

Supporting Information
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Electronic Supporting Information

Sustainable *N*-Formylation of Anilines: Harnessing Aleuritic Acid as a Renewable Formyl Source

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Mechanistic study

Radical scavenging experiment in the presence of TEMPO (2,2,6,6-Tetramethylpiperidin-1-yl)oxyl

A clean washed reaction tube equipped with a magnetic stir bar was charged with aniline **1a** (46.5 mg, 0.5 mmol), aleuritic acid **2** (228.3 mg, 1.5 mmol), TEMPO (156.25 mg, 1 mmol) and solvent methanol (1.0 mL), the above mixture was stirred for 12h at 60°C. The expected product **3a** was not obtained, it proves the evidence for the involvement of a radical mechanism in the reaction pathway. Unfortunately, no adduct resulting from the interaction between TEMPO and **1a** or aleuritic acid was detected during the analysis.

Radical scavenging experiment in the presence of BHT 3,5-Di-tert-4-butylhydroxytoluene

A clean washed reaction tube equipped with a magnetic stir bar was charged with aniline **1a** (46.5 mg, 0.5 mmol), aleuritic acid **2** (228.3 mg, 1.5 mmol), BHT (220.25 mg, 1 mmol) and solvent methanol (1.0 mL), the above mixture was stirred for 12h at 60°C. However, the expected product **3a** was not obtained, providing further evidence for the involvement of a radical mechanism in the reaction pathway. To investigate possible intermediates, a sample was withdrawn for GC-MS analysis before the reaction completion. Intriguingly, after just 6 hours, a BHT-linked adduct **4**, was identified (Figure S1).

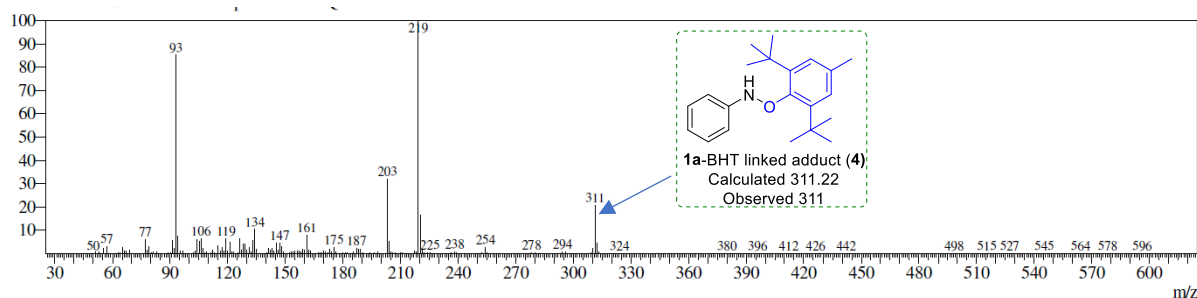


Figure S1: GC-MS data of **1a**-BHT linked adduct

Experimental section

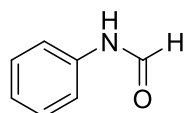
General information: All commercially available chemicals and reagents were used without any further purification unless otherwise indicated. ^1H and ^{13}C { ^1H } NMR spectra were recorded at 600/500 and 150/125 MHz respectively. The spectra were recorded in CDCl_3 , $\text{DMDO-}d_6$ and CD_3CN as solvent. Multiplicity was indicated as follows: s (singlet); d (doublet); t (triplet); m (multiplet); dd (doublet of doublets), etc. and coupling constants (J) were given in Hz. Chemical shifts are reported in ppm relative to TMS as an internal standard for ^1H NMR. Chemical shifts were reported in ppm on the δ scale relative to Me_4Si ($\delta = 0.00$ for ^1H -NMR), CDCl_3 ($\delta = 7.26$ for ^1H NMR and $\delta = 77.160$ for $^{13}\text{C}\{^1\text{H}\}$ -NMR) and $\text{DMSO-}d_6$ ($\delta = 2.50$ for ^1H NMR and $\delta = 39.52$ for $^{13}\text{C}\{^1\text{H}\}$ -NMR). Additional peaks at $\delta = 1.56 - 1.61$ ppm in ^1H -NMR spectra of compounds recorded in CDCl_3 and $\delta = 3.39$ ppm in ^1H -NMR spectra of compounds recorded in $\text{DMSO-}d_6$ correspond to water, present if any. GC spectral data were recorded on a Shimadzu GC-2014. HRMS (SI) spectra were recorded on a Micromass Q-ToF microTM instrument. GCMS spectral data were acquired on a Shimadzu GC-2010 Plus coupled with GCMS-TQ8040 instrument. Progress of the reactions were monitored by thin layer chromatography (TLC). All products were purified through column chromatography using silica gel 100-200 mesh size using hexane/ethyl acetate as eluent, unless otherwise indicated.

General procedure (A) for the synthesis of *N*-Phenyl formamide derivatives:

A clean-washed reaction tube equipped with a magnetic stir bar was charged with aniline **1a** (0.5 mmol), aleuritic acid **2a** (0.75 mmol), $K_2Cr_2O_7$ (10 mol%), and Methanol (1 ml), the above mixture was stirred for 12 h at 60 °C in a closed tube. After the completion of reaction, the product was extracted with ethyl acetate and dried with anhydrous Na_2SO_4 . The solvent was removed under reduced pressure and the residue was purified through column chromatography using silica gel, eluting with (20% EtOAc/hexane) to obtain the product **3a**.

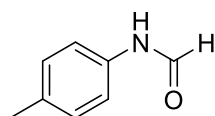
Characterization data:

N-Phenyl formamide (**3a**)¹



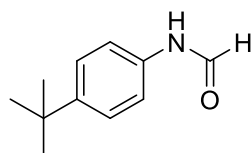
(Eluent: 20% EtOAc/hexane); 70% yield (42.3 mg); Dark brown liquid. The compound is a mixture of rotamers. ¹H NMR (600 MHz, CHLOROFORM-*D*) δ 9.30 (d, *J* = 11.5 Hz, 1H), 8.69 (d, *J* = 11.5 Hz, 2H), 8.31 (s, 1H), 7.56 (s, 2H), 7.31 (dt, *J* = 20.7, 8.0 Hz, 4H), 7.17 (t, *J* = 7.5 Hz, 1H), 7.10 (d, *J* = 9.2 Hz, 3H). ¹³C NMR (151 MHz, CHLOROFORM-*D*) δ 163.43, 160.10, 137.24, 136.99, 129.83, 129.83, 125.37, 124.88, 120.36, 118.88.

N-(*p*-Tolyl) formamide (**3b**)¹



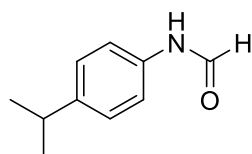
(Eluent: 20% EtOAc/hexane); 67% yield (45.3 mg); Brown solid. The compound is a mixture of rotamers. ¹H NMR (600 MHz, CHLOROFORM-*D*) δ 8.62 (d, *J* = 11.5 Hz, 1H), 8.34 (s, 1H), 7.92 (s, 1H), 7.42 (s, 1H), 7.41 (s, 1H), 7.17 – 7.13 (m, 4H), 6.98 (d, *J* = 8.6 Hz, 2H), 2.33 (d, *J* = 10.9 Hz, 6H). ¹³C NMR (151 MHz, CHLOROFORM-*D*) δ 162.65, 158.94, 135.31, 134.60, 134.37, 134.09, 130.31, 129.61, 120.10, 119.28, 20.97, 20.88.

N-(4-*tert*butylphenyl) formamide (**3c**)²



(Eluent: 20% EtOAc/hexane); 62% yield (55 mg); Brown liquid. The compound is a mixture of rotamers. ¹H NMR (600 MHz, CHLOROFORM-*D*) δ 9.20 (d, *J* = 10.6 Hz, 1H), 8.69 (s, 1H), 8.54 (d, *J* = 11.5 Hz, 1H), 8.17 (d, *J* = 2.2 Hz, 1H), 7.37 (d, *J* = 8.8 Hz, 2H), 7.19 (dd, *J* = 20.3, 8.8 Hz, 4H), 6.91 (d, *J* = 8.8 Hz, 2H), 1.17 (s, 9H), 1.15 (s, 9H). ¹³C NMR (151 MHz, CHLOROFORM-*D*) δ 163.30, 159.90, 148.26, 147.57, 134.54, 134.27, 126.43, 125.71, 120.08, 118.69, 34.31, 34.28, 31.26.

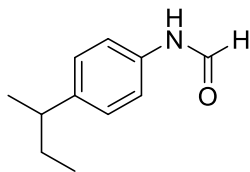
N-(4-isopropylphenyl) formamide (**3d**)³



(Eluent: 20% EtOAc/hexane); 77% yield (63 mg); Brown liquid. The compound is a mixture of rotamers. ¹H NMR (600 MHz, CHLOROFORM-*D*) δ 8.63 (d, *J* = 11.5 Hz, 1H), 8.35 (s, 1H), 7.88 (s, 1H), 7.45 (d, *J* = 8.3 Hz, 2H), 7.29 (s, 1H), 7.20 (dd, *J* = 14.7, 8.3 Hz, 4H), 7.02 (d, *J* = 8.6 Hz, 2H), 2.95 – 2.84 (m, 2H), 1.24 (t, *J* =

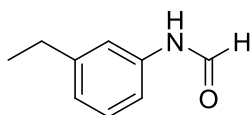
6.9 Hz, 12H). ^{13}C NMR (151 MHz, CHLOROFORM-*D*) δ 162.74, 159.00, 146.46, 145.77, 134.62, 134.38, 127.82, 127.14, 120.27, 119.46, 33.71, 24.10.

***N*-(4-secbutylphenyl) formamide (3e)**



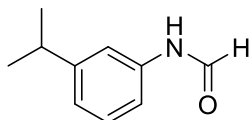
(Eluent: 20% EtOAc/hexane); 57% yield (50.5 mg); Brown liquid. The compound is a mixture of rotamers. ^1H NMR (600 MHz, CHLOROFORM-*D*) δ 8.63 (d, J = 11.5 Hz, 1H), 8.36 (s, 1H), 7.70 (s, 1H), 7.45 (s, 2H), 7.16 (dd, J = 13.5, 8.3 Hz, 4H), 7.01 (d, J = 8.3 Hz, 2H), 2.58 (dt, J = 10.6, 7.0 Hz, 2H), 1.60 – 1.56 (m, 4H), 1.22 (t, J = 6.5 Hz, 6H), 0.81 (td, J = 7.5, 4.9 Hz, 6H). ^{13}C NMR (151 MHz, CHLOROFORM-*D*) δ 162.58, 158.87, 145.23, 144.53, 143.82, 134.57, 134.29, 128.39, 127.72, 121.59, 120.14, 119.39, 41.27, 31.20, 21.92, 12.24.

***N*-(3-ethylphenyl) formamide (3f)⁴**



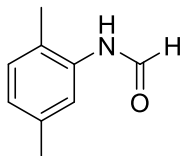
(Eluent: 20% EtOAc/hexane); 49% yield (36.5 mg); Dark Brown liquid. The compound is a mixture of rotamers. ^1H NMR (600 MHz, CHLOROFORM-*D*) δ 8.68 (d, J = 11.5 Hz, 1H), 8.37 (s, 1H), 7.75 (s, 1H), 7.41 (s, 1H), 7.34 (dd, J = 7.9, 2.1 Hz, 1H), 7.28 – 7.23 (m, 3H), 7.04 (d, J = 7.6 Hz, 1H), 6.99 (d, J = 7.5 Hz, 1H), 6.90 (d, J = 5.6 Hz, 2H), 2.67 – 2.63 (m, 4H), 1.24 (q, J = 7.3 Hz, 6H). ^{13}C NMR (151 MHz, CHLOROFORM-*D*) δ 162.44, 158.88, 146.40, 129.77, 129.11, 124.53, 119.54, 118.62, 117.36, 116.26, 28.91, 28.83, 15.53, 15.46.

***N*-(3-isopropylphenyl) formamide (3g)⁴**



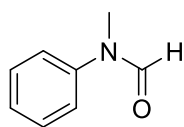
(Eluent: 20% EtOAc/hexane); 42% yield (34.3 mg); Brown liquid. The compound is a mixture of rotamers. ^1H NMR (600 MHz, CHLOROFORM-*D*) δ 8.68 (d, J = 11.5 Hz, 1H), 8.36 (s, 1H), 7.41 – 7.34 (m, 2H), 7.26 (p, J = 7.8 Hz, 3H), 7.07 (d, J = 8.0 Hz, 1H), 7.01 (d, J = 8.0 Hz, 1H), 6.91 (d, J = 7.5 Hz, 3H), 2.89 (dt, J = 13.2, 6.6 Hz, 2H), 1.25 (d, J = 6.9 Hz, 12H). ^{13}C NMR (151 MHz, CHLOROFORM-*D*) δ 162.74, 159.02, 151.07, 150.24, 136.93, 136.69, 129.76, 129.11, 123.61, 123.04, 118.23, 117.58, 117.32, 116.40, 34.17, 23.98, 23.93.

***N*-(2,5-dimethylphenyl) formamide (3h)⁵**



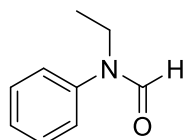
(Eluent: 20% EtOAc/hexane); 45% yield (33.6 mg); White Solid. The compound is a mixture of rotamers. ^1H NMR (600 MHz, CHLOROFORM-*D*) δ 8.52 (d, J = 11.3 Hz, 1H), 8.41 (s, 1H), 7.99 (s, 1H), 7.72 (s, 1H), 7.11 (d, J = 7.5 Hz, 1H), 7.07 (d, J = 7.8 Hz, 1H), 6.96 (d, J = 9.9 Hz, 3H), 6.90 (d, J = 9.5 Hz, 1H), 2.32 (d, J = 10.6 Hz, 6H), 2.24 (d, J = 14.5 Hz, 6H). ^{13}C NMR (151 MHz, CHLOROFORM-*D*) δ 163.52, 159.22, 137.07, 136.75, 134.89, 134.52, 131.18, 131.09, 130.49, 126.78, 126.59, 125.50, 123.67, 121.55, 121.44, 21.18, 21.05, 17.33.

***N*-methyl-*N*-phenyl formamide (3i)³**



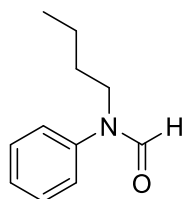
(Eluent: 20% EtOAc/hexane); 39% yield (26.3 mg); yellowish liquid. ^1H NMR (600 MHz, CHLOROFORM-*D*) δ 8.39 (d, $J = 3.3$ Hz, 1H), 7.33 (t, $J = 7.8$ Hz, 2H), 7.19 (t, $J = 7.5$ Hz, 1H), 7.09 (d, $J = 8.6$ Hz, 2H), 3.23 (s, 3H). ^{13}C NMR (151 MHz, CHLOROFORM-*D*) δ 162.32, 142.23, 122.42, 129.89, 126.65, 32.11.

***N*-ethyl-*N*-Phenyl formamide (3j)⁶**



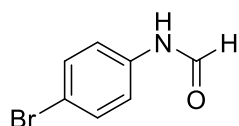
(Eluent: 10% EtOAc/hexane); 29% yield (21.6 mg); colourless liquid. The compound is a mixture of rotamers. ^1H NMR (200 MHz, CDCl_3) δ 8.36 (s, 1H), 7.47 – 7.37 (m, 2H), 7.34 – 7.25 (m, 1H), 7.21 – 7.13 (m, 2H), 3.87 (q, $J = 7.2$ Hz, 2H), 1.16 (t, $J = 7.2$ Hz, 3H). ^{13}C NMR (50 MHz, CDCl_3) δ 162.04, 139.74, 129.67, 129.25, 126.87, 126.11, 124.25, 44.96, 40.08, 15.04, 13.06.

***N*-butyl-*N*-Phenyl formamide (3k)⁷**



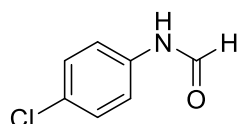
(Eluent: 20% EtOAc/hexane); 17% yield (15.0 mg); yellowish liquid. ^1H NMR (200 MHz, CDCl_3) δ 8.36 (s, 1H), 7.46 – 7.36 (m, 2H), 7.33 – 7.25 (m, 1H), 7.20 – 7.12 (m, 2H), 3.86 – 3.77 (m, 2H), 1.59 – 1.42 (m, 2H), 1.40 – 1.21 (m, 2H), 0.88 (t, $J = 7.2$ Hz, 3H). ^{13}C NMR (50 MHz, CDCl_3) δ 162.26, 140.99, 129.61, 126.77, 124.15, 44.62, 29.64, 19.96, 13.69.

***N*-(4-bromophenyl) formamide (3l)⁸**



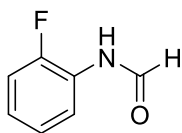
(Eluent: 20% EtOAc/hexane); 48% yield (48 mg); Light Brown Solid. ^1H NMR (600 MHz, CHLOROFORM-*D*) δ 8.38 (s, 1H), 7.46 (d, $J = 15.5$ Hz, 4H), 6.97 (d, $J = 8.6$ Hz, 1H). ^{13}C NMR (151 MHz, CHLOROFORM-*D*) δ 162.06, 158.83, 135.96, 132.94, 132.21, 121.54, 120.51.

