**Supporting Information**

# Pd/C-Catalyzed Reductive Carbonylation of Nitroaromatics for the Synthesis of Unsymmetrical Ureas: One-Step Synthesis of Neburon

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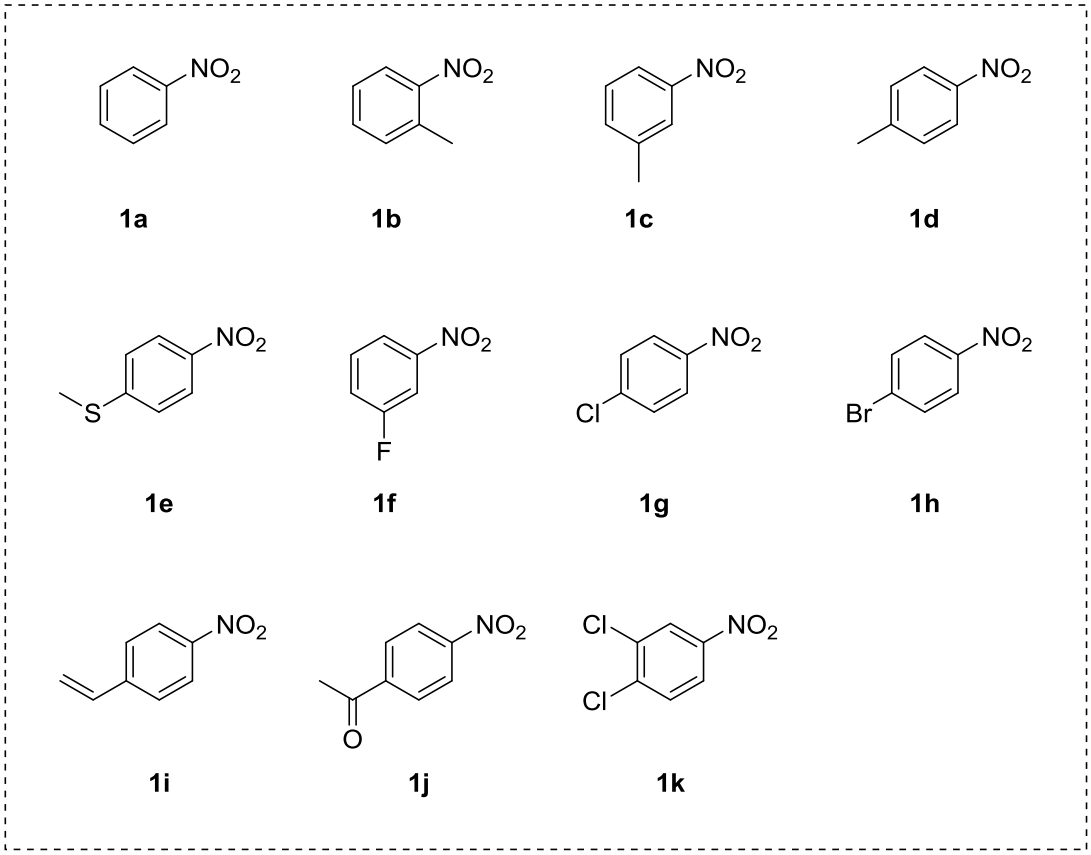
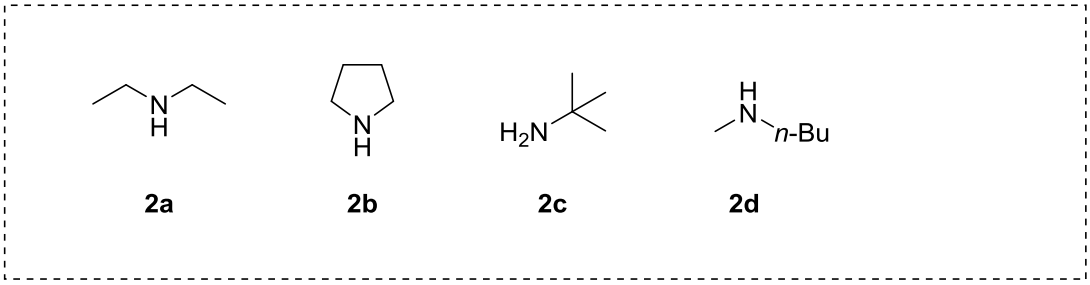
## CONTENTS

## 1. General details and materials

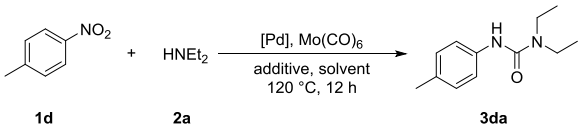
All reactions were carried out under $N_2$ atmosphere. All reagents were from commercial sources and used as received without further purification. All solvents were dried by standard techniques, and distilled prior to use. Column chromatography was performed on silica gel (200-300 meshes) using petroleum ether (b.p. 60~90 °C) and ethyl acetate as eluent. $^{1}H$ and $^{13}C$ NMR spectra were taken on 400 MHz instruments and spectral data were reported in ppm relative to tetramethylsilane (TMS) as internal standard and $CDCl_3$($^{1}H$ NMR $\delta$ 7.26, $^{13}C$ NMR $\delta$ 77.0) as solvent. All coupling constants (*J*) are reported in Hz with the following abbreviations: s = singlet, d = doublet, dd = double doublet, t = triplet, dt = double triplet, q = quatriplet, m = multiplet, br = broad.

## The structure of the starting materials:



## 2. Optimization of the Reaction Condition[a]




1d 2a 3da

| Entry | [Pd] | Ligand | additive | Solvent | Base | Yield (%)[b] |
|---|---|---|---|---|---|---|
| 1 | $Pd(OAc)_2$ (3%) | BINAP (3%) | - | 1,4-dioxane | - | 20 |
| 2 | $Pd(OAc)_2$ (3%) | BINAP (3%) | MeI | 1,4-dioxane | - | 62 |
| 3 | $Pd(OAc)_2$ (3%) | BINAP (3%) | TBAI | 1,4-dioxane | - | 55 |
| 4 | $Pd(OAc)_2$ (3%) | BINAP (3%) | NaI | 1,4-dioxane | - | 78 |
| 5 | $Pd(OAc)_2$ (3%) | BINAP (3%) | KI | 1,4-dioxane | - | 52 |
| 6 | $Pd(OAc)_2$ (3%) | Xantphos (3%) | NaI | 1,4-dioxane | - | 58 |
| 7 | $Pd(OAc)_2$ (3%) | dppp (3%) | NaI | 1,4-dioxane | - | 54 |
| 8 | $Pd(OAc)_2$ (3%) | $PPh_3$ (6) | NaI | 1,4-dioxane | - | 51 |
| 9 | $Pd(OAc)_2$ (3%) | $PCy_3$ (6) | NaI | 1,4-dioxane | - | 70 |
| **10** | **Pd/C (10 mg)** | **-** | **NaI** | **1,4-dioxane** | **-** | **79** |
| 11 | $Pd(PPh_3)_2Cl_2$ (2%) | - | NaI | 1,4-dioxane | - | 72 |
| 12 | $Pd(PPh_3)_4$ (2%) | - | NaI | 1,4-dioxane | - | 78 |
| 13 | $PdCl_2$ (2%) | BINAP (5) | NaI | 1,4-dioxane | - | 72 |
| 14 | - | - | NaI | 1,4-dioxane | - | 63 |
| 15[c] | Pd/C (10 mg) | - | NaI | 1,4-dioxane | | 0 |
| 16 | Pd/C (10 mg) | - | NaI | toluene | | 67 |
| 17 | Pd/C (10 mg) | - | NaI | $CH_3CN$ | | 38 |
| 18 | Pd/C (10 mg) | - | NaI | DMF | | 15 |
| 19 | Pd/C (10 mg) | - | NaI | Cyclohexane | | 56 |
| 20[d] | Pd/C (10 mg) | - | NaI | 1,4-dioxane | DABCO | 16 |
| 21[d] | Pd/C (10 mg) | - | NaI | 1,4-dioxane | $K_3PO_4$ | trace |
| 22[d] | Pd/C (10 mg) | - | NaI | 1,4-dioxane | DBU | 6% |

[a]Reaction conditions: **1d** (1.5 mmol), **2a** (1.0 mmol), $Mo(CO)_6$ (1.0 mmol), additive (0.2 mmol), solvent (2 mL), 120 °C, 12 h.

[b]Isolated yield.

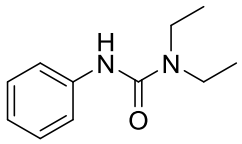
[c]1.0 mmol $H_2O$ was added.

[d] base (1.5 mmol), 1,4-dioxane (4 mL)

## 3. General Procedure

An oven-dried tube, which was equipped with a magnetic stir bar, was charged with Pd/C (10 mg), $Mo(CO)_6$ (1.0 equiv.), NaI (0.2 equiv.) and nitroarenes (1.5 equiv.) at room temperature. The tube was evacuated and backfilled with $N_2$ (this process was repeated 3 times). Then, a solution of diethylamine (1.0 mmol, 1.0 equiv.) in 1,4-dioxane (2 mL) was added to the reaction tube via syringe. The tube was sealed and the mixture was stirred at 120 ℃ for 12 h. After the reaction was completed, the reaction mixture was cooled to room temperature and filtered through a pad of Celite using excess EtOAc. The crude product was purified via flash chromatography (petroleum ether / ethyl acetate 5:1) to provide the pure product.

## 4. Spectroscopic Data of Products

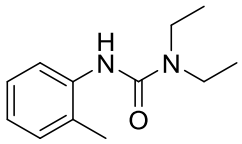


**1,1-Diethyl-3-phenylurea, 3aa, 56% yield**

Following general procedure, using nitrobenzene (155 μL, 1.5 mmol) and diethylamine (105 μL, 1.0 mmol), Compound 3aa (107.6 mg, 56% yield) was a yellow oil.

**$^{1}$H NMR (400 MHz, $CDCl_3$)** δ 7.43 (d, *J* = 8.1 Hz, 2H), 7.31 (t, *J* = 7.9 Hz, 2H), 7.05 (t, *J* = 7.3 Hz, 1H), 6.39 (s, 1H), 3.41 (q, *J* = 7.1 Hz, 4H), 1.26 (t, *J* = 7.2 Hz, 6H).

**$^{13}$C NMR (101 MHz, $CDCl_3$)** δ 154.54, 139.26, 128.72, 122.68, 119.75, 41.54, 13.87.

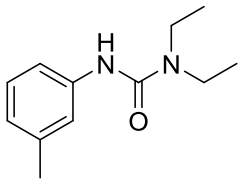


**1,1-Diethyl-3-(*o*-tolyl)urea, 3ba, 64% yield**

Following general procedure, using 1-methyl-2-nitrobenzene (179 μL, 1.5 mmol) and diethylamine (105 μL, 1.0 mmol), Compound **3ba** (131.8 mg, 64% yield) was a yellow powder.

**$^{1}$H NMR (400 MHz, $CDCl_3$)** δ 7.76 (d, *J* = 8.1 Hz, 1H), 7.16 (dd, *J* = 18.3, 7.7 Hz, 2H), 6.98 (t, *J* = 7.4 Hz, 1H), 6.16 (s, 1H), 3.37 (q, *J* = 7.2 Hz, 4H), 2.24 (s, 3H), 1.23 (t, *J* = 7.2 Hz, 6H).

**$^{13}$C NMR (101 MHz, $CDCl_3$)** δ 154.70, 137.37, 130.19, 127.91, 126.71, 123.43, 122.33, 41.70, 17.81, 13.93.

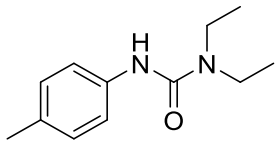


**1,1-Diethyl-3-(*m*-tolyl)urea, 3ca, 71% yield**

Following general procedure, using 1-methyl-3-nitrobenzene (180 μL, 1.5 mmol) and diethylamine (105 μL, 1.0 mmol), Compound **3cg** (146.3 mg, 71% yield) was a yellow powder.

