Supporting Information

Iron-Catalyzed C-H Bond Functionalization into Oxime Ethers via Photo-Induced Ligand-to-Metal Charge Transfer

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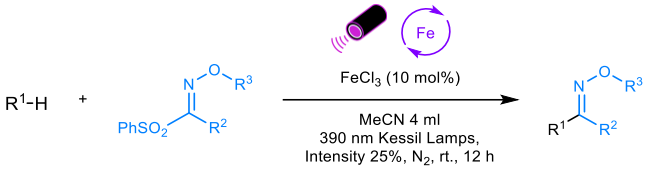
1. General Information

All commercial reagents were used without further purification unless otherwise noted. Unless otherwise stated, all experiments were conducted in a sealed tube under N_2 atmosphere. Reactions were monitored by TLC or GC-MS analysis. Proton nuclear magnetic resonance (^{1}H NMR) spectra, carbon nuclear magnetic resonance (^{13}C NMR) spectra, and fluorine nuclear magnetic resonance (^{19}F NMR) were recorded on Bruker AV-400 (400 MHz), JEOL-500 (500 MHz) spectrometers. Chemical shifts for protons are reported in parts per million downfield from tetramethylsilane and are referenced to residual protium in the NMR solvent ($CHCl_3$ = δ 7.26). Chemical shifts for carbon are reported in parts per million downfield from tetramethylsilane and are referenced to the carbon resonances. NMR data are reported as follows: chemical shift (δ) (multiplicity, coupling constants (J, Hz) and integration). HRMS were obtained on an Exactive Plus LC-MS (ESI) mass spectrometer with the use of a quadrupole analyzer.

2. General procedures for iron catalyzed LMCT reaction



General procedure:

A dry 10 mL sealed tube equipped with a stirring bar was charged with a sulfonyl oxime (0.2 mmol, 1.0 equiv), $FeCl_3$(0.02 mmol, 0.1 equiv, 3.2 mg), 4 mL MeCN in glovebox. Alkanes (2 mmol, 10.0 equiv) were added subsequently via syringe. The reaction mixture was stirred for 12 h under the irradiation of 40W 390 nm Kessil Lamps with fan cooling. After the reaction is completed, the mixture was transferred to a 25 mL round bottom flask via syringe. The combined organic layers were concentrated with a rotary evaporator. The crude product was purified by flash column chromatography over neutral alumina using a hexane/ethyl acetate solvent system as the eluent.

Figure S1. Reaction equipment

Procedure for scale-up reaction：

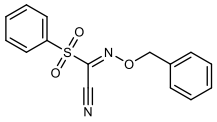
A dry 50 mL sealed tube equipped with a stirring bar was charged with a sulfonyl oxime (2.0 mmol, 1.0 equiv, 600.0 mg), $FeCl_3$(0.2 mmol, 0.1 equiv 32.0 mg), 40 mL MeCN in glovebox. Cyclohexane (20 mmol, 10.0 equiv, 2.16 mL) were added subsequently via syringe. The reaction mixture was stirred for 12 h under the irradiation of 390 nm Kessil Lamps with fan cooling. After the reaction is completed, the mixture was transferred to a 100 mL round bottom flask via syringe. The combined organic layers were concentrated with a rotary evaporator. The product was purified by column chromatography on neutral alumina using hexane/ethyl acetate as eluent to afford 451 mg (93%) of the desired compound.

Procedure for synthesis of 5

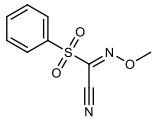
To a solution of **3a** (48.4 mg, 1equiv, 0.2 mmol) in water/2-propanol (2:1, 6 mL) were added sodium azide (39.0 mg, 3.0 equiv, 0.6 mmol) and $ZnBr_2$ (45.0 mg, 1.0 equiv, 0.2 mmol) at room temperature. While stirring, the reaction mixture was heated under Inert gas at 120 ℃ for 72 hours. The mixture was cool to room temperature, HCl (1N solution) and ethyl acetate were added, and the resulting mixture was stirred until the solid was entirely dissolved. The organic layer was separated, and the aqueous layer was extracted with ethyl acetate. The combined organic layer was washed with brine, dried with Na_2SO_4, filtered, and concentrated under reduced pressure. The residue was purified by chromatography on a silica gel column (DCM: MeOH = 10:1) to afford the title compound **5** (23.4 mg, 41%) in an inseparable mixture of rotamers and Z/E isomers (of each rotamer) as an oil.

3. General procedures for synthesis of substrates

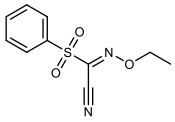
Sulfonyl-oxime ethers **2a-2g** were synthesized using reported procedures. [1-2]



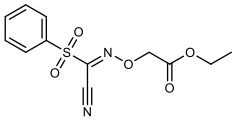
2a



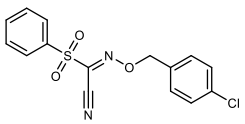
2b



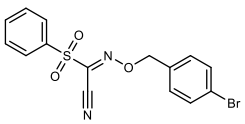
2c



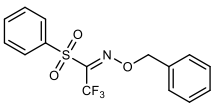
2d



2e



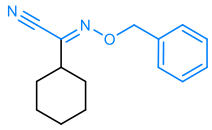
2f



2g

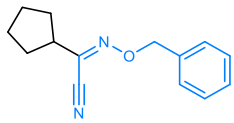
4. Spectroscopic Data of the Products

N-(benzyloxy)cyclohexanecarbimidoyl cyanide (3a)



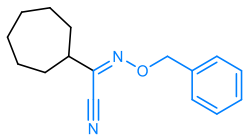
Yield: 96% (46.5 mg), colorless oil. ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.41 – 7.29 (m, 5H), 5.23 (s, 2H), 2.43 (tt, *J* = 11.6, 3.6 Hz, 1H), 1.93 – 1.76 (m, 4H), 1.74 – 1.67 (m, 1H), 1.49 – 1.36 (m, 2H), 1.35 – 1.17 (m, 3H). ^{13}C NMR (126 MHz, $CDCl_3$) δ 137.3, 136.2, 128.5, 128.4, 128.3, 109.9, 77.6, 40.8, 29.9, 25.4, 25.4. Data in accordance with the literature[1].

N-(benzyloxy)cyclopentanecarbimidoyl cyanide (3b)



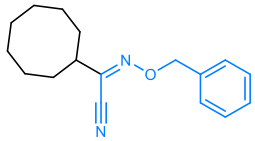
Yield: 67% (30.6 mg), colorless oil, E/Z = 3:1. ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.45 – 7.28 (m, 5H), 5.40 – 5.04 (m, 2H), 3.42 – 3.28 (m, 0.23H), 2.87 (p, *J* = 8.0 Hz, 0.71H), 2.00 – 1.87 (m, 2H), 1.79 – 1.53 (m, 6H). ^{13}C NMR (126 MHz, $CDCl_3$) δ 144.4, 136.9, 136.3, 136.1, 128.7, 128.65, 128.62, 128.59, 128.49, 128.45, 113.8, 110.0, 78.3, 77.7, 42.1, 36.9, 30.6, 30.4, 25.5, 25.3. Data in accordance with the literature[1].

N-(benzyloxy)cycloheptanecarbimidoyl cyanide (3c)



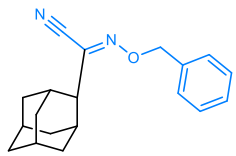
Yield: 94% (48.2 mg), colorless oil. ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.36 (m, 5H), 5.22 (s, 2H), 2.60 (tt, *J* = 9.6, 4.2 Hz, 1H), 1.92 – 1.85 (m, 2H), 1.82 – 1.71 (m, 2H), 1.69 – 1.45 (m, 8H). ^{13}C NMR (126 MHz, CDCl3) δ 138.4, 136.3, 128.5, 128.33, 128.31, 110.2, 77.6, 41.1, 29.5, 26.7, 25.9, 24.8. Data in accordance with the literature[1].

N-(benzyloxy)cyclooctanecarbimidoyl cyanide (3d)



Yield: 73% (39.4 mg), colorless oil. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.47 – 7.32 (m, 5H), 5.25 (s, 2H), 2.71 (tt, *J* = 8.6, 3.8 Hz, 1H), 1.91 – 1.68 (m, 6H), 1.59 (m, 8H). ^{13}C NMR (126 MHz, $CDCl_3$) δ 138.1, 136.3, 128.6, 128.4, 110.2, 77.6, 42.7, 31.9, 28.0, 26.1. Data in accordance with the literature[1].

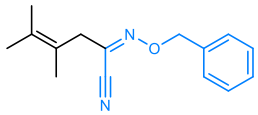
N-(benzyloxy)adamantane-2-carbimidoyl cyanide (3e)



Yield: 42% (24.7 mg), colorless oil, E/Z = 3.5:1. ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.41 – 7.28 (m, 5H),

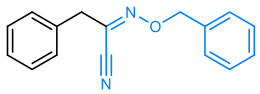
5.26 (s, 0.76H), 5.22 (s, 1.24H), 2.68 (s, 0.36H), 2.29 (s, 0.76H), 2.12 – 1.48 (m, 15H) ^{13}C NMR (126 MHz, $CDCl_3$) δ 141.2, 136.5, 136.3, 135.9, 128.7, 128.6, 128.5, 128.4, 110.1, 109.4, 77.8, 77.7, 47.1, 39.7, 38.2, 37.5, 36.3, 32.1, 29.7, 27.9, 27.7, 27.5. Data in accordance with the literature[1].

N-(benzyloxy)-3,4-dimethylpent-3-enimidoyl cyanide (3f)



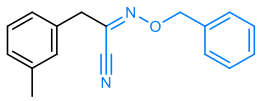
Yield: 45% (21.8 mg), colorless oil, E/Z = 1.1:1. ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.40 – 7.28 (m, 5H), 5.26 – 5.23 (m, 2H), 3.22 (s, 1.41H), 3.13 (s, 1.59H), 1.76 – 1.66 (m, 6H), 1.64 – 1.56 (m, 3H). ^{13}C NMR (126 MHz, $CDCl_3$) δ 138.5, 136.4, 136.0, 131.5, 131.2, 131.1, 128.7, 128.6, 128.4, 119.8, 114.6, 110.6, 78.4, 77.7, 36.9, 33.3, 21.1, 20.9, 20.8, 20.7, 19.1, 18.1. Data in accordance with the literature[1].

N-(benzyloxy)-2-phenylacetimidoyl cyanide (3g)



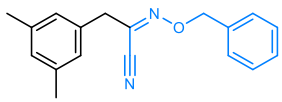
Yield: 42% (21.0mg), colorless oil, E/Z = 2.3:1. ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.48 – 7.29 (m, 8H), 7.27 – 7.19 (m, 2H), 5.33 – 5.27 (m, 2H), 3.81 (s, 0.60), 3.71 (s, 1.40H). ^{13}C NMR (126 MHz, $CDCl_3$) δ 137.6, 136.1, 135.8, 133.6, 133.4, 131.9, 129.2, 129.1, 129.1, 129.1, 128.8, 128.8, 128.7, 128.7, 128.6, 128.5, 127.9, 127.8, 114.5, 110.3, 78.7, 78.0, 38.3, 34.5. Data in accordance with the literature[4].

N-(benzyloxy)-2-(m-tolyl)acetimidoyl cyanide (3h)



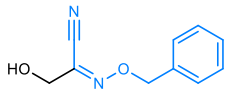
Yield: 63% (33.3 mg), colorless oil, E/Z = 1.7:1. ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.44 – 7.34 (m, 5H), 7.27 – 7.19 (m, 1H), 7.14 – 7.08 (m, 1H), 7.05 – 6.99 (m, 2H), 5.33 – 5.28 (m, 2H), 3.77 (s, 0.73H), 3.68 (s, 1.27H), 2.36 – 2.30 (m, 3H). ^{13}C NMR (126 MHz, $CDCl_3$) δ 138.9, 138.8, 137.8, 136.2, 135.9, 133.5, 133.2, 132.0, 129.9, 129.8, 129.02, 128.99, 128.82, 128.77, 128.69, 128.67, 128.57, 128.53, 126.2, 126.1, 114.6, 110.3, 78.7, 78.0, 38.2, 34.4, 21.5, 21.4. Data in accordance with the literature[1].

N-(benzyloxy)-2-(3,5-dimethylphenyl)acetimidoyl cyanide (3i)



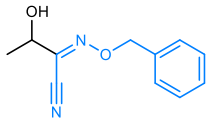
Yield: 83% (47.2 mg), colorless oil, E/Z = 1.7:1. ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.42 – 7.36 (m, 5H), 6.96 – 6.92 (m, 1H), 6.84 – 6.81 (m, 2H), 5.34 – 5.29 (m, 2H), 3.74 (s, 0.75H), 3.64 (s, 1.25H), 2.33 – 2.24 (m, 6H). ^{13}C NMR (126 MHz, $CDCl_3$) δ 138.73, 138.67, 137.9, 136.3, 135.9, 133.4, 133.1, 132.1, 129.6, 129.4, 128.80, 128.76, 128.68, 128.55, 128.52, 127.0, 126.9, 114.7, 110.4, 78.7, 78.0, 38.1, 34.3, 21.34, 21.32. Data in accordance with the literature[1].

N-(benzyloxy)-2-hydroxyacetimidoyl cyanide (3j)



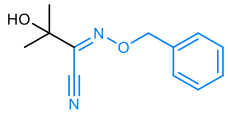
Yield: 52% (19.8 mg), colorless oil, E/Z = 1.8:1. ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.41 – 7.30 (m, 5H), 5.28 – 5.24 (m, 2H), 4.43 (s, 0.72H), 4.36 (s, 1.28H), 2.71 – 2.39 (m, 1H). ^{13}C NMR (126 MHz, $CDCl_3$) δ 140.3, 135.7, 135.4, 131.9, 129.0, 128.83, 128.81, 128.77, 128.74, 128.66, 113.1, 109.6, 79.2, 78.5, 61.1, 57.2. Data in accordance with the literature[1].

N-(benzyloxy)-2-hydroxypropanimidoyl cyanide (3k)



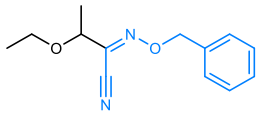
Yield: 58% (23.7 mg), colorless oil, E/Z = 4:1. ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.48 – 7.30 (m, 5H), 5.25 (s, 2H), 4.96 (q, *J* = 6.6 Hz, 0.2H), 4.56 (q, *J* = 6.6 Hz, 0.78H), 2.29 (s, 1H), 1.45 (d, *J* = 6.6 Hz, 2.41H), 1.38 (d, *J* = 6.7 Hz, 0.63H). ^{13}C NMR (126 MHz, $CDCl_3$) δ 143.8, 136.0, 135.8, 135.5, 129.0, 128.8, 128.8, 128.7, 128.6, 112.7, 109.0, 79.1, 78.4, 66.8, 62.3, 20.7, 19.6. Data in accordance with the literature[1].

N-(benzyloxy)-2-hydroxy-2-methylpropanimidoyl cyanide (3l)



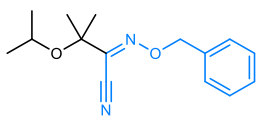
Yield: 85% (37.1 mg), colorless oil. ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.40 – 7.32 (m, 5H), 5.25 (s, 2H), 2.22 (s, 1H), 1.49 (s, 6H). ^{13}C NMR (126 MHz, $CDCl_3$) δ 138.8, 135.8, 128.69, 128.67, 109.2, 78.4, 71.7, 27.8. Data in accordance with the literature[3].

(N-(benzyloxy)-2-ethoxypropanimidoyl cyanide (3m)



Yield: 62% (28.8 mg), colorless oil, E/Z = 6:1. ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.42 – 7.28 (m, 5H), 5.34 – 5.19 (m,2H), 4.68 (q, *J* = 6.6 Hz, 0.14H), 4.14 (q, *J* = 6.6 Hz, 0.82H), 3.51 – 3.33 (m, 2H), 1.42 (d, *J* = 6.6 Hz, 2.58H), 1.31 (d, *J* = 6.6 Hz, 0.42H), 1.21 – 1.14 (m, 3H). ^{13}C NMR (126 MHz, $CDCl_3$) δ 143.6, 135.9, 135.6, 135.3, 128.9, 128.8, 128.7, 128.6, 128.5, 112.6, 108.8, 78.9, 78.3, 76.9, 73.5, 68.8, 65.8, 64.7, 19.2, 18.0, 15.15, 15.12. Data in accordance with the literature[1].

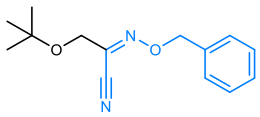
N-(benzyloxy)-2-isopropoxy-2-methylpropanimidoyl cyanide (3n)



Yield: 71% (36.9 mg), colorless oil. ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.40 – 7.26 (m, 5H), 5.27 (s, 2H), 3.56 (p, *J* = 6.1 Hz, 1H), 1.42 (s, 6H), 1.08 (d, *J* = 6.2 Hz, 6H). ^{13}C NMR (126 MHz, $CDCl_3$) δ 138.2, 136.1, 128.62, 128.57, 109.5, 78.2, 75.6, 66.3, 25.4, 24.5. IR (ATR): $\tilde{\nu}$ = 2978, 2929, 1455, 1370, 1171, 1110, 996, 804, 740, 697, 599 cm^{-1}. HRMS (ESI) exact mass calculated for [M+H^{+}]

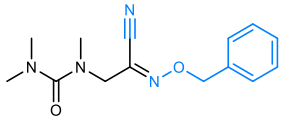
($C_{15}H_{21}N_2O_2^+$): m/z 261.1598; found: 261.1594.

N-(benzyloxy)-2-(tert-butoxy)acetimidoyl cyanide (3o)



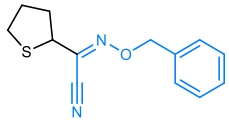
Yield: 60% (29.5 mg), colorless oil, E/Z = 3.3:1. ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.40 – 7.31 (m, 5H), 5.27 – 5.22 (m, 2H), 4.22 (s, 0.47H), 4.13 (s, 1.53H), 1.28 – 1.10 (m, 9H). ^{13}C NMR (126 MHz, $CDCl_3$) δ 140.4, 135.9, 135.7, 131.7, 128.9, 128.8, 128.8, 128.7, 128.6, 128.6, 113.1, 109.9, 79.0, 78.3, 75.2, 75.2, 60.7, 56.5, 27.5, 27.3. Data in accordance with the literature[1].

N-(benzyloxy)-2-(1,3,3-trimethylureido)acetimidoyl cyanide (3p)



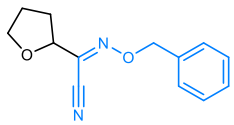
Yield: 51% (28.0 mg), colorless oil. ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.37 – 7.31 (m, 5H), 5.29 – 5.20 (m, 2H), 4.17 – 4.12 (m, 1H), 4.12 – 4.07 (m, 1H), 3.19 – 2.62 (m, 9H). ^{13}C NMR (126 MHz, $CDCl_3$) δ 164.63, 164.59, 139.0, 135.9, 135.6, 130.5, 128.8, 128.73, 128.67, 128.64, 128.58, 113.5, 109.7, 79.0, 78.3, 50.5, 47.5, 39.1, 38.6, 38.5, 37.7. Data in accordance with the literature[1].

N-(benzyloxy)tetrahydrothiophene-2-carbimidoyl cyanide (3q)



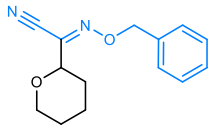
Yield: 64% (31.5 mg), colorless oil, E/Z = 2.6:1. ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.42 – 7.30 (m, 5H), 5.25 (s, 0.56H), 5.21 (s, 1.44H), 4.66 (t, J = 6.7 Hz, 0.14H), 4.24 (t, J = 6.8 Hz, 0.71H), 3.08 – 2.98 (m, 1H), 2.95 – 2.87 (m, 1H), 2.35 – 2.20 (m, 2H), 2.14 – 1.92 (m, 2H). ^{13}C NMR (126 MHz, $CDCl_3$) δ 141.9, 135.9, 135.7, 135.0, 128.8, 128.73, 128.67, 128.64, 128.59, 128.55, 113.3, 109.4, 78.8, 78.1, 47.6, 45.9, 40.8, 35.0, 33.9, 31.2. Data in accordance with the literature[3].

N-(benzyloxy)tetrahydrofuran-2-carbimidoyl cyanide (3r)



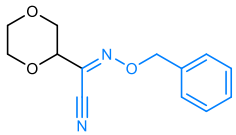
Yield: 74% (34.1 mg), colorless oil, E/Z = 2.7:1. ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.39 – 7.31 (m, 5H), 5.27 – 5.22 (m, 2H), 4.97 (t, J = 7.1 Hz, 0.27H), 4.61 (t, J = 6.7 Hz, 0.73H), 4.08 – 3.94 (m, 1H), 3.92 – 3.84 (m, 1H), 2.29 – 1.77 (m, 4H). ^{13}C NMR (126 MHz, $CDCl_3$) δ 143.2, 135.8, 135.7, 134.3, 128.8, 128.8, 128.7, 128.6, 128.6, 112.9, 109.3, 79.0, 78.4, 76.6, 72.6, 69.5, 69.5, 30.8, 30.3, 26.0, 25.9. Data in accordance with the literature[3].

N-(benzyloxy)tetrahydro-2H-pyran-2-carbimidoyl cyanide (3s)



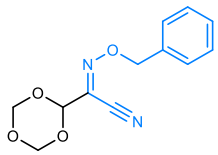
Yield: 56% (27.3 mg), colorless oil, E/Z = 9:1. ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.41 – 7.30 (m, 5H), 5.26 (s, 1.8H), 5.23 (s, 0.2H), 4.55 (dd, *J* = 11.0, 2.3 Hz, 0.08H), 4.12 (dd, *J* = 9.8, 3.8 Hz, 0.89H), 4.04 (ddt, *J* = 11.4, 4.0, 1.8 Hz, 1H), 3.58 – 3.40 (m, 1H), 1.95 – 1.88 (m, 1H), 1.79 – 1.68 (m, 2H), 1.66 – 1.44 (m, 3H). ^{13}C NMR (126 MHz, $CDCl_3$) δ 141.0, 135.8, 135.7, 133.8, 128.8, 128.8, 128.7, 128.6, 128.5, 112.8, 109.2, 79.0, 78.4, 75.4, 71.4, 68.7, 68.5, 29.8, 29.2, 27.8, 25.2, 22.6, 22.5. Data in accordance with the literature[3].

N-(benzyloxy)-1,4-dioxane-2-carbimidoyl cyanide (3t)



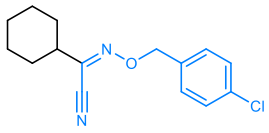
Yield: 81% (38.4 mg), colorless oil, E/Z = 7.8:1. ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.40 – 7.31 (m, 5H), 5.41 – 5.11 (m, 1H), 4.82 (dd, *J* = 9.9, 2.8 Hz, 0.11H), 4.36 (dd, *J* = 9.6, 2.9 Hz, 0.86H), 3.87 (td, *J* = 11.5, 2.6 Hz, 3H), 3.82 – 3.60 (m, 3.93H), 3.38 (dd, *J* = 11.4, 9.9 Hz, 0.07H). ^{13}C NMR (126 MHz, $CDCl_3$) δ 137.2, 135.4, 135.2, 130.3, 128.82, 128.76, 128.7, 112.4, 108.7, 78.9, 78.8, 72.8, 72.7, 70.1, 70.0, 67.9, 66.7, 66.23, 66.18. Data in accordance with the literature[3].