***N*-(4-chlorophenyl) formamide (3m)¹**



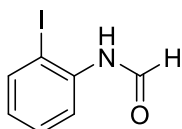
(Eluent: 30% EtOAc/hexane); 41% yield (32 mg); White Solid. The compound is a mixture of rotamers. ^1H NMR (600 MHz, CHLOROFORM-*D*) δ 8.80 (s, 1H), 8.66 (d, $J = 11.2$ Hz, 1H), 8.35 (d, $J = 1.9$ Hz, 1H), 7.91 (s, 1H), 7.50 (d, $J = 8.9$ Hz, 2H), 7.30 (dd, $J = 25.1, 8.8$ Hz, 3H), 7.05 (d, $J = 8.8$ Hz, 2H). ^{13}C NMR (151 MHz, CHLOROFORM-*D*) δ 162.82, 159.36, 135.55, 135.46, 130.83, 129.92, 129.21, 121.40, 120.15.

***N*-(2-fluorophenyl) formamide (3n)³**



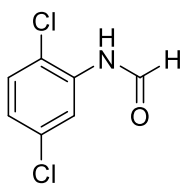
(Eluent: 20% EtOAc/hexane); 46% yield (32 mg); Light Brown Solid. The compound is a mixture of rotamers. ^1H NMR (600 MHz, CHLOROFORM-*D*) δ 8.68 (d, J = 11.2 Hz, 1H), 8.46 (d, J = 1.9 Hz, 2H), 8.28 (t, J = 8.0 Hz, 2H), 8.18 (s, 1H), 7.22 – 7.08 (m, 6H). ^{13}C NMR (151 MHz, CHLOROFORM-*D*) δ 162.96, 162.80, 159.76, 159.49, 153.37, 151.75, 125.52, 125.45, 125.19, 125.11, 125.00, 124.94, 124.84, 124.82, 124.49, 122.60, 122.38, 120.35, 120.09.

***N*-(2-iodophenyl) formamide (3o)¹**



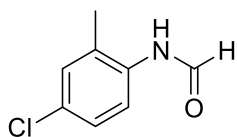
(Eluent: 30% EtOAc/hexane); 43% yield (53.1 mg); Light Brown Solid. The compound is a mixture of rotamers. ^1H NMR (600 MHz, CHLOROFORM-*D*) δ 8.66 (d, J = 10.9 Hz, 1H), 8.49 (s, 1H), 8.29 (d, J = 8.0 Hz, 1H), 7.85 (d, J = 8.0 Hz, 1H), 7.80 (d, J = 8.0 Hz, 1H), 7.47 (s, 1H), 7.36 (d, J = 7.5 Hz, 2H), 7.21 (d, J = 8.0 Hz, 1H), 6.94 (t, J = 7.8 Hz, 1H), 6.88 (d, J = 8.0 Hz, 1H). ^{13}C NMR (151 MHz, CHLOROFORM-*D*) δ 161.89, 158.90, 140.07, 139.06, 137.88, 137.38, 129.73, 129.47, 127.12, 126.49, 122.32, 119.32, 90.73, 89.29.

***N*-(2,5-dichlorophenyl) formamide (3p)⁸**



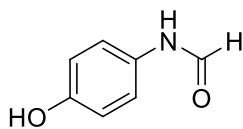
(Eluent: 30% EtOAc/hexane); 40% yield (38 mg); White Solid. The compound is a mixture of rotamers. ^1H NMR (600 MHz, CHLOROFORM-*D*) δ 8.74 (d, J = 12 Hz, 1H), 8.54 – 8.49 (m, 2H), 7.69 (s, 1H), 7.37 (d, J = 6 Hz, 1H), 7.31 (d, J = 8.6 Hz, 1H), 7.12 (d, J = 6 Hz, 1H), 7.07 (dd, J = 8.6, 2.9 Hz, 1H). ^{13}C NMR (151 MHz, CHLOROFORM-*D*) δ 160.87, 158.75, 134.54, 133.73, 131.19, 129.85, 125.82, 125.17, 121.83, 120.55, 118.29.

***N*-(2-methyl, 4-chlorophenyl) formamide (3q)**



(Eluent: 20% EtOAc/hexane); 47% yield (40 mg); White Solid. The compound is a mixture of rotamers. ^1H NMR (600 MHz, CHLOROFORM-*D*) δ 8.49 (d, J = 11.5 Hz, 1H), 8.43 (s, 1H), 7.93 (s, 1H), 7.86 (d, J = 9.8 Hz, 1H), 7.23 (s, 1H), 7.19 (d, J = 5.2 Hz, 3H), 7.07 (d, J = 8.0 Hz, 1H), 2.27 (d, J = 17.8 Hz, 6H). ^{13}C NMR (151 MHz, CHLOROFORM-*D*) δ 163.14, 159.08, 133.69, 133.27, 131.75, 131.49, 131.20, 130.59, 130.44, 130.40, 127.21, 126.94, 124.25, 122.03, 17.74, 17.70.

***N*-(4-hydroxyphenyl) formamide (3r)²**

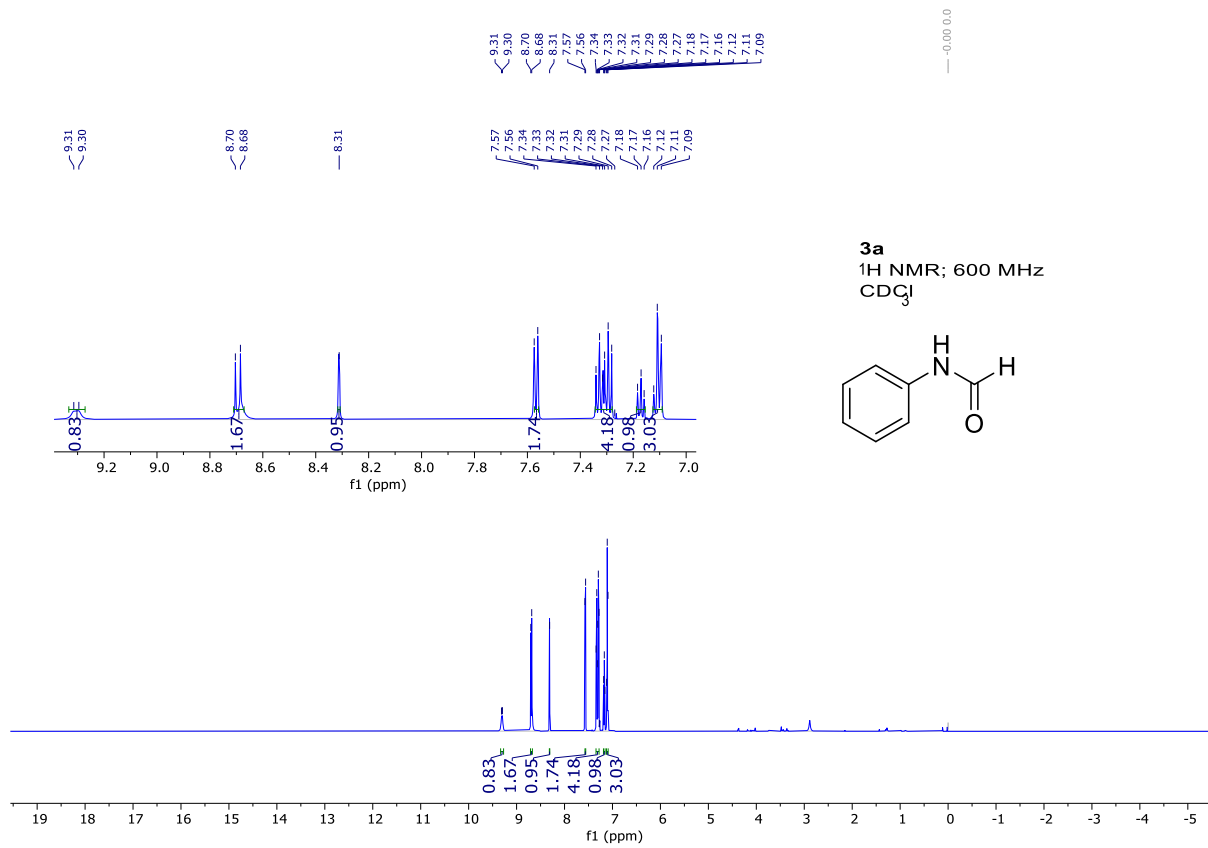


(Eluent: 30% EtOAc/hexane); 31% yield (21.2 mg); brown solid. The compound is a mixture of rotamers. ^1H NMR (200 MHz, DMSO) δ 9.95 (s, 3H), 9.33 (s, 3H), 8.20 (d, J = 2.1 Hz, 2H), 7.44 – 7.39 (m, 4H), 7.06 – 6.98 (m, 2H), 6.75 (dd, J = 8.7, 1.9 Hz, 6H). ^{13}C NMR (50 MHz, DMSO) δ 163.11, 159.39, 154.69, 154.02, 130.42, 130.09, 121.33, 120.72, 116.30, 116.04, 115.68.

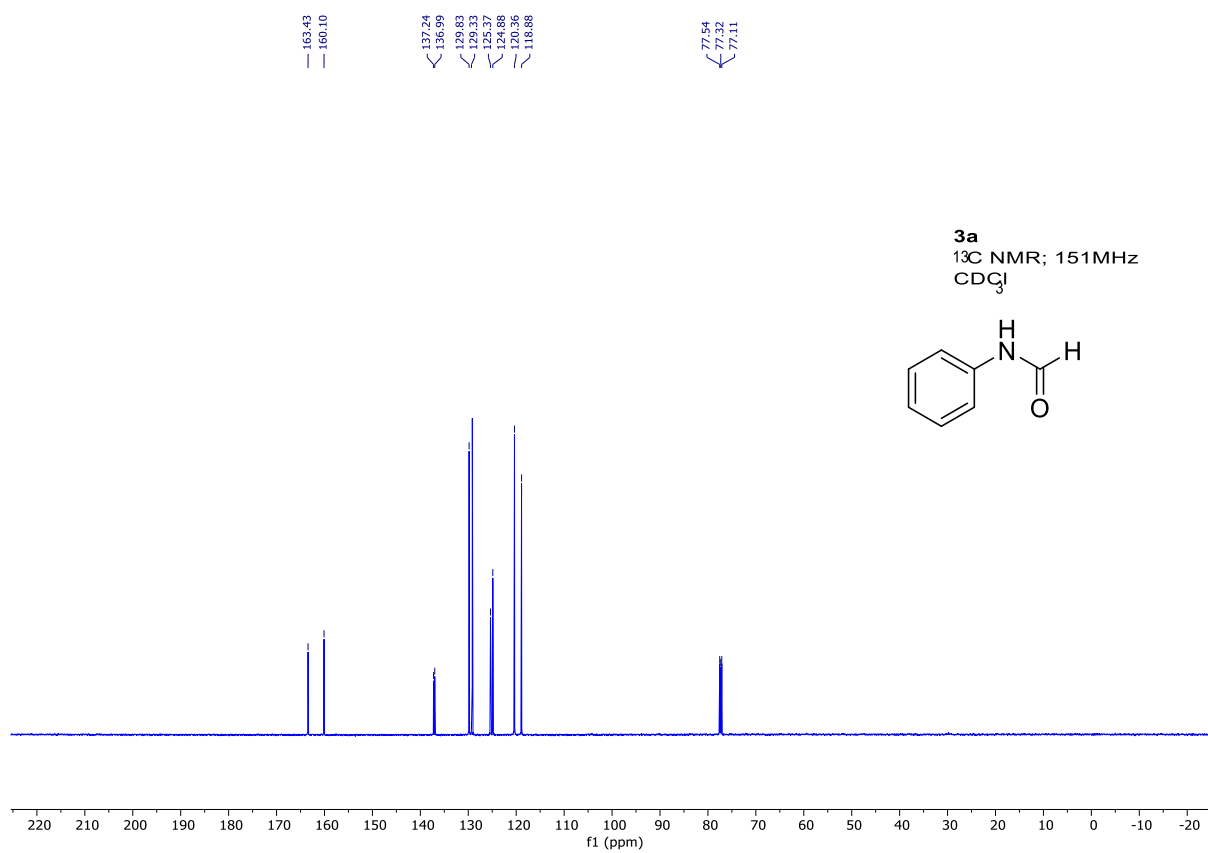
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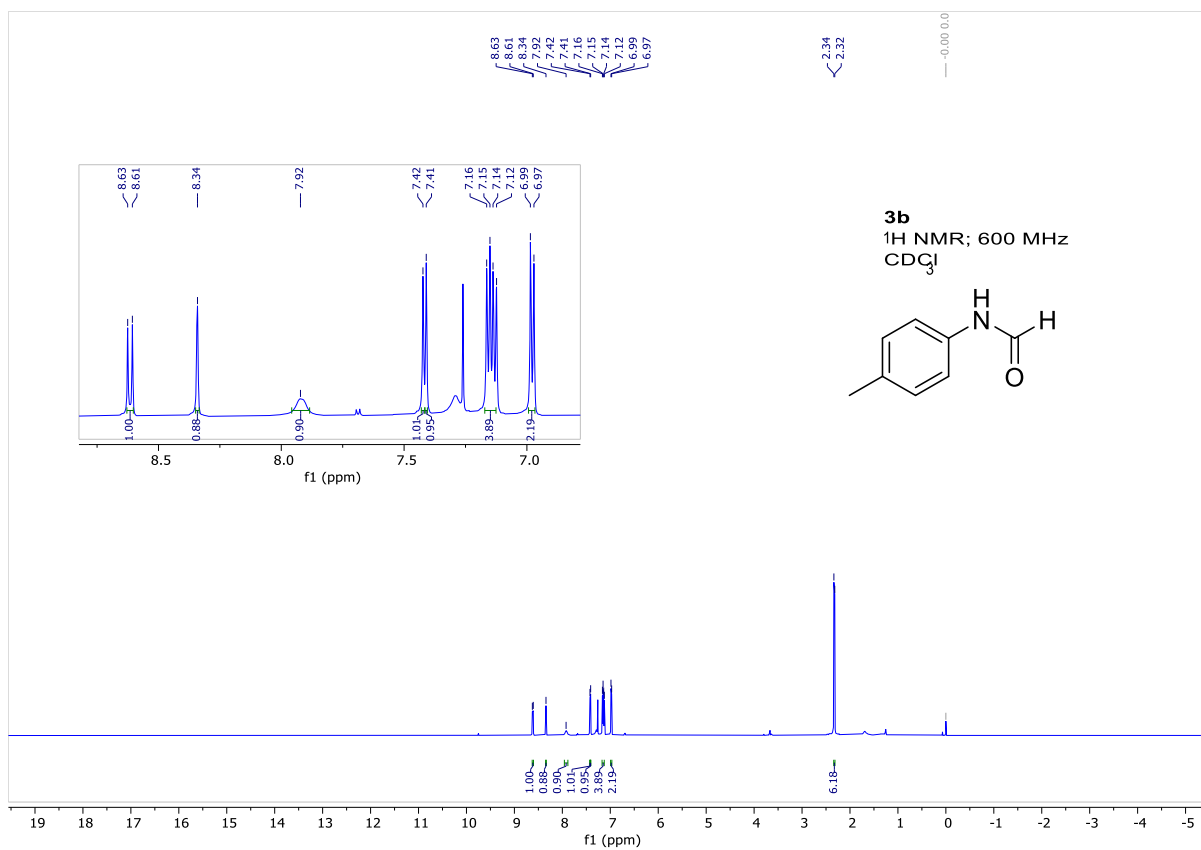
Copies of ^1H & ^{13}C NMR



