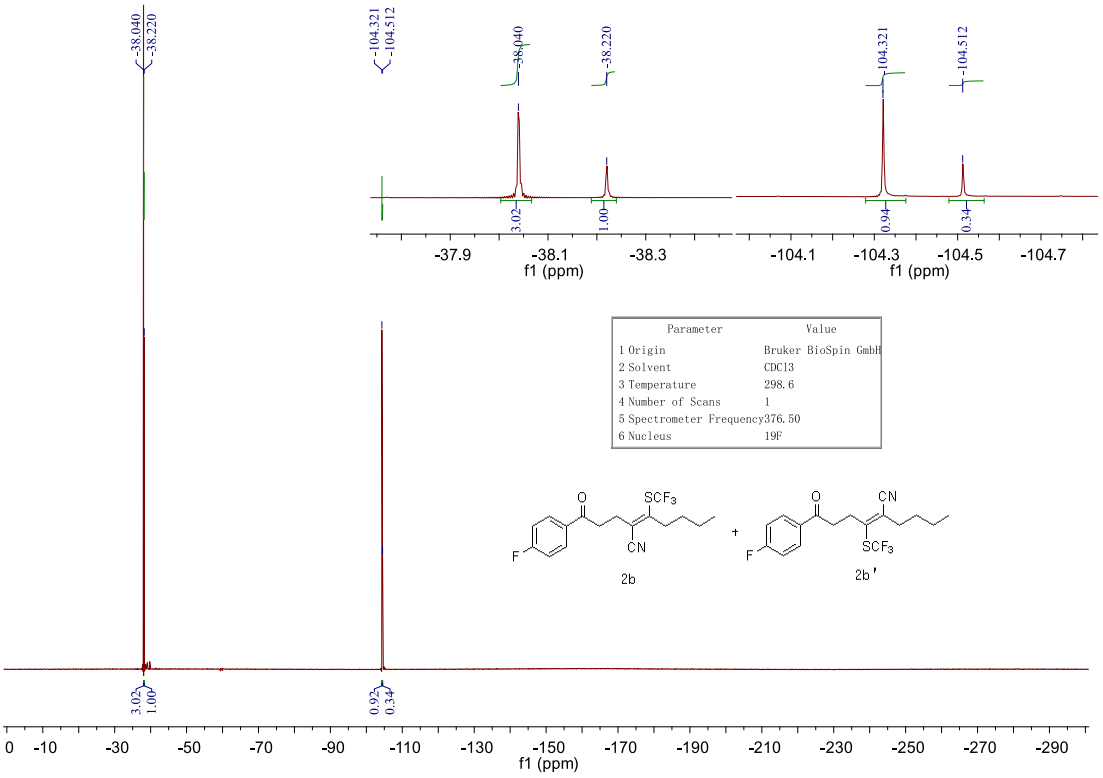

-38.046
-38.224
Parameter Value
1 Origin Bruker BioSpin GmbH
2 Solvent CDCl3
3 Temperature 298.2
4 Number of Scans 4
5 Spectrometer Frequency 376.44
6 Nucleus 19F
SCF3
CN
2a
2a'
3.02
1.00
f1 (ppm)

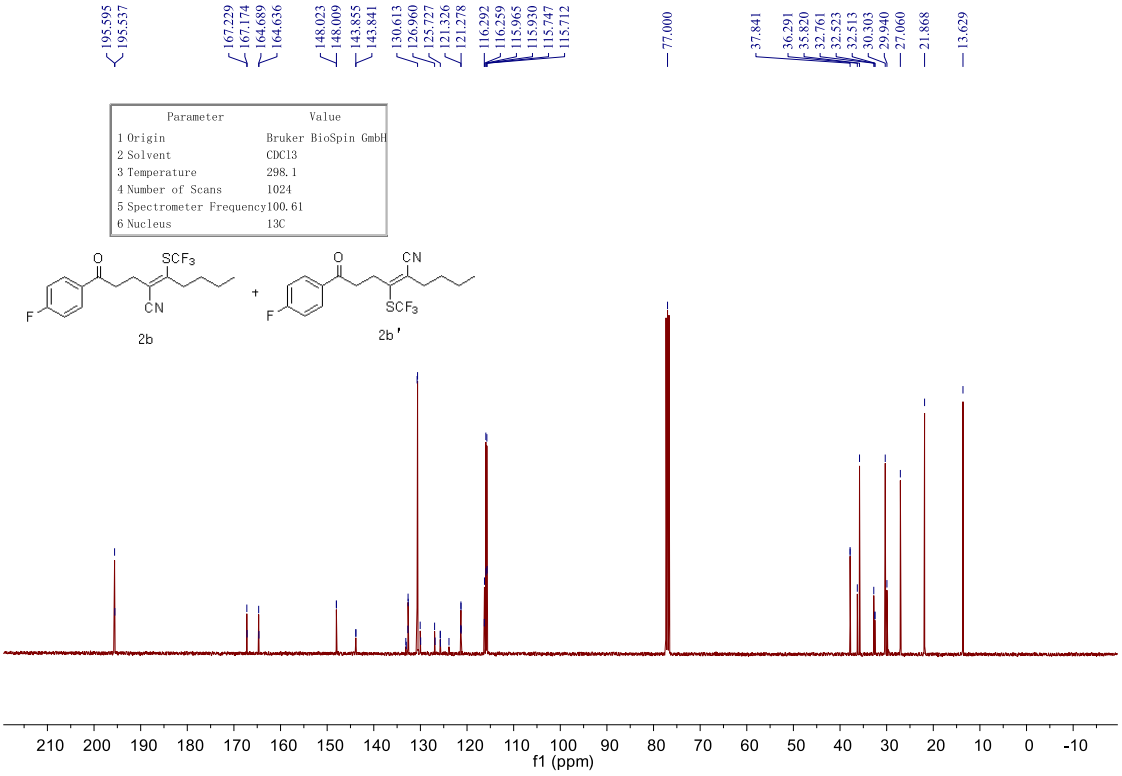

197.241
197.171
147.956
147.942
144.053
128.706
126.995
125.628
121.474
121.439
116.319
77.000
37.858
37.849
36.414
35.941
32.786
32.581
32.571
30.326
29.963
27.148
21.895
13.664
Parameter Value
1 Origin Bruker BioSpin GmbH
2 Solvent CDCl3
3 Temperature 298.1
4 Number of Scans 1024
5 Spectrometer Frequency 100.61
6 Nucleus 13C
SCF3
CN
2a
2a'
f1 (ppm)

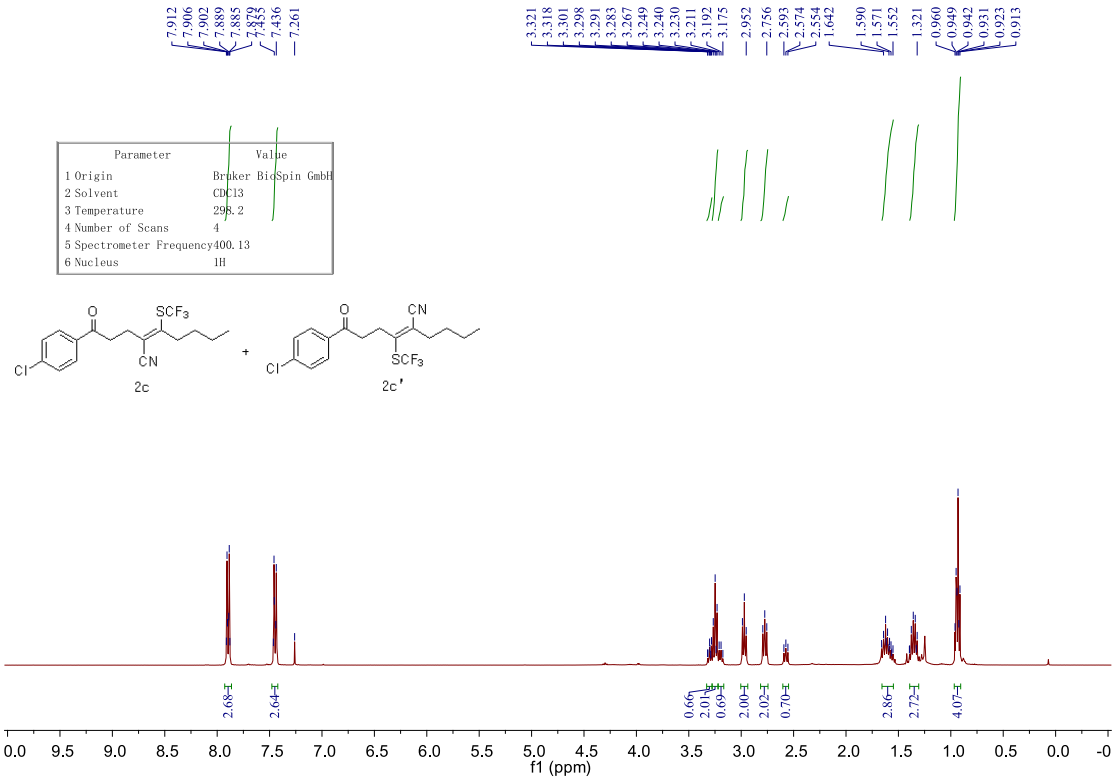
HMBC

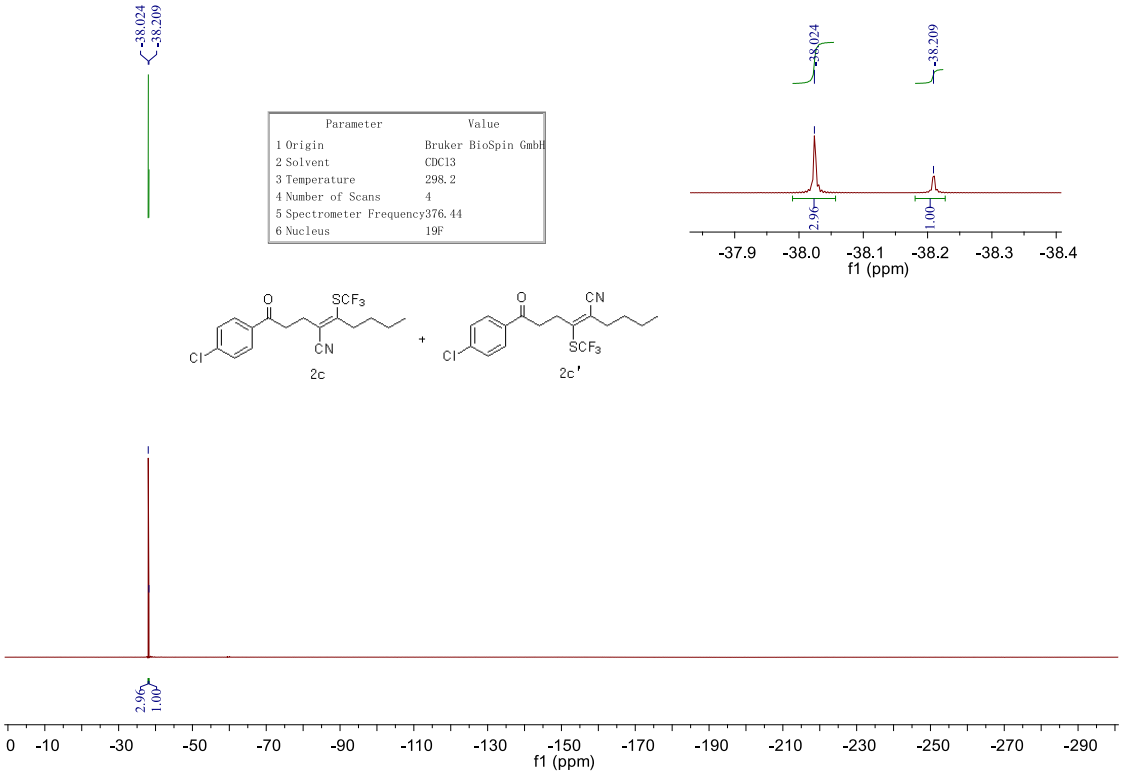

Parameter Value (f2, f1)
1 Origin Bruker BioSpin GmbH
2 Solvent CDCl3
3 Temperature 298.2
4 Number of Scans 8
5 Spectrometer Frequency (400.13, 100.61)
6 Nucleus (1H, 13C)
SCF3
CN
2a
2a'
f1 (ppm)

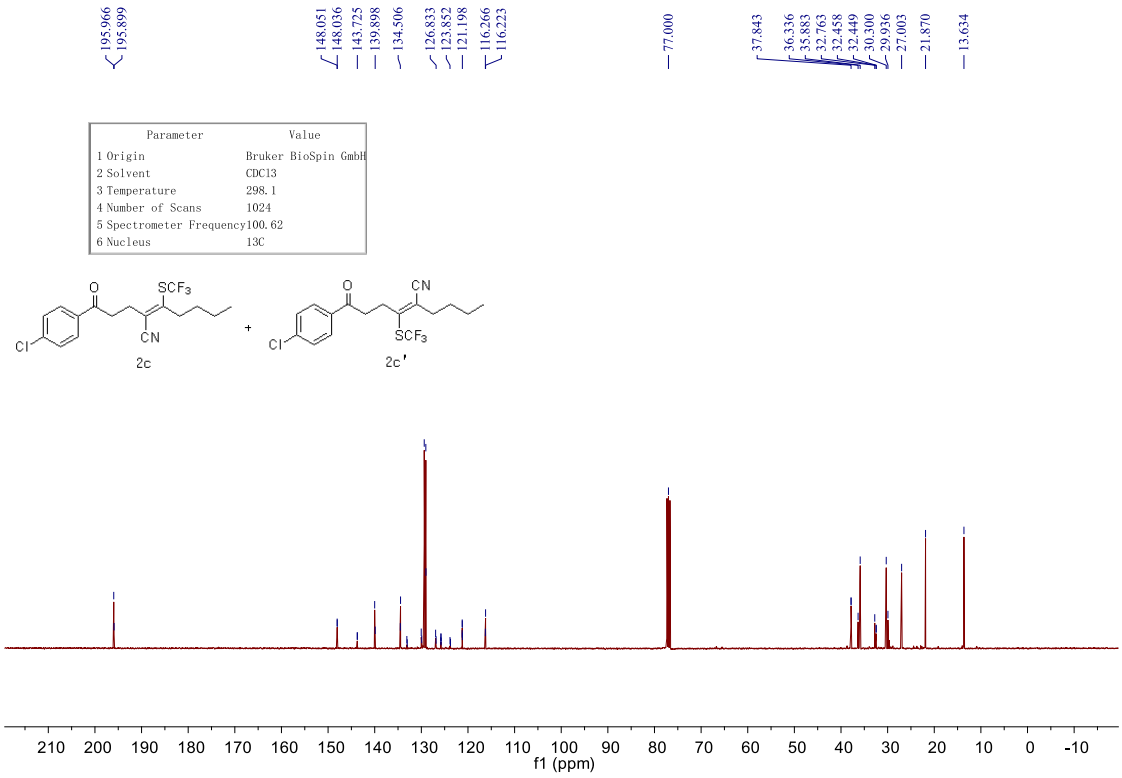

Parameter Value
1 Origin Bruker BioSpin GmbH
2 Solvent CDCl3
3 Temperature 298.6
4 Number of Scans 2
5 Spectrometer Frequency 400.13
6 Nucleus 1H
2b
2b'
f1 (ppm)

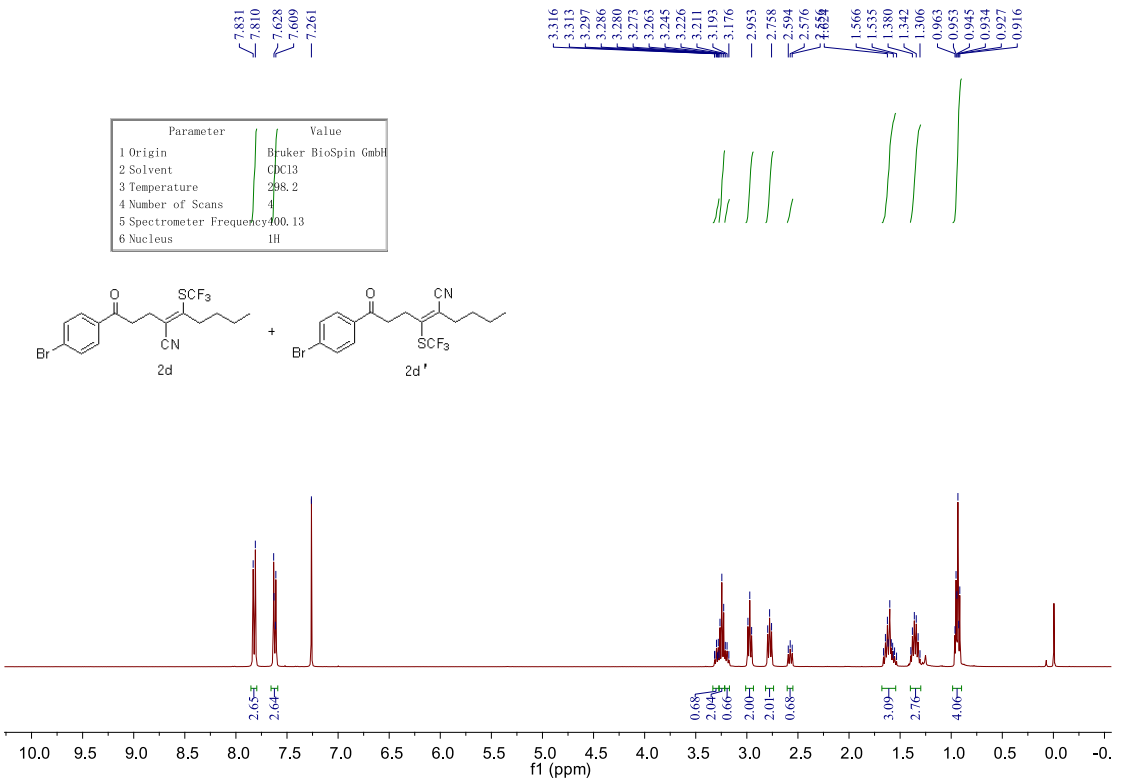

-38.040
-38.220
-104.321
-104.512
3.02
1.00
0.92
0.34
f1 (ppm)
Parameter Value
1 Origin Bruker BioSpin GmbH
2 Solvent CDCl3
3 Temperature 298.6
4 Number of Scans 1
5 Spectrometer Frequency 376.50
6 Nucleus 19F
SCF3
CN
F
2b
2b'

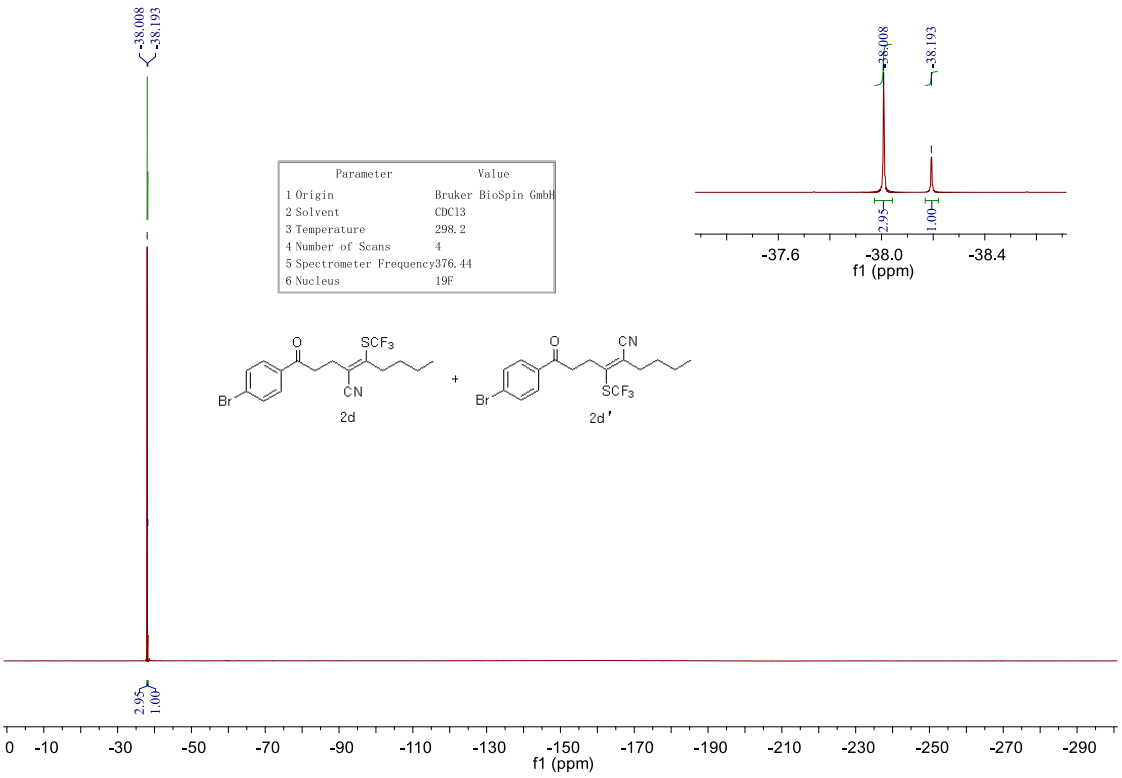

195.595
195.537
167.229
167.174
164.689
164.636
148.023
148.009
143.855
143.841
130.613
126.960
125.727
121.326
121.278
116.292
116.259
115.965
115.930
115.747
115.712
77.000
37.841
36.291
35.820
32.761
32.523
32.513
30.303
29.940
27.060
21.868
13.629
Parameter Value
1 Origin Bruker BioSpin GmbH
2 Solvent CDCl3
3 Temperature 298.1
4 Number of Scans 1024
5 Spectrometer Frequency 100.61
6 Nucleus 13C
SCF3
CN
F
2b
2b'
f1 (ppm)

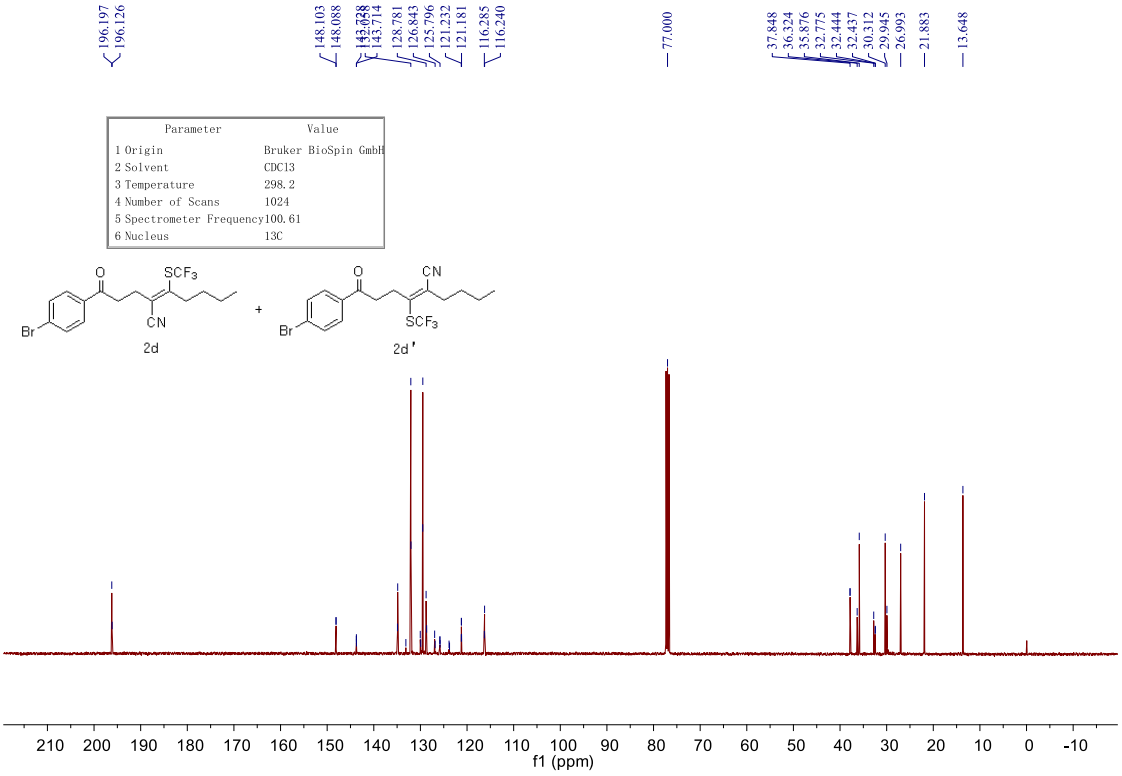

7.912
7.906
7.902
7.889
7.885
7.879
7.455
7.436
7.261
3.321
3.318
3.301
3.298
3.291
3.283
3.267
3.249
3.240
3.230
3.211
3.192
3.175
2.952
2.756
2.593
2.574
2.554
1.642
1.590
1.571
1.552
1.321
0.960
0.949
0.942
0.931
0.923
0.913
Parameter Value
1 Origin Bruker BioSpin GmbH
2 Solvent CDCl3
3 Temperature 298.2
4 Number of Scans 4
5 Spectrometer Frequency 400.13
6 Nucleus 1H
2c
2c'
2.68
2.64
0.66
2.01
0.69
2.00
2.02
0.70
2.86
2.72
4.07
f1 (ppm)

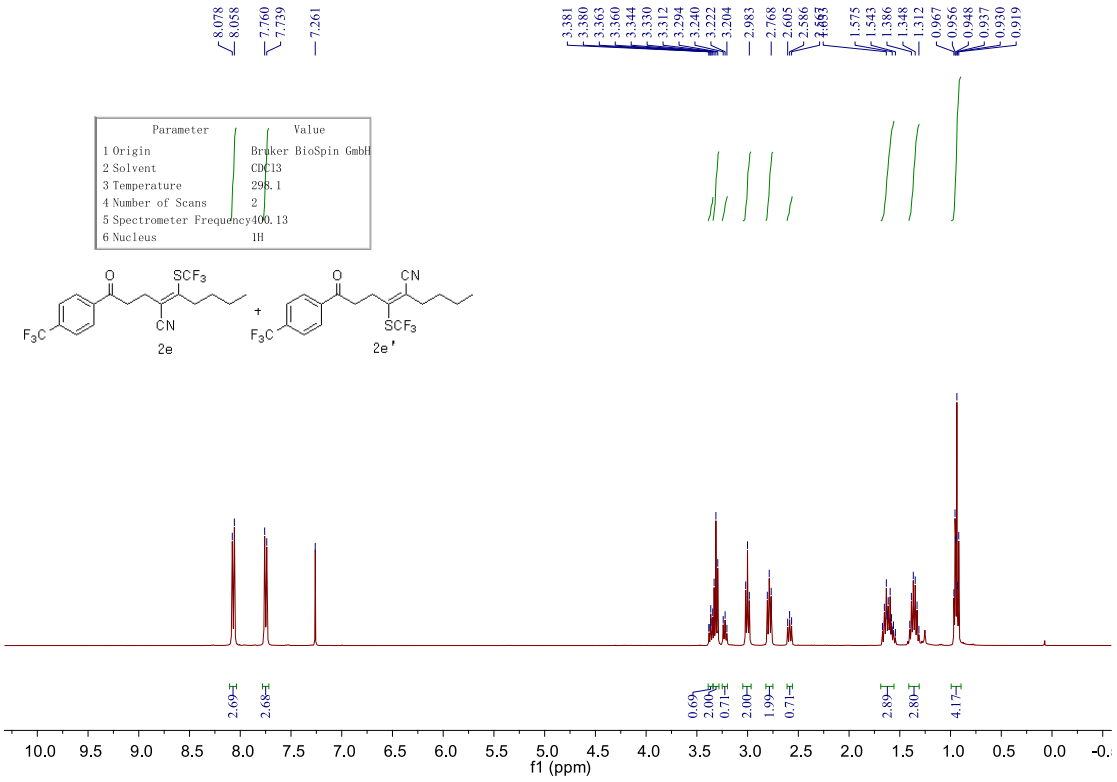

-38.024
-38.209
Parameter Value
1 Origin Bruker BioSpin GmbH
2 Solvent CDCl3
3 Temperature 298.2
4 Number of Scans 4
5 Spectrometer Frequency 376.44
6 Nucleus 19F
2c
2c'
2.96
1.00
f1 (ppm)

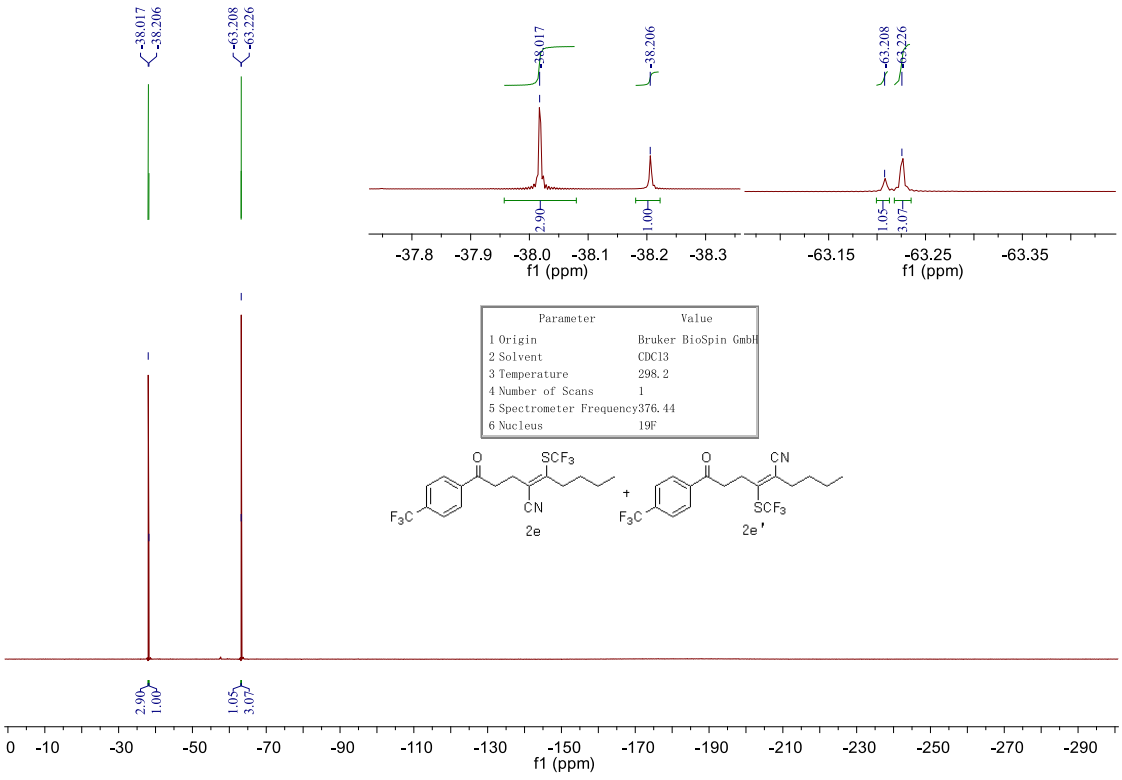

195.966
195.899
148.051
148.036
143.725
139.898
134.506
126.833
123.852
121.198
116.266
116.223
77.000
37.843
36.336
35.883
32.763
32.458
32.449
30.300
29.936
27.003
21.870
13.634
Parameter Value
1 Origin Bruker BioSpin GmbH
2 Solvent CDCl3
3 Temperature 298.1
4 Number of Scans 1024
5 Spectrometer Frequency 100.62
6 Nucleus 13C
O
SCF3
CN
Cl
2c
+
O
CN
SCF3
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
f1 (ppm)

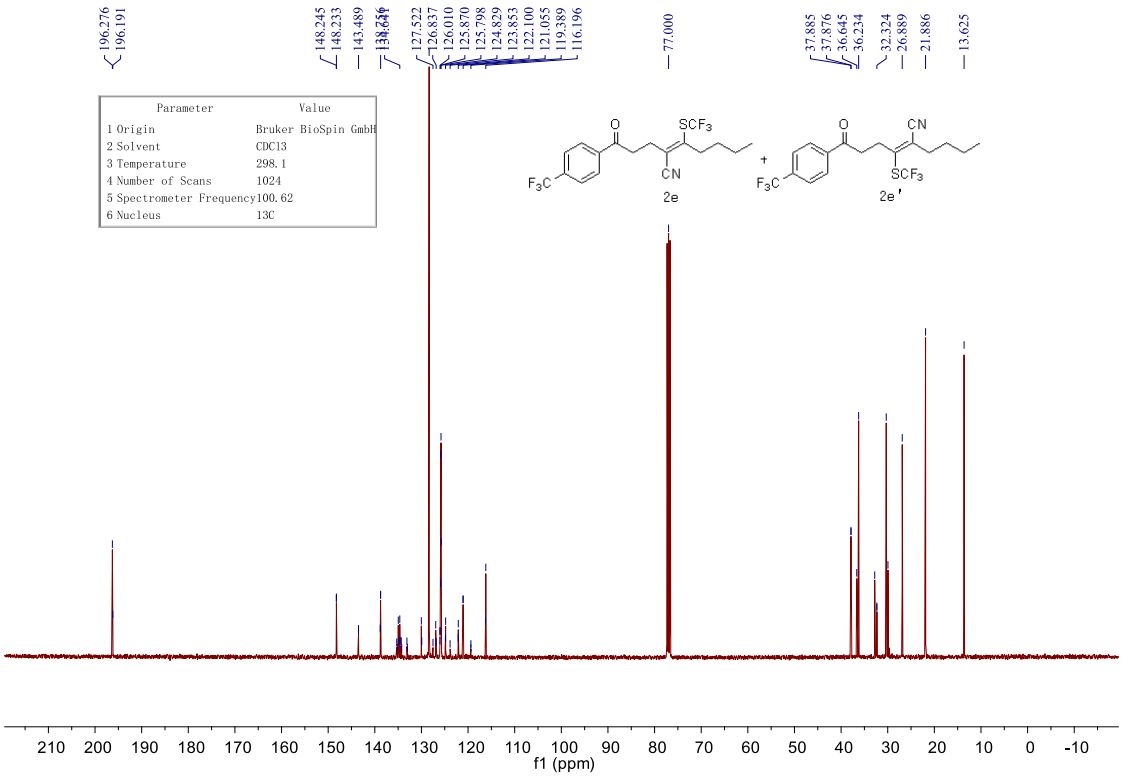

7.831
7.810
7.628
7.609
7.261
3.316
3.313
3.297
3.286
3.280
3.273
3.263
3.245
3.226
3.211
3.193
3.176
2.953
2.758
2.594
2.576
1.566
1.535
1.380
1.342
1.306
0.963
0.953
0.945
0.934
0.927
0.916
Parameter Value
1 Origin Bruker BioSpin GmbH
2 Solvent CDCl3
3 Temperature 298.2
4 Number of Scans 4
5 Spectrometer Frequency 400.13
6 Nucleus 1H
O
SCF3
CN
Br
2d
+
O
CN
SCF3
Br
2d'
2.65
2.64
0.68
2.04
0.66
2.00
2.01
0.68
3.09
2.76
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.
f1 (ppm)