N-(benzyloxy)-1,3,5-trioxane-2-carbimidoyl cyanide (3u)



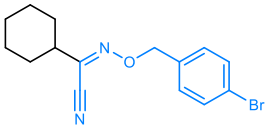
Yield: 78% (38.7 mg), colorless oil, E/Z = 9:1. ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.38 – 7.36 (m, 5H), 6.04 (s, 0.1H), 5.59 (s, 0.9H), 5.37 – 5.23 (m, 4H), 5.18 – 5.12 (m, 2H). ^{13}C NMR (126 MHz, $CDCl_3$) δ 135.1, 135.0, 134.3, 129.3, 129.1, 128.94, 128.89, 128.86, 128.79, 128.70, 111.7, 107.7, 96.7, 93.2, 93.1, 90.7, 80.0, 79.4. Data in accordance with the literature[3].

N-((4-chlorobenzyl)oxy)cyclohexanecarbimidoyl cyanide (4a)



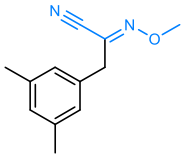
Yield: 84% (46.4 mg), colorless oil, E/Z = 9:1. ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.36 – 7.23 (m, 4H), 5.16 (s, 2H), 3.01 (tt, *J* = 11.9, 3.6 Hz, 0.10H), 2.41 (tt, *J* = 11.6, 3.6 Hz, 0.86H), 1.94 – 1.74 (m, 4H), 1.71 – 1.64 (m, 1H), 1.47 – 1.32 (m, 2H), 1.30 – 1.11 (m, 3H). ^{13}C NMR (126 MHz, $CDCl_3$) δ 144.5, 137.8, 134.8, 134.63, 134.59, 134.3, 129.9, 129.8, 128.8, 128.8, 113.6, 109.9, 76.8, 76.7, 40.9, 36.0, 30.0, 28.8, 25.4, 25.3. Data in accordance with the literature[1].

N-((4-bromobenzyl)oxy)cyclohexanecarbimidoyl cyanide (4b)



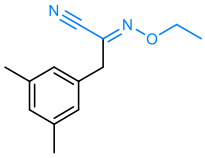
Yield: 80% (51.2 mg), colorless oil, E/Z = 10:1. ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.52 – 7.45 (m, 2H), 7.33 – 7.17 (m, 2H), 5.15 (s, 2H), 3.01 (tt, *J* = 11.9, 3.6 Hz, 0.09H), 2.41 (tt, *J* = 11.6, 3.5 Hz, 0.9H), 1.91 – 1.75 (m, 4H), 1.71 – 1.64 (m, 1H), 1.38 (m, 2H), 1.32 – 1.13 (m, 3H). ^{13}C NMR (126 MHz, $CDCl_3$) δ 144.5, 137.8, 135.3, 135.1, 131.9, 131.8, 130.2, 130.1, 122.8, 122.5, 113.6, 109.8, 76.8, 76.7, 40.9, 36.0, 30.0, 28.8, 25.4, 25.3. Data in accordance with the literature[1].

2-(3,5-dimethylphenyl)-N-methoxyacetimidoyl cyanide (4c)



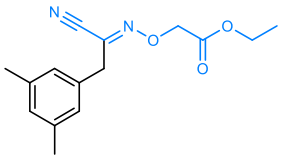
Yield: 64% (25.9 mg), colorless oil, E/Z = 3.5:1. ^{1}H NMR (400 MHz, $CDCl_3$) δ 6.85 (s, 1H), 6.80 – 6.73 (m, 2H), 4.04 – 3.97 (m, 3H), 3.62 (s, 0.64H), 3.55 (s, 2.23H), 2.23 (s, 6H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 138.7, 138.6, 137.4, 133.4, 133.1, 131.4, 129.5, 129.3, 126.8, 126.7, 114.4, 110.2, 64.0, 63.6, 37.9, 33.9, 29.7, 21.2. IR (ATR): $\tilde{\nu}$ = 2922, 1606, 1462, 1380, 1157, 1044, 936, 849, 739 cm^{-1}. HRMS (ESI) exact mass calculated for [M+H$^+$] ($C_{12}H_{15}N_2O^+$): m/z 203.1179; found: 203.1177.

2-(3,5-dimethylphenyl)-N-ethoxyacetimidoyl cyanide (4d)



Yield: 87% (37.6 mg), colorless oil, E/Z = 2:1. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.01 – 6.86 (m, 3H), 4.38 (dq, *J* = 10.2, 7.1 Hz, 2H), 3.75 (s, 0.66H), 3.68 (s, 1.34H), 2.35 (s, 6H), 1.39 (t, *J* = 7.1 Hz, 3H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 138.6, 138.5, 137.0, 133.6, 133.3, 131.0, 129.4, 129.3, 126.8, 126.7, 114.7, 110.4, 72.3, 71.9, 38.0, 34.0, 29.7, 21.2, 14.5, 14.3. IR (ATR): $\tilde{\nu}$ = 2920, 1606, 1463, 1383, 1159, 1040, 998, 848, 765, 736 cm^{-1}. HRMS (ESI) exact mass calculated for [M+H$^+$] ($C_{13}H_{17}N_2O^+$): m/z 217.1335; found: 217.1334.

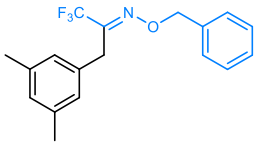
ethyl 2-(((1-cyano-2-(3,5-dimethylphenyl)ethylidene)amino)oxy)acetate (4e)



Yield: 81% (44.4 mg), colorless oil, E/Z = 3:1. ^{1}H NMR (400 MHz, $CDCl_3$) δ 6.97 (s, 1H), 6.94 – 6.88 (m, 2H), 4.87 – 4.78 (m, 2H), 4.29 (qd, *J* = 7.3, 2.7 Hz, 2H), 3.84 (s, 0.49H), 3.70 (s, 1.51H), 2.34 (s, 6H), 1.40 – 1.29 (m, 3H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 164.52, 164.49, 138.9, 135.8, 135.6, 130.5,

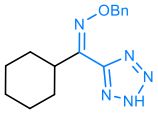
128.7, 128.63, 128.60, 128.57, 128.53, 128.45, 113.4, 109.6, 78.9, 78.3, 50.5, 47.4, 38.9, 38.5, 38.4, 37.6. IR (ATR): $\tilde{\nu}$ = 2987, 2924, 1756, 1606, 1466, 1378, 1208, 1079, 1024, 938, 852, 742 cm^{-1}. HRMS (ESI) exact mass calculated for [M+H^+] ($C_{15}H_{19}N_2O_3^+$): m/z 275.1390; found: 275.1386.

3-(3,5-dimethylphenyl)-1,1,1-trifluoropropan-2-one O-benzyl oxime (4f)



Yield: 46% (29.5 mg), colorless oil. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.30 – 7.18 (m, 5H), 6.77 (s, 1H), 6.70 (s, 2H), 5.16 (s, 2H), 3.64 (s, 2H), 2.15 (s, 6H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 148.0 (q, J = 31.8 Hz), 138.1, 136.3, 134.1, 128.5, 128.4, 126.7, 120.9 (q, J = 274.7 Hz), 77.9, 30.4, 21.2. ^{19}F NMR (376 MHz, $CDCl_3$) δ -68.08. IR (ATR): $\tilde{\nu}$ = 2927, 1606, 1456, 1371, 1188, 1130, 1090, 1014, 848, 741, 697, 610 cm^{-1}. HRMS (ESI) exact mass calculated for [M+H^+] ($C_{18}H_{19}F_3NO^+$): m/z 322.1413; found: 322.1412.

cyclohexyl(2H-tetrazol-5-yl)methanone O-benzyl oxime (5)

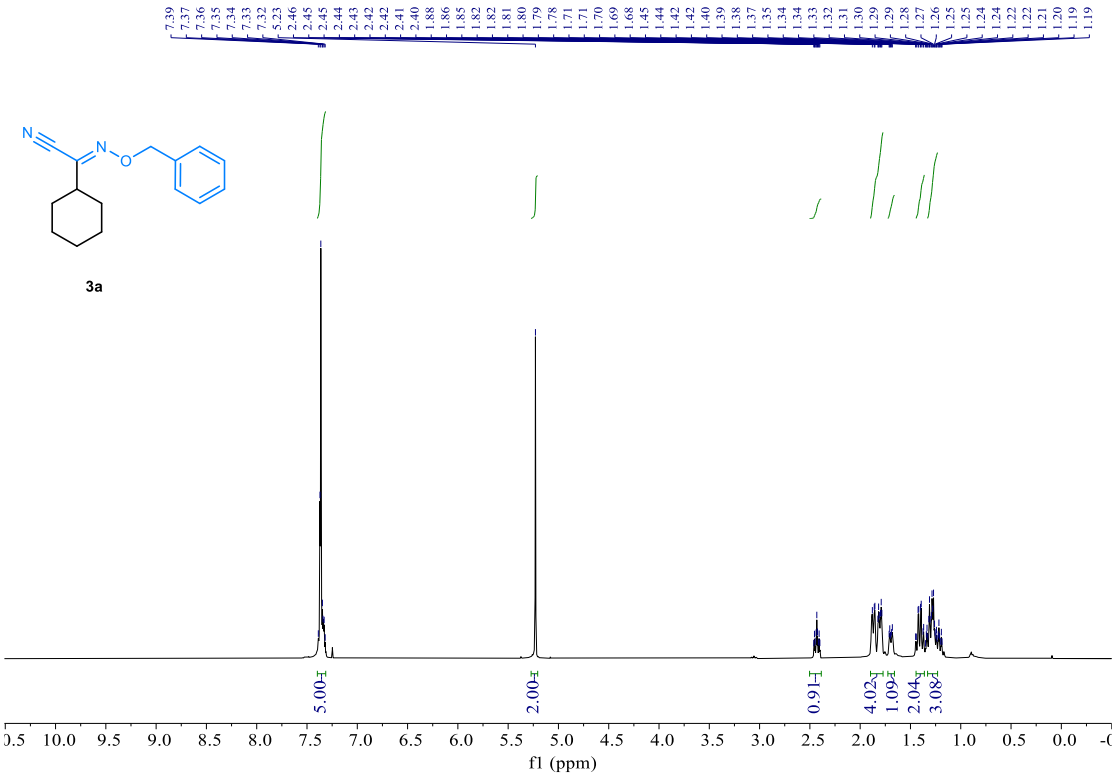


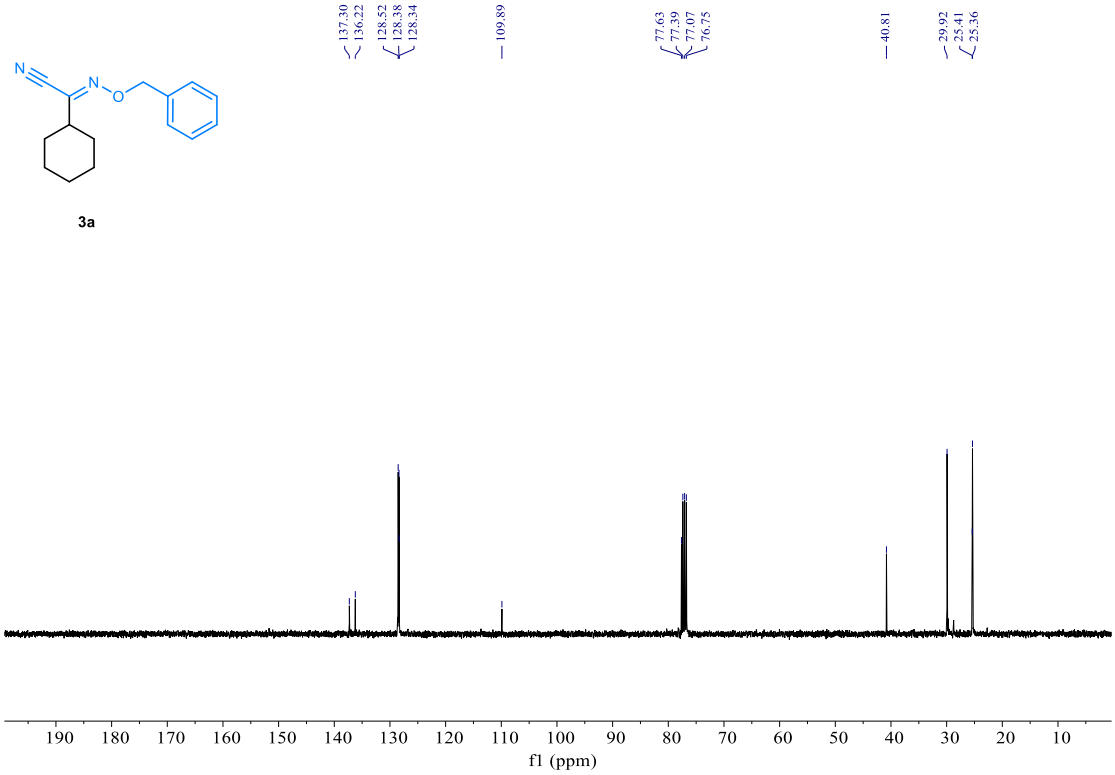
Yield: 41% (23.4 mg), colorless oil. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.45 – 7.35 (m, 5H), 5.38 (s, 0.72H), 5.27 (s, 1.28H), 3.51 (t, J = 12.3 Hz, 0.67H), 3.22 (t, J = 11.5 Hz, 0.33H), 2.21 – 2.01 (m, 2H), 1.95 – 1.73 (m, 3H), 1.64 – 1.40 (m, 3H), 1.36 – 1.23 (m, 2H).^{13}C NMR (101 MHz, $CDCl_3$) δ 144.2, 137.4, 136.4, 136.2, 132.0, 128.9, 128.7, 128.7, 128.6, 128.5, 113.8, 110.0, 78.3, 77.8, 40.9, 36.0, 30.0, 28.9, 25.5, 25.5, 25.4. IR (ATR): $\tilde{\nu}$ = 2961, 2920, 1753, 1454, 1258, 1081, 1014, 866, 792, 698 cm^{-1}. HRMS (ESI) exact mass calculated for [M+H^+] ($C_{15}H_{20}N_5O^+$): m/z 286.1662; found: 286.1661.

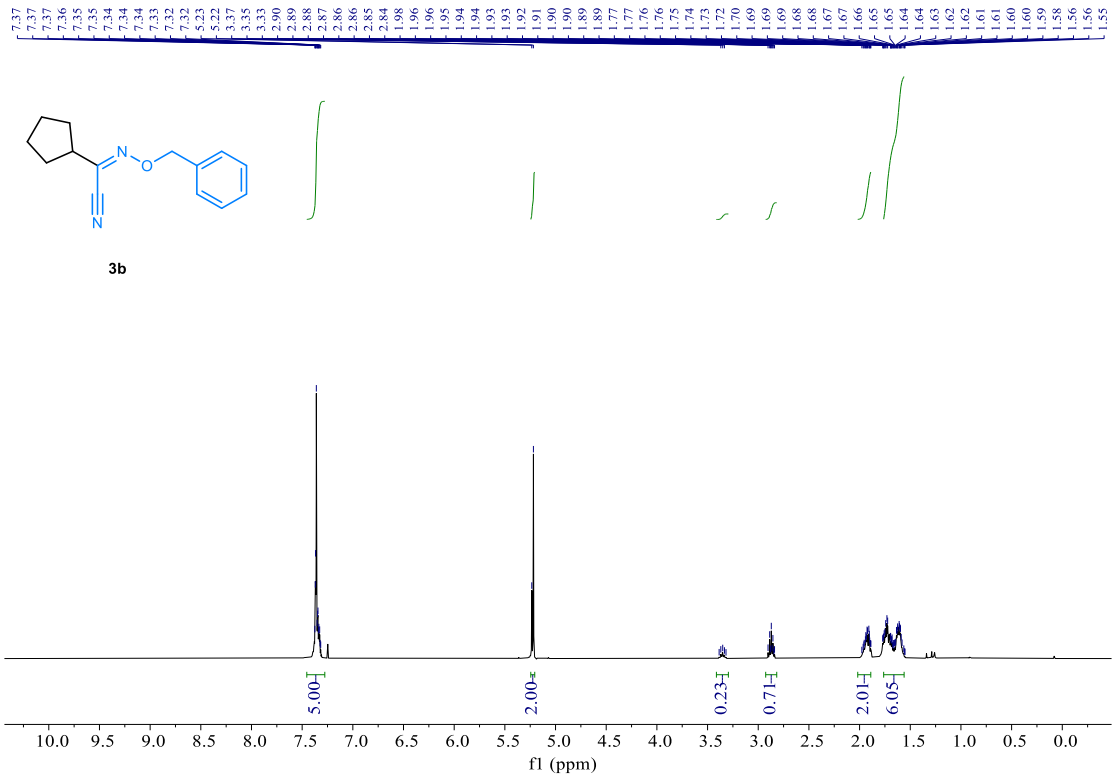
5. References

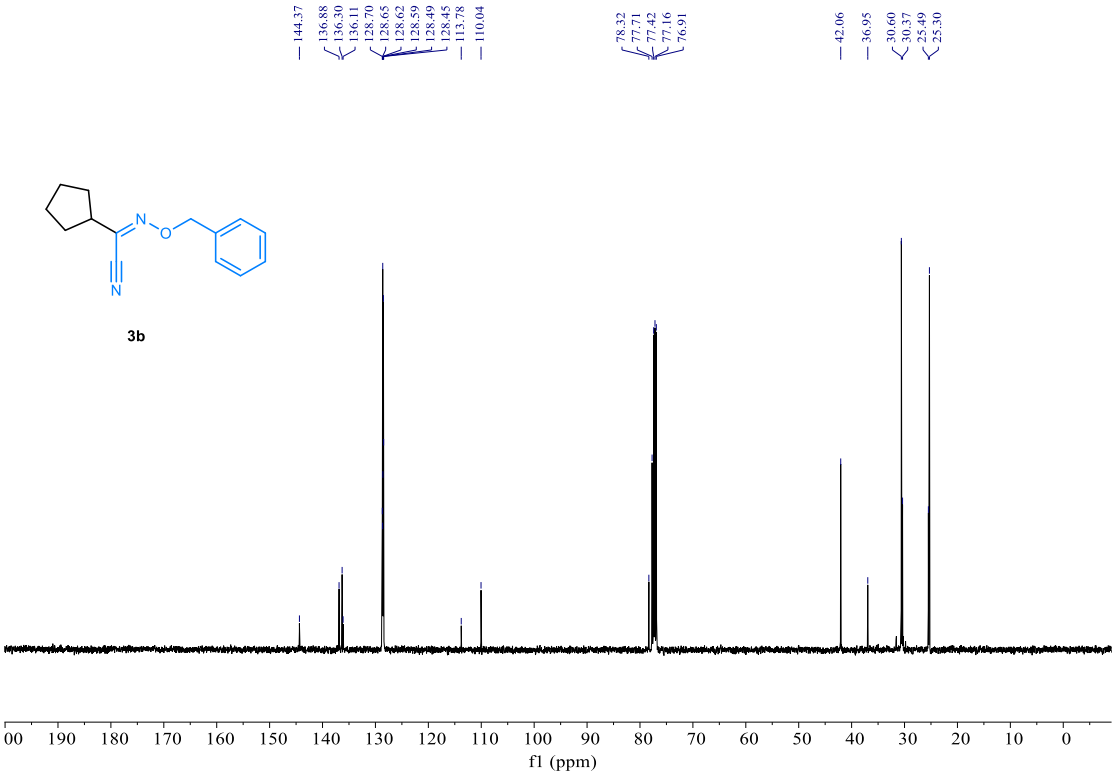
1 X. Wang, M. Yu, H. Song, Y. Liu and Q. Wang, *Org. Lett.*, 2021, **23**, 8353-8358.
2 J. Dey, N. Banerjee, S. Daw and J. Guin, *Angew. Chem. Int. Ed.* 2023, **62,** e20231238.
3 J. Dey, S. Paul, M. Bhakat and J. Guin, *Org. Lett.*, 2022, **24**, 8047-8051.
4 L.-J. Li, Y. Wei, Y.-L. Zhao, Y. Gao and X.-Q. Hu, *Org. Lett.*, 2024, **26**, 1110-1115.

