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Supporting Information

Radical trifunctionalization of hexenenitrile by remote cyano migration

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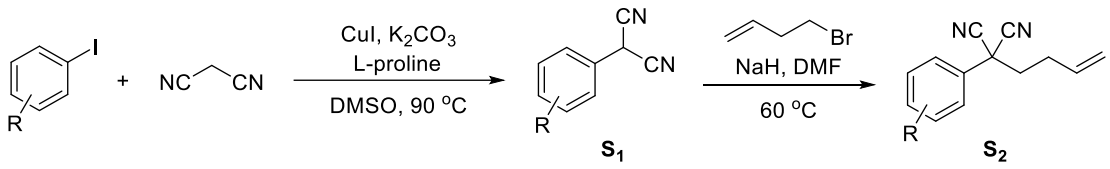
1. General Experimental Details

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

2. General procedures for synthesis of starting materials

The starting materials **1a-1h, 1o-1ad** were prepared according to **General Procedure B**.
The starting materials **1i-1n** were prepared according to **General Procedure A**.

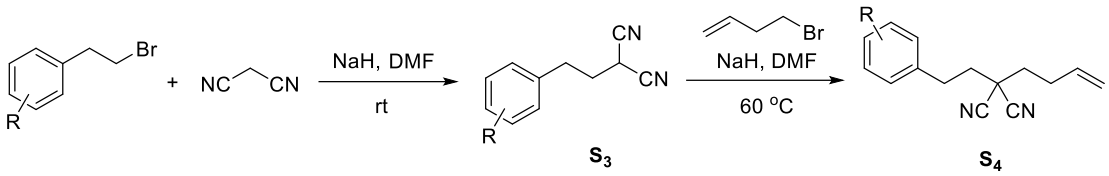
General Procedure A



Step 1: To a dry round bottom flask was added malononitrile (30 mmol, 3.0 equiv.), cuprous iodide (1 mmol, 10 mol %), L-proline (2 mmol, 20 mol %), potassium carbonate (40 mmol, 4.0 equiv.), iodobenzene (10 mmol, 1.0 equiv.), and DMSO (40 mL) at rt. The reaction mixture was stirred at 90 °C overnight under N_2 and quenched with HCl (2 M, 20 mL). The reaction was extracted with ethyl acetate, and the combined organic layer was washed with brine, dried over $MgSO_4$, filtered, concentrated in vacuum, and purified by flash column chromatography on silica gel (ethyl acetate/ petroleum ether) to give **S1**.

Step 2: To a dry round bottom flask was sequentially added sodium hydride (6 mmol, 1.2 equiv.), DMF (20 mL), and then **S1** (5 mmol, 1.0 equiv.) at 0 °C. The reaction mixture was stirred at rt for 1 h under N_2 and then 4-bromo-1-butene (6 mmol, 1.2 equiv.) was added dropwise at rt. The reaction mixture was stirred at 60 °C overnight and quenched with sat. NH_4Cl (20 mL). The reaction was extracted with ethyl acetate, concentrated in vacuum, and purified by flash column chromatography on silica gel (ethyl acetate/ petroleum ether) to give **S2**.

General Procedure B



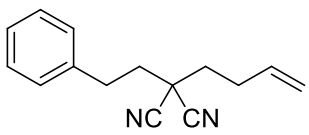
Step 1: To a dry round bottom flask was added sodium hydride (10 mmol, 1.0 equiv.), malononitrile (20 mmol, 2.0 equiv.), and DMF (30 mL) at 0 °C. The reaction mixture was stirred at 0 °C for 2 h under N_2 and then phenethyl bromide (10 mmol, 1.0 equiv.) was added dropwise. The reaction mixture was stirred at rt overnight. After the reaction was complete, the mixture was quenched with sat. NH_4Cl (20 mL). The reaction was extracted with ethyl acetate, and the combined organic layer was washed with brine, dried over $MgSO_4$, filtered, concentrated in vacuum, and purified by flash column chromatography on silica gel (ethyl acetate/ petroleum ether) to give **S3**.

Step 2: To a dry round bottom flask was sequentially added sodium hydride (6 mmol, 1.2 equiv.), DMF (20 mL), and then **S3** (5 mmol, 1.0 equiv.) at 0 °C. The reaction mixture was stirred at rt for 1 h under N_2 and then 4-bromo-1-butene (6 mmol, 1.2 equiv.) was added dropwise at rt. The reaction mixture was stirred at 60 °C overnight and quenched with sat. NH_4Cl (20 mL). The reaction was extracted with ethyl acetate, concentrated in vacuum, and purified by flash column chromatography on silica gel (ethyl acetate/ petroleum ether) to give **S4**.

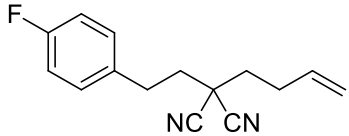
3. General procedure for radical trifunctionalization of hexenenitriles

Hexenenitrile **1** (0.2 mmol, 1.0 equiv.) and PIFA (0.4 mmol, 2.0 equiv.) were loaded in a flame-dried glass reaction vial which was subjected to evacuation/ flushing with N_2 for three times. DCM (2.0 mL) was added to the mixture via syringe and then $TMSN_3$ (0.8 mmol, 4.0 equiv.) was added. The mixture was then stirred at rt until the starting material had been consumed as determined by TLC. The mixture was extracted with ethyl acetate (3 × 10 mL). The combined organic extracts were washed by brine, dried over $MgSO_4$, filtered, concentrated, and purified by flash column chromatography on silica gel (ethyl acetate/ petroleum ether) to give the product **2.**

4. Characterization of starting materials

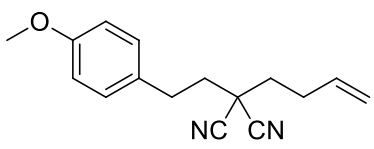


1a: 80% yield, yellow oil. Purification by flash column chromatography on silica gel (eluent: EtOAc/Petroleum ether = 1/15). ^1H NMR (400 MHz, $CDCl_3$) δ 7.38-7.32 (m, 2H), 7.31-7.26 (m, 1H), 7.26-7.22 (m, 2H), 5.89-5.78 (m, 1H), 5.24-5.12 (m, 2H), 3.05-2.97 (m, 2H), 2.52-2.44 (m, 2H), 2.28-2.20 (m, 2H), 2.11-2.04 (m, 2H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 138.4, 134.5, 128.9, 128.4, 127.0, 117.5, 115.3, 39.7, 37.2, 37.0, 31.9, 29.7. FT-IR: ν (cm^{-1}) 3029, 2932, 2863, 2359, 1644, 1455. HRMS [ESI] m/z: $[M+Na]^+$ calcd for $C_{15}H_{16}NaN_2$ 247.1206; found 247.1203.

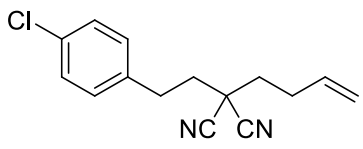


1b: 70% yield, yellow oil. Purification by flash column chromatography on silica gel (eluent: EtOAc/Petroleum ether = 1/15). ^1H NMR (400 MHz, $CDCl_3$) δ 7.22-7.15 (m, 2H),

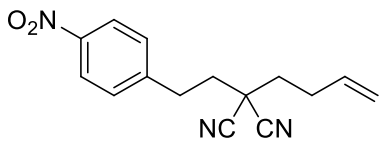
7.06-6.98 (m, 2H), 5.88-5.76 (m, 1H), 5.21-5.10 (m, 2H), 3.01-2.94 (m, 2H), 2.51-2.42 (m, 2H), 2.24-2.16 (m, 2H), 2.10-2.03 (m, 2H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 161.9 (d, J_{C-F} = 244.1 Hz), 134.4, 134.0 (d, J_{C-F} = 3.2 Hz), 129.9 (d, J_{C-F} = 7.9 Hz), 117.5, 115.7 (d, J_{C-F} = 21.2 Hz), 115.2, 39.8, 37.1, 37.1, 31.2, 29.7; ^{19}F NMR (376 MHz, $CDCl_3$) δ -115.6 (s). FT-IR: ν (cm^{-1}) 3079, 2934, 2863, 1603, 1510, 1455, 1222. HRMS [ESI] m/z: $[M+Na]^+$ calcd for $C_{15}H_{15}NaFN_2$ 265.1111; found 265.1115.



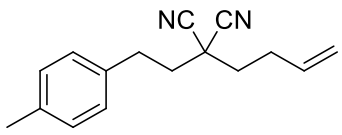
1c: 36% yield, yellow oil. Purification by flash column chromatography on silica gel (eluent: EtOAc/Petroleum ether = 1/15). ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.16-7.11 (m, 2H), 6.88-6.84 (m, 2H), 5.88-5.76 (m, 1H), 5.20-5.10 (m, 2H), 3.80 (s, 3H), 2.97-2.91 (m, 2H), 2.50-2.42 (m, 2H), 2.22-2.16 (m, 2H), 2.09-2.03 (m, 2H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 158.6, 134.5, 130.4, 129.4, 117.5, 115.3, 114.3, 55.3, 40.0, 37.1, 37.1, 31.1, 29.7. FT-IR: ν (cm^{-1}) 2959, 2933, 2838, 2359, 2335, 1612, 1513, 1247. HRMS [ESI] m/z: $[M+Na]^+$ calcd for $C_{16}H_{18}ONaN_2$ 277.1311; found 277.1309.



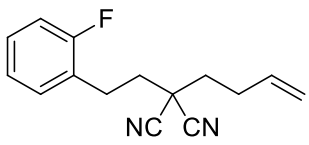
1d: 76% yield, yellow oil. Purification by flash column chromatography on silica gel (eluent: EtOAc/Petroleum ether = 1/5). ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.33-7.27 (m, 2H), 7.19-7.13 (m, 2H), 5.87-5.76 (m, 1H), 5.21-5.10 (m, 2H), 3.00-2.94 (m, 2H), 2.51-2.43 (m, 2H), 2.23-2.16 (m, 2H), 2.09-2.03 (m, 2H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 136.8, 134.4, 132.9, 129.8, 129.1, 117.6, 115.1, 39.6, 37.2, 37.1, 31.3, 29.7. FT-IR: ν (cm^{-1}) 3082, 2932, 2858, 1734, 1644, 1493, 1454. HRMS [ESI] m/z: $[M+Na]^+$ calcd for $C_{15}H_{15}ClNaN_2$ 281.0816; found 281.0825.



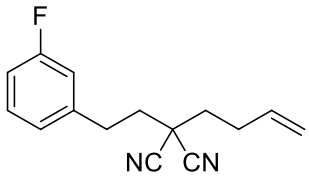
1e: 54% yield, yellow oil. Purification by flash column chromatography on silica gel (eluent: EtOAc/Petroleum ether = 1/15). ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.23-8.18 (m, 2H), 7.43-7.39 (m, 2H), 5.88-5.76 (m, 1H), 5.22-5.11 (m, 2H), 3.16-3.09 (m, 2H), 2.52-2.44 (m, 2H), 2.29-2.23 (m, 2H), 2.12-2.06 (m, 2H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 147.2, 145.8, 134.2, 129.4, 124.2, 117.7, 114.9, 39.0, 37.2, 31.8, 29.7. FT-IR: ν (cm^{-1}) 2962, 2952, 2159, 2027, 1976, 1518, 1345. HRMS [ESI] m/z: $[M+Na]^+$ calcd for $C_{15}H_{15}N_3NaO_2$ 292.1056; found 292.1060.



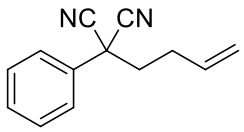
1f: 31% yield, yellow oil. Purification by flash column chromatography on silica gel (eluent: EtOAc/Petroleum ether = 1/15). ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.17-7.09 (m, 4H), 5.88-5.77 (m, 1H), 5.22-5.10 (m, 2H), 3.00-2.92 (m, 2H), 2.51-2.43 (m, 2H), 2.34 (s, 3H), 2.24-2.17 (m, 2H), 2.10-2.03 (m, 2H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 136.6, 135.3, 134.5, 129.5, 128.3, 117.4, 115.3, 39.8, 37.2, 37.1, 31.5, 29.7, 21.0. FT-IR: ν (cm^{-1}) 3385, 2977, 2928, 2360, 2341, 1644, 1516, 1455. HRMS [ESI] m/z: $[M+Na]^+$ calcd for $C_{16}H_{18}NaN_2$ 261.1362; found 261.1359.



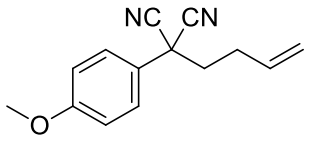
1g: 62% yield, yellow oil. Purification by flash column chromatography on silica gel (eluent: EtOAc/Petroleum ether = 1/15). ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.33-7.25 (m, 2H), 7.18-7.06 (m, 2H), 5.92-5.81 (m, 1H), 5.25-5.14 (m, 2H), 3.09-3.03 (m, 2H), 2.54-2.46 (m, 2H), 2.31-2.25 (m, 2H), 2.14-2.08 (m, 2H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 161.1 (d, $J_{C\text{-}F}$ = 244.1 Hz), 134.5, 130.7 (d, $J_{C\text{-}F}$ = 4.5 Hz), 129.0 (d, $J_{C\text{-}F}$ = 8.2 Hz), 125.3 (d, $J_{C\text{-}F}$ = 15.6 Hz), 124.5 (d, $J_{C\text{-}F}$ = 3.6 Hz), 117.5, 115.6 (d, $J_{C\text{-}F}$ = 21.6 Hz), 115.1, 37.8 (d, $J_{C\text{-}F}$ = 1.3 Hz), 37.1, 36.9, 29.7, 25.8 (d, $J_{C\text{-}F}$ = 2.6 Hz); ^{19}F NMR (376 MHz, $CDCl_3$) δ -118.4 (s). FT-IR: ν (cm^{-1}) 3406, 2977, 2935, 2159, 2030, 1976, 1454. HRMS [ESI] m/z: $[M+Na]^+$ calcd for $C_{15}H_{15}FNaN_2$ 265.1111; found 265.1113.



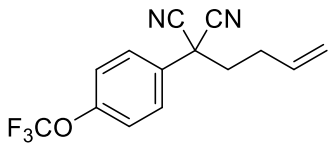
1h: 33% yield, yellow oil. Purification by flash column chromatography on silica gel (eluent: EtOAc/Petroleum ether = 1/15). ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.34-7.26 (m, 1H), 7.04-6.90 (m, 3H), 5.88-5.77 (m, 1H), 5.22-5.11 (m, 2H), 3.03-2.97 (m, 2H), 2.51-2.43 (m, 2H), 2.25-2.19 (m, 2H), 2.10-2.04 (m, 2H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 163.0 (d, $J_{C\text{-}F}$ = 245.2 Hz), 140.8 (d, $J_{C\text{-}F}$ = 7.2 Hz), 134.4, 130.5 (d, $J_{C\text{-}F}$ = 8.4 Hz), 124.1 (d, $J_{C\text{-}F}$ = 2.9 Hz), 117.5, 115.4 (d, $J_{C\text{-}F}$ = 21.4 Hz), 115.1, 114.0 (d, $J_{C\text{-}F}$ = 20.7 Hz), 39.3, 37.1, 37.1, 31.6, 29.7; ^{19}F NMR (376 MHz, $CDCl_3$) δ -112.6 (s). FT-IR: ν (cm^{-1}) 3083, 2935, 2864, 2359, 2249, 1590, 1489, 1252. HRMS [ESI] m/z: $[M+Na]^+$ calcd for $C_{15}H_{15}NaFN_2$ 265.1111; found 265.1118.



1i: 75% yield, yellow oil. Purification by flash column chromatography on silica gel (eluent: EtOAc/Petroleum ether = 1/5). ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.60-7.55 (m, 2H), 7.53-7.44 (m, 3H), 5.83-5.71 (m, 1H), 5.15-5.06 (m, 2H), 2.42-2.34 (m, 2H), 2.34-2.28 (m, 2H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 134.3, 132.0, 130.0, 129.8, 125.8, 117.3, 114.9, 42.0, 41.7, 29.7. FT-IR: ν (cm^{-1}) 2979, 2936, 2361, 2159, 1559, 1541. HRMS [ESI] m/z: $[M+Na]^+$ calcd for $C_{13}H_{12}NaN_2$ 219.0893; found 219.0898.

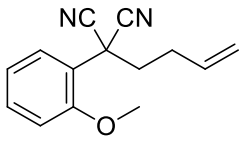


1j: 90% yield, yellow oil. Purification by flash column chromatography on silica gel (eluent: EtOAc/Petroleum ether = 1/5). ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.50-7.44 (m, 2H), 7.01-6.96 (m, 2H), 5.82-5.70 (m, 1H), 5.14-5.05 (m, 2H), 3.84 (s, 3H), 2.40-2.32 (m, 2H), 2.31-2.25 (m, 2H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 160.6, 134.4, 127.1, 123.6, 117.2, 115.1, 115.0, 55.5, 41.7, 41.3, 29.6. FT-IR: ν (cm^{-1}) 2976, 2936, 2842, 2159, 2029, 1609, 1511, 1257. HRMS [ESI] m/z: $[M+H]^+$ calcd for $C_{14}H_{15}N_2O$ 227.1179; found 227.1184.

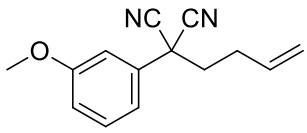


1k: 60% yield, yellow oil. Purification by flash column chromatography on silica gel (eluent: EtOAc/Petroleum ether = 1/5). ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.65-7.60 (m, 2H), 7.38-7.33 (m, 2H), 5.82-5.70 (m, 1H), 5.16-5.08 (m, 2H), 2.44-2.36 (m, 2H), 2.34-2.27 (m, 2H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 150.2 (q, J = 1.8 Hz), 134.0, 130.6, 127.6, 122.0, 120.3 (q, J = 257.1 Hz), 117.5, 114.5, 41.7, 41.4, 29.7; ^{19}F NMR (376 MHz, $CDCl_3$) δ -57.9

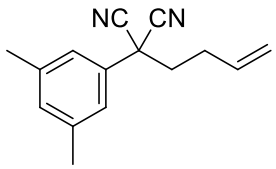
(s). FT-IR: ν (cm^{-1}) 2976, 2935, 2361, 2159, 1734, 1509, 1212. HRMS [ESI] m/z: $[M+H]^+$ calcd for $C_{14}H_{12}F_3N_2O$ 281.0896; found 281.0887.



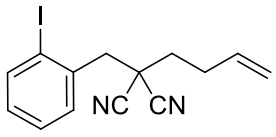
1l: 69% yield, yellow oil. Purification by flash column chromatography on silica gel (eluent: EtOAc/Petroleum ether = 1/5). ^1H NMR (400 MHz, $CDCl_3$) δ 7.55 (dd, 8.0, 1.6 Hz, 1H), 7.48-7.42 (m, 1H), 7.08-7.00 (m, 2H), 5.84-5.73 (m, 1H), 5.14-5.04 (m, 2H), 3.96 (s, 3H), 2.48-2.41 (m, 2H), 2.41-2.33 (m, 2H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 156.4, 134.9, 131.7, 127.6, 121.3, 119.1, 116.9, 114.8, 112.6, 56.0, 39.6, 36.6, 29.8. FT-IR: ν (cm^{-1}) 3082, 2978, 2940, 2159, 2029, 1976, 1599, 1494, 1464, 1257. HRMS [ESI] m/z: $[M+Na]^+$ calcd for $C_{14}H_{14}NaN_2O$ 249.0998; found 249.0991.



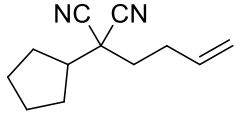
1m: 44% yield, yellow oil. Purification by flash column chromatography on silica gel (eluent: EtOAc/Petroleum ether = 1/5). ^1H NMR (400 MHz, $CDCl_3$) δ 7.43-7.37 (m, 1H), 7.17-7.12 (m, 1H), 7.11-7.06 (m, 1H), 7.00-6.96 (m, 1H), 5.82-5.71 (m, 1H), 5.15-5.06 (m, 2H), 3.86 (s, 3H), 2.42-2.34 (m, 2H), 2.33-2.27 (m, 2H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 160.5, 134.3, 133.3, 130.9, 117.8, 117.3, 115.2, 114.8, 111.8, 55.5, 41.9, 41.6, 29.7. FT-IR: ν (cm^{-1}) 3082, 2973, 2938, 2359, 2341, 1588, 1492, 1295, 1259. HRMS [ESI] m/z: $[M+Na]^+$ calcd for $C_{14}H_{14}NaN_2O$ 249.0998; found 249.0989.



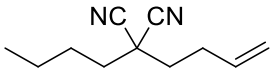
1n: 86% yield, yellow oil. Purification by flash column chromatography on silica gel (eluent: EtOAc/Petroleum ether = 1/5). ^1H NMR (400 MHz, $CDCl_3$) δ 7.15 (s, 2H), 7.07 (s, 1H), 5.83-5.71 (m, 1H), 5.15-5.06 (m, 2H), 2.42-2.34 (m, 2H), 2.37 (s, 6H), 2.32-2.24 (m, 2H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 139.7, 134.4, 131.7, 131.5, 123.4, 117.2, 115.1, 41.8, 41.7, 29.7, 21.3. FT-IR: ν (cm^{-1}) 2954, 2923, 2854, 2362, 2330, 1721, 1605, 1456, 1378, 1215. HRMS [ESI] m/z: $[M+Na]^+$ calcd for $C_{15}H_{16}NaN_2$ 247.1206; found 247.1196.



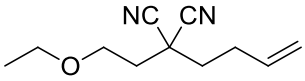
1o: 10% yield, yellow oil. Purification by flash column chromatography on silica gel (eluent: EtOAc/Petroleum ether = 1/15). ^1H NMR (400 MHz, $CDCl_3$) δ 7.93 (dd, *J* = 8.0, 1.2 Hz, 1H), 7.57 (dd, *J* = 7.6, 1.6 Hz, 1H), 7.44-7.39 (m, 1H), 7.10-7.04 (m, 1H), 5.89-5.78 (m, 1H), 5.22-5.10 (m, 2H), 3.51 (s, 2H), 2.54-2.46 (m, 2H), 2.19-2.12 (m, 2H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 140.5, 135.4, 134.5, 130.8, 130.5, 129.0, 117.4, 114.9, 102.4, 46.2, 38.5, 36.8, 29.9. FT-IR: ν (cm^{-1}) 2973, 2928, 2884, 2360, 2342, 1380. HRMS [ESI] m/z: $[M+Na]^+$ calcd for $C_{14}H_{13}NaIN_2$ 359.0016; found 359.0008.



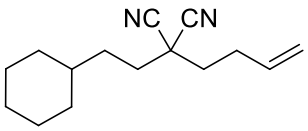
1p: 83% yield, yellow oil. Purification by flash column chromatography on silica gel (eluent: EtOAc/Petroleum ether = 1/15). ^1H NMR (400 MHz, $CDCl_3$) δ 5.87-5.76 (m, 1H), 5.19-5.08 (m, 2H), 2.48-2.41 (m, 2H), 2.39-2.29 (m, 1H), 2.05-1.95 (m, 4H), 1.87-1.75 (m, 2H), 1.69-1.59 (m, 3H), 1.57-1.53 (m, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 134.8, 117.2, 115.3, 46.6, 41.9, 36.3, 30.0, 29.2, 25.2. FT-IR: ν (cm^{-1}) 2961, 2927, 2872, 2159, 2031, 1976, 1453. HRMS [ESI] m/z: $[M+Na]^+$ calcd for $C_{12}H_{16}NaN_2$ 211.1206; found 211.1199.



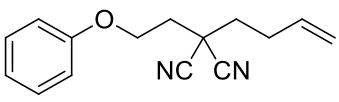
1q: 73% yield, yellow oil. Purification by flash column chromatography on silica gel (eluent: EtOAc/Petroleum ether = 1/15). ^{1}H NMR (400 MHz, $CDCl_3$) δ 5.87-5.75 (m, 1H), 5.19-5.08 (m, 2H), 2.47-2.39 (m, 2H), 2.04-1.97 (m, 2H), 1.96-1.90 (m, 2H), 1.70-1.62 (m, 2H), 1.49-1.38 (m, 2H), 0.97 (t, *J* = 7.2 Hz, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 134.7, 117.3, 115.6, 37.6, 37.4, 37.0, 29.7, 27.6, 22.0, 13.6. FT-IR: ν (cm^{-1}) 2963, 2933, 2874, 2159, 2029, 1976, 1645, 1454. HRMS [ESI] m/z: $[M+Na]^+$ calcd for $C_{11}H_{16}NaN_2$ 199.1206; found 199.1213.



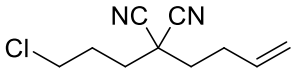
1r: 52% yield, yellow oil. Purification by flash column chromatography on silica gel (eluent: EtOAc/Petroleum ether = 1/15). ^{1}H NMR (400 MHz, $CDCl_3$) δ 5.86-5.75 (m, 1H), 5.18-5.07 (m, 2H), 3.72 (t, *J* = 6.0 Hz, 2H), 3.53 (q, *J* = 7.2 Hz, 2H), 2.47-2.39 (m, 2H), 2.21 (t, *J* = 6.0 Hz, 2H), 2.10-2.04 (m, 2H), 1.21 (t, *J* = 7.2 Hz, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 134.7, 117.2, 115.3, 66.9, 65.9, 37.3, 37.1, 35.1, 29.6, 14.9. FT-IR: ν (cm^{-1}) 2978, 2935, 2873, 2359, 2342, 1644, 1380. HRMS [ESI] m/z: $[M+Na]^+$ calcd for $C_{11}H_{16}NaON_2$ 215.1155; found 215.1155.



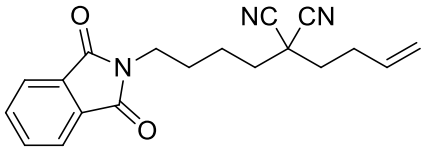
1s: 94% yield, yellow oil. Purification by flash column chromatography on silica gel (eluent: EtOAc/Petroleum ether = 1/15). ^{1}H NMR (400 MHz, $CDCl_3$) δ 5.87-5.75 (m, 1H), 5.19-5.09 (m, 2H), 2.47-2.40 (m, 2H), 2.04-1.98 (m, 2H), 1.98-1.92 (m, 2H), 1.76-1.62 (m, 5H), 1.60-1.52 (m, 2H), 1.28-1.14 (m, 4H), 1.02-0.90 (m, 2H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 134.7, 117.3, 115.6, 37.5, 37.2, 36.9, 35.7, 33.0, 32.8, 29.7, 26.4, 26.1. FT-IR: ν (cm^{-1}) 3083, 2923, 2853, 2159, 2029, 1976, 1644, 1453. HRMS [ESI] m/z: $[M+Na]^+$ calcd for $C_{15}H_{22}NaN_2$ 253.1675; found 253.1679.



1t: 48% yield, yellow oil. Purification by flash column chromatography on silica gel (eluent: EtOAc/Petroleum ether = 1/15). ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.35-7.29 (m, 2H), 7.04-6.99 (m, 1H), 6.97-6.92 (m, 2H), 5.87-5.75 (m, 1H), 5.22-5.11 (m, 2H), 4.31 (t, *J* = 6.0 Hz, 2H), 2.54-2.44 (m, 4H), 2.18-2.12 (m, 2H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 157.8, 134.5, 129.7, 121.7, 117.5, 115.0, 114.5, 63.3, 37.3, 36.8, 35.1, 29.6. FT-IR: ν (cm^{-1}) 2977, 2935, 2159, 2029, 1588, 1497, 1239. HRMS [ESI] m/z: $[M+Na]^+$ calcd for $C_{15}H_{16}NaN_2O$ 263.1155; found 263.1145.

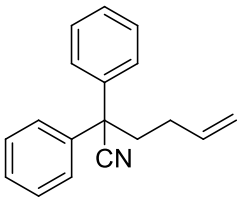


1u: 41% yield, yellow oil. Purification by flash column chromatography on silica gel (eluent: EtOAc/Petroleum ether = 1/15). ^{1}H NMR (400 MHz, $CDCl_3$) δ 5.86-5.75 (m, 1H), 5.20-5.08 (m, 2H), 3.65-3.61 (m, 1H), 3.50-3.45 (m, 1H), 2.47-2.39 (m, 2H), 2.27-2.16 (m, 1H), 2.16-2.08 (m, 3H), 2.07-2.00 (m, 2H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 134.4, 117.5, 115.1, 43.2, 37.0, 36.9, 35.4, 29.7, 28.4. FT-IR: ν (cm^{-1}) 3082, 2966, 2937, 2857, 1644, 1452, 1296. HRMS [ESI] m/z: $[M+Na]^+$ calcd for $C_{10}H_{13}ClNaN_2$ 219.0659; found 219.0663.

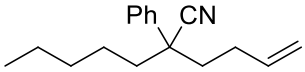


1v: 85% yield, white solid. Purification by flash column chromatography on silica gel (eluent: EtOAc/Petroleum

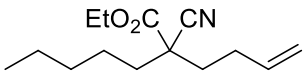
ether = 1/5). ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.88-7.82 (m, 2H), 7.75-7.69 (m, 2H), 5.86-5.75 (m, 1H), 5.20-5.08 (m, 2H), 3.74 (t, *J* = 6.8 Hz, 2H), 2.48-2.40 (m, 2H), 2.06-1.99 (m, 4H), 1.86-1.68 (m, 4H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 168.3, 134.5, 134.1, 132.0, 123.4, 117.4, 115.3, 37.2, 37.2, 36.9, 29.7, 27.7, 22.6. FT-IR: ν (cm^{-1}) 3420, 2975, 2938, 2359, 2342, 1773, 1713, 1439. HRMS [ESI] m/z: $[M+Na]^+$ calcd for $C_{19}H_{19}NaO_2N_3$ 344.1369; found 344.1368.



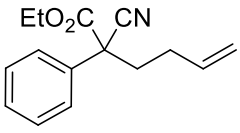
1w: 73% yield, yellow oil. Purification by flash column chromatography on silica gel (eluent: EtOAc/Petroleum ether = 1/20). ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.42-7.33 (m, 8H), 7.33-7.27 (m, 2H), 5.87-5.76 (m, 1H), 5.08-4.98 (m, 2H), 2.50-2.44 (m, 2H), 2.22-2.14 (m, 2H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 140.0, 136.7, 128.9, 127.9, 126.9, 122.2, 115.7, 51.5, 38.9, 29.9. FT-IR: ν (cm^{-1}) 3063, 3028, 2935, 2236, 1493, 1449. HRMS [ESI] m/z: $[M+Na]^+$ calcd for $C_{18}H_{17}NNa$ 270.1253; found 270.1242.



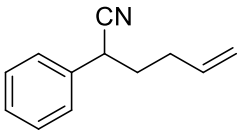
1x: 73% yield, yellow oil. Purification by flash column chromatography on silica gel (eluent: EtOAc/Petroleum ether = 1/20). ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.40-7.35 (m, 2H), 7.35-7.29 (m, 2H), 7.27-7.21 (m, 1H), 5.73-5.62 (m, 1H), 4.96-4.86 (m, 2H), 2.23-2.12 (m, 1H), 2.10-2.00 (m, 1H), 2.00-1.76 (m, 4H), 1.51-1.39 (m, 1H), 1.27-1.02 (m, 5H), 0.83-0.74 (m, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 138.4, 136.9, 128.9, 127.7, 125.9, 122.3, 115.4, 48.1, 41.1, 40.3, 31.6, 29.6, 24.9, 22.3, 13.9. FT-IR: ν (cm^{-1}) 3064, 2930, 2862, 2361, 2343, 1642, 1449. HRMS [ESI] m/z: $[M+Na]^+$ calcd for $C_{17}H_{23}NaN$ 264.1723; found 264.1717.



1y: 84% yield, yellow oil. Purification by flash column chromatography on silica gel (eluent: EtOAc/Petroleum ether = 1/10). ^{1}H NMR (400 MHz, $CDCl_3$) δ 5.81-5.69 (m, 1H), 5.10-4.98 (m, 2H), 4.26 (q, *J* = 6.8 Hz, 2H), 2.37-2.26 (m, 1H), 2.15-1.95 (m, 2H), 1.94-1.71 (m, 3H), 1.63-1.50 (m, 1H), 1.37-1.23 (m, 8H), 0.88 (t, *J* = 6.4 Hz, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 169.1, 136.0, 119.2, 116.2, 62.6, 49.6, 37.6, 36.6, 31.3, 29.7, 25.0, 22.3, 14.1, 13.9. FT-IR: ν (cm^{-1}) 2959, 2931, 2864, 2359, 2342, 1739, 1643, 1451, 1218. HRMS [ESI] m/z: $[M+Na]^+$ calcd for $C_{14}H_{23}NaO_2N$ 260.1621; found 260.1612.

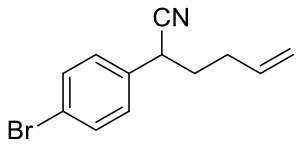


1z: 52% yield, yellow oil. Purification by flash column chromatography on silica gel (eluent: EtOAc/Petroleum ether = 1/5). ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.57-7.53 (m, 2H), 7.44-7.35 (m, 3H), 5.83-5.73 (m, 1H), 5.11-4.98 (m, 2H), 4.30-4.16 (m, 2H), 2.52-2.42 (m, 1H), 2.30-2.12 (m, 3H), 1.25 (t, *J* = 7.2 Hz, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 167.5, 136.0, 134.5, 129.2, 128.9, 126.0, 118.3, 116.1, 63.2, 53.8, 37.3, 29.7, 13.8. FT-IR: ν (cm^{-1}) 3068, 2982, 2936, 2247, 1741, 1449, 1223. HRMS [ESI] m/z: $[M+Na]^+$ calcd for $C_{15}H_{17}NaO_2N$ 266.1151; found 266.1140.

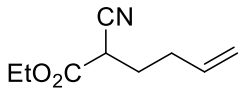


1aa: 43% yield, yellow oil. Purification by flash column chromatography on silica gel (eluent: EtOAc/Petroleum ether = 1/20). ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.42-7.36 (m, 2H), 7.36-7.30 (m, 3H), 5.84-5.73 (m, 1H), 5.15-5.05 (m, 2H), 3.81 (dd, *J* = 8.8, 6.4 Hz, 1H), 2.29-2.21 (m, 2H),

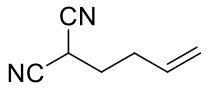
2.10-2.00 (m, 1H), 2.00-1.89 (m, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 136.2, 135.8, 129.1, 128.1, 127.3, 120.7, 116.6, 36.5, 34.9, 31.0. FT-IR: ν (cm^{-1}) 3067, 3032, 2980, 2931, 2862, 2241, 1736, 1642, 1494, 1454, 1242. HRMS [ESI] m/z: $[M+Na]^+$ calcd for $C_{12}H_{13}NaN$ 194.0940; found 194.0942.



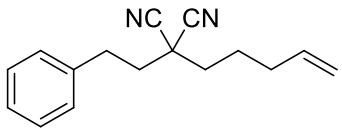
1ab: 47% yield, colorless oil. Purification by flash column chromatography on silica gel (eluent: EtOAc/Petroleum ether = 1/20). ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.53-7.49 (m, 2H), 7.23-7.18 (m, 2H), 5.82-5.71 (m, 1H), 5.14-5.05 (m, 2H), 3.77 (dd, *J* = 8.8, 6.4 Hz, 1H), 2.27-2.19 (m, 2H), 2.08-1.97 (m, 1H), 1.96-1.86 (m, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 135.8, 134.8, 132.3, 129.0, 122.2, 120.2, 116.9, 36.0, 34.8, 30.8. FT-IR: ν (cm^{-1}) 3079, 3019, 2979, 2931, 2862, 2242, 1641, 1488, 1439. HRMS [ESI] m/z: $[M+Na]^+$ calcd for $C_{12}H_{12}NaNBr$ 272.0045; found 272.0050.



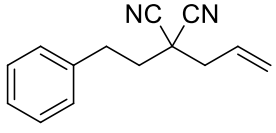
1ac: 42% yield, colorless oil. Purification by flash column chromatography on silica gel (eluent: EtOAc/Petroleum ether = 1/10). ^{1}H NMR (400 MHz, $CDCl_3$) δ 5.79-5.68 (m, 1H), 5.15-5.04 (m, 2H), 4.24 (q, *J* = 7.2 Hz, 2H), 3.50 (dd, *J* = 8.0, 6.4 Hz, 1H), 2.35-2.18 (m, 2H), 2.10-1.96 (m, 2H), 1.30 (t, *J* = 7.2 Hz, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 166.1, 135.3, 117.3, 116.3, 62.8, 36.7, 30.6, 28.9, 14.0. FT-IR: ν (cm^{-1}) 3082, 2980, 2939, 2159, 2018, 1976, 1742, 1453, 1255. HRMS [ESI] m/z: $[M+Na]^+$ calcd for $C_9H_{13}NNaO_2S$ 190.0838; found 190.0834.



1ad: 36% yield, colorless oil. Purification by flash column chromatography on silica gel (eluent: EtOAc/Petroleum ether = 1/5). ^{1}H NMR (400 MHz, $CDCl_3$) δ 5.78-5.66 (m, 1H), 5.20-5.11 (m, 2H), 3.76 (t, *J* = 7.2 Hz, 1H), 2.38-2.30 (m, 2H), 2.13-2.06 (m, 2H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 134.0, 118.5, 112.8, 30.2, 29.7, 21.7. FT-IR: ν (cm^{-1}) 2974, 2935, 2102, 1243. HRMS [ESI] m/z: $[M+Na]^+$ calcd for $C_7H_8NaN_2$ 143.0580; found 143.0572.



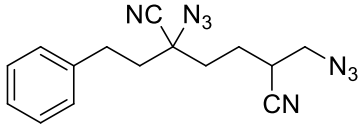
3: 28% yield, yellow oil. Purification by flash column chromatography on silica gel (eluent: EtOAc/Petroleum ether = 1/15). ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.41-7.33 (m, 2H), 7.32-7.28 (m, 1H), 7.27-7.23 (m, 2H), 5.87-5.75 (m, 1H), 5.14-5.06 (m, 2H), 3.05-2.98 (m, 2H), 2.27-2.18 (m, 4H), 2.03-1.97 (m, 2H), 1.89-1.79 (m, 2H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 138.5, 136.6, 128.9, 128.4, 127.0, 116.4, 115.4, 39.6, 37.5, 37.2, 32.6, 31.9, 24.6. FT-IR: ν (cm^{-1}) 2977, 2932, 2866, 2159, 2028, 1643, 1455. HRMS [ESI] m/z: $[M+Na]^+$ calcd for $C_{16}H_{18}N_2Na$ 261.1362; found 261.1364.



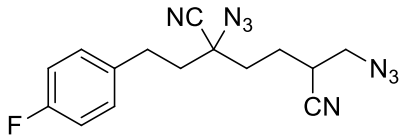
5: 45% yield, yellow oil. Purification by flash column chromatography on silica gel (eluent: EtOAc/Petroleum ether = 1/15). ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.40-7.34 (m, 2H), 7.32-7.27 (m, 1H), 7.27-7.23 (m, 2H), 6.00-5.88 (m, 1H), 5.49-5.40 (m, 2H), 3.05-2.98 (m, 2H), 2.75 (d,

J = 7.2 Hz, 2H), 2.26-2.19 (m, 2H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 138.5, 128.9, 128.5, 128.5, 127.0, 123.4, 115.1, 41.6, 38.8, 37.3, 31.9. FT-IR: ν (cm^{-1}) 2975, 2933, 2159, 2029, 1976, 1455. HRMS [ESI] m/z: $[M+Na]^+$ calcd for $C_{14}H_{14}NaN_2$ 233.1049; found 233.1046.

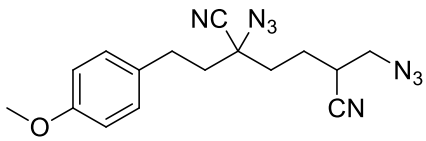
5. Characterization of products



2a: *d.r.* = 1:1, 49.2 mg, 80%, yellow oil, Purification by flash column chromatography on silica gel (eluent: EtOAc/Petroleum ether = 1/5). ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.38-7.29 (m, 2H, two isomers), 7.29-7.18 (m, 3H, two isomers), 3.65-3.45 (m, 2H, two isomers), 3.96-2.76 (m, 3H, two isomers), 2.22-2.12 (m, 2H, two isomers), 2.10-1.81 (m, 4H, two isomers); ^{13}C NMR (100 MHz, $CDCl_3$) δ 139.0 & 139.0 (overlap, two isomers), 128.9 & 128.9 (overlap, two isomers), 128.3 & 128.3 (overlap, two isomers), 126.8 & 126.8 (overlap, two isomers), 118.7 & 118.7 (two isomers), 116.9 & 116.8 (two isomers), 62.4 & 62.2 (two isomers), 51.7 & 51.6 (two isomers), 40.2 & 40.2 (two isomers), 35.4 & 35.3 (two isomers), 31.8 & 31.7 (two isomers), 30.7 & 30.7 (two isomers), 24.8 & 24.7 (two isomers). FT-IR: ν (cm^{-1}) 2974, 2930, 2102, 1732, 1455, 1242. HRMS [ESI] m/z: $[M+Na]^+$ calcd for $C_{15}H_{16}NaN_8$ 331.1390; found 331.1388.

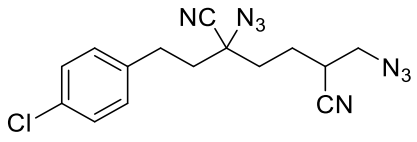


2b: *d.r.* = 1:1, 39.8 mg, 61%, yellow oil, Purification by flash column chromatography on silica gel (eluent: EtOAc/Petroleum ether = 1/5). ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.20-7.14 (m, 2H, two isomers), 7.05-6.97 (m, 2H, two isomers), 3.65-3.54 (m, 2H, two isomers), 2.92-2.78 (m, 3H, two isomers), 2.20-2.08 (m, 2H, two isomers), 2.07-1.82 (m, 4H, two isomers); ^{13}C NMR (100 MHz, $CDCl_3$) δ 161.2 (d, $J_{C\text{-}F}$ = 243.5 Hz) (overlap, two isomers), 134.6 (d, $J_{C\text{-}F}$ = 3.1 Hz, one isomer) & 134.6 (d, $J_{C\text{-}F}$ = 3.2 Hz, one isomer), 129.8 (d, $J_{C\text{-}F}$ = 7.9 Hz) (overlap, two isomers), 118.6 & 118.6 (two isomers), 116.8 & 116.7 (two isomers), 115.7 (d, $J_{C\text{-}F}$ = 21.2 Hz) (overlap, two isomers), 62.3 & 62.1 (two isomers), 51.7 & 51.6 (two isomers), 40.4 & 40.3 (two isomers), 35.5 & 35.4 (two isomers), 31.8 & 31.7 (two isomers), 30.0 & 29.9 (two isomers), 24.9 & 24.6 (two isomers); ^{19}F NMR (376 MHz, $CDCl_3$) δ -116.0 (s, one isomer), -116.0 (s, one isomer). FT-IR: ν (cm^{-1}) 2936, 2103, 1732, 1510, 1241, 1222. HRMS [ESI] m/z: $[M+Na]^+$ calcd for $C_{15}H_{15}FNaN_8$ 349.1296; found 349.1313.

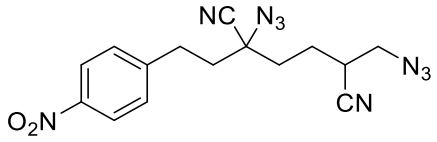


2c: *d.r.* = 1:1, 35.2 mg, 52%, yellow oil, Purification by flash column chromatography on silica gel (eluent: EtOAc/Petroleum ether = 1/5). ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.15-7.09 (m, 2H, two isomers), 6.89-6.83 (m, 2H, two isomers), 3.79 (s, 3H, two isomers), 3.61-3.53 (m, 2H, two isomers), 2.88-2.74 (m, 3H, two isomers), 2.15-2.09 (m, 2H, two isomers), 2.03-1.80 (m, 4H, two isomers); ^{13}C NMR (100 MHz, $CDCl_3$) δ 158.5 & 158.5 (overlap, two isomers), 131.0 & 131.0 (overlap, two isomers), 129.3 & 129.3 (overlap, two isomers), 118.7 & 118.7 (two isomers), 117.0 & 116.8 (two isomers), 114.3 & 114.3 (overlap, two isomers), 62.4 & 62.2 (two isomers), 55.3 & 55.3 (overlap, two isomers), 51.7 & 51.7 (two isomers), 40.5 & 40.4 (two isomers), 35.4 & 35.3 (two isomers), 31.8 & 31.7 (two isomers), 29.9 & 29.8 (two isomers), 24.9 & 24.7 (two isomers). FT-IR: ν (cm^{-1})

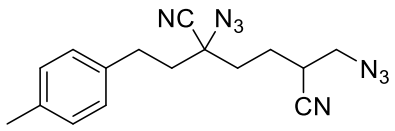
3020, 2932, 2103, 1612, 1513, 1246. HRMS [ESI] m/z: $[M+Na]^+$ calcd for $C_{16}H_{18}N_8NaO$ 361.1496; found 361.1476.



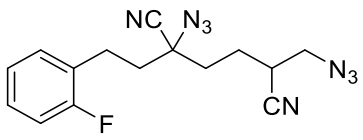
2d: *d.r.* = 1:1, 44.7 mg, 65%, yellow oil, Purification by flash column chromatography on silica gel (eluent: EtOAc/Petroleum ether = 1/5). ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.32-7.27 (m, 2H, two isomers), 7.16-7.12 (m, 2H, two isomers), 3.64-3.54 (m, 2H, two isomers), 2.89-2.80 (m, 3H, two isomers), 2.16-2.07 (m, 2H, two isomers), 2.06-1.82 (m, 4H, two isomers); ^{13}C NMR (100 MHz, $CDCl_3$) δ 137.4 & 137.4 (overlap, two isomers), 132.6 & 132.6 (overlap, two isomers), 129.7 & 129.7 (overlap, two isomers), 129.0 & 129.0 (overlap, two isomers), 118.6 & 118.6 (two isomers), 116.8 & 116.6 (two isomers), 62.3 & 62.1 (two isomers), 51.7 & 51.6 (two isomers), 40.2 & 40.1 (two isomers), 35.5 & 35.4 (two isomers), 31.8 & 31.7 (two isomers), 30.1 & 30.0 (two isomers), 24.9 & 24.6 (two isomers). FT-IR: ν (cm^{-1}) 2924, 2853, 2246, 2103, 1735, 1493, 1248. HRMS [ESI] m/z: $[M+Na]^+$ calcd for $C_{15}H_{15}ClN_8Na$ 365.1000; found 365.1001.



2e: *d.r.* = 1:1, 32.7 mg, 46%, yellow oil. Purification by flash column chromatography on silica gel (eluent: EtOAc/Petroleum ether = 1/5). ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.21-8.16 (m, 2H, two isomers), 7.41-7.36 (m, 2H, two isomers), 3.66-3.57 (m, 2H, two isomers), 3.06-2.93 (m, 2H, two isomers), 2.90-2.82 (m, 1H, two isomers) , 2.24-2.06 (m, 3H, two isomers), 2.06-1.87 (m, 3H, two isomers); ^{13}C NMR (100 MHz, $CDCl_3$) δ 147.0 & 147.0 (overlap, two isomers), 146.6 & 146.6 (overlap, two isomers), 129.3 & 129.3 (overlap, two isomers), 124.1 & 124.1 (overlap, two isomers), 118.6 & 118.6 (two isomers), 116.5 & 116.4 (two isomers), 62.2 & 62.1 (two isomers), 51.7 & 51.6 (two isomers), 39.6 & 39.6 (two isomers), 35.7 & 35.6 (two isomers), 31.8 & 31.7 (two isomers), 30.6 & 30.6 (two isomers), 24.9 & 24.6 (two isomers). FT-IR: ν (cm^{-1}) 2924, 2853, 2103, 1601, 1518, 1456, 1346, 1246. HRMS [ESI] m/z: $[M+Na]^+$ calcd for $C_{15}H_{15}N_9NaO_2$ 376.1241; found 376.1221.

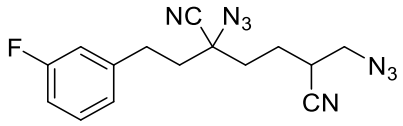


2f: *d.r.* = 1:1, 39.3 mg, 61%, yellow oil. Purification by flash column chromatography on silica gel (eluent: EtOAc/Petroleum ether = 1/5). ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.19-7.05 (m, 4H, two isomers), 3.63-3.53 (m, 2H, two isomers), 2.90-2.77 (m, 3H, two isomers), 2.34 (s, 3H, two isomers), 2.18-2.09 (m, 2H, two isomers), 2.05-1.82 (m, 4H, two isomers); ^{13}C NMR (100 MHz, $CDCl_3$) δ 136.4 & 136.4 (overlap, two isomers), 135.9 & 135.9 (overlap, two isomers), 129.5 & 129.5 (overlap, two isomers), 128.2 & 128.2 (overlap, two isomers), 118.7 & 118.6 (two isomers), 116.9 & 116.8 (two isomers), 62.4 & 62.2 (two isomers), 51.7 & 51.7 (overlap, two isomers), 40.4 & 40.3 (two isomers), 35.4 & 35.3 (two isomers), 31.8 & 31.7 (two isomers), 30.3 & 30.2 (two isomers), 24.9 & 24.7 (two isomers), 21.0 & 21.0 (overlap, two isomers). FT-IR: ν (cm^{-1}) 3021, 2925, 2867, 2246, 2103, 1515, 1455, 1247. HRMS [ESI] m/z: $[M+Na]^+$ calcd for $C_{16}H_{18}N_8Na$ 345.1547; found 345.1552.

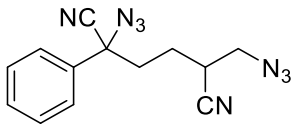


2g: *d.r.* = 1:1, 30.6 mg, 47%, yellow oil. Purification by flash column chromatography on silica gel (eluent: EtOAc/Petroleum

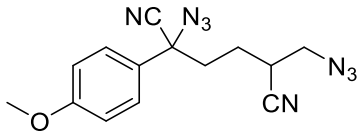
ether = 1/5). ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.28-7.19 (m, 2H, two isomers), 7.13-7.02 (m, 2H, two isomers), 3.65-3.55 (m, 2H, two isomers), 2.93-2.87 (m, 2H, two isomers), 2.87-2.79 (m, 1H, two isomers), 2.20-2.11 (m, 2H, two isomers), 2.08-1.87 (m, 4H, two isomers); ^{13}C NMR (100 MHz, $CDCl_3$) δ 161.1 (d, J_{C-F} = 243.8 Hz) (overlap, two isomers), 130.6 (d, J_{C-F} = 4.8 Hz) (overlap, two isomers), 128.8 (d, J_{C-F} = 8.1 Hz) (overlap, two isomers), 125.9 (d, J_{C-F} = 15.5 Hz) (overlap, two isomers), 124.5 (d, J_{C-F} = 3.6 Hz) (overlap, two isomers), 118.6 & 118.6 (two isomers), 116.8 & 116.7 (two isomers), 115.6 (d, J_{C-F} = 21.4 Hz) (overlap, two isomers), 62.3 & 62.1 (two isomers), 51.7 & 51.7 (two isomers), 38.4 (d, J_{C-F} = 5.1 Hz, one isomer) & 38.4 (d, J_{C-F} = 4.8 Hz, one isomer), 35.2 & 35.1 (two isomers), 31.8 & 31.7 (two isomers), 24.8 & 24.6 (two isomers), 24.5 (d, J_{C-F} = 7.6 Hz, one isomer) & 24.5 (d, J_{C-F} = 7.6 Hz, one isomer)); ^{19}F NMR (376 MHz, $CDCl_3$) δ -118.5 & -118.5 (overlap, two isomers). FT-IR: ν (cm^{-1}) 2983, 2934, 2104, 1732, 1493, 1373, 1239. HRMS [ESI] m/z: $[M+Na]^+$ calcd for $C_{15}H_{15}FNaN_8$ 349.1296; found 349.1284.



2h: *d.r.* = 1:1, 31.1 mg, 48%, yellow oil. Purification by flash column chromatography on silica gel (eluent: EtOAc/Petroleum ether = 1/5). ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.33-7.26 (m, 1H, two isomers), 7.01-6.89 (m, 3H, two isomers), 3.65-3.55 (m, 2H, two isomers), 2.94-2.79 (m, 3H, two isomers), 2.20-2.10 (m, 2H, two isomers), 2.00-1.83 (m, 4H, two isomers); ^{13}C NMR (100 MHz, $CDCl_3$) δ 163.0 (d, J_{C-F} = 244.9 Hz) (overlap, two isomers), 141.5 (d, J_{C-F} = 7.2 Hz) (overlap, two isomers), 130.4 (d, J_{C-F} = 8.5 Hz) (overlap, two isomers), 124.0 (d, J_{C-F} = 2.8 Hz) (two isomers), 118.6 & 118.6 (two isomers), 116.7 & 116.6 (two isomers), 115.3 (d, J_{C-F} = 21.1 Hz) (overlap, two isomers), 113.8 (d, J_{C-F} = 20.8 Hz) (overlap, two isomers), 62.3 & 62.1 (two isomers), 51.7 & 51.6 (two isomers), 40.0 & 39.9 (two isomers), 35.5 & 35.4 (two isomers), 31.8 & 31.7 (two isomers), 30.5 (d, J_{C-F} = 7.8 Hz, one isomer) & 30.4 (d, J_{C-F} = 7.9 Hz, one isomer), 24.9 & 24.7 (two isomers); ^{19}F NMR (376 MHz, $CDCl_3$) δ -112.7 (s, one isomer), -112.7 (s, one isomer). FT-IR: ν (cm^{-1}) 3021, 2932, 2245, 2102, 1589, 1453, 1248. HRMS [ESI] m/z: $[M+Na]^+$ calcd for $C_{15}H_{15}FNaN_8$ 349.1296; found 349.1307.

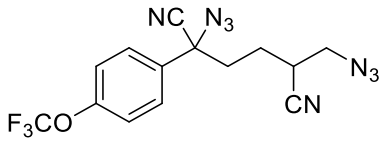


2i: *d.r.* = 1:1, 42.6 mg, 76%, yellow oil. Purification by flash column chromatography on silica gel (eluent: EtOAc/Petroleum ether = 1/5). ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.59-7.45 (m, 5H, two isomers), 3.58-3.48 (m, 2H, two isomers), 2.87-2.70 (m, 1H, two isomers), 2.35-2.02 (m, 2H, two isomers), 2.00-1.89 (m, 1H, two isomers), 1.84-1.69 (m, 1H, two isomers); ^{13}C NMR (100 MHz, $CDCl_3$) δ 134.8 & 134.7 (two isomers), 130.4 & 130.3 (two isomers), 129.7 & 129.7 (overlap, two isomers), 125.5 & 125.5 (overlap, two isomers), 118.7 & 118.7 (two isomers), 117.0 & 116.9 (two isomers), 66.4 & 66.3 (two isomers), 51.7 & 51.6 (two isomers), 39.0 & 38.9 (two isomers), 31.7 & 31.5 (two isomers), 25.1 & 25.0 (two isomers). FT-IR: ν (cm^{-1}) 3021, 2932, 2245, 2099, 1492, 1224. HRMS [ESI] m/z: $[M+Na]^+$ calcd for $C_{13}H_{12}N_8Na$ 303.1077; found 303.1079.

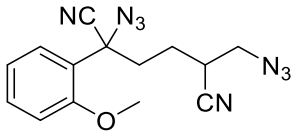


2j: *d.r.* = 1:1, 45.5 mg, 73%, yellow oil. Purification by flash column chromatography on silica gel (eluent: EtOAc/Petroleum ether = 1/5). ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.50-7.44 (m, 2H, two isomers), 7.02-6.97 (m, 2H, two isomers), 3.85 (s, 3H, two

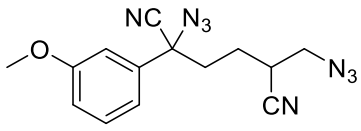
isomers), 3.58-3.48 (m, 2H, two isomers), 2.87-2.69 (m, 1H, two isomers), 2.34-2.00 (m, 2H, two isomers), 1.99-1.86 (m, 1H, one isomer), 1.80-1.65 (m, 1H, one isomer); ^{13}C NMR (100 MHz, $CDCl_3$) δ 160.9 & 160.9 (two isomers), 127.1 & 127.0 (two isomers), 126.5 & 126.3 (two isomers), 118.7 & 118.7 (two isomers), 117.2 & 117.2 (two isomers), 114.9 & 114.9 (two isomers), 66.1 & 65.9 (two isomers), 55.5 & 55.5 (overlap, two isomers), 51.7 & 51.6 (two isomers), 38.8 & 38.7 (two isomers), 31.7 & 31.5 (two isomers), 25.2 & 25.0 (two isomers). FT-IR: ν (cm^{-1}) 2932, 2362, 2331, 2102, 1512, 1256. HRMS [ESI] m/z: $[M+Na]^+$ calcd for $C_{14}H_{14}N_8NaO$ 333.1183; found 333.1196.



2k: *d.r.* = 1:1, 44.0 mg, 60%, yellow oil. Purification by flash column chromatography on silica gel (eluent: EtOAc/Petroleum ether = 1/5). ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.64-7.59 (m, 2H, two isomers), 7.38-7.33 (m, 2H, two isomers), 3.61-3.50 (m, 2H, two isomers), 2.88-2.73 (m, 1H, one isomer), 2.33-2.19 (m, 1H, one isomer), 2.18-2.06 (m, 1H, one isomer), 2.06-1.91 (m, 1H, one isomer), 1.86-1.71 (m, 1H, one isomer); ^{13}C NMR (100 MHz, $CDCl_3$) δ 150.4 (q, J_{C-F} = 1.9 Hz) (overlap, two isomers), 133.6 & 133.4 (two isomers), 127.4 & 127.4 (overlap, two isomers), 121.9 & 121.9 (overlap, two isomers), 120.3 & 120.3 (q, J = 257.2 Hz) (overlap, two isomers), 118.6 &.118.5 (two isomers), 116.5 & 116.5 (two isomers), 65.8 & 65.6 (two isomers), 51.6 & 51.6 (two isomers), 39.2 & 39.0 (two isomers), 31.7 & 31.5 (two isomers), 25.1 & 25.0 (two isomers); ^{19}F NMR (376 MHz, $CDCl_3$) δ -57.8 (s, one isomer), -57.8 (s, one isomer). FT-IR: ν (cm^{-1}) 2933, 2246, 2103, 1734, 1509, 1254, 1211. HRMS [ESI] m/z: $[M+Na]^+$ calcd for $C_{14}H_{11}F_3N_8NaO$ 387.0900; found 387.0902.

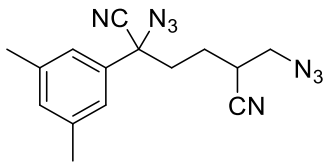


2l: *d.r.* = 1:1, 43.9 mg, 71%, yellow oil. Purification by flash column chromatography on silica gel (eluent: EtOAc/Petroleum ether = 1/5). ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.51-7.41 (m, 2H, two isomers), 7.09-7.01 (m, 2H, two isomers), 3.95 (s, 3H, two isomers), 3.56-3.47 (m, 2H, two isomers), 2.82-2.71 (m, 1H, two isomers), 2.56-2.20 (m, 2H, two isomers), 1.88-1.72 (m, 2H, two isomers); ^{13}C NMR (100 MHz, $CDCl_3$) δ 156.4 & 156.3 (two isomers), 131.6 & 131.6 (two isomers), 127.1 & 126.9 (two isomers), 122.2 & 122.0 (two isomers), 121.3 & 121.3 (two isomers), 118.9 & 118.8 (two isomers), 116.9 &.116.9 (overlap, two isomers), 112.5 & 112.5 (overlap, two isomers), 64.0 & 63.7 (two isomers), 55.9 & 55.9 (overlap, two isomers), 51.7 & 51.7 (two isomers), 35.3 & 35.2 (two isomers), 31.8 & 31.6 (two isomers), 24.9 & 24.7 (two isomers). FT-IR: ν (cm^{-1}) 2926, 2846, 2360, 2244, 2103, 1490, 1252. HRMS [ESI] m/z: $[M+Na]^+$ calcd for $C_{14}H_{14}N_8NaO$ 333.1183; found 333.1200.

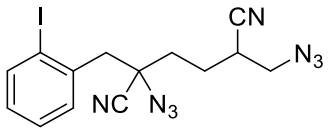


2m: *d.r.* = 1:1, 46.1 mg, 74%, yellow solid. Purification by flash column chromatography on silica gel (eluent: EtOAc/Petroleum ether = 1/5). ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.44-7.38 (m, 1H, two isomers), 7.15-7.11 (m, 1H, two isomers), 7.07-7.04 (m, 1H, two isomers), 7.01-6.97 (m, 1H, two isomers), 3.86 (s, 3H, two isomers), 3.58-3.48 (m, 2H, two isomers), 2.85-2.69 (m, 1H, two isomers), 2.33-2.02 (m, 2H, two isomers), 1.99-1.87 (m, 1H, two isomer), 1.83-1.67 (m, 1H, two isomer); ^{13}C NMR (100 MHz, $CDCl_3$) δ 160.4 & 160.4 (two isomers), 136.2 & 136.1 (two isomers), 130.8 & 130.8 (two isomers), 118.7 &

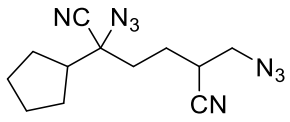
118.7 (two isomers), 117.6 & 117.6 (two isomers), 116.9 & 116.9 (two isomers), 115.5 & 115.4 (two isomers), 111.5 & 111.5 (two isomers), 66.3 & 66.2 (two isomers), 55.5 & 55.5 (overlap, two isomers), 51.7 & 51.6 (two isomers), 38.9 & 38.8 (two isomers), 31.7 & 31.5 (two isomers), 25.1 & 24.9 (two isomers). FT-IR: ν (cm^{-1}) 3021, 2939, 2245, 2104, 1735, 1261, 1225. HRMS [ESI] m/z: $[M+Na]^+$ calcd for $C_{14}H_{14}N_8NaO$ 333.1183; found 333.1197.



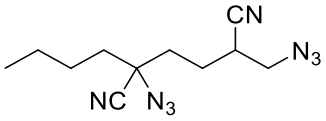
2n: *d.r.* = 1:1, 35.8 mg, 58%, yellow oil. Purification by flash column chromatography on silica gel (eluent: EtOAc/Petroleum ether = 1/5). ^1H NMR (400 MHz, $CDCl_3$) δ 7.14 (s, 2H, two isomers), 7.09 (s, 1H, two isomers), 3.58-3.49 (m, 2H, two isomers), 2.86-2.68 (m, 1H, two isomers), 2.38 (s, 6H, two isomers), 2.32-2.00 (m, 2H, two isomers), 2.00-1.88 (m, 1H, one isomer), 1.83-1.69 (m, 1H, one isomer); ^{13}C NMR (100 MHz, $CDCl_3$) δ 139.5 & 139.5 (overlap, two isomers), 134.6 & 134.5 (two isomers), 132.0 & 131.9 (two isomers), 123.2 & 123.2 (overlap, two isomers), 118.7 & 118.7 (two isomers), 117.2 & 117.1 (two isomers), 66.4 & 66.3 (two isomers), 51.7 & 51.6 (two isomers), 38.9 & 38.8 (two isomers), 31.7 & 31.6 (two isomers), 25.2 & 25.0 (two isomers), 21.4 & 21.4 (overlap, two isomers). FT-IR: ν (cm^{-1}) 3020, 2924, 2247, 2104, 1609, 1455, 1219. HRMS [ESI] m/z: $[M+Na]^+$ calcd for $C_{15}H_{16}N_8Na$ 331.1390; found 331.1405.