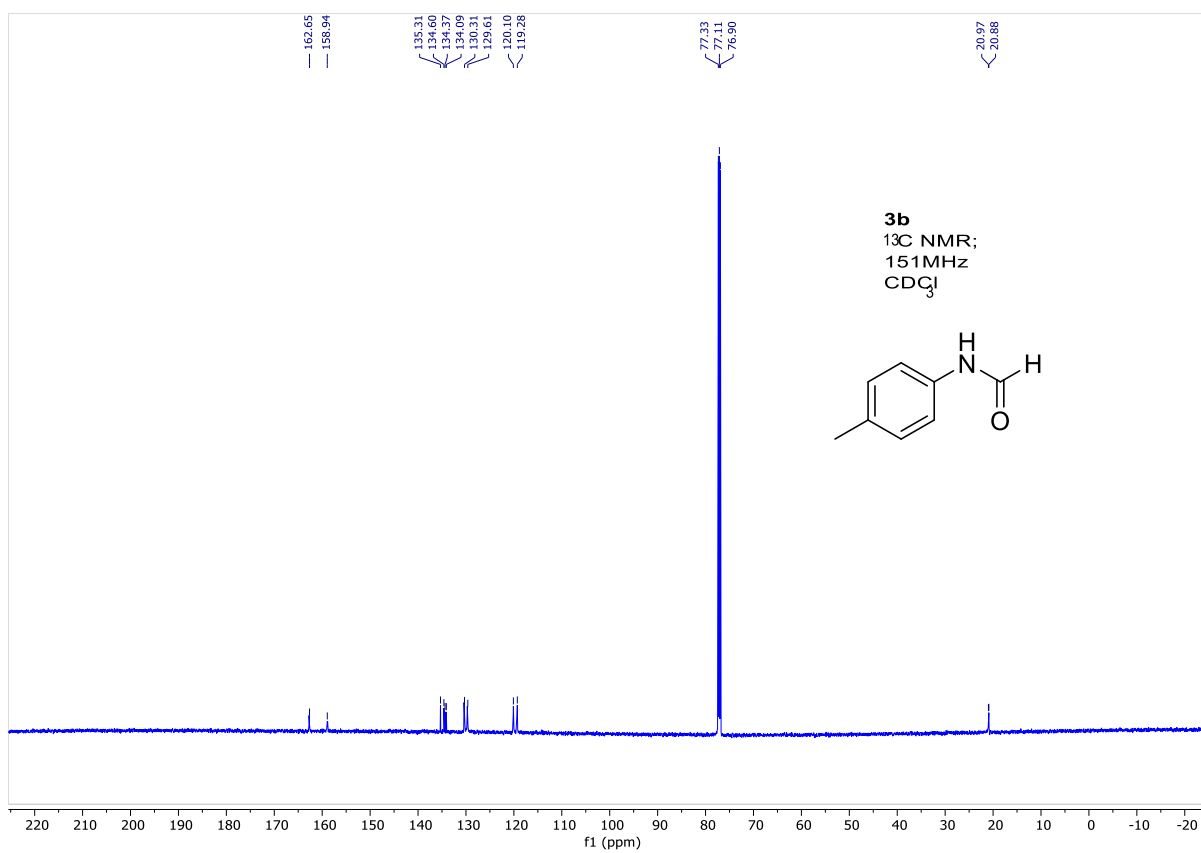
$^1\text{H NMR}$ 3a



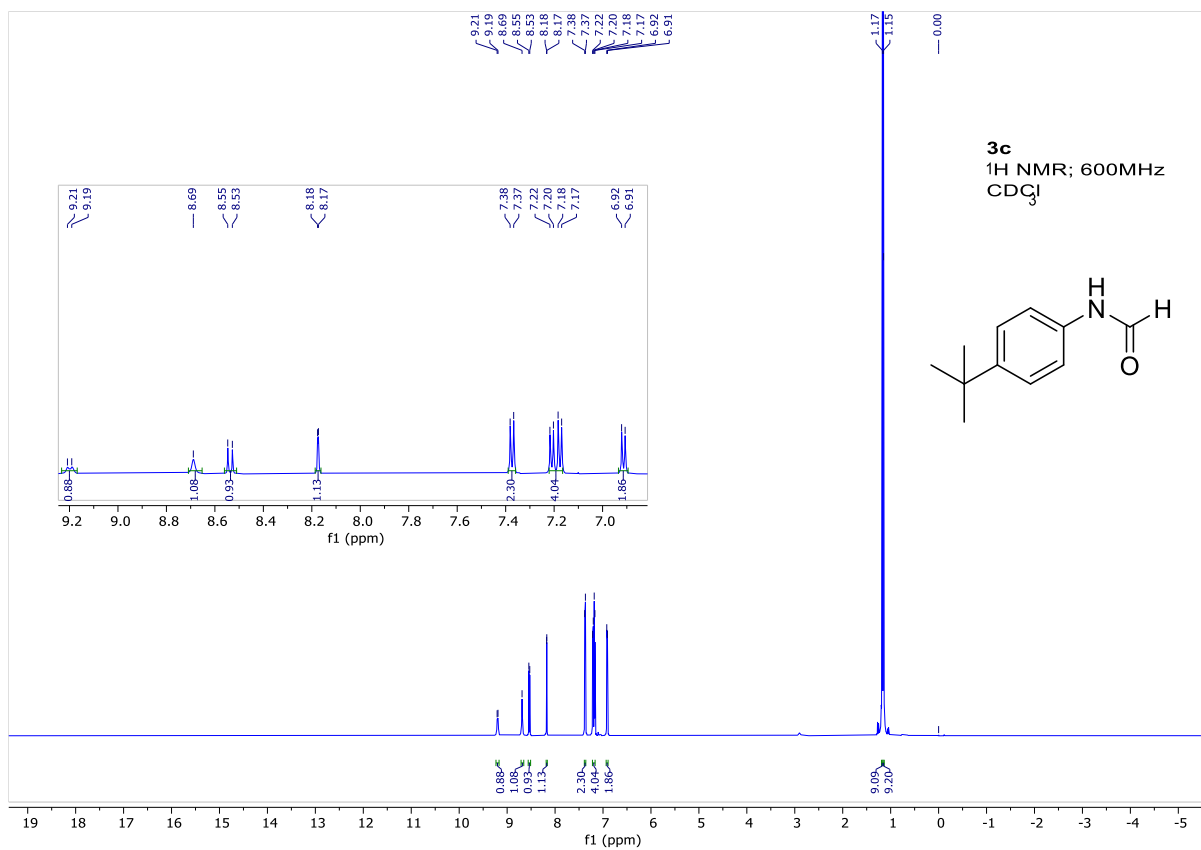
$^{13}\text{C NMR}$ 3a



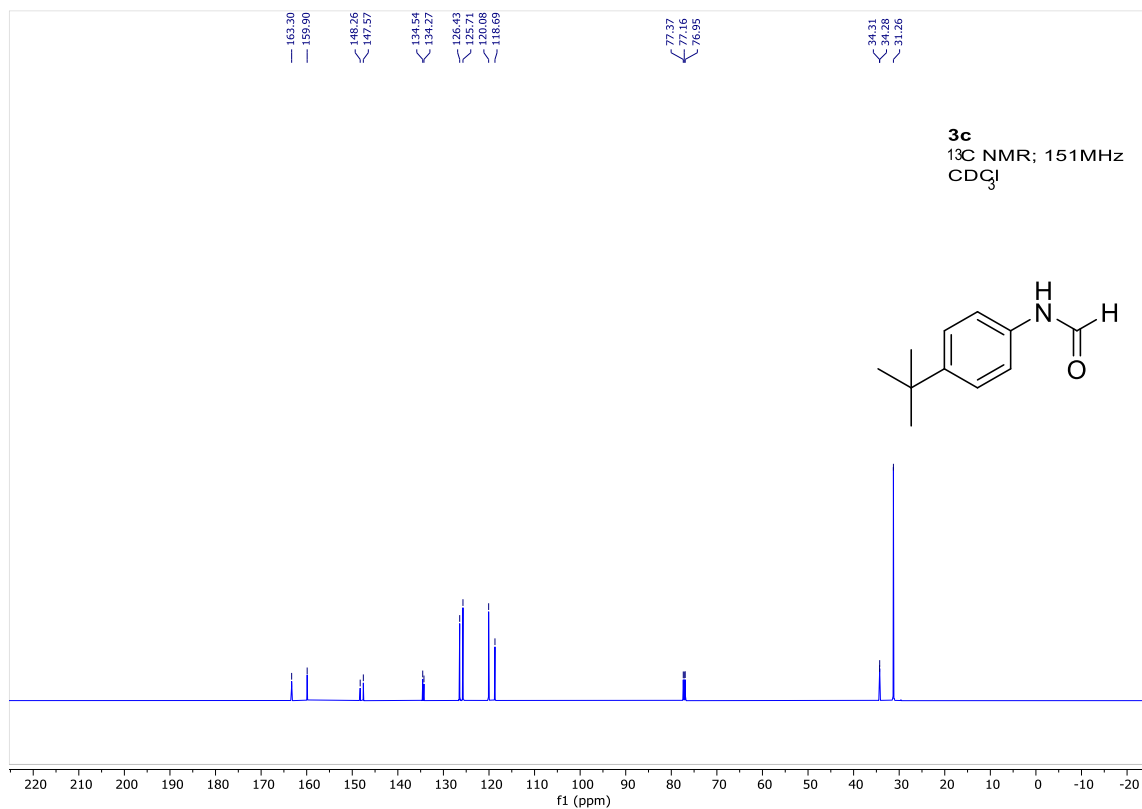
$^1\text{H NMR}$ 3b



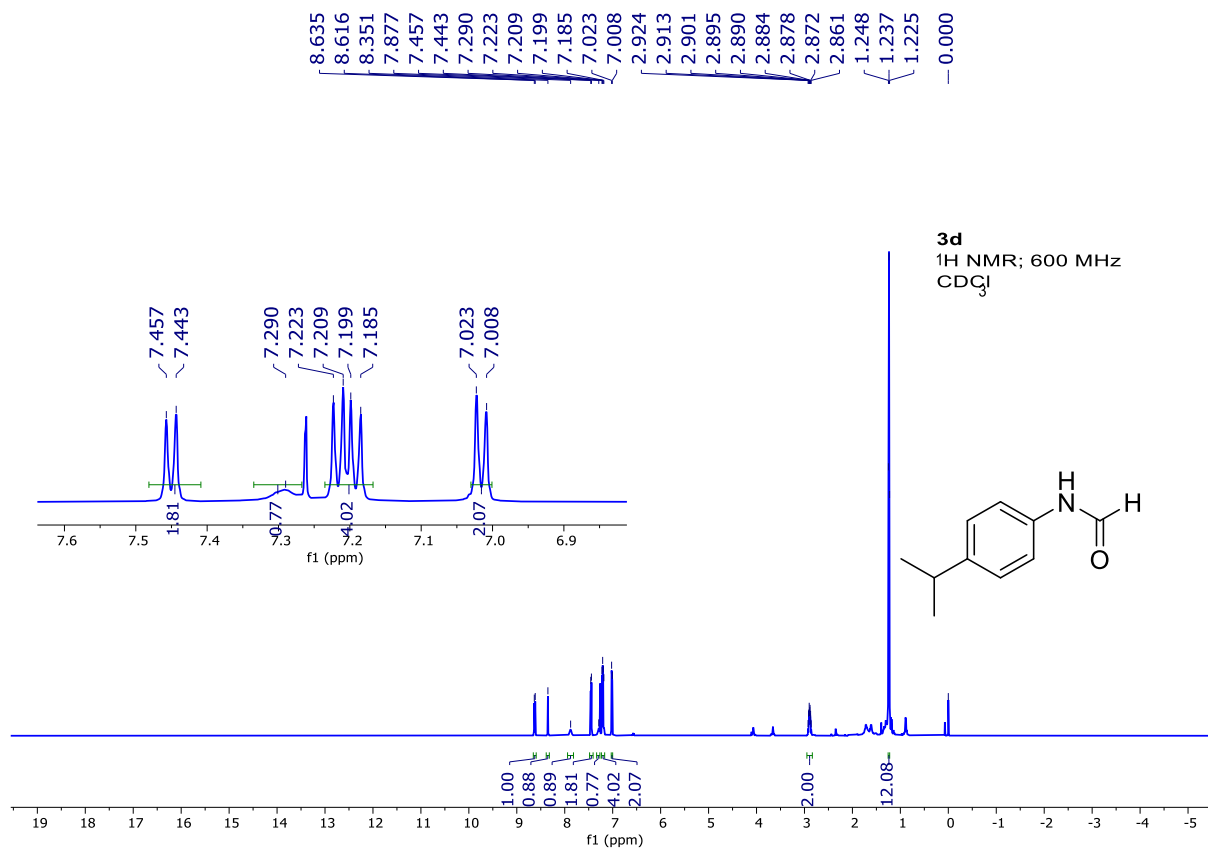
$^{13}\text{C NMR}$ 3b



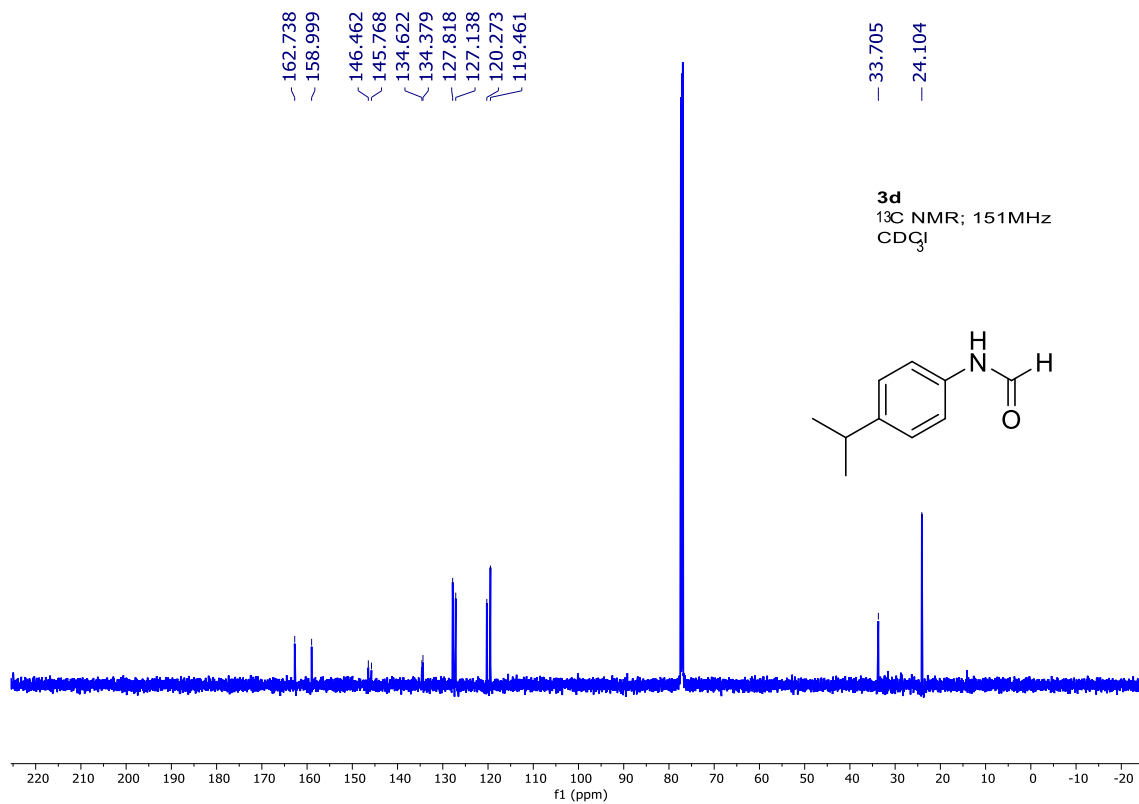
¹H NMR 3c



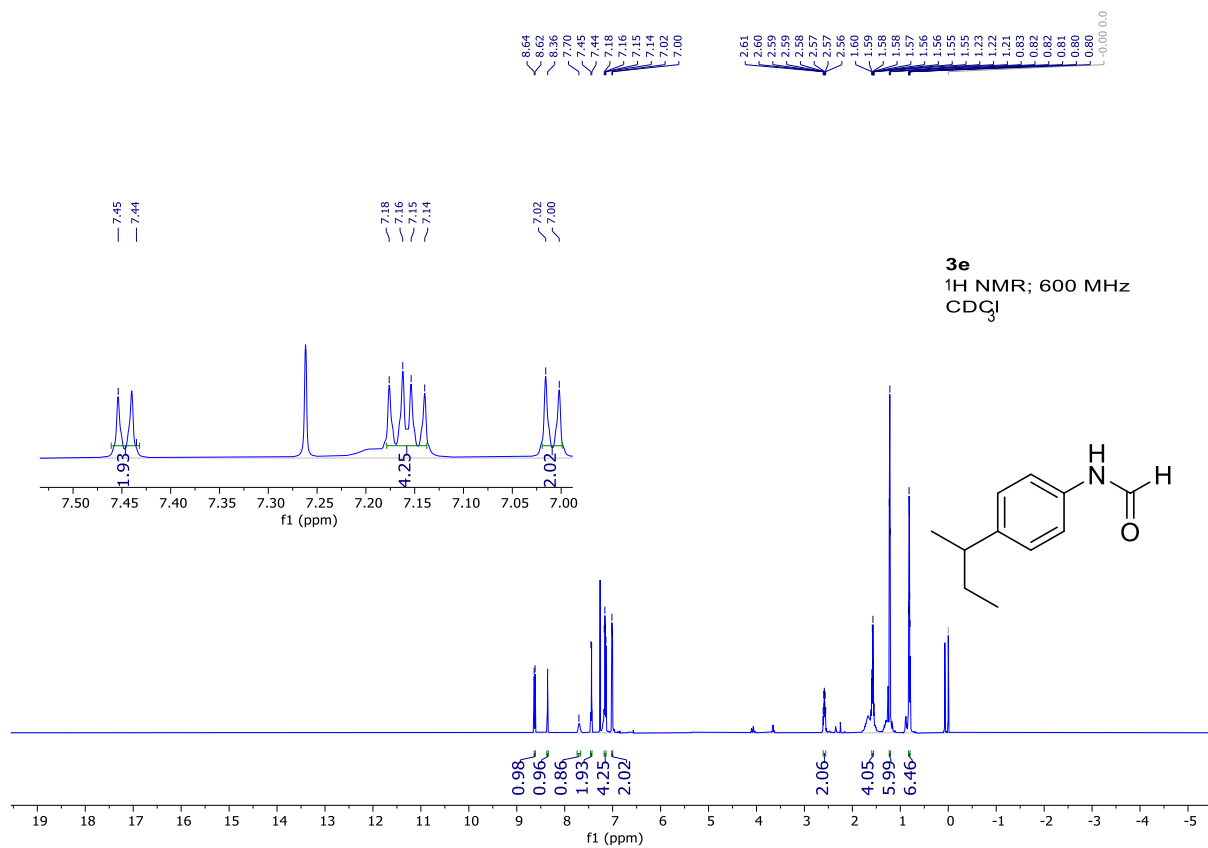