**$^{1}$H NMR (400 MHz, $CDCl_3$)** δ 7.36 – 7.22 (m, 3H), 6.90 (s, 1H), 6.36 (s, 1H), 3.44 (q, *J* = 7.2 Hz, 4H), 2.39 (s, 3H), 1.29 (t, *J* = 7.2 Hz, 6H).

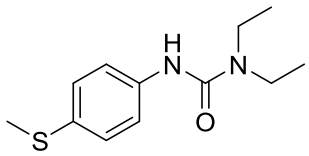
**$^{13}$C NMR (101 MHz, $CDCl_3$)** δ 154.56, 139.16, 138.59, 128.53, 123.50, 120.42, 116.73, 41.56, 21.42, 13.88.



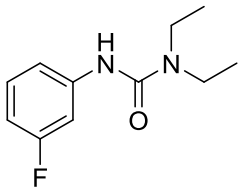
**1,1-Diethyl-3-(*p*-tolyl)urea, 3da, 79% yield**

Following general procedure, using 1-methyl-4-nitrobenzene (207.8 mg, 1.5 mmol) and diethylamine (105 μL, 1.0 mmol), Compound **3da** (162.7 mg, 79% yield) was a yellow powder.

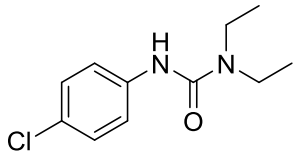
**$^{1}$H NMR (400 MHz, $CDCl_3$)** δ 7.31 (d, *J* = 8.2 Hz, 2H), 7.11 (d, *J* = 8.2 Hz, 2H), 6.32 (s, 1H), 3.40 (q, *J* = 7.2 Hz, 4H), 2.33 (s, 3H), 1.25 (t, *J* = 7.2 Hz, 6H).
**$^{13}$C NMR (101 MHz, $CDCl_3$)** δ 154.80, 136.73, 132.24, 129.27, 120.07, 41.56, 20.69, 13.92.



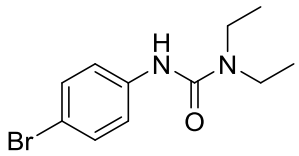
**1,1-Diethyl-3-(4-(methylthio)phenyl)urea, 3ea, 65% yield**
Following general procedure, using methyl(4-nitrophenyl)sulfane (256.3 mg, 1.5 mmol) and diethylamine (105 μL, 1.0 mmol), Compound **3ea** (154.7 mg, 65% yield) was a yellow powder.
**$^{1}$H NMR (400 MHz, $CDCl_3$)** δ 7.33 (d, *J* = 8.5 Hz, 2H), 7.21 (d, *J* = 8.6 Hz, 2H), 6.27 (s, 1H), 3.36 (q, *J* = 7.1 Hz, 4H), 2.44 (s, 3H), 1.21 (t, *J* = 7.1 Hz, 6H).
**$^{13}$C NMR (101 MHz, $CDCl_3$)** δ 154.46, 137.21, 131.43, 128.57, 120.44, 41.59, 17.24, 14.03.



**1,1-Diethyl-3-(3-fluorophenyl)urea, 3fa, 70% yield**
Following general procedure, using 1-fluoro-3-nitrobenzene (161 μL, 1.5 mmol) and diethylamine (105 μL, 1.0 mmol), Compound **3fa** (147.0 mg, 70% yield) was a yellow powder.
**$^{1}$H NMR (400 MHz, $CDCl_3$)** δ 7.35 (d, *J* = 11.5 Hz, 1H), 7.15 (dd, *J* = 14.9, 8.1 Hz, 1H), 7.01 (d, *J* = 8.1 Hz, 1H), 6.66 (td, *J* = 8.3, 1.8 Hz, 1H), 6.59 (s, 1H), 3.33 (q, *J* = 7.1 Hz, 4H), 1.18 (t, *J* = 7.2 Hz, 6H).
**$^{13}$C NMR (101 MHz, $CDCl_3$)** δ 162.96 (d, $J_{CF}$ = 243.3 Hz), 154.22, 141.05 (d, $J_{CF}$ = 11.2 Hz), 129.55 (d, $J_{CF}$ = 9.6 Hz), 114.82, 109.07 (d, $J_{CF}$ = 21.4 Hz), 106.97 (d, $J_{CF}$ = 26.3 Hz), 41.47, 13.76.



**3-(4-Chlorophenyl)-1,1-diethylurea, 3ga, 73% yield**
Following general procedure, using 1-chloro-4-nitrobenzene (238.7 mg, 1.5 mmol) and diethylamine (105 μL, 1.0 mmol), Compound **3ga** (165.0 mg, 73% yield) was a yellow powder.
**$^{1}$H NMR (400 MHz, $CDCl_3$)** δ 7.32 (d, *J* = 8.8 Hz, 2H), 7.19 (d, *J* = 8.8 Hz, 2H), 6.44 (s, 1H), 3.33 (q, *J* = 7.1 Hz, 4H), 1.18 (t, *J* = 7.1 Hz, 6H).
**$^{13}$C NMR (101 MHz, $CDCl_3$)** δ 154.42, 137.99, 128.66, 127.58, 121.12, 41.57, 13.89.

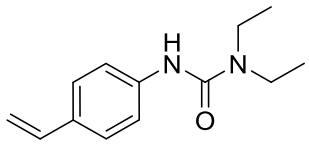


**3-(4-Bromophenyl)-1,1-diethylurea, 3ha, 83% yield**

Following general procedure, using 1-bromo-4-nitrobenzene (306.1 mg, 1.5 mmol) and diethylamine (105 μL, 1.0 mmol), Compound **3ha** (224.9 mg, 83% yield) was a yellow powder.

**$^1$H NMR (400 MHz, $CDCl_3$)** δ 7.39 (d, *J* = 8.7 Hz, 2H), 7.32 (d, *J* = 8.8 Hz, 2H), 6.43 (s, 1H), 3.39 (q, *J* = 7.1 Hz, 4H), 1.24 (t, *J* = 7.1 Hz, 6H).

**$^{13}$C NMR (101 MHz, $CDCl_3$)** δ 154.27, 138.43, 131.57, 121.34, 115.06, 41.55, 13.85.

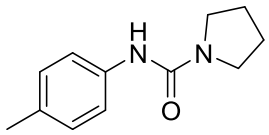


**1,1-Diethyl-3-(4-vinylphenyl)urea, 3ia, 46% yield**

Following general procedure, using 4-nitrostyrene (194 μL, 1.5 mmol) and diethylamine (105 μL, 1.0 mmol), Compound **3cg** (100.3 mg, 46% yield) was a yellow powder.

**$^1$H NMR (400 MHz, $CDCl_3$)** δ 7.34 (m, *J* = 8.7 Hz, 4H), 6.65 (dd, *J* = 17.6, 10.9 Hz, 1H), 6.33 (s, 1H), 5.64 (d, *J* = 17.6 Hz, 1H), 5.14 (d, *J* = 10.9 Hz, 1H), 3.37 (q, *J* = 7.1 Hz, 4H), 1.22 (t, *J* = 7.1 Hz, 6H).

**$^{13}$C NMR (101 MHz, $CDCl_3$)** δ 154.39, 138.95, 136.30, 132.21, 126.68, 119.53, 112.04, 41.61, 13.91.

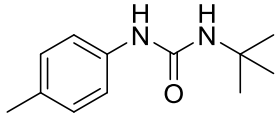


**N-(*p*-tolyl)pyrrolidine-1-carboxamide, 3db, 58% yield**

Following general procedure, using 1-methyl-4-nitrobenzene (207.8 mg, 1.5 mmol) and tetrahydropyrrole (83 μL, 1.0 mmol), Compound **3db** (118.3 mg, 58% yield) was a yellow powder.

**$^1$H NMR (400 MHz, $CDCl_3$)** δ 7.28 (d, *J* = 8.3 Hz, 2H), 7.06 (d, *J* = 8.2 Hz, 2H), 6.17 (s, 1H), 3.43 (t, *J* = 6.5 Hz, 4H), 2.28 (s, 3H), 1.93 (t, *J* = 6.5 Hz, 4H).

**$^{13}$C NMR (101 MHz, $CDCl_3$)** δ 154.09, 136.62, 132.10, 129.23, 119.69, 45.70, 25.54, 20.65.

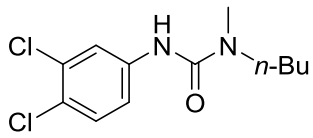


**1-(*tert*-Butyl)-3-(*p*-tolyl)urea, 3dc, 69% yield**

Following general procedure, using 1-methyl-4-nitrobenzene (207.8 mg, 1.5 mmol) and *tert*-butylamine (106 μL, 1.0 mmol), Compound **3dc** (142.1 mg, 69% yield) was a yellow powder.

**$^1$H NMR (400 MHz, $CDCl_3$)** δ 7.17 (s, 1H), 7.16 (d, *J* = 8.2 Hz, 2H), 7.04 (d, *J* = 8.2 Hz, 2H), 5.38 (s, 1H), 2.26 (s, 3H), 1.32 (s, 9H).

