Electronic Supplementary Material (ESI) for Chemical Communications.


# Supporting Information

## Amine organocatalysts for highly *ortho*-selective chlorination of anilines with sulfuryl chloride

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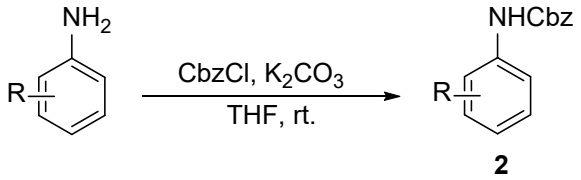
## (A) General information

Commercially available reagents were used directly without further purification. For others, we prepared them in suitable reaction conditions. NMR spectra were recorded on a Brucker ADVANCE III 400MHz spectrometer ($^{1}$H NMR: 400 MHz, $^{13}$C NMR: 100 MHz). Chemical shifts (δ) were reported in ppm relative to $CDCl_3$ (δ 7.26) for the $^{1}$H NMR and to $CDCl_3$ (δ 77.16) for the $^{13}$C NMR measurements. Mass spectra were recorded on Therno Finnigan MAT 95 XL spectrometer and Bruker solariX 9.4 Tesla FTICR spectrometer. GC/MS analysis was conducted on a Shimadzu GCMSQP2010 instrument equipped with a Restec-5HT column (30 m × 0.25 mm, Hewlett-Packard). IR spectra were recorded on a PerkinElmer FT-IR spectrophotometer and reported in terms of wavenumber of absorption ($cm^{-1}$). Flash column chromatography was performed on 300-400 mesh silica gel from Qingdao Haiyang Chemical Co., Ltd. Reactions were monitored by thin-layer chromatography (TLC) using 254 nm UV light to visualize the progress of the reactions.

## (B) Substrate preparation

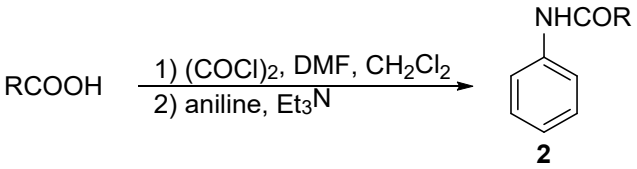
**General Procedure for the preparation of *N*-Cbz aniline 2**




**2**

To a solution of aniline (5.0 mmol, 1.0 eq) and $K_2CO_3$ (828 mg, 6.0 mmol, 1.2 eq) in dry THF (30 mL) was added dropwise CbzCl (937.7 mg, 5.5 mmol, 1.1 eq) over 10 min at 0°C and the reaction mixture was stirred overnight at 25 °C under $N_2$. The reaction mixture was quenched with $H_2O$ (20 mL), then extracted with $CH_2Cl_2$ (10 mL × 3). The combined organic layers were dried over sodium sulfate, filtered, and concentrated to dryness *in vacuo*. The residue was purified over silica gel chromatography eluted with *n*-hexane/ethyl acetate (5:1-1:1) to yield *N*-Cbz aniline **2**.

**General Procedure for the preparation of *N*-carbonyl aniline 2**




**2**

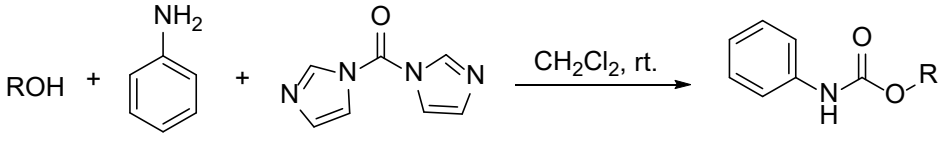
**Step-1**

To a solution of carboxylic acid (5.0 mmol, 1.0 eq) and catalytic amount of DMF in dry $CH_2Cl_2$ (20 mL) was added dropwise oxalyl chloride (6.5 mmol, 1.3 eq) over 10 min at 0°C, and the resulting reaction mixture was stirred for 4 h at 25 °C under $N_2$. The resulting mixture was concentrated under reduced pressure to afford acid chloride quantitatively which was used directly without further purification for the next step.

**Step-2**

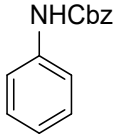
To a solution of aniline (4.2 mmol, 1.0 eq) and $Et_3N$ (6.3 mmol, 1.5 eq) in dry $CH_2Cl_2$ (20 mL) was added dropwise acid chloride (5.0 mmol, 1.2 eq) over 15 min at 0°C and the resulting reaction mixture was stirred for 12 h at 25 °C under $N_2$. Then the reaction was quenched with $H_2O$ (20 mL), then extracted with $CH_2Cl_2$ (10 mL × 3). The combined organic layers were washed with saturated aqueous $NaHCO_3$ (20 mL) followed by $H_2O$ (20 mL). After that, the organic layer was dried over sodium sulfate, filtered, and concentrated to dryness *in vacuo*. The residue was purified over silica gel chromatography eluted with *n*-hexane/ethyl acetate (5:1-1:1) to yield aniline **2**.

**General Procedure for the preparation of aniline 2**

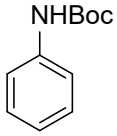



**2**

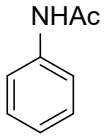
To a stirred solution of aniline (5.0 mmol, 1.0 eq) in $CH_3CN$ (15 mL) were added carbonyldiimidazole (CDI) (20.0 mmol, 4.0 eq) and DMAP (1.0 mmol, 0.2 eq). The reaction mixture was heated at reflux for 5 h. After this time, the appropriate ROH (75.0 mmol, 15 eq) was then added and reflux continued for a further 24 h under the same conditions. The reaction mixture was then cooled to room temperature, concentrated *in vacuo* and the resulting crude product purified by flash column chromatography eluted with *n*-hexane/ethyl acetate (5:1-1:1) to yield aniline **2**.



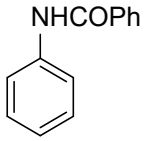

**benzyl phenylcarbamate (2a)**
White solid. $^1$H NMR (400 MHz, $CDCl_3$) δ 5.21 (s, 2H), 6.70 (s, 1H), 7.07 (t, *J* = 8.0 Hz, 1H), 7.28-7.33 (m, 2H), 7.34-7.43 (m, 7H); $^{13}$C NMR (100 MHz, $CDCl_3$) δ 153.6, 137.9, 136.1, 129.0, 128.5, 128.3, 128.2, 123.4, 118.8, 66.9.
The analytical data are in accordance with those reported in the literature.[1]




**tert-butyl phenylcarbamate (2b)**
White solid. $^1$H NMR (400 MHz, $CDCl_3$) δ 1.44 (s, 9H), 6.50 (s, 1H), 6.95 (t, *J* = 8.0 Hz, 1H), 7.20 (t, *J* = 8.0 Hz, 2H), 7.28 (d, *J* = 8.0 Hz, 2H); $^{13}$C NMR (100 MHz, $CDCl_3$) δ 152.9, 138.4, 129.1, 123.1, 118.6, 80.6, 28.5.
The analytical data are in accordance with those reported in the literature.[2]

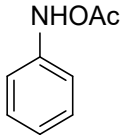



**N-phenylacetamide (2c)**
White solid. $^1$H NMR (400 MHz, $CDCl_3$) δ 2.15 (s, 3H), 7.09 (t, *J* = 8.0 Hz, 1H), 7.30 (t, *J* = 8.0 Hz, 2H), 7.51 (d, *J* = 8.0 Hz, 2H), 7.84 (s, 1H); $^{13}$C NMR (100 MHz, $CDCl_3$) δ 168.9, 138.1, 129.0, 124.4, 120.1, 24.6.
The analytical data are in accordance with those reported in the literature.[2]

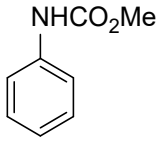



**N-phenylbenzamide (2d)**
White solid. $^1$H NMR (400 MHz, $CDCl_3$) δ 7.16 (t, *J* = 8.0 Hz, 1H), 7.39 (t, *J* = 8.0

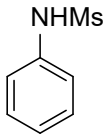
Hz, 2H), 7.50 (t, *J* = 8.0 Hz, 2H), 7.55-7.58 (m, 1H), 7.65 (d, *J* = 8.0 Hz, 2H), 7.80 (s, 1H), 7.88 (d, *J* = 8.0 Hz, 2H); $^{13}$C NMR (100 MHz, $CDCl_3$) δ 166.0, 138.1, 135.1, 132.0, 129.2, 128.9, 127.2, 124.7, 120.4.
The analytical data are in accordance with those reported in the literature.[2]



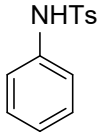

**O-acetyl-N-phenylhydroxylamine (2e)**
White solid. $^{1}$H NMR (400 MHz, $CDCl_3$) δ 2.15 (s, 3H), 7.09 (t, *J* = 8.0 Hz, 1H), 7.30 (t, *J* = 8.0 Hz, 2H), 7.51 (t, *J* = 8.0 Hz, 2H), 7.82 (s, 1H); $^{13}$C NMR (100 MHz, $CDCl_3$) δ 168.9, 138.1, 129.0, 124.4, 120.1, 24.6.



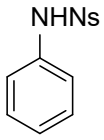

**methyl phenylcarbamate (2f)**
White solid. $^{1}$H NMR (400 MHz, $CDCl_3$) δ 3.78 (s, 3H), 6.59 (s, 1H), 7.07 (t, *J* = 8.0 Hz, 1H), 7.31 (t, *J* = 8.0 Hz, 2H), 7.38 (d, *J* = 8.0 Hz, 2H); $^{13}$C NMR (100 MHz, $CDCl_3$) δ 154.2, 138.0, 129.2, 123.6, 118.8, 52.5.
The analytical data are in accordance with those reported in the literature.[3]




**N-phenylmethanesulfonamide (2g)**
White solid. $^{1}$H NMR (400 MHz, $CDCl_3$) δ 3.01 (s, 3H), 7.16-7.20 (m, 2H), 7.25 (d, *J* = 8.0 Hz, 2H), 7.34 (t, *J* = 8.0 Hz, 2H); $^{13}$C NMR (100 MHz, $CDCl_3$) δ 136.9, 129.8, 125.5, 120.9, 39.3.
The analytical data are in accordance with those reported in the literature.[2]



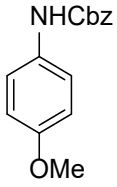

**4-methyl-N-phenylbenzenesulfonamide (2h)**
White solid. $^{1}$H NMR (400 MHz, $CDCl_3$) δ 3.36 (s, 3H), 7.07-7.11 (m, 3H), 7.20-7.26 (m, 4H), 7.30 (s, 3H), 7.70 (t, *J* = 8.0 Hz, 2H); $^{13}$C NMR (100 MHz, $CDCl_3$) δ 144.0, 136.7, 136.1, 129.8, 129.4, 127.4, 125.3, 121.5, 21.7.
The analytical data are in accordance with those reported in the literature.[2]




**4-nitro-N-phenylbenzenesulfonamide (2i)**

Pale yellow solid. $^{1}$H NMR (400 MHz, $CDCl_3$) δ 6.62 (s, 1H), 7.08 (d, *J* = 8.0 Hz, 2H), 7.20 (t, *J* = 8.0 Hz, 1H), 7.29 (t, *J* = 8.0 Hz, 2H), 7.92 (d, *J* = 8.0 Hz, 2H), 8.28 (d, *J* = 8.0 Hz, 2H); $^{13}$C NMR (100 MHz, $CDCl_3$) δ 150.4, 144.7, 135.4, 129.8, 128.7, 126.7, 124.4, 122.6.

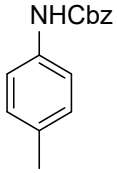
The analytical data are in accordance with those reported in the literature.[2]




**benzyl (4-methoxyphenyl)carbamate (2j)**

White solid. $^{1}$H NMR (400 MHz, $CDCl_3$) δ 3.78 (s, 3H), 5.19 (s, 2H), 6.67 (s, 1H), 6.85 (d, *J* = 8.0 Hz, 2H), 7.29-7.42 (m, 7H); $^{13}$C NMR (100 MHz, $CDCl_3$) δ 156.1, 153.8, 136.3, 130.9, 128.7, 128.4, 120.8, 114.3, 67.0, 55.6.

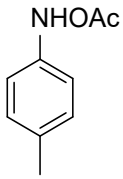
The analytical data are in accordance with those reported in the literature.[1]




**benzyl p-tolylcarbamate (2k)**

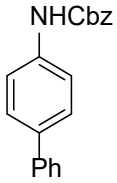
White solid. $^{1}$H NMR (400 MHz, $CDCl_3$) δ 2.22 (s, 3H), 5.10 (s, 2H), 6.87 (s, 1H), 7.01 (d, *J* = 8.0 Hz, 2H), 7.20-7.31 (m, 7H); $^{13}$C NMR (100 MHz, $CDCl_3$) δ 153.6, 136.2, 135.3, 133.0, 129.5, 128.6, 128.3, 118.9, 66.9, 20.8.

The analytical data are in accordance with those reported in the literature.[1]




**O-acetyl-N-(p-tolyl)hydroxylamine (2l)**

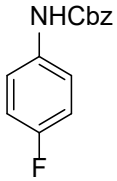
White solid. $^{1}$H NMR (400 MHz, $CDCl_3$) δ 2.16 (s, 3H), 2.31 (s, 3H), 7.11 (d, *J* = 8.0 Hz, 2H), 7.37 (d, *J* = 8.0 Hz, 2H); $^{13}$C NMR (100 MHz, $CDCl_3$) δ 168.8, 135.5, 134.0, 129.5, 120.3, 24.5, 21.0. HRMS(ESI) calcd for $C_9H_{11}NO_2Na$ *m/z* $[M+Na]^+$: 188.0682, found: 188.0682.




**benzyl [1,1'-biphenyl]-4-ylcarbamate (2m)**

White solid. $^{1}$H NMR (400 MHz, $CDCl_3$) δ 5.23 (s, 2H), 6.74 (s, 1H), 7.31-7.48 (m, 10H)，7.54-7.58 (m, 4H); $^{13}$C NMR (100 MHz, $CDCl_3$) δ 153.4, 140.6, 137.2, 136.6, 136.1, 128.9, 128.8, 128.6, 128.5, 127.9, 127.2, 126.9, 119.1, 67.3.

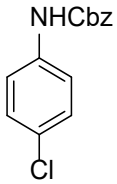
The analytical data are in accordance with those reported in the literature.[4]




**benzyl (4-fluorophenyl)carbamate (2n)**

White solid. $^{1}$H NMR (400 MHz, $CDCl_3$) δ 5.20 (s, 2H), 6.72 (s, 1H), 7.00 (t, $J$ = 8.0 Hz, 2H), 7.32-7.41 (m, 7H); $^{13}$C NMR (100 MHz, $CDCl_3$) δ 160.4, 157.9, 153.6, 136.1, 133.8, 128.8, 128.6, 128.5, 120.6, 115.9, 115.7, 67.2.

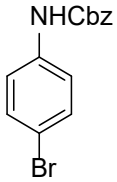
The analytical data are in accordance with those reported in the literature.[1]




**benzyl (4-chlorophenyl)carbamate (2o)**

White solid. $^{1}$H NMR (400 MHz, $CDCl_3$) δ 5.20 (s, 2H), 6.70 (s, 1H), 7.25-7.27 (m, 2H), 7.33-7.42 (m, 7H); $^{13}$C NMR (100 MHz, $CDCl_3$) δ 153.3, 136.5, 135.9, 129.2, 128.8, 128.6, 128.5, 120.0, 67.3.

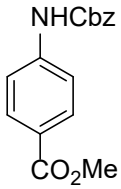
The analytical data are in accordance with those reported in the literature.[1]




**benzyl (4-bromophenyl)carbamate (2p)**

White solid. $^{1}$H NMR (400 MHz, $CDCl_3$) δ 5.20 (s, 2H), 6.69 (s, 1H), 7.26-7.29 (m, 2H), 7.34-7.42 (m, 7H); $^{13}$C NMR (100 MHz, $CDCl_3$) δ 153.2, 137.0, 135.9, 132.1, 128.8, 128.6, 128.5, 120.3, 116.2, 67.4.

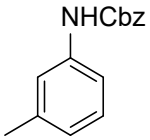
The analytical data are in accordance with those reported in the literature.[1]




**methyl 4-(((benzyloxy)carbonyl)amino)benzoate (2q)**

White solid. $^{1}$H NMR (400 MHz, $CDCl_3$) δ 3.89 (s, 3H), 5.22 (s, 2H), 6.82 (s, 1H), 7.35-7.42 (m, 5H), 7.46 (d, *J* = 8.0 Hz, 2H), 7.99 (d, *J* = 8.0 Hz, 2H); $^{13}$C NMR (100 MHz, $CDCl_3$) δ 166.9, 153.1, 142.4, 135.8, 131.0, 128.7, 128.5, 128.4, 124.8, 117.7, 67.3, 52.1.

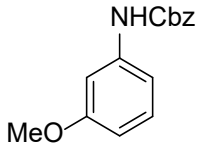
The analytical data are in accordance with those reported in the literature.[5]




**benzyl m-tolylcarbamate (2r)**

White solid. $^{1}$H NMR (400 MHz, $CDCl_3$) δ 2.31 (s, 3H), 5.20 (s, 2H), 6.65 (s, 1H), 7.11 (d, *J* = 8.0 Hz, 2H), 7.26-7.42 (m, 7H); $^{13}$C NMR (100 MHz, $CDCl_3$) δ 153.6, 136.2, 135.3, 133.2, 129.7, 128.7, 128.5, 128.4, 118.9, 67.1, 20.9.

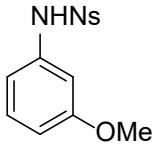
The analytical data are in accordance with those reported in the literature.[5]




**benzyl (3-methoxyphenyl)carbamate (2s)**

White solid. $^{1}$H NMR (400 MHz, $CDCl_3$) δ 3.80 (s, 3H), 5.20 (s, 2H), 6.63 (dd, *J* = 4.0, 8.0 Hz, 1H), 6.78 (s, 1H), 6.88 (d, *J* = 8.0 Hz, 1H), 7.14 (s, 1H), 7.19 (t, *J* = 8.0 Hz, 1H), 7.33-7.42 (m, 5H); $^{13}$C NMR (100 MHz, $CDCl_3$) δ 160.4, 153.4, 139.2, 136.1, 129.9, 128.8, 128.5, 128.4, 111.0, 109.4, 104.5, 67.2, 53.4.

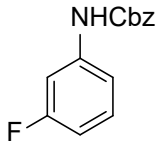
The analytical data are in accordance with those reported in the literature.[1]




**N-(3-methoxyphenyl)-4-nitrobenzenesulfonamide (2t)**

White solid. $^{1}$H NMR (400 MHz, $CDCl_3$) δ 3.76 (s, 3H), 6.61 (d, *J* = 8.0 Hz, 1H), 6.70-6.72 (m, 2H), 6.89 (s, 1H), 7.16 (t, *J* = 8.0 Hz, 1H), 7.96 (d, *J* = 8.0 Hz, 2H), 8.29 (d, *J* = 8.0 Hz, 2H); $^{13}$C NMR (100 MHz, $CDCl_3$) δ 160.6, 150.4, 144.6, 136.7, 130.5, 128.7, 124.5, 113.9, 111.6, 108.0, 55.5.

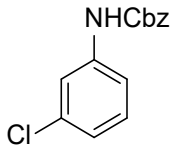
The analytical data are in accordance with those reported in the literature.[2]




**benzyl (3-fluorophenyl)carbamate (2u)**

White solid. $^{1}$H NMR (400 MHz, $CDCl_3$) δ 5.21 (s, 2H), 6.71 (s, 1H), 6.76 (t, *J* = 8.0 Hz, 1H), 7.01 (d, *J* = 8.0 Hz, 1H), 7.21-7.25 (m, 1H), 7.33-7.43 (m, 6H); $^{13}$C NMR (100 MHz, $CDCl_3$) δ 164.4, 162.0, 153.3, 139.6, 139.4, 135.9, 130.3, 130.2, 128.7, 128.5, 128.4, 114.0, 110.3, 110.1, 106.3, 106.0, 67.3.

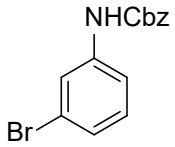
The analytical data are in accordance with those reported in the literature.[6]




**benzyl (3-chlorophenyl)carbamate (2v)**

White solid. $^{1}$H NMR (400 MHz, $CDCl_3$) δ 5.20 (s, 2H), 6.77 (s, 1H), 7.03-7.05 (m, 1H), 7.19-7.22 (m, 2H), 7.33-7.40 (m, 5H), 7.52 (s, 1H); $^{13}$C NMR (100 MHz, $CDCl_3$) δ 153.2, 139.1, 135.9, 134.9, 130.2, 128.8, 128.6, 128.5, 123.7, 118.8, 116.7, 67.4.

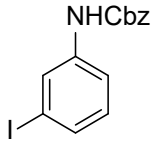
The analytical data are in accordance with those reported in the literature.[7]




**benzyl (3-bromophenyl)carbamate (2w)**

White solid. $^{1}$H NMR (400 MHz, $CDCl_3$) δ 5.20 (s, 2H), 6.70 (s, 1H), 6.13-6.20 (m, 2H), 7.26-7.28 (m, 1H), 7.34-7.40 (m, 5H), 7.66 (s, 1H); $^{13}$C NMR (100 MHz, $CDCl_3$) δ 153.1, 139.2, 135.9, 130.5, 128.8, 128.6, 128.5, 126.6, 122.9, 121.6, 117.2, 67.4.

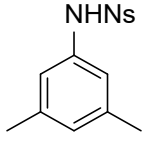
The analytical data are in accordance with those reported in the literature.[7]




**benzyl (3-iodophenyl)carbamate (2x)**

White solid. $^{1}$H NMR (400 MHz, $CDCl_3$) δ 5.20 (s, 2H), 6.61 (s, 1H), 7.02 (t, *J* = 8.0 Hz, 1H), 7.31-7.40 (m, 7H), 7.82 (s, 1H); $^{13}$C NMR (100 MHz, $CDCl_3$) δ 153.1, 139.1, 135.9, 132.7, 130.6, 128.8, 128.6, 128.5, 127.4, 117.9, 94.4, 67.4.

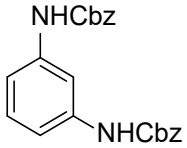
The analytical data are in accordance with those reported in the literature.[8]



**N-(3,5-dimethylphenyl)-4-nitrobenzenesulfonamide (2y)**

White solid. $^1$H NMR (400 MHz, $CDCl_3$) δ 2.24 (s, 6H), 6.42 (s, 1H), 6.68 (s, 2H), 6.82 (s, 1H), 7.93 (d, *J* = 8.0 Hz, 2H), 8.29 (d, *J* = 8.0 Hz, 2H); $^{13}$C NMR (100 MHz, $CDCl_3$) δ 150.3, 144.8, 139.7, 135.3, 128.6, 128.2, 124.4, 119.8, 21.4.

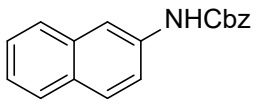
The analytical data are in accordance with those reported in the literature.[2]




**dibenzyl 1,3-phenylenedicarbamate (2z)**

White solid. $^1$H NMR (400 MHz, $CDCl_3$) δ 5.19 (s, 4H), 6.68 (s, 2H), 7.08 (d, *J* = 8.0 Hz, 2H), 7.22 (t, *J* = 8.0 Hz, 1H), 7.33-7.42 (m, 10H), 7.57 (s, 1H); $^{13}$C NMR (100 MHz, $CDCl_3$) δ 152.5, 138.6, 136.0, 129.6, 128.6, 128.3(2), 113.6, 109.0, 67.0.

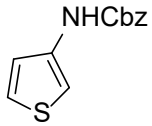
The analytical data are in accordance with those reported in the literature.[9]




**benzyl naphthalen-2-ylcarbamate (2aa)**

White solid. $^1$H NMR (400 MHz, $CDCl_3$) δ 5.25 (s, 2H), 6.84 (s, 1H), 7.34-7.48 (m, 8H), 7.78 (dd, *J* = 4.0, 8.0 Hz, 3H), 8.01 (s, 1H); $^{13}$C NMR (100 MHz, $CDCl_3$) δ 153.5, 136.1, 135.3, 134.1, 130.4, 129.1, 128.8, 128.6, 128.5, 127.7, 127.6, 126.7, 124.9, 119.2, 115.0, 67.3.

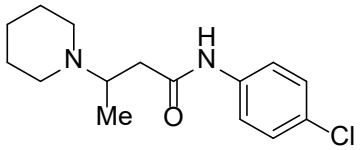
The analytical data are in accordance with those reported in the literature.[7]




**benzyl thiophen-3-ylcarbamate (2ab)**

White solid. $^1$H NMR (400 MHz, $CDCl_3$) δ 5.21 (s, 2H), 6.88 (s, 1H), 6.93 (d, *J* = 4.0 Hz, 1H), 7.21-7.26 (m, 2H), 7.32-7.42 (m, 5H); $^{13}$C NMR (100 MHz, $CDCl_3$) δ 153.6, 136.0, 135.7, 128.6, 128.4, 128.2, 124.8, 120.8, 108.1, 67.1.

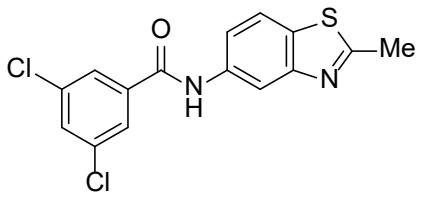
The analytical data are in accordance with those reported in the literature.[10]



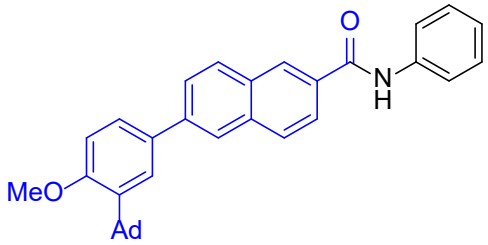

**N-(4-chlorophenyl)-3-(piperidin-1-yl)butanamide (2a')**

White solid. $R_f$ = 0.30 (PE:EtOAc = 2:1); $^1$H NMR (400 MHz, $CDCl_3$) δ 1.02 (d, *J* = 6.4 Hz, 3H), 1.54-1.60 (m, 2H), 1.63-1.76 (m, 4H), 2.21 (dd, *J* = 2.8, 8.6 Hz, 1H ), 2.44-2.49 (m, 2H), 2.55-2.63 (m, 1H), 2.72-2.78 (m, 2H), 3.04-3.09 (m, 1H), 7.26 (d,

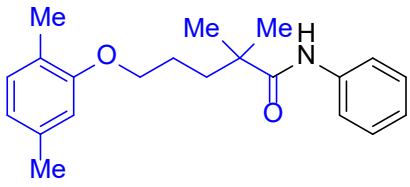
$J$ = 8.0 Hz, 2H), 7.52 (d, $J$ = 8.0 Hz, 2H), 11.79 (s, 1H); $^{13}$C NMR (100 MHz, $CDCl_3$) δ 170.6, 137.8, 129.1, 128.3, 120.8, 56.9, 48.6, 39.5, 26.8, 24.7, 13.3.
The analytical data are in accordance with those reported in the literature.[15]




**3,5-dichloro-N-(2-methylbenzo[d]thiazol-5-yl)benzamide (2b')**
White solid. $R_f$ = 0.30 (PE:EtOAc = 2:1); $^1$H NMR (400 MHz, $CDCl_3$) δ 2.84 (s, 3H), 7.54 (s, 1H), 7.69 (d, $J$ = 8.0 Hz, 1H), 7.77 (s, 2H), 7.80 (d, $J$ = 8.0 Hz, 1H), 7.93 (s, 1H), 8.15 (s, 1H); $^{13}$C NMR (100 MHz, $CDCl_3$) δ 168.9, 163.4, 154.0, 137.8, 135.9, 135.8, 132.3, 131.9, 125.9, 121.9, 118.4, 114.2, 20.4.
The analytical data are in accordance with those reported in the literature.[11]

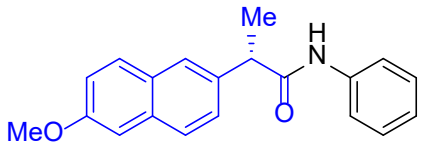



**6-(3-((3s)-adamantan-1-yl)-4-methoxyphenyl)-N-phenyl-2-naphthamide (2c')**
White solid. $R_f$ = 0.35 (PE:EtOAc = 4:1); $^1$H NMR (400 MHz, DMSO-*d6*) δ 1.76 (s, 6H), 2.07 (s, 3H), 2.14 (s, 6H), 3.86 (s, 3H), 7.12 (d, $J$ = 8.0 Hz, 2H), 7.38 (t, $J$ = 8.0 Hz, 2H), 7.59 (s, 1H), 7.66 (d, $J$ = 8.0 Hz, 1H), 7.85 (d, $J$ = 8.0 Hz, 2H), 7.91 (d, $J$ = 8.0 Hz, 1H), 8.02-8.05 (m, 1H), 8.13 (dd, $J$ = 4.0, 8.0 Hz, 2H), 8.24 (s, 1H), 8.59 (s, 1H), 10.44 (s, 1H); $^{13}$C NMR (100 MHz, $CDCl_3$) δ 165.9, 159.1, 141.2, 139.2, 138.2, 135.5, 132.6, 131.8, 131.5, 129.5, 129.3, 129.0, 127.5, 127.0, 126.1, 125.9, 124.9, 124.7, 124.0, 120.4, 112.3, 55.3, 40.8, 37.4, 37.3, 29.2. HRMS(ESI) calcd for $C_{34}H_{34}NO_2$ *m/z* $[M+H]^+$: 488.2584, found: 488.2584.



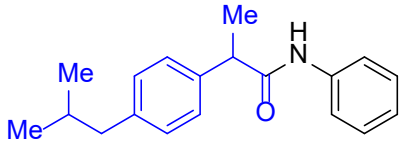

**5-(2,5-dimethylphenoxy)-2,2-dimethyl-N-phenylpentanamide (2d')**
White solid. $R_f$ = 0.35 (PE:EtOAc = 10:1); $^1$H NMR (400 MHz, $CDCl_3$) δ 1.35 (s, 6H), 1.82-1.83 (m, 4H), 2.18 (s, 3H), 2.30 (s, 3H), 3.95 (t, $J$ = 4.0 Hz, 2H), 6.61 (s, 1H), 6.67 (d, $J$ = 8.0 Hz, 1H), 7.01 (d, $J$ = 4.0 Hz, 1H), 7.11 (t, $J$ = 8.0 Hz, 1H), 7.32 (t, $J$ = 8.0 Hz, 2H), 7.38 (s, 1H), 7.52 (d, $J$ = 8.0 Hz, 2H); $^{13}$C NMR (100 MHz, $CDCl_3$) δ 175.8, 156.9, 137.9, 136.7, 130.4, 129.1, 124.4, 123.6, 120.9, 120.2, 112.2, 67.9, 42.9,

37.8, 25.8, 25.3, 21.5, 15.9. HRMS(ESI) calcd for $C_{21}H_{27}NO_2Na$ *m/z* [M+ Na]$^+$: 348.1934, found: 213.9865.



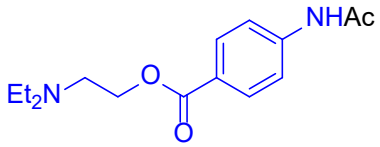

**(S)-2-(6-methoxynaphthalen-2-yl)-N-phenylpropanamide (2e')**

White solid. $R_f$ = 0.55 (PE:EtOAc = 2:1); $^1$H NMR (400 MHz, $CDCl_3$) δ 1.62 (d, *J* = 4.0 Hz, 3H), 3.81 (q, *J* = 8.0 Hz, 1H), 3.88 (s, 3H), 7.01 (t, *J* = 8.0 Hz, 1H), 7.10 (s, 1H), 7.14 (dd, *J* = 4.0, 8.0 Hz, 1H), 7.21 (t, *J* = 8.0 Hz, 2H), 7.38 (d, *J* = 8.0 Hz, 3H), 7.67-7.72 (m, 3H); $^{13}$C NMR (100 MHz, $CDCl_3$) δ 172.7, 157.9, 137.9, 136.1, 133.9, 129.4, 129.1, 128.9, 127.9, 126.4, 126.3, 124.3, 119.8, 119.4, 105.8, 55.4, 48.1, 18.7. HRMS(ESI) calcd for $C_{20}H_{20}NO_2$ *m/z* [M+H]$^+$: 306.1489, found: 306.1490.



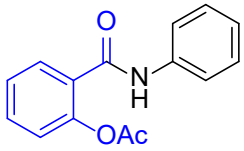

**2-(4-isobutylphenyl)-N-phenylpropanamide (2f')**

White solid. $R_f$ = 0.41 (PE:EtOAc = 3:1); $^1$H NMR (400 MHz, $CDCl_3$) δ 0.94 (d, *J* = 4.0 Hz, 6H), 1.62 (d, *J* = 8.0 Hz, 3H), 1.86-1.92 (m, 1H), 2.50 (d, *J* = 8.0 Hz, 2H), 3.73 (q, *J* = 8.0 Hz, 1H), 7.08 (d, *J* = 8.0 Hz, 1H), 7.17 (d, *J* = 8.0 Hz, 2H), 7.26-7.30 (m, 5H), 7.45 (d, *J* = 8.0 Hz, 2H); $^{13}$C NMR (100 MHz, $CDCl_3$) δ 172.7, 141.2, 138.2, 138.0, 130.0, 129.0, 127.6, 124.3, 119.7, 47.9, 45.1, 30.3, 22.5, 18.6. HRMS(ESI) calcd for $C_{19}H_{23}NONa$ *m/z* [M+Na]$^+$: 304.1672, found: 304.1672.




**2-(diethylamino)ethyl 4-acetamidobenzoate (2g')**

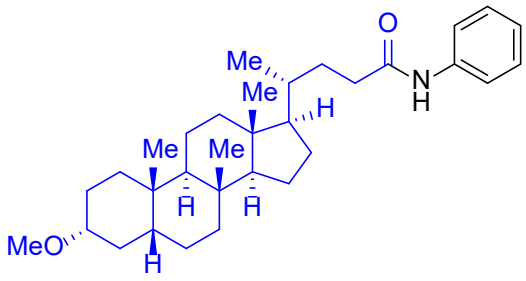
White solid. $R_f$ = 0.37 (DCM:MeOH = 3:1); $^1$H NMR (400 MHz, $CDCl_3$) δ 1.06 (t, *J* = 8.0 Hz, 6H), 2.18 (s, 3H), 2.64 (q, *J* = 8.0 Hz, 4H), 2.86 (t, *J* = 6.0 Hz, 2H), 4.37 (t, *J* = 6.0 Hz, 2H), 7.59 (d, *J* = 8.0 Hz, 2H), 7.96 (d, *J* = 8.0 Hz, 2H); $^{13}$C NMR (100 MHz, $CDCl_3$) δ 168.9, 166.3, 142.4, 130.9, 125.6, 118.9, 63.2, 51.0, 47.8, 24.8, 11.9. HRMS(ESI) calcd for $C_{15}H_{23}N_2O_3$ *m/z* [M+H]$^+$: 279.1703, found: 279.1703.



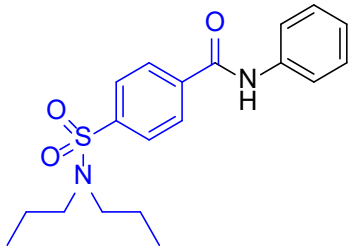

**2-(phenylcarbamoyl)phenyl acetate (2h')**

White solid. $R_f$ = 0.45 (PE:EtOAc = 5:1); $^1$H NMR (400 MHz, $CDCl_3$) δ 2.31 (s, 3H),

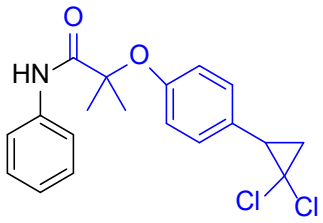
7.15 (t, $J$ = 8.0 Hz, 2H), 7.30-7.37 (m, 3H), 7.49 (t, $J$ = 8.0 Hz, 1H), 7.60 (d, $J$ = 8.0 Hz, 2H), 7.81 (d, $J$ = 8.0 Hz, 1H), 8.14 (s, 1H); $^{13}$C NMR (100 MHz, $CDCl_3$) δ 169.4, 163.8, 147.9, 137.9, 132.2, 129.9, 129.2, 128.9, 126.6, 124.8, 123.4, 120.0, 21.1.
The analytical data are in accordance with those reported in the literature.[12]




**(*R*)-4-((3*R*,5*R*,8*R*,9*R*,10*S*,13*R*,14*R*,17*R*)-3-methoxy-8,10,13-trimethylhexadecahydro-1H-cyclopenta[a]phenanthren-17-yl)-N-phenylpentanamide (2i')**
White solid. $R_f$ = 0.35 (PE:EtOAc = 2:1); $^1$H NMR (400 MHz, $CDCl_3$) δ 0.64 (s, 3H), 0.83-0.96 (m, 10H), 1.03-1.15 (m, 6H), 1.33-1.43 (m, 9H), 1.64-1.97 (m, 9H), 2.21-2.29 (m, 1H), 2.38-2.46 (m, 1H), 3.13-3.20 (m, 1H), 3.35 (s, 3H), 7.08 (d, $J$ = 8.0 Hz, 1H), 7.11 (s, 1H), 7.32 (t, $J$ = 8.0 Hz, 2H), 7.51 (d, $J$ = 8.0 Hz, 2H); $^{13}$C NMR (100 MHz, $CDCl_3$) δ 171.9, 138.2, 129.1, 124.3, 119.9, 80.6, 56.6, 56.2, 55.7, 42.9, 42.2, 40.4, 36.0, 35.6, 35.5, 35.1, 34.8, 32.9, 31.8, 29.8, 28.4, 27.5, 27.0, 26.5, 24.4, 23.6, 21.0, 18.6, 12.2. HRMS(ESI) calcd for $C_{32}H_{49}NO_2Na$ *m/z* $[M+Na]^+$: 502.3656, found: 502.3656.

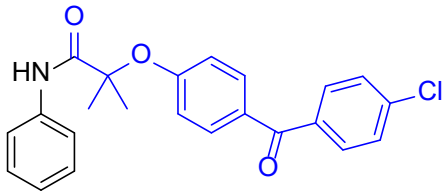



**4-(N,N-dipropylsulfamoyl)-N-phenylbenzamide (2j')**
White solid. $R_f$ = 0.55 (PE:EtOAc = 3:1); $^1$H NMR (400 MHz, $CDCl_3$) δ 0.83 (t, $J$ = 8.0 Hz, 6H), 1.45-1.54 (m, 4H), 3.02 (t, $J$ = 8.0 Hz, 4H), 7.12 (t, $J$ = 8.0 Hz, 1H), 7.30 (t, $J$ = 8.0 Hz, 2H), 7.62 (d, $J$ = 8.0 Hz, 2H), 7.70 (d, $J$ = 8.0 Hz, 2H), 7.88 (d, $J$ = 8.0 Hz, 2H), 8.98 (s, 1H); $^{13}$C NMR (100 MHz, $CDCl_3$) δ 165.1, 142.2, 138.8, 138.0, 128.9, 128.2, 127.0, 124.8, 120.5, 49.9, 21.9, 11.1. HRMS(ESI) calcd for $C_{19}H_{25}N_2O_3S$ *m/z* $[M+H]^+$: 361.1580, found: 361.1580.



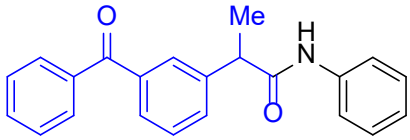
**2-(4-(2,2-dichlorocyclopropyl)phenoxy)-2-methyl-N-phenylpropanamide (2k')**

White solid. $R_f$ = 0.40 (PE:EtOAc = 3:1); $^1$H NMR (400 MHz, $CDCl_3$) δ 1.60 (s, 6H), 1.81 (t, *J* = 8.0 Hz, 1H), 1.95-2.00 (m, 1H), 2.87 (t, *J* = 8.0 Hz, 1H), 6.99 (t, *J* = 8.0 Hz, 2H), 7.14 (t, *J* = 8.0 Hz, 1H), 7.19 (d, *J* = 8.0 Hz, 2H), 7.35 (t, *J* = 8.0 Hz, 2H), 7.59 (dd, *J* = 4.0, 8.0 Hz, 2H), 8.56 (s, 1H); $^{13}$C NMR (100 MHz, $CDCl_3$) δ 172.9, 153.4, 137.6, 130.2, 130.0, 129.2, 124.6, 121.7, 119.9, 82.2, 60.8, 34.9, 26.0, 25.1, 25.0. HRMS(ESI) calcd for $C_{19}H_{19}NO_2Cl_2Na$ *m/z* $[M+Na]^+$: 386.0685, found: 386.0685.



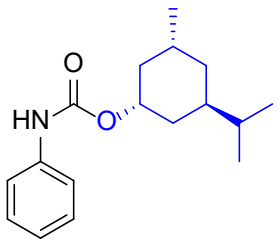

**2-(4-(4-chlorobenzoyl)phenoxy)-2-methyl-N-phenylpropanamide (2l')**

White solid. $R_f$ = 0.35 (PE:EtOAc = 5:1); $^1$H NMR (400 MHz, $CDCl_3$) δ 1.68 (s, 6H), 7.05 (t, *J* = 8.0 Hz, 2H), 7.14 (t, *J* = 8.0 Hz, 1H), 7.34 (t, *J* = 8.0 Hz, 2H), 7.45 (d, *J* = 8.0 Hz, 2H), 7.54 (d, *J* = 8.0 Hz, 2H), 7.67-7.78 (m, 4H), 8.30 (s, 1H); $^{13}$C NMR (100 MHz, $CDCl_3$) δ 194.4, 172.4, 158.3, 138.8, 137.3, 136.1, 132.1, 131.3, 129.2, 128.7(2), 124.9, 120.1(2), 82.4, 25.2. HRMS(ESI) calcd for $C_{23}H_{21}NClO_3$ *m/z* $[M+H]^+$: 394.1205, found: 394.1204.




**2-(3-benzoylphenyl)-N-phenylpropanamide (2m')**

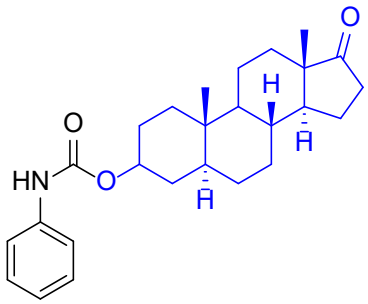
White solid. $R_f$ = 0.40 (PE:EtOAc = 5:1); $^1$H NMR (400 MHz, $CDCl_3$) δ 1.55 (d, *J* = 8.0 Hz, 3H), 3.79 (d, *J* = 8.0 Hz, 1H), 7.05 (t, *J* = 8.0 Hz, 1H), 7.22-7.25 (m, 2H), 7.41-7.49 (m, 5H), 7.58 (t, *J* = 8.0 Hz, 1H), 7.65 (dd, *J* = 4.0, 8.0 Hz, 2H), 7.76 (d, *J* = 8.0 Hz, 2H), 7.83 (s, 1H), 8.04 (d, *J* = 8.0 Hz, 1H); $^{13}$C NMR (100 MHz, $CDCl_3$) δ 197.0, 172.1, 141.8, 138.0(2), 137.3, 132.8, 131.6, 130.2, 129.4, 129.3, 128.9(2), 128.4, 124.4, 120.0, 47.7, 18.9. HRMS(ESI) calcd for $C_{22}H_{19}NO_2Na$ *m/z* $[M+Na]^+$: 352.1308, found: 352.1308.




**(3*R*)-3-isopropyl-5-methylcyclohexyl phenylcarbamate (2n')**

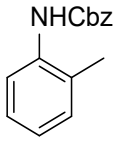
White solid. $R_f$ = 0.55 (PE:EtOAc = 2:1); $^1$H NMR (400 MHz, $CDCl_3$) δ 0.81 (d, *J* = 8.0 Hz, 3H), 0.92 (dd, *J* = 4.0, 8.0 Hz, 6H), 0.97-1.13 (m, 2H), 1.33-1.41 (m, 1H),

1.48-1.55 (m, 1H), 1.66-1.72 (m, 2H), 1.94-1.99 (m, 1H), 2.09-2.14 (m, 1H), 4.67 (dt, $J$ = 4.0, 8.0 Hz, 1H), 6.54 (s, 1H), 7.05 (t, $J$ = 8.0 Hz, 1H), 7.30 (t, $J$ = 8.0 Hz, 2H), 7.39 (d, $J$ = 8.0 Hz, 2H); $^{13}$C NMR (100 MHz, $CDCl_3$) δ 153.4, 138.3, 129.2, 123.3, 118.5, 75.2, 47.5, 41.5, 34.4, 31.5, 26.4, 23.6, 22.2, 20.9, 16.6. HRMS(ESI) calcd for $C_{17}H_{25}NO_2Na$ *m/z* $[M+Na]^+$: 298.1778, found: 298.1778.




**(5*S*,8*R*,10*S*,13*S*,14*S*)-10,13-dimethyl-17-oxohexadecahydro-1H-cyclopenta[a]phenanthren-3-yl phenylcarbamate (2o')**

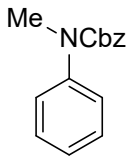
White solid. $R_f$ = 0.35 (PE:EtOAc = 2:1); $^1$H NMR (400 MHz, $CDCl_3$) δ 0.71 (dd, $J$ = 4.0, 8.0 Hz, 1H), 0.84 (s, 3H), 0.85 (s, 3H), 0.92-1.08 (m, 2H), 1.17-1.43 (m, 7H), 1.45-1.58 (m, 3H), 1.62-1.83 (m, 5H), 1.88-1.95 (m, 2H), 2.02-2.11 (m, 1H), 2.39-2.46 (m, 1H), 4.63-4.72 (m, 1H), 6.74 (s, 1H), 7.03 (t, $J$ = 8.0 Hz, 1H), 7.26-7.30 (m, 2H), 7.38 (d, $J$ = 8.0 Hz, 2H); $^{13}$C NMR (100 MHz, $CDCl_3$) δ 153.3, 138.2, 129.1, 123.3, 118.6, 74.5, 54.3, 51.4, 47.9, 44.7, 36.8, 35.9, 35.7, 35.1, 34.3, 31.6, 30.9, 28.3, 27.8, 21.8, 20.5, 13.9, 12.3. HRMS(ESI) calcd for $C_{26}H_{36}NO_3$ *m/z* $[M+H]^+$: 410.2690, found: 410.2690.




**benzyl o-tolylcarbamate (6)**

White solid. $^1$H NMR (400 MHz, $CDCl_3$) δ 2.15 (s, 3H), 5.14 (s, 2H), 6.52 (s, 1H), 6.97 (t, $J$ = 8.0 Hz, 1H), 7.08 (d, $J$ = 8.0 Hz, 1H), 7.14 (t, $J$ = 8.0 Hz, 1H), 7.26-7.36 (m, 5H), 7.75 (s, 1H); $^{13}$C NMR (100 MHz, $CDCl_3$) δ 153.8, 136.1, 135.8, 130.4, 128.7, 128.6, 128.3(2), 126.8, 124.2, 121.3, 67.0, 17.6.

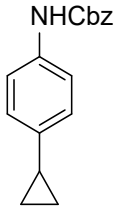
The analytical data are in accordance with those reported in the literature.[9]




**benzyl methyl(phenyl)carbamate (8)**

White solid. $^1$H NMR (400 MHz, $CDCl_3$) δ 3.23 (s, 3H), 5.17 (s, 1H), 7.22-7.37 (m, 10H); $^{13}$C NMR (100 MHz, $CDCl_3$) δ 155.6, 143.3, 136.8, 129.0, 128.5, 128.0, 127.8, 126.3, 125.9, 67.4, 37.9.

The analytical data are in accordance with those reported in the literature.[13]




**benzyl (4-cyclopropylphenyl)carbamate (13)**
White solid. $^{1}$H NMR (400 MHz, $CDCl_3$) δ 0.62-0.66 (m, 2H), 0.90-0.95 (m, 2H), 1.83-1.89 (m, 1H), 5.19 (s, 1H), 6.61 (s, 1H), 7.02 (t, $J$ = 8.0 Hz, 2H), 7.33-7.42 (m, 5H); $^{13}$C NMR (100 MHz, $CDCl_3$) δ 153.5, 139.3, 136.2, 135.3, 128.7, 128.4(2), 126.4, 118.9, 67.1, 15.0, 9.0. HRMS(ESI) calcd for $C_{17}H_{18}NO_2$ *m/z* $[M+H]^+$: 268.1332, found: 268.1333.

## (C) General procedure for the *ortho*-chlorination of aniline catalyzed by 1f

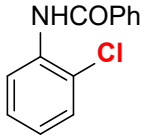
To a solution of secondary amine **1f** (0.02 mmol) and aniline **2** (0.2 mmol) in toluene (2 mL) in the dark was added $SO_2Cl_2$ (0.4 mmol). The resulting mixture was stirred at room temperature and monitored by TLC. Upon completion, the reaction was quenched with saturated $Na_2SO_3$ (3 mL). The organic layer was extracted with dichloromethane (3×10 mL), the combined organic layers were dried over anhydrous $Na_2SO_4$ and evaporated under vacuum. The residue was purified by silica gel column chromatography (hexane/EA = 5:1 to 1:1) to yield the corresponding chlorinated product **3**.


**benzyl (2-chlorophenyl)carbamate (3a)**
White solid. $R_f$ = 0.45 (PE:EtOAc = 10:1); $^{1}$H NMR (400 MHz, $CDCl_3$) δ 5.24 (s, 2H), 7.01 (dt, $J$ = 4.0, 8.0 Hz, 1H), 7.24 (s, 1H), 7.28 (t, $J$ = 8.0 Hz, 1H), 7.34-7.45 (m, 6H), 8.21 (d, $J$ = 8.0 Hz, 1H); $^{13}$C NMR (100 MHz, $CDCl_3$) δ 153.1, 137.1, 134.7, 129.2, 128.8, 128.6, 128.5, 127.9, 123.9, 122.1, 119.9, 67.4.
The analytical data are in accordance with those reported in the literature.[14]

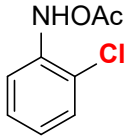

**tert-butyl (2-chlorophenyl)carbamate (3b)**
White solid. $R_f$ = 0.46 (PE:EtOAc = 20:1); $^{1}$H NMR (400 MHz, $CDCl_3$) δ 1.53 (s, 9H),

6.96 (t, $J$ = 8.0 Hz, 1H), 7.01 (s, 1H), 7.24 (t, $J$ = 8.0 Hz, 1H), 7.33 (d, $J$ = 8.0 Hz, 1H); $^{13}$C NMR (100 MHz, $CDCl_3$) δ 152.5, 135.3, 129.1, 127.8, 123.4, 121.9, 119.9, 81.2, 28.4.
The analytical data are in accordance with those reported in the literature.[2]

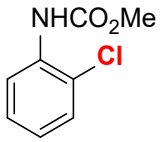

**N-(2-chlorophenyl)acetamide (3c)**
White solid. $R_f$ = 0.42 (PE:EtOAc = 2:1); $^1$H NMR (400 MHz, $CDCl_3$) δ 2.24 (s, 3H), 7.03 (t, $J$ = 8.0 Hz, 1H), 7.27 (t, $J$ = 8.0 Hz, 1H), 7.36 (d, $J$ = 8.0 Hz, 1H), 7.63 (s, 1H), 8.35 (d, $J$ = 8.0 Hz, 1H); $^{13}$C NMR (100 MHz, $CDCl_3$) δ 168.4, 134.7, 129.1, 127.9, 124.7, 122.6, 121.7, 25.0.
The analytical data are in accordance with those reported in the literature.[2]




**N-(2-chlorophenyl)benzamide (3d)**
White solid. $R_f$ = 0.50 (PE:EtOAc = 5:1); $^1$H NMR (400 MHz, $CDCl_3$) δ 7.09 (t, $J$ = 8.0 Hz, 1H), 7.34 (t, $J$ = 8.0 Hz, 1H), 7.42 (d, $J$ = 8.0 Hz, 1H), 7.51-7.55 (m, 2H), 7.59 (t, $J$ = 8.0 Hz, 1H), 7.92-7.95 (m, 2H), 8.46 (s, 1H), 8.58 (dd, $J$ = 4.0, 8.0 Hz, 1H); $^{13}$C NMR (100 MHz, $CDCl_3$) δ 165.4, 134.9, 134.7, 132.4, 129.2, 129.1, 128.0, 127.2, 124.9, 123.1, 121.6, 81.2, 28.4.
The analytical data are in accordance with those reported in the literature.[2]

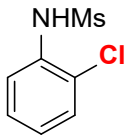



**O-acetyl-N-(2-chlorophenyl)hydroxylamine (3e)**
White solid. $R_f$ = 0.45 (PE:EtOAc = 2:1); $^1$H NMR (400 MHz, $CDCl_3$) δ 2.23 (s, 3H), 7.03 (t, $J$ = 8.0 Hz, 1H), 7.26 (t, $J$ = 8.0 Hz, 1H), 7.35 (d, $J$ = 8.0 Hz, 1H), 7.64 (s, 1H), 8.35 (d, $J$ = 8.0 Hz, 1H); $^{13}$C NMR (100 MHz, $CDCl_3$) δ 168.4, 134.7, 129.1, 127.8, 124.7, 122.7, 121.8, 24.9. HRMS (ESI) calcd for $C_8H_8NO_2ClNa$ *m/z* $[M+Na]^+$: 208.0136, found: 208.0136.




**methyl (2-chlorophenyl)carbamate (3f)**

White solid. $R_f$ = 0.55 (PE:EtOAc = 10:1); $^1$H NMR (400 MHz, $CDCl_3$) δ 3.81 (s, 3H), 7.00 (dt, *J* = 4.0, 8.0 Hz, 1H), 7.15 (s, 1H), 7.27 (t, *J* = 8.0 Hz, 1H), 7.35 (dd, *J* = 4.0, 8.0 Hz, 1H), 8.16 (d, *J* = 8.0 Hz, 1H); $^{13}$C NMR (100 MHz, $CDCl_3$) δ 153.8, 134.8, 129.2, 127.9, 123.9, 122.2, 119.9, 52.7. HRMS (EI) calcd for $C_{15}H_{14}NO_2Cl$ *m/z* $[M]^+$: 275.0708, found: 241.0095.




**N-(2-chlorophenyl)methanesulfonamide (3g)**

White solid. $R_f$ = 0.45 (PE:EtOAc = 5:1); $^1$H NMR (400 MHz, $CDCl_3$) δ 3.02 (s, 3H), 6.80 (s, 1H), 7.15 (t, *J* = 8.0 Hz, 1H), 7.32 (t, *J* = 8.0 Hz, 1H), 7.43 (d, *J* = 8.0 Hz, 1H), 7.66 (d, *J* = 8.0 Hz, 1H); $^{13}$C NMR (100 MHz, $CDCl_3$) δ 133.7, 129.9, 128.5, 126.4, 125.1, 122.5, 40.0.

The analytical data are in accordance with those reported in the literature.[2]


**N-(2-chlorophenyl)-4-methylbenzenesulfonamide (3h)**

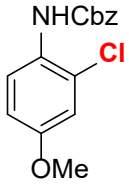
White solid. $R_f$ = 0.35 (PE:EtOAc = 10:1); $^1$H NMR (400 MHz, $CDCl_3$) δ 2.38 (s, 3H), 6.99 (s, 1H), 7.04 (t, *J* =8.0 Hz, 1H), 7.21-7.27 (t, 4H), 7.65-7.67 (m, 3H); $^{13}$C NMR (100 MHz, $CDCl_3$) δ 144.4, 135.9, 133.6, 129.8, 129.5, 128.0, 127.4, 125.9, 125.1, 122.4, 21.7.

The analytical data are in accordance with those reported in the literature.[2]


**N-(2-chlorophenyl)-4-nitrobenzenesulfonamide (3i)**

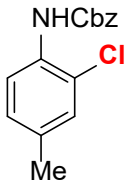
White solid. $R_f$ = 0.45 (PE:EtOAc = 3:1); $^1$H NMR (400 MHz, $CDCl_3$) δ 7.07 (s, 1H), 7.13 (t, *J* =6.0 Hz, 1H), 7.26-7.32 (m, 2H), 7.69 (t, *J* =8.0 Hz, 1H), 7.92 (d, *J* =8.0 Hz, 2H), 8.27 (t, *J* =8.0 Hz, 2H); $^{13}$C NMR (100 MHz, $CDCl_3$) δ 150.5, 144.6, 132.4, 129.8, 128.7, 128.4, 127.4, 126.4, 124.4, 124.1.

The analytical data are in accordance with those reported in the literature.[2]



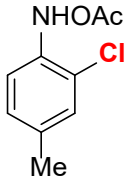
**benzyl (2-chloro-4-methoxyphenyl)carbamate (3j)**

Yellow solid. $R_f$ = 0.50 (PE:EtOAc = 8:1); $^1$H NMR (400 MHz, $CDCl_3$) δ 3.78 (s, 3H), 5.21 (s, 2H), 6.83 (dd, *J* = 4.0, 8.0 Hz, 1H), 6.92 (d, *J* = 4.0 Hz, 1H), 6.96 (s, 1H), 7.35-7.44 (m, 5H), 8.01 (s, 1H); $^{13}$C NMR (100 MHz, $CDCl_3$) δ 155.9, 153.5, 136.0, 128.8, 128.7, 128.5, 128.0, 123.6, 121.7, 114.6, 113.5, 67.4, 55.8. HRMS (ESI) calcd for $C_{15}H_{15}ClNO_3$ *m/z* $[M+H]^+$: 292.0741, found: 292.0742.



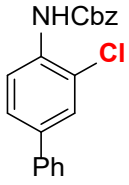

**benzyl (2-chloro-4-methylphenyl)carbamate (3k)**

White solid. $R_f$ = 0.45 (PE:EtOAc = 8:1); $^1$H NMR (400 MHz, $CDCl_3$) δ 2.99 (s, 3H), 5.23 (s, 2H), 7.08 (dd, *J* = 8.0 Hz, 1H), 7.13 (s, 1H), 7.17 (s, 1H), 7.37-7.42 (m, 5H), 8.05 (d, *J* = 8.0 Hz, 1H); $^{13}$C NMR (100 MHz, $CDCl_3$) δ 153.2, 136.0, 133.9, 132.1, 129.5, 128.8, 128.6, 128.5, 128.4, 122.1, 120.0, 67.3, 20.6. HRMS (ESI) calcd for $C_{15}H_{14}NO_2ClNa$ *m/z* $[M+Na]^+$: 298.0605, found: 298.0605.



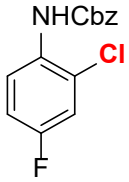

**O-acetyl-N-(2-chloro-4-methylphenyl)hydroxylamine (3l)**

White solid. $R_f$ = 0.45 (PE:EtOAc = 3:1); $^1$H NMR (400 MHz, $CDCl_3$) δ 2.22 (s, 3H), 2.29 (s, 3H), 7.06 (d, *J* = 8.4 Hz, 2H), 7.17 (s, 1H), 7.53 (s, 1H), 8.19 (d, *J* = 8.4 Hz, 1H); $^{13}$C NMR (100 MHz, $CDCl_3$) δ 168.3, 134.9, 132.1, 129.4, 128.5, 122.6, 121.7, 24.9, 20.8. HRMS (ESI) calcd for $C_9H_{11}ClNO_2$ *m/z* $[M+H]^+$: 200.0478, found: 200.0473.



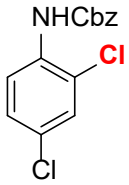

**benzyl (3-chloro-[1,1'-biphenyl]-4-yl)carbamate (3m)**

White solid. $R_f$ = 0.49 (PE:EtOAc = 10:1); $^1$H NMR (400 MHz, $CDCl_3$) δ 5.21 (s, 2H), 7.21 (d, *J* = 8.0 Hz, 1H), 7.29-7.55 (m, 12H), 8.23 (d, *J* = 8.0 Hz, 1H); $^{13}$C NMR (100 MHz, $CDCl_3$) δ 153.1, 139.3, 137.1, 135.8, 133.8, 129.0, 128.8, 128.7, 128.6, 127.7, 127.6, 126.8, 126.5m 122.5, 67.5. HRMS (ESI) calcd for $C_{20}H_{16}NO_2ClNa$ *m/z* $[M+Na]^+$: 360.0762, found: 360.0762.




**benzyl (2-chloro-4-fluorophenyl)carbamate (3n)**

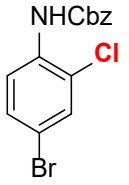
White solid. $R_f$ = 0.41 (PE:EtOAc = 30:1); $^1$H NMR (400 MHz, $CDCl_3$) δ 5.22 (s, 2H), 7.01 (dt, *J* = 4.0, 8.0 Hz, 1H), 7.07 (s, 1H), 7.12 (dd, *J* = 4.0, 8.0 Hz, 1H), 7.34-7.44 (m, 5H), 8.14 (t, *J* = 8.0 Hz, 1H); $^{13}$C NMR (100 MHz, $CDCl_3$) δ 159.3, 156.9, 153.3, 135.8, 131.2(2), 128.8, 128.7, 128.6, 122.9, 121.3, 116.6, 116.3, 114.9, 114.7, 67.6. HRMS (ESI) calcd for $C_{14}H_{11}ClFNO_2Na$ *m/z* $[M+Na]^+$: 302.0355, found: 302.0355.




**benzyl (2,4-dichlorophenyl)carbamate (3o)**

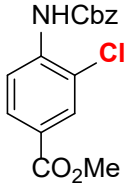
White solid. $R_f$ = 0.40 (PE:EtOAc = 30:1); $^1$H NMR (400 MHz, $CDCl_3$) δ 5.22 (s, 2H), 7.16 (s, 1H), 7.25 (dd, *J* = 4.0, 8.0 Hz, 1H), 7.35-7.44 (m, 6H), 8.16 (d, *J* = 8.0 Hz, 1H); $^{13}$C NMR (100 MHz, $CDCl_3$) δ 152.9, 135.7, 133.6, 128.9, 128.8, 128.7, 128.6, 128.4, 128.1, 122.7, 120.8, 67.7.

The analytical data are in accordance with those reported in the literature.[15]




**benzyl (4-bromo-2-chlorophenyl)carbamate (3p)**

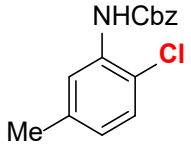
White solid. $R_f$ = 0.42 (PE:EtOAc = 30:1); $^1$H NMR (400 MHz, $CDCl_3$) δ 5.22 (s, 2H), 7.16 (s, 1H), 7.36-7.43 (m, 6H), 7.49 (d, *J* = 4.0 Hz, 1H), 8.11 (d, *J* = 8.0 Hz, 1H); $^{13}$C NMR (100 MHz, $CDCl_3$) δ 152.9, 135.7, 134.1, 131.6, 130.9, 128.9, 128.8, 128.6, 122.8, 121.1, 115.4, 67.7. HRMS (ESI) calcd for $C_{14}H_{11}BrClNO_2Na$ *m/z* $[M+Na]^+$: 361.9554, found: 361.9556.




**methyl 4-(((benzyloxy)carbonyl)amino)-3-chlorobenzoate (3q)**

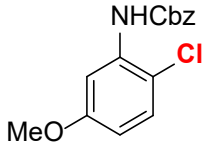
White solid. $R_f$ = 0.40 (PE:EtOAc = 8:1); $^1$H NMR (400 MHz, $CDCl_3$) δ 3.89 (s, 3H), 5.24 (s, 2H), 7.36-7.42 (m, 6H), 7.94 (d, *J* = 8.4 Hz, 1H), 8.03 (s, 1H), 8.33 (d, *J* = 8.4

Hz, 1H); $^{13}$C NMR (100 MHz, $CDCl_3$) δ 165.8, 152.8, 138.9, 135.6, 130.7, 129.6, 128.9, 128.8, 128.7, 125.5, 121.6, 118.8, 67.9, 52.4. HRMS (ESI) calcd for $C_{16}H_{14}ClNO_4Na$ *m/z* $[M+Na]^+$: 342.0504, found: 342.0509.



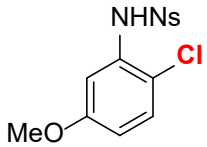

**benzyl (2-chloro-5-methylphenyl)carbamate (3r)**

White solid. $R_f$ = 0.46 (PE:EtOAc = 8:1); $^1$H NMR (400 MHz, $CDCl_3$) δ 2.29 (s, 3H), 5.21 (s, 2H), 7.06 (d, *J* = 8.8 Hz, 1H), 7.11 (s, 1H), 7.16 (s, 1H), 7.35-7.43 (m, 5H), 8.03 (d, *J* = 8.0 Hz, 1H); $^{13}$C NMR (100 MHz, $CDCl_3$) δ 153.2, 135.9, 133.9, 132.1, 129.5, 128.8, 128.6(2), 128.5, 122.1, 120.1, 67.4, 20.7. HRMS (ESI) calcd for $C_{15}H_{14}ClNO_2Na$ *m/z* $[M+Na]^+$: 298.0605, found: 298.0603.