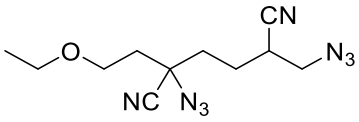
2o: *d.r.* = 1:1, 55.6 mg, 66%, yellow solid. Purification by flash column chromatography on silica gel (eluent: EtOAc/Petroleum ether = 1/5). ^1H NMR (400 MHz, $CDCl_3$) δ 7.93 (dd, *J* = 7.6, 0.4 Hz, 1H, two isomers), 7.49 (dd, *J* = 7.6, 0.4 Hz, 1H, two isomers), 7.39 (ddd, *J* = 7.6, 7.6, 0.8 Hz, 1H, two isomers), 7.05 (ddd, *J* = 7.6, 7.6, 1.2 Hz, 1H, two isomers), 3.62-3.53 (m, 2H, two isomers), 3.42 (s, 2H, two isomers), 2.90-2.78 (m, 1H, two isomers), 2.21-1.86 (m, 4H, two isomers); ^{13}C NMR (100 MHz, $CDCl_3$) δ 140.5 & 140.5 (overlap, two isomers), 135.7 & 135.6 (two isomers), 131.3 & 131.3 (two isomers), 130.2 & 130.2 (overlap, two isomers), 128.9 & 128.9 (overlap, two isomers), 118.7 & 118.6 (two isomers), 116.4 & 116.2 (two isomers), 102.6 & 102.6 (overlap, two isomers), 63.4 & 63.3 (two isomers), 51.7 & 51.7 (overlap, two isomers), 48.1 & 48.0 (two isomers), 35.7 & 35.6 (two isomers), 31.8 & 31.7 (two isomers), 25.1 & 25.0 (two isomers). FT-IR: ν (cm^{-1}) 2977, 2935, 2361, 2106, 1732, 1243. HRMS [ESI] m/z: $[M+Na]^+$ calcd for $C_{14}H_{13}N_8NaI$ 443.0200; found 443.0202.



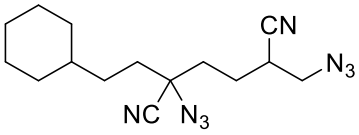
2p: *d.r.* = 1:1, 34.2 mg, 63%, yellow oil. Purification by flash column chromatography on silica gel (eluent: EtOAc/Petroleum ether = 1/5). ^1H NMR (400 MHz, $CDCl_3$) δ 3.64-3.54 (m, 2H, two isomers), 2.92-2.76 (m, 1H, two isomers), 2.76-2.54 (m, 1H, two isomers), 2.34-2.22 (m, 1H, two isomers), 2.15-1.85 (m, 5H, two isomers), 1.85-1.68 (m, 3H, two isomers), 1.68-1.55 (m, 3H, two isomers); ^{13}C NMR (100 MHz, $CDCl_3$) δ 118.7 & 118.7 (two isomers), 116.5 & 116.4 (two isomers), 66.5 & 66.5 (overlap, two isomers), 51.7 & 51.7 (two isomers), 48.4 & 48.4 (overlap, two isomers), 35.1 & 34.9 (two isomers), 31.9 &.31.9 (two isomers), 28.8 & 28.8 (two isomers), 28.1 & 27.9 (two isomers), 25.4 & 25.3 (two isomers), 25.2 & 25.2 (two isomers), 25.0 & 24.8 (two isomers). FT-IR: ν (cm^{-1}) 3649, 2972, 2253, 2109, 1717, 1259. HRMS [ESI] m/z: $[M+Na]^+$ calcd for $C_{12}H_{16}N_8Na$ 295.1390; found 295.1390.



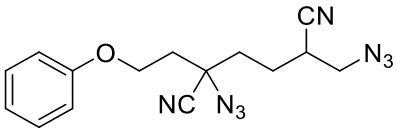
2q: *d.r.* = 1:1, 33.1 mg, 64%, yellow oil. Purification by flash column chromatography on silica gel (eluent: EtOAc/Petroleum ether = 1/5). ^{1}H NMR (400 MHz, $CDCl_3$) δ 3.64-3.53 (m, 2H, two isomers), 2.91-2.75 (m, 1H, two isomers), 2.12-1.70 (m, 6H, two isomers), 1.60-1.47 (m, 2H, two isomers), 1.47-1.35 (m, 2H, two isomers), 0.96 (t, *J* = 7.2 Hz, 3H, two isomers); ^{13}C NMR (100 MHz, $CDCl_3$) δ 118.7 & 118.7 (two isomers), 117.2 & 117.1 (two isomers), 62.6 & 62.4 (two isomers), 51.7 & 51.7 (two isomers), 38.2 & 38.2 (overlap, two isomers), 35.2 & 35.1 (two isomers), 31.8 &.31.8 (two isomers), 26.4 & 26.3 (two isomers), 24.9 & 24.7 (two isomers), 22.3 & 22.3 (overlap, two isomers), 13.8 & 13.8 (overlap, two isomers). FT-IR: ν (cm^{-1}) 2969, 2922, 2361, 2104, 1497, 1259. HRMS [ESI] m/z: $[M+Na]^+$ calcd for $C_{11}H_{16}N_8Na$ 283.1390; found 283.1389.



2r: *d.r.* = 1:1, 24.3 mg, 44%, yellow oil. Purification by flash column chromatography on silica gel (eluent: EtOAc/Petroleum ether = 1/5). ^{1}H NMR (400 MHz, $CDCl_3$) δ 3.66 (t, *J* = 6.0 Hz, 2H, two isomers), 3.63-3.54 (m, 2H, two isomers), 3.51 (q, *J* = 7.2 Hz, 2H, two isomers), 2.87-2.77 (m, 1H, two isomers), 2.23-1.80 (m, 6H, two isomers), 1.22 (t, *J* = 7.2 Hz, 3H, two isomers); ^{13}C NMR (100 MHz, $CDCl_3$) δ 118.7 & 118.7 (two isomers), 117.0 & 116.9 (two isomers), 66.8 & 66.8 (overlap, two isomers), 65.4 & 65.4 (two isomers), 61.5 & 61.3 (two isomers), 51.8 & 51.8 (two isomers), 38.0 & 38.0 (overlap, two isomers), 35.9 & 35.8 (two isomers), 31.8 & 31.8 (two isomers), 24.8 & 24.6 (two isomers), 15.0 & 15.0 (overlap, two isomers). FT-IR: ν (cm^{-1}) 2923, 2851, 2358, 2148, 1459, 1261. HRMS [ESI] m/z: $[M+Na]^+$ calcd for $C_{11}H_{16}N_8NaO$ 299.1339; found 299.1349.

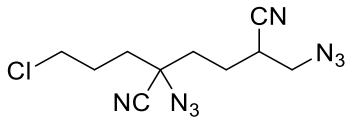


2s: *d.r.* = 1:1, 45.9 mg, 73%, yellow oil. Purification by flash column chromatography on silica gel (eluent: EtOAc/Petroleum ether = 1/5). ^{1}H NMR (400 MHz, $CDCl_3$) δ 3.64-3.54 (m, 2H, two isomers), 2.90-2.70 (m, 1H, two isomers), 2.00-1.84 (m, 5H, two isomers), 1.83-1.62 (m, 6H, two isomers), 1.50-1.35 (m, 2H, two isomers), 1.33-1.09 (m, 5H, two isomers), 1.02-0.85 (m, 1H, two isomers); ^{13}C NMR (100 MHz, $CDCl_3$) δ 118.7 & 118.7 (two isomers), 117.2 & 117.1 (two isomers), 62.8 & 62.6 (two isomers), 51.7 & 51.7 (two isomers), 37.4 & 37.4 (overlap, two isomers), 36.0 & 36.0 (overlap, two isomers), 35.1 &.35.0 (two isomers), 33.1 & 33.1 (two isomers), 31.8 & 31.8 (two isomers), 31.6 & 31.5 (two isomers), 26.4 & 26.4 (overlap, two isomers), 26.1 & 26.1 (overlap, two isomers), 24.9 & 24.6 (two isomers). FT-IR: ν (cm^{-1}) 2975, 2925, 2362, 2103, 1734, 1489, 1245. HRMS [ESI] m/z: $[M+Na]^+$ calcd for $C_{15}H_{22}N_8Na$ 337.1860; found 337.1852.

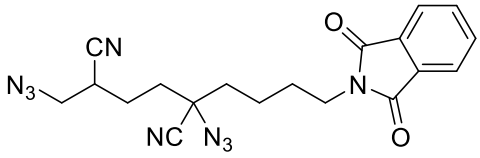


2t: *d.r.* = 1:1, 44.7 mg, 70%, yellow oil. Purification by flash column chromatography on silica gel (eluent: EtOAc/Petroleum ether = 1/5). ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.35-7.28 (m, 2H, two isomers), 7.03-6.98 (m, 1H, two isomers), 6.95-6.90 (m, 2H, two isomers), 4.29-4.19 (m, 2H, two isomers), 3.64-3.54 (m, 2H, two isomers), 2.88-2.79 (m, 1H, two isomers), 2.46-2.30 (m, 2H, two isomers), 2.30-2.10 (m, 1H, two

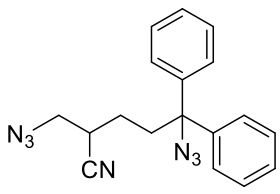
isomers), 2.04-1.91 (m, 3H, two isomers); ^{13}C NMR (100 MHz, $CDCl_3$) δ 157.8 & 157.8 (overlap, two isomers), 129.7 & 129.7 (overlap, two isomers), 121.6 & 121.6 (overlap, two isomers), 118.7 & 118.7 (overlap, two isomers), 116.8 & 116.7 (two isomers), 114.5 & 114.5 (overlap, two isomers), 62.7 & 62.7 (two isomers), 61.2 & 61.0 (two isomers), 51.7 & 51.7 (overlap, two isomers), 37.5 & 37.4 (two isomers), 35.9 & 35.8 (two isomers), 31.8 & 31.8 (two isomers), 24.8 & 24.7 (two isomers). FT-IR: ν (cm^{-1}) 2979, 2937, 2341, 2104, 1732, 1239. HRMS [ESI] m/z: $[M+Na]^+$ calcd for $C_{15}H_{16}N_8NaO$ 347.1339; found 347.1322.



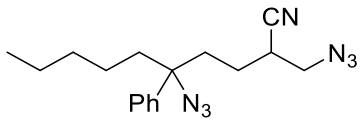
2u: *d.r.* = 1:1, 48.1 mg, 86%, yellow oil. Purification by flash column chromatography on silica gel (eluent: EtOAc/Petroleum ether = 1/5). ^{1}H NMR (400 MHz, $CDCl_3$) δ 3.66-3.55 (m, 3H, two isomers), 3.51-3.44 (m, 1H, two isomers), 2.88-2.80 (m, 1H, two isomers), 2.20-1.99 (m, 5H, two isomers), 1.99-1.81 (m, 3H, two isomers); ^{13}C NMR (100 MHz, $CDCl_3$) δ 118.6 & 118.6 (two isomers), 116.7 & 116.6 (two isomers), 62.1 & 61.9 (two isomers), 51.7 & 51.6 (two isomers), 43.6 & 43.6 (overlap, two isomers), 35.8 & 35.8 (two isomers), 35.5 & 35.3 (two isomers), 31.8 & 31.7 (two isomers), 27.3 & 27.2 (two isomers), 24.8 & 24.6 (two isomers). FT-IR: ν (cm^{-1}) 2983, 2938, 2106, 1733, 1240. HRMS [ESI] m/z: $[M+Na]^+$ calcd for $C_{10}H_{14}ClN_8$ 281.1024; found 281.1015.



2v: *d.r.* = 1:1, 72.8 mg, 90%, yellow oil. Purification by flash column chromatography on silica gel (eluent: EtOAc/Petroleum ether = 1/5). ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.86-7.83 (m, 2H), 7.73-7.71 (m, 2H), 3.72 (t, *J* = 6.8 Hz, 2H), 3.59 (dd, *J* = 6.4, 2.8 Hz, 2H), 2.86-2.82 (m, 1H), 1.98-1.89 (m, 5H), 1.81-1.75 (m, 3H), 1.63-1.56 (m, 2H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 168.4 & 168.4 (overlap, two isomers), 134.1 & 134.1 (overlap, two isomers), 132.0 & 132.0 (overlap, two isomers), 123.4 & 123.4 (overlap, two isomers), 118.7 & 118.6 (two isomers), 117.0 & 116.9 (two isomers), 62.4 & 62.3 (two isomers), 51.7 & 51.7 (overlap, two isomers), 37.7 & 37.6 (two isomers), 37.0 & 37.0 (overlap, two isomers), 35.2 & 35.0 (two isomers), 31.8 & 31.8 (two isomers), 28.0 & 28.0 (overlap, two isomers), 24.8 & 24.6 (two isomers), 21.4 & 21.3 (two isomers). FT-IR: ν (cm^{-1}) 3021, 2939, 2869, 2104, 1771, 1706, 1438. HRMS [ESI] m/z: $[M+Na]^+$ calcd for $C_{19}H_{19}N_9NaO_2$ 428.1554; found 428.1571.

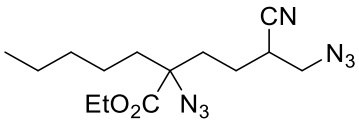


2w: 41.5 mg, 63%, yellow oil. Purification by flash column chromatography on silica gel (eluent: EtOAc/Petroleum ether = 1/5). ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.40-7.34 (m, 4H), 7.34-7.28 (m, 6H), 3.50-3.39 (m, 2H), 2.74-2.62 (m, 2H), 2.53-2.44 (m, 1H), 1.61-1.50 (m, 2H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 142.0, 141.8, 128.7, 128.0, 128.0, 127.0, 126.9, 119.4, 72.0, 51.9, 36.3, 32.3, 24.7. FT-IR: ν (cm^{-1}) 3060, 2933, 2244, 2097, 1773, 1493, 1447, 1252. HRMS [ESI] m/z: $[M+Na]^+$ calcd for $C_{18}H_{17}N_7Na$ 354.1438; found 354.1441.

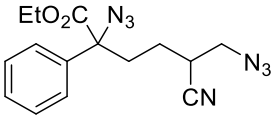


2x: *d.r.* = 1:1, 36.4 mg, 56%, yellow solid. Purification by flash column chromatography on silica gel (eluent: EtOAc/Petroleum

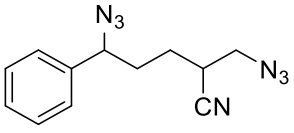
ether = 1/5). ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.44-7.26 (m, 5H, two isomers), 3.50-3.36 (m, 2H, two isomers), 2.78-2.48 (m, 1H, two isomers), 2.26-2.12 (m, 1H, two isomers), 2.06-1.88 (m, 2H, two isomers), 1.74-1.56 (m, 1H, two isomers), 1.44-1.20 (m, 7H, two isomers), 1.14-1.00 (m, 1H, two isomers), 0.84 (t, *J* = 6.8 Hz, 3H, two isomers); ^{13}C NMR (100 MHz, $CDCl_3$) δ 140.5 & 140.5 (overlap, two isomers), 128.7 & 128.7 (overlap, two isomers), 127.5 & 127.4 (two isomers), 125.7 & 125.7 (overlap, two isomers), 119.3 & 119.3 (overlap, two isomers), 69.6 & 69.4 (two isomers), 51.9 & 51.7 (two isomers), 40.3 & 40.0 (two isomers), 37.5 & 37.3 (two isomers), 32.3 & 32.1 (two isomers), 31.8 & 31.8 (overlap, two isomers), 24.4 & 24.3 (two isomers), 23.4 & 23.4 (overlap, two isomers), 22.4 & 22.4 (overlap, two isomers), 13.9 & 13.9 (overlap, two isomers). FT-IR: ν (cm^{-1}) 2932, 2872, 2099, 1976, 1375, 1259. HRMS [ESI] m/z: $[M+Na]^+$ calcd for $C_{17}H_{23}N_7Na$ 348.1907; found 348.1898.



2y: *d.r.* = 1:1, 47.8 mg, 75%, yellow oil. Purification by flash column chromatography on silica gel (eluent: EtOAc/Petroleum ether = 1/5). ^{1}H NMR (400 MHz, $CDCl_3$) δ 4.26 (q, *J* = 7.2 Hz, 2H, two isomers), 3.58-3.47 (m, 2H, two isomers), 2.81-2.70 (m, 1H, two isomers), 2.12-1.54 (m, 6H, two isomers), 1.45-1.20 (m, 9H, two isomers), 0.89 (t, *J* = 6.0 Hz, 3H, two isomers); ^{13}C NMR (100 MHz, $CDCl_3$) δ 171.6 & 171.5 (two isomers), 119.2 & 119.2 (two isomers), 69.3 & 69.0 (two isomers), 62.2 & 62.2 (overlap, two isomers), 51.8 & 51.7 (two isomers), 37.1 & 36.8 (two isomers), 33.4 & 33.2 (two isomers), 32.2 & 32.1 (two isomers), 31.7 & 31.7 (overlap, two isomers), 24.6 & 24.4 (two isomers), 23.5 & 23.5 (two isomers), 22.3 & 22.3 (overlap, two isomers), 14.2 & 14.2 (overlap, two isomers), 13.9 & 13.9 (overlap, two isomers). FT-IR: ν (cm^{-1}) 2962, 2935, 2105, 1976, 1733, 1456, 1259. HRMS [ESI] m/z: $[M+Na]^+$ calcd for $C_{14}H_{23}N_7NaO_2$ 344.1805; found 344.1817.

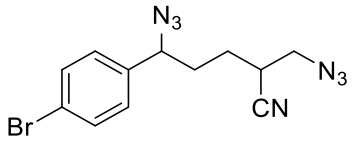


2z: *d.r.* = 1:1, 57.5 mg, 88%, yellow oil. Purification by flash column chromatography on silica gel (eluent: EtOAc/Petroleum ether = 1/5). ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.46-7.34 (m, 5H, two isomers), 4.37-4.28 (m, 2H, two isomers), 3.54-3.44 (m, 2H, two isomers), 2.78-2.69 (m, 1H, two isomers), 2.41-2.04 (m, 2H, two isomers), 1.78-1.59 (m, 2H, two isomers), 1.32 (t, *J* = 7.2 Hz, 3H, one isomer), 1.31 (t, *J* = 7.2 Hz, 3H, one isomer); ^{13}C NMR (100 MHz, $CDCl_3$) δ 170.6 & 170.6 (two isomers), 137.4 & 137.3 (two isomers), 129.2 & 129.2 (overlap, two isomers), 128.9 & 128.9 (two isomers), 125.5 & 125.5 (overlap, two isomers), 119.2 & 119.2 (two isomers), 72.4 & 72.3 (two isomers), 62.7 & 62.7 (overlap, two isomers), 51.8 & 51.7 (two isomers), 36.0 & 36.0 (two isomers), 32.1 & 32.1 (two isomers), 24.7 & 24.6 (two isomers), 14.1 & 14.1 (overlap, two isomers). FT-IR: ν (cm^{-1}) 2983, 2938, 2244, 2106, 1733, 1448, 1241. HRMS [ESI] m/z: $[M+Na]^+$ calcd for $C_{15}H_{17}N_7O_2Na$ 350.1336; found 350.1347.

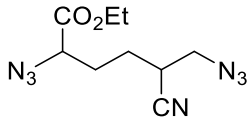


2aa: *d.r.* = 1:1, 27.6 mg, 54%, yellow oil. Purification by flash column chromatography on silica gel (eluent: EtOAc/Petroleum ether = 1/5). ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.48-7.35 (m, 3H, two isomers), 7.35-7.29 (m, 2H, two isomers), 4.50 (dt, *J* = 8.0, 5.6 Hz, 1H, two isomers), 3.56-3.45 (m, 2H, two isomers), 2.80-2.71 (m, 1H, two isomers), 2.10-1.75 (m, 3H, two isomers), 1.71-1.60 (m, 1H, two isomers); ^{13}C NMR (100 MHz, $CDCl_3$) δ 138.6 & 138.6 (overlap,

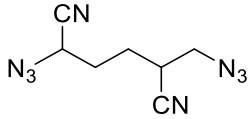
two isomers), 129.1 & 129.1 (overlap, two isomers), 128.8 & 128.7 (two isomers), 126.8 & 126.8 (overlap, two isomers), 119.3 & 119.2 (two isomers), 65.7 & 65.3 (two isomers), 51.9 & 51.8 (two isomers), 33.6 & 33.4 (two isomers), 32.1 & 31.9 (two isomers), 26.6 & 26.2 (two isomers). FT-IR: ν (cm^{-1}) 3024, 2933, 2356, 2245, 2095, 1741, 1454, 1246. HRMS [ESI] m/z: $[M+Na]^+$ calcd for $C_{12}H_{13}N_7Na$ 278.1125; found 278.1130.



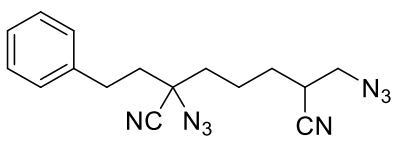
2ab: *d.r.* = 1:1, 28.6 mg, 43%, yellow oil. Purification by flash column chromatography on silica gel (eluent: EtOAc/Petroleum ether = 1/5). ^1H NMR (400 MHz, $CDCl_3$) δ 7.56-7.52 (m, 2H), 7.21-7.17 (m, 2H), 4.51-4.44 (m, 1H), 3.54-3.47 (m, 2H), 2.79-2.73 (m, 1H), 2.04-1.76 (m, 3H), 1.69-1.61 (m, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 137.7 & 137.7 (overlap, two isomers), 132.3 & 132.3 (overlap, two isomers), 128.4 & 128.4 (overlap, two isomers), 122.7 & 122.7 (two isomers), 119.2 & 119.1 (two isomers), 65.1 & 64.7 (two isomers), 51.8 & 51.7 (two isomers), 33.6 & 33.4 (two isomers), 32.1 & 31.8 (two isomers), 26.5 & 26.0 (two isomers). FT-IR: ν (cm^{-1}) 2929, 2095, 1507, 1455, 1245. HRMS [ESI] m/z: $[M+Na]^+$ calcd for $C_{12}H_{12}N_7NaBr$ 356.0230; found 356.0214.



2ac: *d.r.* = 1:1, 20.8 mg, 41%, yellow oil. Purification by flash column chromatography on silica gel (eluent: EtOAc/Petroleum ether = 1/5). ^1H NMR (400 MHz, $CDCl_3$) δ 4.28 (q, *J* = 7.2 Hz, 2H, two isomers), 4.02-3.94 (m, 1H, two isomers), 3.60-3.50 (m, 2H, two isomers), 2.85-2.75 (m, 1H, two isomers), 2.15-1.84 (m, 2H, two isomers), 1.84-1.70 (m, 2H, two isomers), 1.33 (t, *J* = 7.2 Hz, 3H, two isomers); ^{13}C NMR (100 MHz, $CDCl_3$) δ 169.6 & 169.6 (two isomers), 119.1 & 119.0 (two isomers), 62.3 & 62.3 (overlap, two isomers), 61.4 & 61.1 (two isomers), 51.8 & 51.7 (two isomers), 32.0 & 31.8 (two isomers), 28.6 & 28.4 (two isomers), 26.0 & 25.6 (two isomers), 14.2 & 14.2 (overlap, two isomers). FT-IR: ν (cm^{-1}) 2920, 2851, 2362, 2335, 2104, 1736, 1647, 1260. HRMS [ESI] m/z: $[M+Na]^+$ calcd for $C_9H_{13}N_7NaO_2$ 274.1023; found 274.1037.



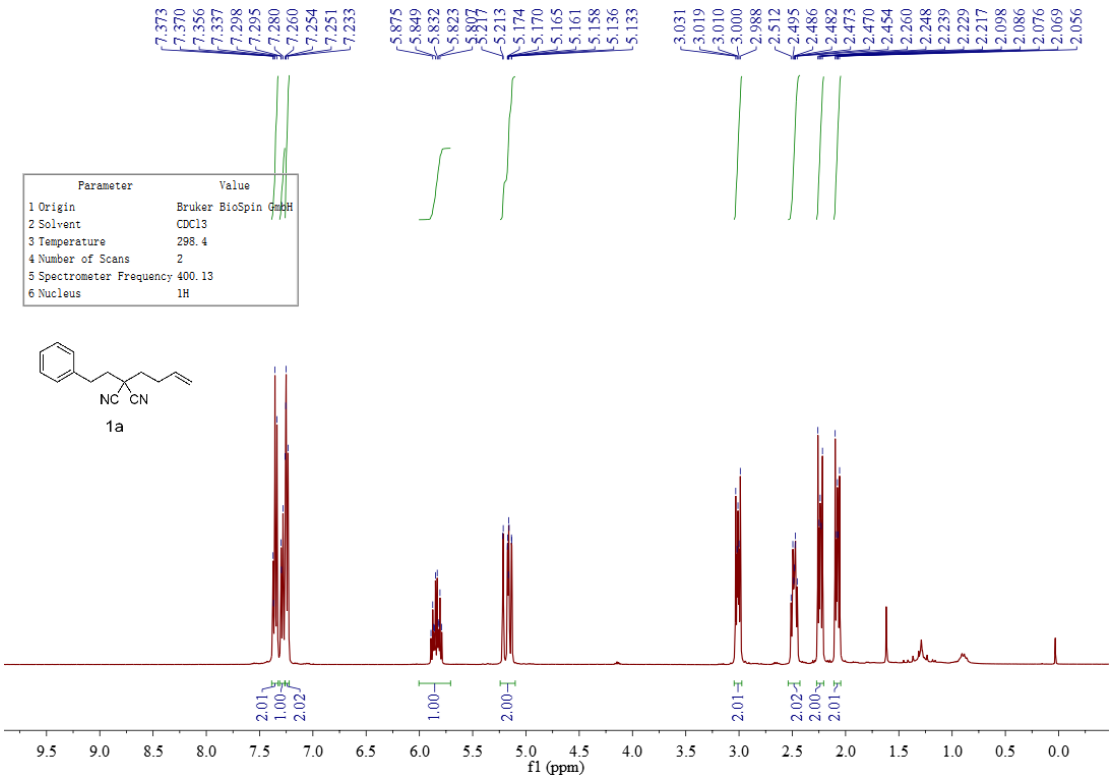
2ad: *d.r.* = 1:1, 22.9 mg, 56%, yellow oil. Purification by flash column chromatography on silica gel (eluent: EtOAc/Petroleum ether = 1/5). ^1H NMR (400 MHz, $CDCl_3$) δ 4.41-4.36 (m, 1H, two isomers), 3.64-3.54 (m, 2H, two isomers), 2.88-2.79 (m, 1H, two isomers), 2.18-2.07 (m, 1H, two isomers), 2.04-1.93 (m, 1H, two isomers), 1.93-1.85 (m, 2H, two isomers); ^{13}C NMR (100 MHz, $CDCl_3$) δ 118.6 & 118.6 (overlap, two isomers), 115.4 & 115.4 (overlap, two isomers), 51.6 & 51.6 (overlap, two isomers), 50.5 & 50.4 (two isomers), 31.6 & 31.6 (two isomers), 30.1 & 30.0 (two isomers), 25.3 & 25.2 (two isomers). FT-IR: ν (cm^{-1}) 2974, 2935, 2361, 2102, 1419, 1243. HRMS [ESI] m/z: $[M+Na]^+$ calcd for $C_7H_7N_8Na$ 227.0764; found 227.0772.

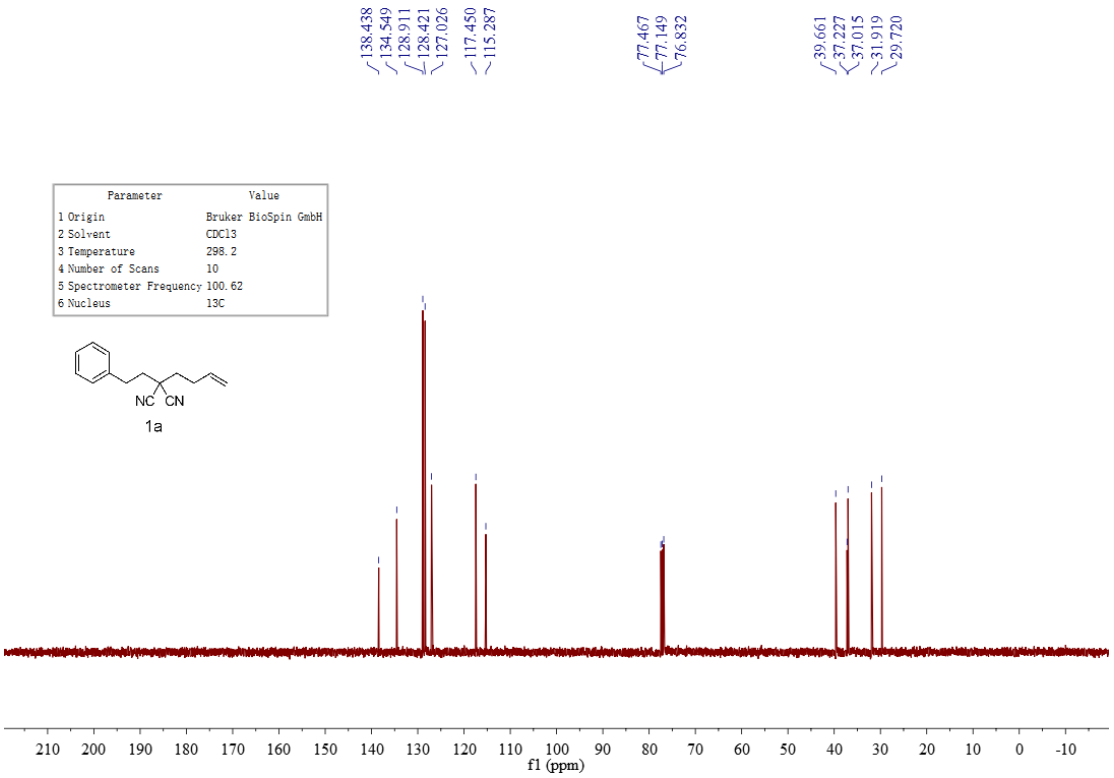


4: *d.r.* = 1:1, 28.0 mg, 44%, yellow oil. Purification by flash column chromatography on silica gel (eluent: EtOAc/Petroleum ether = 1/5). ^1H NMR (400 MHz, $CDCl_3$) δ 7.36-7.29 (m, 2H, two isomers), 7.26-7.17 (m, 3H, two isomers), 3.61-3.51 (m, 2H, two isomers), 2.93-2.72 (m, 3H, two isomers), 2.18-2.05 (m, 2H, two isomers), 1.96-1.78 (m, 3H, two isomers), 1.78-1.64 (m, 3H, two isomers); ^{13}C NMR (100 MHz,

$CDCl_3$) δ 139.3 & 139.3 (overlap, two isomers), 128.8 & 128.8 (overlap, two isomers), 128.4 & 128.4 (overlap, two isomers), 126.7 & 126.7 (overlap, two isomers), 119.1 & 119.1 (overlap, two isomers), 117.3 & 117.3 (overlap, two isomers), 62.6 & 62.6 (two isomers), 51.7 & 51.7 (two isomers), 40.1 & 40.0 (two isomers), 37.5 & 37.5 (two isomers), 32.1 & 32.1 (two isomers), 30.8 & 30.8 (overlap, two isomers), 29.0 & 29.0 (overlap, two isomers), 22.0 & 21.9 (two isomers). FT-IR: ν (cm^{-1}) 2975, 2933, 2361, 2103, 1976, 1497, 1258. HRMS [ESI] m/z: $[M+Na]^+$ calcd for $C_{16}H_{18}N_8Na$ 345.1547; found 345.1541.

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

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128.911
128.421
127.026
117.450
115.287
77.467
77.149
76.832
39.661
37.227
37.015
31.919
29.720
Parameter Value
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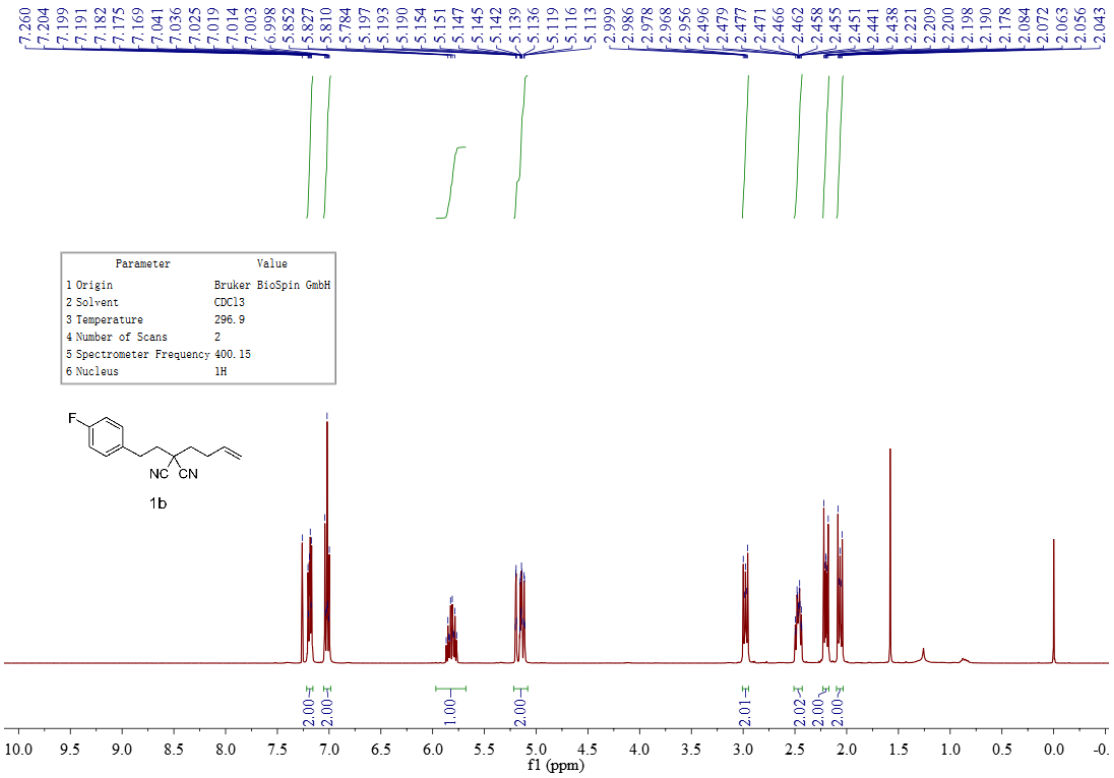
2 Solvent CDCl3
3 Temperature 298.2
4 Number of Scans 10
5 Spectrometer Frequency 100.62
6 Nucleus 13C
NC CN
1a
f1 (ppm)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7.199
7.191
7.182
7.175
7.169
7.041
7.036
7.025
7.019
7.014
7.003
6.998
5.852
5.827
5.810
5.784
5.197
5.193
5.190
5.154
5.151
5.147
5.145
5.142
5.139
5.136
5.119
5.116
5.113
2.999
2.986
2.978
2.968
2.956
2.496
2.479
2.477
2.471
2.466
2.462
2.458
2.455
2.451
2.441
2.438
2.221
2.209
2.200
2.198
2.190
2.178
2.084
2.072
2.063
2.056
2.043
Parameter Value
1 Origin Bruker BioSpin GmbH
2 Solvent CDCl3
3 Temperature 296.9
4 Number of Scans 2
5 Spectrometer Frequency 400.15
6 Nucleus 1H
F
NC CN
1b
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1.00
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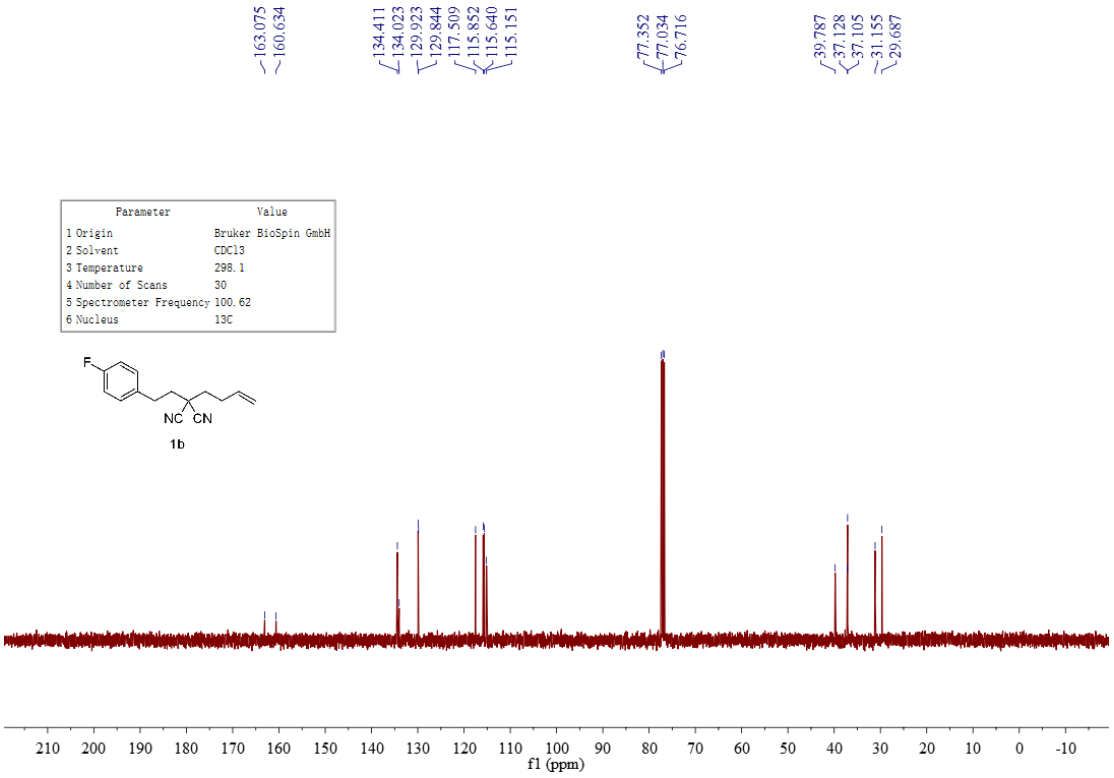
2.02
2.00
2.00
f1 (ppm)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160.634
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134.023
129.923
129.844
117.509
115.852
115.640
115.151
77.352
77.034
76.716
39.787
37.128
37.105
31.155
29.687
Parameter Value
1 Origin Bruker BioSpin GmbH
2 Solvent CDCl3
3 Temperature 298.1
4 Number of Scans 30
5 Spectrometer Frequency 100.62
6 Nucleus 13C
F
NC CN
1b
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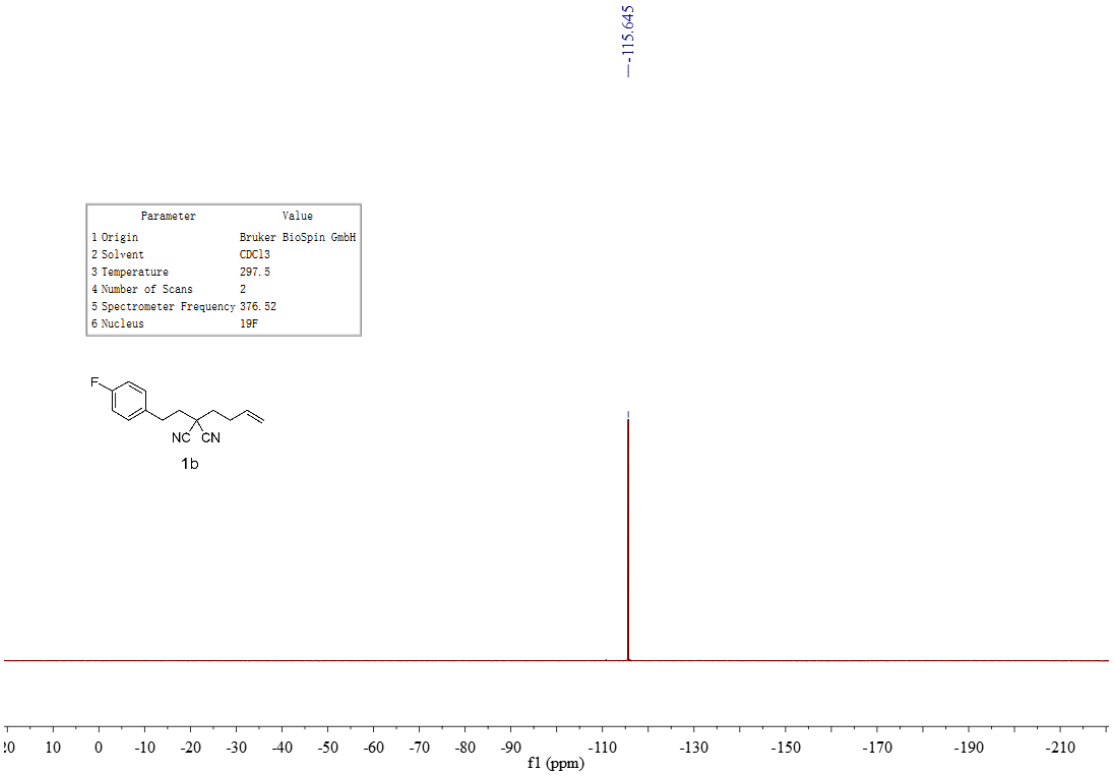
f1 (ppm)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3 Temperature 297.5
4 Number of Scans 2
5 Spectrometer Frequency 376.52
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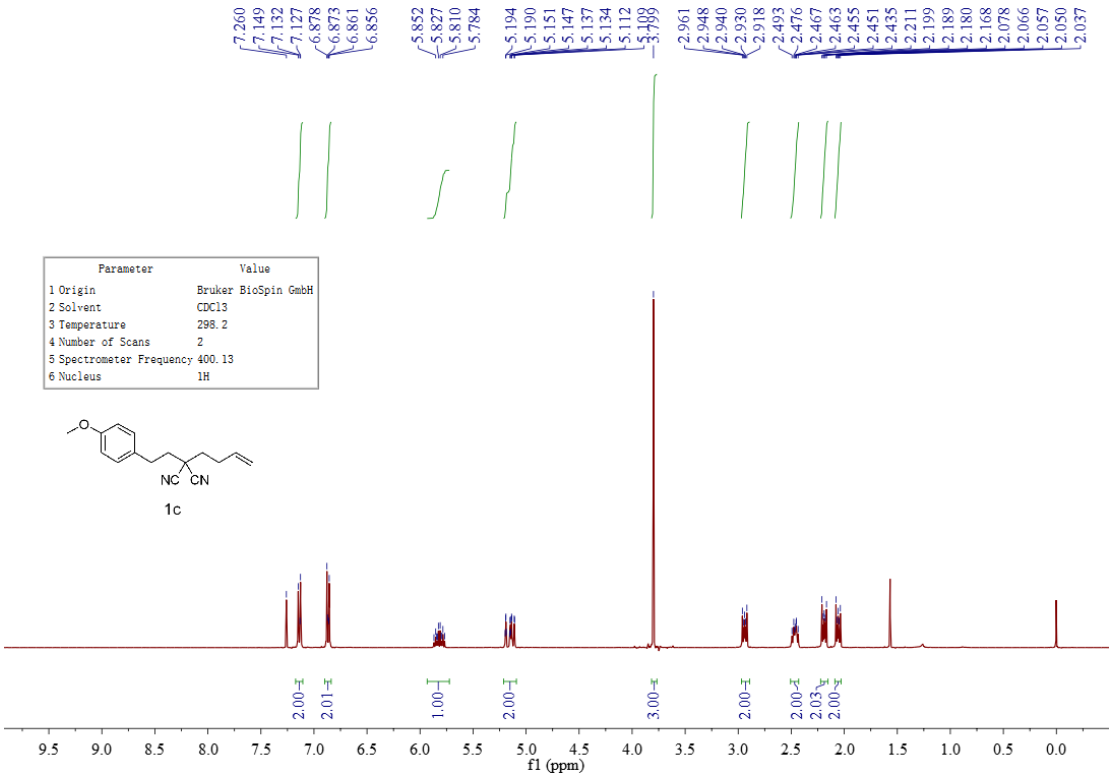
NC CN
1b
10 10 0 -10 -20 -30 -40 -50 -60 -70 -80 -90 -110 -130 -150 -170 -190 -210
f1 (ppm)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6.861
6.856
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5.827
5.810
5.784
5.194
5.190
5.151
5.147
5.137
5.134
5.112
5.109
3.799
2.961
2.948
2.940
2.930
2.918
2.493
2.476
2.467
2.463
2.455
2.451
2.435
2.211
2.199
2.189
2.180
2.168
2.078
2.066
2.057
2.050
2.037
Parameter Value
1 Origin Bruker BioSpin GmbH
2 Solvent CDCl3
3 Temperature 298.2
4 Number of Scans 2
5 Spectrometer Frequency 400.13
6 Nucleus 1H
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1c
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1.00
2.00
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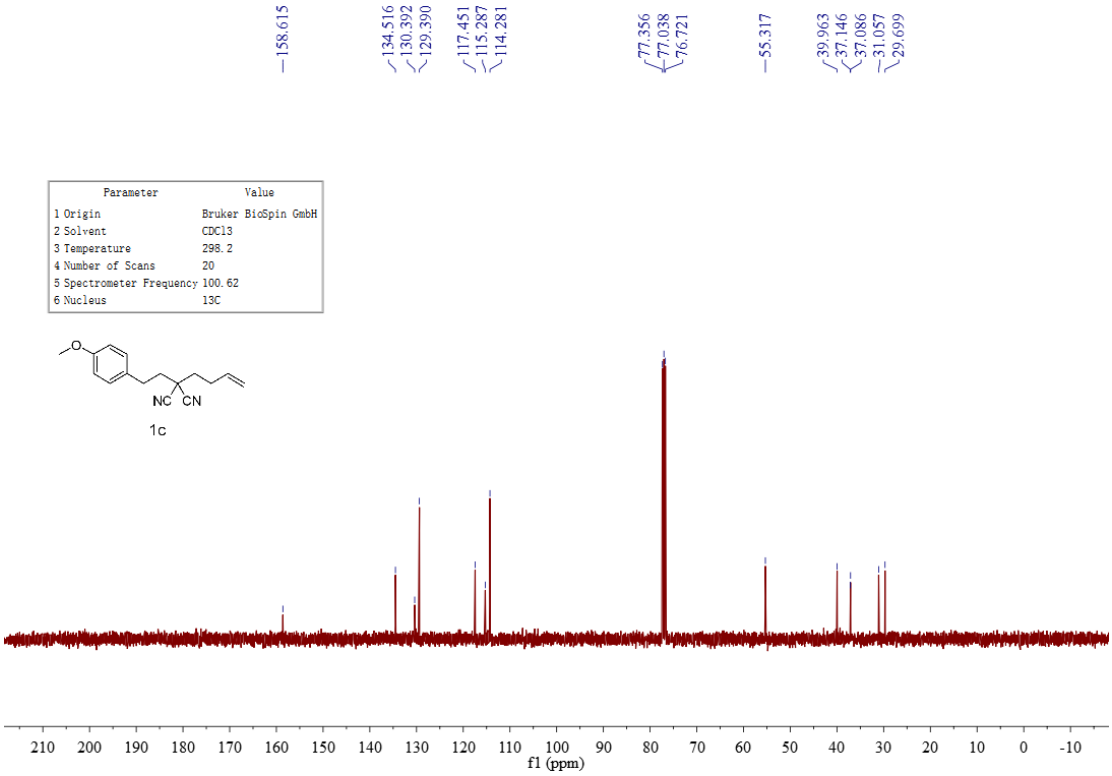
2.00
2.00
2.03
2.00
f1 (ppm)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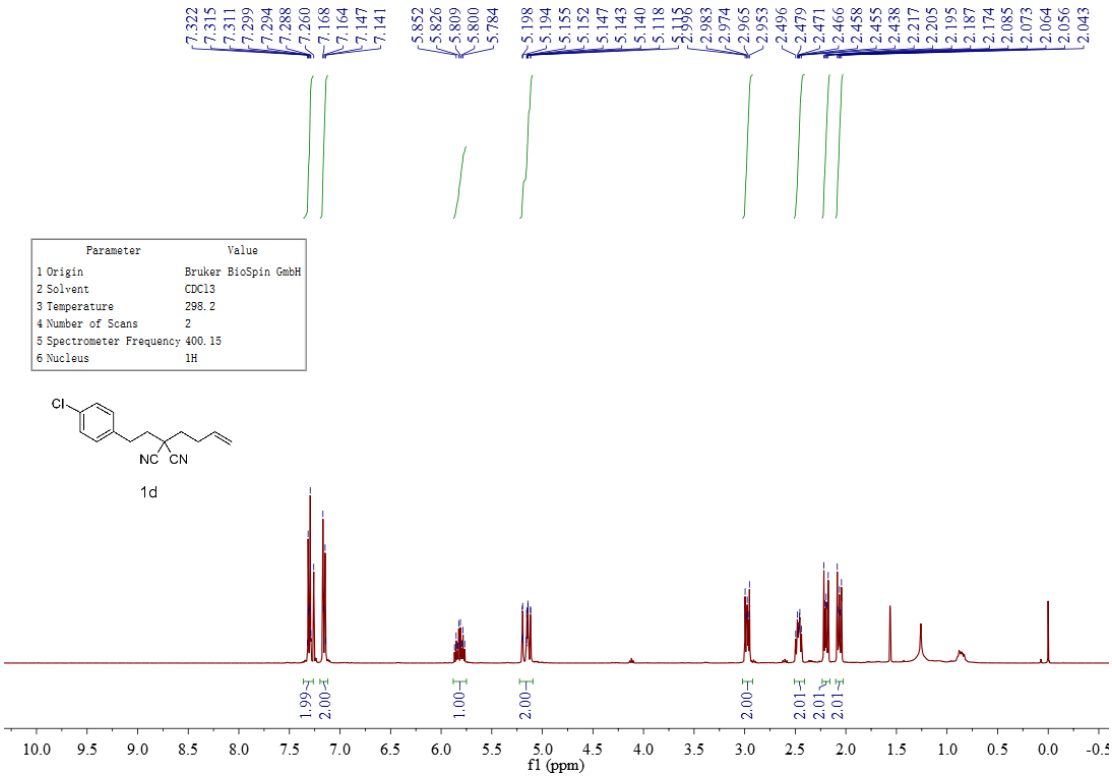
115.287
114.281
77.356
77.038
76.721
55.317
39.963
37.146
37.086
31.057
29.699
Parameter Value
1 Origin Bruker BioSpin GmbH
2 Solvent CDCl3
3 Temperature 298.2
4 Number of Scans 20
5 Spectrometer Frequency 100.62
6 Nucleus 13C
NC CN
1c
f1 (ppm)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7.294
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7.164
7.147
7.141
5.852
5.826
5.809
5.800
5.784
5.198
5.194
5.155
5.152
5.147
5.143
5.140
5.118
2.983
2.974
2.965
2.953
2.496
2.479
2.471
2.466
2.458
2.455
2.438
2.217
2.205
2.195
2.187
2.174
2.085
2.073
2.064
2.056
2.043
Parameter Value
1 Origin Bruker BioSpin GmbH
2 Solvent CDCl3
3 Temperature 298.2
4 Number of Scans 2
5 Spectrometer Frequency 400.15
6 Nucleus 1H
Cl
NC CN
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1.00
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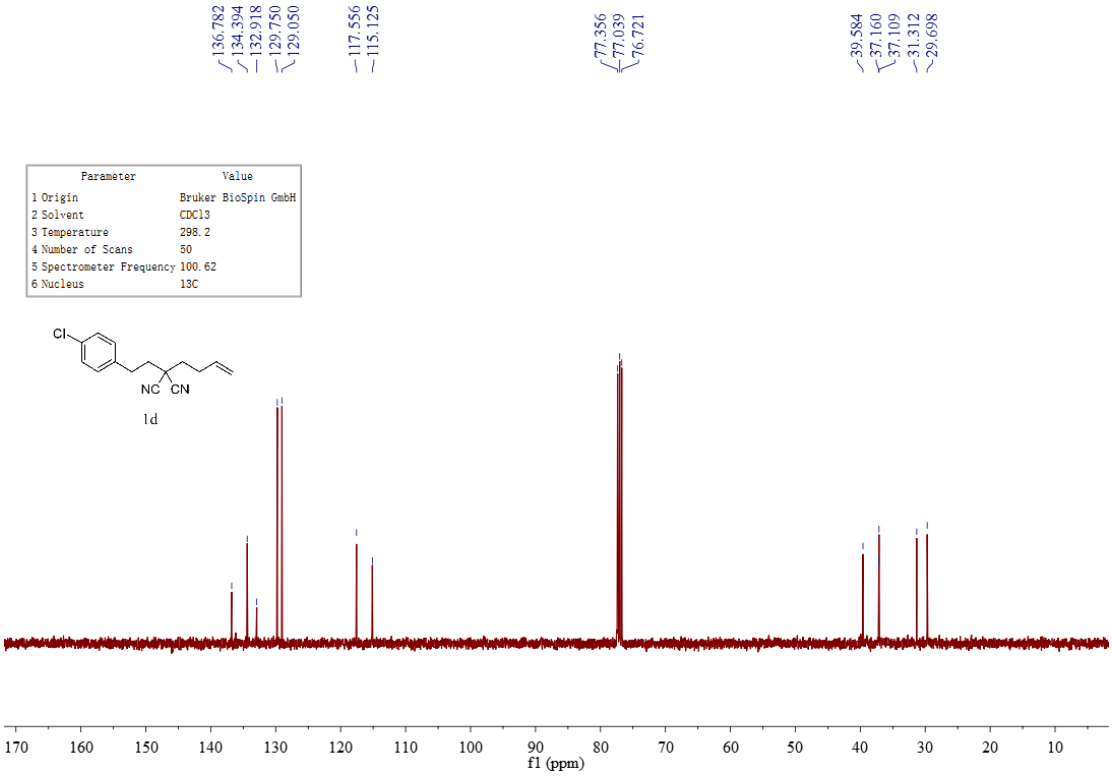
2.01
2.01
f1 (ppm)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115.125
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37.160
37.109
31.312
29.698
Parameter Value
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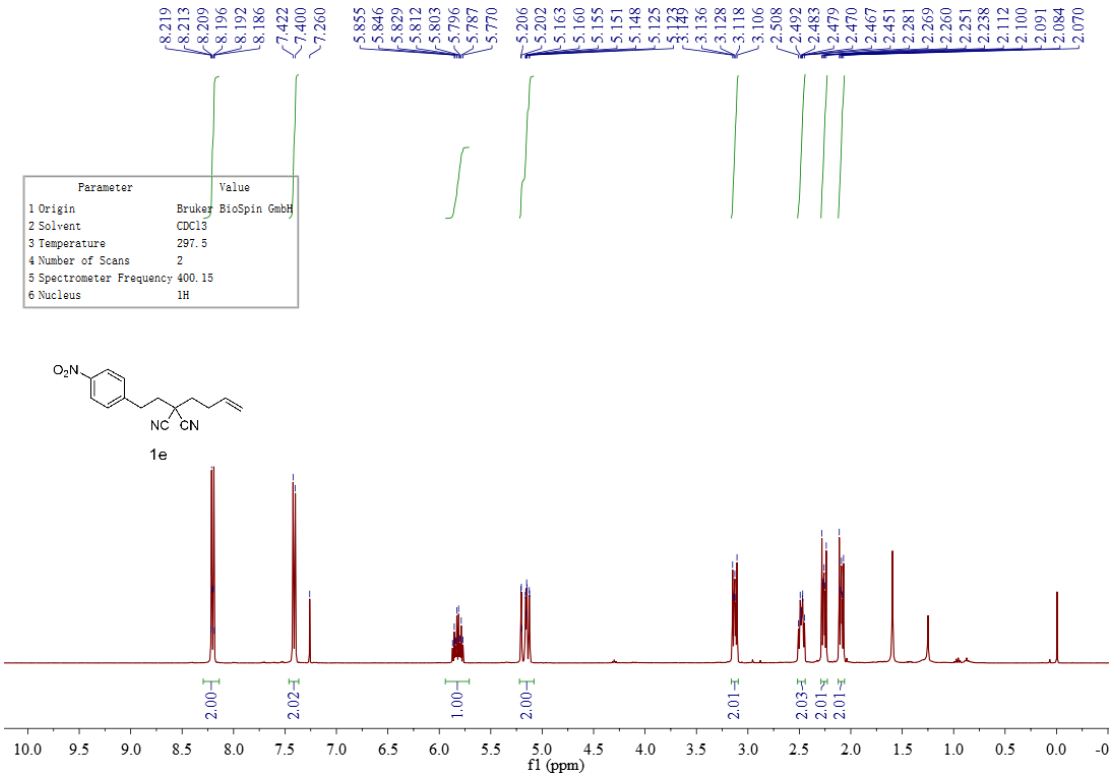
4 Number of Scans 50
5 Spectrometer Frequency 100.62
6 Nucleus 13C
Cl
NC CN
1d
f1 (ppm)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5.812
5.803
5.796
5.787
5.770
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5.202
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5.160
5.155
5.151
5.148
5.125
5.123
3.149
3.136
3.128
3.118
3.106
2.508
2.492
2.483
2.479
2.470
2.467
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2.269
2.260
2.251
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2.100
2.091
2.084
2.070
Parameter Value
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2 Solvent CDCl3
3 Temperature 297.5
4 Number of Scans 2
5 Spectrometer Frequency 400.15
6 Nucleus 1H
O2N
NC CN
1e
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2.02
1.00
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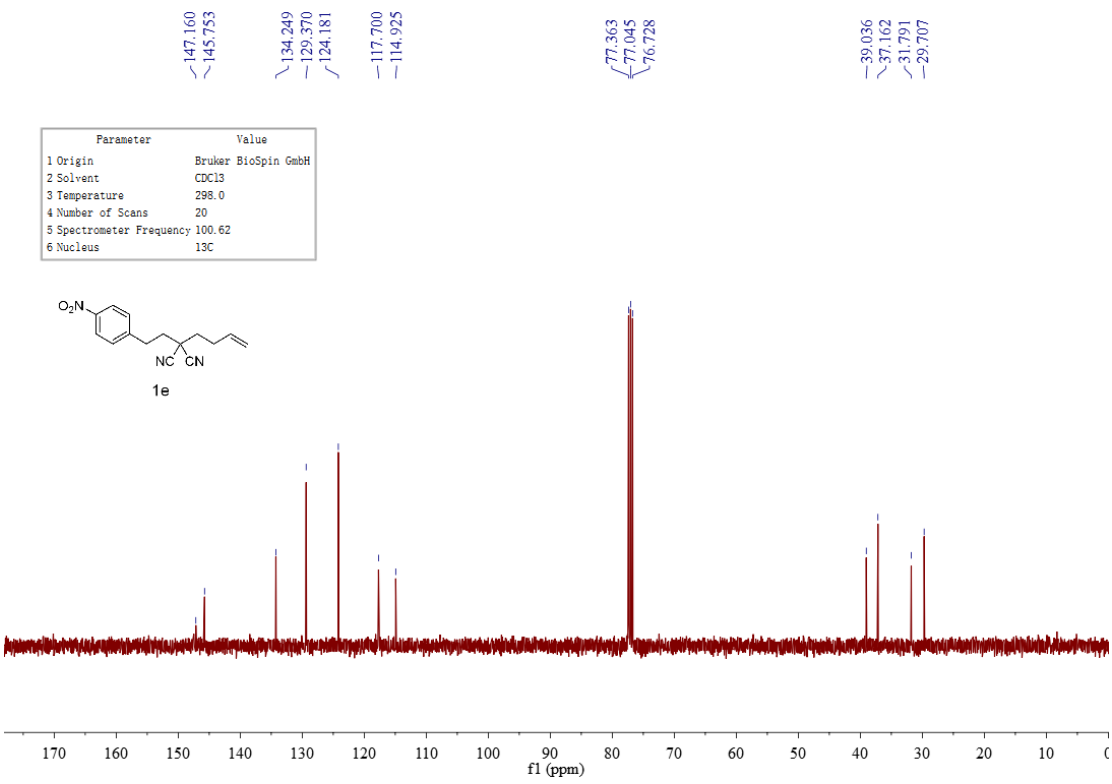
2.01
2.01
10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0
f1 (ppm)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76.728
39.036
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31.791
29.707
Parameter Value
1 Origin Bruker BioSpin GmbH
2 Solvent CDCl3
3 Temperature 298.0
4 Number of Scans 20
5 Spectrometer Frequency 100.62
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O2N
NC CN
1e
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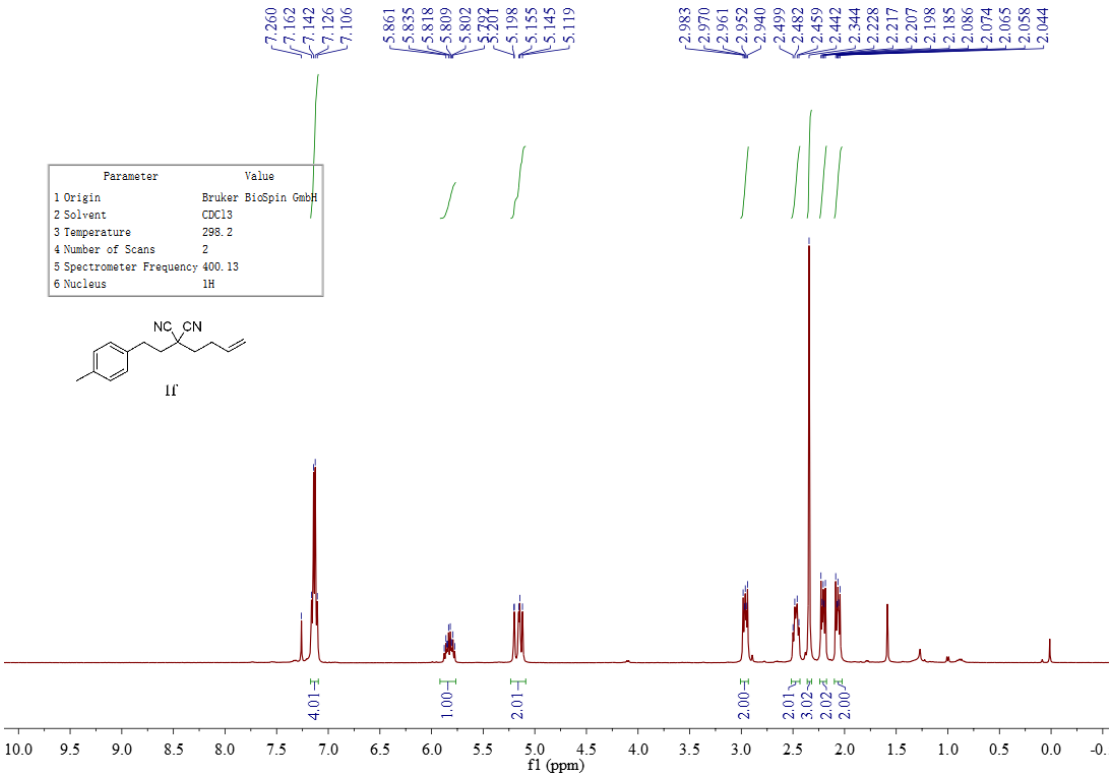
f1 (ppm)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5.155
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2.970
2.961
2.952
2.940
2.499
2.482
2.459
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2.344
2.228
2.217
2.207
2.198
2.185
2.086
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2.065
2.058
2.044
Parameter Value
1 Origin Bruker BioSpin GmbH
2 Solvent CDCl3
3 Temperature 298.2
4 Number of Scans 2
5 Spectrometer Frequency 400.13
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NC CN
1f
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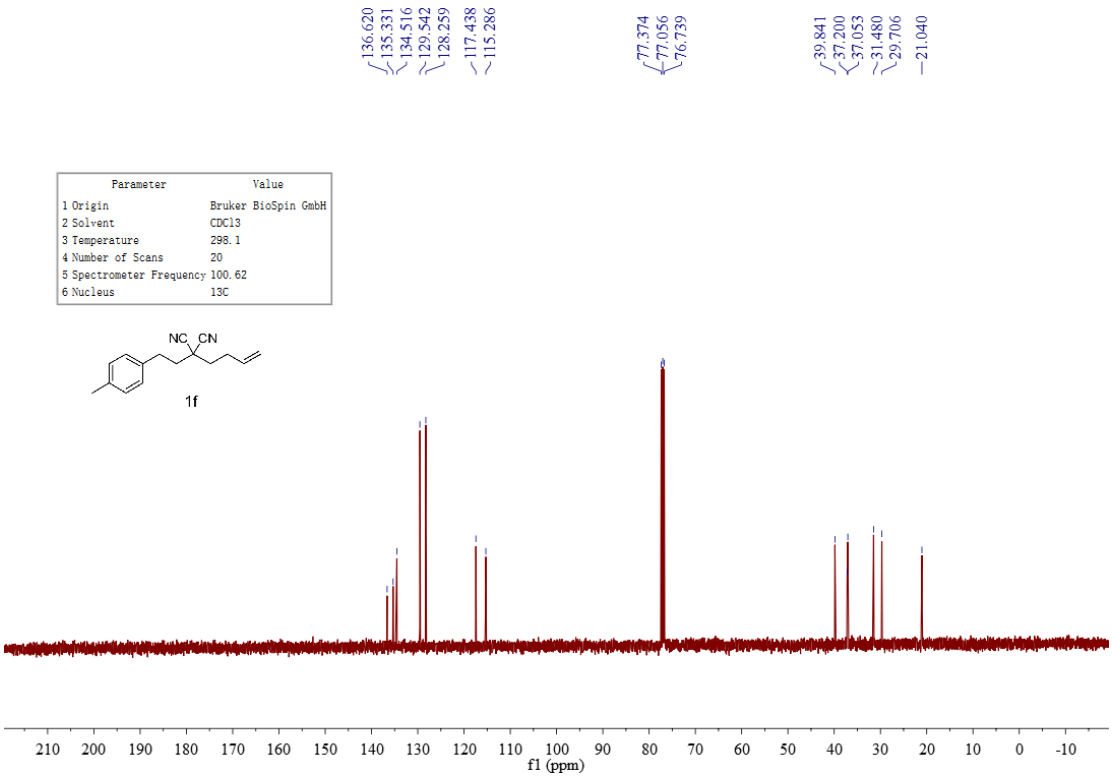
2.01
2.00
2.01
3.02
2.02
2.00
f1 (ppm)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128.259
117.438
115.286
77.374
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76.739
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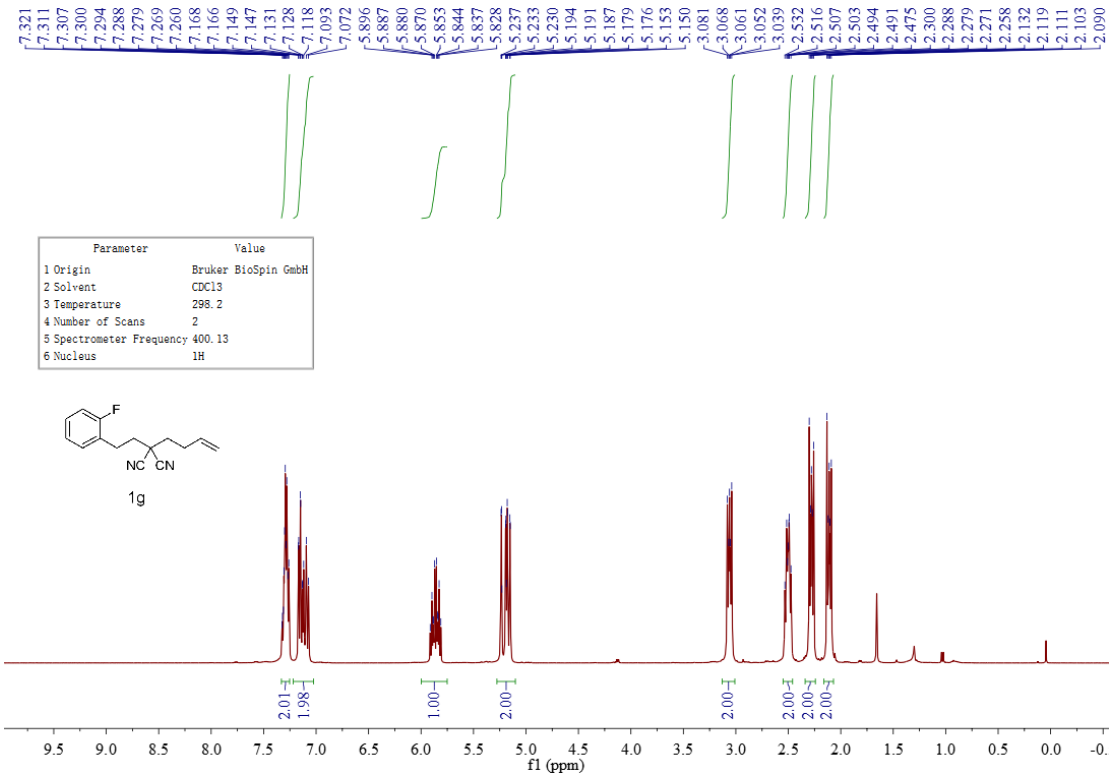
37.200
37.053
31.480
29.706
21.040
Parameter Value
1 Origin Bruker BioSpin GmbH
2 Solvent CDCl3
3 Temperature 298.1
4 Number of Scans 20
5 Spectrometer Frequency 100.62
6 Nucleus 13C
NC CN
1f
f1 (ppm)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7.147
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7.128
7.118
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7.072
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5.880
5.870
5.853
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5.233
5.230
5.194
5.191
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5.179
5.176
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5.150
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3.068
3.061
3.052
3.039
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2.516
2.507
2.503
2.494
2.491
2.475
2.300
2.288
2.279
2.271
2.258
2.132
2.119
2.111
2.103
2.090
Parameter Value
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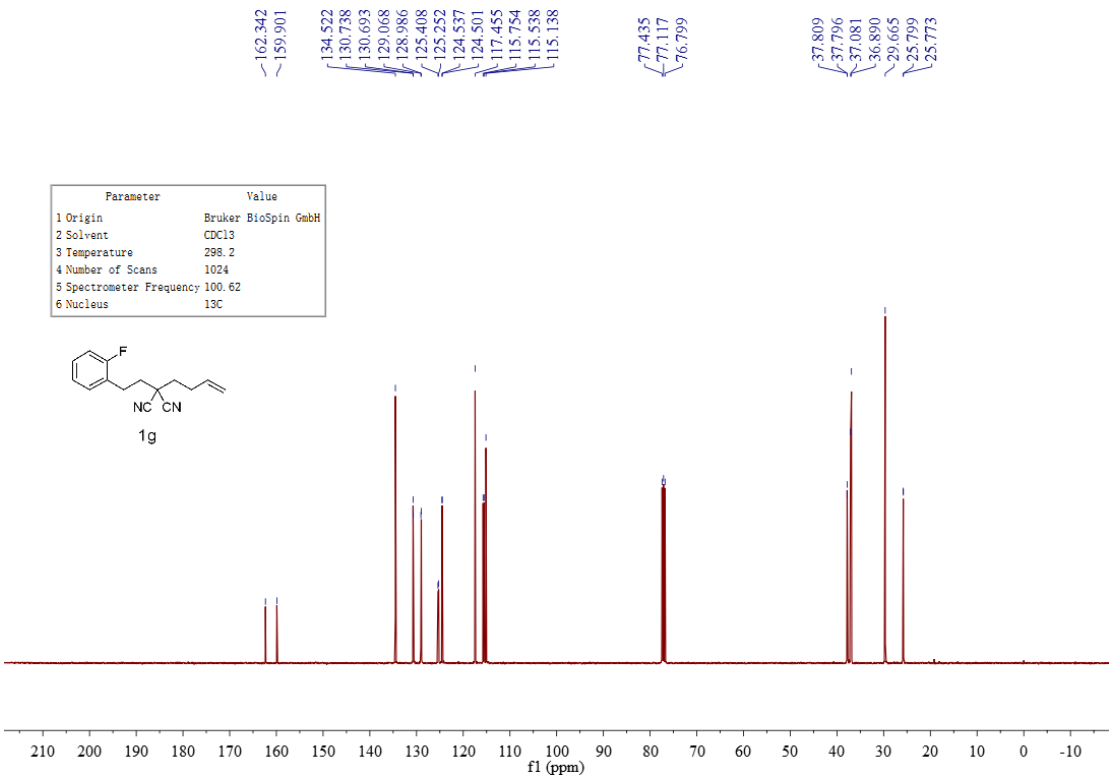
2 Solvent CDCl3
3 Temperature 298.2
4 Number of Scans 2
5 Spectrometer Frequency 400.13
6 Nucleus 1H
F
NC CN
1g
2.01
1.98
1.00
2.00
2.00
2.00
2.00
2.00
9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.
f1 (ppm)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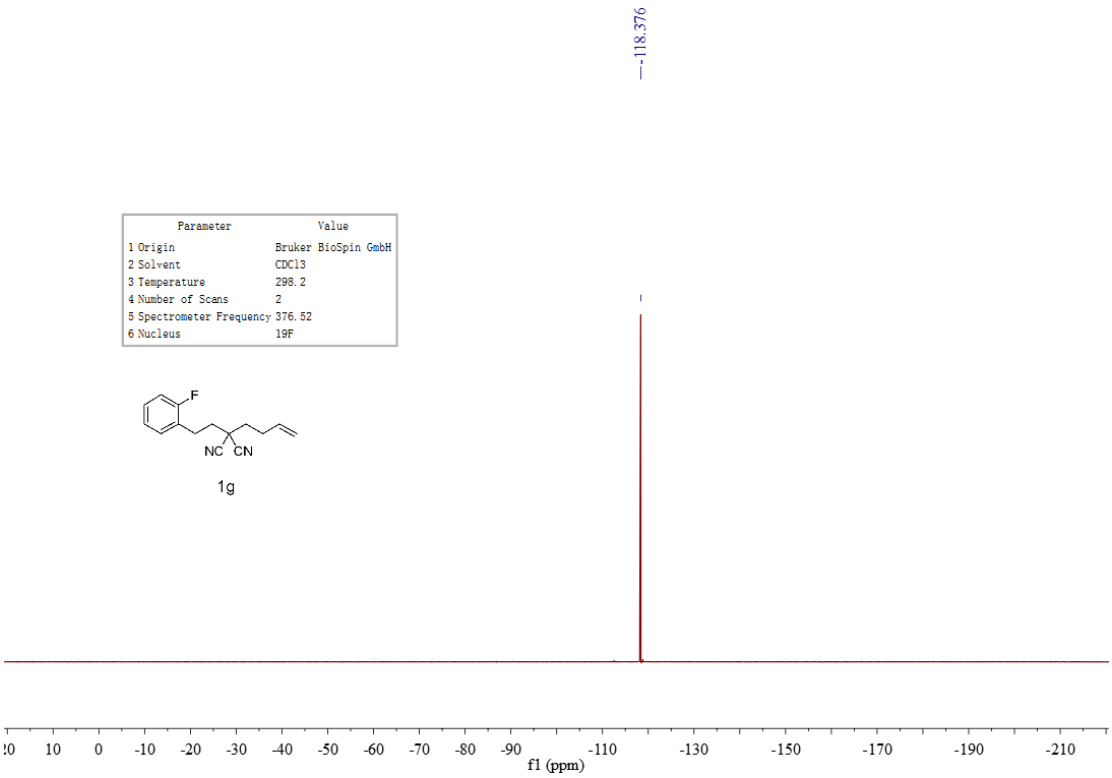
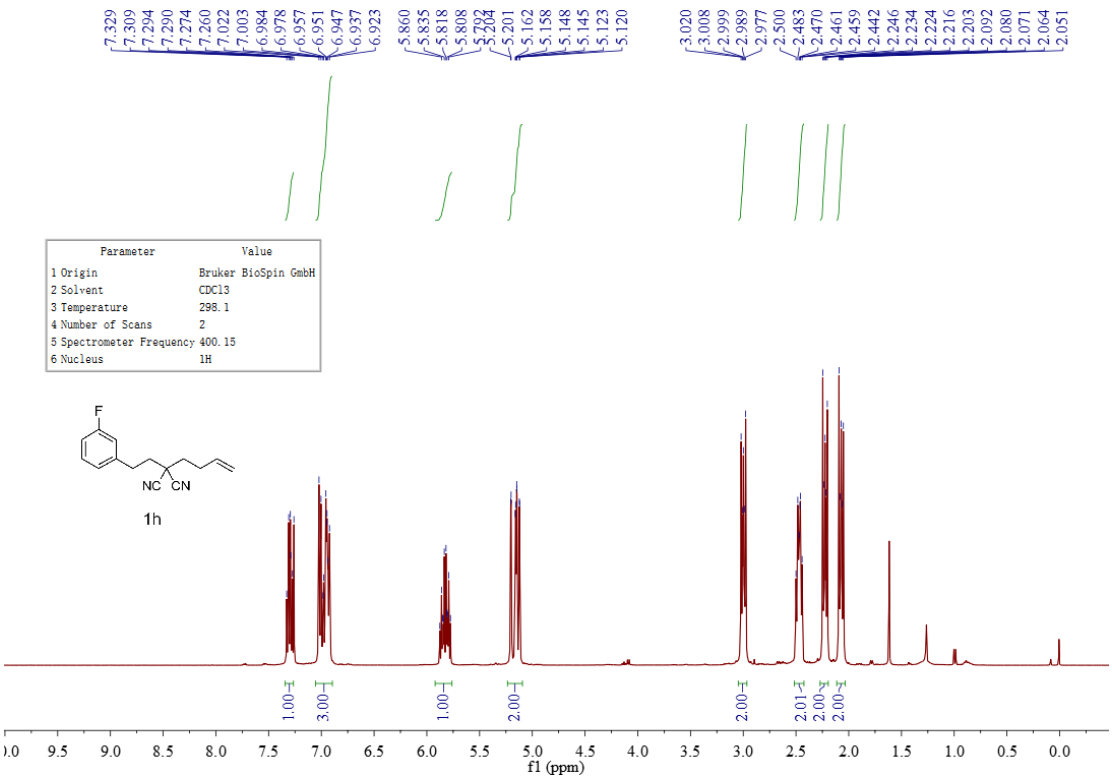
77.117
76.799
37.809
37.796
37.081
36.890
29.665
25.799
25.773
Parameter Value
1 Origin Bruker BioSpin GmbH
2 Solvent CDCl3
3 Temperature 298.2
4 Number of Scans 1024
5 Spectrometer Frequency 100.62
6 Nucleus 13C
F
NC CN
1g
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)