**$^{13}$C NMR (101 MHz, $CDCl_3$)** δ 155.75, 136.52, 132.54, 129.53, 120.57, 50.36, 29.30, 20.68.



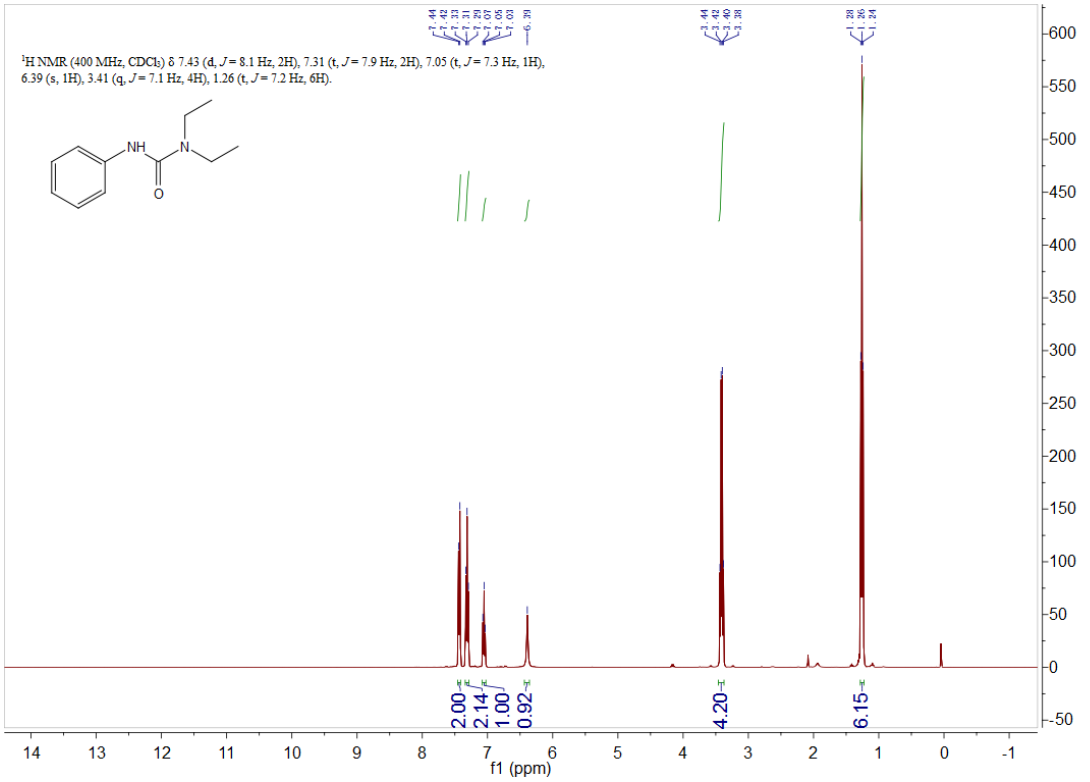

**1-Butyl-3-(3,4-dichlorophenyl)-1-methylurea, 3kd, 64% yield**

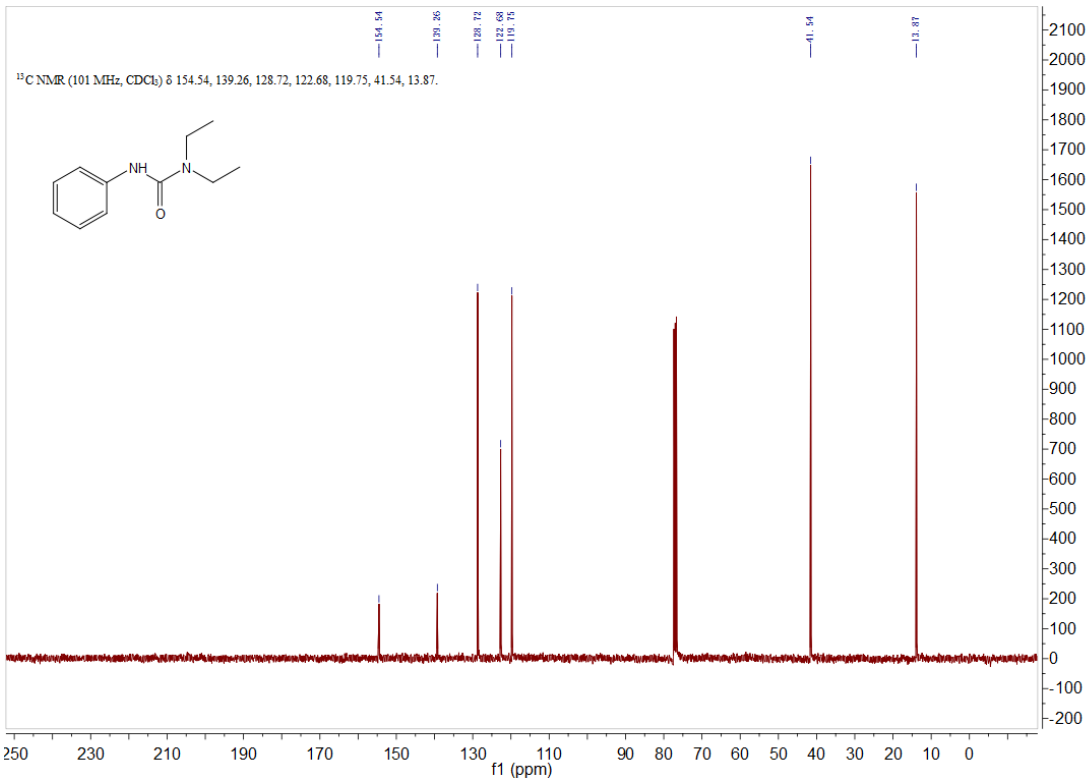
Following general procedure, using 3,4-dichloronitrobenzene (290.9 mg, 1.5 mmol) and N-butylmethylamine (93%, 128 μL, 1.0 mmol), Compound **3kd** (175.4 mg, 64% yield) was a white powder.

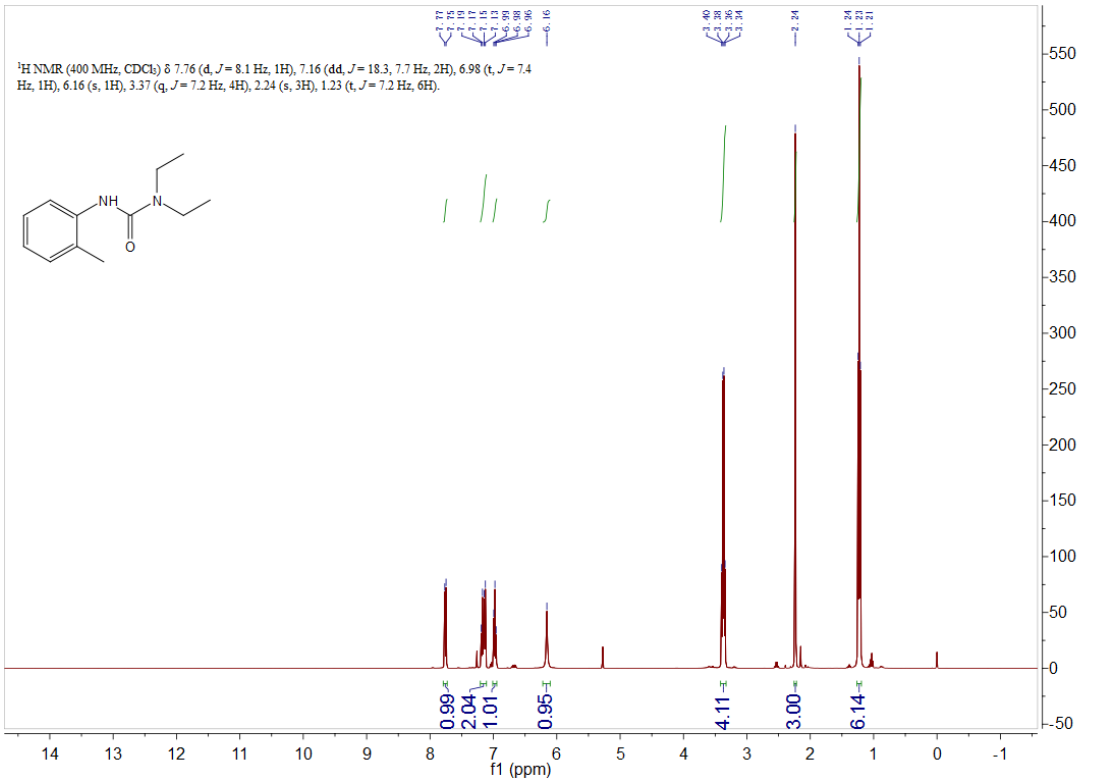
**$^{1}$H NMR (400 MHz, $CDCl_3$)** δ 7.61 (d, *J* = 2.4 Hz, 1H), 7.27 (d, *J* = 8.7 Hz, 1H), 7.20 (dd, *J* = 8.7, 2.4 Hz, 1H), 6.73 (s, 1H), 3.36 – 3.30 (m, 2H), 2.98 (s, 3H), 1.60 – 1.50 (m, 2H), 1.33 (dq, *J* = 14.6, 7.3 Hz, 2H), 0.95 (t, *J* = 7.3 Hz, 3H).

**$^{13}$C NMR (101 MHz, $CDCl_3$)** δ 154.86, 138.96, 132.18, 129.97, 125.59, 121.43, 119.16, 48.79, 34.49, 30.01, 19.96, 13.77.

## 5. Copy of $^{1}H$ and $^{13}C$ NMR Spectra of Products




$^1$H NMR (400 MHz, CDCl$_3$) δ 7.76 (d, $J$ = 8.1 Hz, 1H), 7.16 (dd, $J$ = 18.3, 7.7 Hz, 2H), 6.98 (t, $J$ = 7.4 Hz, 1H), 6.16 (s, 1H), 3.37 (q, $J$ = 7.2 Hz, 4H), 2.24 (s, 3H), 1.23 (t, $J$ = 7.2 Hz, 6H).
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N
O
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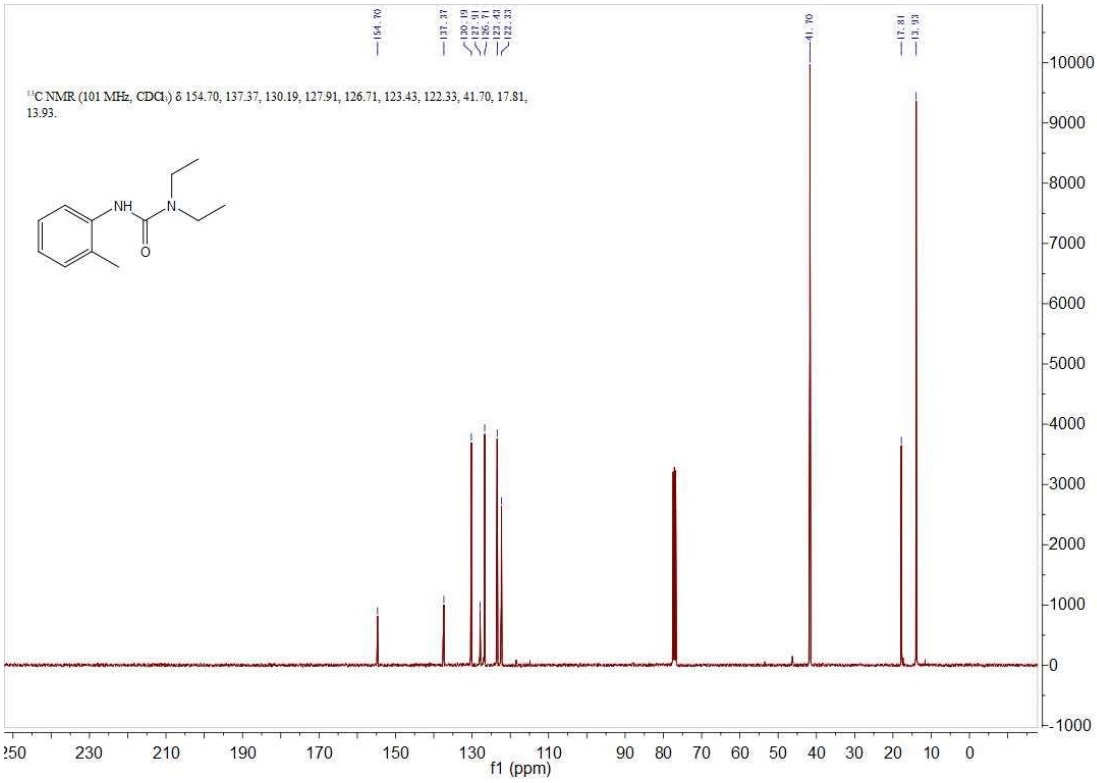
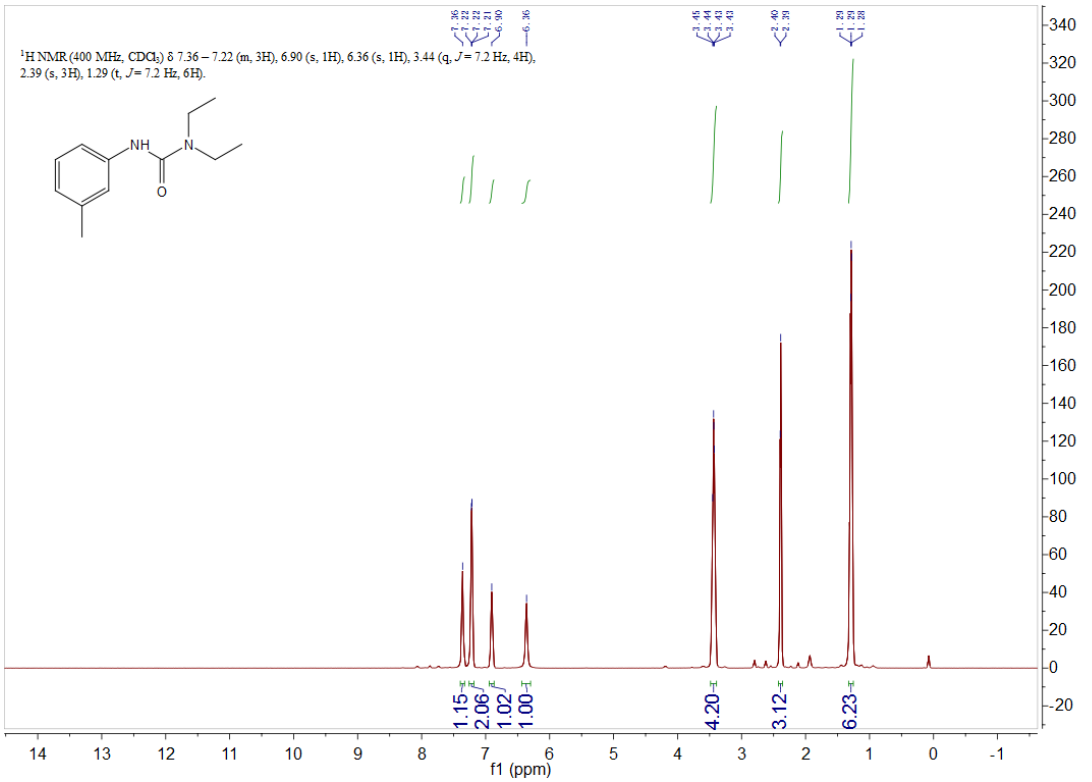
1.01
0.95
4.11
3.00
6.14
f1 (ppm)