**benzyl (2-chloro-5-methoxyphenyl)carbamate (3s)**

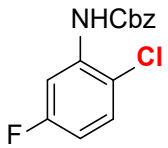
White solid. $R_f$ = 0.45 (PE:EtOAc = 8:1); $^1$H NMR (400 MHz, $CDCl_3$) δ 3.80 (s, 3H), 5.23 (s, 2H), 6.57 (dd, *J* = 4.0, 8.0 Hz, 1H), 7.20-7.22 (m, 2H), 7.36-7.45 (m, 5H), 7.87 (s, 1H); $^{13}$C NMR (100 MHz, $CDCl_3$) δ 159.3, 153.0, 135.8, 135.4, 129.4, 128.8, 128.7, 128.6, 113.3, 110.4, 104.9, 67.5, 55.7. HRMS (ESI) calcd for $C_{15}H_{14}ClNO_3Na$ *m/z* $[M+Na]^+$: 314.0554, found: 314.0554.




**N-(2-chloro-5-methoxyphenyl)-4-nitrobenzenesulfonamide (3t)**

White solid. $^1$H NMR (400 MHz, $CDCl_3$) δ 3.75 (s, 3H), 6.60 (dd, *J* = 4.0, 8.0 Hz, 2H), 6.96 (s, 1H), 7.08 (d, *J* = 12.0 Hz, 1H), 7.18 (d, *J* = 4.0 Hz, 1H), 7.87 (d, *J* = 8.0 Hz, 2H), 8.21 (d, *J* = 8.0 Hz, 2H); $^{13}$C NMR (100 MHz, $CDCl_3$) δ 159.3, 150.5, 144.5, 133.0, 130.1, 128.7, 124.4, 117.2, 113.2, 109.3, 55.9.

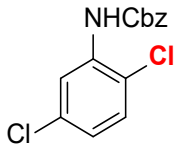
The analytical data are in accordance with those reported in the literature.[2]




**benzyl (2-chloro-5-fluorophenyl)carbamate (3u)**

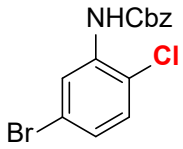
White solid. $R_f$ = 0.40 (PE:EtOAc = 30:1); $^1$H NMR (400 MHz, $CDCl_3$) δ 5.22 (s, 2H), 6.71 (dt, *J* = 4.0, 8.0 Hz, 1H), 7.24 (s, 1H), 7.28 (dd, *J* = 4.0, 8.0 Hz, 1H), 7.35-7.44

(m, 5H), 8.04 (dd, $J$ = 4.0, 12.0 Hz, 1H); $^{13}$C NMR (100 MHz, $CDCl_3$) δ 163.1, 160.6, 152.8, 136.0, 135.9, 135.6, 129.9, 129.8, 128.9, 1228.8, 128.7, 128.6, 116.7, 116.6, 110.8, 110.5, 107.5, 107.2, 67.7. HRMS (ESI) calcd for $C_{14}H_{11}ClFNO_2Na$ *m/z* $[M+Na]^+$: 302.0355, found: 302.0355.



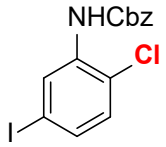

**benzyl (2,5-dichlorophenyl)carbamate (3v)**

White solid. $R_f$ = 0.40 (PE:EtOAc = 30:1); $^1$H NMR (400 MHz, $CDCl_3$) δ 5.23 (s, 2H), 6.98 (dd, $J$ = 4.0, 8.0 Hz, 1H), 7.21 (s, 1H), 7.26 (d, $J$ = 8.0 Hz, 1H), 7.37-7.45 (m, 5H), 8.30 (s, 1H); $^{13}$C NMR (100 MHz, $CDCl_3$) δ 152.8, 135.6(2), 133.8, 129.8, 128.8(2), 128.7, 123.8, 120.0, 119.8, 67.7. HRMS (ESI) calcd for $C_{14}H_{12}Cl_2NO_2$ *m/z* $[M+H]^+$: 296.0240, found: 296.0240.



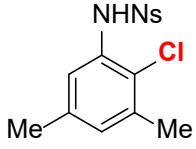

**benzyl (5-bromo-2-chlorophenyl)carbamate (3w)**

White solid. $R_f$ = 0.40 (PE:EtOAc = 30:1); $^1$H NMR (400 MHz, $CDCl_3$) δ 5.23 (s, 2H), 7.12 (d, $J$ = 8.0 Hz, 1H), 7.19-7.21 (m, 2H), 7.36-7.45 (m, 5H), 8.44 (s, 1H); $^{13}$C NMR (100 MHz, $CDCl_3$) δ 152.8, 135.8, 135.6, 130.2, 128.9, 128.8, 128.6, 126.7, 122.6, 121.5, 120.8, 67.7. HRMS (ESI) calcd for $C_{14}H_{11}ClBrNO_2Na$ *m/z* $[M+Na]^+$: 361.9554, found: 361.9556.




**benzyl (2-chloro-5-iodophenyl)carbamate (3x)**

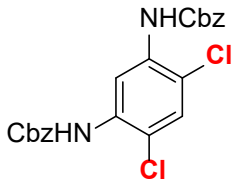
White solid. $R_f$ = 0.40 (PE:EtOAc = 30:1); $^1$H NMR (400 MHz, $CDCl_3$) δ 5.22 (s, 2H), 7.05 (d, $J$ = 8.0 Hz, 1H), 7.16 (s, 1H), 7.26 (d, $J$ = 8.0 Hz, 1H), 7.31 (d, $J$ = 8.0 Hz, 1H), 7.37-7.44 (m, 5H), 8.58 (d, $J$ = 4.0 Hz, 1H); $^{13}$C NMR (100 MHz, $CDCl_3$) δ 152.8, 135.8, 135.6, 132.8, 130.5, 128.8, 128.7, 128.6, 128.4, 121.9, 92.4, 67.7. HRMS (ESI) calcd for $C_{14}H_{11}ClINO_2Na$ *m/z* $[M+Na]^+$: 409.9415, found: 409.9415.



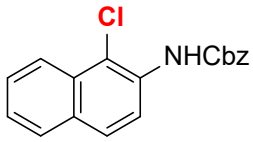

**N-(2-chloro-3,5-dimethylphenyl)-4-nitrobenzenesulfonamide (3y)**

White solid. $R_f$ = 0.40 (PE:EtOAc = 5:1); $^1$H NMR (400 MHz, $CDCl_3$) δ 2.22 (s, 3H),

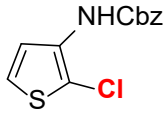
2.30 (s, 3H), 6.87 (s, 1H), 7.03 (s, 1H), 7.35 (s, 1H), 7.92 (d, $J$ = 8.0 Hz, 2H), 8.27 (d, $J$ = 12.0 Hz, 2H); $^{13}$C NMR (100 MHz, $CDCl_3$) δ 150.5, 144.8, 137.6, 136.9, 132.0, 129.5, 128.7, 124.3, 123.3, 121.8, 21.2, 20.6.
The analytical data are in accordance with those reported in the literature.[2]



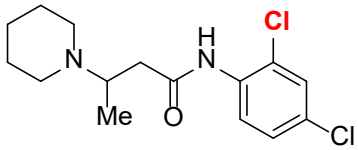

**dibenzyl (4,6-dichloro-1,3-phenylene)dicarbamate (3z)**
White solid. $R_f$ = 0.45 (PE:EtOAc = 10:1); $^1$H NMR (400 MHz, $CDCl_3$) δ 5.25 (s, 4H), 7.13 (s, 2H), 7.33 (s, 1H), 7.36-7.45 (m, 10H), 9.22 (s, 1H); $^{13}$C NMR (100 MHz, $CDCl_3$) δ 152.8, 135.8, 134.4, 128.8(2), 128.7, 115.9, 110.9, 67.7. HRMS (ESI) calcd for $C_{22}H_{18}Cl_2N_2O_4Na$ *m/z* $[M+Na]^+$: 467.0536, found: 467.0536.




**benzyl (1-chloronaphthalen-2-yl)carbamate (3aa)**
White solid. $R_f$ = 0.45 (PE:EtOAc = 10:1); $^1$H NMR (400 MHz, $CDCl_3$) δ 5.27 (s, 2H), 7.37-7.42 (m, 7H), 7.46 (t, $J$ = 7.8 Hz, 1H), 7.80 (t, $J$ = 10.0 Hz, 2H), 8.16 (d, $J$ = 8.0 Hz, 1H), 8.41 (d, $J$ = 9.2 Hz, 1H); $^{13}$C NMR (100 MHz, $CDCl_3$) δ 153.4, 135.9, 132.8, 130.9, 130.8, 128.8, 128.7, 128.6, 128.2, 127.9, 127.7, 125.4, 123.8, 119.2, 117.3, 67.6. HRMS (ESI) calcd for $C_{18}H_{15}ClNO_2$ *m/z* $[M+H]^+$: 312.0786, found: 312.0789.

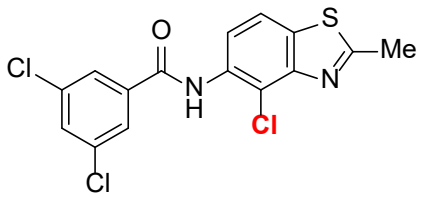



**benzyl (2-chlorothiophen-3-yl)carbamate (3ab)**
White solid. $R_f$ = 0.50 (PE:EtOAc = 10:1); $^1$H NMR (400 MHz, $CDCl_3$) δ 5.21 (s, 2H), 6.79 (s, 1H), 7.08 (d, $J$ = 8.0 Hz, 1H), 7.34-7.43 (m, 5H), 7.60 (s, 1H); $^{13}$C NMR (100 MHz, $CDCl_3$) δ 152.9, 135.8, 132.9, 128.8, 128.7, 128.6, 122.0, 121.3 67.7. HRMS (ESI) calcd for $C_{12}H_{11}ClNO_2S$ *m/z* $[M+H]^+$: 268.0194, found: 268.0194.

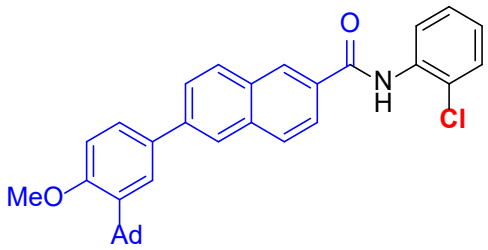



**N-(2,4-dichlorophenyl)-3-(piperidin-1-yl)butanamide (4a)**
Pale yellow solid. $R_f$ = 0.35 (PE:EtOAc = 2:1); $^1$H NMR (400 MHz, $CDCl_3$) δ 1.05 (d, $J$ = 4.0 Hz, 3H), 1.44-1.50 (m, 2H), 1.57-1.65 (m, 2H), 1.67-1.74 (m, 2H), 2.34 (dd, $J$ = 4.0, 16.0 Hz, 1H), 2.42-2.48 (m, 2H), 2.63-2.72 (m, 3H), 3.04-3.09 (m, 1H), 7.21

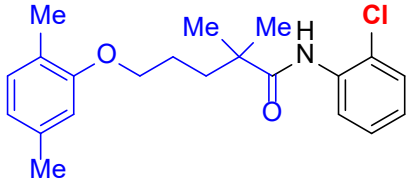
(dd, $J$ = 4.0, 8.0 Hz, 1H), 7.36 (d, $J$ = 4.0 Hz, 1H), 8.15 (d, $J$ = 8.0 Hz, 1H), 11.08 (s, 1H); $^{13}$C NMR (100 MHz, $CDCl_3$) δ 171.2, 134.4, 129.2, 129.0, 127.5, 124.9(2), 56.8, 49.0, 40.1, 26.0, 24.6, 13.3.
The analytical data are in accordance with those reported in the literature.[15]




**3,5-dichloro-N-(6-chloro-2-methylbenzo[d]thiazol-5-yl)benzamide (4b)**
White solid. $R_f$ = 0.50 (PE:EtOAc = 2:1); $^1$H NMR (400 MHz, $CDCl_3$) δ 2.90 (s, 3H), 7.58 (d, $J$ = 4.0 Hz, 1H), 7.77 (d, $J$ = 8.0 Hz, 1H), 7.81 (s, 2H), 8.42 (s, 1H), 8.50 (d, $J$ = 8.0 Hz, 1H); $^{13}$C NMR (100 MHz, $CDCl_3$) δ 170.2, 163.0, 150.5, 137.5, 136.1, 132.6, 132.5, 132.3, 125.9, 120.2, 118.9, 116.3, 20.6. HRMS (ESI) calcd for $C_{15}H_{10}Cl_3N_2OS$ $m/z$ $[M+H]^+$: 370.9574, found: 370.9574.

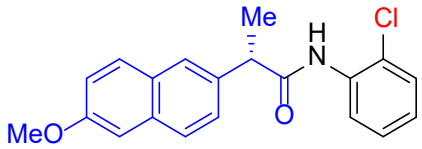



**6-(3-((3s)-adamantan-1-yl)-4-methoxyphenyl)-N-(2-chlorophenyl)-2-naphthamide (4c)**
White solid. $R_f$ = 0.32 (PE:EtOAc = 30:1); $^1$H NMR (400 MHz, DMSO-*d6*) δ 1.79 (s, 6H), 2.08 (s, 3H), 2.16 (s, 6H), 3.92 (s, 3H), 7.00 (d, $J$ = 8.0 Hz, 2H), 7.13 (dd, $J$ = 4.0, 8.0 Hz, 1H), 7.39 (dt, $J$ = 4.0, 8.0 Hz, 2H), 7.45 (t, $J$ = 8.0 Hz, 2H), 7.60 (d, $J$ = 12.0 Hz, 1H), 7.94 (d, $J$ = 8.0 Hz, 1H), 8.09 (d, $J$ = 4.0, 8.0 Hz, 1H), 8.47 (d, $J$ = 4.0 Hz, 1H), 8.54 (d, $J$ = 8.0 Hz, 1H), 8.62-8.64 (m, 2H); $^{13}$C NMR (100 MHz, $CDCl_3$) δ 165.1, 158.7, 140.6, 138.3, 134.8, 133.3, 132.8, 132.2, 131.6, 130.4, 129.6, 129.2, 128.7, 128.2, 128.1, 127.9, 126.4, 125.1, 124.7, 123.3, 121.7, 111.3, 55.19, 40.7, 37.3(2), 29.2. HRMS(ESI) calcd for $C_{34}H_{32}ClNO_2Na$ $m/z$ $[M+Na]^+$: 544.2014, found: 544.2014.



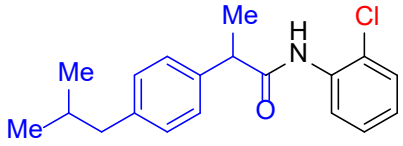

**N-(2-chlorophenyl)-5-(2,5-dimethylphenoxy)-2,2-dimethylpentanamide (4d)**
White solid. $R_f$ = 0.50 (PE:EtOAc = 5:1); $^1$H NMR (400 MHz, $CDCl_3$) δ 1.34 (s, 6H), 1.79-1.83 (m, 4H), 2.14 (s, 3H), 2.29 (s, 3H), 3.92 (t, $J$ = 8.0 Hz, 2H), 6.61 (s, 1H),

7.07 (s, 1H), 7.11 (t, $J$ = 8.0 Hz, 1H), 7.30-7.34 (m, 3H), 7.51 (d, $J$ = 8.0 Hz, 2H); $^{13}$C NMR (100 MHz, $CDCl_3$) δ 175.7, 155.6, 137.9, 133.9, 130.7, 129.1(2), 125.9, 125.0, 124.5, 121.4, 120.2, 113.7, 68.4, 42.9, 37.8, 25.8, 25.2, 20.2, 15.8. HRMS (ESI) calcd for $C_{21}H_{26}ClNO_2Na$ *m/z* $[M+Na]^+$: 382.1544, found: 382.1544.



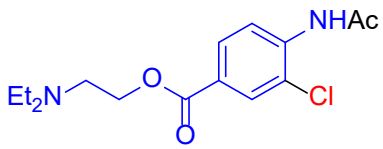

**(S)-N-(2-chlorophenyl)-2-(6-methoxynaphthalen-2-yl)propenamide (4e)**

White solid. $R_f$ = 0.55 (PE:EtOAc = 5:1); $^1$H NMR (400 MHz, $CDCl_3$) δ 1.72 (d, $J$ = 8.0 Hz, 3H), 3.95 (q, $J$ = 8.0 Hz, 1H), 4.04 (s, 3H), 6.98 (dt, $J$ = 4.0, 8.0 Hz, 1H), 7.22-7.26 (m, 2H), 7.32-7.35 (m, 1H), 7.58 (d, $J$ = 8.0 Hz, 1H), 7.68 (s, 1H), 7.79 (d, $J$ = 8.0 Hz, 1H), 7.81 (s, 1H), 8.25 (d, $J$ = 8.0 Hz, 1H), 8.37 (d, $J$ = 8.0 Hz, 1H); $^{13}$C NMR (100 MHz, $CDCl_3$) δ 172.3, 152.9, 136.4, 134.6, 131.4, 129.7, 129.0, 127.9, 127.8, 127.5, 126.8, 124.9, 124.7, 122.8, 121.4, 116.9, 114.3, 57.1, 48.3, 18.3. HRMS (ESI) calcd for $C_{20}H_{18}ClNO_2K$ *m/z* $[M+K]^+$: 378.0658, found: 378.0658.



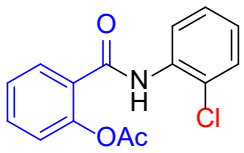

**N-(2-chlorophenyl)-2-(4-isobutylphenyl)propanamide (4f)**

White solid. $R_f$ = 0.32 (PE:EtOAc = 8:1); $^1$H NMR (400 MHz, $CDCl_3$) δ 0.89 (d, $J$ = 8.0 Hz, 6H), 1.65 (s, 3H), 1.84-1.88 (m, 1H), 2.48 (d, $J$ = 8.0 Hz, 2H), 3.77 (q, $J$ = 8.0 Hz, 1H), 6.97 (dt, $J$ = 4.0, 8.0 Hz, 1H), 7.17-7.30 (m, 6H), 7.63 (s, 1H), 8.38 (d, $J$ = 8.0 Hz, 1H); $^{13}$C NMR (100 MHz, $CDCl_3$) δ 172.9, 141.5, 137.5, 134.8, 130.1, 128.9, 127.8(2), 124.4, 122.7, 121.1, 48.2, 45.1, 30.4, 22.4, 18.0. HRMS (ESI) calcd for $C_{19}H_{22}ClNONa$ *m/z* $[M+Na]^+$: 338.1282, found: 338.1288.



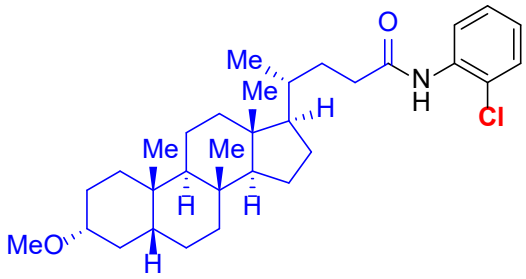

**2-(diethylamino)ethyl 4-acetamido-3-chlorobenzoate (4g)**

White solid. $R_f$ = 0.45 (DCM:MeOH = 8:1); $^1$H NMR (400 MHz, $CDCl_3$) δ 1.06 (t, $J$ = 8.0 Hz, 6H), 2.27 (s, 3H), 2.63 (q, $J$ = 8.0 Hz, 4H), 2.85 (d, $J$ = 8.4 Hz, 2H), 4.37 (d, $J$ = 8.0 Hz, 2H), 7.81 (s, 1H), 7.92 (d, $J$ = 8.4 Hz, 1H), 8.04 (s, 1H), 8.52 (d, $J$ = 12.0 Hz, 1H); $^{13}$C NMR (100 MHz, $CDCl_3$) δ 168.6, 165.2, 138.6, 130.5, 129.5, 126.2, 121.9, 120.3, 63.6, 51.0, 47.9, 25.2, 12.0. HRMS (ESI) calcd for $C_{15}H_{22}ClN_2O_3$ *m/z* $[M+H]^+$: 313.1314, found: 313.1313.



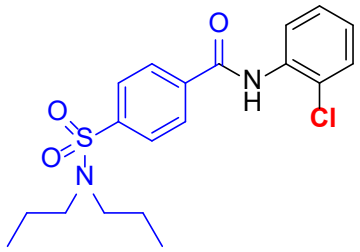

**2-((2-chlorophenyl)carbamoyl)phenyl acetate (4h)**

White solid. $R_f$ = 0.50 (PE:EtOAc = 5:1); $^1$H NMR (400 MHz, $CDCl_3$) δ 2.38 (s, 3H), 7.09 (t, *J* = 8.0 Hz, 1H), 7.19 (d, *J* = 8.0 Hz, 1H), 7.31-7.42 (m, 3H), 7.36 (t, *J* = 8.0 Hz, 2H), 7.98 (d, *J* = 8.0 Hz, 1H), 8.58 (t, *J* = 8.0 Hz, 1H), 8.74 (s, 1H); $^{13}$C NMR (100 MHz, $CDCl_3$) δ 169.0, 163.4, 148.1, 134.9, 132.8, 130.7, 129.2, 128.1, 127.9, 126.7, 125.0, 123.7, 122.8, 121.9, 21.5. HRMS (ESI) calcd for $C_{15}H_{12}ClNO_3Na$ *m/z* $[M+Na]^+$: 312.0398, found: 312.0398.




**(*R*)-*N*-(2-chlorophenyl)-4-((3*R*,5*R*,8*R*,9*R*,10*S*,13*R*,14*R*,17*R*)-3-methoxy-8,10,13-trimethylhexadecahydro-1H-cyclopenta[a]phenanthren-17-yl)pentanamide (4i)**

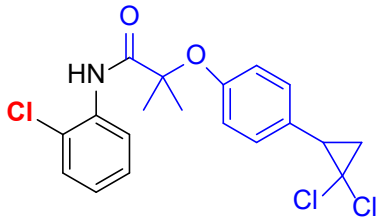
White solid. $R_f$ = 0.42 (PE:EtOAc = 8:1); $^1$H NMR (400 MHz, $CDCl_3$) δ 0.65 (s, 3H), 0.93 (s, 3H), 0.97 (d, *J* = 8.0 Hz, 3H), 1.02-1.17 (m, 6H), 1.20-1.51 (m, 13H), 1.54-.162 (m, 2H), 1.64-1.75 (m, 1H), 1.74-1.98 (m, 6H), 2.29-2.36 (m, 1H), 2.45-2.53 (m, 1H), 3.12-3.20 (m, 1H), 3.35 (s, 3H), 7.03 (t, *J* = 8.0 Hz, 1H), 7.24-7.27 (m, 1H), 7.36 (d, *J* = 8.0 Hz, 1H), 7.62 (s, 1H), 8.38 (d, *J* = 8.0 Hz, 1H); $^{13}$C NMR (100 MHz, $CDCl_3$) δ 171.9, 134.8, 129.1, 127.9, 124.6, 122.6, 121.7, 80.5, 56.6, 56.1, 55.7, 42.9, 42.2, 40.5, 40.3, 35.9, 35.5, 35.4, 35.0, 32.9, 31.7, 28.4, 27.5, 26.9, 26.5, 24.4, 23.6, 20.9, 18.5, 12.2. HRMS(ESI) calcd for $C_{32}H_{48}ClNO_2Na$ *m/z* $[M+Na]^+$: 536.3266, found: 356.3266.




**N-(2-chlorophenyl)-4-(N,N-dipropylsulfamoyl)benzamide (4j)**

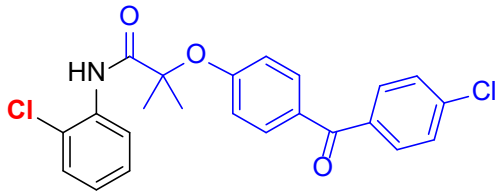
White solid. $R_f$ = 0.50 (PE:EtOAc = 6:1); $^1$H NMR (400 MHz, $CDCl_3$) δ 0.88 (t, *J* = 8.0 Hz, 6H), 1.54-1.61 (m, 4H), 3.12(t, *J* = 8.0 Hz, 4H), 7.13 (t, *J* = 8.0 Hz, 1H), 7.36 (t, *J* = 8.0 Hz, 1H), 7.44 (d, *J* = 8.0 Hz, 1H), 7.95 (d, *J* = 8.0 Hz, 2H), 8.03 (d, *J* =8.0 Hz, 2H), 8.44 (s, 1H), 8.52 (*J* = 8.0 Hz, 1H); $^{13}$C NMR (100 MHz, $CDCl_3$) δ 163.9, 143.8, 138.0, 134.4, 129.3, 128.1, 127.9, 127.8, 125.5, 123.4, 121.8, 50.1, 22.1, 11.3.

HRMS (ESI) calcd for $C_{19}H_{23}ClN_2O_3SNa$ *m/z* $[M+Na]^+$: 417.1010, found: 417.1010.



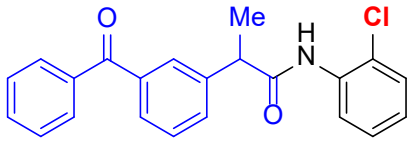

**N-(2-chlorophenyl)-2-(4-(2,2-dichlorocyclopropyl)phenoxy)-2-methylpropanamide (4k)**

White solid. $R_f$ = 0.45 (PE:EtOAc = 6:1); $^1$H NMR (400 MHz, $CDCl_3$) δ 1.62 (s, 6H), 1.81 (t, *J* = 8.0 Hz, 1H), 1.95-2.00 (s, 1H), 2.85 (t, *J* = 8.0 Hz, 1H), 7.01 (d, *J* = 8.0 Hz, 2H), 7.07 (dt, *J* = 4.0, 8.0 Hz, 1H), 7.19 (d, *J* = 8.0 Hz, 2H), 7.31 (t, *J* = 8.0 Hz, 1H), 7.37 (d, *J* =8.0 Hz, 1H), 8.45 (d, *J* =8.0 Hz, 1H), 9.28 (s, 1H); $^{13}$C NMR (100 MHz, $CDCl_3$) δ 173.2, 153.6, 134.4, 130.3, 130.0, 129.3, 127.8, 124.9, 123.6, 121.7, 121.4, 82.4, 60.8, 35.0, 26.0, 25.2 (2). HRMS (ESI) calcd for $C_{19}H_{18}Cl_3NO_2Na$ *m/z* $[M+Na]^+$: 420.0295, found: 420.0295.



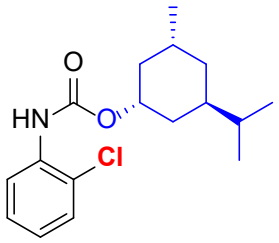

**N-(2-chlorophenyl)-2-methyl-2-(4-(4-methylbenzoyl)phenoxy)propenamide (4l)**

White solid. $R_f$ = 0.50 (PE:EtOAc = 10:1); $^1$H NMR (400 MHz, $CDCl_3$) δ 1.71 (s, 6H), 7.05-7.09 (m, 3H), 7.31 (t, *J* = 8.0 Hz, 1H), 7.37 (dd, *J* = 4.0, 8.0 Hz, 1H), 7.45 (d, *J* = 8.0 Hz, 2H), 7.72 (d, *J* = 8.0 Hz, 2H), 7.77 (d, *J* =8.0 Hz, 2H), 8.41 (d, *J* =8.0 Hz, 1H), 9.02 (s, 1H); $^{13}$C NMR (100 MHz, $CDCl_3$) δ 194.4, 172.5, 158.4, 138.8, 136.2, 134.2, 132.2, 132.1, 131.4, 129.3, 128.8, 127.9, 125.2, 123.5, 121.5, 120.1, 82.7, 25.3. HRMS (ESI) calcd for $C_{23}H_{20}Cl_2NO_3$ *m/z* $[M+H]^+$: 428.0815, found: 428.0815.



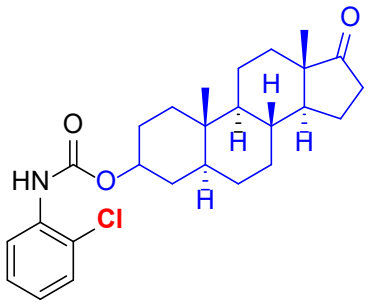

**2-(3-benzoylphenyl)-N-(2-chlorophenyl)propenamide (4m)**

White solid. $R_f$ = 0.45 (PE:EtOAc = 5:1); $^1$H NMR (400 MHz, $CDCl_3$) δ 1.67 (d, *J* = 8.0 Hz, 3H), 3.87 (q, *J* = 8.0 Hz, 1H), 7.02 (dt, *J* = 4.0, 8.0 Hz, 1H), 7.23-7.27 (m, 1H), 7.30 (d, *J* = 8.0 Hz, 1H), 7.45-7.50 (m, 2H), 7.53 (d, *J* = 8.0 Hz, 1H), 7.58-7.67 (m, 3H), 7.73 (d, *J* =8.0 Hz, 1H), 7.80 (d, *J* = 8.0 Hz, 2H), 7.84 (s, 1H), 8.36 (dd, *J* = 4.0, 8.0 Hz, 1H); $^{13}$C NMR (100 MHz, $CDCl_3$) δ 196.5, 171.8, 141.0, 138.5, 137.5, 134.5, 132.8, 131.8, 130.2, 129.7, 129.4, 129.3, 129.1, 128.5, 127.9, 124.9, 122.9, 121.4, 48.4, 18.4. HRMS (ESI) calcd for $C_{22}H_{19}ClNO_2$ *m/z* $[M+H]^+$: 364.1099, found: 364.1099.



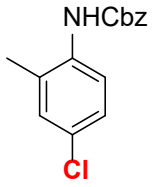

**(1*R*,3*R*,5*R*)-3-isopropyl-5-methylcyclohexyl (2-chlorophenyl)carbamate (5n)**

White solid. $R_f$ = 0.45 (PE:EtOAc = 5:1); $^1$H NMR (400 MHz, $CDCl_3$) δ 0.82 (d, *J* = 8.0 Hz, 3H), 0.87-0.97 (m, 1H), 0.93 (d, *J* = 4.0 Hz, 6H), 1.01-1.14 (m, 2H), 1.37-1.45 (m, 1H), 1.48-1.57 (m, 1H), 1.67-1.73 (m, 2H), 1.94-2.00 (m, 1H), 2.08-2.14 (m, 1H), 4.69 (dt, *J* = 4.0, 8.0 Hz, 1H), 6.98 (dt, *J* = 4.0, 8.0 Hz, 1H), 7.10 (s, 1H), 7.26 (t, *J* = 8.0 Hz, 1H), 7.34 (d, *J* = 8.0 Hz, 1H), 8.20 (d, *J* = 8.0 Hz, 1H); $^{13}$C NMR (100 MHz, $CDCl_3$) δ 153.1, 135.1, 129.1, 127.9, 123.6, 121.9, 119.9, 75.7, 47.3, 41.4, 34.4, 31.6, 26.4, 23.6, 22.2, 20.9, 16.5. HRMS (ESI) calcd for $C_{17}H_{25}ClNO_2$ *m/z* $[M+H]^+$: 310.1568, found: 310.1568.




**(5*S*,8*R*,10*S*,13*S*,14*S*)-10,13-dimethyl-17-oxohexadecahydro-1H-cyclopenta[a]phenanthren-3-yl (2-chlorophenyl)carbamate (5o)**

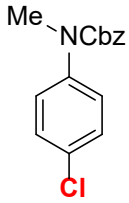
White solid. $R_f$ = 0.40 (PE:EtOAc = 5:1); $^1$H NMR (400 MHz, $CDCl_3$) δ 0.74 (dt, *J* = 4.0, 8.0 Hz, 1H), 0.86 (s, 3H), 0.87 (s, 3H), 0.94-1.11 (m, 2H), 1.20-1.41 (m, 6H), 1.43-1.62 (m, 4H), 1.64-1.82 (m, 5H), 1.90-1.97 (m, 2H), 2.03-2.12 (m, 1H), 2.40-2.47 (m, 1H), 4.67-4.75 (m, 1H), 6.98 (dt, *J* = 4.0, 8.0 Hz, 1H), 7.09 (s, 1H), 7.26 (t, *J* = 8.0 Hz, 1H), 7.34 (d, *J* = 8.0 Hz, 1H), 8.15 (d, *J* = 8.0 Hz, 1H); $^{13}$C NMR (100 MHz, $CDCl_3$) δ 152.9, 135.0, 129.7, 127.9, 123.6, 122.0, 119.9, 75.0, 54.4, 51.5, 47.9, 44.8, 36.9, 36.0, 35.8, 35.2, 34.3, 31.7, 31.0, 28.4, 27.9, 21.9, 20.6, 14.0, 12.4. HRMS (ESI) calcd for $C_{26}H_{35}ClNO_3$ *m/z* $[M+H]^+$: 444.2300, found: 444.2300.




**benzyl (4-chloro-2-methylphenyl)carbamate (7)**

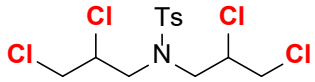
White solid. $R_f$ = 0.45 (PE:EtOAc = 10:1); $^1$H NMR (400 MHz, $CDCl_3$) δ 2.38 (s, 3H), 5.20 (s, 2H), 6.41 (s, 1H), 7.17 (dt, *J* = 4.0, 8.0 Hz, 2H), 7.34-7.43 (m, 5H), 7.79 (s, 1H); $^{13}$C NMR (100 MHz, $CDCl_3$) δ 153.6, 135.9, 134.5, 130.3, 128.8, 128.6(2),

126.9, 67.4, 17.7. HRMS (ESI) calcd for $C_{15}H_{14}ClNO_2Na$ *m/z* $[M+Na]^+$: 298.0605, found: 298.0607.




**benzyl (4-chlorophenyl)(methyl)carbamate (9)**

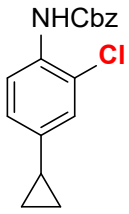
White solid. $R_f$ = 0.50 (PE:EtOAc = 10:1); $^1$H NMR (400 MHz, $CDCl_3$) δ 3.31 (s, 3H), 5.18 (s, 2H), 7.20 (d, *J* = 8.0 Hz, 2H), 7.30-7.35 (m, 7H); $^{13}$C NMR (100 MHz, $CDCl_3$) δ 155.3, 141.9, 136.5, 131.6, 129.0, 128.6, 128.1, 127.9, 127.0, 67.6, 37.7. HRMS (ESI) calcd for $C_{15}H_{14}ClNO_2Na$ *m/z* $[M+Na]^+$: 298.0605, found: 298.0605.




**N,N-bis(2,3-dichloropropyl)-4-methylbenzenesulfonamide (11)**

White solid. $R_f$ = 0.32 (PE:EtOAc = 10:1); $^1$H NMR (400 MHz, $CDCl_3$) δ 2.46 (s, 3H), 3.12-3.18 (m, 1H), 3.34-3.40 (m, 1H), 3.75-3.82 (m, 3H), 3.84-3.90 (m, 3H), 4.48-4.56 (m, 2H), 7.38 (dd, *J* = 4.0, 8.0 Hz, 2H), 7.73 (dd, *J* = 4.0, 8.0 Hz, 2H); $^{13}$C NMR (100 MHz, $CDCl_3$) δ 144.9, 144.8, 134.6, 134.1, 130.3(2), 127.8(2), 58.6, 58.4, 54.8(2), 46.5, 46.4, 21.8.

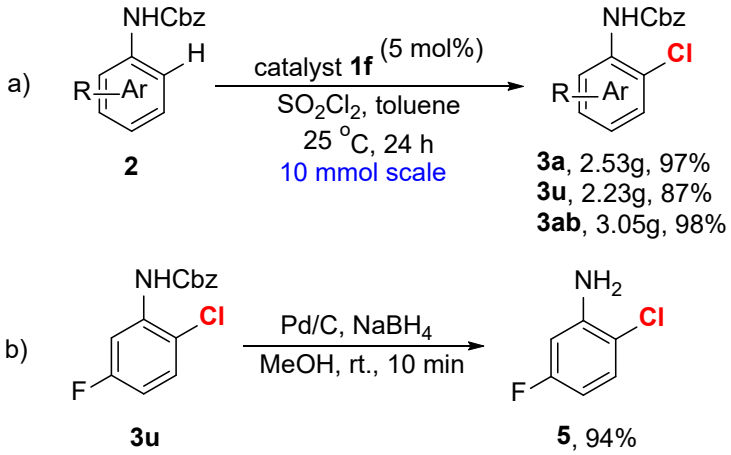
The analytical data are in accordance with those reported in the literature.[15]




**benzyl (2-chloro-4-cyclopropylphenyl)carbamate (14)**

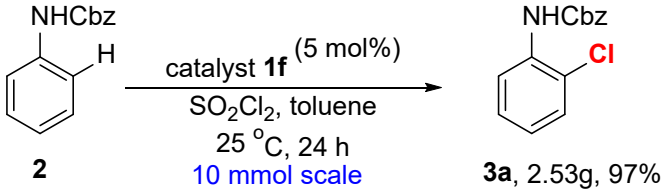
White solid. $R_f$ = 0.50 (PE:EtOAc = 10:1); $^1$H NMR (400 MHz, $CDCl_3$) δ 0.62-0.66 (m, 2H), 0.92-0.97 (m, 2H), 3.34-3.40 (m, 1H), 1.80-1.87 (m, 1H), 5.21 (s, 2H), 6.98 (dd, *J* = 4.0, 8.0 Hz, 2H), 7.05 (s, 1H), 7.09 (s, 1H), 7.35-7.44 (s, 5H), 8.02 (d, *J* = 8.0 Hz, 1H); $^{13}$C NMR (100 MHz, $CDCl_3$) δ 153.2, 140.3, 136.0, 132.1, 128.8, 128.6(2), 126.4, 125.3, 122.3, 120.2, 67.4, 14.8, 9.1. HRMS (ESI) calcd for $C_{17}H_{17}ClNO_2$ *m/z* $[M+H]^+$: 302.0942, found: 302.0942.

**(D) Scale-Up of the Chlorination and Deprotection**



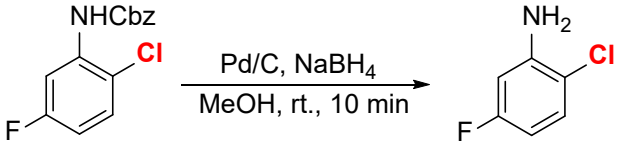

Furthermore, this catalytic protocol could be easily scaled up without selectivity deterioration and the catalyst loading could also be further decreased. The *ortho*-chlorination of **2a**, **2u** and **2ab** on a 10 mmol scale were completed in 24 h with only 5 mol% secondary amine **1f** to furnish the corresponding products **3a**, **3u** and **3ab** in excellent yield. The benzyloxycarbonyl group of the *ortho*-chlorinated product **3u** can be efficiently removed using $NaBH_4$ in the presence of Pd/C in methanol to give aniline **5** in 98% yield. The advantages of practical and environmental benign features make this chlorination methodology more attractive in the industrial synthesis.

**(E) Representative procedure for the large scale preparation of 3a**




To a solution of catalyst **1f** (50.5 mg, 0.5 mmol) and substrate **2a** (2.27 g, 10.0 mmol) in toluene (80 mL) was added dropwise $SO_2Cl_2$ (2.7 g, 20.0 mmol) over 30 min in the absence of light at 0 °C. Then the resulting mixture was stirred at 25 °C for 24 h. Upon completion, the reaction was quenched with saturated aqueous $Na_2SO_3$ (30 mL). The organic layer was separated, and the aqueous layer was extracted with dichloromethane (3×15 mL). The combined organic layers were dried over anhydrous $Na_2SO_4$, filtered, and concentrated under reduced pressure. The residue was purified by silica gel column chromatography (hexane/EtOAc = 20:1) to yield **3a** as white solid (97%, 2.53 g).

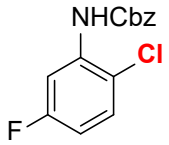
**(F) General procedure for *N*-Cbz deprotection**



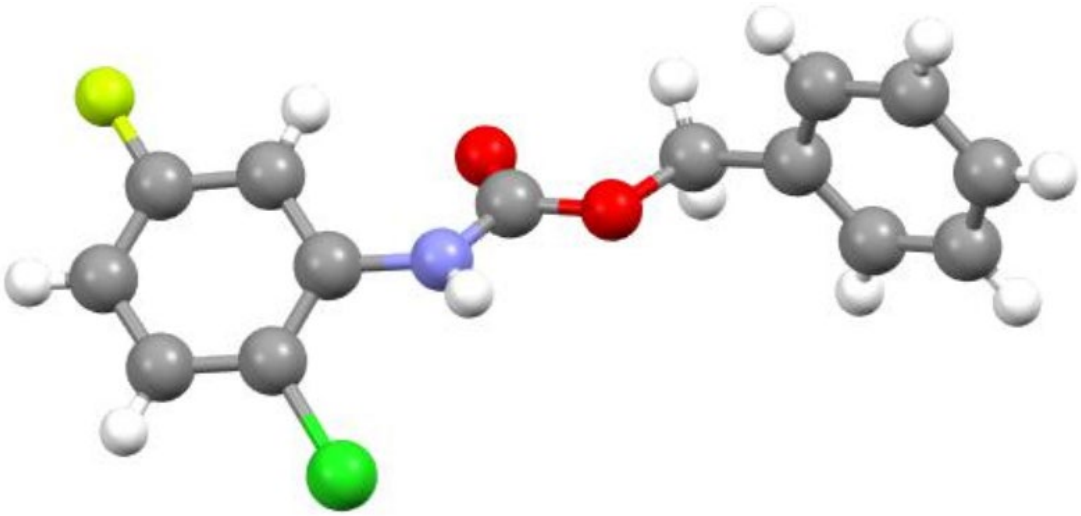

**3u** **5**, 94%

To a stirred solution of substrate **3u** (0.28 g, 1 mmol) and 10 % Pd/C (20 mg, 10 wt%) in MeOH (20 mL) was added $NaBH_4$ (56.8 mg, 1.5 mmol) portion wise using solid addition funnel. A septum with an empty balloon was placed to avoid the loss of generated hydrogen and overpressure in the flask. After completion of reaction (10 min), reaction mixture was filtered through celite and filtrate was evaporated to dryness to afford crude amine which upon purification using flash chromatography (hexane/EtOAc = 30:1) afforded pure amine **5** (136.3 mg, 94%). $R_f$ = 0.50 (PE:EtOAc = 10:1); $^1$H NMR (400 MHz, $CDCl_3$) δ 4.14 (s, 2H), 6.40 (t, $J$ = 4.0, 8.0 Hz, 1H), 6.47 (d, $J$ = 8.0 Hz, 1H), 7.15-7.19 (m, 1H); $^{13}$C NMR (100 MHz, $CDCl_3$) δ 163.5, 161.1, 144.3, 144.2, 130.4, 130.3, 114.3(2), 106.0, 105.8, 102.8, 102.5. The analytical data are in accordance with those reported in the literature.[16]

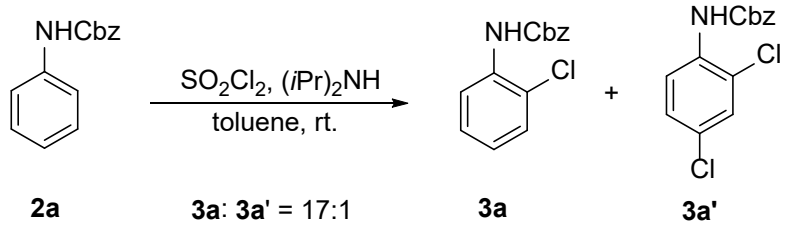
**(G) X-ray diffraction data of 3u (CCDC 2158109)**

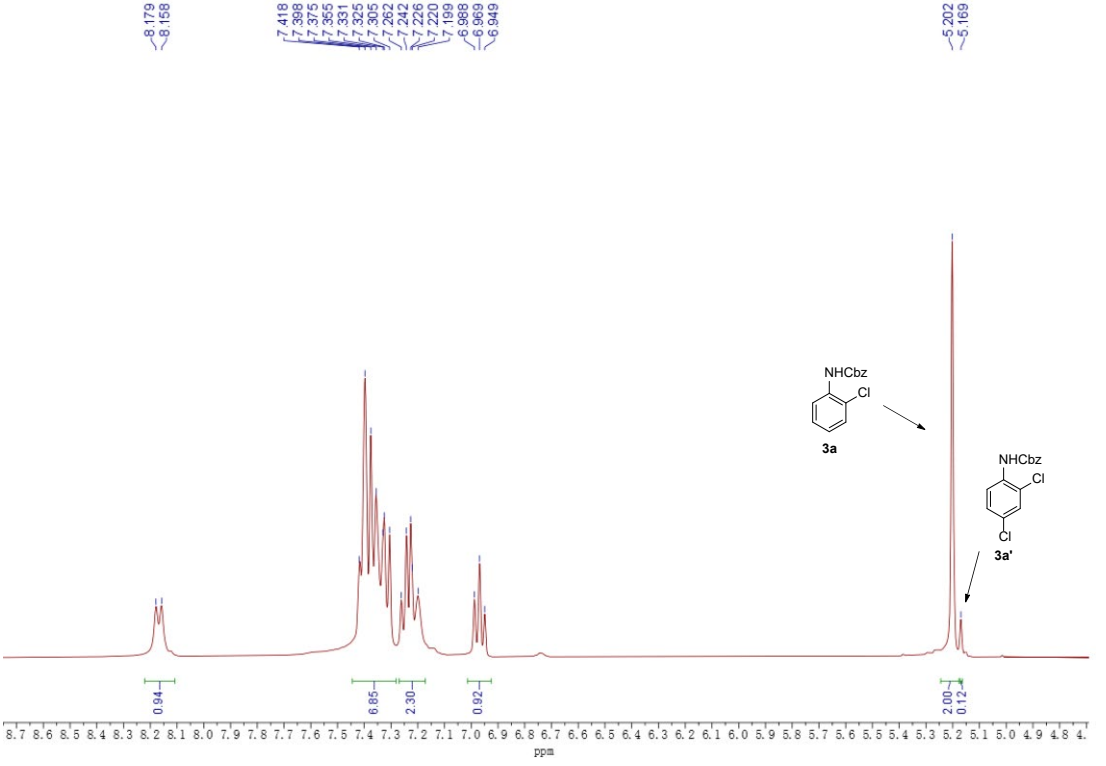


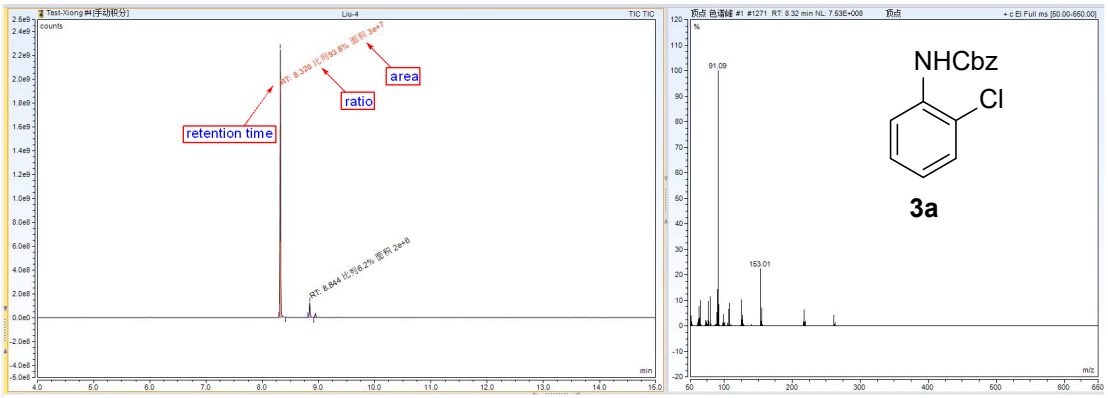

**3u**

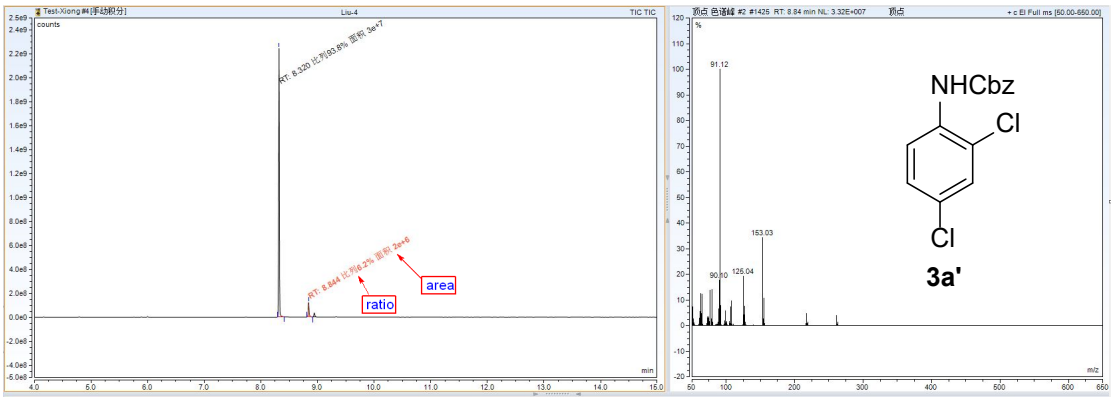


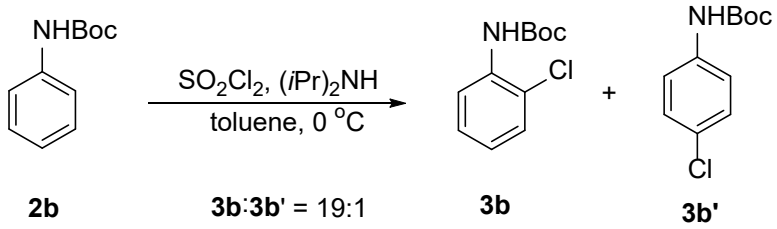
## (H) Examples of crude NMR and GC/MS spectra for determination of the regioselectivity of the *ortho*-chlorination

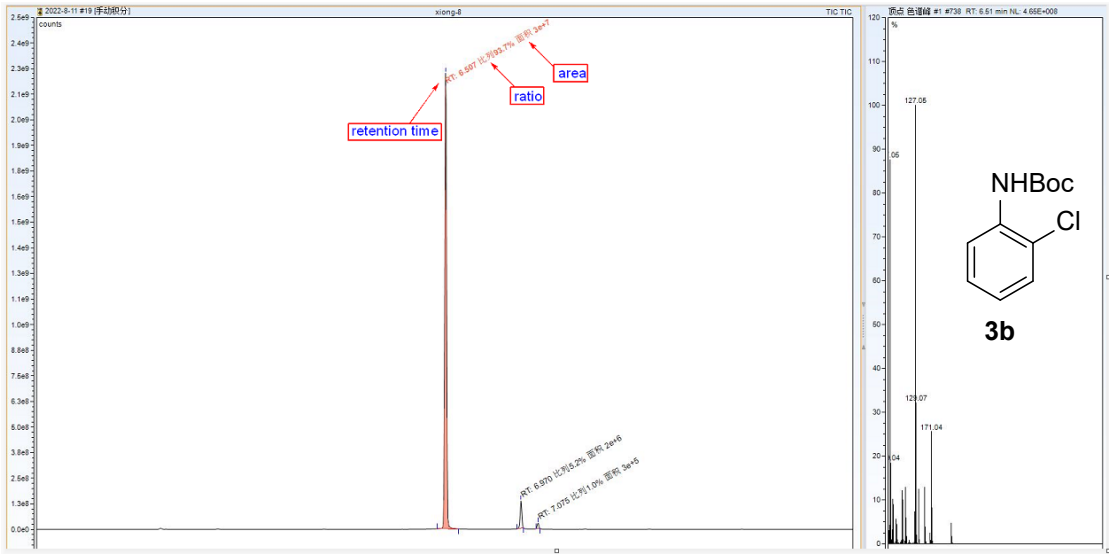


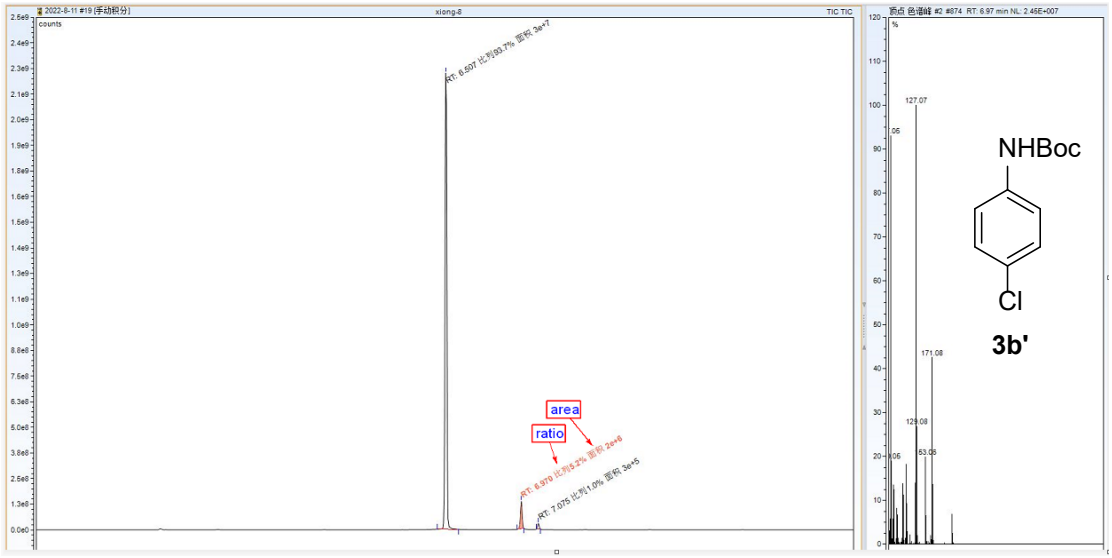



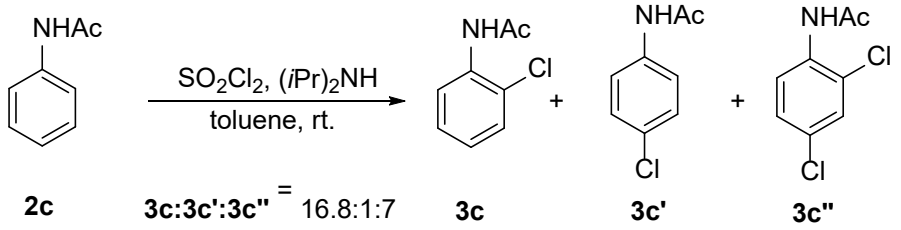



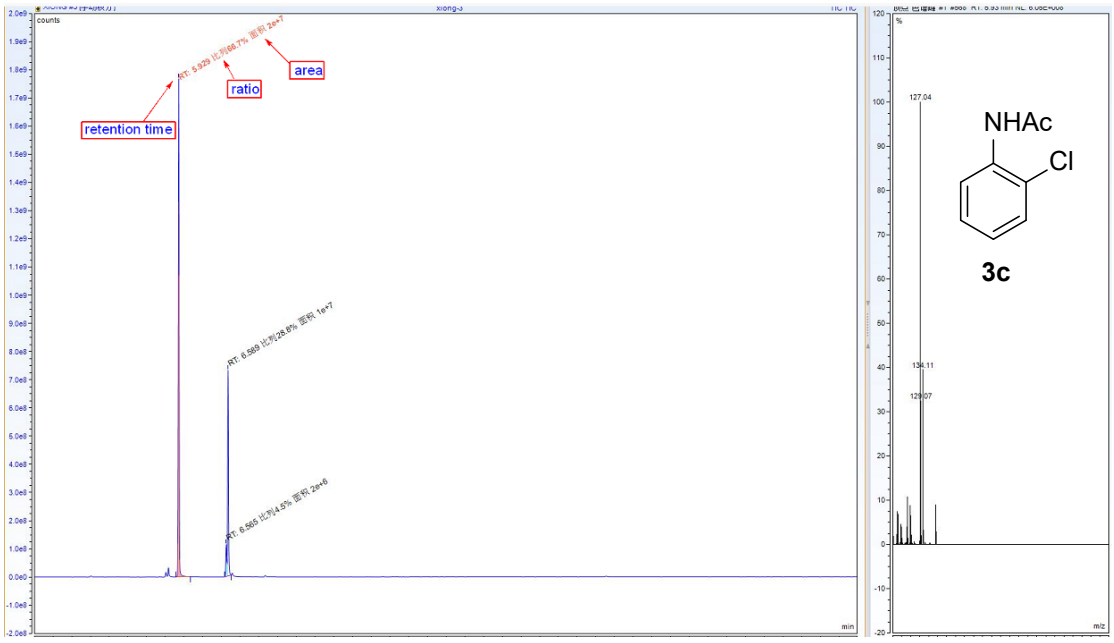

area
ratio
NHCbz
Cl
Cl
3a'

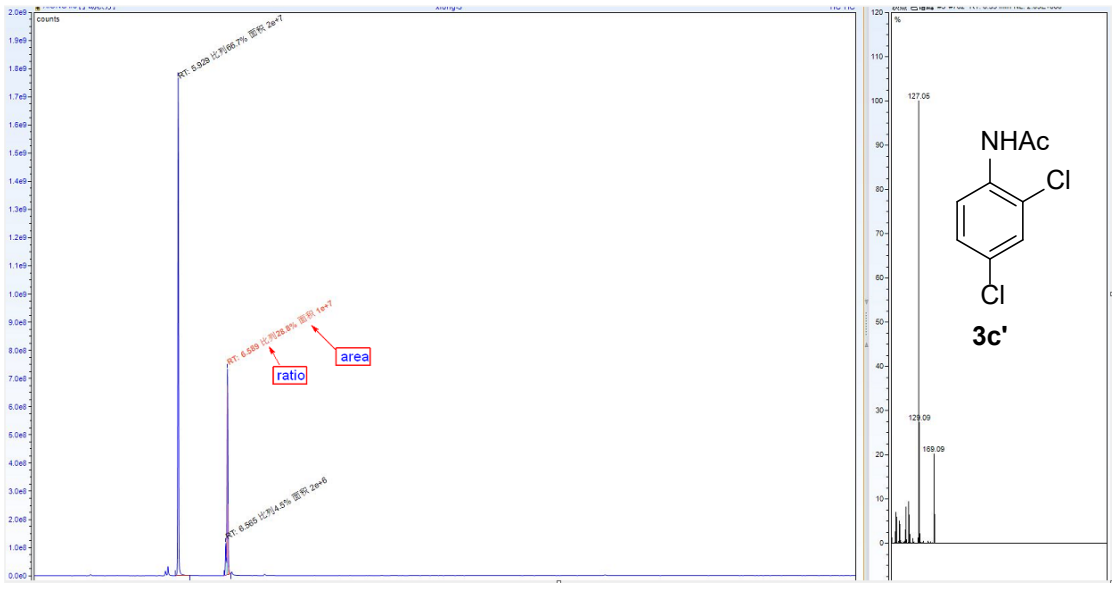

NHBoc
SO2Cl2, (iPr)2NH
toluene, 0 °C
NHBoc
Cl
+
NHBoc
Cl
2b
3b:3b' = 19:1
3b
3b'

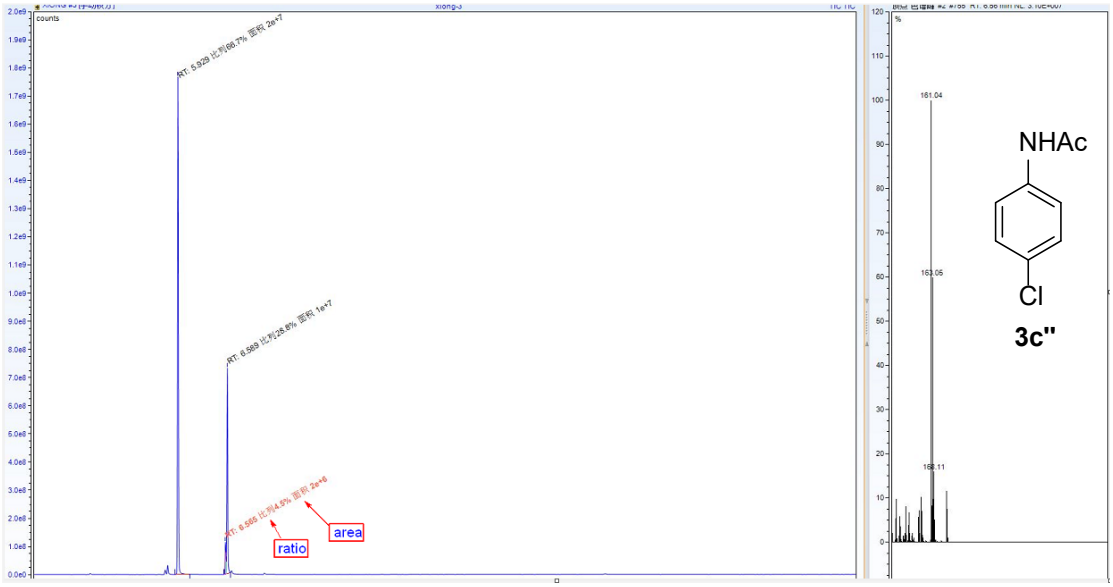

retention time
area
ratio
NHBoc
Cl
3b

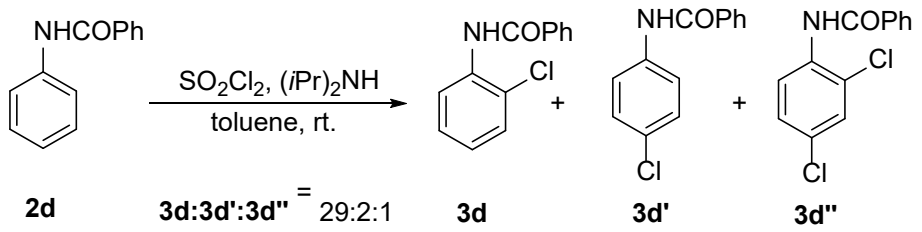

area
ratio
NHBoc
Cl
3b'

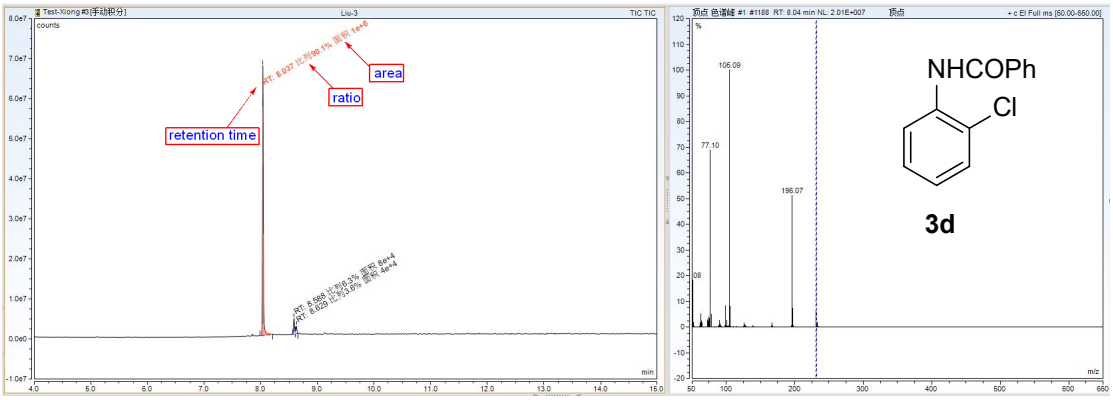

NHAc
SO2Cl2, (iPr)2NH
toluene, rt.
NHAc
Cl
NHAc
Cl
NHAc
Cl
Cl
2c
3c:3c':3c'' = 16.8:1:7
3c
3c'
3c''