¹³C NMR 3c



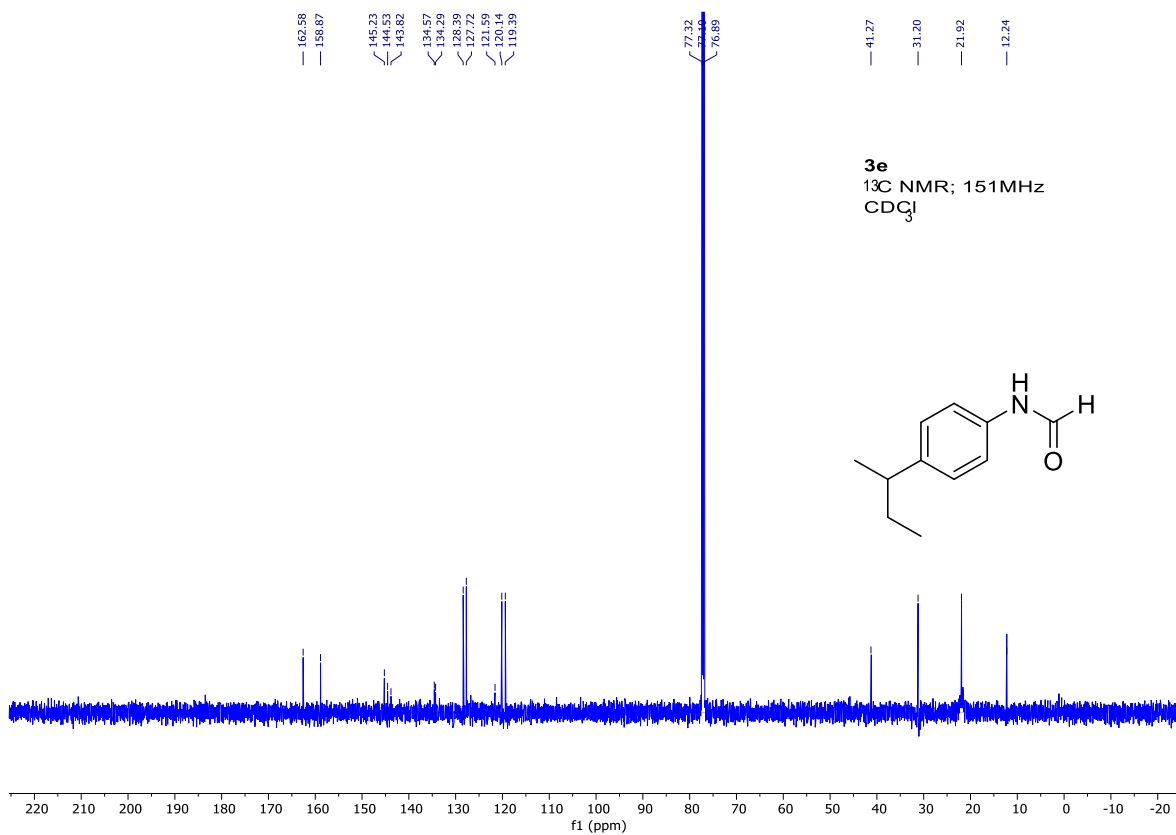
^1H NMR 3d



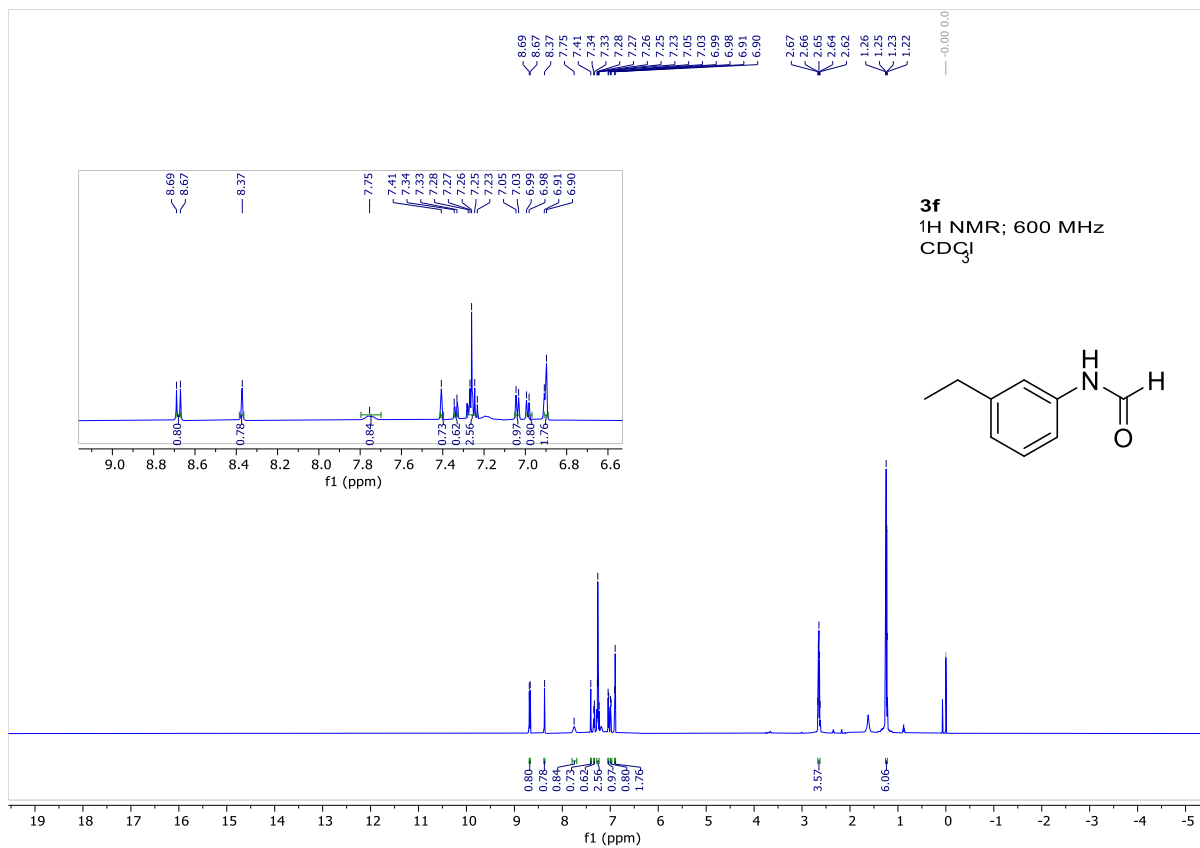
^{13}C NMR 3d



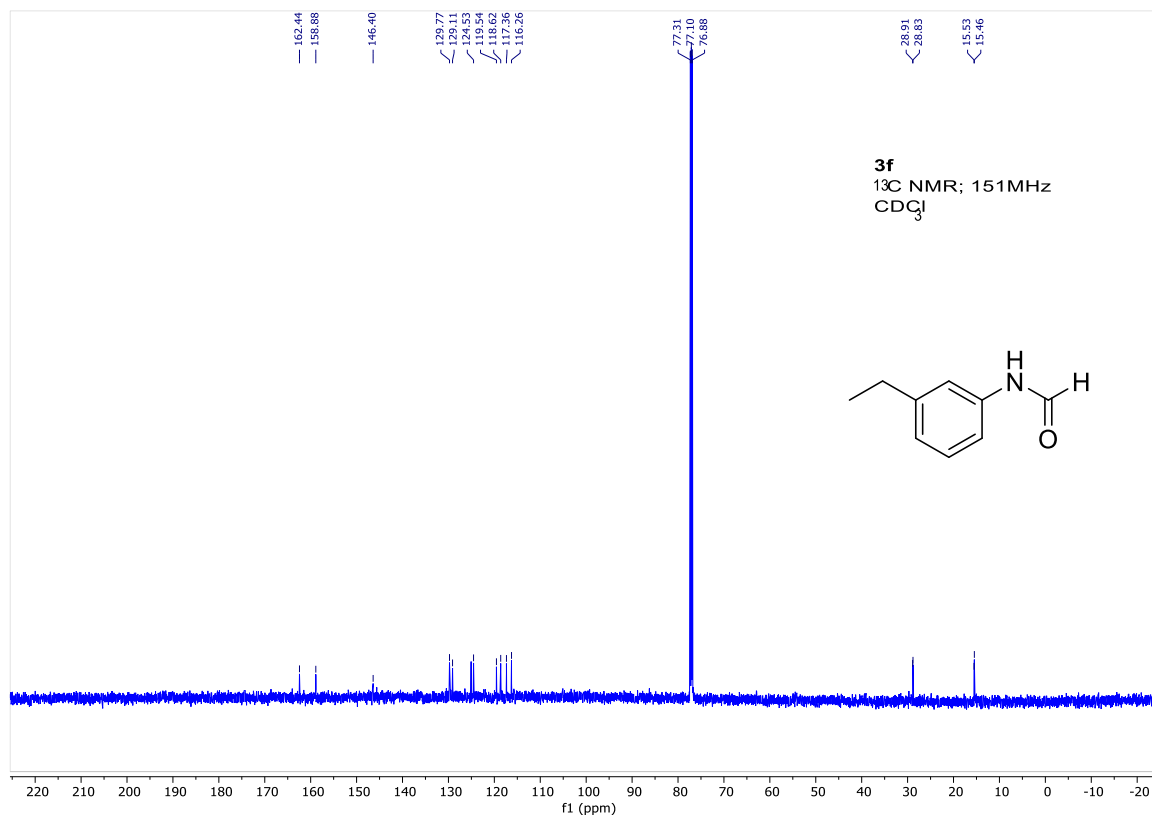
¹H NMR 3e



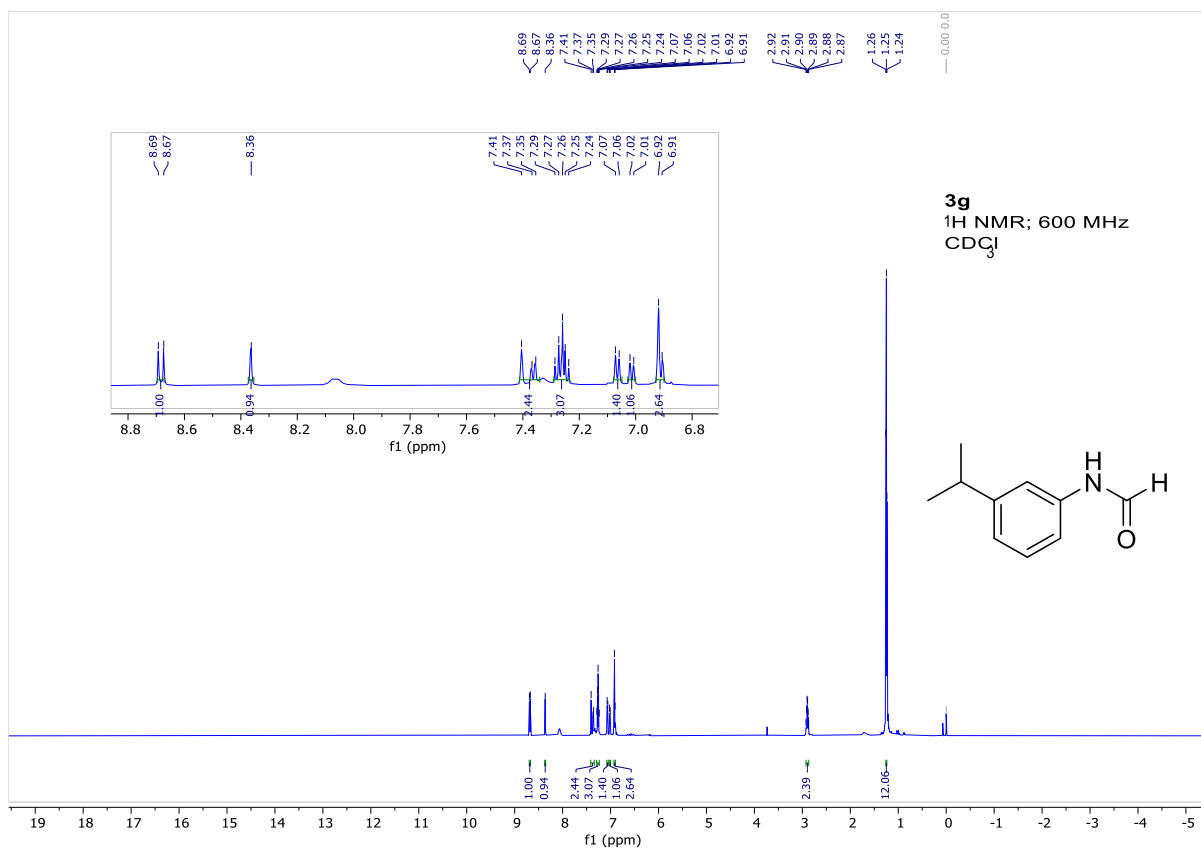
¹³C NMR 3e



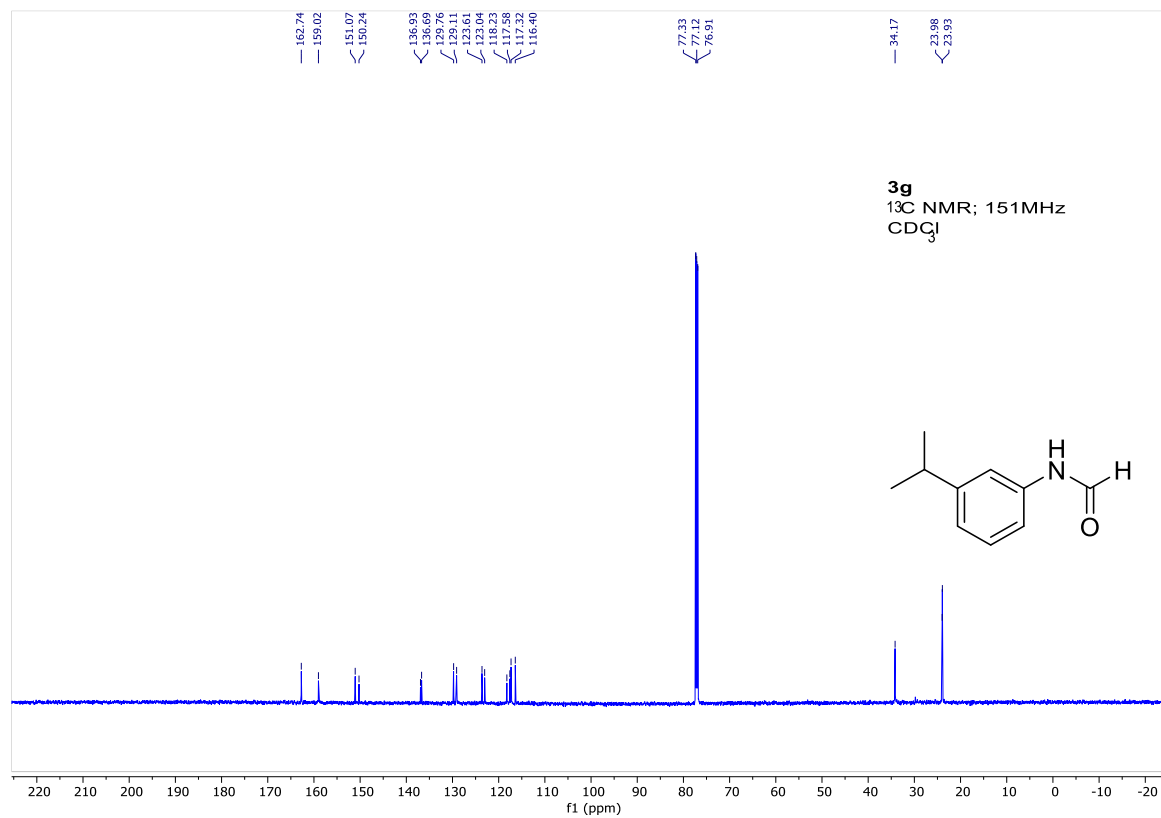
^1H NMR 3f



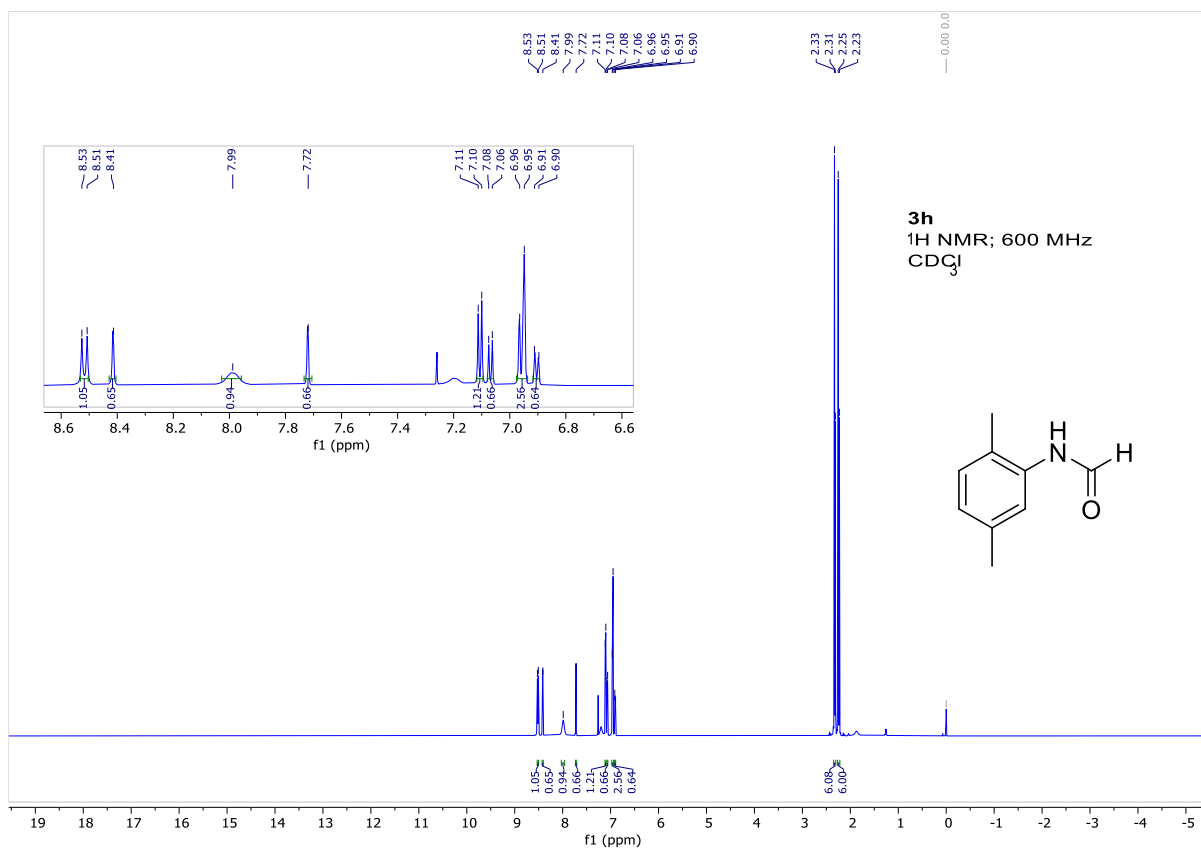
^{13}C NMR 3f



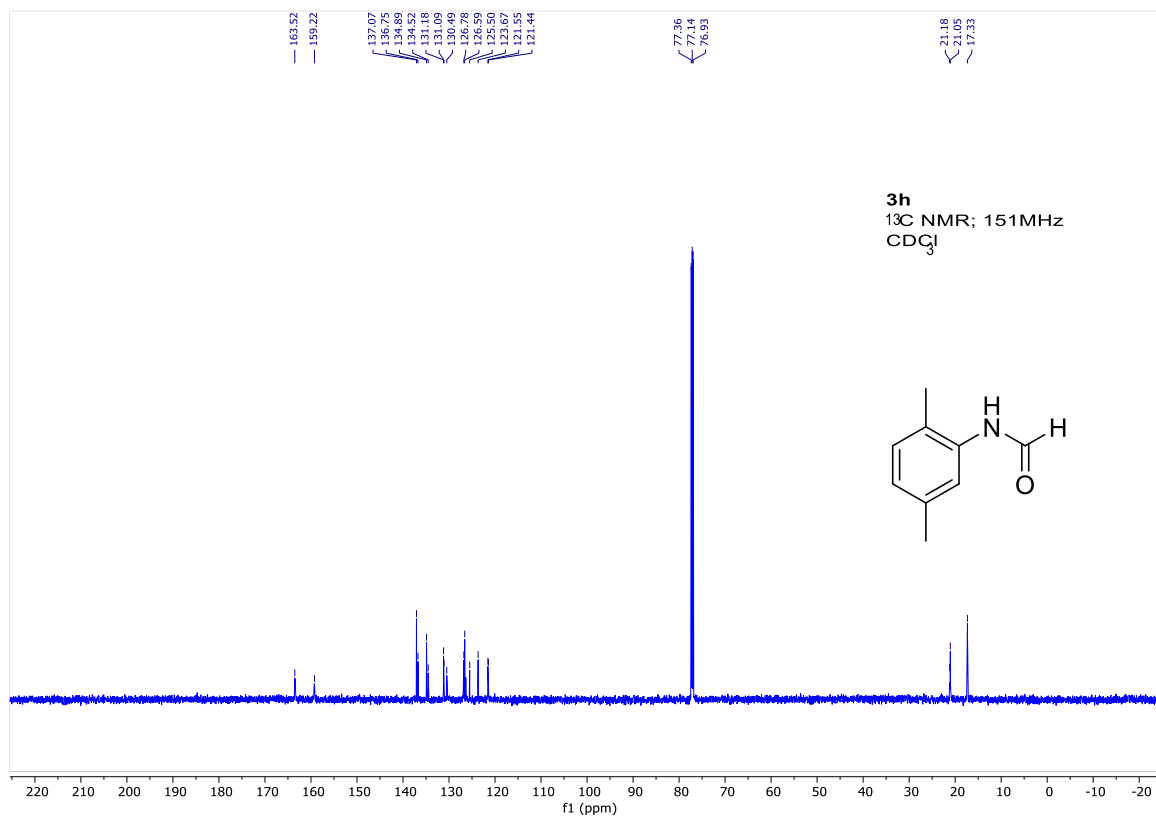