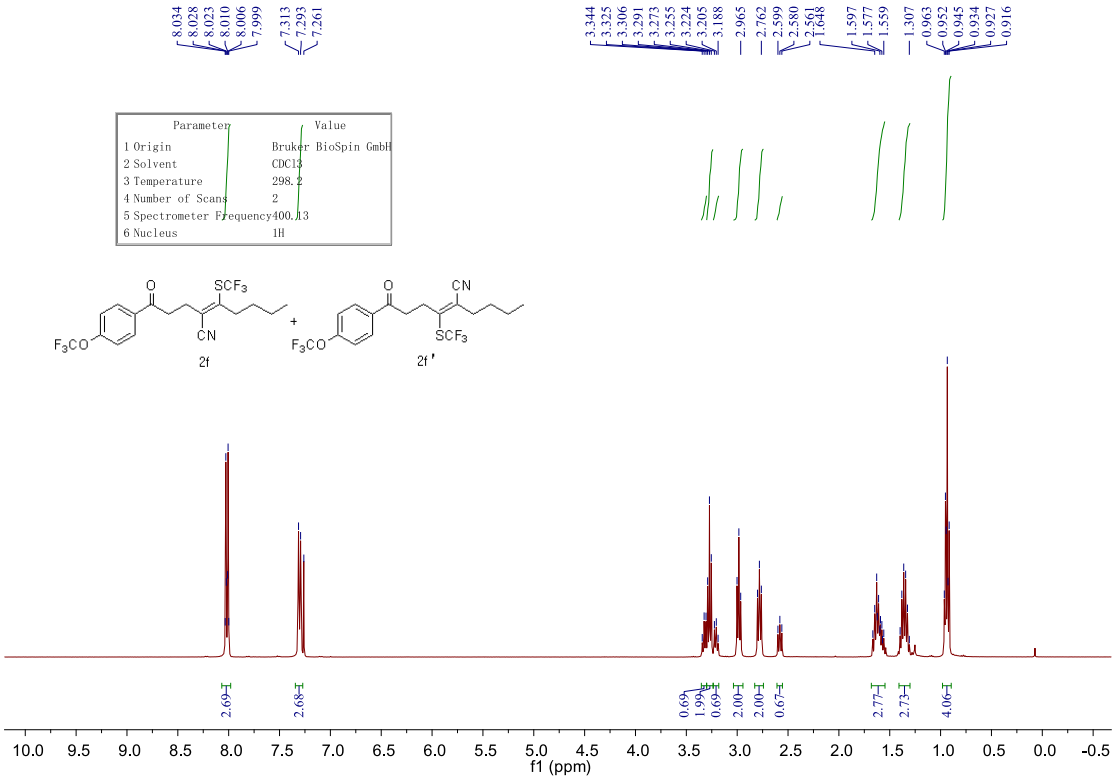

-38.008
-38.193
Parameter Value
1 Origin Bruker BioSpin GmbH
2 Solvent CDCl3
3 Temperature 298.2
4 Number of Scans 4
5 Spectrometer Frequency 376.44
6 Nucleus 19F
2.95
1.00
f1 (ppm)
2d
2d'

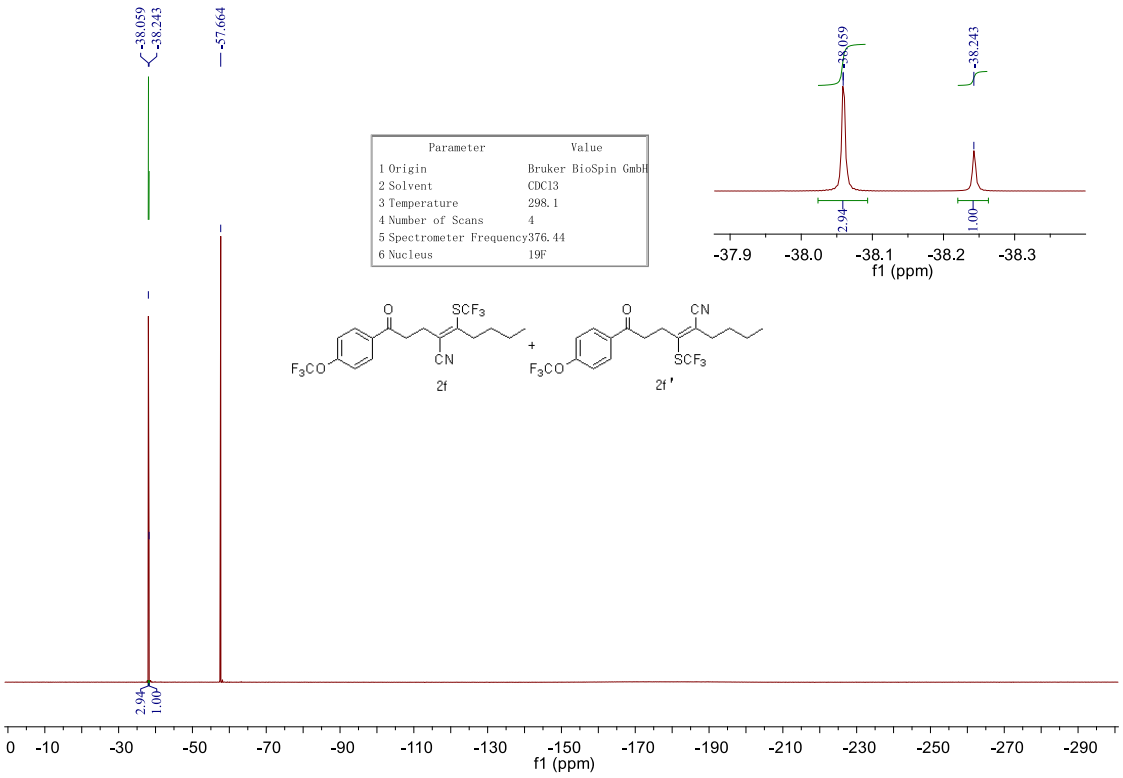

196.197
196.126
148.103
148.088
128.781
126.843
125.796
121.232
121.181
116.285
116.240
77.000
37.848
36.324
35.876
32.775
32.444
32.437
30.312
29.945
26.993
21.883
13.648
Parameter Value
1 Origin Bruker BioSpin GmbH
2 Solvent CDCl3
3 Temperature 298.2
4 Number of Scans 1024
5 Spectrometer Frequency 100.61
6 Nucleus 13C
f1 (ppm)
2d
2d'

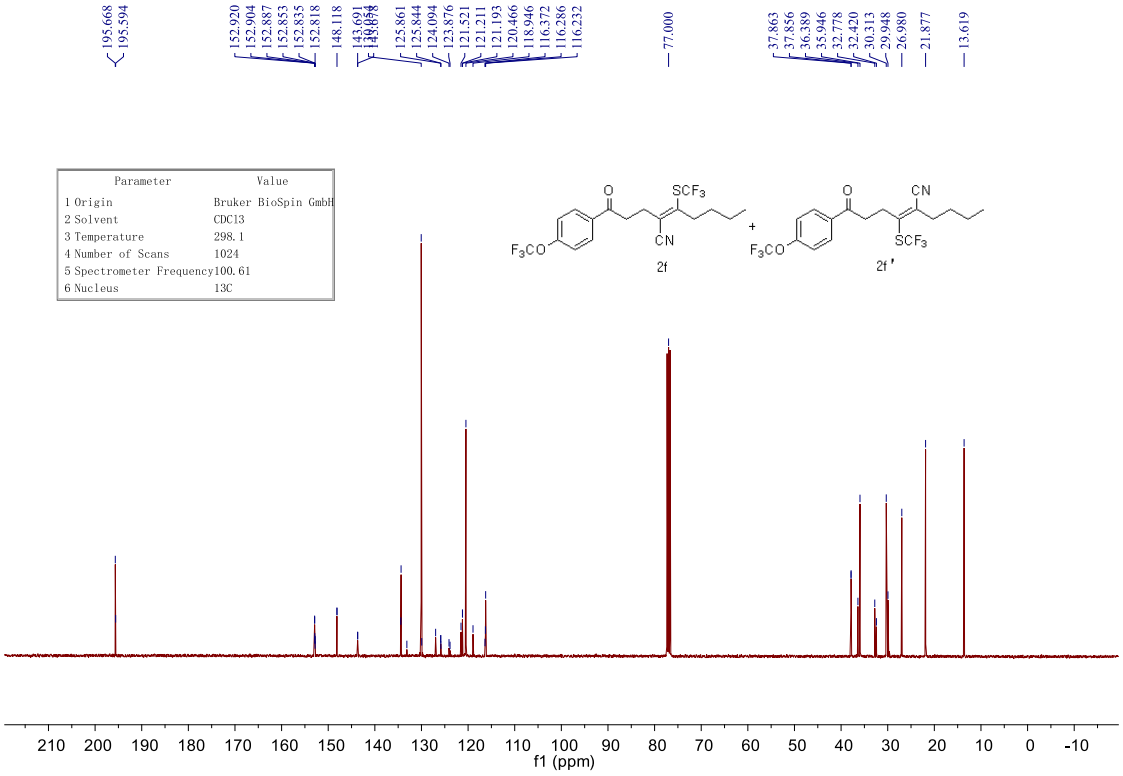

8.078
8.058
7.760
7.739
7.261
3.381
3.380
3.363
3.360
3.344
3.330
3.312
3.294
3.240
3.222
3.204
2.983
2.768
2.605
2.586
1.575
1.543
1.386
1.348
1.312
0.967
0.956
0.948
0.937
0.930
0.919
Parameter Value
1 Origin Bruker BioSpin GmbH
2 Solvent CDCl3
3 Temperature 298.1
4 Number of Scans 2
5 Spectrometer Frequency 400.13
6 Nucleus 1H
SCF3
CN
F3C
2e
2e'
2.69
2.68
0.69
2.00
0.71
2.00
1.99
0.71
2.89
2.80
4.17
f1 (ppm)

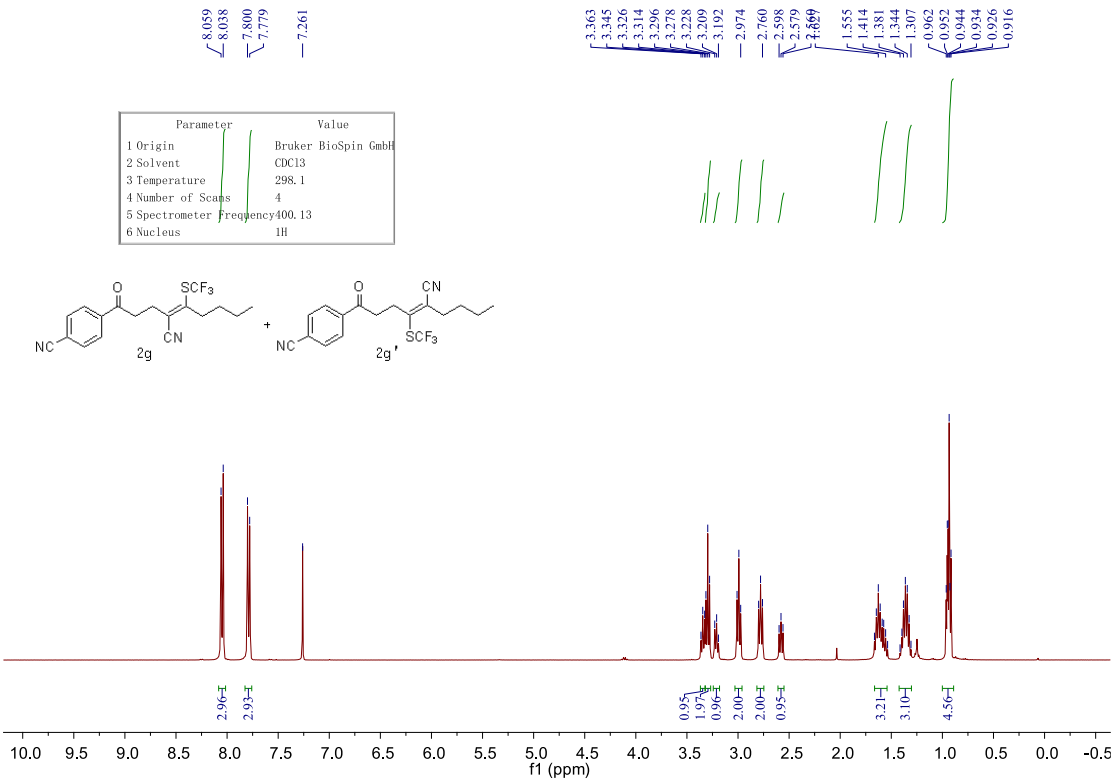

-38.017
-38.206
-63.208
-63.226
2.90
1.00
1.05
3.07
f1 (ppm)
Parameter Value
1 Origin Bruker BioSpin GmbH
2 Solvent CDCl3
3 Temperature 298.2
4 Number of Scans 1
5 Spectrometer Frequency 376.44
6 Nucleus 19F
SCF3
CN
F3C
2e
2e'

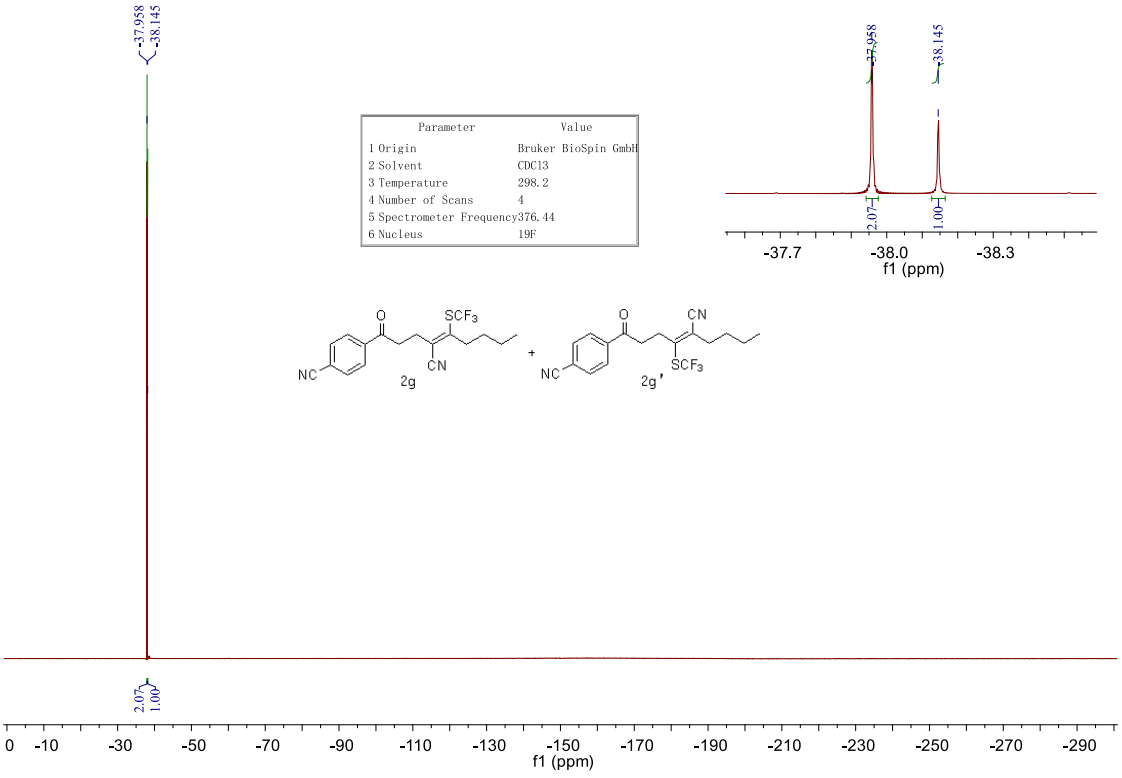

196.276
196.191
148.245
148.233
143.489
127.522
126.837
126.010
125.870
125.798
124.829
123.853
122.100
121.055
119.389
116.196
77.000
37.885
37.876
36.645
36.234
32.324
26.889
21.886
13.625
Parameter Value
1 Origin Bruker BioSpin GmbH
2 Solvent CDCl3
3 Temperature 298.1
4 Number of Scans 1024
5 Spectrometer Frequency 100.62
6 Nucleus 13C
2e
2e'
f1 (ppm)

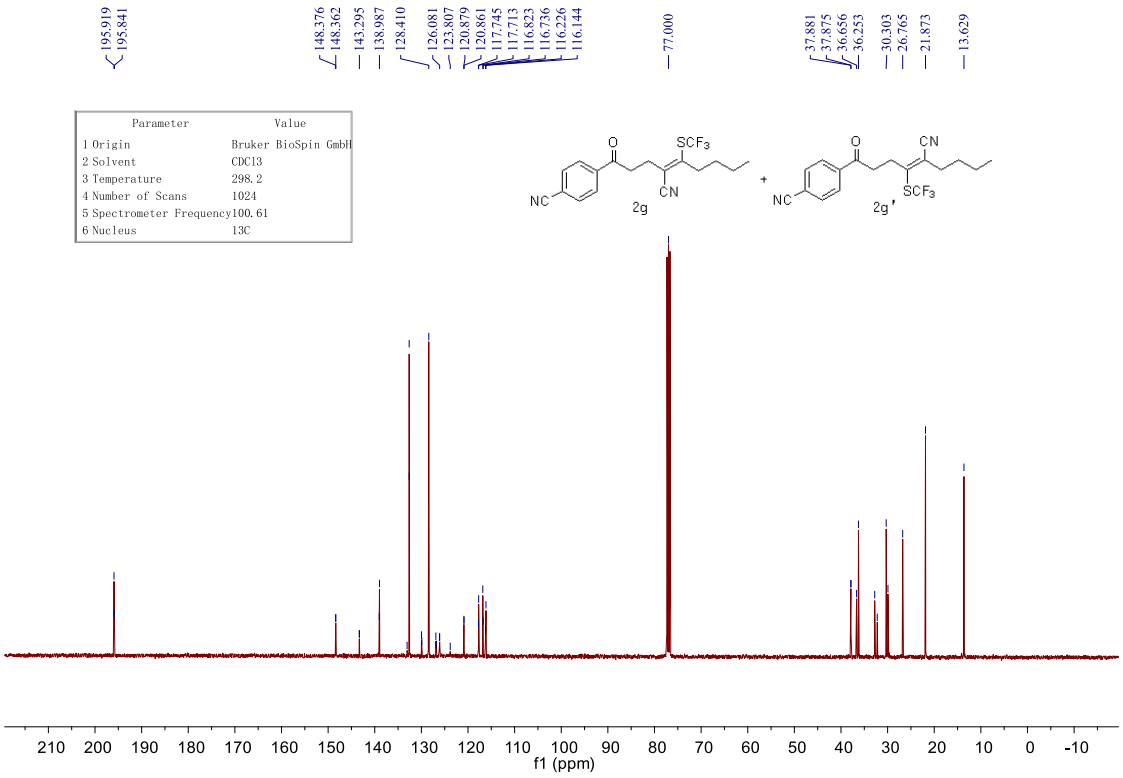

8.034
8.028
8.023
8.010
8.006
7.999
7.313
7.293
7.261
3.344
3.325
3.306
3.291
3.273
3.255
3.224
3.205
3.188
2.965
2.762
2.599
2.580
2.561
1.648
1.597
1.577
1.559
1.307
0.963
0.952
0.945
0.934
0.927
0.916
Parameter Value
1 Origin Bruker BioSpin GmbH
2 Solvent CDCl3
3 Temperature 298.2
4 Number of Scans 2
5 Spectrometer Frequency 400.13
6 Nucleus 1H
2f
2f'
2.69
2.68
0.69
1.99
0.69
2.00
2.00
0.67
2.77
2.73
4.06
f1 (ppm)

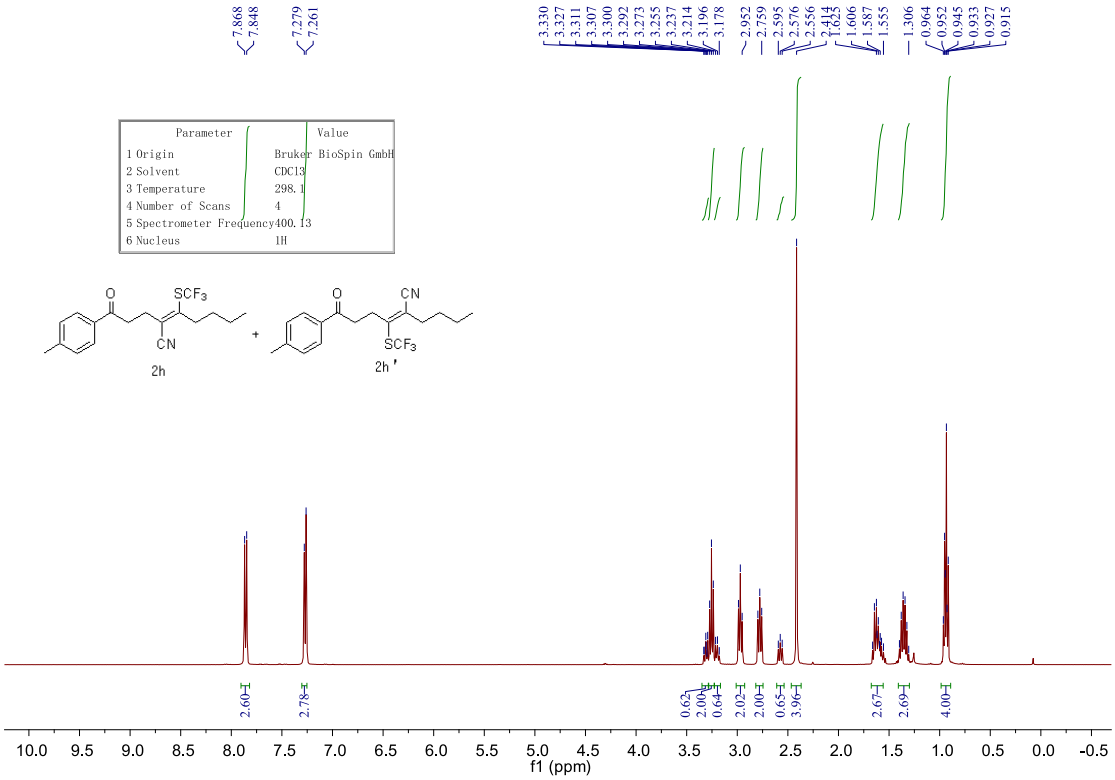

-38.059
-38.243
-57.664
Parameter Value
1 Origin Bruker BioSpin GmbH
2 Solvent CDCl3
3 Temperature 298.1
4 Number of Scans 4
5 Spectrometer Frequency 376.44
6 Nucleus 19F
2.94
1.00
f1 (ppm)
2f
2f'

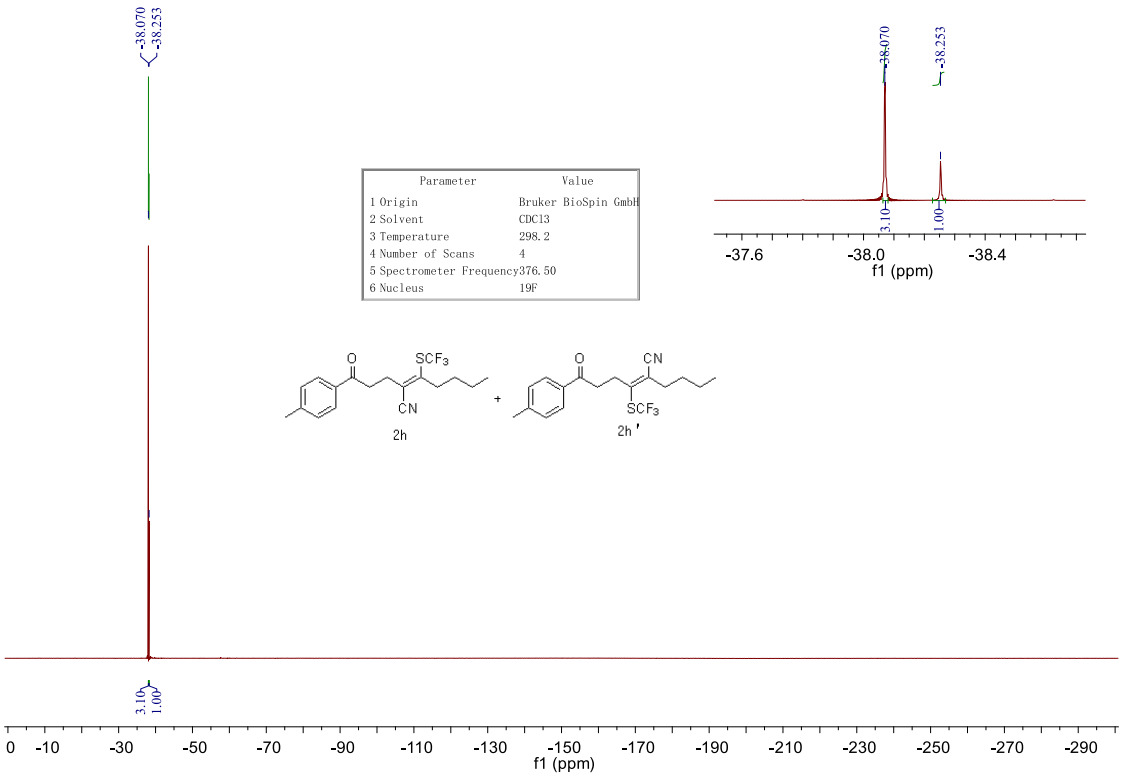

195.668
195.594
152.920
152.904
152.887
152.853
152.835
152.818
148.118
125.861
125.844
124.094
123.876
121.521
121.211
121.193
120.466
118.946
116.372
116.286
116.232
77.000
37.863
37.856
36.389
35.946
32.778
32.420
30.313
29.948
26.980
21.877
13.619
Parameter Value
1 Origin Bruker BioSpin GmbH
2 Solvent CDCl3
3 Temperature 298.1
4 Number of Scans 1024
5 Spectrometer Frequency 100.61
6 Nucleus 13C
f1 (ppm)
2f
2f'

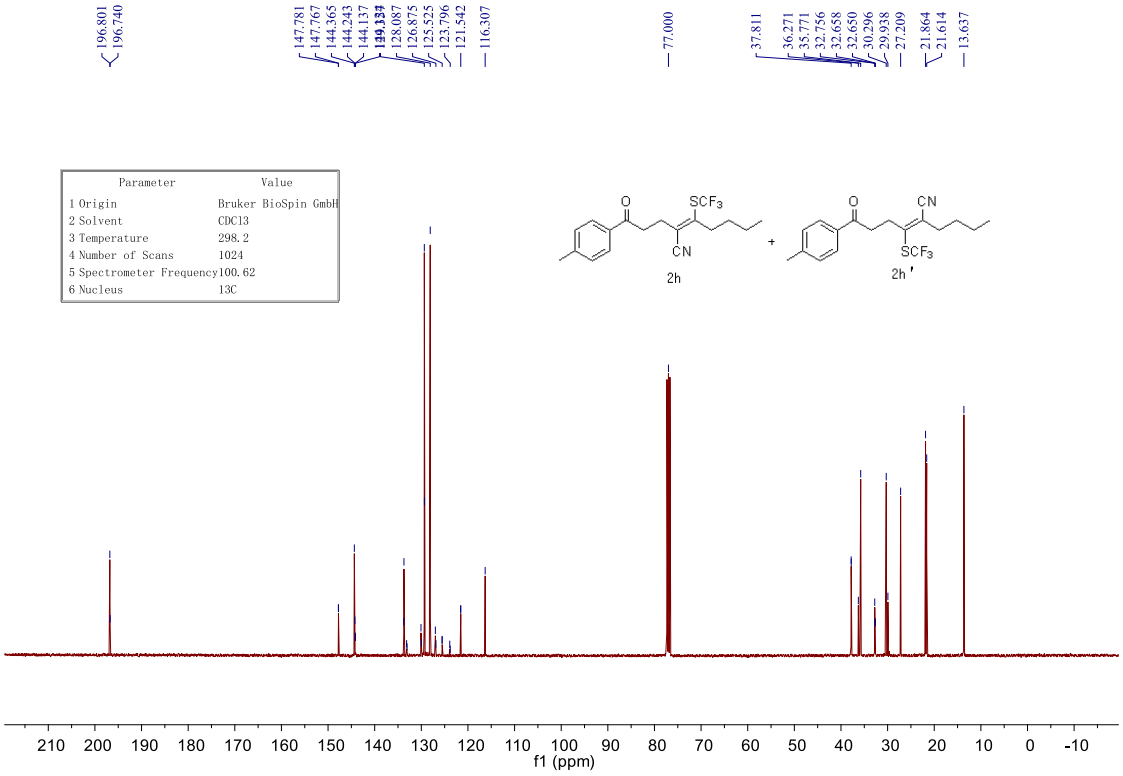

8.059
8.038
7.800
7.779
7.261
3.363
3.345
3.326
3.314
3.296
3.278
3.228
3.209
3.192
2.974
2.760
2.598
2.579
1.555
1.414
1.381
1.344
1.307
0.962
0.952
0.944
0.934
0.926
0.916
Parameter Value
1 Origin Bruker BioSpin GmbH
2 Solvent CDCl3
3 Temperature 298.1
4 Number of Scans 4
5 Spectrometer Frequency 400.13
6 Nucleus 1H
NC
O
SCF3
CN
2g
2g'
2.96
2.93
0.95
1.97
0.90
2.00
2.00
0.95
3.21
3.10
4.56
f1 (ppm)

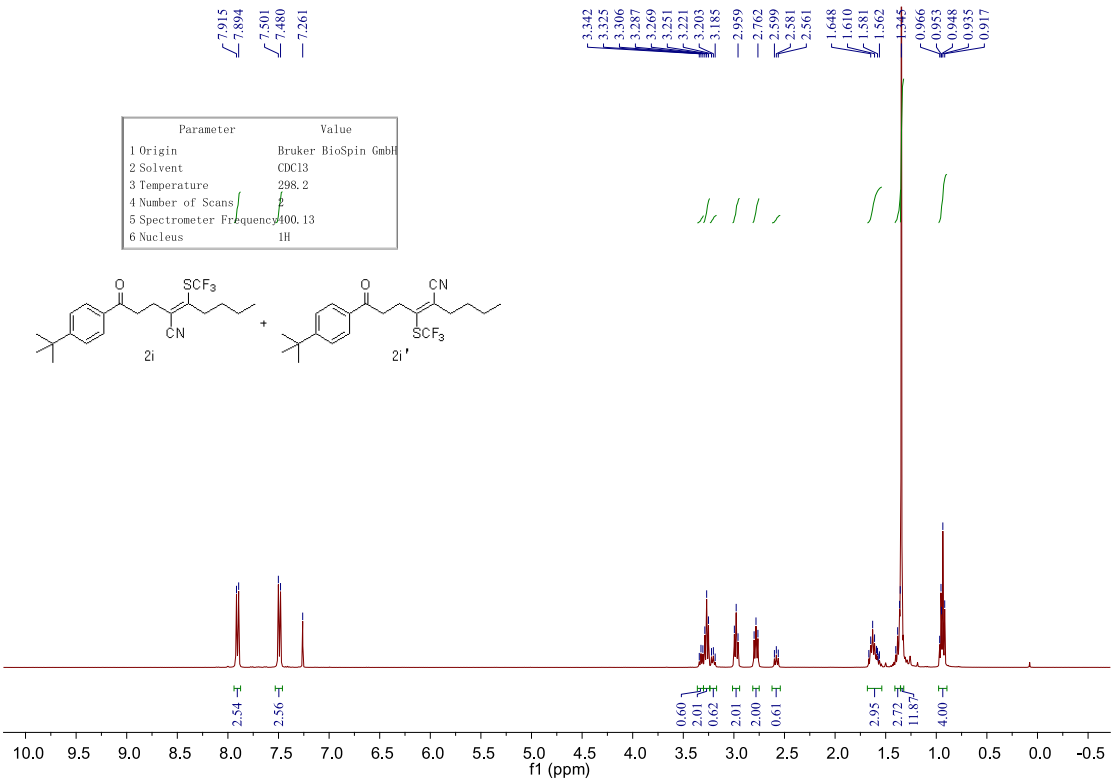

-37.958
-38.145
Parameter Value
1 Origin Bruker BioSpin GmbH
2 Solvent CDCl3
3 Temperature 298.2
4 Number of Scans 4
5 Spectrometer Frequency 376.44
6 Nucleus 19F
2.07
1.00
f1 (ppm)

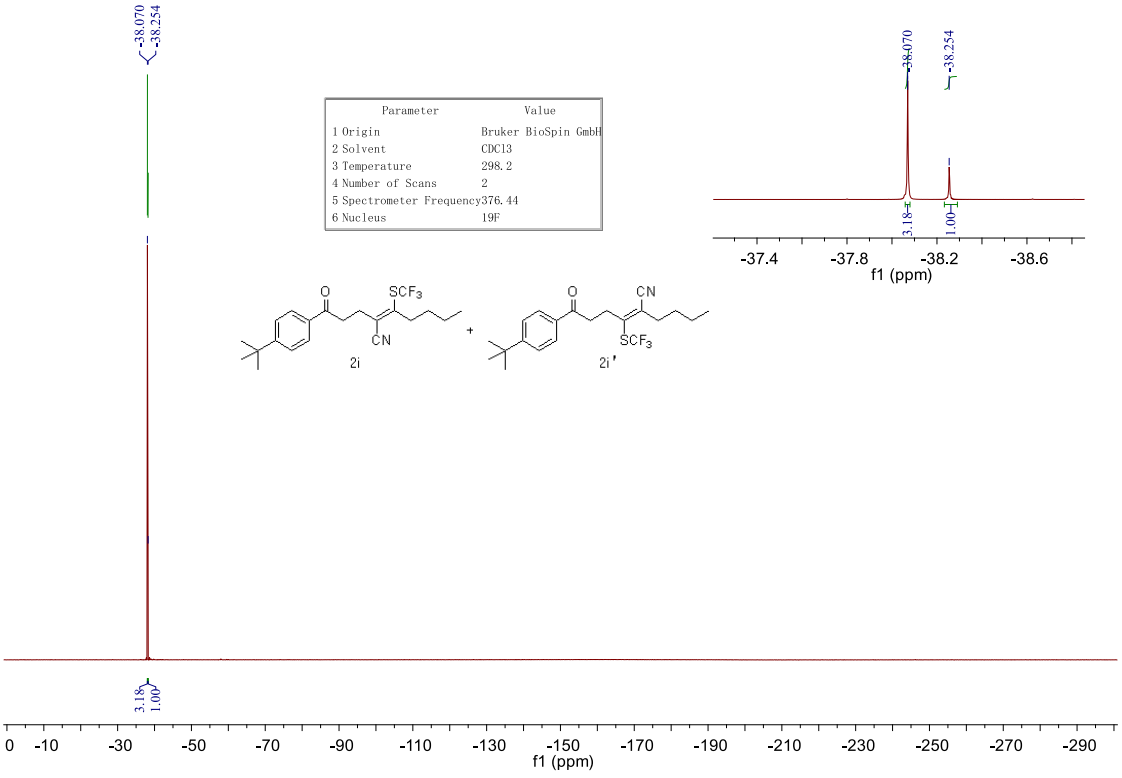

195.919
195.841
148.376
148.362
143.295
138.987
128.410
126.081
123.807
120.879
120.861
117.745
117.713
116.823
116.736
116.226
116.144
77.000
37.881
37.875
36.656
36.253
30.303
26.765
21.873
13.629
Parameter Value
1 Origin Bruker BioSpin GmbH
2 Solvent CDCl3
3 Temperature 298.2
4 Number of Scans 1024
5 Spectrometer Frequency 100.61
6 Nucleus 13C
NC
O
SCF3
CN
2g
2g'
f1 (ppm)