$^{13}$C NMR (101 MHz, CDCl$_3$) δ 154.70, 137.37, 130.19, 127.91, 126.71, 123.43, 122.33, 41.70, 17.81, 13.93.
NH
N
O
f1 (ppm)


$^1$H NMR (400 MHz, $CDCl_3$) δ 7.36 – 7.22 (m, 3H), 6.90 (s, 1H), 6.36 (s, 1H), 3.44 (q, $J$ = 7.2 Hz, 4H), 2.39 (s, 3H), 1.29 (t, $J$ = 7.2 Hz, 6H).
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N
O
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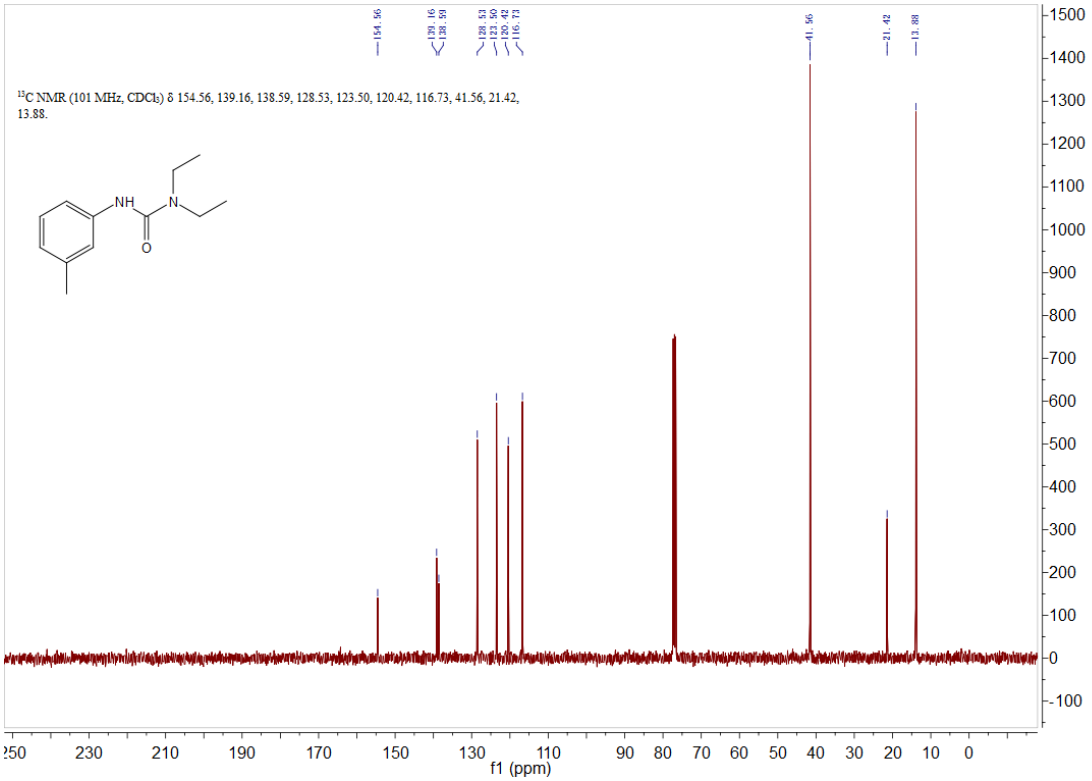
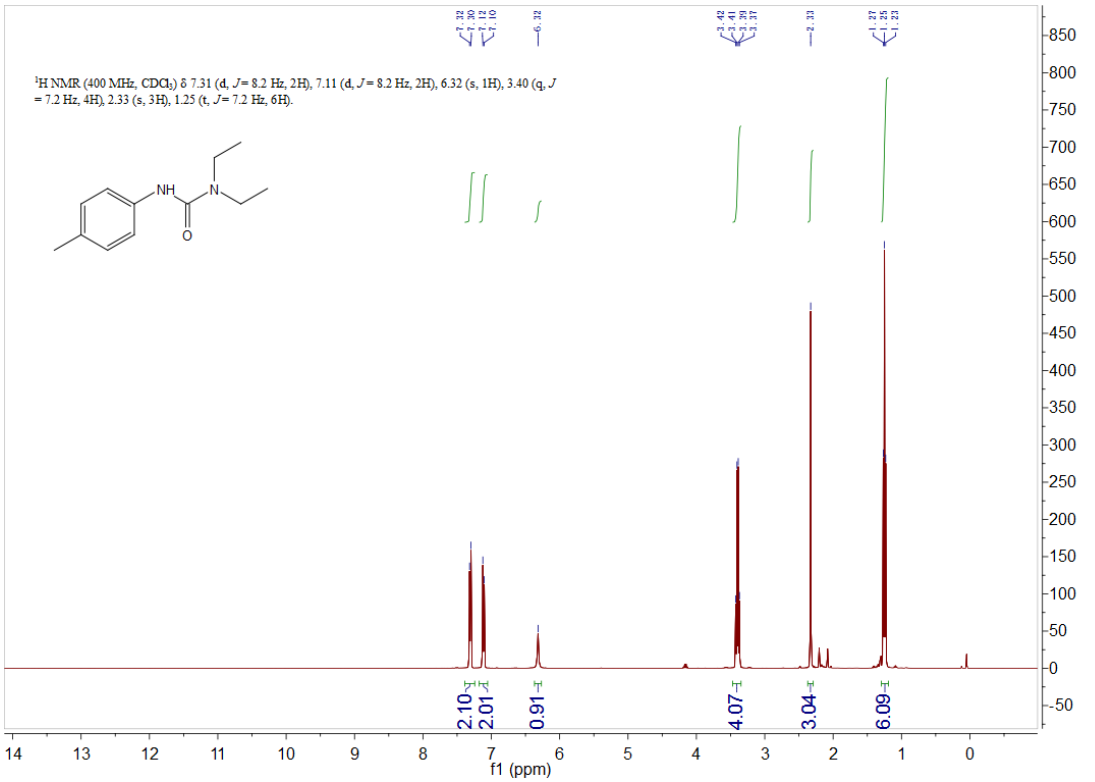
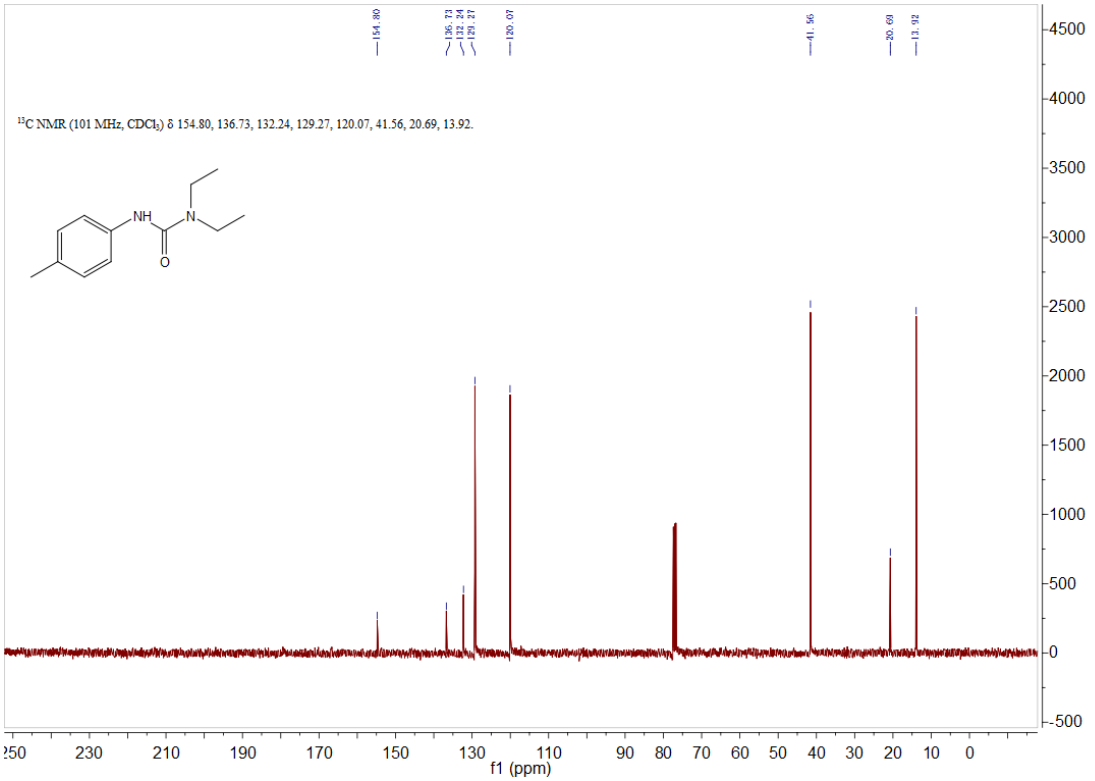
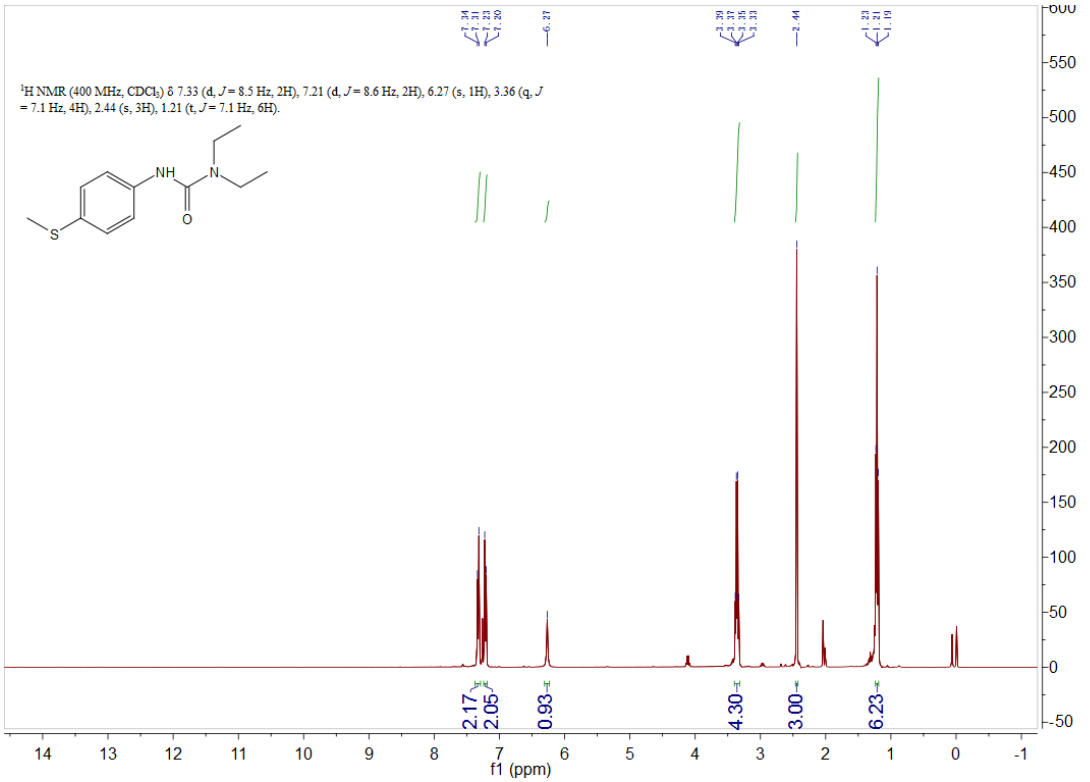
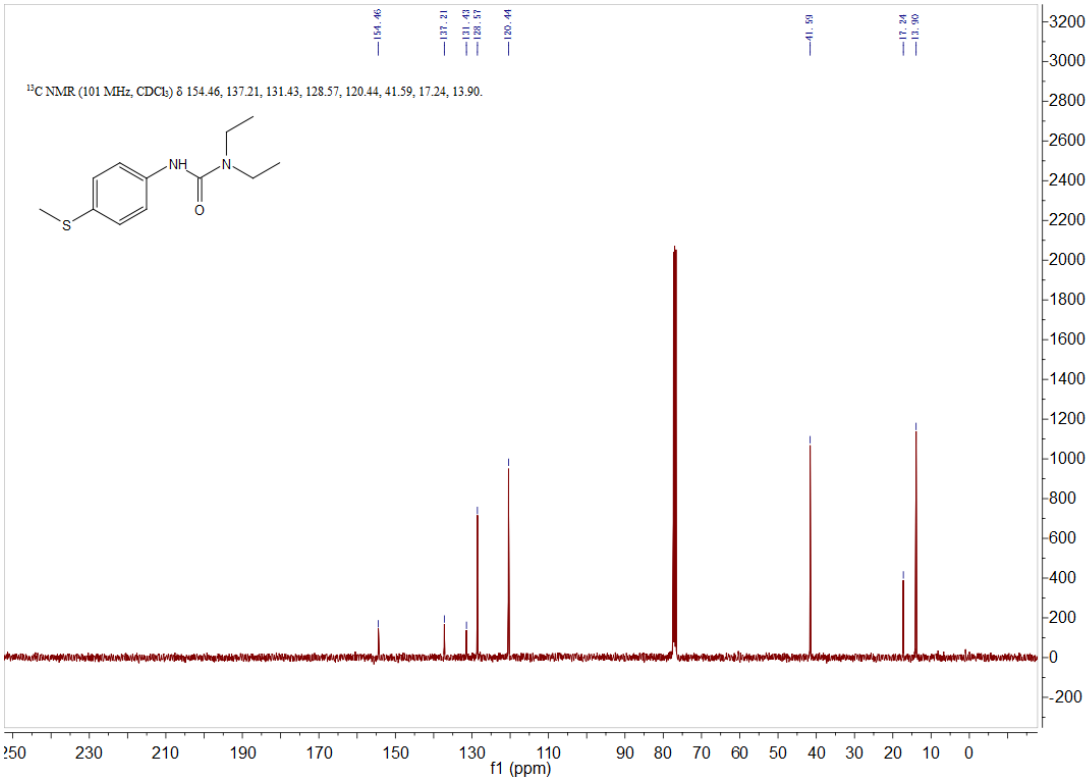
f1 (ppm)