¹H NMR **3g**



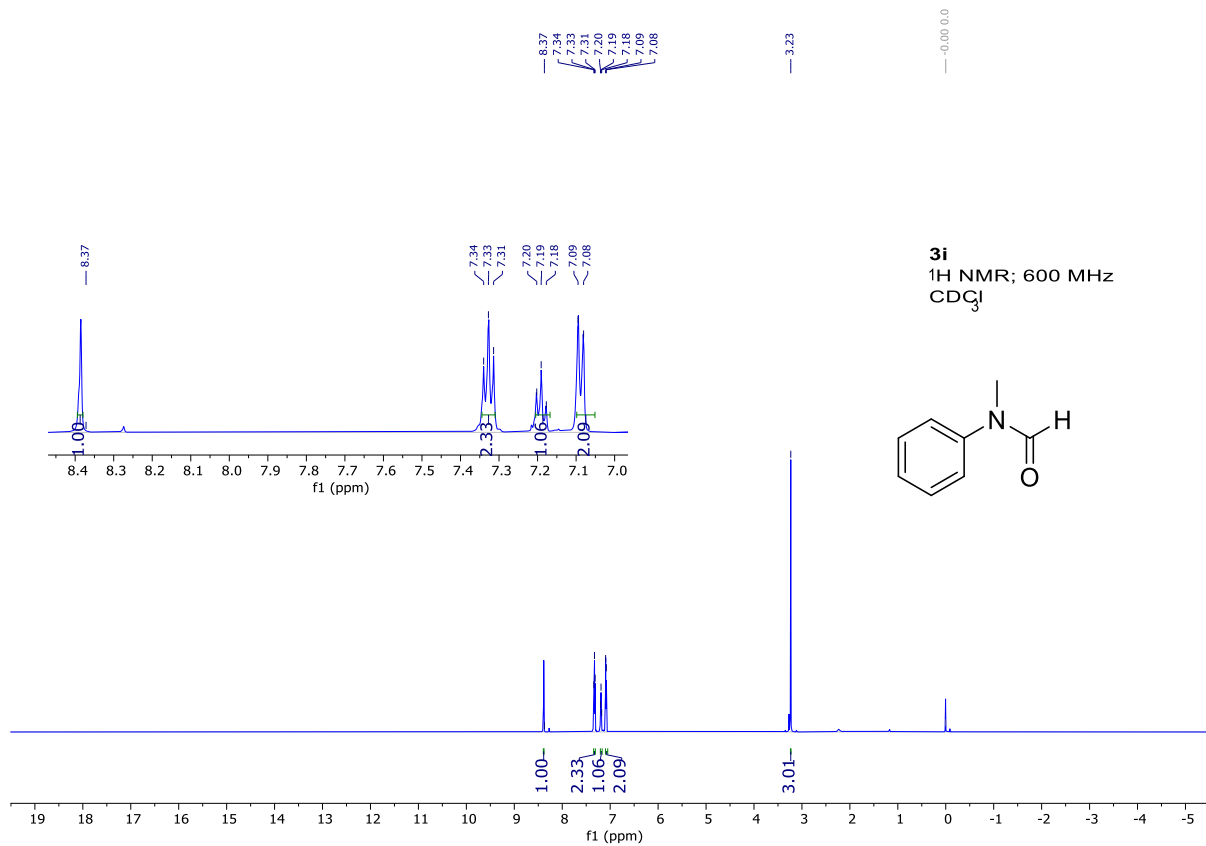
¹³C NMR **3g**



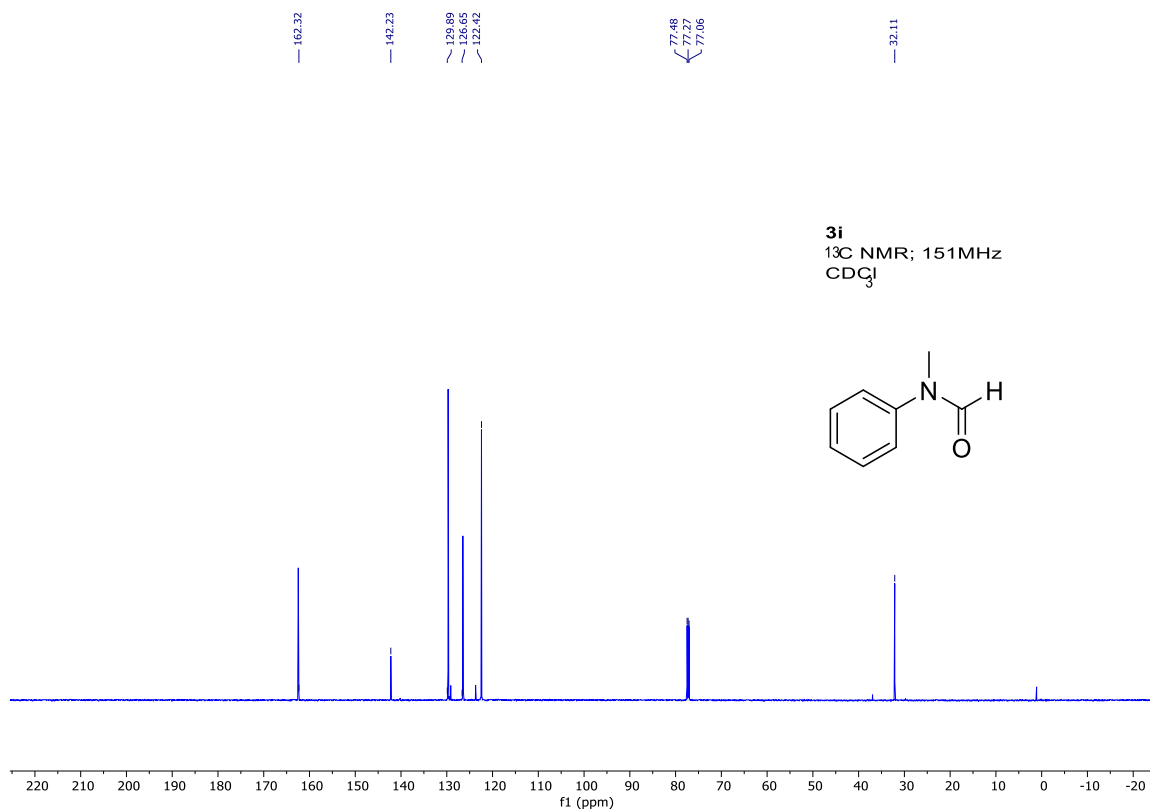
^1H NMR 3h



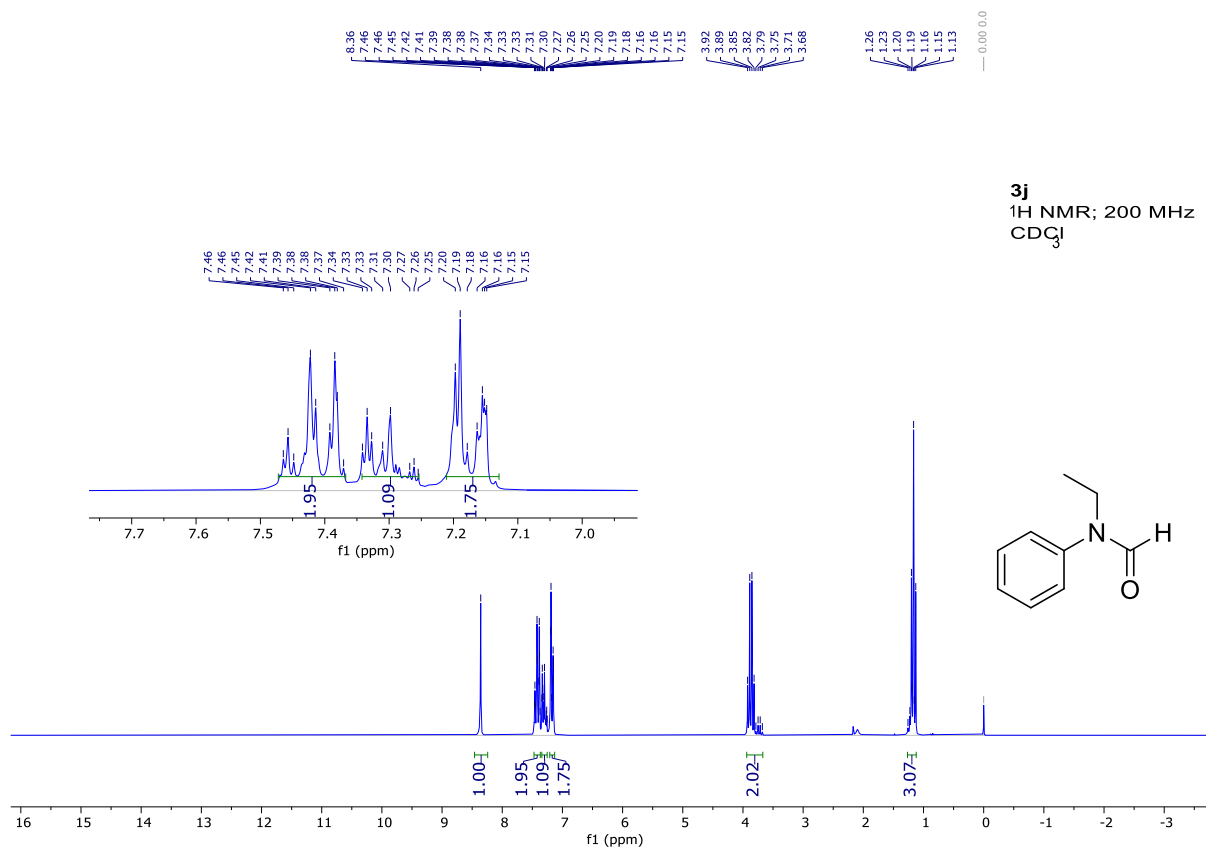
^{13}C NMR 3h



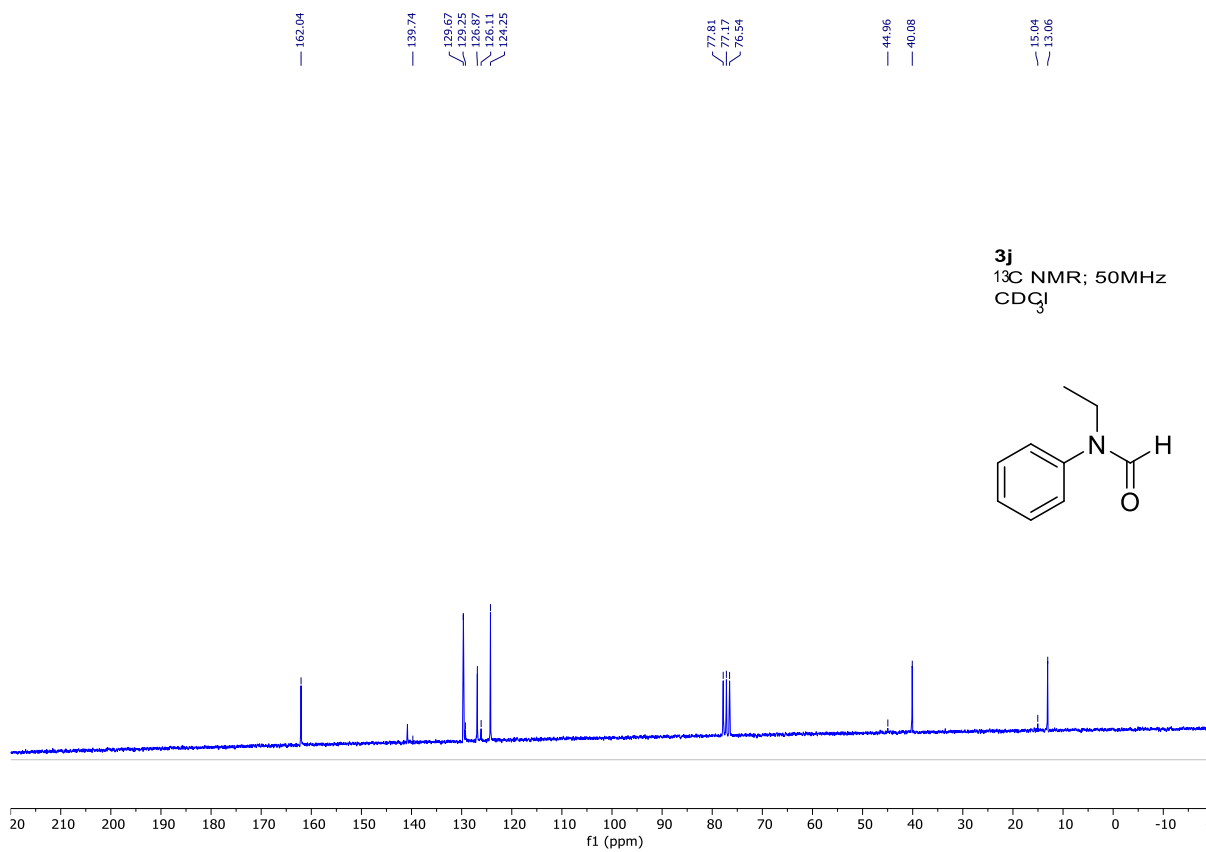
^1H NMR 3i



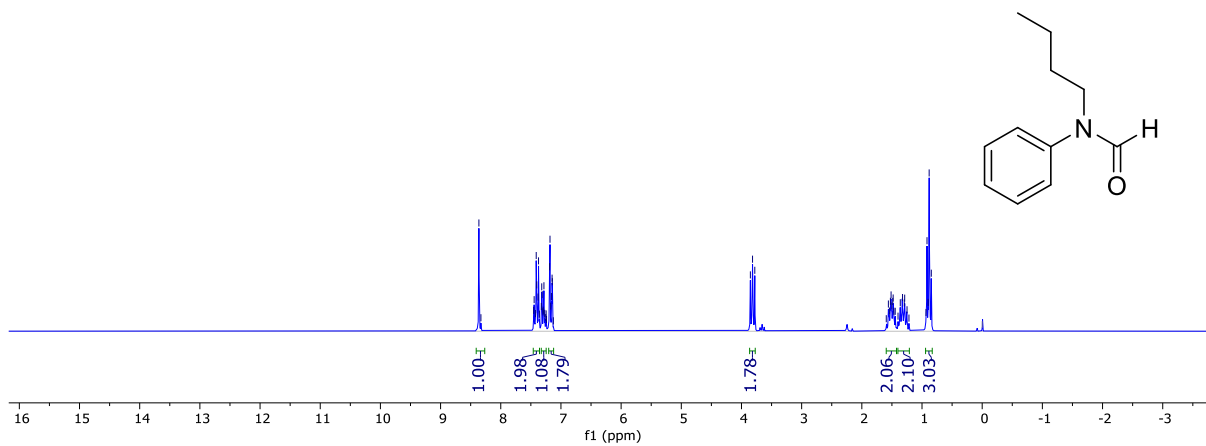
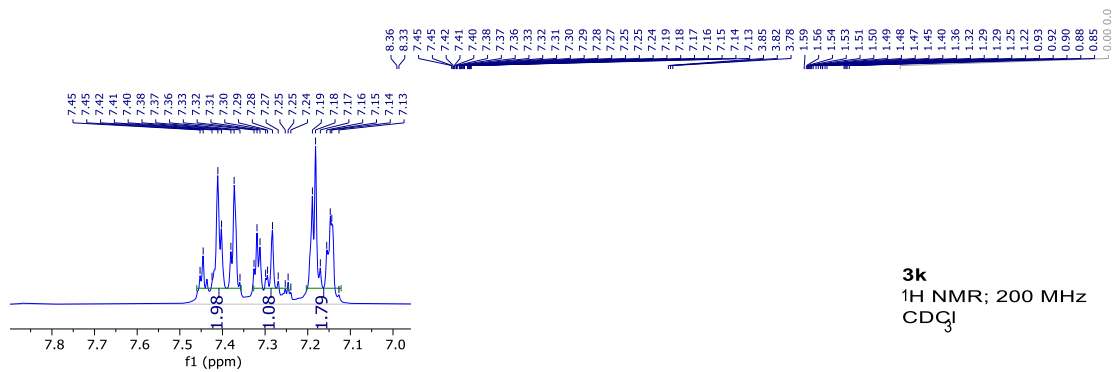
^{13}C NMR 3i