-118.376
Parameter Value
1 Origin Bruker BioSpin GmbH
2 Solvent CDCl3
3 Temperature 298.2
4 Number of Scans 2
5 Spectrometer Frequency 376.52
6 Nucleus 19F
F
NC CN
1g
f1 (ppm)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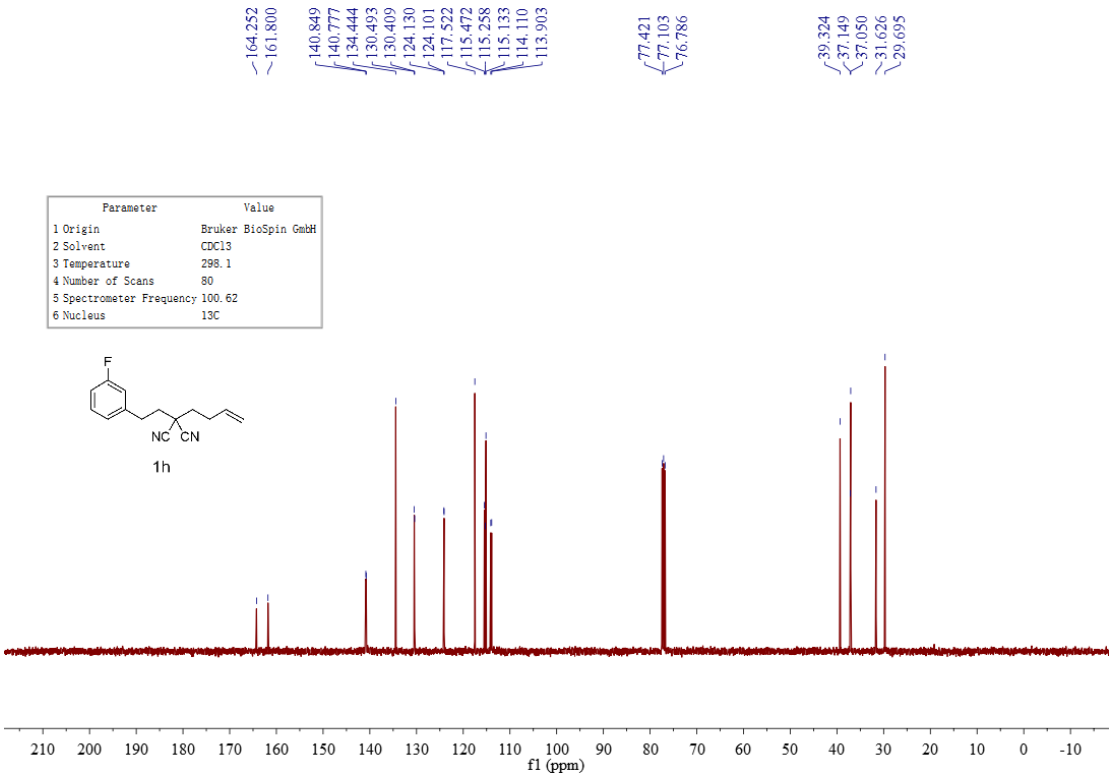
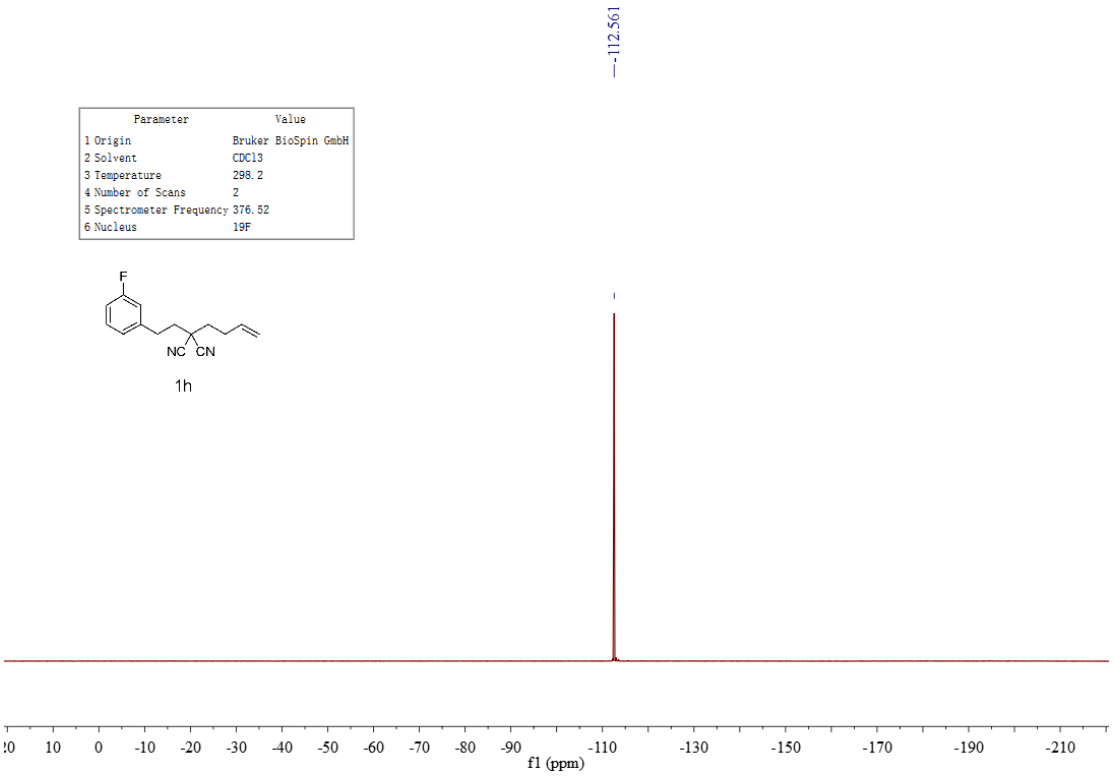
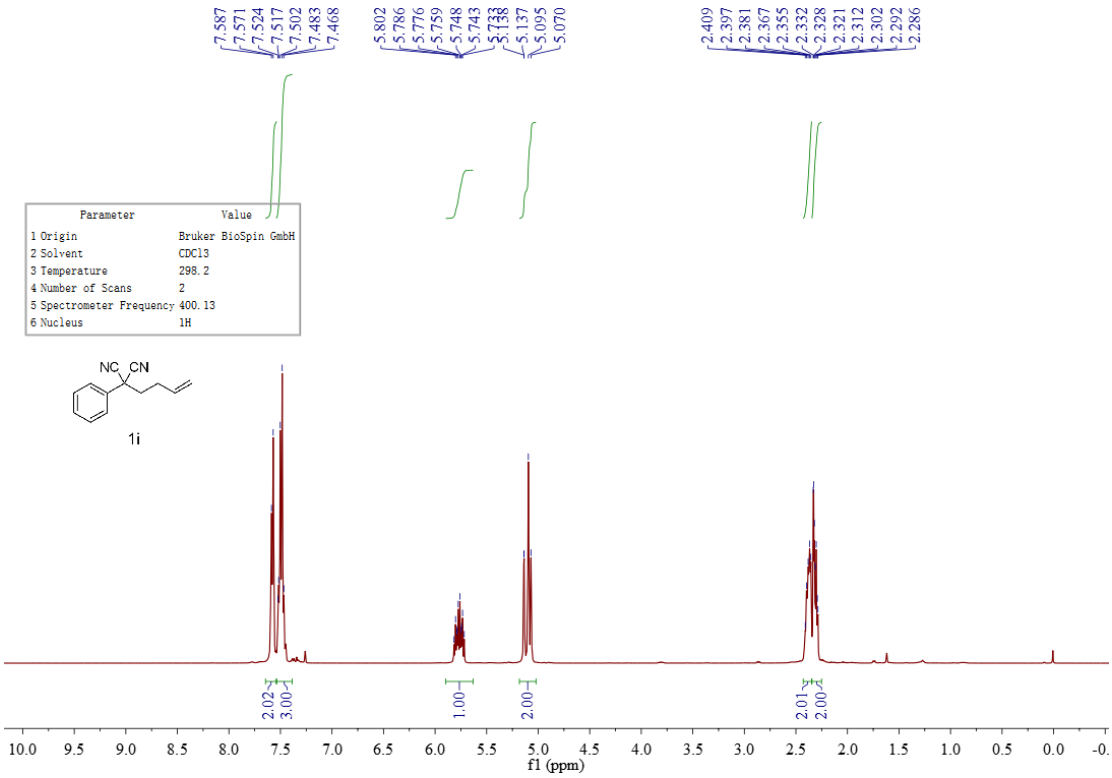
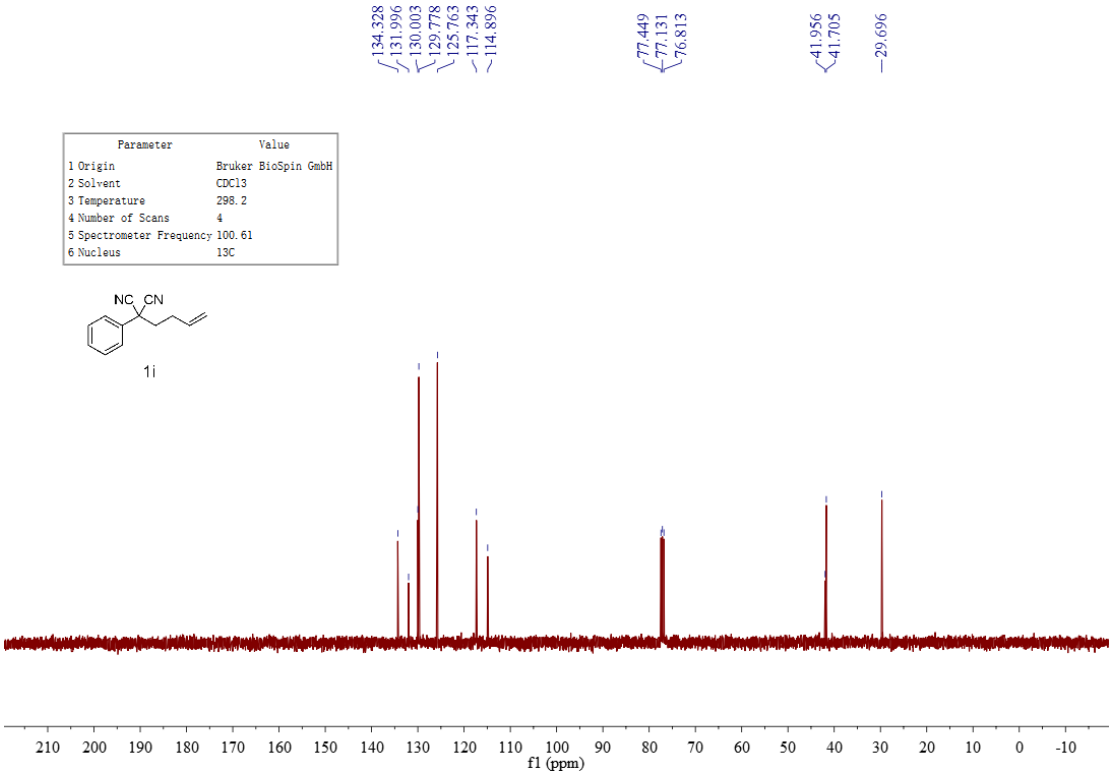
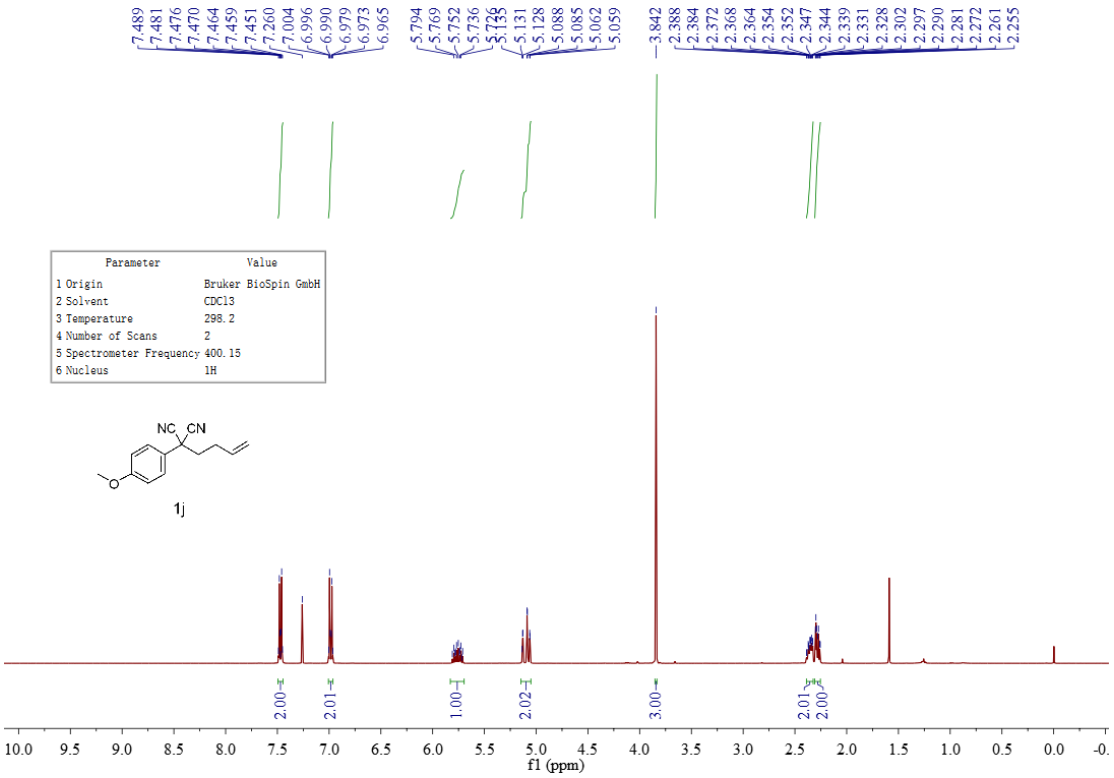
7.309
7.294
7.290
7.274
7.260
7.022
7.003
6.984
6.978
6.957
6.951
6.947
6.937
6.923
5.860
5.835
5.818
5.808
5.792
5.204
5.201
5.162
5.158
5.148
5.145
5.123
5.120
3.020
3.008
2.999
2.989
2.977
2.500
2.483
2.470
2.461
2.459
2.442
2.246
2.234
2.224
2.216
2.203
2.092
2.080
2.071
2.064
2.051
Parameter Value
1 Origin Bruker BioSpin GmbH
2 Solvent CDCl3
3 Temperature 298.1
4 Number of Scans 2
5 Spectrometer Frequency 400.15
6 Nucleus 1H
F
NC CN
1h
1.00
3.00
1.00
2.00
2.00
2.01
2.00
2.00
f1 (ppm)

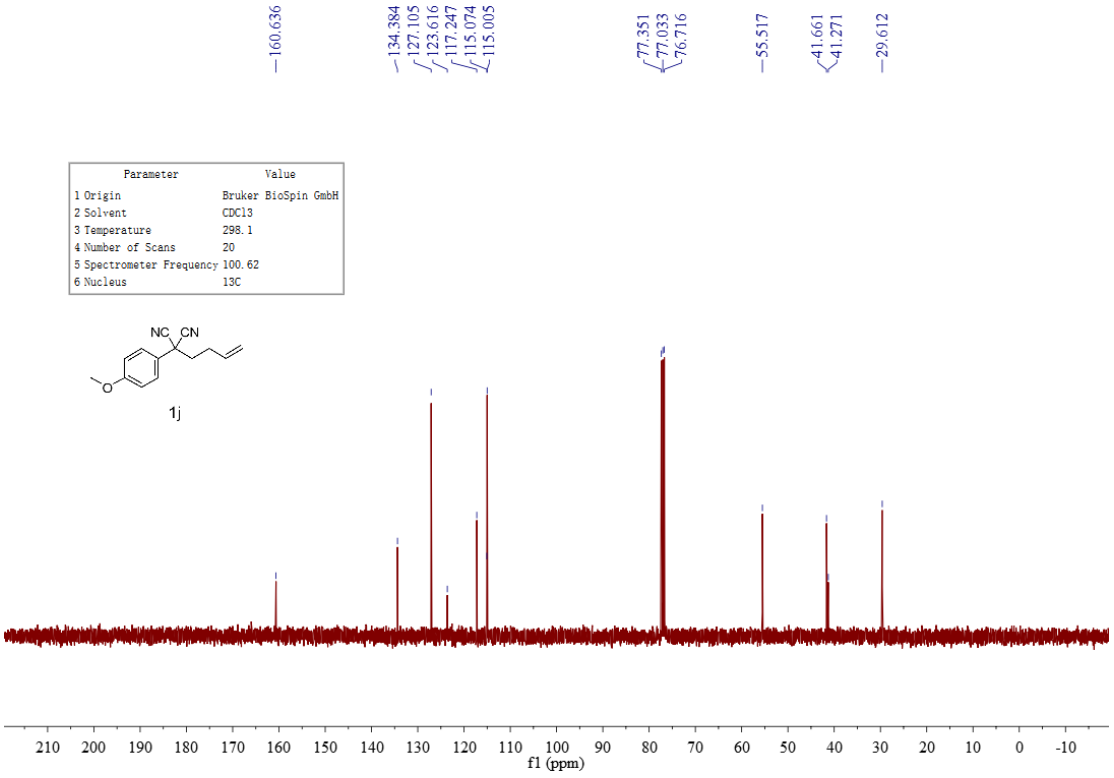

164.252
161.800
140.849
140.777
134.444
130.493
130.409
124.130
124.101
117.522
115.472
115.258
115.133
114.110
113.903
77.421
77.103
76.786
39.324
37.149
37.050
31.626
29.695
Parameter Value
1 Origin Bruker BioSpin GmbH
2 Solvent CDCl3
3 Temperature 298.1
4 Number of Scans 80
5 Spectrometer Frequency 100.62
6 Nucleus 13C
F
NC CN
1h
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)

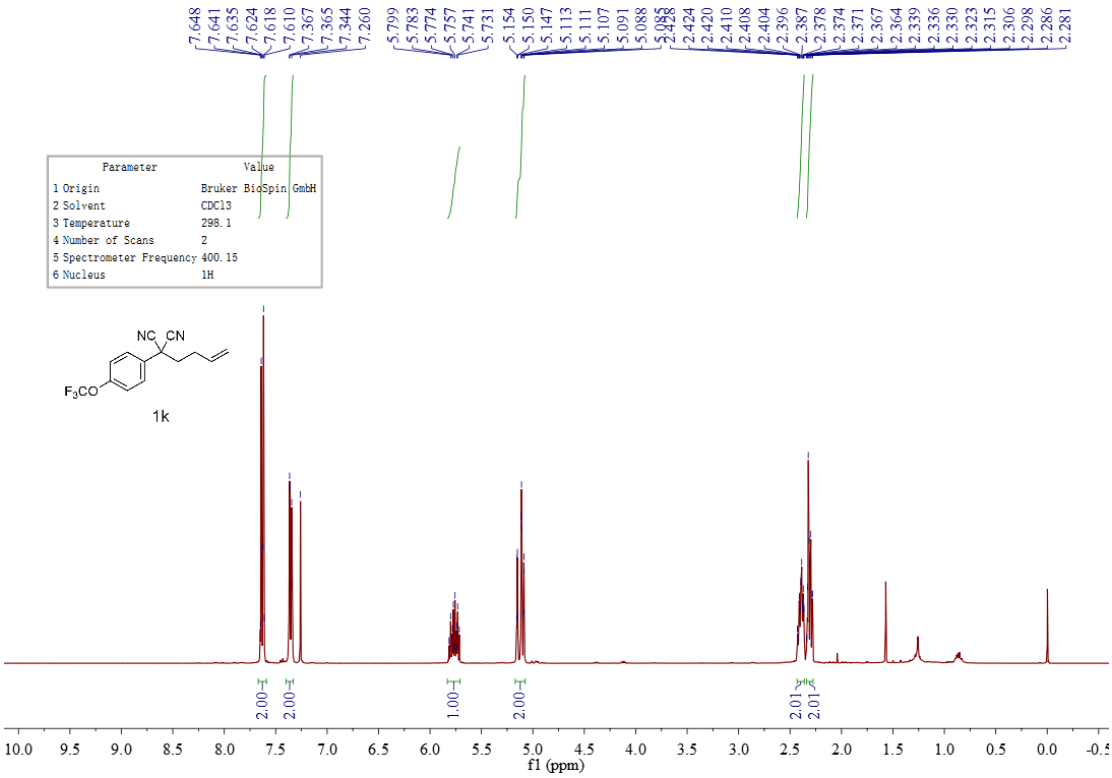

-112.561
Parameter Value
1 Origin Bruker BioSpin GmbH
2 Solvent CDCl3
3 Temperature 298.2
4 Number of Scans 2
5 Spectrometer Frequency 376.52
6 Nucleus 19F
F
NC CN
1h
10 10 0 -10 -20 -30 -40 -50 -60 -70 -80 -90 -110 -130 -150 -170 -190 -210
f1 (ppm)

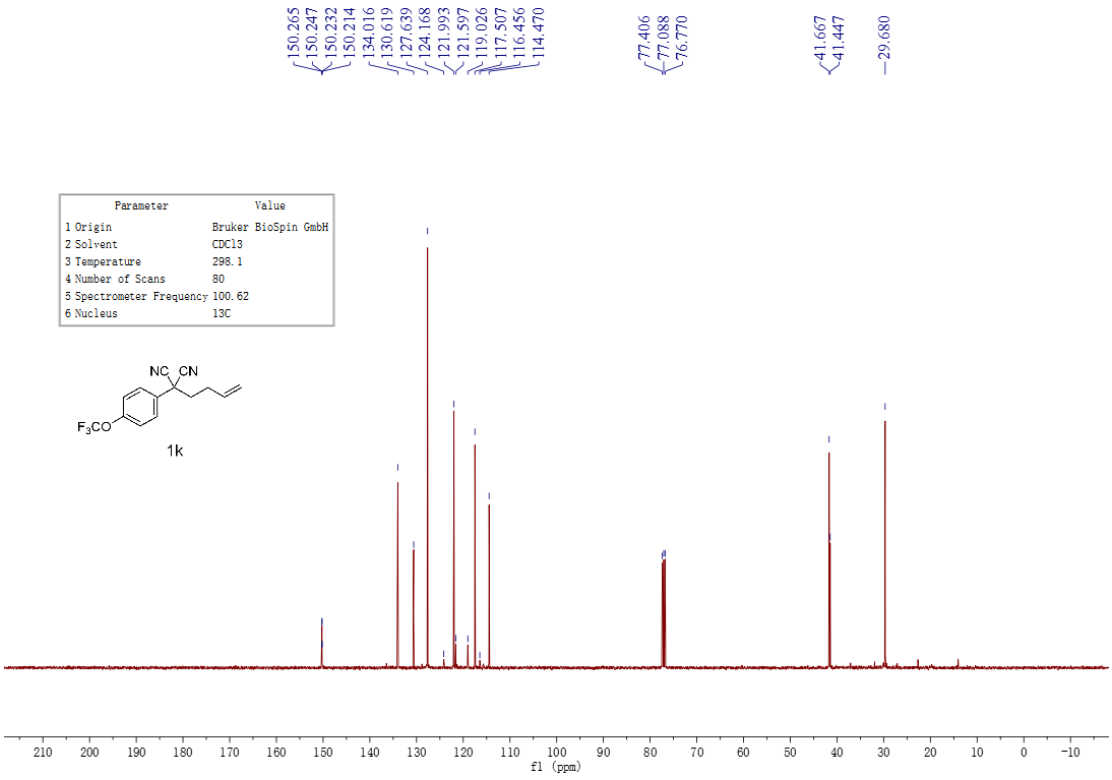

7.587
7.571
7.524
7.517
7.502
7.483
7.468
5.802
5.786
5.776
5.759
5.748
5.743
5.138
5.137
5.095
5.070
2.409
2.397
2.381
2.367
2.355
2.332
2.328
2.321
2.312
2.302
2.292
2.286
Parameter Value
1 Origin Bruker BioSpin GmbH
2 Solvent CDCl3
3 Temperature 298.2
4 Number of Scans 2
5 Spectrometer Frequency 400.13
6 Nucleus 1H
NC CN
1i
2.02
3.00
1.00
2.00
2.01
2.00
f1 (ppm)

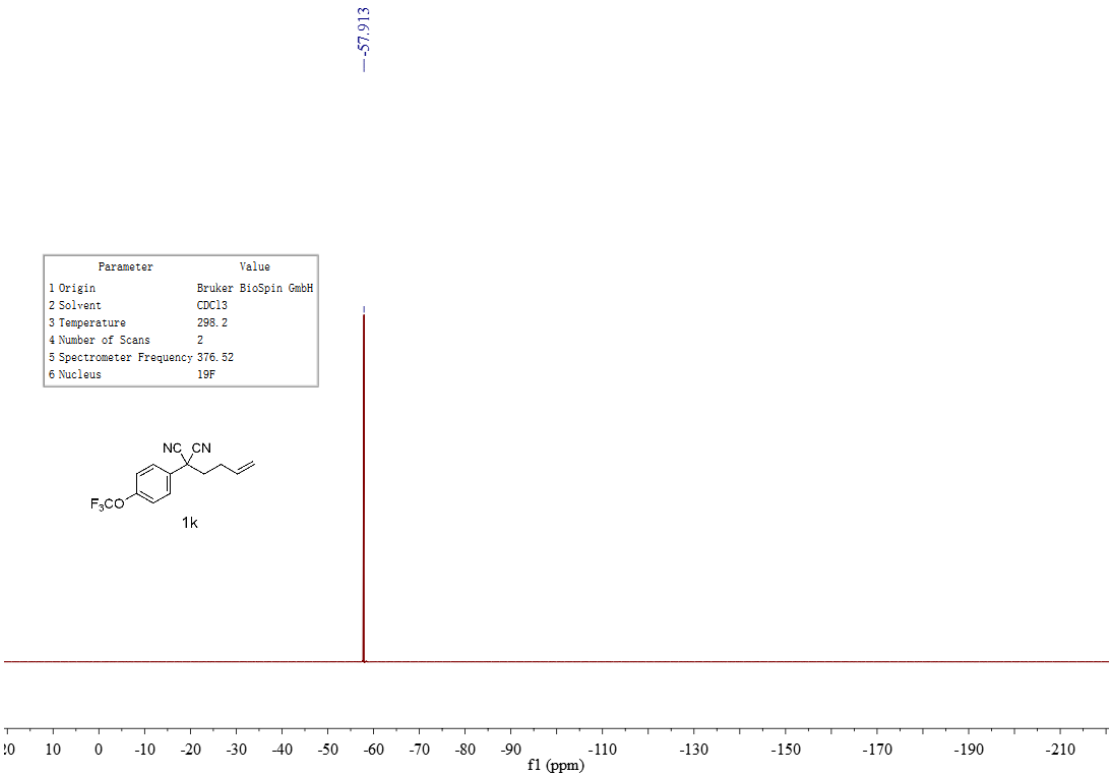

134.328
131.996
130.003
129.778
125.763
117.343
114.896
77.449
77.131
76.813
41.956
41.705
29.696
Parameter Value
1 Origin Bruker BioSpin GmbH
2 Solvent CDCl3
3 Temperature 298.2
4 Number of Scans 4
5 Spectrometer Frequency 100.61
6 Nucleus 13C
NC CN
1i
f1 (ppm)

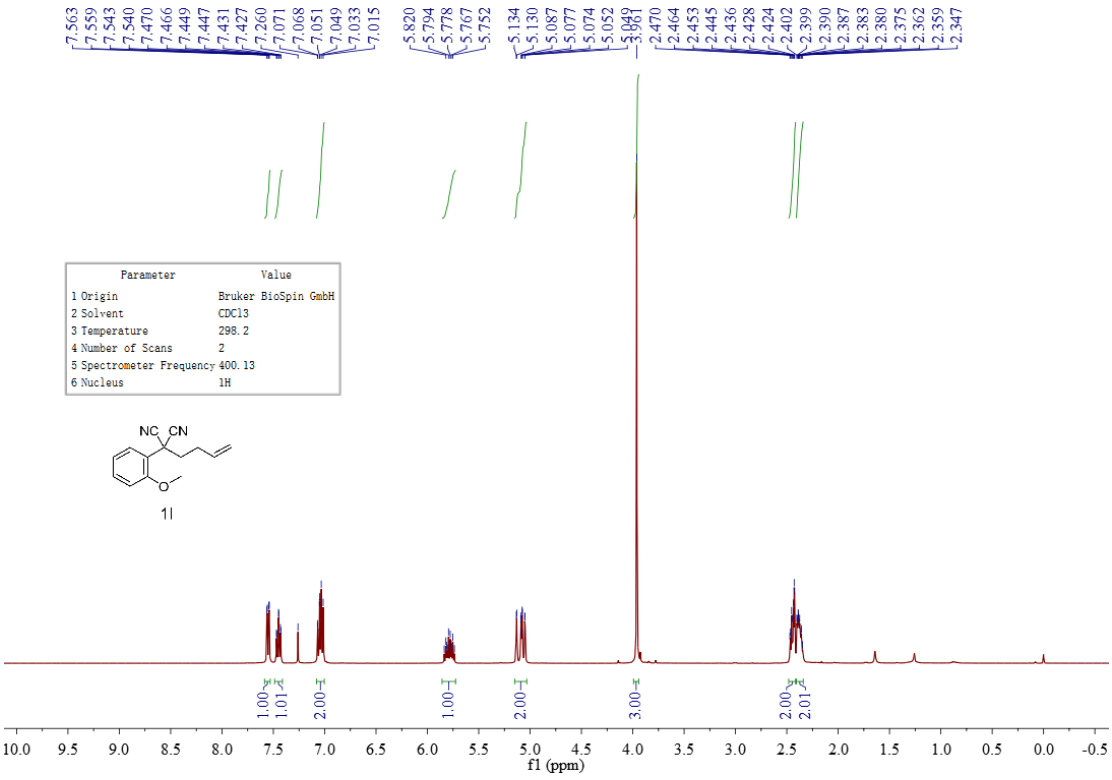

7.489
7.481
7.476
7.470
7.464
7.459
7.451
7.260
7.004
6.996
6.990
6.979
6.973
6.965
5.794
5.769
5.752
5.736
5.131
5.128
5.088
5.085
5.062
5.059
3.842
2.388
2.384
2.372
2.368
2.364
2.354
2.352
2.347
2.344
2.339
2.331
2.328
2.302
2.297
2.290
2.281
2.272
2.261
2.255
Parameter Value
1 Origin Bruker BioSpin GmbH
2 Solvent CDCl3
3 Temperature 298.2
4 Number of Scans 2
5 Spectrometer Frequency 400.15
6 Nucleus 1H
NC CN
O
1j
2.00
2.01
1.00
2.02
3.00
2.01
2.00
f1 (ppm)

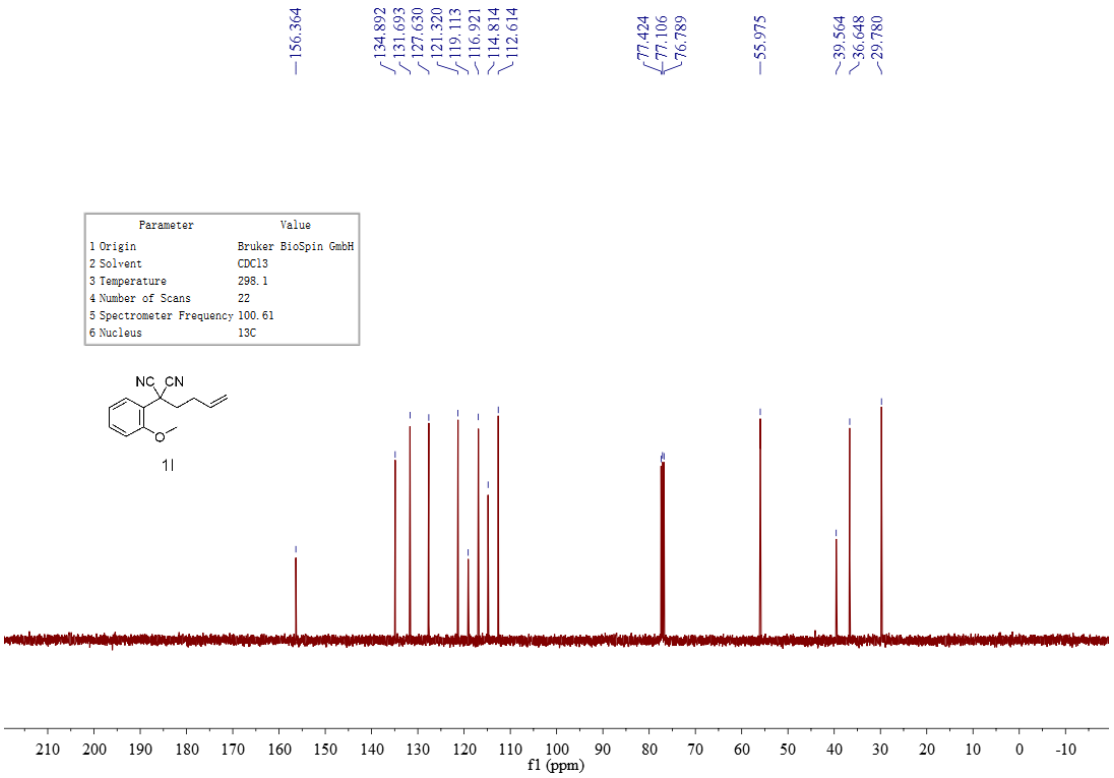

160.636
134.384
127.105
123.616
117.247
115.074
115.005
77.351
77.033
76.716
55.517
41.661
41.271
29.612
Parameter Value
1 Origin Bruker BioSpin GmbH
2 Solvent CDCl3
3 Temperature 298.1
4 Number of Scans 20
5 Spectrometer Frequency 100.62
6 Nucleus 13C
NC CN
O
1j
f1 (ppm)

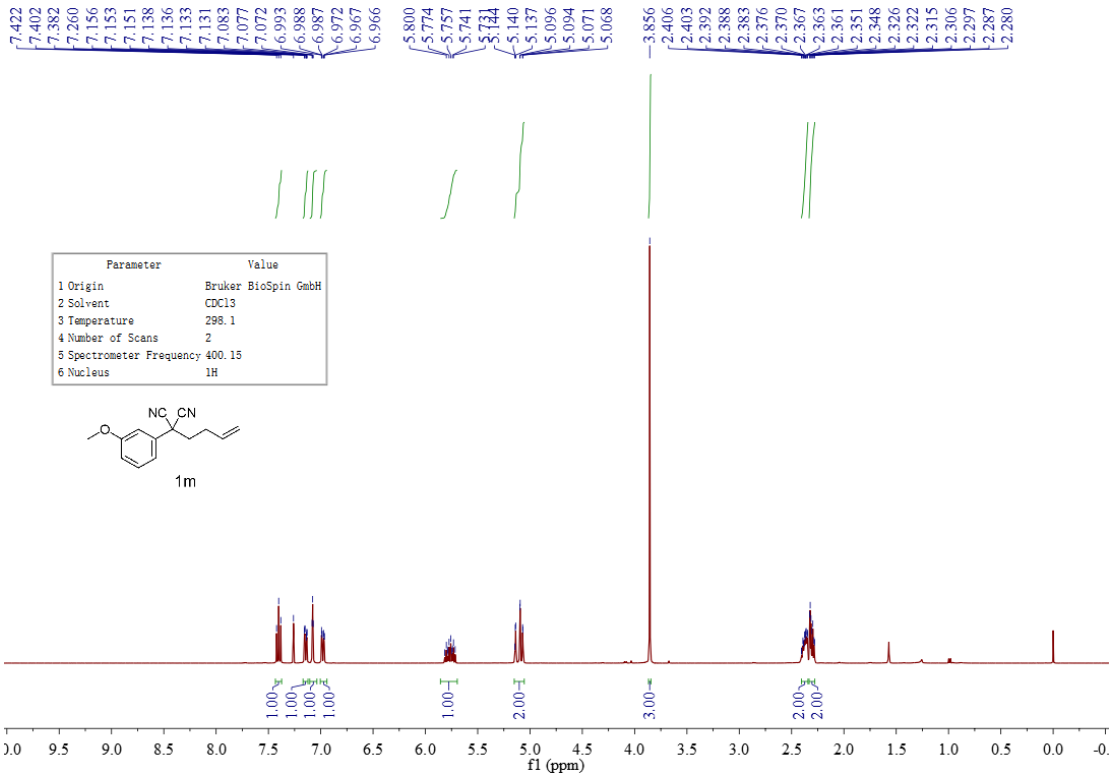

7.648 7.641 7.635 7.624 7.618 7.610 7.367 7.365 7.344 7.260
5.799 5.783 5.774 5.757 5.741 5.731 5.154 5.150 5.147 5.113 5.111 5.107 5.091 5.088 5.085
2.428 2.424 2.420 2.410 2.408 2.404 2.396 2.387 2.378 2.374 2.371 2.367 2.364 2.339 2.336 2.330 2.323 2.315 2.306 2.298 2.286 2.281
Parameter Value
1 Origin Bruker BioSpin GmbH
2 Solvent CDCl3
3 Temperature 298.1
4 Number of Scans 2
5 Spectrometer Frequency 400.15
6 Nucleus 1H
NC CN
F3CO
1k
2.00 2.00 1.00 2.00 2.01 2.01
f1 (ppm)


150.265 150.247 150.232 150.214 134.016 130.619 127.639 124.168 121.993 121.597 119.026 117.507 116.456 114.470
77.406 77.088 76.770
41.667 41.447
29.680
Parameter Value
1 Origin Bruker BioSpin GmbH
2 Solvent CDCl3
3 Temperature 298.1
4 Number of Scans 80
5 Spectrometer Frequency 100.62
6 Nucleus 13C
NC CN
F3CO
1k
f1 (ppm)


-57.913
Parameter Value
1 Origin Bruker BioSpin GmbH
2 Solvent CDCl3
3 Temperature 298.2
4 Number of Scans 2
5 Spectrometer Frequency 376.52
6 Nucleus 19F
NC CN
F3CO
1k
10 0 -10 -20 -30 -40 -50 -60 -70 -80 -90 -110 -130 -150 -170 -190 -210
f1 (ppm)


7.563 7.559 7.543 7.540 7.470 7.466 7.449 7.447 7.431 7.427 7.260 7.071 7.068 7.051 7.049 7.033 7.015
5.820 5.794 5.778 5.767 5.752
5.134 5.130 5.087 5.077 5.074 5.052 5.049 3.961
2.470 2.464 2.453 2.445 2.436 2.428 2.424 2.402 2.399 2.390 2.387 2.383 2.380 2.375 2.362 2.359 2.347
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
NC CN
O
1l
1.00 1.01 2.00 1.00 2.00 3.00 2.00 2.01
10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5
f1 (ppm)


156.364
134.892
131.693
127.630
121.320
119.113
116.921
114.814
112.614
77.424
77.106
76.789
55.975
39.564
36.648
29.780
Parameter Value
1 Origin Bruker BioSpin GmbH
2 Solvent CDCl3
3 Temperature 298.1
4 Number of Scans 22
5 Spectrometer Frequency 100.61
6 Nucleus 13C
NC CN
O
1l
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)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7.402
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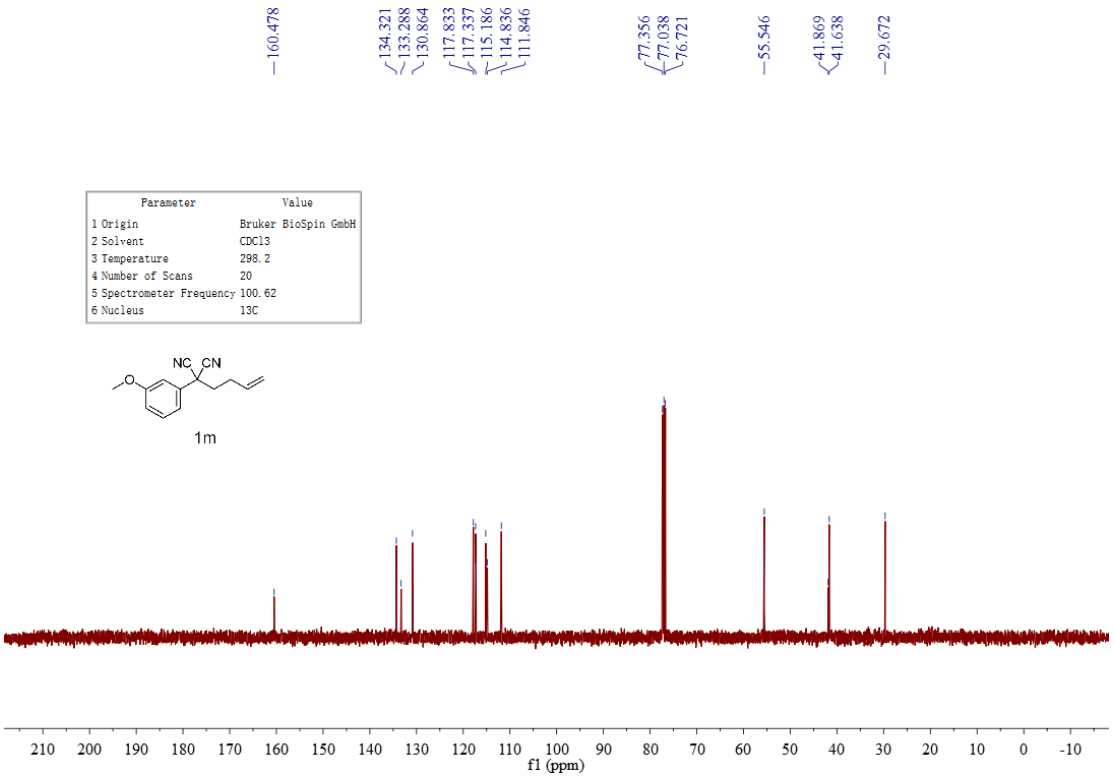
7.260
7.156
7.153
7.151
7.138
7.136
7.133
7.131
7.083
7.077
7.072
6.993
6.988
6.987
6.972
6.967
6.966
5.800
5.774
5.757
5.741
5.731
5.144
5.140
5.137
5.096
5.094
5.071
5.068
3.856
2.406
2.403
2.392
2.388
2.383
2.376
2.370
2.367
2.363
2.361
2.351
2.348
2.326
2.322
2.315
2.306
2.297
2.287
2.280
Parameter Value
1 Origin Bruker BioSpin GmbH
2 Solvent CDCl3
3 Temperature 298.1
4 Number of Scans 2
5 Spectrometer Frequency 400.15
6 Nucleus 1H
NC CN
O
1m
1.00
1.00
1.00
1.00
1.00
2.00
3.00
2.00
2.00
f1 (ppm)


160.478
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117.337
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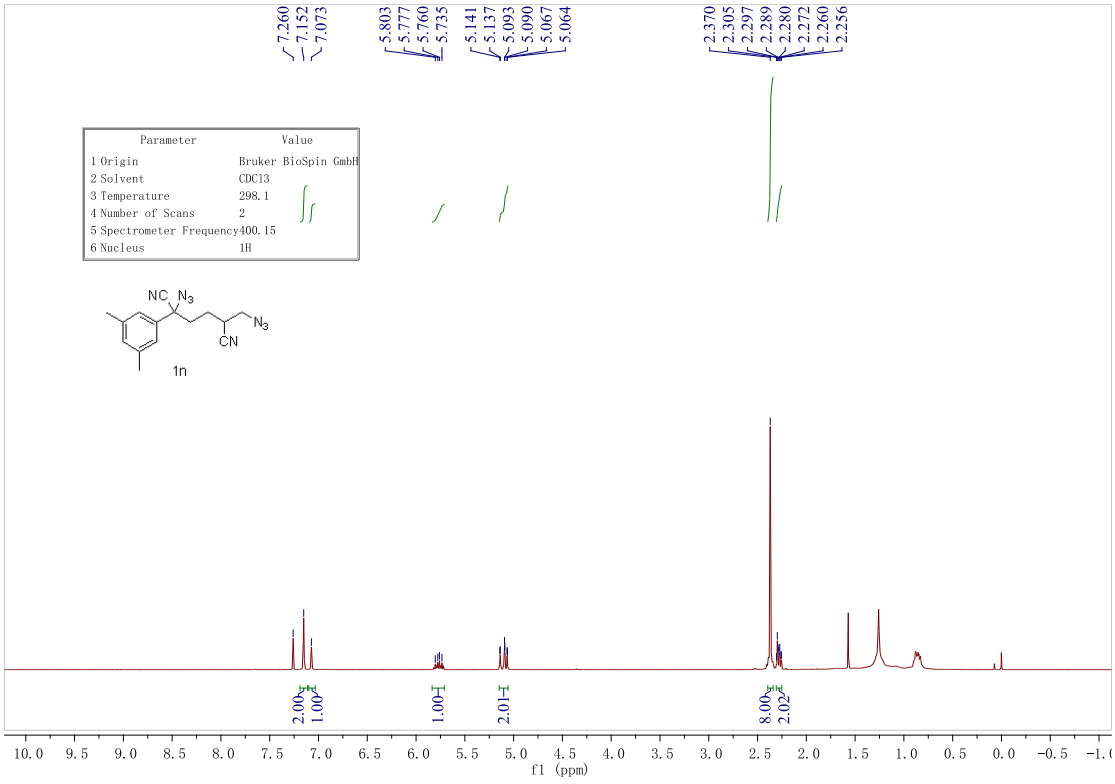
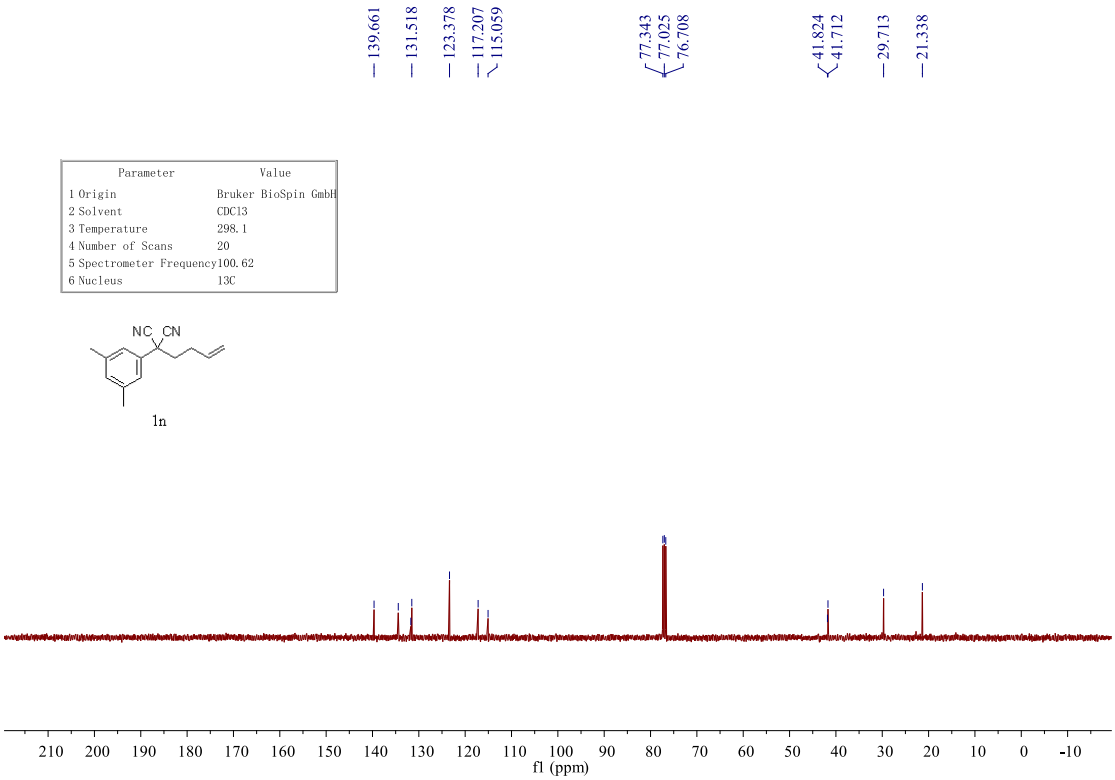
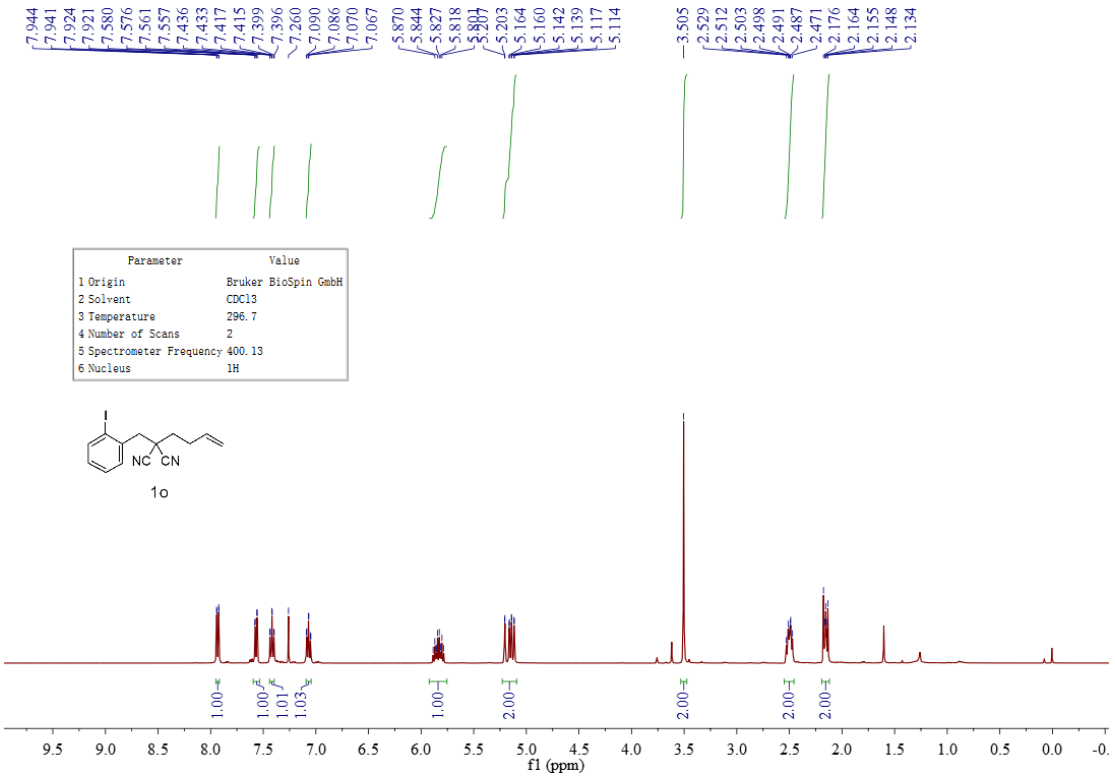
114.836
111.846
77.356
77.038
76.721
55.546
41.869
41.638
29.672
Parameter Value
1 Origin Bruker BioSpin GmbH
2 Solvent CDCl3
3 Temperature 298.2
4 Number of Scans 20
5 Spectrometer Frequency 100.62
6 Nucleus 13C
NC CN
O
1m
f1 (ppm)