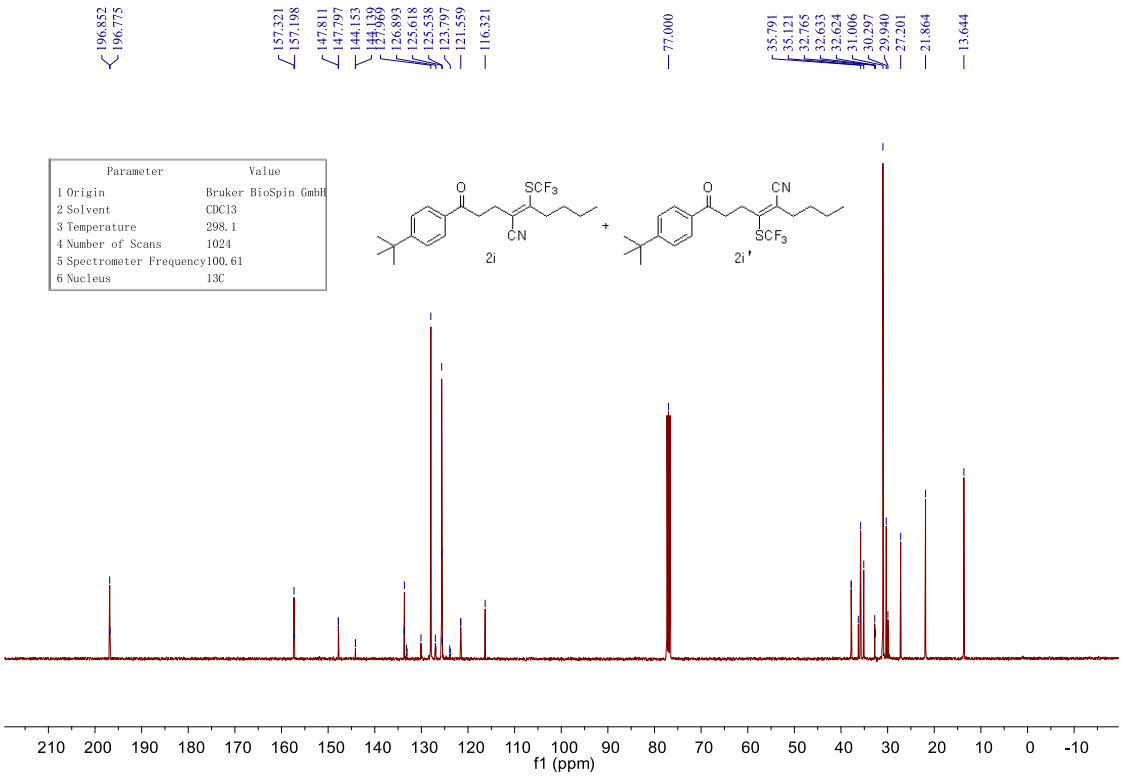

7.868
7.848
7.279
7.261
3.330
3.327
3.311
3.307
3.300
3.292
3.273
3.255
3.237
3.214
3.196
3.178
2.952
2.759
2.595
2.576
2.556
2.414
1.625
1.606
1.587
1.555
1.306
0.964
0.952
0.945
0.933
0.927
0.915
Parameter Value
1 Origin Bruker BioSpin GmbH
2 Solvent CDCl3
3 Temperature 298.1
4 Number of Scans 4
5 Spectrometer Frequency 400.13
6 Nucleus 1H
2h
2h'
2.60
2.78
0.62
2.00
0.64
2.02
2.00
0.65
3.96
2.67
2.69
4.00
f1 (ppm)

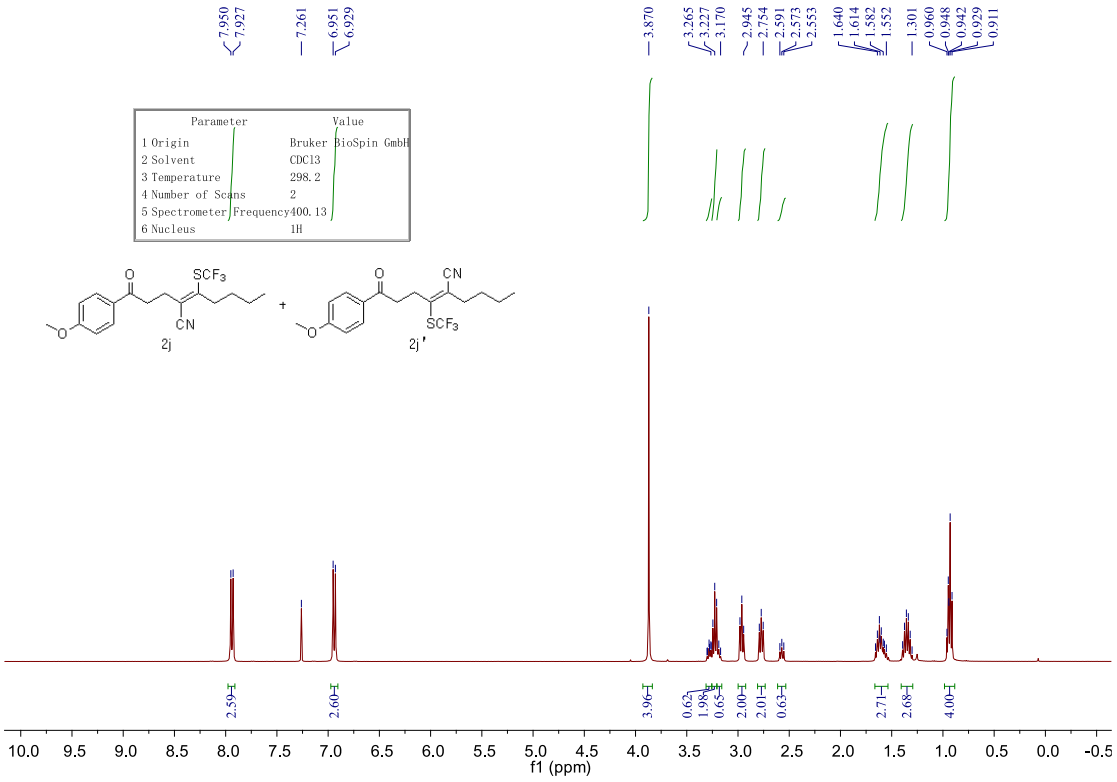

-38.070
-38.253
Parameter Value
1 Origin Bruker BioSpin GmbH
2 Solvent CDCl3
3 Temperature 298.2
4 Number of Scans 4
5 Spectrometer Frequency 376.50
6 Nucleus 19F
3.10
1.00
f1 (ppm)
2h
2h'

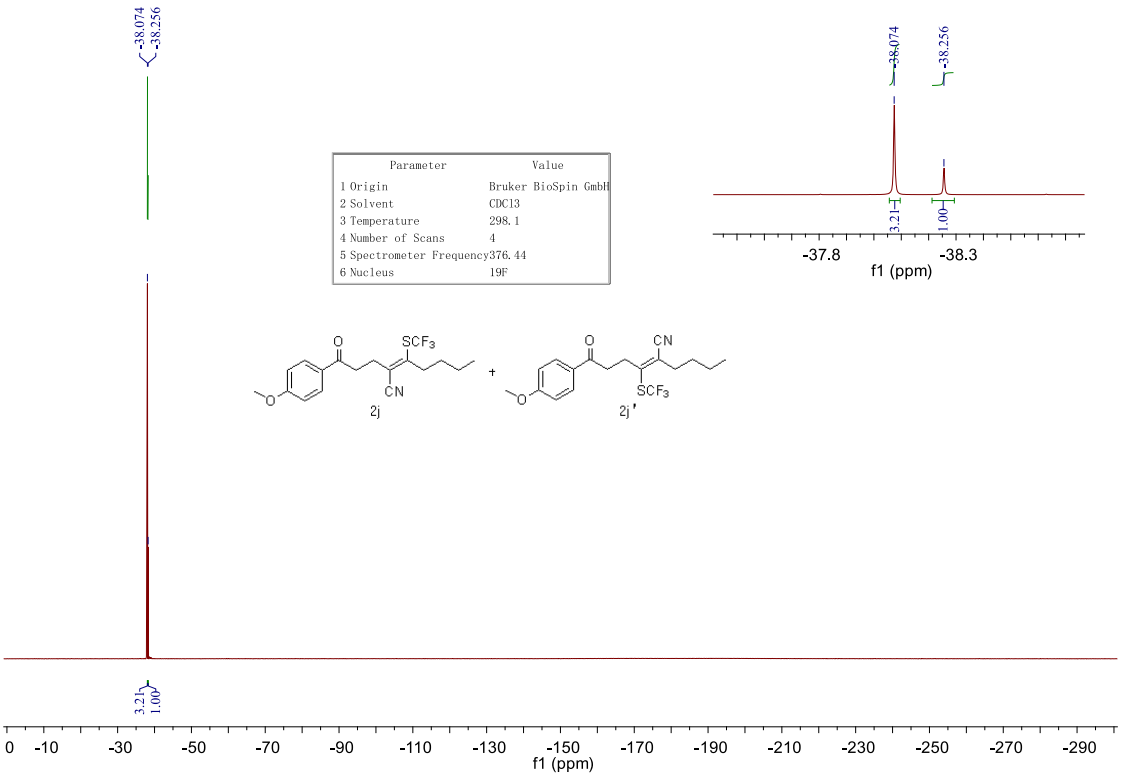

196.801
196.740
147.781
147.767
144.365
144.243
144.137
128.087
126.875
125.525
123.796
121.542
116.307
77.000
37.811
36.271
35.771
32.756
32.658
32.650
30.296
29.938
27.209
21.864
21.614
13.637
Parameter Value
1 Origin Bruker BioSpin GmbH
2 Solvent CDCl3
3 Temperature 298.2
4 Number of Scans 1024
5 Spectrometer Frequency 100.62
6 Nucleus 13C
f1 (ppm)
2h
2h'

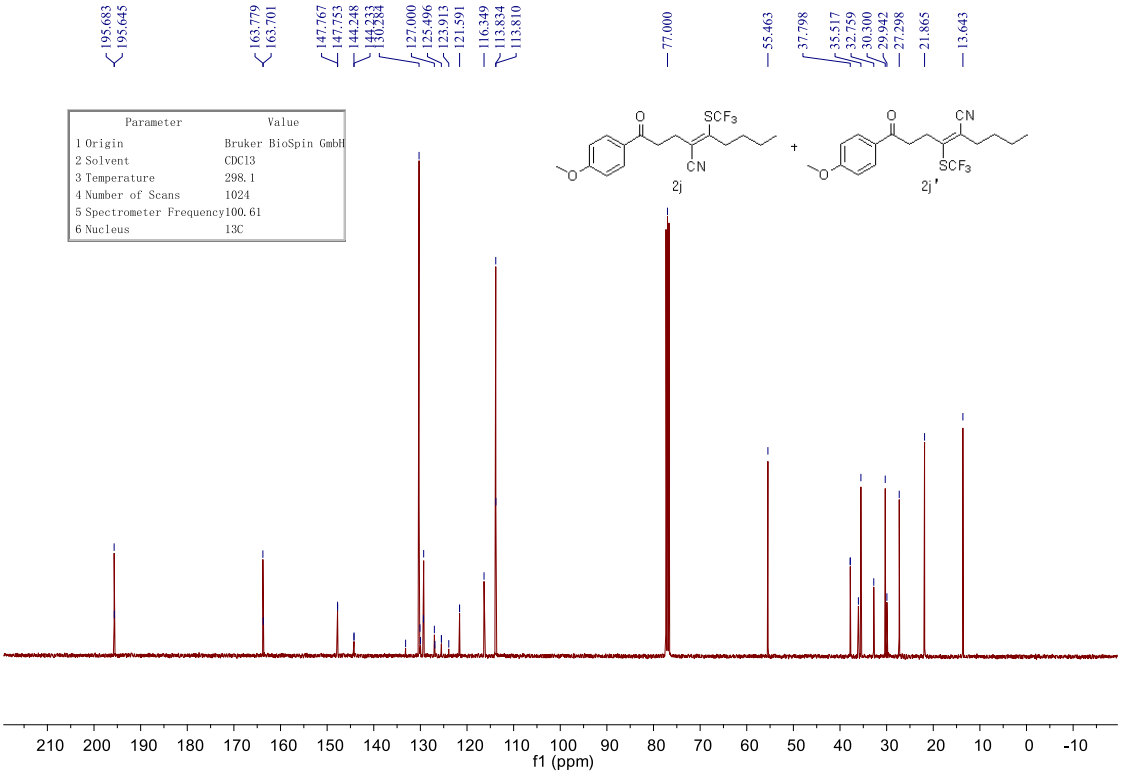

7.915
7.894
7.501
7.480
7.261
3.342
3.325
3.306
3.287
3.269
3.251
3.221
3.203
3.185
2.959
2.762
2.599
2.581
2.561
1.648
1.610
1.581
1.562
1.345
0.966
0.953
0.948
0.935
0.917
Parameter Value
1 Origin Bruker BioSpin GmbH
2 Solvent CDCl3
3 Temperature 298.2
4 Number of Scans 2
5 Spectrometer Frequency 400.13
6 Nucleus 1H
O
SCF3
CN
2i
+
O
CN
SCF3
2i'
2.54
2.56
0.60
2.01
0.62
2.01
2.00
0.61
2.95
2.72
11.87
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
f1 (ppm)

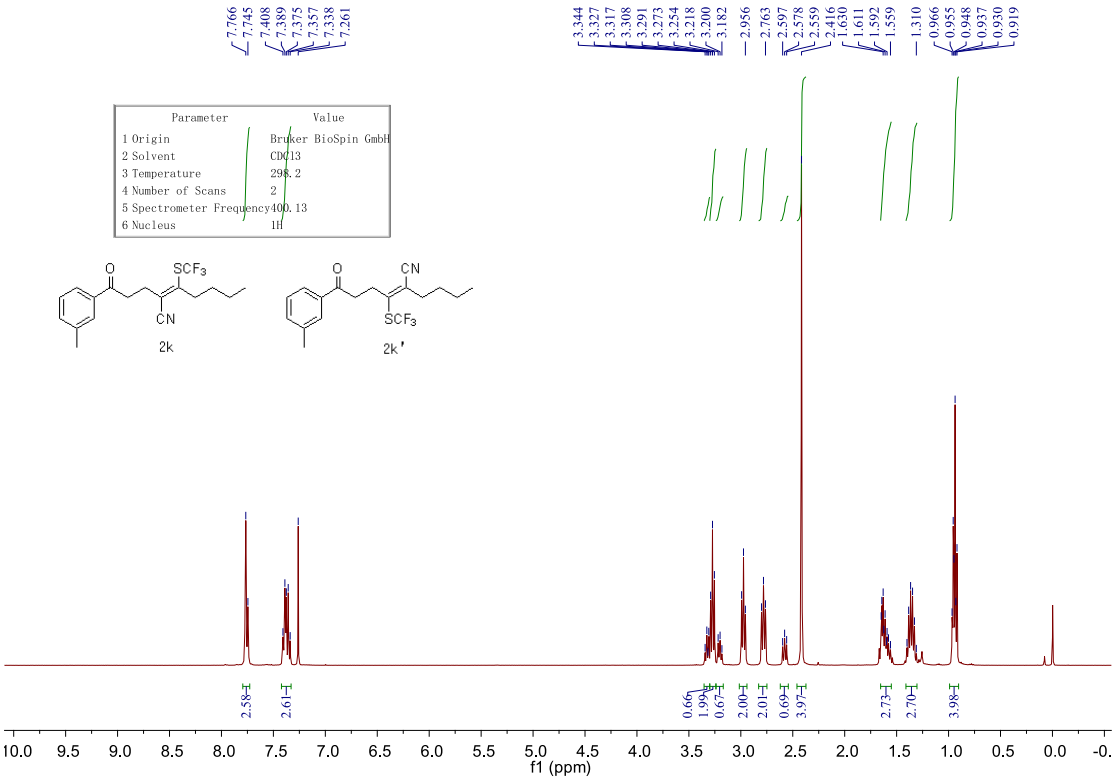

-38.070
-38.254
Parameter Value
1 Origin Bruker BioSpin GmbH
2 Solvent CDCl3
3 Temperature 298.2
4 Number of Scans 2
5 Spectrometer Frequency 376.44
6 Nucleus 19F
O
SCF3
CN
2i
+
O
CN
SCF3
2i'
3.18
1.00
-37.4 -37.8 -38.2 -38.6
f1 (ppm)
3.18
1.00
0 -10 -30 -50 -70 -90 -110 -130 -150 -170 -190 -210 -230 -250 -270 -290
f1 (ppm)

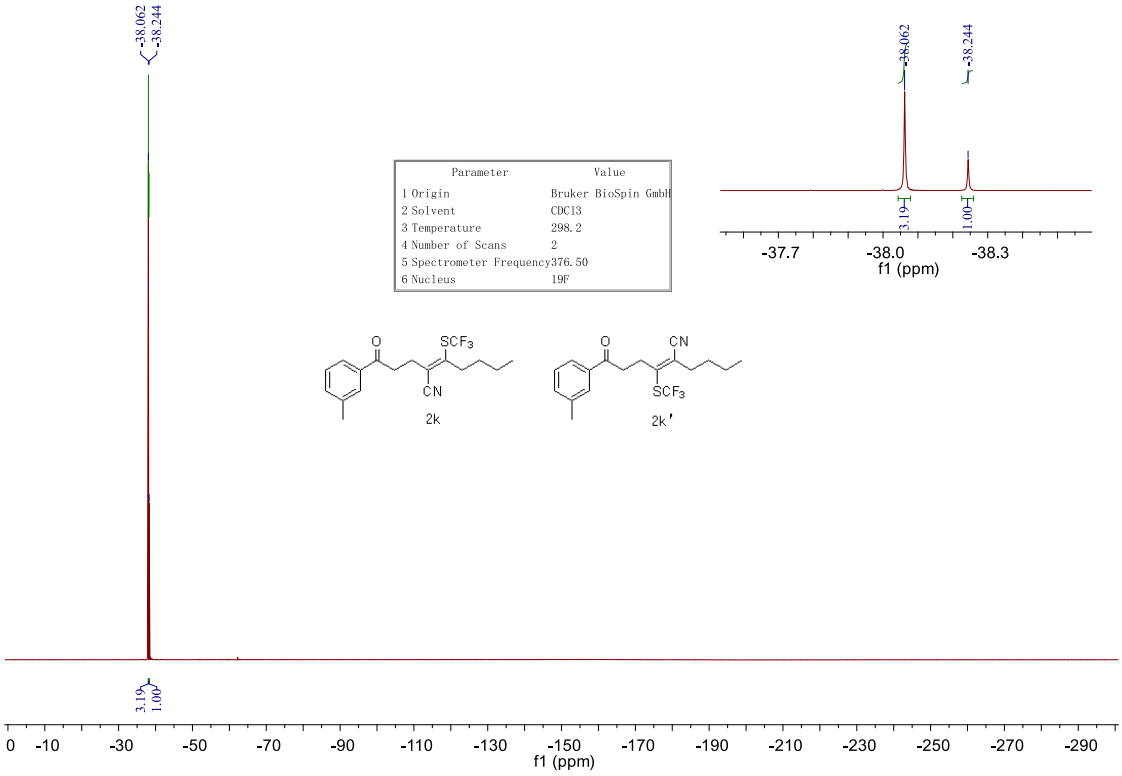

196.852
196.775
157.321
157.198
147.811
147.797
144.153
127.969
126.893
125.618
125.538
123.797
121.559
116.321
77.000
35.791
35.121
32.765
32.633
32.624
31.006
30.297
29.940
27.201
21.864
13.644
Parameter Value
1 Origin Bruker BioSpin GmbH
2 Solvent CDCl3
3 Temperature 298.1
4 Number of Scans 1024
5 Spectrometer Frequency 100.61
6 Nucleus 13C
SCF3
CN
2i
2i'
f1 (ppm)

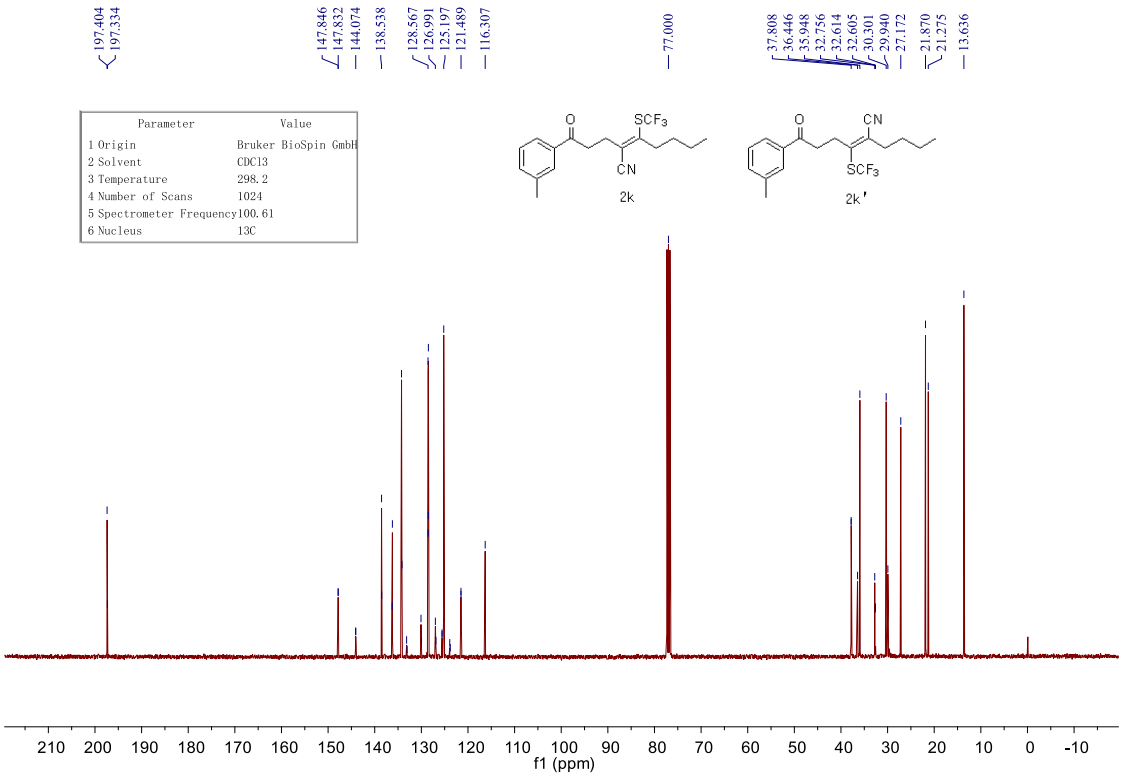

7.950
7.927
7.261
6.951
6.929
3.870
3.265
3.227
3.170
2.945
2.754
2.591
2.573
2.553
1.640
1.614
1.582
1.552
1.301
0.960
0.948
0.942
0.929
0.911
Parameter Value
1 Origin Bruker BioSpin GmbH
2 Solvent CDCl3
3 Temperature 298.2
4 Number of Scans 2
5 Spectrometer Frequency 400.13
6 Nucleus 1H
SCF3
CN
2j
2j'
2.59
2.60
3.96
0.62
1.98
0.65
2.00
2.01
0.63
2.71
2.68
4.00
f1 (ppm)

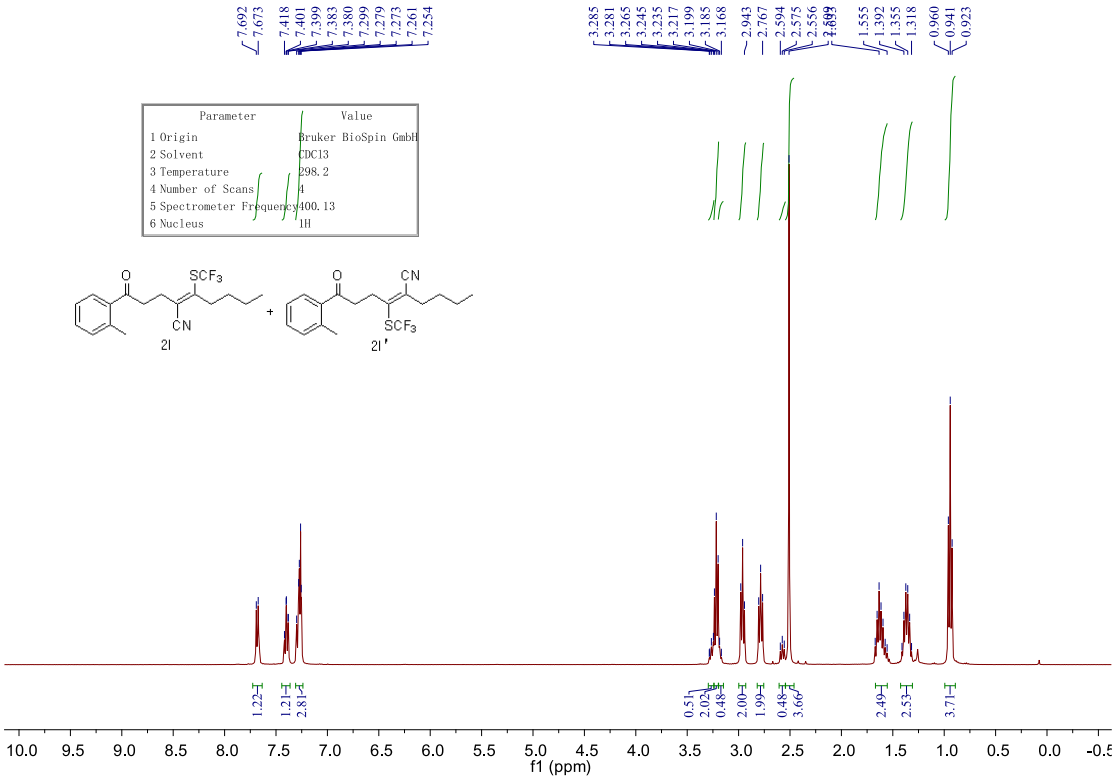

-38.074
-38.256
Parameter Value
1 Origin Bruker BioSpin GmbH
2 Solvent CDCl3
3 Temperature 298.1
4 Number of Scans 4
5 Spectrometer Frequency 376.44
6 Nucleus 19F
3.21
1.00
-37.8
-38.3
f1 (ppm)
SCF3
CN
2j
2j'
0 -10 -30 -50 -70 -90 -110 -130 -150 -170 -190 -210 -230 -250 -270 -290
f1 (ppm)

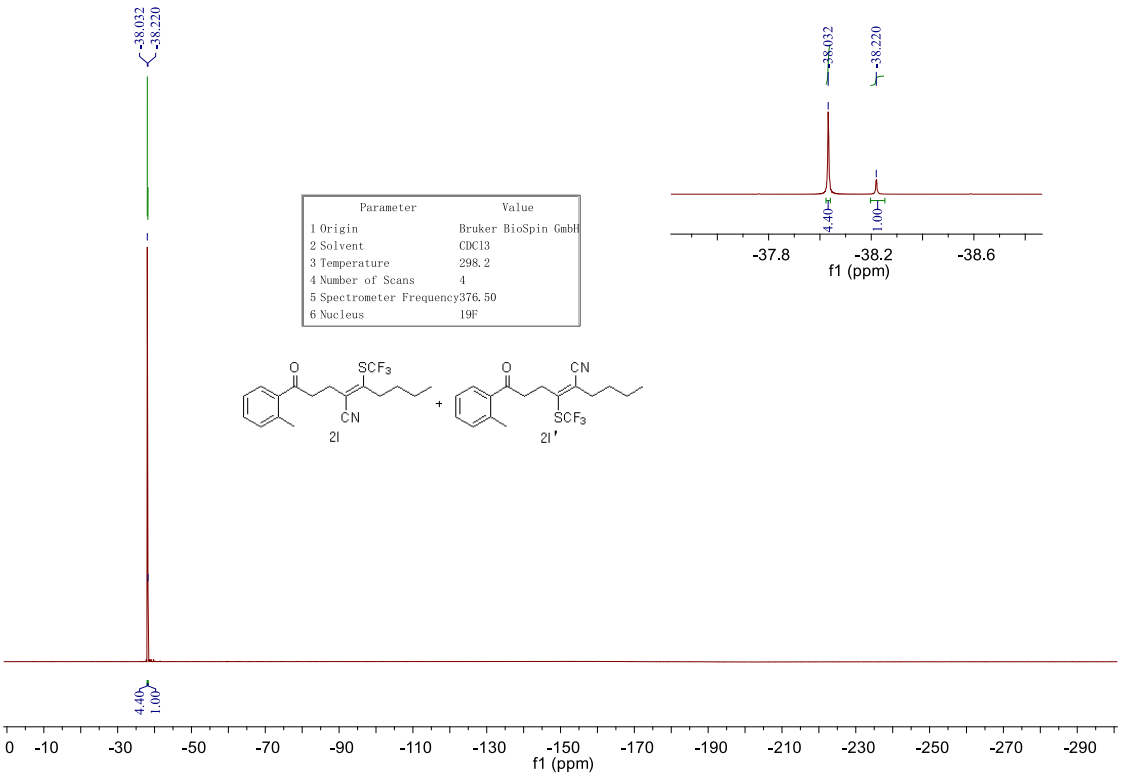

195.683
195.645
163.779
163.701
147.767
147.753
144.248
144.233
130.284
127.000
125.496
123.913
121.591
116.349
113.834
113.810
77.000
55.463
37.798
35.517
32.759
30.300
29.942
27.298
21.865
13.643
Parameter Value
1 Origin Bruker BioSpin GmbH
2 Solvent CDCl3
3 Temperature 298.1
4 Number of Scans 1024
5 Spectrometer Frequency 100.61
6 Nucleus 13C
SCF3
CN
2j
2j'
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)

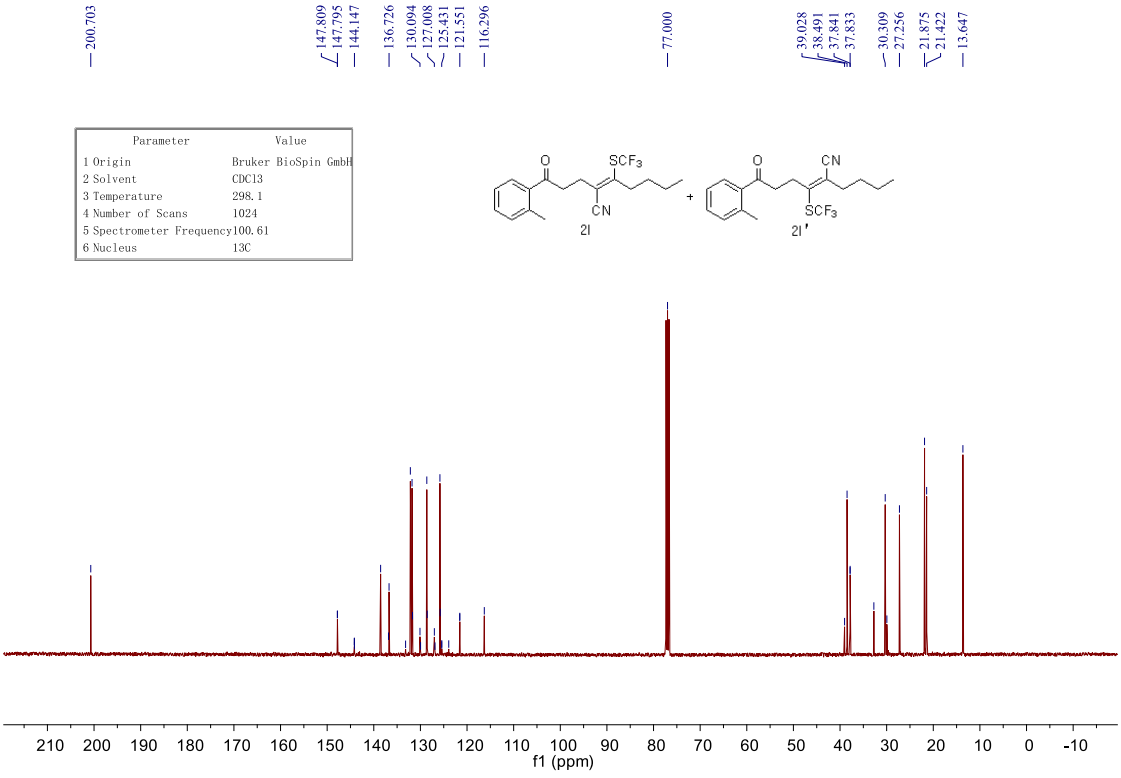

7.766
7.745
7.408
7.389
7.375
7.357
7.338
7.261
3.344
3.327
3.317
3.308
3.291
3.273
3.254
3.218
3.200
3.182
2.956
2.763
2.597
2.578
2.559
2.416
1.630
1.611
1.592
1.559
1.310
0.966
0.955
0.948
0.937
0.930
0.919
Parameter Value
1 Origin Bruker BioSpin GmbH
2 Solvent CDCl3
3 Temperature 298.2
4 Number of Scans 2
5 Spectrometer Frequency 400.13
6 Nucleus 1H
SCF3
CN
2k
CN
SCF3
2k'
2.58
2.61
0.66
1.99
0.67
2.00
2.01
0.69
3.97
2.73
2.70
3.98
f1 (ppm)

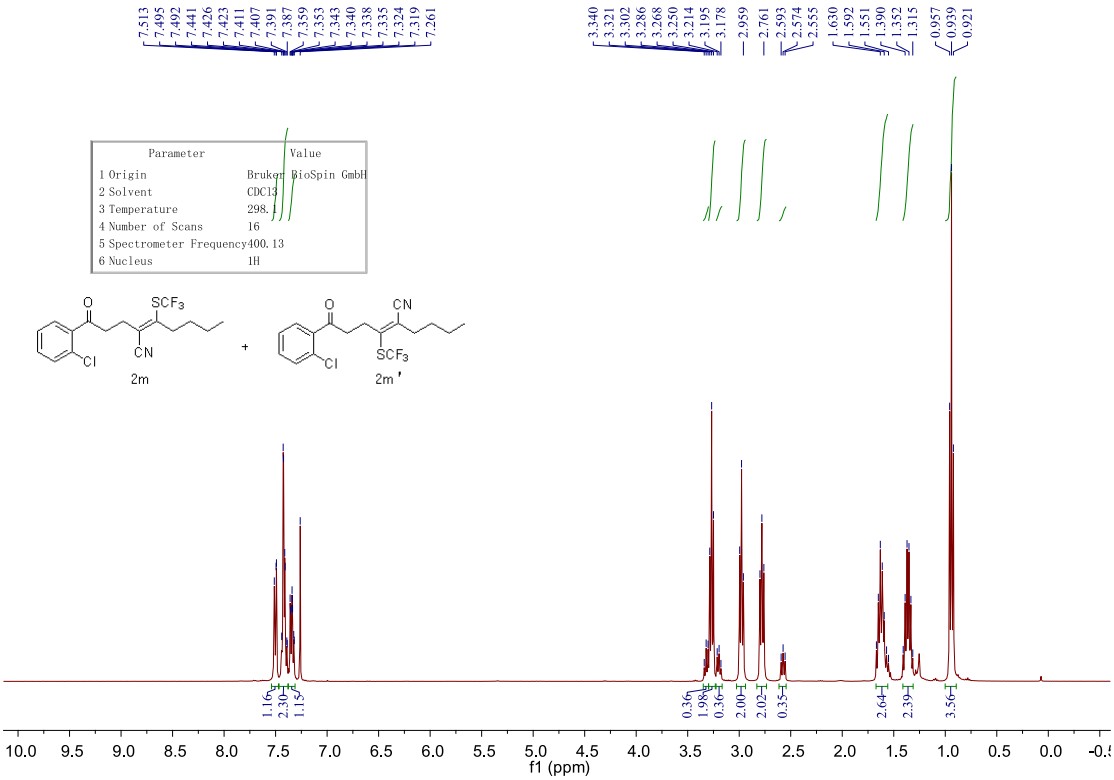

-38.062
-38.244
Parameter Value
1 Origin Bruker BioSpin GmbH
2 Solvent CDCl3
3 Temperature 298.2
4 Number of Scans 2
5 Spectrometer Frequency 376.50
6 Nucleus 19F
SCF3
CN
2k
CN
SCF3
2k'
3.19
1.00
f1 (ppm)