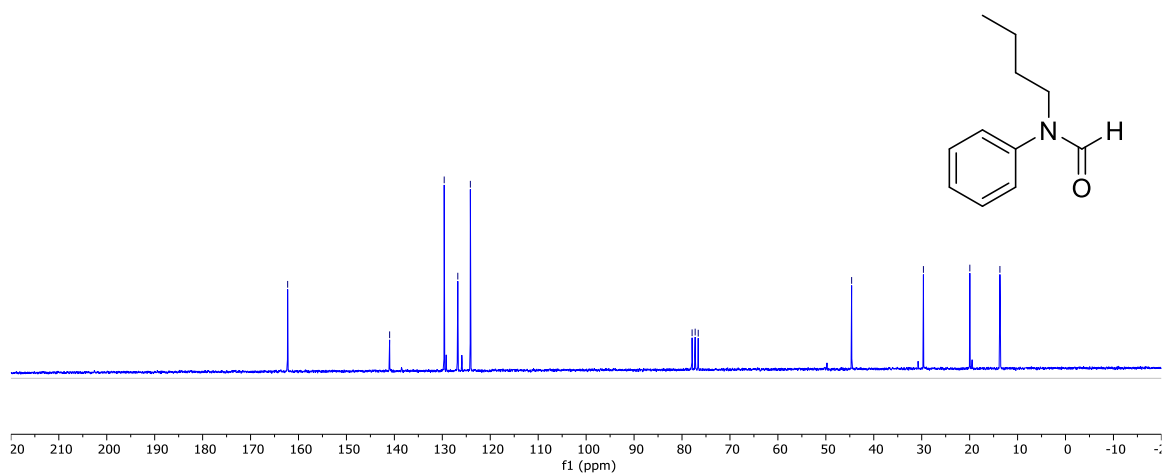
^1H NMR 3j



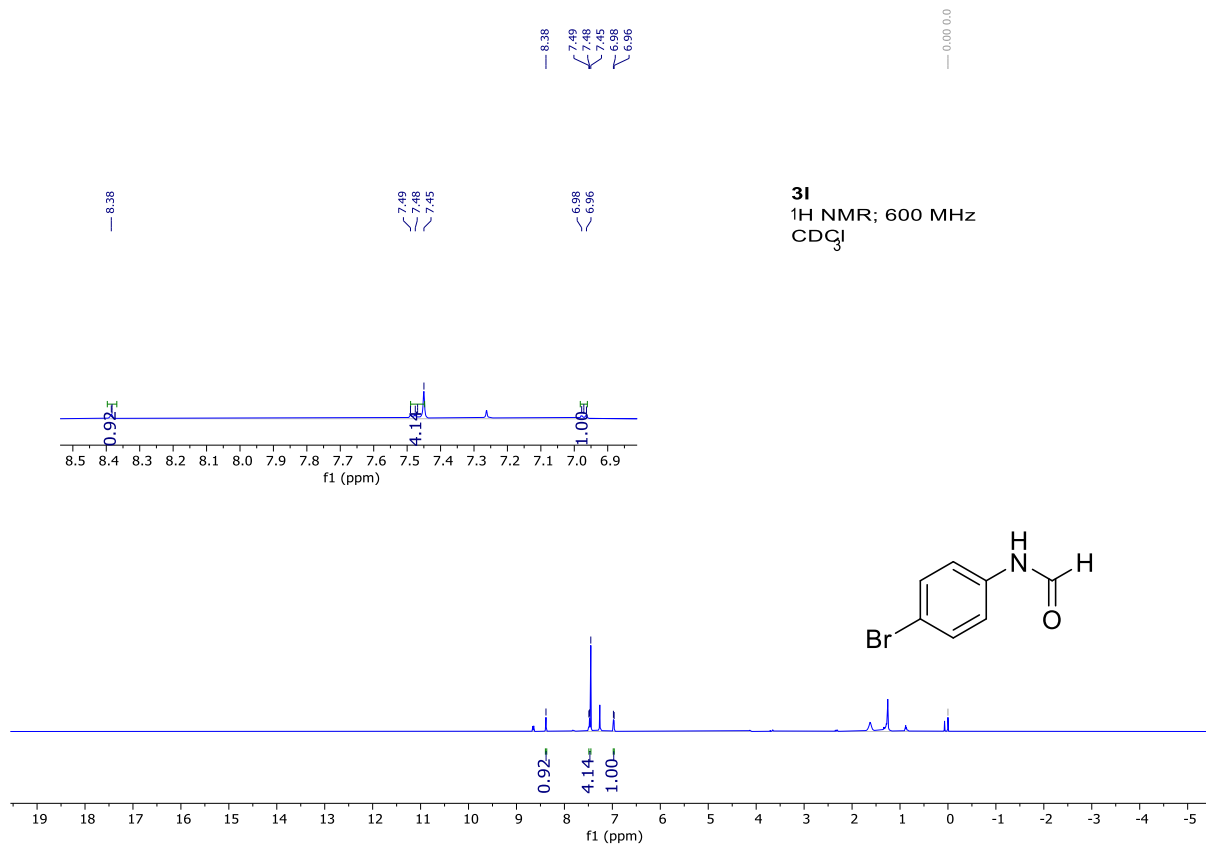
^{13}C NMR 3j



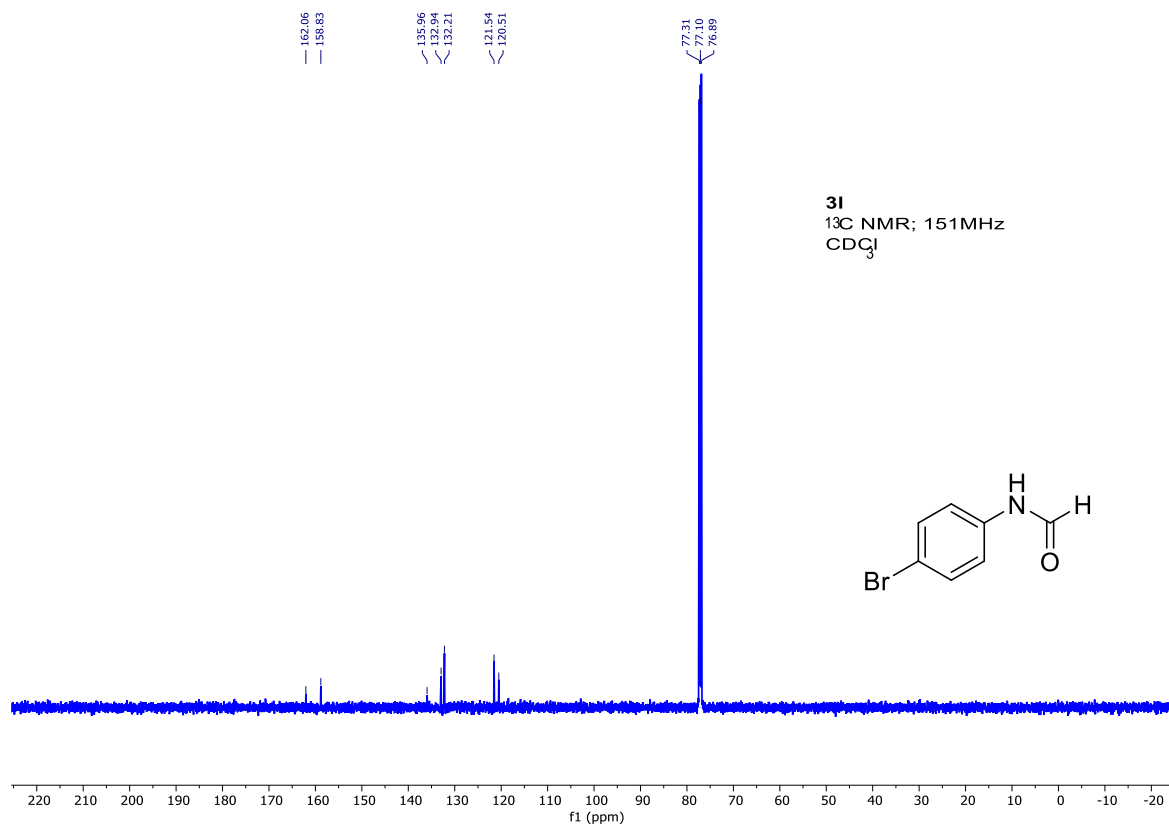
^1H NMR 3k



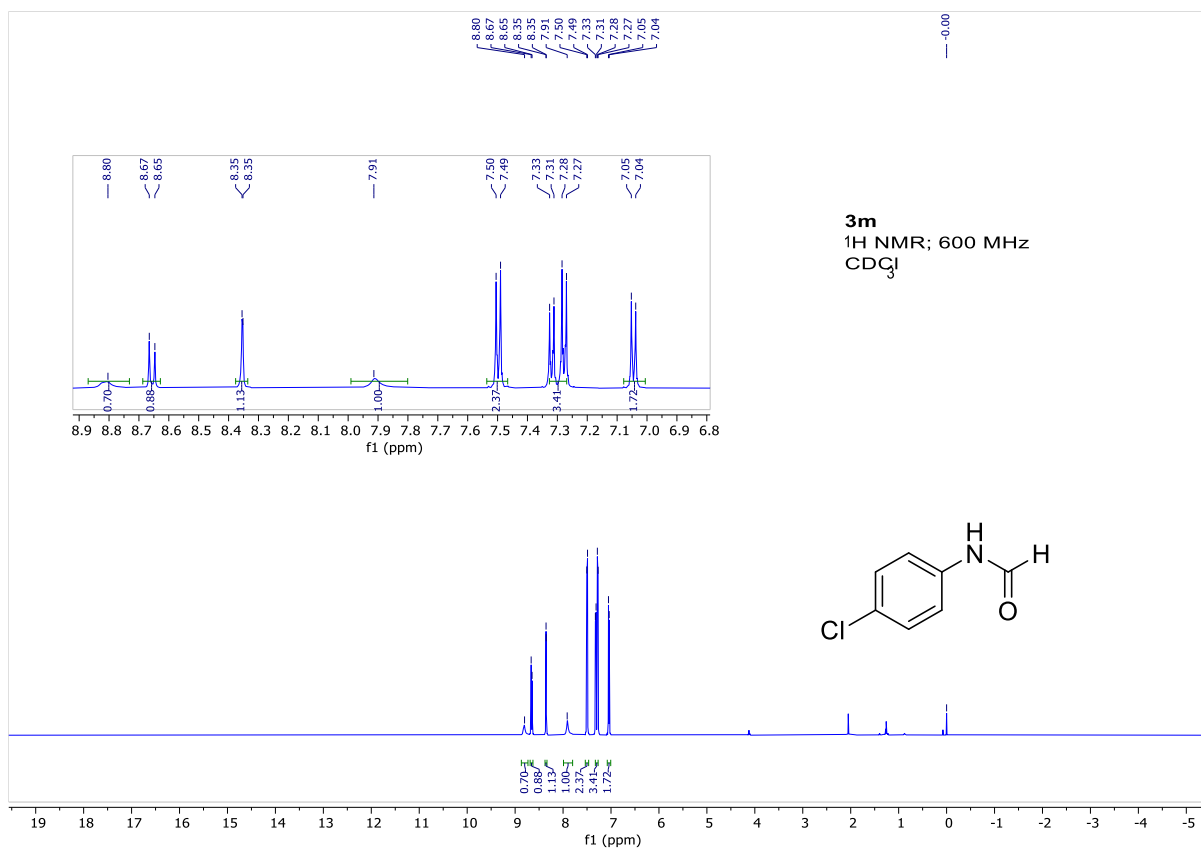
^{13}C NMR 3k



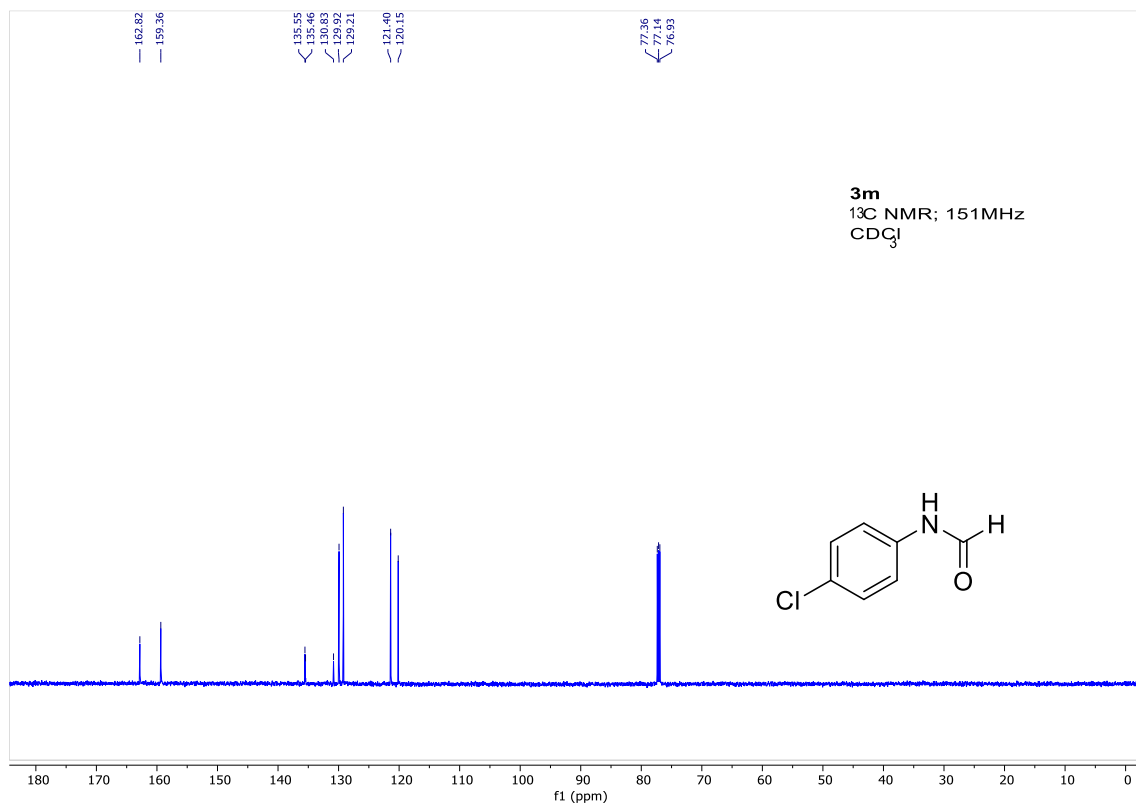
¹H NMR 3I



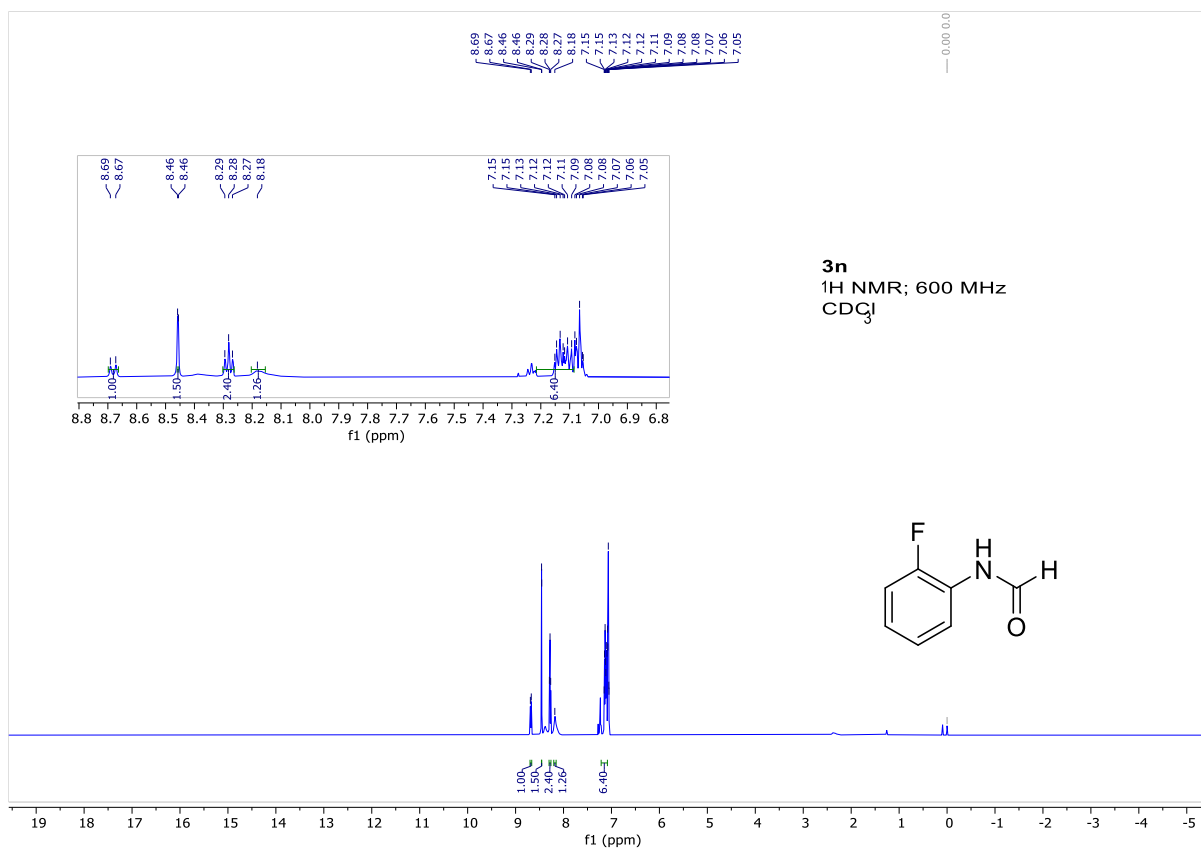
¹³C NMR 3I



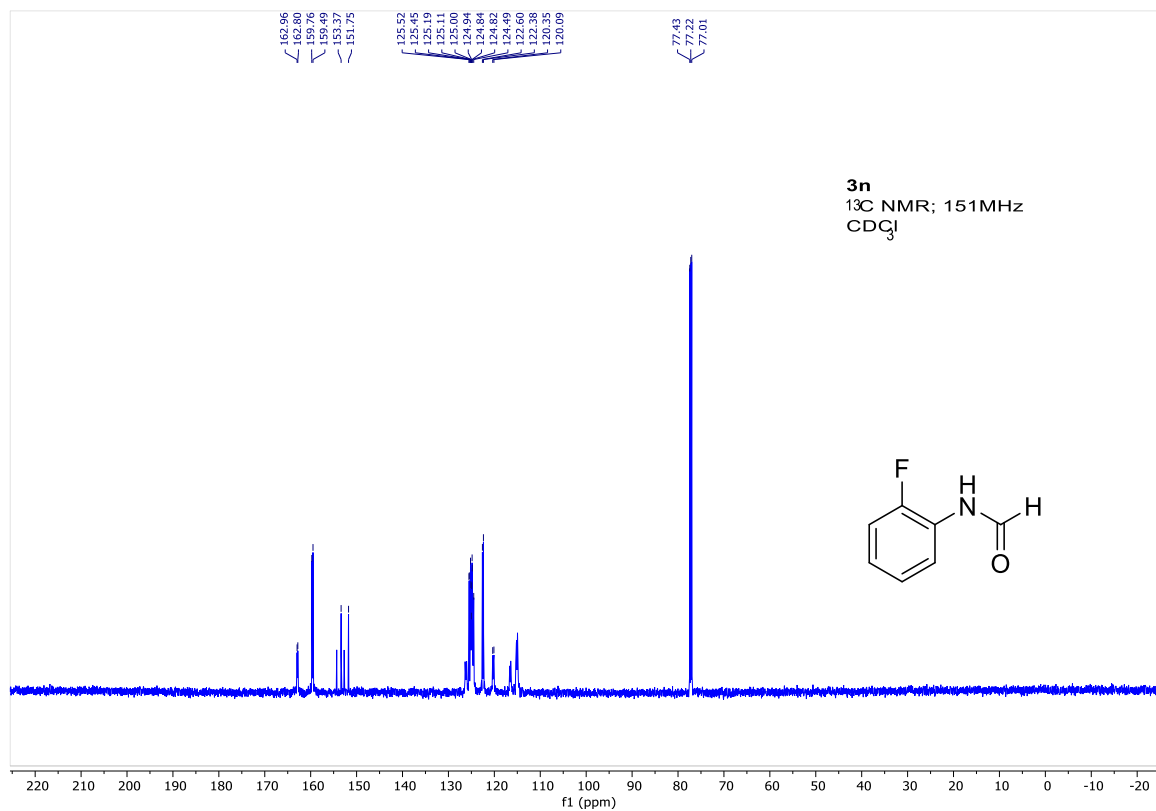