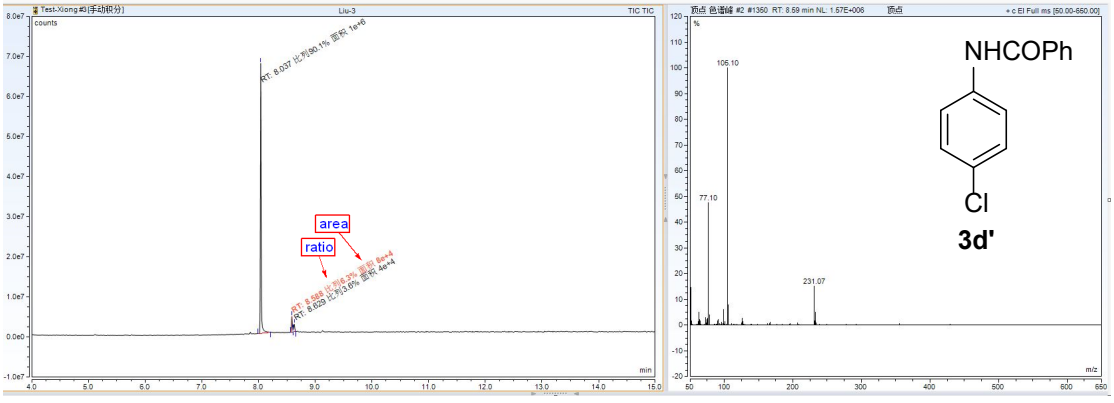

counts
retention time
ratio
area
min
127.04
134.11
129.07
NHAc
Cl
3c
m/z

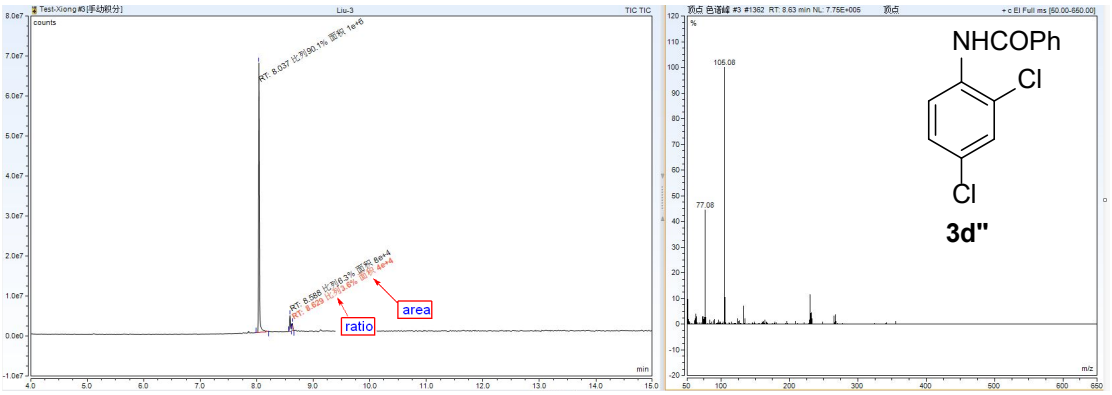

counts
ratio
area
min
127.05
129.09
169.09
NHAc
Cl
Cl
3c'
m/z

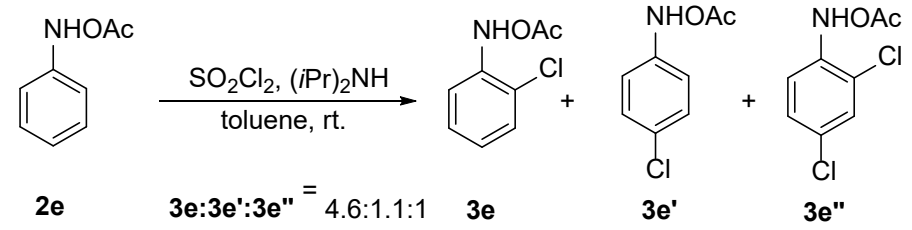

counts
area
ratio
NHAc
Cl
3c''

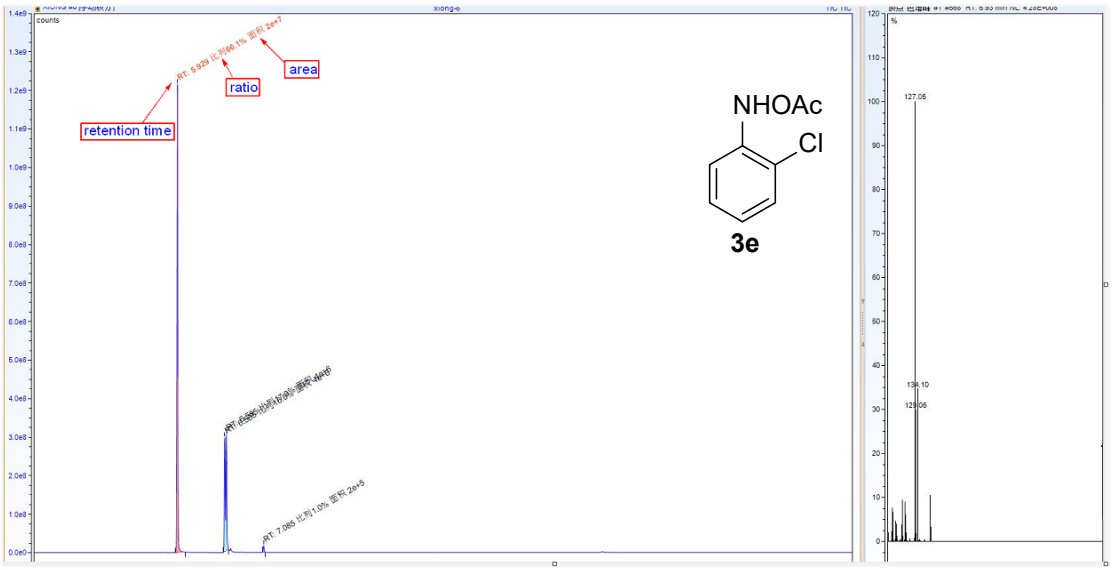

NHCOPh
SO2Cl2, (iPr)2NH
toluene, rt.
NHCOPh
Cl
NHCOPh
Cl
NHCOPh
Cl
2d
3d:3d':3d'' = 29:2:1
3d
3d'
3d''

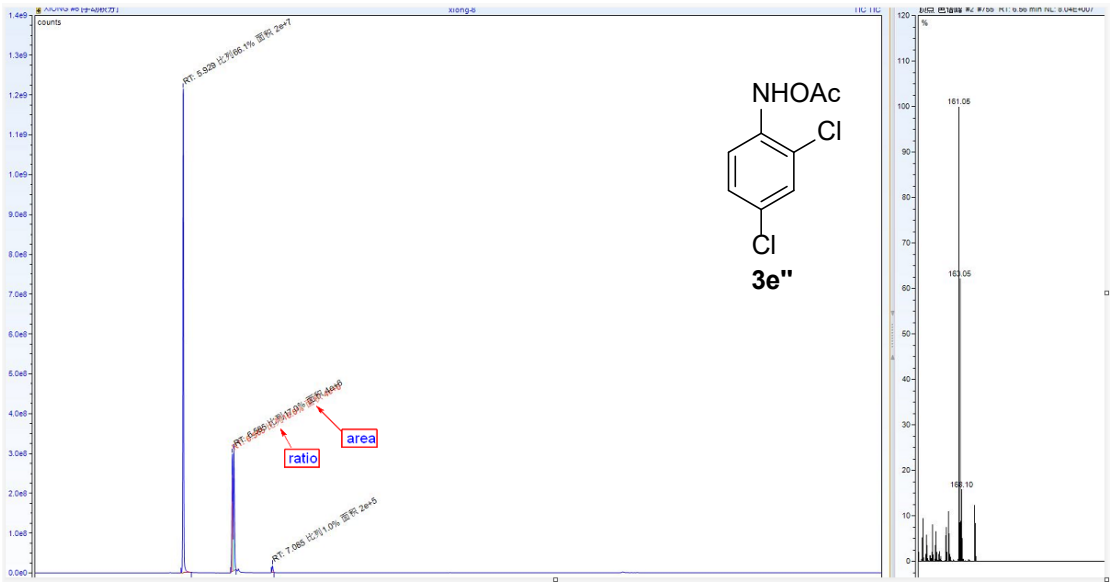

counts
area
ratio
retention time
NHCOPh
Cl
3d

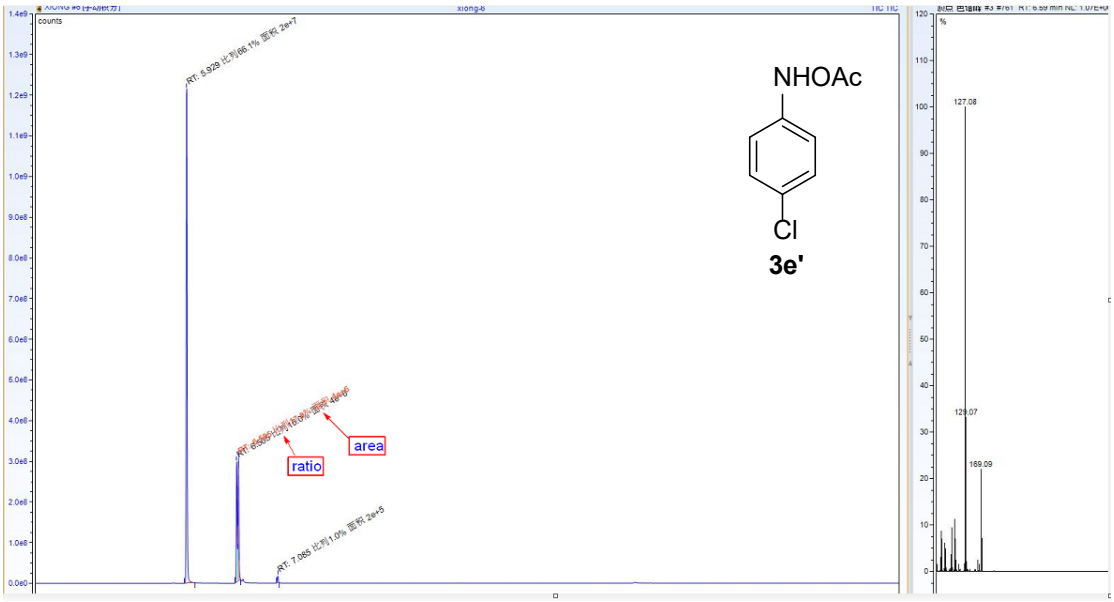

counts
area
ratio
NHCOPh
Cl
3d'

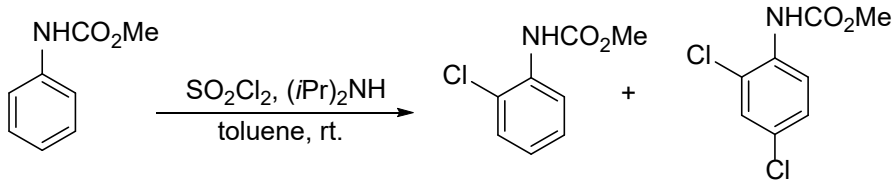

area
ratio
NHCOPh
Cl
Cl
3d"


NHOAc
SO2Cl2, (iPr)2NH
toluene, rt.
NHOAc
Cl
NHOAc
Cl
NHOAc
Cl
2e
3e:3e':3e" = 4.6:1.1:1
3e
3e'
3e"

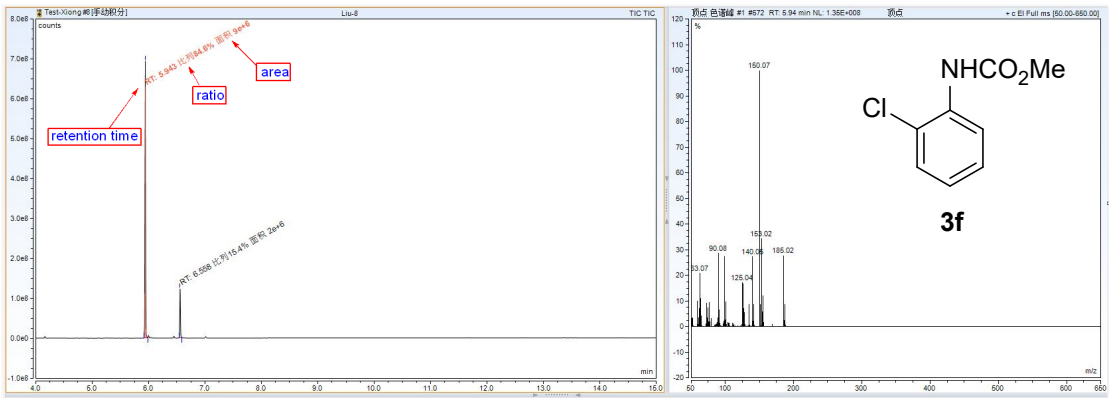

retention time
ratio
area
NHOAc
Cl
3e

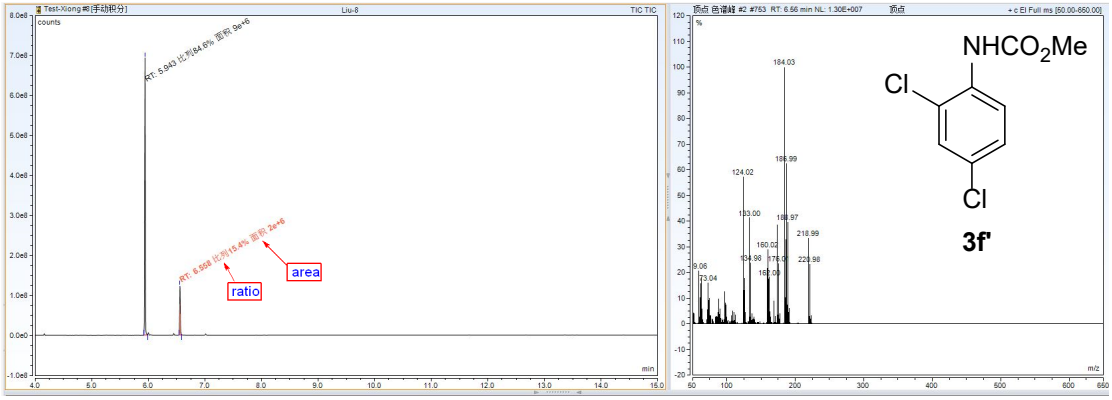


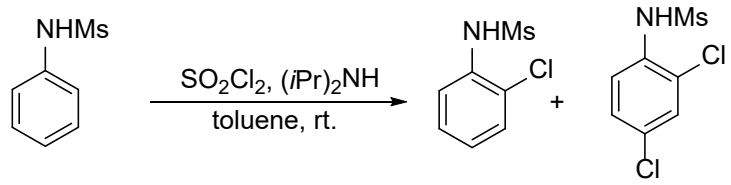



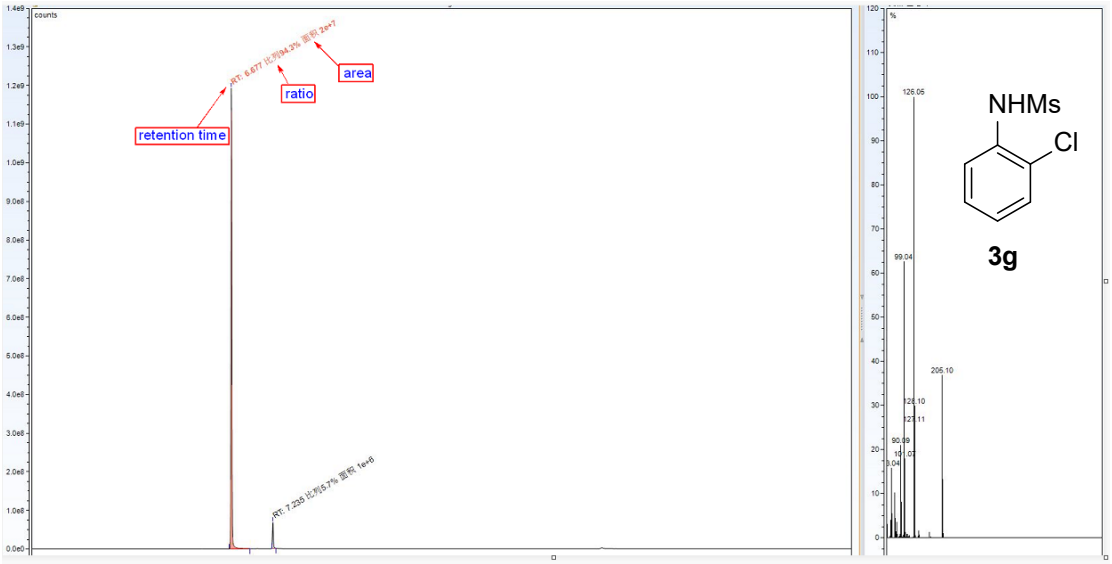



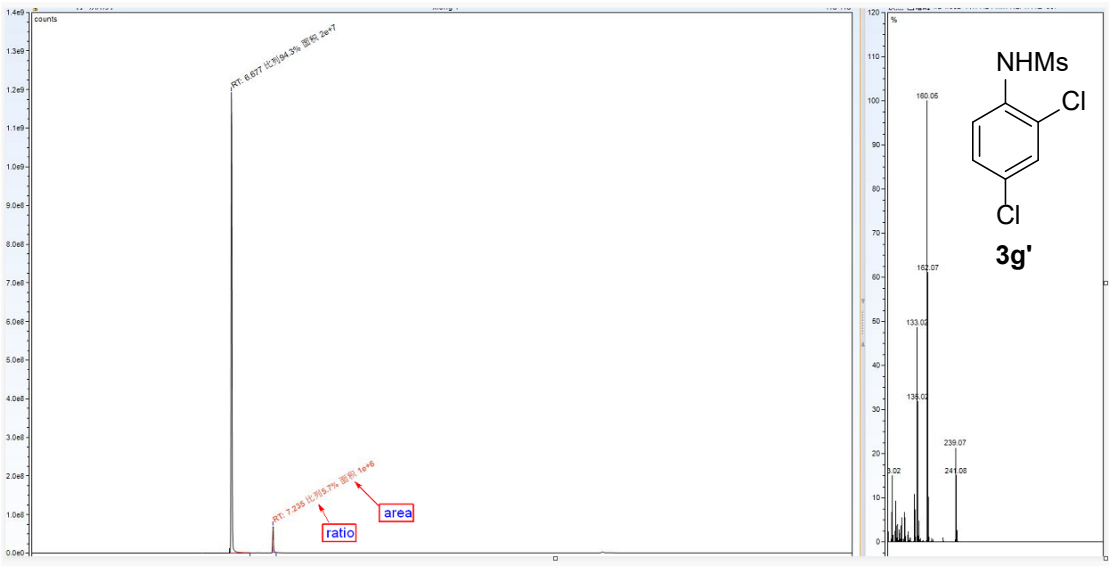

**2f** **3f**:**3f'** = 6.7:1 **3f** **3f'**

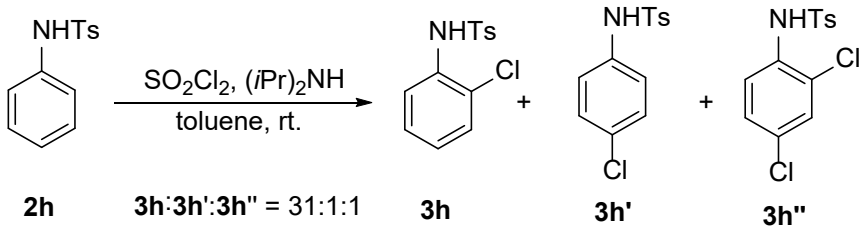

retention time
ratio
area
NHCO2Me
Cl
3f

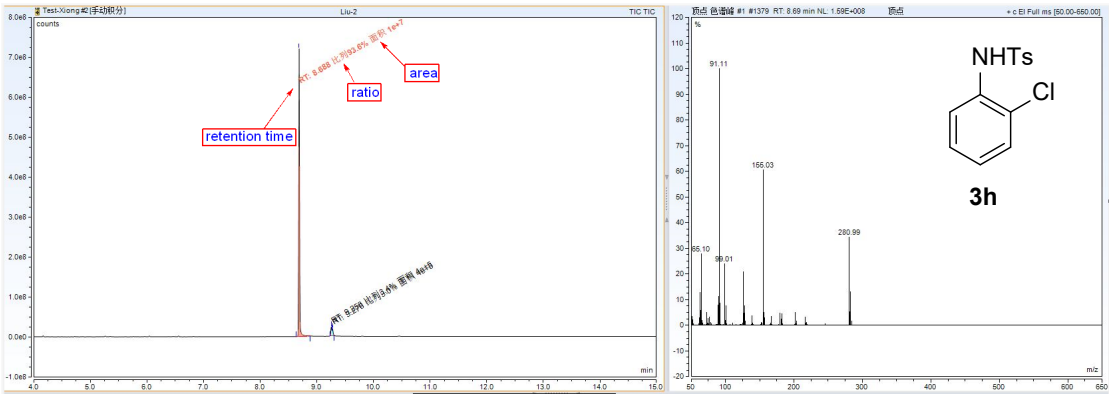

ratio
area
NHCO2Me
Cl
Cl
3f'

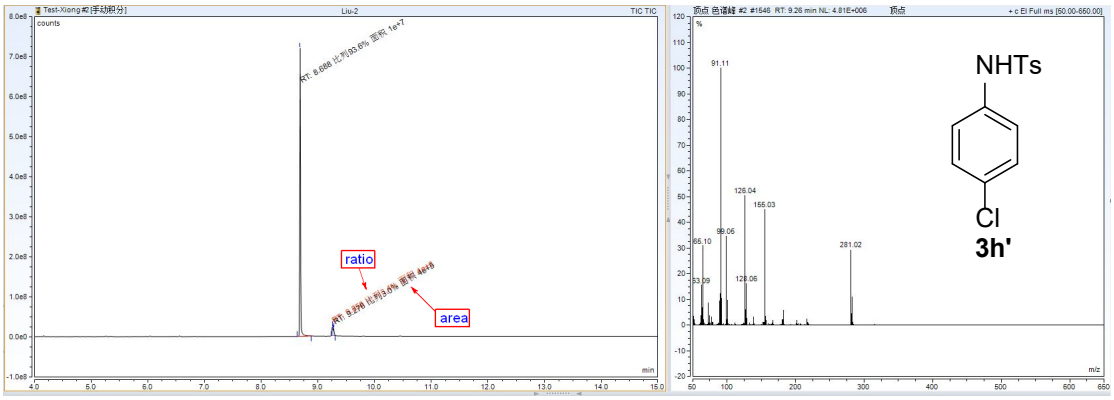

NHMs
SO2Cl2, (iPr)2NH
toluene, rt.
NHMs
Cl
+
NHMs
Cl
Cl
2g
3g:3g' = 19.3:1
3g
3g'

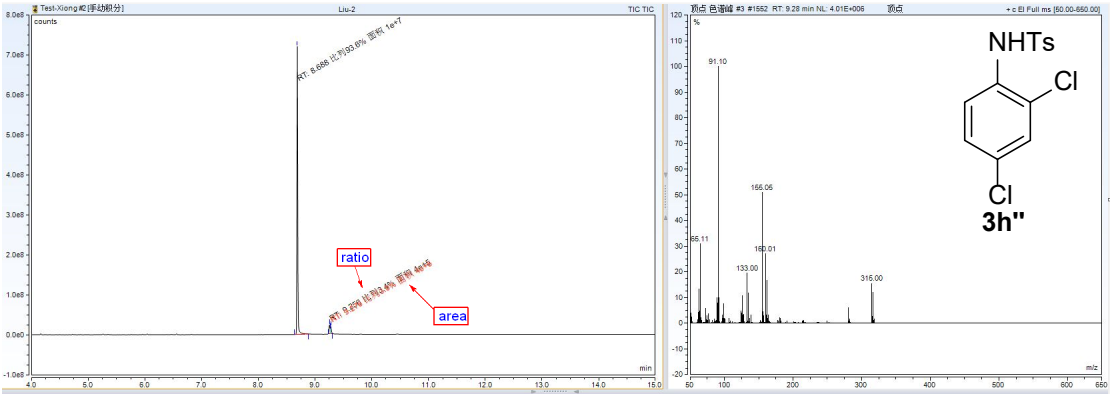

retention time
ratio
area
NHMs
Cl
3g

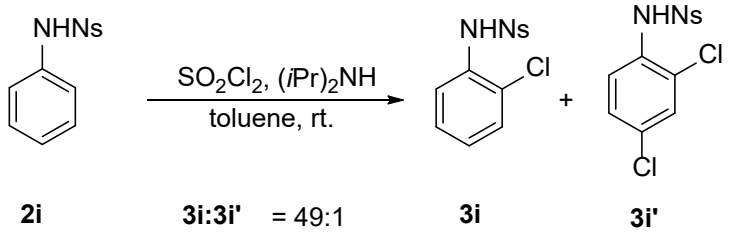

counts
ratio
area
NHMs
Cl
Cl
3g'


NHTs
SO2Cl2, (iPr)2NH
toluene, rt.
NHTs
Cl
+
NHTs
Cl
+
NHTs
Cl
2h
3h:3h':3h'' = 31:1:1
3h
3h'
3h''

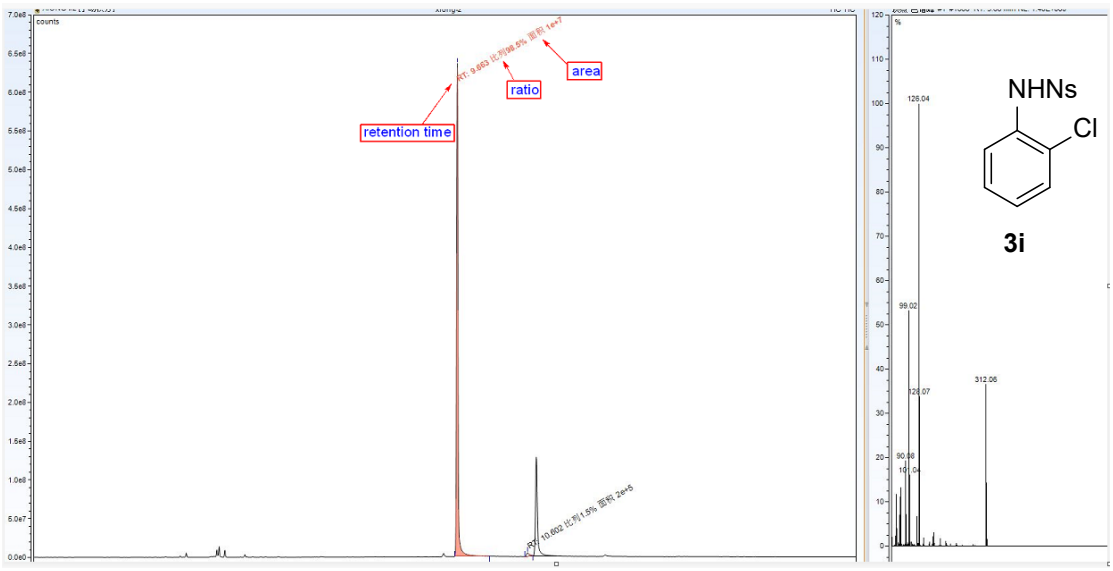

counts
retention time
ratio
area
NHTs
Cl
3h

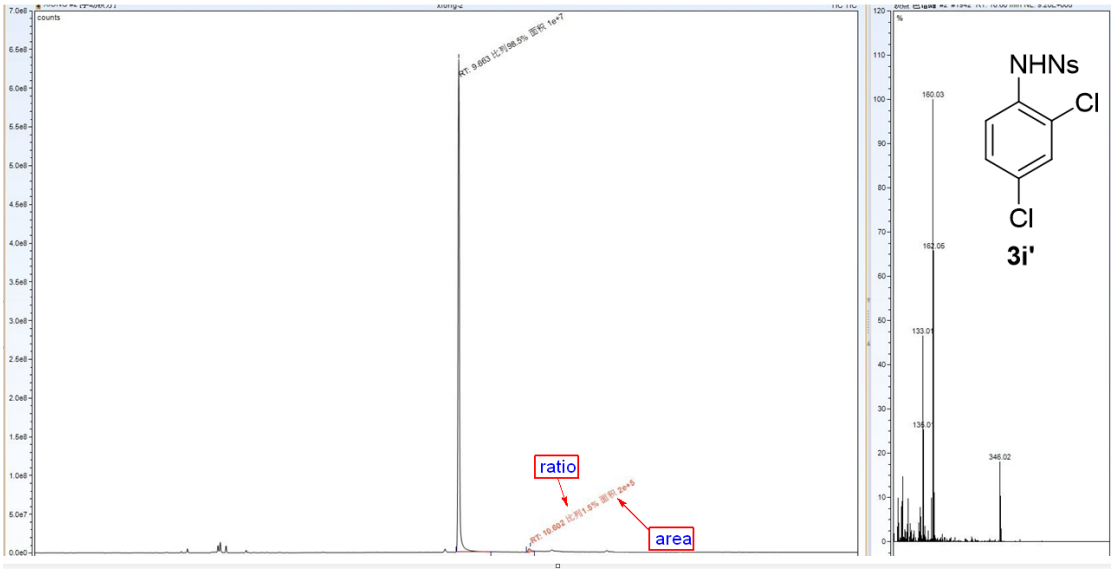

counts
ratio
area
NHTs
Cl
3h'

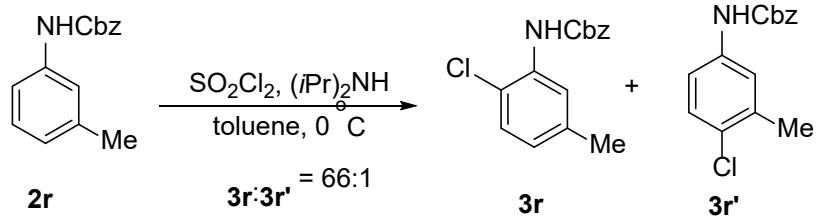


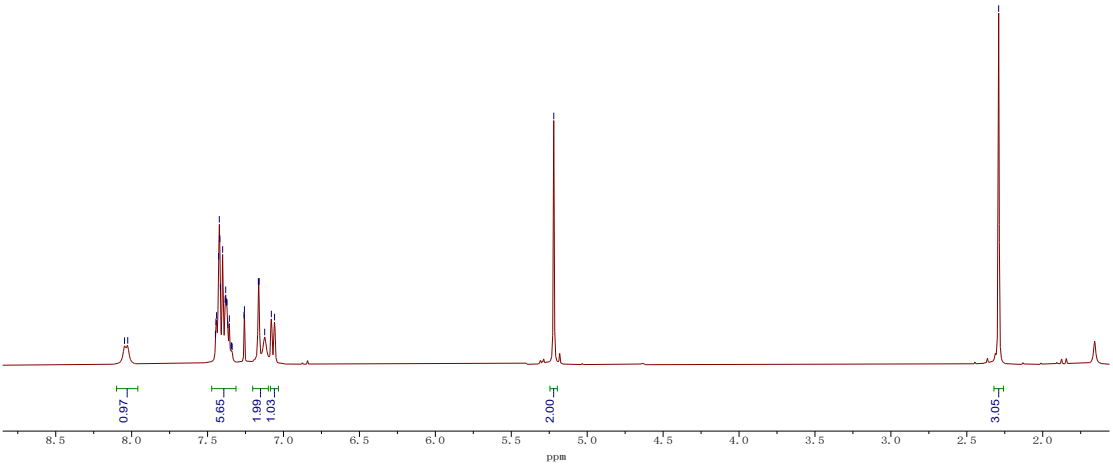

**2i** **3i:3i'** = 49:1 **3i** **3i'**

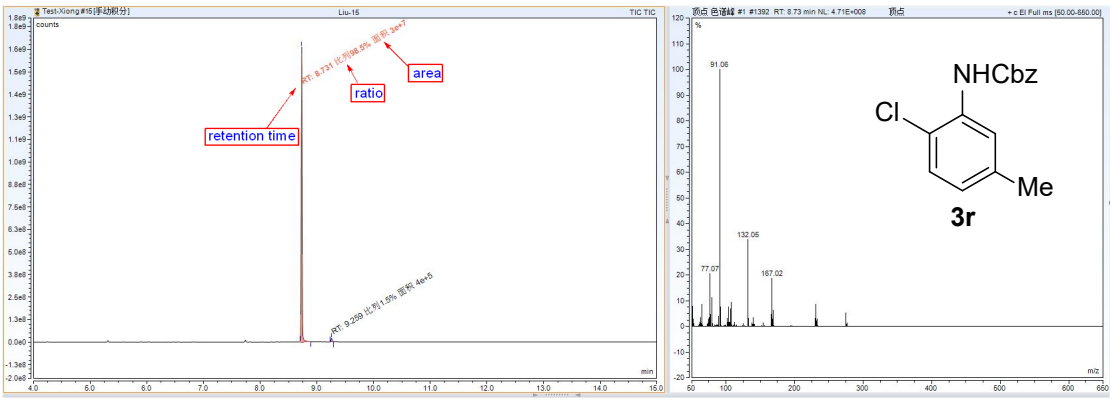


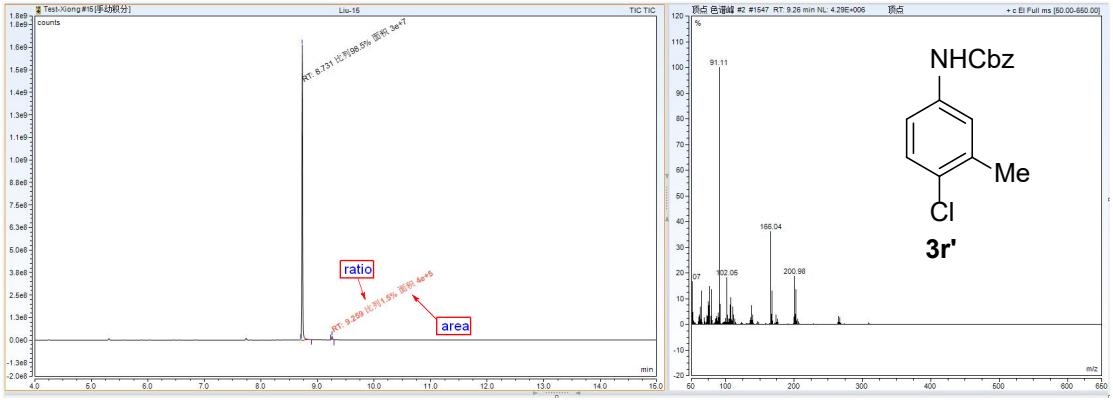

counts
ratio
area
NHNs
Cl
Cl
3i'
160.03
162.06
133.01
136.0
346.02

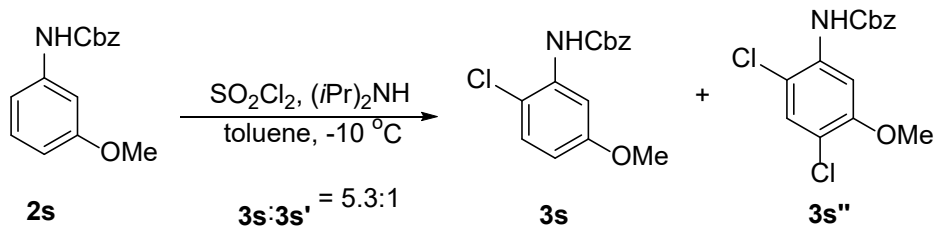

NHCbz
Me
2r
SO2Cl2, (iPr)2NH
toluene, 0 °C
3r:3r' = 66:1
NHCbz
Cl
Me
3r
+
NHCbz
Me
Cl
3r'

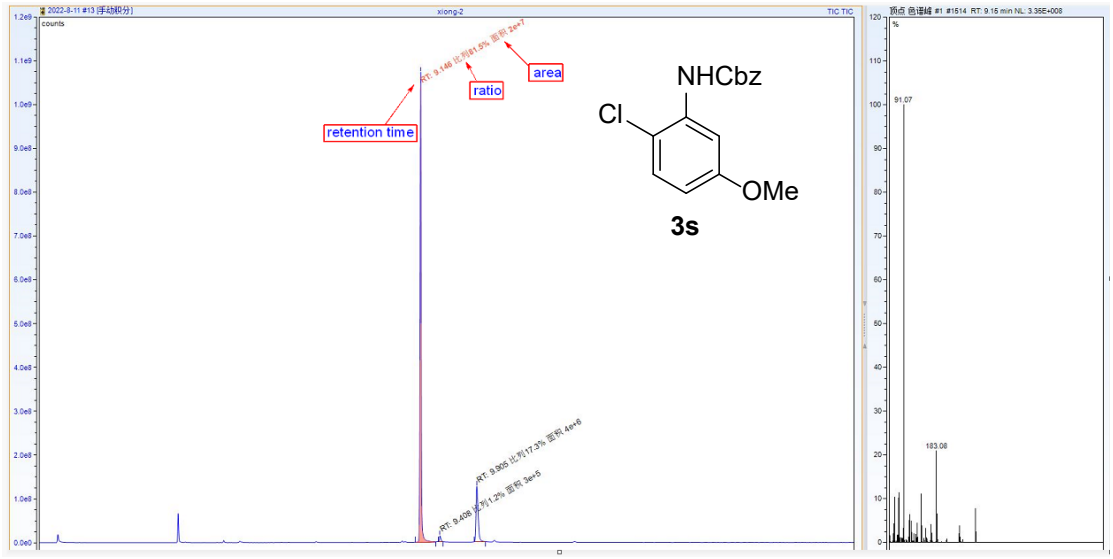

8.047
8.026
7.448
7.445
7.441
7.427
7.423
7.419
7.415
7.401
7.384
7.381
7.375
7.372
7.366
7.357
7.345
7.342
7.338
7.260
7.257
7.166
7.161
7.124
7.080
7.059
5.220
2.290

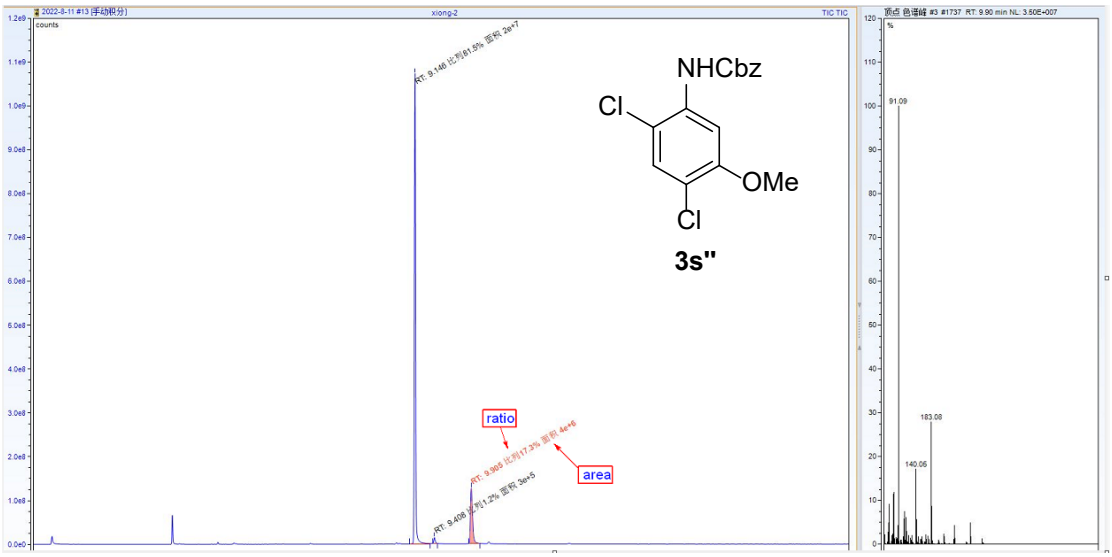

0.97
5.65
1.99
1.03
2.00
3.05
ppm

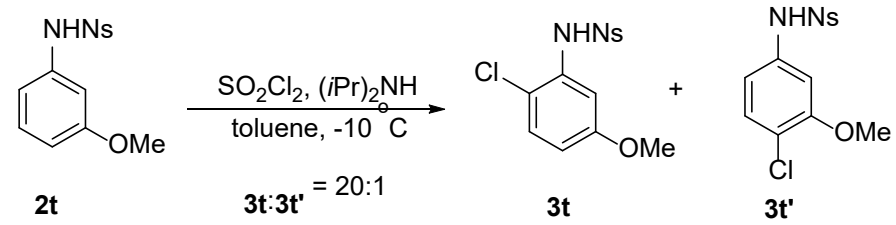

retention time
ratio
area
NHCbz
Cl
Me
3r

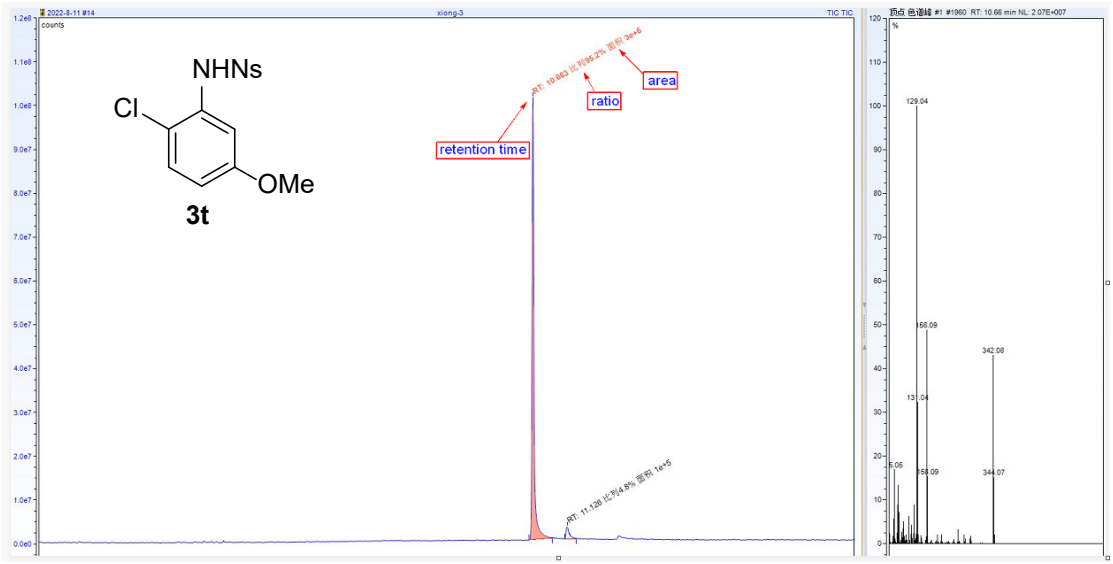

ratio
area
NHCbz
Me
Cl
3r'

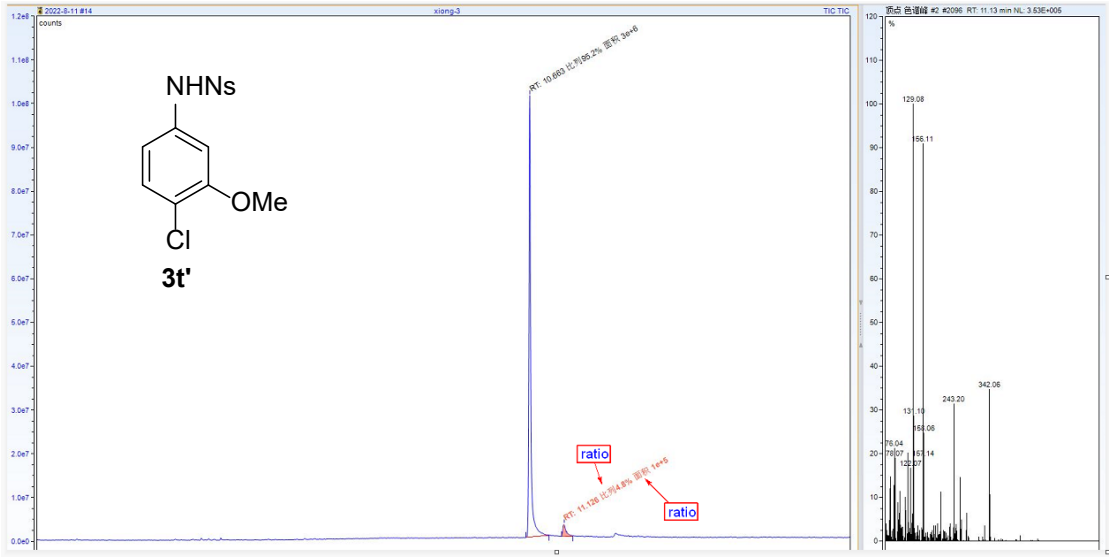

NHCbz
OMe
SO2Cl2, (iPr)2NH
toluene, -10 °C
NHCbz
Cl
OMe
+
NHCbz
Cl
OMe
Cl
2s
3s:3s' = 5.3:1
3s
3s''

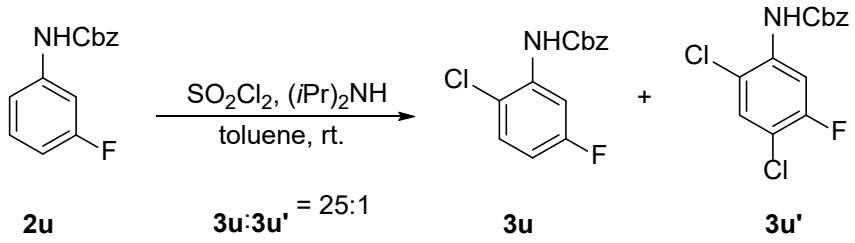

retention time
ratio
area
NHCbz
Cl
OMe
3s

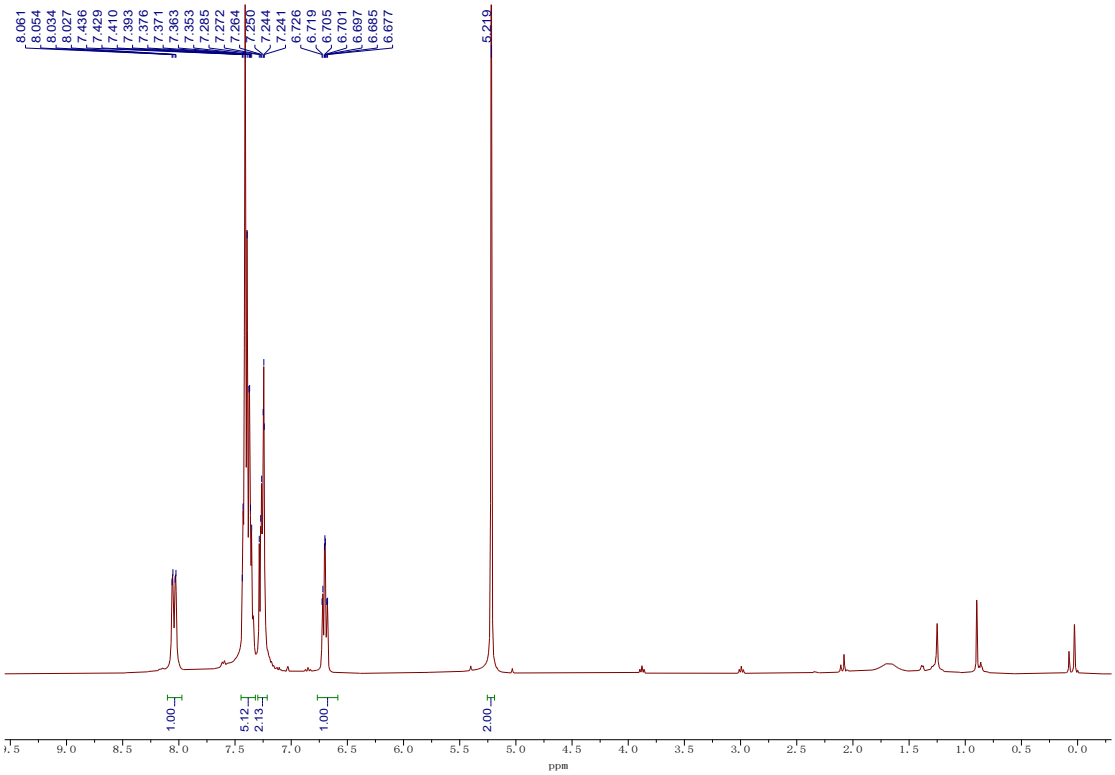

NHCbz
Cl
OMe
Cl
3s''
ratio
area

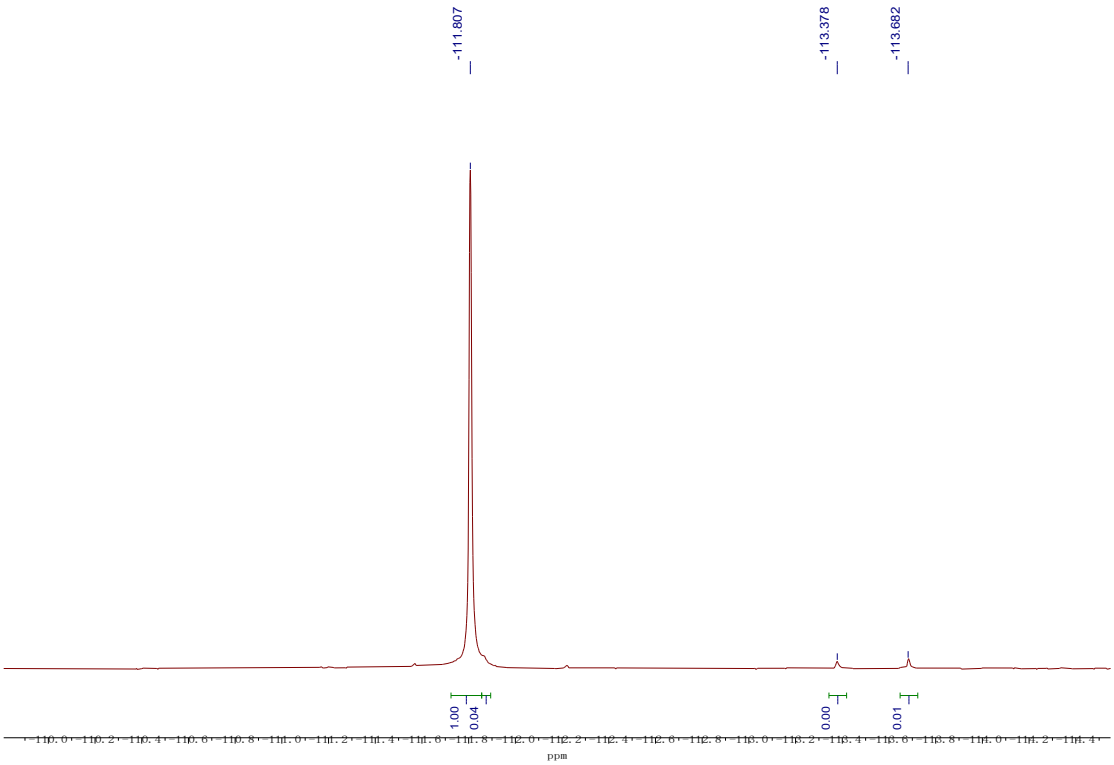

NHNs
OMe
SO2Cl2, (iPr)2NH
toluene, -10 °C
NHNs
Cl
OMe
+
NHNs
OMe
Cl
2t
3t:3t' = 20:1
3t
3t'

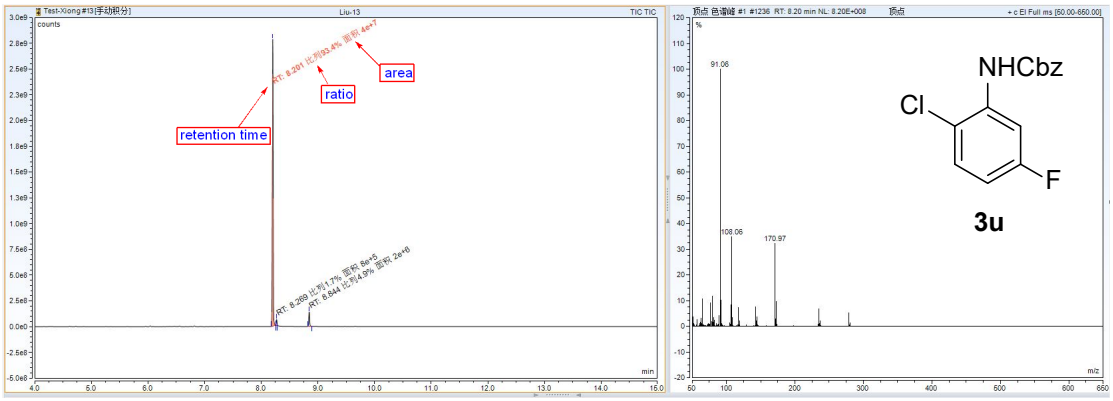

NHNs
Cl
OMe
3t
area
ratio
retention time

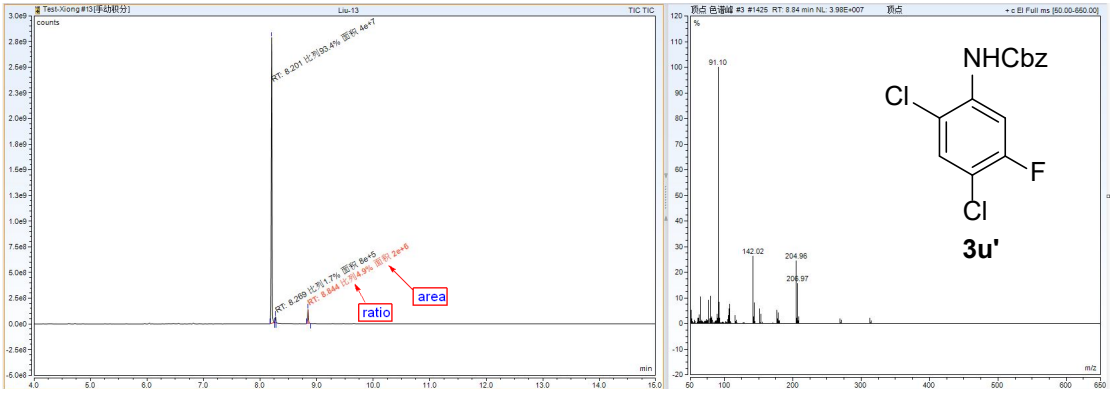

NHNs
OMe
Cl
3t'
ratio
ratio

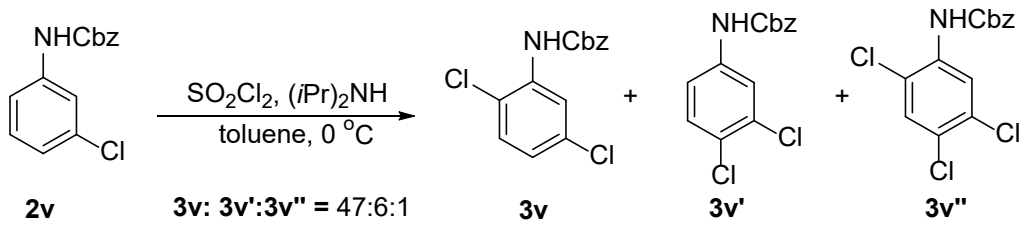

NHCbz
F
SO2Cl2, (iPr)2NH
toluene, rt.
NHCbz
Cl
F
+
NHCbz
Cl
F
Cl
2u
3u:3u' = 25:1
3u
3u'


8.061
8.054
8.034
8.027
7.436
7.429
7.410
7.393
7.376
7.371
7.363
7.353
7.285
7.272
7.264
7.250
7.244
7.241
6.726
6.719
6.705
6.701
6.697
6.685
6.677
5.219
1.00
5.12
2.13
1.00
2.00
ppm

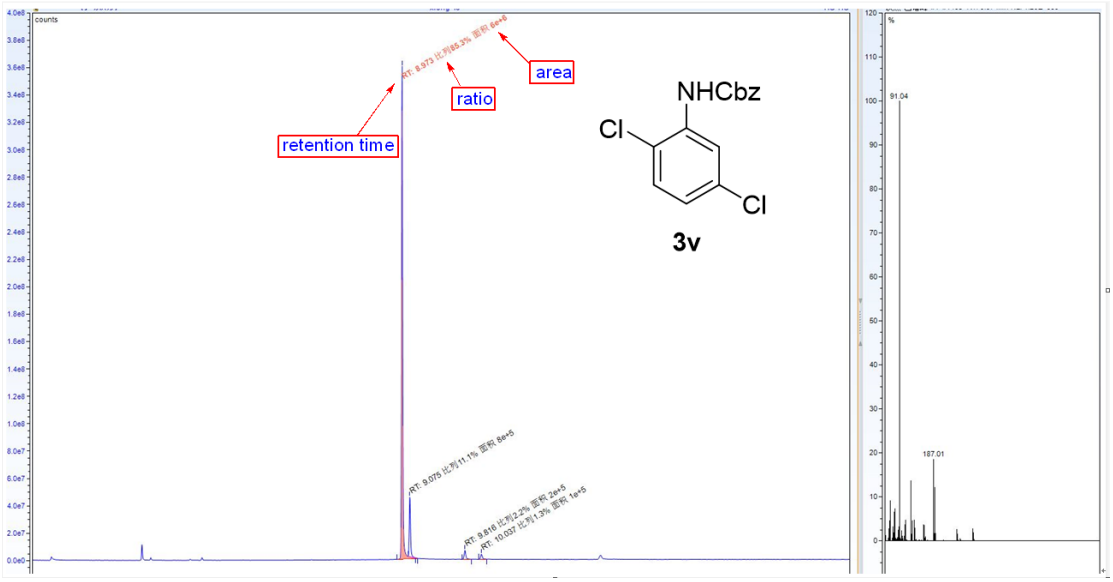

-111.807
-113.378
-113.682
1.00
0.04
0.00
0.01
ppm

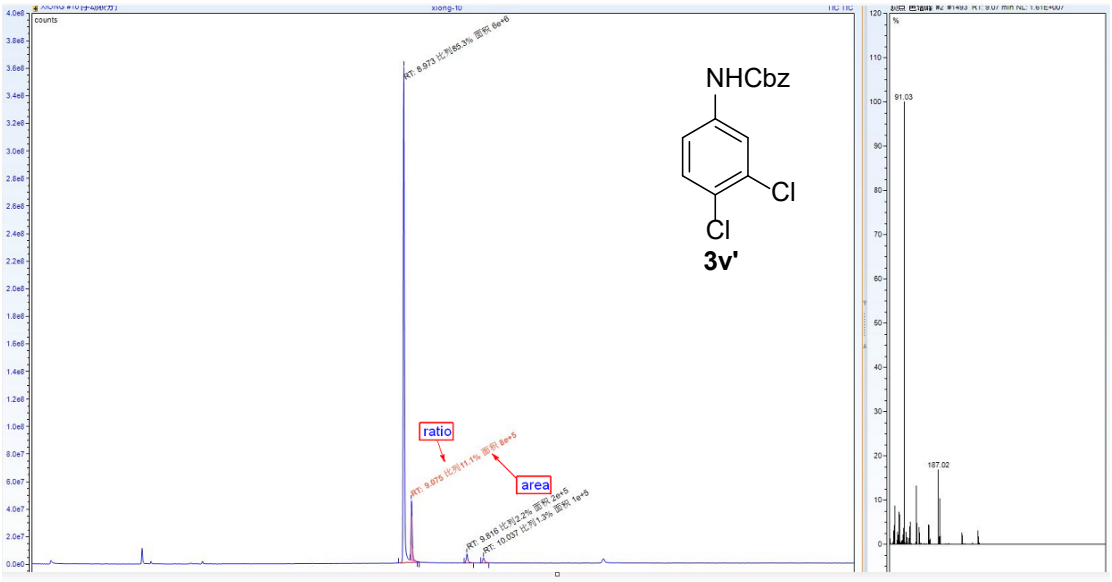

retention time
ratio
area
NHCbz
Cl
F
3u

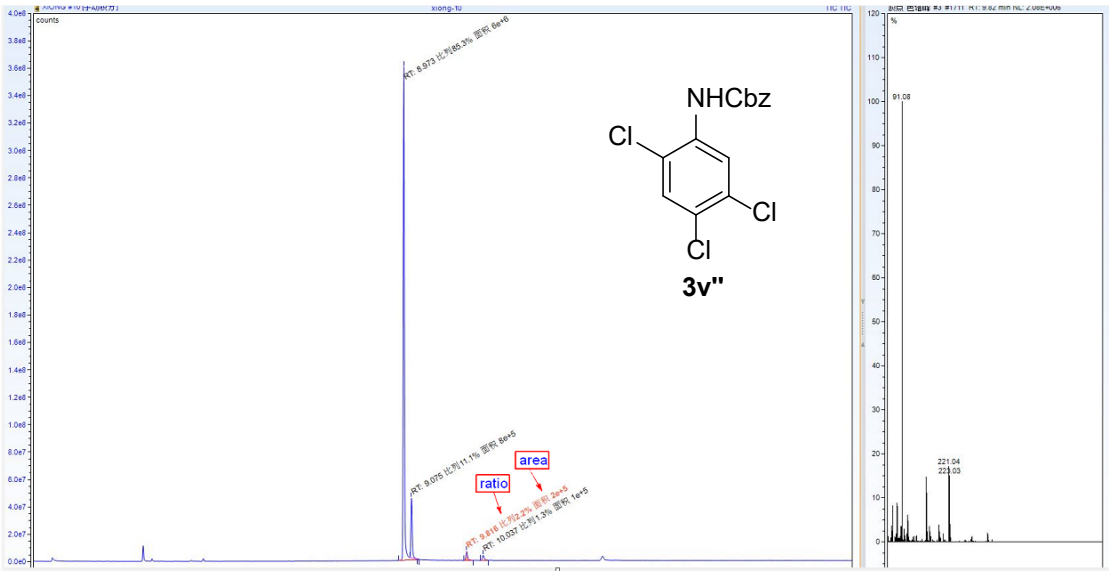

ratio
area
NHCbz
Cl
F
Cl
3u'

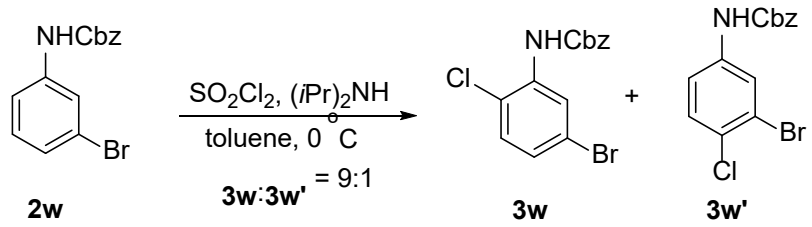


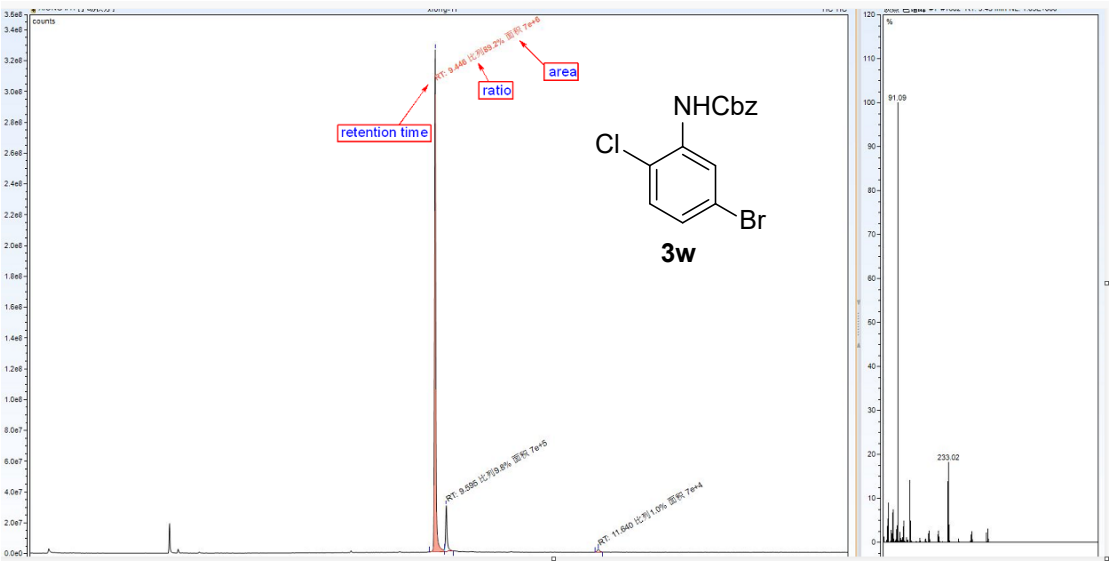

**2v** **3v: 3v':3v'' =** 47:6:1 **3v** **3v'** **3v''**

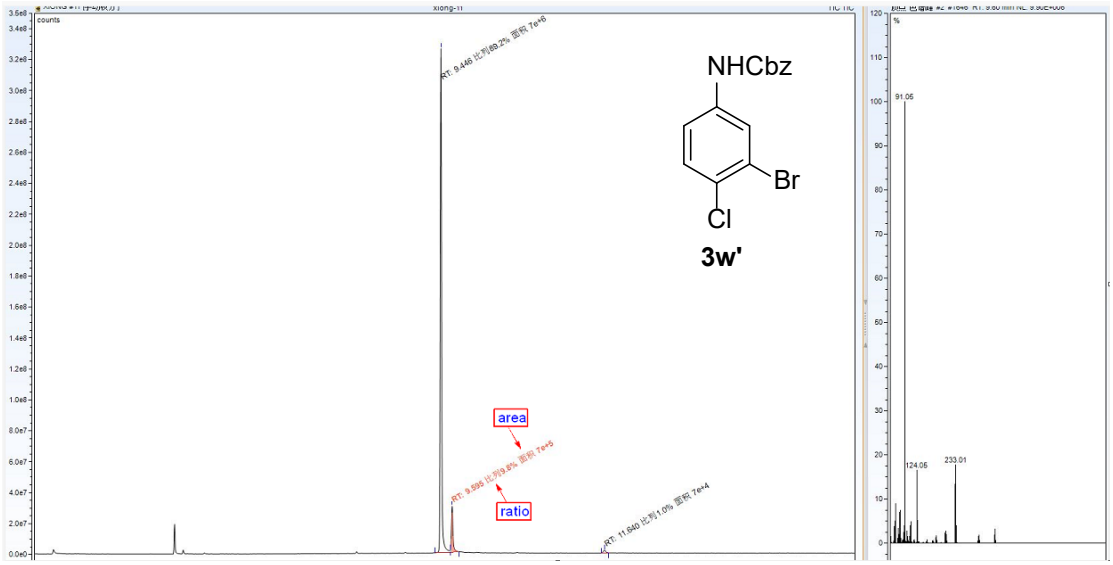


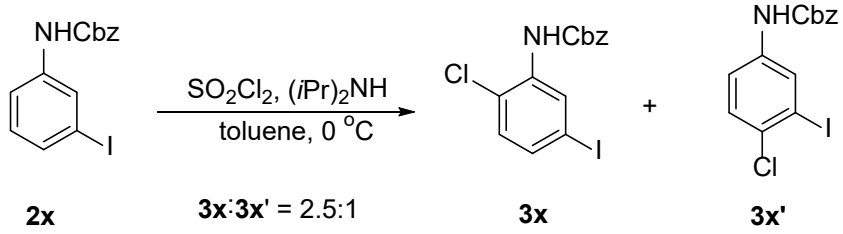



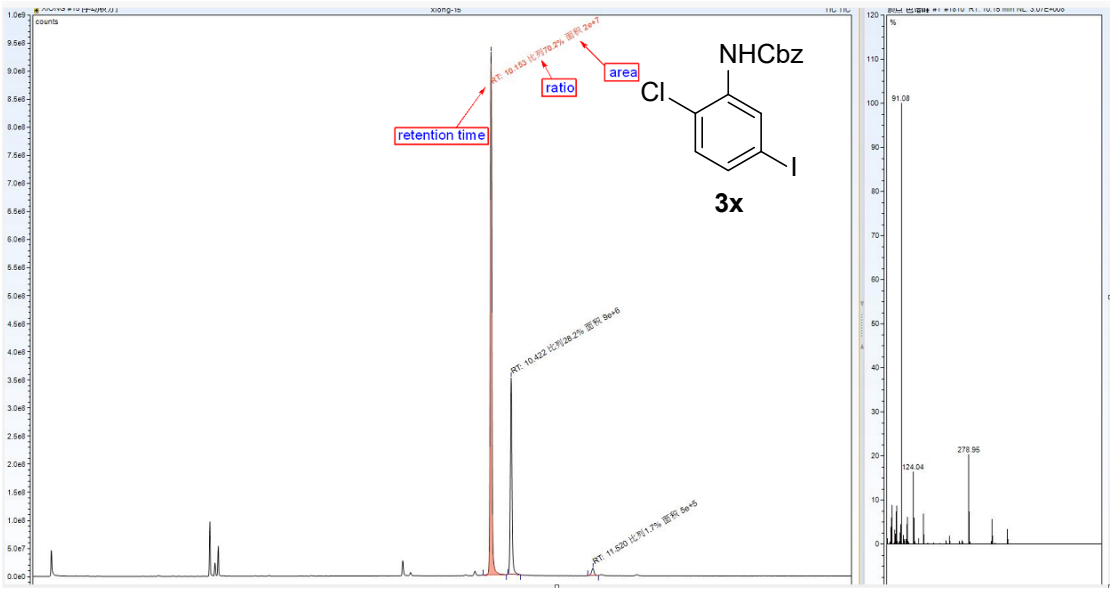

counts
area
ratio
NHCbz
Cl
Cl
Cl
3v''