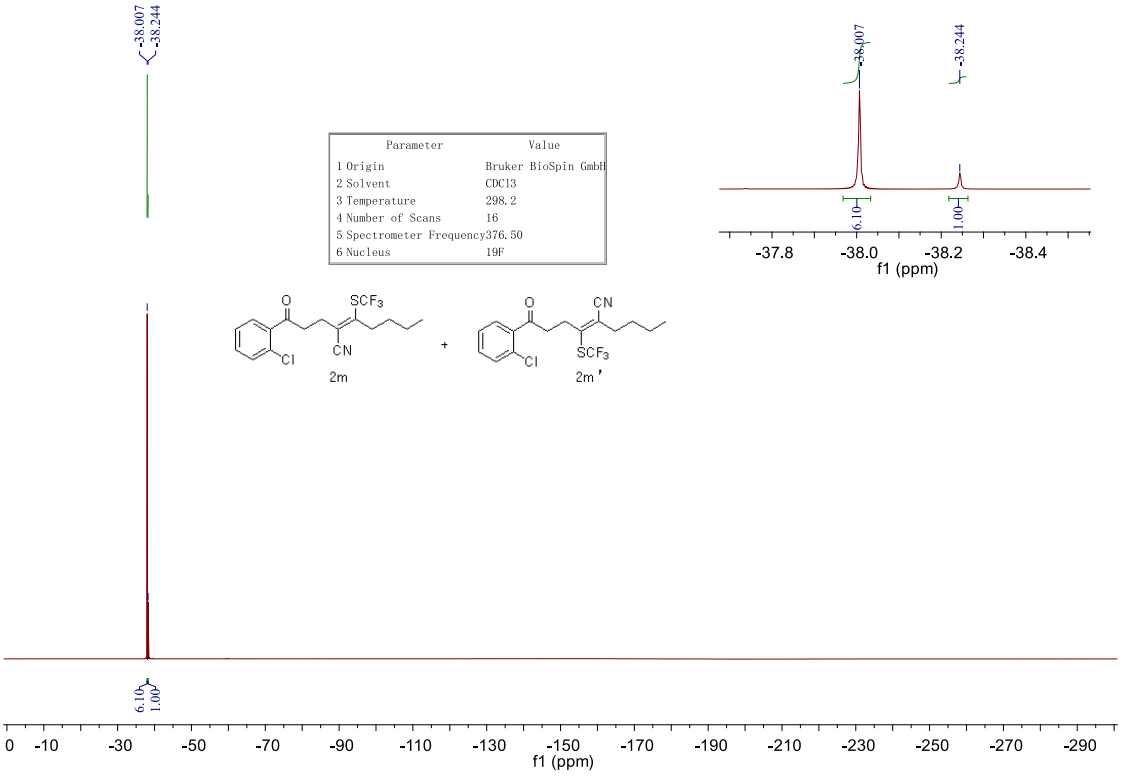

197.404
197.334
147.846
147.832
144.074
138.538
128.567
126.991
125.197
121.489
116.307
77.000
37.808
36.446
35.948
32.756
32.614
32.605
30.301
29.940
27.172
21.870
21.275
13.636
Parameter Value
1 Origin Bruker BioSpin GmbH
2 Solvent CDCl3
3 Temperature 298.2
4 Number of Scans 1024
5 Spectrometer Frequency 100.61
6 Nucleus 13C
O
SCF3
CN
2k
O
CN
SCF3
2k'
f1 (ppm)

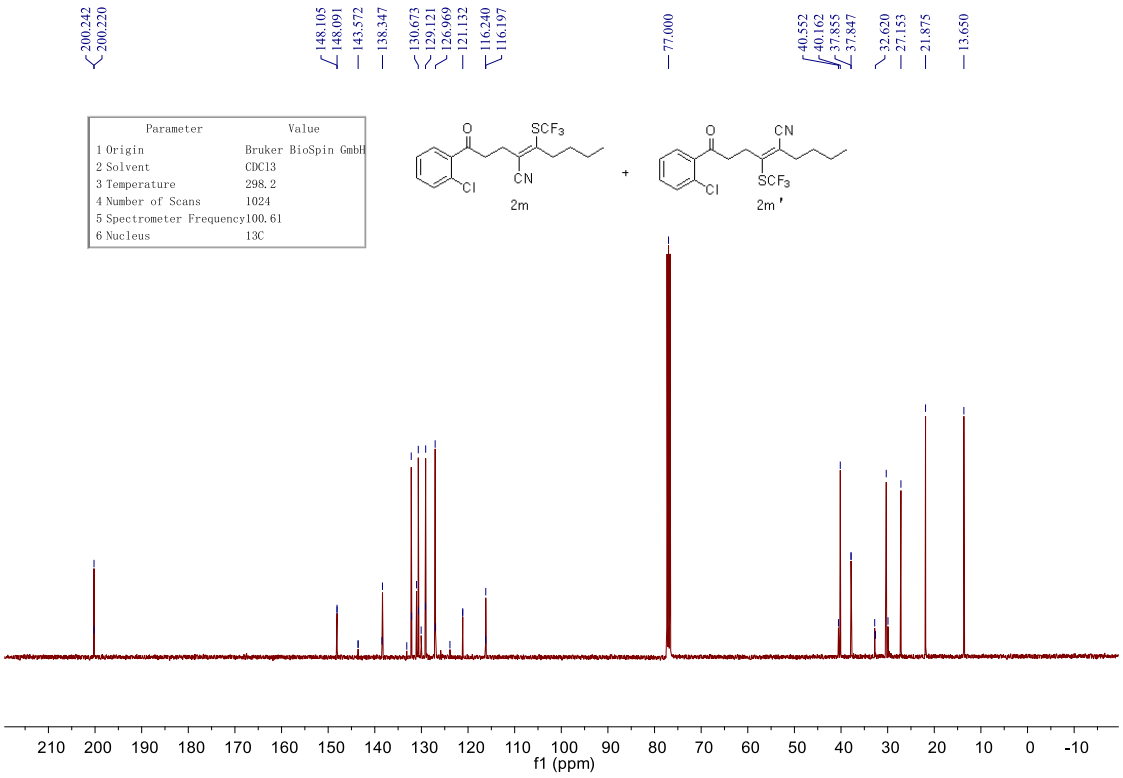

7.692
7.673
7.418
7.401
7.399
7.383
7.380
7.299
7.279
7.273
7.261
7.254
3.285
3.281
3.265
3.245
3.235
3.217
3.199
3.185
3.168
2.943
2.767
2.594
2.575
2.556
1.555
1.392
1.355
1.318
0.960
0.941
0.923
Parameter Value
1 Origin Bruker BioSpin GmbH
2 Solvent CDCl3
3 Temperature 298.2
4 Number of Scans 4
5 Spectrometer Frequency 400.13
6 Nucleus 1H
O
SCF3
CN
2l
+
O
CN
SCF3
2l'
1.22
1.21
2.81
0.51
2.02
0.48
2.00
1.99
0.48
3.66
2.49
2.53
3.71
f1 (ppm)

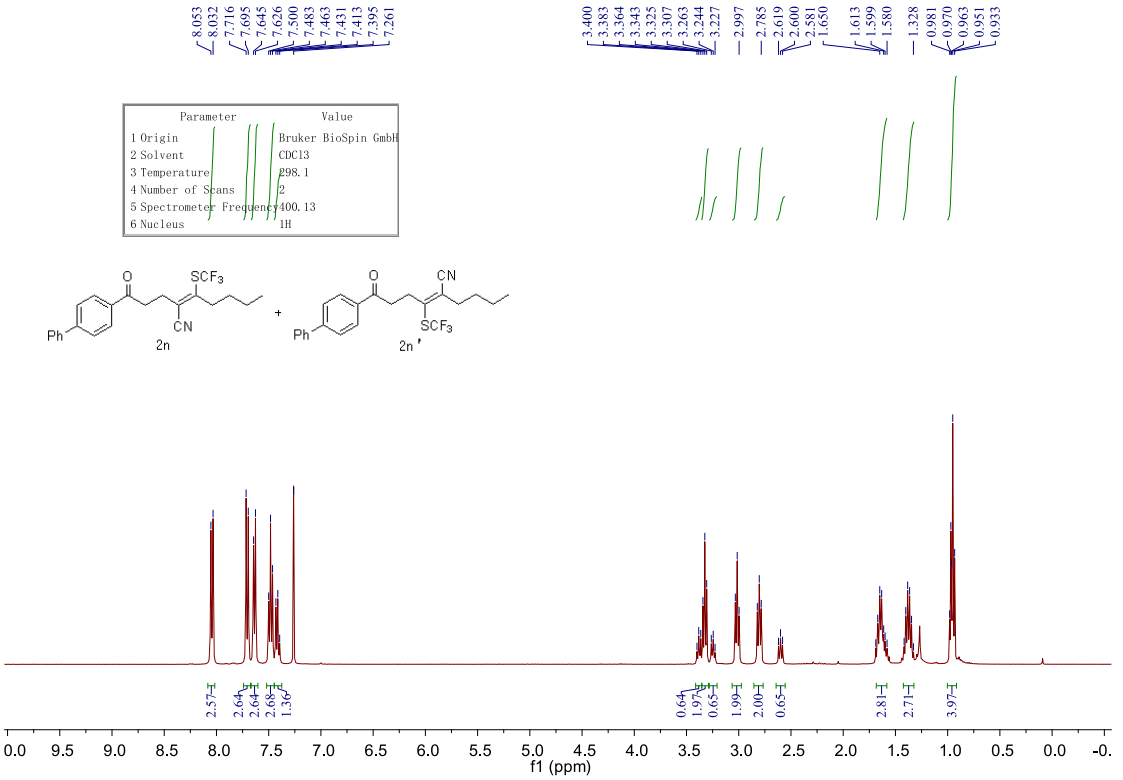

-38.032
-38.220
4.40
1.00
-37.8
-38.2
-38.6
f1 (ppm)
Parameter Value
1 Origin Bruker BioSpin GmbH
2 Solvent CDCl3
3 Temperature 298.2
4 Number of Scans 4
5 Spectrometer Frequency 376.50
6 Nucleus 19F
SCF3
CN
2l
2l'
0 -10 -30 -50 -70 -90 -110 -130 -150 -170 -190 -210 -230 -250 -270 -290
f1 (ppm)

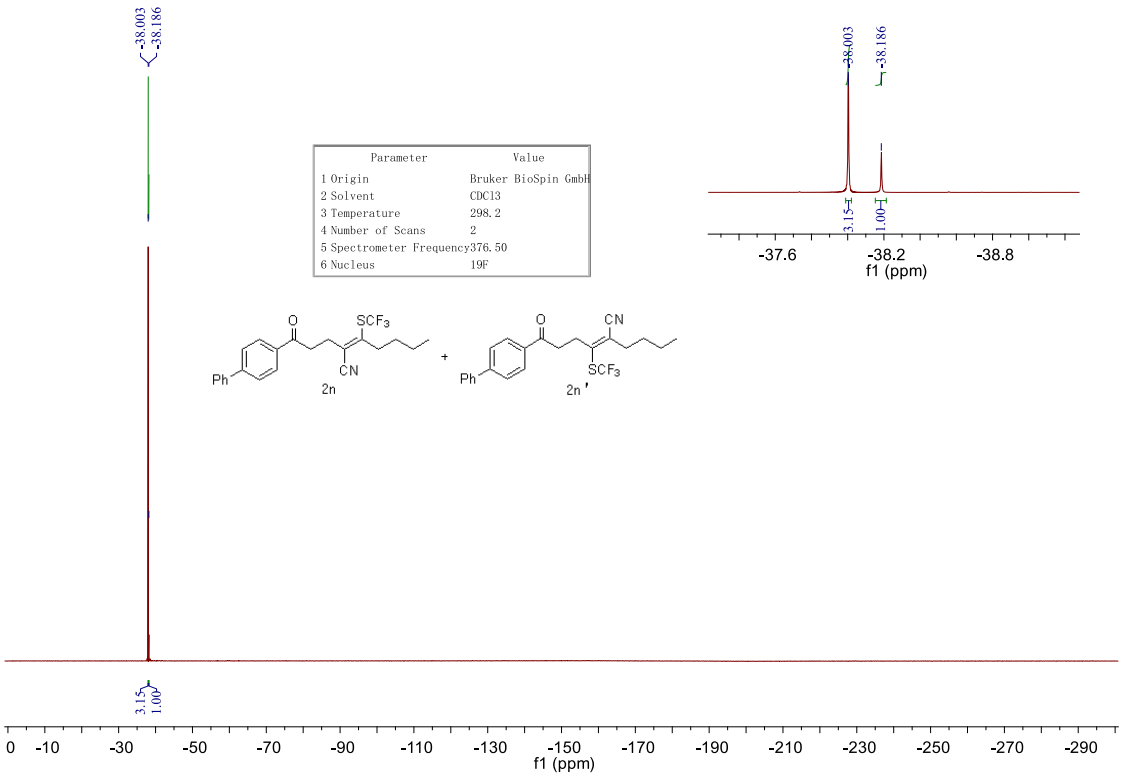

200.703
147.809
147.795
144.147
136.726
130.094
127.008
125.431
121.551
116.296
77.000
39.028
38.491
37.841
37.833
30.309
27.256
21.875
21.422
13.647
Parameter Value
1 Origin Bruker BioSpin GmbH
2 Solvent CDCl3
3 Temperature 298.1
4 Number of Scans 1024
5 Spectrometer Frequency 100.61
6 Nucleus 13C
SCF3
CN
2l
2l'
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)

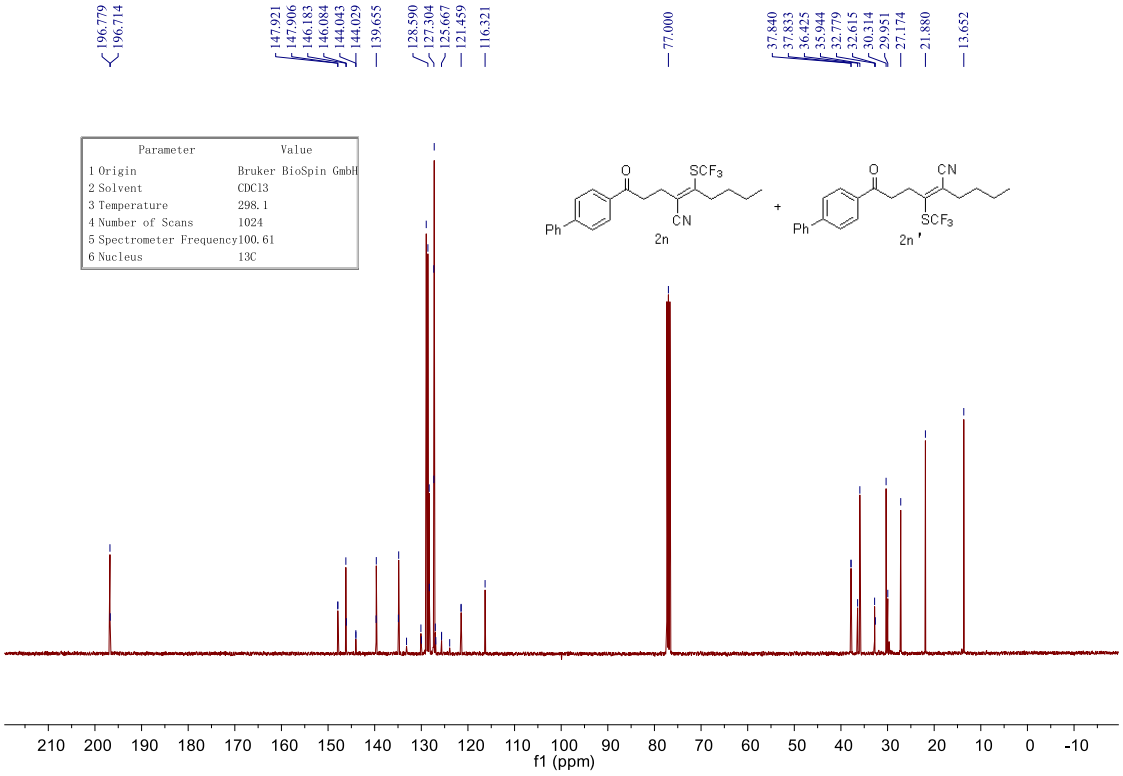

7.513
7.495
7.492
7.441
7.426
7.423
7.411
7.407
7.391
7.387
7.359
7.353
7.343
7.340
7.338
7.335
7.324
7.319
7.261
3.340
3.321
3.302
3.286
3.268
3.250
3.214
3.195
3.178
2.959
2.761
2.593
2.574
2.555
1.630
1.592
1.551
1.390
1.352
1.315
0.957
0.939
0.921
Parameter Value
1 Origin Bruker BioSpin GmbH
2 Solvent CDCl3
3 Temperature 298.1
4 Number of Scans 16
5 Spectrometer Frequency 400.13
6 Nucleus 1H
O
SCF3
CN
Cl
2m
+
O
CN
SCF3
Cl
2m'
1.16
2.30
1.15
0.36
1.98
0.36
2.00
2.02
0.35
2.64
2.39
3.56
10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)

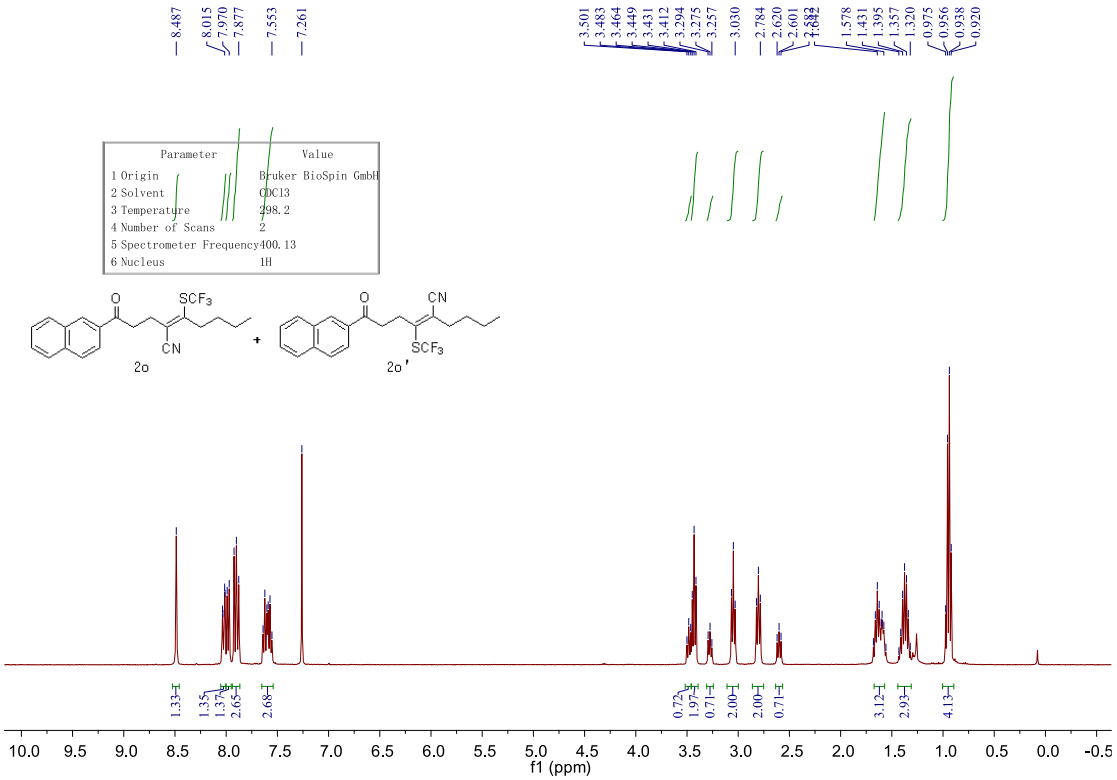

-38.007
-38.244
Parameter Value
1 Origin Bruker BioSpin GmbH
2 Solvent CDCl3
3 Temperature 298.2
4 Number of Scans 16
5 Spectrometer Frequency 376.50
6 Nucleus 19F
O
SCF3
CN
Cl
2m
+
O
CN
SCF3
Cl
2m'
6.10
1.00
-37.8 -38.0 -38.2 -38.4
f1 (ppm)
0 -10 -30 -50 -70 -90 -110 -130 -150 -170 -190 -210 -230 -250 -270 -290
f1 (ppm)

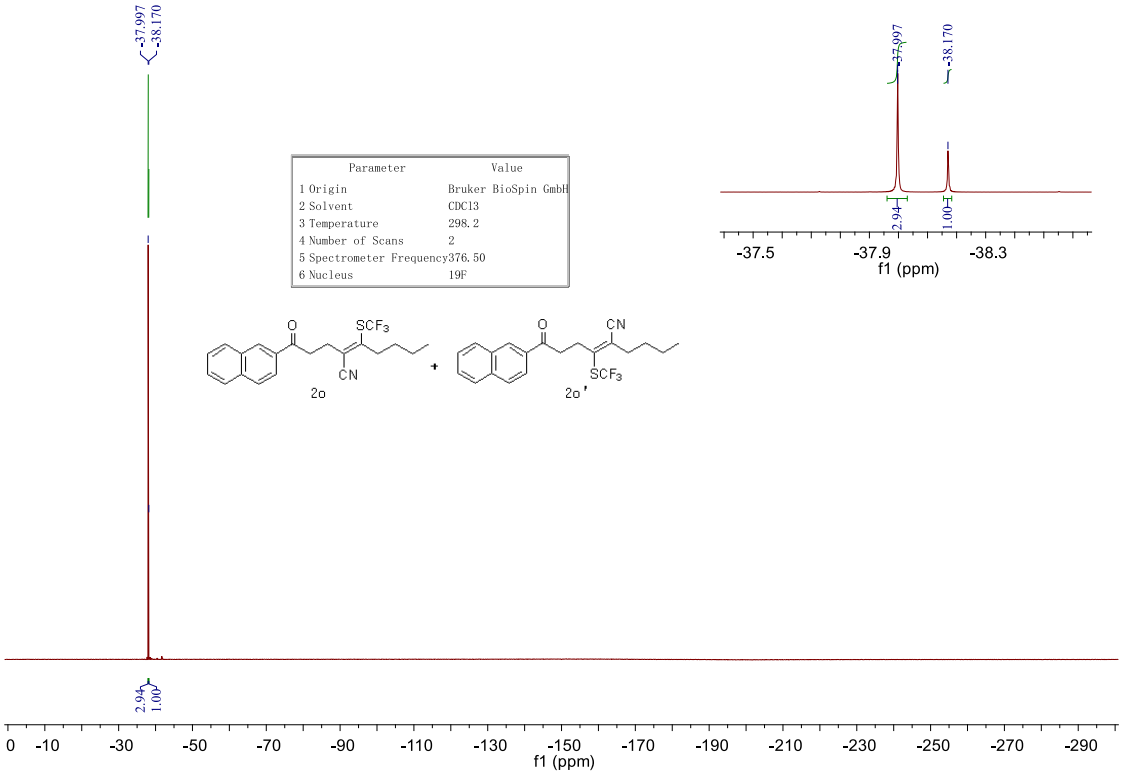

200.242
200.220
148.105
148.091
143.572
138.347
130.673
129.121
126.969
121.132
116.240
116.197
77.000
40.552
40.162
37.855
37.847
32.620
27.153
21.875
13.650
Parameter Value
1 Origin Bruker BioSpin GmbH
2 Solvent CDCl3
3 Temperature 298.2
4 Number of Scans 1024
5 Spectrometer Frequency 100.61
6 Nucleus 13C
SCF3
CN
Cl
2m
2m'
f1 (ppm)

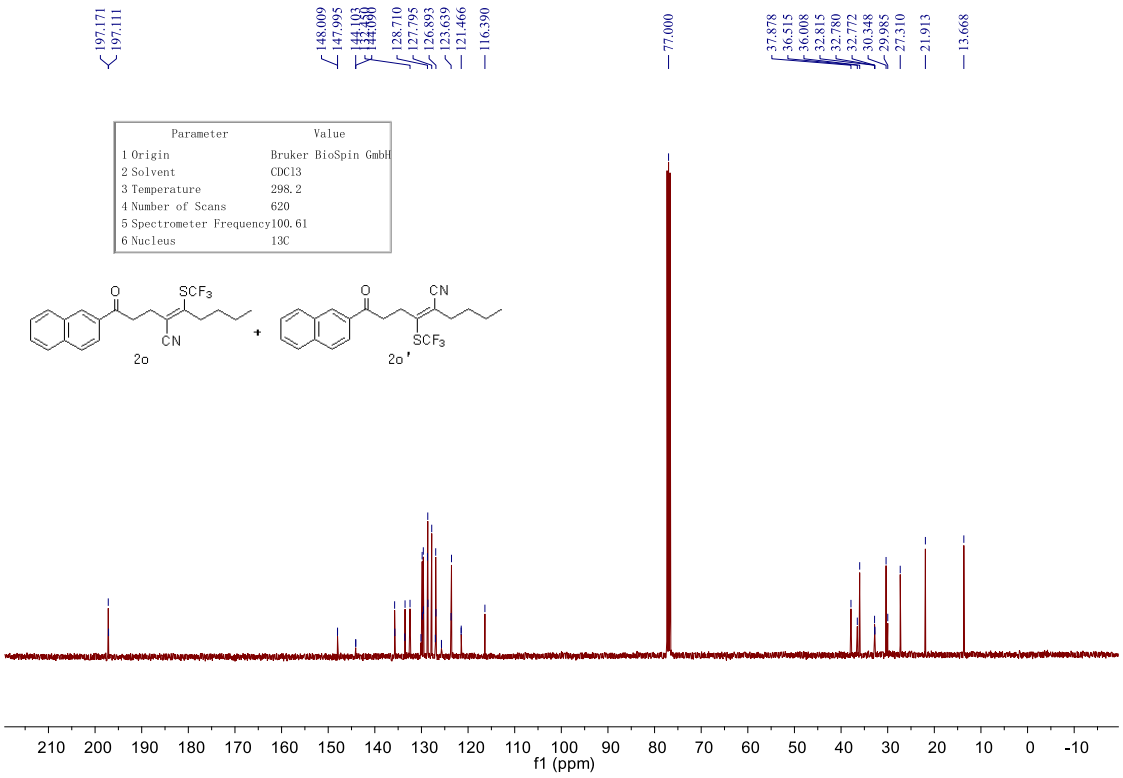

8.053
8.032
7.716
7.695
7.645
7.626
7.500
7.483
7.463
7.431
7.413
7.395
7.261
3.400
3.383
3.364
3.343
3.325
3.307
3.263
3.244
3.227
2.997
2.785
2.619
2.600
2.581
1.650
1.613
1.599
1.580
1.328
0.981
0.970
0.963
0.951
0.933
Parameter Value
1 Origin Bruker BioSpin GmbH
2 Solvent CDCl3
3 Temperature 298.1
4 Number of Scans 2
5 Spectrometer Frequency 400.13
6 Nucleus 1H
Ph
SCF3
CN
2n
2n'
2.57
2.64
2.64
2.68
1.36
0.64
1.97
0.65
1.99
2.00
0.65
2.81
2.71
3.97
f1 (ppm)

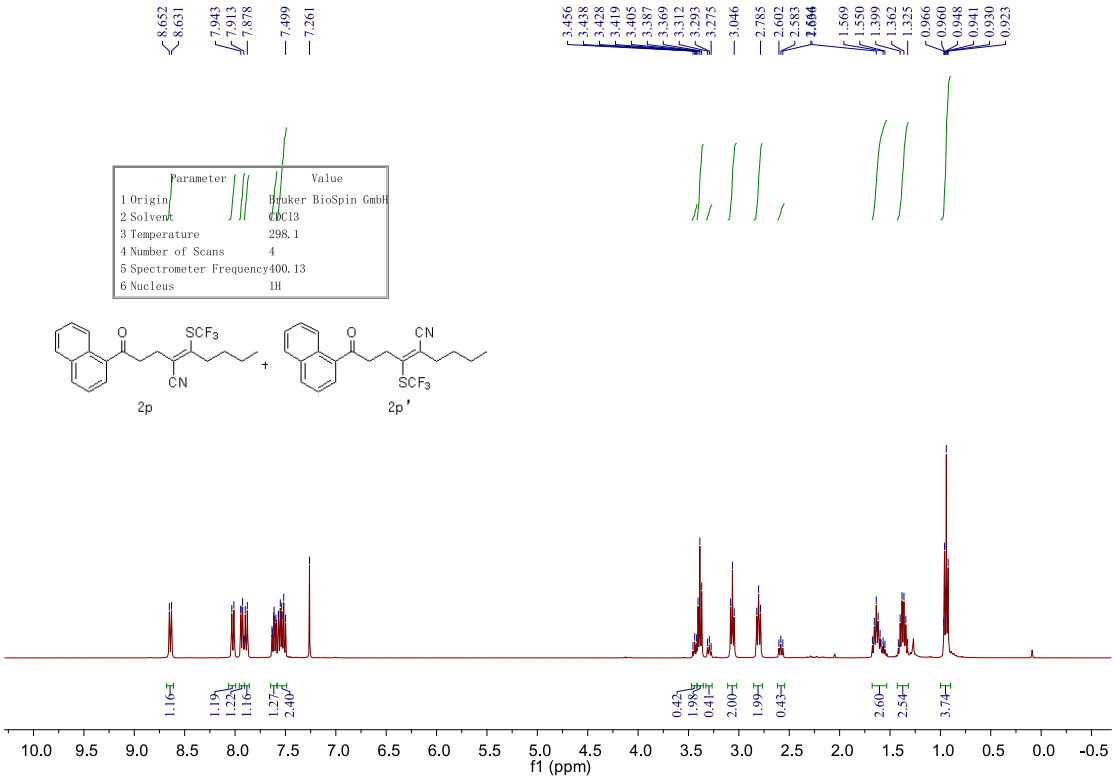

-38.003
-38.186
Parameter Value
1 Origin Bruker BioSpin GmbH
2 Solvent CDCl3
3 Temperature 298.2
4 Number of Scans 2
5 Spectrometer Frequency376.50
6 Nucleus 19F
3.15
1.00
-37.6
-38.2
-38.8
f1 (ppm)
SCF3
CN
Ph
2n
2n'
0 -10 -30 -50 -70 -90 -110 -130 -150 -170 -190 -210 -230 -250 -270 -290
f1 (ppm)

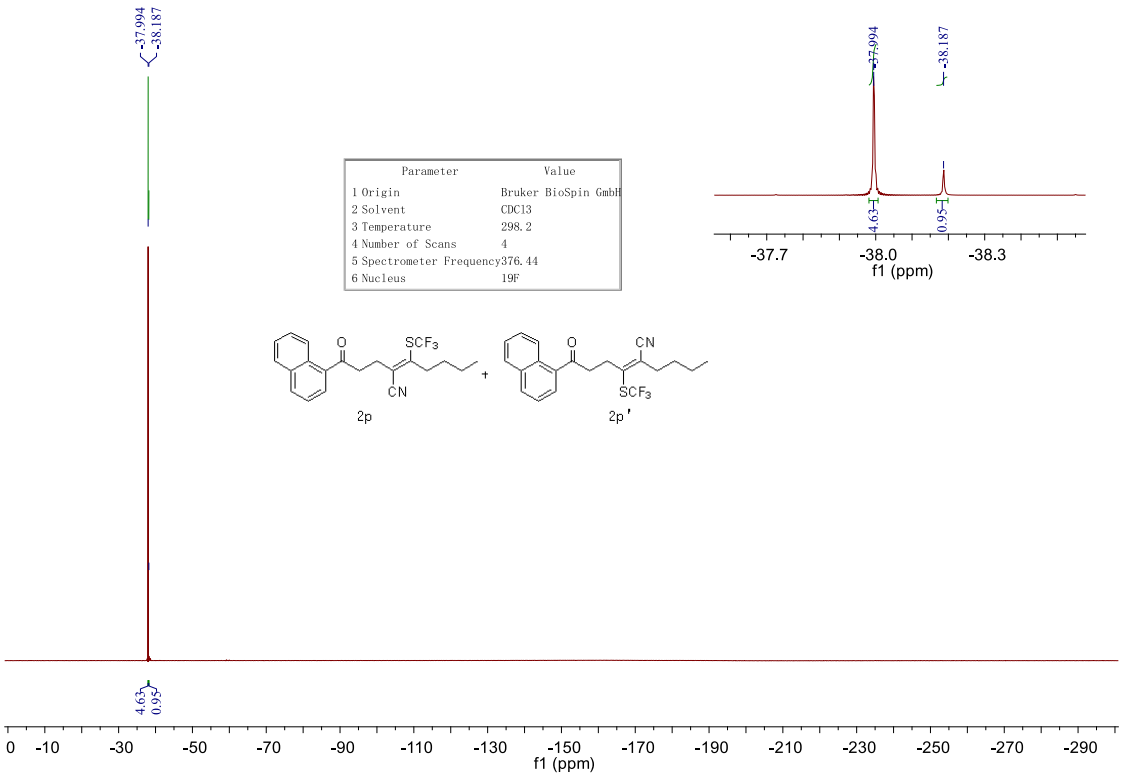

196.779
196.714
147.921
147.906
146.183
146.084
144.043
144.029
139.655
128.590
127.304
125.667
121.459
116.321
77.000
37.840
37.833
36.425
35.944
32.779
32.615
30.314
29.951
27.174
21.880
13.652
Parameter Value
1 Origin Bruker BioSpin GmbH
2 Solvent CDCl3
3 Temperature 298.1
4 Number of Scans 1024
5 Spectrometer Frequency100.61
6 Nucleus 13C
SCF3
CN
Ph
2n
2n'
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)