¹H NMR 3m



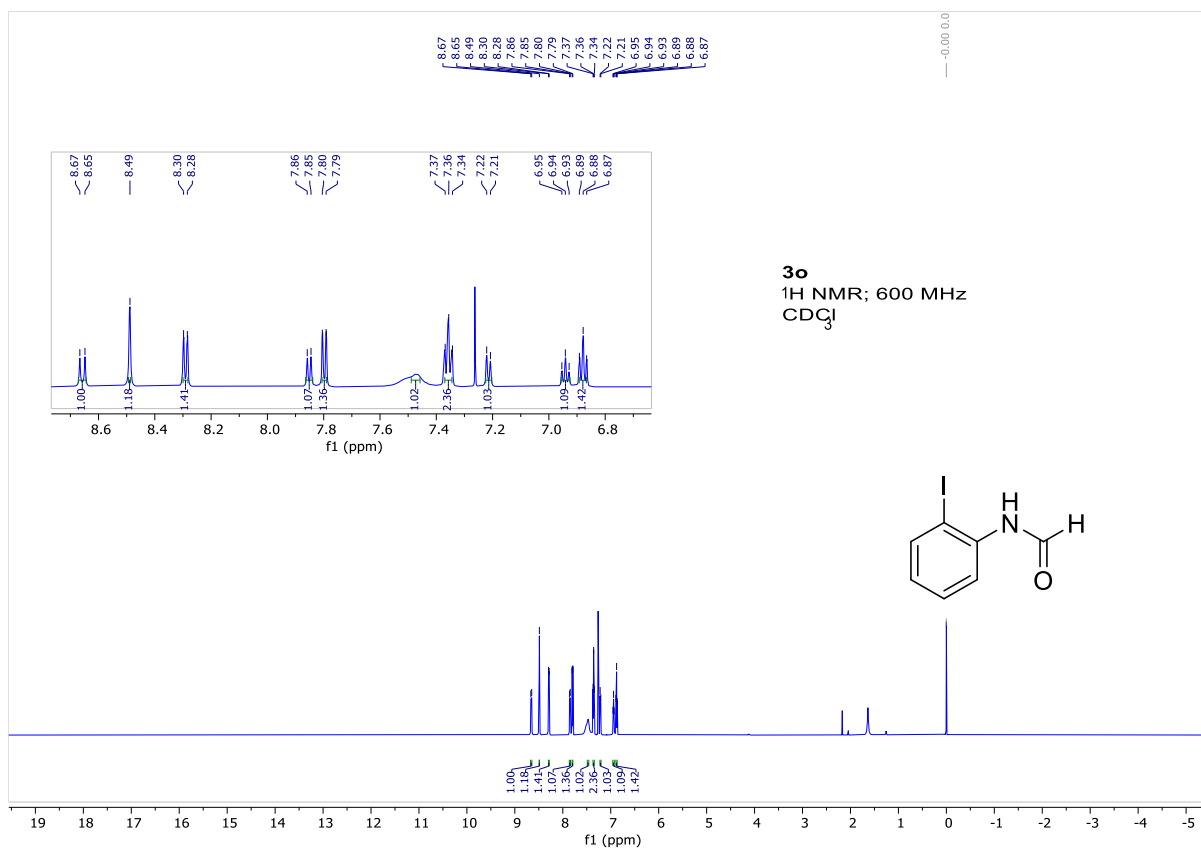
¹³C NMR 3m



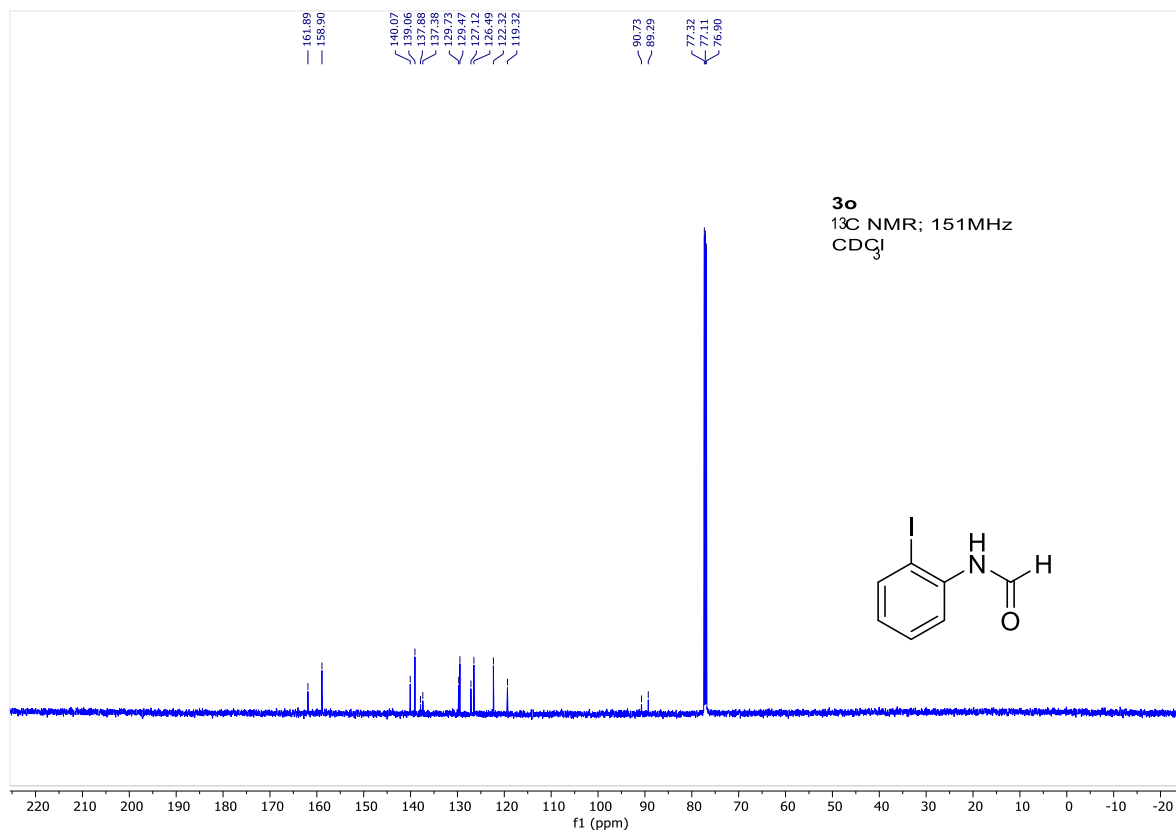
¹H NMR 3n



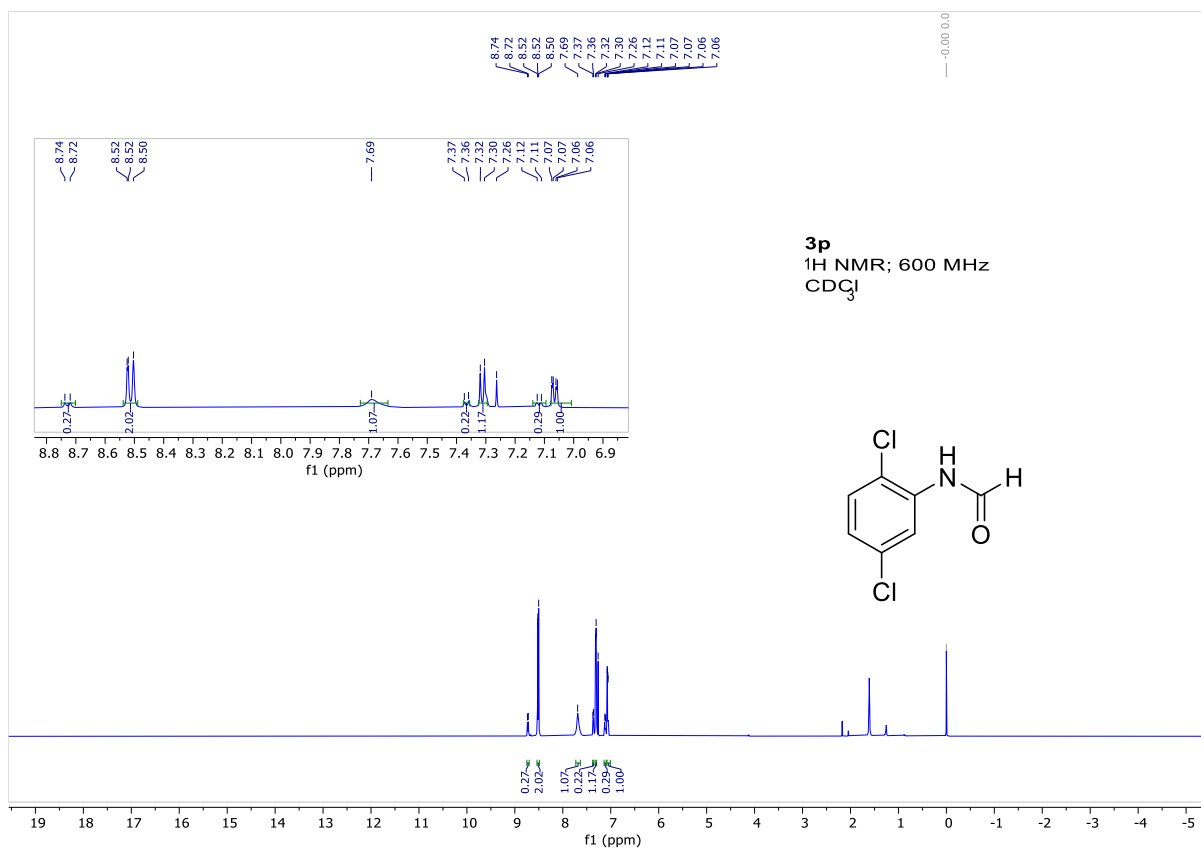
¹³C NMR 3n



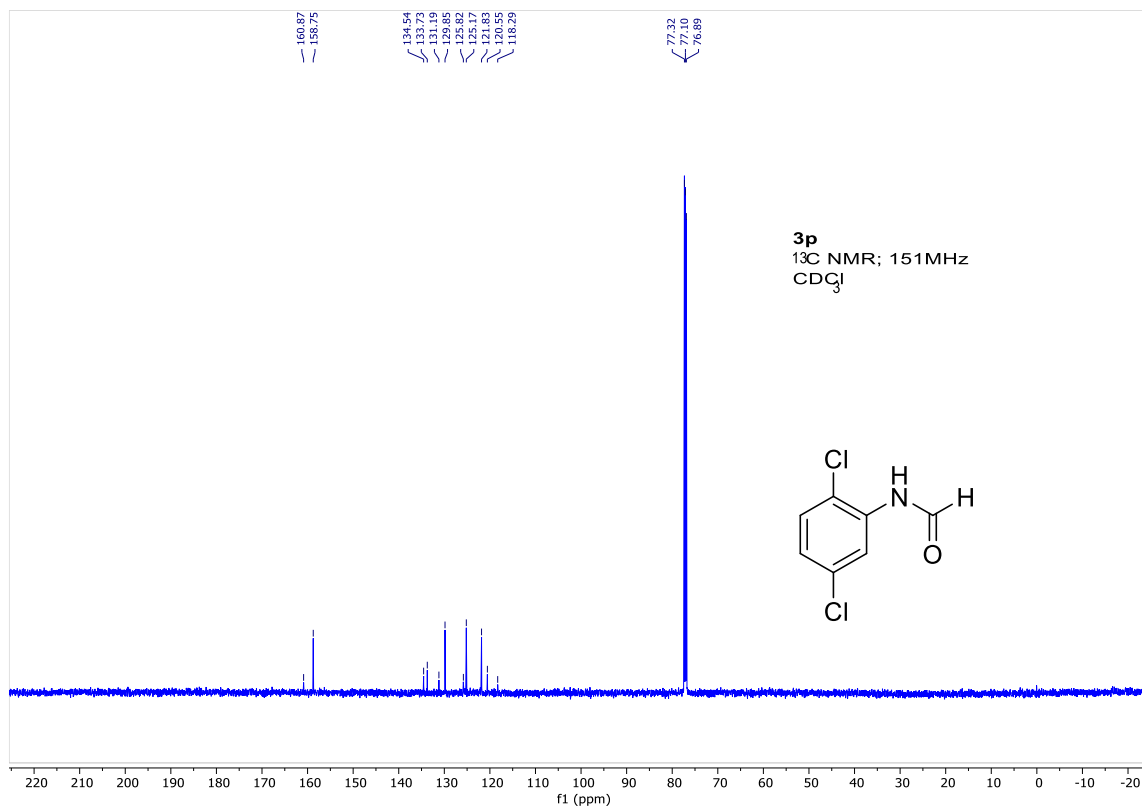
$^1\text{H NMR}$ 3o



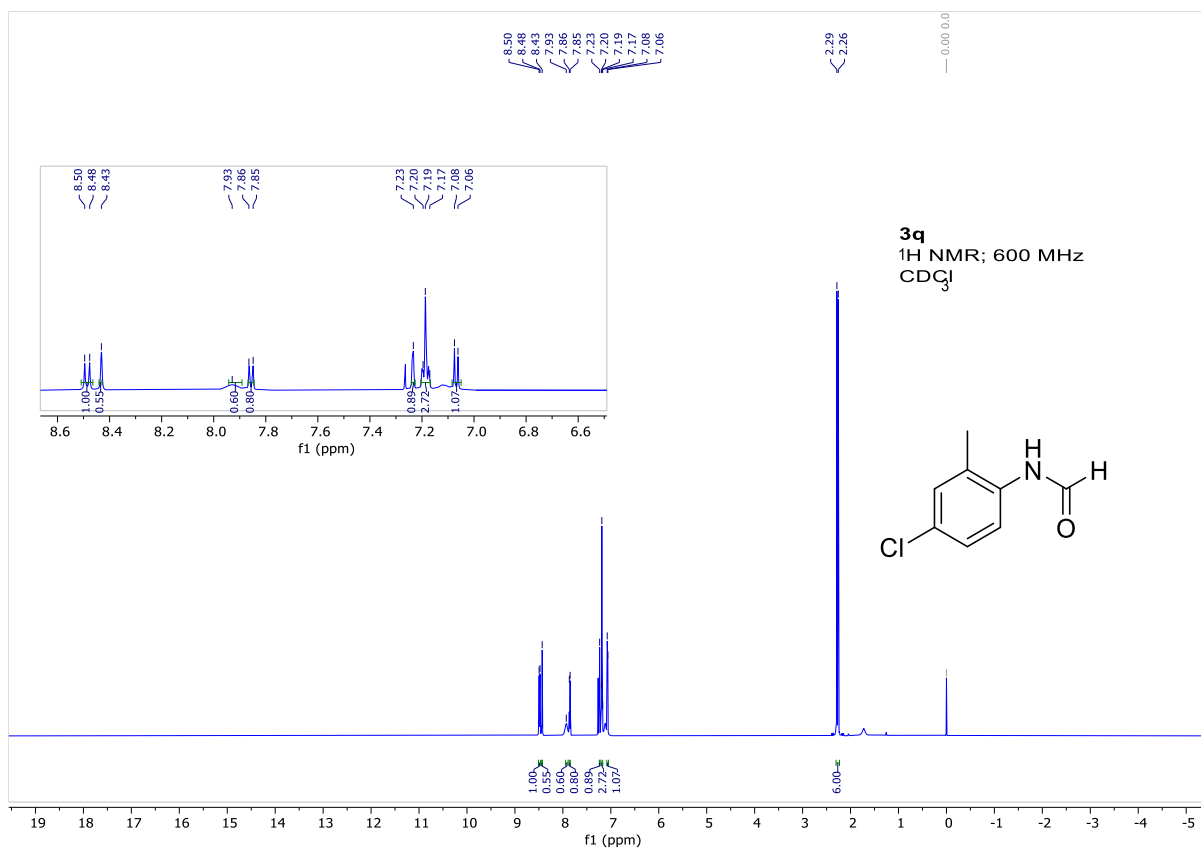
$^{13}\text{C NMR}$ 3o



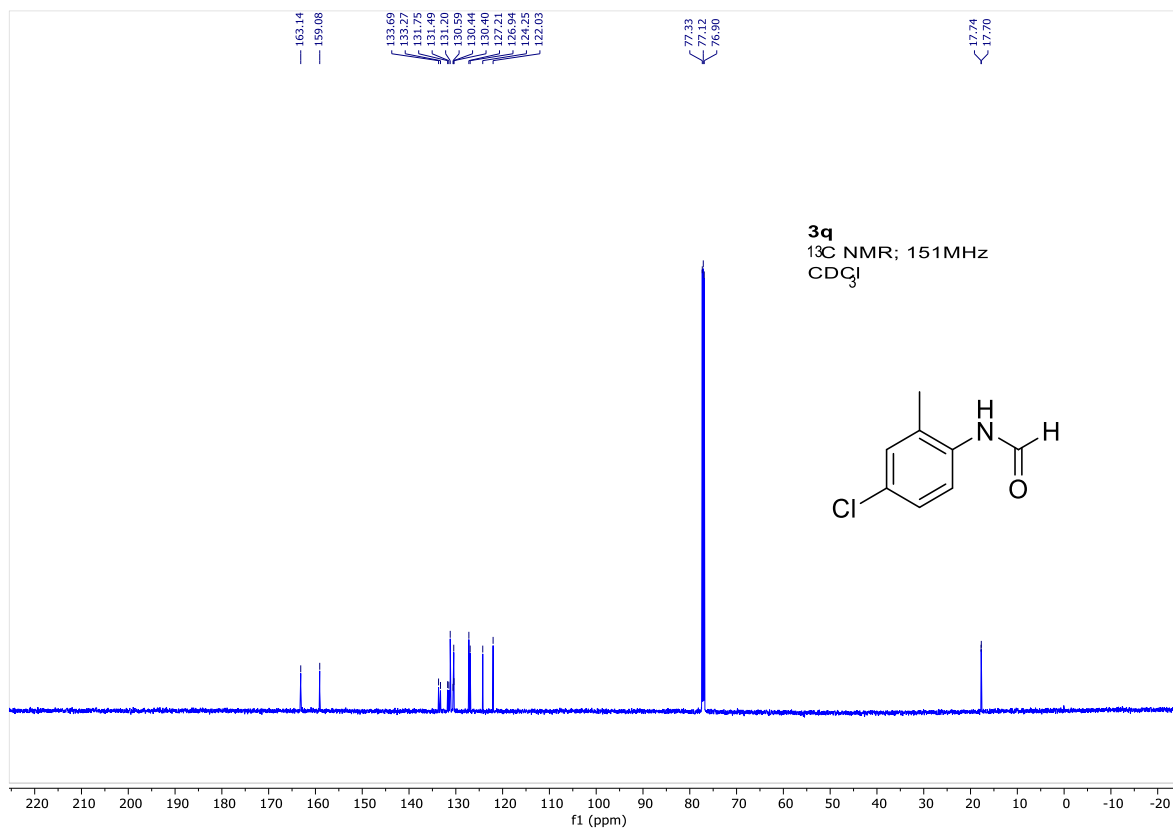