7.260
7.152
7.073
5.803
5.777
5.760
5.735
5.141
5.137
5.093
5.090
5.067
5.064
2.370
2.305
2.297
2.289
2.280
2.272
2.260
2.256
Parameter Value
1 Origin Bruker BioSpin GmbH
2 Solvent CDCl3
3 Temperature 298.1
4 Number of Scans 2
5 Spectrometer Frequency 400.15
6 Nucleus 1H
NC N3
N3
CN
1n
2.00
1.00
1.00
2.01
8.00
2.02
f1 (ppm)


139.661
131.518
123.378
117.207
115.059
77.343
77.025
76.708
41.824
41.712
29.713
21.338
Parameter Value
1 Origin Bruker BioSpin GmbH
2 Solvent CDCl3
3 Temperature 298.1
4 Number of Scans 20
5 Spectrometer Frequency 100.62
6 Nucleus 13C
NC CN
1n
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)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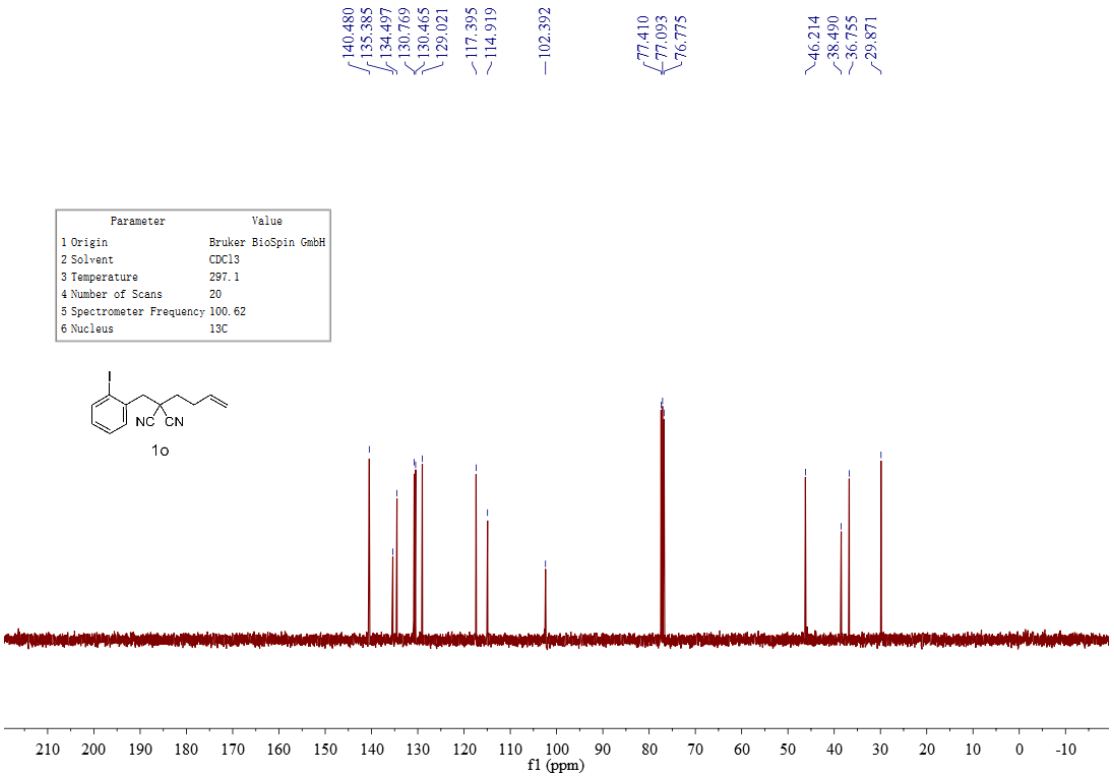
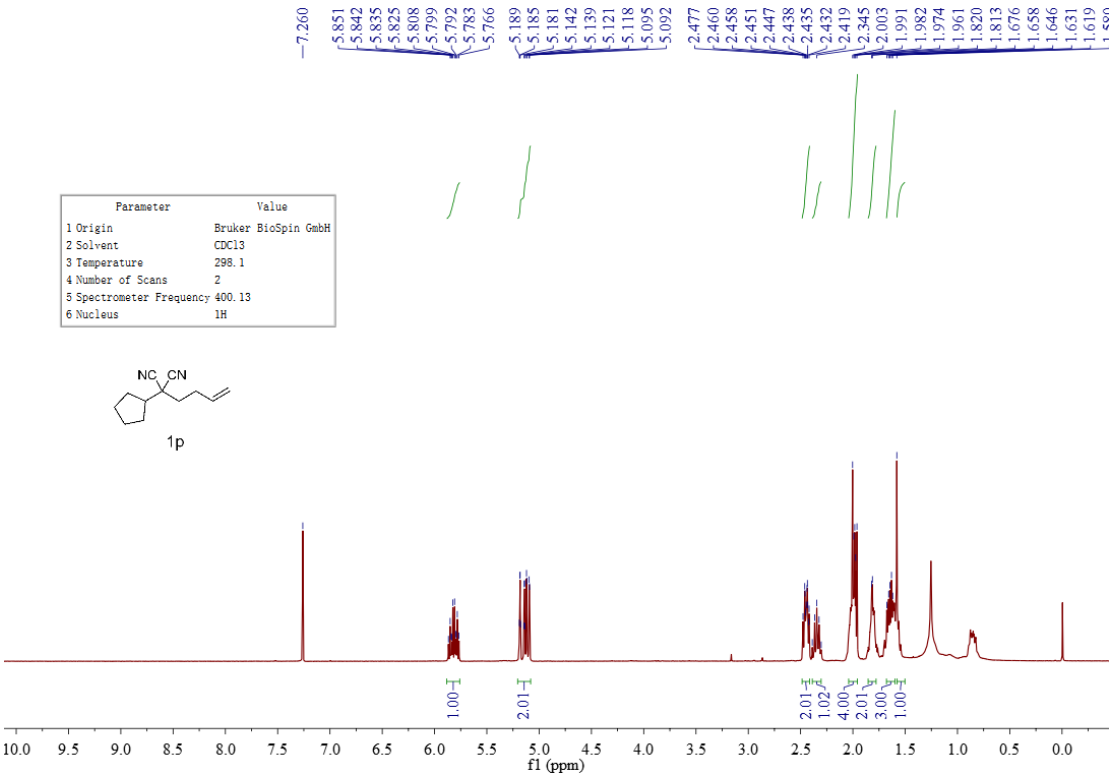
7.924
7.921
7.580
7.576
7.561
7.557
7.436
7.433
7.417
7.415
7.399
7.396
7.260
7.090
7.086
7.070
7.067
5.870
5.844
5.827
5.818
5.203
5.164
5.160
5.142
5.139
5.117
5.114
3.505
2.529
2.512
2.503
2.498
2.491
2.487
2.471
2.176
2.164
2.155
2.148
2.134
Parameter Value
1 Origin Bruker BioSpin GmbH
2 Solvent CDCl3
3 Temperature 296.7
4 Number of Scans 2
5 Spectrometer Frequency 400.13
6 Nucleus 1H
I
NC CN
1o
1.00
1.00
1.01
1.03
1.00
2.00
2.00
2.00
2.00
9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.
f1 (ppm)


140.480
135.385
134.497
130.769
130.465
129.021
117.395
114.919
102.392
77.410
77.093
76.775
46.214
38.490
36.755
29.871
Parameter Value
1 Origin Bruker BioSpin GmbH
2 Solvent CDCl3
3 Temperature 297.1
4 Number of Scans 20
5 Spectrometer Frequency 100.62
6 Nucleus 13C
NC CN
1o
f1 (ppm)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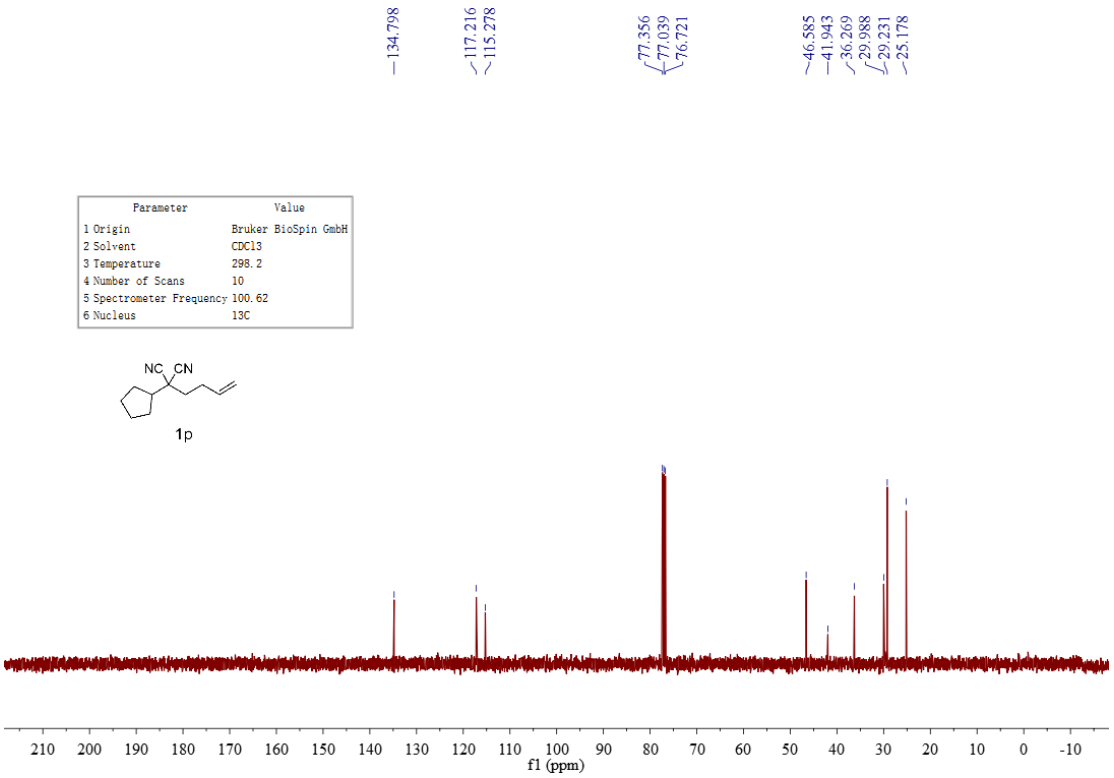
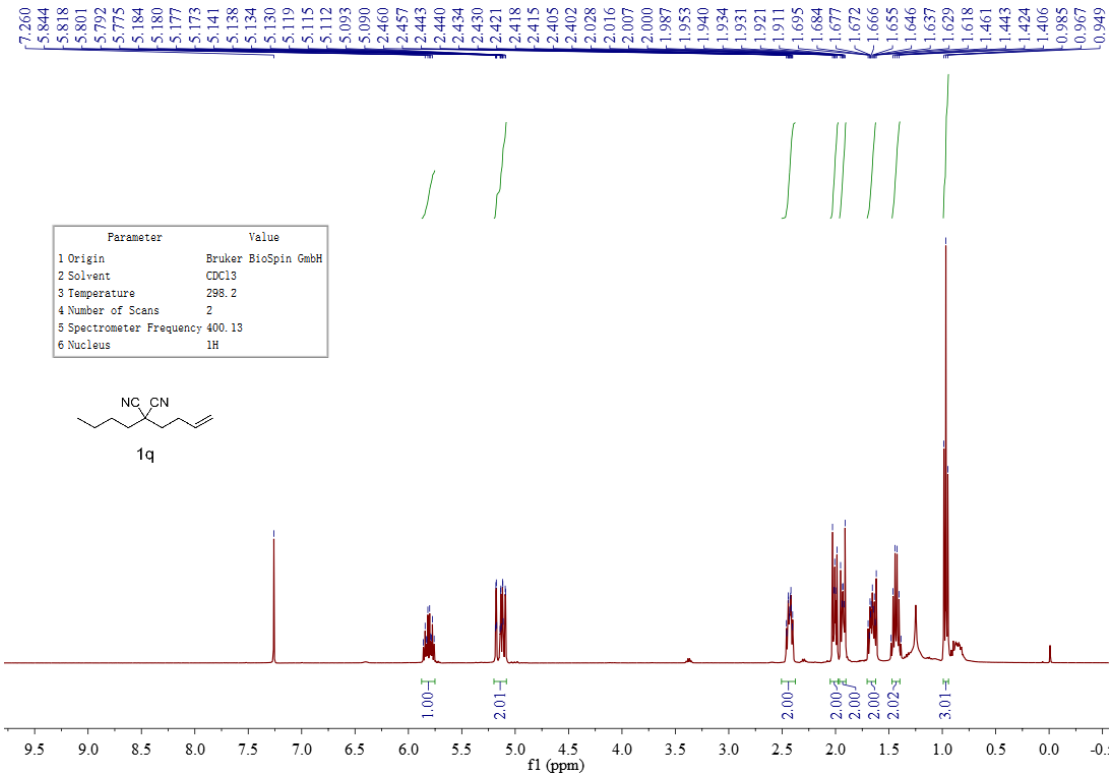
5.842
5.835
5.825
5.808
5.799
5.792
5.783
5.766
5.189
5.185
5.181
5.142
5.139
5.121
5.118
5.095
5.092
2.477
2.460
2.458
2.451
2.447
2.438
2.435
2.432
2.419
2.345
2.003
1.991
1.982
1.974
1.961
1.820
1.813
1.676
1.658
1.646
1.631
1.619
Parameter Value
1 Origin Bruker BioSpin GmbH
2 Solvent CDCl3
3 Temperature 298.1
4 Number of Scans 2
5 Spectrometer Frequency 400.13
6 Nucleus 1H
NC CN
1p
1.00
2.01
2.01
1.02
4.00
2.01
3.00
1.00
f1 (ppm)


134.798
117.216
115.278
77.356
77.039
76.721
46.585
41.943
36.269
29.988
29.231
25.178
Parameter Value
1 Origin Bruker BioSpin GmbH
2 Solvent CDCl3
3 Temperature 298.2
4 Number of Scans 10
5 Spectrometer Frequency 100.62
6 Nucleus 13C
NC CN
1p
f1 (ppm)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5.775
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5.180
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5.173
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5.138
5.134
5.130
5.119
5.115
5.112
5.093
5.090
2.460
2.457
2.443
2.440
2.434
2.430
2.421
2.418
2.415
2.405
2.402
2.028
2.016
2.007
2.000
1.987
1.953
1.940
1.934
1.931
1.921
1.911
1.695
1.684
1.677
1.672
1.666
1.655
1.646
1.637
1.629
1.618
1.461
1.443
1.424
1.406
0.985
0.967
0.949
Parameter Value
1 Origin Bruker BioSpin GmbH
2 Solvent CDCl3
3 Temperature 298.2
4 Number of Scans 2
5 Spectrometer Frequency 400.13
6 Nucleus 1H
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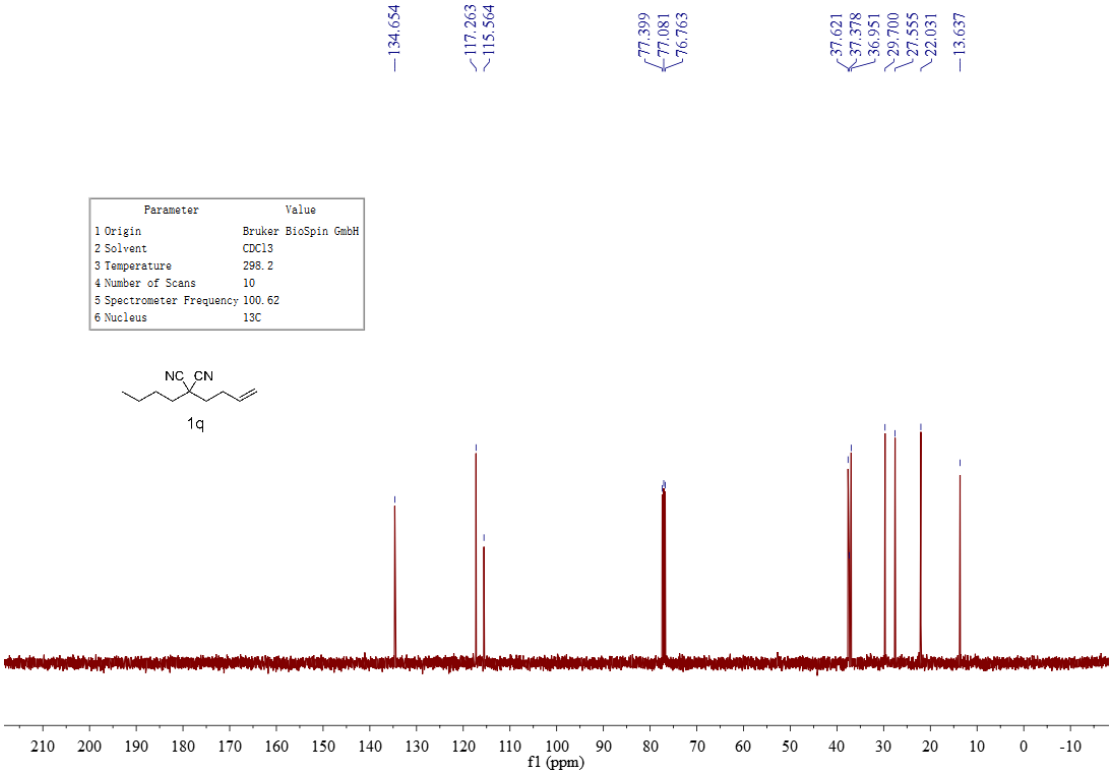
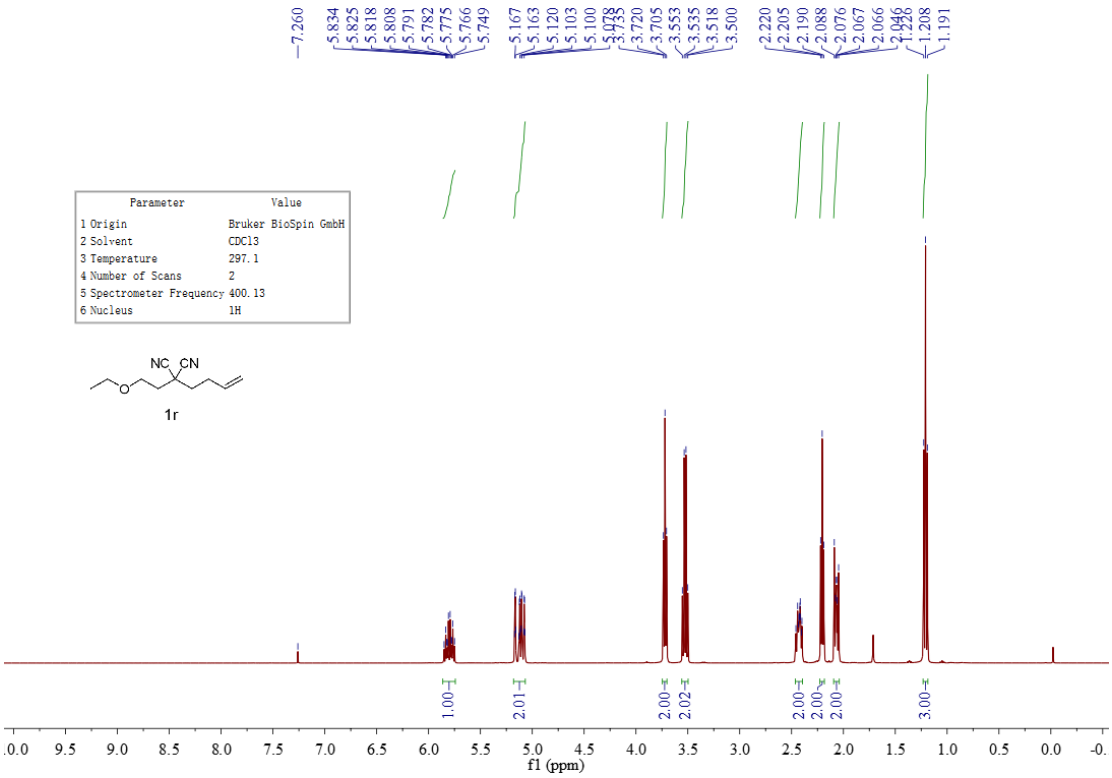
2.00
2.02
3.01
f1 (ppm)


134.654
117.263
115.564
77.399
77.081
76.763
37.621
37.378
36.951
29.700
27.555
22.031
13.637
Parameter Value
1 Origin Bruker BioSpin GmbH
2 Solvent CDCl3
3 Temperature 298.2
4 Number of Scans 10
5 Spectrometer Frequency 100.62
6 Nucleus 13C
NC CN
1q
f1 (ppm)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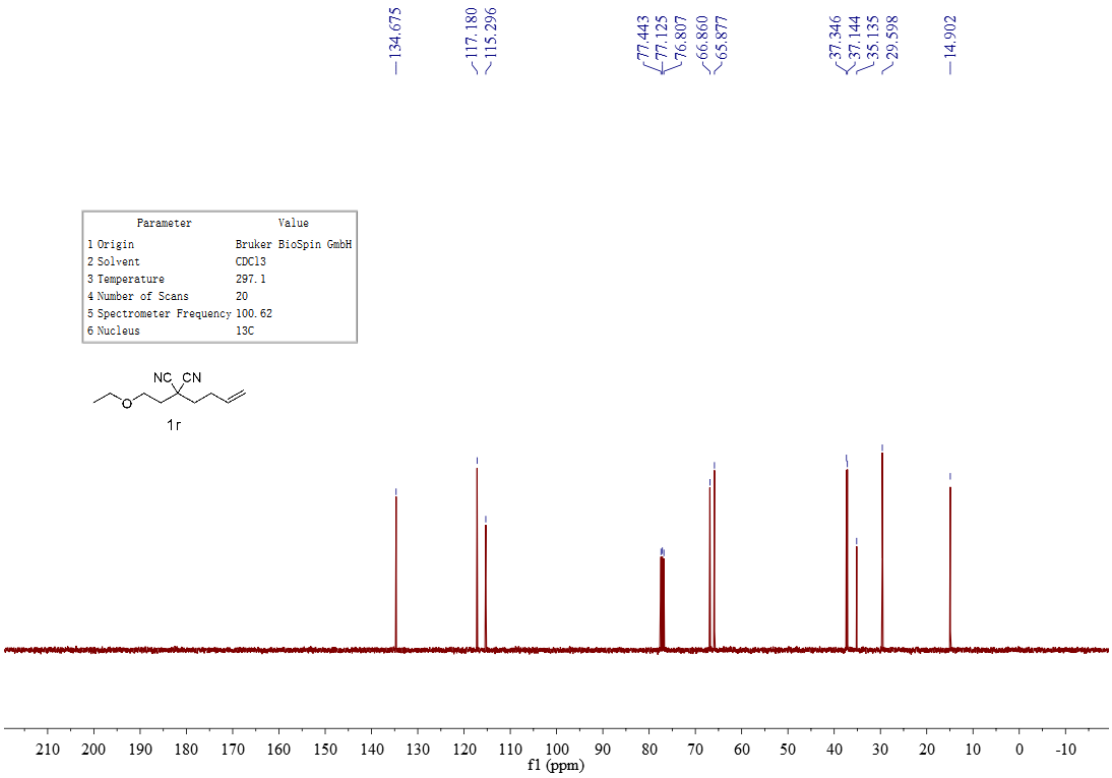
5.825
5.818
5.808
5.791
5.782
5.775
5.766
5.749
5.167
5.163
5.120
5.103
5.100
3.735
3.720
3.705
3.553
3.535
3.518
3.500
2.220
2.205
2.190
2.088
2.076
2.067
2.066
1.208
1.191
Parameter Value
1 Origin Bruker BioSpin GmbH
2 Solvent CDCl3
3 Temperature 297.1
4 Number of Scans 2
5 Spectrometer Frequency 400.13
6 Nucleus 1H
NC CN
O
1r
1.00
2.01
2.00
2.02
2.00
2.00
2.00
3.00
f1 (ppm)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117.180
115.296
77.443
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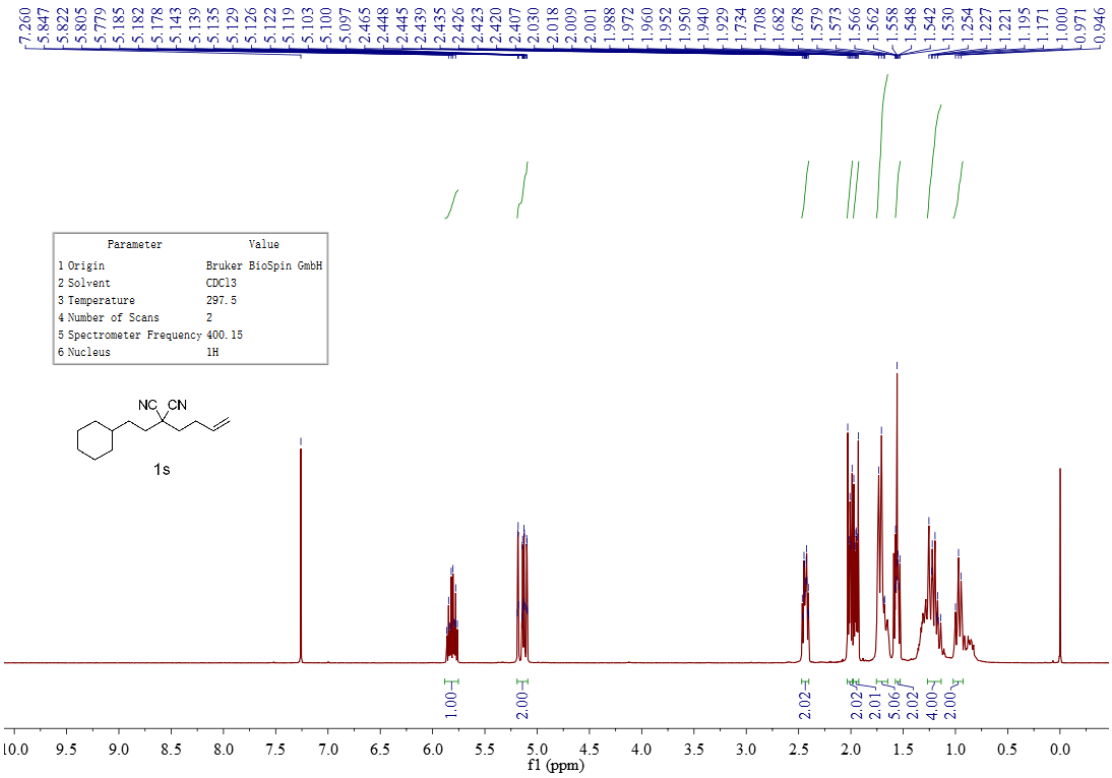
76.807
66.860
65.877
37.346
37.144
35.135
29.598
14.902
Parameter Value
1 Origin Bruker BioSpin GmbH
2 Solvent CDCl3
3 Temperature 297.1
4 Number of Scans 20
5 Spectrometer Frequency 100.62
6 Nucleus 13C
NC CN
O
1r
f1 (ppm)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5.822
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5.178
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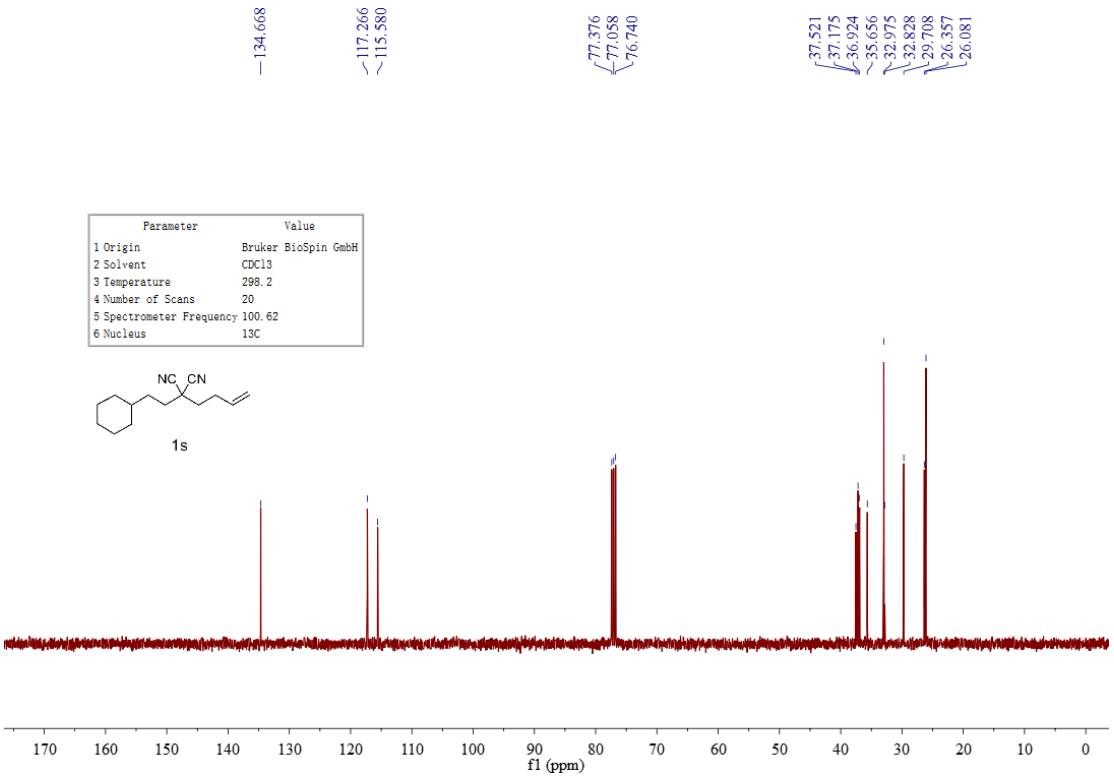
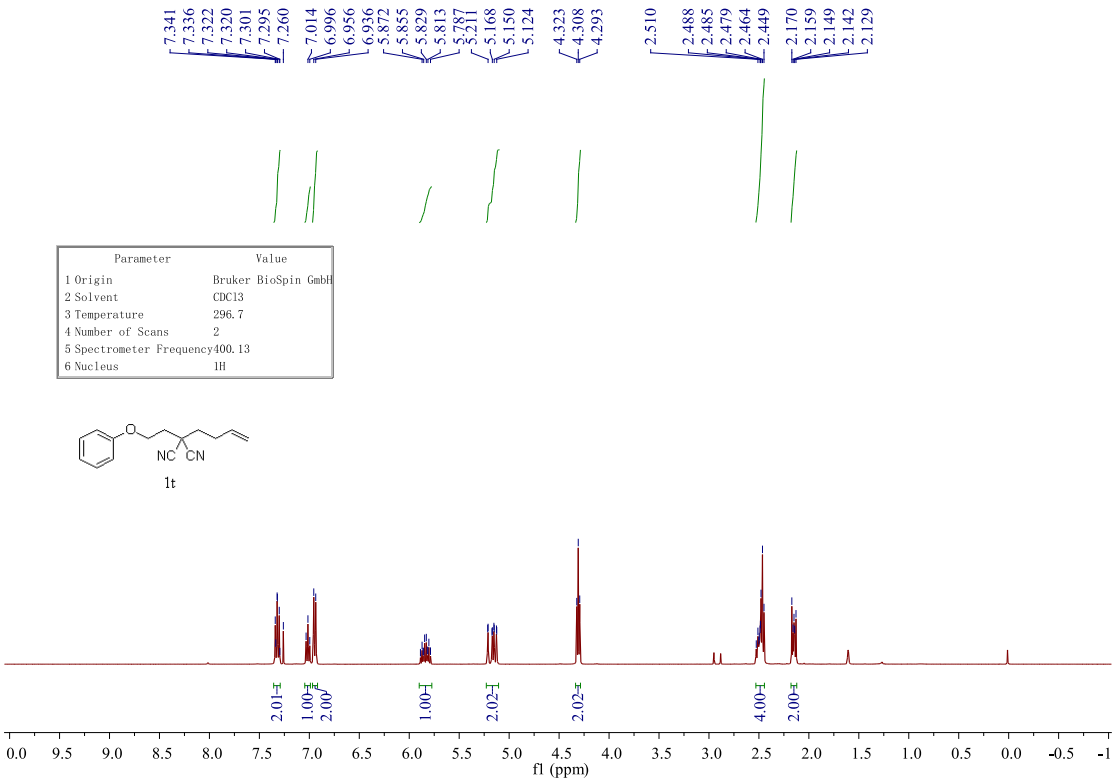
5.139
5.135
5.129
5.126
5.122
5.119
5.103
5.100
5.097
2.465
2.448
2.445
2.439
2.435
2.426
2.423
2.420
2.407
2.030
2.018
2.009
2.001
1.988
1.972
1.960
1.952
1.950
1.940
1.929
1.734
1.708
1.682
1.678
1.579
1.573
1.566
1.562
1.558
1.548
1.542
1.530
1.254
1.227
1.221
1.195
1.171
1.000
0.971
0.946
Parameter Value
1 Origin Bruker BioSpin GmbH
2 Solvent CDCl3
3 Temperature 297.5
4 Number of Scans 2
5 Spectrometer Frequency 400.15
6 Nucleus 1H
NC CN
1s
1.00
2.00
2.02
2.02
2.01
5.06
2.02
4.00
2.00
f1 (ppm)


134.668
117.266
115.580
77.376
77.058
76.740
37.521
37.175
36.924
35.656
32.975
32.828
29.708
26.357
26.081
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
NC CN
1s
f1 (ppm)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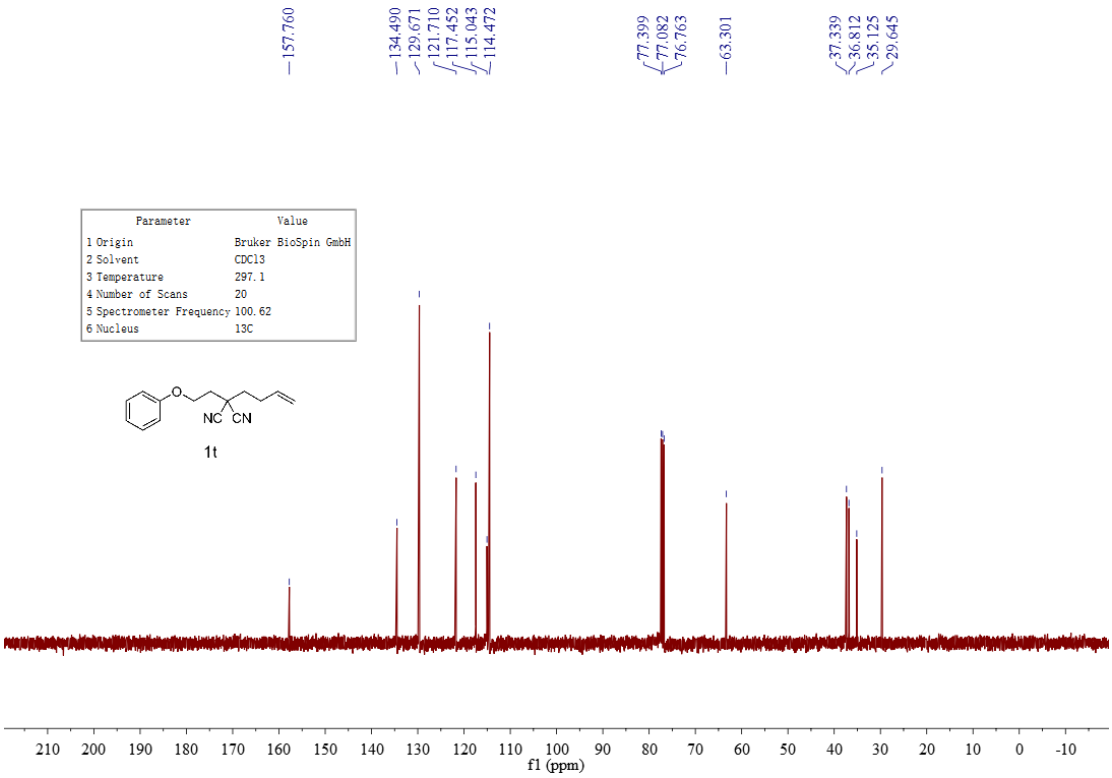
7.336
7.322
7.320
7.301
7.295
7.260
7.014
6.996
6.956
6.936
5.872
5.855
5.829
5.813
5.787
5.211
5.168
5.150
5.124
4.323
4.308
4.293
2.510
2.488
2.485
2.479
2.464
2.449
2.170
2.159
2.149
2.142
2.129
Parameter Value
1 Origin Bruker BioSpin GmbH
2 Solvent CDCl3
3 Temperature 296.7
4 Number of Scans 2
5 Spectrometer Frequency 400.13
6 Nucleus 1H
O
NC CN
1t
2.01
1.00
2.00
1.00
2.02
2.02
4.00
2.00
f1 (ppm)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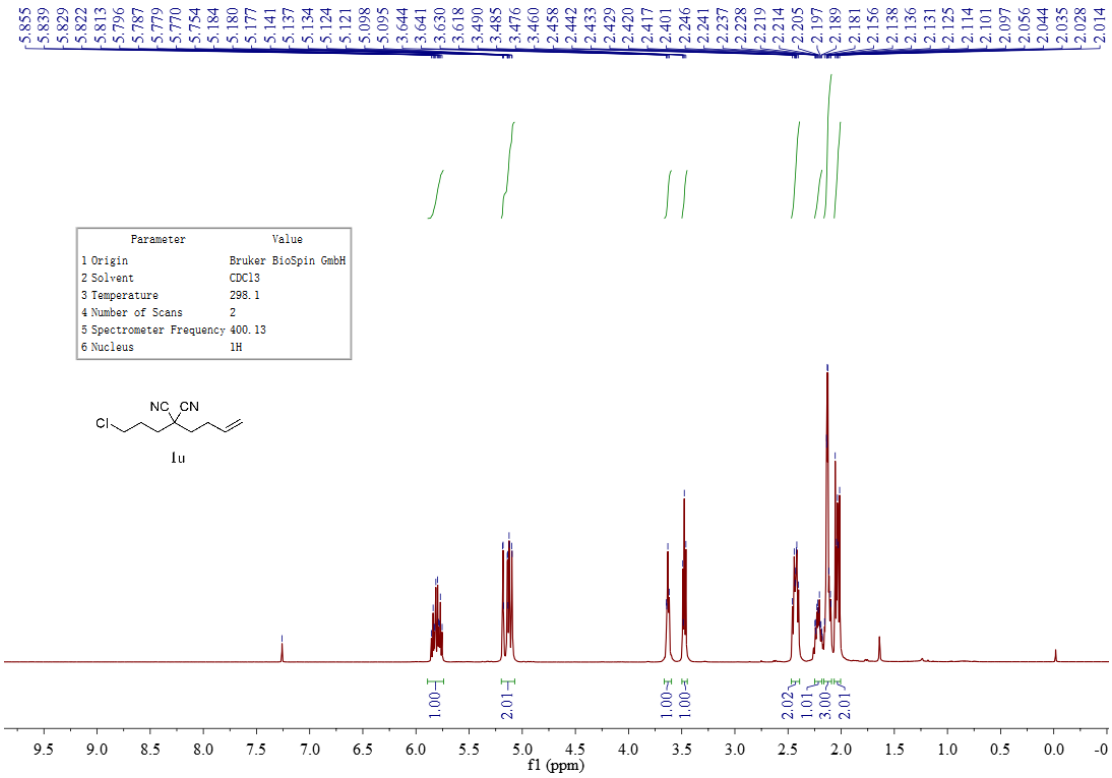
129.671
121.710
117.452
115.043
114.472
77.399
77.082
76.763
63.301
37.339
36.812
35.125
29.645
Parameter Value
1 Origin Bruker BioSpin GmbH
2 Solvent CDCl3
3 Temperature 297.1
4 Number of Scans 20
5 Spectrometer Frequency 100.62
6 Nucleus 13C
O
NC CN
1t
f1 (ppm)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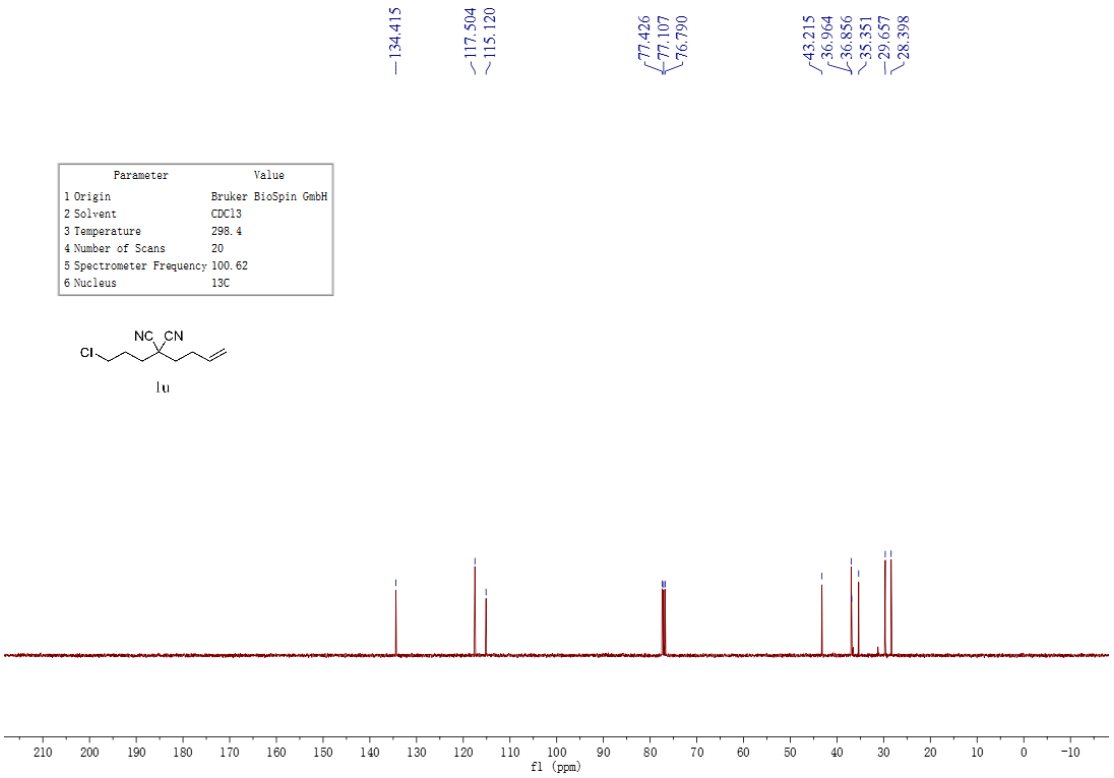
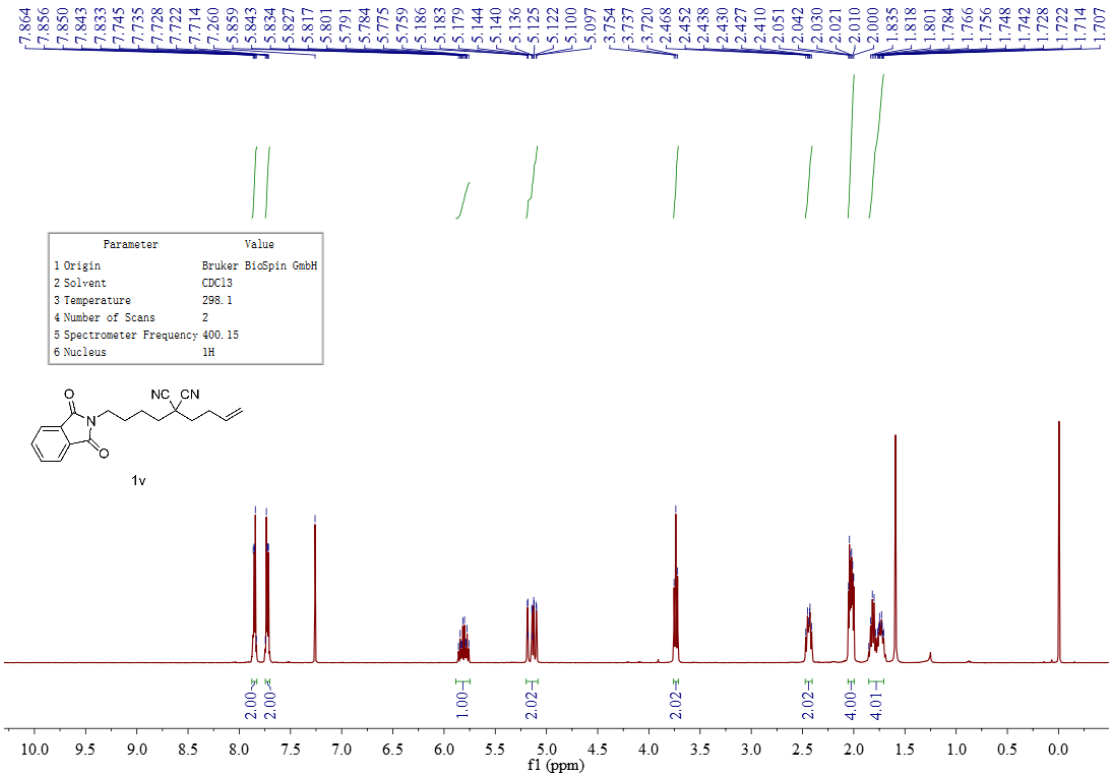
5.839
5.829
5.822
5.813
5.796
5.787
5.779
5.770
5.754
5.184
5.180
5.177
5.141
5.137
5.134
5.124
5.121
5.098
5.095
3.644
3.641
3.630
3.618
3.490
3.485
3.476
3.460
2.458
2.442
2.433
2.429
2.420
2.417
2.401
2.246
2.241
2.237
2.228
2.219
2.214
2.205
2.197
2.189
2.181
2.156
2.138
2.136
2.131
2.125
2.114
2.101
2.097
2.056
2.044
2.035
2.028
2.014
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
NC CN
Cl
1u
1.00
2.01
1.00
1.00
2.02
1.01
3.00
2.01
f1 (ppm)


134.415
117.504
115.120
77.426
77.107
76.790
43.215
36.964
36.856
35.351
29.657
28.398
Parameter Value
1 Origin Bruker BioSpin GmbH
2 Solvent CDCl3
3 Temperature 298.4
4 Number of Scans 20
5 Spectrometer Frequency 100.62
6 Nucleus 13C
NC CN
Cl
1u
f1 (ppm)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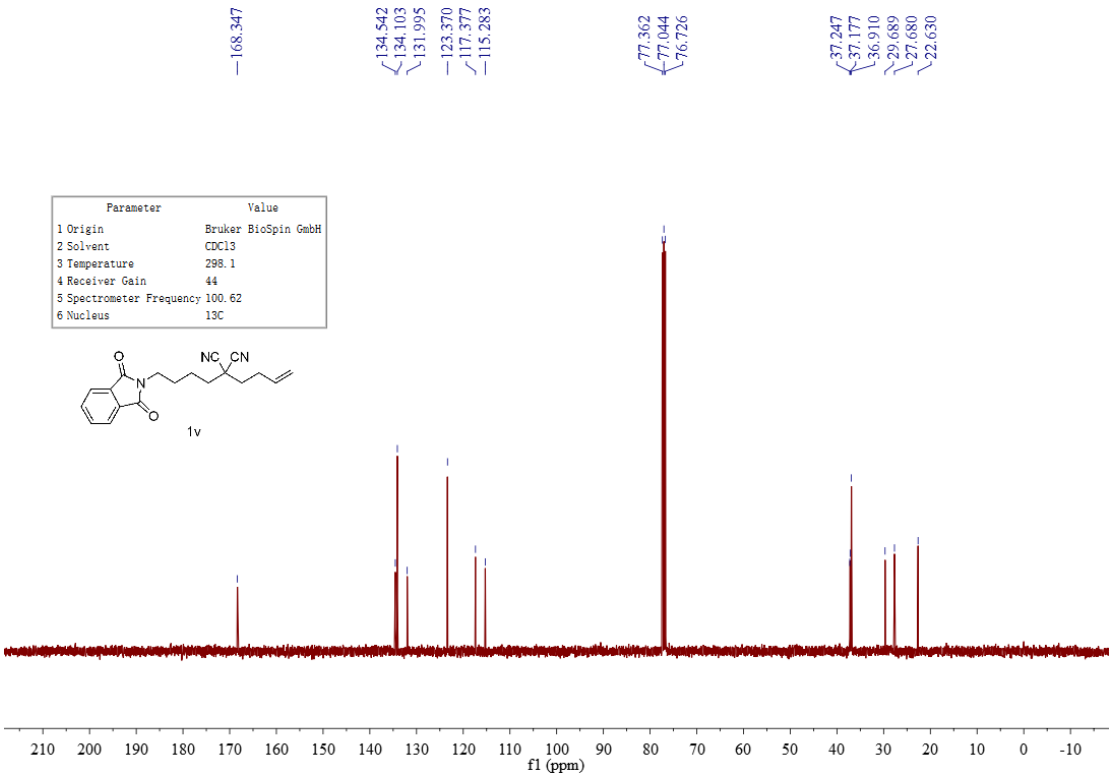
7.856
7.850
7.843
7.833
7.745
7.735
7.728
7.722
7.714
7.260
5.859
5.843
5.834
5.827
5.817
5.801
5.791
5.784
5.775
5.759
5.186
5.183
5.179
5.144
5.140
5.136
5.125
5.122
5.100
5.097
3.754
3.737
3.720
2.468
2.452
2.438
2.430
2.427
2.410
2.051
2.042
2.030
2.021
2.010
2.000
1.835
1.818
1.801
1.784
1.766
1.756
1.748
1.742
1.728
1.722
1.714
1.707
Parameter Value
1 Origin Bruker BioSpin GmbH
2 Solvent CDCl3
3 Temperature 298.1
4 Number of Scans 2
5 Spectrometer Frequency 400.15
6 Nucleus 1H
NC CN
1v
2.00
2.00
1.00
2.02
2.02
2.02
4.00
4.01
f1 (ppm)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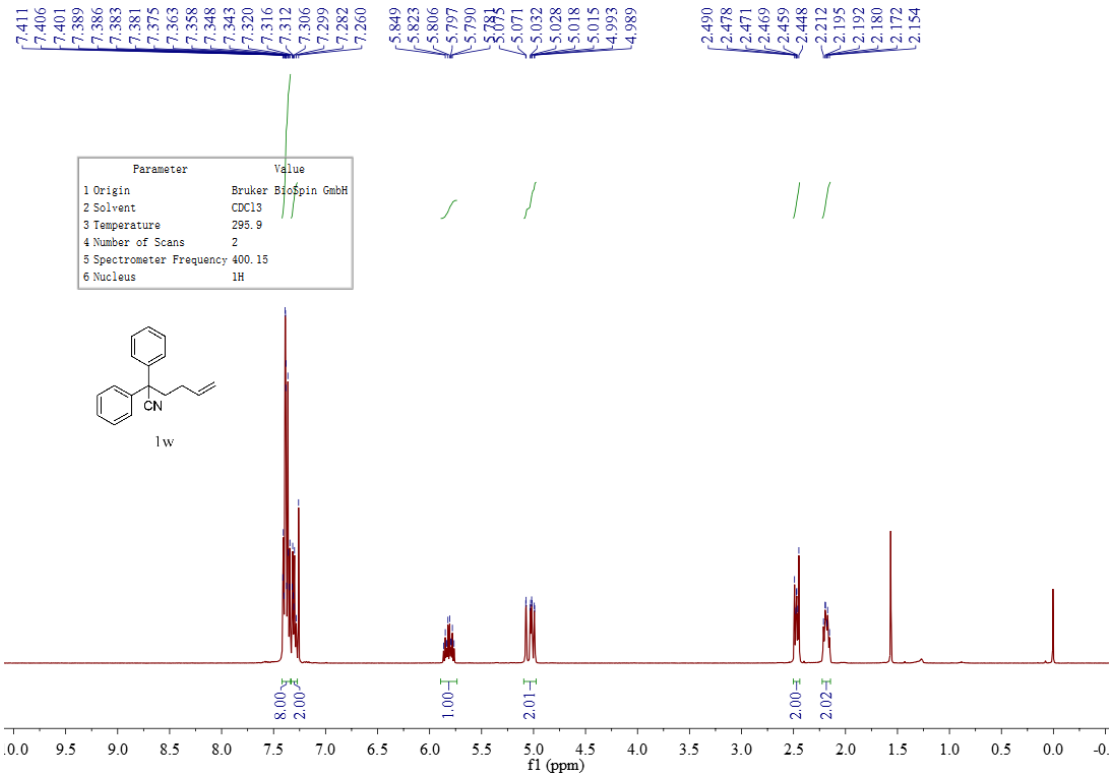
134.103
131.995
123.370
117.377
115.283
77.362
77.044
76.726
37.247
37.177
36.910
29.689
27.680
22.630
Parameter Value
1 Origin Bruker BioSpin GmbH
2 Solvent CDCl3
3 Temperature 298.1
4 Receiver Gain 44
5 Spectrometer Frequency 100.62
6 Nucleus 13C
NC CN
O
N
O
1v
f1 (ppm)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7.401
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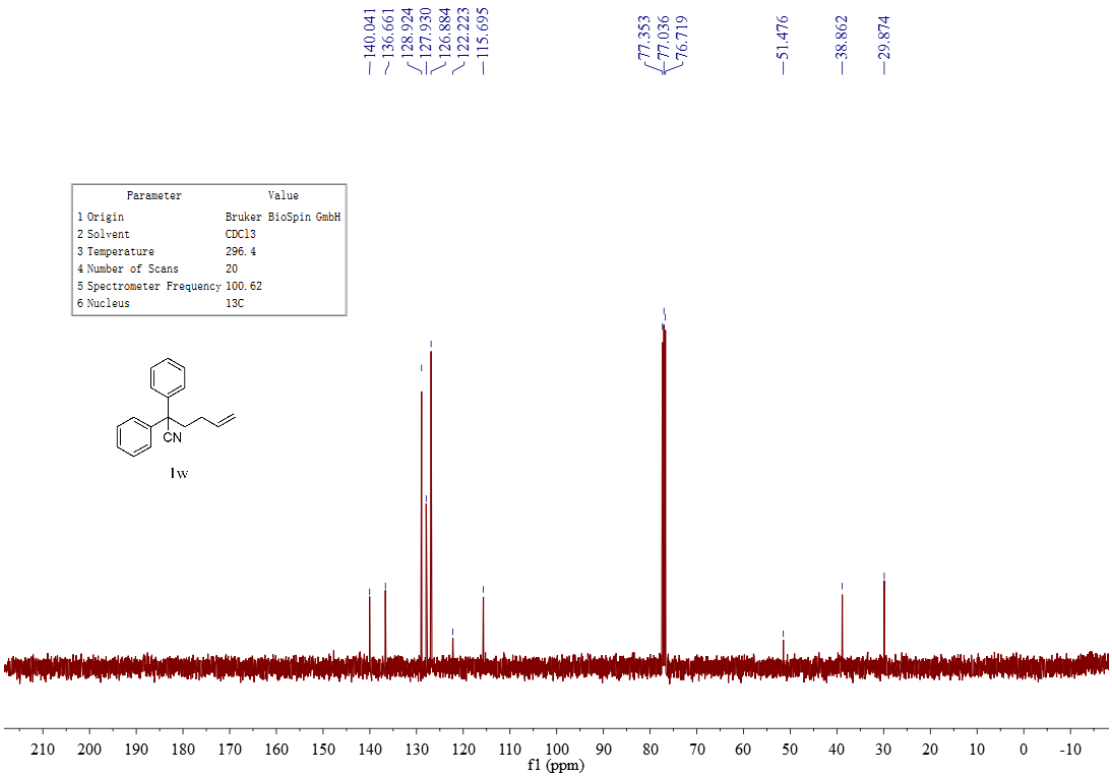
7.383
7.381
7.375
7.363
7.358
7.348
7.343
7.320
7.316
7.312
7.306
7.299
7.282
7.260
5.849
5.823
5.806
5.797
5.790
5.781
5.075
5.071
5.032
5.028
5.018
5.015
4.993
4.989
2.490
2.478
2.471
2.469
2.459
2.448
2.212
2.195
2.192
2.180
2.172
2.154
Parameter Value
1 Origin Bruker BioSpin GmbH
2 Solvent CDCl3
3 Temperature 295.9
4 Number of Scans 2
5 Spectrometer Frequency 400.15
6 Nucleus 1H
CN
1w
8.00
2.00
1.00
2.01
2.00
2.02
f1 (ppm)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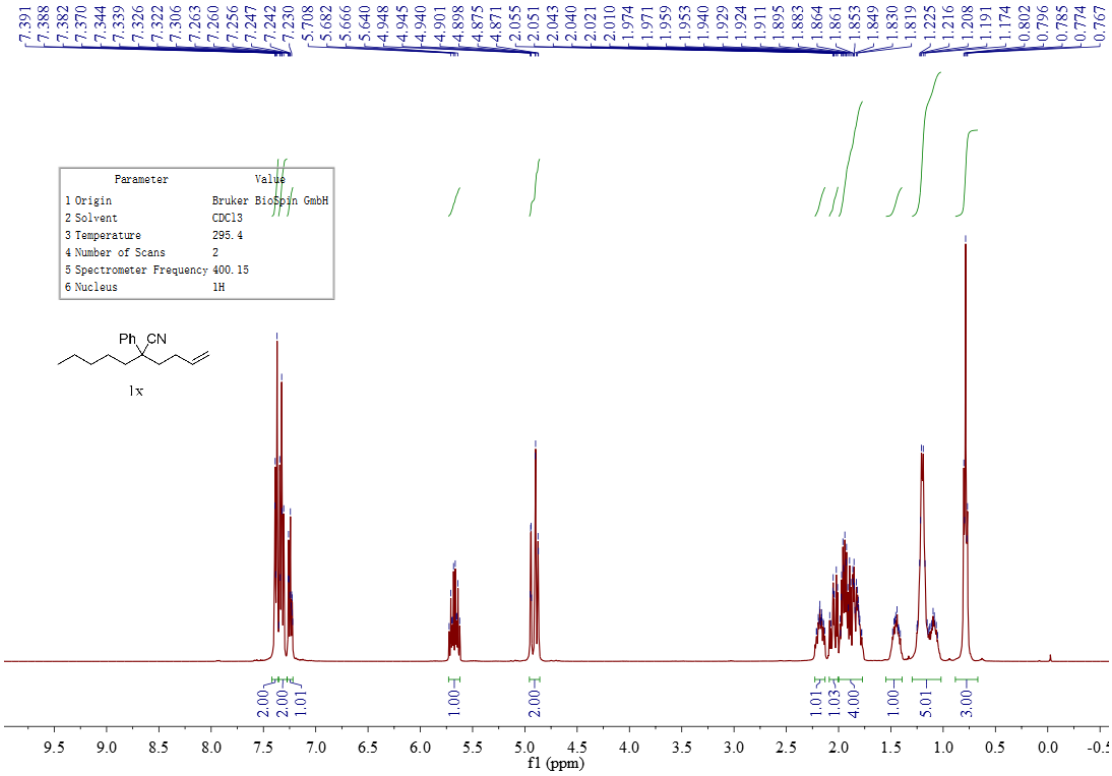
136.661
128.924
127.930
126.884
122.223
115.695
77.353
77.036
76.719
51.476
38.862
29.874
Parameter Value
1 Origin Bruker BioSpin GmbH
2 Solvent CDCl3
3 Temperature 296.4
4 Number of Scans 20
5 Spectrometer Frequency 100.62
6 Nucleus 13C
CN
1w
f1 (ppm)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7.339
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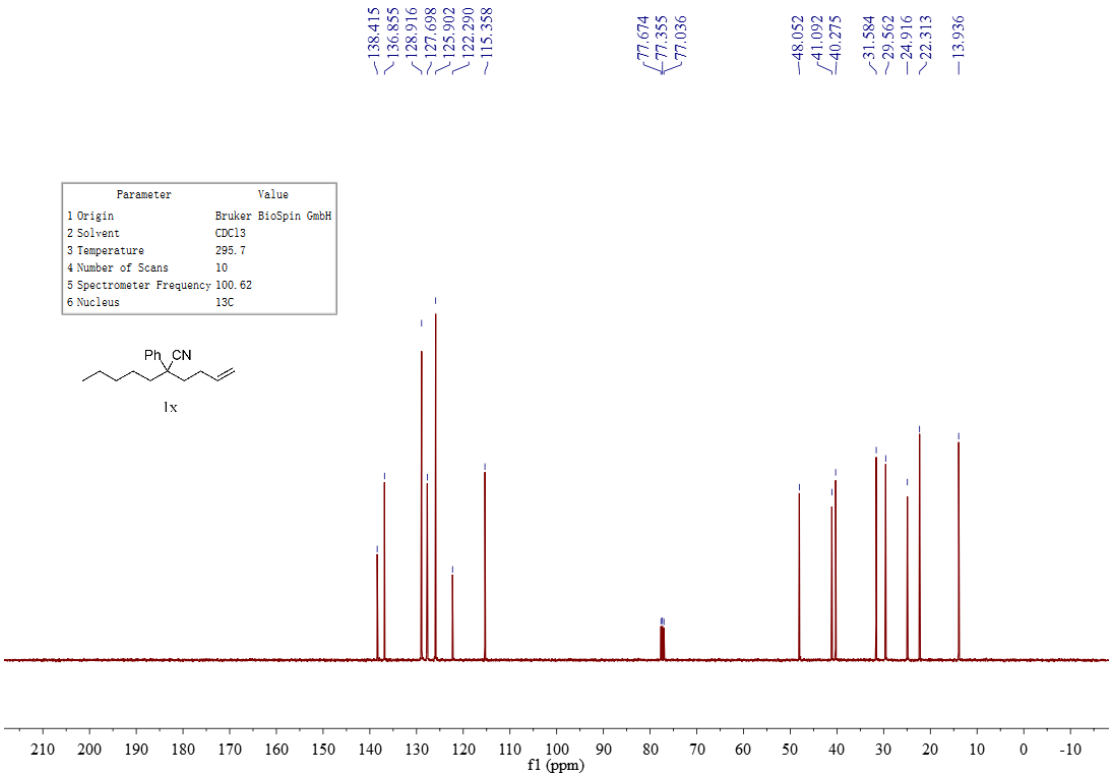
7.322
7.306
7.263
7.260
7.256
7.247
7.242
7.230
5.708
5.682
5.666
5.640
4.948
4.945
4.940
4.901
4.898
4.875
4.871
2.055
2.051
2.043
2.040
2.021
2.010
1.974
1.971
1.959
1.953
1.940
1.929
1.924
1.911
1.895
1.883
1.864
1.861
1.853
1.849
1.830
1.819
1.225
1.216
1.208
1.191
1.174
0.802
0.796
0.785
0.774
0.767
Parameter Value
1 Origin Bruker BioSpin GmbH
2 Solvent CDCl3
3 Temperature 295.4
4 Number of Scans 2
5 Spectrometer Frequency 400.15
6 Nucleus 1H
Ph CN
1x
2.00
2.00
1.01
1.00
2.00
1.01
1.03
4.00
1.00
5.01
3.00
f1 (ppm)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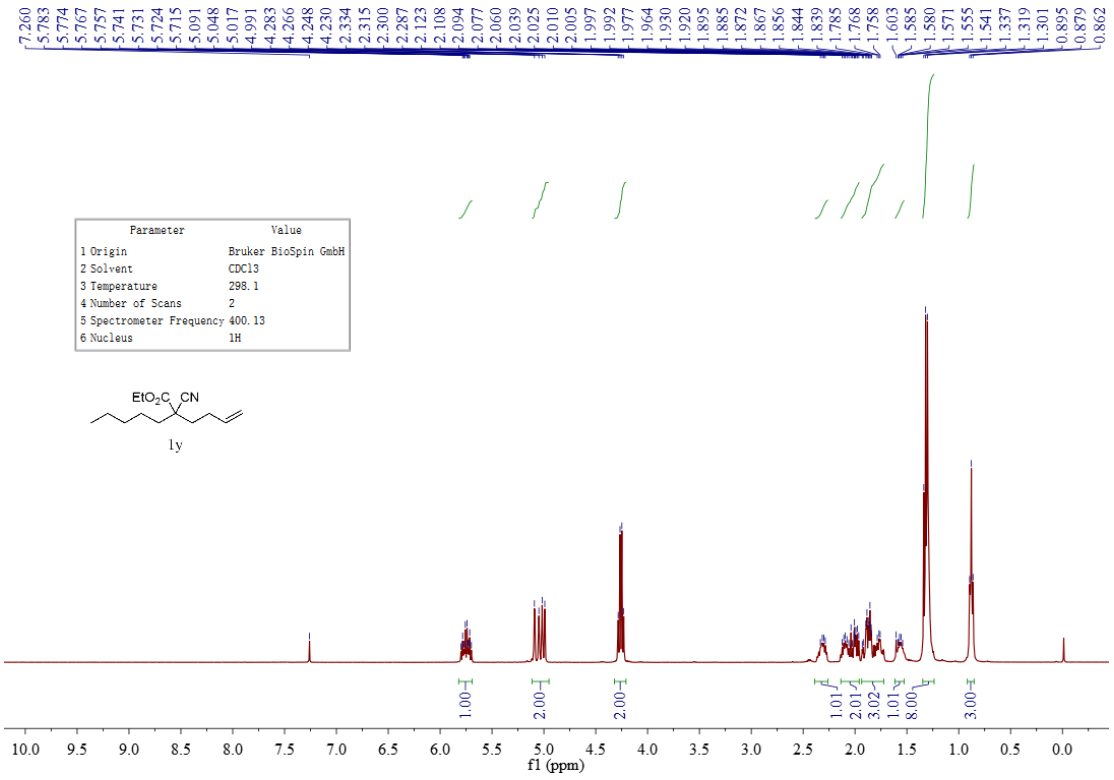
136.855
128.916
127.698
125.902
122.290
115.358
77.674
77.355
77.036
48.052
41.092
40.275
31.584
29.562
24.916
22.313
13.936
Parameter Value
1 Origin Bruker BioSpin GmbH
2 Solvent CDCl3
3 Temperature 295.7
4 Number of Scans 10
5 Spectrometer Frequency 100.62
6 Nucleus 13C
Ph CN
1x
f1 (ppm)