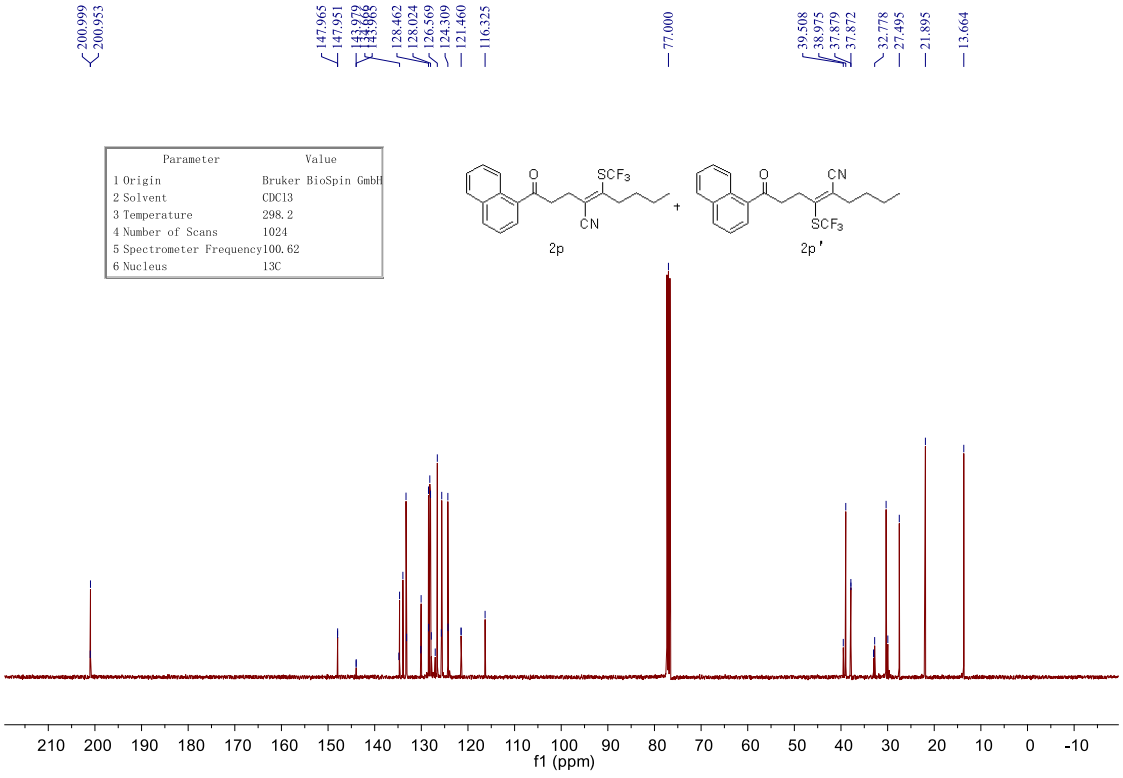

8.487
8.015
7.970
7.877
7.553
7.261
3.501
3.483
3.464
3.449
3.431
3.412
3.294
3.275
3.257
3.030
2.784
2.620
2.601
1.578
1.431
1.395
1.357
1.320
0.975
0.956
0.938
0.920
Parameter Value
1 Origin Bruker BioSpin GmbH
2 Solvent CDCl3
3 Temperature 298.2
4 Number of Scans 2
5 Spectrometer Frequency 400.13
6 Nucleus 1H
SCF3
CN
2o
2o'
1.33
1.35
2.65
2.68
0.72
1.97
0.71
2.00
2.00
0.71
3.12
2.93
4.13
f1 (ppm)

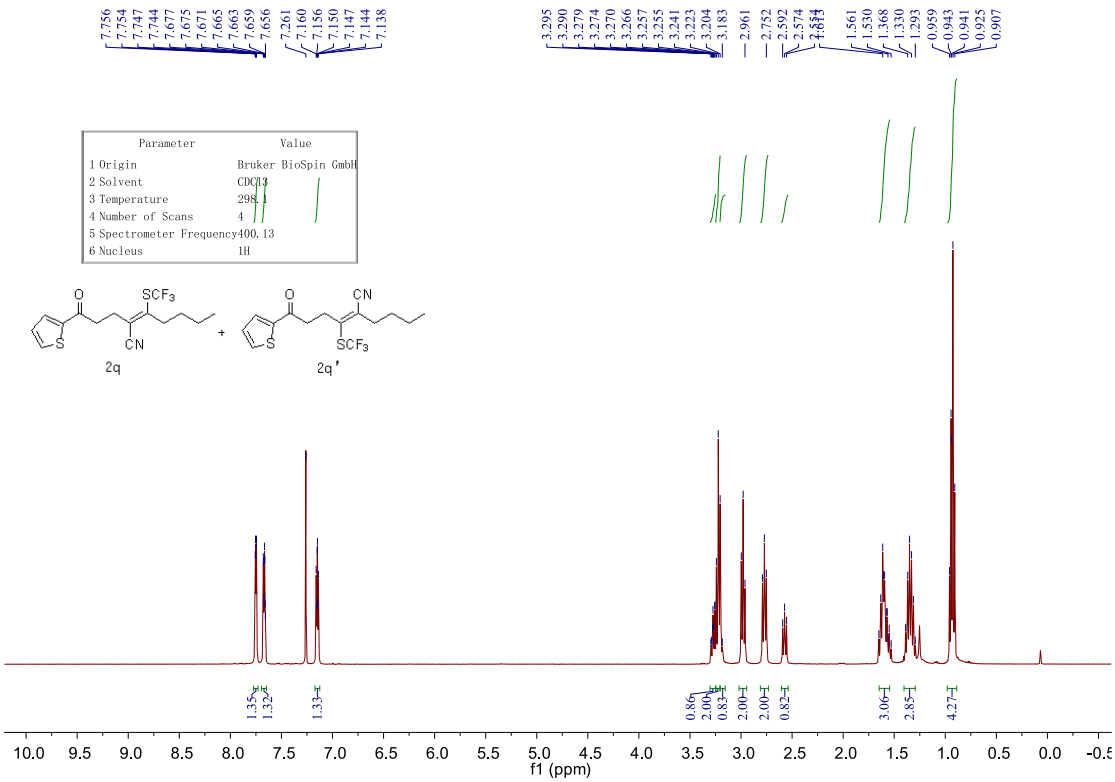

-37.997
-38.170
Parameter Value
1 Origin Bruker BioSpin GmbH
2 Solvent CDCl3
3 Temperature 298.2
4 Number of Scans 2
5 Spectrometer Frequency 376.50
6 Nucleus 19F
SCF3
CN
2o
2o'
2.94
1.00
f1 (ppm)

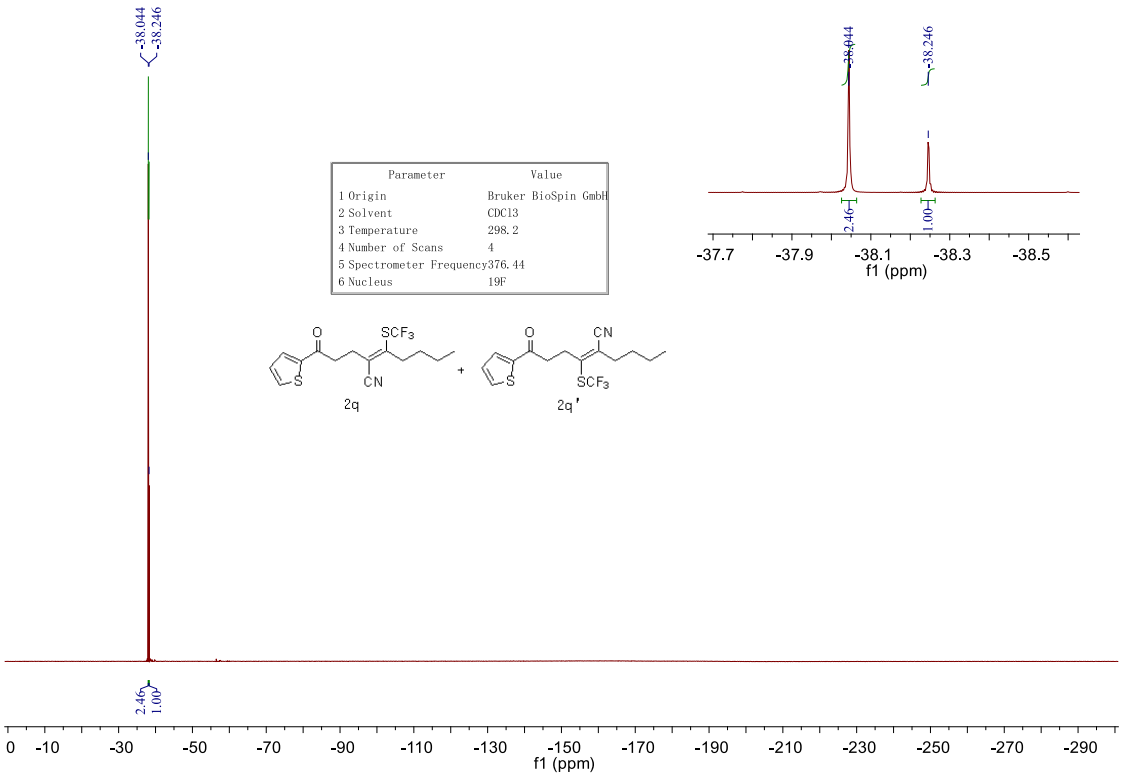

197.171
197.111
148.009
147.995
128.710
127.795
126.893
123.639
121.466
116.390
77.000
37.878
36.515
36.008
32.815
32.780
32.772
30.348
29.985
27.310
21.913
13.668
Parameter Value
1 Origin Bruker BioSpin GmbH
2 Solvent CDCl3
3 Temperature 298.2
4 Number of Scans 620
5 Spectrometer Frequency 100.61
6 Nucleus 13C
O
SCF3
CN
2o
+
O
CN
SCF3
2o'
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)

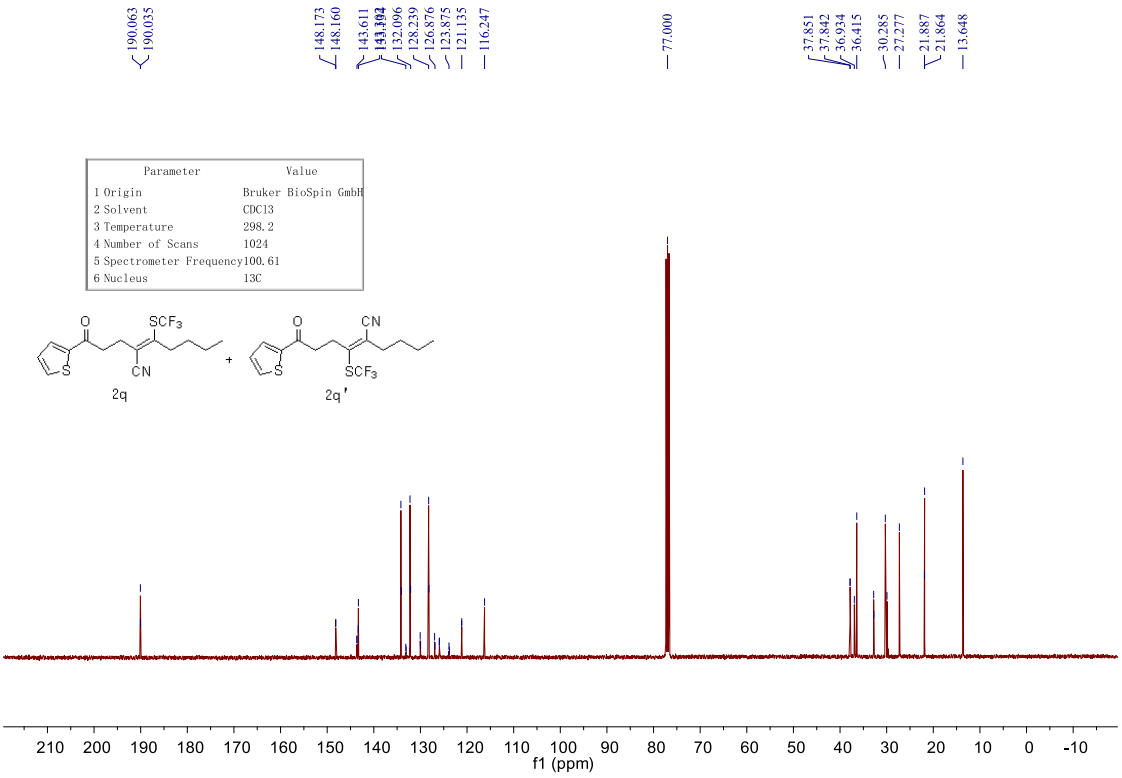

8.652
8.631
7.943
7.913
7.878
7.499
7.261
3.456
3.438
3.428
3.419
3.405
3.387
3.369
3.312
3.293
3.275
3.046
2.785
2.602
2.583
1.569
1.550
1.399
1.362
1.325
0.966
0.960
0.948
0.941
0.930
0.923
Parameter Value
1 Origin Bruker BioSpin GmbH
2 Solvent CDCl3
3 Temperature 298.1
4 Number of Scans 4
5 Spectrometer Frequency 400.13
6 Nucleus 1H
O
SCF3
CN
2p
+
O
CN
SCF3
2p'
1.16
1.19
1.22
1.16
1.27
2.40
0.42
1.98
0.41
2.00
1.99
0.43
2.60
2.54
3.74
10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5
f1 (ppm)

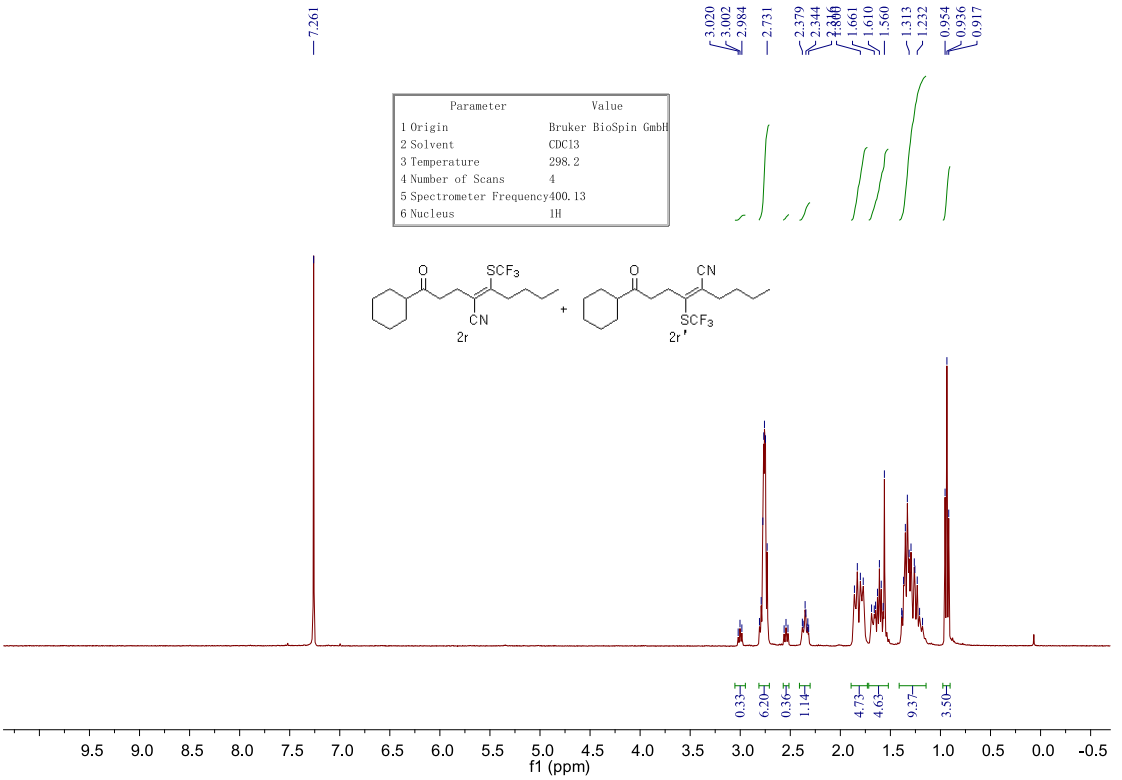

-37.994
-38.187
Parameter Value
1 Origin Bruker BioSpin GmbH
2 Solvent CDCl3
3 Temperature 298.2
4 Number of Scans 4
5 Spectrometer Frequency376.44
6 Nucleus 19F
4.63
0.95
f1 (ppm)
2p
2p'

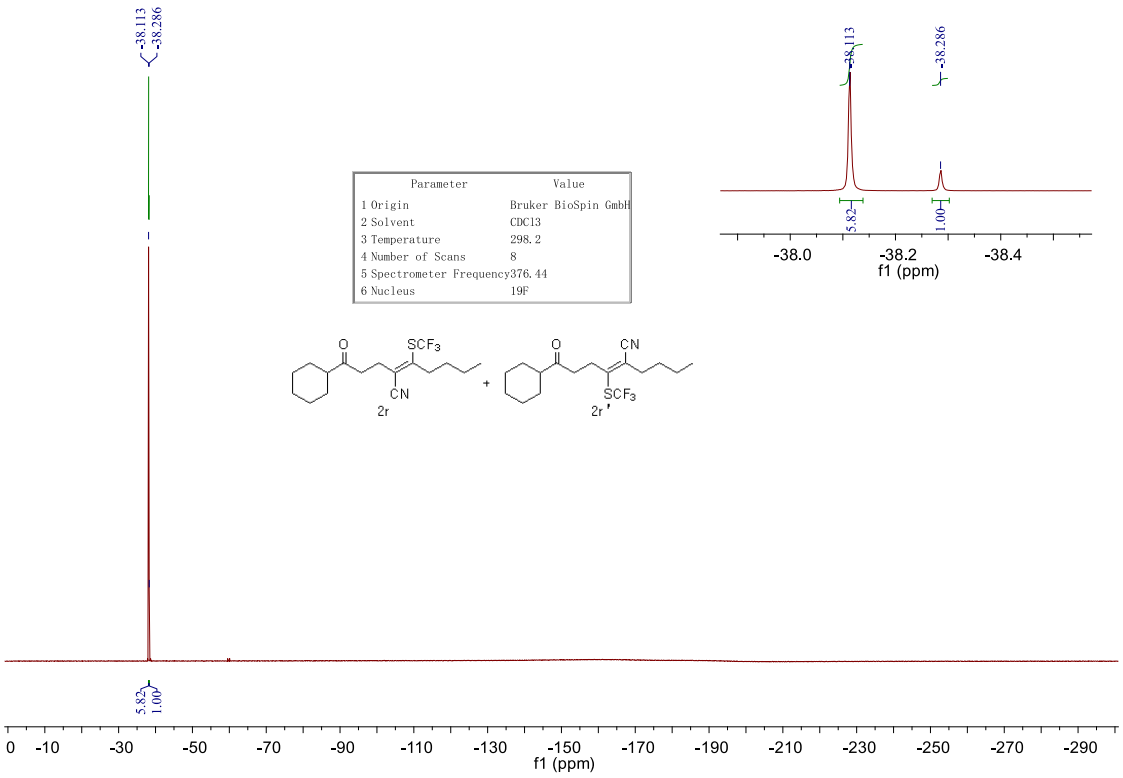

200.999
200.953
147.965
147.951
128.462
128.024
126.569
124.309
121.460
116.325
77.000
39.508
38.975
37.879
37.872
32.778
27.495
21.895
13.664
Parameter Value
1 Origin Bruker BioSpin GmbH
2 Solvent CDCl3
3 Temperature 298.2
4 Number of Scans 1024
5 Spectrometer Frequency100.62
6 Nucleus 13C
f1 (ppm)
2p
2p'

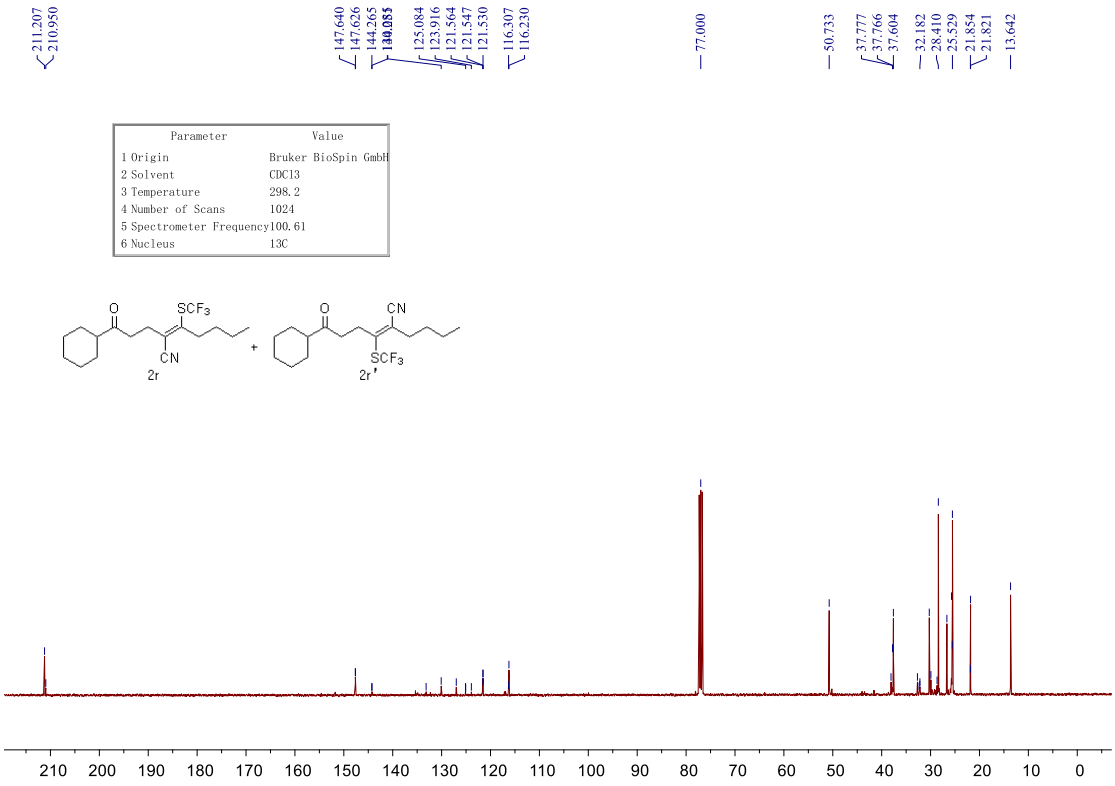

7.756
7.754
7.747
7.744
7.677
7.675
7.671
7.665
7.663
7.659
7.656
7.261
7.160
7.156
7.150
7.147
7.144
7.138
3.295
3.290
3.279
3.274
3.270
3.266
3.257
3.255
3.241
3.223
3.204
3.183
2.961
2.752
2.592
2.574
2.554
1.561
1.530
1.368
1.330
1.293
0.959
0.943
0.941
0.925
0.907
Parameter Value
1 Origin Bruker BioSpin GmbH
2 Solvent CDCl3
3 Temperature 298.1
4 Number of Scans 4
5 Spectrometer Frequency 400.13
6 Nucleus 1H
SCF3
CN
2q
2q'
1.35
1.32
1.33
0.86
2.00
0.83
2.00
2.00
0.82
3.06
2.85
4.27
f1 (ppm)

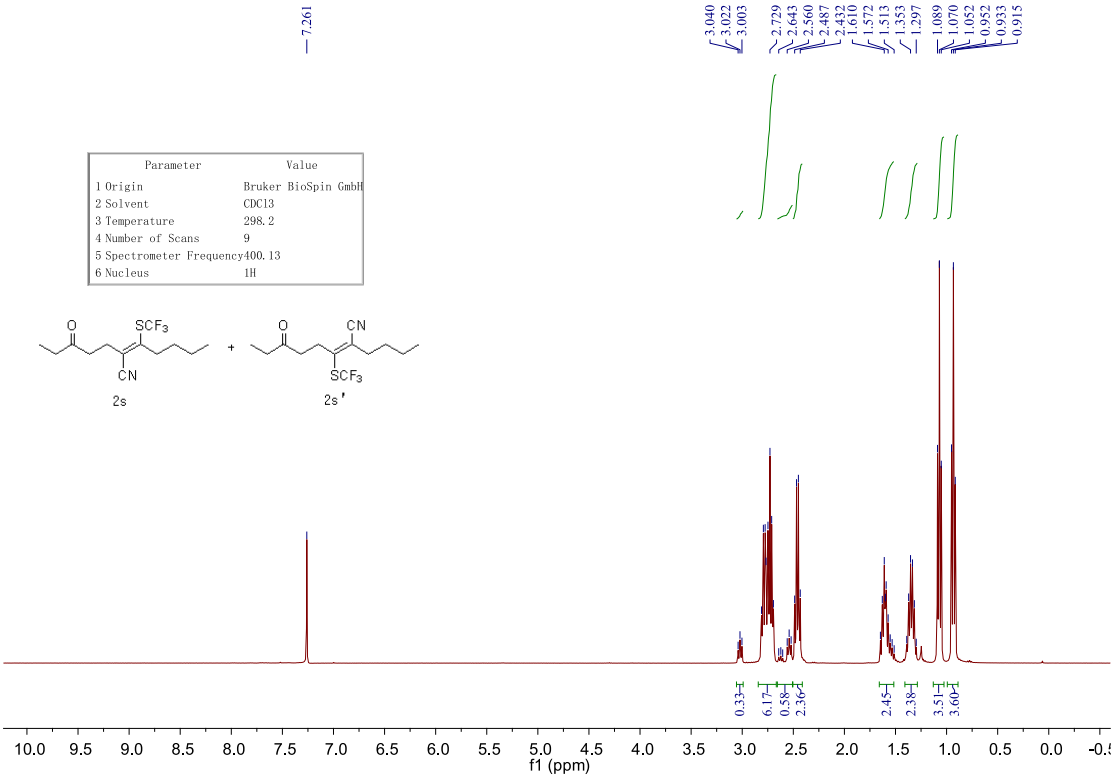

-38.044
-38.246
Parameter Value
1 Origin Bruker BioSpin GmbH
2 Solvent CDCl3
3 Temperature 298.2
4 Number of Scans 4
5 Spectrometer Frequency 376.44
6 Nucleus 19F
SCF3
CN
2q
2q'
2.46
1.00
f1 (ppm)

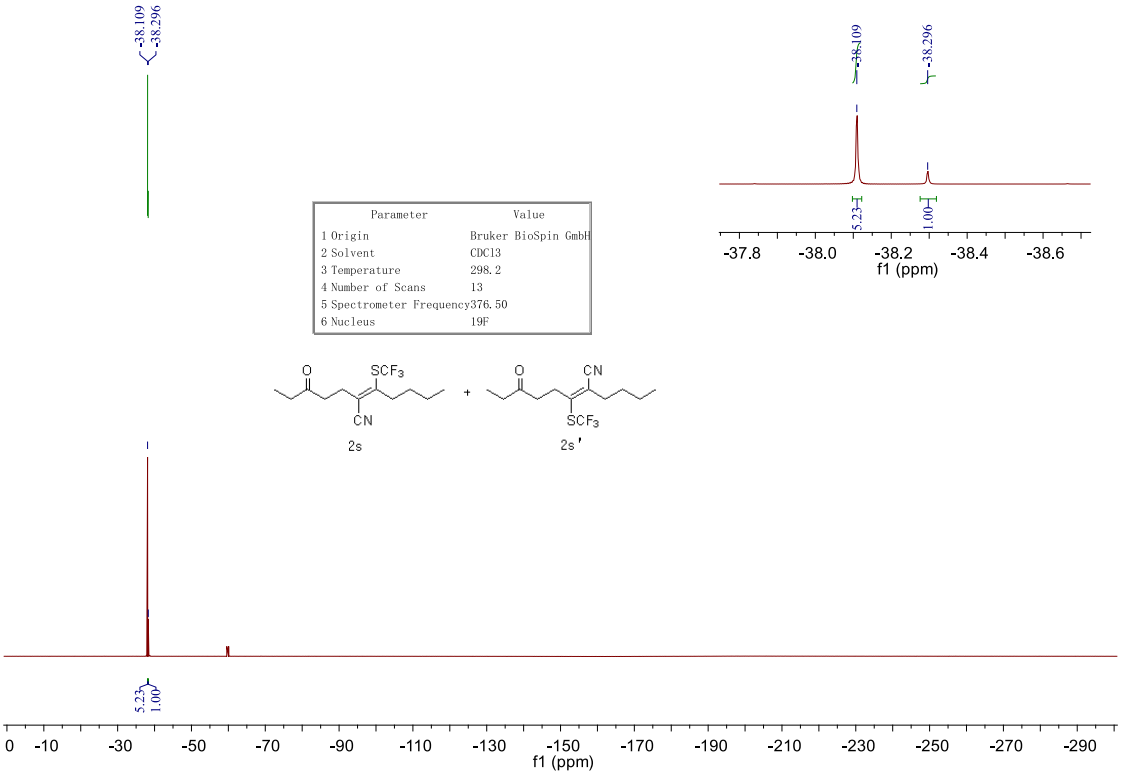

190.063
190.035
148.173
148.160
143.611
132.096
128.239
126.876
123.875
121.135
116.247
77.000
37.851
37.842
36.934
36.415
30.285
27.277
21.887
21.864
13.648
Parameter Value
1 Origin Bruker BioSpin GmbH
2 Solvent CDCl3
3 Temperature 298.2
4 Number of Scans 1024
5 Spectrometer Frequency 100.61
6 Nucleus 13C
O
SCF3
CN
S
2q
2q'
f1 (ppm)

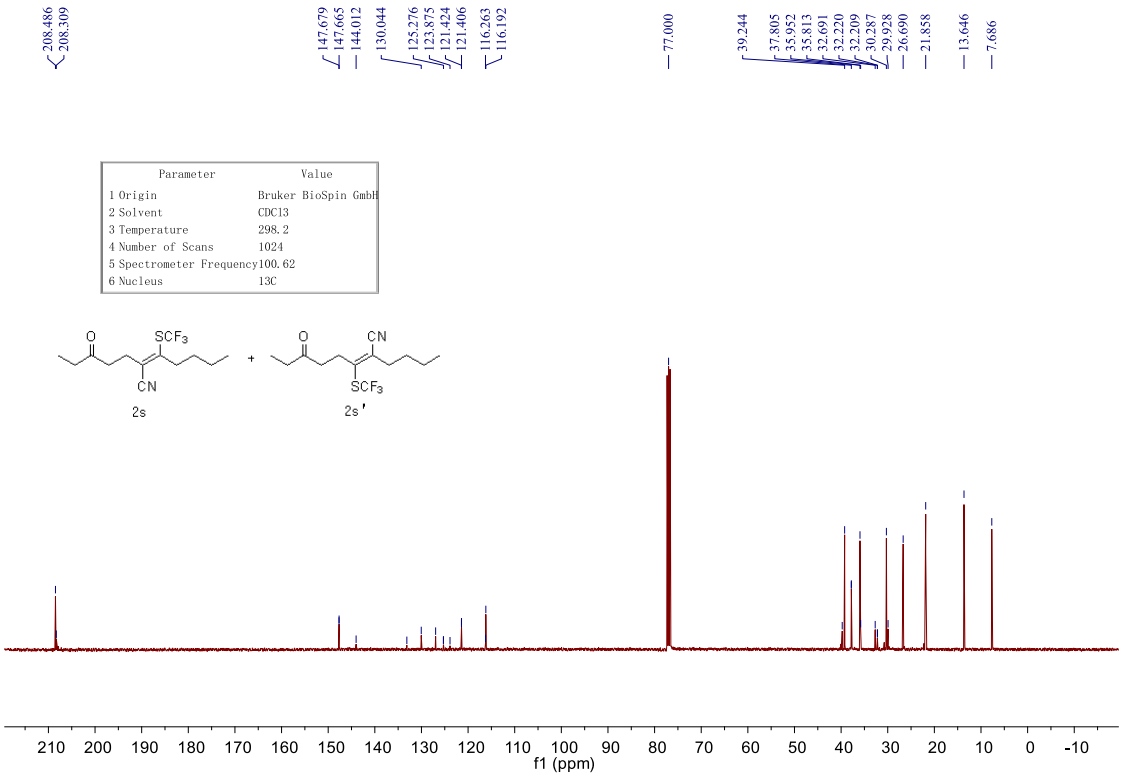

7.261
3.020
3.002
2.984
2.731
2.379
2.344
1.661
1.610
1.560
1.313
1.232
0.954
0.936
0.917
Parameter Value
1 Origin Bruker BioSpin GmbH
2 Solvent CDCl3
3 Temperature 298.2
4 Number of Scans 4
5 Spectrometer Frequency 400.13
6 Nucleus 1H
O
SCF3
CN
2r
2r'
0.33
6.20
0.36
1.14
4.73
4.63
9.37
3.50
f1 (ppm)

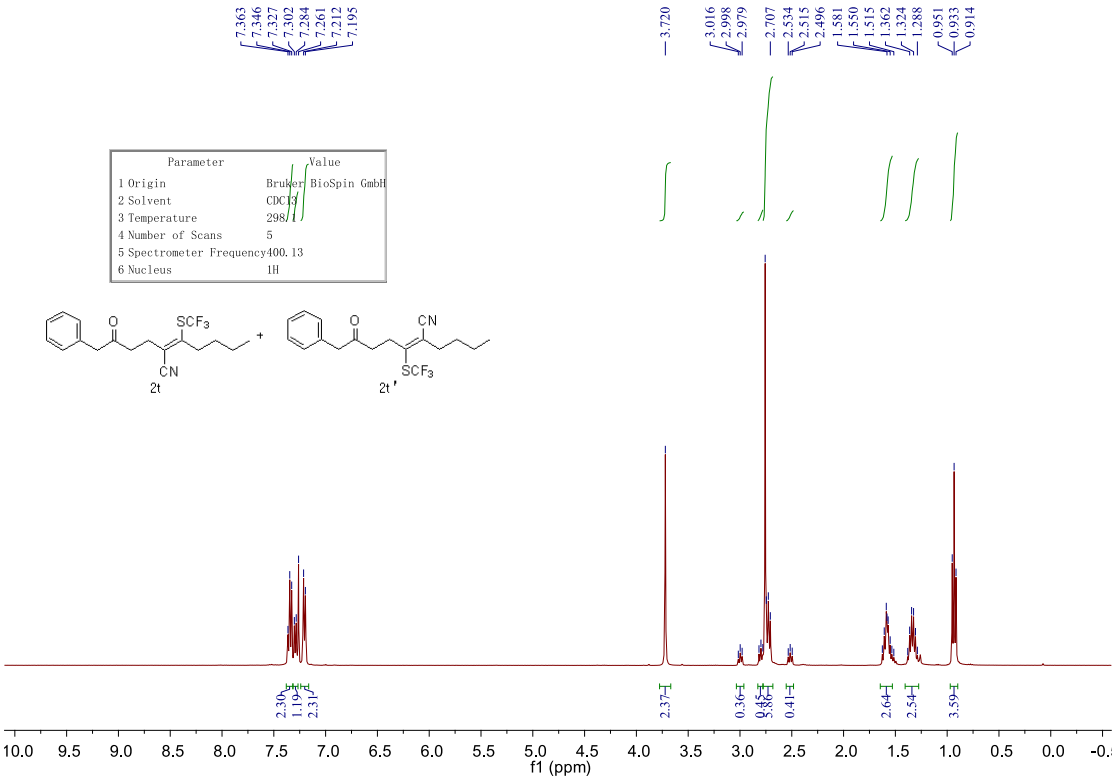

-38.113
-38.286
Parameter Value
1 Origin Bruker BioSpin GmbH
2 Solvent CDCl3
3 Temperature 298.2
4 Number of Scans 8
5 Spectrometer Frequency 376.44
6 Nucleus 19F
5.82
1.00
f1 (ppm)
2r
2r'