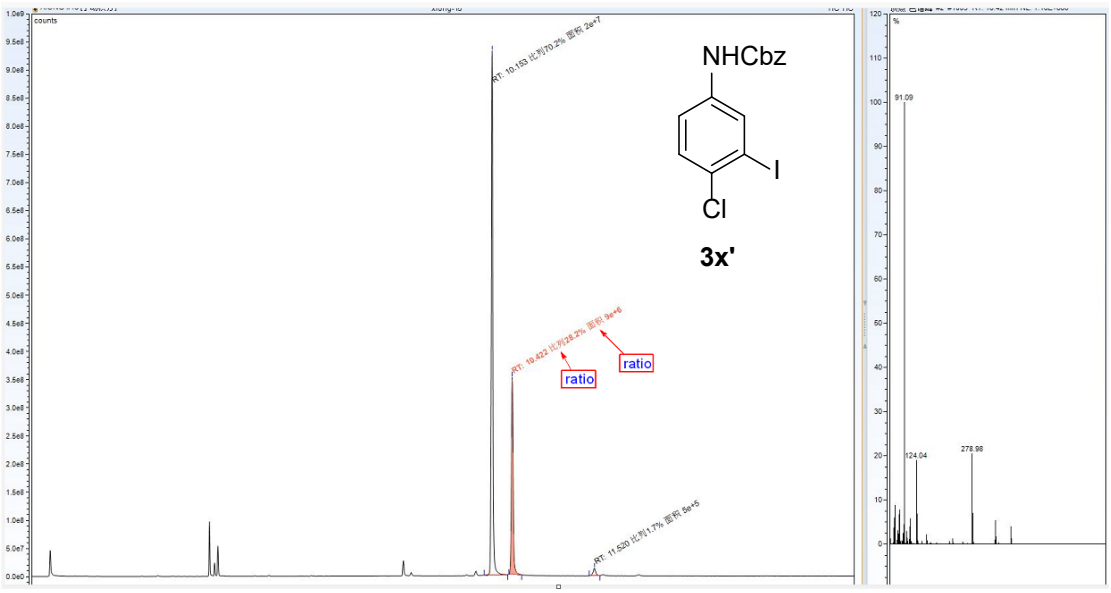

NHCbz
Br
2w
SO2Cl2, (iPr)2NH
toluene, 0 °C
3w:3w' = 9:1
NHCbz
Cl
Br
3w
+
NHCbz
Br
Cl
3w'

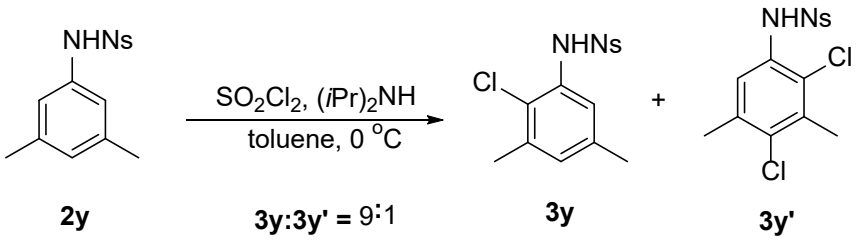

counts
retention time
ratio
area
NHCbz
Cl
Br
3w

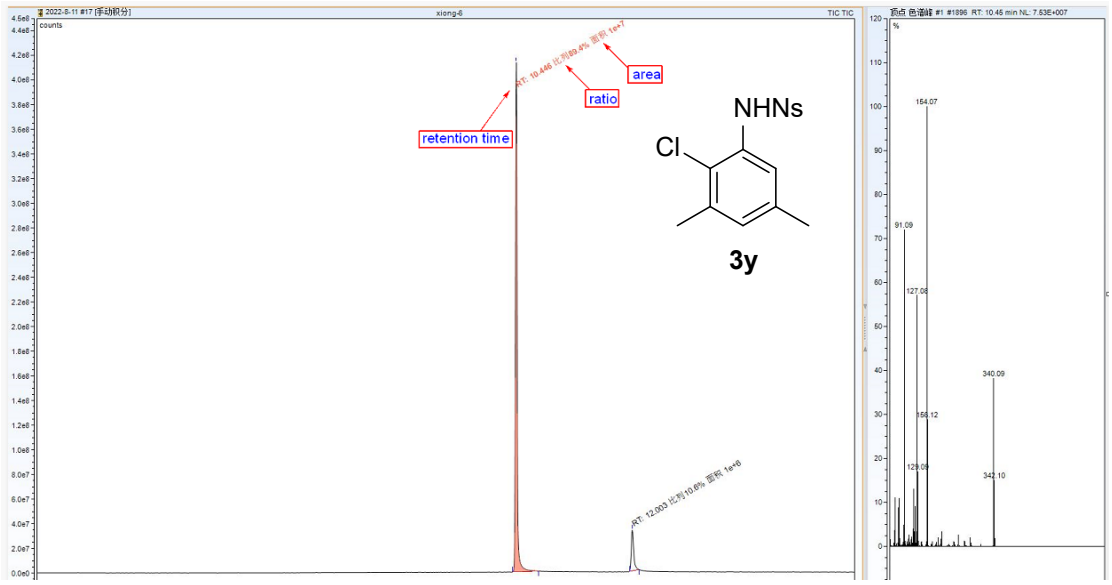

NHCbz
Br
Cl
3w'
area
ratio

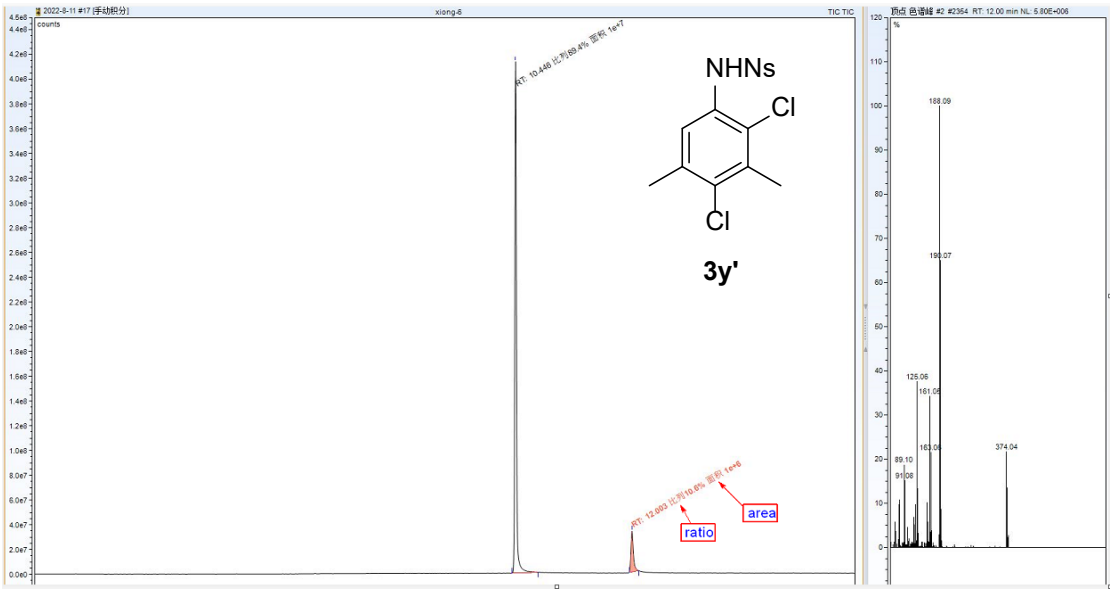

NHCbz
I
2x
SO2Cl2, (iPr)2NH
toluene, 0 °C
3x:3x' = 2.5:1
NHCbz
Cl
I
3x
+
NHCbz
I
Cl
3x'

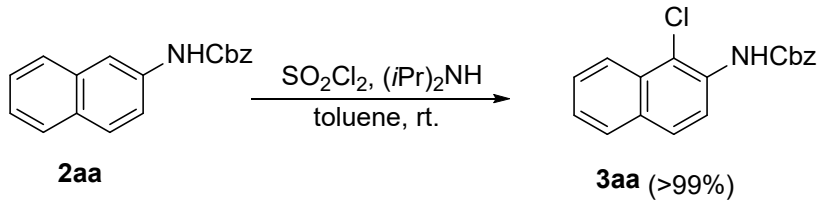

retention time
ratio
area
NHCbz
Cl
I
3x


NHCbz
I
Cl
3x'
ratio
ratio
91.09
124.04
278.98

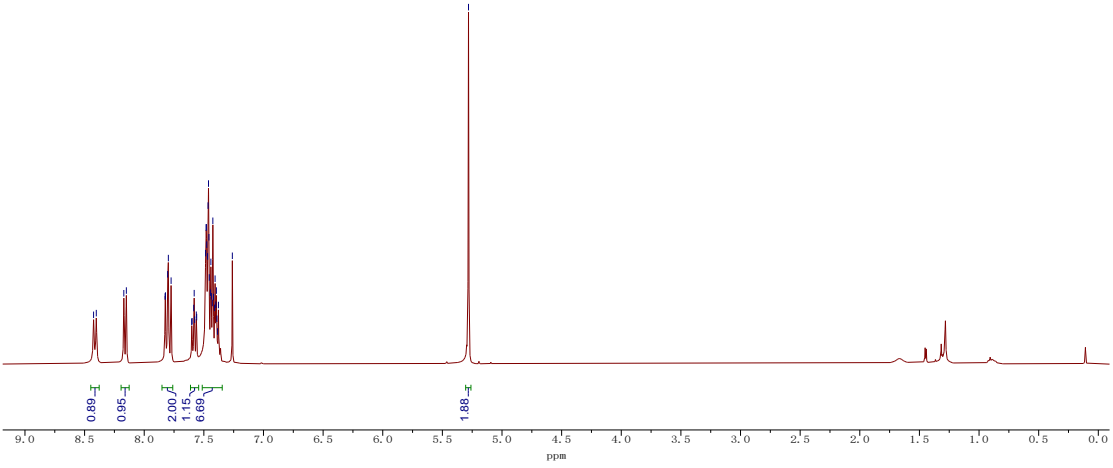

NHNs
2y
SO2Cl2, (iPr)2NH
toluene, 0 °C
3y:3y' = 9:1
NHNs
Cl
3y
+
NHNs
Cl
Cl
3y'


retention time
ratio
area
NHNs
Cl
3y
154.07
91.09
127.08
340.09
166.12
129.09
342.10


NHNs
Cl
Cl
3y'
ratio
area

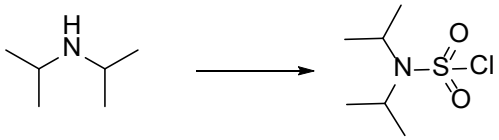

NHCbz
SO2Cl2, (iPr)2NH
toluene, rt.
Cl
NHCbz
2aa
3aa (>99%)


8.425
8.402
8.171
8.150
7.825
7.822
7.803
7.798
7.775
7.602
7.599
7.585
7.581
7.577
7.563
7.560
7.485
7.481
7.479
7.475
7.469
7.465
7.461
7.458
7.455
7.445
7.441
7.437
7.429
7.425
7.419
7.410
7.406
7.399
7.395
7.391
7.385
7.378
7.261
5.281

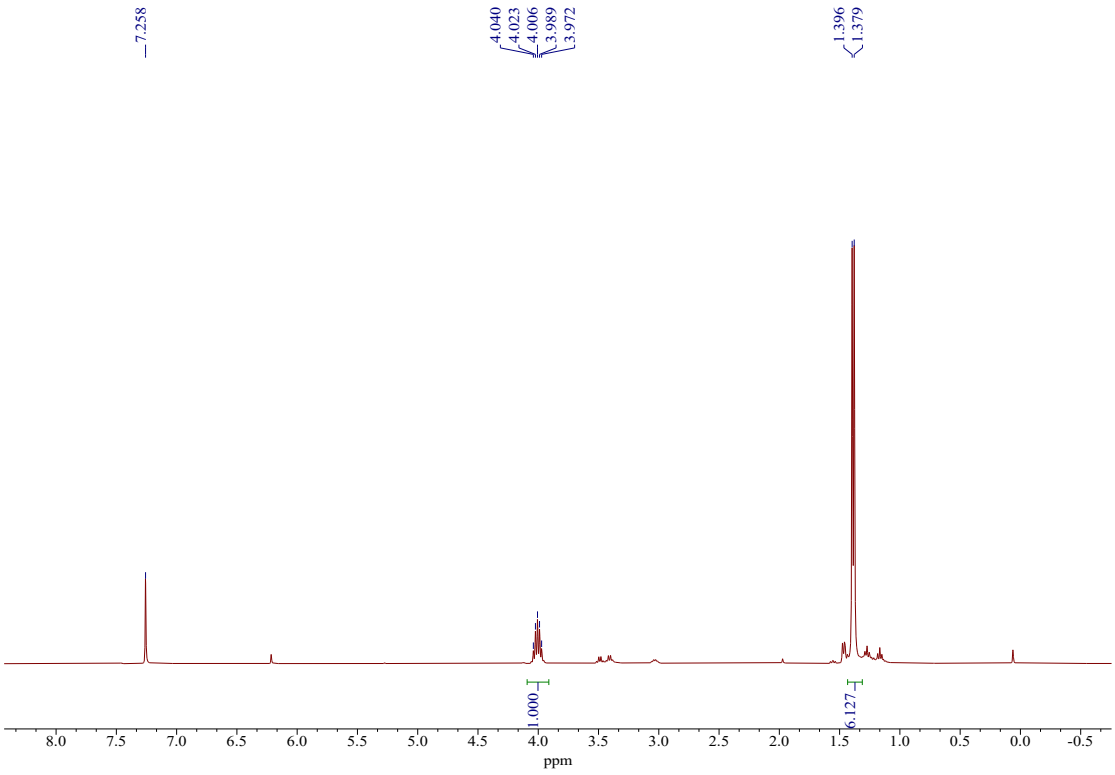

0.89
0.95
2.00
1.15
6.69
1.88
ppm

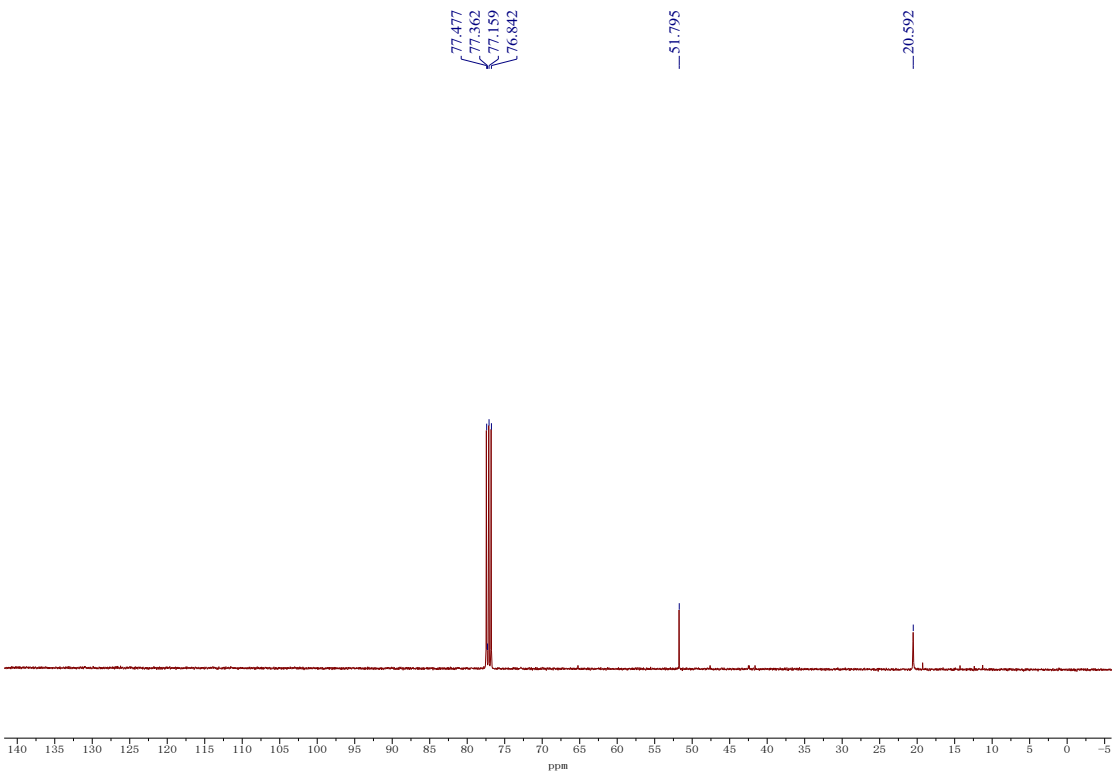
**Mechanistic study:**

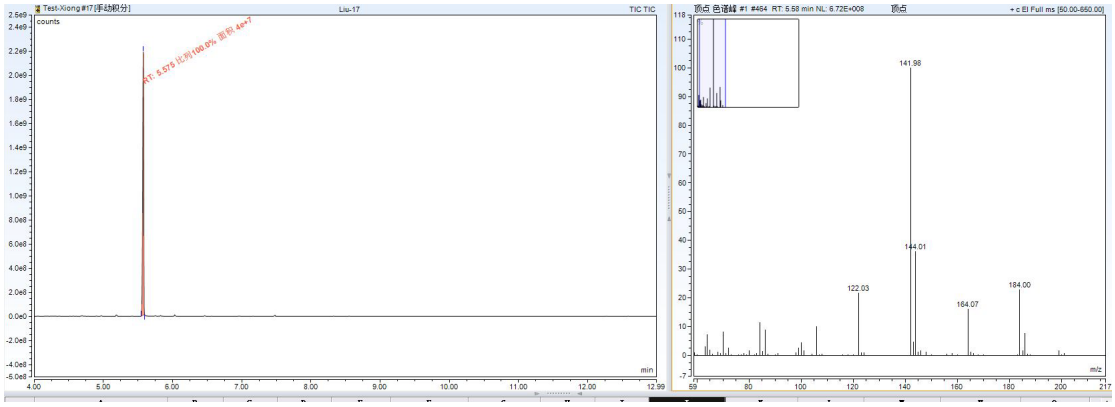
**(I) Preparation for species E**



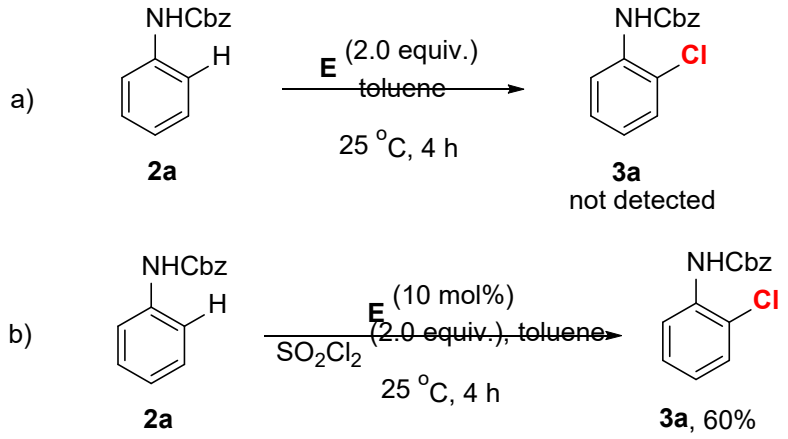

A solution of dry diisopropylamine (2.9 mL, 20 mmol) in dry $Et_2O$ (10 mL) was added dropwise to a stirred solution of sulfuryl chloride (0.81 mL, 10 mmol) and $Et_3N$ (2.5 mL, 20 mmol) in $Et_2O$ (20 mL) at -10 ℃ under $N_2$. After 2 h, the reaction mixture was diluted with $Et_2O$ (10 mL) and vacuum-filtered through Celite. The filtrate was evaporated to give **E** as a yellow oil (0.59 g, 30%). $^1$H NMR (400 MHz, $CDCl_3$) δ 1.39 (d, $J$ = 8.0 Hz, 12H), 3.96-4.06 (m, 2H); $^{13}$C NMR (100 MHz, $CDCl_3$) δ 51.8, 20.6.




77.477
77.362
77.159
76.842
51.795
20.592
ppm

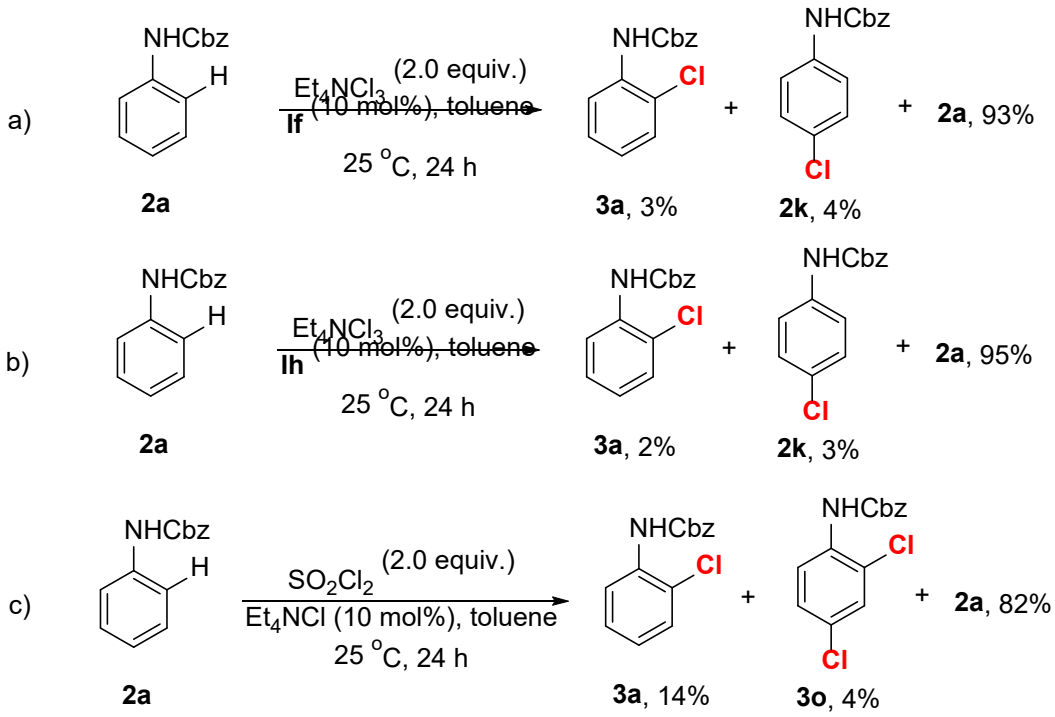

Test-Xiong #17[手动积分]
Liu-17
TIC TIC
counts
min
顶点 色谱峰 #1 #464 RT: 5.58 min NL: 6.72E+008
顶点
+ c EI Full ms [60.00-650.00]
141.98
144.01
122.03
164.07
184.00
m/z

**(J) Species E as halogen source and catalyst for *ortho*-chlorination**



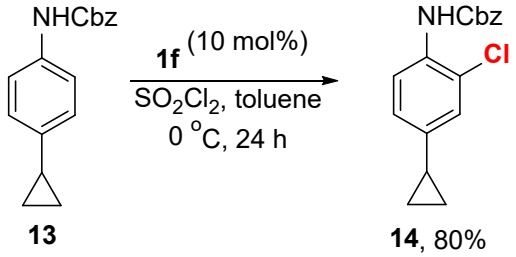

*Notes: The ortho-chlorination of **2a** was carried out using species **E** as chlorinating reagent at room temperature, ortho-chlorinated product **3a** was not detected. However, the ortho-chlorination of **2a** worked in the presence of species **E** and sulfuryl chloride, providing the desired product **3a** in 60% yield.*

**(K) Mioskowski reagent as halogen source for *ortho*-chlorination**




*Notes: The ortho-chlorination of **2a** was carried out using Mioskowski reagent as chlorinating reagent at room temperature in the presence of **1f** and **1h**, providing the desired product **3a** in 3% yield and 2% yield, respectively. These results indicated that the larger tetraethylammonium cation could provide stable environment for allowing the anion $Cl_3^-$ to approach in lowest energy form, whereas the smaller cations offer the unstable conditions.*

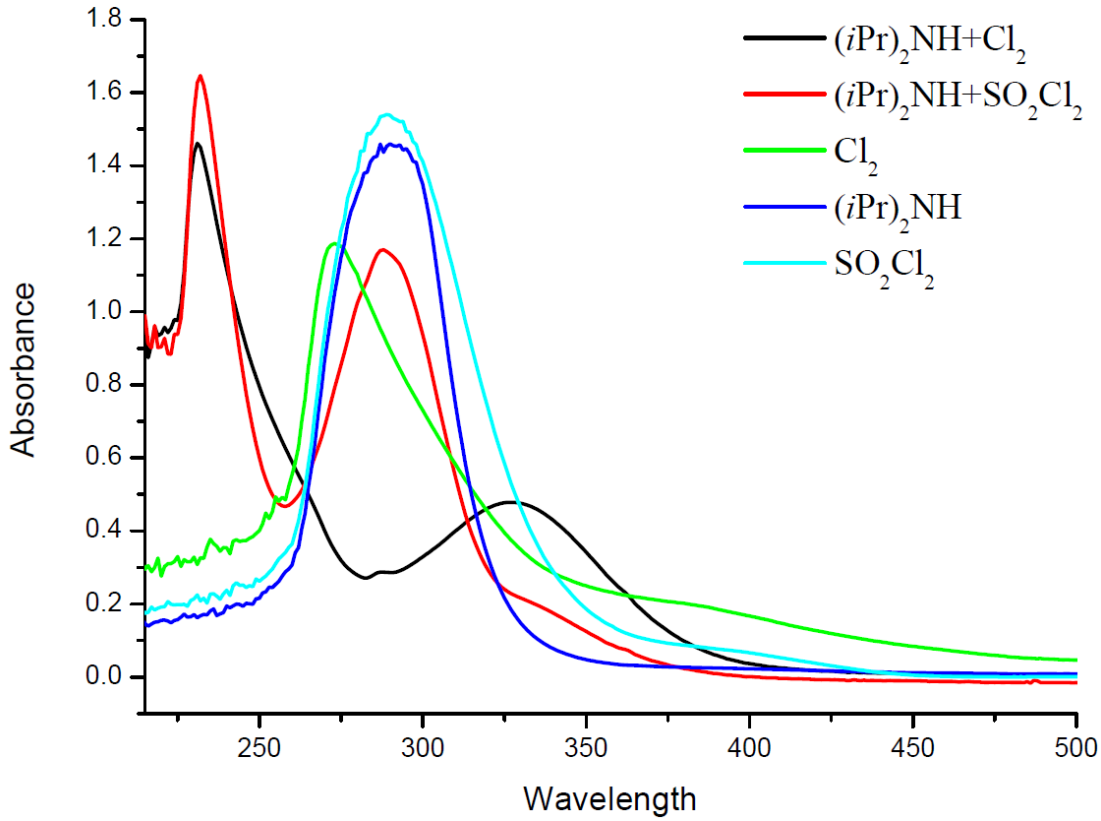
See (a) Evans, J. C.; Lo, Y.-S. Vibrational Spectra of the $Cl_3^-$ Ion and Evidence for the Existence of $Cl_5^-$. ***J. Chem. Phys***. **1966**, 44, 3638−3639. (b) Daniel, F.; Hoyle, G. Perhalides of Quaternary Ammonium Salts. *J. Chem. Soc. Trans*. **1923**, *123*, 654−662.




**13** **14**, 80%

*Notes: The chlorination of cyclopropane **13** provides the corresponding ortho-chlorinated compound **14** in 80% yield, and the product with cyclopropane opened was not observed. This result further suggests the involvement of radical pathway was impossible.*

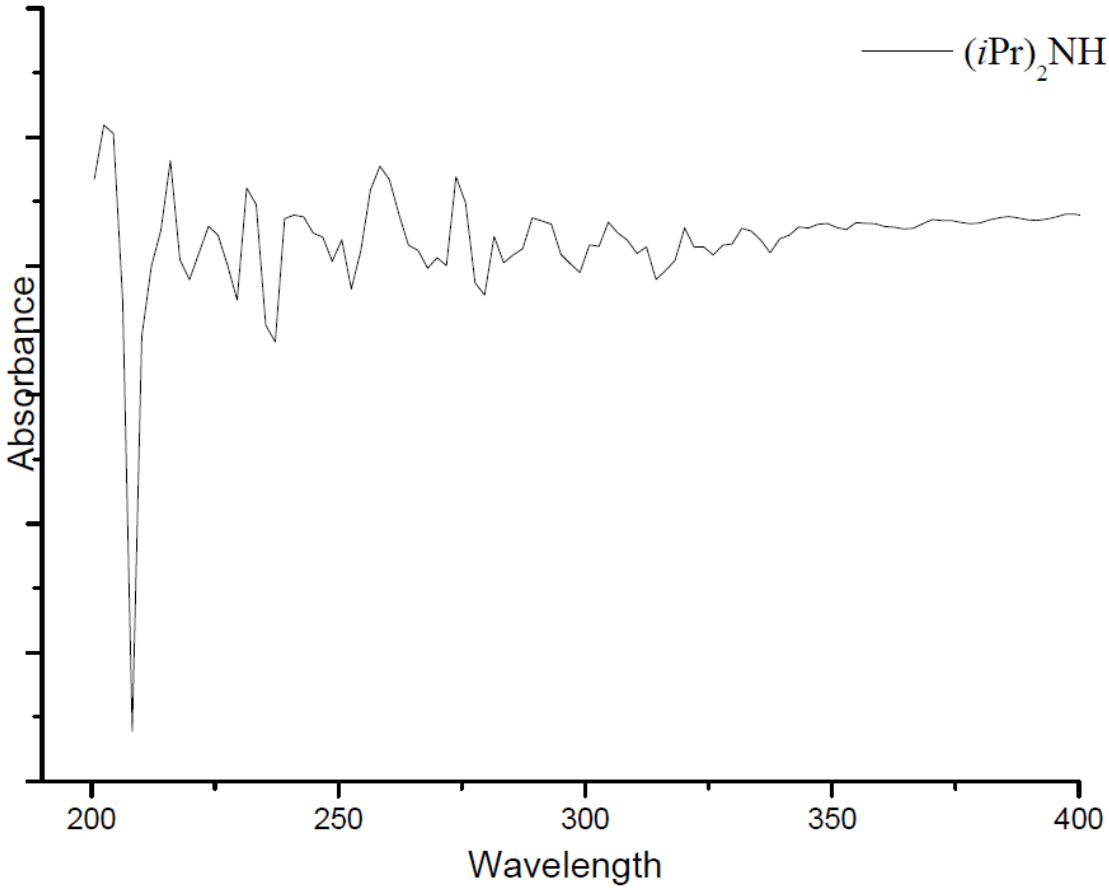
**(L) Determine the species A**

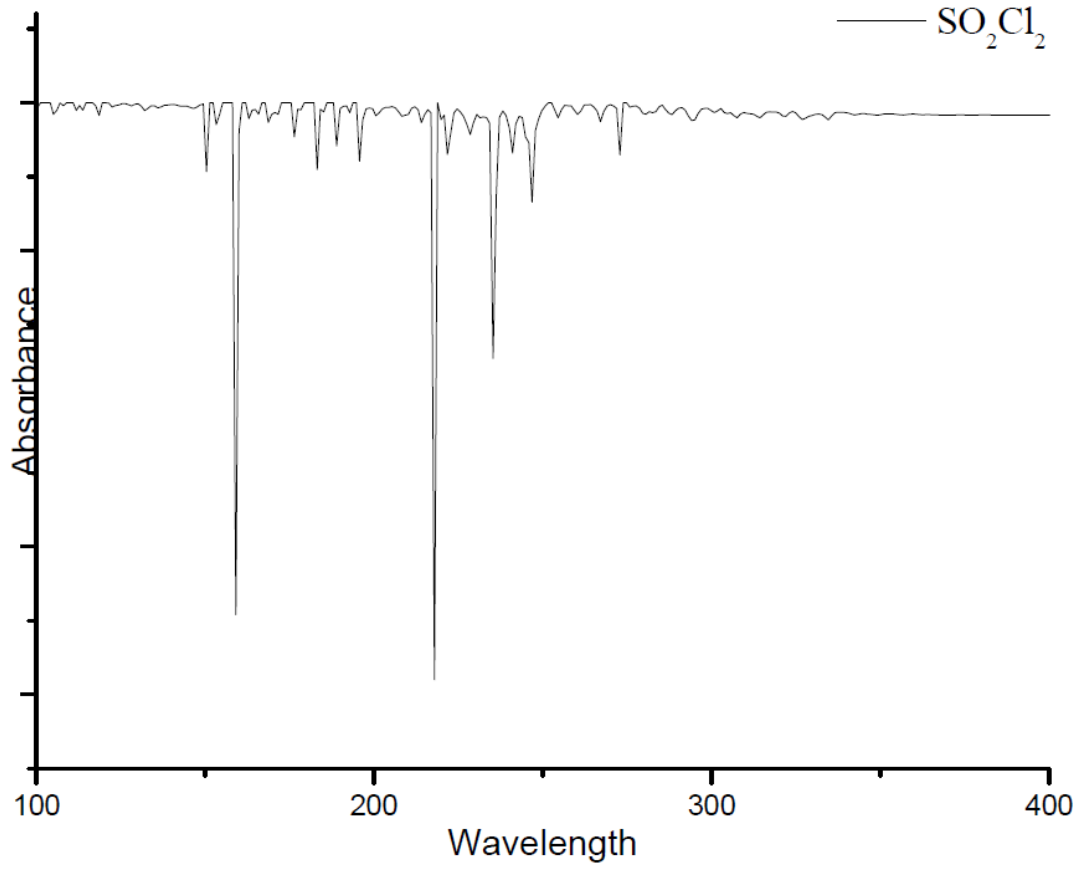


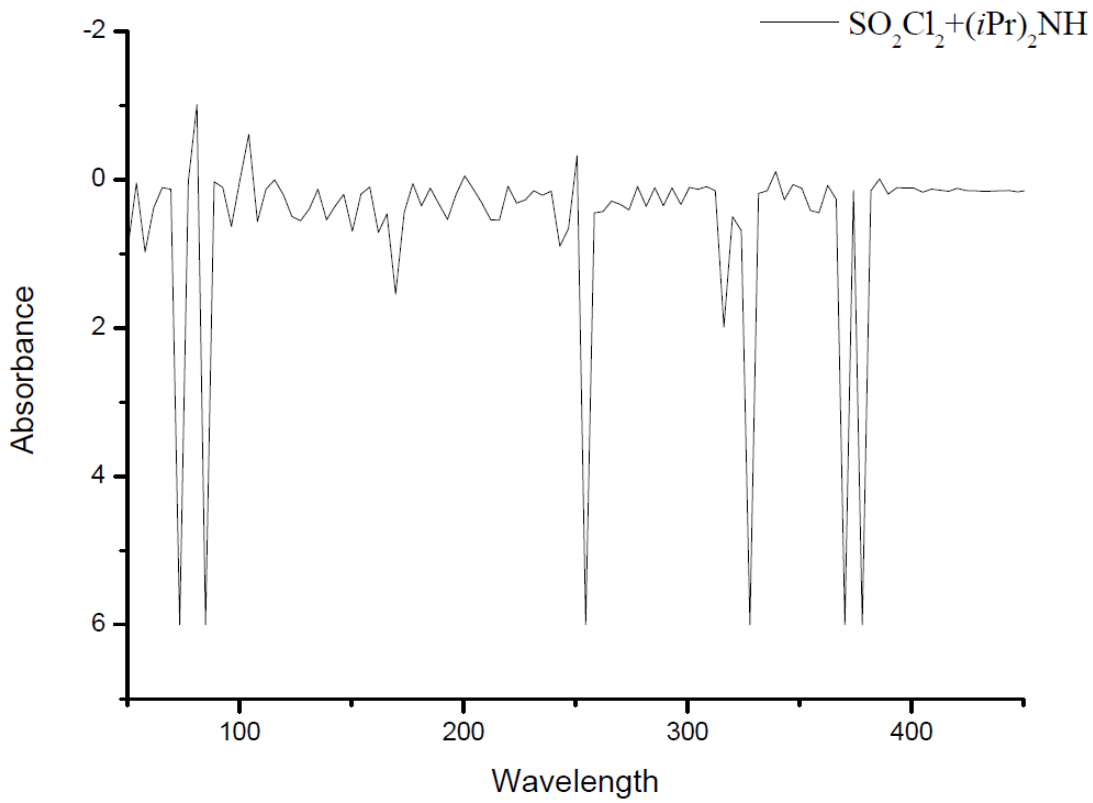

*Notes: The UV-vis experiment was conducted using **1f** (0.1 eq.) and $SO_2Cl_2$ (1.0 eq.) in $CH_2Cl_2$ at 25 °C. The new signal could be attributed to the strong intense absorption of the species **A** at 232 nm.*

**Figure S1**. UV-vis experiment studies

See (a) Brown, D. M.; Dainton, F. S. Matrix Isolation of Unstable Halogen Radical Ions. *Nature* **1966**, *209*, 195−196. (b) Andrews, L. Optical Spectra of the Difluoride, Dichloride, and Trichloride Ions in the Matrix-Isolated $M^+F_2^-$, $M^+Cl_2^-$, and $M^+Cl_3^-$ Species. *J. Am. Chem. Soc.* **1976**, *98*, 2147−2152.


(iPr)2NH
Absorbance
200
250
300
350
400
Wavelength

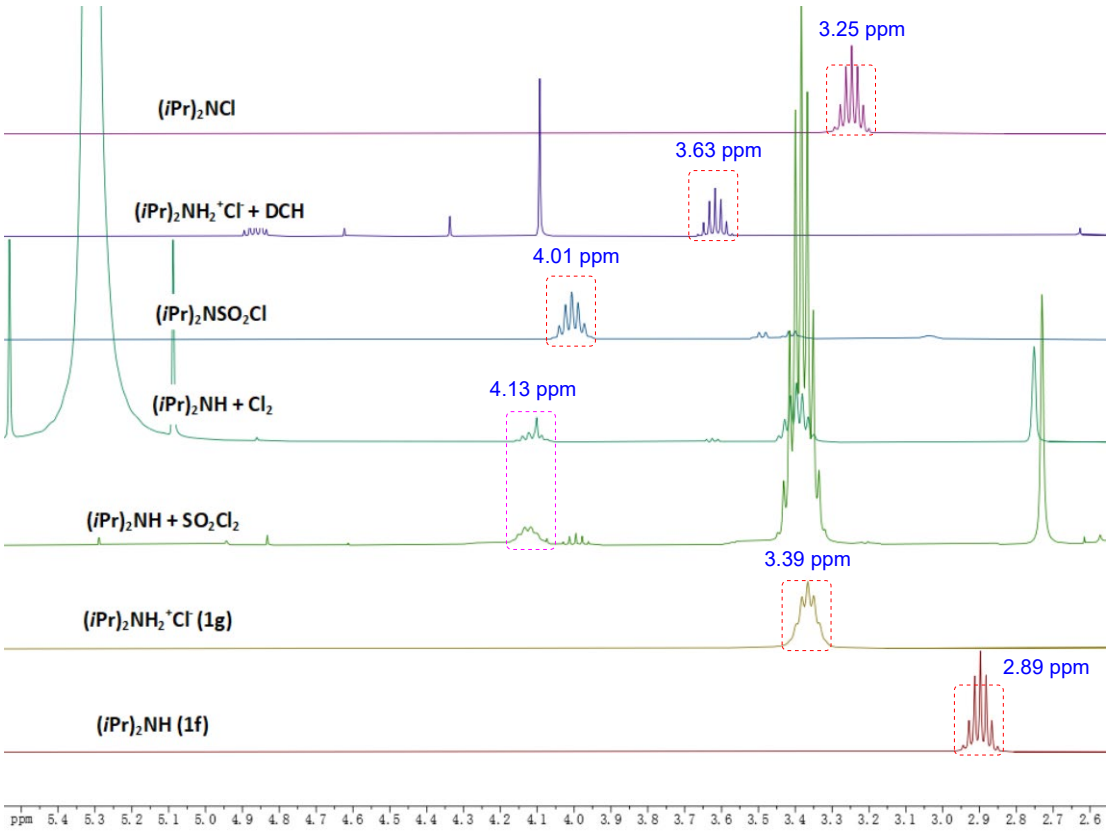

SO2Cl2
Absorbance
100
200
300
400
Wavelength




*Notes:* ***1f*** *(0.1 eq.) and $SO_2Cl_2$ (1.0 eq.) were solved in $CH_2Cl_2$ at 25 °C, then the solvent was removed to afford white solid, which was used to conduct the IR experiment. The new signal could be attributed to the sharp band of the species* ***A*** *at 254 $cm^{-1}$.*

**Figure S2**. IR experiment studies

See (a) Evans, J, C.; Lo, G. Y-S. Vibrational Spectra of the $Cl_3^-$ Ion and Evidence for the Existence of $Cl_5^-$. *J. Chem. Phys*. **1966**, *44*, 3638−3639. (b) Redeker, F. A.; Riedel, S. Matrix-isolation and comparative far-IR investigation of free linear $[Cl_3]^-$ and a series of alkali trichlorides. *Chem. Commun*. **2017**, *53*, 12958−12961.




*Notes: The NMR experiment was conducted using **1f** (0.1 eq.) and $SO_2Cl_2$ (1.0 eq.) in $CDCl_3$ at 25 °C. The signal of the methine proton of **1g** (3.4 ppm) and a new signal (4.1 ppm) appeared concurrently. The new signal could be attributed to the methine proton of the species **A**.*

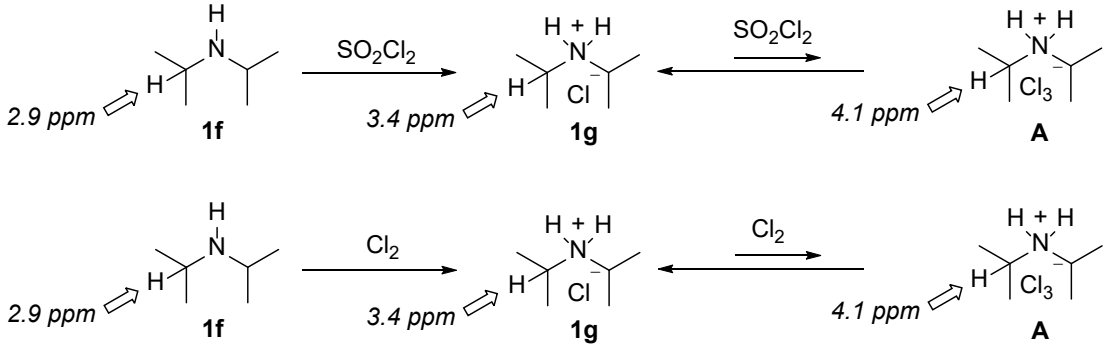
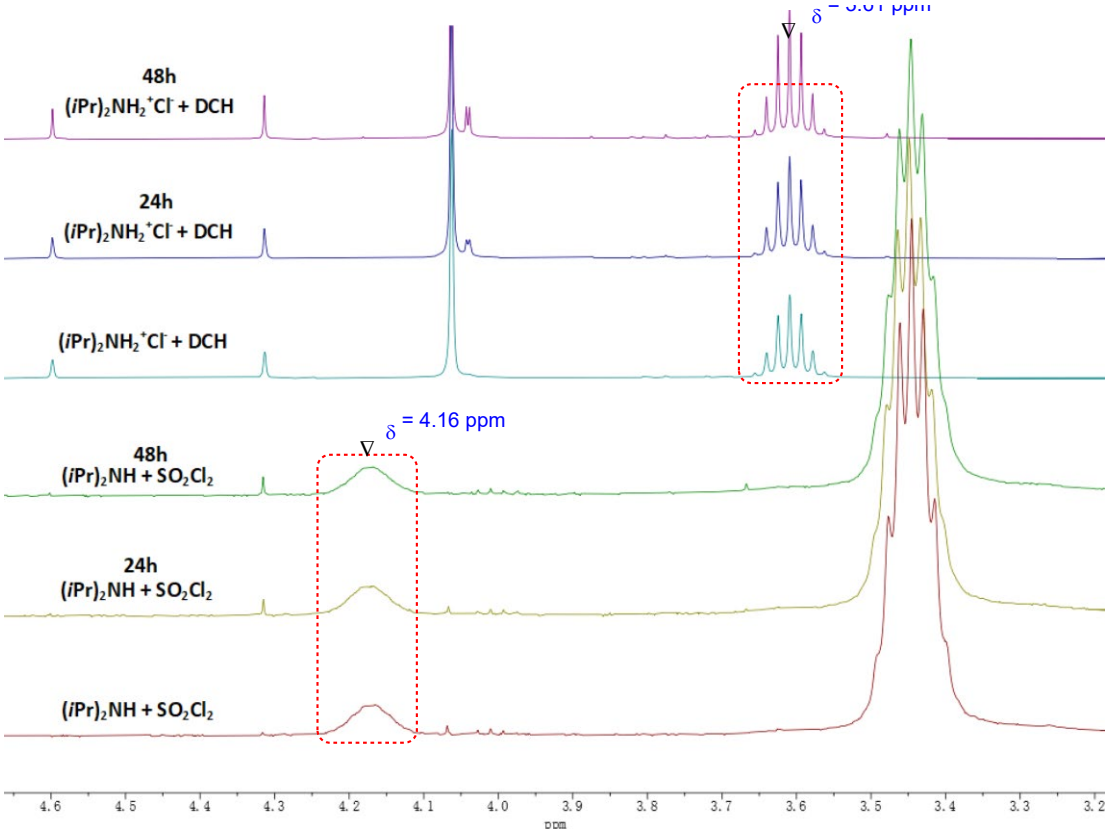
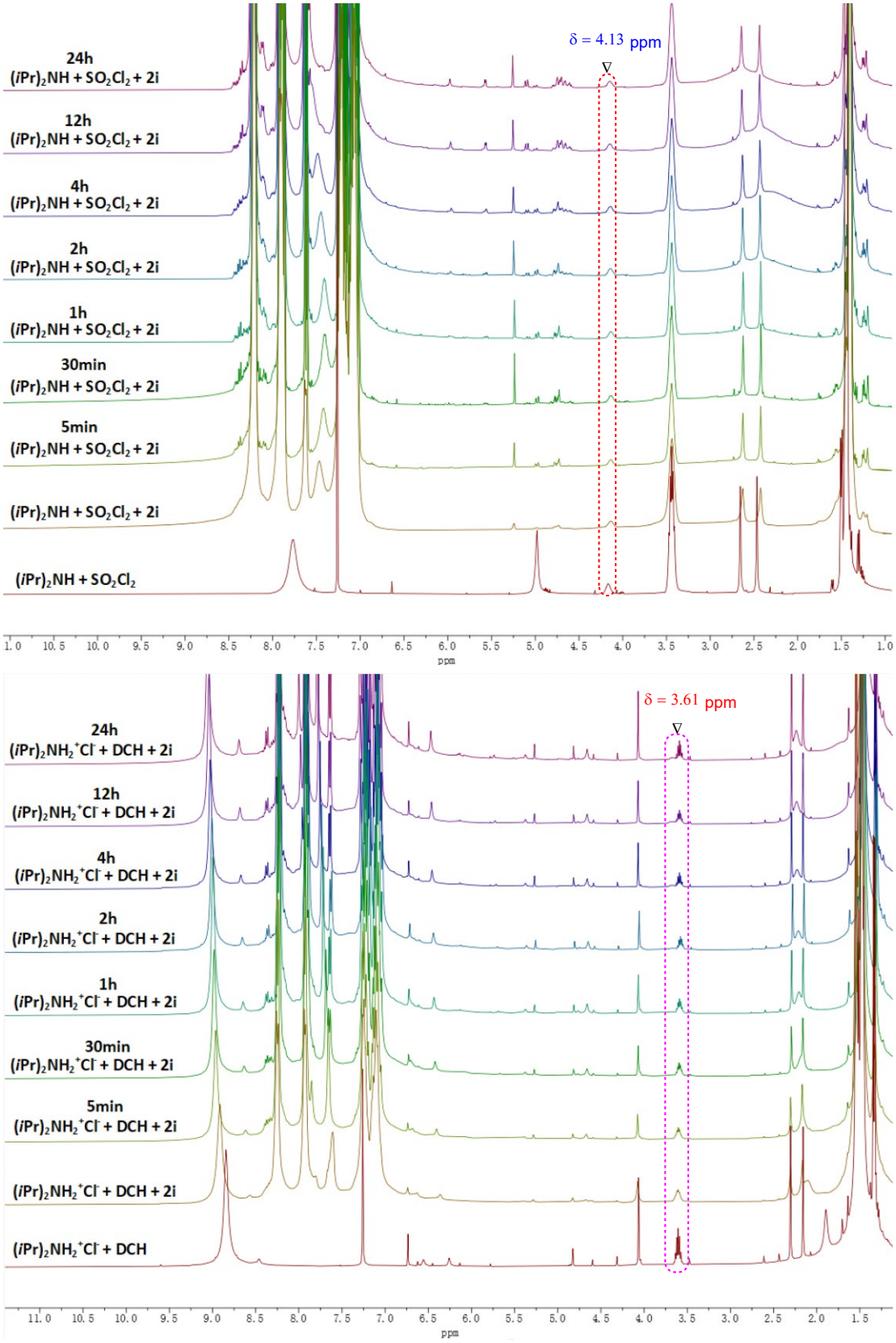



**Figure S3.** $^1$H NMR experiment on a mixture of **1f** and $SO_2Cl_2$ in $CDCl_3$




*Notes: The NMR experiments were conducted using **1f** (0.1 eq.) and $SO_2Cl_2$ (1.0 eq.), **1h** (0.1 eq.) and DCH (1.0 eq.) in $CDCl_3$ at 25 °C. These results suggested that the species **A** (4.1 ppm) and the active cationic species (3.6 ppm) were stable at 25 °C.*

**Figure S4.** $^1$H NMR experiment on a mixture of **1f** and $SO_2Cl_2$, **1h** and DCH in $CDCl_3$ at 25 °C




*Notes: The NMR experiments were conducted using species **A** and the active cationic species with substrate **2i** in $CDCl_3$ at 25 °C, respectively. These results suggested that the species **A** (4.1 ppm) and the active cationic species (3.6 ppm) were not interchangeable with substrate at 25 °C.*

## (M) References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6. W. B. Im.; S. H. Choi.; J.-Y. Park.; S. H. Choi.; J. Finn.; S.-H. Yoon. *Eur. J. Med. Chem*. **2011**, *46*, 1027–1039.
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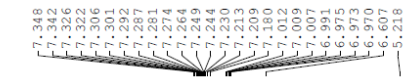
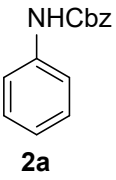
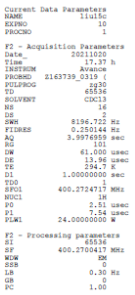
16. A. N. Dinh.; S. M. Maddox.; S. D. Vaidya.; M. A. Saputra.; C. J. Nalbandian.; J. L. Gustafson. *J. Org. Chem*. **2020**, *85*, 13895–13905.

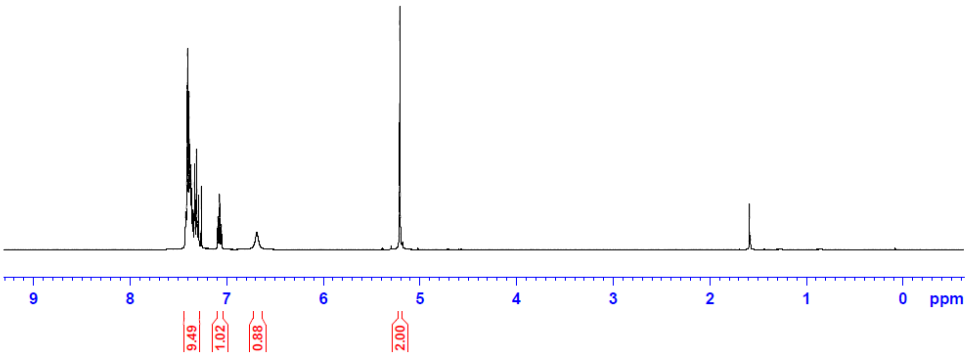
## (N) $^{1}H$ and $^{13}C$ Spectra



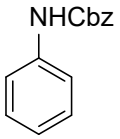




2a

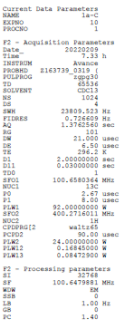


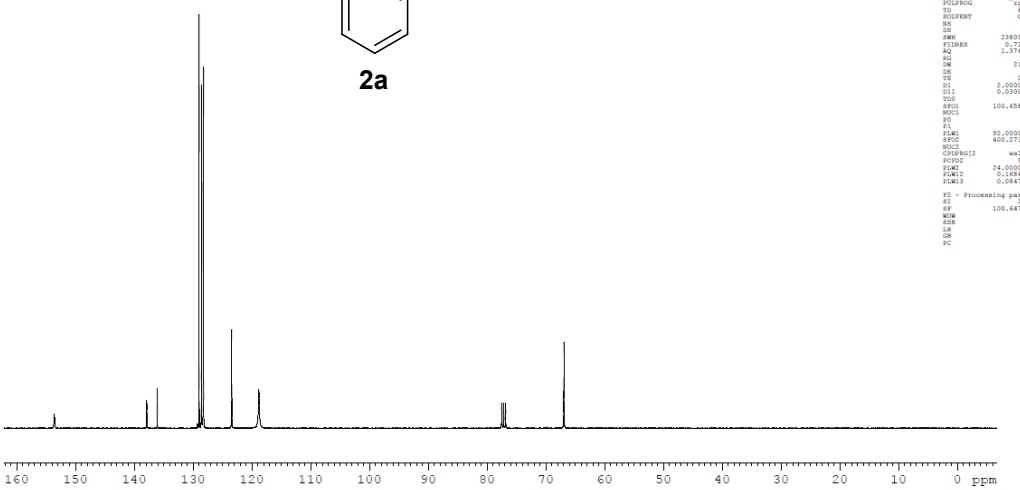


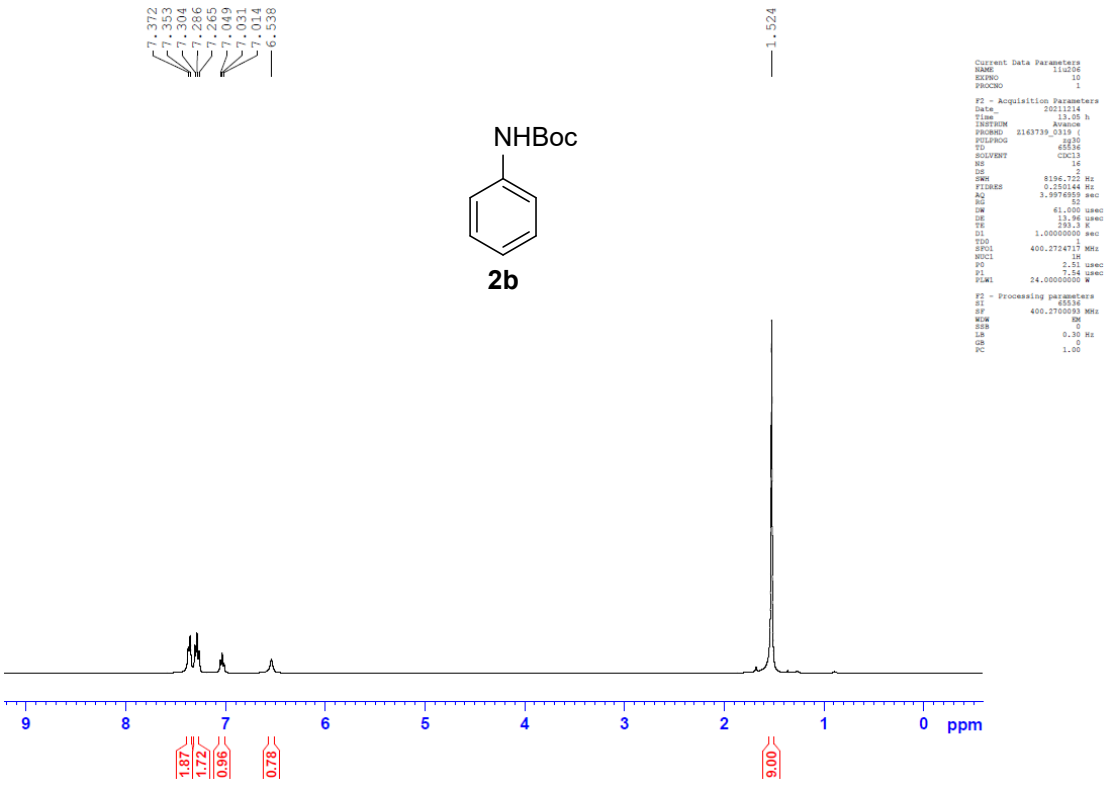





2a



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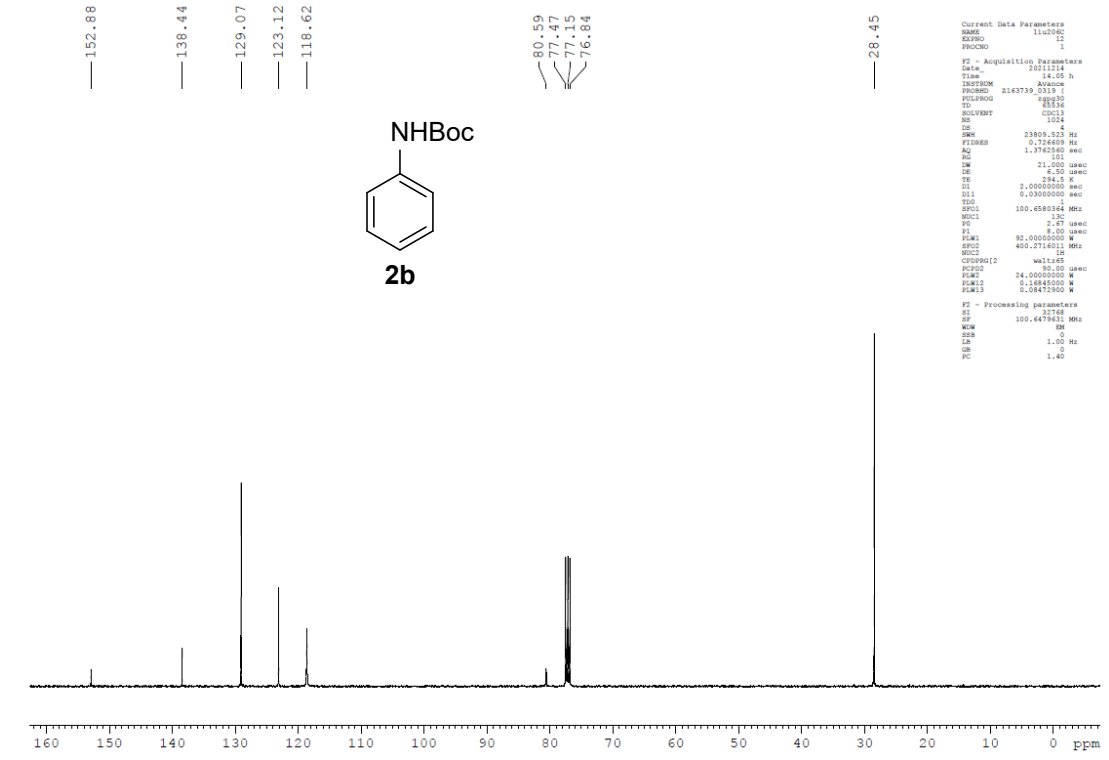
7.353
7.304
7.286
7.265
7.049
7.031
7.014
6.538
1.524
NHBoc
2b
9
8
7
6
5
4
3
2
1
0
ppm
1.87
1.72
0.96
0.78
9.00