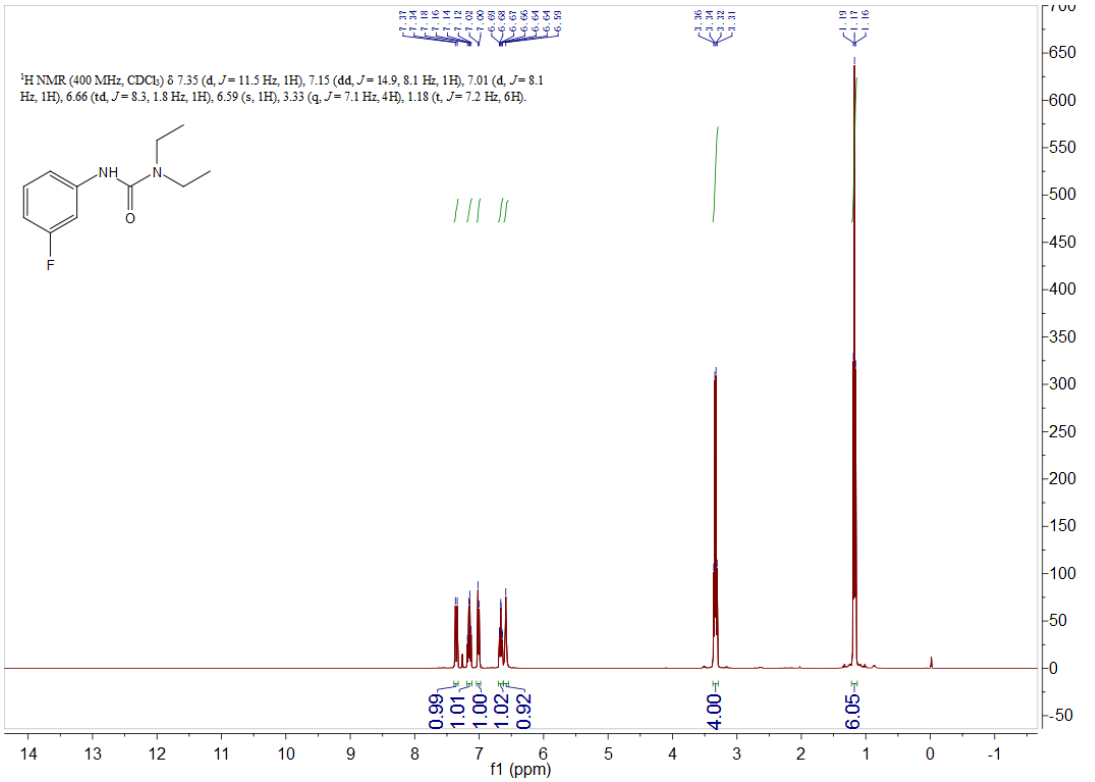

$^{13}$C NMR (101 MHz, $CDCl_3$) δ 154.56, 139.16, 138.59, 128.53, 123.50, 120.42, 116.73, 41.56, 21.42, 13.88.
NH
N
O
154.56
139.16
138.59
128.53
123.50
120.42
116.73
41.56
21.42
13.88
f1 (ppm)

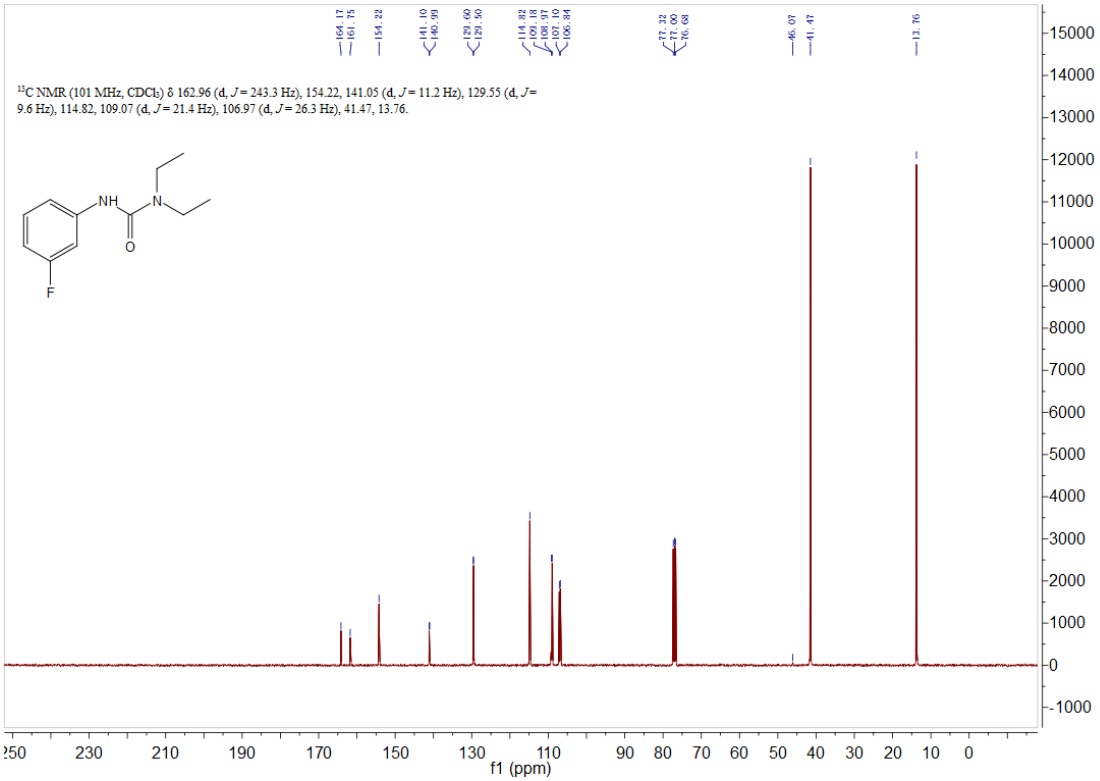

$^1$H NMR (400 MHz, $CDCl_3$) δ 7.31 (d, $J$ = 8.2 Hz, 2H), 7.11 (d, $J$ = 8.2 Hz, 2H), 6.32 (s, 1H), 3.40 (q, $J$ = 7.2 Hz, 4H), 2.33 (s, 3H), 1.25 (t, $J$ = 7.2 Hz, 6H).
NH
N
O
2.10
2.01
0.91
4.07
3.04
6.09
f1 (ppm)

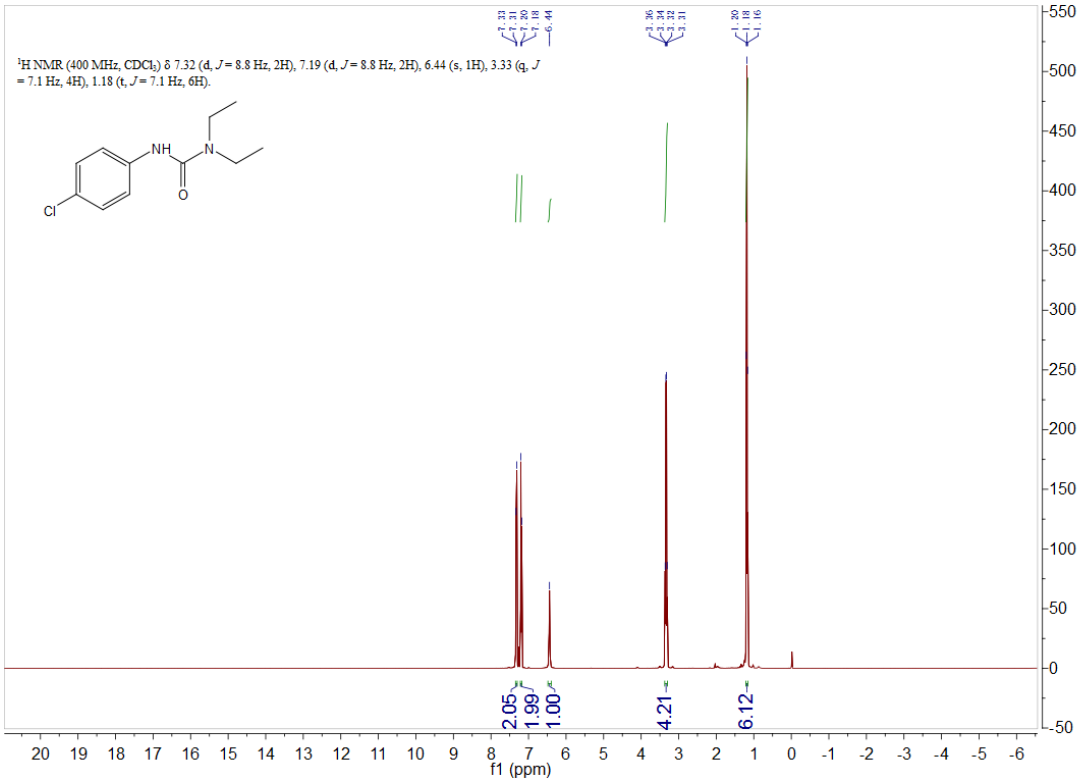

$^{13}$C NMR (101 MHz, $CDCl_3$) δ 154.80, 136.73, 132.24, 129.27, 120.07, 41.56, 20.69, 13.92.
NH
N
O
f1 (ppm)