7.260
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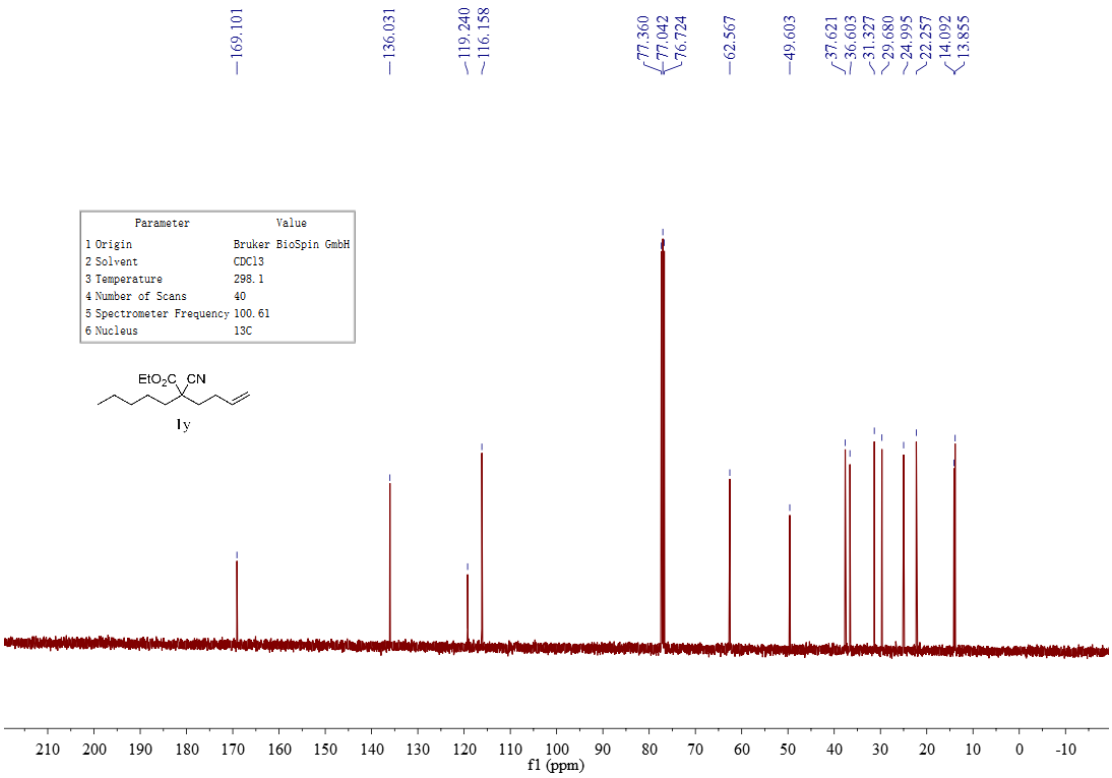
5.774
5.767
5.757
5.741
5.731
5.724
5.715
5.091
5.048
5.017
4.991
4.283
4.266
4.248
4.230
2.334
2.315
2.300
2.287
2.123
2.108
2.094
2.077
2.060
2.039
2.025
2.010
2.005
1.997
1.992
1.977
1.964
1.930
1.920
1.895
1.885
1.872
1.867
1.856
1.844
1.839
1.785
1.768
1.758
1.603
1.585
1.580
1.571
1.555
1.541
1.337
1.319
1.301
0.895
0.879
0.862
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
EtO2C CN
1y
1.00
2.00
2.00
1.01
2.01
3.02
1.01
8.00
3.00
f1 (ppm)


169.101
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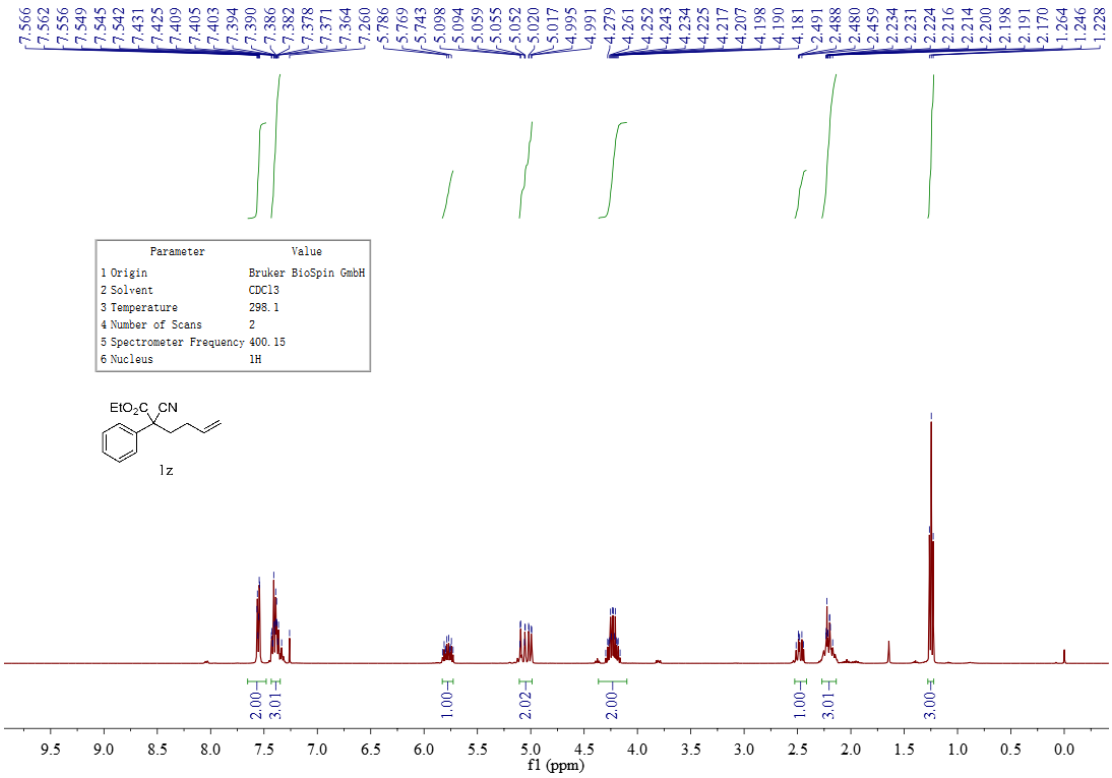
116.158
77.360
77.042
76.724
62.567
49.603
37.621
36.603
31.327
29.680
24.995
22.257
14.092
13.855
Parameter Value
1 Origin Bruker BioSpin GmbH
2 Solvent CDCl3
3 Temperature 298.1
4 Number of Scans 40
5 Spectrometer Frequency 100.61
6 Nucleus 13C
EtO2C CN
1y
f1 (ppm)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7.403
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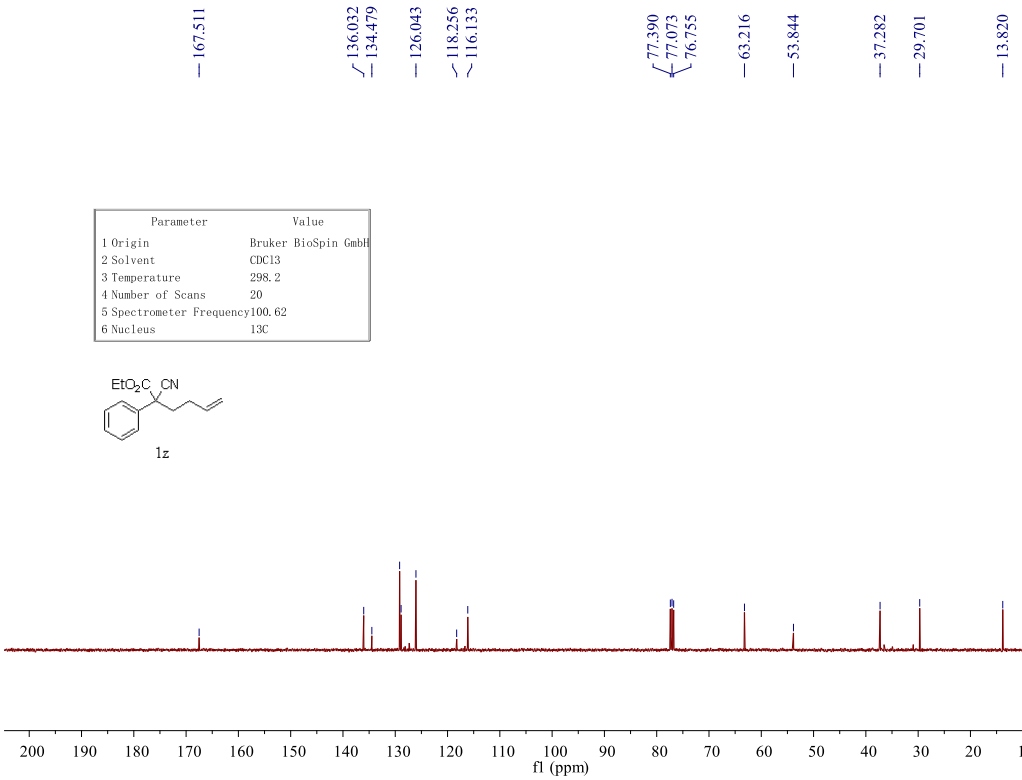
7.390
7.386
7.382
7.378
7.371
7.364
7.260
5.786
5.769
5.743
5.098
5.094
5.059
5.055
5.052
5.020
5.017
4.995
4.991
4.279
4.261
4.252
4.243
4.234
4.225
4.217
4.207
4.198
4.190
4.181
2.491
2.488
2.480
2.459
2.234
2.231
2.224
2.216
2.214
2.200
2.198
2.191
2.170
1.264
1.246
1.228
Parameter Value
1 Origin Bruker BioSpin GmbH
2 Solvent CDCl3
3 Temperature 298.1
4 Number of Scans 2
5 Spectrometer Frequency 400.15
6 Nucleus 1H
EtO2C CN
1z
2.00
3.01
1.00
2.02
2.00
1.00
3.01
3.00
f1 (ppm)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116.133
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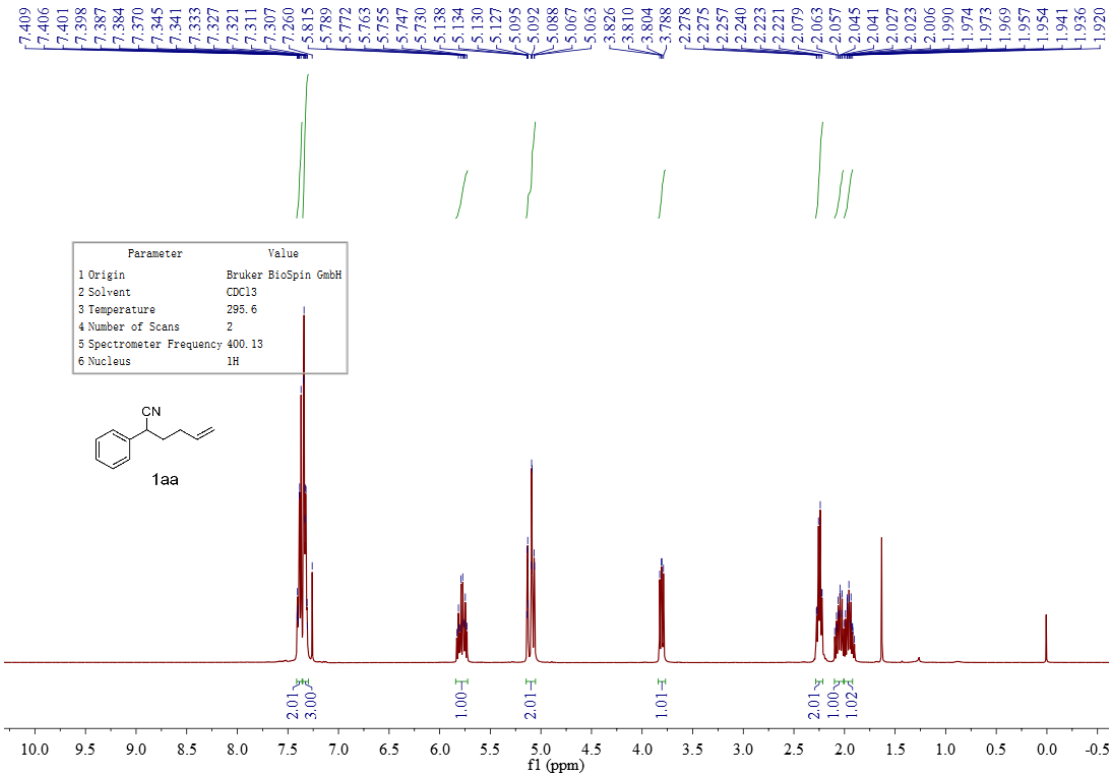
77.073
76.755
63.216
53.844
37.282
29.701
13.820
Parameter Value
1 Origin Bruker BioSpin GmbH
2 Solvent CDCl3
3 Temperature 298.2
4 Number of Scans 20
5 Spectrometer Frequency 100.62
6 Nucleus 13C
EtO2C CN
1z
200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)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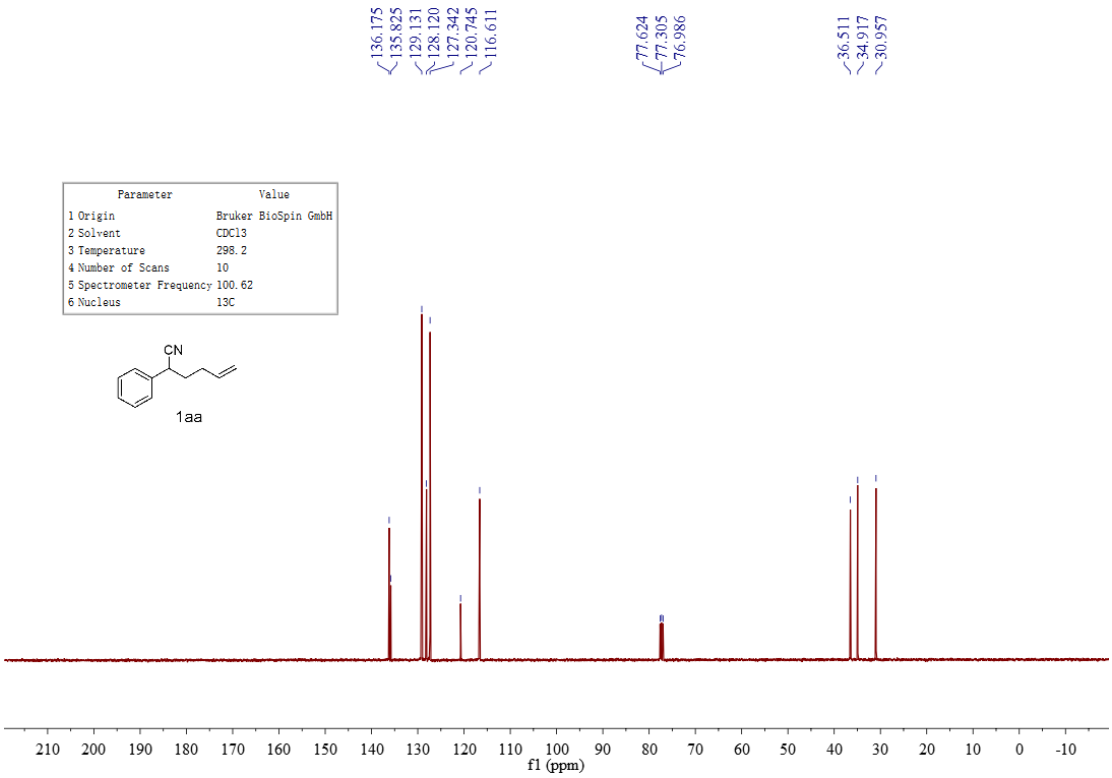
Parameter Value
1 Origin Bruker BioSpin GmbH
2 Solvent CDCl3
3 Temperature 295.6
4 Number of Scans 2
5 Spectrometer Frequency 400.13
6 Nucleus 1H
CN
1aa
2.01 3.00 1.00 2.01 1.01 2.01 1.00 1.02
10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5
f1 (ppm)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135.825
129.131
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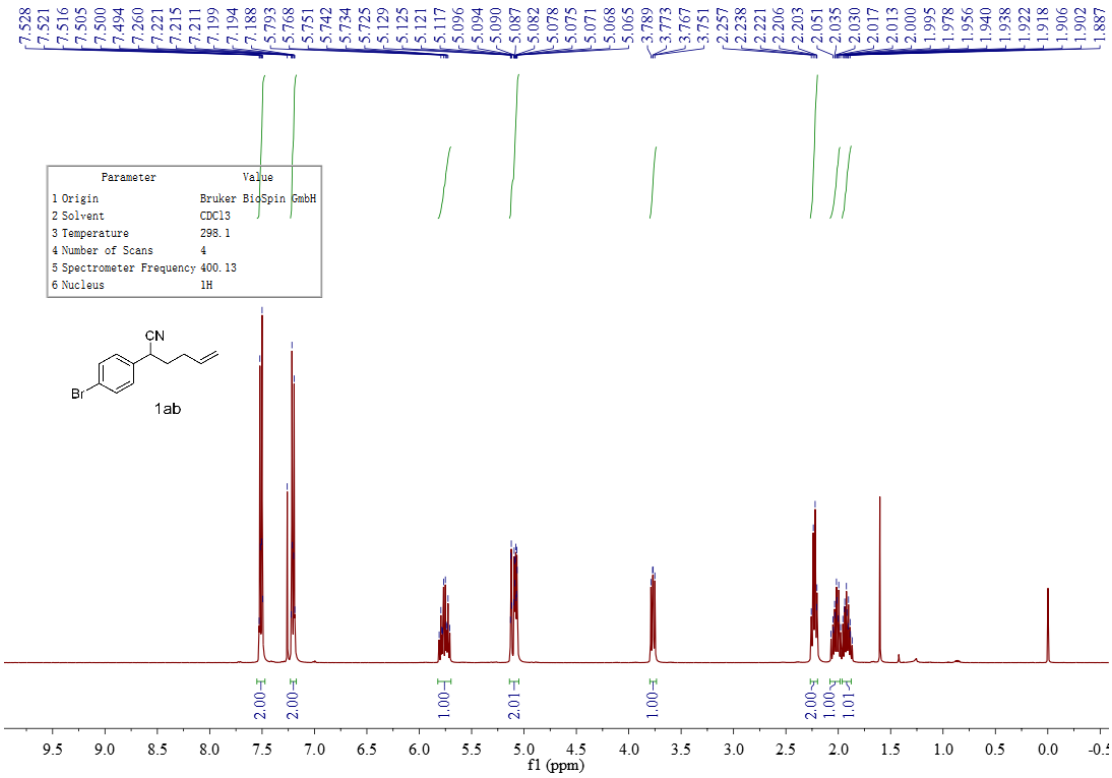
127.342
120.745
116.611
77.624
77.305
76.986
36.511
34.917
30.957
Parameter Value
1 Origin Bruker BioSpin GmbH
2 Solvent CDCl3
3 Temperature 298.2
4 Number of Scans 10
5 Spectrometer Frequency 100.62
6 Nucleus 13C
CN
1aa
f1 (ppm)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5.768
5.751
5.742
5.734
5.725
5.129
5.125
5.121
5.117
5.096
5.094
5.090
5.087
5.082
5.078
5.075
5.071
5.068
5.065
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2.203
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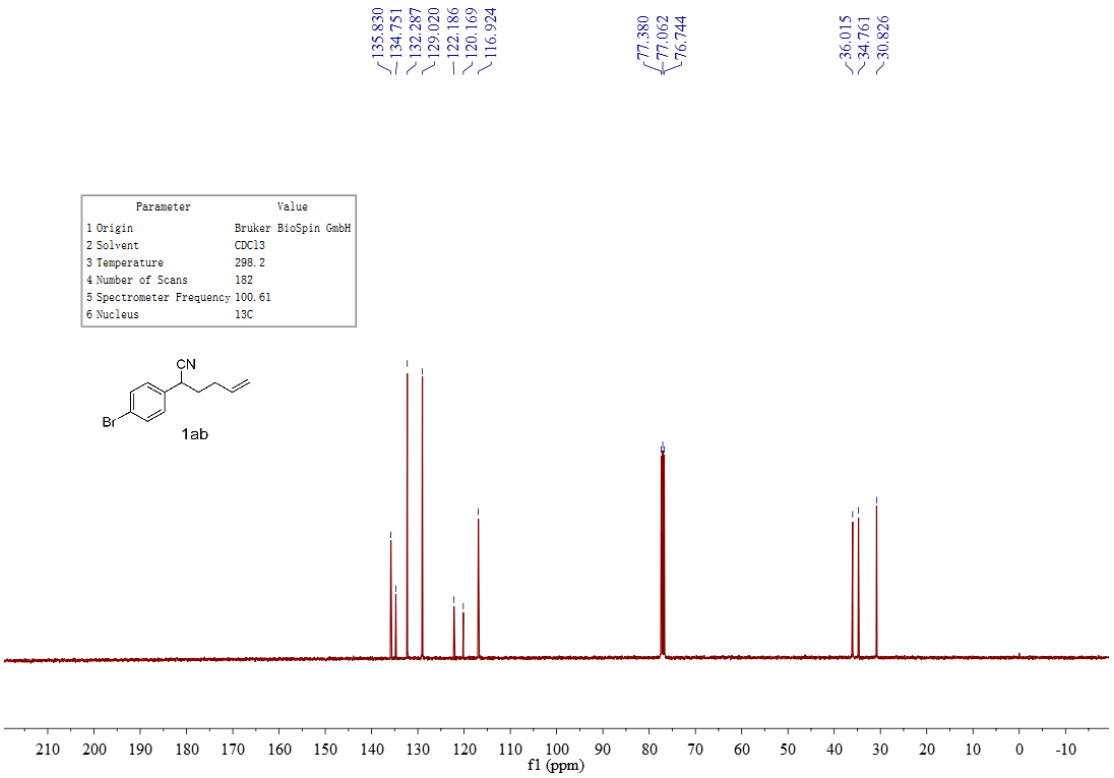
1.956
1.940
1.938
1.922
1.918
1.906
1.902
1.887
Parameter Value
1 Origin Bruker BioSpin GmbH
2 Solvent CDCl3
3 Temperature 298.1
4 Number of Scans 4
5 Spectrometer Frequency 400.13
6 Nucleus 1H
CN
Br
1ab
2.00
2.00
1.00
2.01
1.00
2.00
1.00
1.01
f1 (ppm)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132.287
129.020
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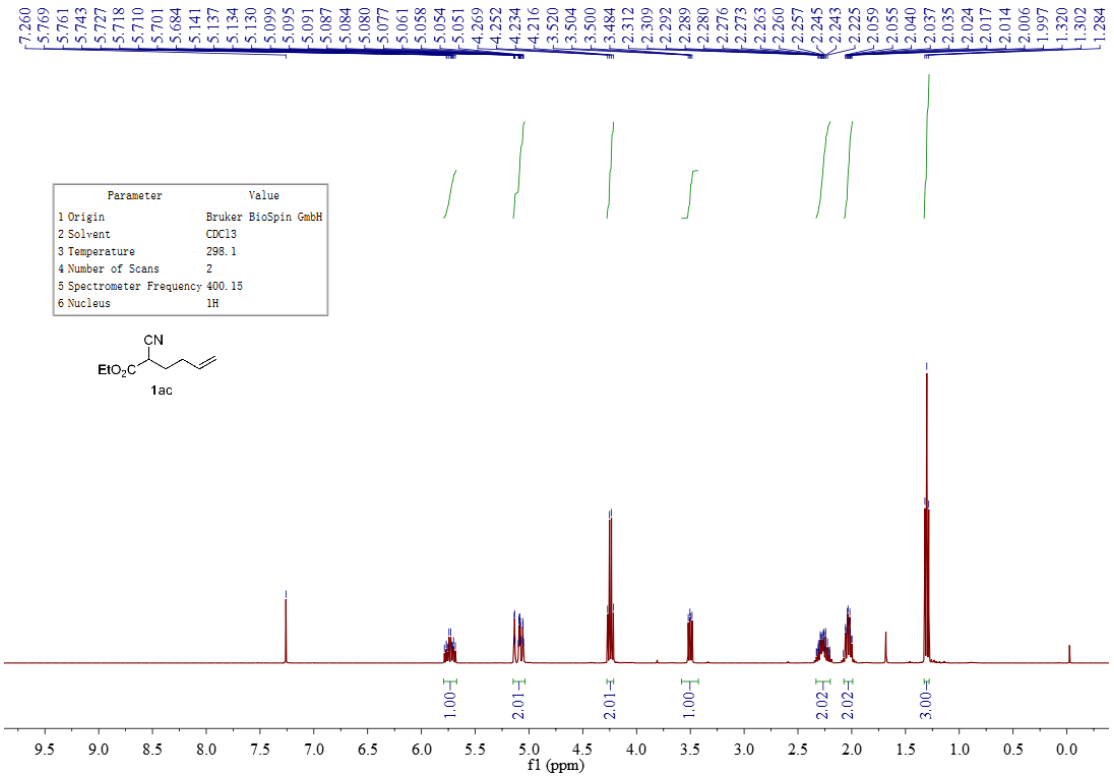
120.169
116.924
77.380
77.062
76.744
36.015
34.761
30.826
Parameter Value
1 Origin Bruker BioSpin GmbH
2 Solvent CDCl3
3 Temperature 298.2
4 Number of Scans 182
5 Spectrometer Frequency 100.61
6 Nucleus 13C
CN
Br
1ab
f1 (ppm)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5.761
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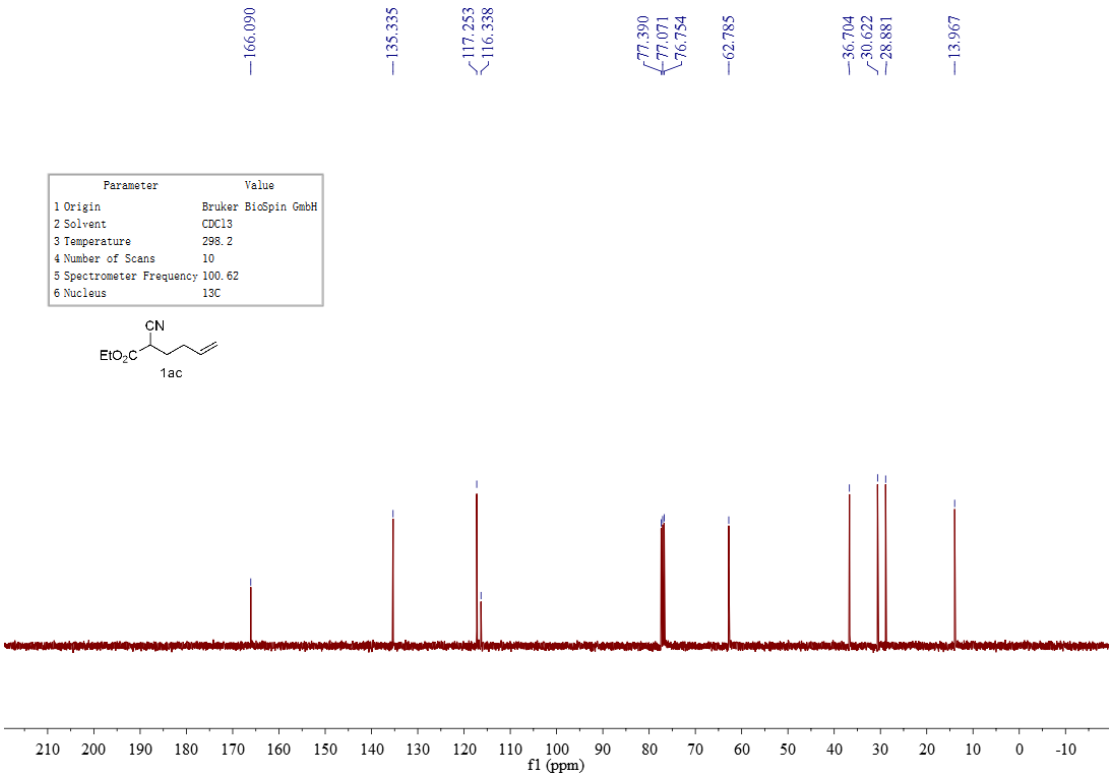
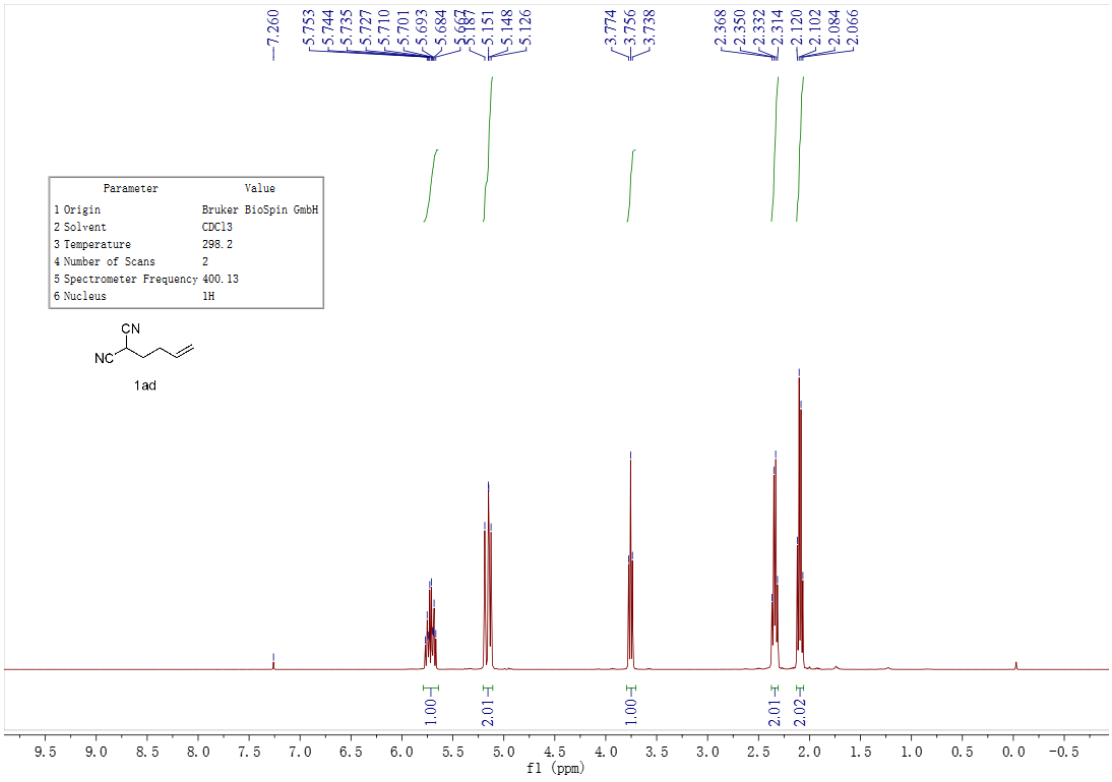
5.727
5.718
5.710
5.701
5.684
5.141
5.137
5.134
5.130
5.099
5.095
5.091
5.087
5.084
5.080
5.077
5.061
5.058
5.054
5.051
4.269
4.252
4.234
4.216
3.520
3.504
3.500
3.484
2.312
2.309
2.292
2.289
2.280
2.276
2.273
2.263
2.260
2.257
2.245
2.243
2.225
2.059
2.055
2.040
2.037
2.035
2.024
2.017
2.014
2.006
1.997
1.320
1.302
1.284
Parameter Value
1 Origin Bruker BioSpin GmbH
2 Solvent CDCl3
3 Temperature 298.1
4 Number of Scans 2
5 Spectrometer Frequency 400.15
6 Nucleus 1H
CN
EtO2C
1ac
1.00
2.01
2.01
1.00
2.02
2.02
3.00
f1 (ppm)


166.090
135.335
117.253
116.338
77.390
77.071
76.754
62.785
36.704
30.622
28.881
13.967
Parameter Value
1 Origin Bruker BioSpin GmbH
2 Solvent CDCl3
3 Temperature 298.2
4 Number of Scans 10
5 Spectrometer Frequency 100.62
6 Nucleus 13C
CN
EtO2C
1ac
f1 (ppm)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5.744
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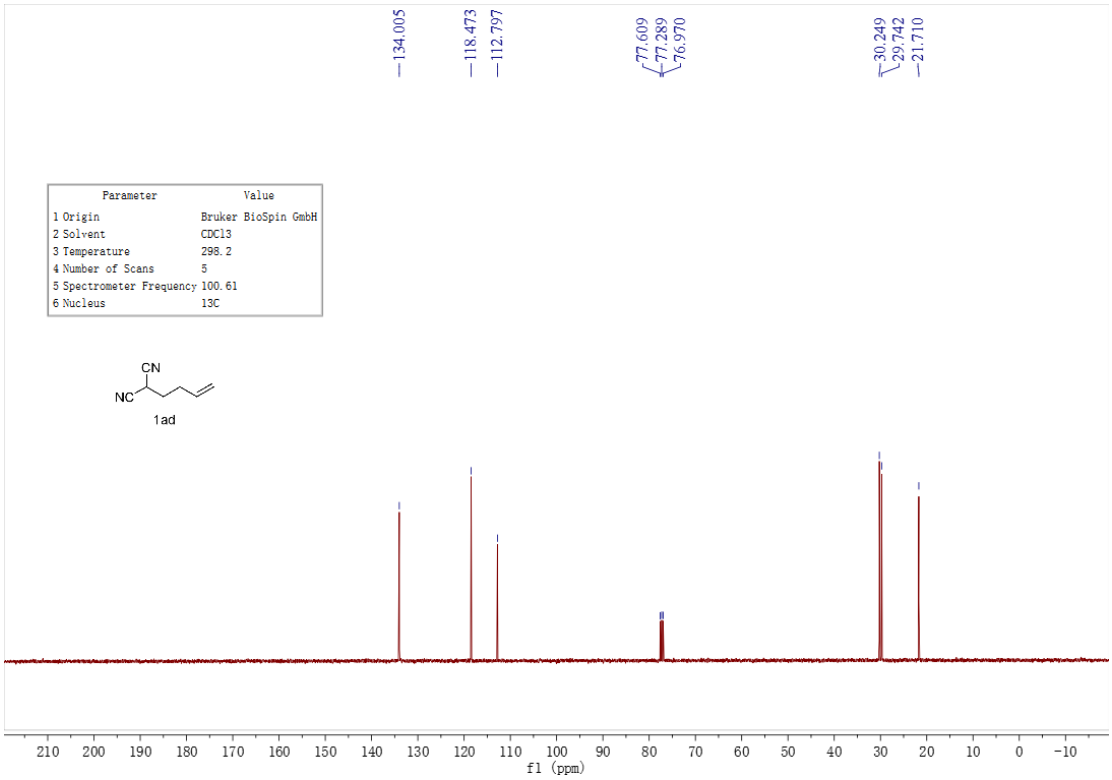
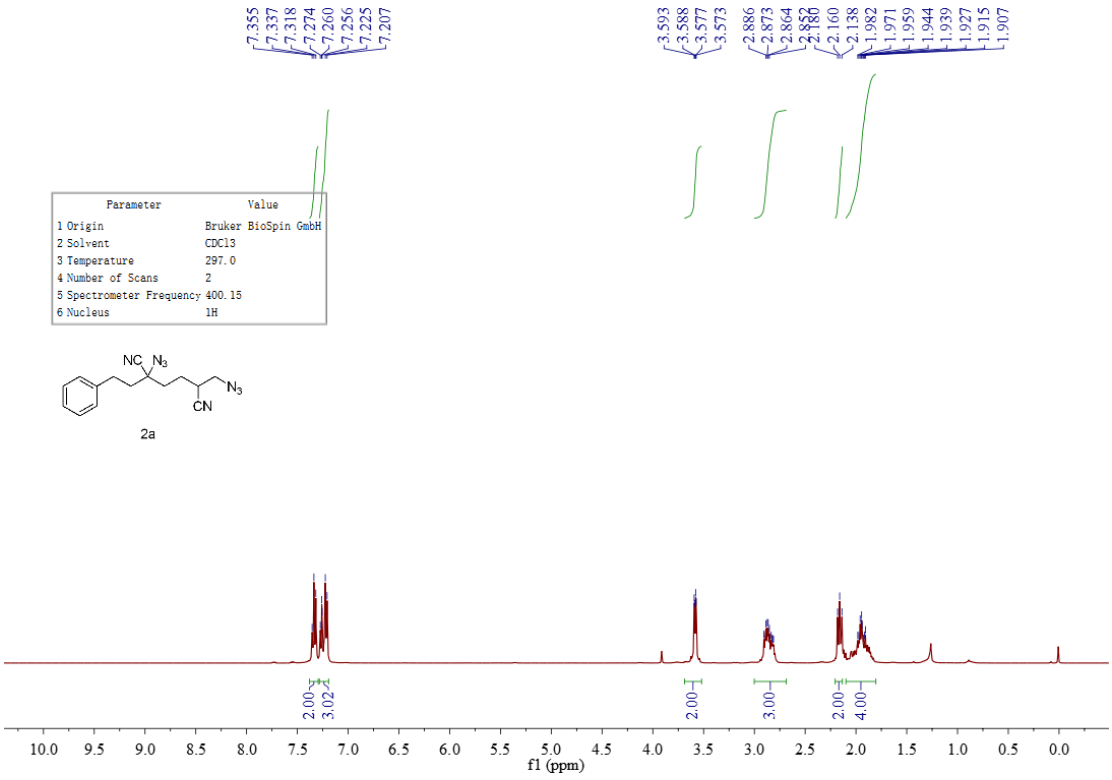
5.701
5.693
5.684
5.667
5.187
5.151
5.148
5.126
3.774
3.756
3.738
2.368
2.350
2.332
2.314
2.120
2.102
2.084
2.066
Parameter Value
1 Origin Bruker BioSpin GmbH
2 Solvent CDCl3
3 Temperature 298.2
4 Number of Scans 2
5 Spectrometer Frequency 400.13
6 Nucleus 1H
CN
NC
1ad
1.00
2.01
1.00
2.01
2.02
f1 (ppm)


134.005
118.473
112.797
77.609
77.289
76.970
30.249
29.742
21.710
Parameter Value
1 Origin Bruker BioSpin GmbH
2 Solvent CDCl3
3 Temperature 298.2
4 Number of Scans 5
5 Spectrometer Frequency 100.61
6 Nucleus 13C
CN
NC
1ad
f1 (ppm)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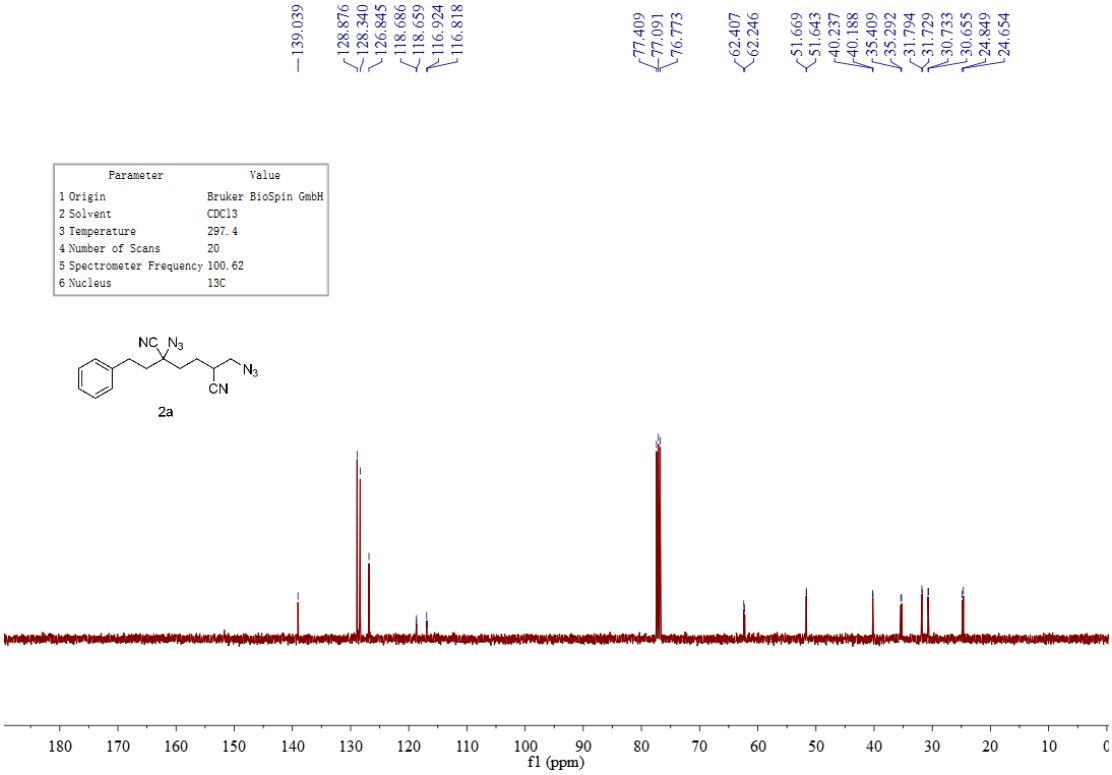
7.337
7.318
7.274
7.260
7.256
7.225
7.207
3.593
3.588
3.577
3.573
2.886
2.873
2.864
2.160
2.138
1.982
1.971
1.959
1.944
1.939
1.927
1.915
1.907
Parameter Value
1 Origin Bruker BioSpin GmbH
2 Solvent CDCl3
3 Temperature 297.0
4 Number of Scans 2
5 Spectrometer Frequency 400.15
6 Nucleus 1H
NC N3
N3
CN
2a
2.00
3.02
2.00
3.00
2.00
4.00
f1 (ppm)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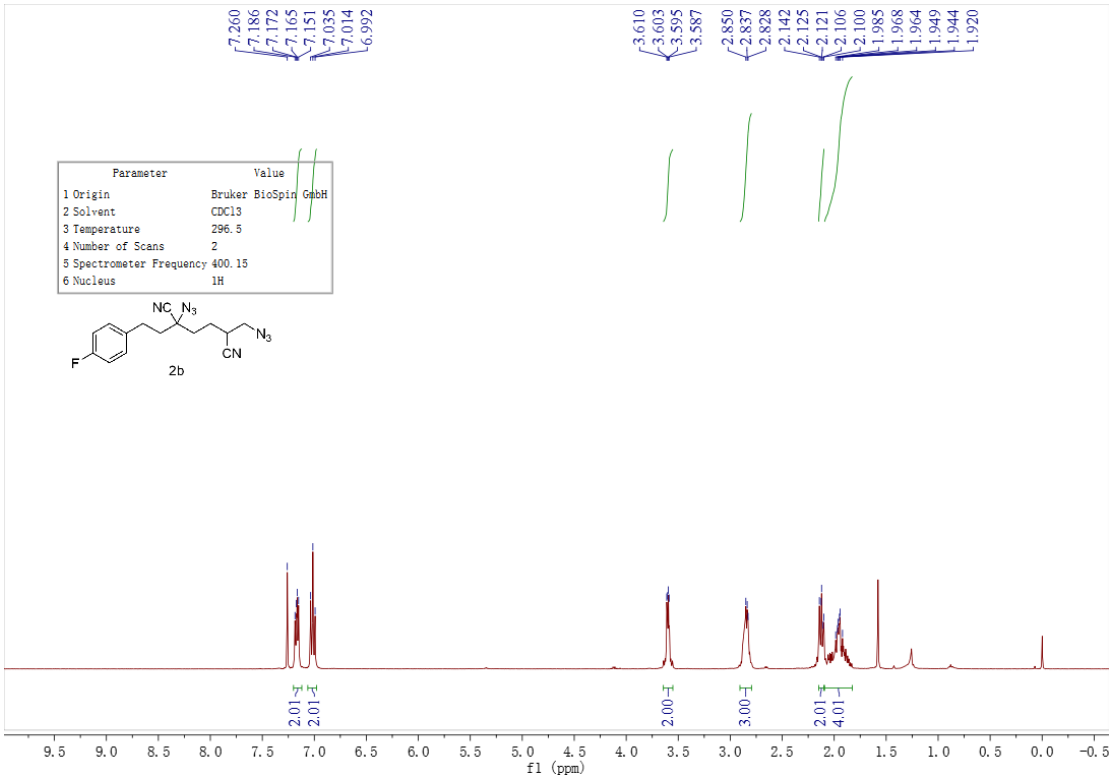
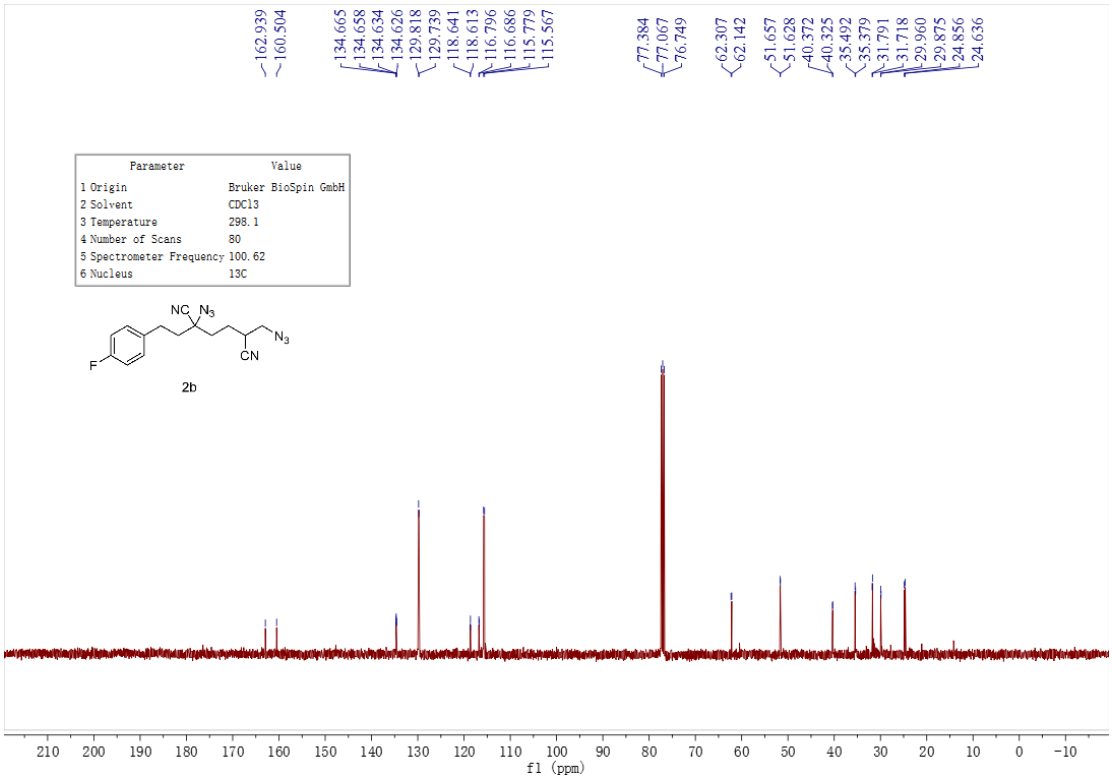
128.876
128.340
126.845
118.686
118.659
116.924
116.818
77.409
77.091
76.773
62.407
62.246
51.669
51.643
40.237
40.188
35.409
35.292
31.794
31.729
30.733
30.655
24.849
24.654
Parameter Value
1 Origin Bruker BioSpin GmbH
2 Solvent CDCl3
3 Temperature 297.4
4 Number of Scans 20
5 Spectrometer Frequency 100.62
6 Nucleus 13C
NC N3
N3
CN
2a
f1 (ppm)


7.260
7.186
7.172
7.165
7.151
7.035
7.014
6.992
3.610
3.603
3.595
3.587
2.850
2.837
2.828
2.142
2.125
2.121
2.106
2.100
1.985
1.968
1.964
1.949
1.944
1.920
Parameter Value
1 Origin Bruker BioSpin GmbH
2 Solvent CDCl3
3 Temperature 296.5
4 Number of Scans 2
5 Spectrometer Frequency 400.15
6 Nucleus 1H
NC N3
N3
CN
F
2b
2.01
2.01
2.00
3.00
2.01
4.01
f1 (ppm)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160.504
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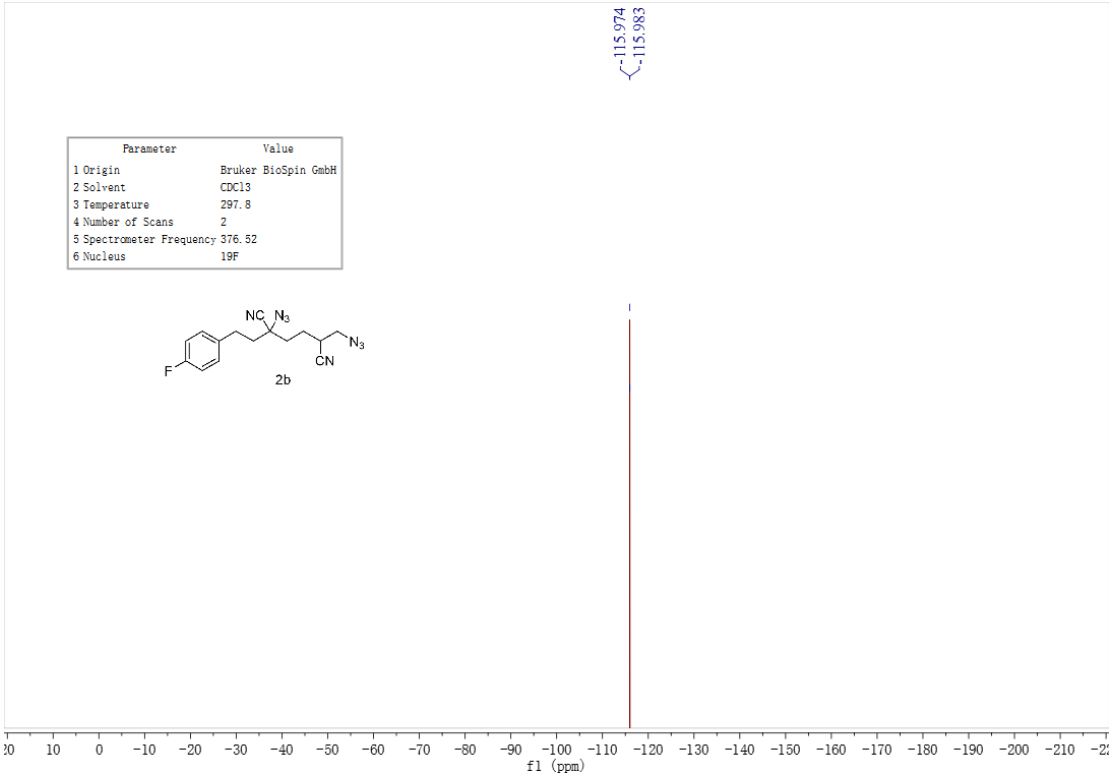
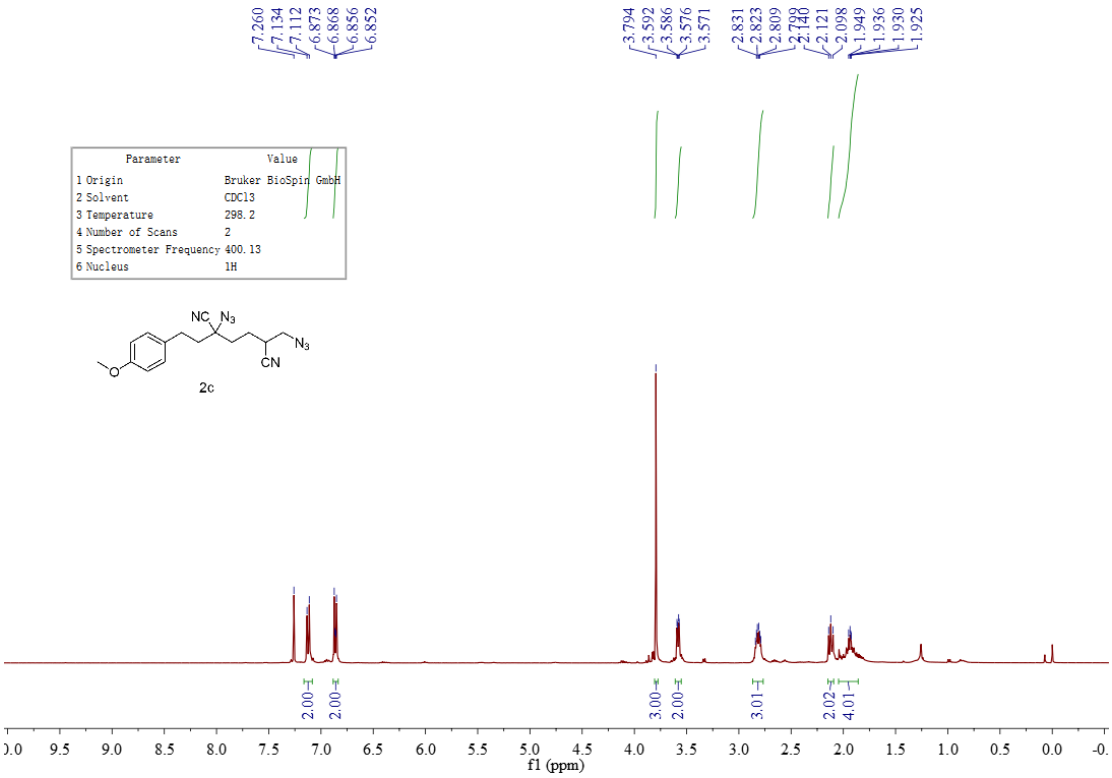
134.658
134.634
134.626
129.818
129.739
118.641
118.613
116.796
116.686
115.779
115.567
77.384
77.067
76.749
62.307
62.142
51.657
51.628
40.372
40.325
35.492
35.379
31.791
31.718
29.960
29.875
24.856
24.636
Parameter Value
1 Origin Bruker BioSpin GmbH
2 Solvent CDCl3
3 Temperature 298.1
4 Number of Scans 80
5 Spectrometer Frequency 100.62
6 Nucleus 13C
NC N3
N3
CN
F
2b
f1 (ppm)