6. NMR Spectrum






7.37 7.37 7.37 7.36 7.35 7.35 7.34 7.34 7.34 7.33 7.32 7.32 5.23 5.22 3.37 3.35 3.33 2.90 2.89 2.88 2.87 2.86 2.86 2.85 2.84 1.98 1.96 1.96 1.95 1.94 1.94 1.93 1.93 1.92 1.91 1.90 1.90 1.89 1.89 1.77 1.77 1.76 1.76 1.75 1.74 1.73 1.72 1.70 1.69 1.69 1.69 1.68 1.68 1.67 1.67 1.66 1.65 1.65 1.64 1.64 1.63 1.62 1.62 1.61 1.61 1.60 1.60 1.59 1.58 1.56 1.56 1.55
N
O
N
3b
5.00
2.00
0.23
0.71
2.01
6.05
10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)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136.88
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136.11
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128.45
113.78
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77.71
77.42
77.16
76.91
42.06
36.95
30.60
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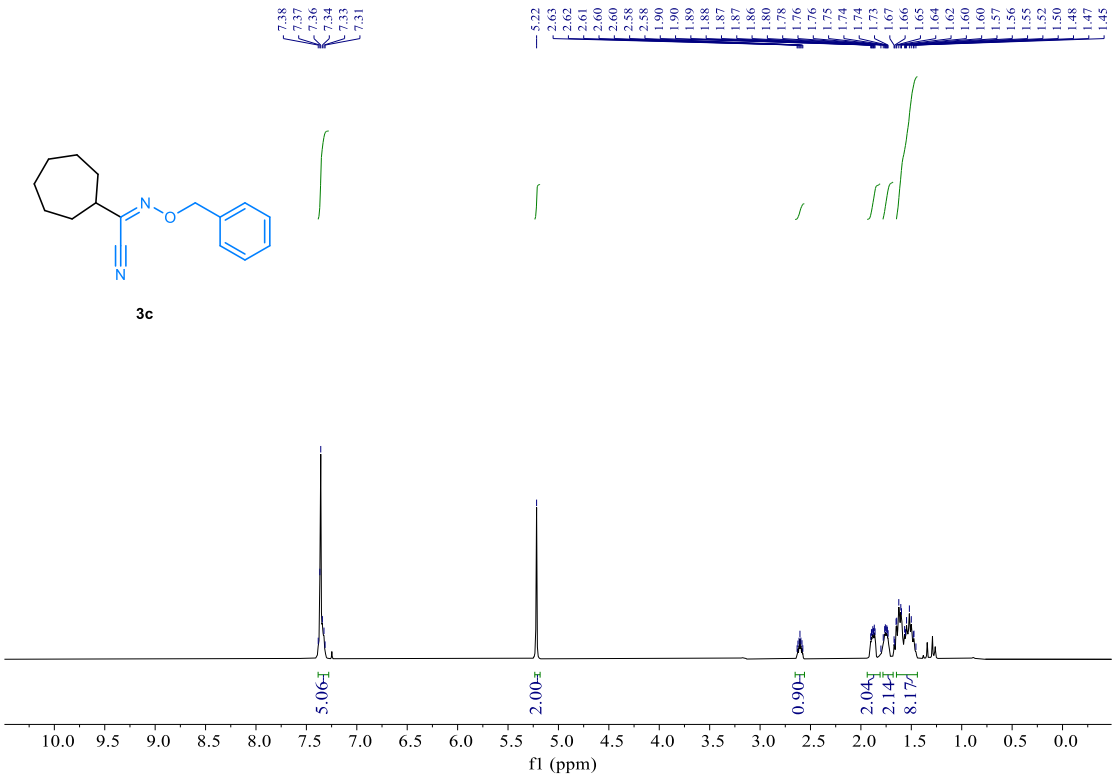
25.30
N
O
N
3b
00 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)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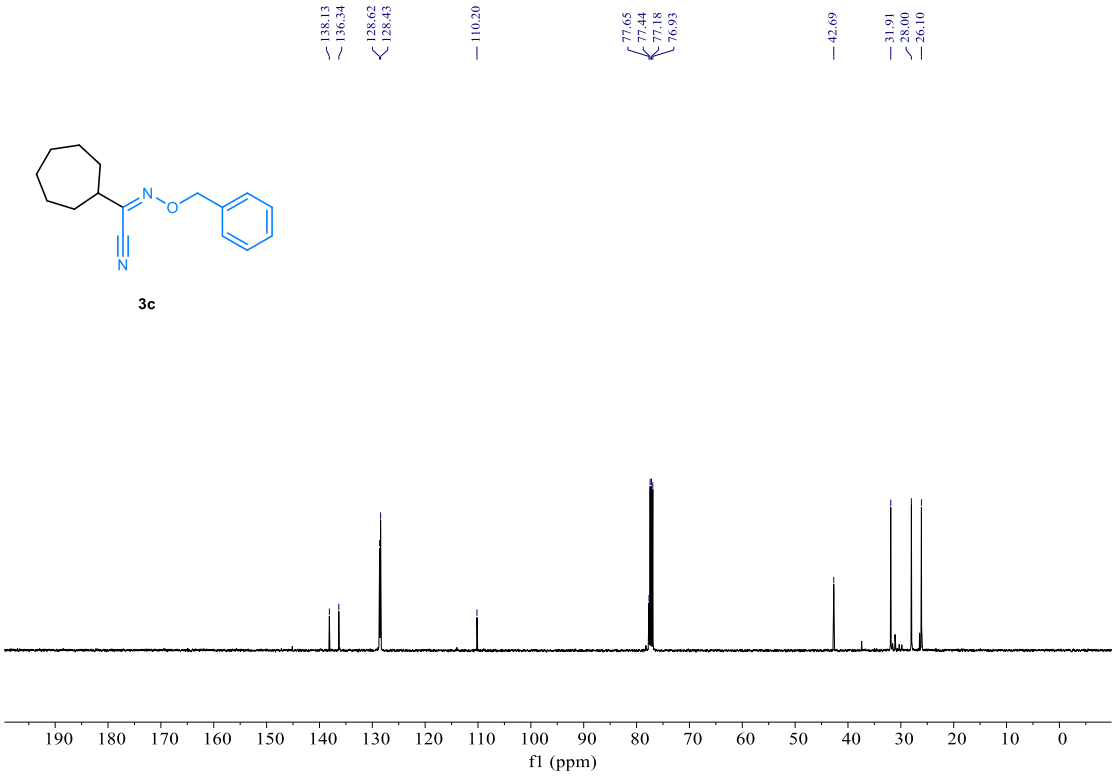
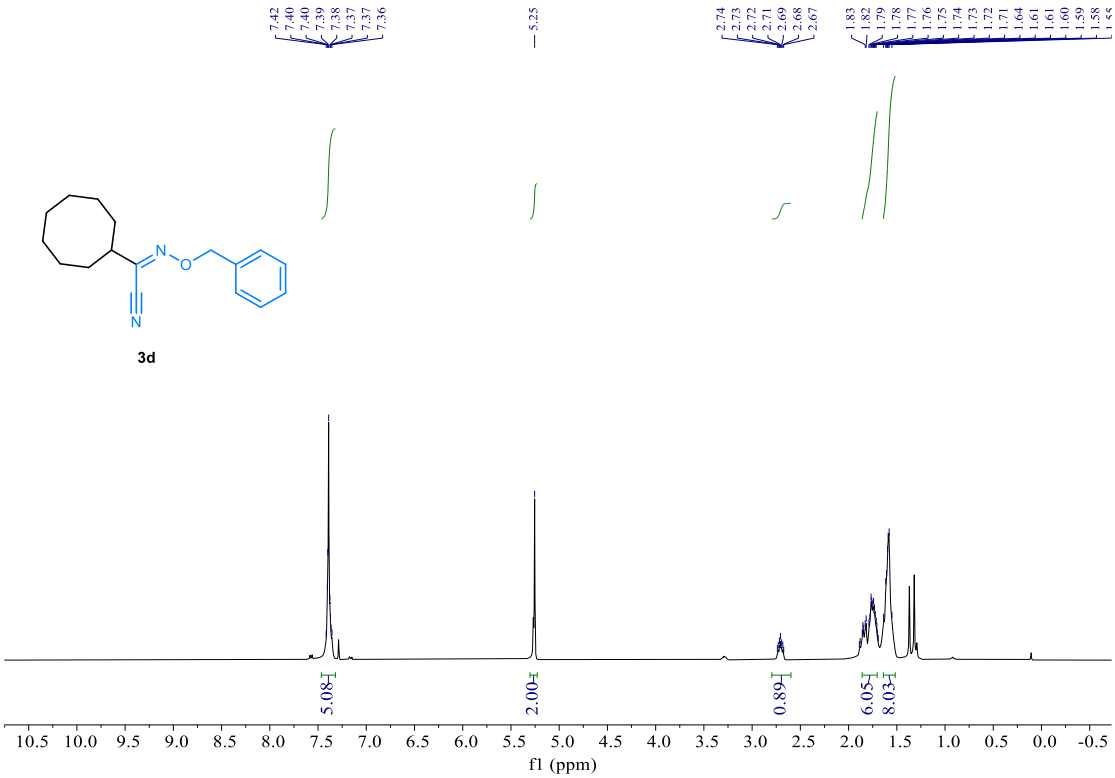
1.56
1.55
1.52
1.50
1.48
1.47
1.45
N
O
N
3c
5.06
2.00
0.90
2.04
2.14
8.17
10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)


138.13
136.34
128.62
128.43
110.20
77.65
77.44
77.18
76.93
42.69
31.91
28.00
26.10
N
O
N
3c
190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)


7.42
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7.40
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7.37
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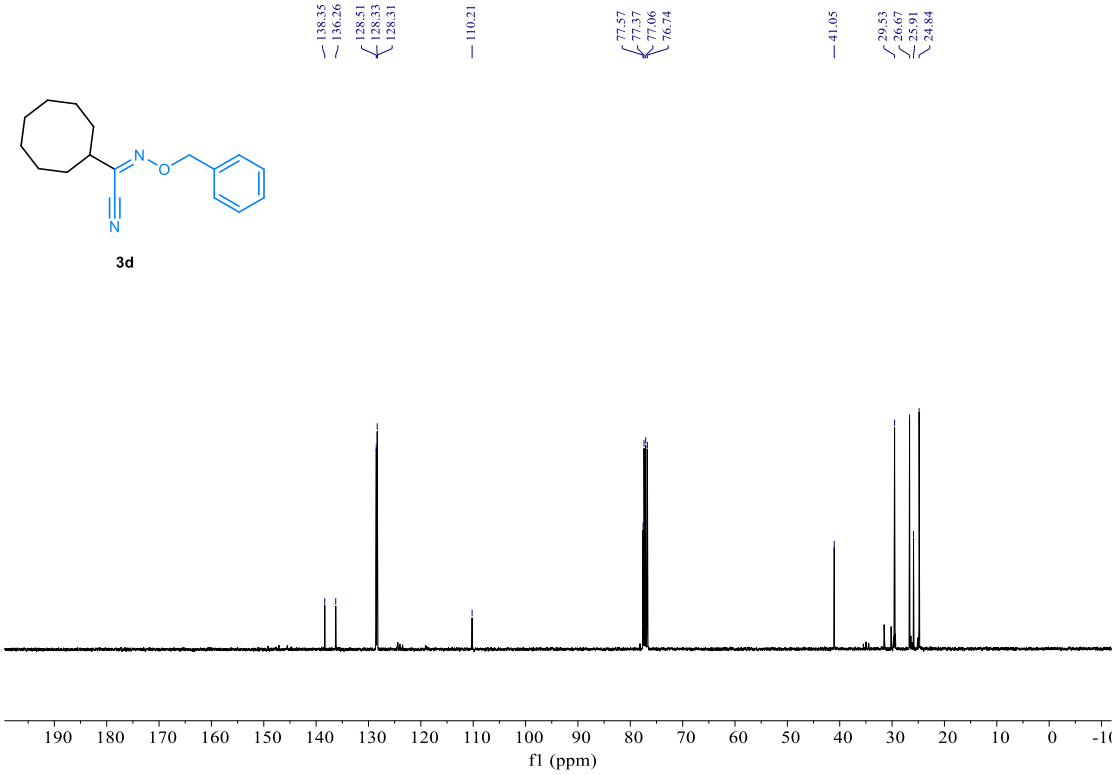
7.36
5.25
2.74
2.73
2.72
2.71
2.69
2.68
2.67
1.83
1.82
1.79
1.78
1.77
1.76
1.75
1.74
1.73
1.72
1.71
1.64
1.61
1.61
1.60
1.59
1.58
N
O
N
3d
5.08
2.00
0.89
6.05
8.03
10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5
f1 (ppm)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136.26
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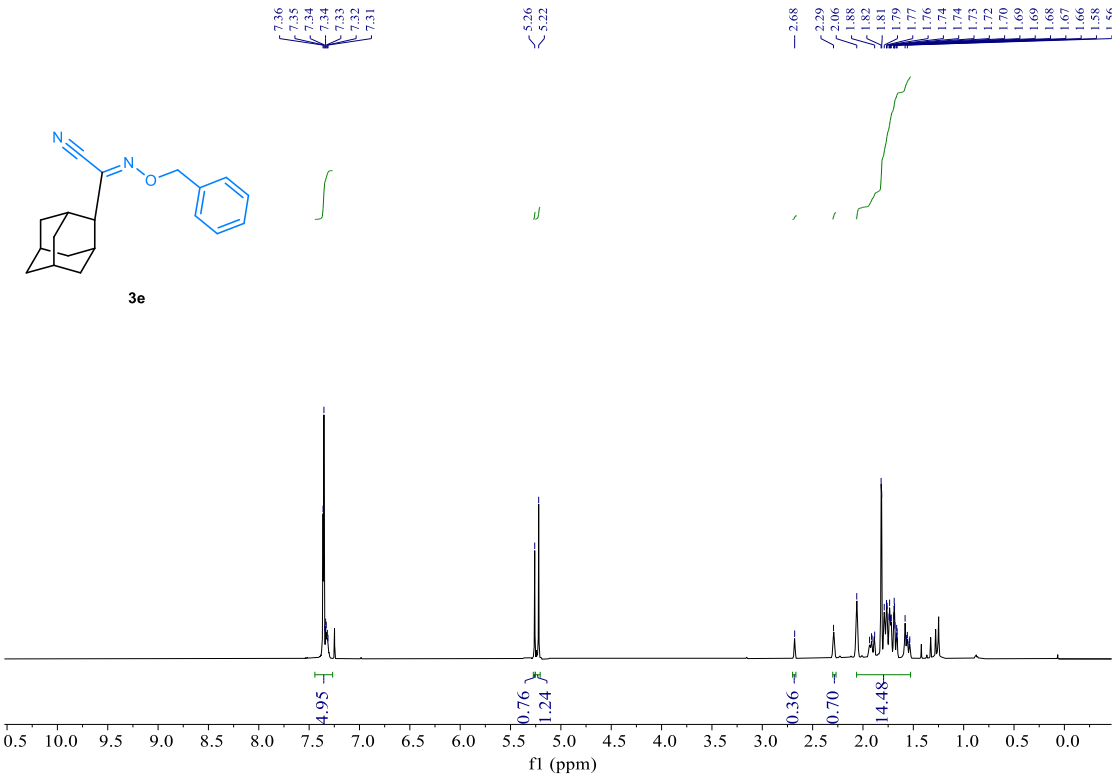
128.33
128.31
110.21
77.57
77.37
77.06
76.74
41.05
29.53
26.67
25.91
24.84
N
O
N
3d
190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -1
f1 (ppm)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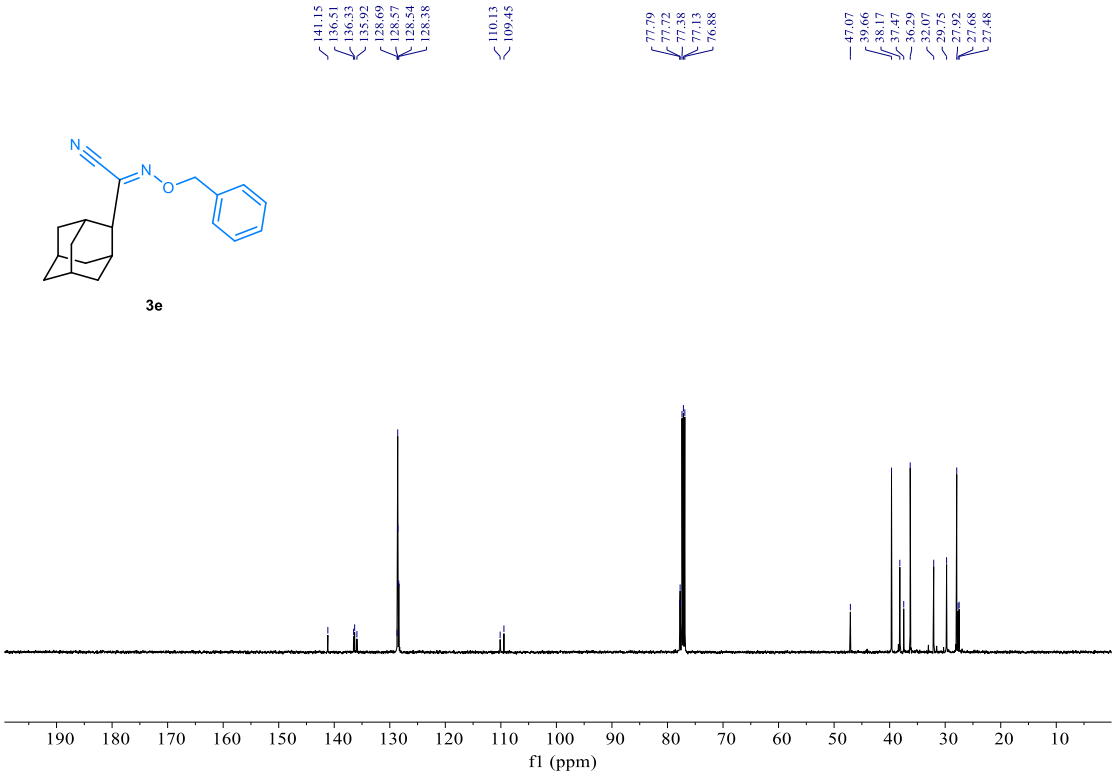
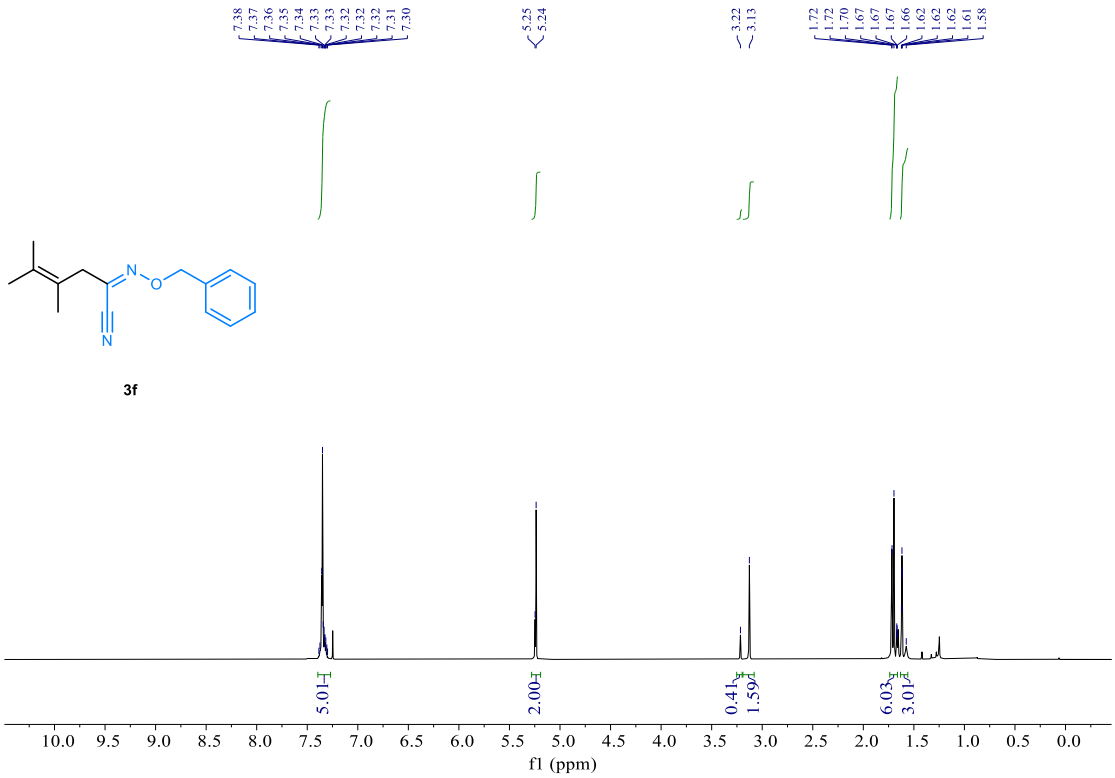
7.32
7.31
5.26
5.22
2.68
2.29
2.06
1.88
1.82
1.81
1.79
1.77
1.76
1.74
1.74
1.73
1.72
1.70
1.69
1.69
1.68
1.67
1.66
1.58
N
N
O
3e
4.95
0.76
1.24
0.36
0.70
14.48
0.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)


141.15
136.51
136.33
135.92
128.69
128.57
128.54
128.38
110.13
109.45
77.79
77.72
77.38
77.13
76.88
47.07
39.66
38.17
37.47
36.29
32.07
29.75
27.92
27.68
27.48
N
N
O
3e
190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10
f1 (ppm)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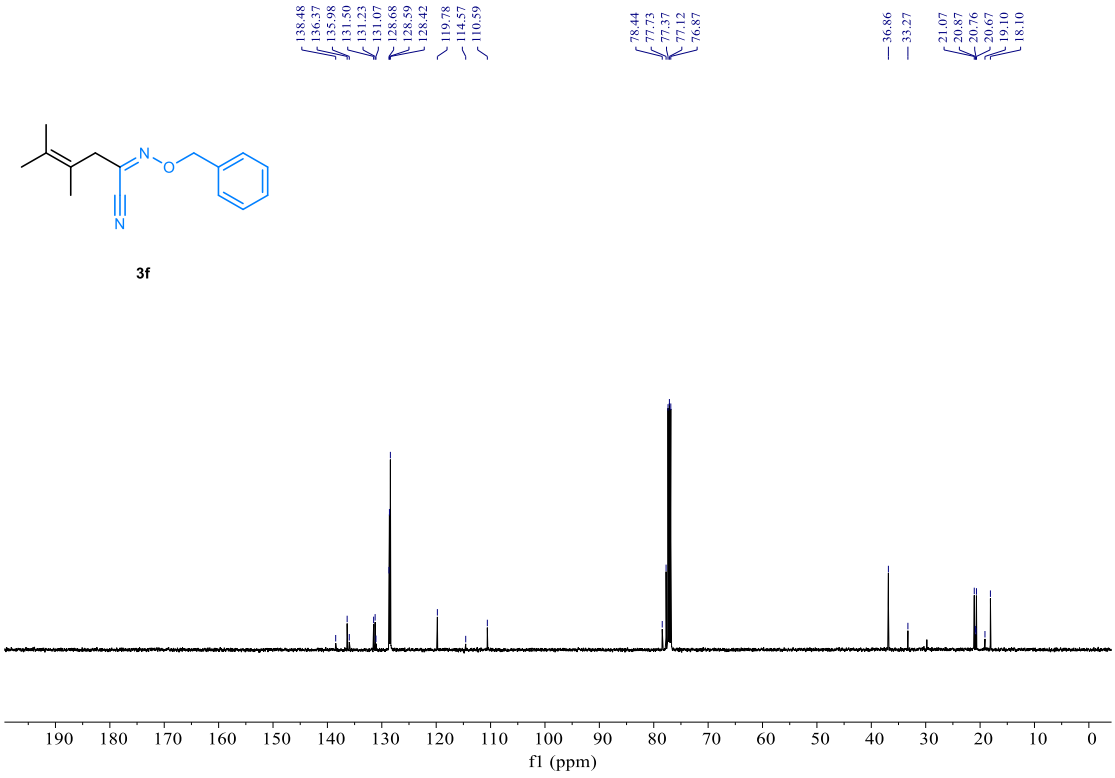
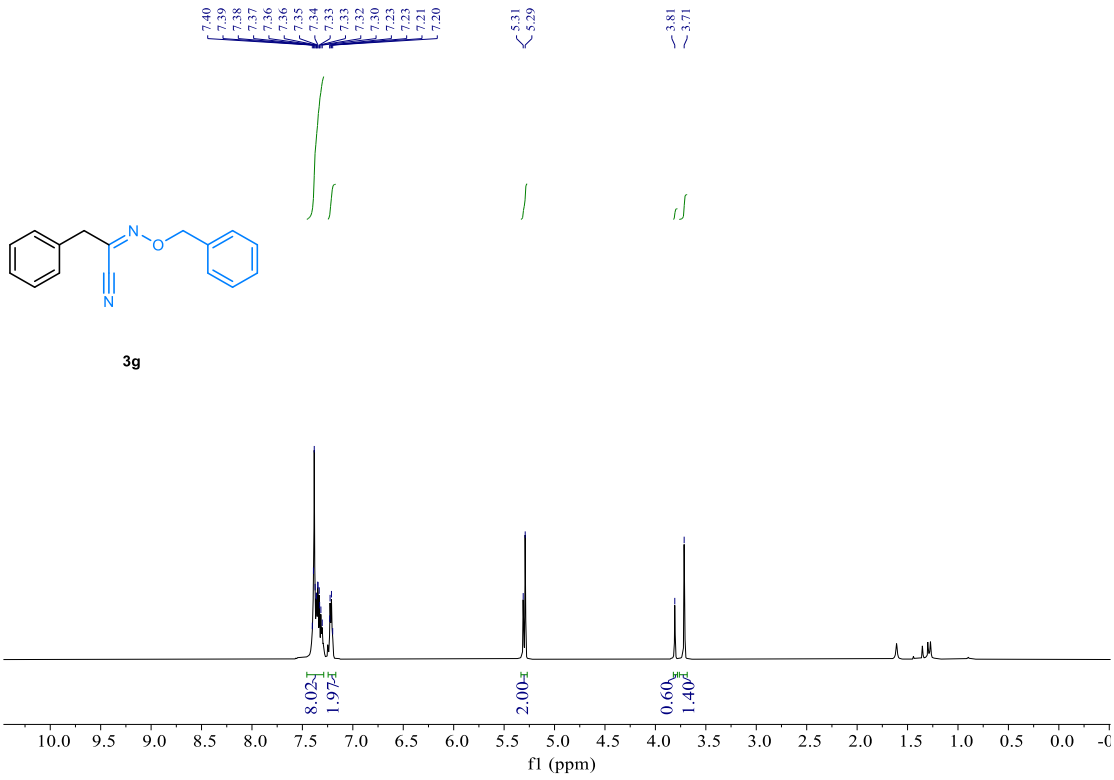
7.33
7.32
7.32
7.32
7.31
7.30
5.25
5.24
3.22
3.13
1.72
1.72
1.70
1.67
1.67
1.67
1.66
1.62
1.62
1.62
1.61
1.58
N
O
N
5.01
2.00
0.41
1.59
6.03
3.01
10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)