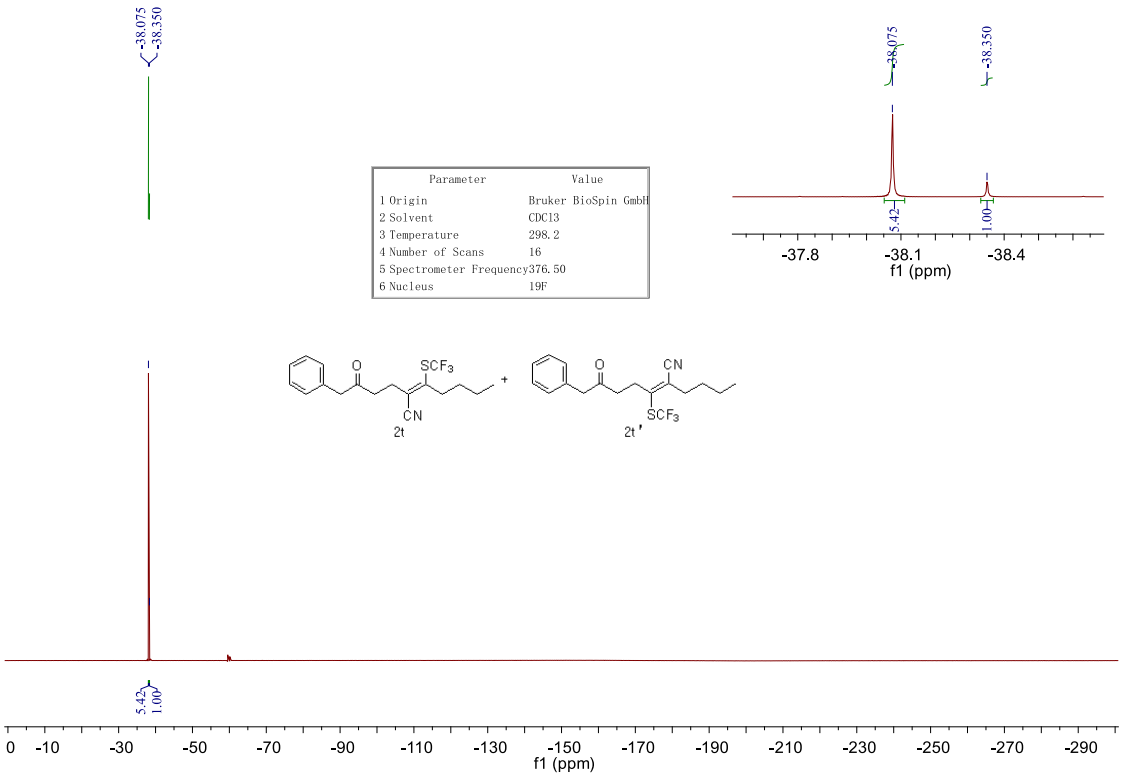

211.207
210.950
147.640
147.626
144.265
125.084
123.916
121.564
121.547
121.530
116.307
116.230
77.000
50.733
37.777
37.766
37.604
32.182
28.410
25.529
21.854
21.821
13.642
Parameter Value
1 Origin Bruker BioSpin GmbH
2 Solvent CDCl3
3 Temperature 298.2
4 Number of Scans 1024
5 Spectrometer Frequency 100.61
6 Nucleus 13C
2r
2r'

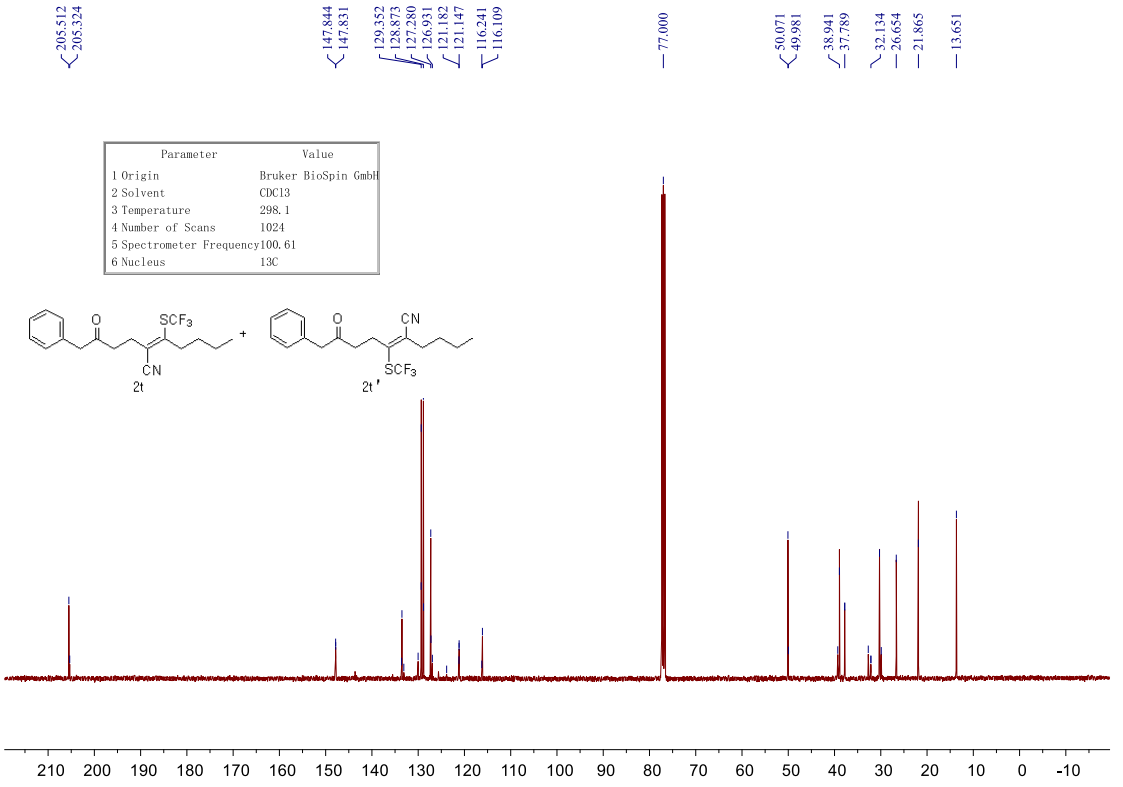

7.261
3.040
3.022
3.003
2.729
2.643
2.560
2.487
2.432
2.410
1.572
1.513
1.353
1.297
1.089
1.070
1.052
0.952
0.933
0.915
Parameter Value
1 Origin Bruker BioSpin GmbH
2 Solvent CDCl3
3 Temperature 298.2
4 Number of Scans 9
5 Spectrometer Frequency 400.13
6 Nucleus 1H
SCF3
CN
2s
2s'
0.33
6.17
0.58
2.36
2.45
2.38
3.51
3.60
f1 (ppm)

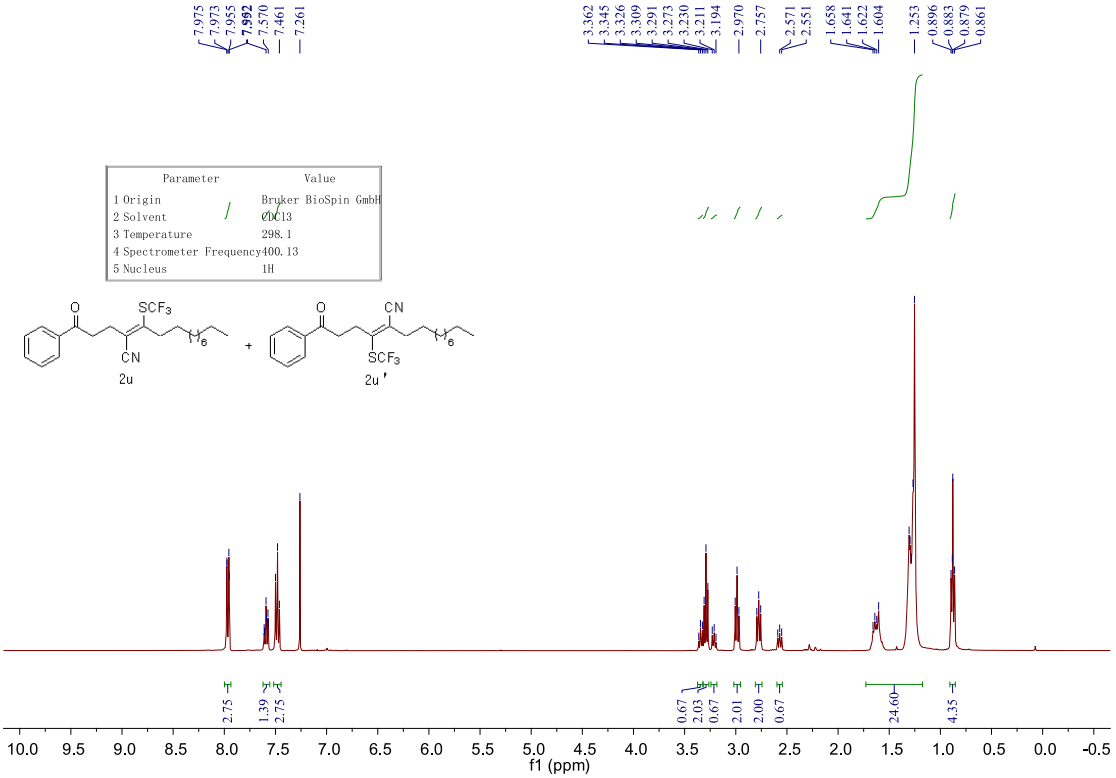

-38.109
-38.296
Parameter Value
1 Origin Bruker BioSpin GmbH
2 Solvent CDCl3
3 Temperature 298.2
4 Number of Scans 13
5 Spectrometer Frequency 376.50
6 Nucleus 19F
SCF3
CN
2s
2s'
5.23
1.00
f1 (ppm)

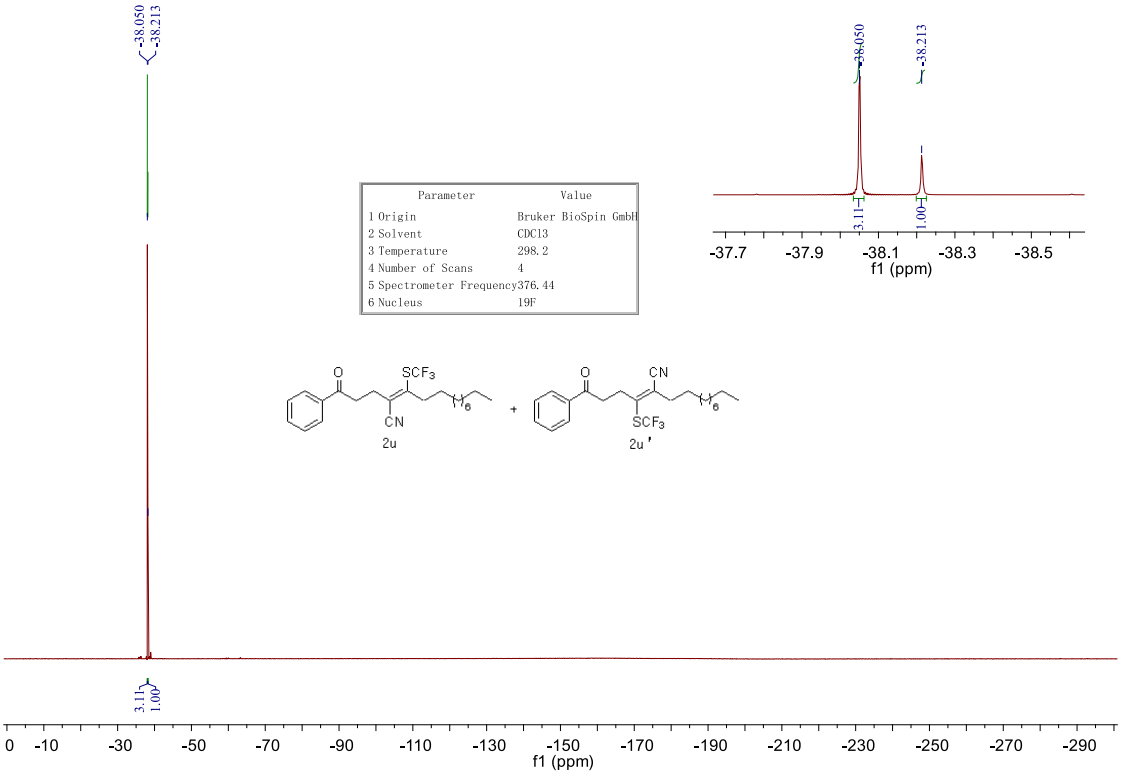

208.486
208.309
147.679
147.665
144.012
130.044
125.276
123.875
121.424
121.406
116.263
116.192
77.000
39.244
37.805
35.952
35.813
32.691
32.220
32.209
30.287
29.928
26.690
21.858
13.646
7.686
Parameter Value
1 Origin Bruker BioSpin GmbH
2 Solvent CDCl3
3 Temperature 298.2
4 Number of Scans 1024
5 Spectrometer Frequency 100.62
6 Nucleus 13C
O
SCF3
CN
2s
+
O
CN
SCF3
2s'
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)

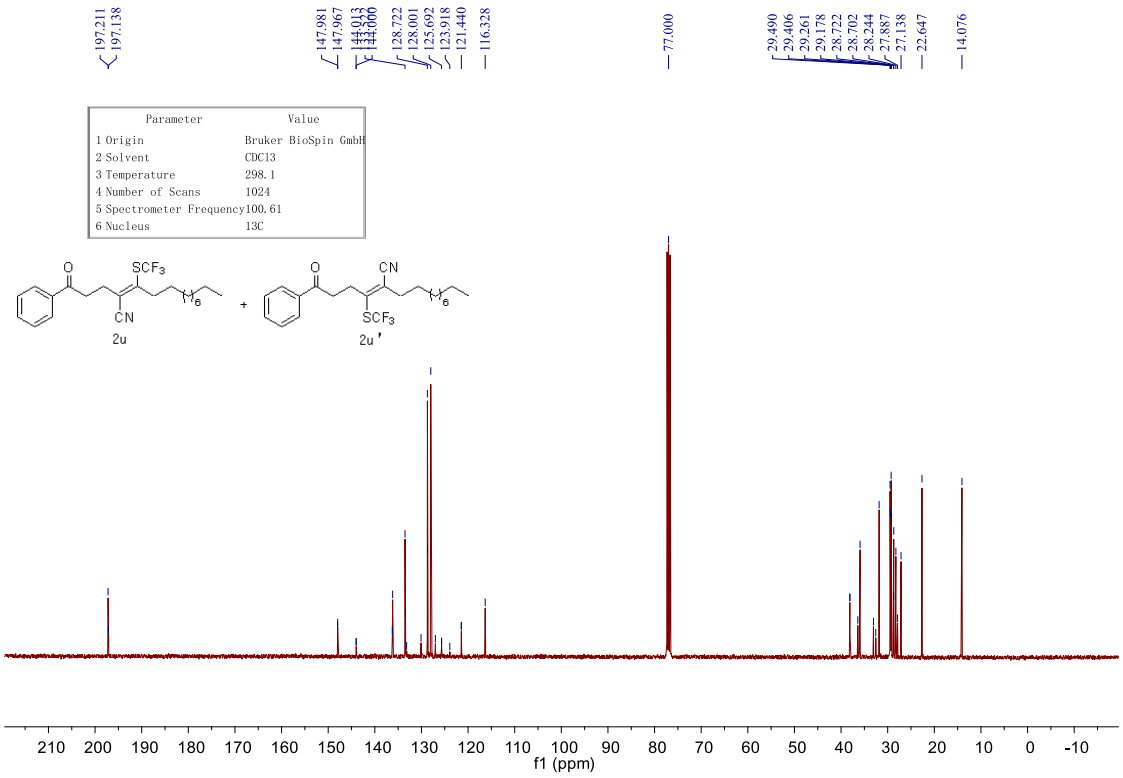

7.363
7.346
7.327
7.302
7.284
7.261
7.212
7.195
3.720
3.016
2.998
2.979
2.707
2.534
2.515
2.496
1.581
1.550
1.515
1.362
1.324
1.288
0.951
0.933
0.914
Parameter Value
1 Origin Bruker BioSpin GmbH
2 Solvent CDCl3
3 Temperature 298.1
4 Number of Scans 5
5 Spectrometer Frequency 400.13
6 Nucleus 1H
O
SCF3
CN
2t
+
O
CN
SCF3
2t'
2.30
1.19
2.31
2.37
0.36
0.45
0.86
0.41
2.64
2.54
3.59
10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)

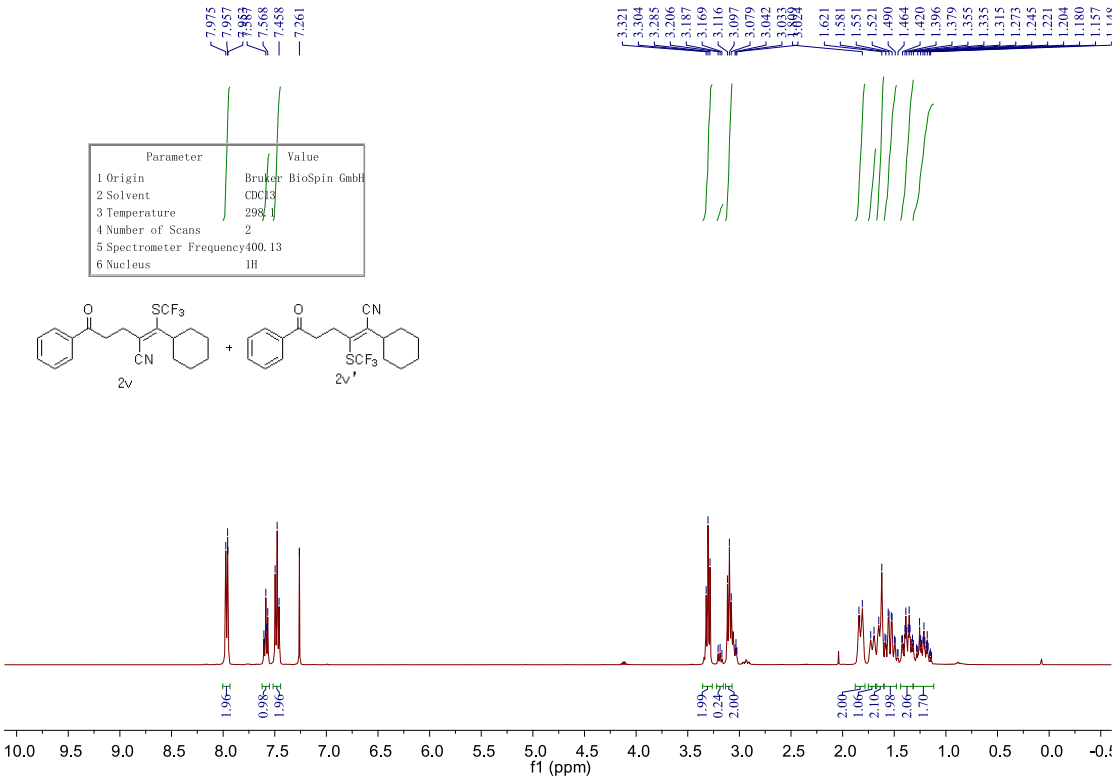

-38.075
-38.350
Parameter Value
1 Origin Bruker BioSpin GmbH
2 Solvent CDCl3
3 Temperature 298.2
4 Number of Scans 16
5 Spectrometer Frequency 376.50
6 Nucleus 19F
5.42
1.00
f1 (ppm)
2t
2t'
f1 (ppm)

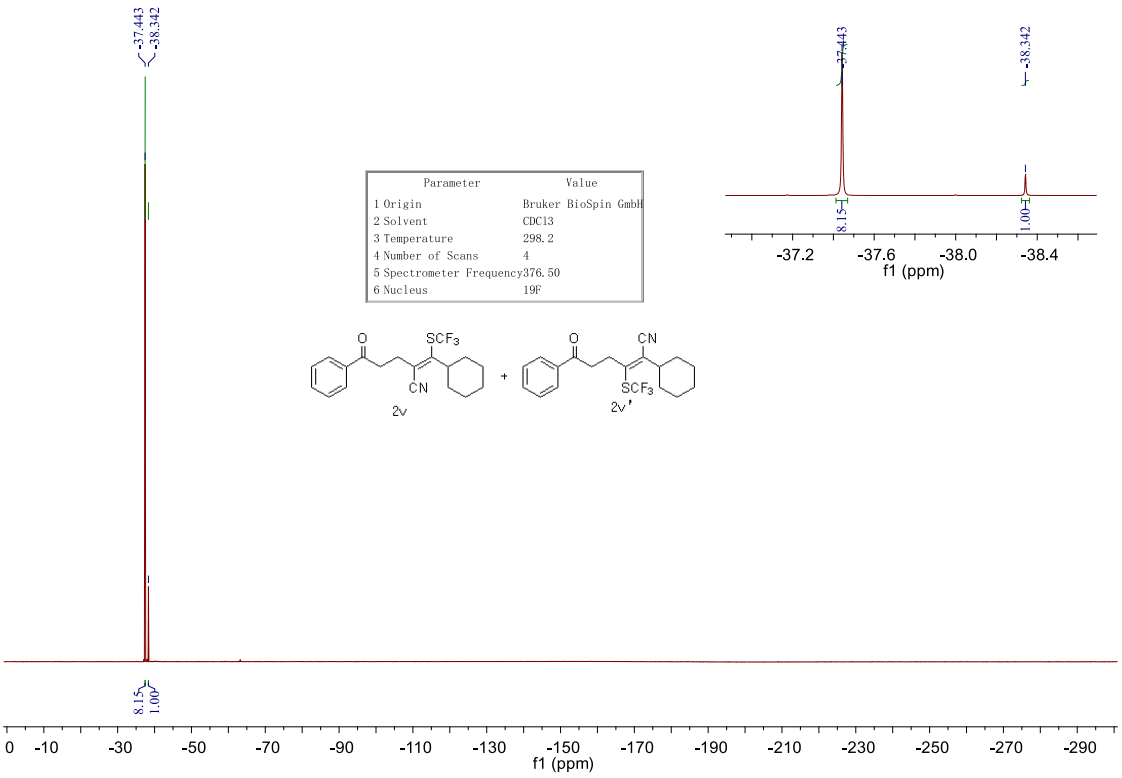

205.512
205.324
147.844
147.831
129.352
128.873
127.280
126.931
121.182
121.147
116.241
116.109
77.000
50.071
49.981
38.941
37.789
32.134
26.654
21.865
13.651
Parameter Value
1 Origin Bruker BioSpin GmbH
2 Solvent CDCl3
3 Temperature 298.1
4 Number of Scans 1024
5 Spectrometer Frequency 100.61
6 Nucleus 13C
2t
2t'

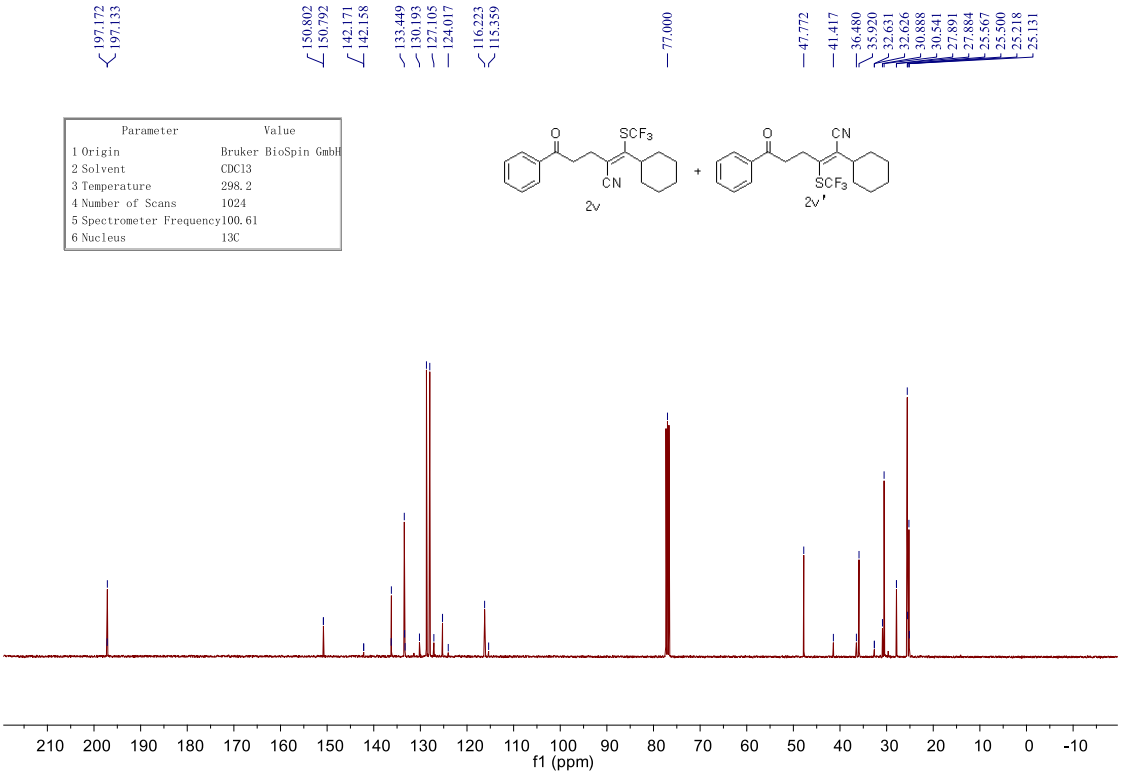

7.975
7.973
7.955
7.592
7.570
7.461
7.261
3.362
3.345
3.326
3.309
3.291
3.273
3.230
3.211
3.194
2.970
2.757
2.571
2.551
1.658
1.641
1.622
1.604
1.253
0.896
0.883
0.879
0.861
Parameter Value
1 Origin Bruker BioSpin GmbH
2 Solvent CDCl3
3 Temperature 298.1
4 Spectrometer Frequency 400.13
5 Nucleus 1H
SCF3
CN
6
2u
2u'
2.75
1.39
2.75
0.67
2.03
0.67
2.01
2.00
0.67
24.60
4.35
f1 (ppm)

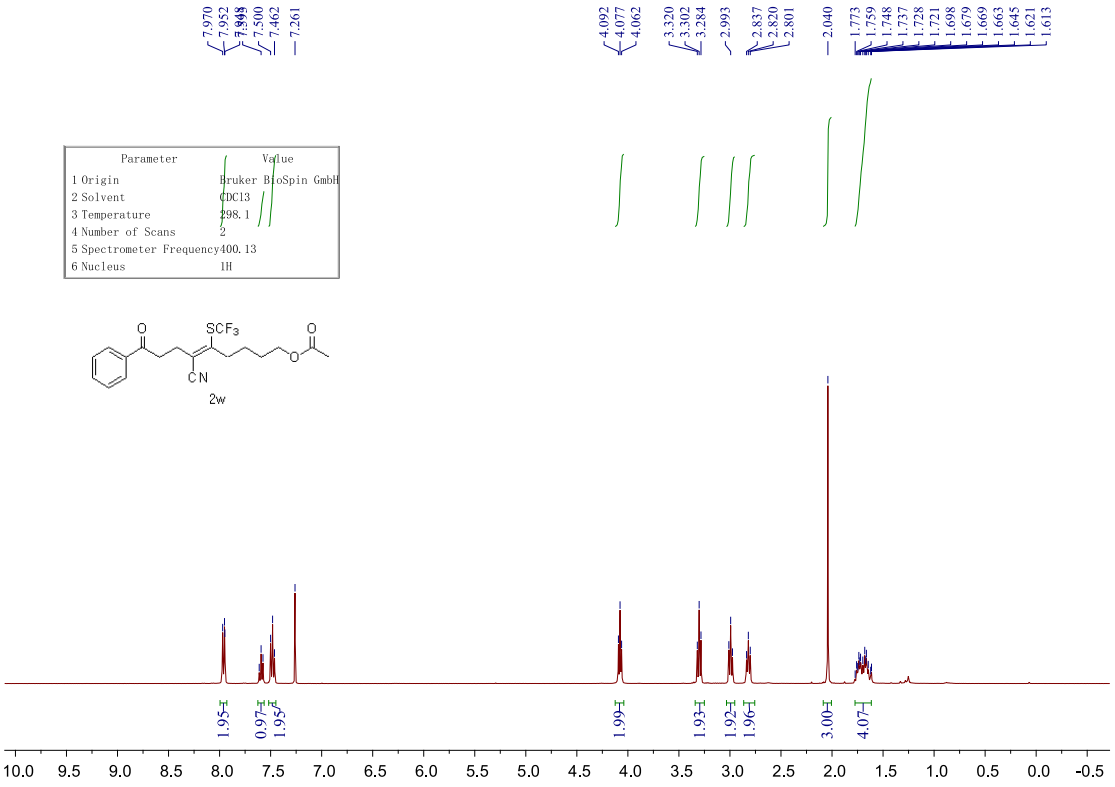

-38.050
-38.213
Parameter Value
1 Origin Bruker BioSpin GmbH
2 Solvent CDCl3
3 Temperature 298.2
4 Number of Scans 4
5 Spectrometer Frequency 376.44
6 Nucleus 19F
SCF3
CN
6
2u
2u'
3.11
1.00
f1 (ppm)

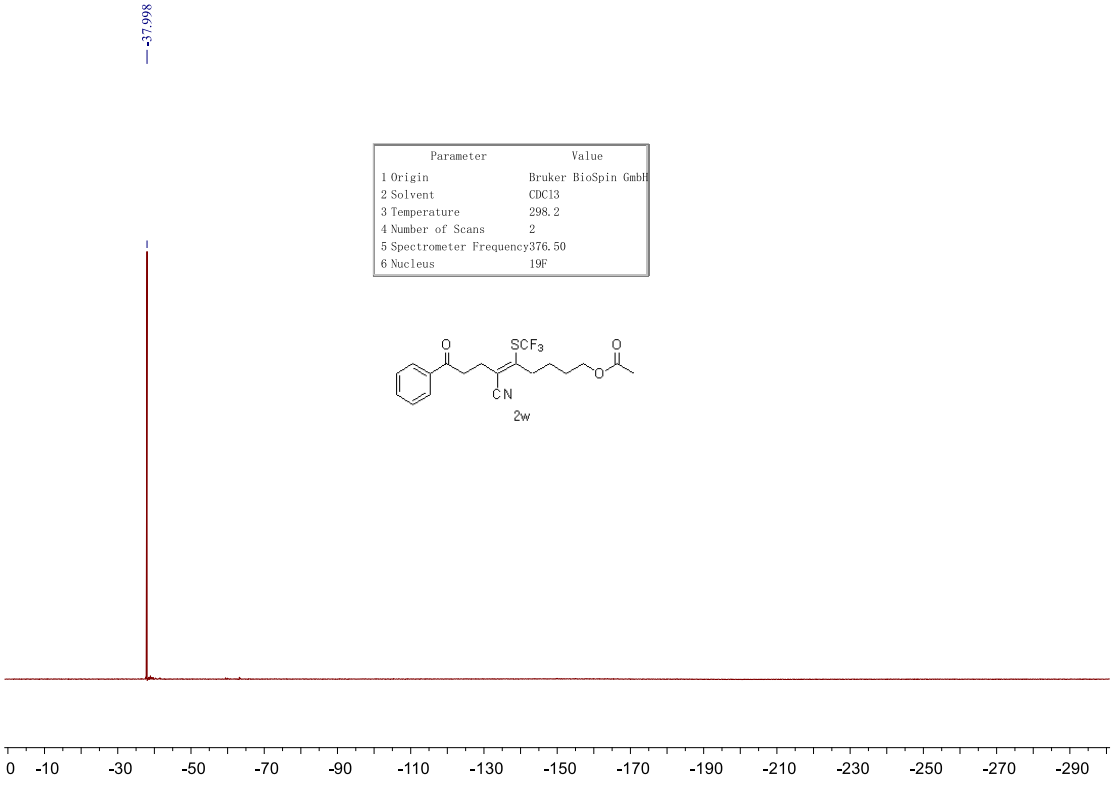

197.211
197.138
147.981
147.967
128.722
128.001
125.692
123.918
121.440
116.328
77.000
29.490
29.406
29.261
29.178
28.722
28.702
28.244
27.887
27.138
22.647
14.076
Parameter Value
1 Origin Bruker BioSpin GmbH
2 Solvent CDCl3
3 Temperature 298.1
4 Number of Scans 1024
5 Spectrometer Frequency 100.61
6 Nucleus 13C
O
SCF3
CN
6
2u
+
O
CN
SCF3
6
2u'
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)

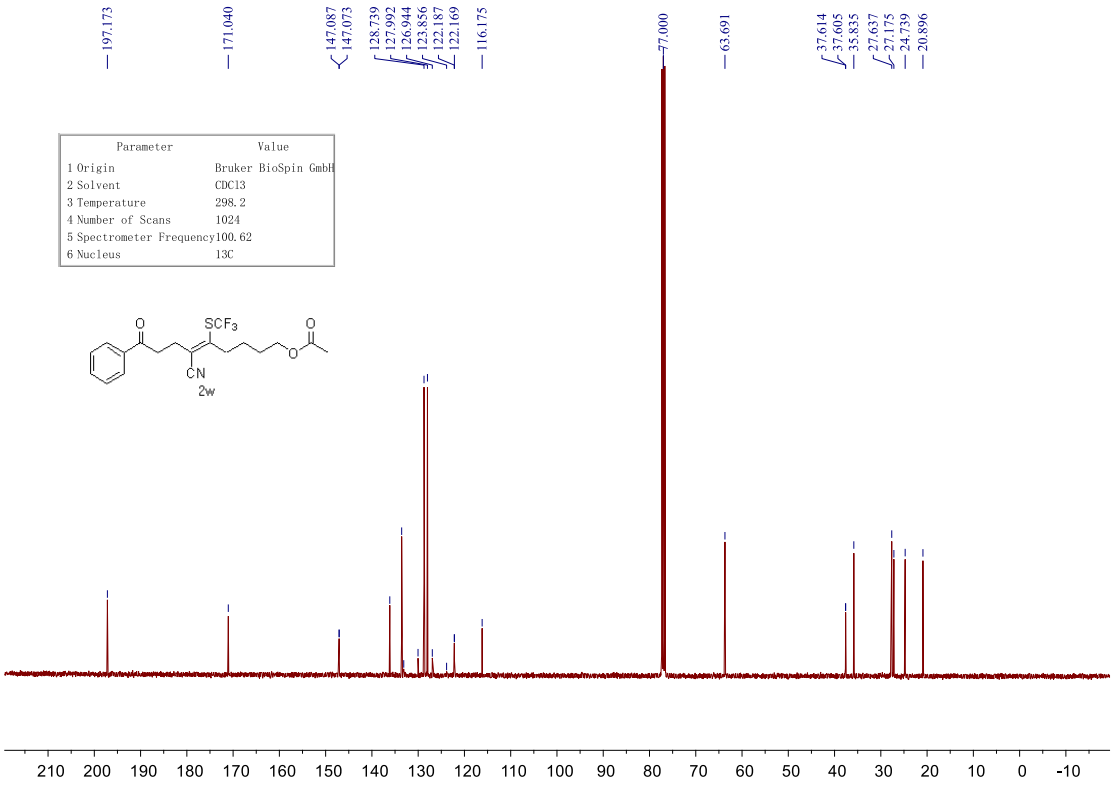

7.975
7.957
7.568
7.458
7.261
3.321
3.304
3.285
3.206
3.187
3.169
3.116
3.097
3.079
3.042
3.033
1.621
1.581
1.551
1.521
1.490
1.464
1.420
1.396
1.379
1.355
1.335
1.315
1.273
1.245
1.221
1.204
1.180
1.157
Parameter Value
1 Origin Bruker BioSpin GmbH
2 Solvent CDCl3
3 Temperature 298.1
4 Number of Scans 2
5 Spectrometer Frequency 400.13
6 Nucleus 1H
O
SCF3
CN
2v
+
O
CN
SCF3
2v'
1.96
0.98
1.96
1.99
0.24
2.00
2.00
1.06
2.10
1.98
2.06
1.70
10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)