152.88
138.44
129.07
123.12
118.62
80.59
77.47
77.15
76.84
28.45
NHBoc
2b
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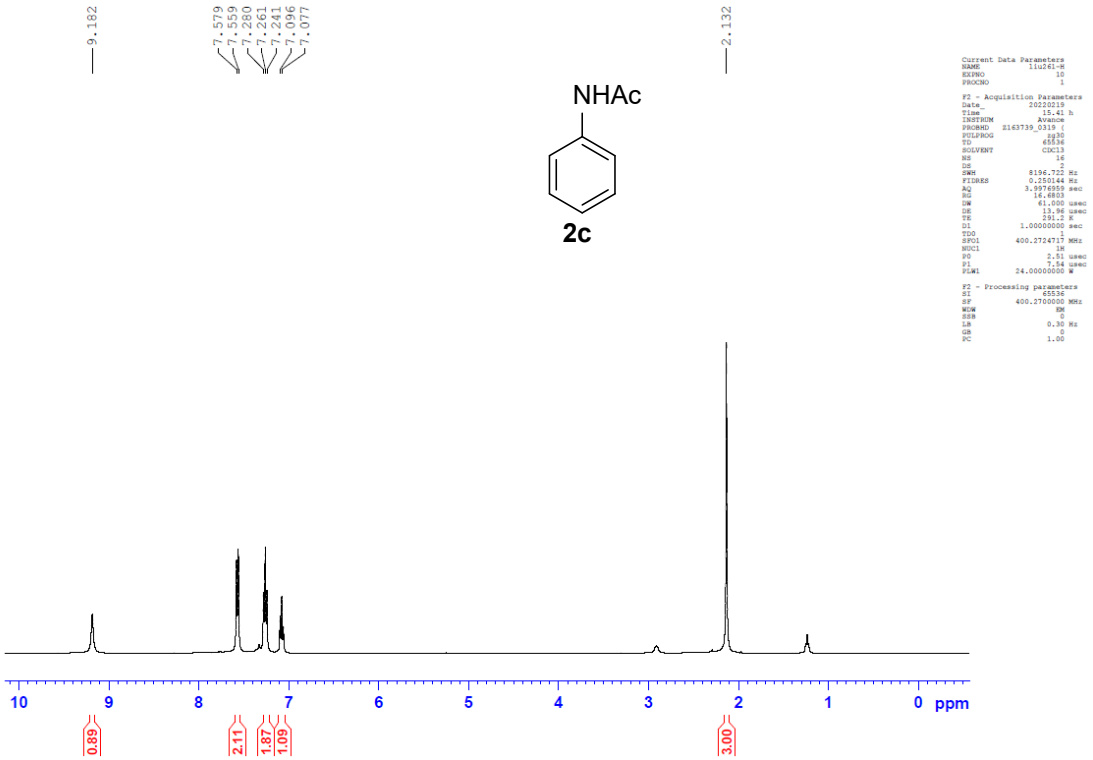
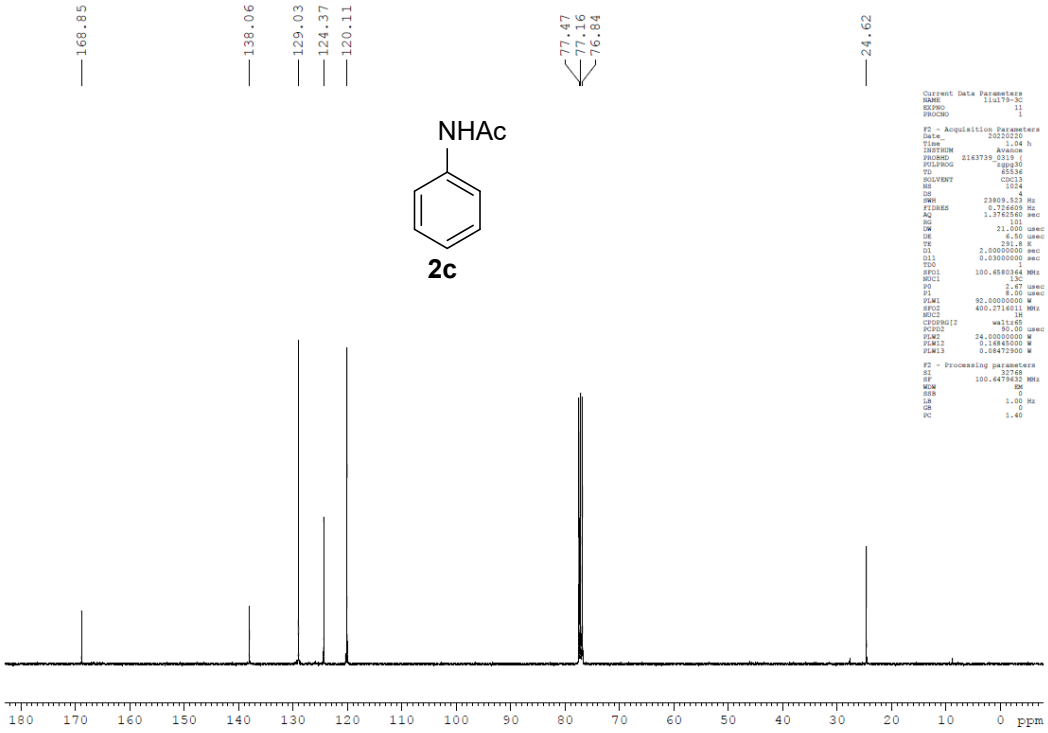
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
ppm


9.182
7.579
7.559
7.280
7.261
7.241
7.096
7.077
2.132
NHAc
2c
10
9
8
7
6
5
4
3
2
1
0
ppm
0.89
2.11
1.87
1.09
3.00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138.06
129.03
124.37
120.11
77.47
77.16
76.84
24.62
NHAc
2c
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170
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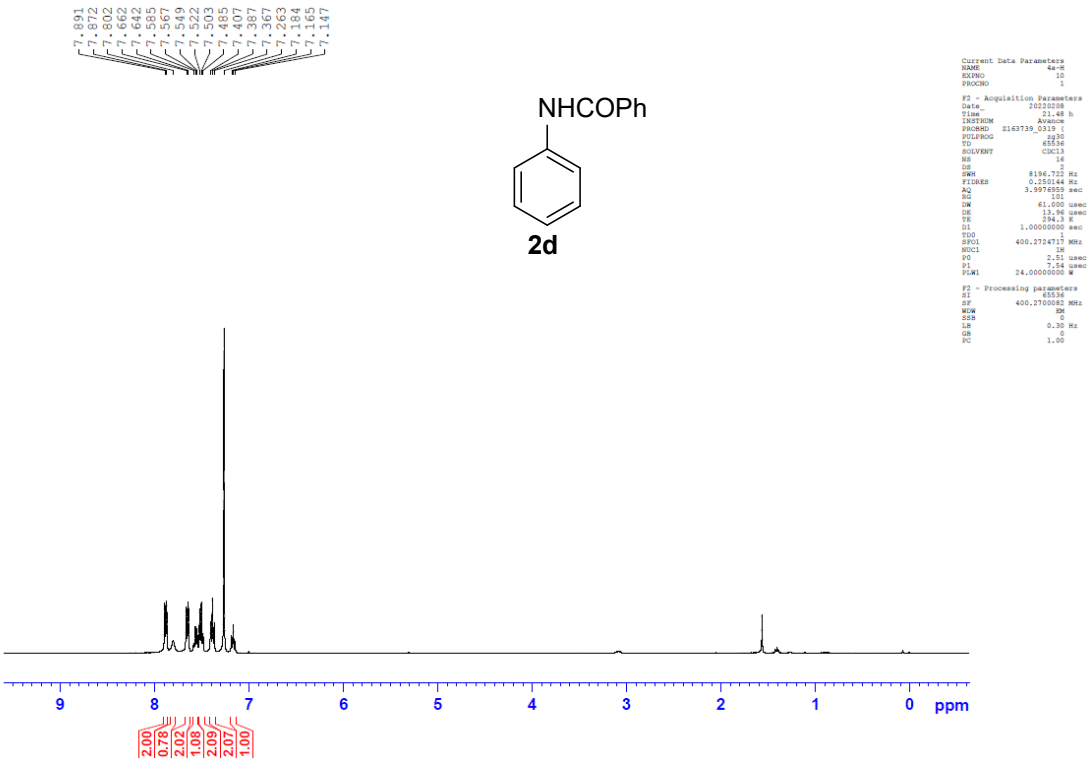
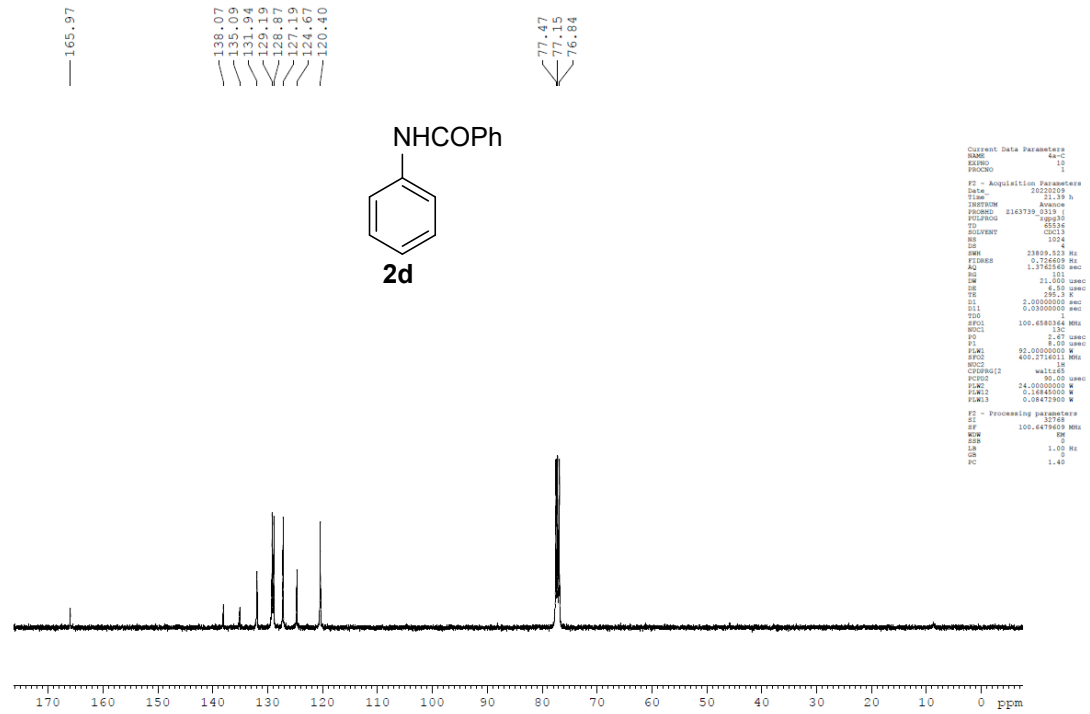
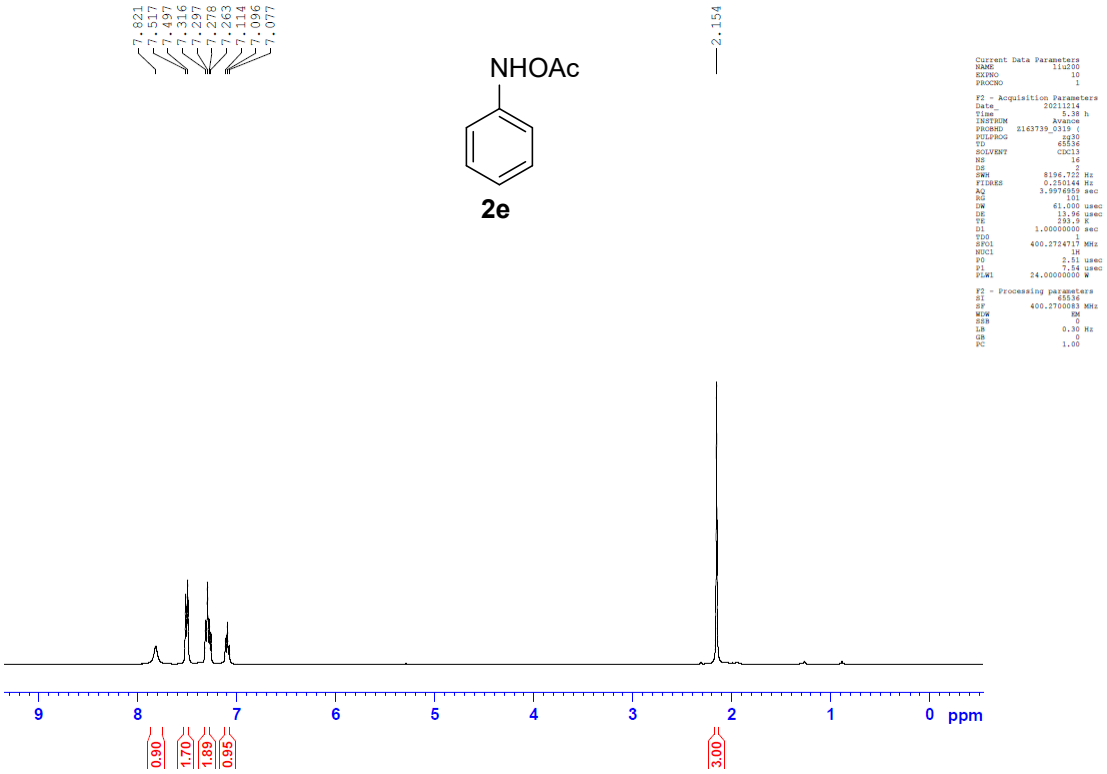
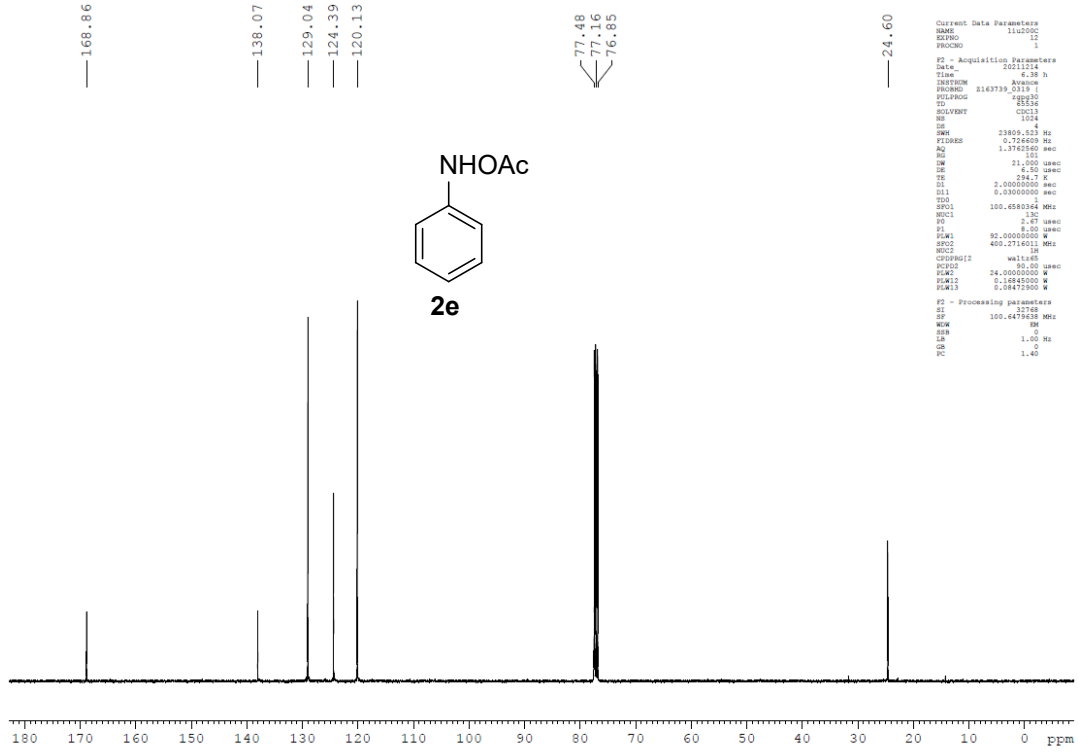
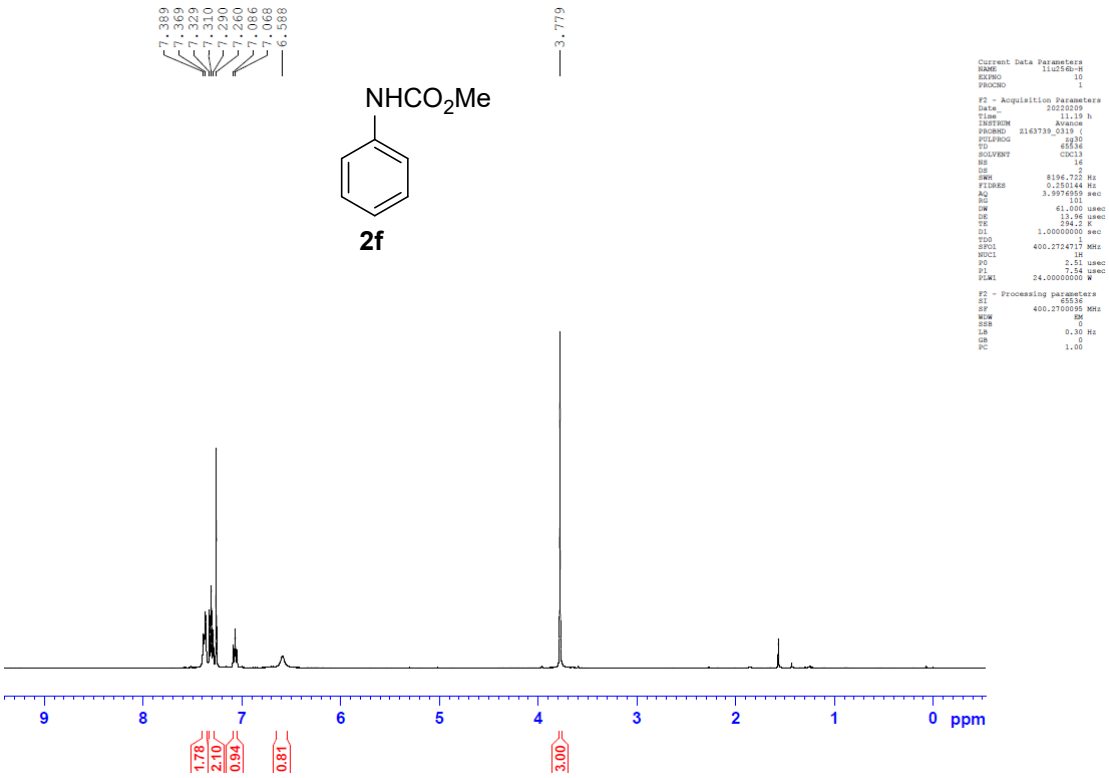
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
ppm

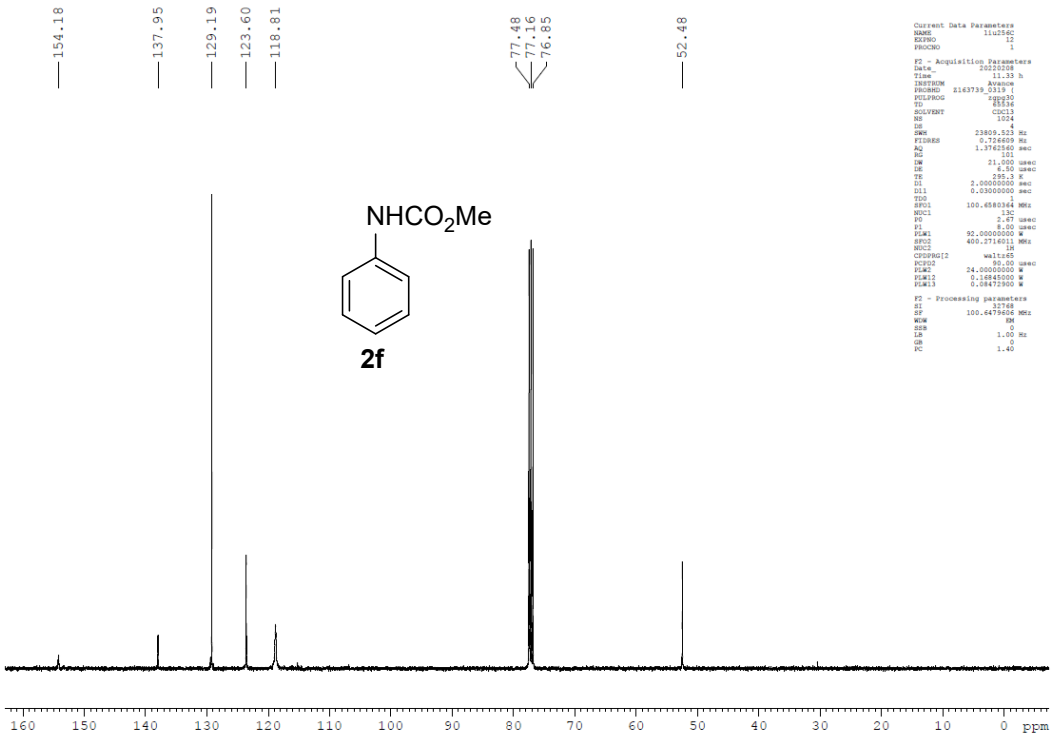

7.891
7.872
7.802
7.662
7.642
7.585
7.567
7.549
7.522
7.503
7.485
7.407
7.387
7.367
7.263
7.184
7.165
7.147
NHCOPh
2d
9
8
7
6
5
4
3
2
1
0
ppm
2.00
0.78
2.02
1.08
2.09
2.07
1.00

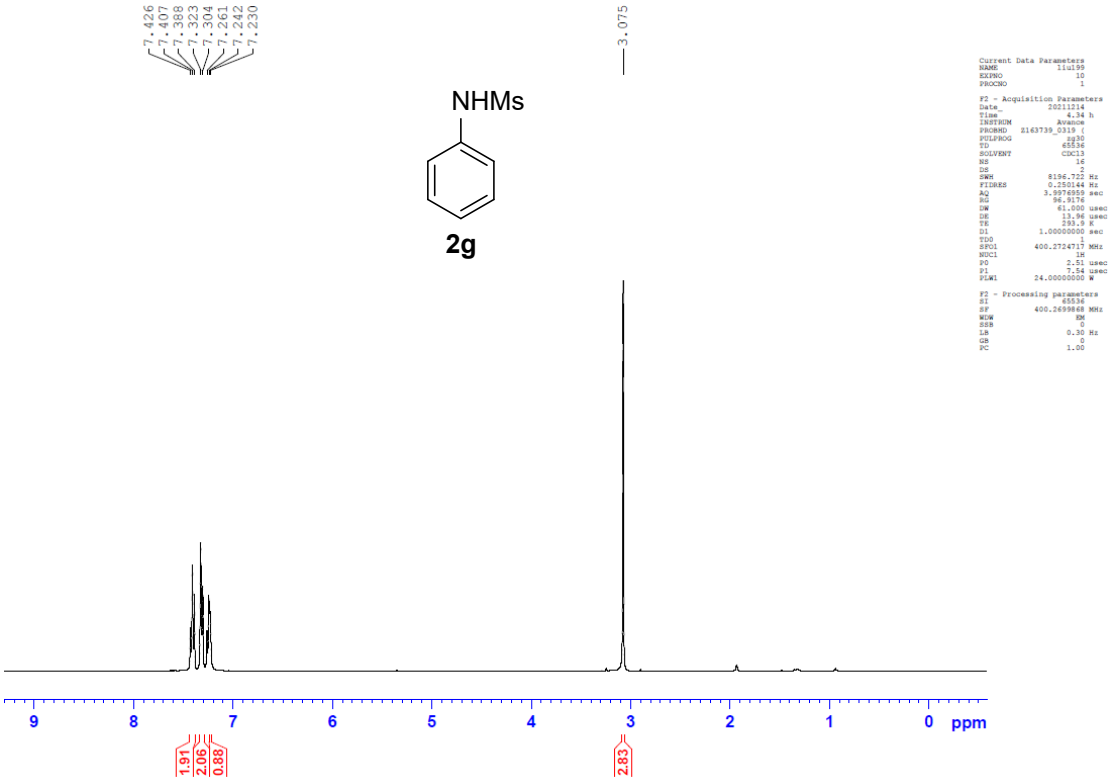

165.97
138.07
135.09
131.94
129.19
128.87
127.19
124.67
120.40
77.47
77.15
76.84
NHCOPh
2d
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
ppm

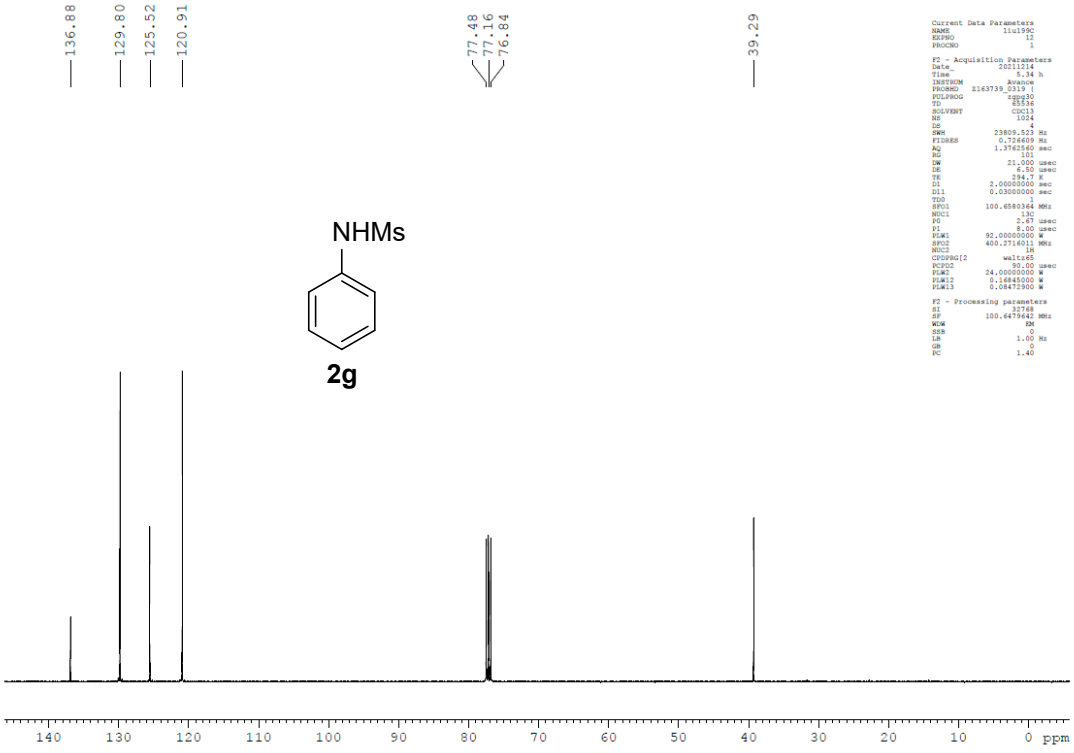

7.821
7.517
7.497
7.316
7.297
7.278
7.263
7.114
7.096
7.077
2.154
NHOAc
2e
9
8
7
6
5
4
3
2
1
0
ppm
0.90
1.70
1.89
0.95
3.00

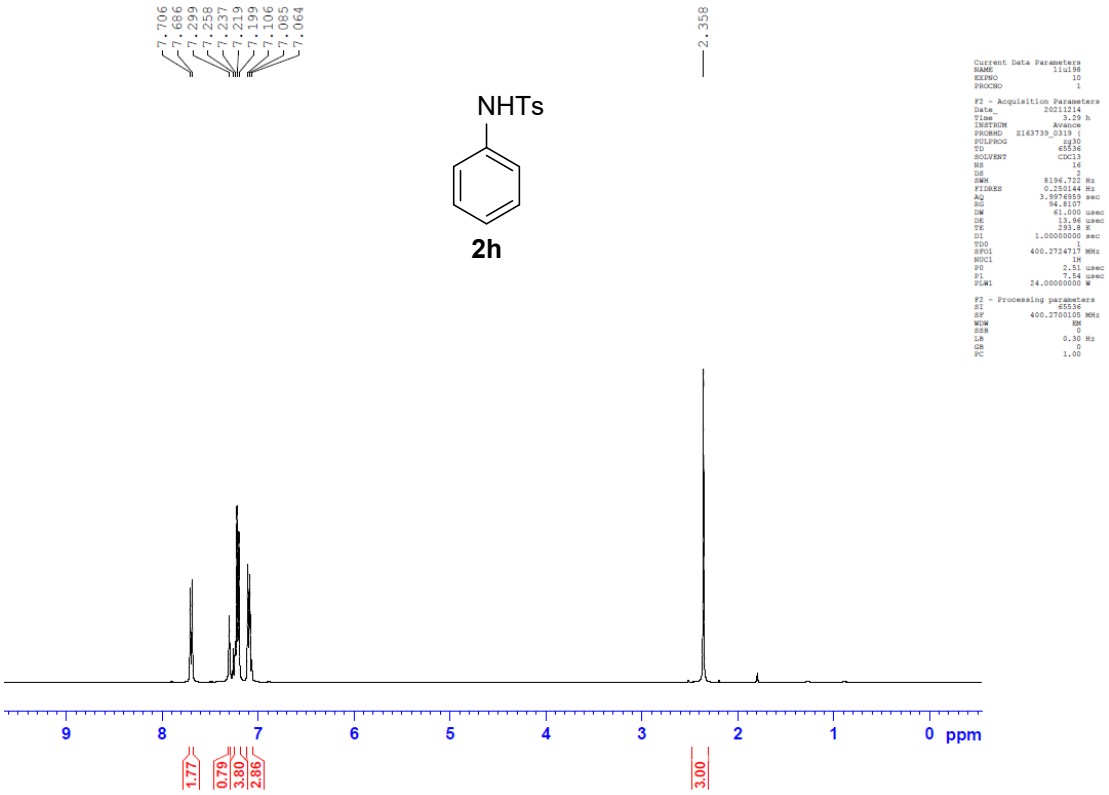

168.86
138.07
129.04
124.39
120.13
77.48
77.16
76.85
24.60
NHOAc
2e
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
ppm

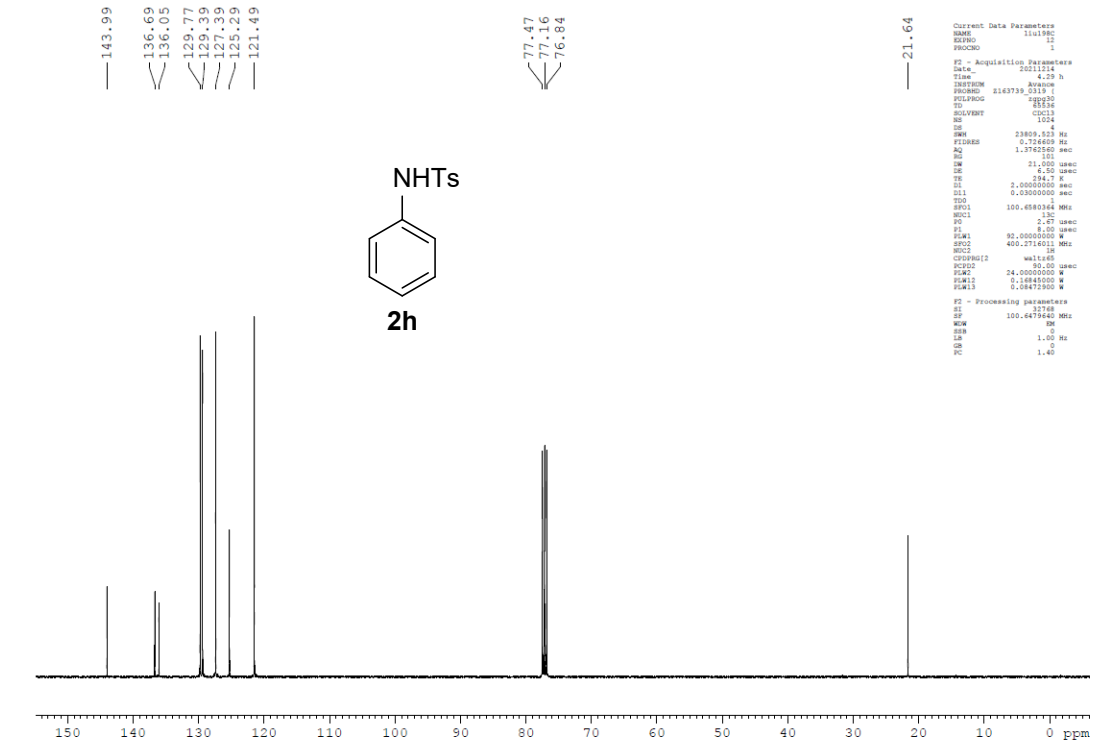

7.389
7.369
7.329
7.310
7.290
7.260
7.086
7.068
6.588
3.779
NHCO2Me
2f
9
8
7
6
5
4
3
2
1
0 ppm
1.78
2.10
0.94
0.81
3.00

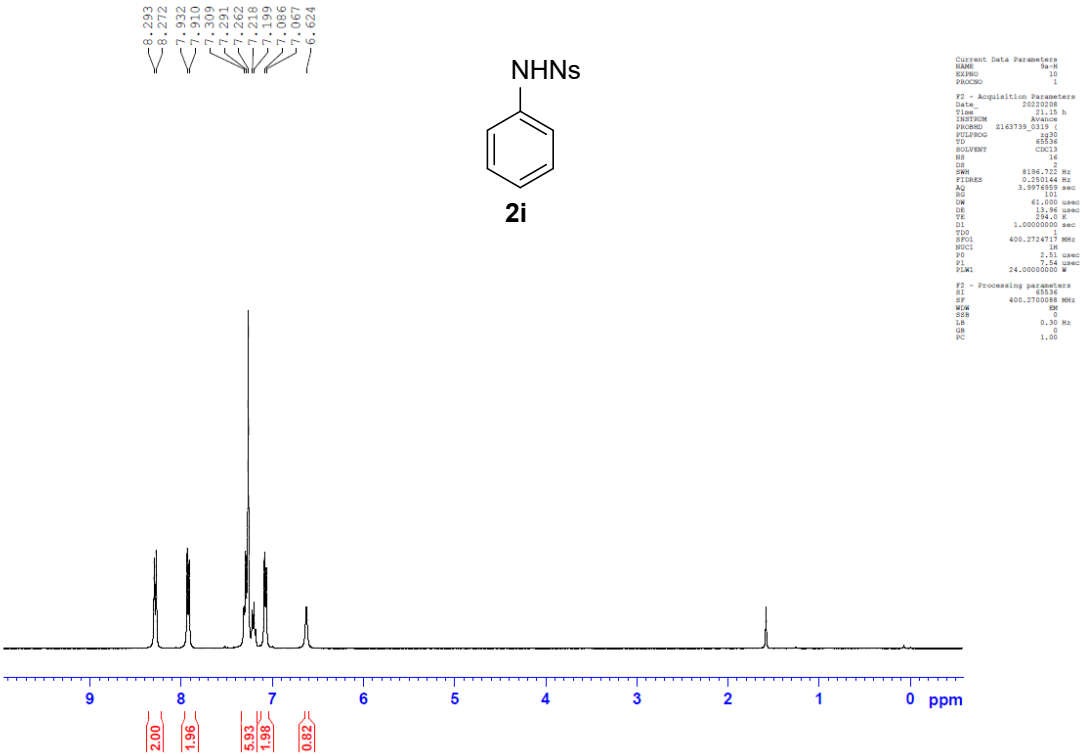

154.18
137.95
129.19
123.60
118.81
77.48
77.16
76.85
52.48
NHCO2Me
2f
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0 ppm

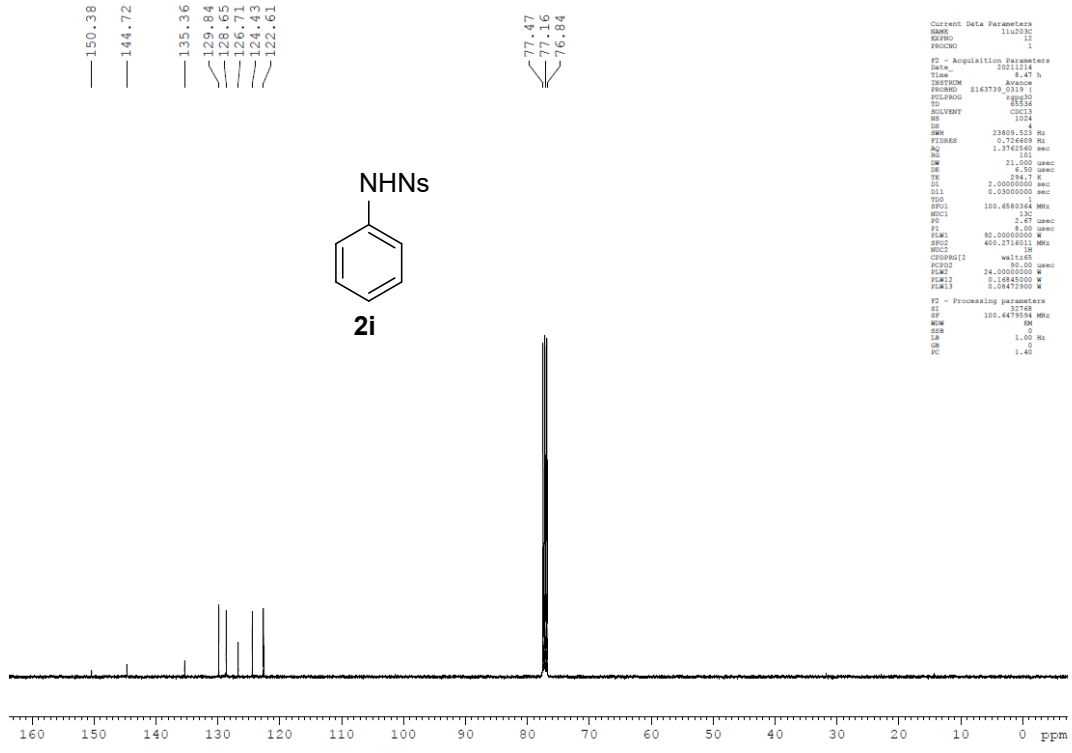

7.426
7.407
7.388
7.323
7.304
7.261
7.242
7.230
3.075
NHMs
2g
9
8
7
6
5
4
3
2
1
0
ppm
1.91
2.06
0.88
2.83

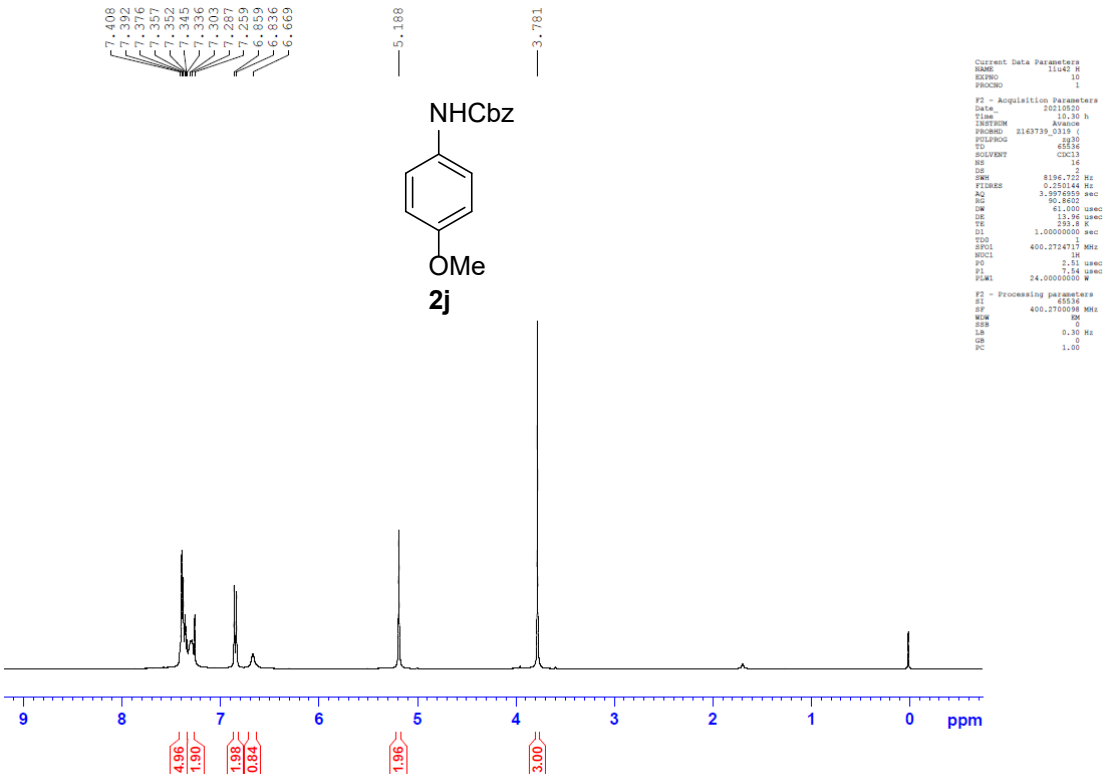

136.88
129.80
125.52
120.91
77.48
77.16
76.84
39.29
NHMs
2g
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
ppm


7.706
7.686
7.299
7.258
7.237
7.219
7.199
7.106
7.085
7.064
2.358
NHTs
2h
9
8
7
6
5
4
3
2
1
0 ppm
1.77
0.79
3.80
2.86
3.00


143.99
136.69
136.05
129.77
129.39
127.39
125.29
121.49
77.47
77.16
76.84
21.64
NHTs
2h
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0 ppm


8.293
8.272
7.932
7.910
7.309
7.291
7.262
7.218
7.199
7.086
7.067
6.624
NHNs
2i
9
8
7
6
5
4
3
2
1
0
ppm
2.00
1.96
5.93
1.98
0.82


150.38
144.72
135.36
129.84
128.65
126.71
124.43
122.61
77.47
77.16
76.84
NHNs
2i
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
ppm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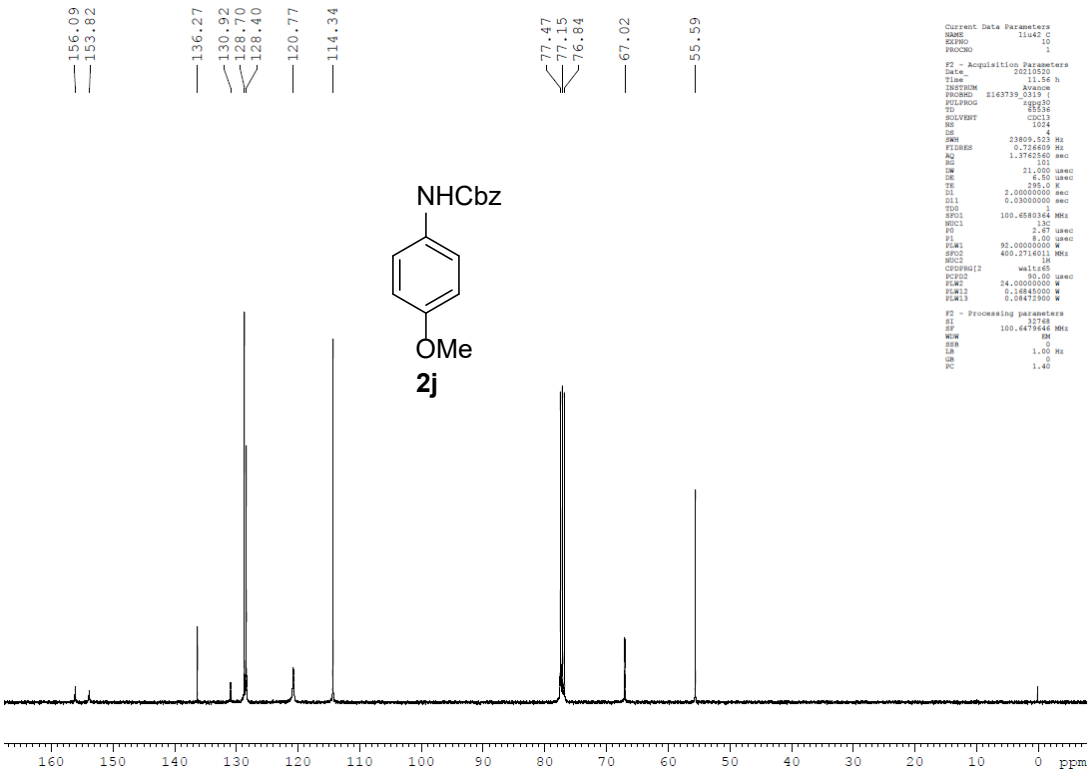
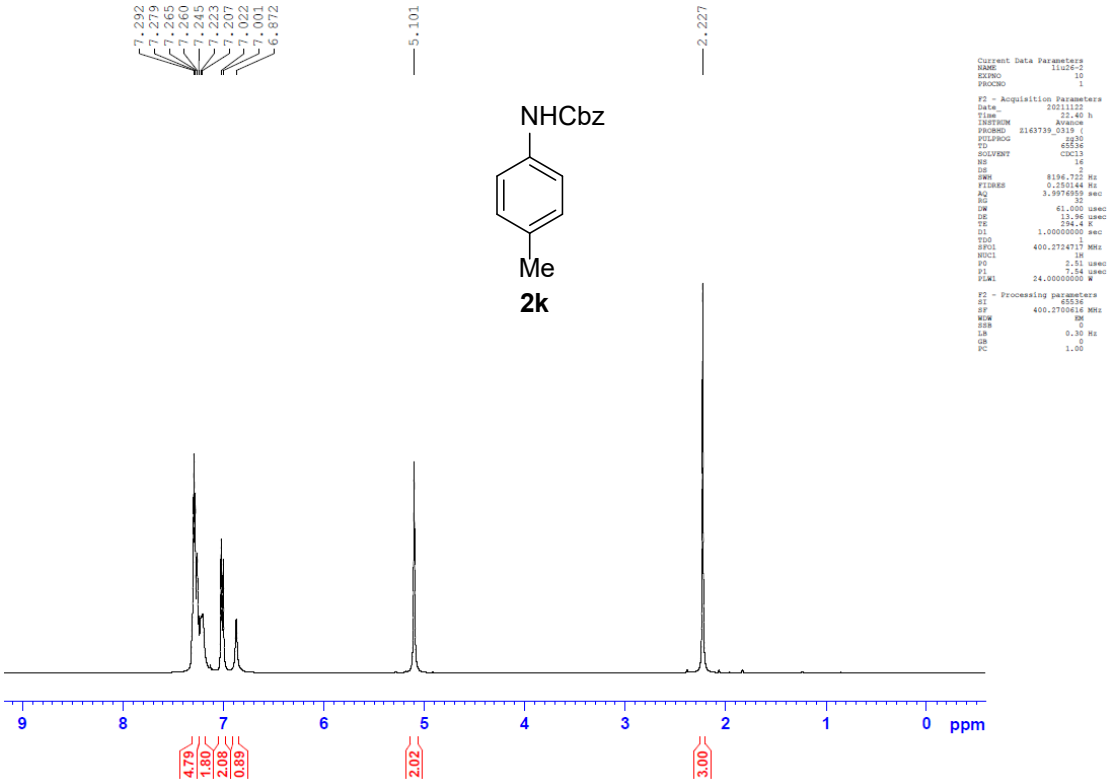
7.376
7.357
7.352
7.345
7.336
7.303
7.287
7.259
6.859
6.836
6.669
5.188
3.781
NHCbz
OMe
2j
9
8
7
6
5
4
3
2
1
0
ppm
4.96
1.90
1.98
0.84
1.96
3.00


156.09
153.82
136.27
130.92
128.70
128.40
120.77
114.34
77.47
77.15
76.84
67.02
55.59
NHCbz
OMe
2j
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
ppm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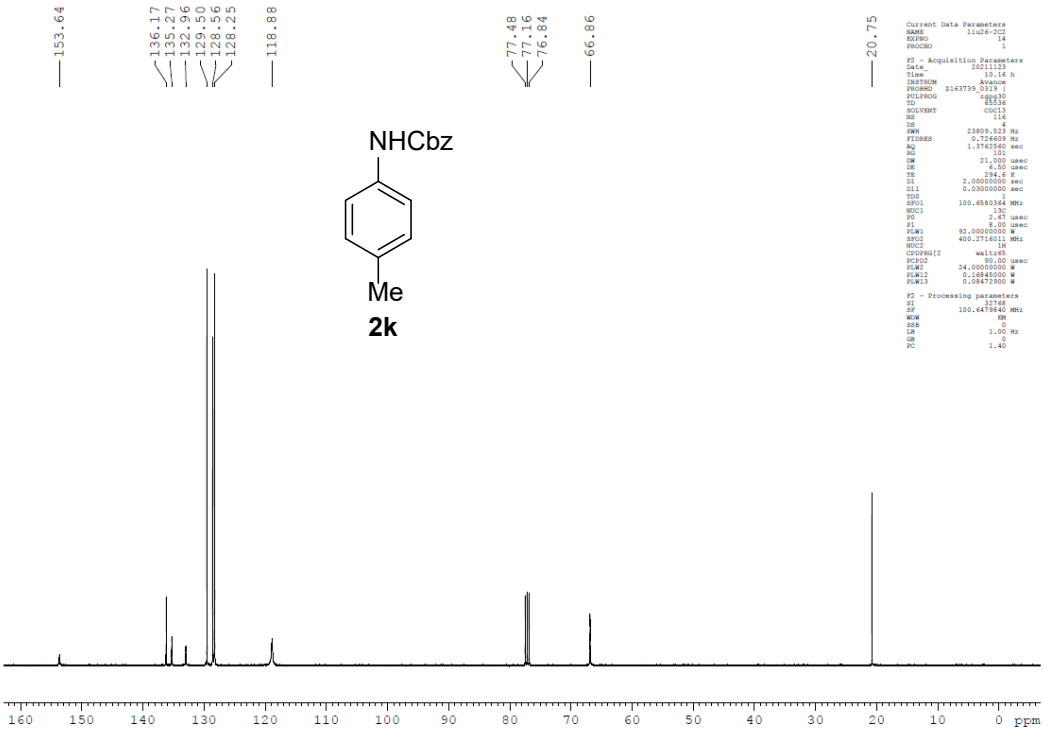
7.279
7.265
7.260
7.245
7.223
7.207
7.022
7.001
6.872
5.101
2.227
NHCbz
Me
2k
9
8
7
6
5
4
3
2
1
0
ppm
4.79
1.80
2.08
0.89
2.02
3.00


153.64
136.17
135.27
132.96
129.50
128.56
128.25
118.88
77.48
77.16
76.84
66.86
20.75
NHCbz
Me
2k
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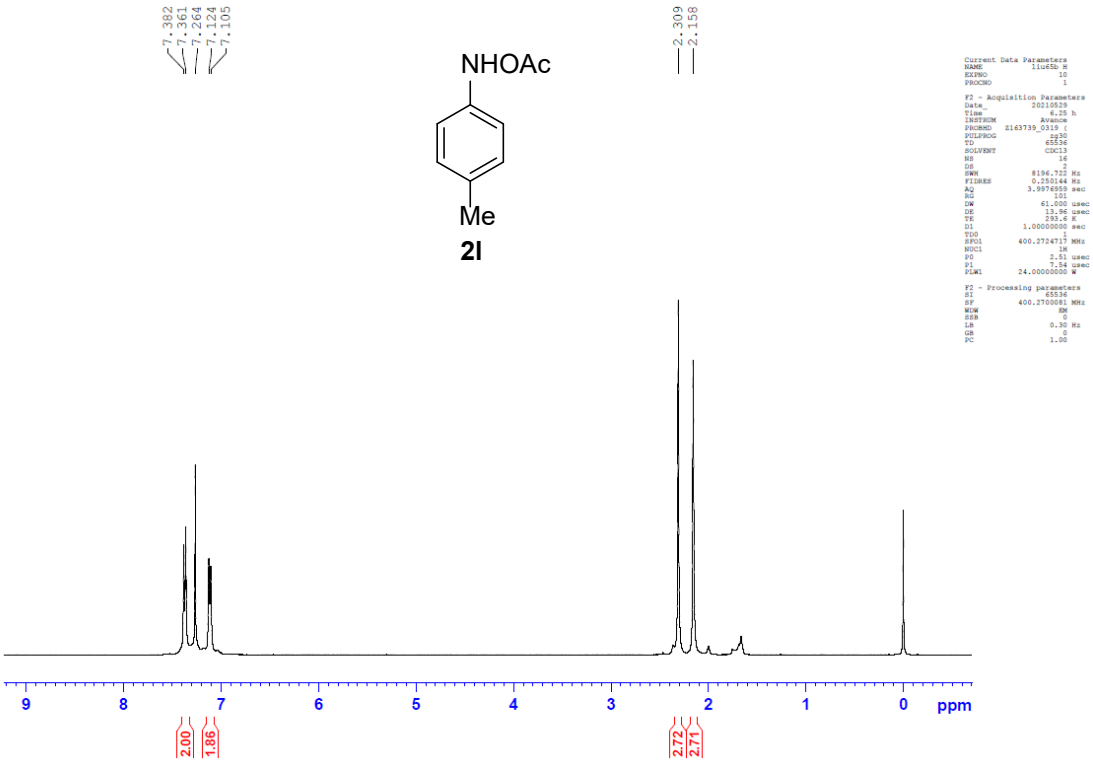
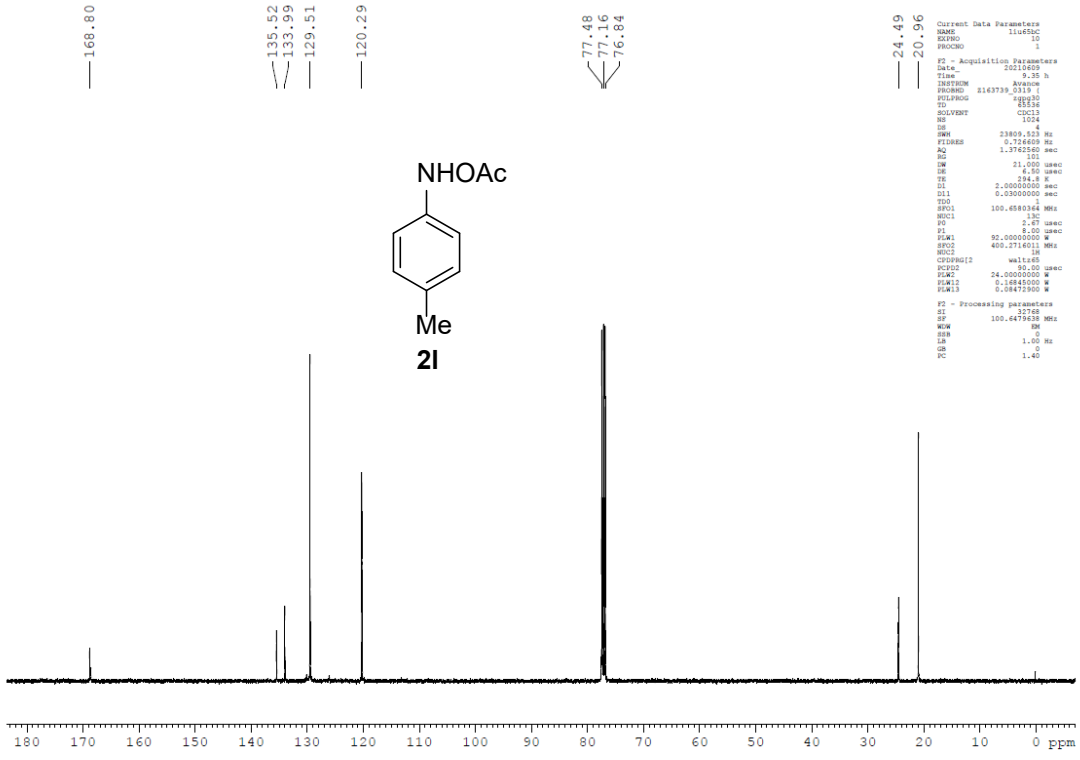
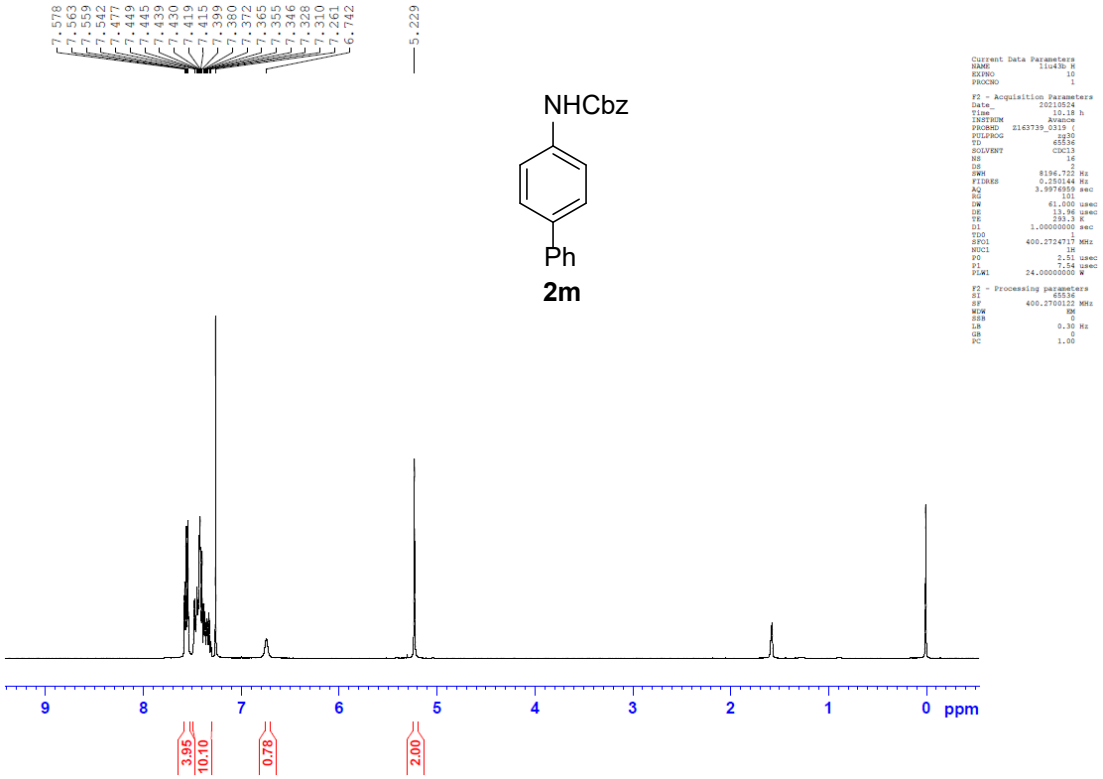
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
ppm


7.382
7.361
7.264
7.124
7.105
2.309
2.158
NHOAc
Me
2l
9
8
7
6
5
4
3
2
1
0
ppm
2.00
1.86
2.72
2.71