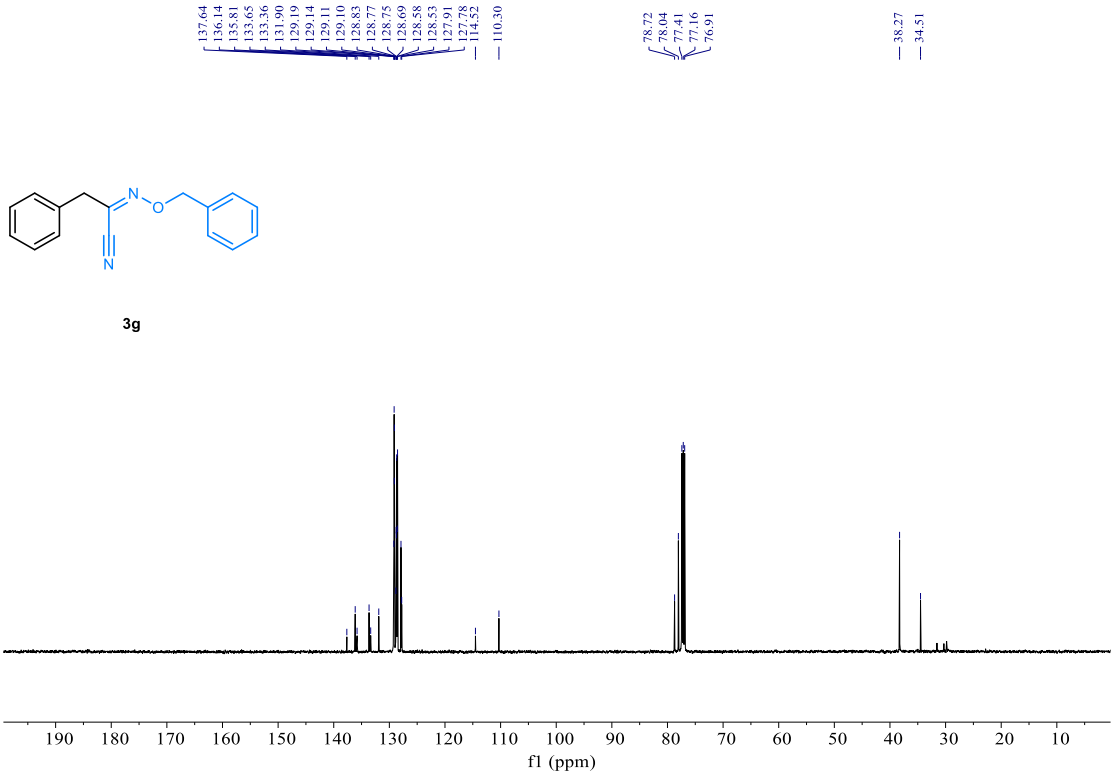
3f


138.48
136.37
135.98
131.50
131.23
131.07
128.68
128.59
128.42
119.78
114.57
110.59
78.44
77.73
77.37
77.12
76.87
36.86
33.27
21.07
20.87
20.76
20.67
19.10
18.10
N
O
N
190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)

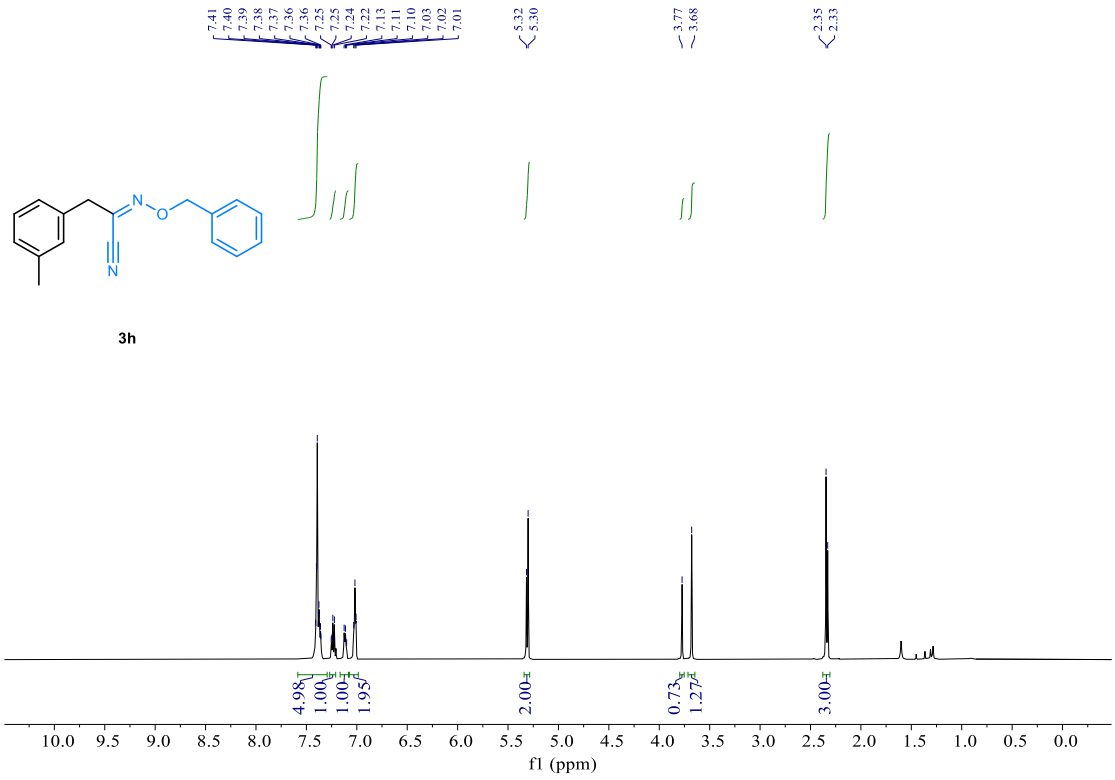
3f


7.40
7.39
7.38
7.37
7.36
7.36
7.35
7.34
7.33
7.33
7.32
7.30
7.23
7.23
7.21
7.20
5.31
5.29
3.81
3.71
N
O
N
8.02
1.97
2.00
0.60
1.40
10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)

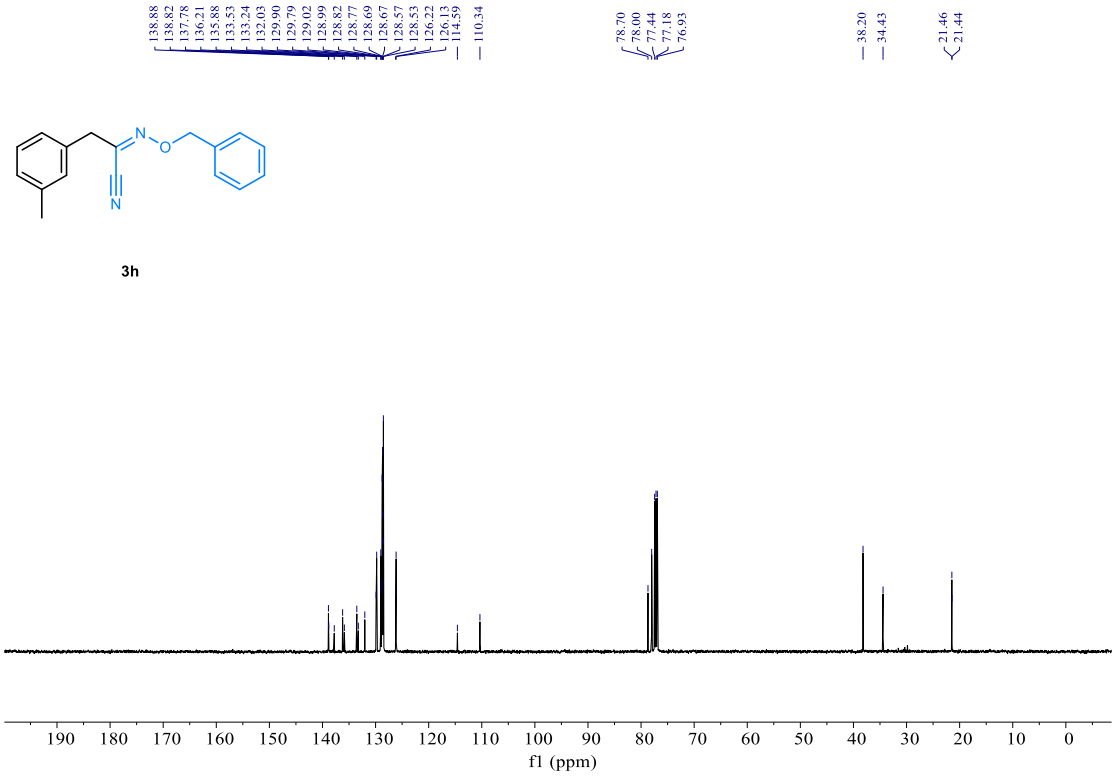
3g


137.64
136.14
135.81
133.65
133.36
131.90
129.19
129.14
129.11
129.10
128.83
128.77
128.75
128.69
128.58
128.53
127.91
127.78
114.52
110.30
78.72
78.04
77.41
77.16
76.91
38.27
34.51
N
O
N
190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10
f1 (ppm)

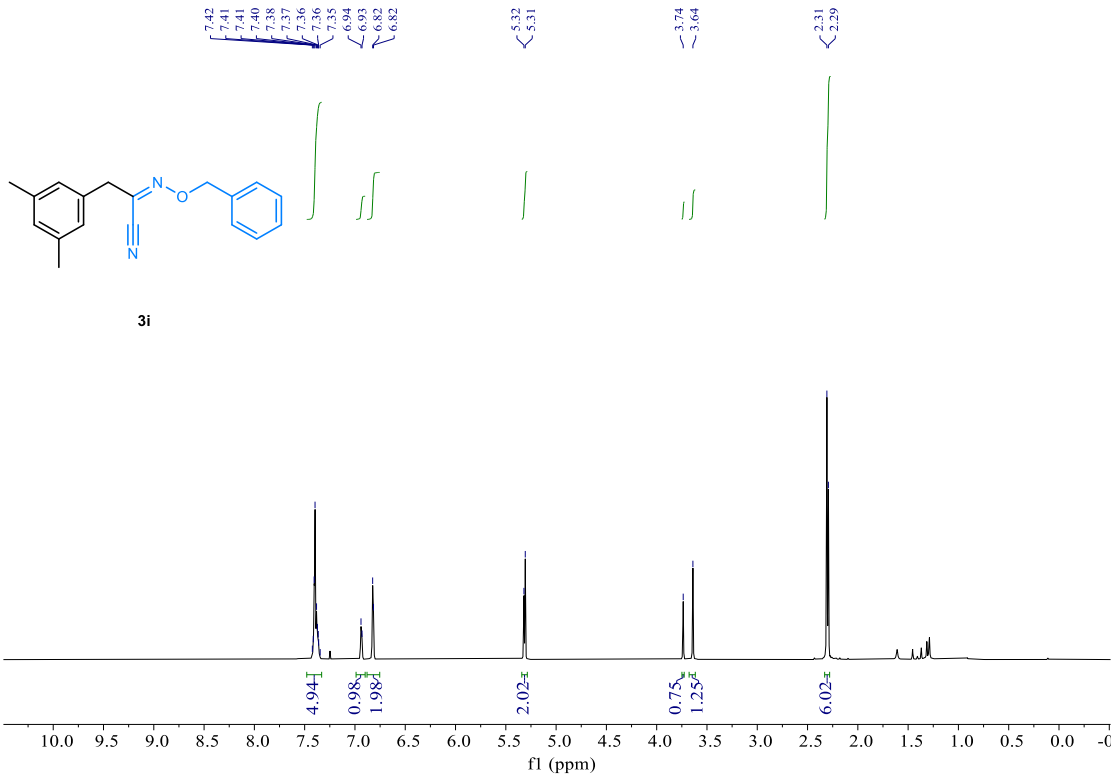
3g


7.41
7.40
7.39
7.38
7.37
7.36
7.36
7.25
7.25
7.24
7.22
7.13
7.11
7.10
7.03
7.02
7.01
5.32
5.30
3.77
3.68
2.35
2.33
N
O
N
4.98
1.00
1.00
1.95
2.00
0.73
1.27
3.00
10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)

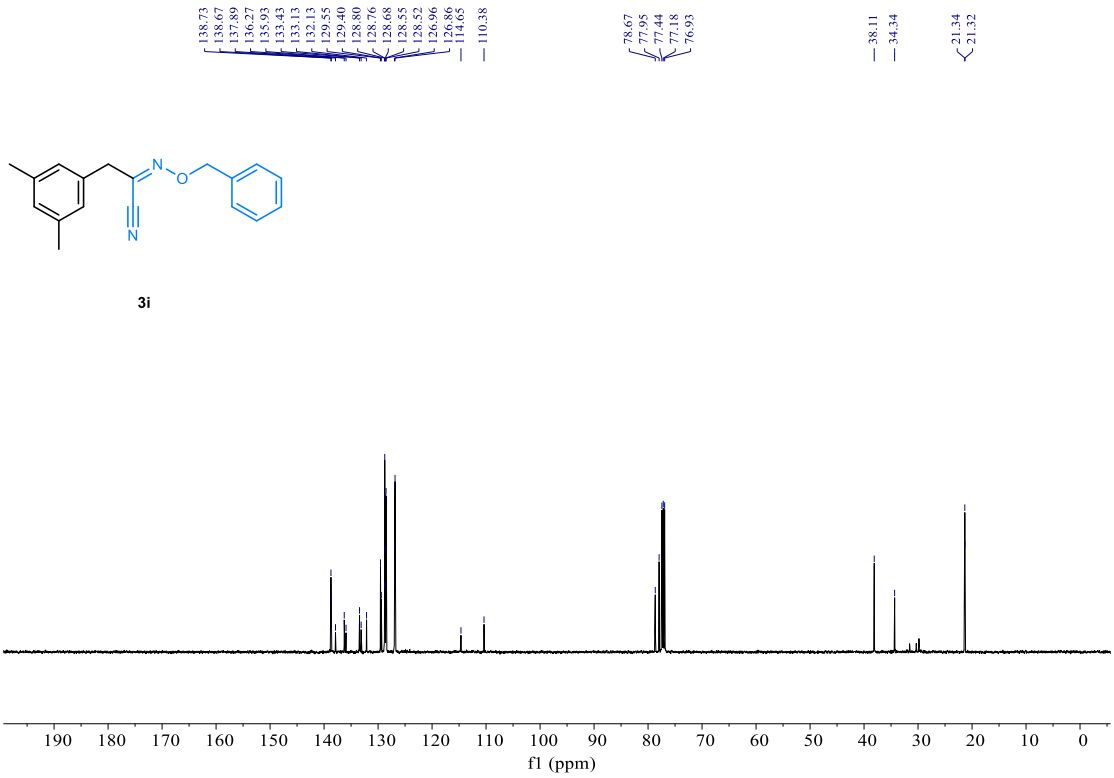
3h


138.88
138.82
137.78
136.21
135.88
133.53
133.24
132.03
129.90
129.79
129.02
128.99
128.82
128.77
128.69
128.67
128.57
128.53
126.22
126.13
114.59
110.34
78.70
78.00
77.44
77.18
76.93
38.20
34.43
21.46
21.44
N
O
N
190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)

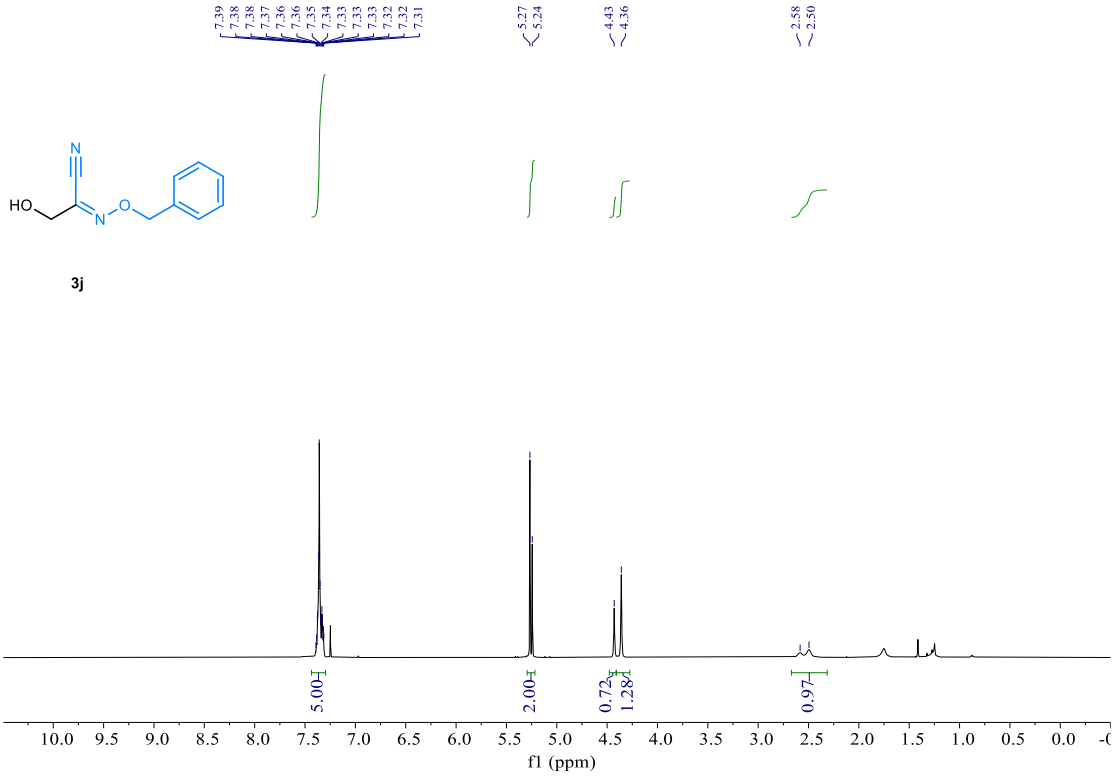
3h


7.42
7.41
7.41
7.40
7.38
7.37
7.36
7.36
7.35
6.94
6.93
6.82
6.82
5.32
5.31
3.74
3.64
2.31
2.29
N
O
N
4.94
0.98
1.98
2.02
0.75
1.25
6.02
10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)

3i


138.73
138.67
137.89
136.27
135.93
133.43
133.13
132.13
129.55
129.40
128.80
128.76
128.68
128.55
128.52
126.96
126.86
114.65
110.38
78.67
77.95
77.44
77.18
76.93
38.11
34.34
21.34
21.32
N
O
N
190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)

3i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7.38
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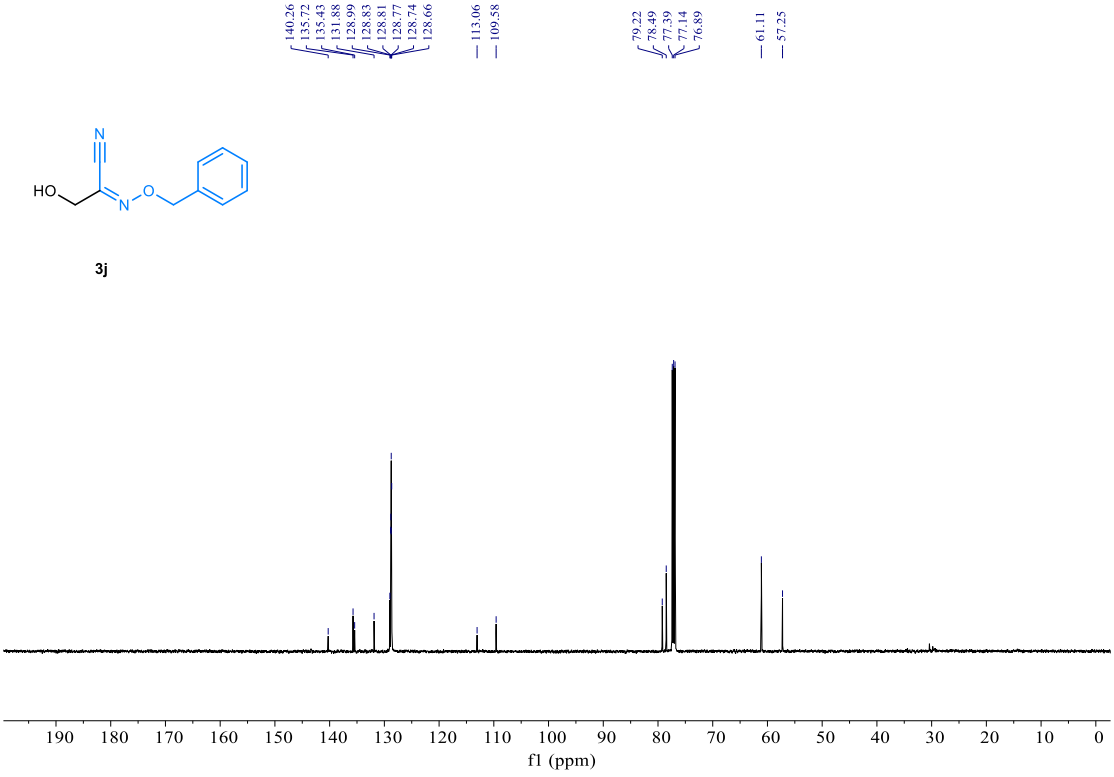
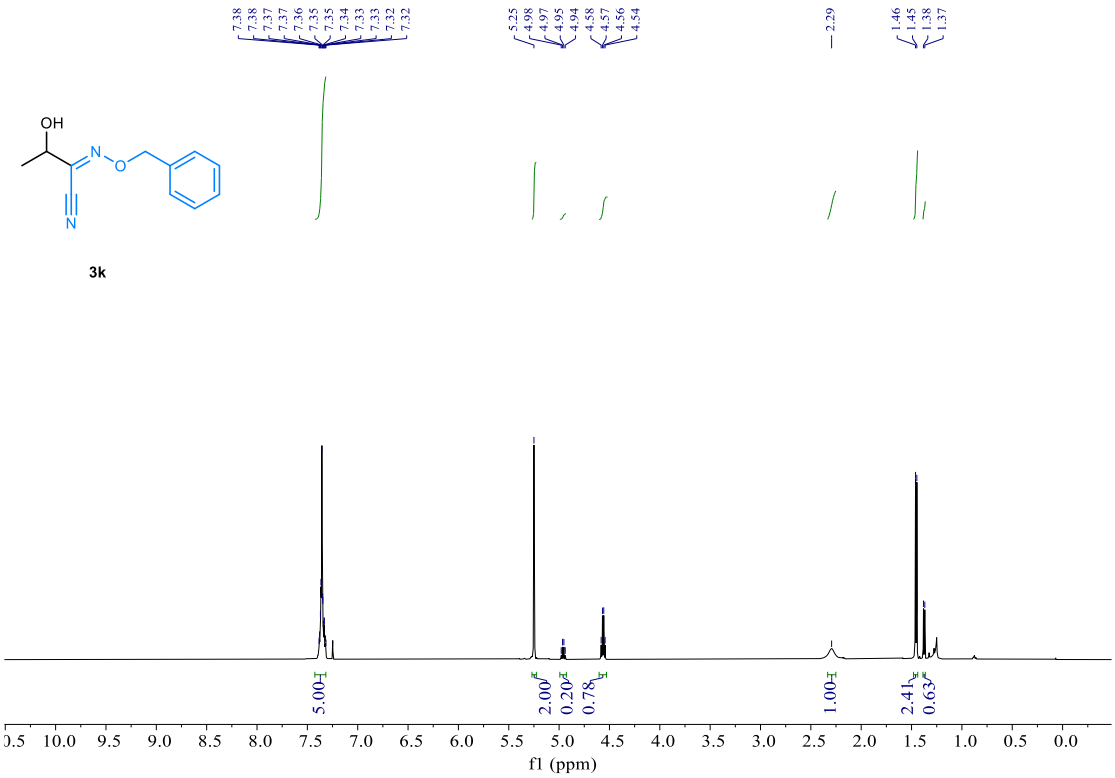
7.36
7.36
7.35
7.34
7.33
7.33
7.33
7.32
7.32
7.31
5.27
5.24
4.43
4.36
2.58
2.50
N
HO
N
O
5.00
2.00
0.72
1.28
0.97
10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)