115.974
115.983
Parameter Value
1 Origin Bruker BioSpin GmbH
2 Solvent CDCl3
3 Temperature 297.8
4 Number of Scans 2
5 Spectrometer Frequency 376.52
6 Nucleus 19F
NC N3
N3
CN
F
2b
f1 (ppm)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6.868
6.856
6.852
3.794
3.592
3.586
3.576
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2.831
2.823
2.809
2.799
2.140
2.121
2.098
1.949
1.936
1.930
1.925
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
NC N3
N3
CN
O
2c
2.00
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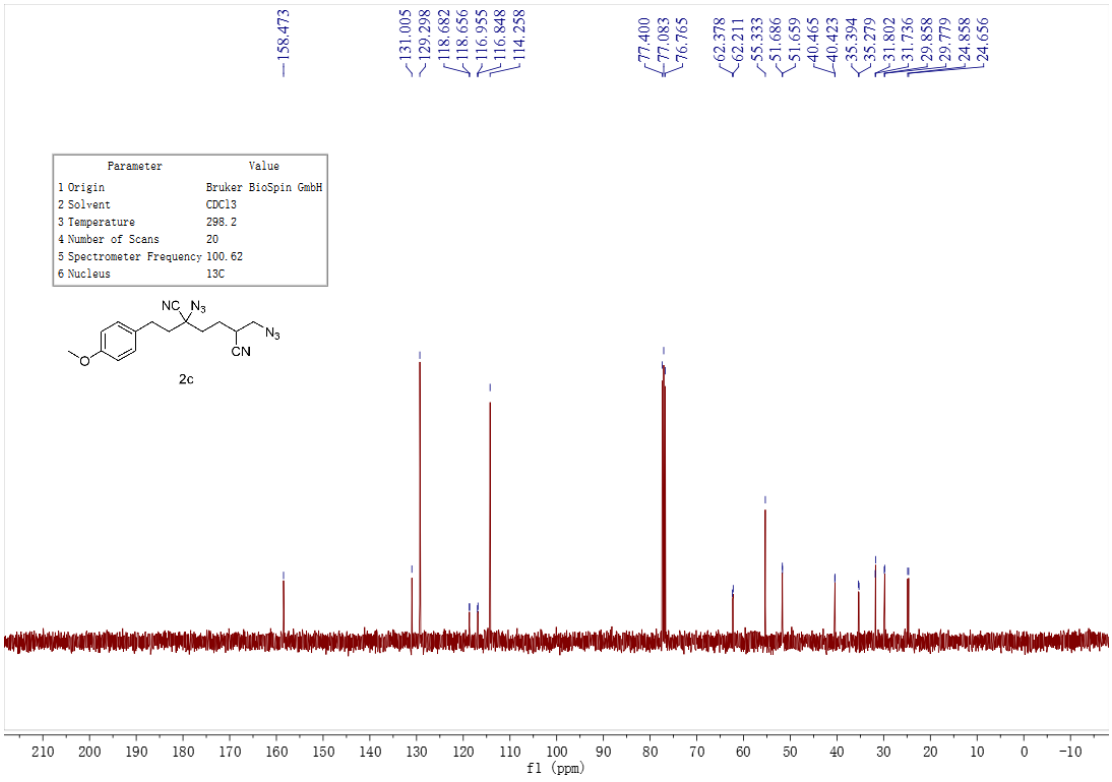
2.00
3.01
2.02
4.01
f1 (ppm)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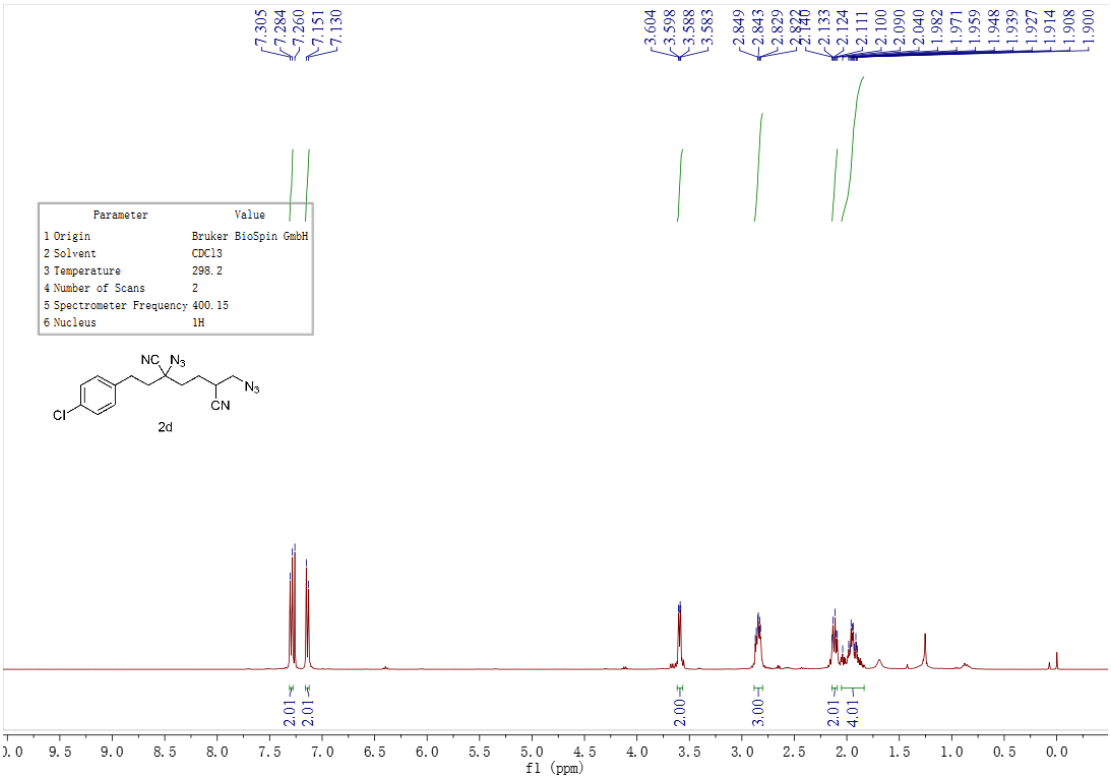
114.258
77.400
77.083
76.765
62.378
62.211
55.333
51.686
51.659
40.465
40.423
35.394
35.279
31.802
31.736
29.858
29.779
24.858
24.656
Parameter Value
1 Origin Bruker BioSpin GmbH
2 Solvent CDCl3
3 Temperature 298.2
4 Number of Scans 20
5 Spectrometer Frequency 100.62
6 Nucleus 13C
NC N3
N3
CN
O
2c
f1 (ppm)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7.260
7.151
7.130
3.604
3.598
3.588
3.583
2.849
2.843
2.829
2.822
2.133
2.124
2.111
2.100
2.090
2.040
1.982
1.971
1.959
1.948
1.939
1.927
1.914
1.908
1.900
Parameter Value
1 Origin Bruker BioSpin GmbH
2 Solvent CDCl3
3 Temperature 298.2
4 Number of Scans 2
5 Spectrometer Frequency 400.15
6 Nucleus 1H
NC
N3
N3
CN
Cl
2d
2.01
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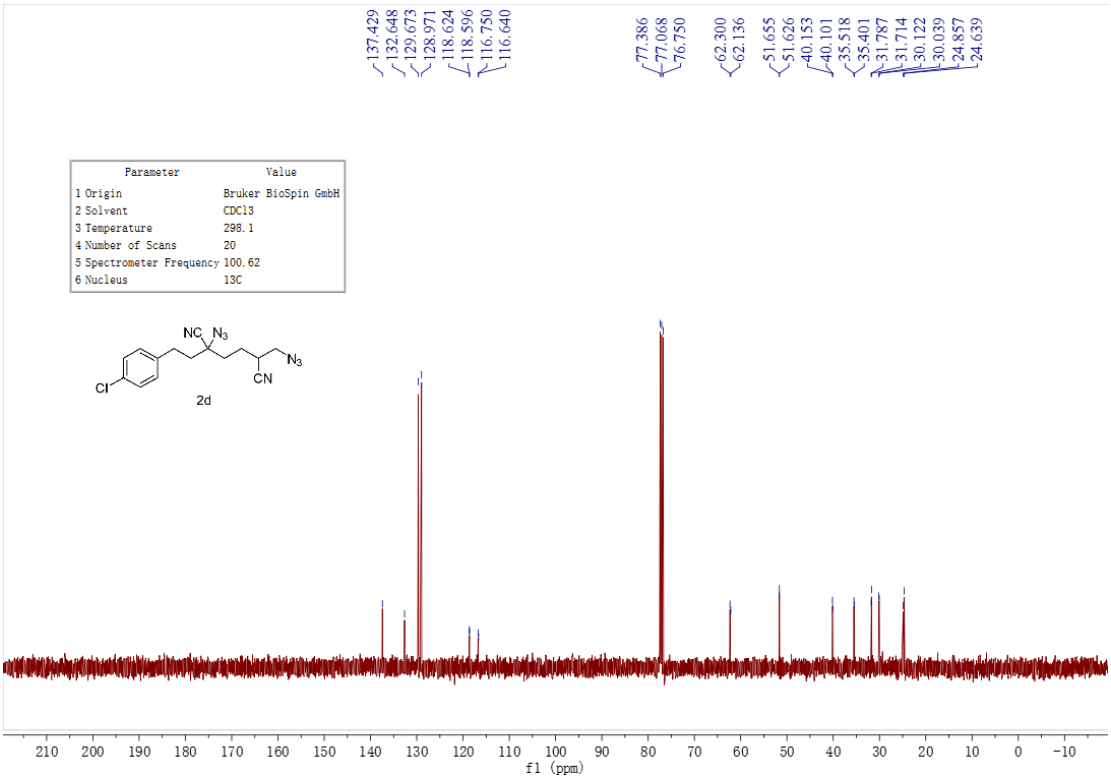
2.00
3.00
2.01
4.01
f1 (ppm)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116.640
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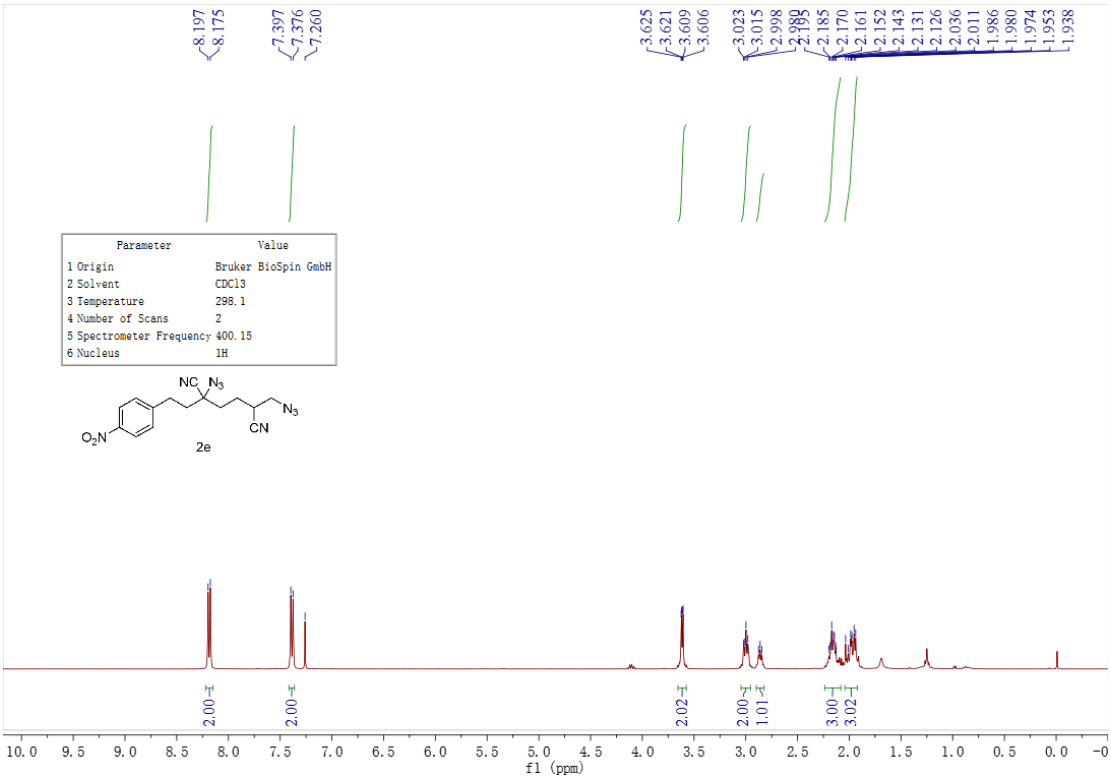
77.068
76.750
62.300
62.136
51.655
51.626
40.153
40.101
35.518
35.401
31.787
31.714
30.122
30.039
24.857
24.639
Parameter Value
1 Origin Bruker BioSpin GmbH
2 Solvent CDCl3
3 Temperature 298.1
4 Number of Scans 20
5 Spectrometer Frequency 100.62
6 Nucleus 13C
NC
N3
N3
CN
Cl
2d
f1 (ppm)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8.175
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7.260
3.625
3.621
3.609
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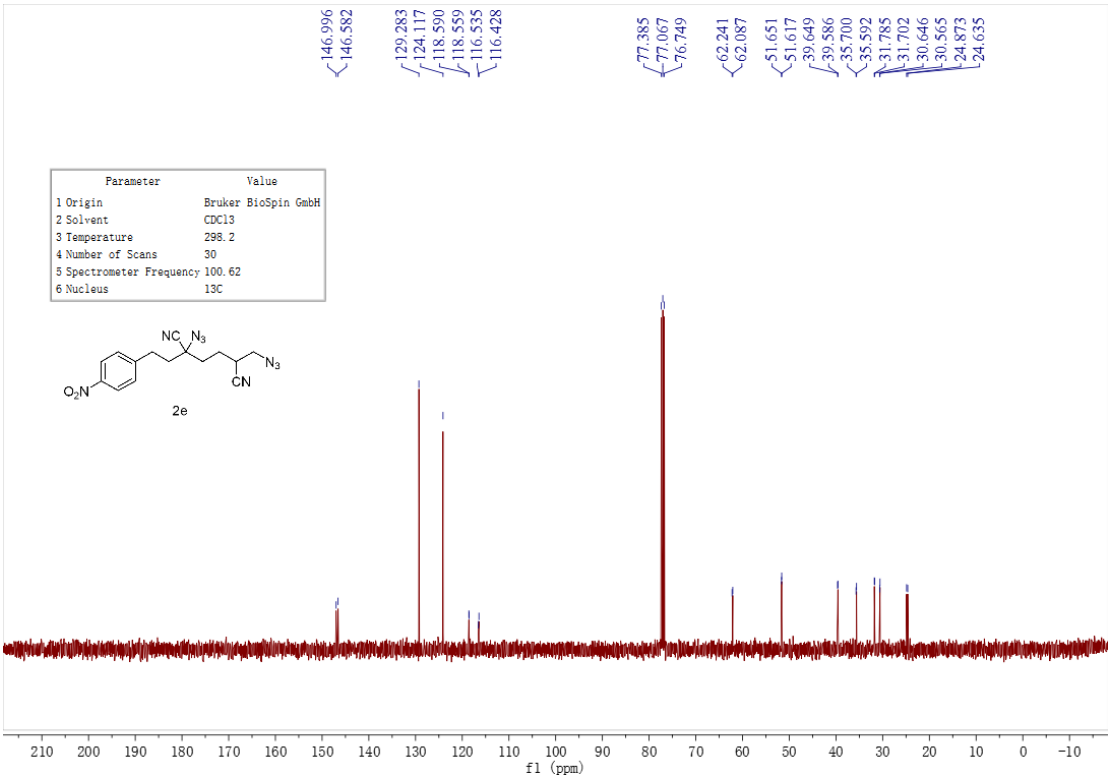
3.023
3.015
2.998
2.980
2.185
2.170
2.161
2.152
2.143
2.131
2.126
2.036
2.011
1.986
1.980
1.974
1.953
1.938
Parameter Value
1 Origin Bruker BioSpin GmbH
2 Solvent CDCl3
3 Temperature 298.1
4 Number of Scans 2
5 Spectrometer Frequency 400.15
6 Nucleus 1H
NC N3
N3
CN
O2N
2e
2.00
2.00
2.02
2.00
1.01
3.00
3.02
f1 (ppm)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116.428
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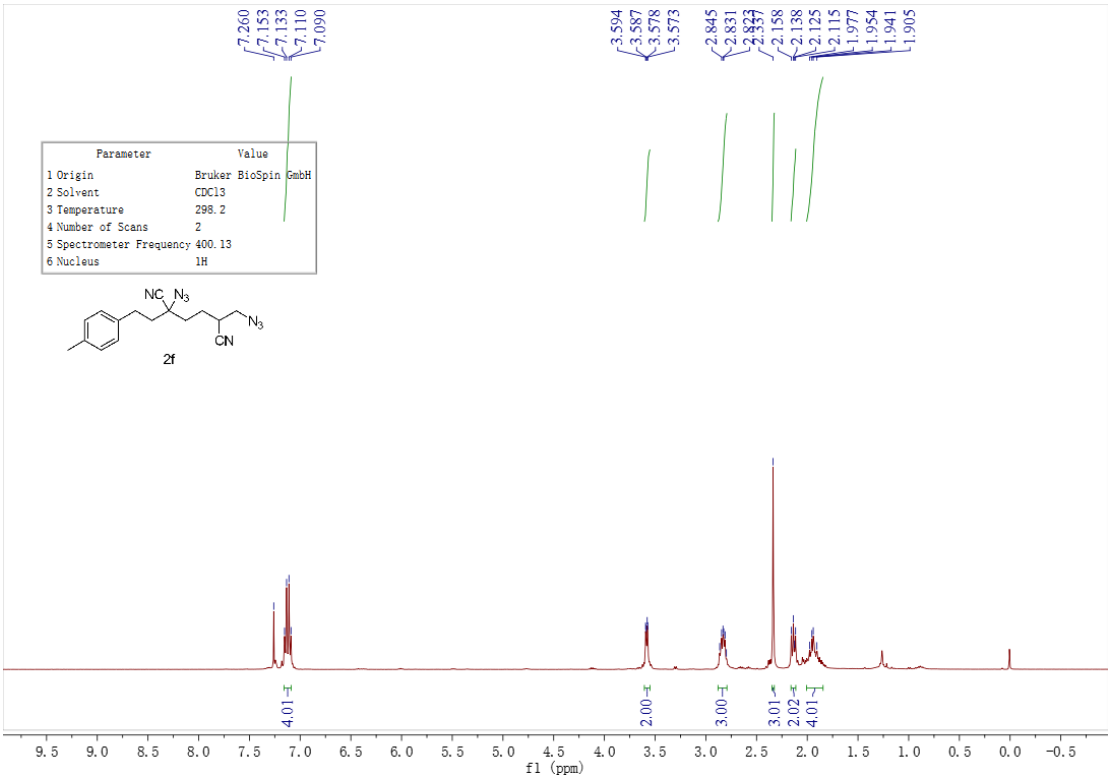
77.067
76.749
62.241
62.087
51.651
51.617
39.649
39.586
35.700
35.592
31.785
31.702
30.646
30.565
24.873
24.635
Parameter Value
1 Origin Bruker BioSpin GmbH
2 Solvent CDCl3
3 Temperature 298.2
4 Number of Scans 30
5 Spectrometer Frequency 100.62
6 Nucleus 13C
NC N3
N3
CN
O2N
2e
f1 (ppm)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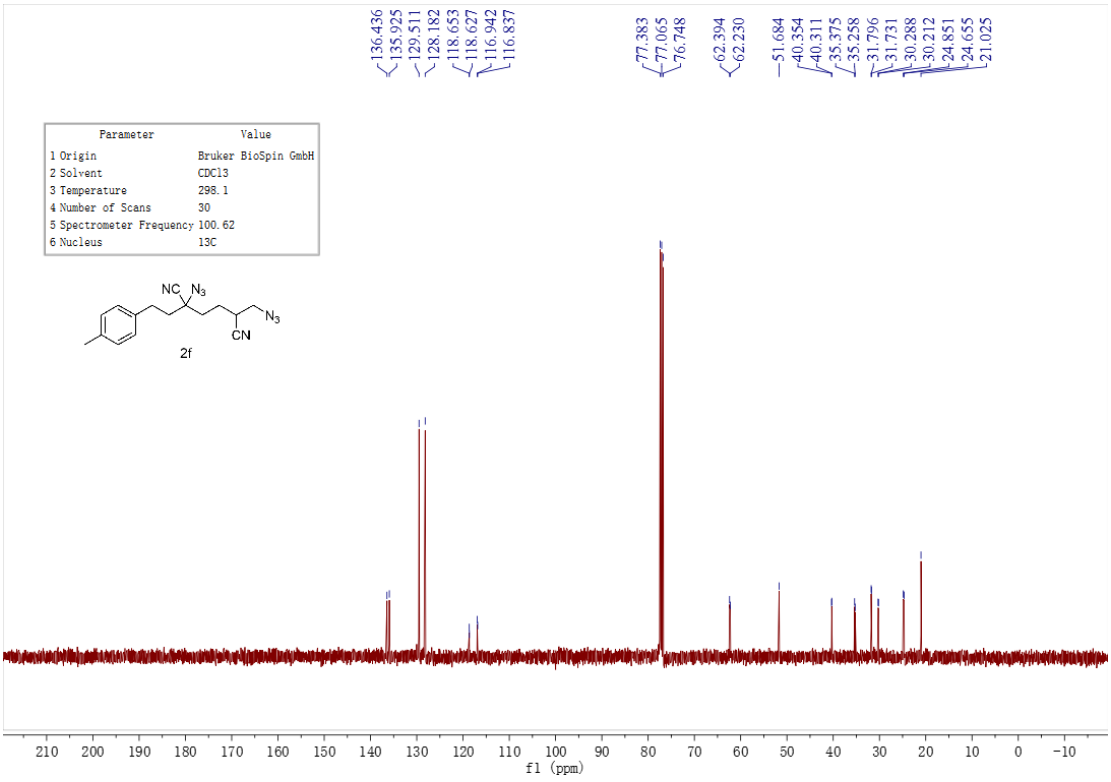
3.587
3.578
3.573
2.845
2.831
2.337
2.158
2.138
2.125
2.115
1.977
1.954
1.941
1.905
Parameter Value
1 Origin Bruker BioSpin GmbH
2 Solvent CDCl3
3 Temperature 298.2
4 Number of Scans 2
5 Spectrometer Frequency 400.13
6 Nucleus 1H
NC N3
N3
CN
2f
4.01
2.00
3.00
3.01
2.02
4.01
f1 (ppm)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116.942
116.837
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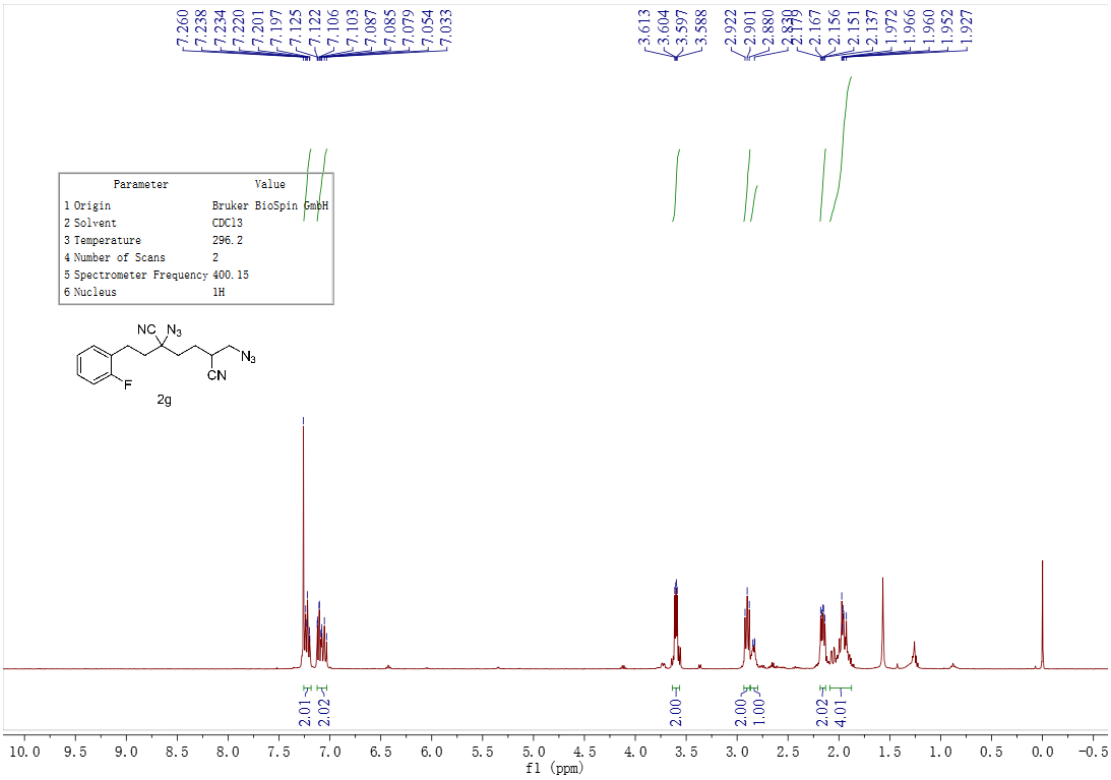
77.065
76.748
62.394
62.230
51.684
40.354
40.311
35.375
35.258
31.796
31.731
30.288
30.212
24.851
24.655
21.025
Parameter Value
1 Origin Bruker BioSpin GmbH
2 Solvent CDCl3
3 Temperature 298.1
4 Number of Scans 30
5 Spectrometer Frequency 100.62
6 Nucleus 13C
NC N3
N3
CN
2f
f1 (ppm)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7.234
7.220
7.201
7.197
7.125
7.122
7.106
7.103
7.087
7.085
7.079
7.054
7.033
3.613
3.604
3.597
3.588
2.922
2.901
2.880
2.838
2.167
2.156
2.151
2.137
1.972
1.966
1.960
1.952
1.927
Parameter Value
1 Origin Bruker BioSpin GmbH
2 Solvent CDCl3
3 Temperature 296.2
4 Number of Scans 2
5 Spectrometer Frequency 400.15
6 Nucleus 1H
NC N3
N3
CN
F
2g
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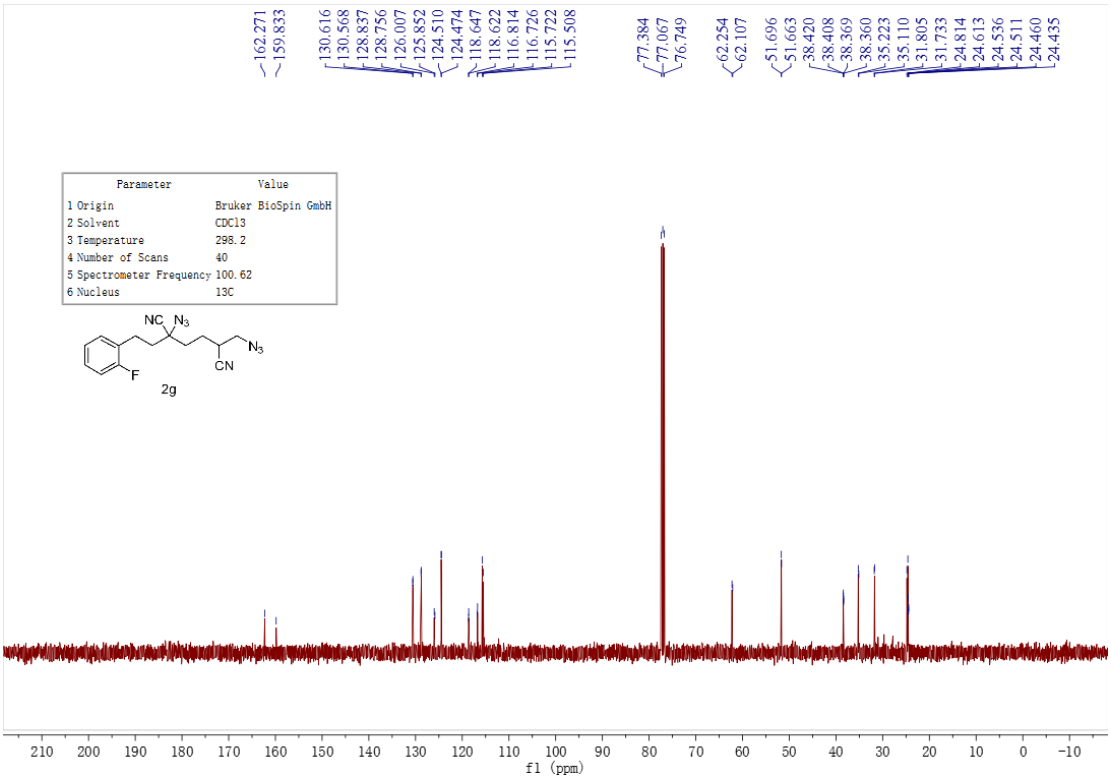
1.00
2.02
4.01
f1 (ppm)


162.271
159.833
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128.756
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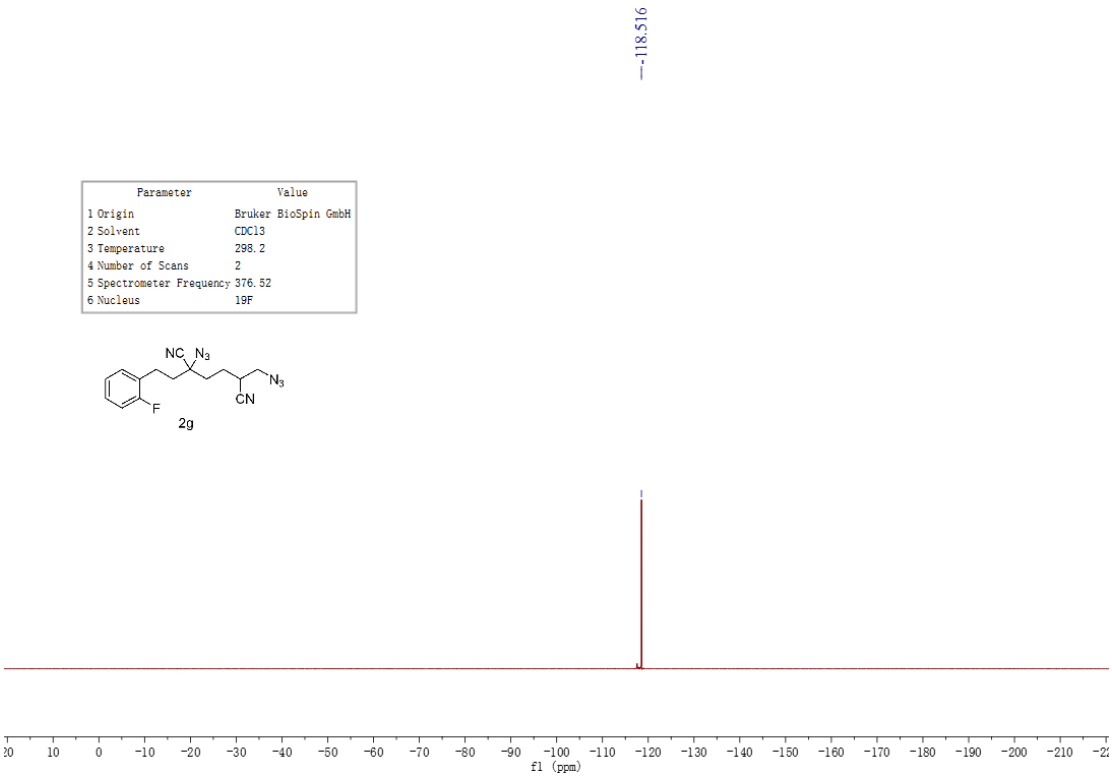
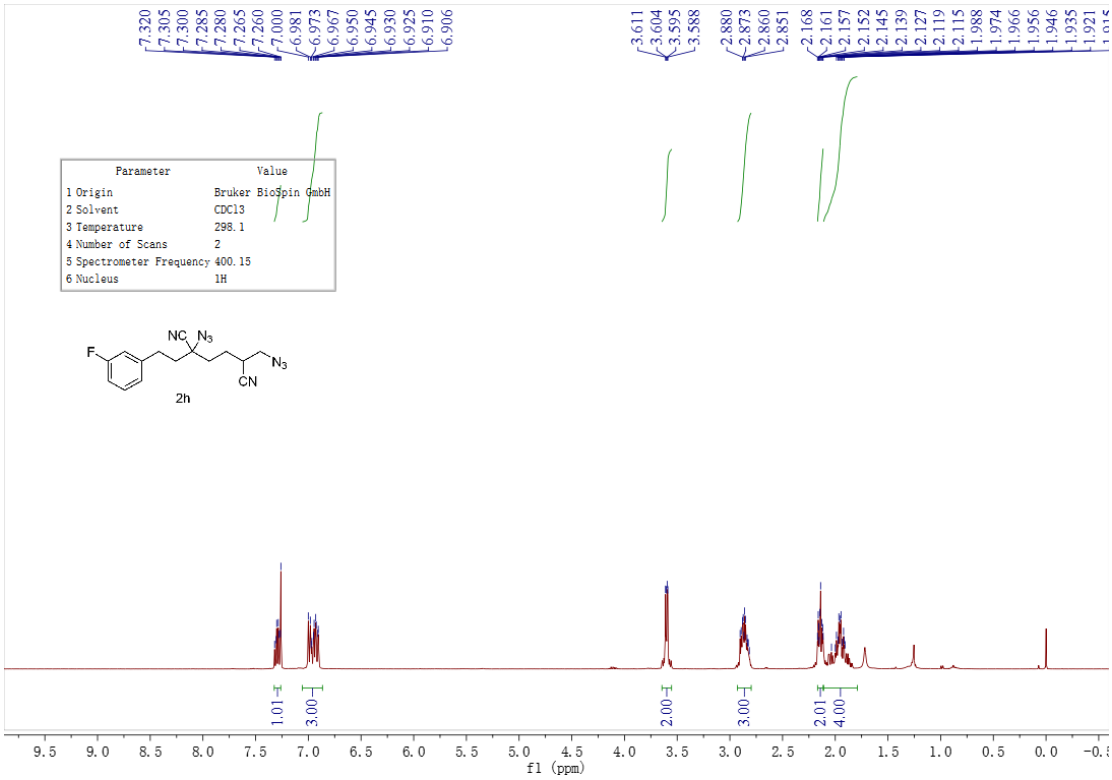
118.647
118.622
116.814
116.726
115.722
115.508
77.384
77.067
76.749
62.254
62.107
51.696
51.663
38.420
38.408
38.369
38.360
35.223
35.110
31.805
31.733
24.814
24.613
24.536
24.511
24.460
24.435
Parameter Value
1 Origin Bruker BioSpin GmbH
2 Solvent CDCl3
3 Temperature 298.2
4 Number of Scans 40
5 Spectrometer Frequency 100.62
6 Nucleus 13C
NC N3
N3
CN
F
2g
f1 (ppm)


-118.516
Parameter Value
1 Origin Bruker BioSpin GmbH
2 Solvent CDCl3
3 Temperature 298.2
4 Number of Scans 2
5 Spectrometer Frequency 376.52
6 Nucleus 19F
NC N3
N3
CN
F
2g
f1 (ppm)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7.000
6.981
6.973
6.967
6.950
6.945
6.930
6.925
6.910
6.906
3.611
3.604
3.595
3.588
2.880
2.873
2.860
2.851
2.168
2.161
2.157
2.152
2.145
2.139
2.127
2.119
2.115
1.988
1.974
1.966
1.956
1.946
1.935
1.921
Parameter Value
1 Origin Bruker BioSpin GmbH
2 Solvent CDCl3
3 Temperature 298.1
4 Number of Scans 2
5 Spectrometer Frequency 400.15
6 Nucleus 1H
NC N3
F
N3
CN
2h
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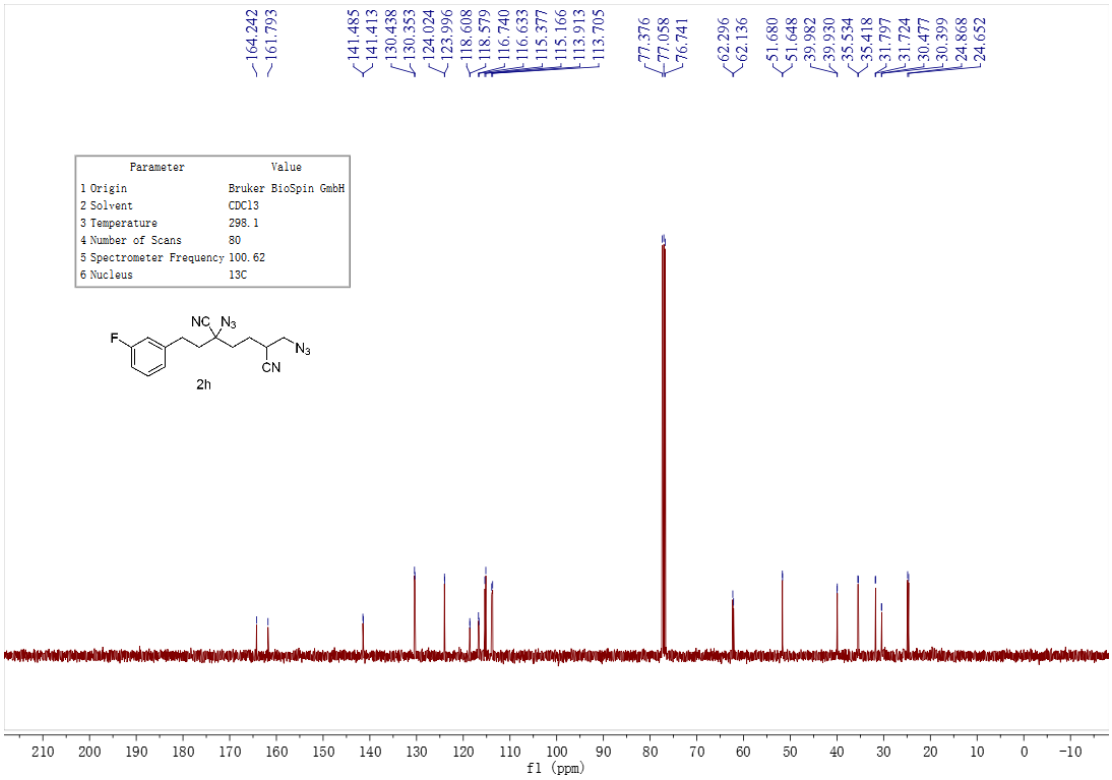
2.01
4.00
f1 (ppm)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123.996
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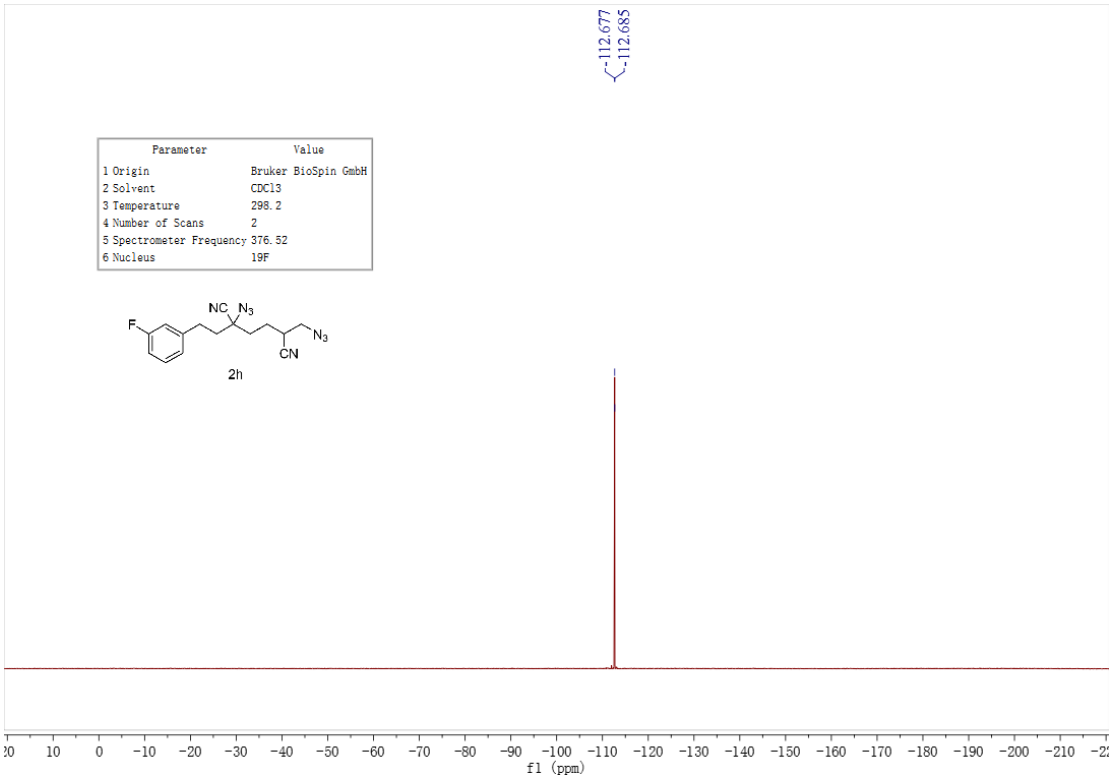
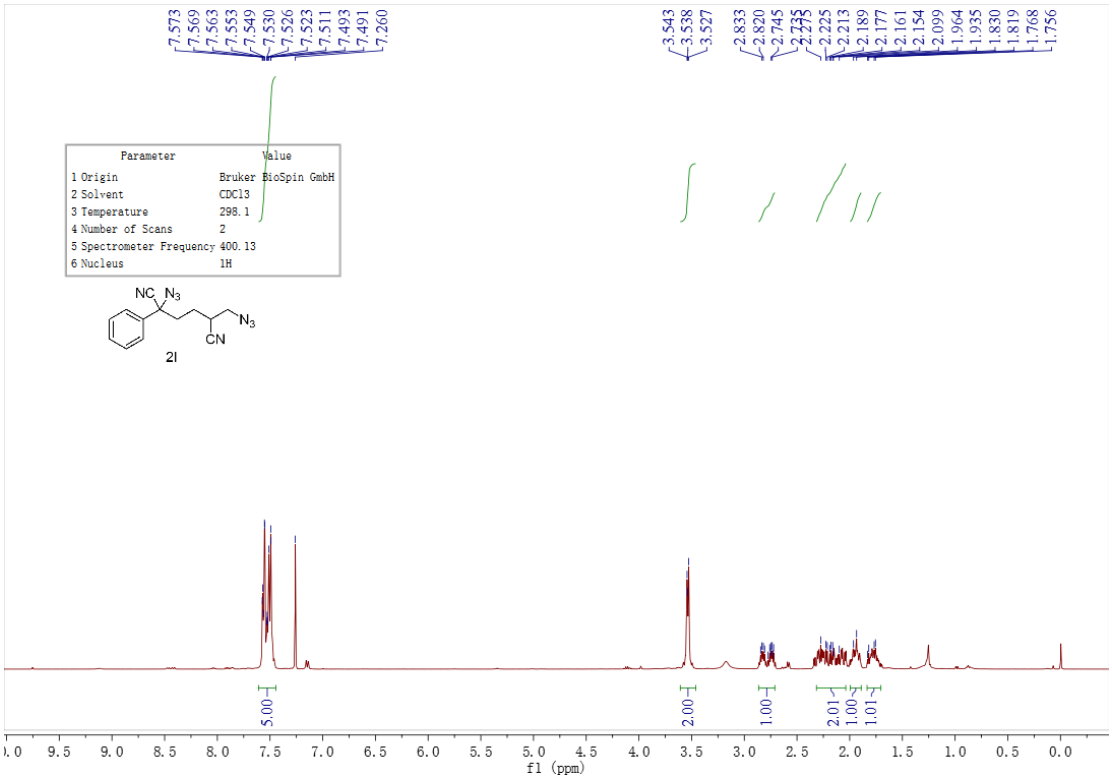
116.633
115.377
115.166
113.913
113.705
77.376
77.058
76.741
62.296
62.136
51.680
51.648
39.982
39.930
35.534
35.418
31.797
31.724
30.477
30.399
24.868
24.652
Parameter Value
1 Origin Bruker BioSpin GmbH
2 Solvent CDCl3
3 Temperature 298.1
4 Number of Scans 80
5 Spectrometer Frequency 100.62
6 Nucleus 13C
NC N3
F
N3
CN
2h
f1 (ppm)


-112.677
-112.685
Parameter Value
1 Origin Bruker BioSpin GmbH
2 Solvent CDCl3
3 Temperature 298.2
4 Number of Scans 2
5 Spectrometer Frequency 376.52
6 Nucleus 19F
NC N3
F
N3
CN
2h
f1 (ppm)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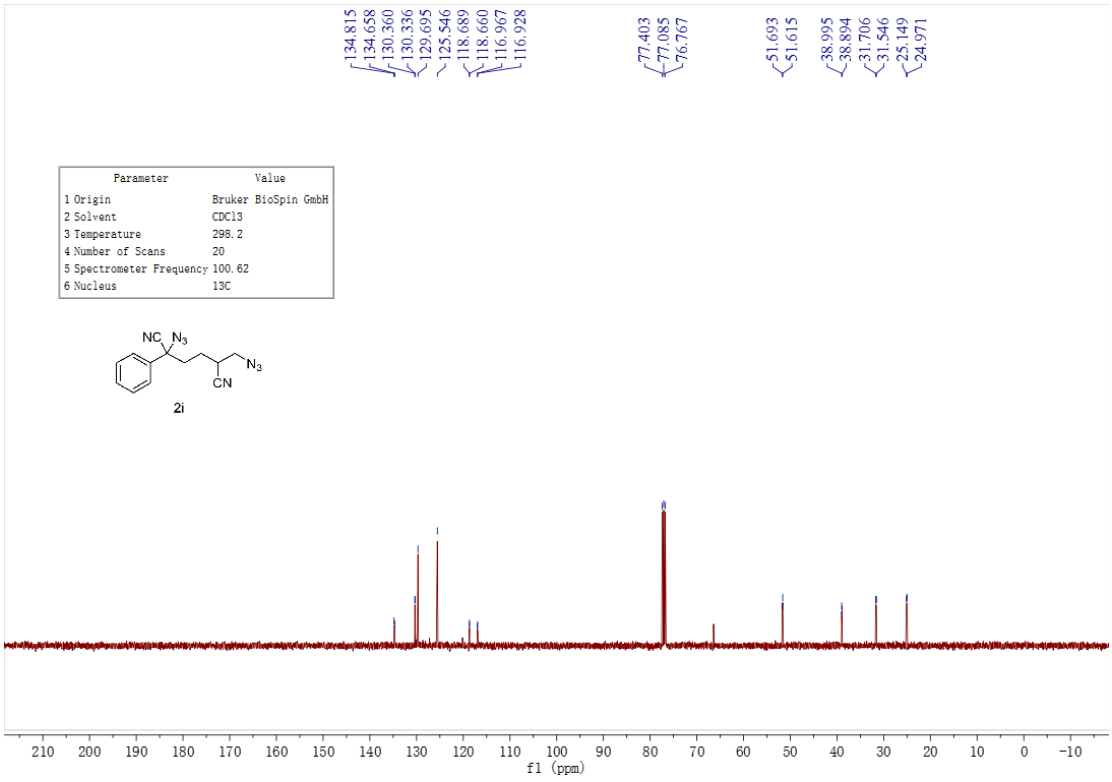
7.530
7.526
7.523
7.511
7.493
7.491
7.260
3.543
3.538
3.527
2.833
2.820
2.745
2.735
2.225
2.213
2.189
2.177
2.161
2.154
2.099
1.964
1.935
1.830
1.819
1.768
1.756
Parameter Value
1 Origin Bruker BioSpin GmbH
2 Solvent CDCl3
3 Temperature 298.1
4 Number of Scans 2
5 Spectrometer Frequency 400.13
6 Nucleus 1H
NC N3
N3
CN
2l
5.00
2.00
1.00
2.01
1.00
1.01
f1 (ppm)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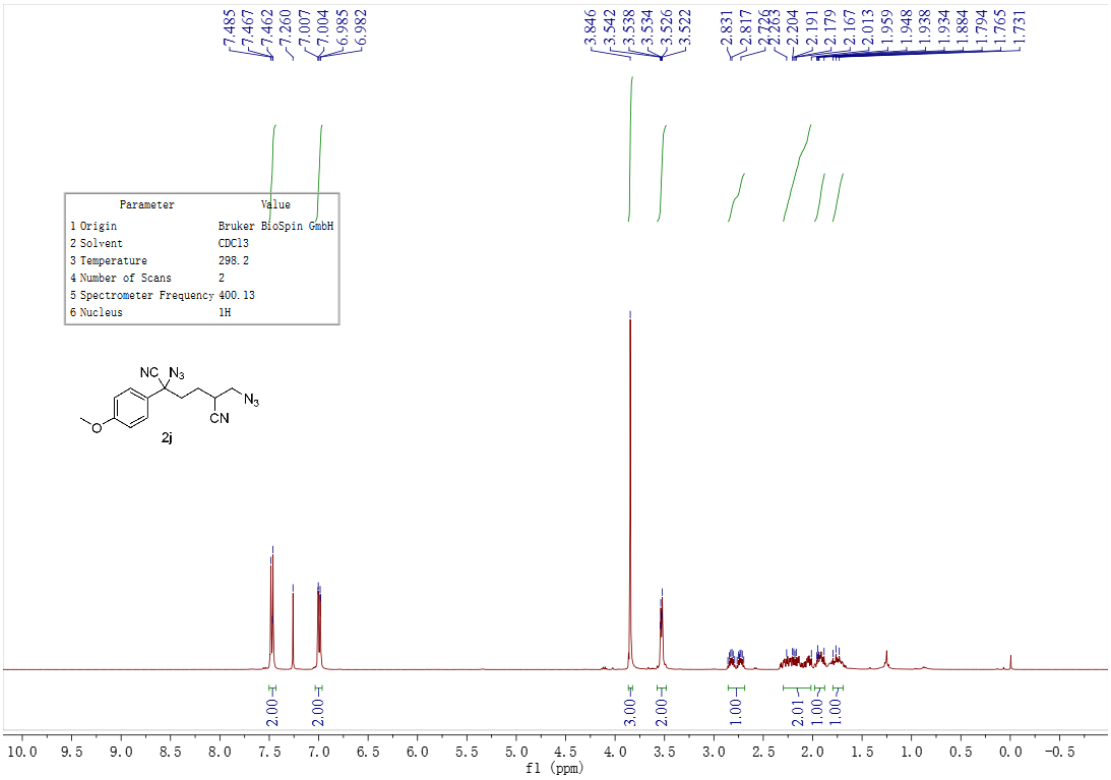
134.658
130.360
130.336
129.695
125.546
118.689
118.660
116.967
116.928
77.403
77.085
76.767
51.693
51.615
38.995
38.894
31.706
31.546
25.149
24.971
Parameter Value
1 Origin Bruker BioSpin GmbH
2 Solvent CDCl3
3 Temperature 298.2
4 Number of Scans 20
5 Spectrometer Frequency 100.62
6 Nucleus 13C
NC N3
N3
CN
2i
f1 (ppm)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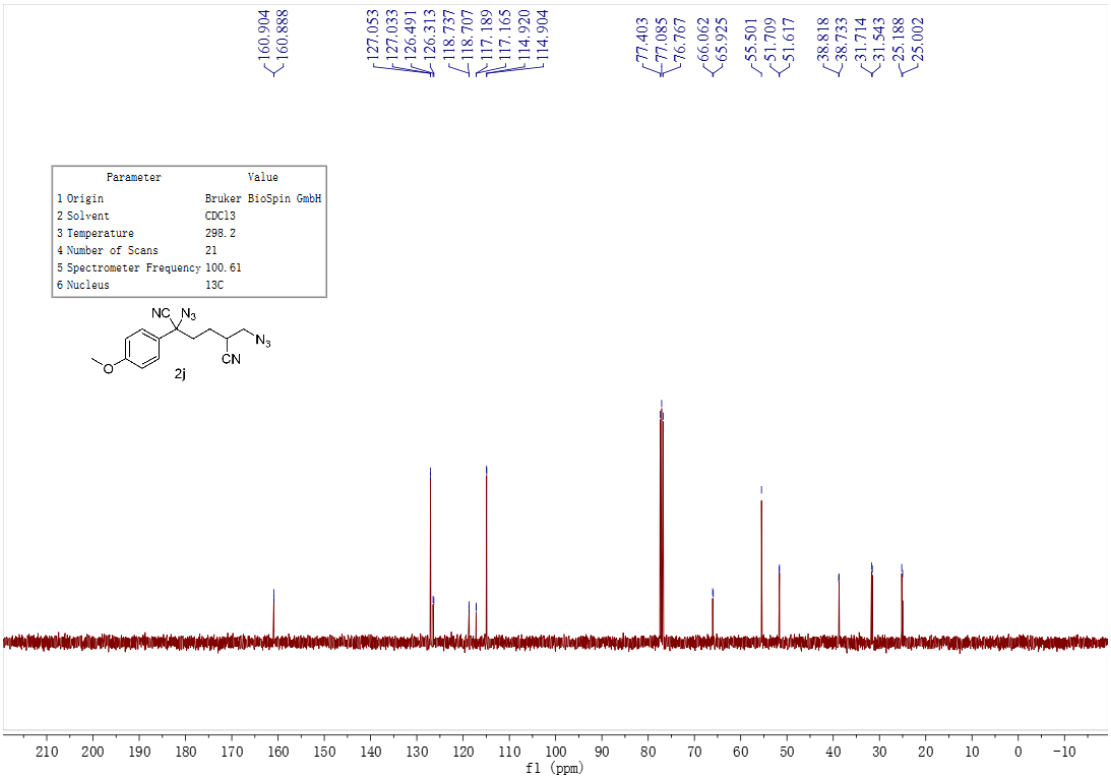
7.467
7.462
7.260
7.007
7.004
6.985
6.982
3.846
3.542
3.538
3.534
3.526
3.522
2.831
2.817
2.726
2.283
2.204
2.191
2.179
2.167
2.013
1.959
1.948
1.938
1.934
1.884
1.794
1.765
1.731
Parameter Value
1 Origin Bruker BioSpin GmbH
2 Solvent CDCl3
3 Temperature 298.2
4 Number of Scans 2
5 Spectrometer Frequency 400.13
6 Nucleus 1H
NC N3
N3
CN
O
2j
2.00
2.00
3.00
2.00
1.00
2.01
1.00
1.00
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)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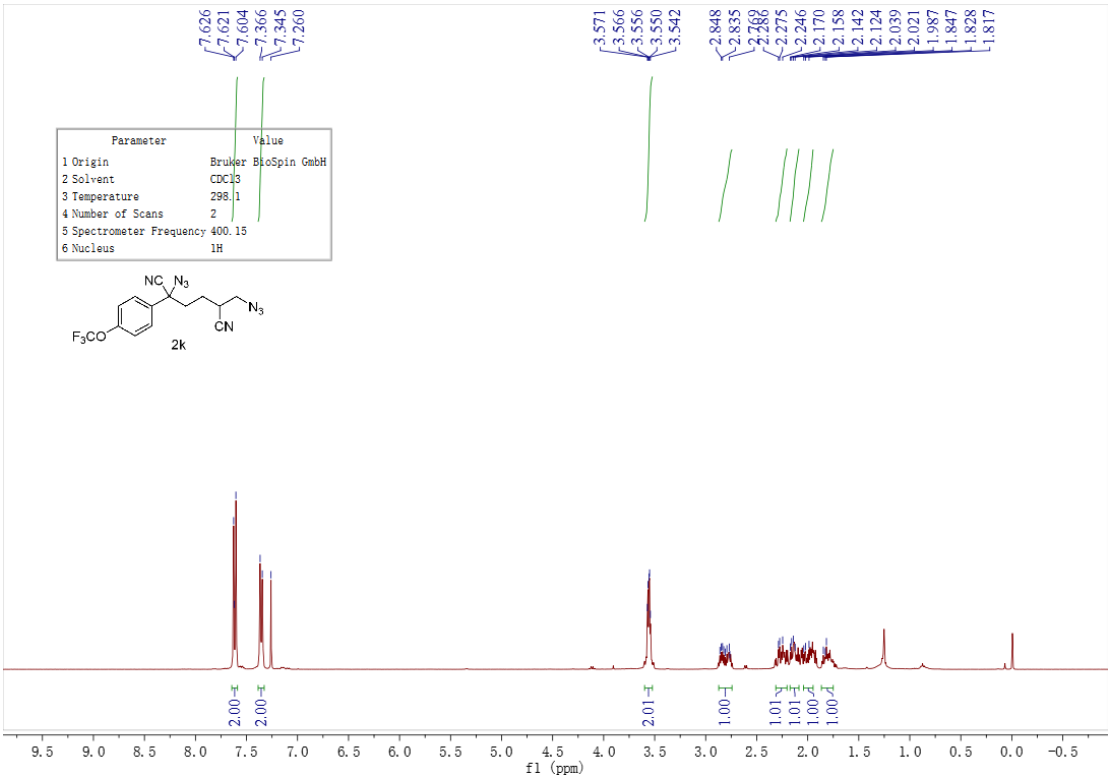
127.053
127.033
126.491
126.313
118.737
118.707
117.189
117.165
114.920
114.904
77.403
77.085
76.767
66.062
65.925
55.501
51.709
51.617
38.818
38.733
31.714
31.543
25.188
25.002
Parameter Value
1 Origin Bruker BioSpin GmbH
2 Solvent CDCl3
3 Temperature 298.2
4 Number of Scans 21
5 Spectrometer Frequency 100.61
6 Nucleus 13C
NC N3
N3
CN
O
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)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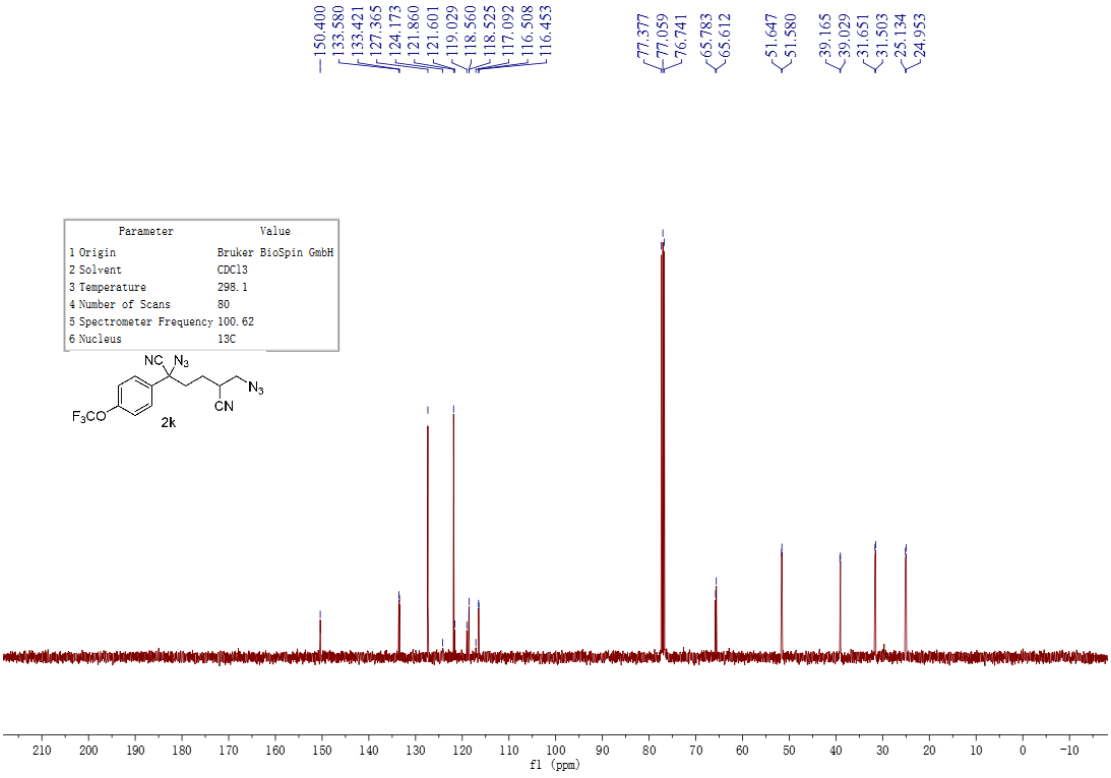
7.345
7.260
3.571
3.566
3.556
3.550
3.542
2.848
2.835
2.769
2.282
2.275
2.246
2.170
2.158
2.142
2.124
2.039
2.021
1.987
1.847
1.828
1.817
Parameter Value
1 Origin Bruker BioSpin GmbH
2 Solvent CDCl3
3 Temperature 298.1
4 Number of Scans 2
5 Spectrometer Frequency 400.15
6 Nucleus 1H
NC N3
N3
CN
F3CO
2k
2.00
2.00
2.01
1.00
1.01
1.01
1.00
1.00
f1 (ppm)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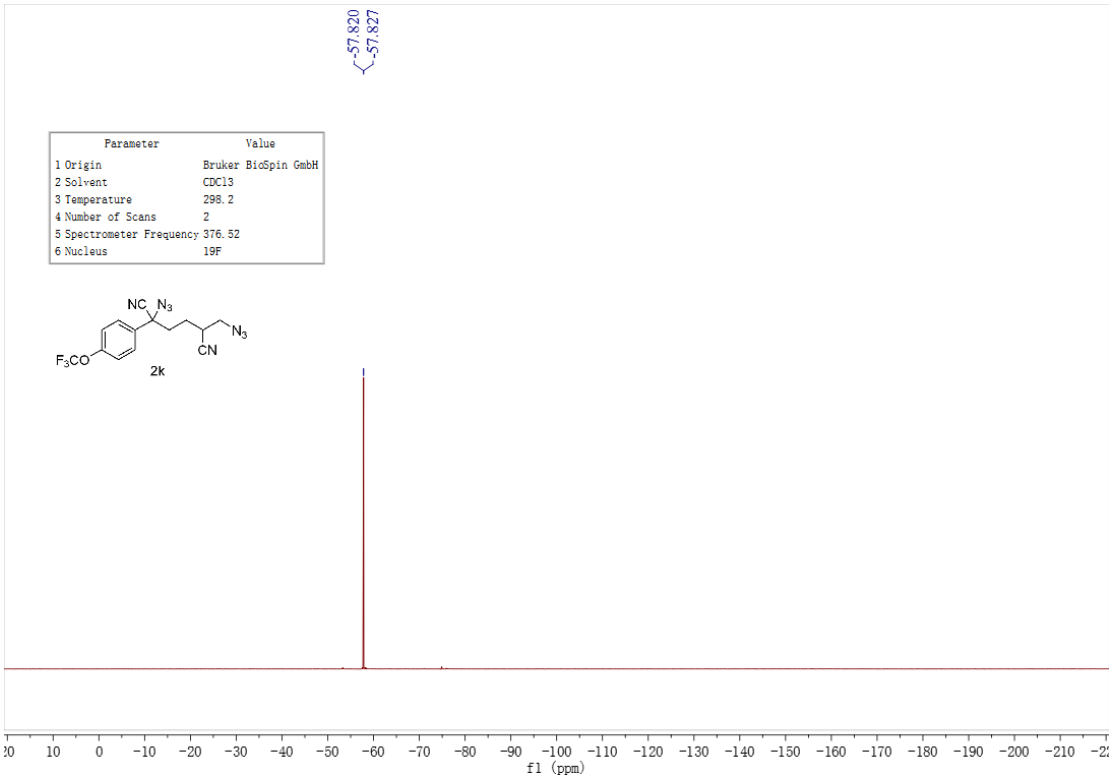
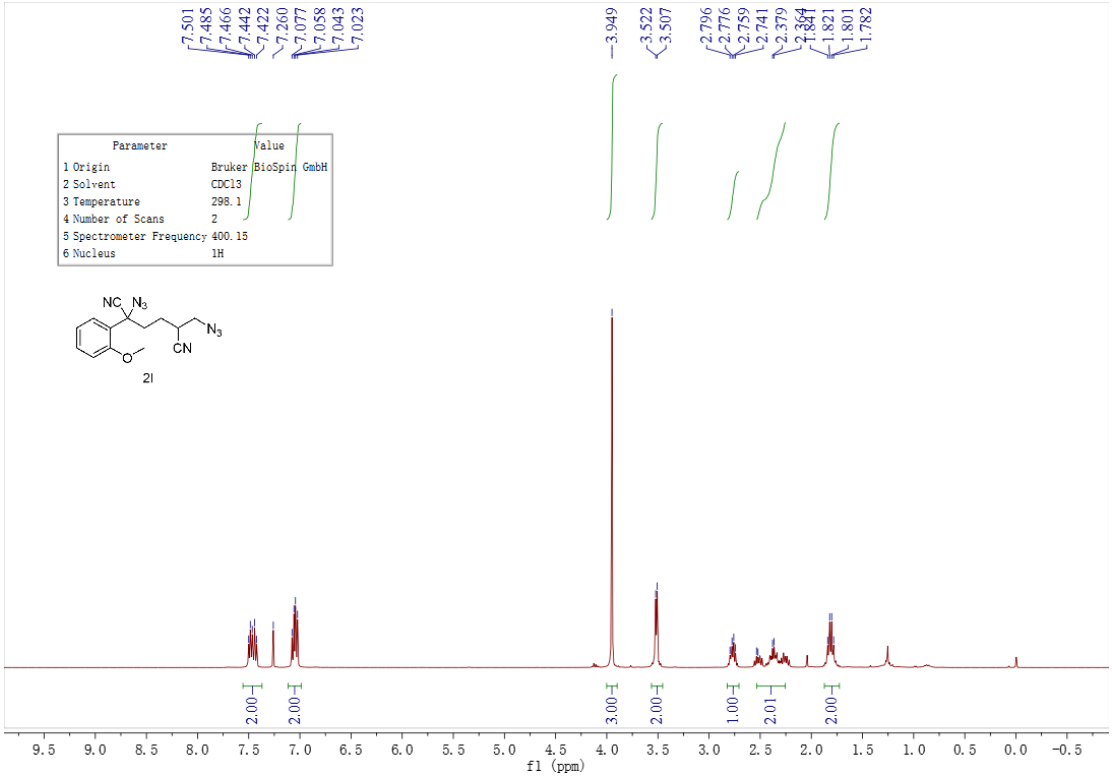
133.580
133.421
127.365
124.173
121.860
121.601
119.029
118.560
118.525
117.092
116.508
116.453
77.377
77.059
76.741
65.783
65.612
51.647
51.580
39.165
39.029
31.651
31.503
25.134
24.953
Parameter Value
1 Origin Bruker BioSpin GmbH
2 Solvent CDCl3
3 Temperature 298.1
4 Number of Scans 80
5 Spectrometer Frequency 100.62
6 Nucleus 13C
NC N3
N3
CN
F3CO
2k
f1 (ppm)