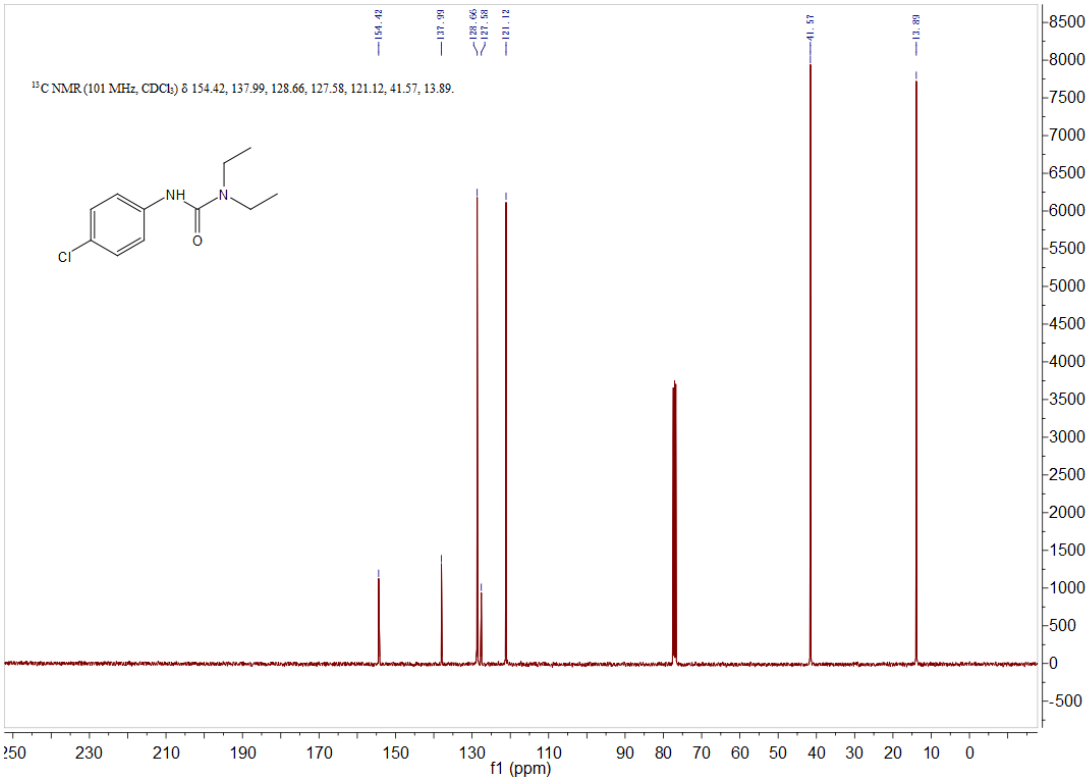

$^1$H NMR (400 MHz, $CDCl_3$) δ 7.33 (d, $J$ = 8.5 Hz, 2H), 7.21 (d, $J$ = 8.6 Hz, 2H), 6.27 (s, 1H), 3.36 (q, $J$ = 7.1 Hz, 4H), 2.44 (s, 3H), 1.21 (t, $J$ = 7.1 Hz, 6H).
NH
N
O
S
7.34
7.31
7.23
7.20
6.27
3.39
3.37
3.35
3.33
2.44
1.23
1.21
1.19
2.17
2.05
0.93
4.30
3.00
6.23
f1 (ppm)

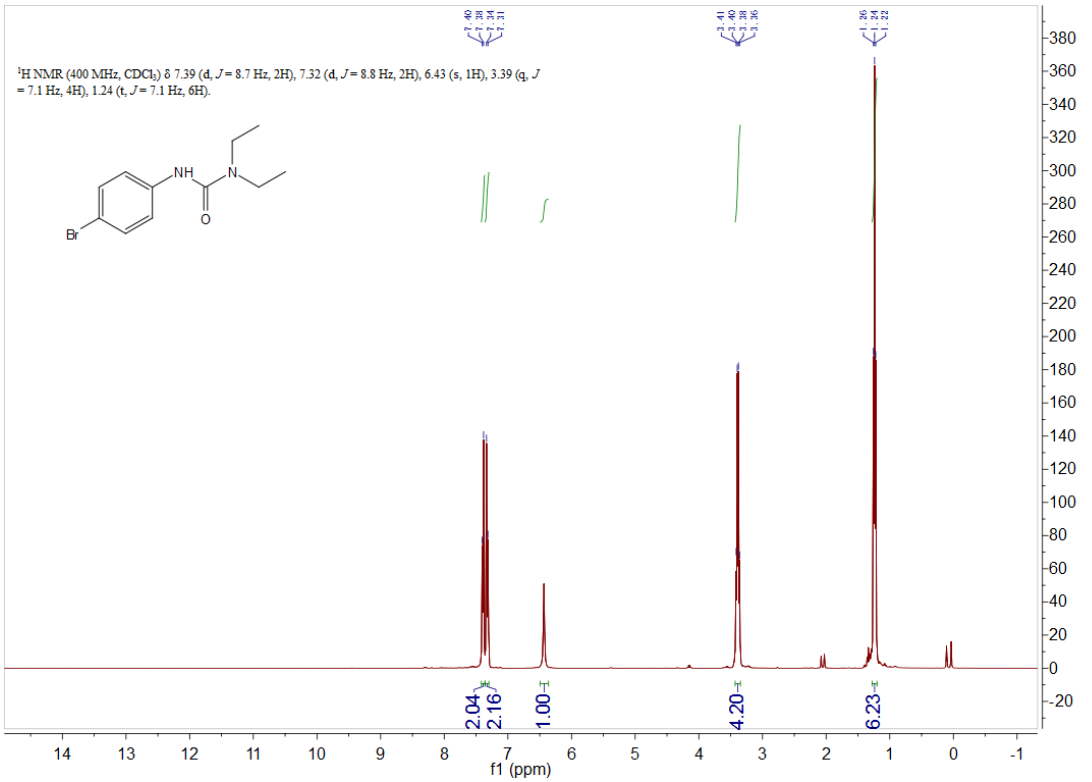

$^{13}$C NMR (101 MHz, $CDCl_3$) δ 154.46, 137.21, 131.43, 128.57, 120.44, 41.59, 17.24, 13.90.
NH
N
O
S
154.46
137.21
131.43
128.57
120.44
41.59
17.24
13.90
f1 (ppm)

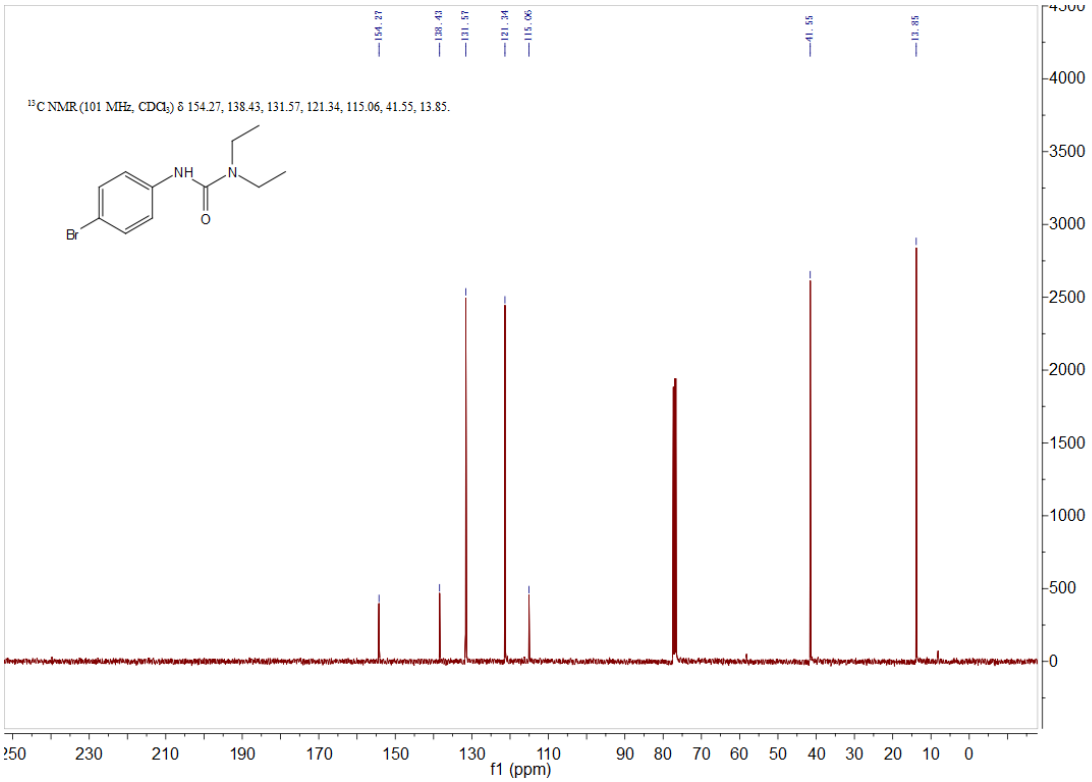

$^1$H NMR (400 MHz, CDCl$_3$) δ 7.35 (d, $J$ = 11.5 Hz, 1H), 7.15 (dd, $J$ = 14.9, 8.1 Hz, 1H), 7.01 (d, $J$ = 8.1 Hz, 1H), 6.66 (td, $J$ = 8.3, 1.8 Hz, 1H), 6.59 (s, 1H), 3.33 (q, $J$ = 7.1 Hz, 4H), 1.18 (t, $J$ = 7.2 Hz, 6H).
NH
N
O
F
0.99
1.01
1.00
1.02
0.92
4.00
6.05
f1 (ppm)

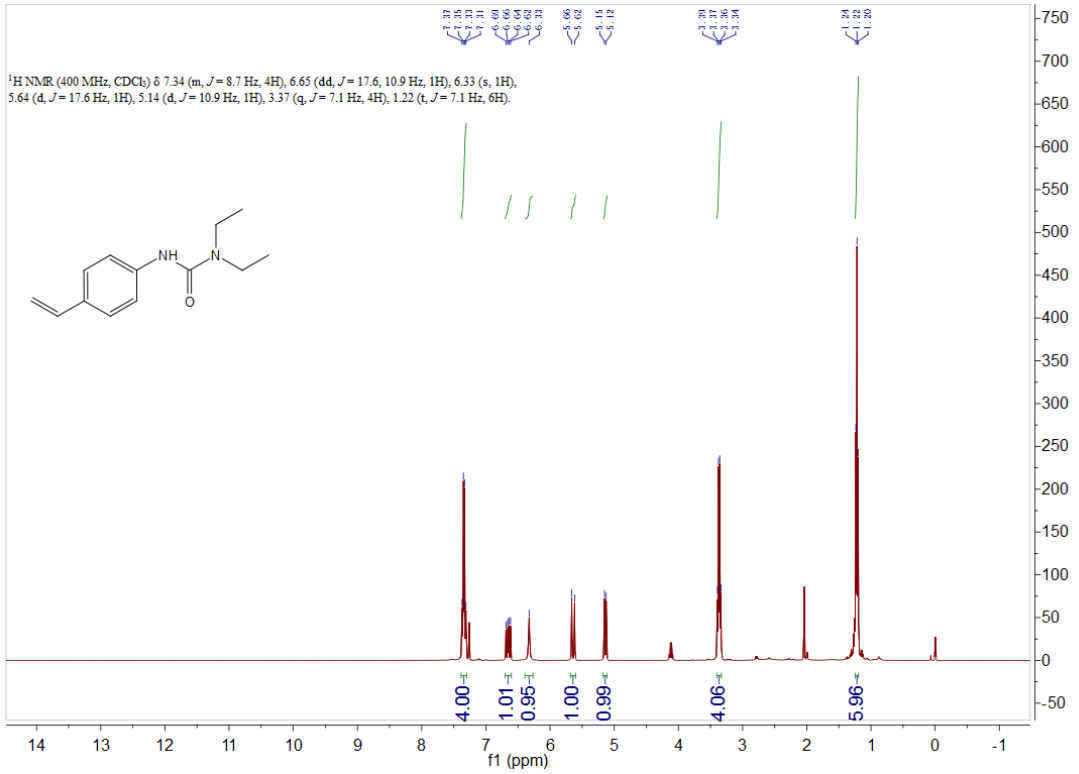

$^{13}$C NMR (101 MHz, CDCl$_3$) δ 162.96 (d, $J$ = 243.3 Hz), 154.22, 141.05 (d, $J$ = 11.2 Hz), 129.55 (d, $J$ = 9.6 Hz), 114.82, 109.07 (d, $J$ = 21.4 Hz), 106.97 (d, $J$ = 26.3 Hz), 41.47, 13.76.
NH
N
O
F
f1 (ppm)