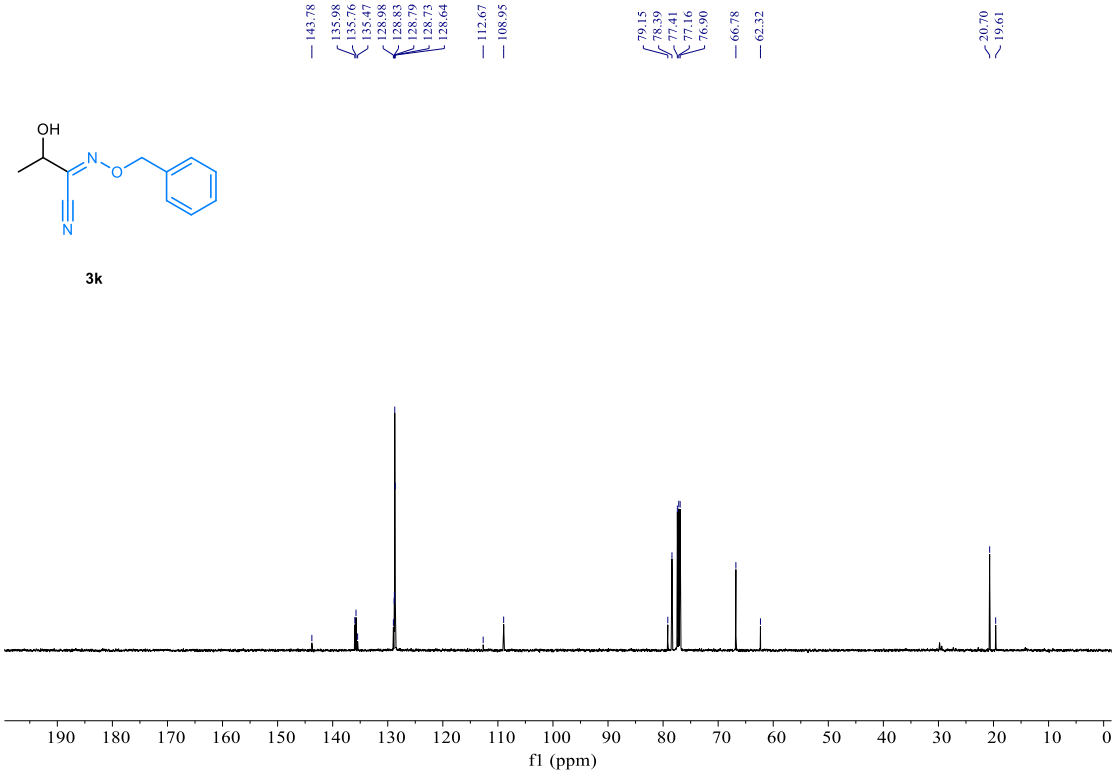
3j


140.26
135.72
135.43
131.88
128.99
128.83
128.81
128.77
128.74
128.66
113.06
109.58
79.22
78.49
77.39
77.14
76.89
61.11
57.25
N
HO
N
O
190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)

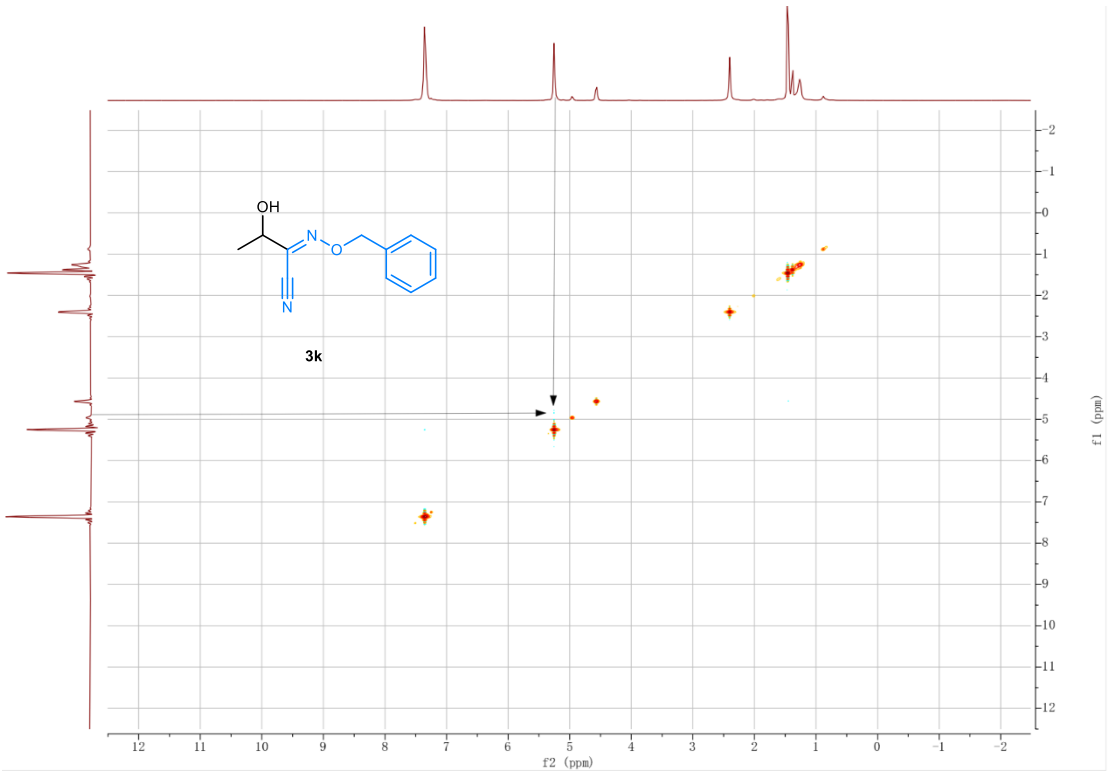
3j

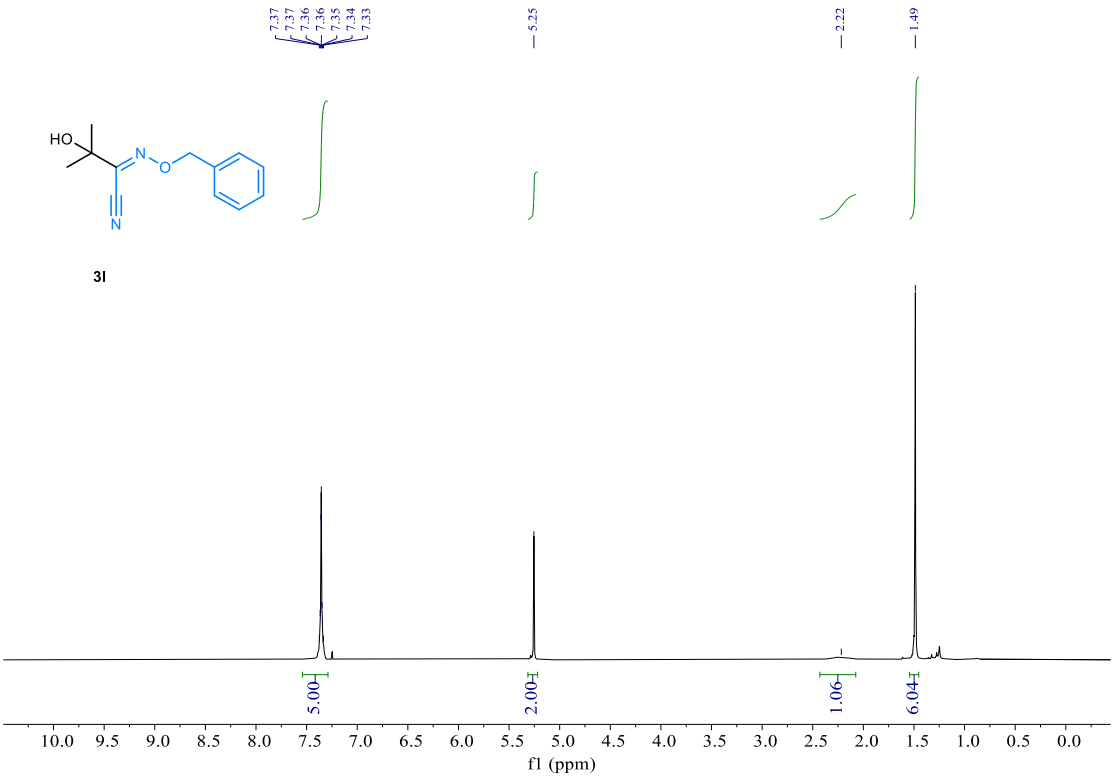

7.38
7.38
7.37
7.37
7.37
7.36
7.35
7.35
7.34
7.33
7.33
7.32
7.32
5.25
4.98
4.97
4.95
4.94
4.58
4.57
4.56
4.54
2.29
1.46
1.45
1.38
1.37
OH
N
O
N
5.00
2.00
0.20
0.78
1.00
2.41
0.63
f1 (ppm)

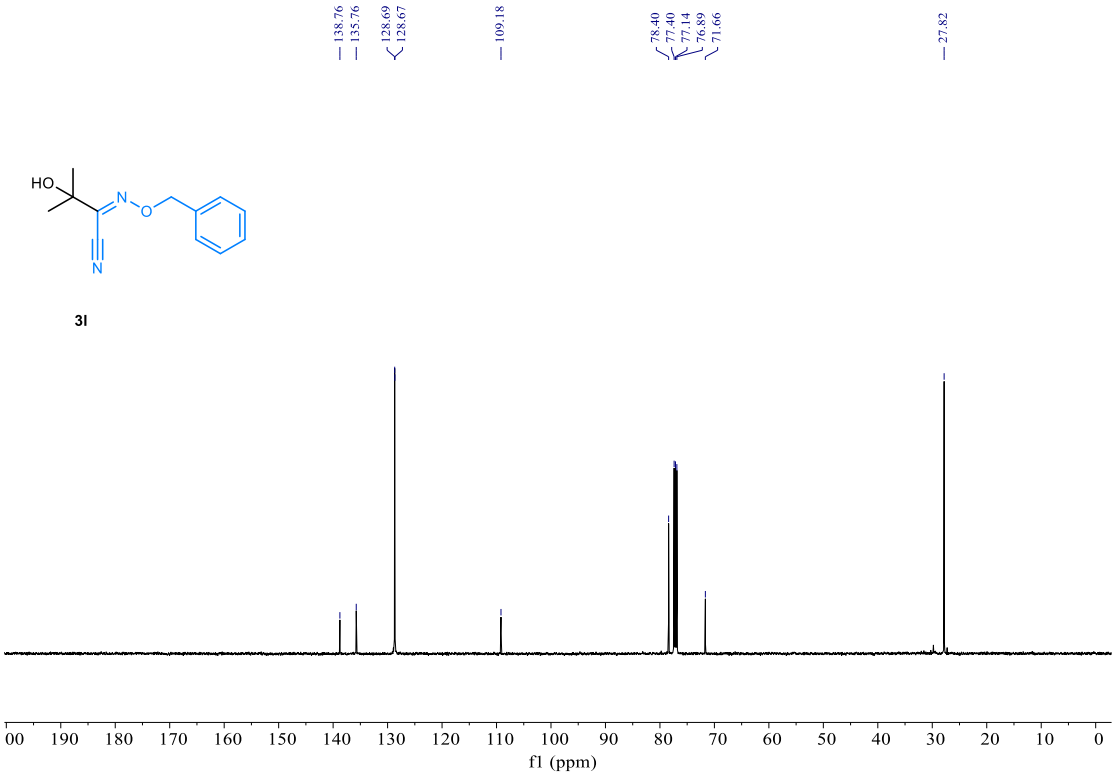
3k

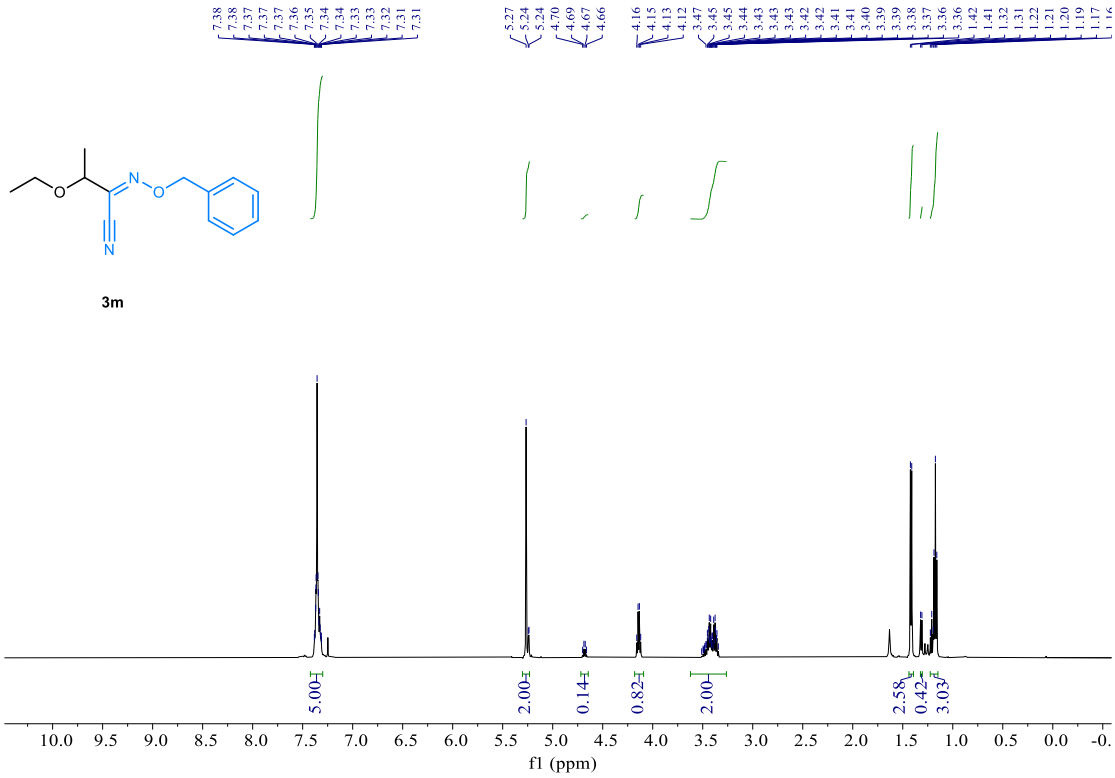

143.78
135.98
135.76
135.47
128.98
128.83
128.79
128.73
128.64
112.67
108.95
79.15
78.39
77.41
77.16
76.90
66.78
62.32
20.70
19.61
OH
N
O
N
f1 (ppm)

3k


OH
N
O
N
3k
f2 (ppm)
f1 (ppm)


7.37
7.37
7.36
7.36
7.35
7.34
7.33
5.25
2.22
1.49
HO
N
O
N
3l
5.00
2.00
1.06
6.04
f1 (ppm)


138.76
135.76
128.69
128.67
109.18
78.40
77.40
77.14
76.89
71.66
27.82
HO
N
O
N
3l
f1 (ppm)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7.38
7.37
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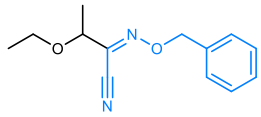
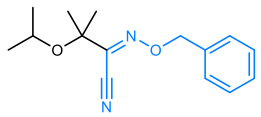
7.36
7.35
7.34
7.34
7.33
7.33
7.32
7.31
7.31
5.27
5.24
5.24
4.70
4.69
4.67
4.66
4.16
4.15
4.13
4.12
3.47
3.45
3.45
3.44
3.43
3.43
3.43
3.42
3.42
3.41
3.41
3.40
3.39
3.39
3.38
3.37
3.36
3.36
1.42
1.41
1.32
1.31
1.22
1.21
1.20
1.19
1.17
O
N
O
N
3m
5.00
2.00
0.14
0.82
2.00
2.58
0.42
3.03
f1 (ppm)



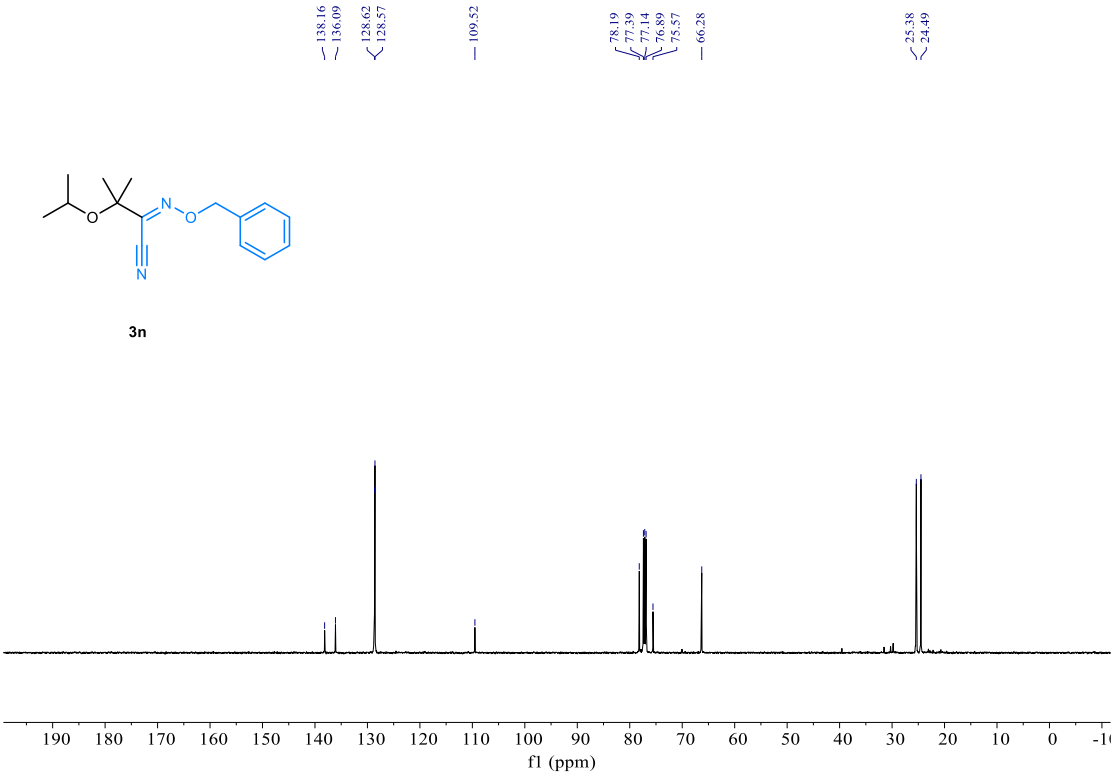
3m

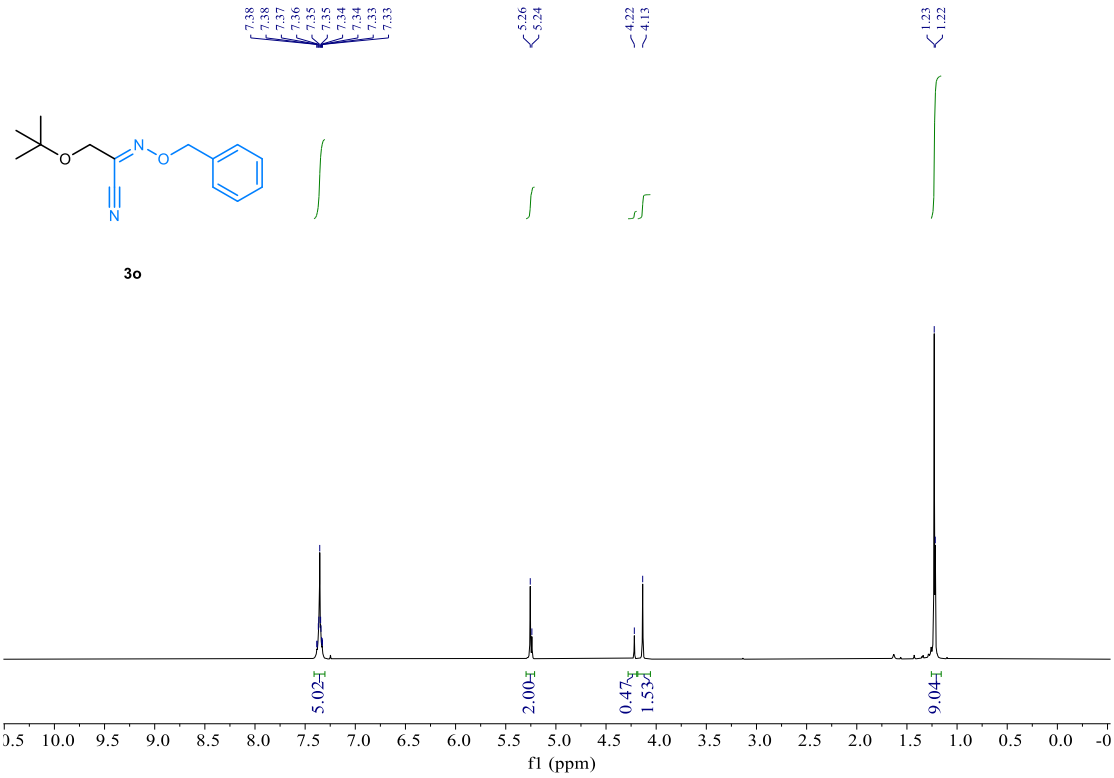
143.64
135.86
135.64
135.26
128.86
128.77
128.67
128.63
128.51
112.64
108.75
78.93
78.29
77.39
77.36
77.14
76.89
73.45
68.81
65.77
64.74
19.15
17.95
15.15
15.12
f1 (ppm)