$^1\text{H NMR}$ 3p



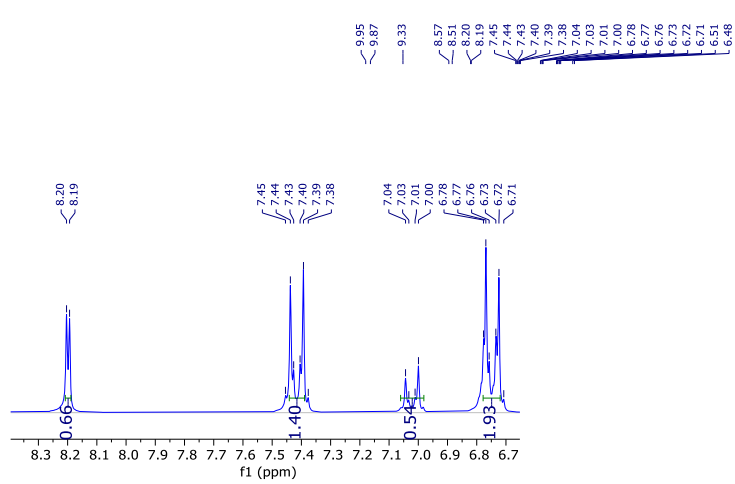
$^{13}\text{C NMR}$ 3p



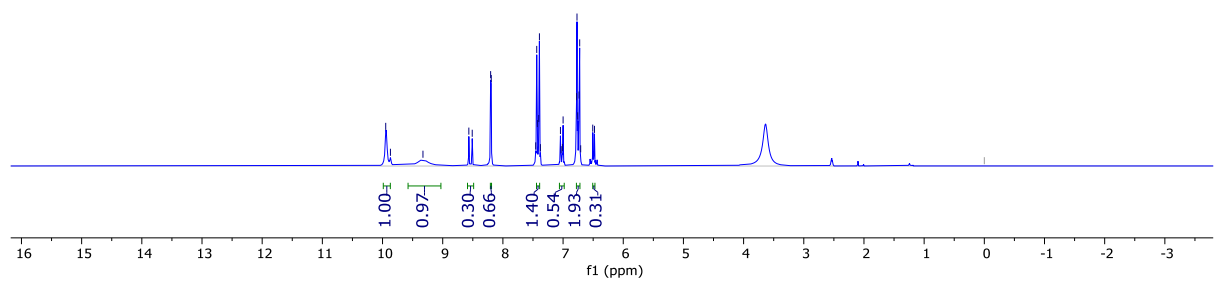
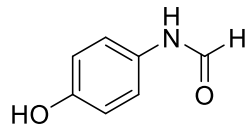
¹H NMR 3q



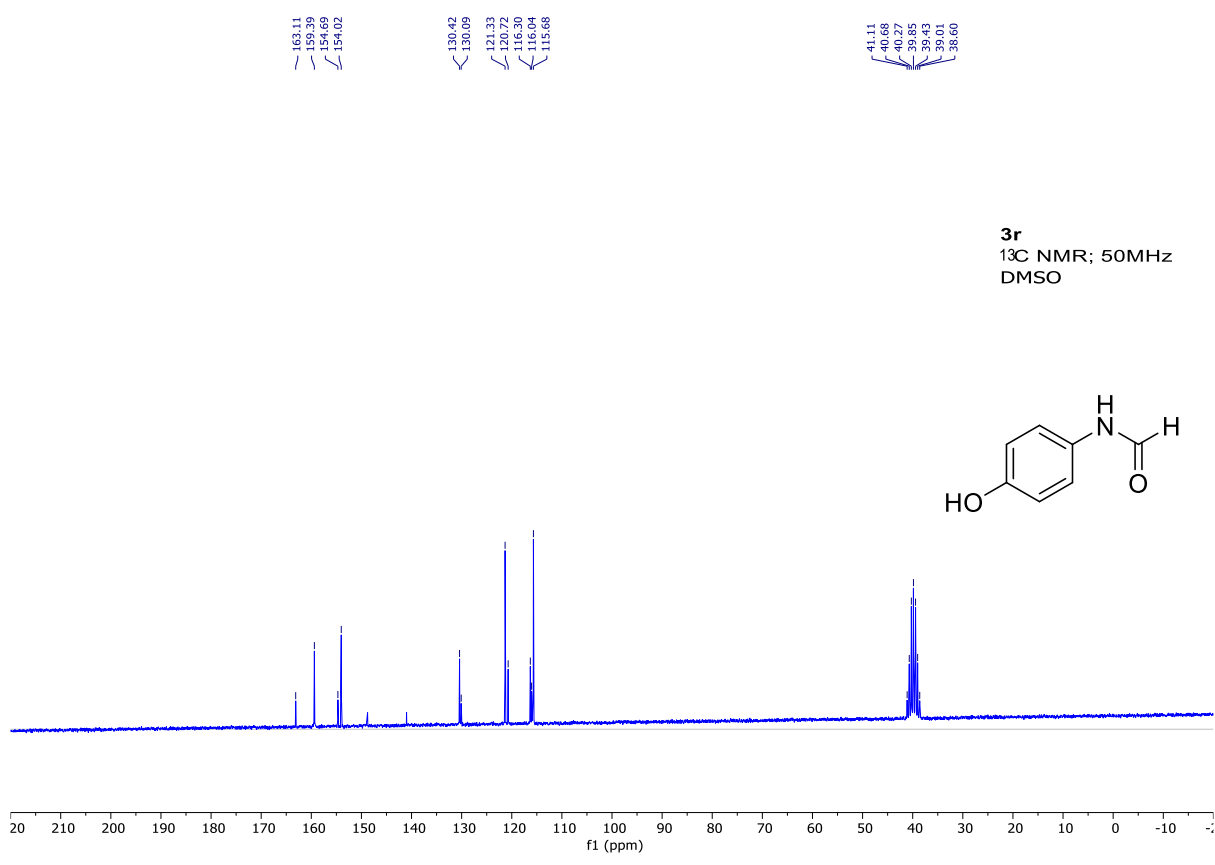
¹³C NMR 3q



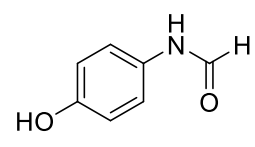
3r
¹H NMR; 200 MHz
 DMSO



¹H NMR 3r



3r
¹³C NMR; 50MHz
 DMSO



¹³C NMR 3r