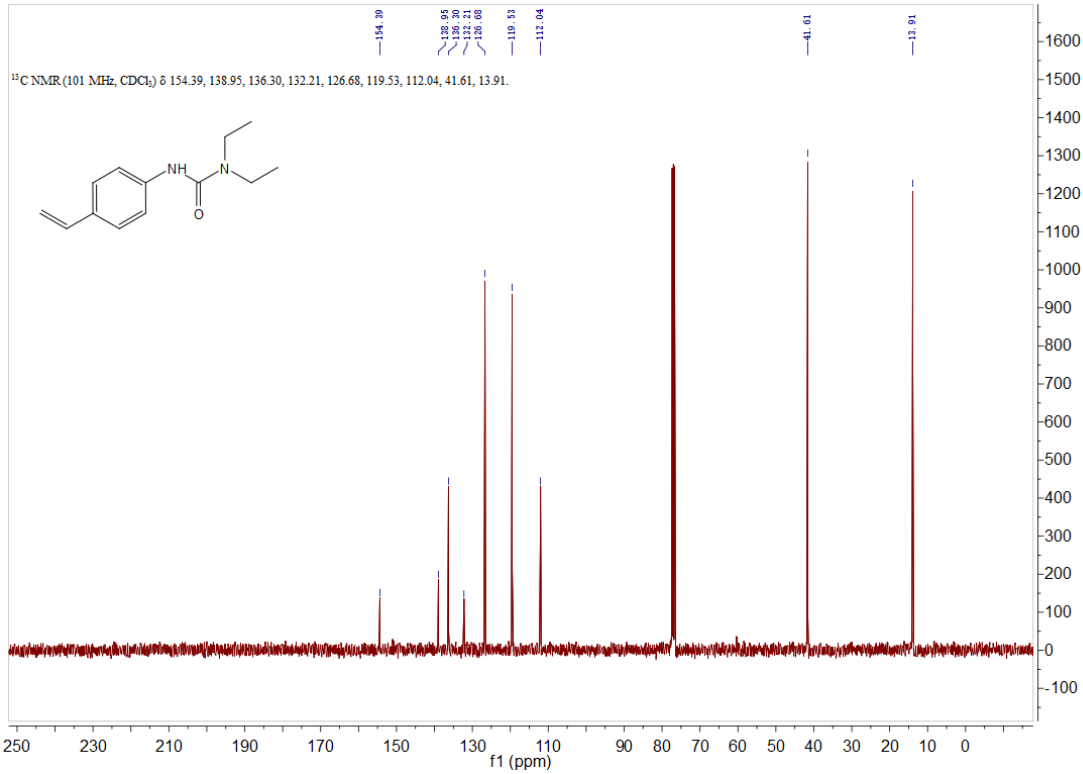

$^1$H NMR (400 MHz, $CDCl_3$) δ 7.32 (d, $J$ = 8.8 Hz, 2H), 7.19 (d, $J$ = 8.8 Hz, 2H), 6.44 (s, 1H), 3.33 (q, $J$ = 7.1 Hz, 4H), 1.18 (t, $J$ = 7.1 Hz, 6H).
NH
N
O
Cl
2.05
1.99
1.00
4.21
6.12
f1 (ppm)

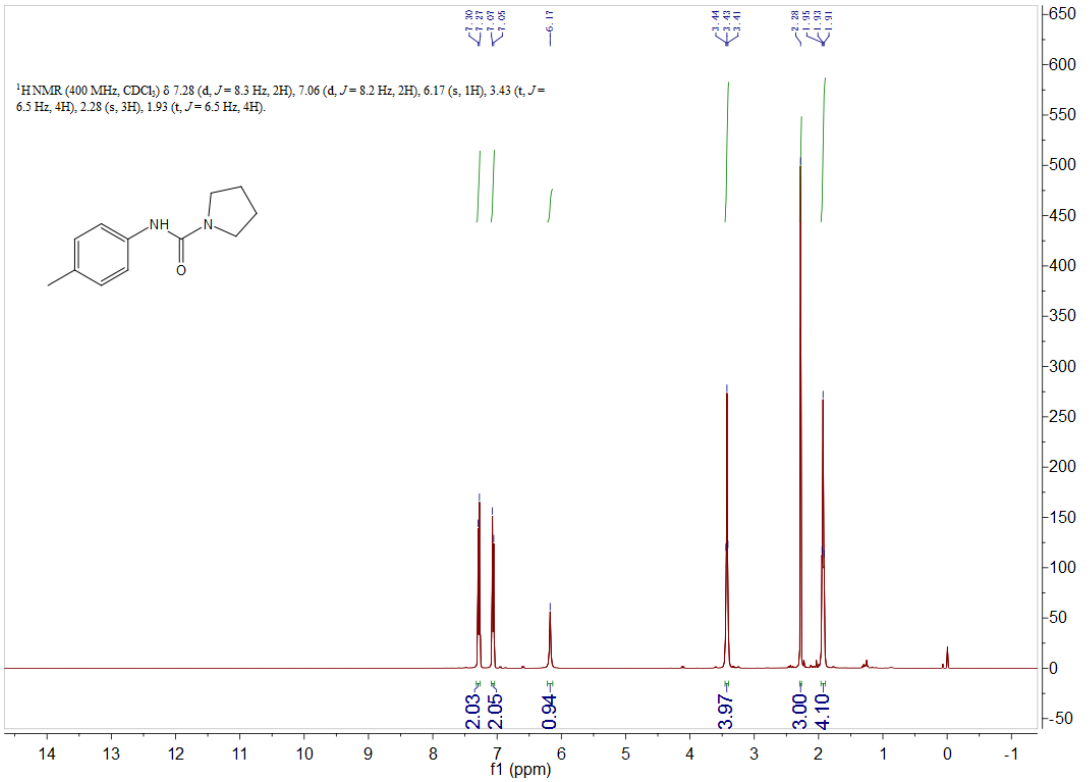

$^{13}$C NMR (101 MHz, $CDCl_3$) δ 154.42, 137.99, 128.66, 127.58, 121.12, 41.57, 13.89.
154.42
137.99
128.66
127.58
121.12
41.57
13.89
NH
N
O
Cl
f1 (ppm)

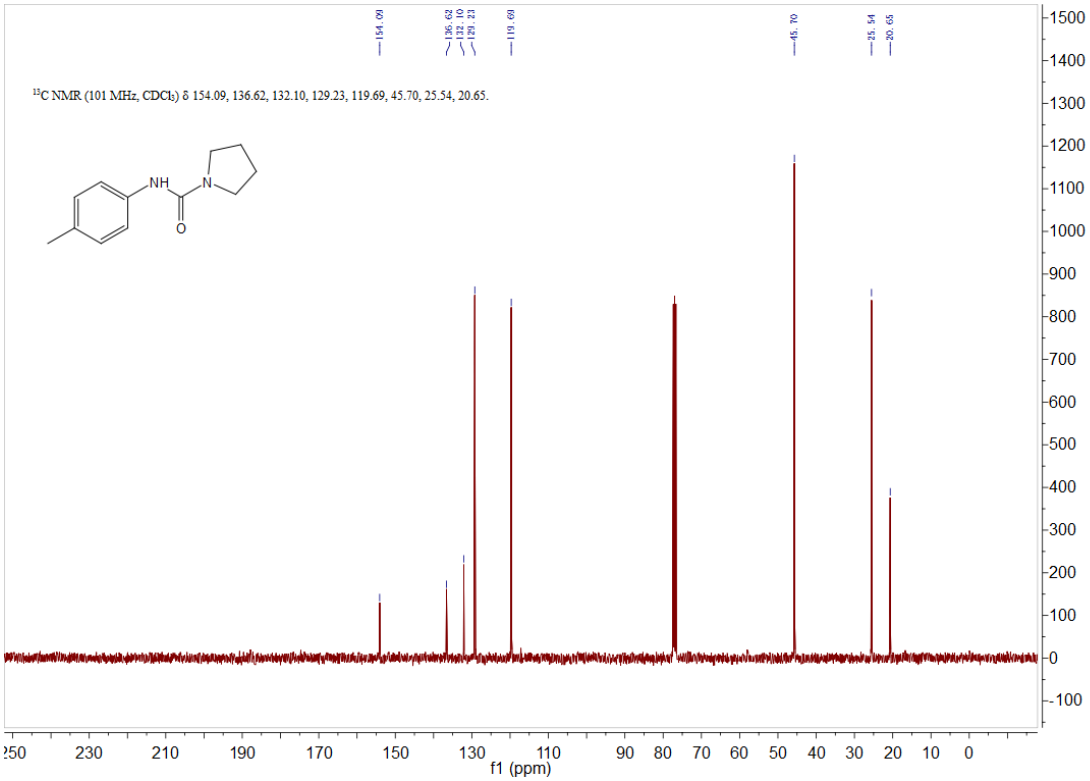

$^1$H NMR (400 MHz, $CDCl_3$) δ 7.39 (d, $J$ = 8.7 Hz, 2H), 7.32 (d, $J$ = 8.8 Hz, 2H), 6.43 (s, 1H), 3.39 (q, $J$ = 7.1 Hz, 4H), 1.24 (t, $J$ = 7.1 Hz, 6H).
NH
N
O
Br
2.04
2.16
1.00
4.20
6.23
f1 (ppm)

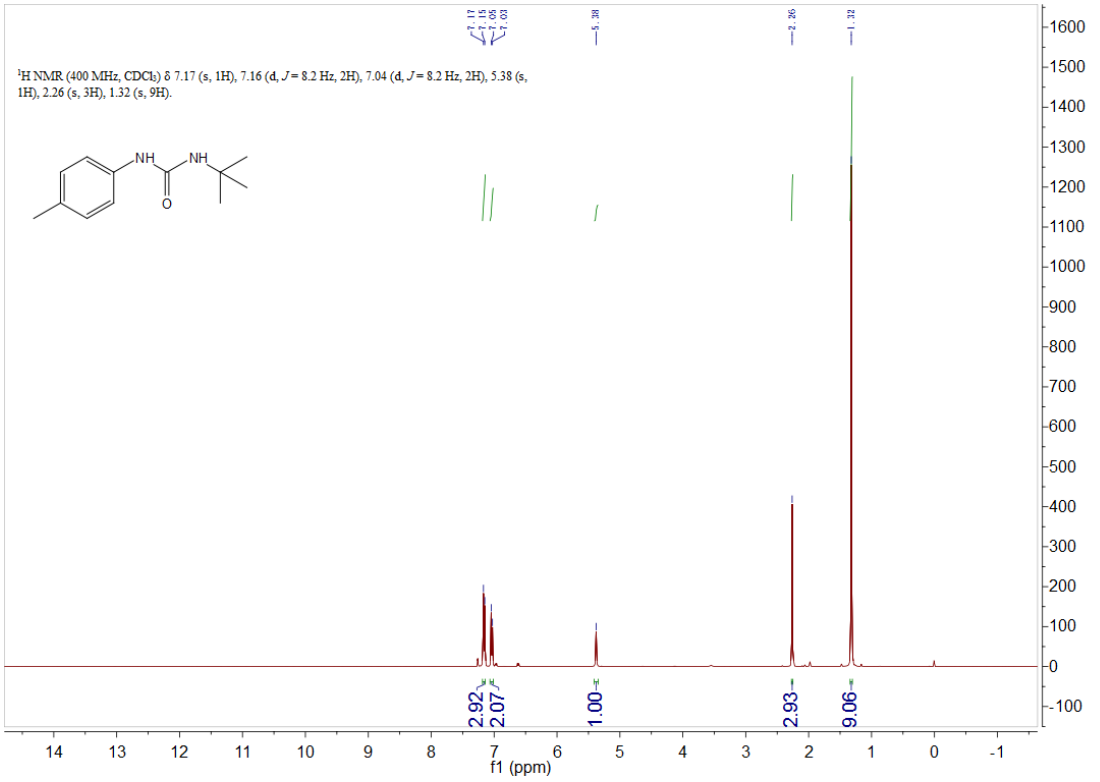

$^{13}$C NMR (101 MHz, $CDCl_3$) δ 154.27, 138.43, 131.57, 121.34, 115.06, 41.55, 13.85.
154.27
138.43
131.57
121.34
115.06
41.55
13.85
NH
N
O
Br
f1 (ppm)