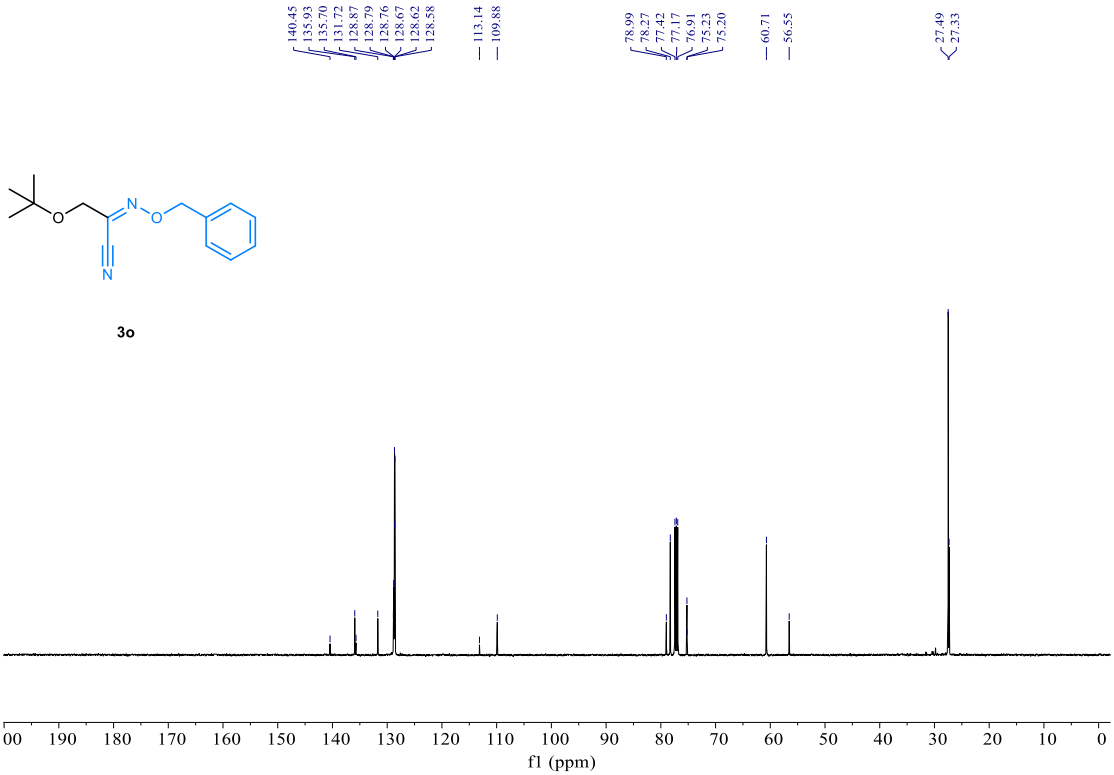


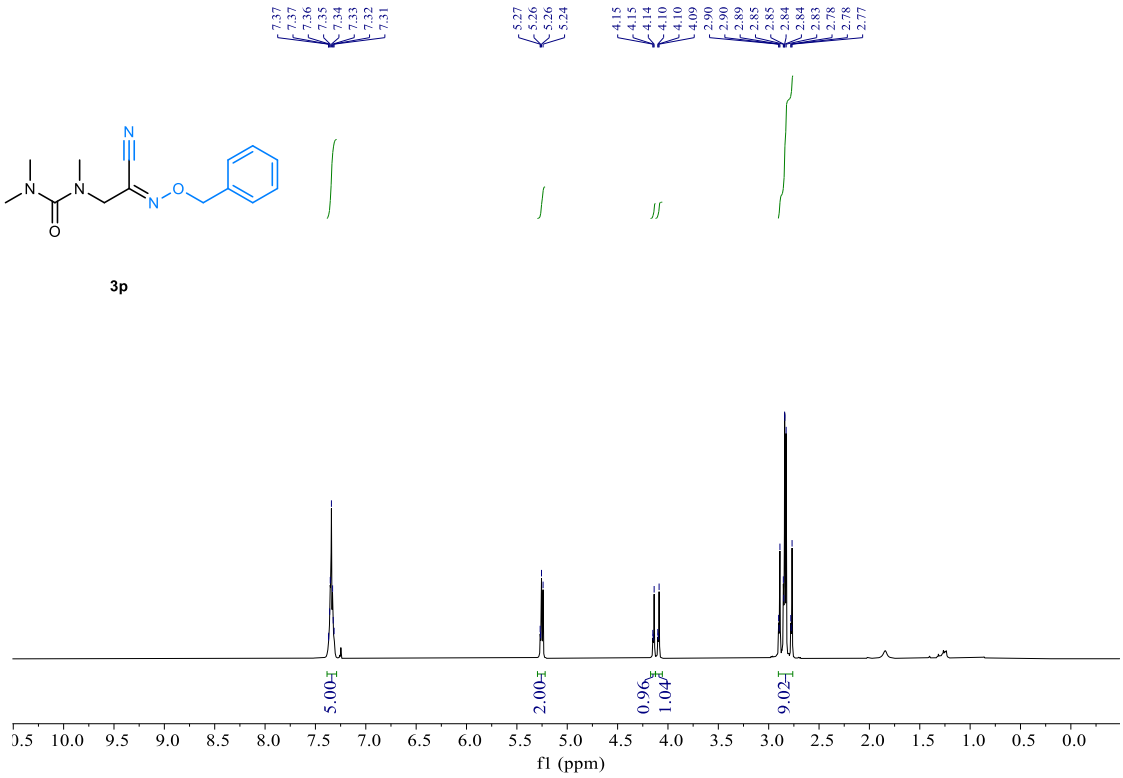
3n

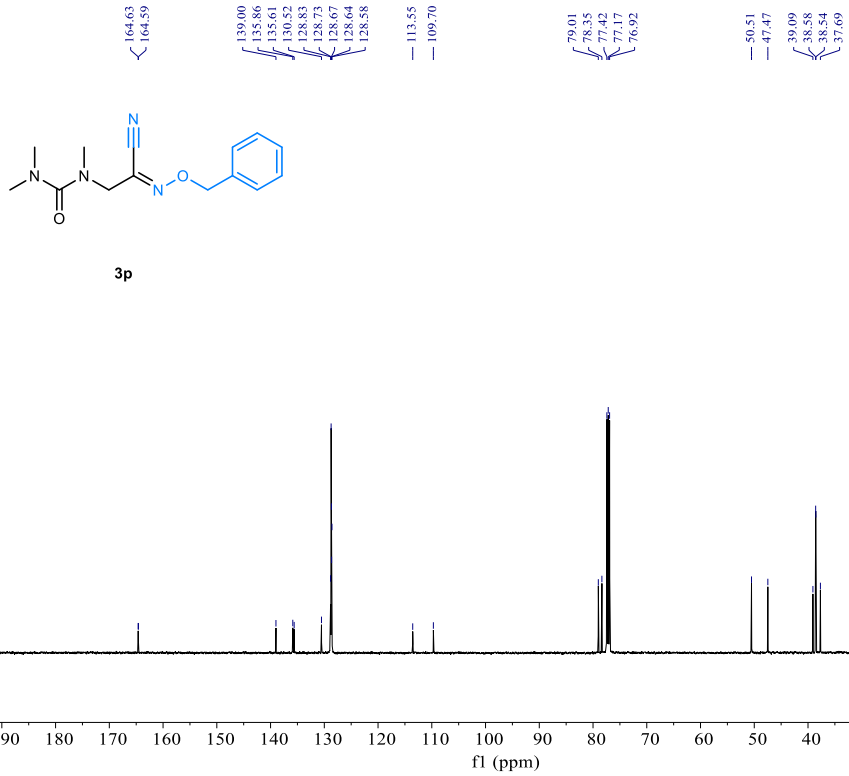
7.38
7.36
7.35
7.34
7.34
7.33
7.33
7.32
7.32
7.31
5.27
3.60
3.59
3.57
3.56
3.55
3.54
3.52
1.42
1.09
1.07
5.03
2.00
0.97
6.02
6.00
f1 (ppm)


138.16
136.09
128.62
128.57
109.52
78.19
77.39
77.14
76.89
75.57
66.28
25.38
24.49
3n
190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)

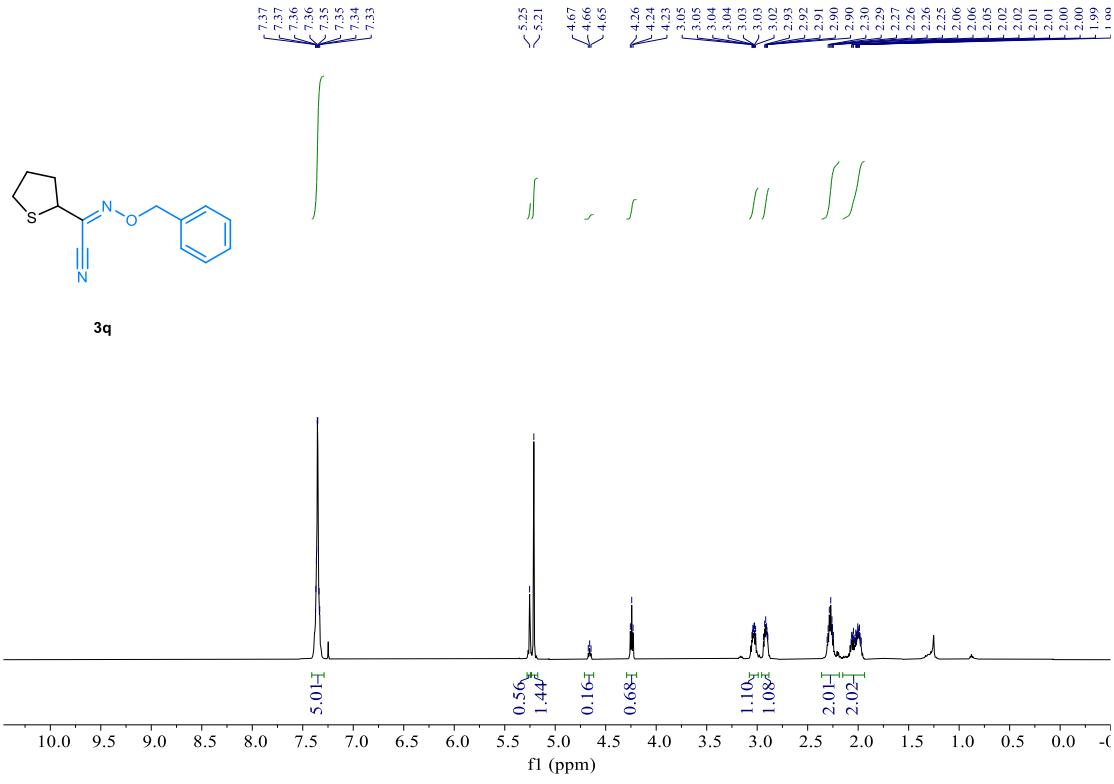

7.38
7.38
7.37
7.36
7.35
7.35
7.34
7.34
7.33
7.33
5.26
5.24
4.22
4.13
1.23
1.22
3o
5.02
2.00
0.47
1.53
9.04
10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)


140.45
135.93
135.70
131.72
128.87
128.79
128.76
128.67
128.62
128.58
113.14
109.88
78.99
78.27
77.42
77.17
76.91
75.23
75.20
60.71
56.55
27.49
27.33
O
N
O
N
3o
00 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)

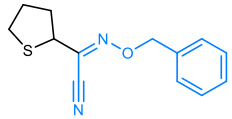

7.37
7.37
7.36
7.35
7.34
7.33
7.32
7.31
5.27
5.26
5.26
5.24
4.15
4.15
4.14
4.10
4.10
4.09
2.90
2.90
2.89
2.85
2.85
2.84
2.84
2.83
2.78
2.78
2.77
N
N
N
O
N
O
3p
5.00
2.00
0.96
1.04
9.02
0.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)


164.63
164.59
139.00
135.86
135.61
130.52
128.83
128.73
128.67
128.64
128.58
113.55
109.70
79.01
78.35
77.42
77.17
76.92
50.51
47.47
39.09
38.58
38.54
37.69
N
N
N
O
N
O
f1 (ppm)

3p

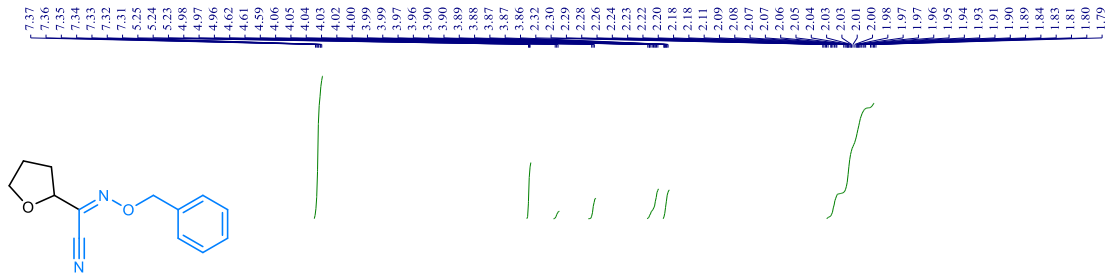

7.37
7.37
7.36
7.36
7.35
7.35
7.34
7.33
5.25
5.21
4.67
4.66
4.65
4.26
4.24
4.23
3.05
3.05
3.04
3.04
3.03
3.03
3.02
2.93
2.92
2.91
2.90
2.90
2.30
2.29
2.27
2.26
2.26
2.25
2.06
2.06
2.05
2.02
2.02
2.01
2.01
2.00
2.00
1.99
S
N
O
N
5.01
0.56
1.44
0.16
0.68
1.10
1.08
2.01
2.02
f1 (ppm)

3q

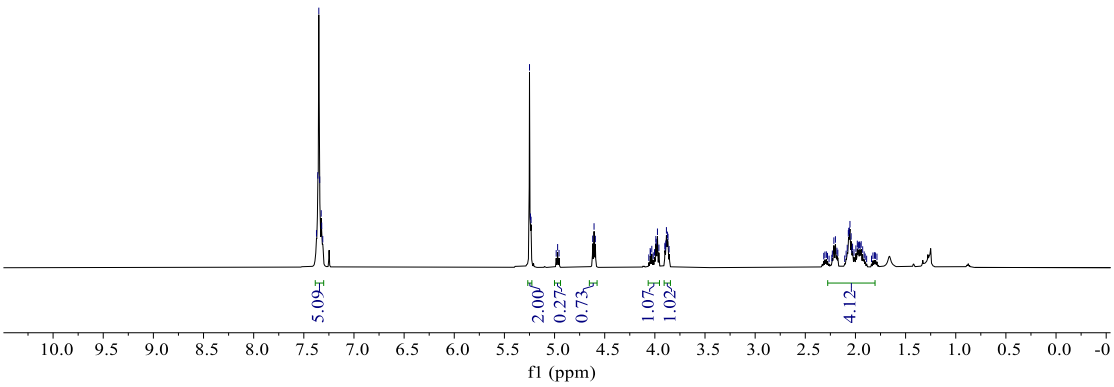


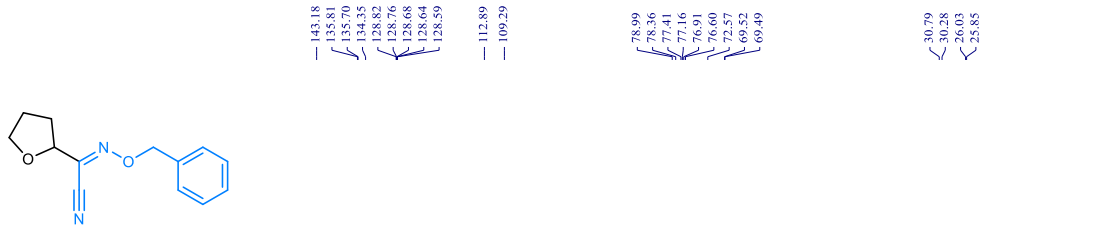
3q

141.89
135.92
135.69
135.05
128.79
128.73
128.67
128.64
128.59
128.55
113.31
109.44
78.81
78.14
77.40
77.14
76.89
47.58
45.86
40.84
35.03
33.90
31.21
190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)

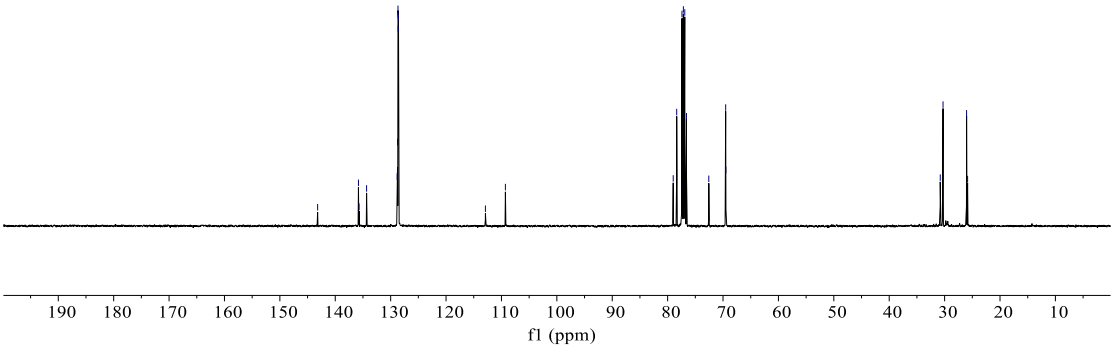


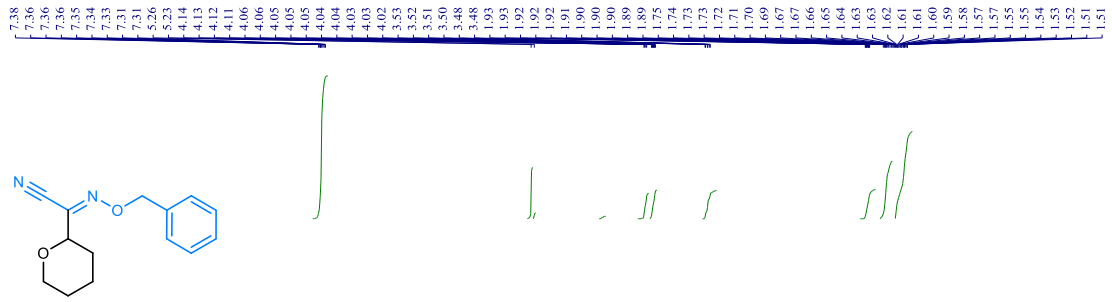
3r


5.09
2.00
0.27
0.73
1.07
1.02
4.12
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)

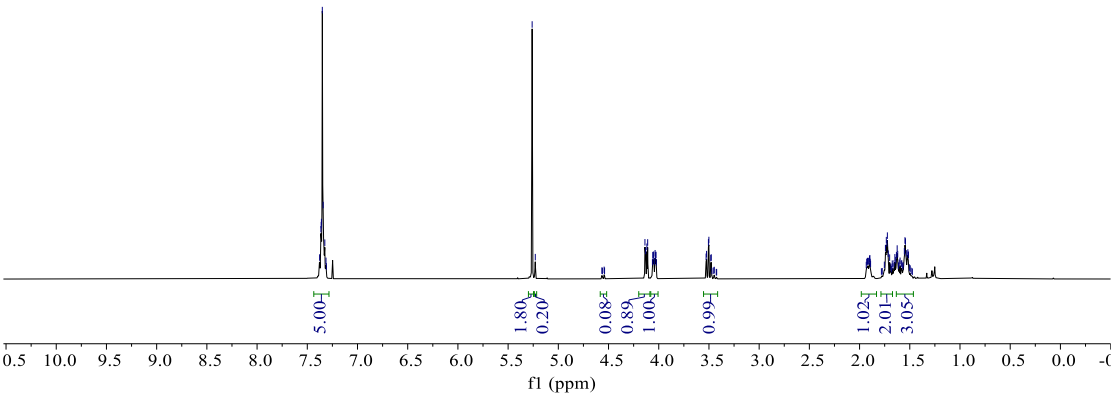

143.18
135.81
135.70
134.35
128.82
128.76
128.68
128.64
128.59
112.89
109.29
78.99
78.36
77.41
77.16
76.91
76.60
72.57
69.52
69.49
30.79
30.28
26.03
25.85

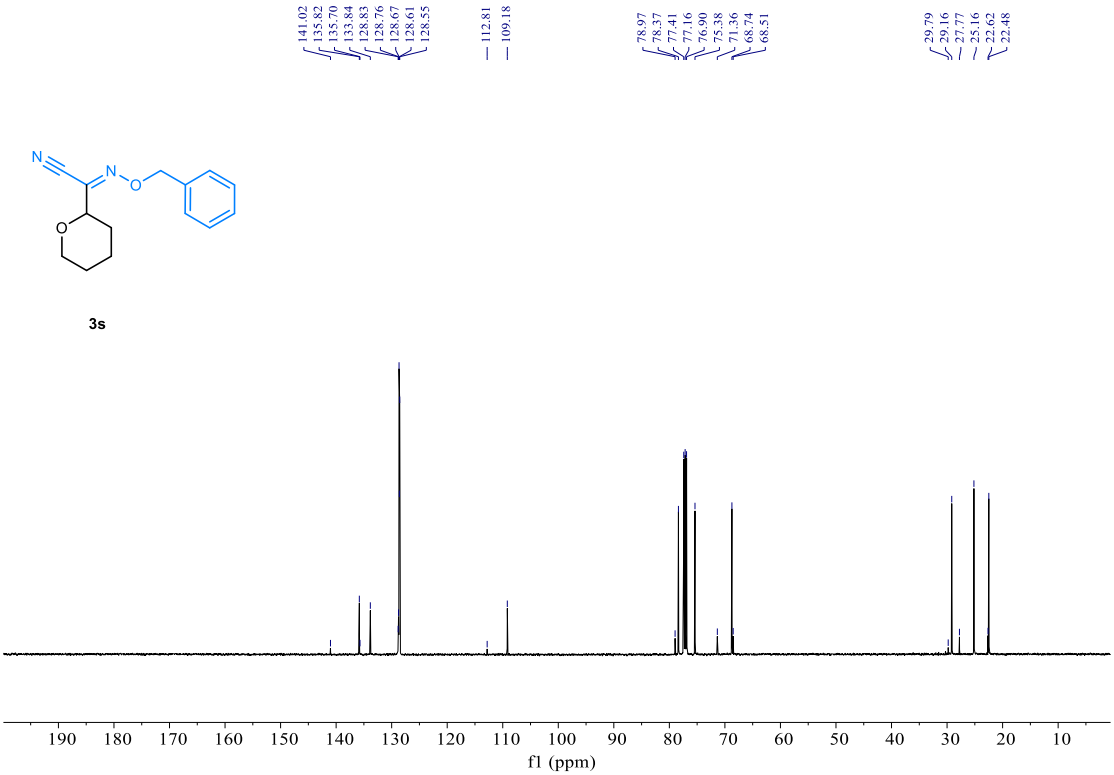
3r

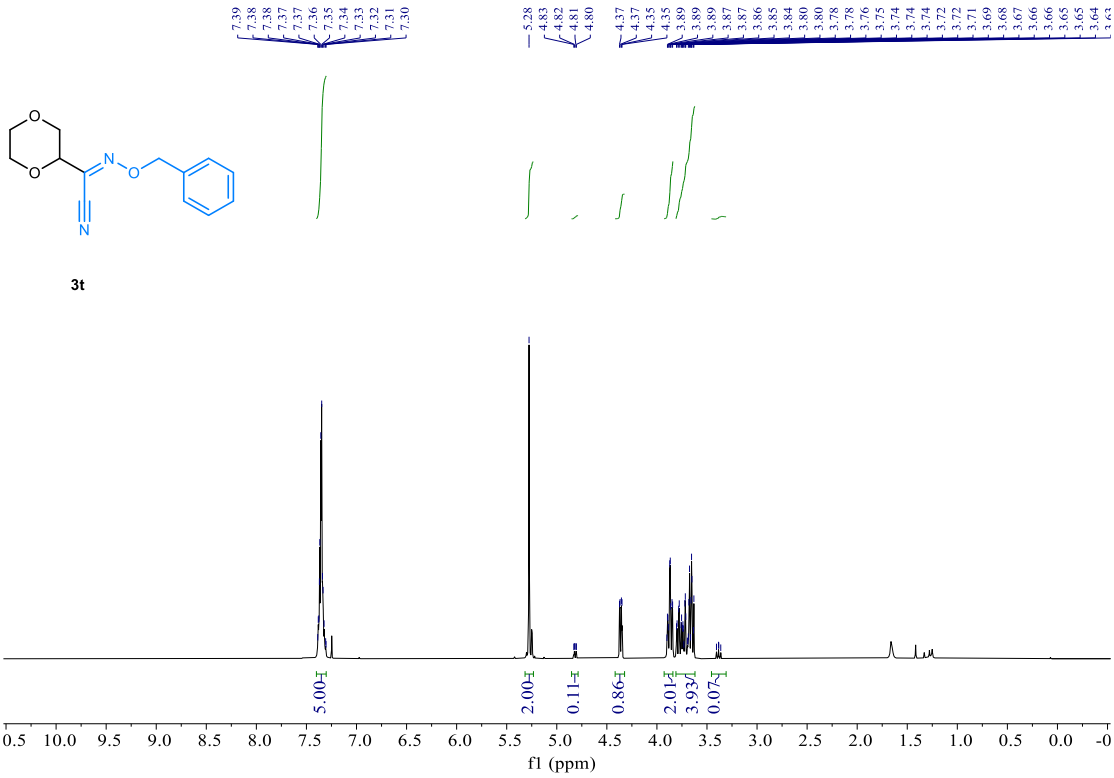

190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10
f1 (ppm)