-57.820
-57.827
Parameter Value
1 Origin Bruker BioSpin GmbH
2 Solvent CDCl3
3 Temperature 298.2
4 Number of Scans 2
5 Spectrometer Frequency 376.52
6 Nucleus 19F
NC N3
N3
CN
F3CO
2k
f1 (ppm)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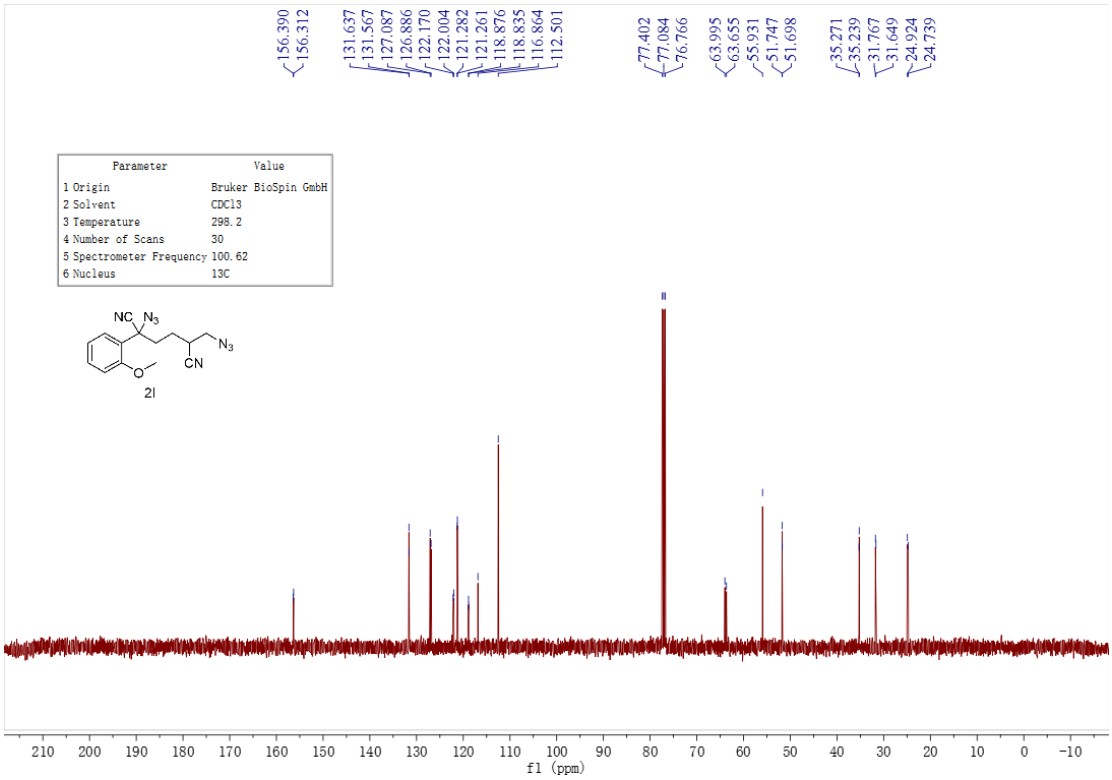
7.485
7.466
7.442
7.422
7.260
7.077
7.058
7.043
7.023
3.949
3.522
3.507
2.796
2.776
2.759
2.741
2.379
2.364
1.821
1.801
1.782
Parameter Value
1 Origin Bruker BioSpin GmbH
2 Solvent CDCl3
3 Temperature 298.1
4 Number of Scans 2
5 Spectrometer Frequency 400.15
6 Nucleus 1H
NC N3
N3
CN
O
2l
2.00
2.00
3.00
2.00
1.00
2.01
2.00
f1 (ppm)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126.886
122.170
122.004
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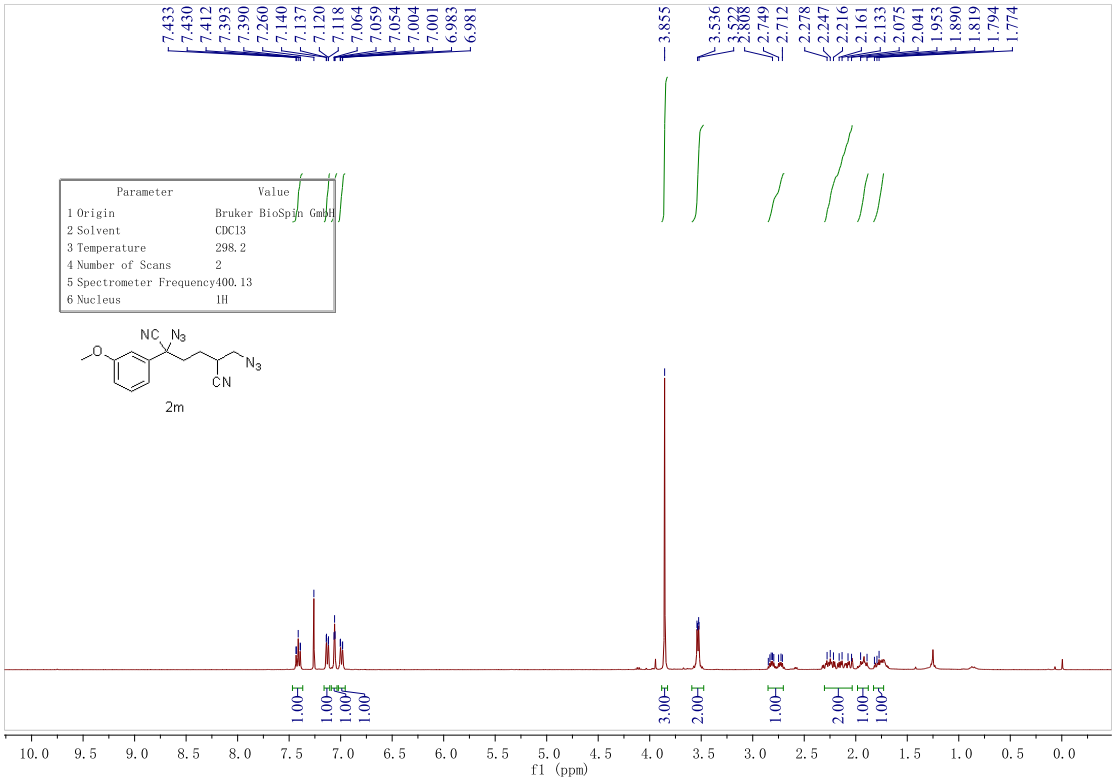
121.261
118.876
118.835
116.864
112.501
77.402
77.084
76.766
63.995
63.655
55.931
51.747
51.698
35.271
35.239
31.767
31.649
24.924
24.739
Parameter Value
1 Origin Bruker BioSpin GmbH
2 Solvent CDCl3
3 Temperature 298.2
4 Number of Scans 30
5 Spectrometer Frequency 100.62
6 Nucleus 13C
NC N3
N3
CN
O
2l
f1 (ppm)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7.260
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7.137
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7.118
7.064
7.059
7.054
7.004
7.001
6.983
6.981
3.855
3.536
2.808
2.749
2.712
2.278
2.247
2.216
2.161
2.133
2.075
2.041
1.953
1.890
1.819
1.794
1.774
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
NC N3
O
N3
CN
2m
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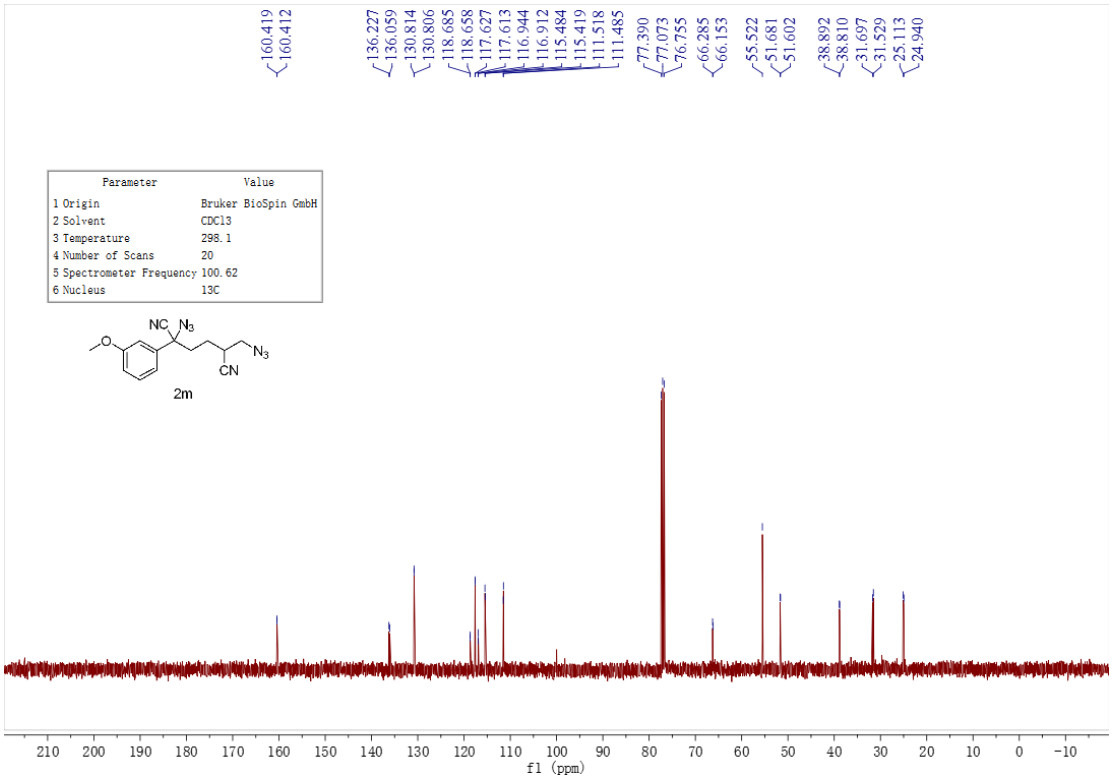
1.00
1.00
3.00
2.00
1.00
2.00
1.00
1.00
f1 (ppm)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117.613
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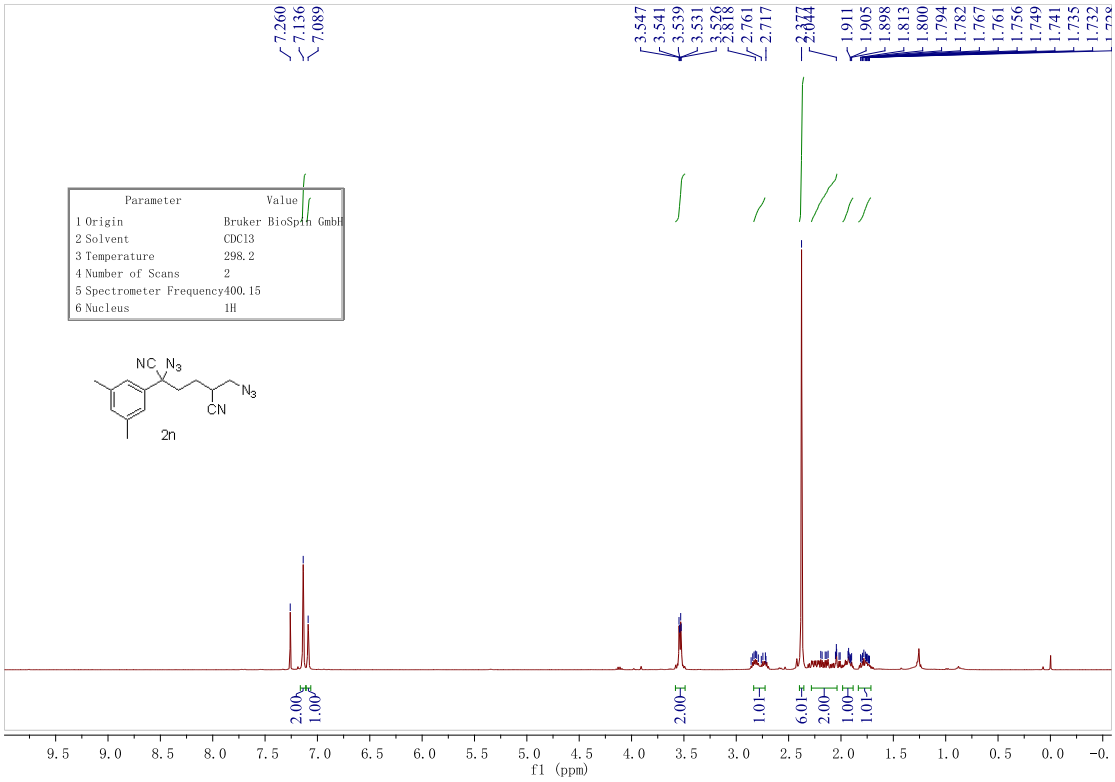
115.484
115.419
111.518
111.485
77.390
77.073
76.755
66.285
66.153
55.522
51.681
51.602
38.892
38.810
31.697
31.529
25.113
24.940
Parameter Value
1 Origin Bruker BioSpin GmbH
2 Solvent CDCl3
3 Temperature 298.1
4 Number of Scans 20
5 Spectrometer Frequency 100.62
6 Nucleus 13C
NC N3
O
N3
CN
2m
f1 (ppm)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3.539
3.531
3.526
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2.761
2.717
2.377
2.044
1.911
1.905
1.898
1.813
1.800
1.794
1.782
1.767
1.761
1.756
1.749
1.741
1.735
1.732
Parameter Value
1 Origin Bruker BioSpin GmbH
2 Solvent CDCl3
3 Temperature 298.2
4 Number of Scans 2
5 Spectrometer Frequency 400.15
6 Nucleus 1H
NC N3
N3
CN
2n
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1.00
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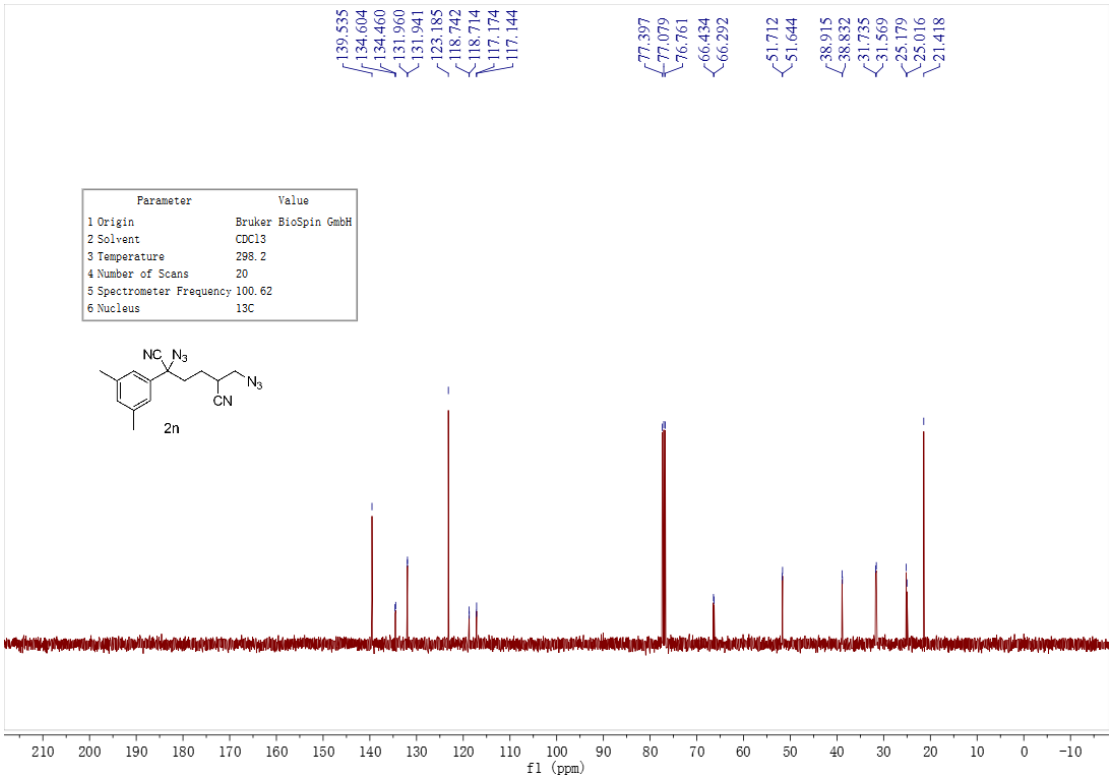
6.01
2.00
1.00
1.01
f1 (ppm)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118.714
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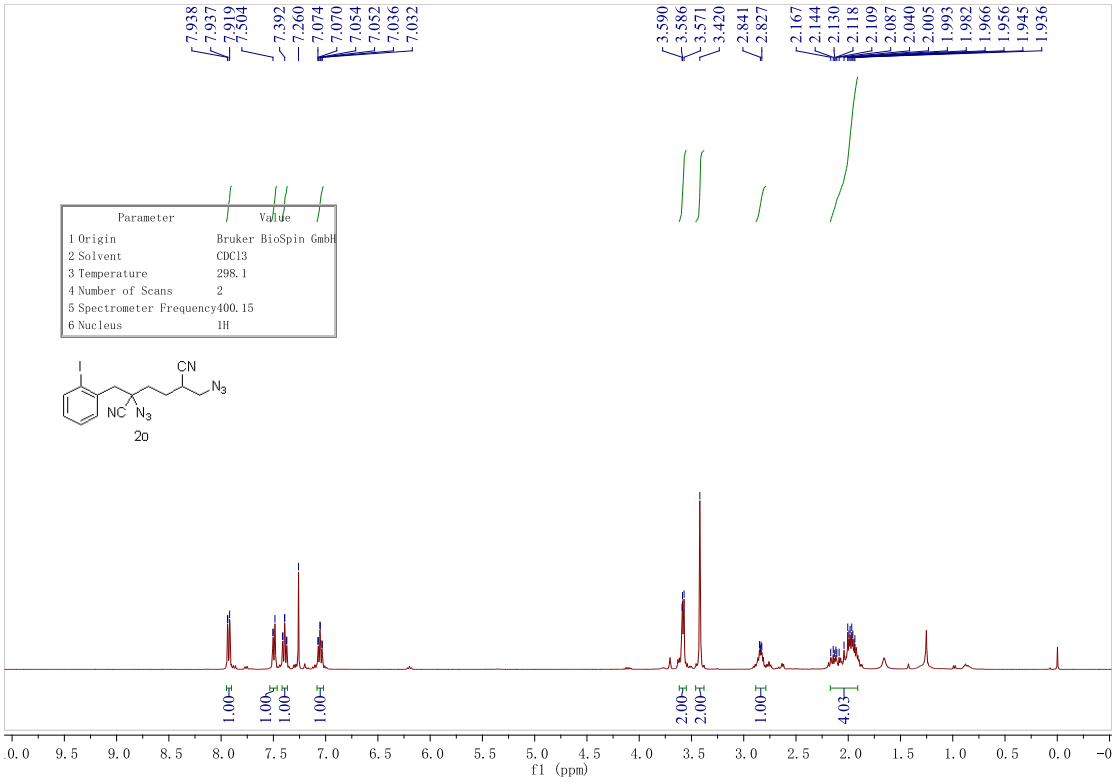
77.079
76.761
66.434
66.292
51.712
51.644
38.915
38.832
31.735
31.569
25.179
25.016
21.418
Parameter Value
1 Origin Bruker BioSpin GmbH
2 Solvent CDCl3
3 Temperature 298.2
4 Number of Scans 20
5 Spectrometer Frequency 100.62
6 Nucleus 13C
NC N3
N3
CN
2n
f1 (ppm)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7.070
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7.052
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7.032
3.590
3.586
3.571
3.420
2.841
2.827
2.167
2.144
2.130
2.118
2.109
2.087
2.040
2.005
1.993
1.982
1.966
1.956
1.945
1.936
Parameter Value
1 Origin Bruker BioSpin GmbH
2 Solvent CDCl3
3 Temperature 298.1
4 Number of Scans 2
5 Spectrometer Frequency 400.15
6 Nucleus 1H
I
CN
N3
NC N3
2o
1.00
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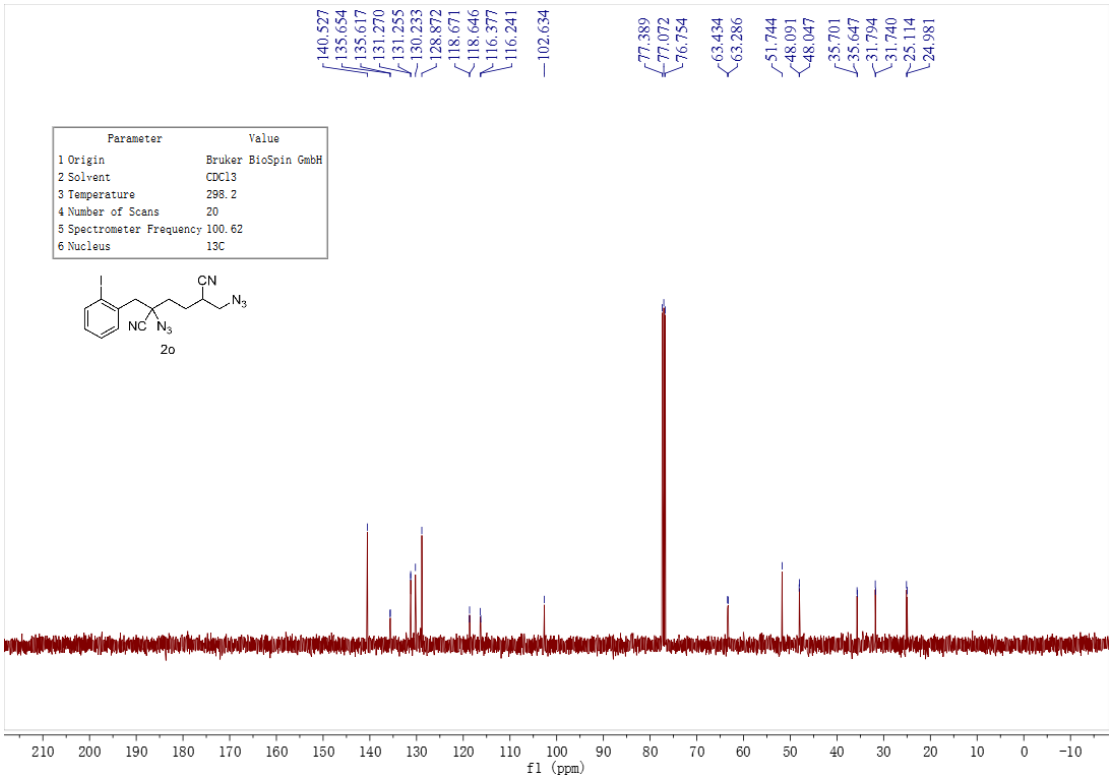
2.00
2.00
1.00
4.03
f1 (ppm)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130.233
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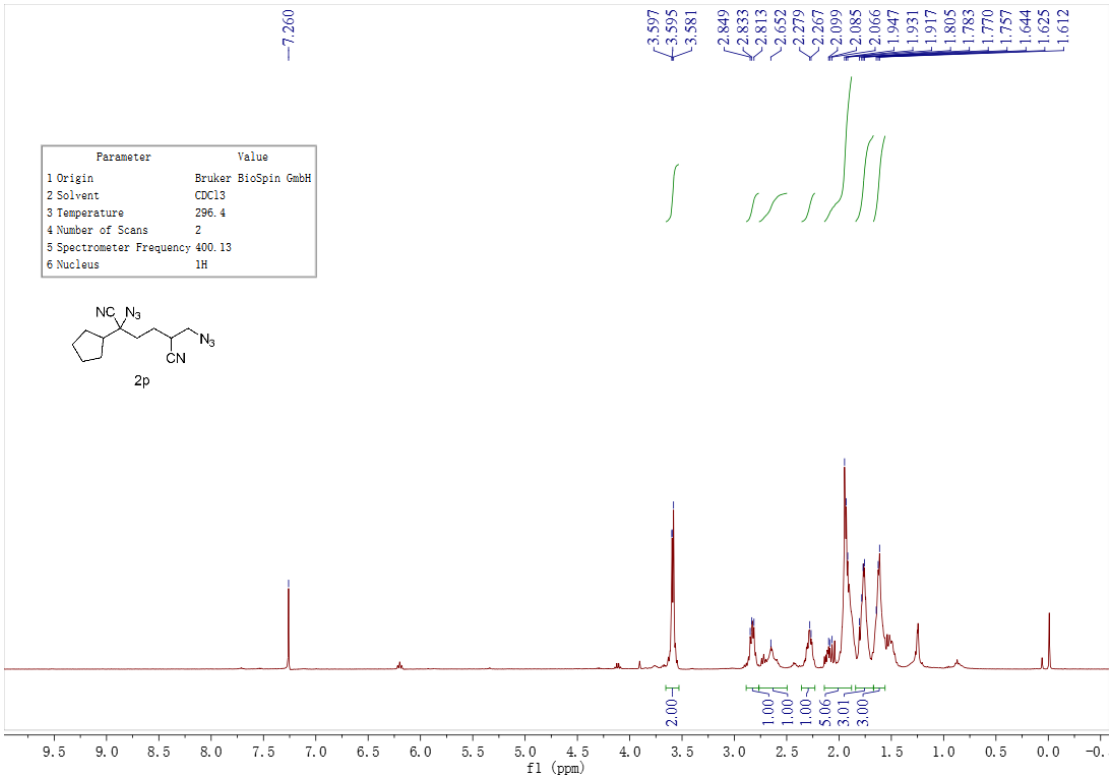
116.377
116.241
102.634
77.389
77.072
76.754
63.434
63.286
51.744
48.091
48.047
35.701
35.647
31.794
31.740
25.114
24.981
Parameter Value
1 Origin Bruker BioSpin GmbH
2 Solvent CDCl3
3 Temperature 298.2
4 Number of Scans 20
5 Spectrometer Frequency 100.62
6 Nucleus 13C
CN
N3
NC
N3
2o
f1 (ppm)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3.595
3.581
2.849
2.833
2.813
2.652
2.279
2.267
2.099
2.085
2.066
1.947
1.931
1.917
1.805
1.783
1.770
1.757
1.644
1.625
1.612
Parameter Value
1 Origin Bruker BioSpin GmbH
2 Solvent CDCl3
3 Temperature 296.4
4 Number of Scans 2
5 Spectrometer Frequency 400.13
6 Nucleus 1H
NC
N3
N3
CN
2p
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1.00
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1.00
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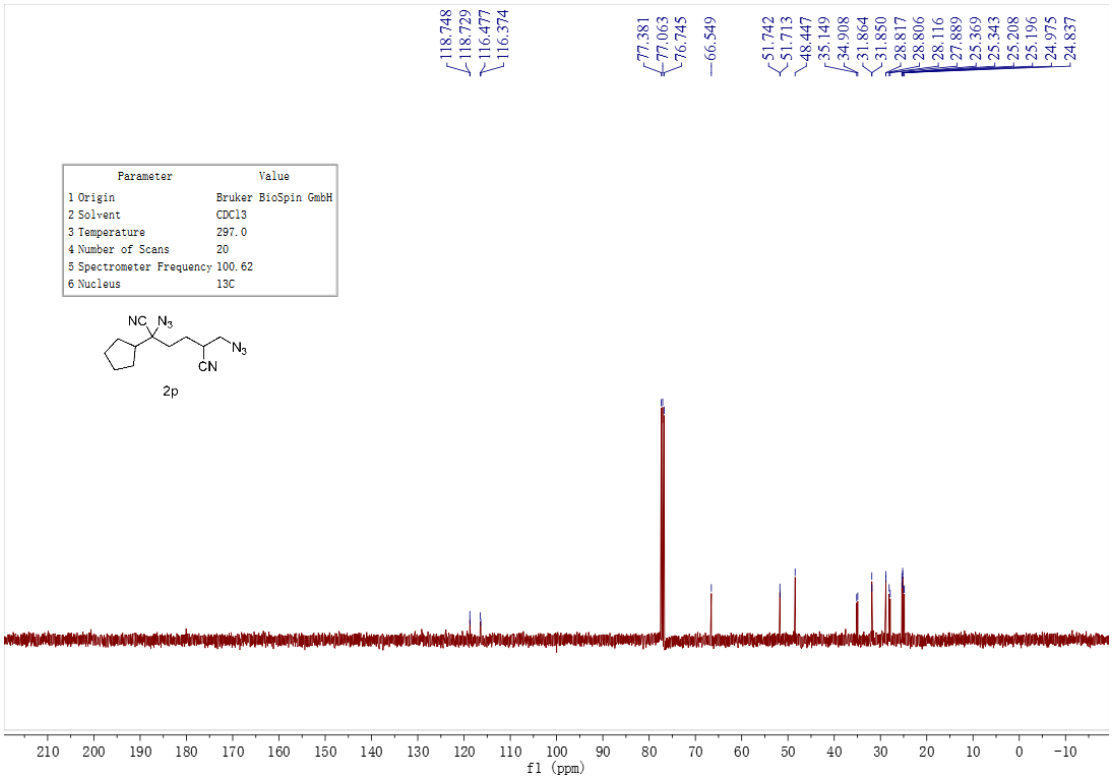
3.01
3.00
f1 (ppm)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77.063
76.745
66.549
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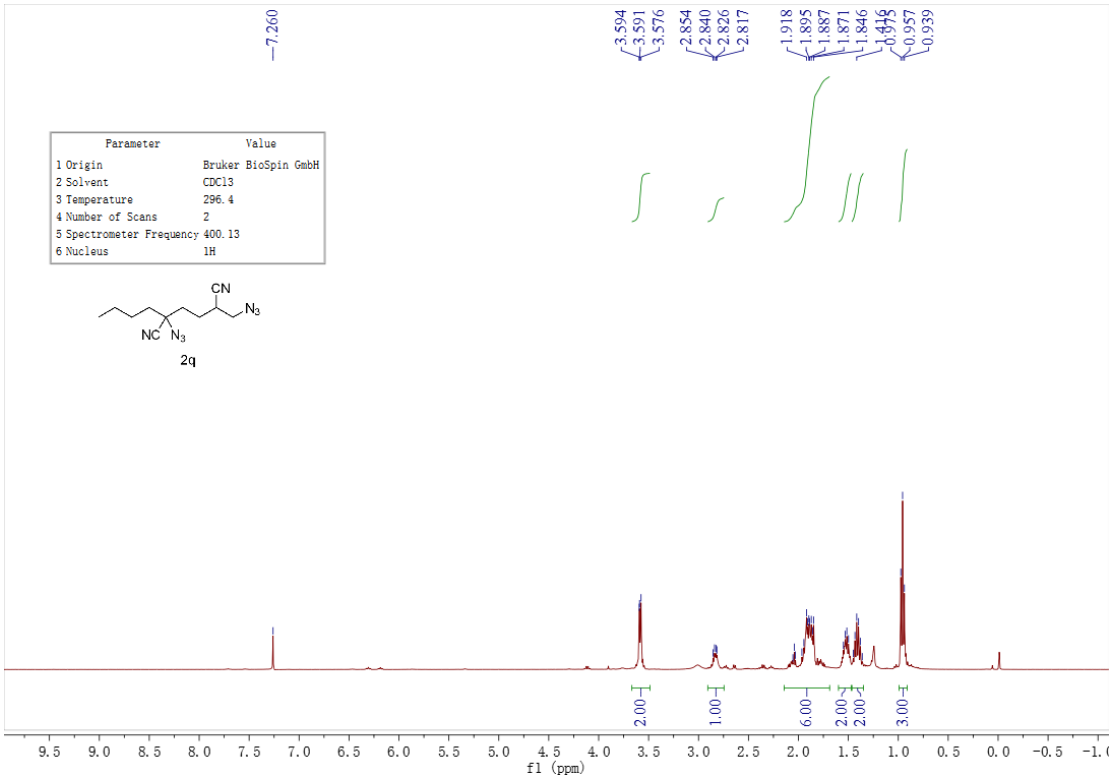
51.713
48.447
35.149
34.908
31.864
31.850
28.817
28.806
28.116
27.889
25.369
25.343
25.208
25.196
24.975
24.837
Parameter Value
1 Origin Bruker BioSpin GmbH
2 Solvent CDCl3
3 Temperature 297.0
4 Number of Scans 20
5 Spectrometer Frequency 100.62
6 Nucleus 13C
NC N3
N3
CN
2p
f1 (ppm)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2.840
2.826
2.817
1.918
1.895
1.887
1.871
1.846
0.957
0.939
Parameter Value
1 Origin Bruker BioSpin GmbH
2 Solvent CDCl3
3 Temperature 296.4
4 Number of Scans 2
5 Spectrometer Frequency 400.13
6 Nucleus 1H
CN
N3
NC N3
2q
2.00
1.00
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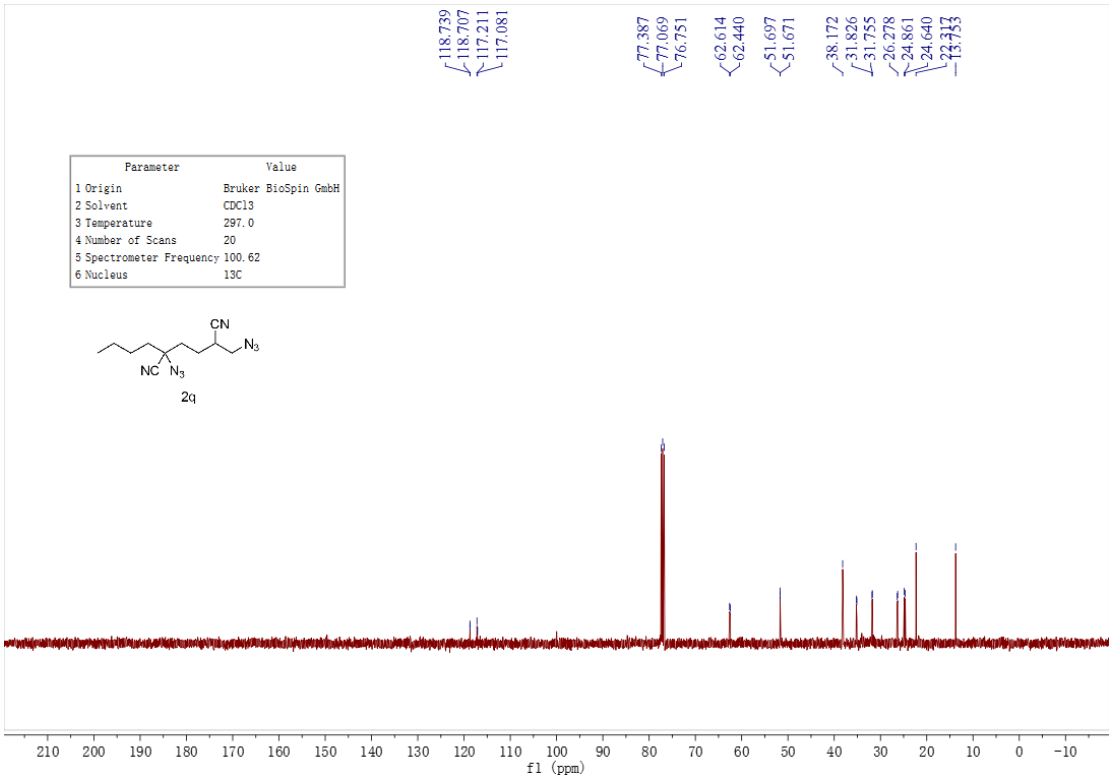
2.00
3.00
f1 (ppm)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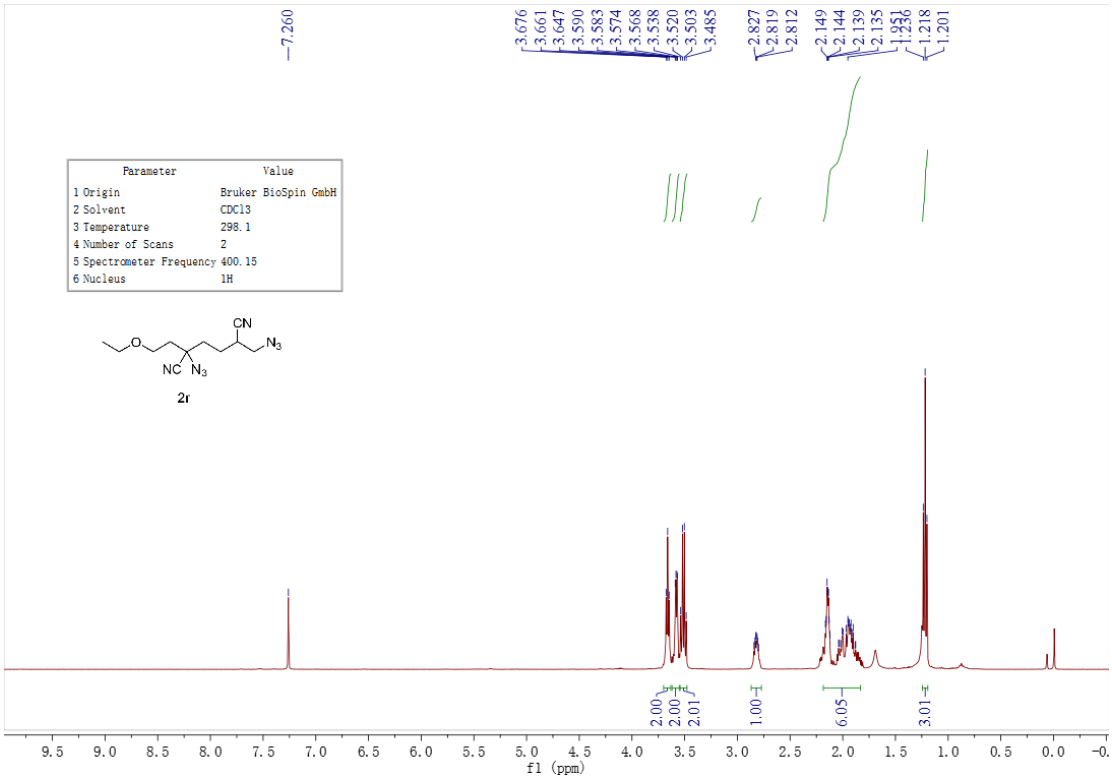
51.697
51.671
38.172
31.826
31.755
26.278
24.861
24.640
22.317
13.753
Parameter Value
1 Origin Bruker BioSpin GmbH
2 Solvent CDCl3
3 Temperature 297.0
4 Number of Scans 20
5 Spectrometer Frequency 100.62
6 Nucleus 13C
CN
N3
NC N3
2q
f1 (ppm)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3.568
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3.520
3.503
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2.827
2.819
2.812
2.149
2.144
2.139
2.135
1.951
1.236
1.218
1.201
Parameter Value
1 Origin Bruker BioSpin GmbH
2 Solvent CDCl3
3 Temperature 298.1
4 Number of Scans 2
5 Spectrometer Frequency 400.15
6 Nucleus 1H
CN
N3
O
NC N3
2r
2.00
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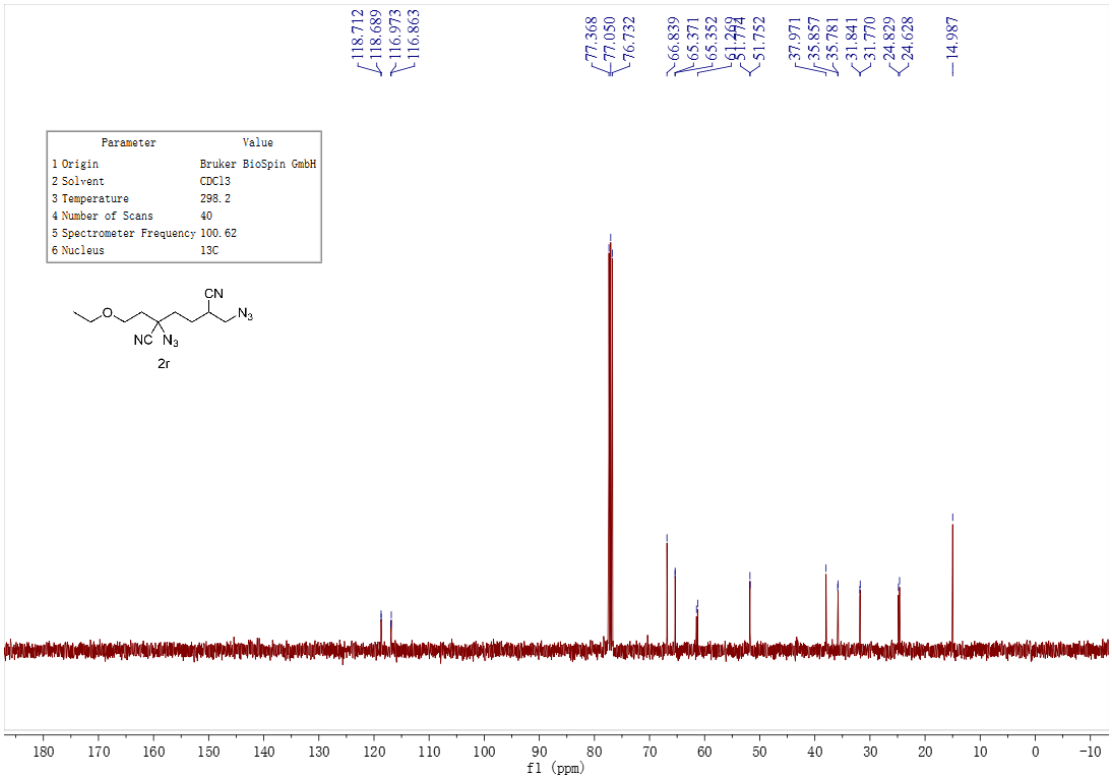
6.05
3.01
f1 (ppm)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116.863
77.368
77.050
76.732
66.839
65.371
65.352
61.269
51.774
51.752
37.971
35.857
35.781
31.841
31.770
24.829
24.628
14.987
Parameter Value
1 Origin Bruker BioSpin GmbH
2 Solvent CDCl3
3 Temperature 298.2
4 Number of Scans 40
5 Spectrometer Frequency 100.62
6 Nucleus 13C
CN
O
N3
NC N3
2r
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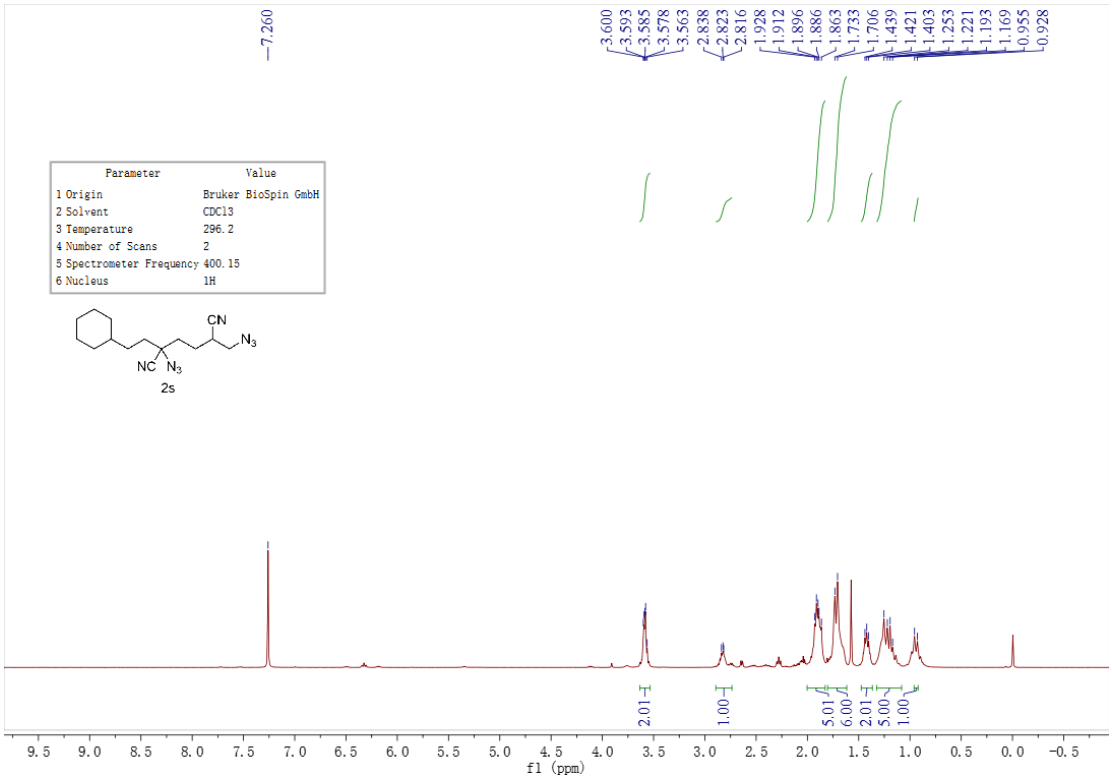
f1 (ppm)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2.823
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1.928
1.912
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1.886
1.863
1.733
1.706
1.439
1.421
1.403
1.253
1.221
1.193
1.169
0.955
0.928
Parameter Value
1 Origin Bruker BioSpin GmbH
2 Solvent CDCl3
3 Temperature 296.2
4 Number of Scans 2
5 Spectrometer Frequency 400.15
6 Nucleus 1H
CN
N3
NC N3
2s
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5.01
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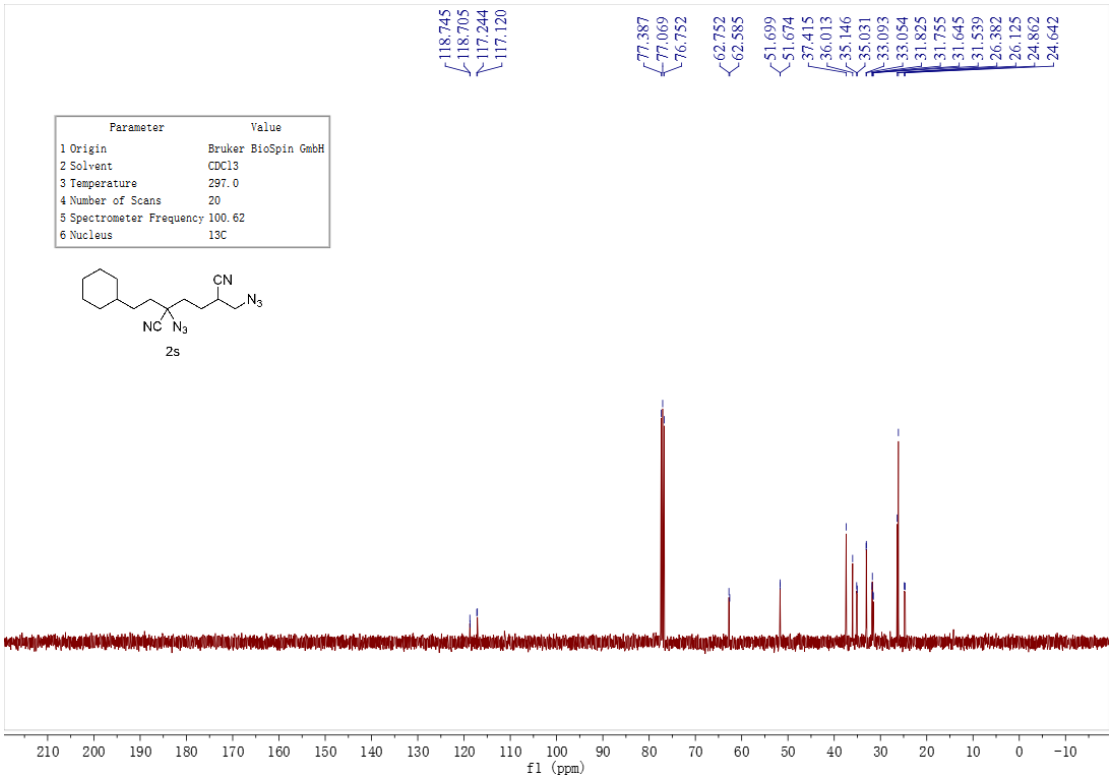
2.01
5.00
1.00
9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5
f1 (ppm)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62.752
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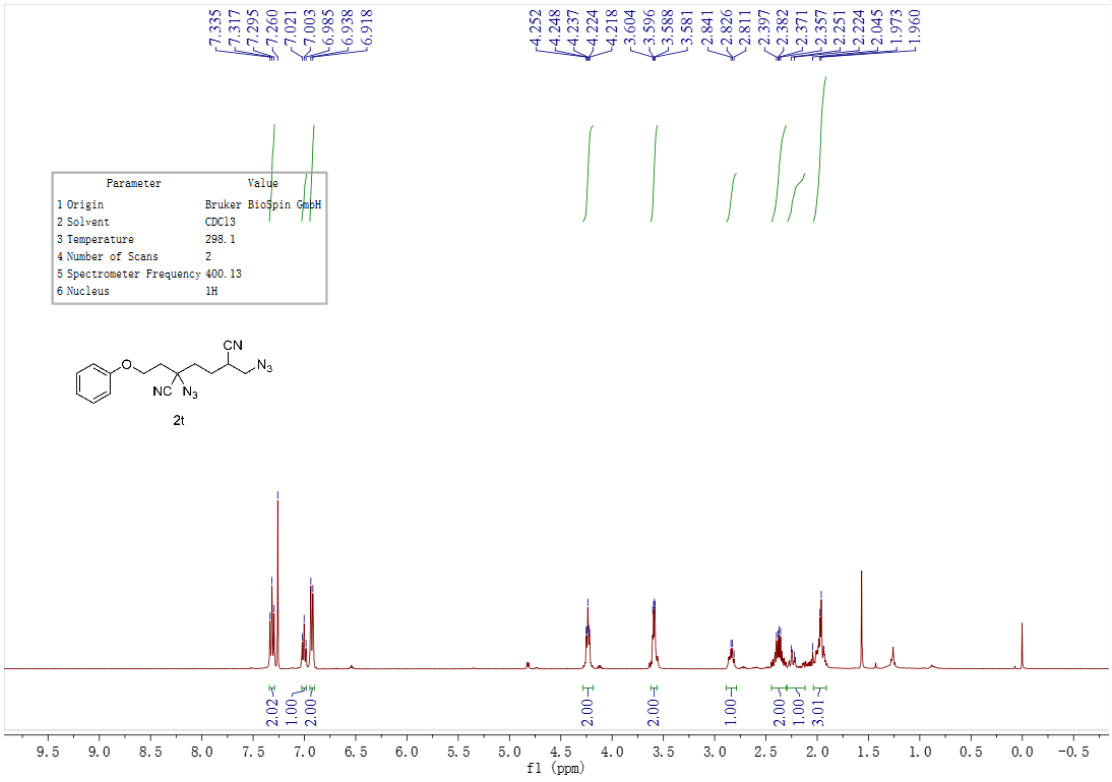
51.674
37.415
36.013
35.146
35.031
33.093
33.054
31.825
31.755
31.645
31.539
26.382
26.125
24.862
24.642
Parameter Value
1 Origin Bruker BioSpin GmbH
2 Solvent CDCl3
3 Temperature 297.0
4 Number of Scans 20
5 Spectrometer Frequency 100.62
6 Nucleus 13C
CN
N3
NC N3
2s
f1 (ppm)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7.003
6.985
6.938
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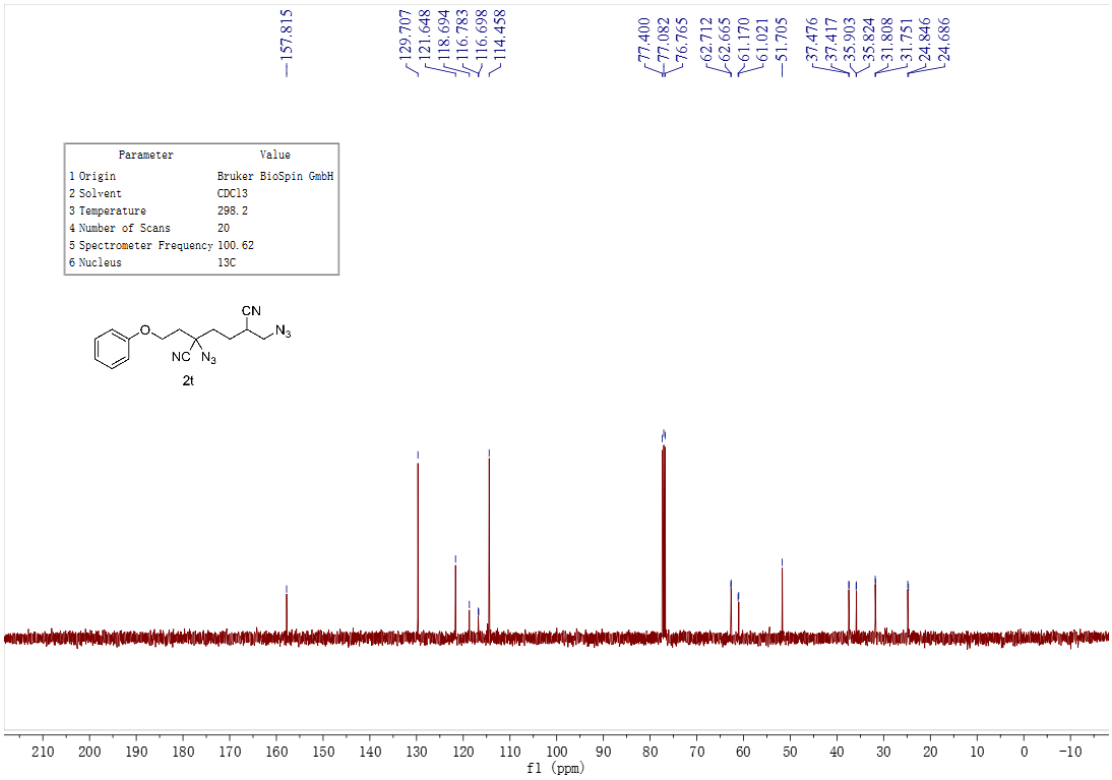
4.252
4.248
4.237
4.224
4.218
3.604
3.596
3.588
3.581
2.841
2.826
2.811
2.397
2.382
2.371
2.357
2.251
2.224
2.045
1.973
1.960
Parameter Value
1 Origin Bruker BioSpin GmbH
2 Solvent CDCl3
3 Temperature 298.1
4 Number of Scans 2
5 Spectrometer Frequency 400.13
6 Nucleus 1H
CN
N3
O
NC N3
2t
2.02
1.00
2.00
2.00
2.00
1.00
2.00
1.00
3.01
f1 (ppm)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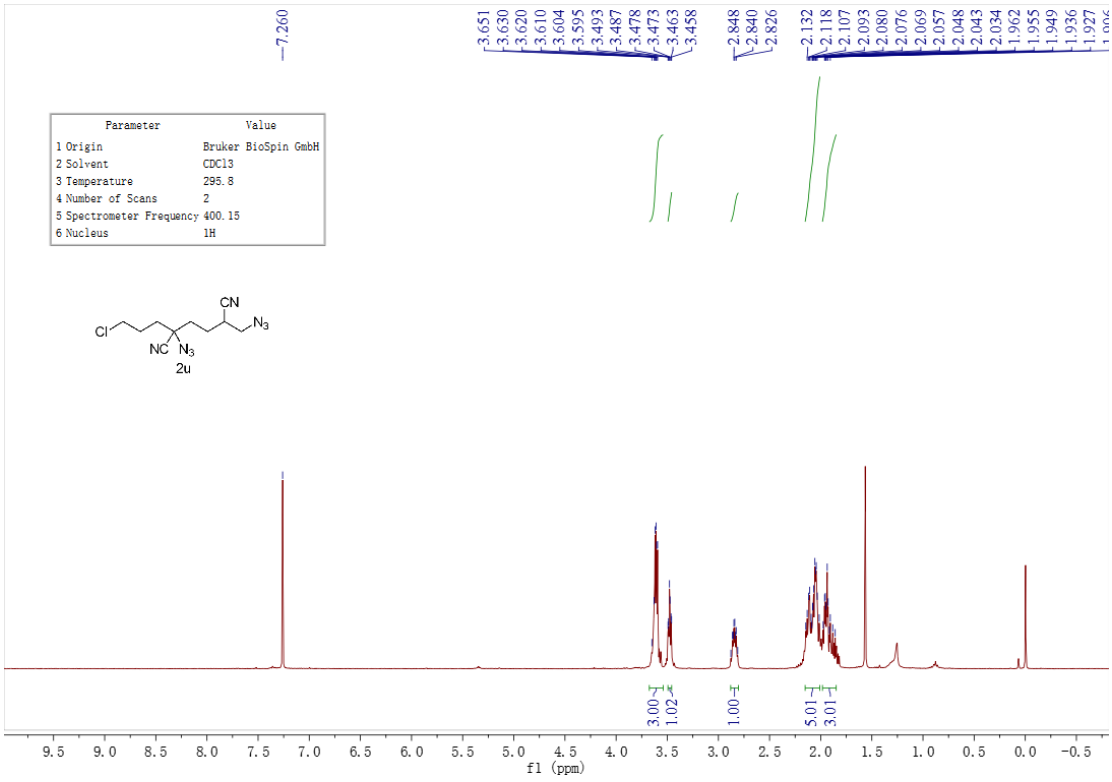
61.170
61.021
51.705
37.476
37.417
35.903
35.824
31.808
31.751
24.846
24.686
Parameter Value
1 Origin Bruker BioSpin GmbH
2 Solvent CDCl3
3 Temperature 298.2
4 Number of Scans 20
5 Spectrometer Frequency 100.62
6 Nucleus 13C
CN
N3
O
NC N3
2t
f1 (ppm)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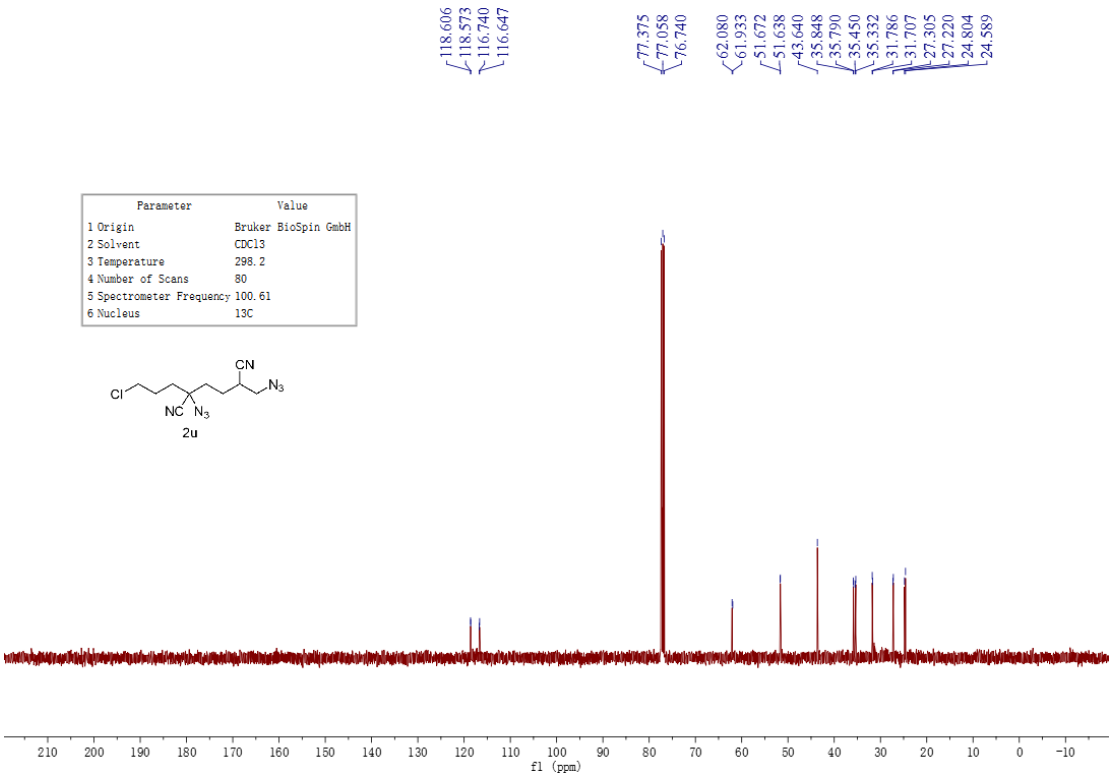
3.620
3.610
3.604
3.595
3.493
3.487
3.478
3.473
3.463
3.458
2.848
2.840
2.826
2.132
2.118
2.107
2.093
2.080
2.076
2.069
2.057
2.048
2.043
2.034
1.962
1.955
1.949
1.936
1.927
Parameter Value
1 Origin Bruker BioSpin GmbH
2 Solvent CDCl3
3 Temperature 295.8
4 Number of Scans 2
5 Spectrometer Frequency 400.15
6 Nucleus 1H
CN
N3
Cl
NC N3
2u
3.00
1.02
1.00
5.01
3.01
f1 (ppm)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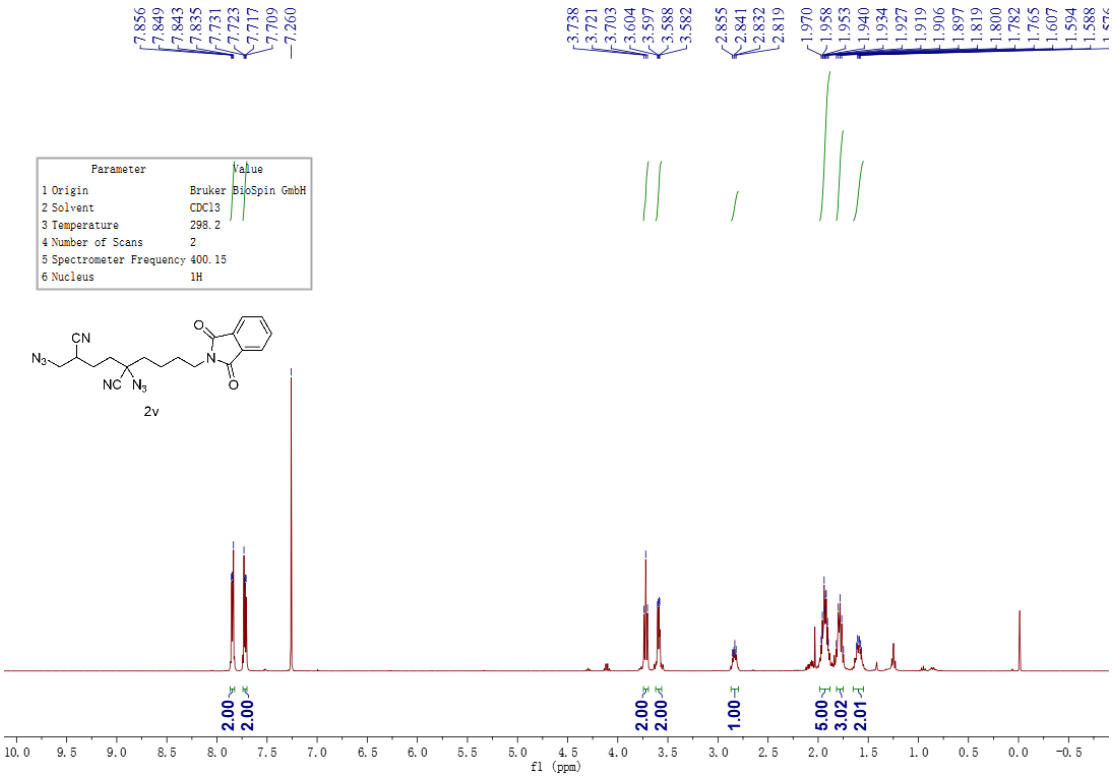
43.640
35.848
35.790
35.450
35.332
31.786
31.707
27.305
27.220
24.804
24.589
Parameter Value
1 Origin Bruker BioSpin GmbH
2 Solvent CDCl3
3 Temperature 298.2
4 Number of Scans 80
5 Spectrometer Frequency 100.61
6 Nucleus 13C
CN
Cl
NC N3
N3
2u
f1 (ppm)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7.723
7.717
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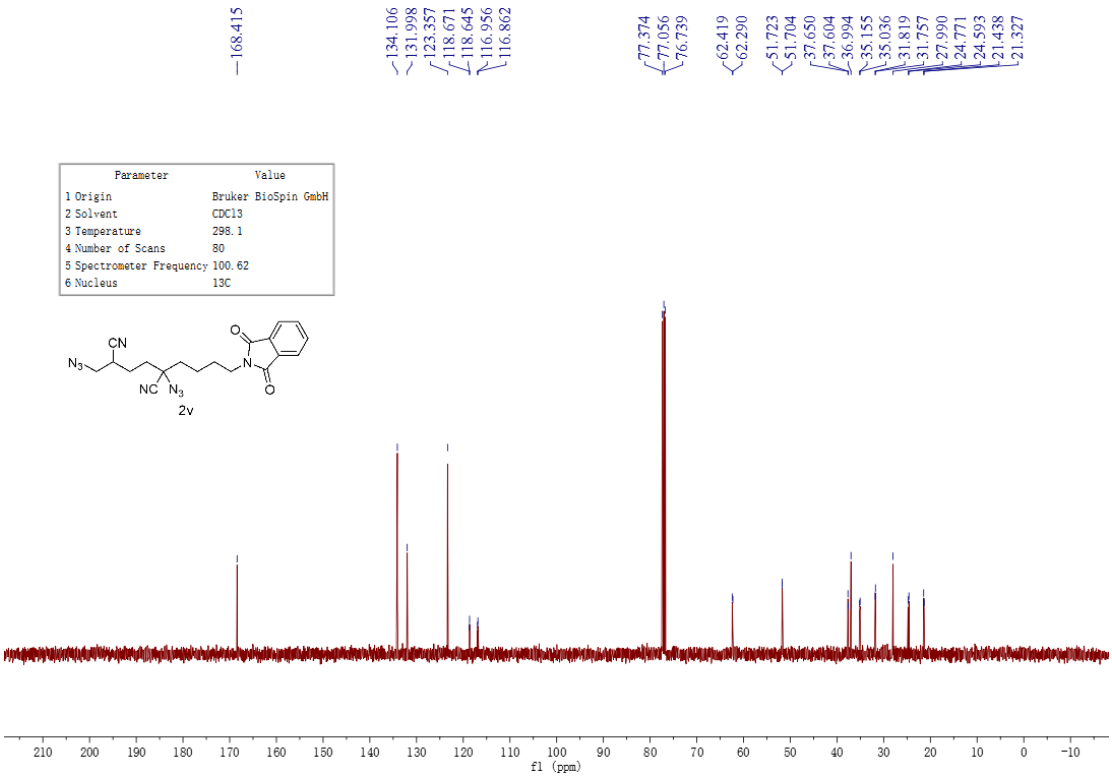
7.260
3.738
3.721
3.703
3.604
3.597
3.588
3.582
2.855
2.841
2.832
2.819
1.970
1.958
1.953
1.940
1.934
1.927
1.919