168.80
135.52
133.99
129.51
120.29
77.48
77.16
76.84
24.49
20.96
NHOAc
Me
2l
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0 ppm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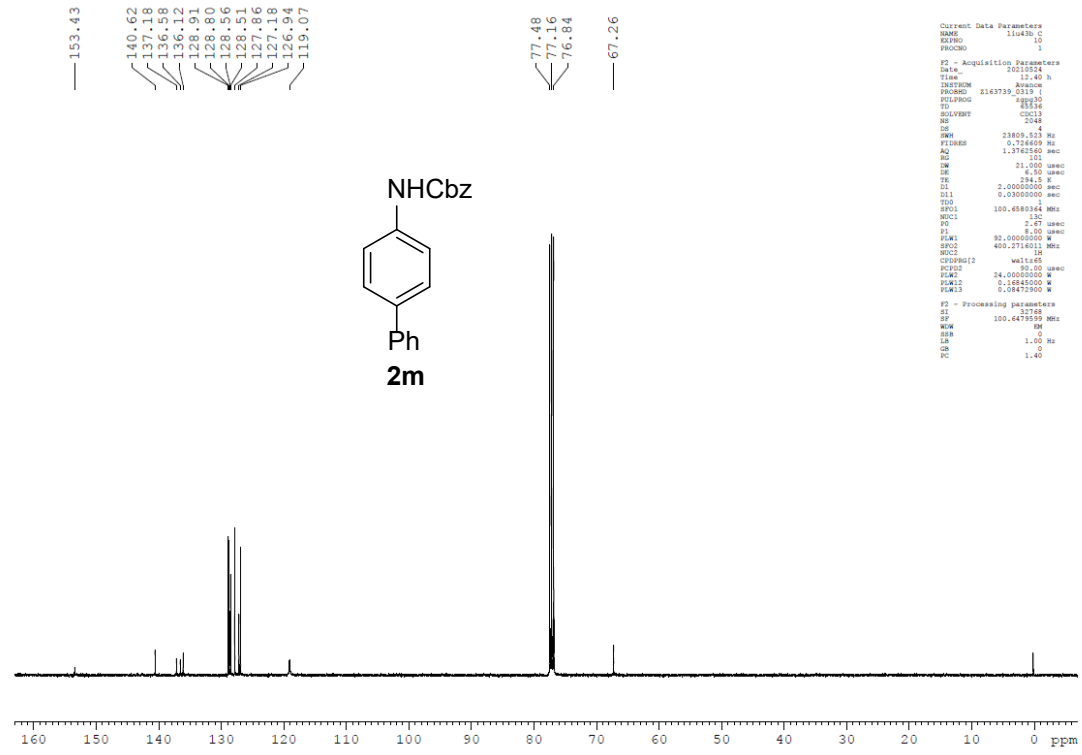
7.445
7.439
7.430
7.419
7.415
7.399
7.380
7.372
7.365
7.355
7.346
7.328
7.310
7.261
6.742
5.229
NHCbz
Ph
2m
9
8
7
6
5
4
3
2
1
0
ppm
3.95
10.10
0.78
2.00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140.62
137.18
136.58
136.12
128.91
128.80
128.56
128.51
127.86
127.18
126.94
119.07
77.48
77.16
76.84
67.26
NHCbz
Ph
2m
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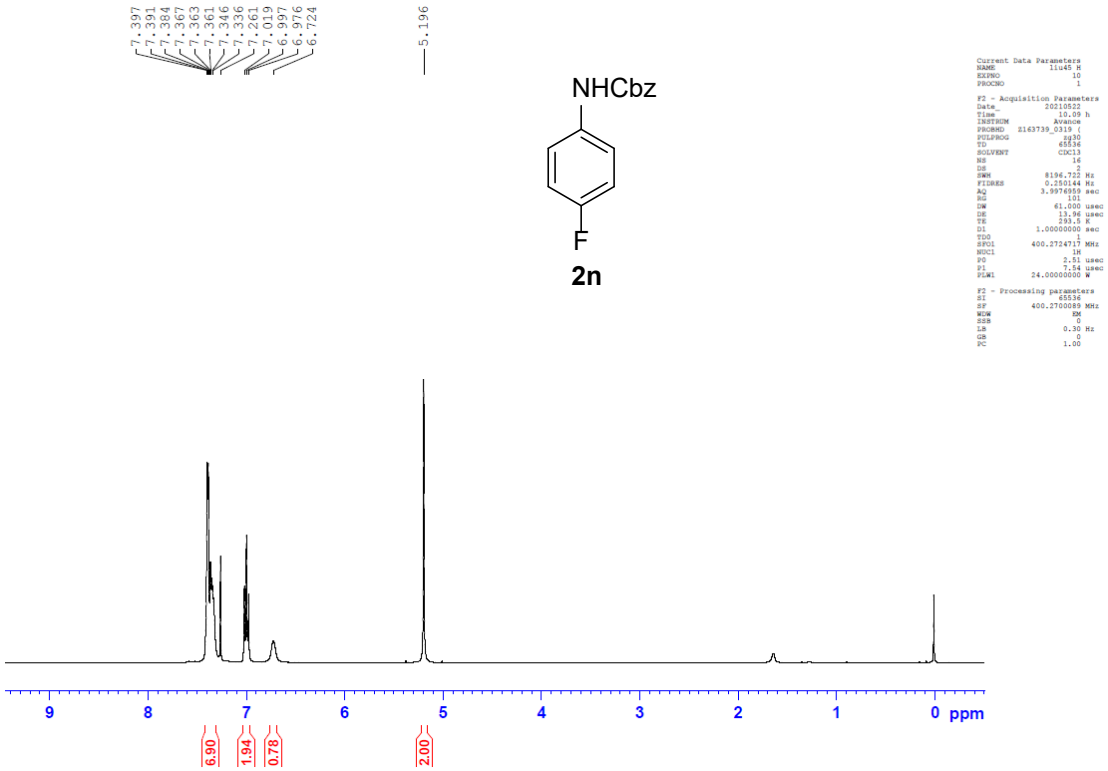
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
ppm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7.391
7.384
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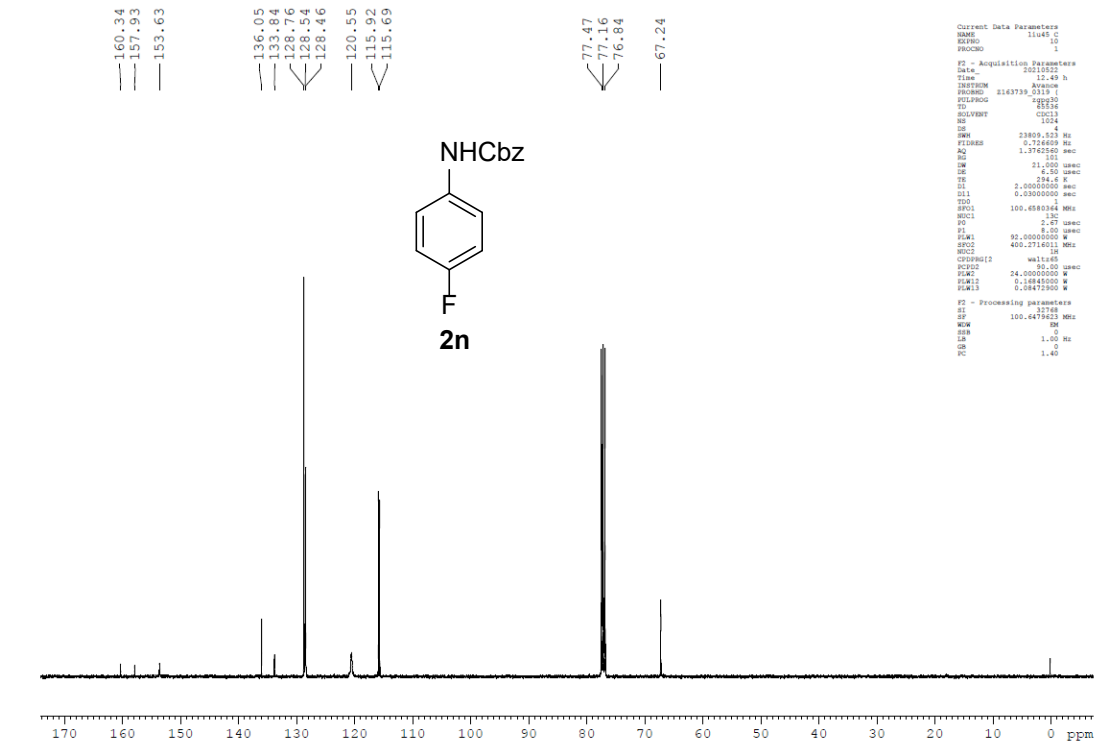
7.363
7.361
7.346
7.336
7.261
7.019
6.997
6.976
6.724
5.196
NHCbz
F
2n
9
8
7
6
5
4
3
2
1
0 ppm
6.90
1.94
0.78
2.00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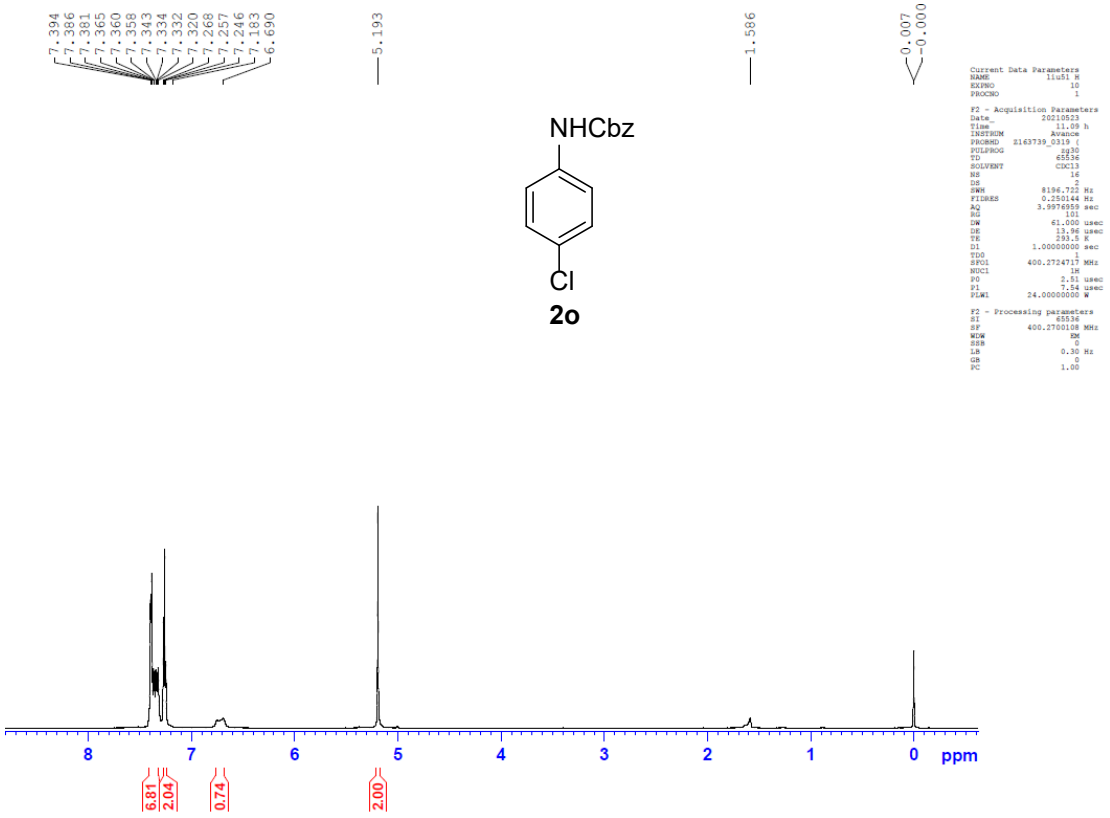
157.93
153.63
136.05
133.84
128.76
128.54
128.46
120.55
115.92
115.69
77.47
77.16
76.84
67.24
NHCbz
F
2n
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0 ppm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7.358
7.343
7.334
7.332
7.320
7.268
7.257
7.246
7.183
6.690
5.193
1.586
0.007
0.000
NHCbz
Cl
2o
8
7
6
5
4
3
2
1
0
ppm
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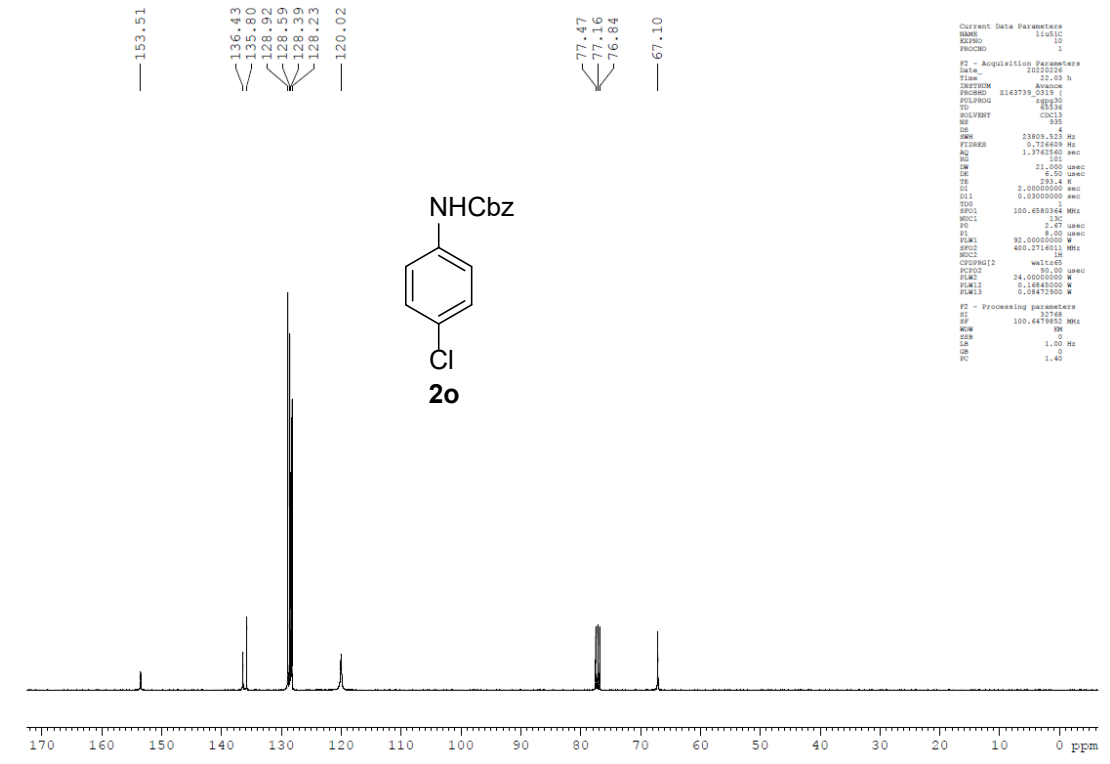
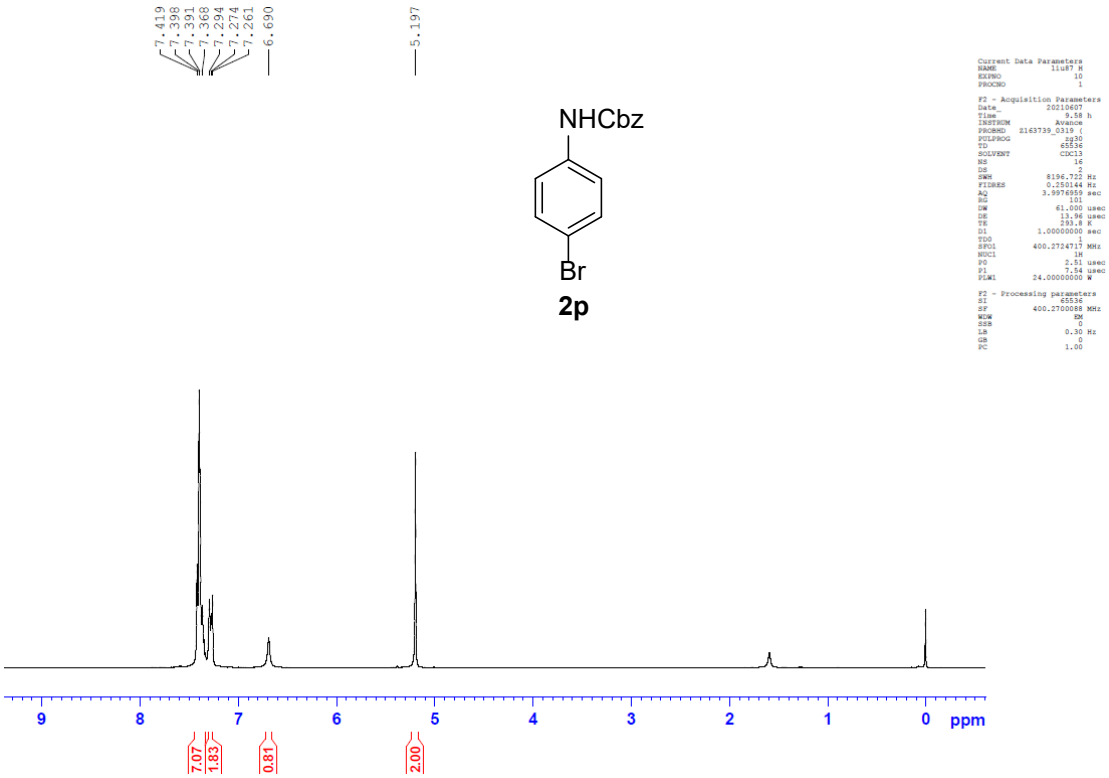
2.04
0.74
2.00


153.51
136.43
135.80
128.92
128.59
128.39
128.23
120.02
77.47
77.16
76.84
67.10
NHCbz
Cl
2o
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0 ppm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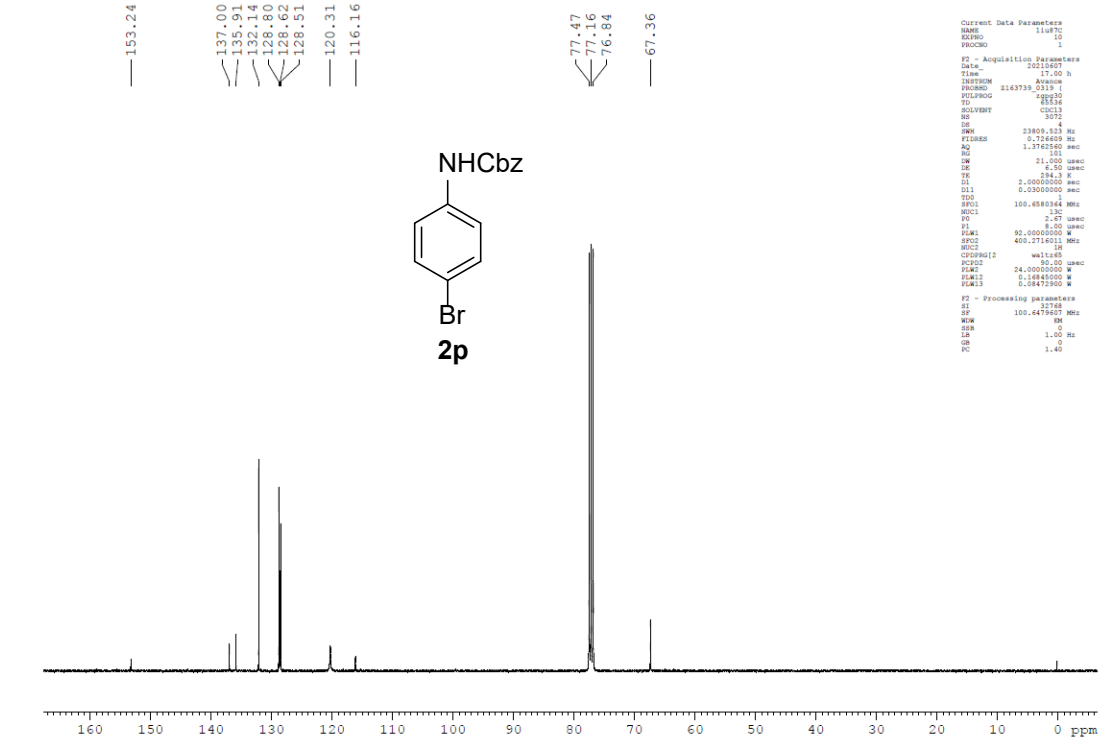
7.294
7.274
7.261
6.690
5.197
NHCbz
Br
2p
9
8
7
6
5
4
3
2
1
0
ppm
7.07
1.83
0.81
2.00


153.24
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135.91
132.14
128.80
128.62
128.51
120.31
116.16
77.47
77.16
76.84
67.36
NHCbz
Br
2p
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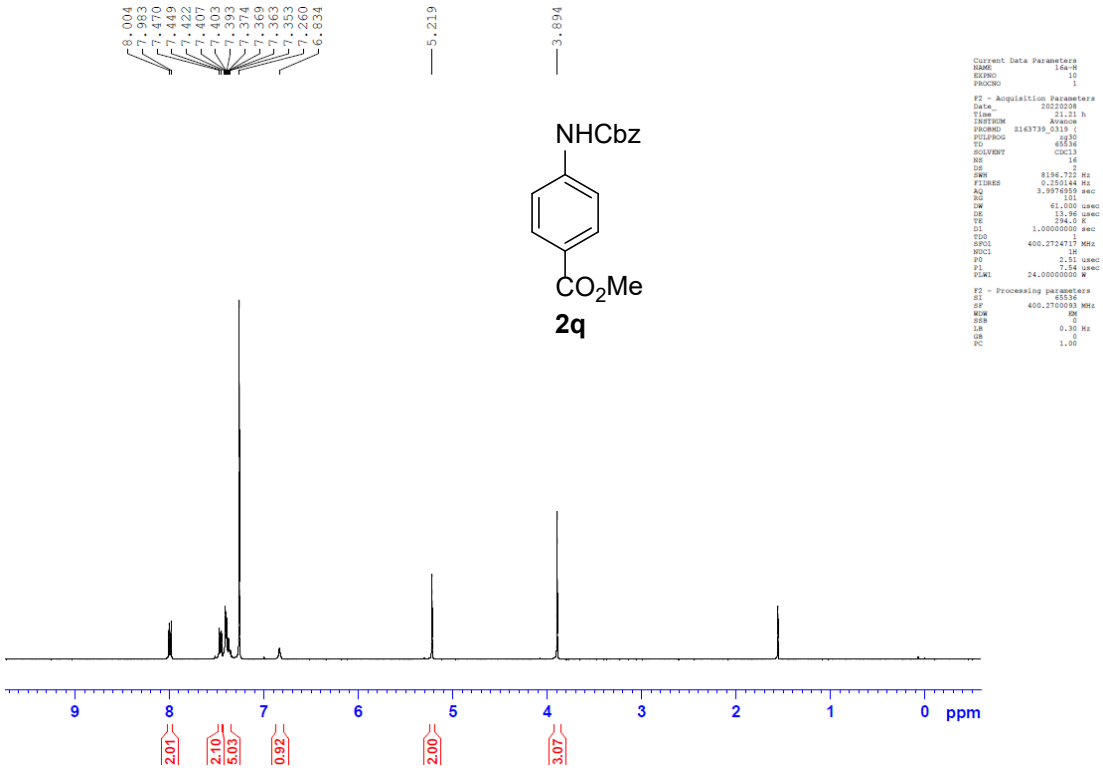
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
ppm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7.983
7.470
7.449
7.422
7.407
7.403
7.393
7.374
7.369
7.363
7.353
7.260
6.834
5.219
3.894
NHCbz
CO2Me
2q
9
8
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6
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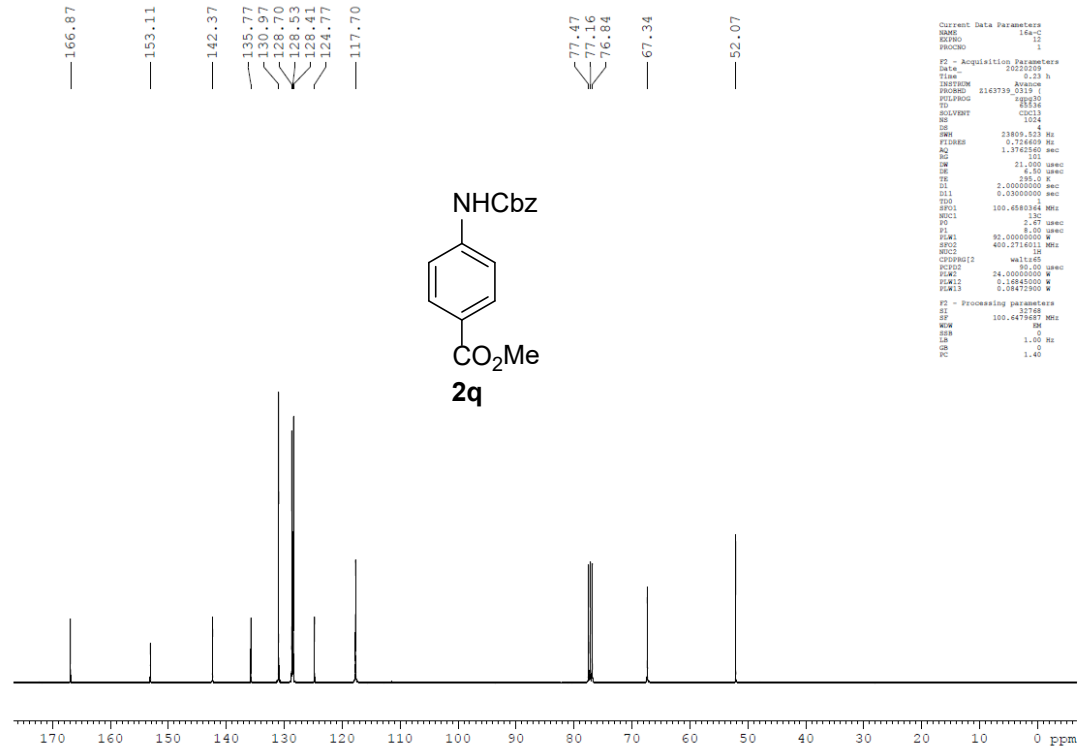
4
3
2
1
0
ppm
2.01
2.10
5.03
0.92
2.00
3.07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142.37
135.77
130.97
128.70
128.53
128.41
124.77
117.70
77.47
77.16
76.84
67.34
52.07
NHCbz
CO2Me
2q
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140
130
120
110
100
90
80
70
60
50
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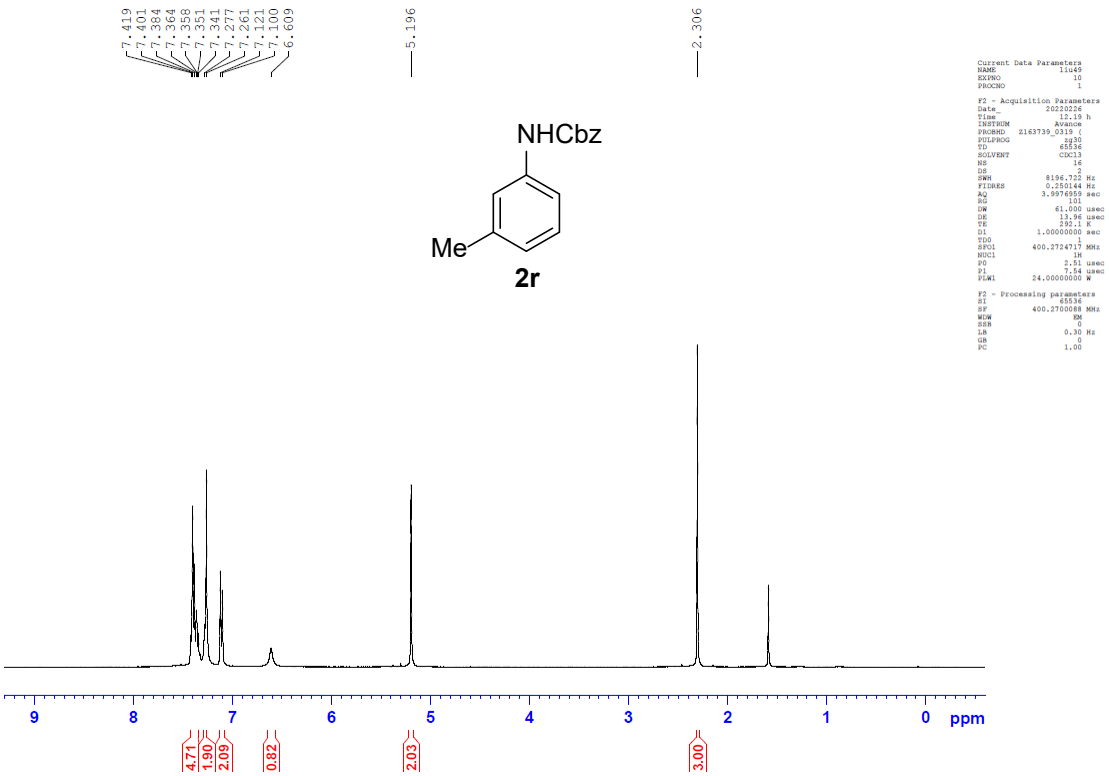
30
20
10
0
ppm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7.364
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7.351
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7.277
7.261
7.121
7.100
6.609
5.196
2.306
NHCbz
Me
2r
9
8
7
6
5
4
3
2
1
0
ppm
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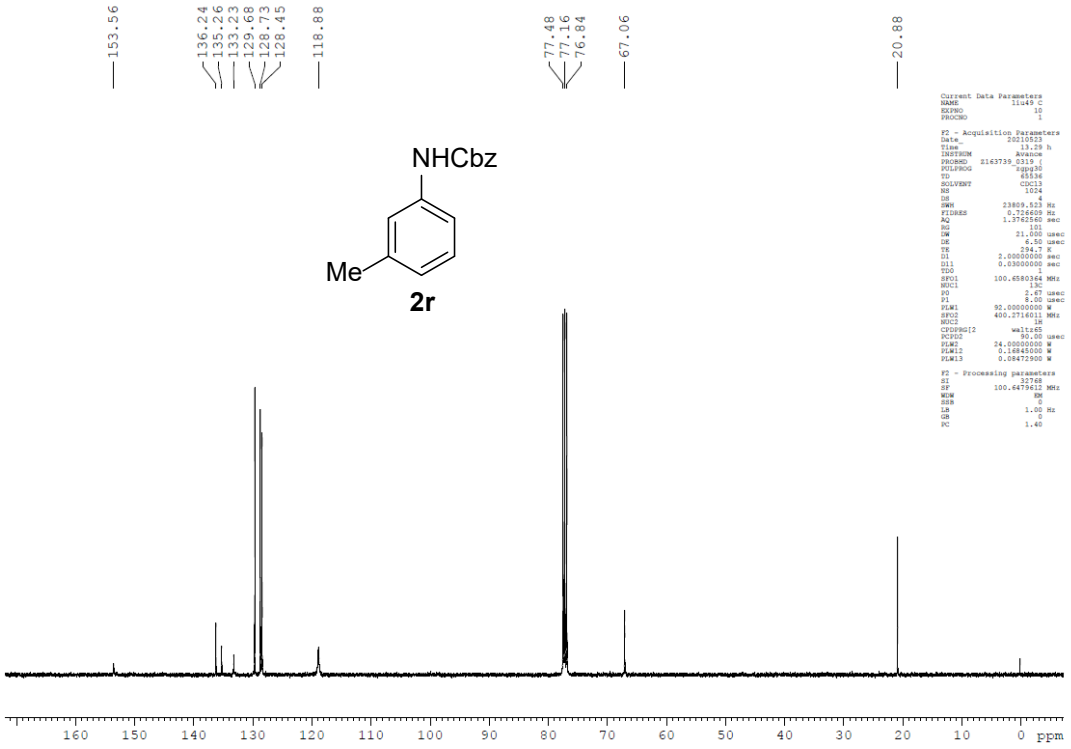
1.90
2.09
0.82
2.03
3.00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136.24
135.26
133.23
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128.73
128.45
118.88
77.48
77.16
76.84
67.06
20.88
NHCbz
Me
2r
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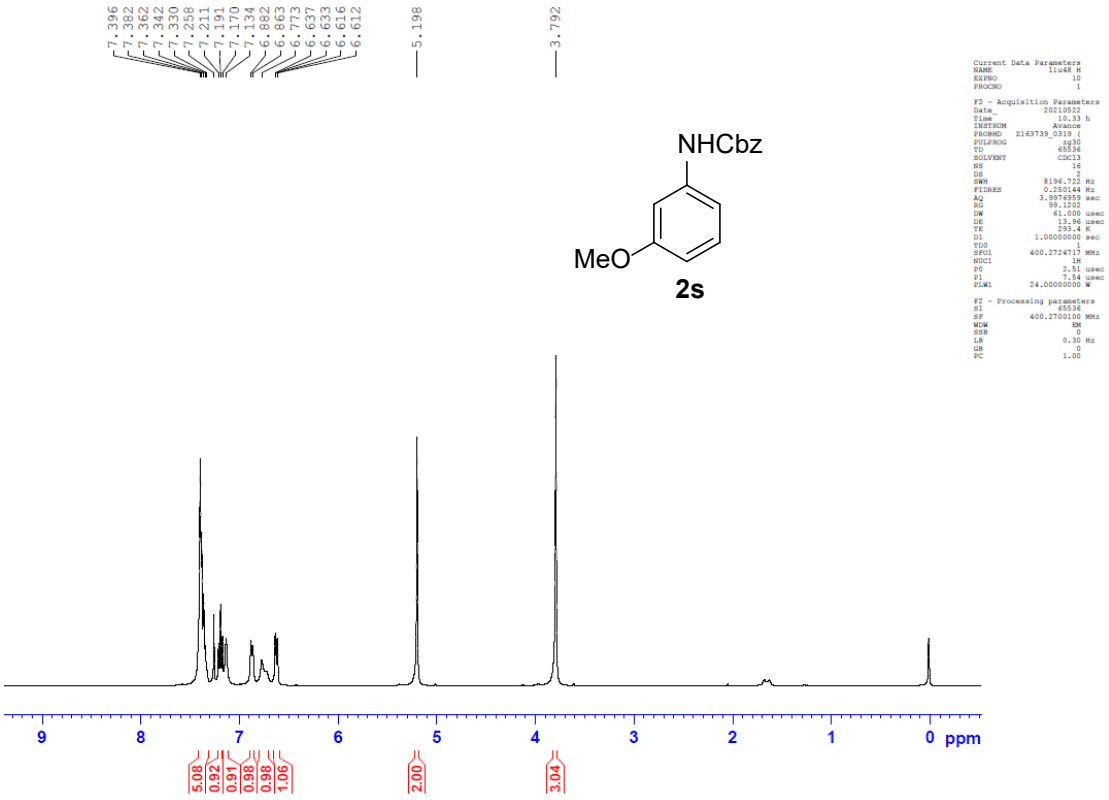
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
ppm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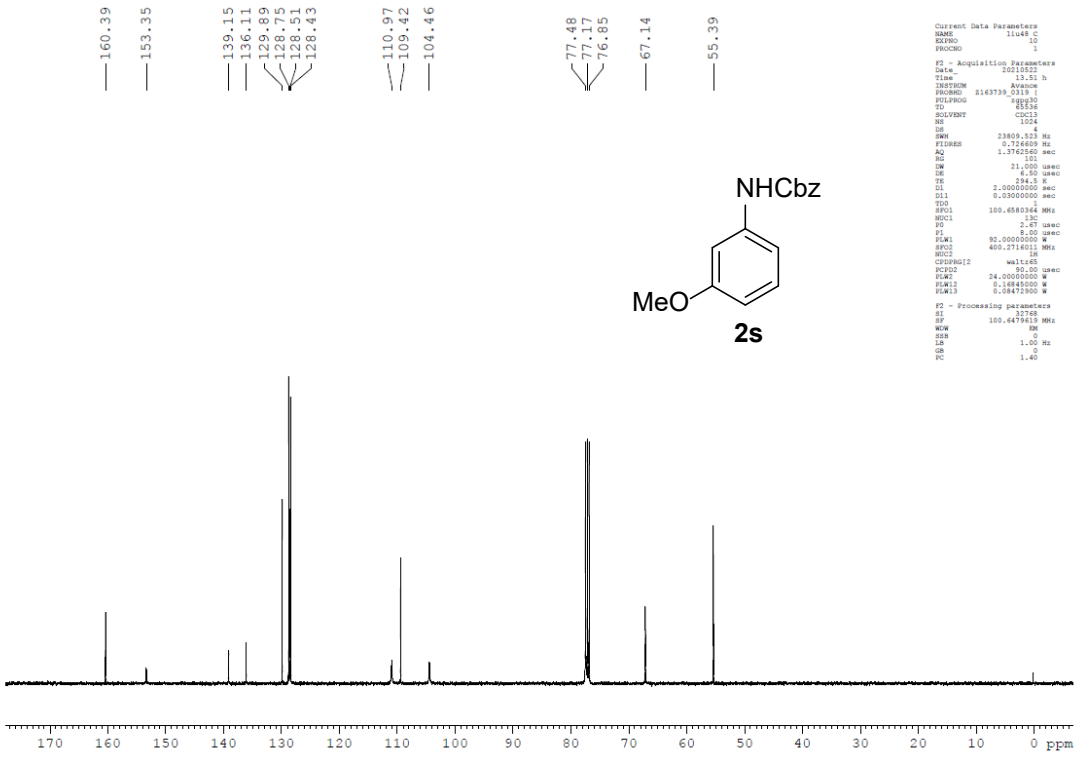
7.382
7.362
7.342
7.330
7.258
7.211
7.191
7.170
7.134
6.882
6.863
6.773
6.637
6.633
6.616
6.612
5.198
3.792
NHCbz
MeO
2s
9
8
7
6
5
4
3
2
1
0 ppm
5.08
0.92
0.91
0.98
0.98
1.06
2.00
3.04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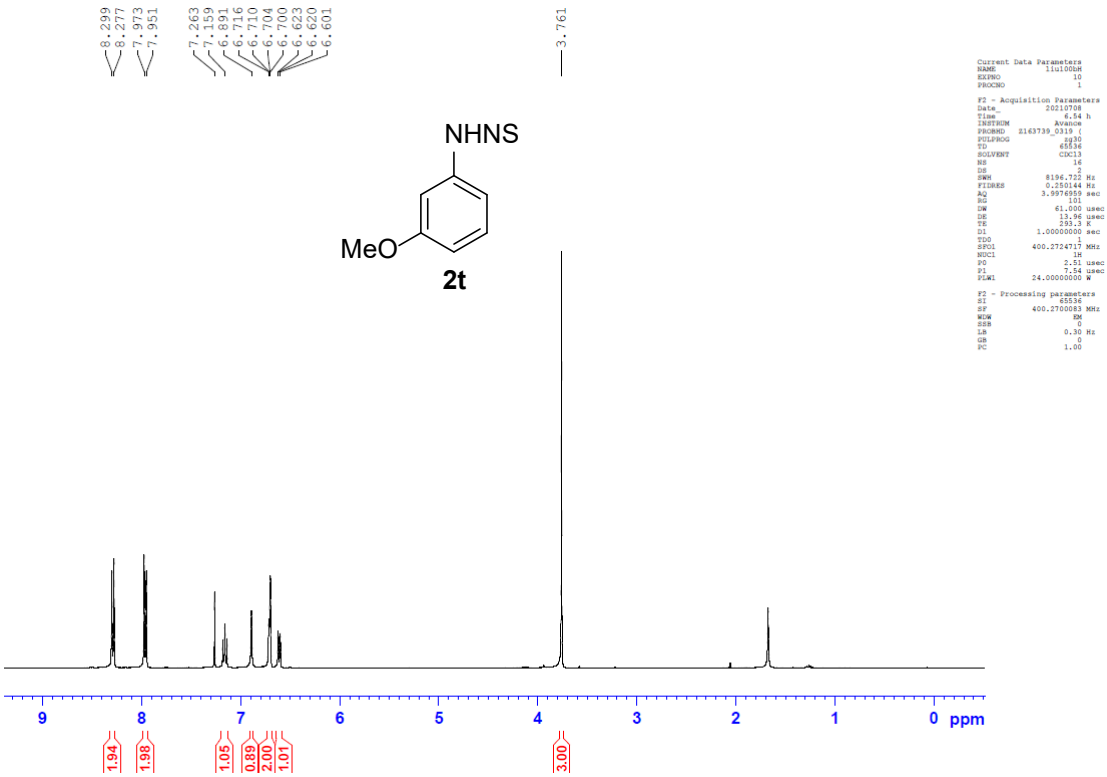
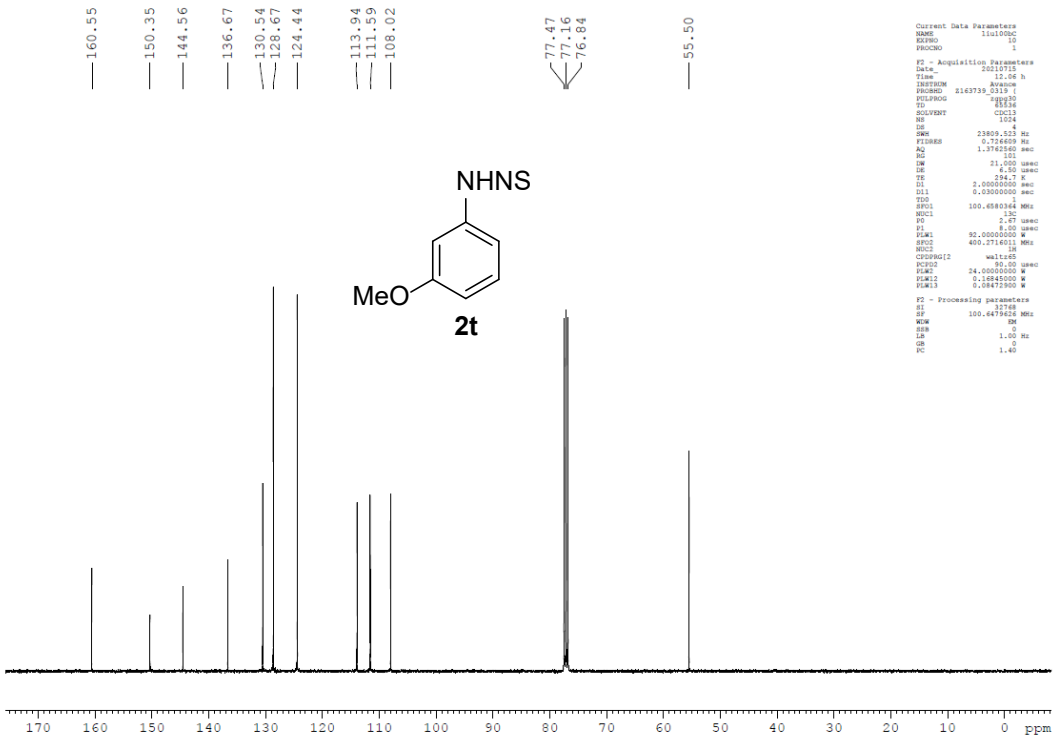
153.35
139.15
136.11
129.89
128.75
128.51
128.43
110.97
109.42
104.46
77.48
77.17
76.85
67.14
55.39
NHCbz
MeO
2s
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0 ppm


8.299
8.277
7.973
7.951
7.263
7.159
6.891
6.716
6.710
6.704
6.700
6.623
6.620
6.601
3.761
NHNS
MeO
2t
9
8
7
6
5
4
3
2
1
0 ppm
1.94
1.98
1.05
0.89
2.00
1.01
3.00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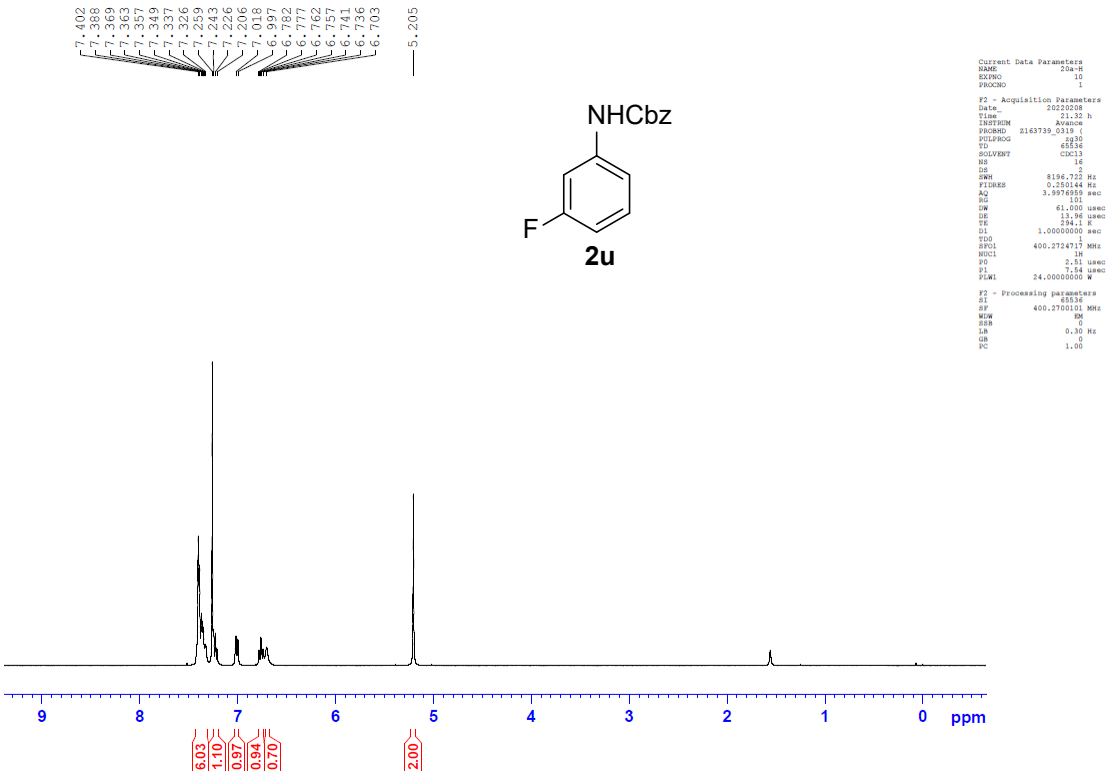
150.35
144.56
136.67
130.54
128.67
124.44
113.94
111.59
108.02
77.47
77.16
76.84
55.50
NHNS
MeO
2t
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0 ppm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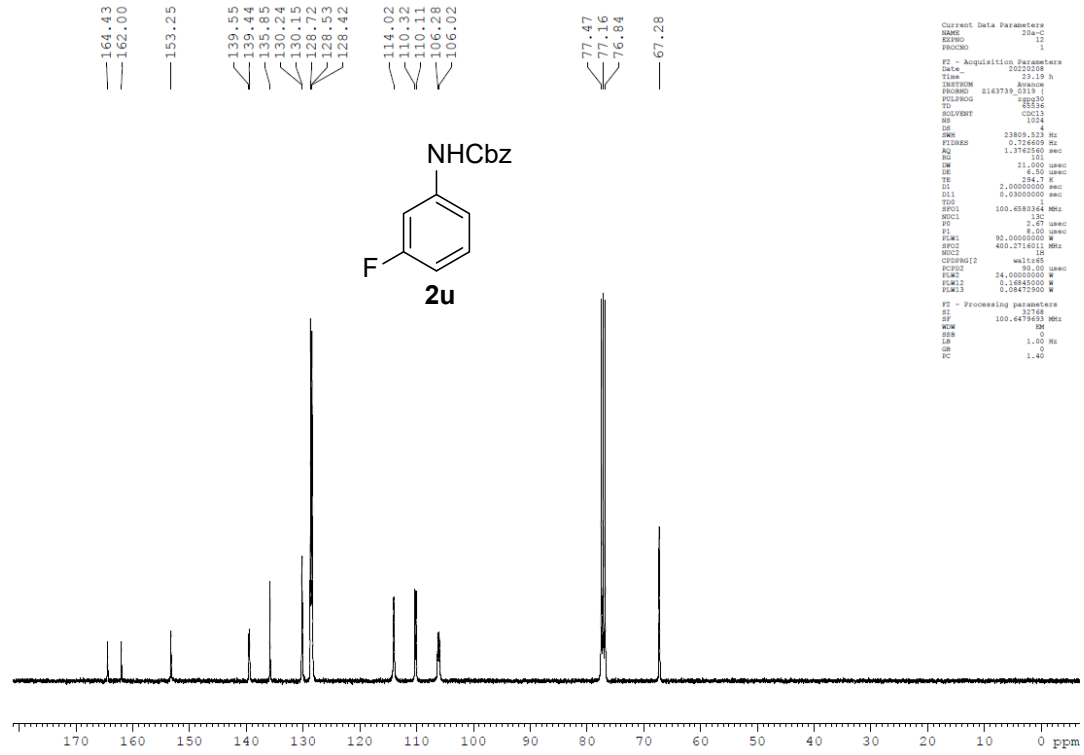
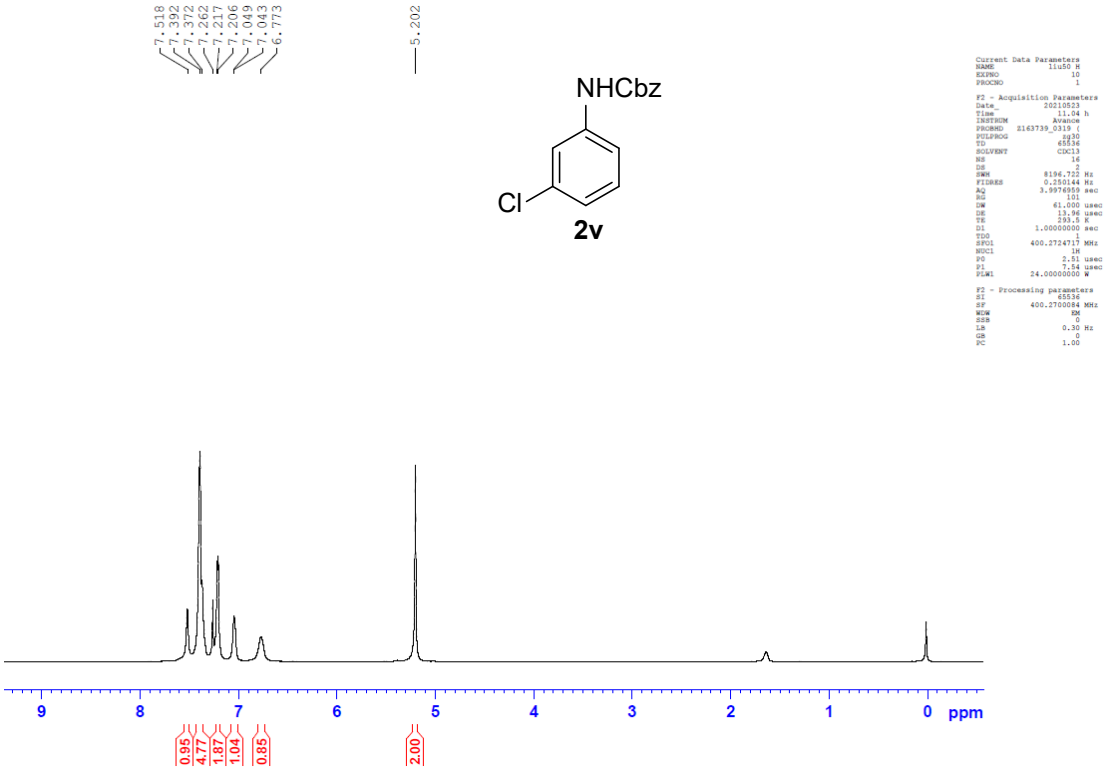
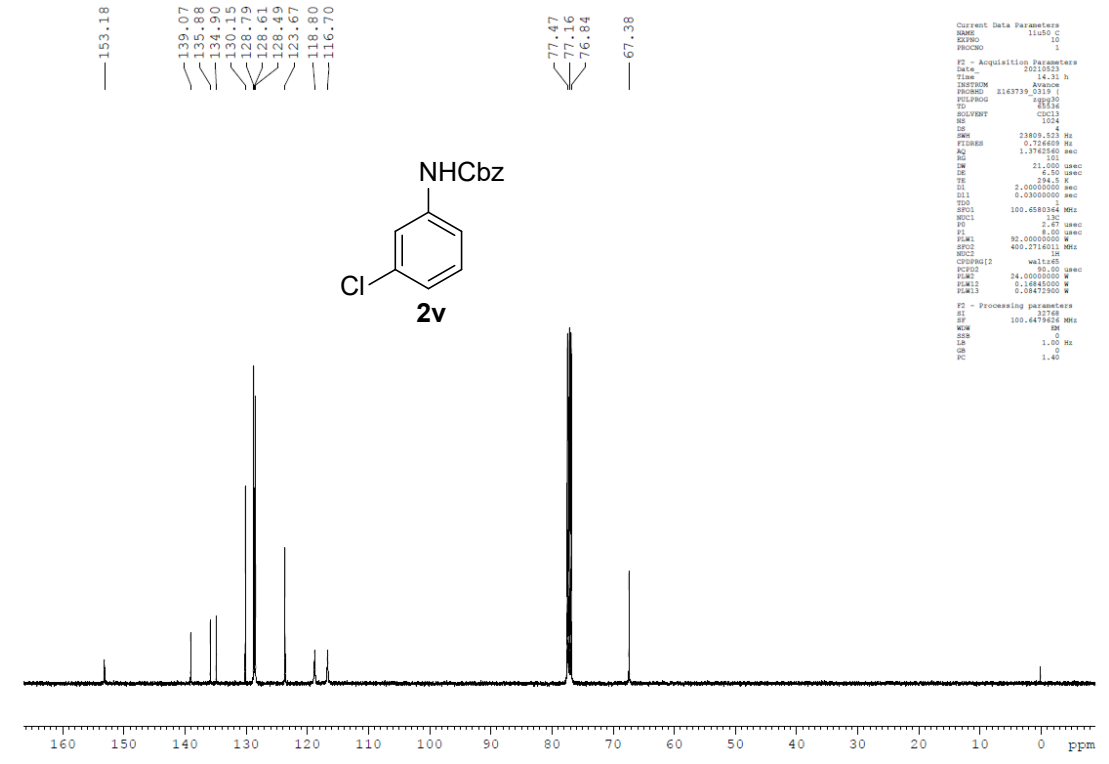
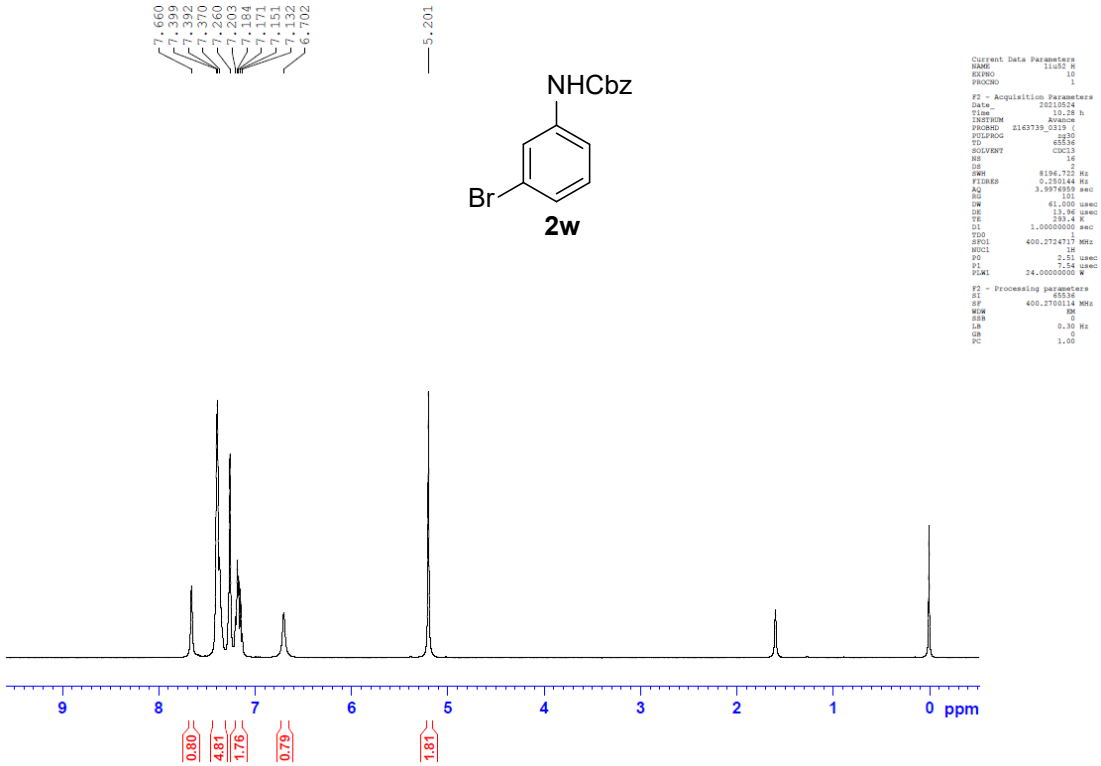
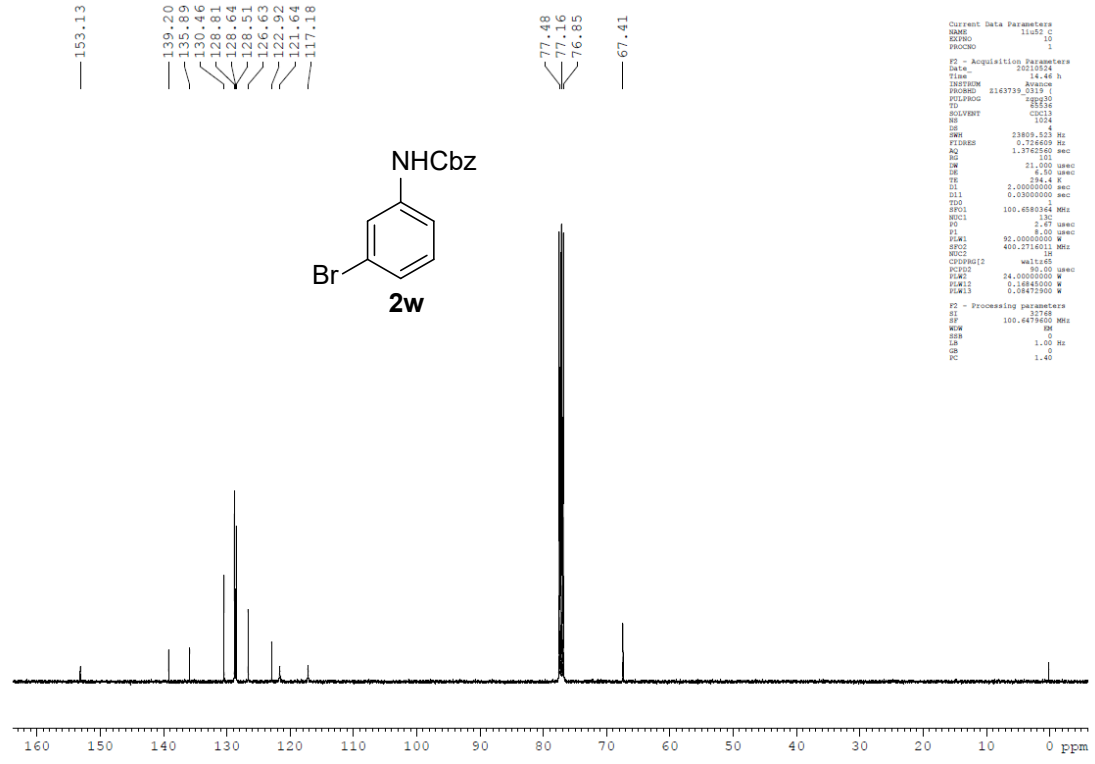
7.388
7.369
7.363
7.357
7.349
7.337
7.326
7.259
7.243
7.226
7.206
7.018
6.997
6.782
6.777
6.762
6.757
6.741
6.736
6.703
5.205
NHCbz
F
2u
9
8
7
6
5
4
3
2
1
0
ppm
6.03
1.10
0.97
0.94
0.70
2.00

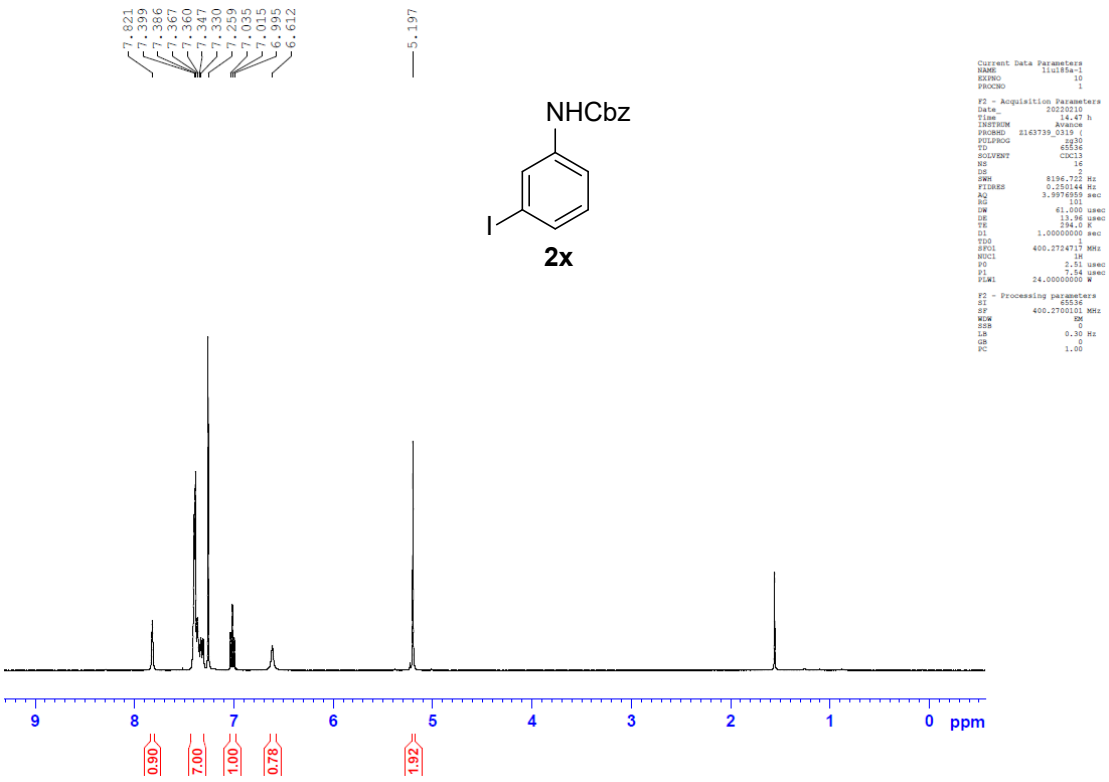

164.43
162.00
153.25
139.55
139.44
135.85
130.24
130.15
128.72
128.53
128.42
114.02
110.32
110.11
106.28
106.02
77.47
77.16
76.84
67.28
NHCbz
F
2u
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0 ppm


7.518
7.392
7.372
7.262
7.217
7.206
7.049
7.043
6.773
5.202
NHCbz
Cl
2v
9
8
7
6
5
4
3
2
1
0
ppm
0.95
4.77
1.87
1.04
0.85
2.00


153.18
139.07
135.88
134.90
130.15
128.79
128.61
128.49
123.67
118.80
116.70
77.47
77.16
76.84
67.38
NHCbz
Cl
2v
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
ppm


7.660
7.399
7.392
7.370
7.260
7.203
7.184
7.171
7.151
7.132
6.702
5.201
NHCbz
Br
2w
9
8
7
6
5
4
3
2
1
0 ppm
0.80
4.81
1.76
0.79
1.81


153.13
139.20
135.89
130.46
128.81
128.64
128.51
126.63
122.92
121.64
117.18
77.48
77.16
76.85
67.41
NHCbz
Br
2w
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0 ppm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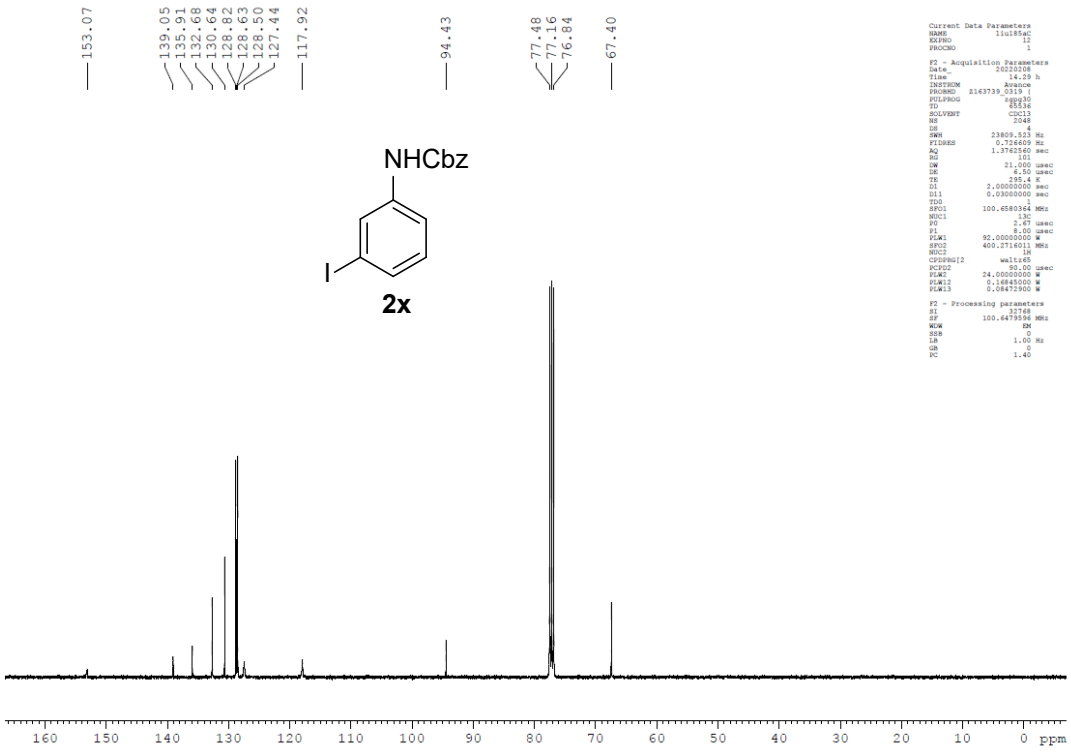
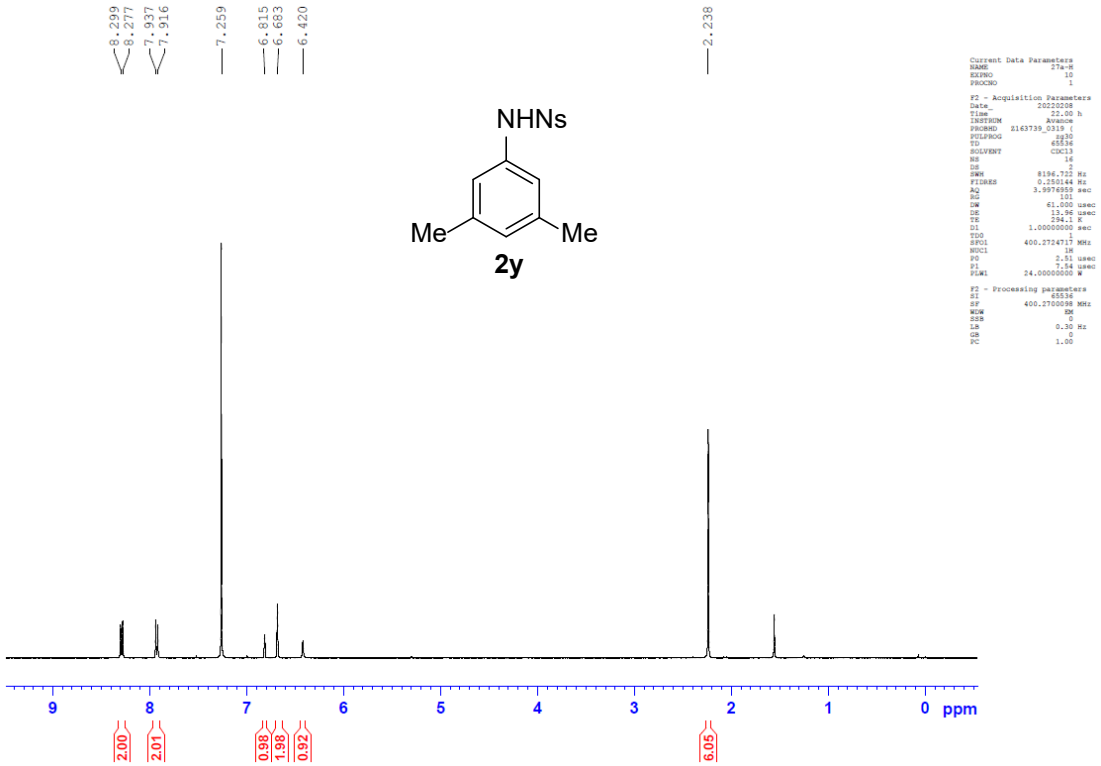
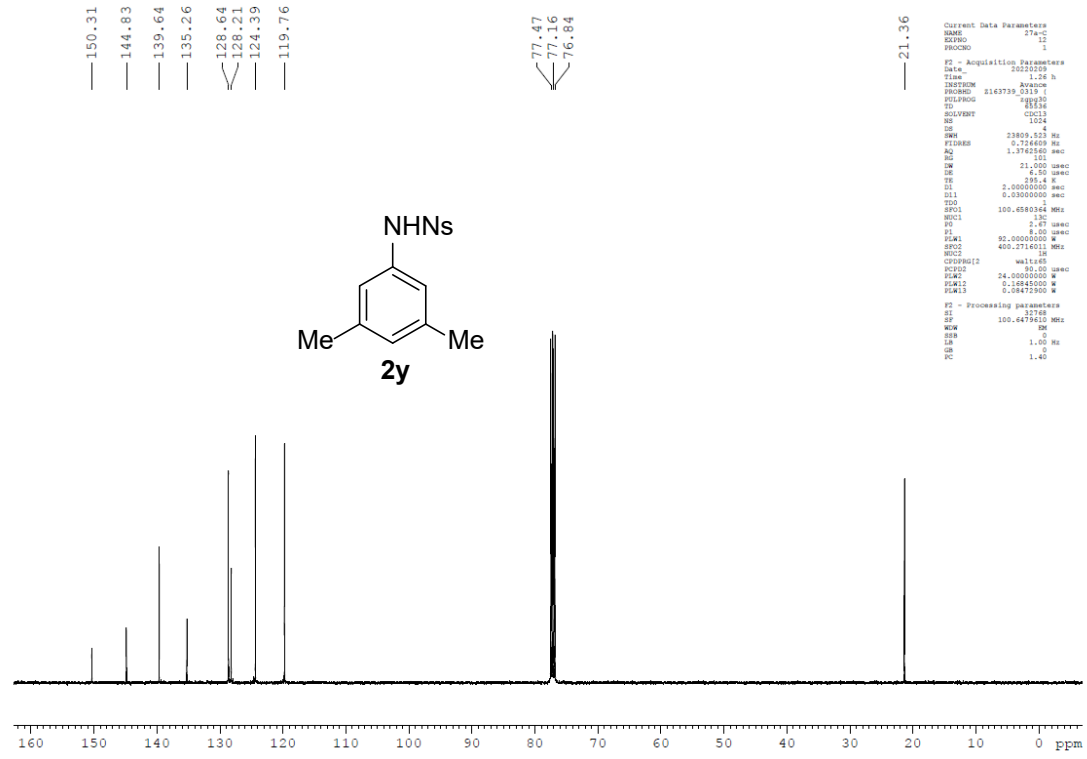
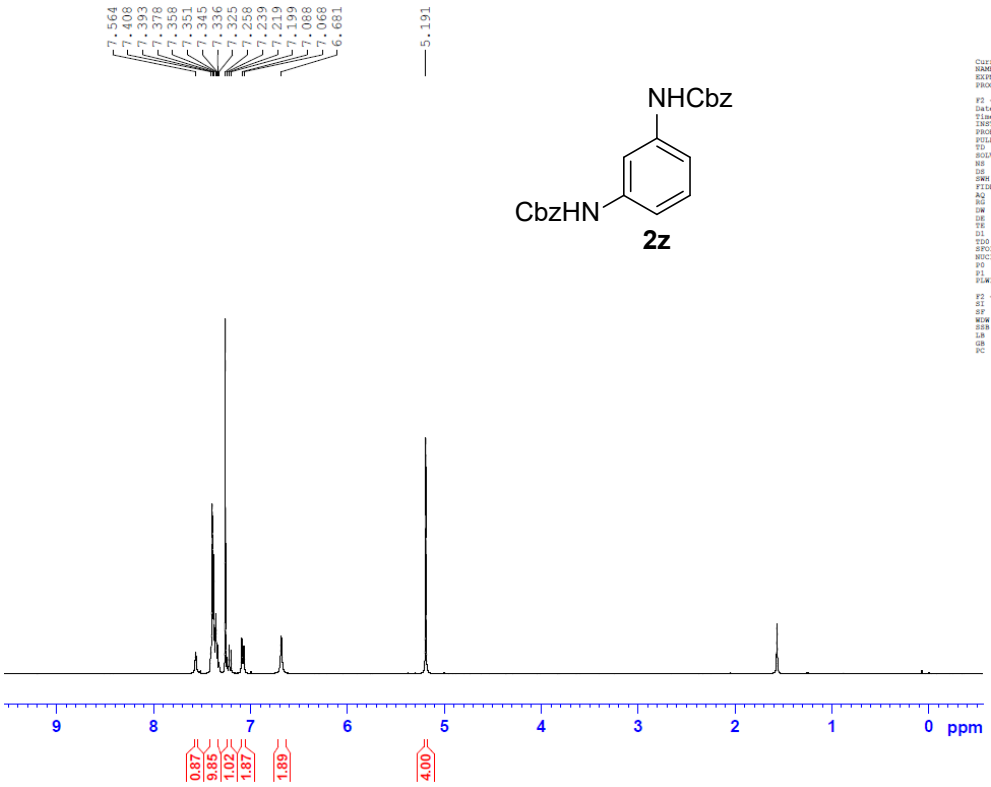
7.399
7.386
7.367
7.360
7.347
7.330
7.259
7.035
7.015
6.995
6.612
5.197
NHCbz
I
2x
9
8
7
6
5
4
3
2
1
0
ppm
0.90
7.00
1.00
0.78
1.92