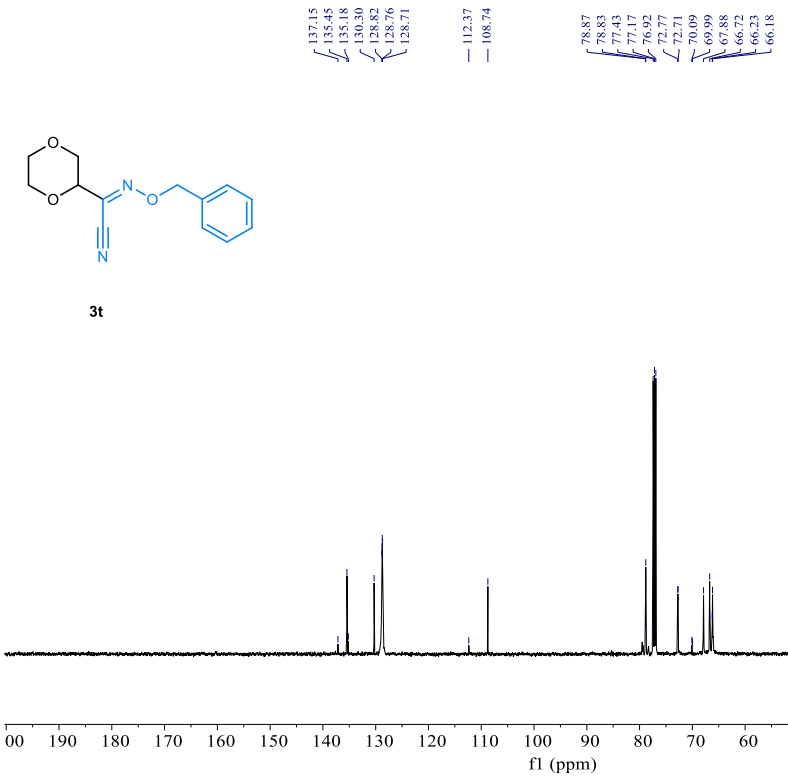

7.38
7.36
7.36
7.36
7.35
7.34
7.33
7.31
7.31
5.26
5.23
4.14
4.13
4.12
4.11
4.06
4.06
4.05
4.05
4.05
4.04
4.04
4.03
4.03
4.02
3.53
3.52
3.51
3.50
3.48
3.48
1.93
1.93
1.92
1.92
1.91
1.90
1.90
1.90
1.89
1.89
1.75
1.74
1.73
1.73
1.72
1.71
1.70
1.69
1.67
1.67
1.66
1.65
1.64
1.63
1.63
1.62
1.61
1.61
1.60
1.59
1.58
1.57
1.57
1.55
1.55
1.54
1.53
1.52
1.51
1.51

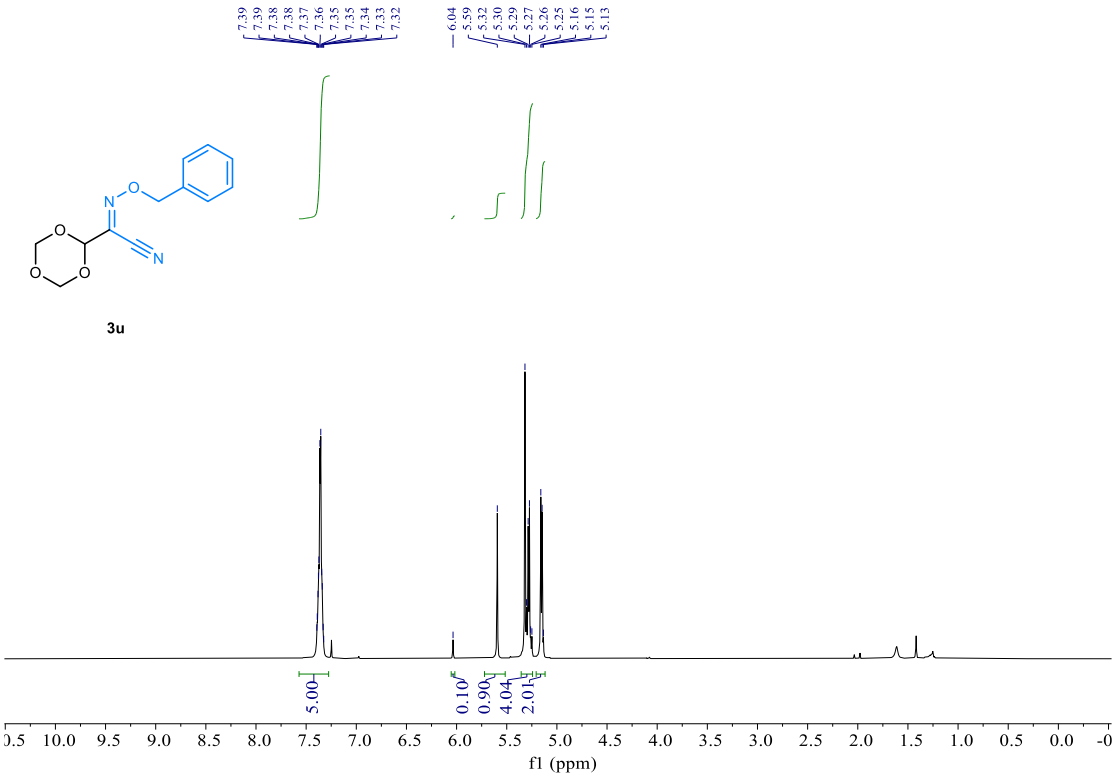
3s

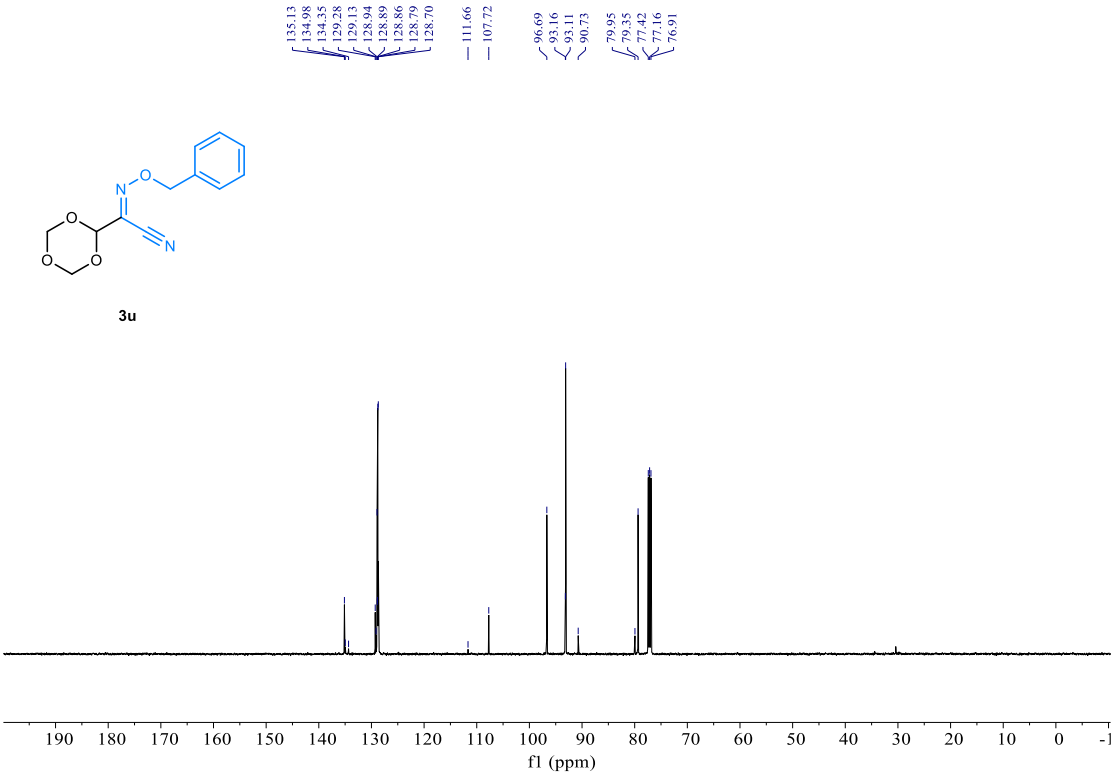

5.00
1.80
0.20
0.08
0.89
1.00
0.99
1.02
2.01
3.05
0.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)

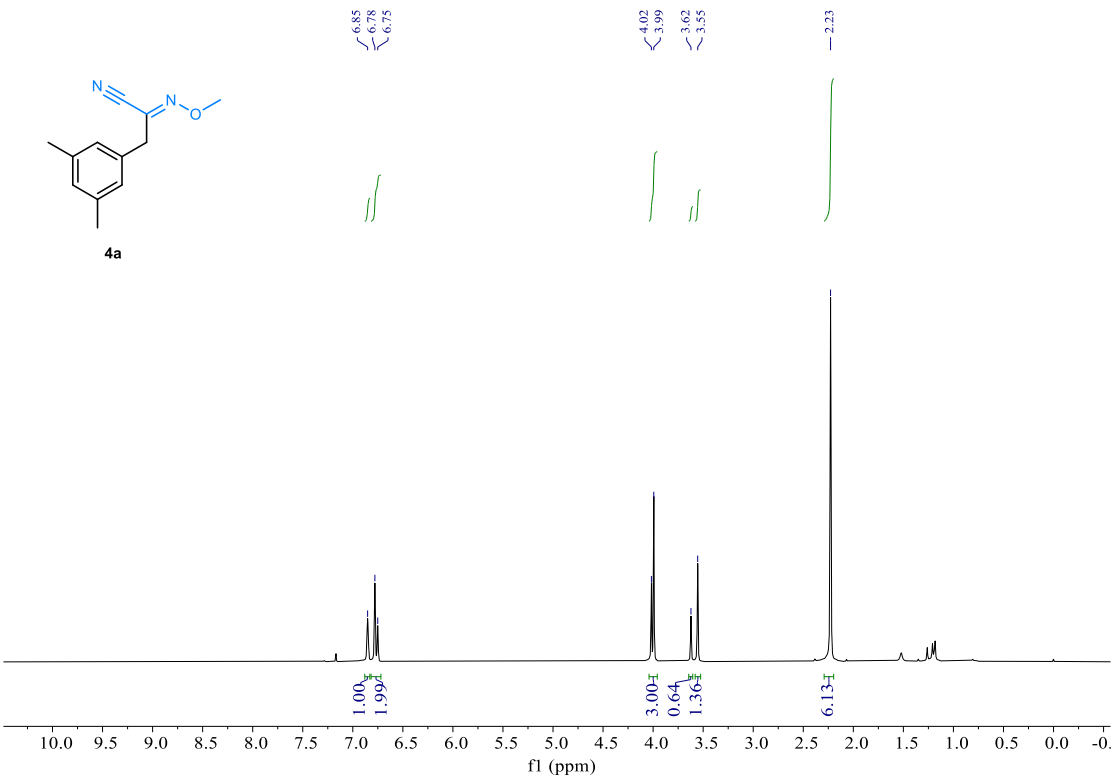

141.02
135.82
135.70
133.84
128.83
128.76
128.67
128.61
128.55
112.81
109.18
78.97
78.37
77.41
77.16
76.90
75.38
71.36
68.74
68.51
29.79
29.16
27.77
25.16
22.62
22.48
N
N
O
O
3s
190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10
f1 (ppm)

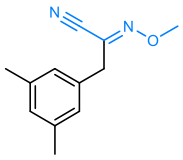

7.39
7.38
7.38
7.37
7.37
7.36
7.35
7.34
7.33
7.32
7.31
7.30
5.28
4.83
4.82
4.81
4.80
4.37
4.37
4.35
4.35
3.89
3.89
3.89
3.87
3.87
3.86
3.85
3.84
3.80
3.80
3.78
3.78
3.76
3.75
3.74
3.74
3.74
3.72
3.72
3.71
3.69
3.68
3.67
3.66
3.66
3.65
3.64
O
O
N
O
N
3t
5.00
2.00
0.11
0.86
2.01
3.93
0.07
0.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0
f1 (ppm)


137.15
135.45
135.18
130.30
128.82
128.76
128.71
112.37
108.74
78.87
78.83
77.43
77.17
76.92
72.77
72.71
70.09
69.99
67.88
66.72
66.23
66.18
3t
00 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)


7.39
7.39
7.38
7.38
7.37
7.36
7.35
7.35
7.34
7.33
7.32
6.04
5.59
5.32
5.30
5.29
5.27
5.26
5.25
5.16
5.15
5.13
3u
5.00
0.10
0.90
4.04
2.01
0.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0
f1 (ppm)

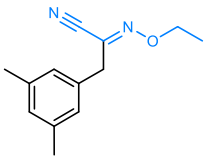

135.13
134.98
134.35
129.28
129.13
128.94
128.89
128.86
128.79
128.70
111.66
107.72
96.69
93.16
93.11
90.73
79.95
79.35
77.42
77.16
76.91
N
O
O
O
O
N
3u
190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -1
f1 (ppm)


6.85
6.78
6.75
4.02
3.99
3.62
3.55
2.23
N
N
O
4a
1.00
1.99
3.00
0.64
1.36
6.13
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)



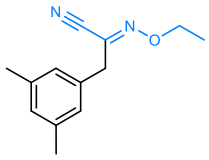
4a

138.66
138.61
137.43
133.39
133.06
131.37
129.47
129.33
126.81
126.74
114.44
110.20
77.37
77.05
76.74
63.98
63.58
37.92
33.92
29.71
21.22
190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)



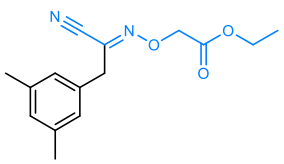
4b

6.97
6.90
6.88
4.42
4.40
4.39
4.38
4.37
4.36
4.34
3.75
3.68
2.35
1.41
1.39
1.37
1.00
1.96
2.02
0.66
1.34
6.15
3.09
10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)



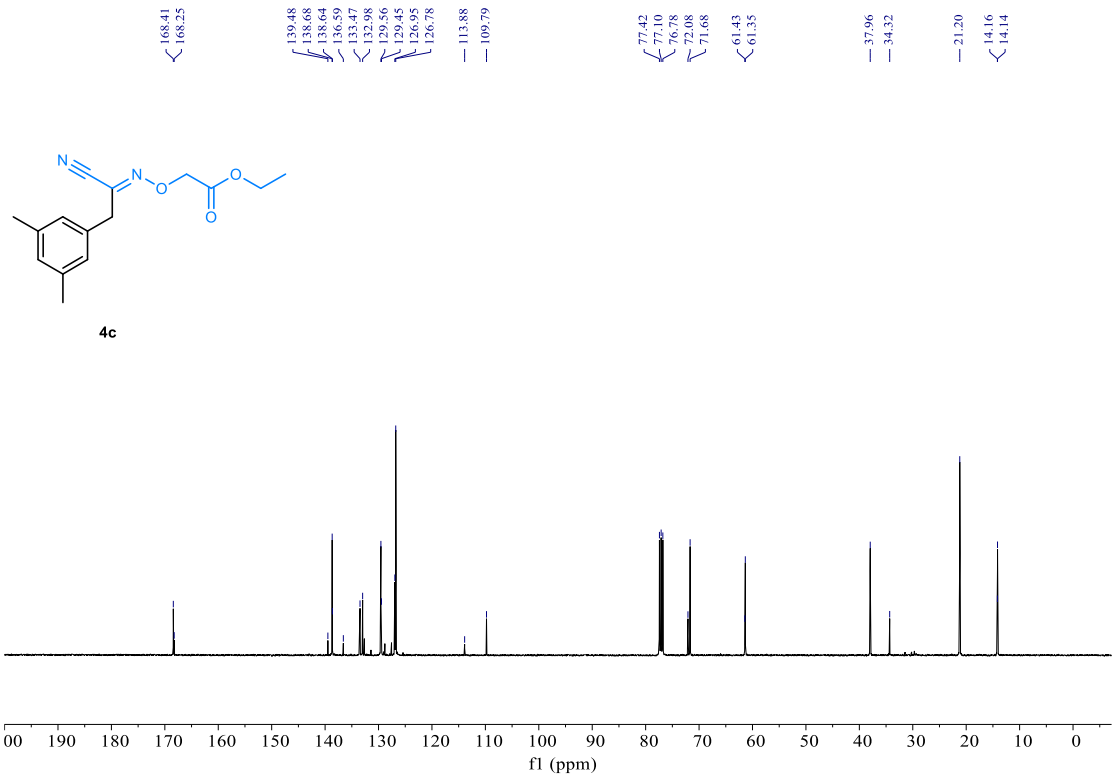
4b

138.62
138.55
137.01
133.60
133.26
130.99
129.41
129.26
126.85
126.73
114.68
110.41
77.38
77.06
76.75
72.32
71.91
38.01
34.00
29.71
21.22
14.47
14.35
190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)

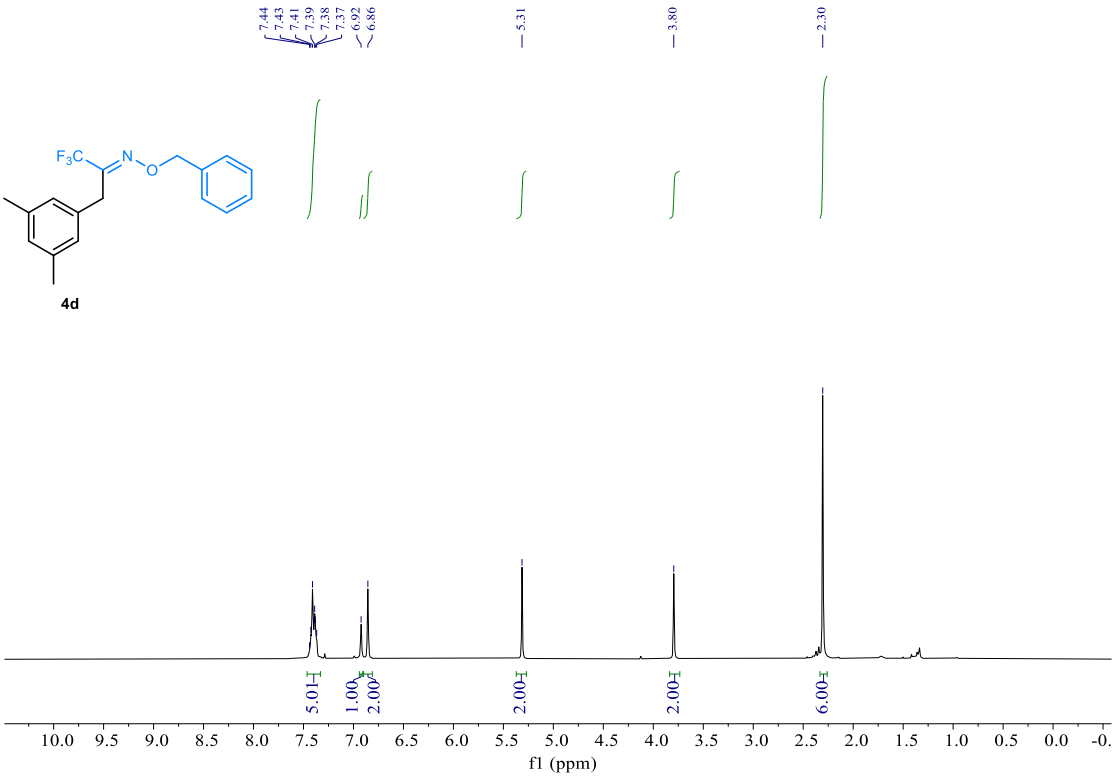


4c

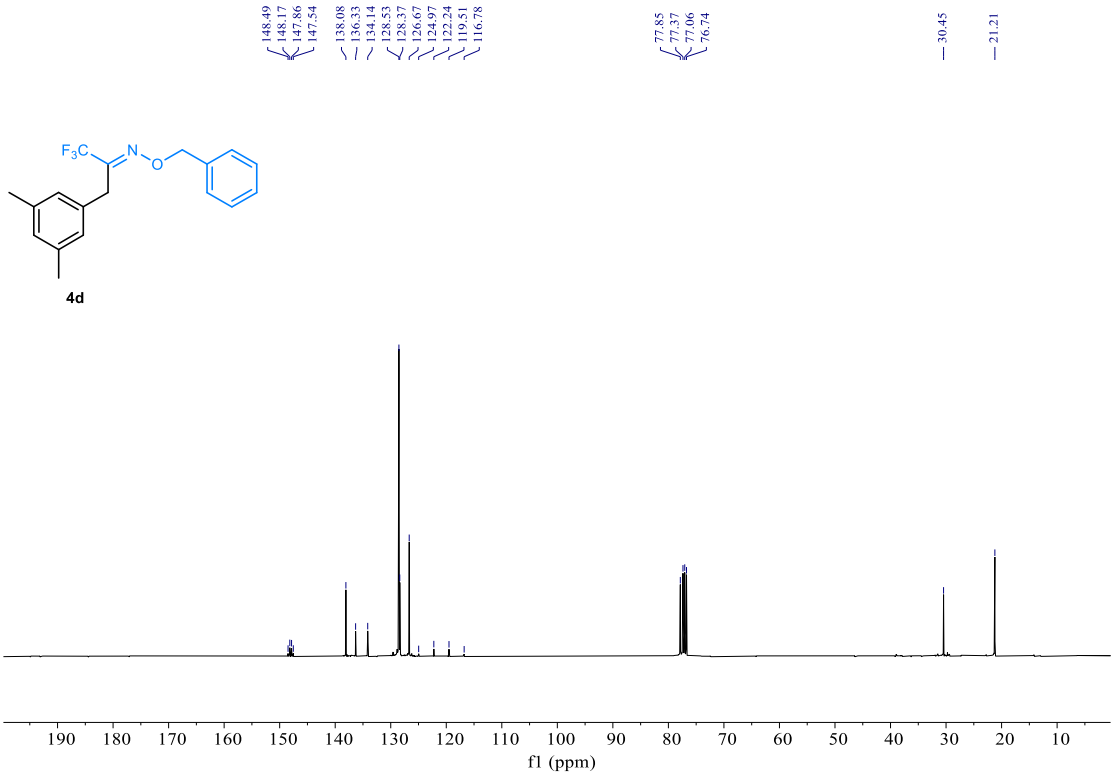
6.97
6.93
6.90
4.85
4.80
4.32
4.32
4.31
4.30
4.29
4.28
4.27
4.26
3.84
3.70
2.34
1.36
1.34
1.34
1.33
1.32
1.31
1.00
1.96
2.00
2.00
0.49
1.51
6.00
3.01
0.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)