1.906
1.897
1.819
1.800
1.782
1.765
1.607
1.594
1.588
Parameter Value
1 Origin Bruker BioSpin GmbH
2 Solvent CDCl3
3 Temperature 298.2
4 Number of Scans 2
5 Spectrometer Frequency 400.15
6 Nucleus 1H
CN
N3
NC N3
O
N
O
2v
2.00
2.00
2.00
2.00
1.00
5.00
3.02
2.01
f1 (ppm)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76.739
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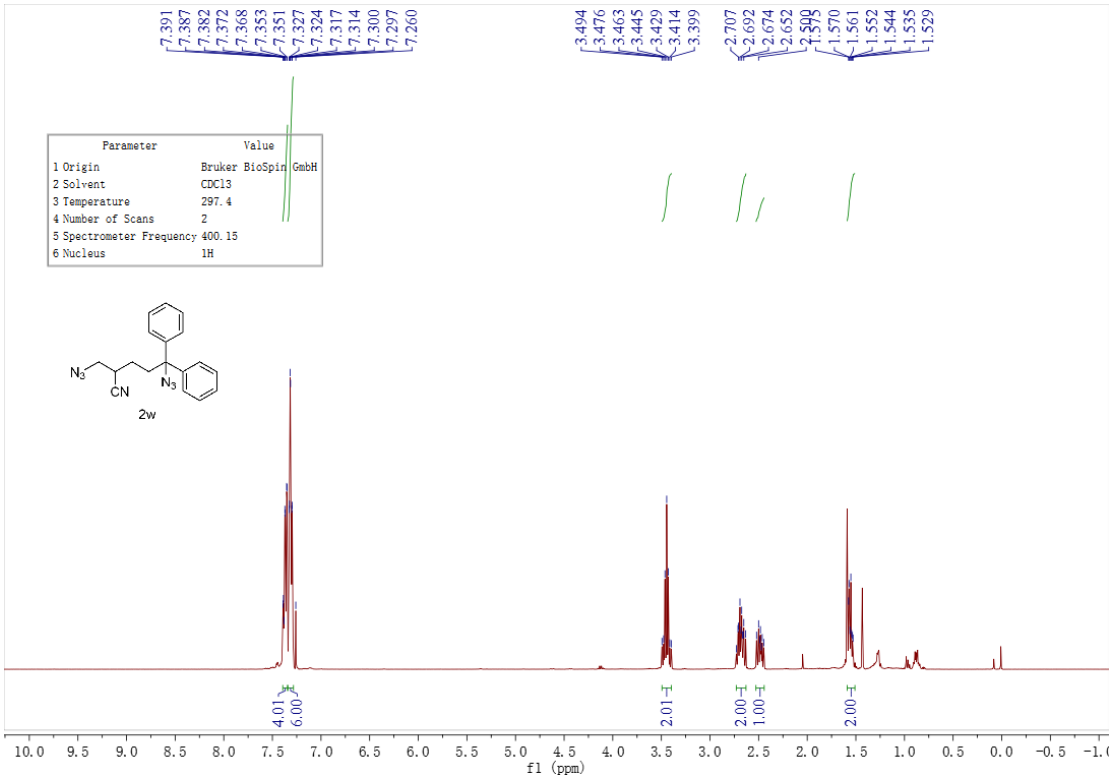
62.290
51.723
51.704
37.650
37.604
36.994
35.155
35.036
31.819
31.757
27.990
24.771
24.593
21.438
21.327
Parameter Value
1 Origin Bruker BioSpin GmbH
2 Solvent CDCl3
3 Temperature 298.1
4 Number of Scans 80
5 Spectrometer Frequency 100.62
6 Nucleus 13C
CN
N3
NC N3
O
N
O
2v
f1 (ppm)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7.382
7.372
7.368
7.353
7.351
7.327
7.324
7.317
7.314
7.300
7.297
7.260
3.494
3.476
3.463
3.445
3.429
3.414
3.399
2.707
2.692
2.674
2.652
1.570
1.561
1.552
1.544
1.535
1.529
Parameter Value
1 Origin Bruker BioSpin GmbH
2 Solvent CDCl3
3 Temperature 297.4
4 Number of Scans 2
5 Spectrometer Frequency 400.15
6 Nucleus 1H
N3
CN
N3
2w
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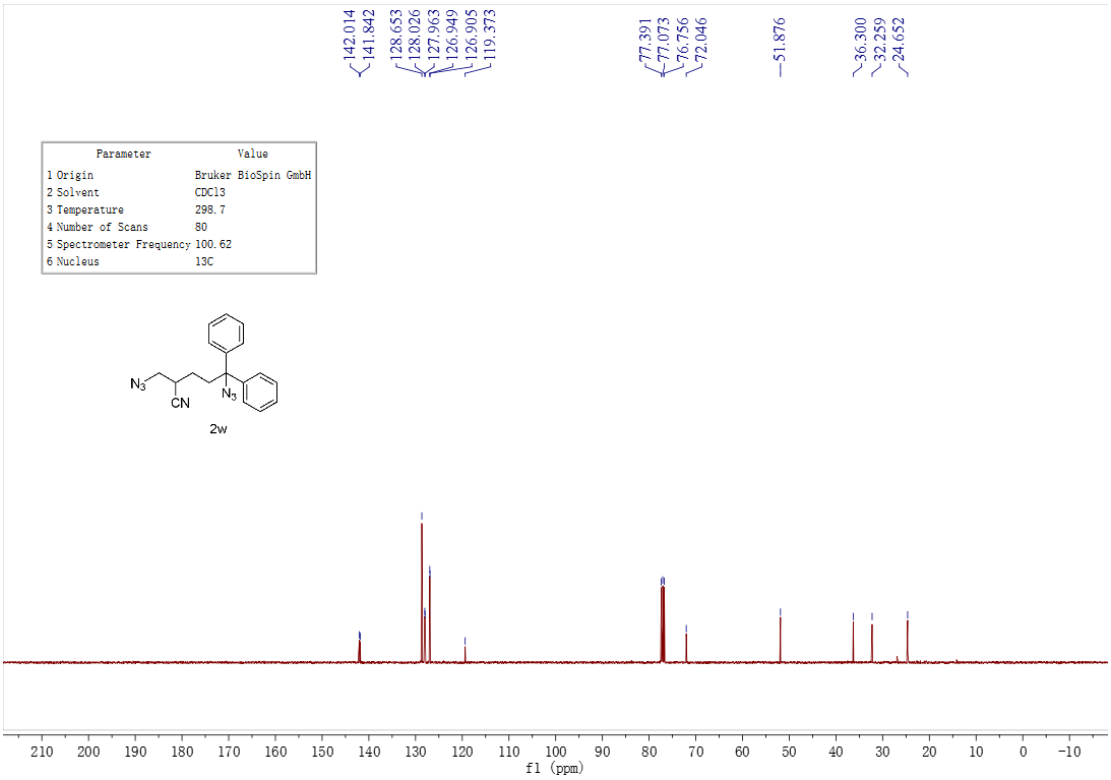
2.01
2.00
1.00
2.00
f1 (ppm)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126.905
119.373
77.391
77.073
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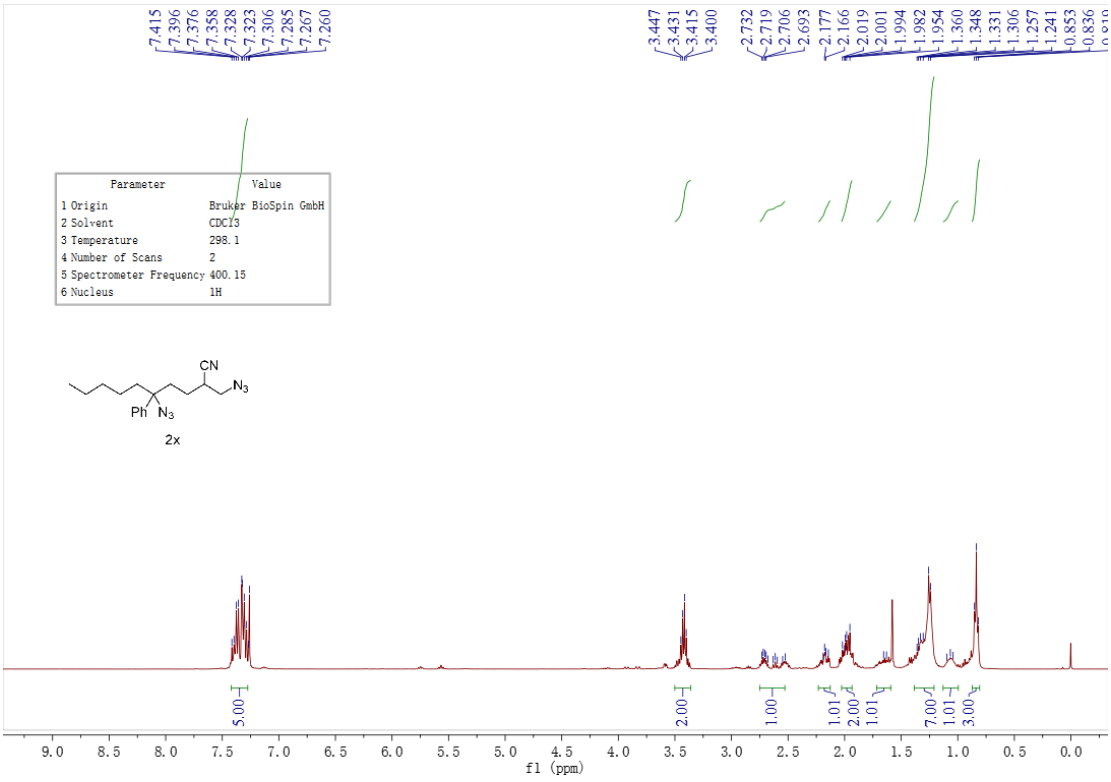
72.046
51.876
36.300
32.259
24.652
Parameter Value
1 Origin Bruker BioSpin GmbH
2 Solvent CDCl3
3 Temperature 298.7
4 Number of Scans 80
5 Spectrometer Frequency 100.62
6 Nucleus 13C
N3
CN
N3
2w
f1 (ppm)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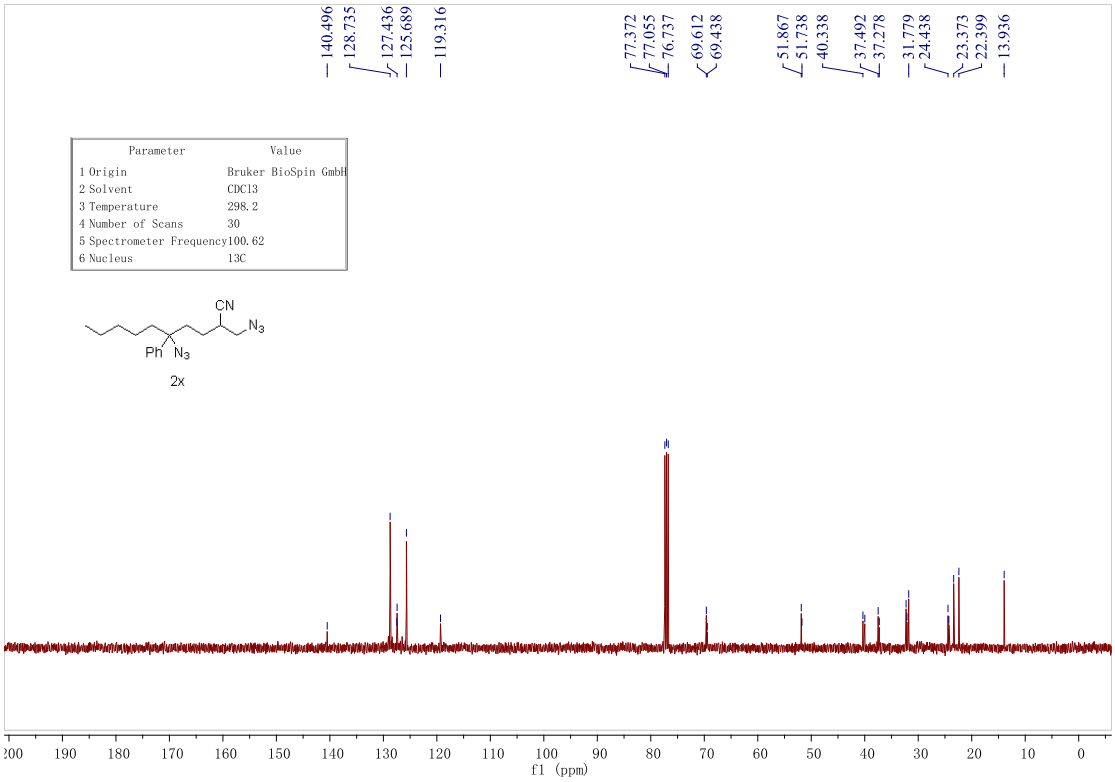
7.376
7.358
7.328
7.323
7.306
7.285
7.267
7.260
3.447
3.431
3.415
3.400
2.732
2.719
2.706
2.693
2.177
2.166
2.019
2.001
1.994
1.982
1.954
1.360
1.348
1.331
1.306
1.257
1.241
0.853
0.836
Parameter Value
1 Origin Bruker BioSpin GmbH
2 Solvent CDCl3
3 Temperature 298.1
4 Number of Scans 2
5 Spectrometer Frequency 400.15
6 Nucleus 1H
CN
N3
Ph N3
2x
5.00
2.00
1.00
1.01
2.00
1.01
7.00
1.01
3.00
f1 (ppm)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77.055
76.737
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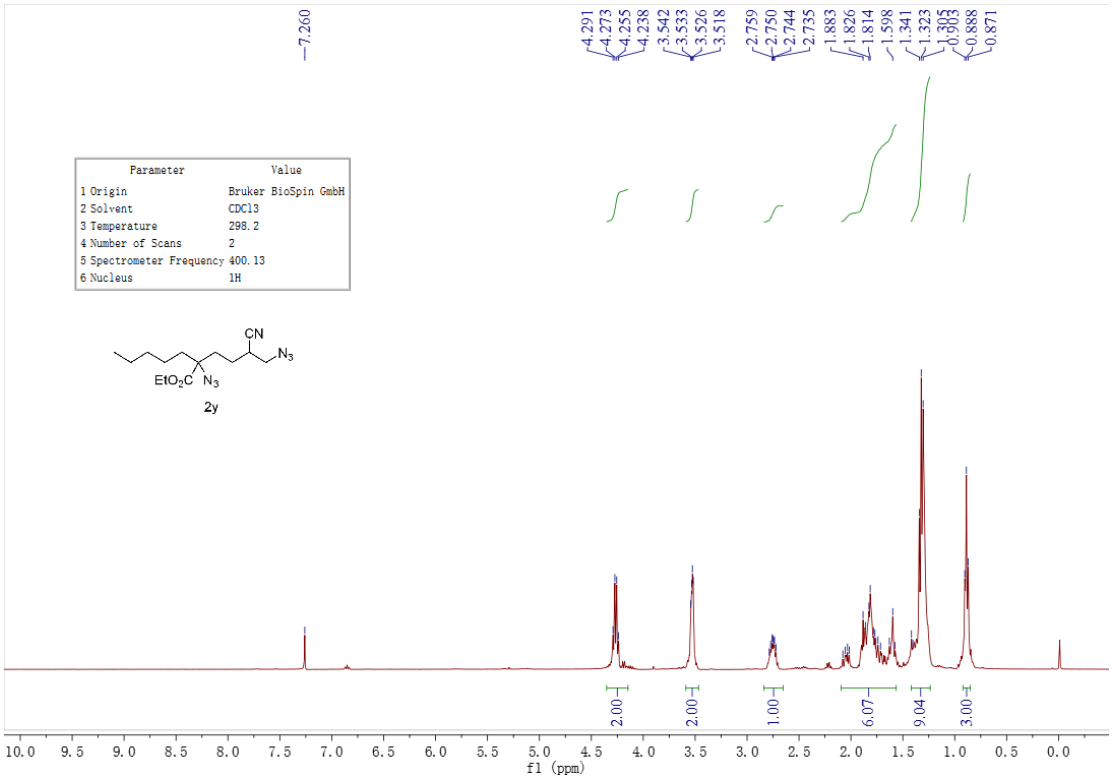
69.438
51.867
51.738
40.338
37.492
37.278
31.779
24.438
23.373
22.399
13.936
Parameter Value
1 Origin Bruker BioSpin GmbH
2 Solvent CDCl3
3 Temperature 298.2
4 Number of Scans 30
5 Spectrometer Frequency 100.62
6 Nucleus 13C
CN
N3
Ph N3
2x
f1 (ppm)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3.526
3.518
2.759
2.750
2.744
2.735
1.883
1.826
1.814
1.598
1.341
1.323
0.903
0.888
0.871
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
CN
N3
EtO2C N3
2y
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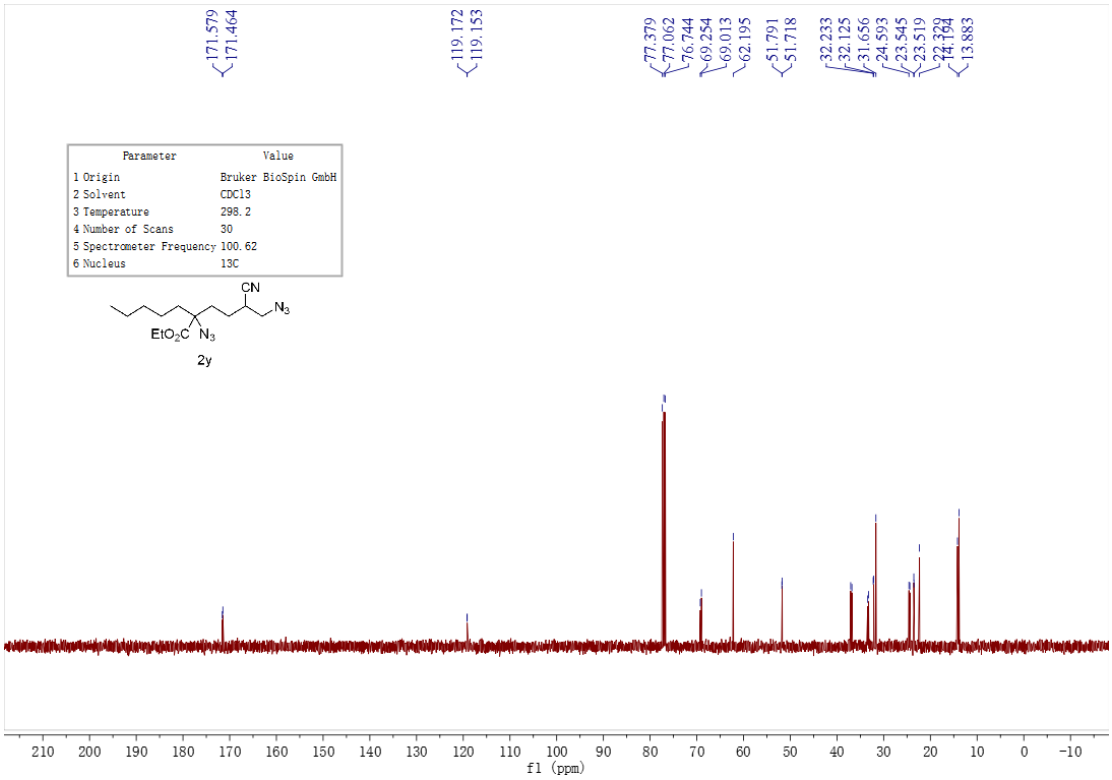
1.00
6.07
9.04
3.00
f1 (ppm)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51.791
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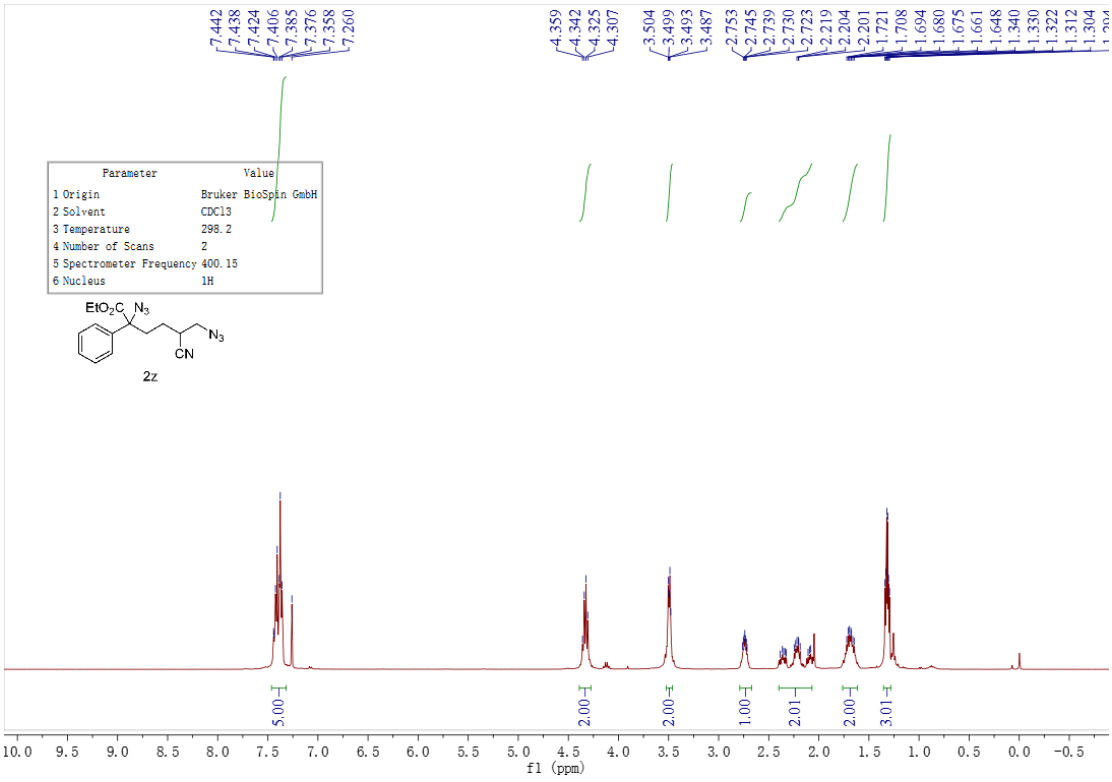
32.233
32.125
31.656
24.593
23.545
23.519
22.329
14.194
13.883
Parameter Value
1 Origin Bruker BioSpin GmbH
2 Solvent CDCl3
3 Temperature 298.2
4 Number of Scans 30
5 Spectrometer Frequency 100.62
6 Nucleus 13C
CN
N3
EtO2C N3
2y
f1 (ppm)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7.260
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4.342
4.325
4.307
3.504
3.499
3.493
3.487
2.753
2.745
2.739
2.730
2.723
2.219
2.204
2.201
1.721
1.708
1.694
1.680
1.675
1.661
1.648
1.340
1.330
1.322
1.312
1.304
Parameter Value
1 Origin Bruker BioSpin GmbH
2 Solvent CDCl3
3 Temperature 298.2
4 Number of Scans 2
5 Spectrometer Frequency 400.15
6 Nucleus 1H
EtO2C N3
N3
CN
2z
5.00
2.00
2.00
1.00
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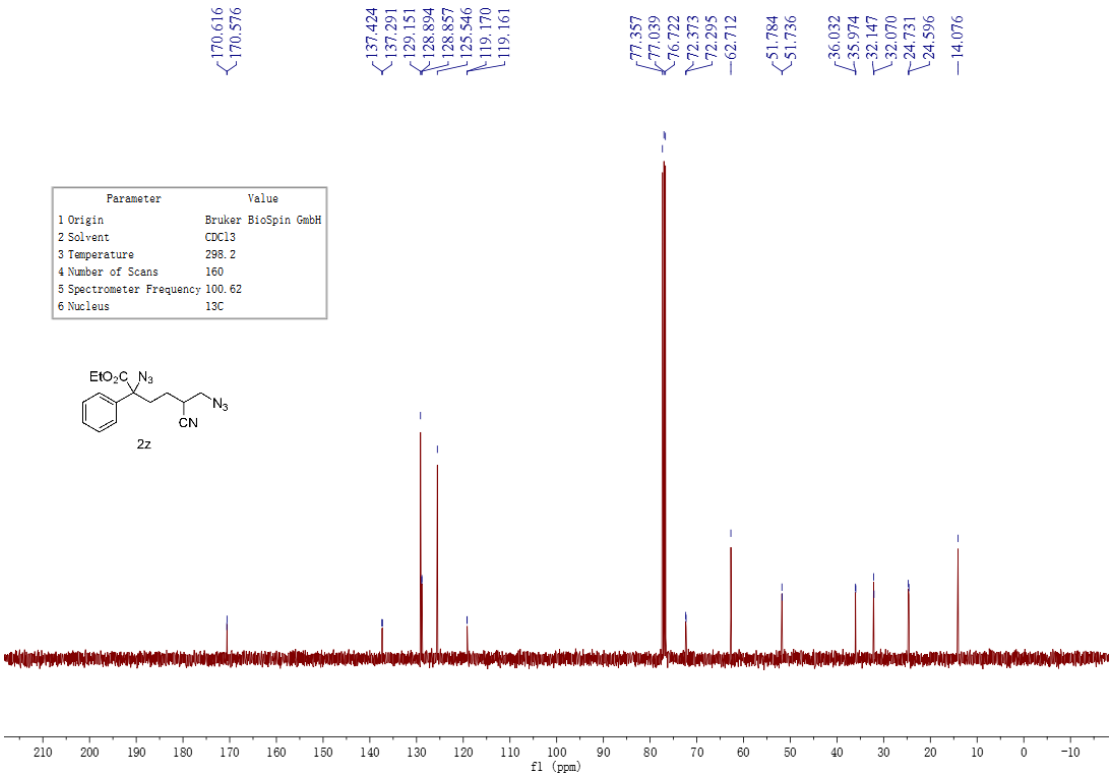
2.00
3.01
f1 (ppm)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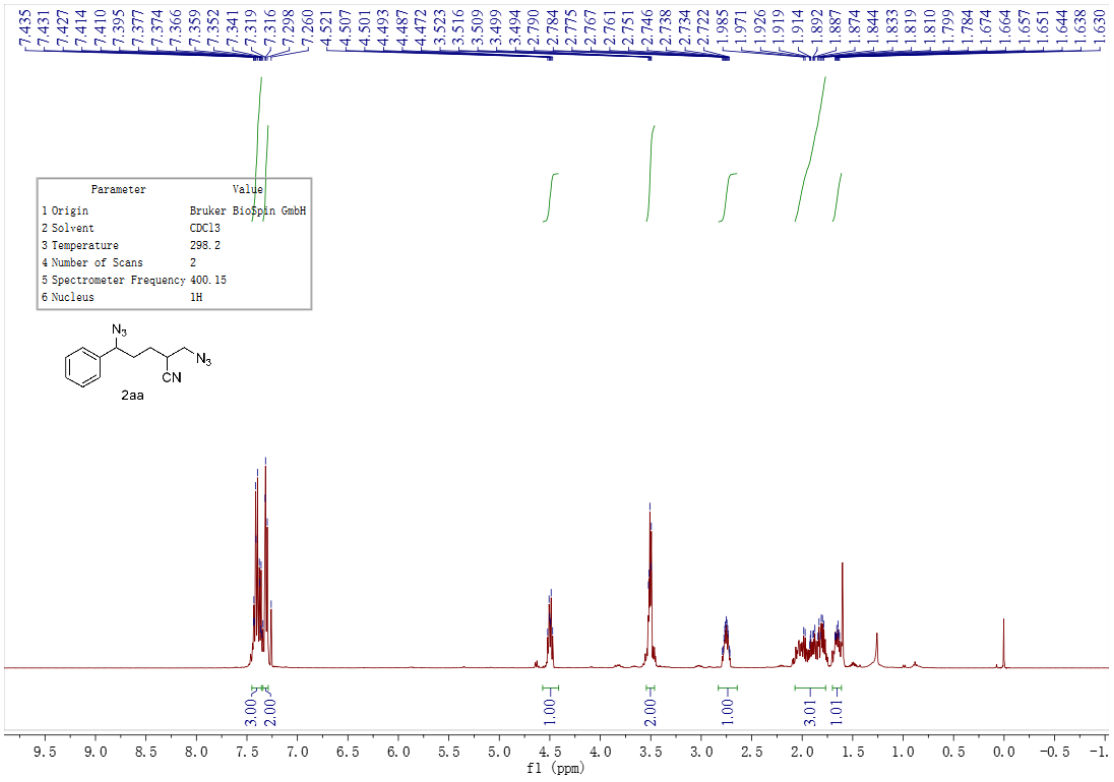
77.357
77.039
76.722
72.373
72.295
62.712
51.784
51.736
36.032
35.974
32.147
32.070
24.731
24.596
14.076
Parameter Value
1 Origin Bruker BioSpin GmbH
2 Solvent CDCl3
3 Temperature 298.2
4 Number of Scans 160
5 Spectrometer Frequency 100.62
6 Nucleus 13C
EtO2C N3
N3
CN
2z
f1 (ppm)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7.316
7.298
7.260
4.521
4.507
4.501
4.493
4.487
4.472
3.523
3.516
3.509
3.499
3.494
2.790
2.784
2.775
2.767
2.761
2.751
2.746
2.738
2.734
2.722
1.985
1.971
1.926
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1.914
1.892
1.887
1.874
1.844
1.833
1.819
1.810
1.799
1.784
1.674
1.664
1.657
1.651
1.644
1.638
1.630
Parameter Value
1 Origin Bruker BioSpin GmbH
2 Solvent CDCl3
3 Temperature 298.2
4 Number of Scans 2
5 Spectrometer Frequency 400.15
6 Nucleus 1H
N3
N3
CN
2aa
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1.00
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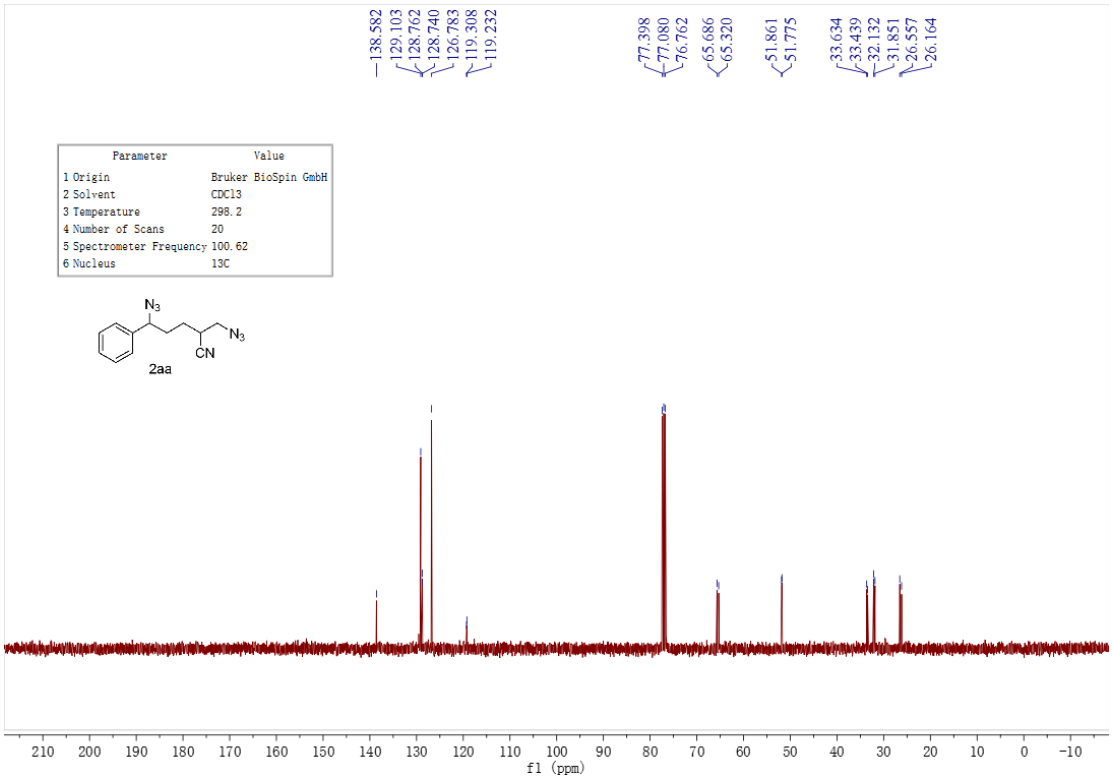
1.01
f1 (ppm)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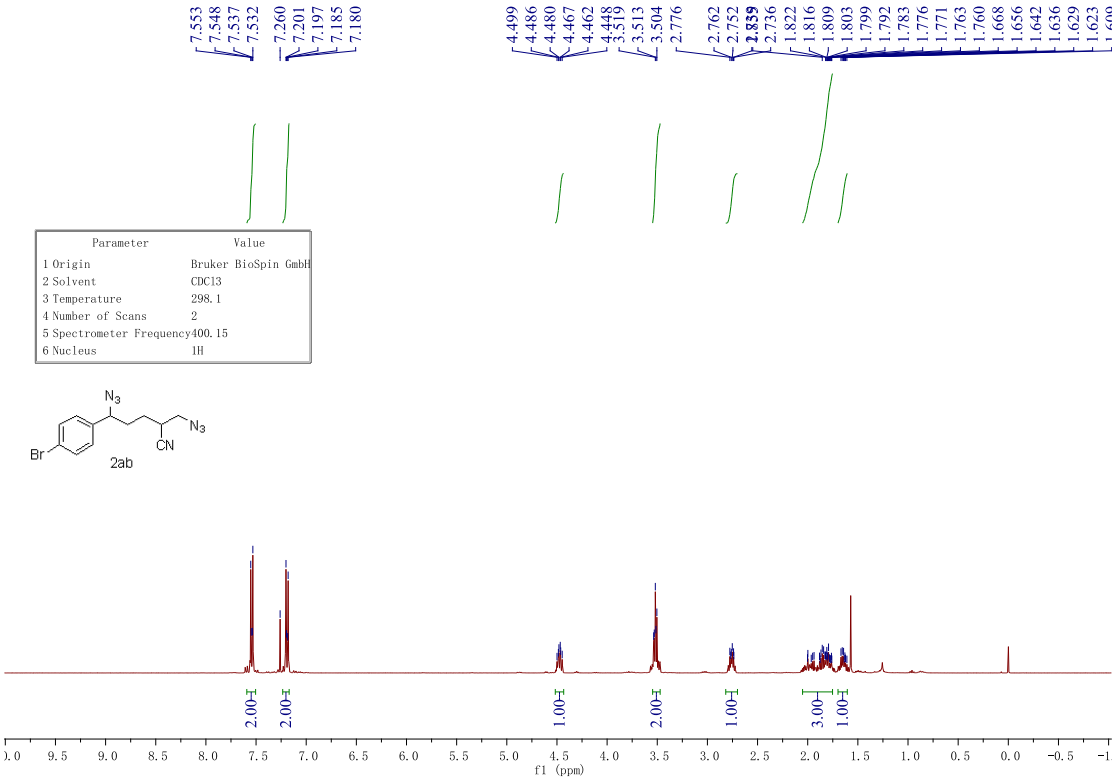
51.861
51.775
33.634
33.439
32.132
31.851
26.557
26.164
Parameter Value
1 Origin Bruker BioSpin GmbH
2 Solvent CDCl3
3 Temperature 298.2
4 Number of Scans 20
5 Spectrometer Frequency 100.62
6 Nucleus 13C
N3
N3
CN
2aa
f1 (ppm)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4.462
4.448
3.519
3.513
3.504
2.776
2.762
2.752
2.736
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1.816
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1.792
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1.771
1.763
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1.656
1.642
1.636
1.629
1.623
Parameter Value
1 Origin Bruker BioSpin GmbH
2 Solvent CDCl3
3 Temperature 298.1
4 Number of Scans 2
5 Spectrometer Frequency 400.15
6 Nucleus 1H
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N3
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Br
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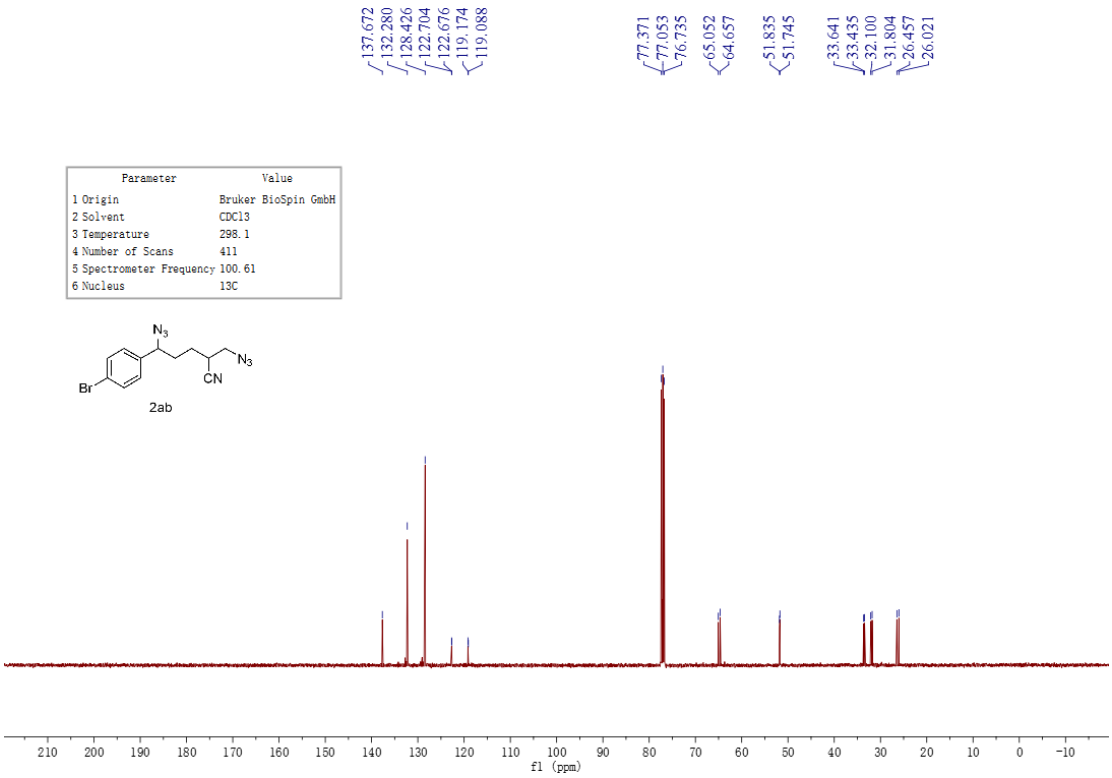
f1 (ppm)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77.371
77.053
76.735
65.052
64.657
51.835
51.745
33.641
33.435
32.100
31.804
26.457
26.021
Parameter Value
1 Origin Bruker BioSpin GmbH
2 Solvent CDCl3
3 Temperature 298.1
4 Number of Scans 411
5 Spectrometer Frequency 100.61
6 Nucleus 13C
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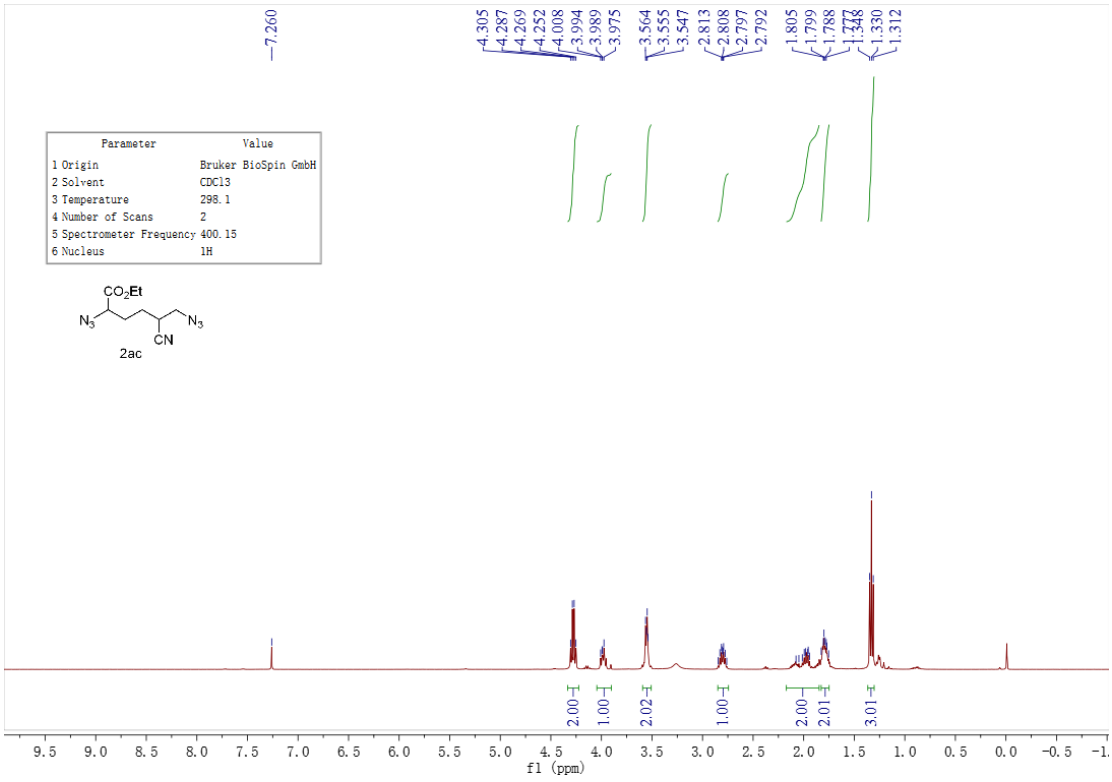
N3
CN
Br
2ab
f1 (ppm)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3.989
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3.564
3.555
3.547
2.813
2.808
2.797
2.792
1.805
1.799
1.788
1.330
1.312
Parameter Value
1 Origin Bruker BioSpin GmbH
2 Solvent CDCl3
3 Temperature 298.1
4 Number of Scans 2
5 Spectrometer Frequency 400.15
6 Nucleus 1H
CO2Et
N3
N3
CN
2ac
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1.00
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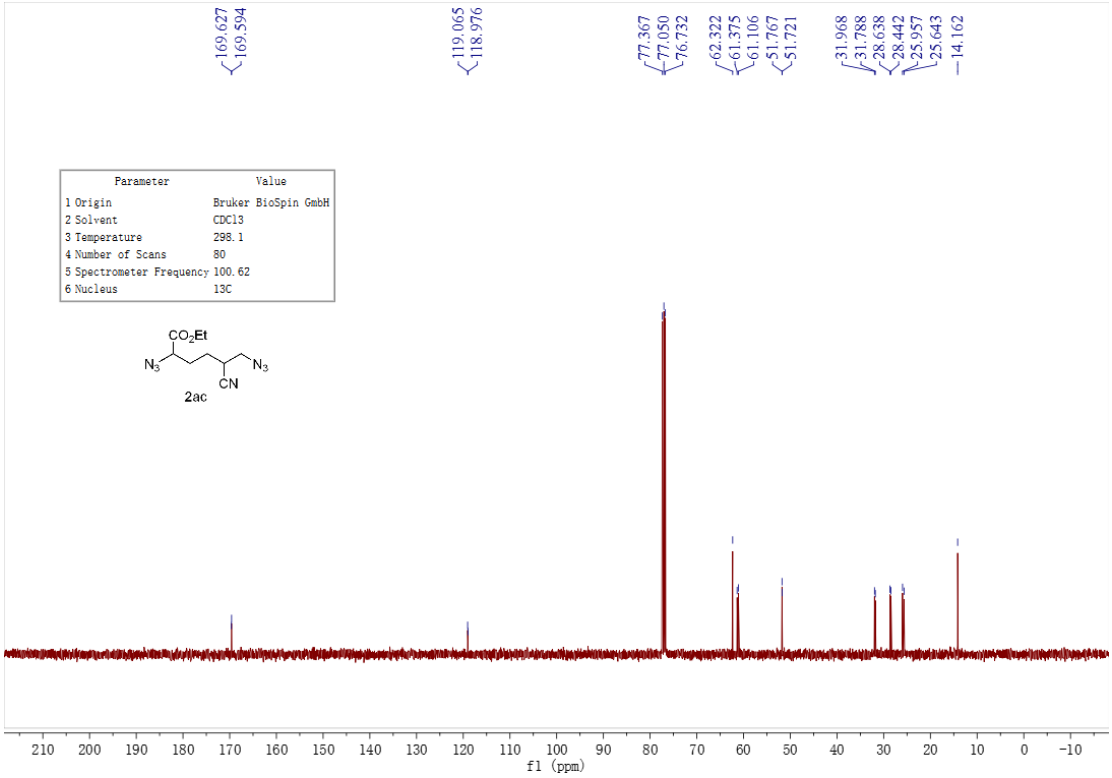
1.00
2.00
2.01
3.01
f1 (ppm)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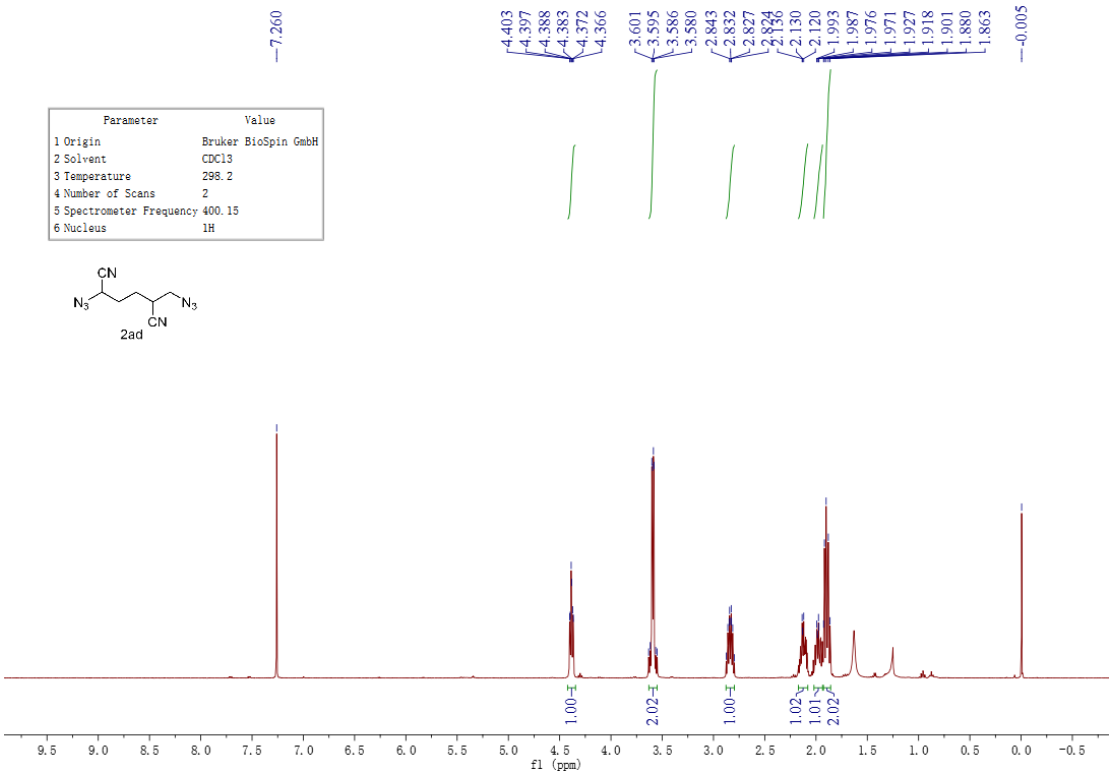
51.767
51.721
31.968
31.788
28.638
28.442
25.957
25.643
14.162
Parameter Value
1 Origin Bruker BioSpin GmbH
2 Solvent CDCl3
3 Temperature 298.1
4 Number of Scans 80
5 Spectrometer Frequency 100.62
6 Nucleus 13C
CO2Et
N3
N3
CN
2ac
f1 (ppm)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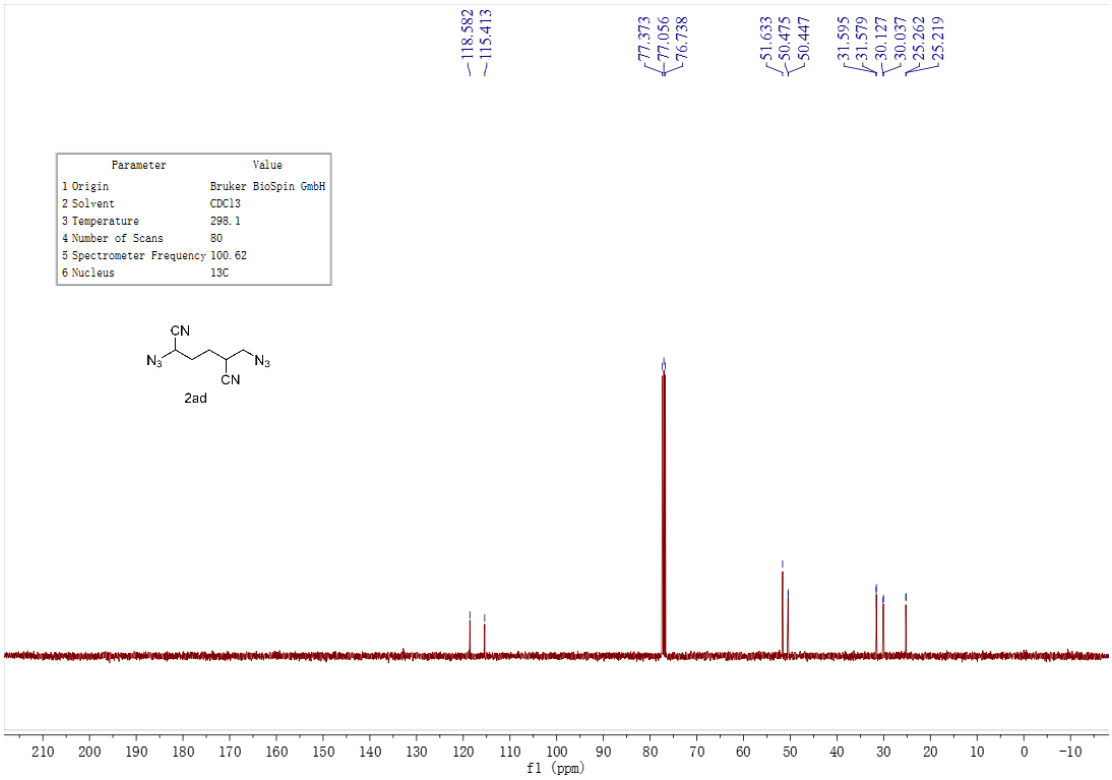
2.832
2.827
2.824
2.136
2.130
2.120
1.993
1.987
1.976
1.971
1.927
1.918
1.901
1.880
1.863
0.005
Parameter Value
1 Origin Bruker BioSpin GmbH
2 Solvent CDCl3
3 Temperature 298.2
4 Number of Scans 2
5 Spectrometer Frequency 400.15
6 Nucleus 1H
CN
N3
N3
CN
2ad
1.00
2.02
1.00
1.02
1.01
2.02
f1 (ppm)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77.056
76.738
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50.447
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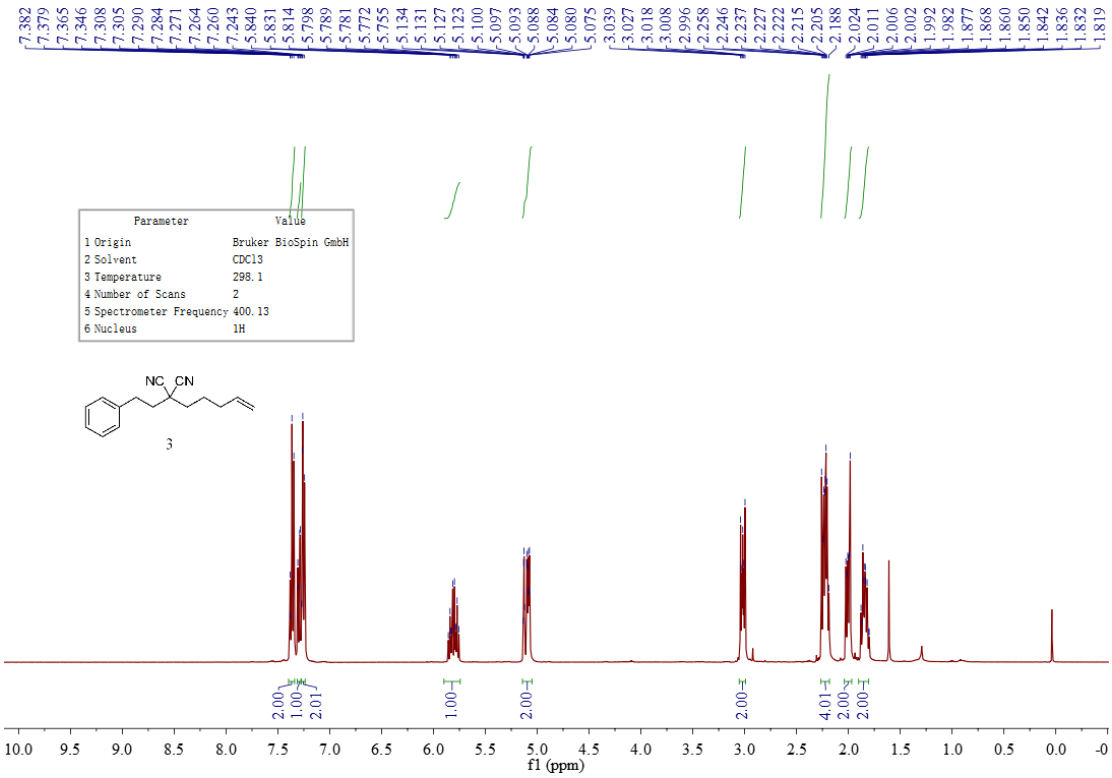
31.579
30.127
30.037
25.262
25.219
Parameter Value
1 Origin Bruker BioSpin GmbH
2 Solvent CDCl3
3 Temperature 298.1
4 Number of Scans 80
5 Spectrometer Frequency 100.62
6 Nucleus 13C
CN
N3
N3
CN
2ad
f1 (ppm)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7.379
7.365
7.346
7.308
7.305
7.290
7.284
7.271
7.264
7.260
7.243
5.840
5.831
5.814
5.798
5.789
5.781
5.772
5.755
5.134
5.131
5.127
5.123
5.100
5.097
5.093
5.088
5.084
5.080
5.075
3.039
3.027
3.018
3.008
2.996
2.258
2.246
2.237
2.227
2.222
2.215
2.205
2.188
2.024
2.011
2.006
2.002
1.992
1.982
1.877
1.868
1.860
1.850
1.842
1.836
1.832
1.819
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
NC CN
3
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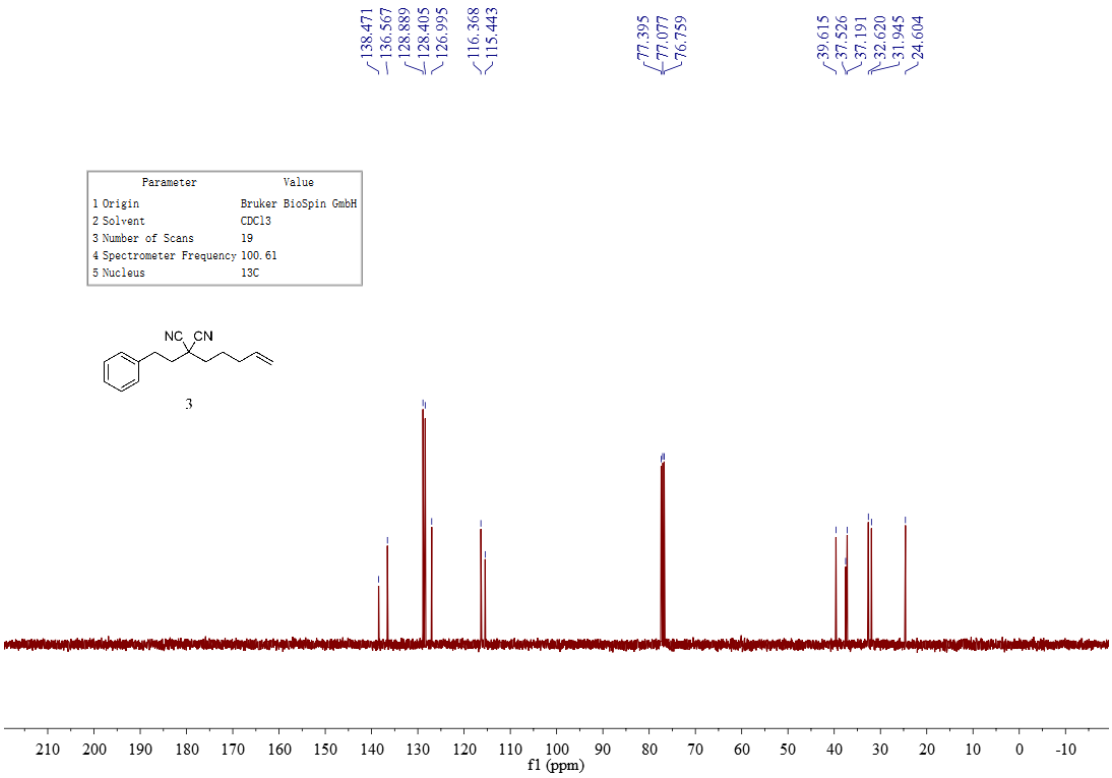
1.00
2.01
1.00
2.00
2.00
4.01
2.00
2.00
f1 (ppm)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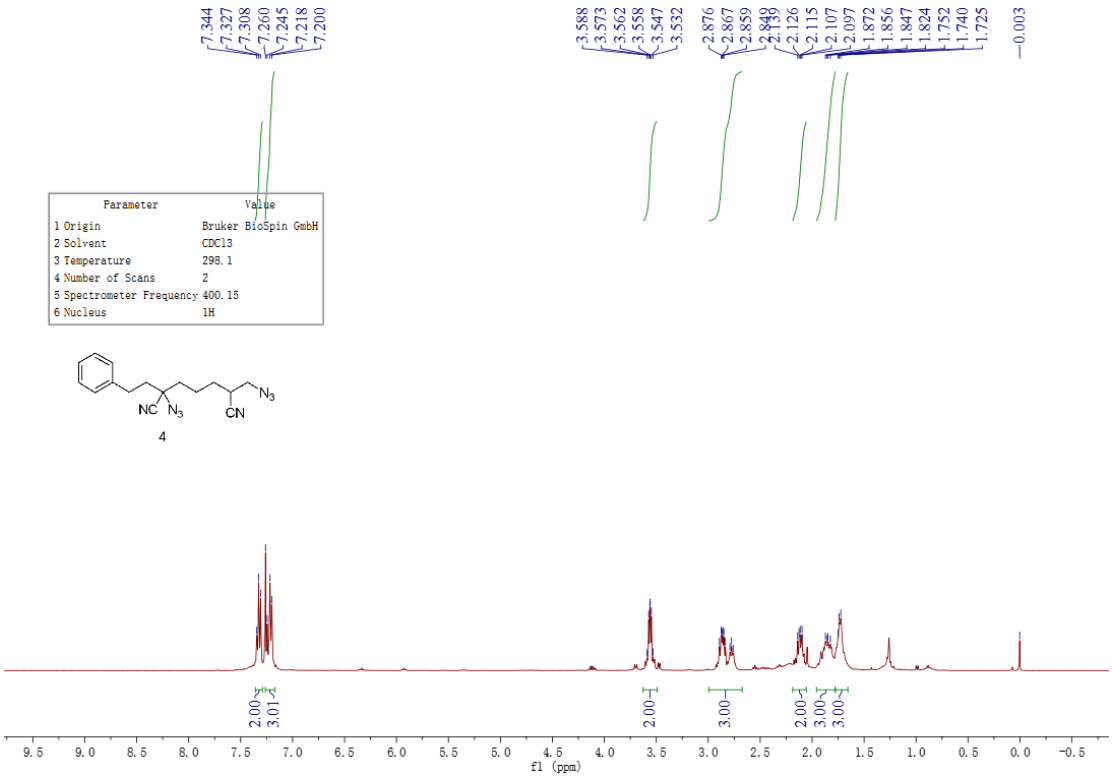
136.567
128.889
128.405
126.995
116.368
115.443
77.395
77.077
76.759
39.615
37.526
37.191
32.620
31.945
24.604
Parameter Value
1 Origin Bruker BioSpin GmbH
2 Solvent CDCl3
3 Number of Scans 19
4 Spectrometer Frequency 100.61
5 Nucleus 13C
NC CN
3
f1 (ppm)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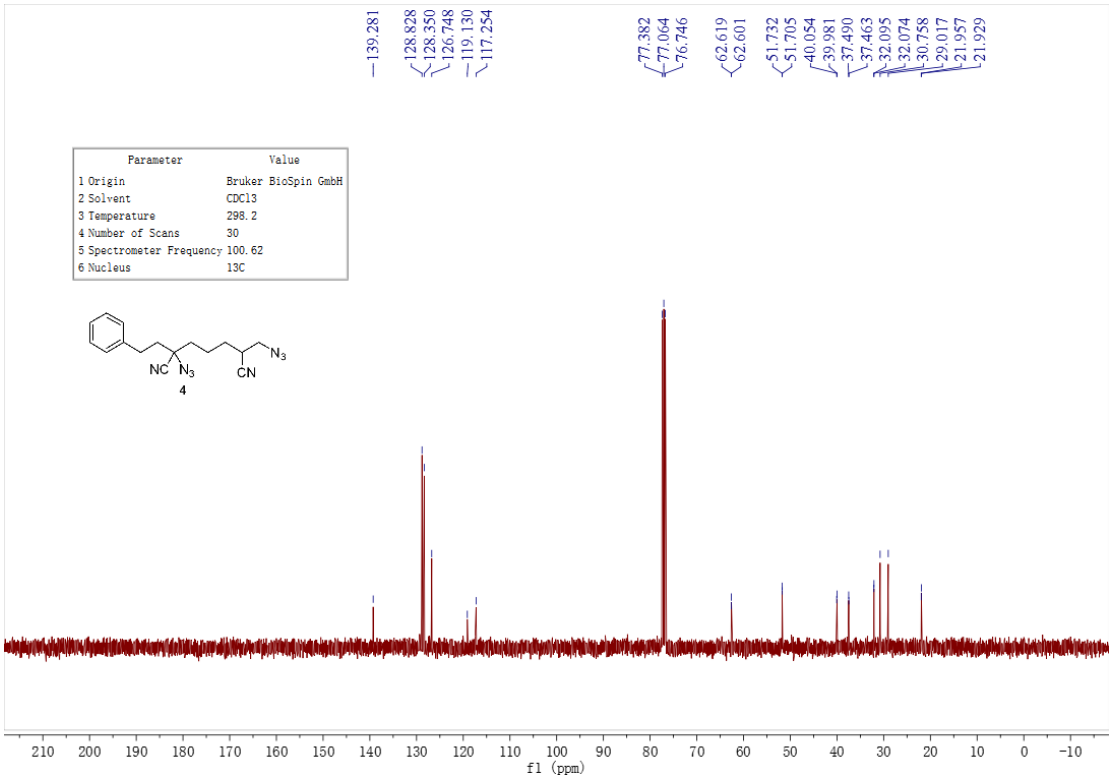
7.327
7.308
7.260
7.245
7.218
7.200
3.588
3.573
3.562
3.558
3.547
3.532
2.876
2.867
2.859
2.849
2.139
2.126
2.115
2.107
2.097
1.872
1.856
1.847
1.824
1.752
1.740
1.725
-0.003
Parameter Value
1 Origin Bruker BioSpin GmbH
2 Solvent CDCl3
3 Temperature 298.1
4 Number of Scans 2
5 Spectrometer Frequency 400.15
6 Nucleus 1H
NC N3 CN N3
4
2.00
3.01
2.00
3.00
2.00
3.00
3.00
f1 (ppm)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128.828
128.350
126.748
119.130
117.254
77.382
77.064
76.746
62.619
62.601
51.732
51.705
40.054
39.981
37.490
37.463
32.095
32.074
30.758
29.017
21.957
21.929
Parameter Value
1 Origin Bruker BioSpin GmbH
2 Solvent CDCl3
3 Temperature 298.2
4 Number of Scans 30
5 Spectrometer Frequency 100.62
6 Nucleus 13C
NC
N3
CN
N3
4
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)