153.07
139.05
135.91
132.68
130.64
128.82
128.63
128.50
127.44
117.92
94.43
77.48
77.16
76.84
67.40
NHCbz
I
2x
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
ppm


8.299
8.277
7.937
7.916
7.259
6.815
6.683
6.420
2.238
NHNs
Me
Me
2y
9
8
7
6
5
4
3
2
1
0
ppm
2.00
2.01
0.98
1.98
0.92
6.05


150.31
144.83
139.64
135.26
128.64
128.21
124.39
119.76
77.47
77.16
76.84
21.36
NHNs
Me
Me
2y
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
ppm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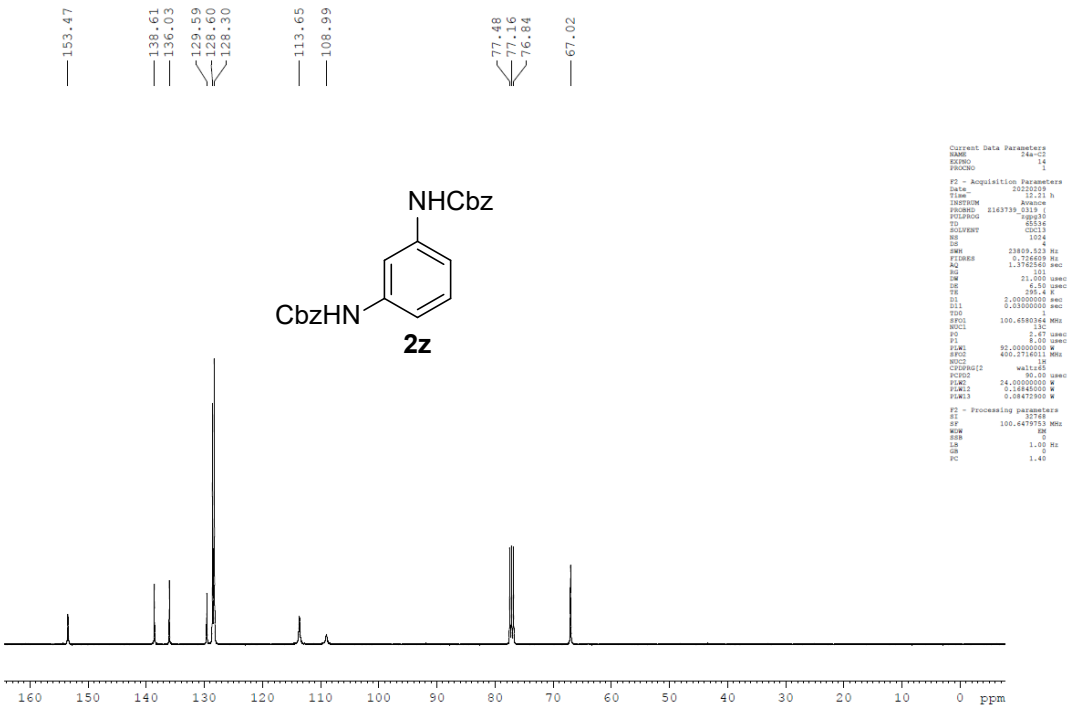
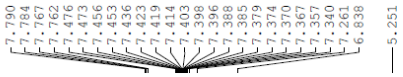
7.408
7.393
7.378
7.358
7.351
7.345
7.336
7.325
7.258
7.239
7.219
7.199
7.088
7.068
6.681
5.191
NHCbz
CbzHN
2z
9
8
7
6
5
4
3
2
1
0
ppm
0.87
9.85
1.02
1.87
1.89
4.00


153.47
138.61
136.03
129.59
128.60
128.30
113.65
108.99
77.48
77.16
76.84
67.02
NHCbz
CbzHN
2z
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
ppm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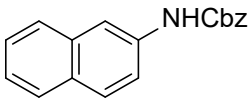
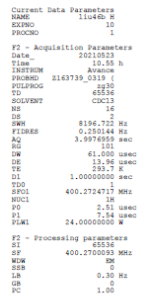
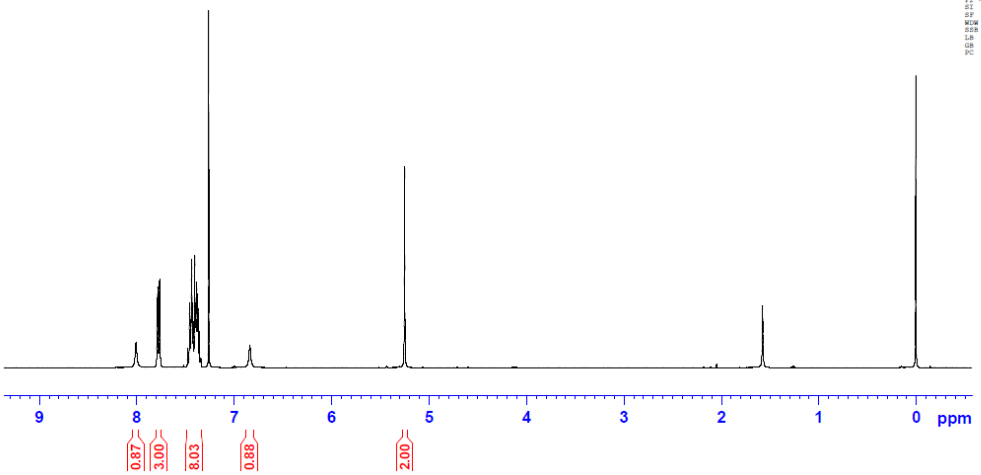
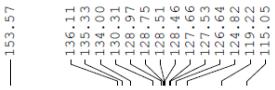
7.784
7.767
7.762
7.476
7.473
7.456
7.453
7.436
7.423
7.419
7.414
7.403
7.398
7.396
7.388
7.385
7.379
7.374
7.370
7.367
7.357
7.340
7.261
6.838
5.251


NHCbz

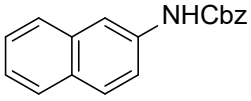
**2aa**



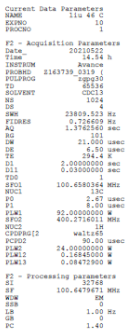

9
8
7
6
5
4
3
2
1
0
ppm
0.87
3.00
8.03
0.88
2.00

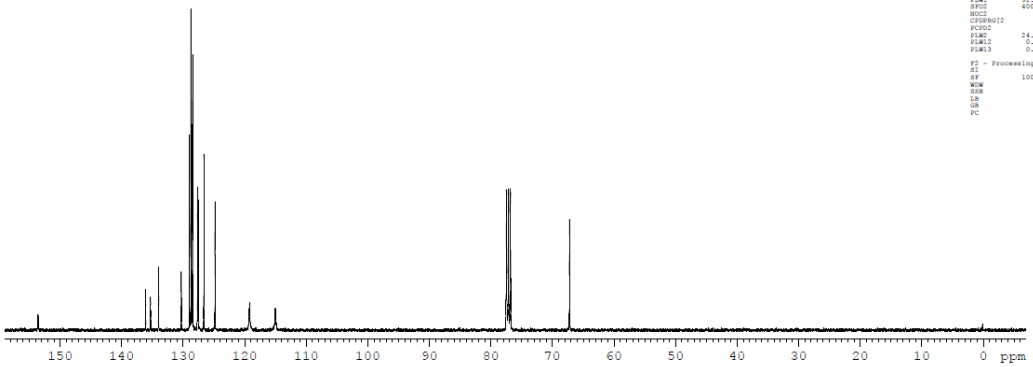

153.57
136.11
135.33
134.00
130.31
128.97
128.75
128.51
128.46
127.66
127.53
126.64
124.82
119.22
115.05

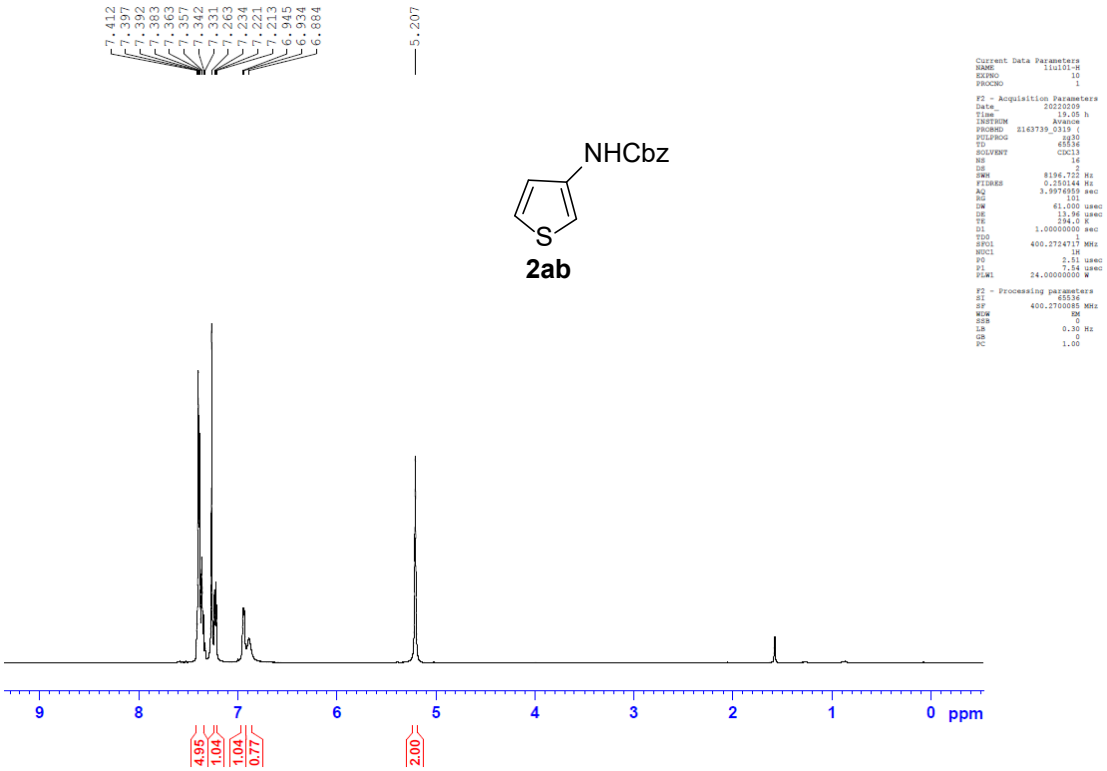

77.48
77.16
76.84
67.22

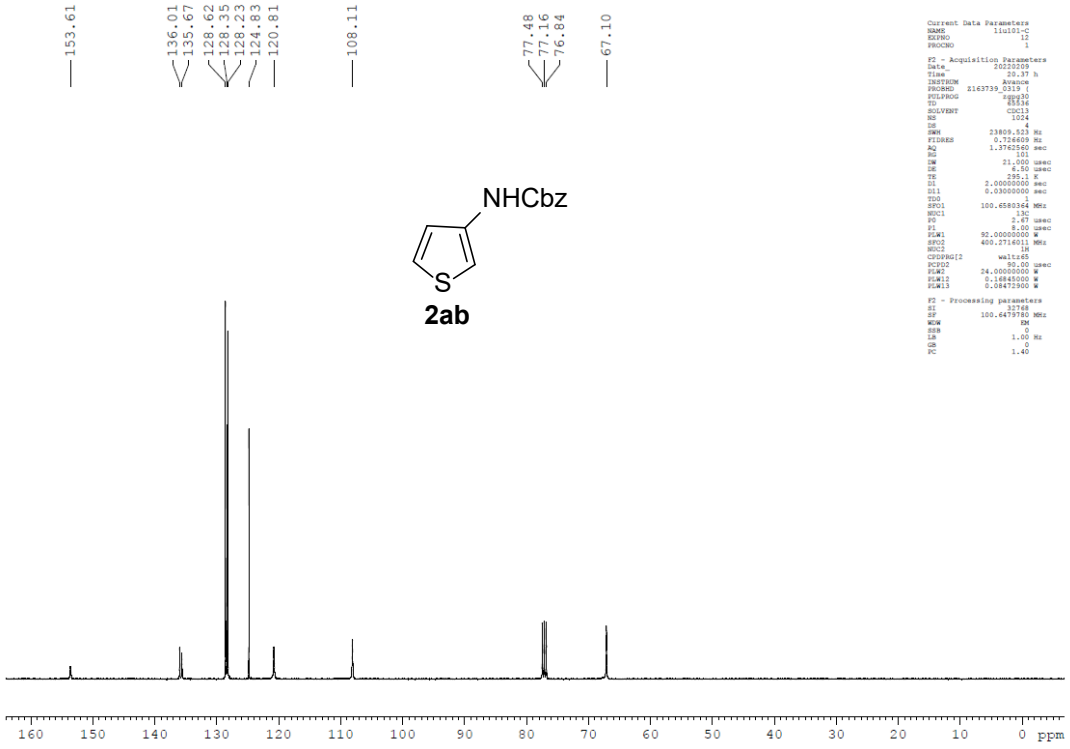

NHCbz

**2aa**

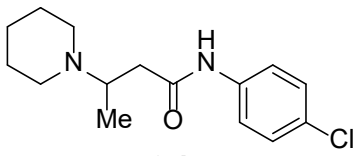



150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
ppm

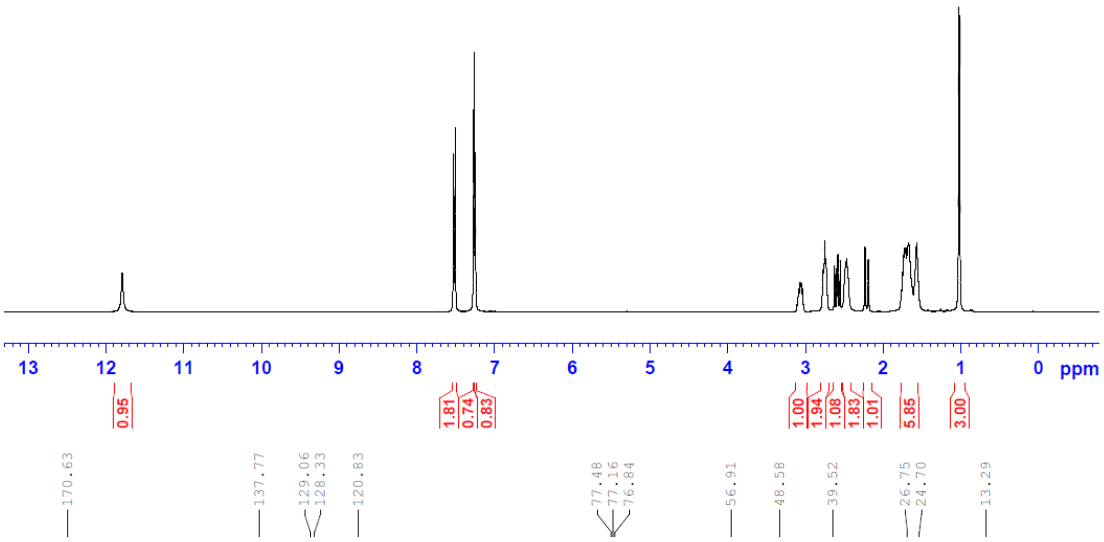

7.412
7.397
7.392
7.383
7.363
7.357
7.342
7.331
7.263
7.234
7.221
7.213
6.945
6.934
6.884
5.207
NHCbz
S
2ab
9
8
7
6
5
4
3
2
1
0
ppm
4.95
1.04
1.04
0.77
2.00


153.61
136.01
135.67
128.62
128.35
128.23
124.83
120.81
108.11
77.48
77.16
76.84
67.10
NHCbz
S
2ab
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
ppm

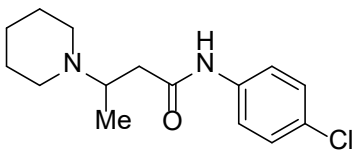

11.789
7.529
7.507
7.269
7.262
7.247
3.107
3.101
3.091
3.084
3.074
3.067
3.063
3.056
3.046
3.039
3.030
3.023
2.771
2.752
2.743
2.734
2.726
2.626
2.597
2.583
2.554
2.471
2.236
2.229
2.193
2.186
1.732
1.723
1.717
1.707
1.691
1.674
1.666


N
H
N
Me
O
Cl

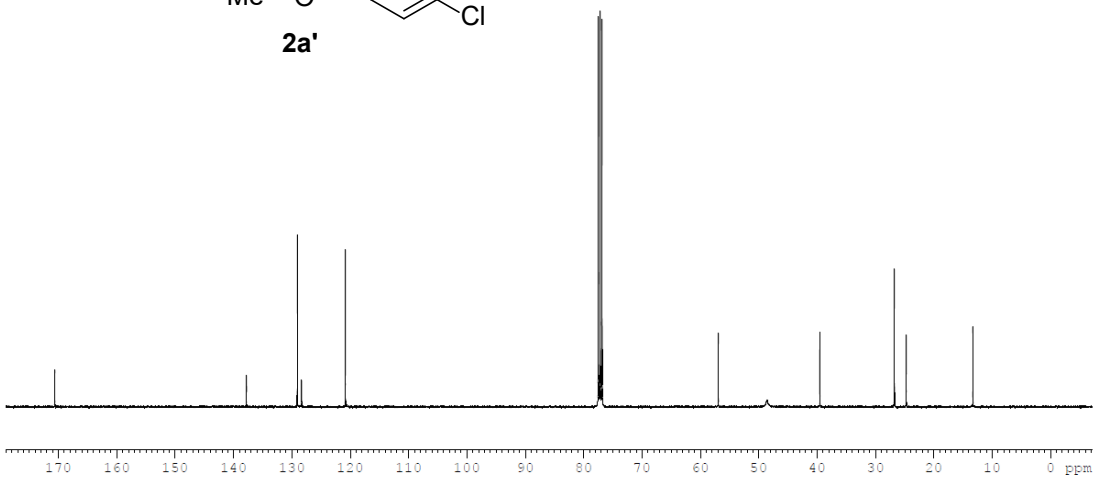
**2a'**

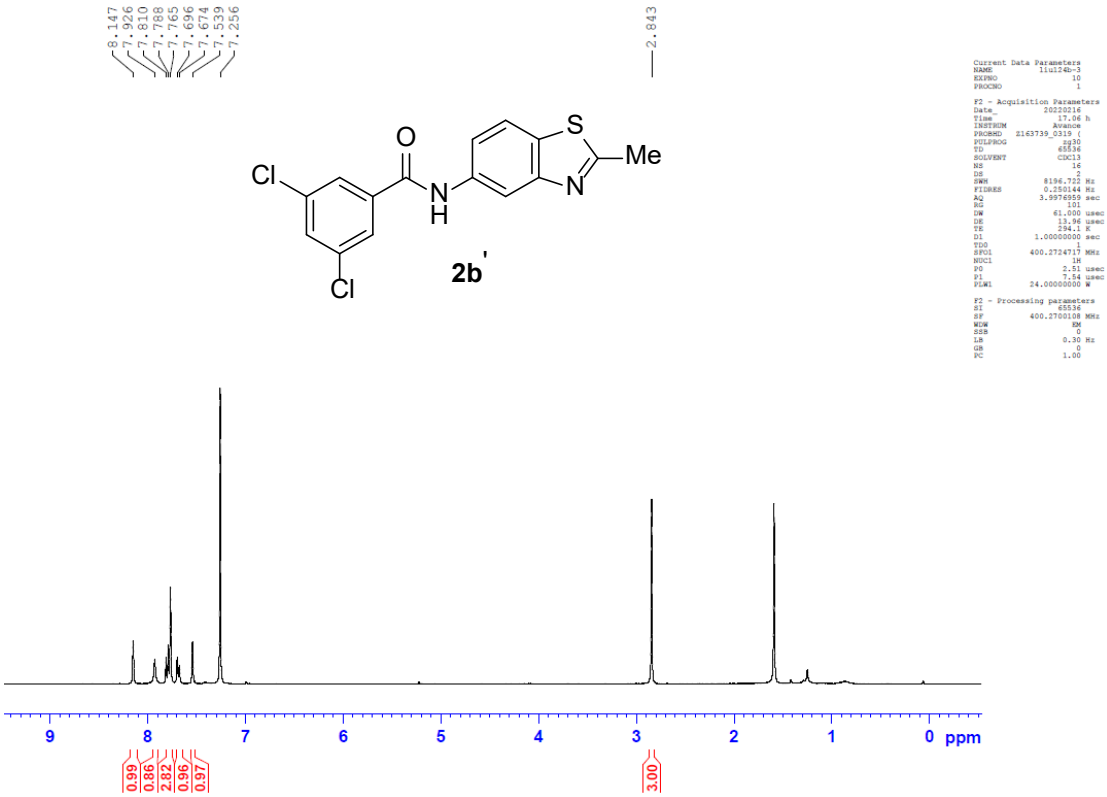

13
12
11
10
9
8
7
6
5
4
3
2
1
0
ppm
0.95
1.81
0.74
0.83
1.00
1.94
1.08
1.83
1.01
5.85
3.00

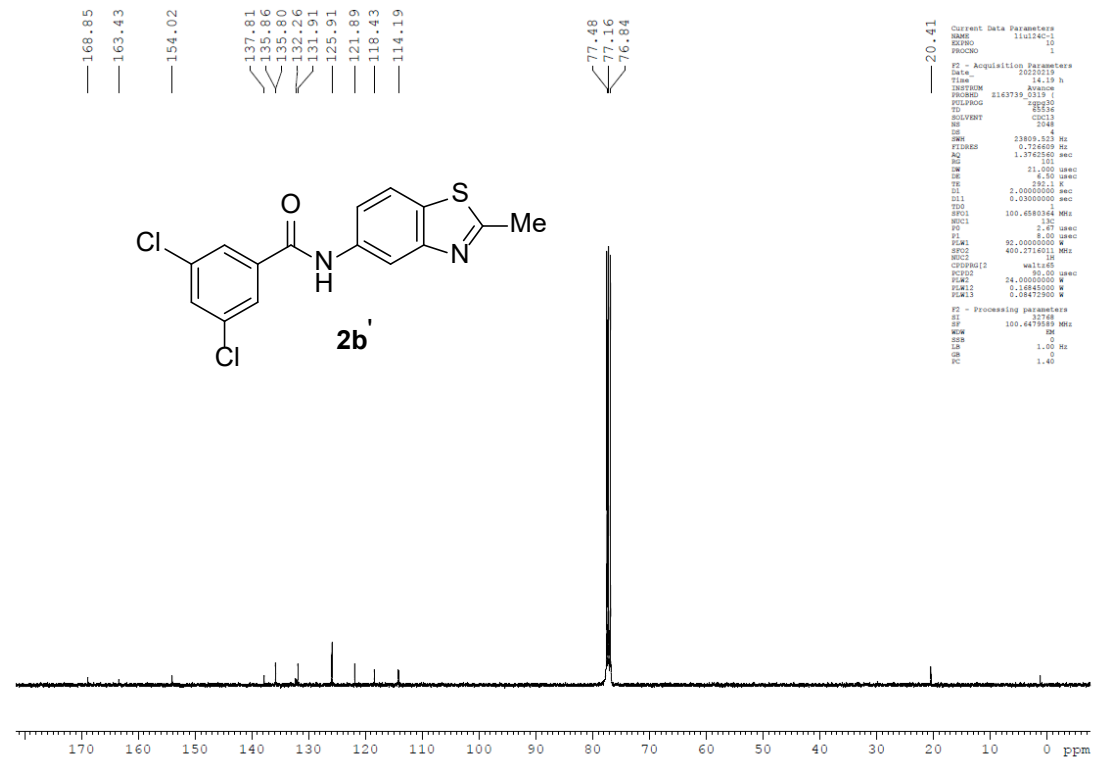

170.63
137.77
129.06
128.33
120.83
77.48
77.16
76.84
56.91
48.58
39.52
26.75
24.70
13.29

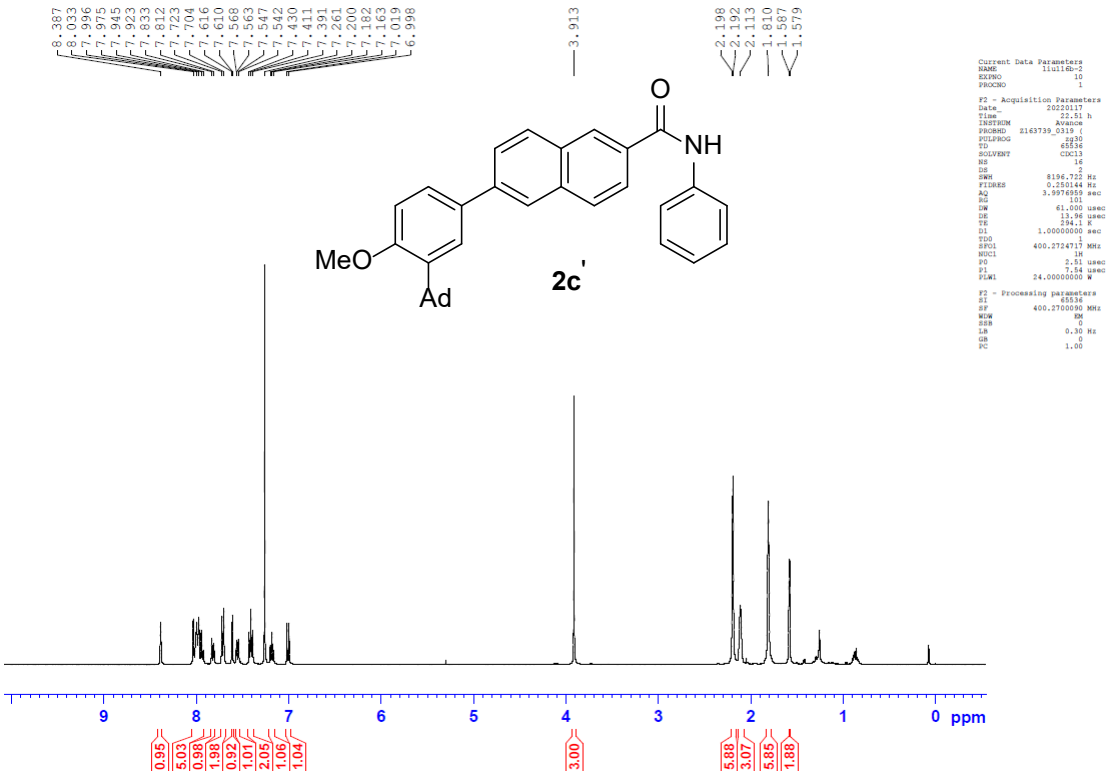

N
H
N
Me
O
Cl

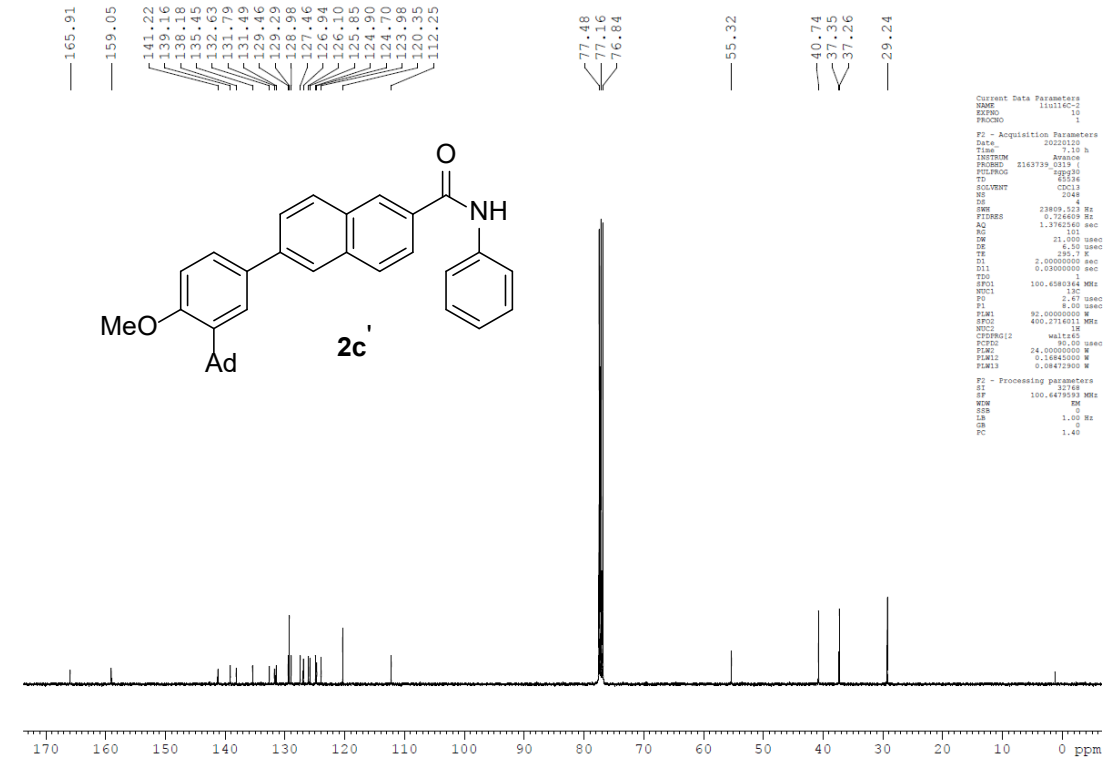
**2a'**

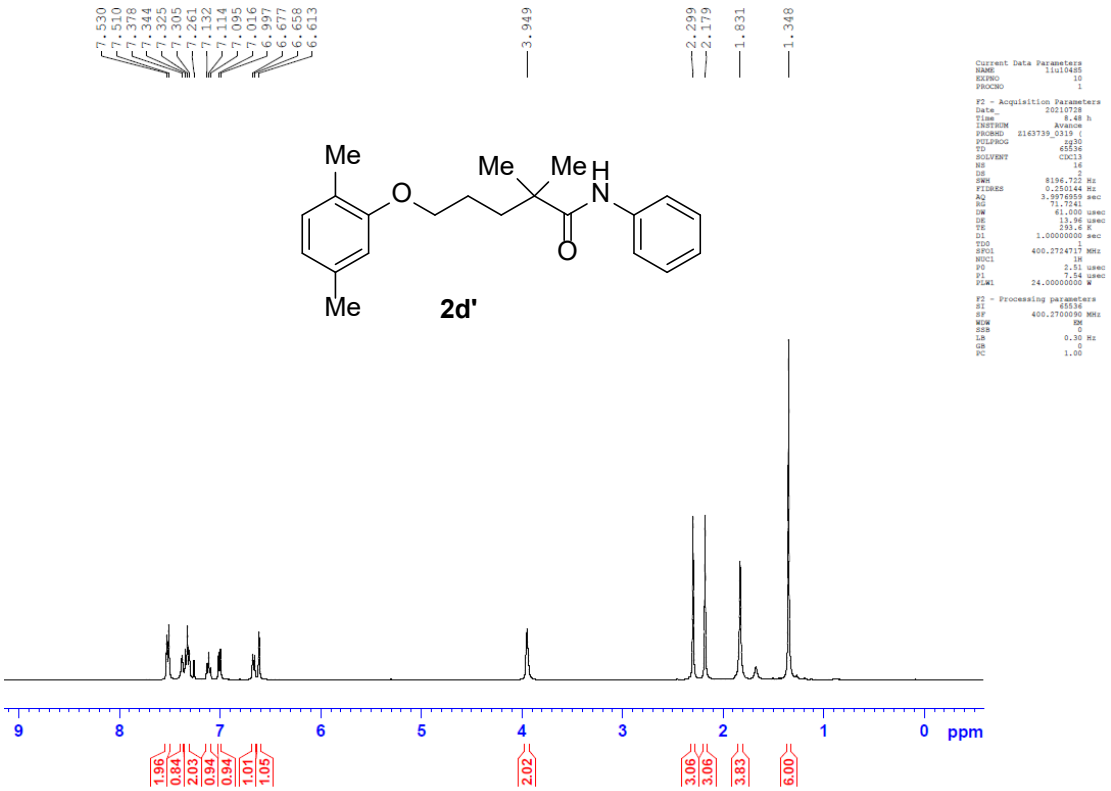

170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
ppm

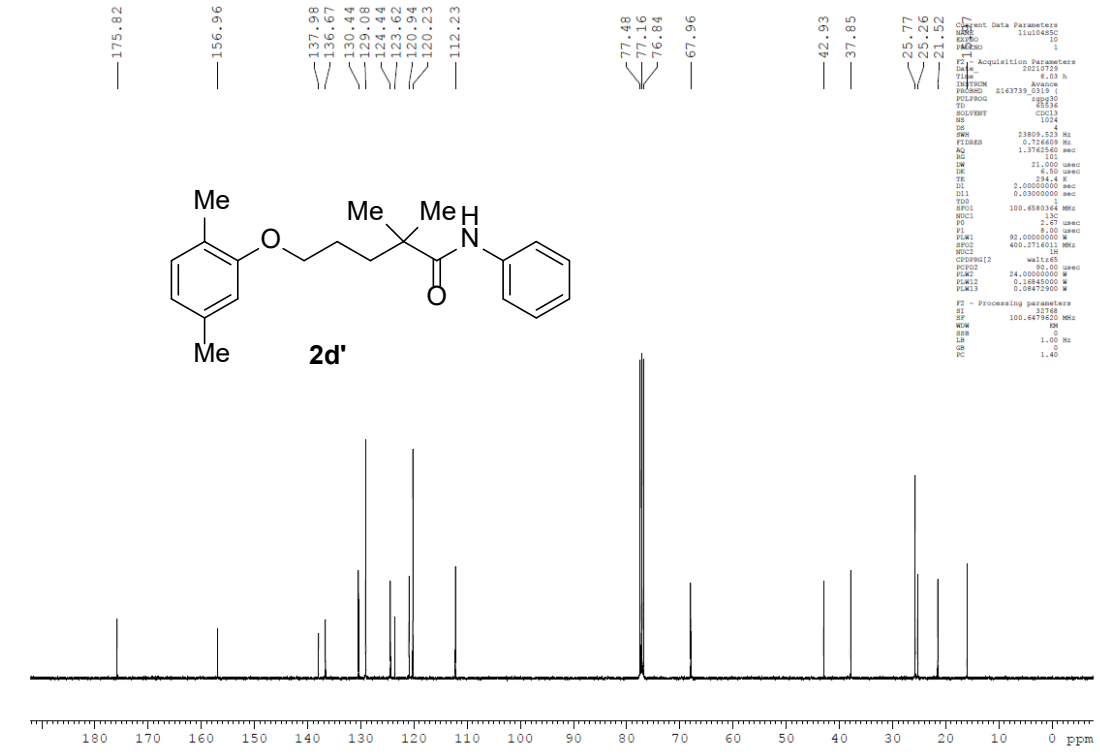

8.147
7.926
7.810
7.788
7.765
7.696
7.674
7.539
7.256
2.643
Cl
O
N
H
S
N
Me
Cl
2b'
9
8
7
6
5
4
3
2
1
0 ppm
0.99
0.86
2.82
0.96
0.97
3.00

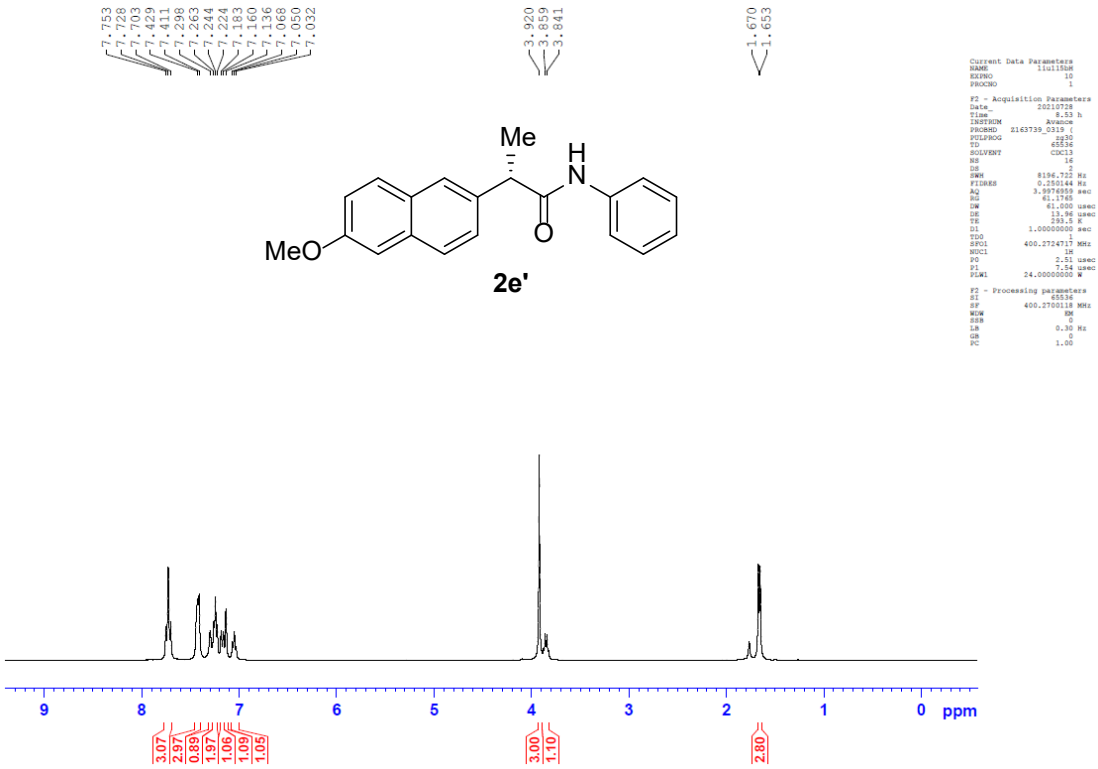

168.85
163.43
154.02
137.81
135.86
135.80
132.26
131.91
125.91
121.89
118.43
114.19
77.48
77.16
76.84
20.41
Cl
O
N
H
S
N
Me
Cl
2b'
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0 ppm

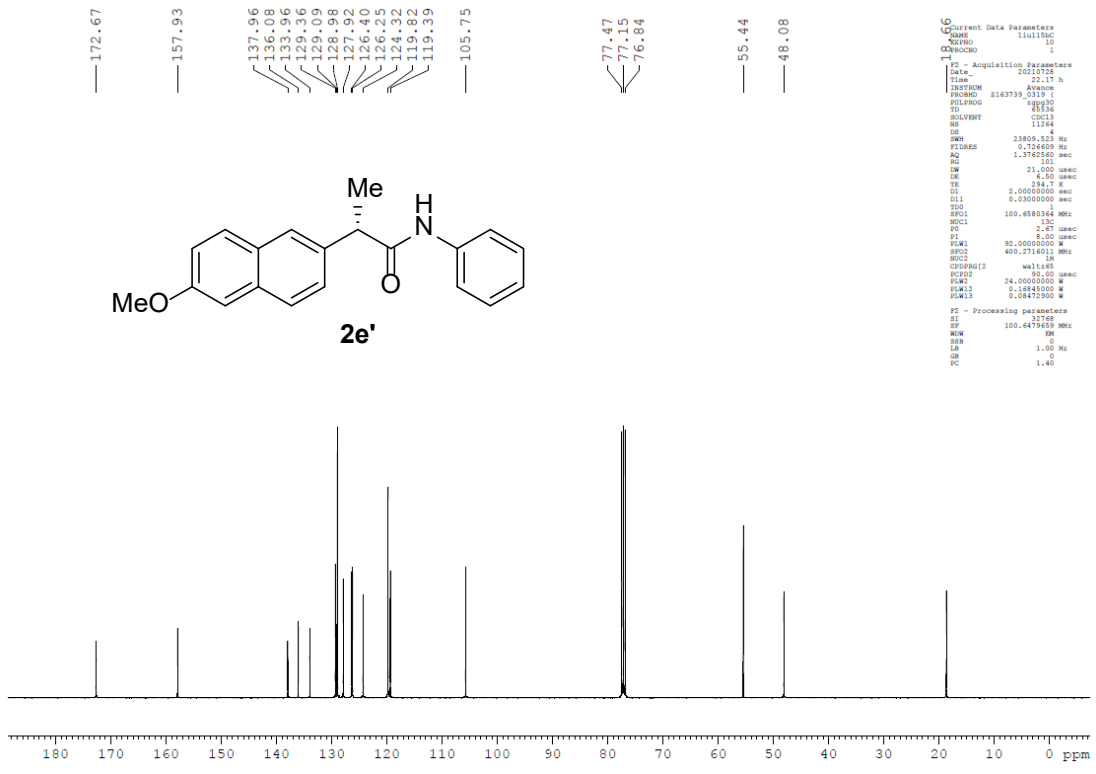

8.387
8.033
7.996
7.975
7.945
7.923
7.833
7.812
7.723
7.704
7.616
7.610
7.568
7.563
7.547
7.542
7.430
7.411
7.391
7.261
7.200
7.182
7.163
7.019
6.998
3.913
2.198
2.192
2.113
1.810
1.587
1.579
O
NH
MeO
Ad
2c'
9
8
7
6
5
4
3
2
1
0 ppm
0.95
5.03
0.98
1.98
0.92
1.01
2.05
1.06
1.04
3.00
5.88
3.07
5.85
1.88


165.91
159.05
141.22
139.16
138.18
135.45
132.63
131.79
131.49
129.46
129.29
128.98
127.46
126.94
126.10
125.85
124.90
124.70
123.98
120.35
112.25
77.48
77.16
76.84
55.32
40.74
37.35
37.26
29.24
O
NH
MeO
Ad
2c'
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0 ppm

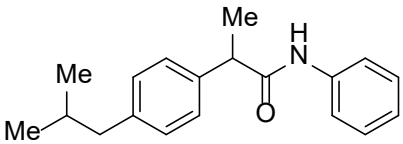

7.530
7.510
7.378
7.344
7.325
7.305
7.261
7.132
7.114
7.095
7.016
6.997
6.677
6.658
6.613
3.949
2.299
2.179
1.831
1.348
Me
Me
Me
H
N
O
O
Me
2d'
9
8
7
6
5
4
3
2
1
0
ppm
1.96
0.84
2.03
0.94
0.94
1.01
1.05
2.02
3.06
3.06
3.83
6.00


175.82
156.96
137.98
136.67
130.44
129.08
124.44
123.62
120.94
120.23
112.23
77.48
77.16
76.84
67.96
42.93
37.85
25.77
25.26
21.52
Me
Me
Me
H
N
O
O
Me
2d'
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
ppm

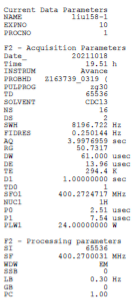

7.753
7.728
7.703
7.429
7.411
7.298
7.263
7.244
7.224
7.183
7.160
7.136
7.068
7.050
7.032
3.920
3.859
3.841
1.670
1.653
Me
H
N
O
MeO
2e'
9
8
7
6
5
4
3
2
1
0
ppm
3.07
2.97
0.89
1.97
1.06
1.09
1.05
3.00
1.10
2.80

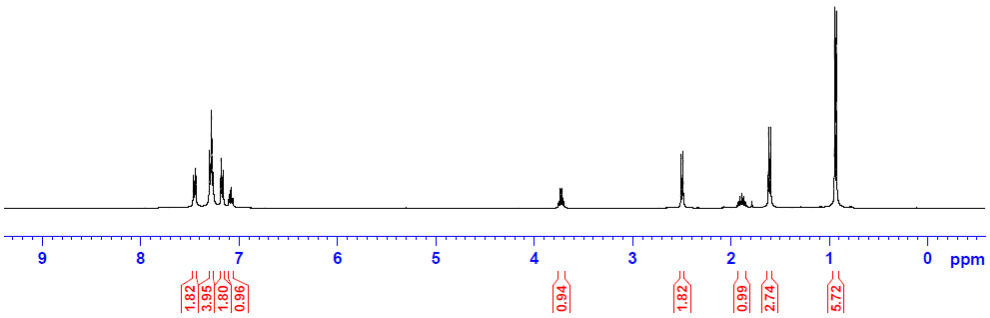

172.67
157.93
137.96
136.08
133.96
129.36
129.09
128.98
127.92
126.40
126.25
124.32
119.82
119.39
105.75
77.47
77.15
76.84
55.44
48.08
Me
H
N
O
MeO
2e'
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
ppm

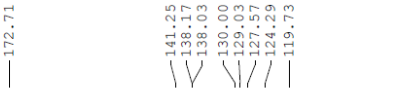

7.461
7.441
7.300
7.280
7.267
7.262
7.182
7.162
7.100
7.081
7.063
3.752
3.734
3.716
3.699
2.506
2.489
1.924
1.907
1.890
1.873
1.856
1.617
1.599
0.946
0.929

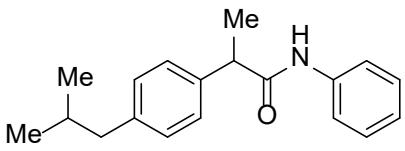

Me
H
N
Me
O
Me

**2f'**

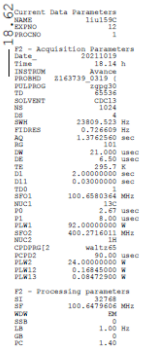


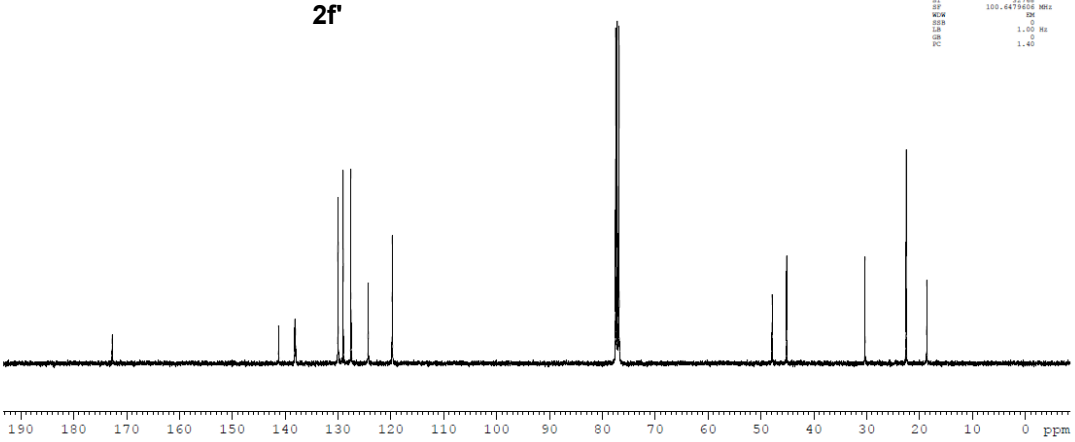

9
8
7
6
5
4
3
2
1
0
ppm
1.82
3.95
1.80
0.96
0.94
1.82
0.99
2.74
5.72

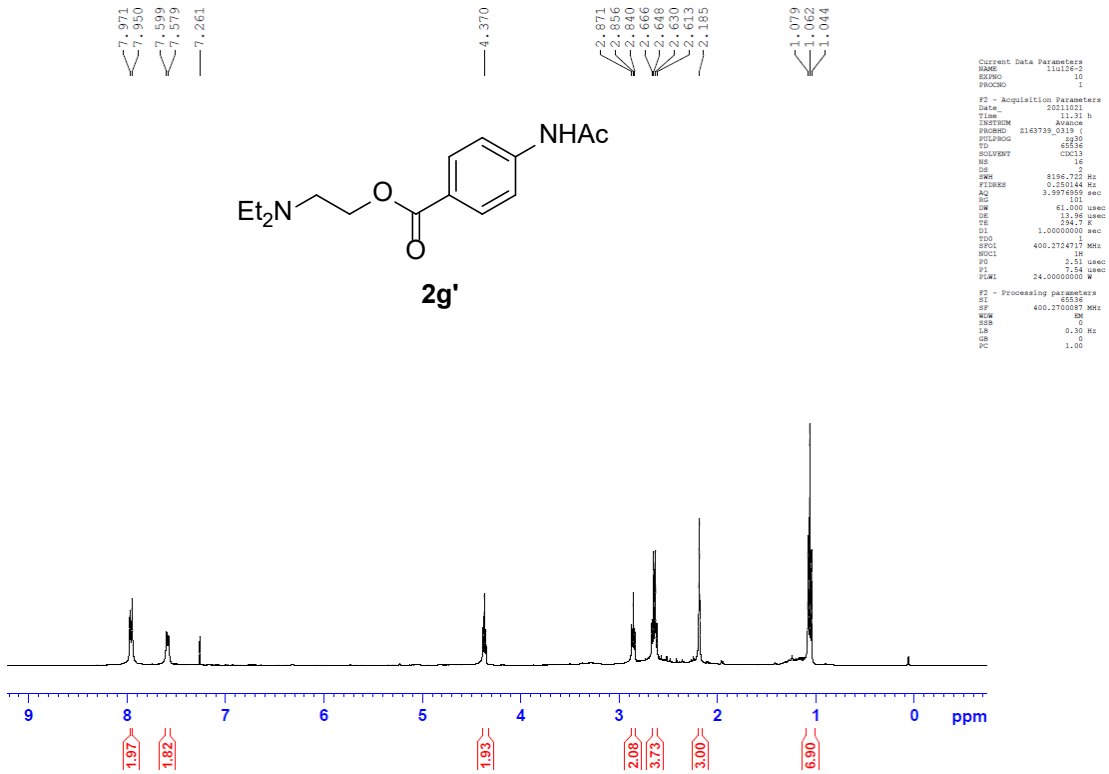

172.71
141.25
138.17
138.03
130.00
129.03
127.57
124.29
119.73
77.48
77.16
76.85
47.89
45.14
30.32
22.52
18.62

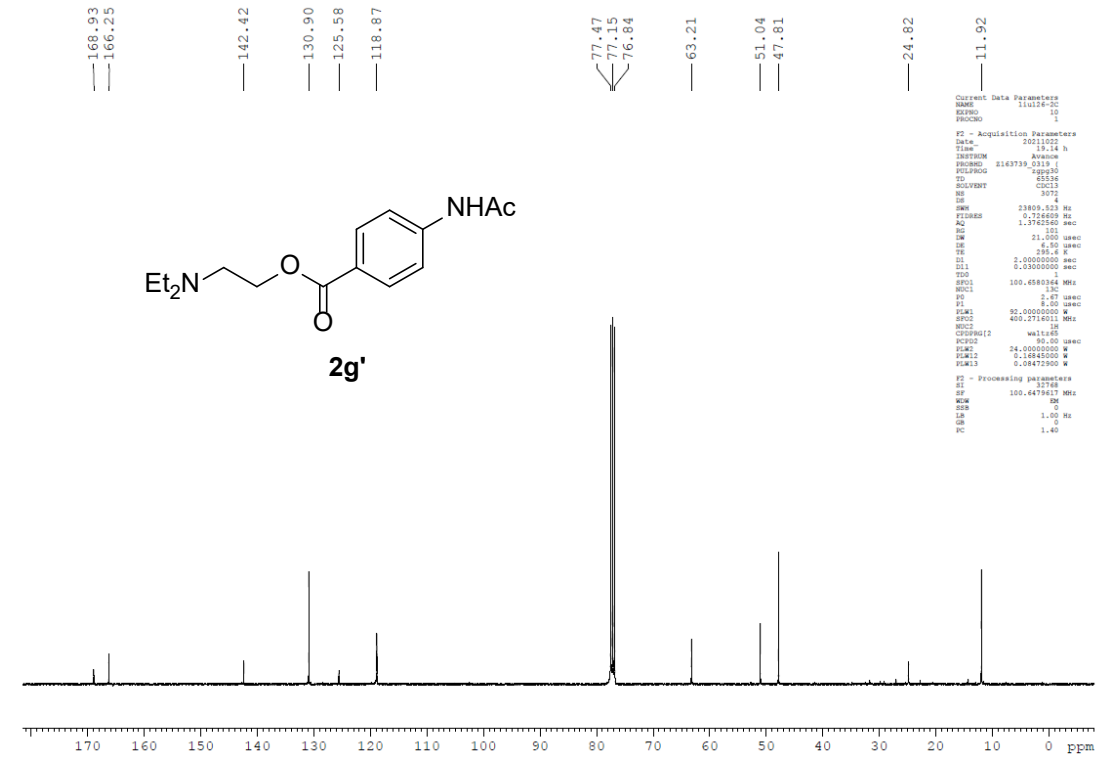

Me
H
N
Me
O
Me

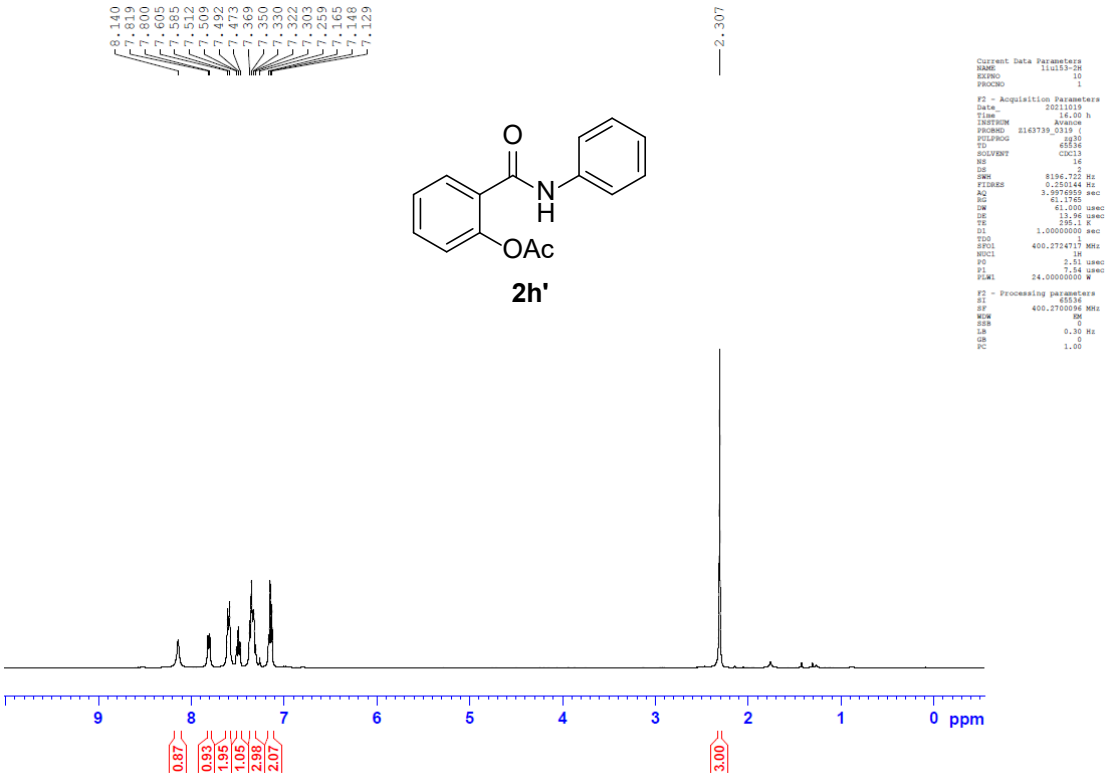
**2f'**

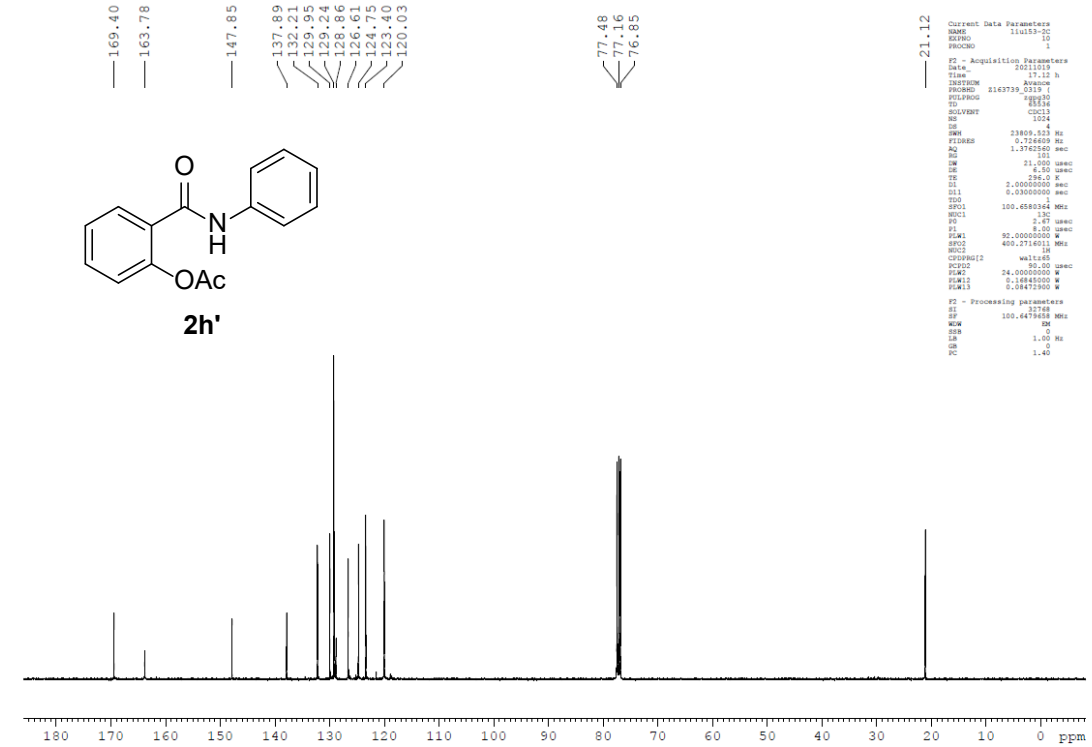


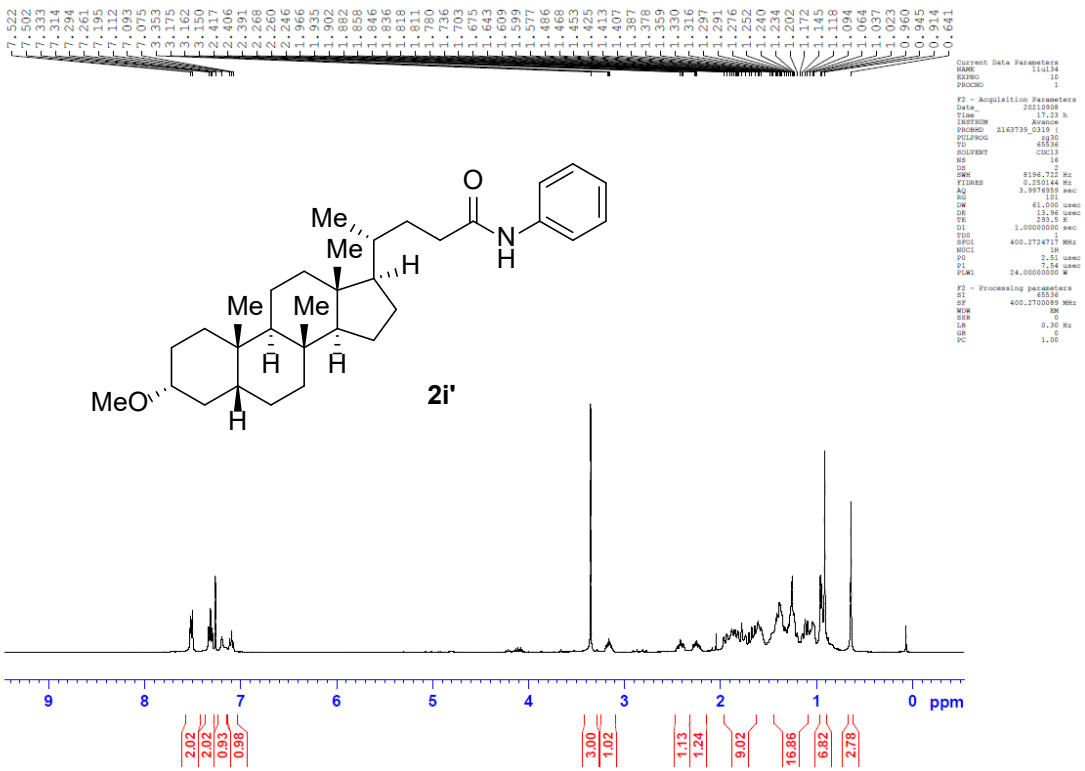

190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
ppm

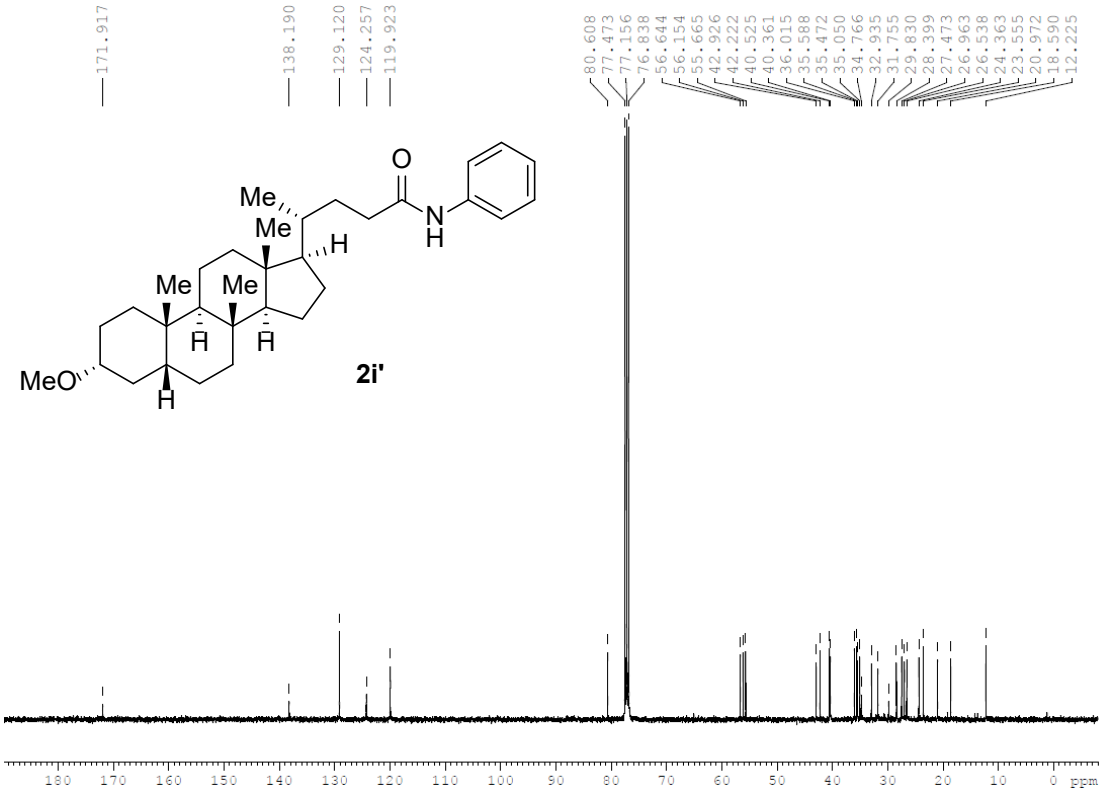

7.971
7.950
7.599
7.579
7.261
4.370
2.871
2.856
2.840
2.666
2.648
2.630
2.613
2.185
1.079
1.062
1.044
NHAc
Et2N
O
O
2g'
9
8
7
6
5
4
3
2
1
0
ppm
1.97
1.82
1.93
2.08
3.73
3.00
6.90