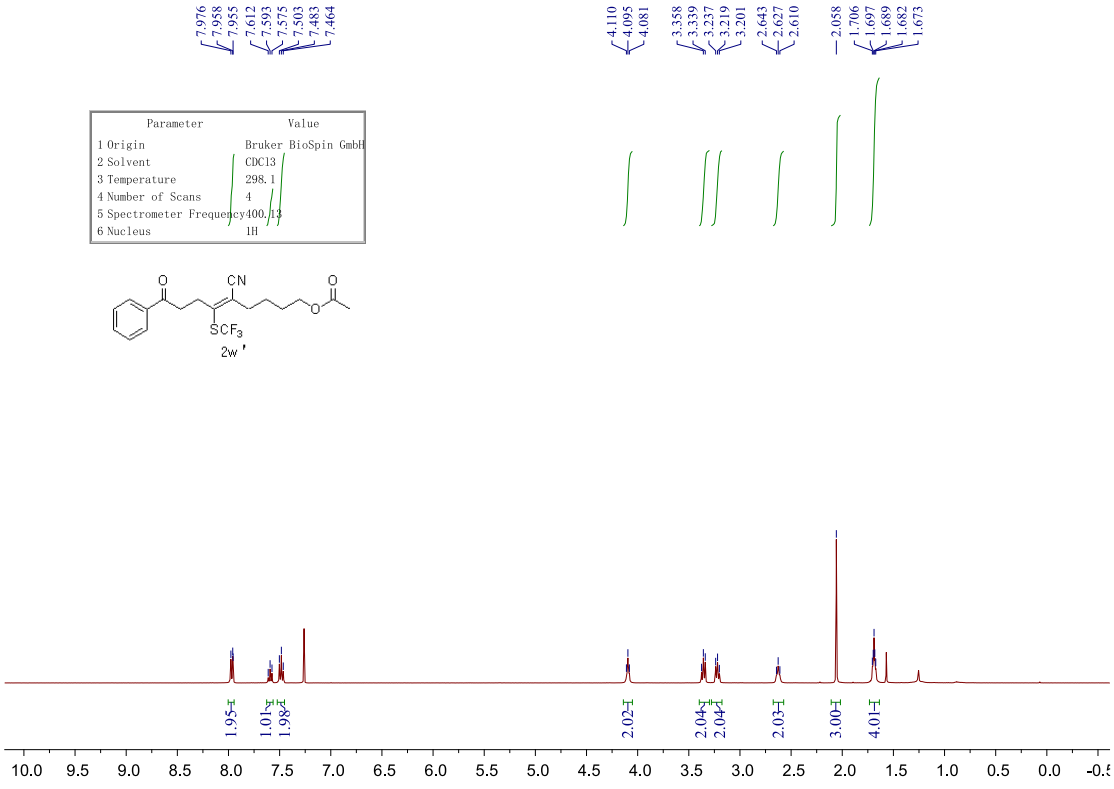

-37.443
-38.342
Parameter Value
1 Origin Bruker BioSpin GmbH
2 Solvent CDCl3
3 Temperature 298.2
4 Number of Scans 4
5 Spectrometer Frequency 376.50
6 Nucleus 19F
8.15
1.00
f1 (ppm)
2v
2v'

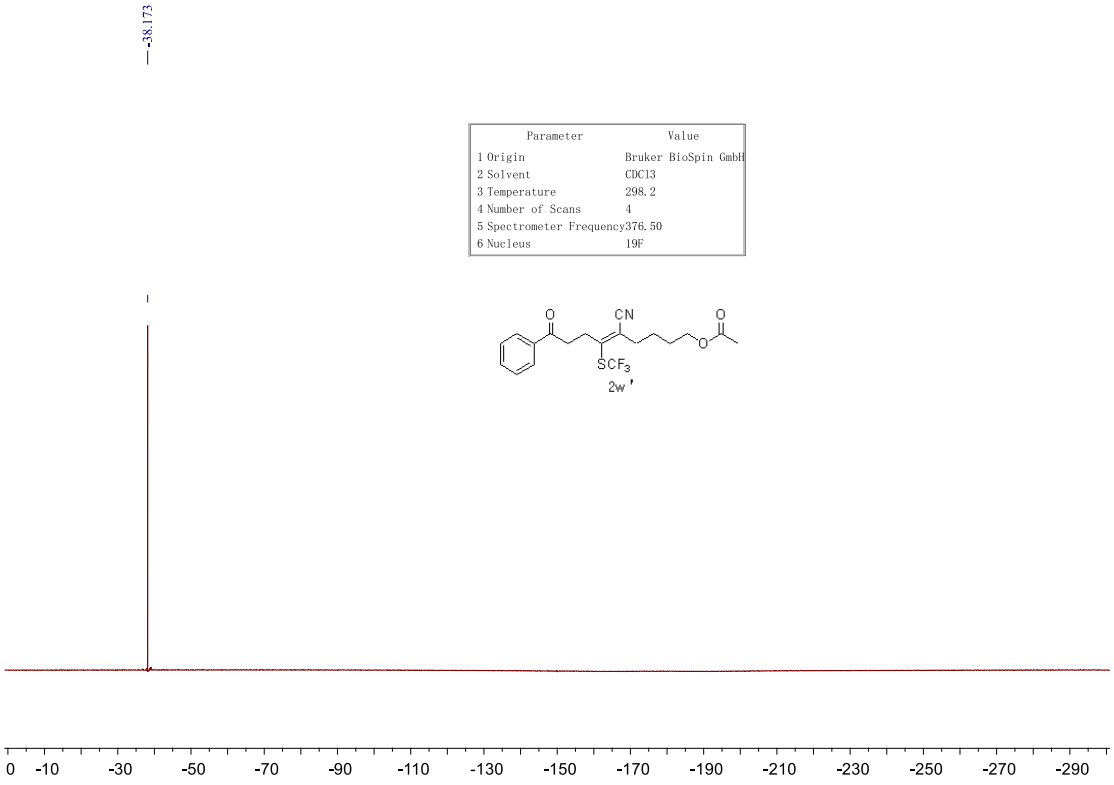

197.172
197.133
150.802
150.792
142.171
142.158
133.449
130.193
127.105
124.017
116.223
115.359
77.000
47.772
41.417
36.480
35.920
32.631
32.626
30.888
30.541
27.891
27.884
25.567
25.500
25.218
25.131
Parameter Value
1 Origin Bruker BioSpin GmbH
2 Solvent CDCl3
3 Temperature 298.2
4 Number of Scans 1024
5 Spectrometer Frequency 100.61
6 Nucleus 13C
f1 (ppm)
2v
2v'

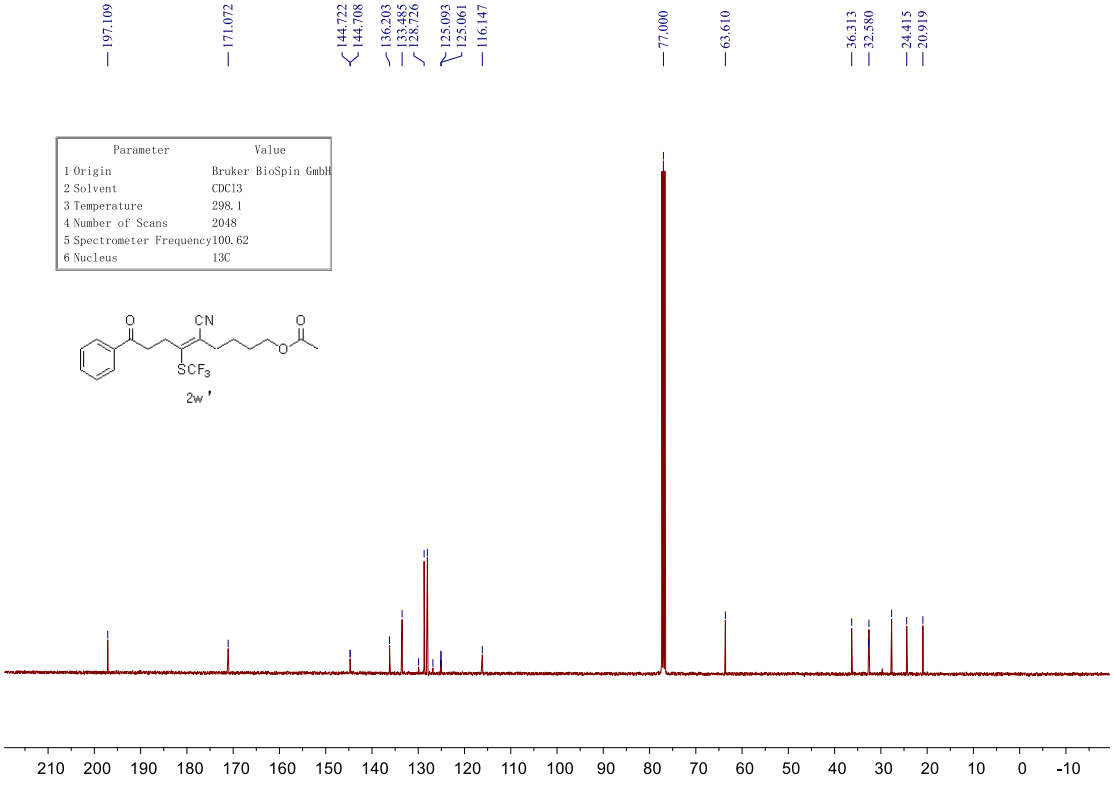

7.970
7.952
7.500
7.462
7.261
4.092
4.077
4.062
3.320
3.302
3.284
2.993
2.837
2.820
2.801
2.040
1.773
1.759
1.748
1.737
1.728
1.721
1.698
1.679
1.669
1.663
1.645
1.621
1.613
Parameter Value
1 Origin Bruker BioSpin GmbH
2 Solvent CDCl3
3 Temperature 298.1
4 Number of Scans 2
5 Spectrometer Frequency 400.13
6 Nucleus 1H
SCF3
O
O
O
CN
2w
1.95
0.97
1.95
1.99
1.93
1.92
1.96
3.00
4.07
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

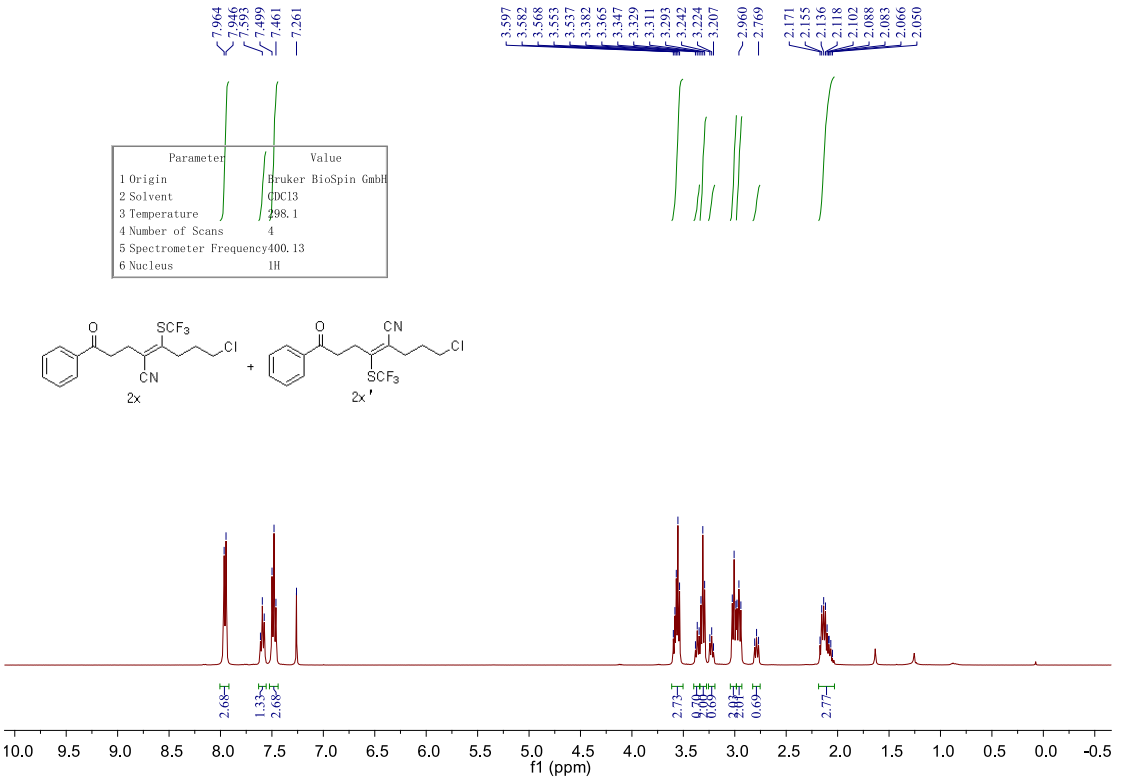

-37.998
Parameter Value
1 Origin Bruker BioSpin GmbH
2 Solvent CDCl3
3 Temperature 298.2
4 Number of Scans 2
5 Spectrometer Frequency 376.50
6 Nucleus 19F
SCF3
O
O
O
CN
2w
0 -10 -30 -50 -70 -90 -110 -130 -150 -170 -190 -210 -230 -250 -270 -290

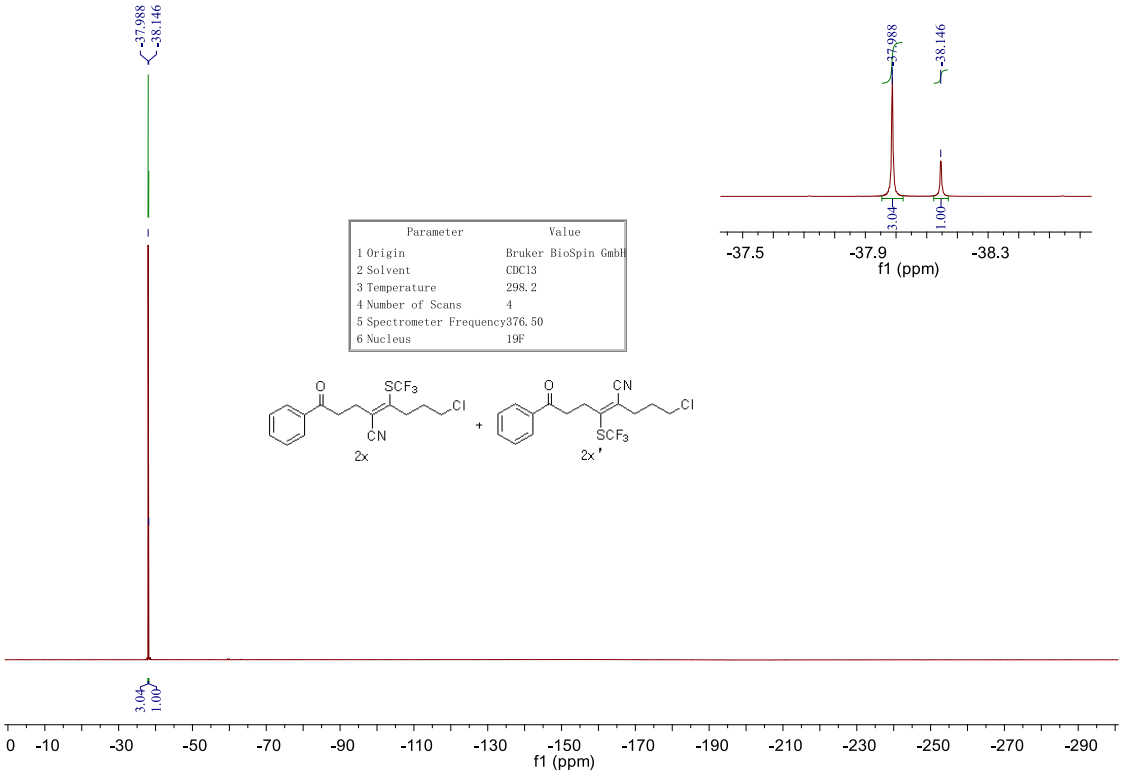

197.173
171.040
147.087
147.073
128.739
127.992
126.944
123.856
122.187
122.169
116.175
77.000
63.691
37.614
37.605
35.835
27.637
27.175
24.739
20.896
Parameter Value
1 Origin Bruker BioSpin GmbH
2 Solvent CDCl3
3 Temperature 298.2
4 Number of Scans 1024
5 Spectrometer Frequency 100.62
6 Nucleus 13C
SCF3
CN
2w

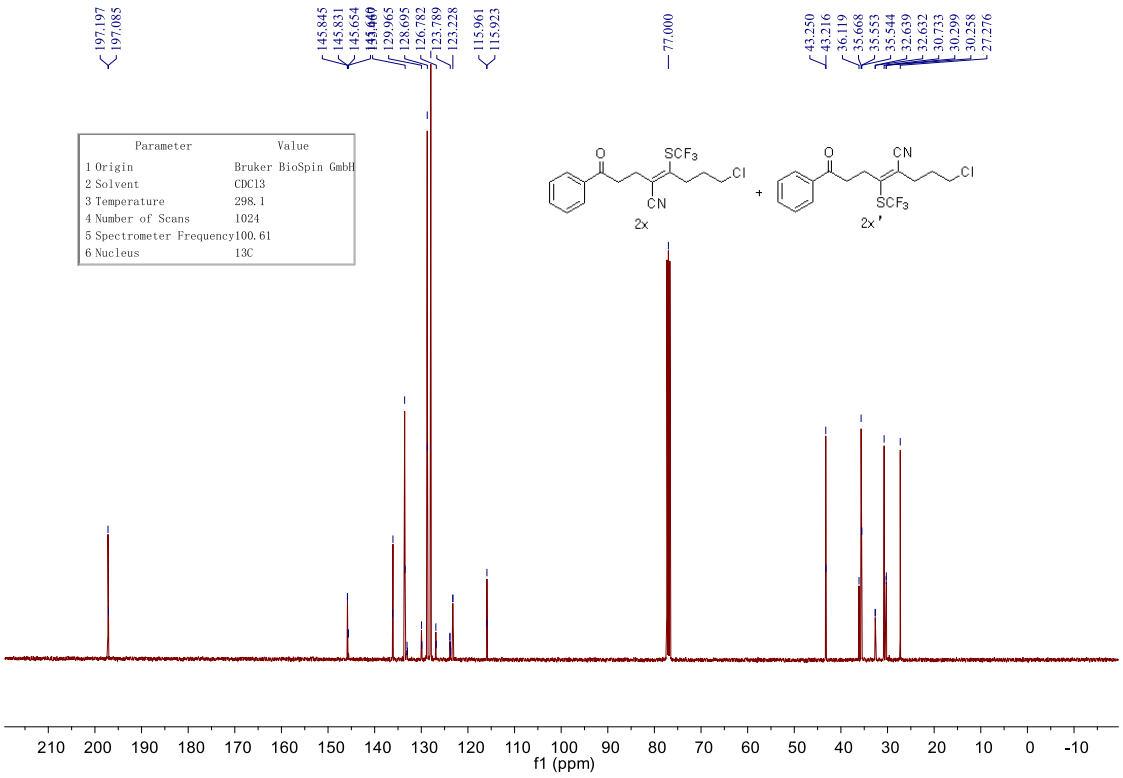

7.976
7.958
7.955
7.612
7.593
7.575
7.503
7.483
7.464
4.110
4.095
4.081
3.358
3.339
3.237
3.219
3.201
2.643
2.627
2.610
2.058
1.706
1.697
1.689
1.682
1.673
Parameter Value
1 Origin Bruker BioSpin GmbH
2 Solvent CDCl3
3 Temperature 298.1
4 Number of Scans 4
5 Spectrometer Frequency 400.13
6 Nucleus 1H
CN
SCF3
2w'
1.95
1.01
1.98
2.02
2.04
2.04
2.03
3.00
4.01

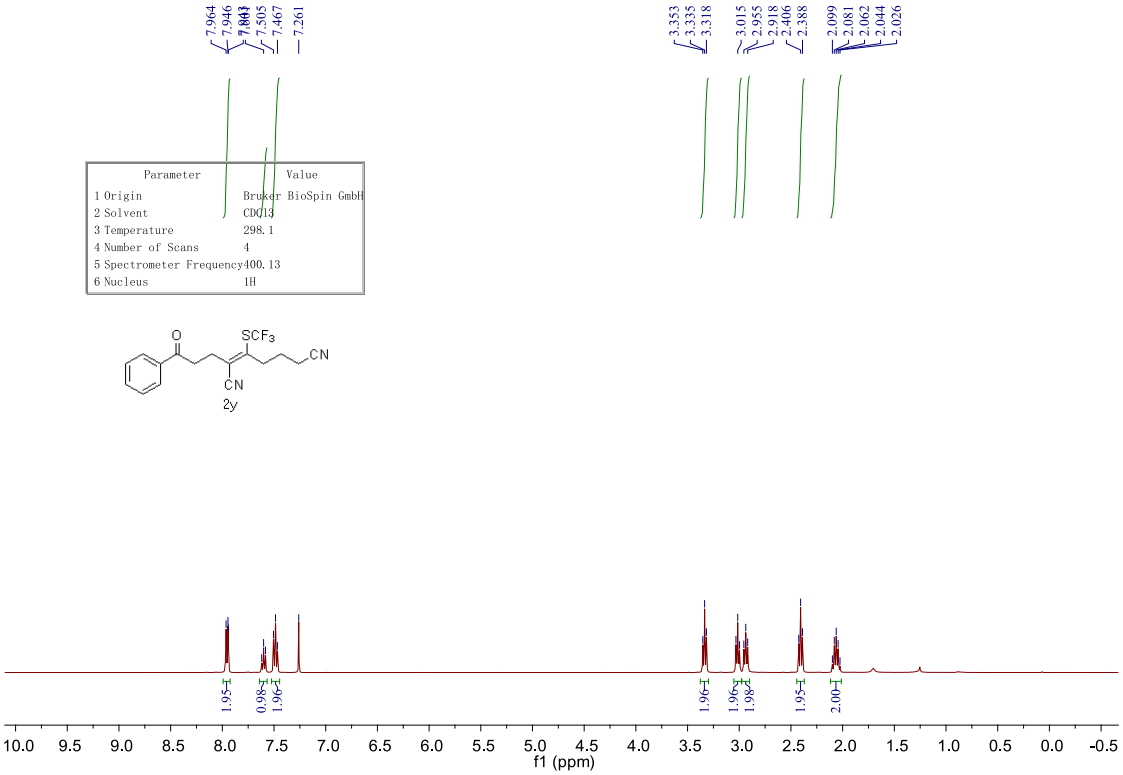

-38.173
Parameter Value
1 Origin Bruker BioSpin GmbH
2 Solvent CDCl3
3 Temperature 298.2
4 Number of Scans 4
5 Spectrometer Frequency 376.50
6 Nucleus 19F
O
CN
O
O
SCF3
2w'
0 -10 -30 -50 -70 -90 -110 -130 -150 -170 -190 -210 -230 -250 -270 -290

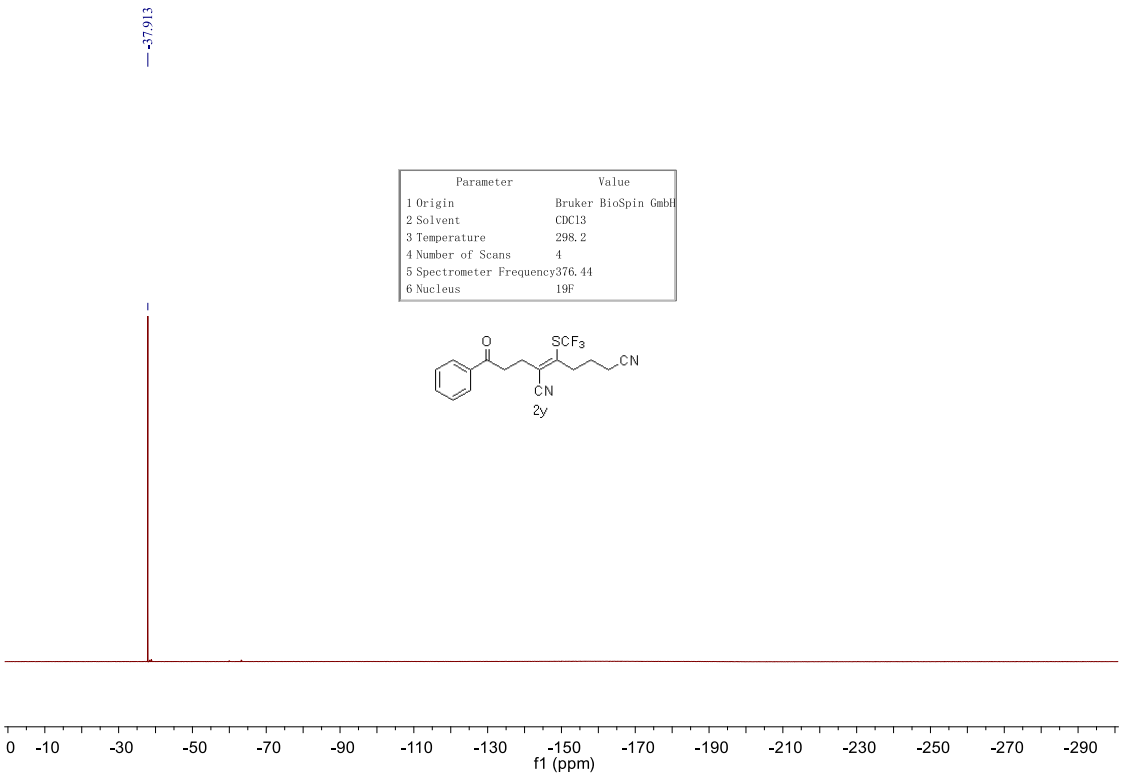

197.109
171.072
144.722
144.708
136.203
133.485
128.726
125.093
125.061
116.147
77.000
63.610
36.313
32.580
24.415
20.919
Parameter Value
1 Origin Bruker BioSpin GmbH
2 Solvent CDCl3
3 Temperature 298.1
4 Number of Scans 2048
5 Spectrometer Frequency 100.62
6 Nucleus 13C
O
CN
O
O
SCF3
2w'
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10

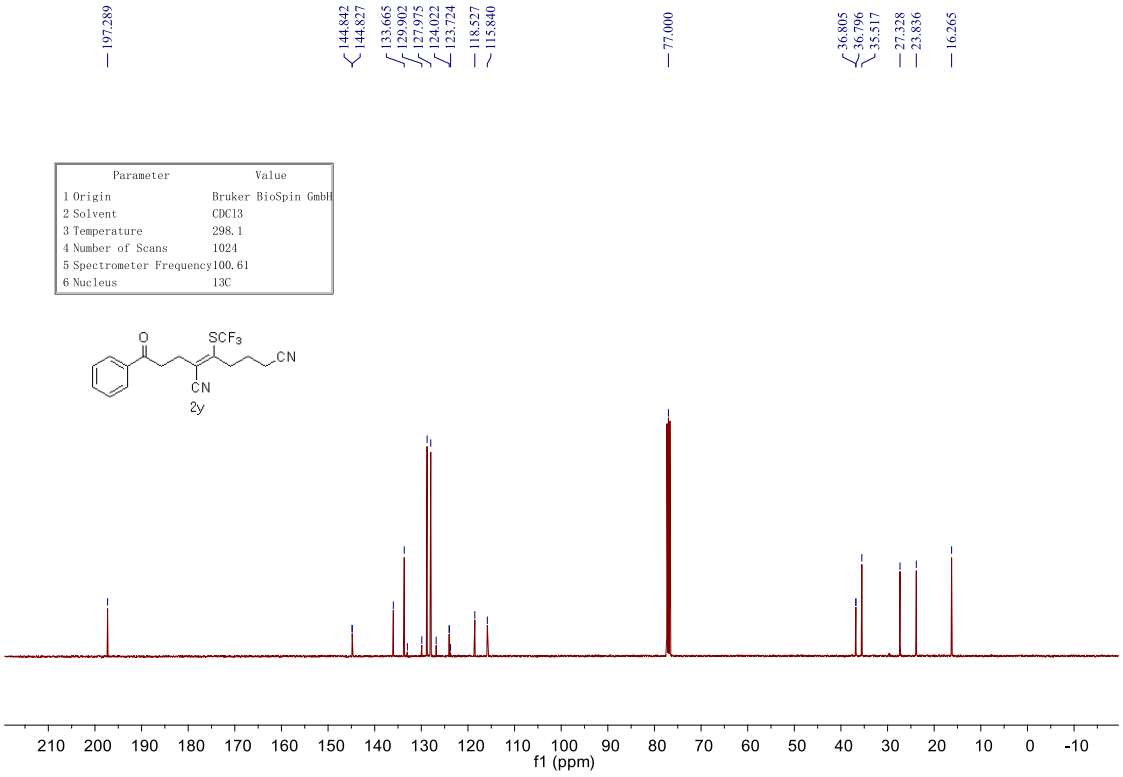

7.964
7.946
7.593
7.499
7.461
7.261
3.597
3.582
3.568
3.553
3.537
3.382
3.365
3.347
3.329
3.311
3.293
3.242
3.224
3.207
2.960
2.769
2.171
2.155
2.136
2.118
2.102
2.088
2.083
2.066
2.050
Parameter Value
1 Origin Bruker BioSpin GmbH
2 Solvent CDCl3
3 Temperature 298.1
4 Number of Scans 4
5 Spectrometer Frequency 400.13
6 Nucleus 1H
SCF3
Cl
CN
2x
CN
Cl
SCF3
2x'
2.68
1.33
2.68
2.73
0.69
2.77
f1 (ppm)

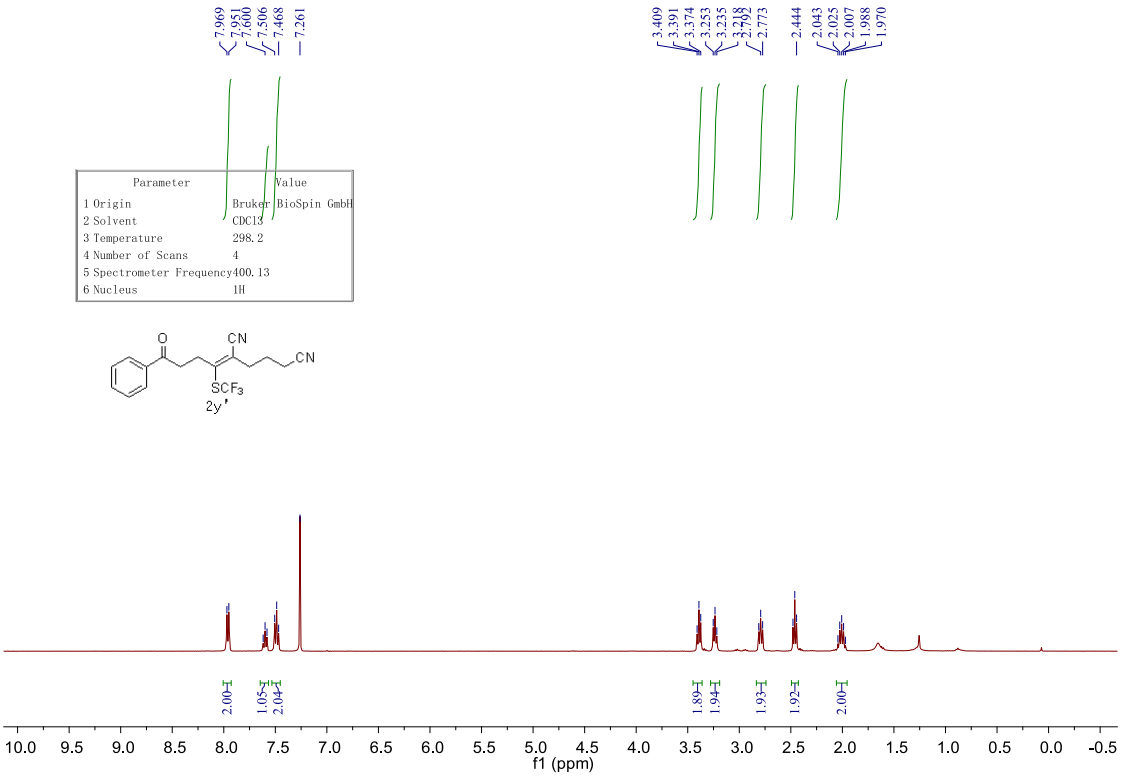

-37.988
-38.146
Parameter Value
1 Origin Bruker BioSpin GmbH
2 Solvent CDCl3
3 Temperature 298.2
4 Number of Scans 4
5 Spectrometer Frequency 376.50
6 Nucleus 19F
SCF3
Cl
CN
2x
CN
Cl
SCF3
2x'
3.04
1.00
f1 (ppm)

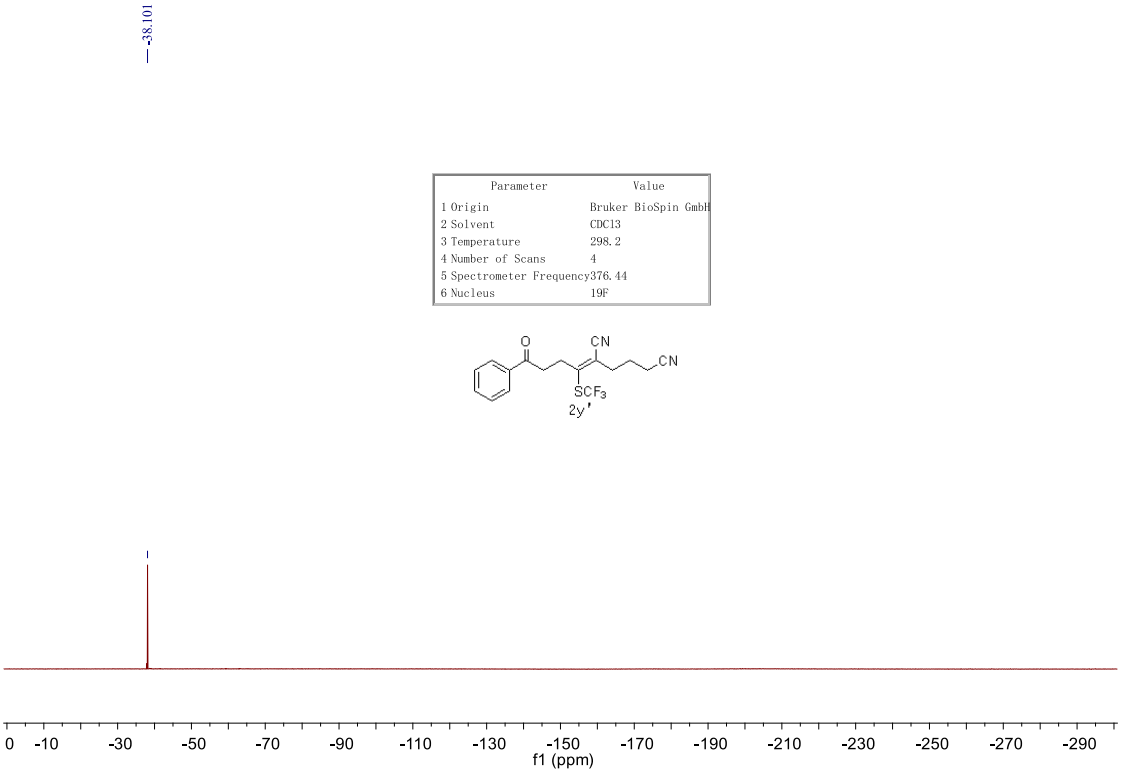

197.197
197.085
145.845
145.831
145.654
129.965
128.695
126.782
123.789
123.228
115.961
115.923
77.000
43.250
43.216
36.119
35.668
35.553
35.544
32.639
32.632
30.733
30.299
30.258
27.276
Parameter Value
1 Origin Bruker BioSpin GmbH
2 Solvent CDCl3
3 Temperature 298.1
4 Number of Scans 1024
5 Spectrometer Frequency 100.61
6 Nucleus 13C
O
SCF3
Cl
CN
2x
+
O
CN
Cl
SCF3
2x'
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)