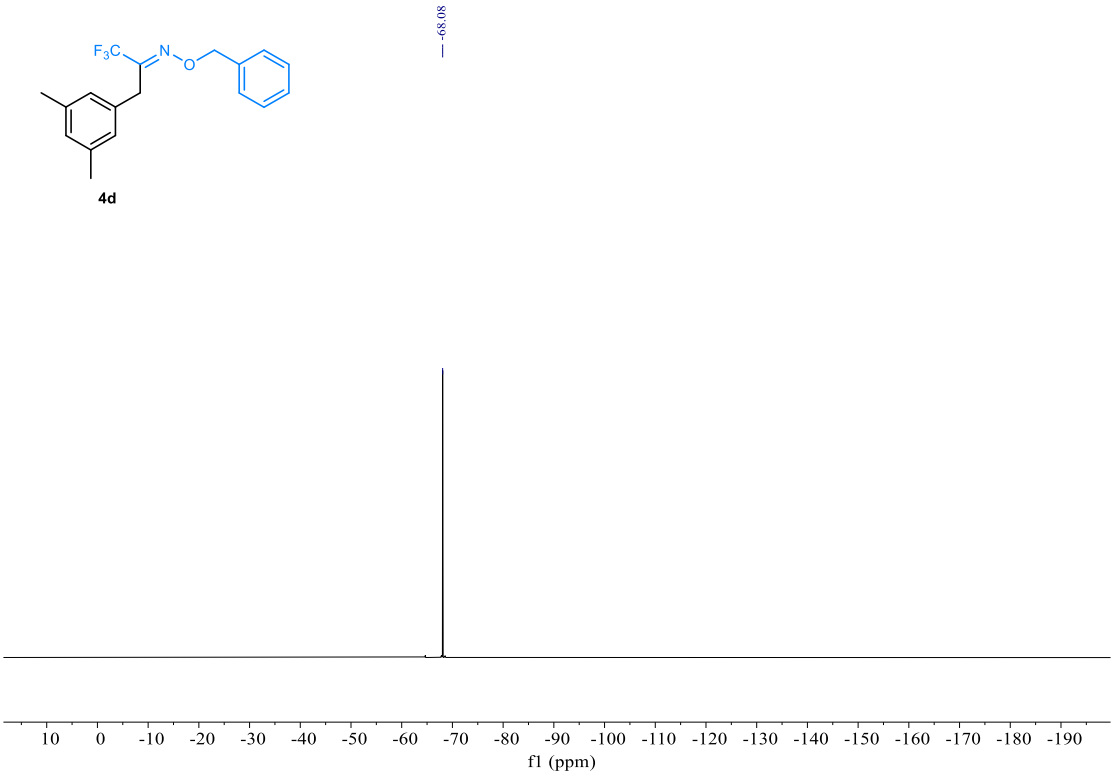

168.41
168.25
139.48
138.68
138.64
136.59
133.47
132.98
129.56
129.45
126.95
126.78
113.88
109.79
77.42
77.10
76.78
72.08
71.68
61.43
61.35
37.96
34.32
21.20
14.16
14.14
N
N
O
O
O
f1 (ppm)

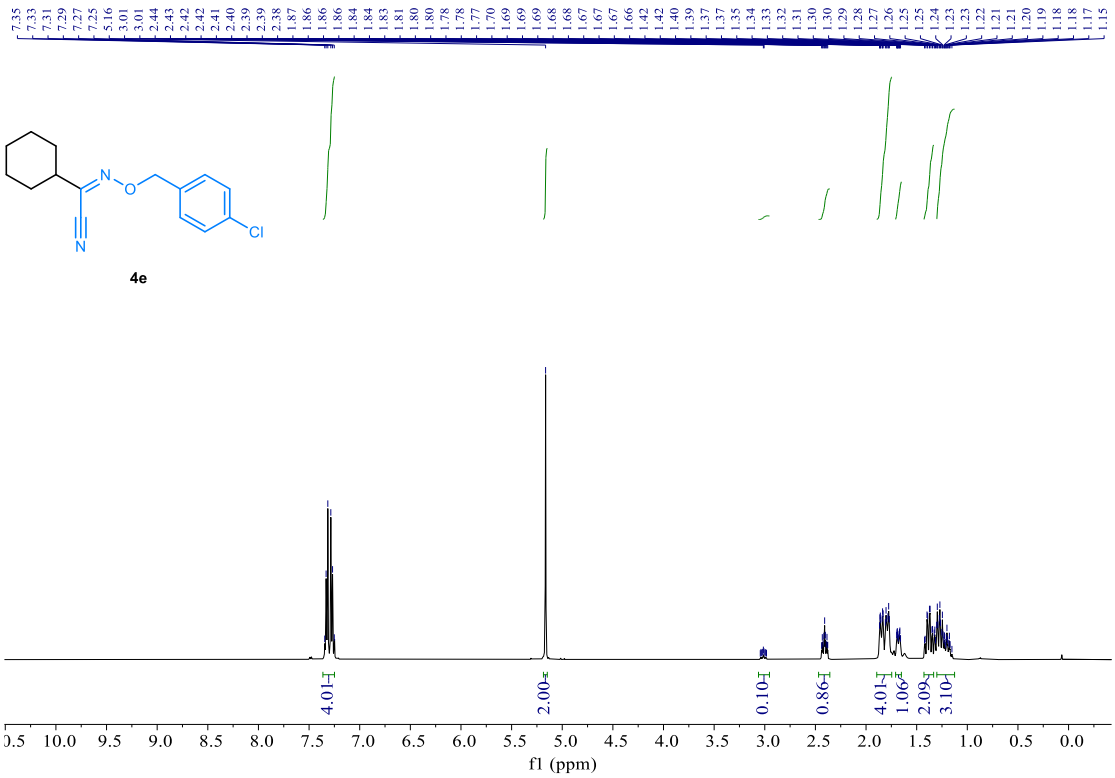
4c

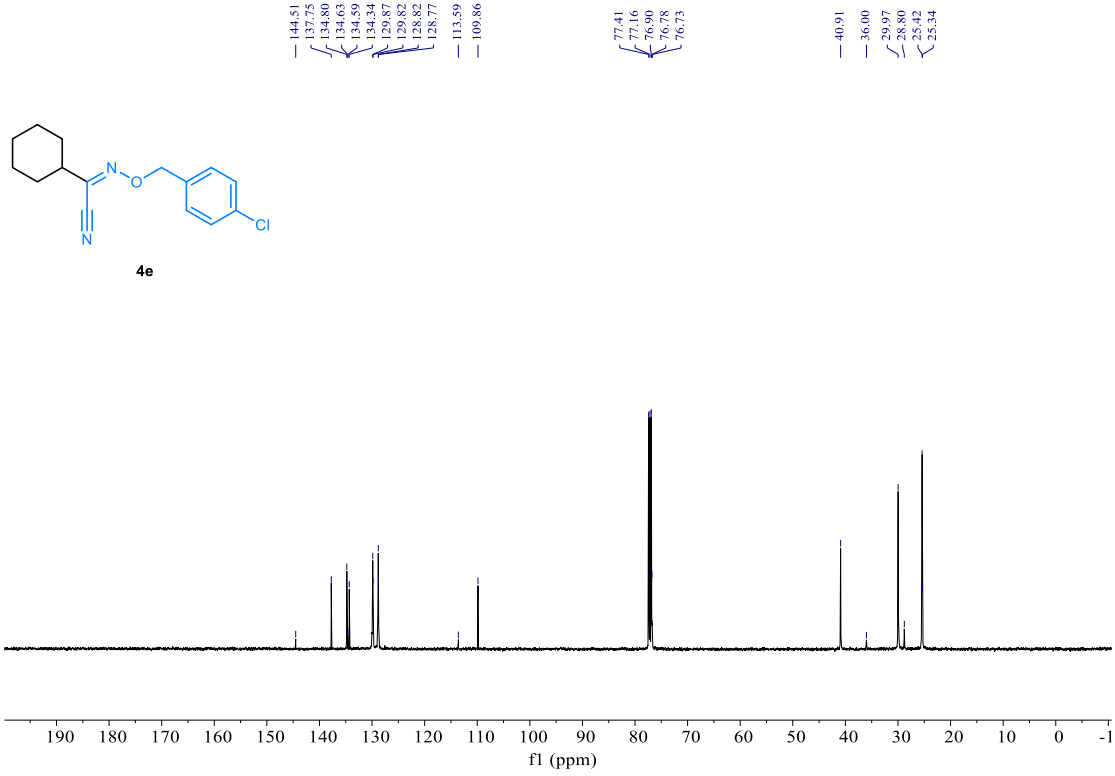

7.44
7.43
7.41
7.39
7.38
7.37
6.92
6.86
5.31
3.80
2.30
F3C
N
O
5.01
1.00
2.00
2.00
2.00
6.00
f1 (ppm)

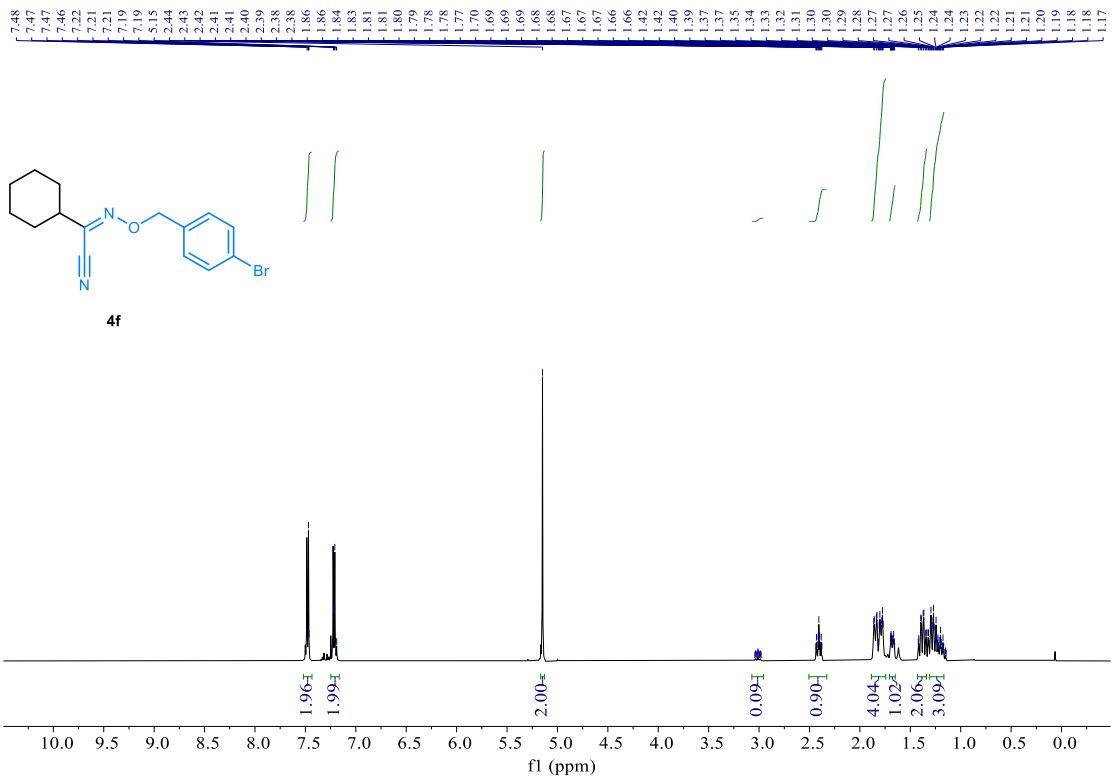
4d

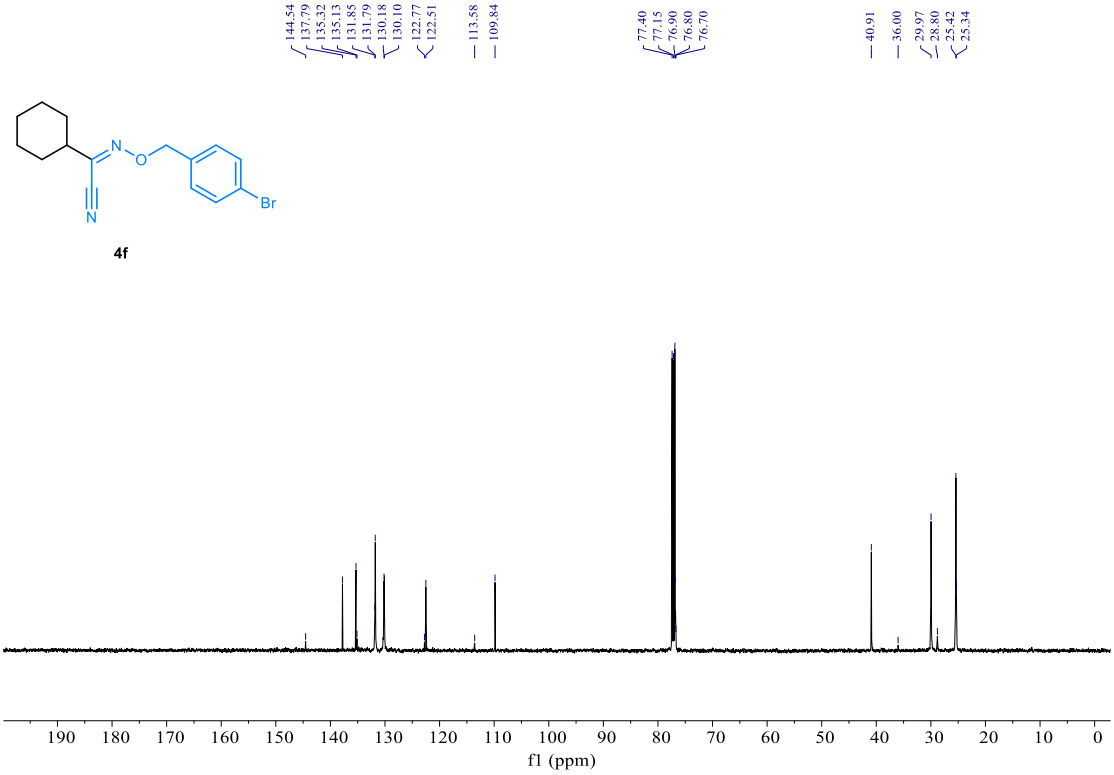

148.49
148.17
147.86
147.54
138.08
136.33
134.14
128.53
128.37
126.67
124.97
122.24
119.51
116.78
77.85
77.37
77.06
76.74
30.45
21.21
F3C
N
O
4d
190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10
f1 (ppm)

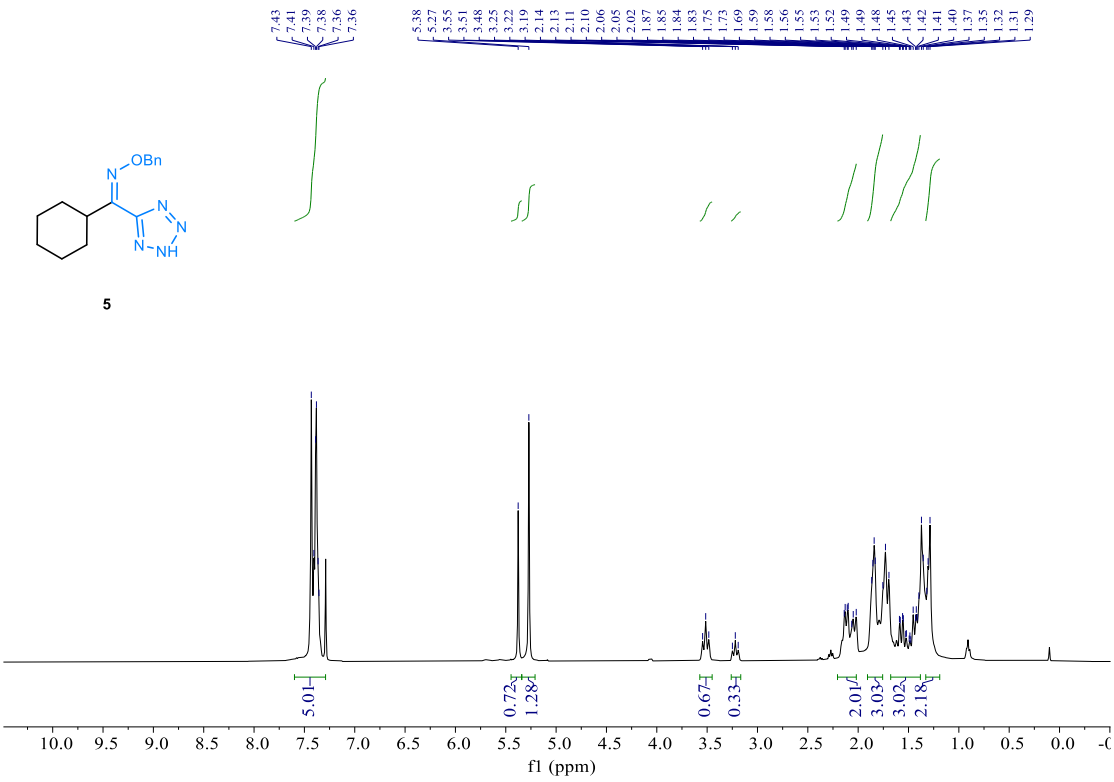

-68.08
F3C
N
O
4d
10 0 -10 -20 -30 -40 -50 -60 -70 -80 -90 -100 -110 -120 -130 -140 -150 -160 -170 -180 -190
f1 (ppm)

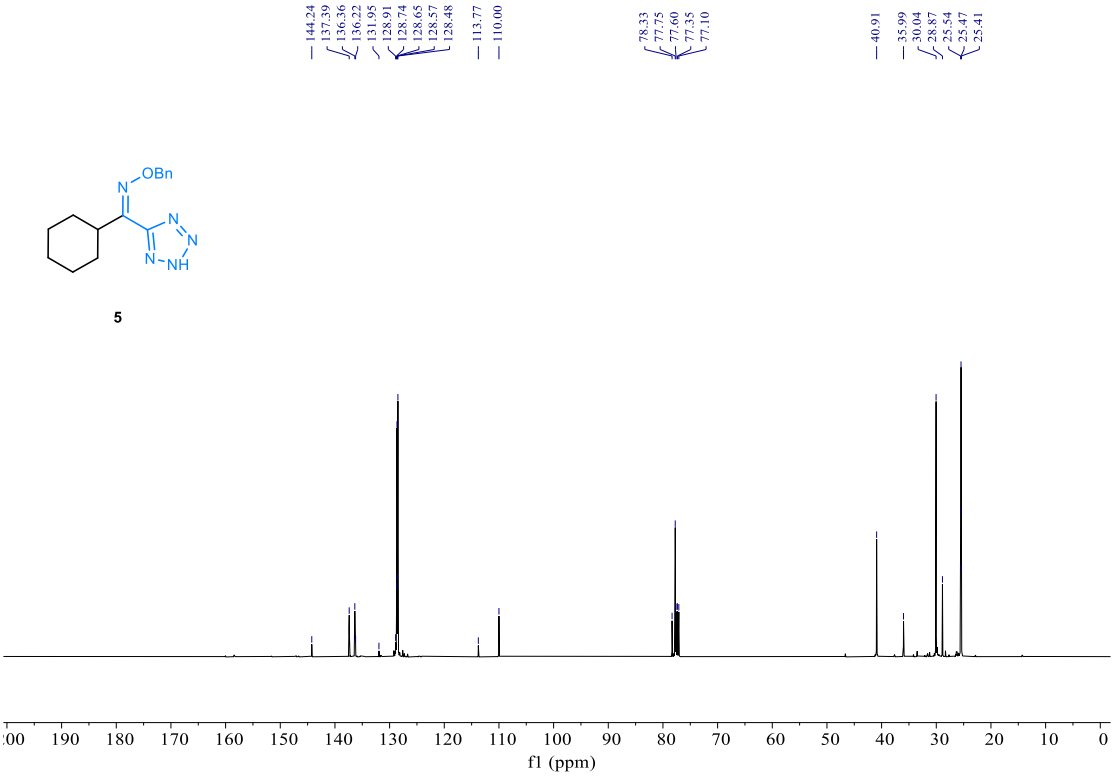

7.35 7.33 7.31 7.29 7.27 7.25 5.16 3.01 3.01 2.44 2.43 2.42 2.42 2.41 2.40 2.39 2.39 2.38 1.87 1.86 1.86 1.86 1.84 1.84 1.83 1.81 1.80 1.80 1.78 1.78 1.77 1.70 1.69 1.69 1.69 1.68 1.68 1.67 1.67 1.67 1.66 1.42 1.42 1.40 1.39 1.37 1.37 1.35 1.34 1.33 1.32 1.31 1.30 1.30 1.29 1.28 1.27 1.26 1.25 1.25 1.24 1.23 1.23 1.22 1.21 1.21 1.20 1.19 1.18 1.18 1.17 1.15
N
O
Cl
N
4e
4.01
2.00
0.10
0.86
4.01
1.06
2.09
3.10
f1 (ppm)


144.51 137.75 134.80 134.63 134.59 134.34 129.87 129.82 128.82 128.77 113.59 109.86 77.41 77.16 76.90 76.78 76.73 40.91 36.00 29.97 28.80 25.42 25.34
N
O
Cl
N
4e
f1 (ppm)


7.48 7.47 7.47 7.46 7.22 7.21 7.21 7.19 7.19 5.15 2.44 2.43 2.42 2.41 2.41 2.40 2.39 2.38 2.38 1.86 1.86 1.84 1.83 1.81 1.81 1.80 1.79 1.78 1.78 1.77 1.70 1.69 1.69 1.68 1.68 1.67 1.67 1.67 1.66 1.66 1.42 1.42 1.40 1.39 1.37 1.37 1.35 1.34 1.33 1.32 1.31 1.30 1.30 1.29 1.28 1.27 1.27 1.26 1.25 1.24 1.24 1.23 1.22 1.22 1.21 1.21 1.20 1.19 1.18 1.18 1.17
N
O
Br
N
4f
1.96
1.99
2.00
0.09
0.90
4.04
1.02
2.06
3.09
10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)


144.54 137.79 135.32 135.13 131.85 131.79 130.18 130.10 122.77 122.51 113.58 109.84 77.40 77.15 76.90 76.80 76.70 40.91 36.00 29.97 28.80 25.42 25.34
N
O
Br
N
4f
190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)


7.43
7.41
7.39
7.38
7.36
7.36
5.38
5.27
3.55
3.51
3.48
3.25
3.22
3.19
2.14
2.13
2.11
2.10
2.06
2.05
2.02
1.87
1.85
1.84
1.83
1.75
1.73
1.69
1.59
1.58
1.56
1.55
1.53
1.52
1.49
1.49
1.48
1.45
1.43
1.42
1.41
1.40
1.37
1.35
1.32
1.31
1.29
OBn
N
N
N
NH
5.01
0.72
1.28
0.67
0.33
2.01
3.03
3.02
2.18
10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)


144.24
137.39
136.36
136.22
131.95
128.91
128.74
128.65
128.57
128.48
113.77
110.00
78.33
77.75
77.60
77.35
77.10
40.91
35.99
30.04
28.87
25.54
25.47
25.41
OBn
N
N
N
NH
5
00 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)