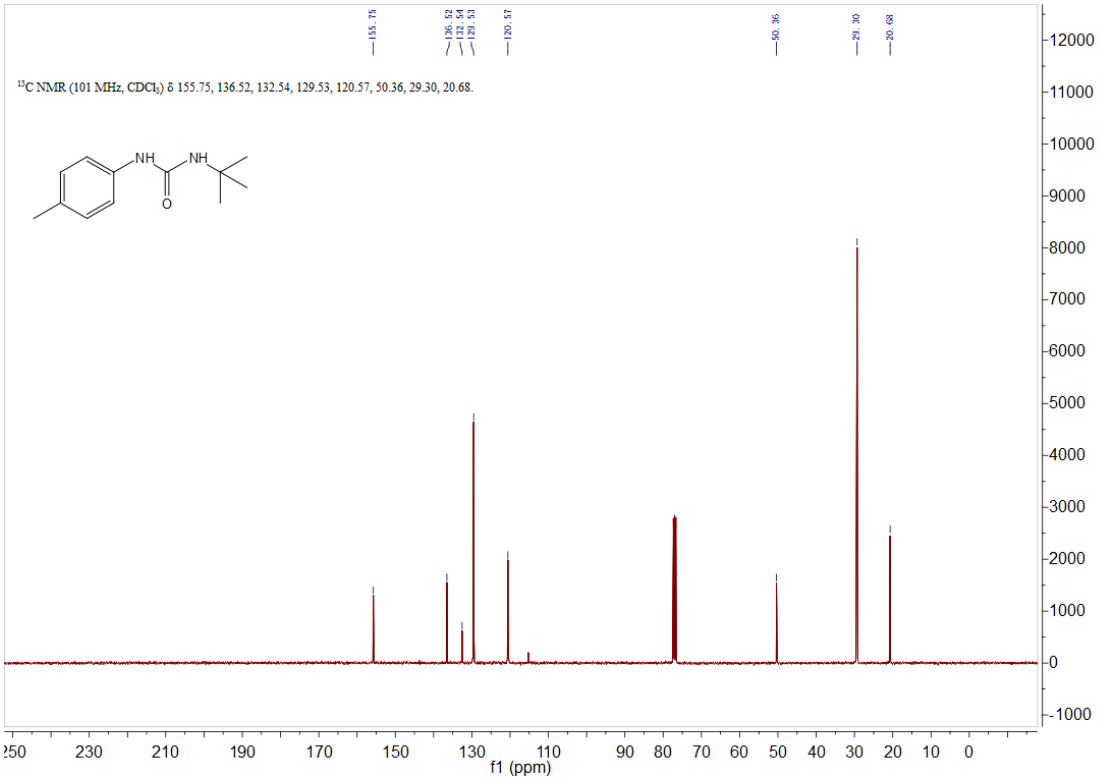

7.37
7.35
7.33
7.31
6.69
6.66
6.64
6.62
6.33
5.66
5.63
5.15
5.12
3.39
3.37
3.36
3.34
1.24
1.22
1.20
[1]H NMR (400 MHz, CDCl3) δ 7.34 (m, J = 8.7 Hz, 4H), 6.65 (dd, J = 17.6, 10.9 Hz, 1H), 6.33 (s, 1H), 5.64 (d, J = 17.6 Hz, 1H), 5.14 (d, J = 10.9 Hz, 1H), 3.37 (q, J = 7.1 Hz, 4H), 1.22 (t, J = 7.1 Hz, 6H).
NH
N
O
4.00
1.01
0.95
1.00
0.99
4.06
5.96
f1 (ppm)

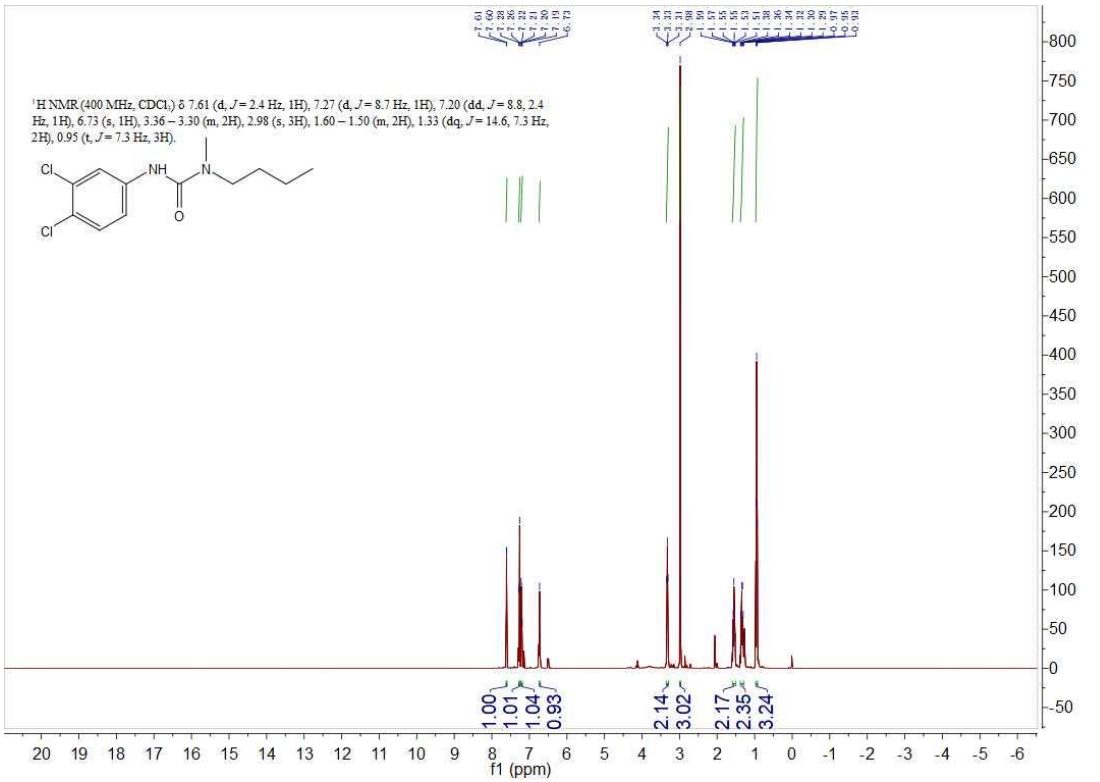

154.39
138.95
136.30
132.21
126.68
119.53
112.04
41.61
13.91
[13]C NMR (101 MHz, CDCl3) δ 154.39, 138.95, 136.30, 132.21, 126.68, 119.53, 112.04, 41.61, 13.91.
NH
N
O
f1 (ppm)

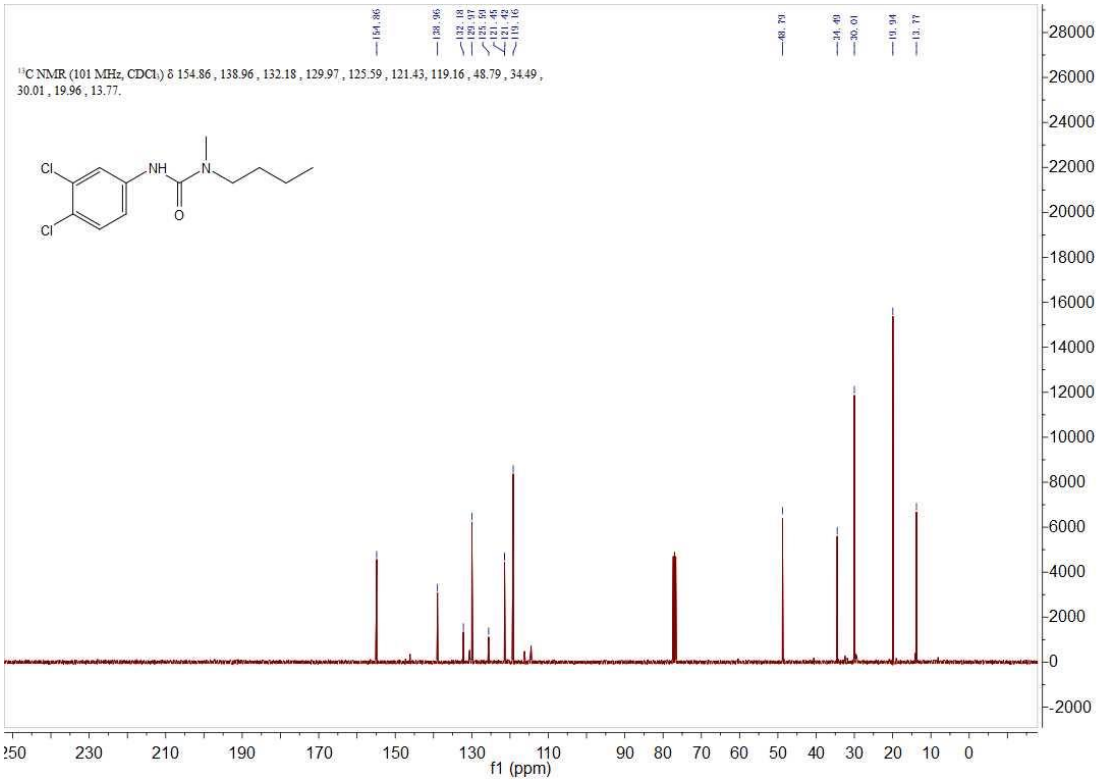

$^1$H NMR (400 MHz, $CDCl_3$) δ 7.28 (d, $J$ = 8.3 Hz, 2H), 7.06 (d, $J$ = 8.2 Hz, 2H), 6.17 (s, 1H), 3.43 (t, $J$ = 6.5 Hz, 4H), 2.28 (s, 3H), 1.93 (t, $J$ = 6.5 Hz, 4H).
NH
N
O
7.30
7.27
7.05
6.17
3.44
3.43
3.41
2.28
1.95
1.93
1.91
2.03
2.05
0.94
3.97
3.00
4.10
f1 (ppm)


$^{13}$C NMR (101 MHz, $CDCl_3$) δ 154.09, 136.62, 132.10, 129.23, 119.69, 45.70, 25.54, 20.65.
NH
N
O
154.09
136.62
132.10
129.23
119.69
45.70
25.54
20.65
f1 (ppm)


7.17
7.15
7.05
7.03
5.38
2.26
1.32
$^1$H NMR (400 MHz, CDCl$_3$) δ 7.17 (s, 1H), 7.16 (d, $J$ = 8.2 Hz, 2H), 7.04 (d, $J$ = 8.2 Hz, 2H), 5.38 (s, 1H), 2.26 (s, 3H), 1.32 (s, 9H).
NH
NH
O
2.92
2.07
1.00
2.93
9.06
f1 (ppm)


155.75
136.52
132.54
129.53
120.57
50.36
29.30
20.68
$^{13}$C NMR (101 MHz, CDCl$_3$) δ 155.75, 136.52, 132.54, 129.53, 120.57, 50.36, 29.30, 20.68.
NH
NH
O
f1 (ppm)


$^1$H NMR (400 MHz, $CDCl_3$) δ 7.61 (d, $J$ = 2.4 Hz, 1H), 7.27 (d, $J$ = 8.7 Hz, 1H), 7.20 (dd, $J$ = 8.8, 2.4 Hz, 1H), 6.73 (s, 1H), 3.36 – 3.30 (m, 2H), 2.98 (s, 3H), 1.60 – 1.50 (m, 2H), 1.33 (dq, $J$ = 14.6, 7.3 Hz, 2H), 0.95 (t, $J$ = 7.3 Hz, 3H).
Cl
Cl
NH
N
O
1.00
1.01
1.04
0.93
2.14
3.02
2.17
2.35
3.24
f1 (ppm)


$^{13}$C NMR (101 MHz, $CDCl_3$) δ 154.86, 138.96, 132.18, 129.97, 125.59, 121.43, 119.16, 48.79, 34.49, 30.01, 19.96, 13.77.
Cl
Cl
NH
N
O
f1 (ppm)