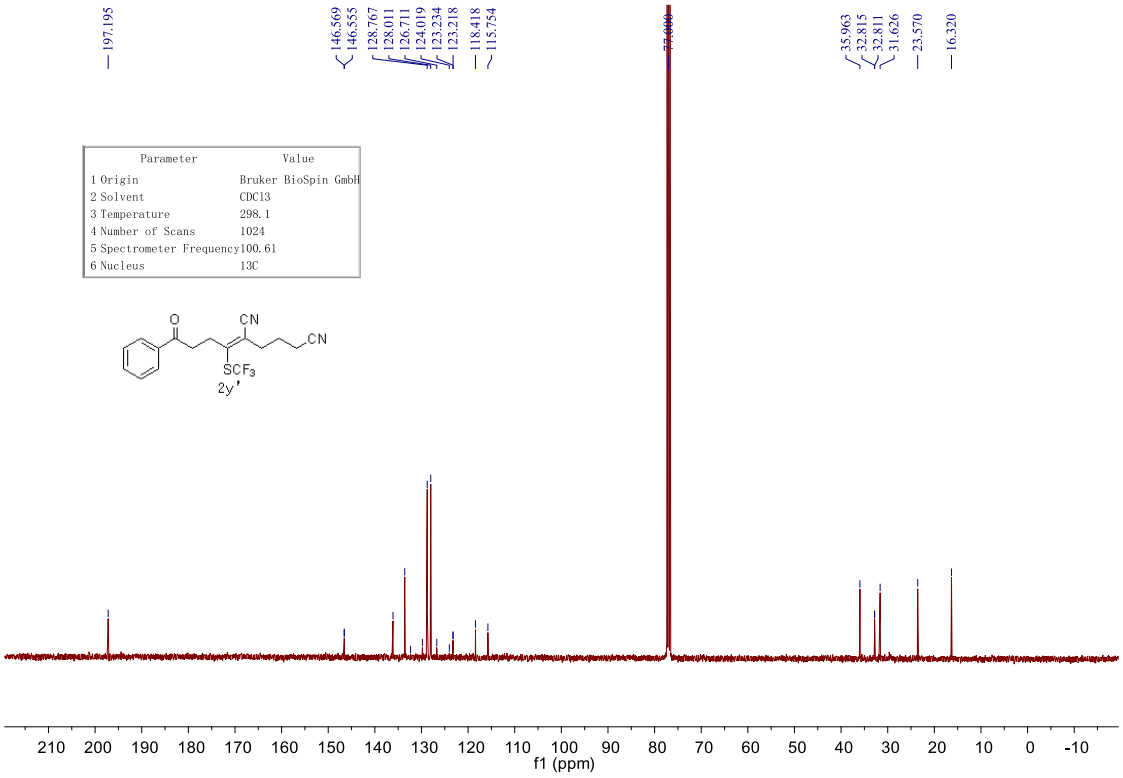

7.964
7.946
7.505
7.467
7.261
3.353
3.335
3.318
3.015
2.955
2.918
2.406
2.388
2.099
2.081
2.062
2.044
2.026
Parameter Value
1 Origin Bruker BioSpin GmbH
2 Solvent CDCl3
3 Temperature 298.1
4 Number of Scans 4
5 Spectrometer Frequency 400.13
6 Nucleus 1H
O
SCF3
CN
CN
2y
1.95
0.98
1.96
1.96
1.96
1.98
1.95
2.00
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
f1 (ppm)

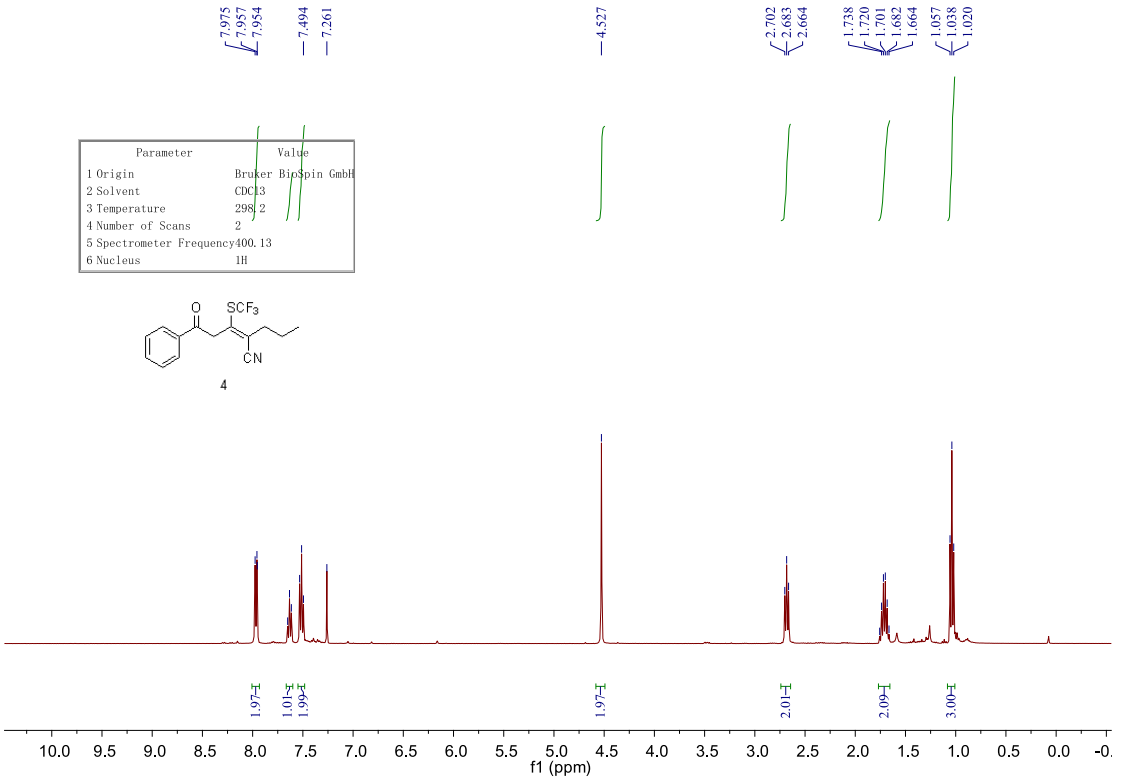

-37.913
Parameter Value
1 Origin Bruker BioSpin GmbH
2 Solvent CDCl3
3 Temperature 298.2
4 Number of Scans 4
5 Spectrometer Frequency 376.44
6 Nucleus 19F
O
SCF3
CN
CN
2y
0 -10 -30 -50 -70 -90 -110 -130 -150 -170 -190 -210 -230 -250 -270 -290
f1 (ppm)

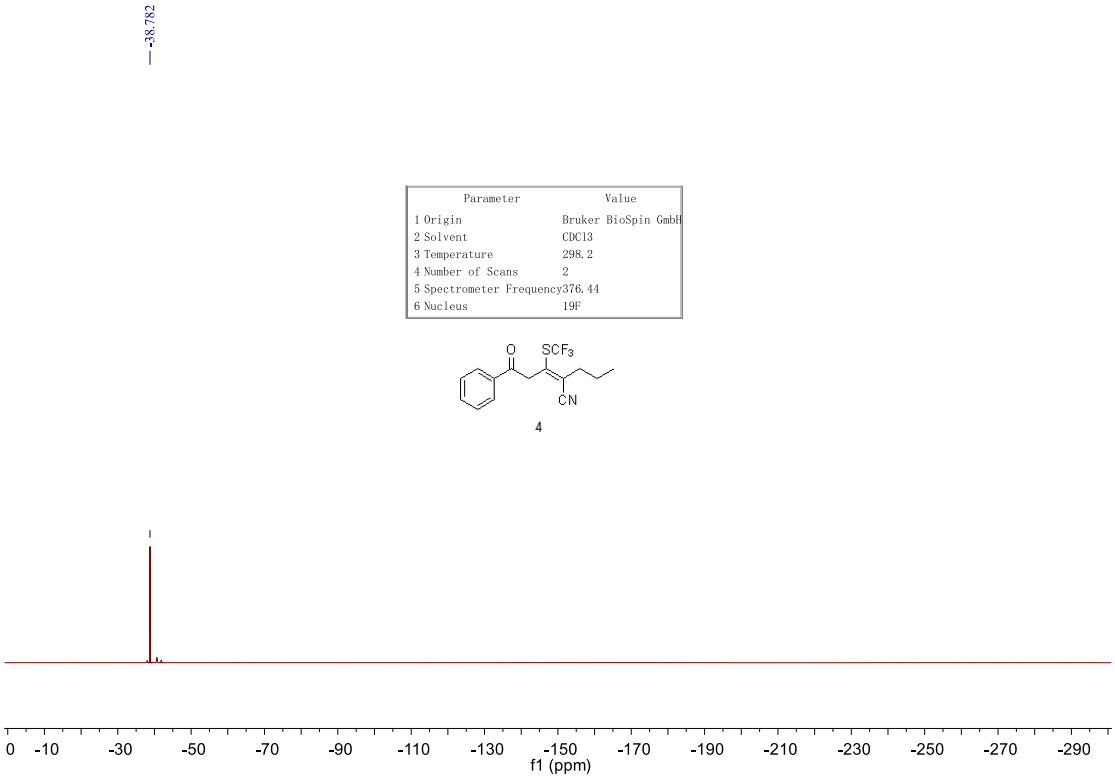

197.289
144.842
144.827
133.665
129.902
127.975
124.022
123.724
118.527
115.840
77.000
36.805
36.796
35.517
27.328
23.836
16.265
Parameter Value
1 Origin Bruker BioSpin GmbH
2 Solvent CDCl3
3 Temperature 298.1
4 Number of Scans 1024
5 Spectrometer Frequency 100.61
6 Nucleus 13C
O
SCF3
CN
CN
2y
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)

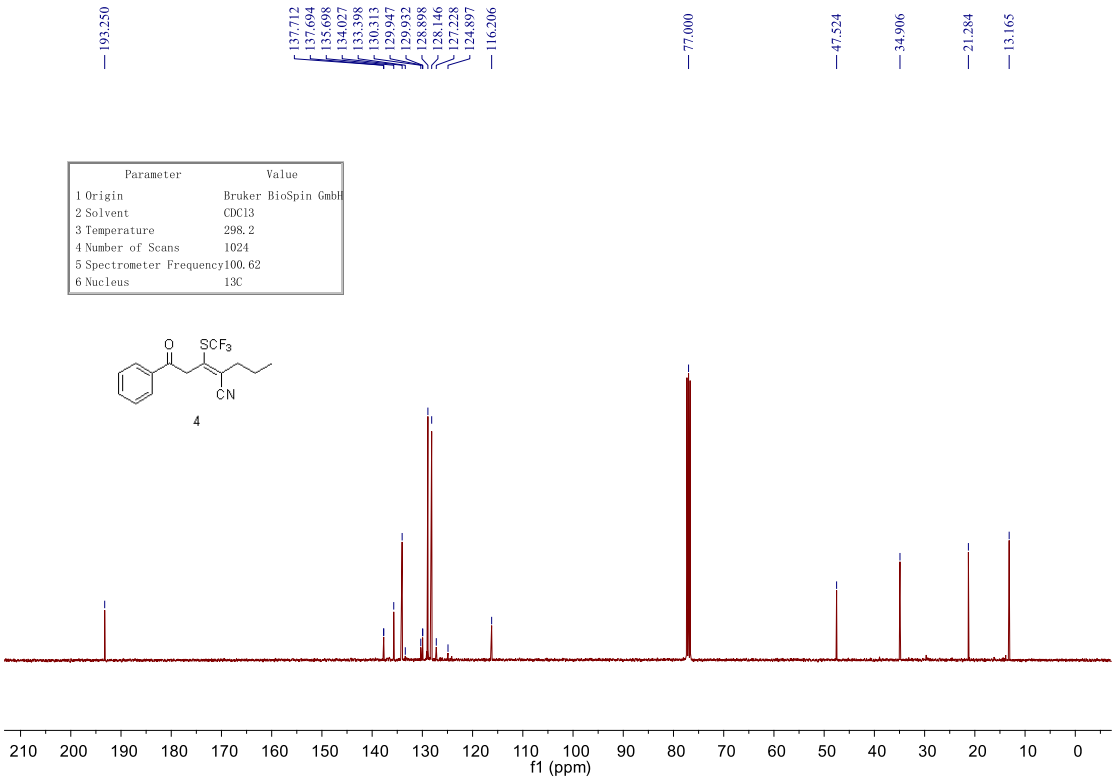

7.969
7.951
7.600
7.506
7.468
7.261
3.409
3.391
3.374
3.253
3.235
3.218
2.792
2.773
2.444
2.043
2.025
2.007
1.988
1.970
Parameter Value
1 Origin Bruker BioSpin GmbH
2 Solvent CDCl3
3 Temperature 298.2
4 Number of Scans 4
5 Spectrometer Frequency 400.13
6 Nucleus 1H
O
CN
CN
SCF3
2y'
2.00
1.05
2.04
1.89
1.94
1.93
1.92
2.00
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
f1 (ppm)


-38.101
Parameter Value
1 Origin Bruker BioSpin GmbH
2 Solvent CDCl3
3 Temperature 298.2
4 Number of Scans 4
5 Spectrometer Frequency 376.44
6 Nucleus 19F
O
CN
CN
SCF3
2y'
0 -10 -30 -50 -70 -90 -110 -130 -150 -170 -190 -210 -230 -250 -270 -290
f1 (ppm)

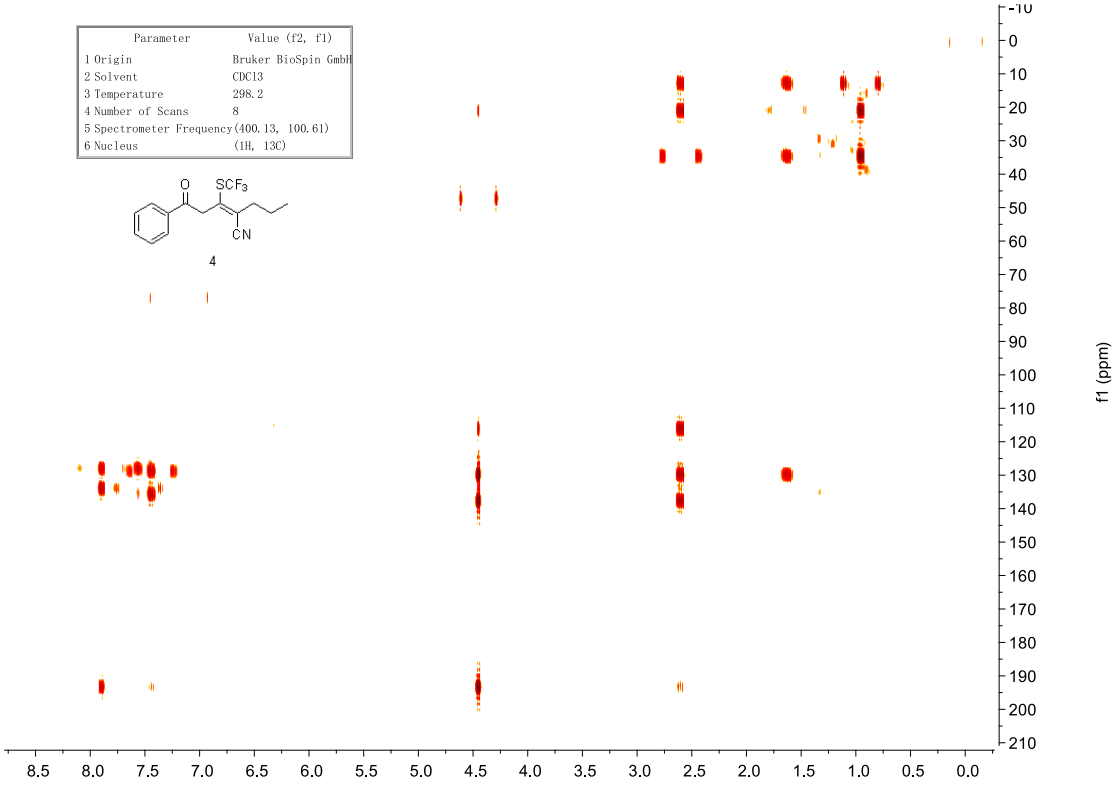

197.195
146.569
146.555
128.767
128.011
126.711
124.019
123.234
123.218
118.418
115.754
77.000
35.963
32.815
32.811
31.626
23.570
16.320
Parameter Value
1 Origin Bruker BioSpin GmbH
2 Solvent CDCl3
3 Temperature 298.1
4 Number of Scans 1024
5 Spectrometer Frequency 100.61
6 Nucleus 13C
O
CN
CN
SCF3
2y'
f1 (ppm)

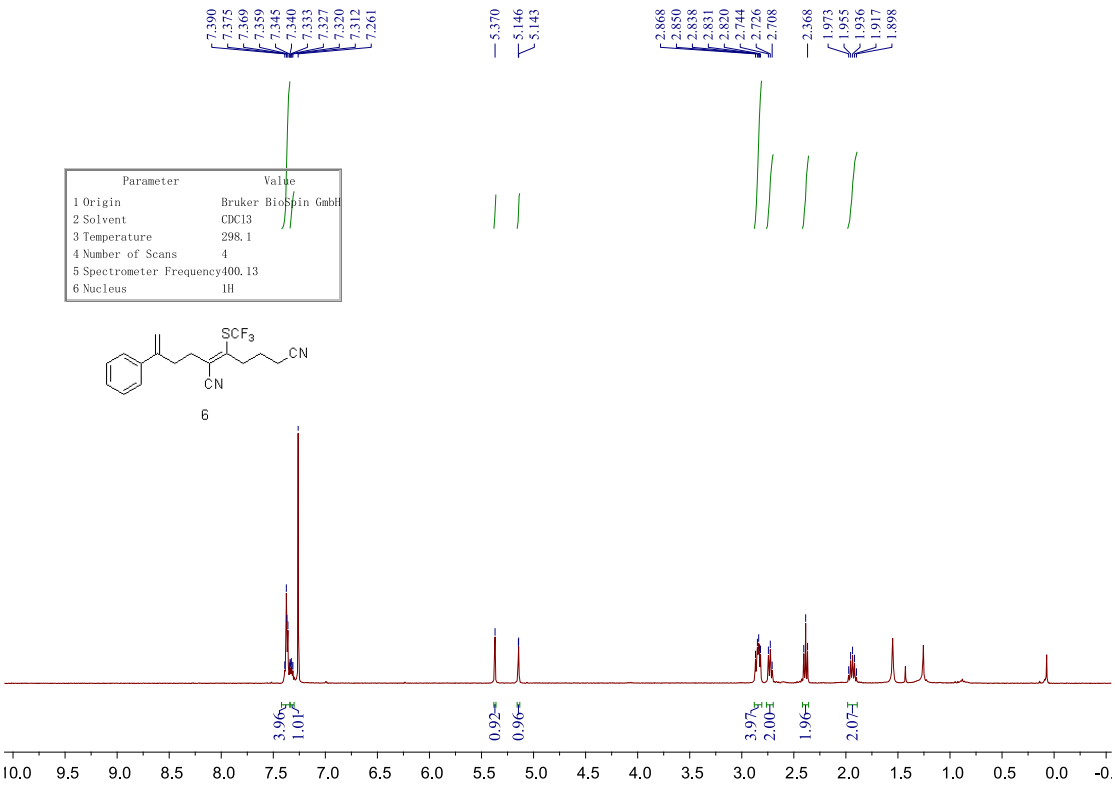

7.975
7.957
7.954
7.494
7.261
4.527
2.702
2.683
2.664
1.738
1.720
1.701
1.682
1.664
1.057
1.038
1.020
Parameter Value
1 Origin Bruker BioSpin GmbH
2 Solvent CDCl3
3 Temperature 298.2
4 Number of Scans 2
5 Spectrometer Frequency 400.13
6 Nucleus 1H
O
SCF3
CN
4
1.97
1.01
1.99
1.97
2.01
2.09
3.00
f1 (ppm)

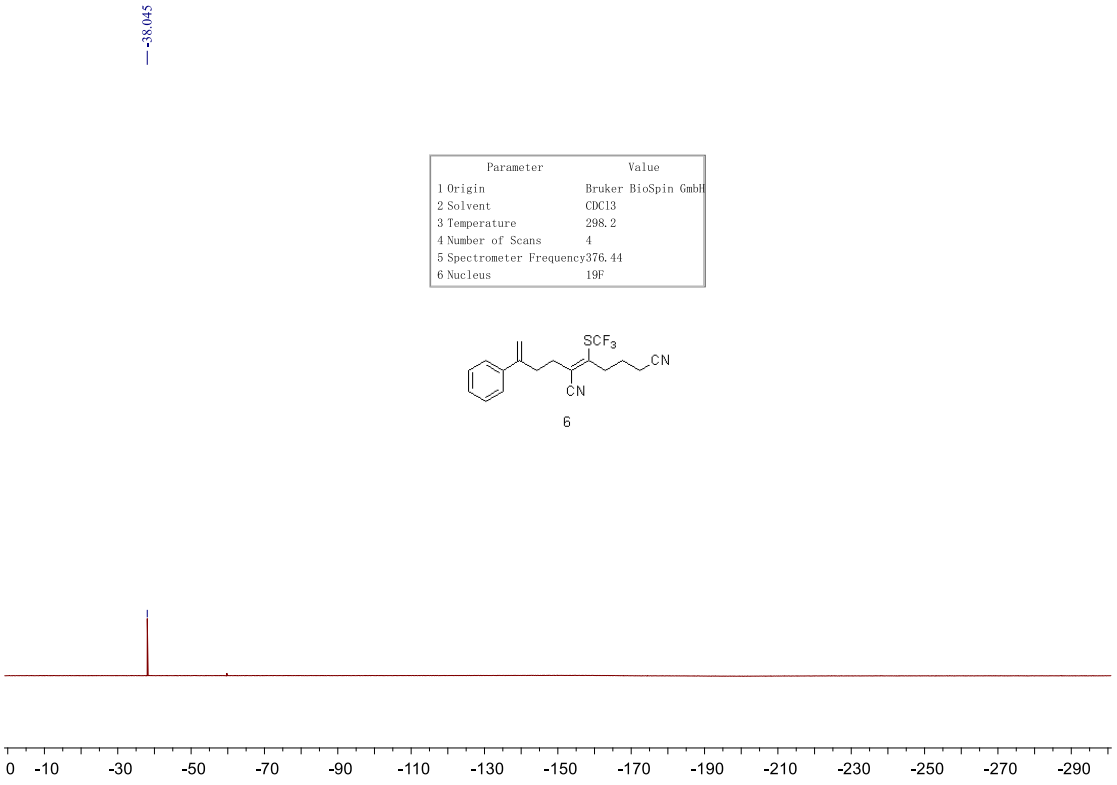

-38.782
Parameter Value
1 Origin Bruker BioSpin GmbH
2 Solvent CDCl3
3 Temperature 298.2
4 Number of Scans 2
5 Spectrometer Frequency376.44
6 Nucleus 19F
O
SCF3
CN
4
0 -10 -30 -50 -70 -90 -110 -130 -150 -170 -190 -210 -230 -250 -270 -290
f1 (ppm)

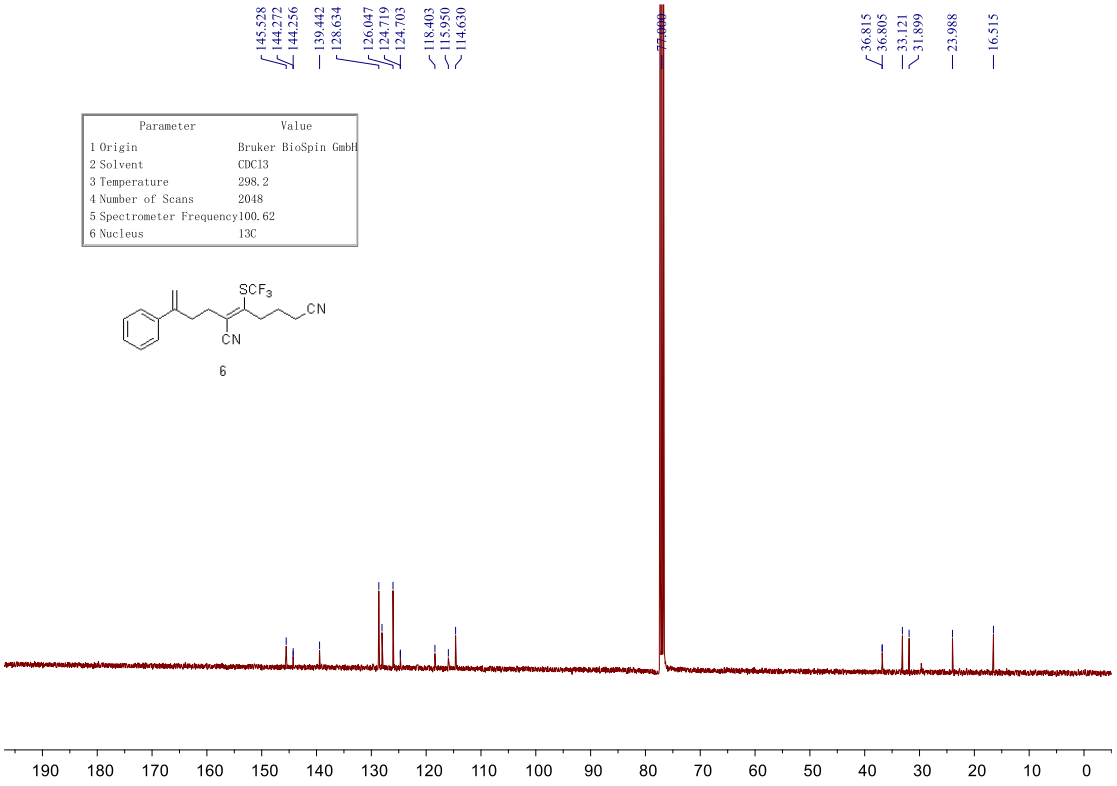

193.250
137.712
137.694
135.698
134.027
133.398
130.313
129.947
129.932
128.898
128.146
127.228
124.897
116.206
77.000
47.524
34.906
21.284
13.165
Parameter Value
1 Origin Bruker BioSpin GmbH
2 Solvent CDCl3
3 Temperature 298.2
4 Number of Scans 1024
5 Spectrometer Frequency100.62
6 Nucleus 13C
O
SCF3
CN
4
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)

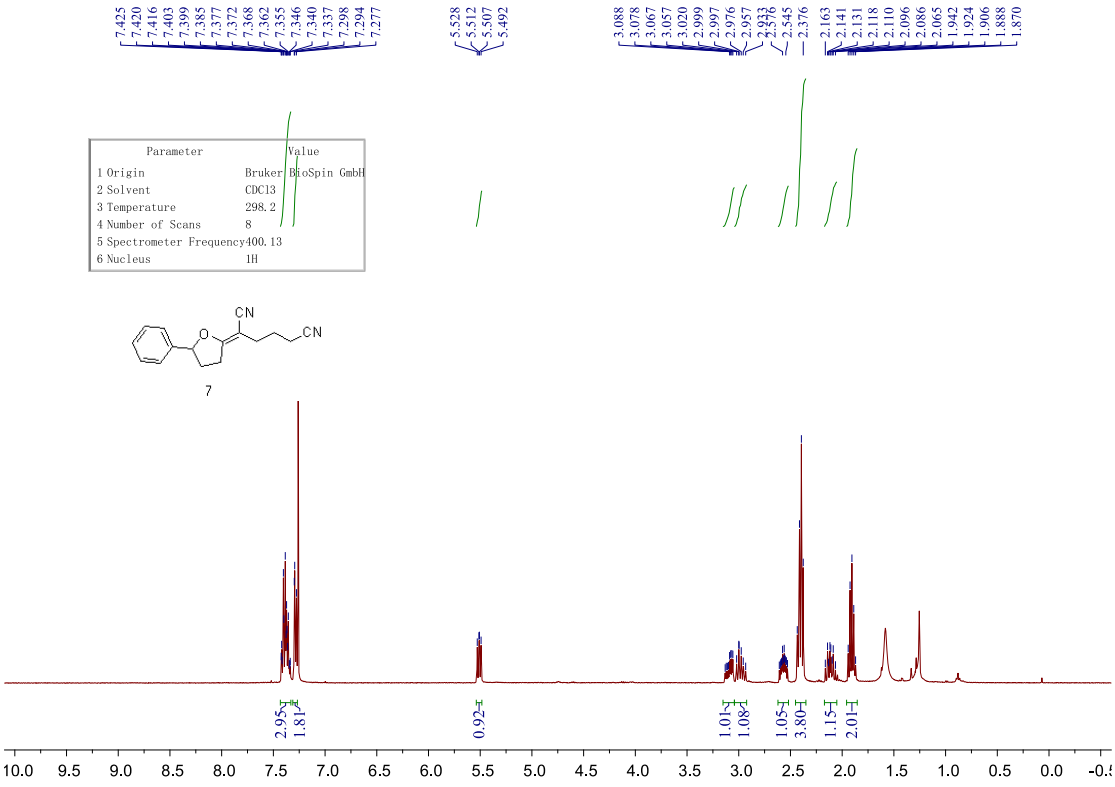
HMBC

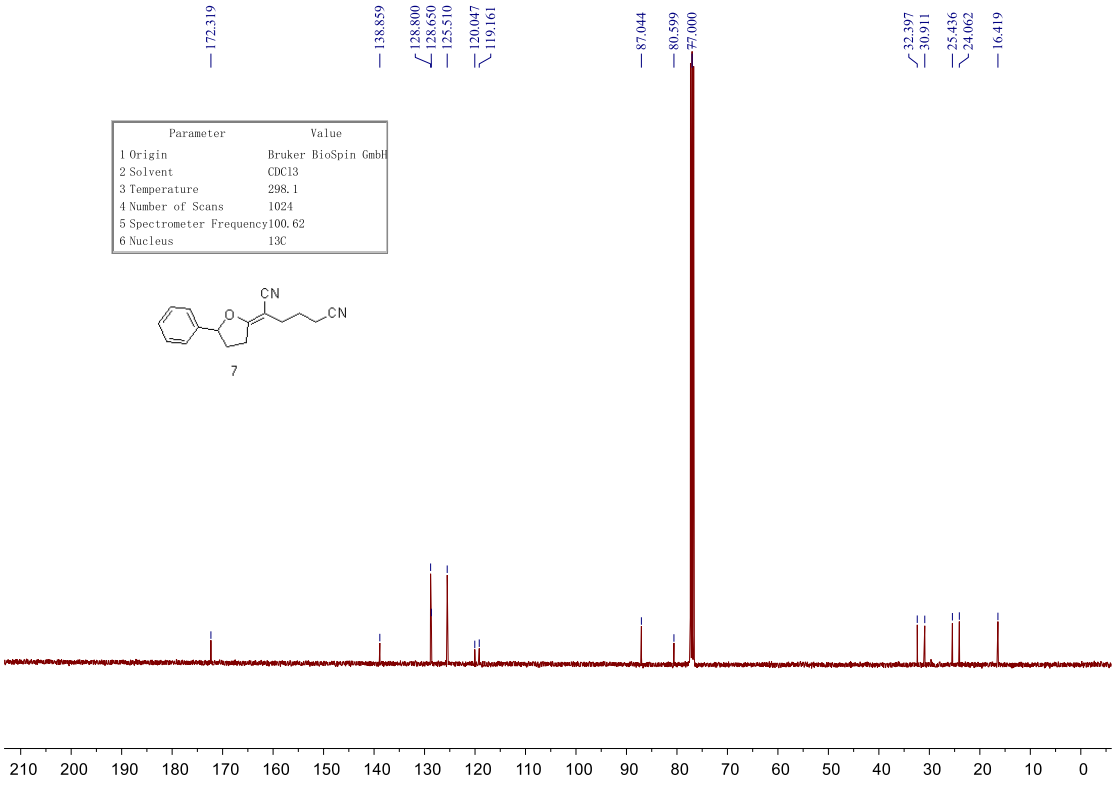

Parameter Value (f2, f1)
1 Origin Bruker BioSpin GmbH
2 Solvent CDCl3
3 Temperature 298.2
4 Number of Scans 8
5 Spectrometer Frequency (400.13, 100.61)
6 Nucleus (1H, 13C)
O
SCF3
CN
4
f1 (ppm)


7.390
7.375
7.369
7.359
7.345
7.340
7.333
7.327
7.320
7.312
7.261
5.370
5.146
5.143
2.868
2.850
2.838
2.831
2.820
2.744
2.726
2.708
2.368
1.973
1.955
1.936
1.917
1.898
Parameter Value
1 Origin Bruker BioSpin GmbH
2 Solvent CDCl3
3 Temperature 298.1
4 Number of Scans 4
5 Spectrometer Frequency 400.13
6 Nucleus 1H
SCF3
CN
CN
6
3.96
1.01
0.92
0.96
3.97
2.00
1.96
2.07


-38.045
Parameter Value
1 Origin Bruker BioSpin GmbH
2 Solvent CDCl3
3 Temperature 298.2
4 Number of Scans 4
5 Spectrometer Frequency 376.44
6 Nucleus 19F
SCF3
CN
CN
6
0 -10 -30 -50 -70 -90 -110 -130 -150 -170 -190 -210 -230 -250 -270 -290


145.528
144.272
144.256
139.442
128.634
126.047
124.719
124.703
118.403
115.950
114.630
77.000
36.815
36.805
33.121
31.899
23.988
16.515
Parameter Value
1 Origin Bruker BioSpin GmbH
2 Solvent CDCl3
3 Temperature 298.2
4 Number of Scans 2048
5 Spectrometer Frequency 100.62
6 Nucleus 13C
SCF3
CN
CN
6
190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0


7.425 7.420 7.416 7.403 7.399 7.385 7.377 7.372 7.368 7.362 7.355 7.346 7.340 7.337 7.298 7.294 7.277
5.528 5.512 5.507 5.492
3.088 3.078 3.067 3.057 3.020 2.999 2.997 2.976 2.957 2.933 2.926 2.545 2.376 2.163 2.141 2.131 2.118 2.110 2.096 2.086 2.065 1.942 1.924 1.906 1.888 1.870
Parameter Value
1 Origin Bruker BioSpin GmbH
2 Solvent CDCl3
3 Temperature 298.2
4 Number of Scans 8
5 Spectrometer Frequency 400.13
6 Nucleus 1H
CN
CN
O
7
2.95 1.81 0.92 1.01 1.08 1.05 3.80 1.15 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


172.319
138.859
128.800
128.650
125.510
120.047
119.161
87.044
80.599
77.000
32.397
30.911
25.436
24.062
16.419
Parameter Value
1 Origin Bruker BioSpin GmbH
2 Solvent CDCl3
3 Temperature 298.1
4 Number of Scans 1024
5 Spectrometer Frequency 100.62
6 Nucleus 13C
CN
CN
O
7
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0