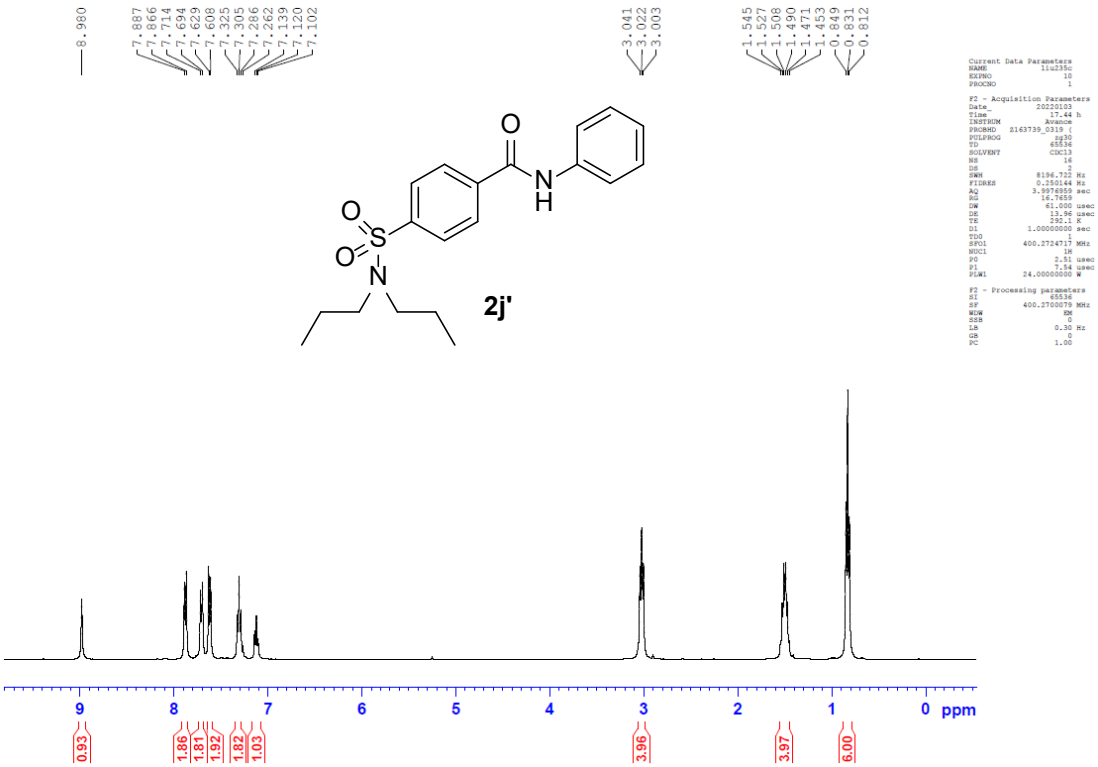

168.93
166.25
142.42
130.90
125.58
118.87
77.47
77.15
76.84
63.21
51.04
47.81
24.82
11.92
NHAc
Et2N
O
O
2g'
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
ppm

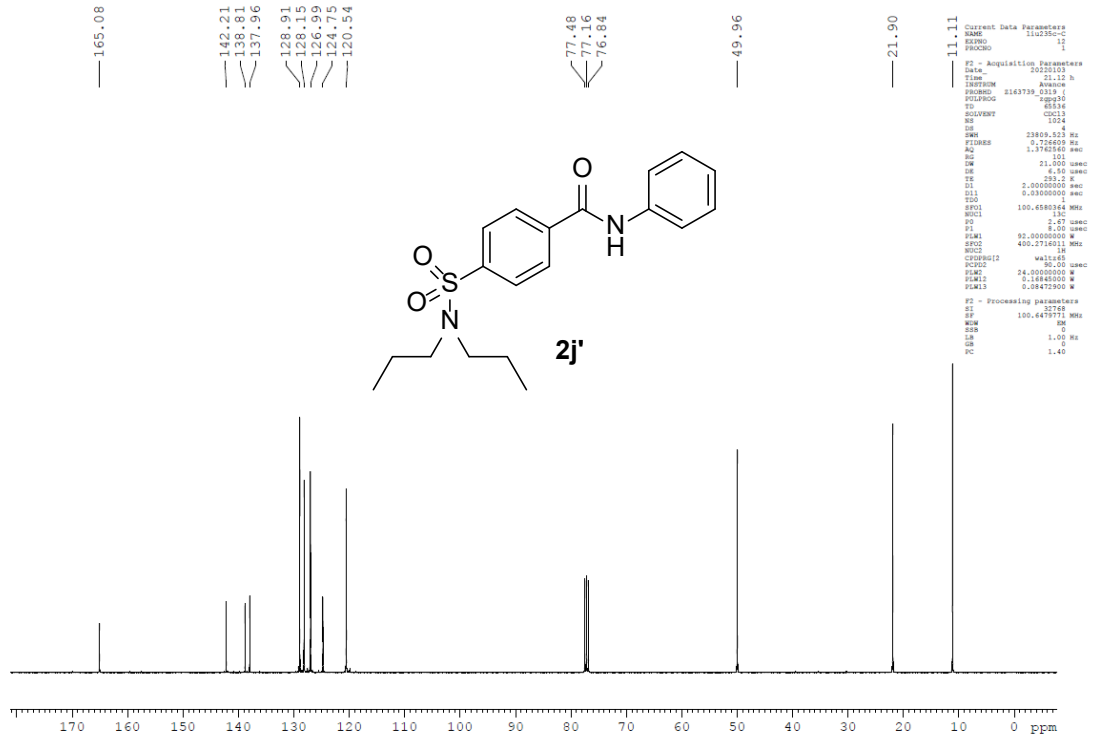

8.140
7.819
7.800
7.605
7.585
7.512
7.509
7.492
7.473
7.369
7.350
7.330
7.322
7.303
7.259
7.165
7.148
7.129
2.307
O
N
H
OAc
2h'
9
8
7
6
5
4
3
2
1
0 ppm
0.87
0.93
1.95
1.05
2.98
2.07
3.00

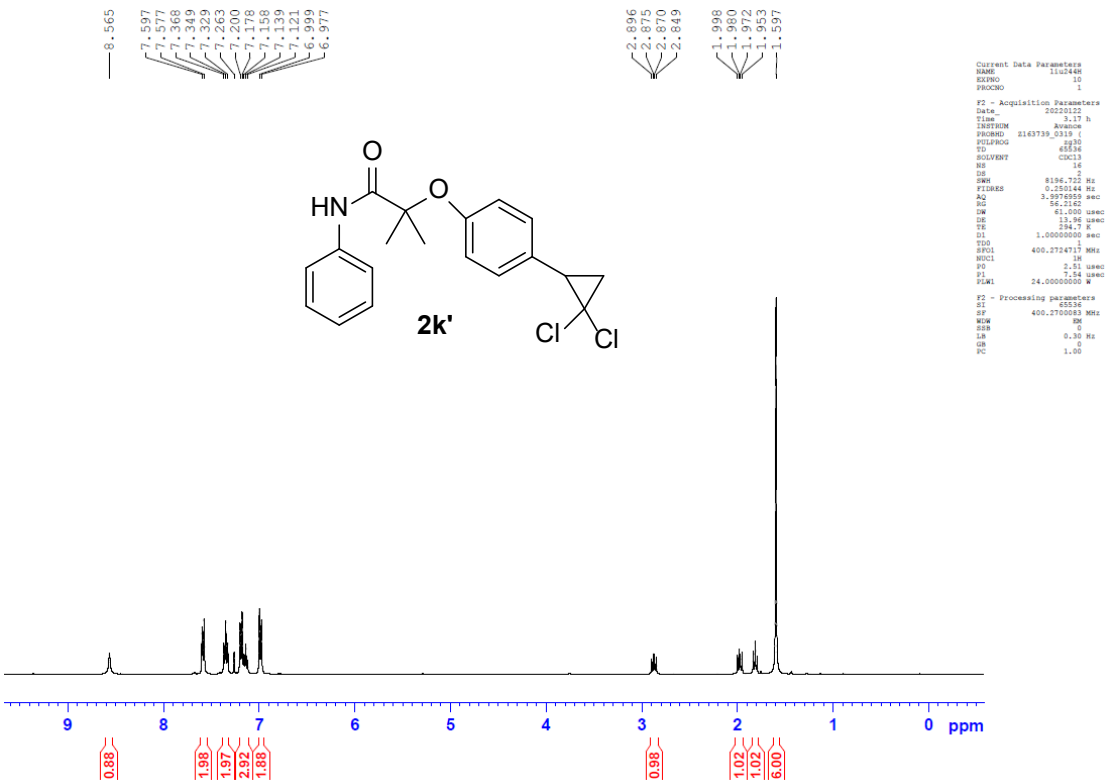

169.40
163.78
147.85
137.89
132.21
129.95
129.24
128.86
126.61
124.75
123.40
120.03
77.48
77.16
76.85
21.12
O
N
H
OAc
2h'
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0 ppm

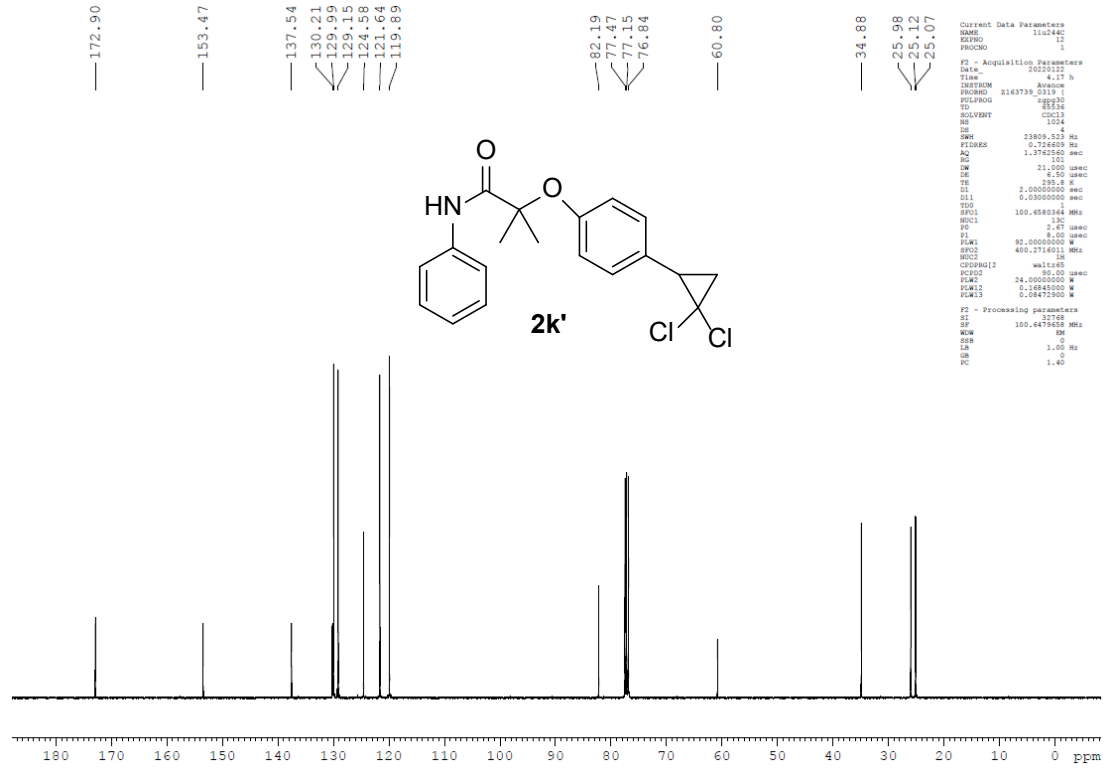

2i'
ppm

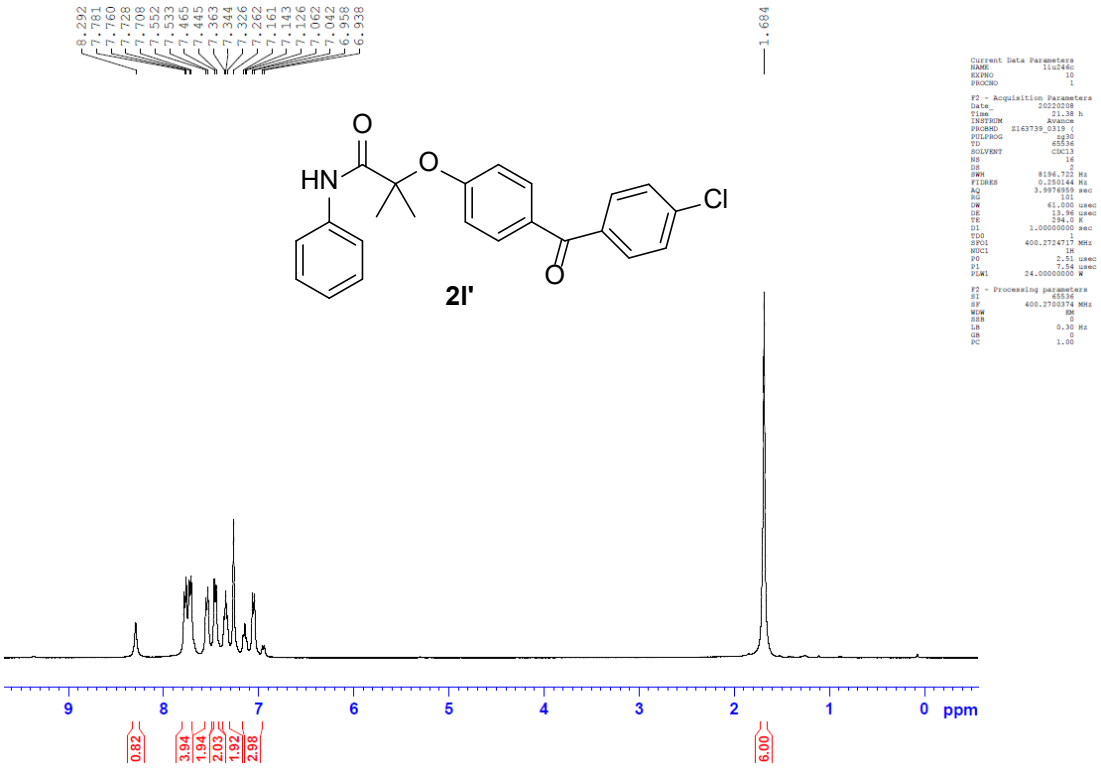

2i'
ppm

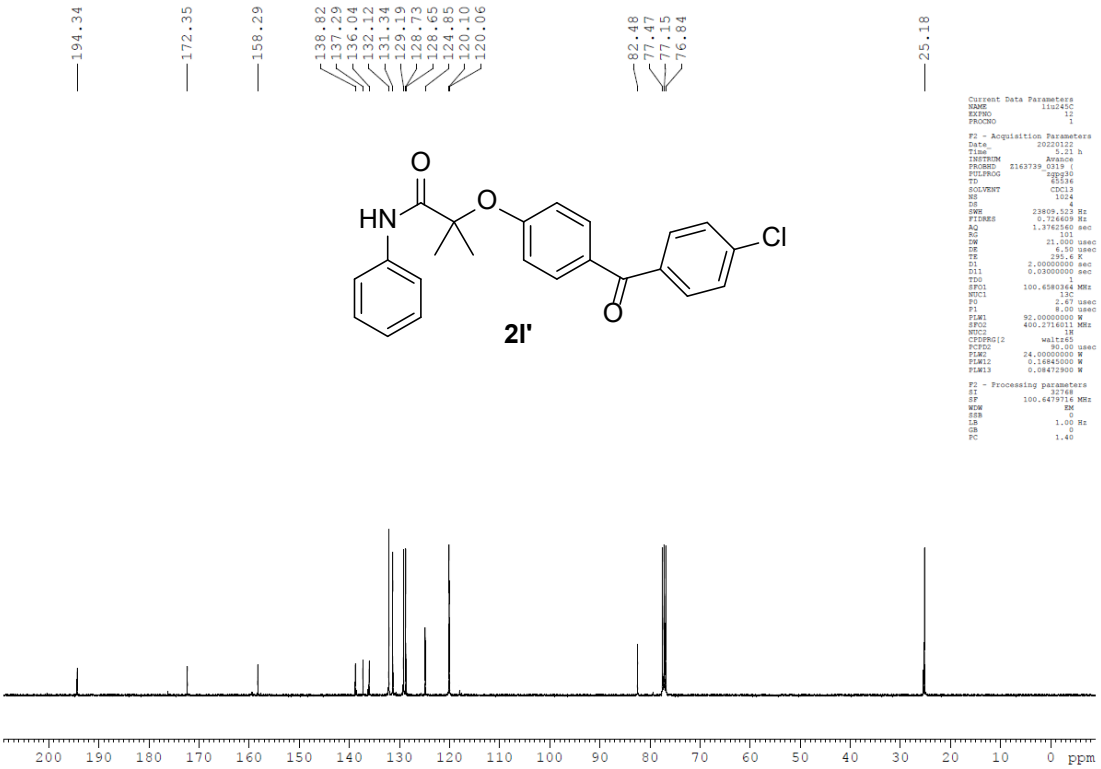

8.980
7.887
7.866
7.714
7.694
7.629
7.608
7.325
7.305
7.286
7.262
7.139
7.120
7.102
3.041
3.022
3.003
1.545
1.527
1.508
1.490
1.471
1.453
0.849
0.831
0.812
2j'
9
8
7
6
5
4
3
2
1
0 ppm
0.93
1.86
1.81
1.92
1.82
1.03
3.96
3.97
6.00

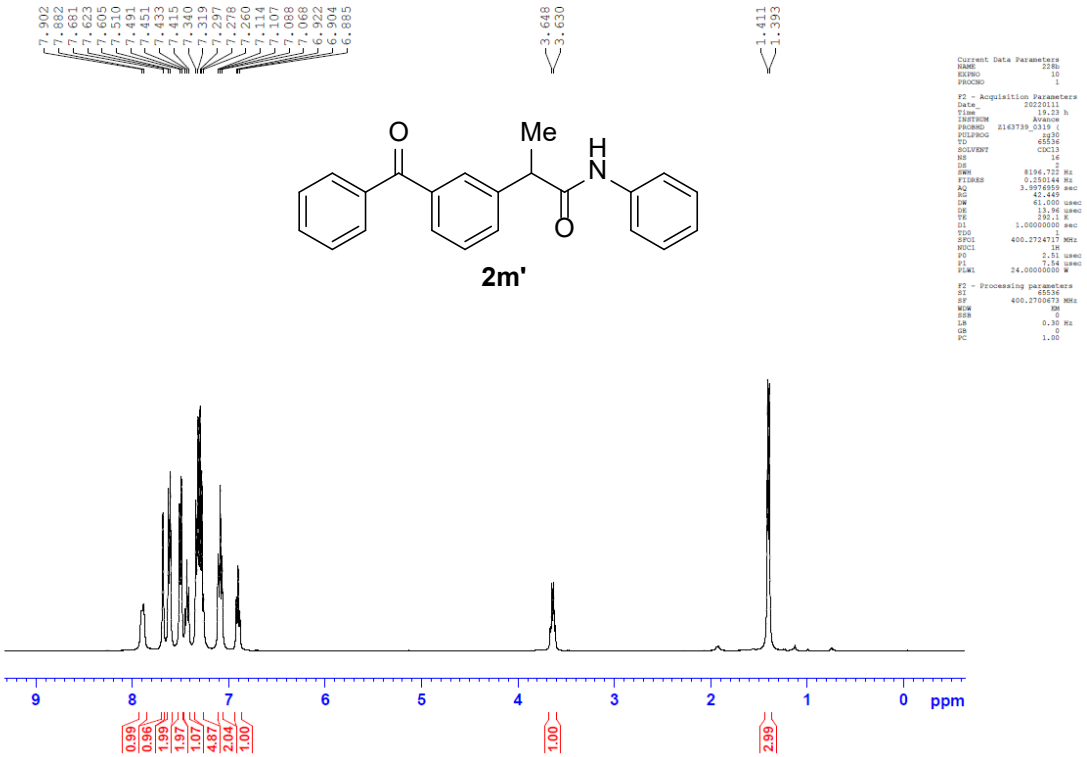

165.08
142.21
138.81
137.96
128.91
128.15
126.99
124.75
120.54
77.48
77.16
76.84
49.96
21.90
11.11
2j'
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0 ppm

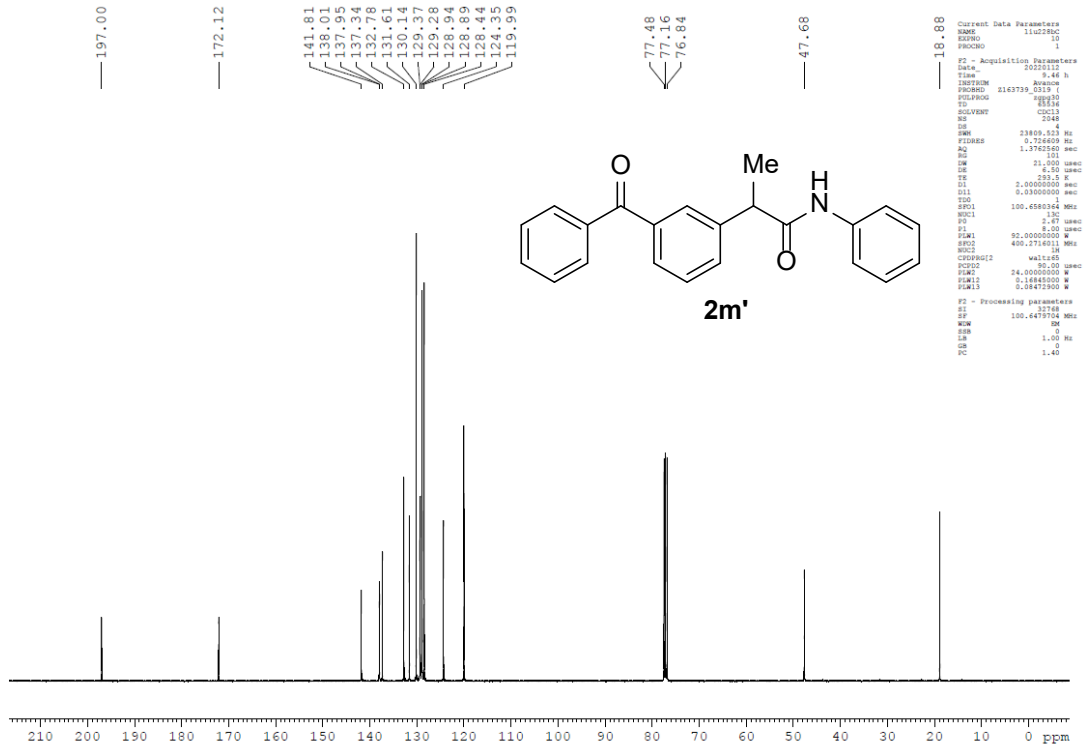

8.565
7.597
7.577
7.368
7.349
7.329
7.263
7.200
7.178
7.158
7.139
7.121
6.999
6.977
2.896
2.875
2.870
2.849
1.998
1.980
1.972
1.953
1.597
HN
O
O
Cl
Cl
2k'
9
8
7
6
5
4
3
2
1
0
ppm
0.88
1.98
1.97
2.92
1.88
0.98
1.02
1.02
6.00

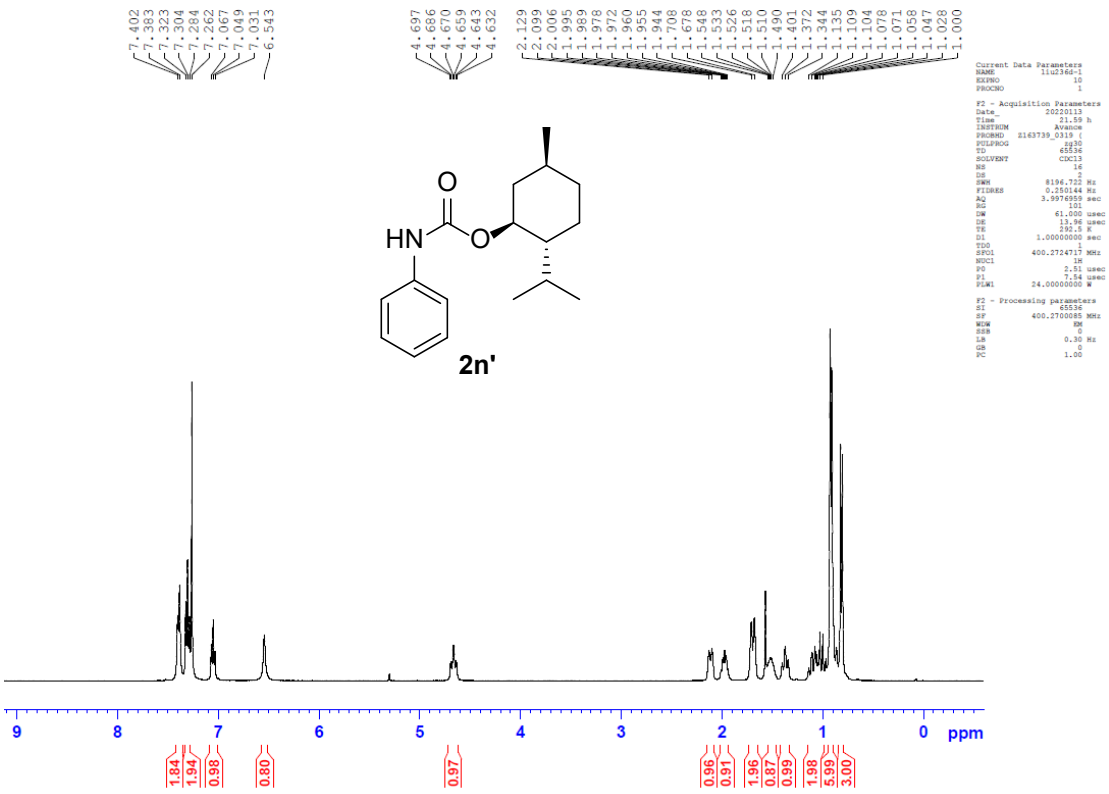

172.90
153.47
137.54
130.21
129.99
129.15
124.58
121.64
119.89
82.19
77.47
77.15
76.84
60.80
34.88
25.98
25.12
25.07
HN
O
O
Cl
Cl
2k'
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
ppm


8.292
7.781
7.760
7.728
7.708
7.552
7.533
7.465
7.445
7.363
7.344
7.326
7.262
7.161
7.143
7.126
7.062
7.042
6.958
6.938
1.684
HN
O
O
Cl
O
2l'
9
8
7
6
5
4
3
2
1
0
ppm
0.82
3.94
1.94
2.03
1.92
2.98
6.00


194.34
172.35
158.29
138.82
137.29
136.04
132.12
131.34
129.19
128.73
128.65
124.85
120.10
120.06
82.48
77.47
77.15
76.84
25.18
HN
O
O
Cl
O
2l'
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
ppm


7.902
7.882
7.681
7.623
7.605
7.510
7.491
7.451
7.433
7.415
7.340
7.319
7.297
7.278
7.260
7.114
7.107
7.088
7.068
6.922
6.904
6.885
3.648
3.630
1.411
1.393
O
Me
H
N
O
2m'
9
8
7
6
5
4
3
2
1
0
ppm
0.99
0.96
1.99
1.97
1.07
4.87
2.04
1.00
1.00
2.99


197.00
172.12
141.81
138.01
137.95
137.34
132.78
131.61
130.14
129.37
129.28
128.94
128.89
128.44
124.35
119.99
77.48
77.16
76.84
47.68
18.88
O
Me
H
N
O
2m'
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0 ppm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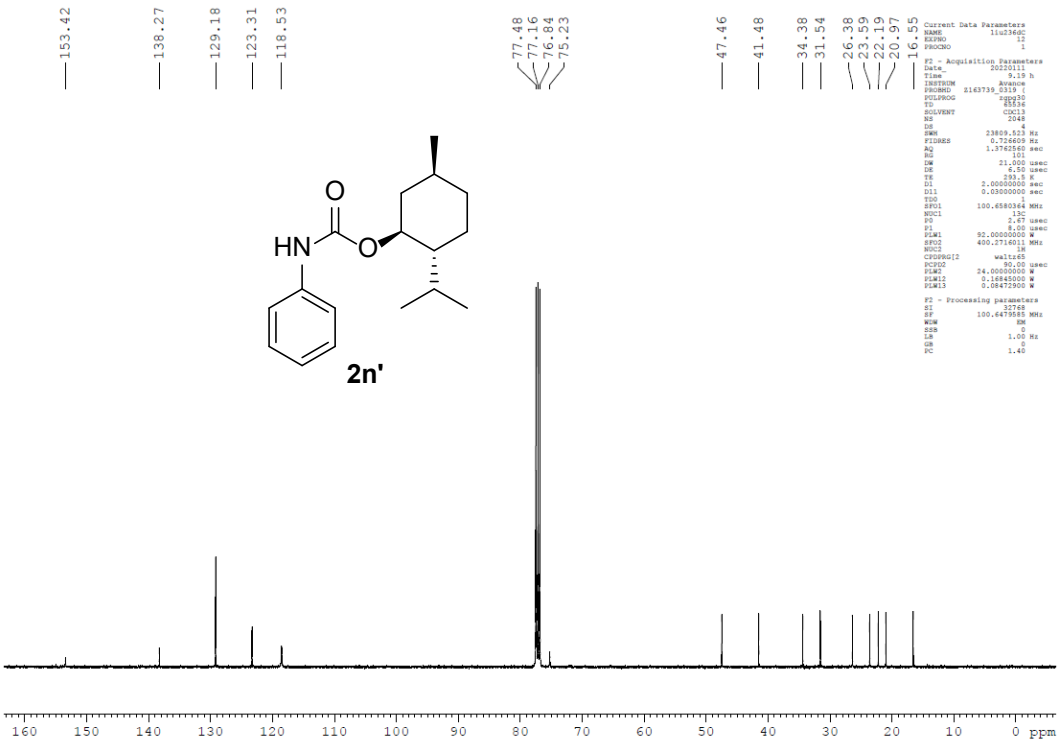
7.383
7.323
7.304
7.284
7.262
7.067
7.049
7.031
6.543
4.697
4.686
4.670
4.659
4.643
4.632
2.129
2.099
2.006
1.995
1.989
1.978
1.972
1.960
1.955
1.944
1.708
1.678
1.548
1.533
1.526
1.518
1.510
1.490
1.401
1.372
1.344
1.135
1.109
1.104
1.078
1.071
1.058
1.047
1.028
1.000
HN
O
O
2n'
9
8
7
6
5
4
3
2
1
0
ppm
1.84
1.94
0.98
0.80
0.97
0.96
0.91
1.96
0.87
0.99
1.98
5.99
3.00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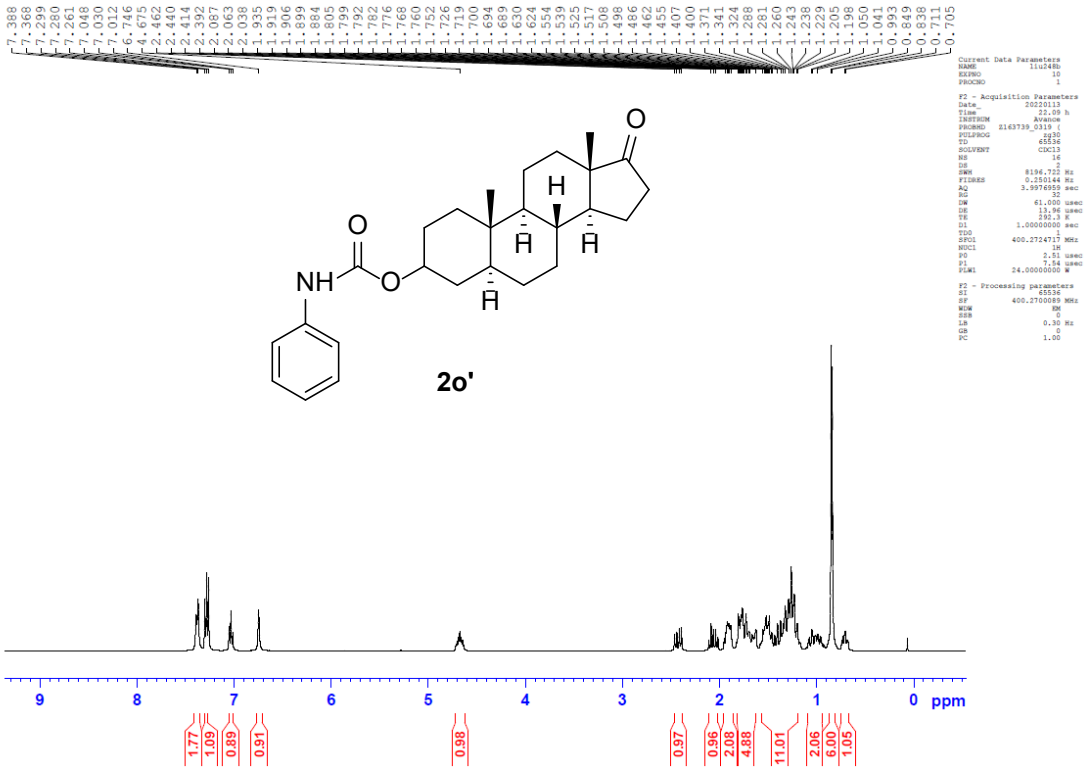
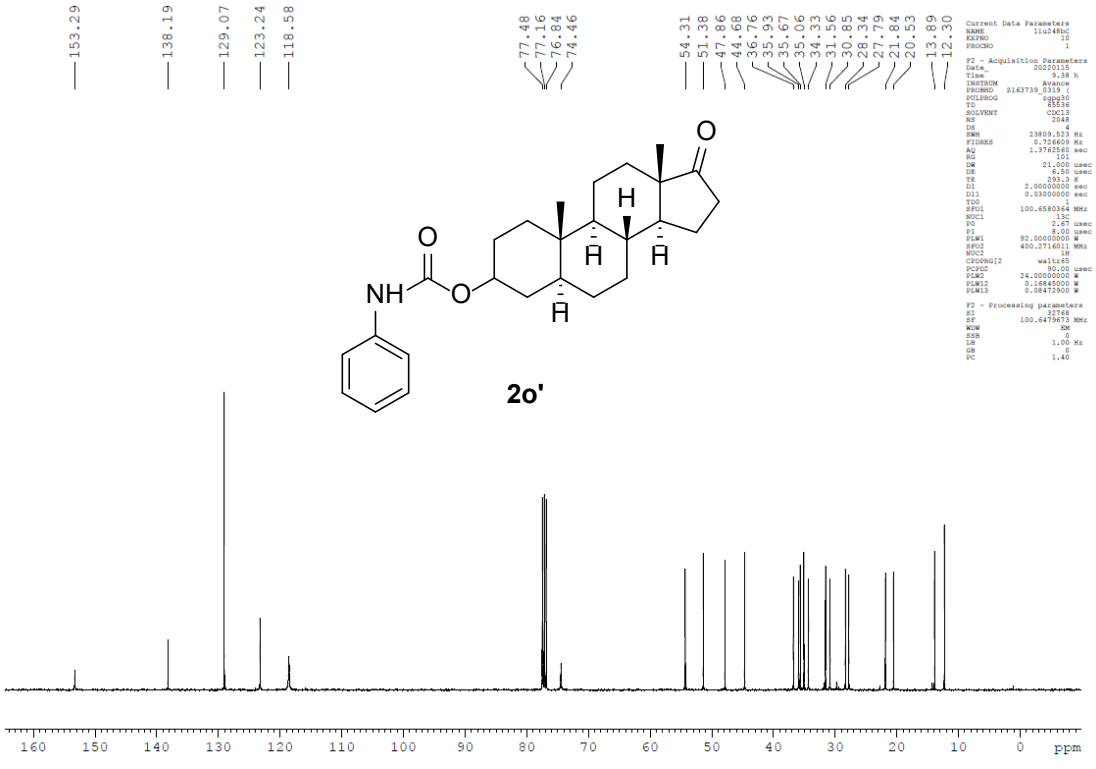
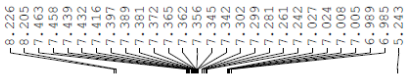
138.27
129.18
123.31
118.53
77.48
77.16
76.84
75.23
47.46
41.48
34.38
31.54
26.38
23.59
22.19
20.97
16.55
HN
O
O
2n'
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
ppm


2o'
ppm


2o'
ppm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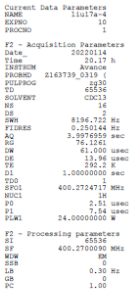
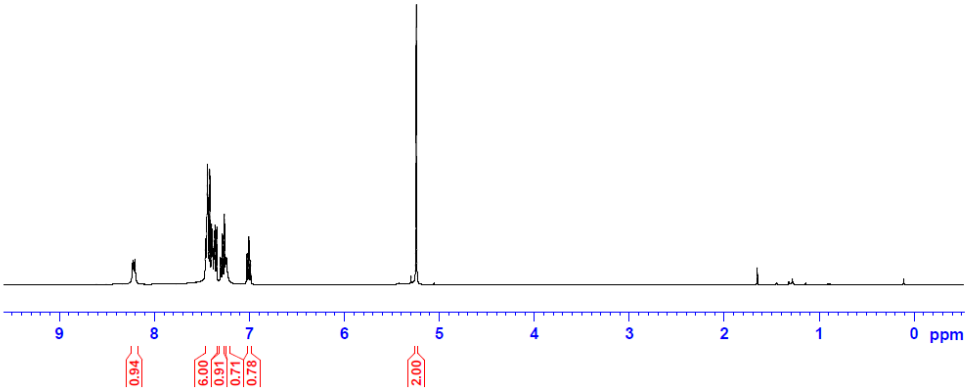
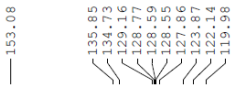
8.205
7.463
7.458
7.439
7.432
7.416
7.397
7.389
7.381
7.372
7.365
7.362
7.356
7.345
7.342
7.302
7.299
7.281
7.261
7.242
7.027
7.024
7.008
7.005
6.989
6.985
5.243


NHCbz
Cl

3a



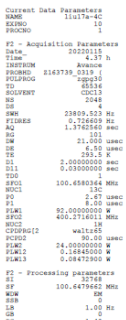

9
8
7
6
5
4
3
2
1
0
ppm
0.94
6.00
0.91
0.71
0.78
2.00

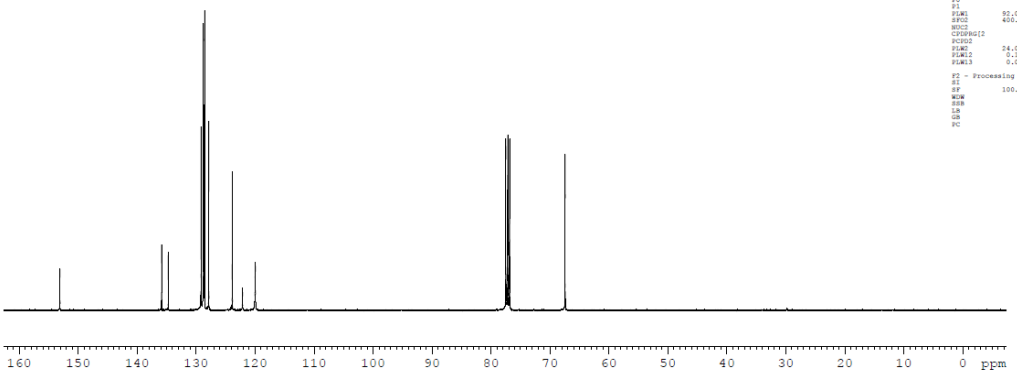

153.08
135.85
134.73
129.16
128.77
128.59
128.55
127.86
123.87
122.14
119.98


77.47
77.16
76.84
67.42


NHCbz
Cl

3a

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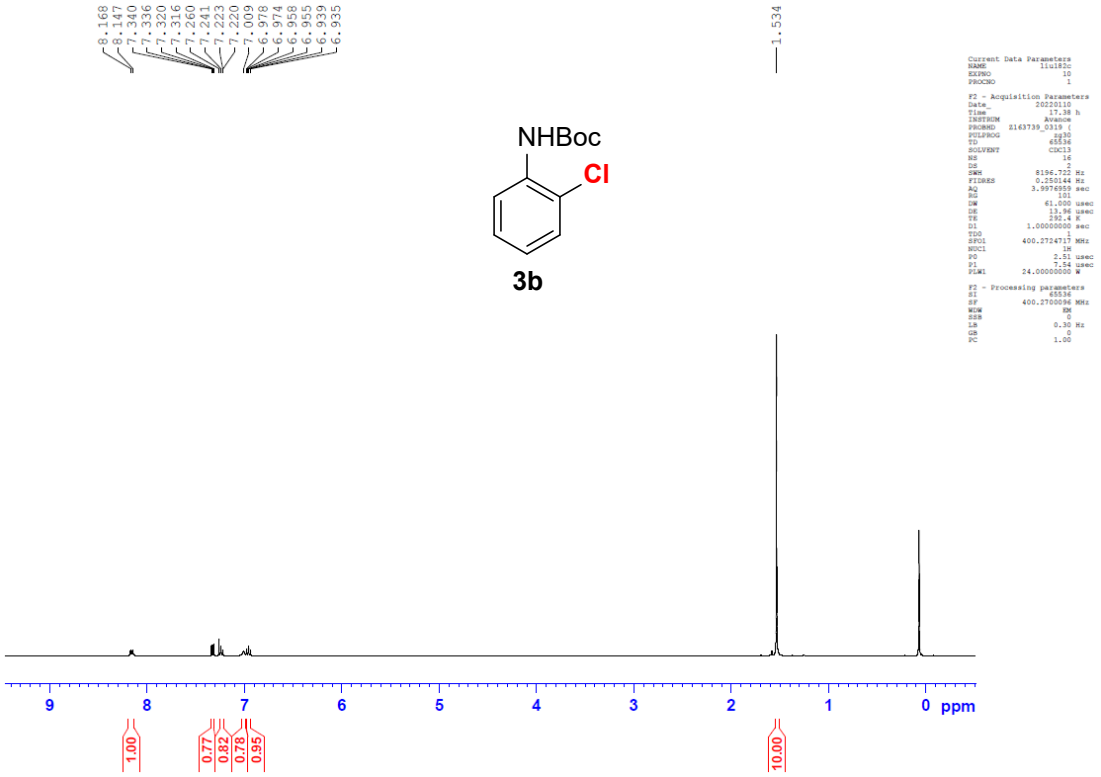
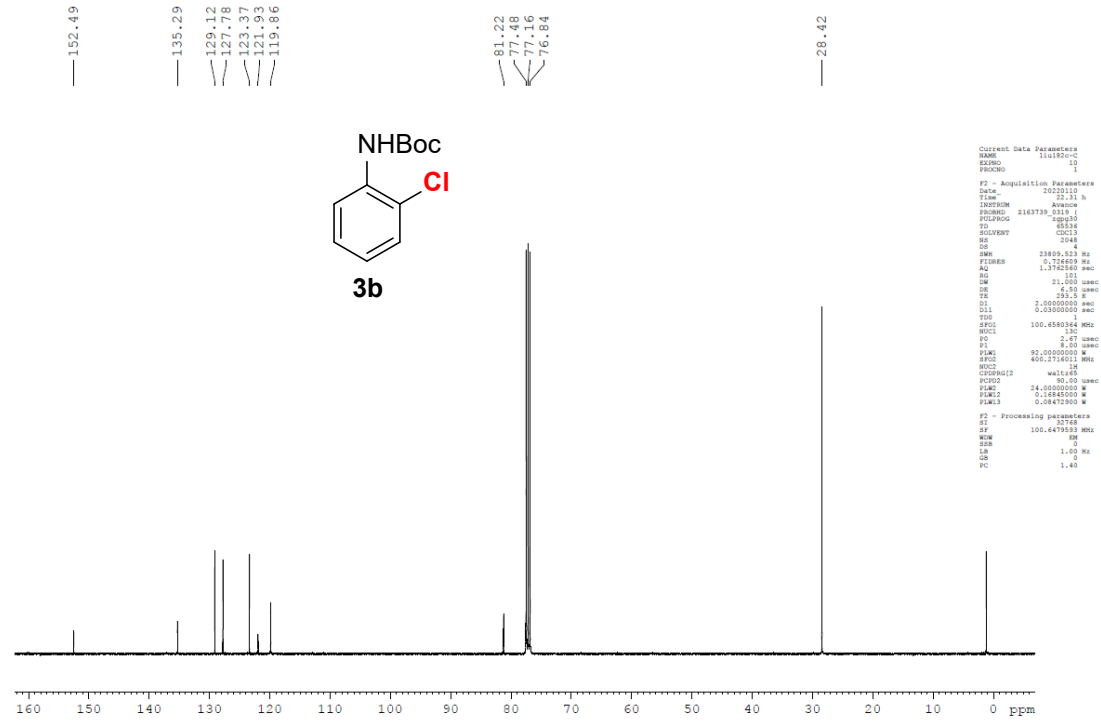
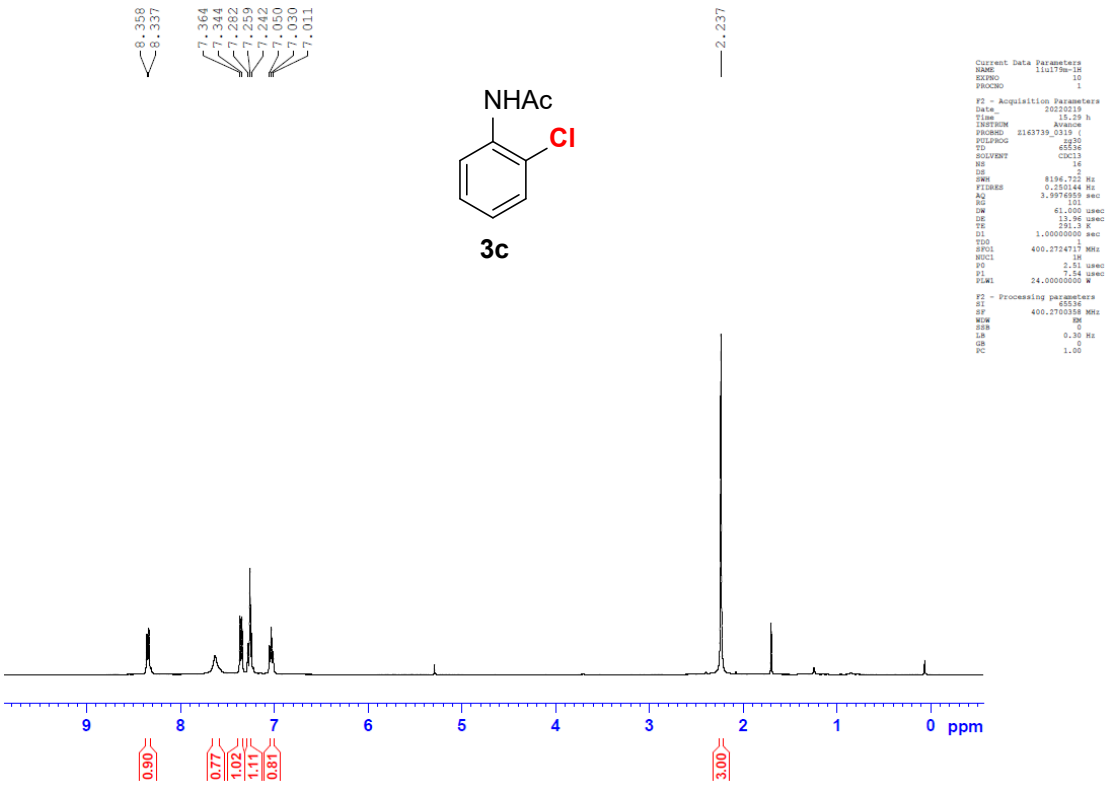
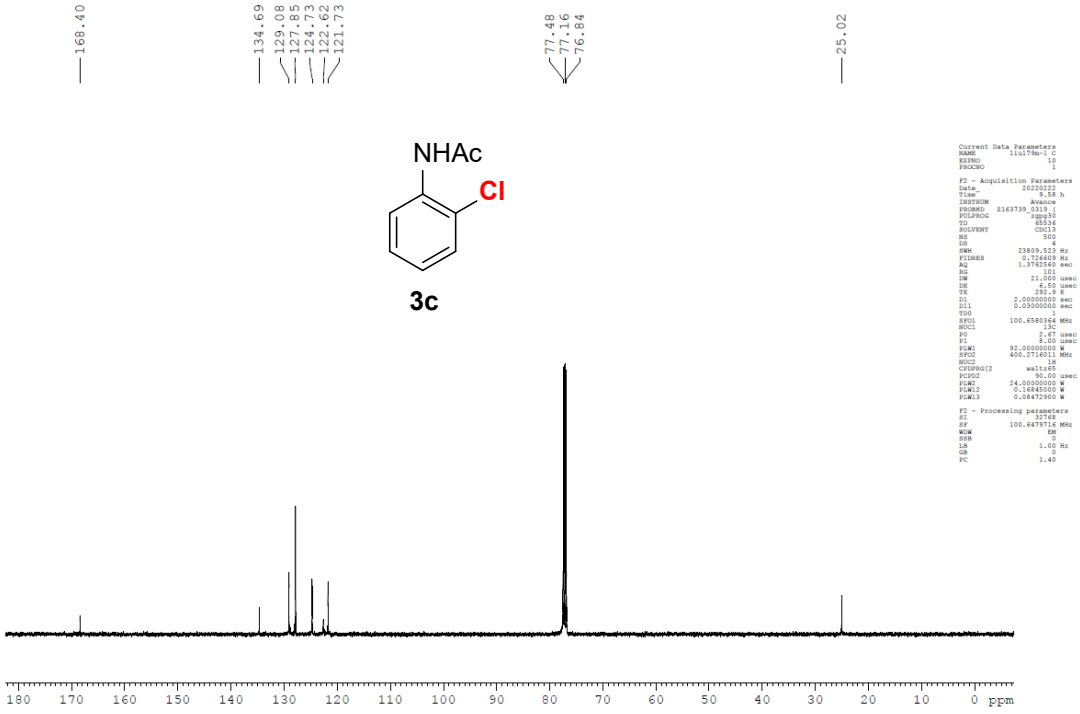
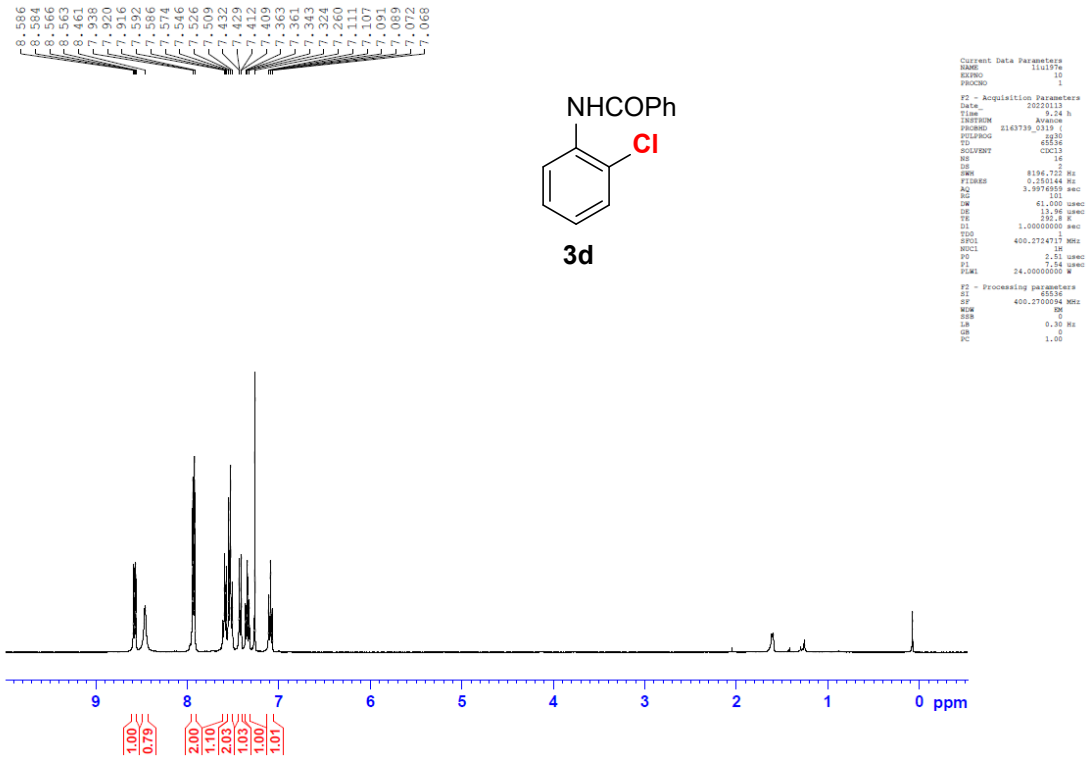
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
ppm


8.168
8.147
7.340
7.336
7.320
7.316
7.260
7.241
7.223
7.220
7.009
6.978
6.974
6.958
6.955
6.939
6.935
1.534
NHBoc
Cl
3b
9
8
7
6
5
4
3
2
1
0 ppm
1.00
0.77
0.82
0.78
0.95
10.00


152.49
135.29
129.12
127.78
123.37
121.93
119.86
81.22
77.48
77.16
76.84
28.42
NHBoc
Cl
3b
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0 ppm


8.358
8.337
7.364
7.344
7.282
7.259
7.242
7.050
7.030
7.011
2.237
NHAc
Cl
3c
9
8
7
6
5
4
3
2
1
0
ppm
0.90
0.77
1.02
1.11
0.81
3.00


168.40
134.69
129.08
127.95
124.73
122.62
121.73
77.48
77.16
76.84
25.02
NHAc
Cl
3c
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
ppm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8.584
8.566
8.563
8.461
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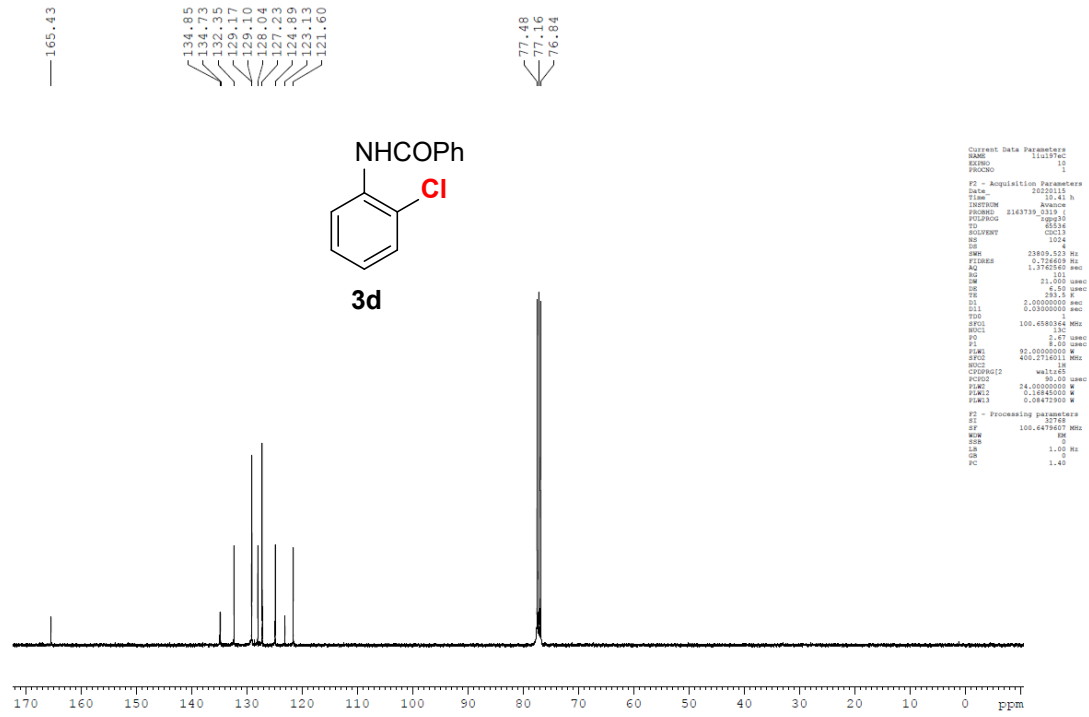
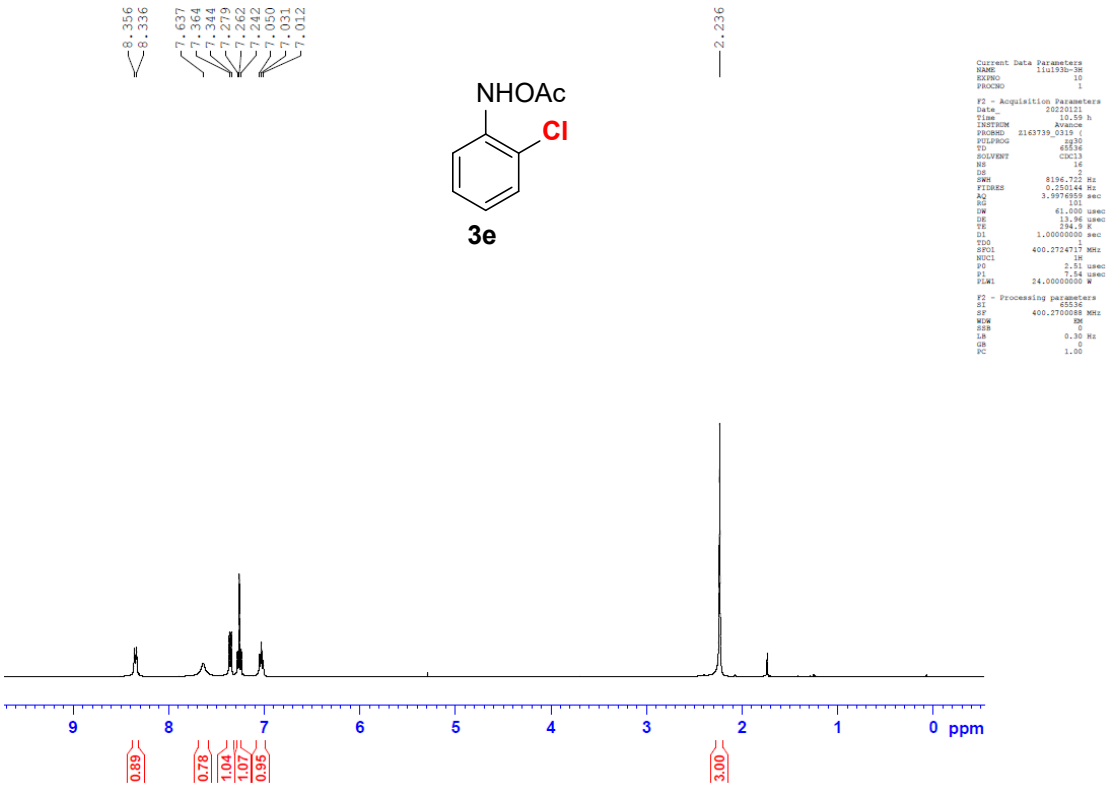
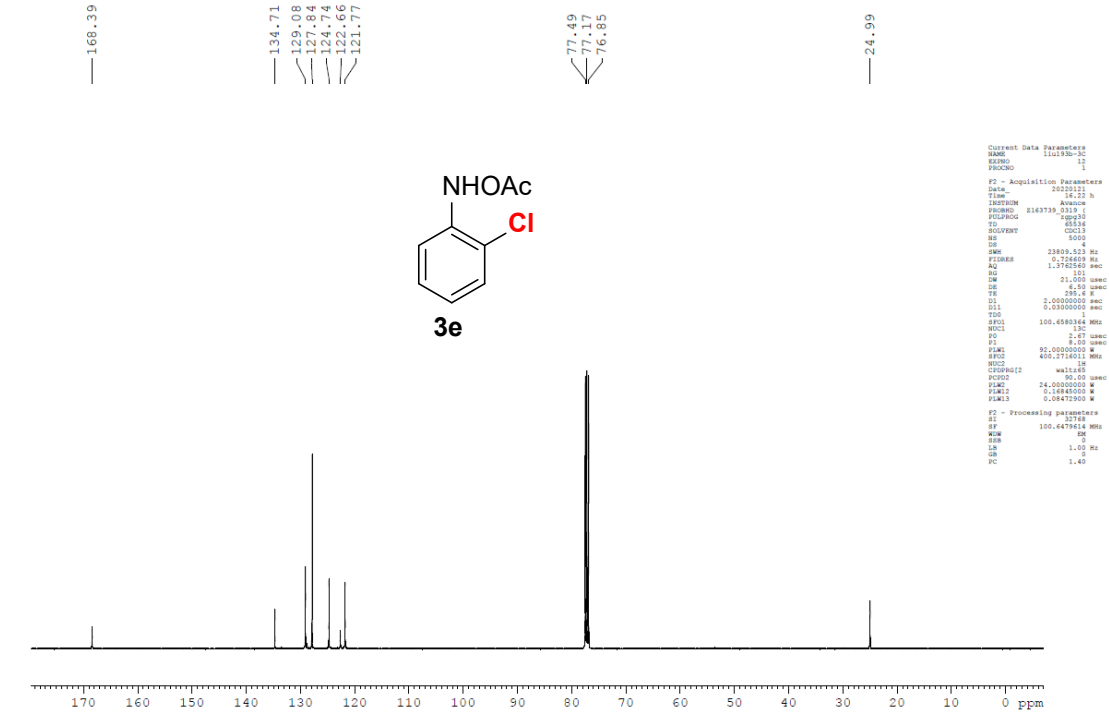
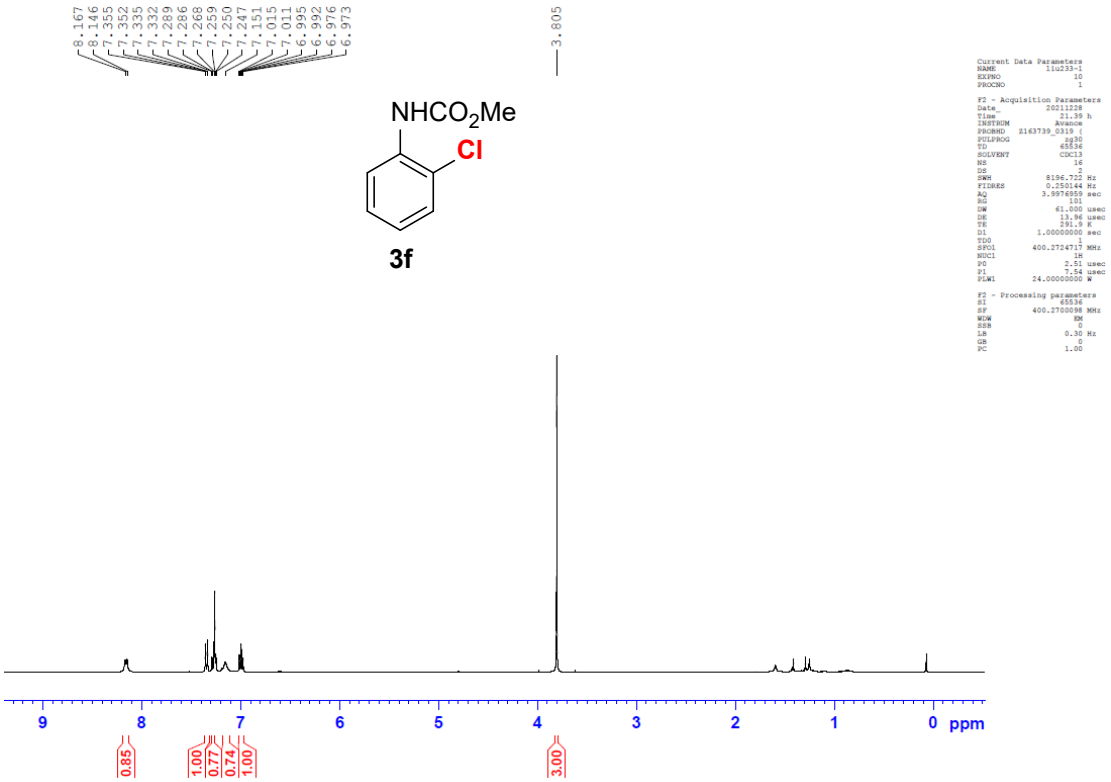
7.920
7.916
7.592
7.586
7.574
7.546
7.526
7.509
7.432
7.429
7.412
7.409
7.363
7.361
7.343
7.324
7.260
7.111
7.107
7.091
7.089
7.072
7.068
NHCOPh
Cl
3d
9
8
7
6
5
4
3
2
1
0 ppm
1.00
0.79
2.00
1.10
2.03
1.03
1.00
1.01


165.43
134.85
134.73
132.35
129.17
129.10
128.04
127.23
124.89
123.13
121.60
77.48
77.16
76.84
NHCOPh
Cl
3d
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
ppm


8.356
8.336
7.637
7.364
7.344
7.279
7.262
7.242
7.050
7.031
7.012
2.236
NHOAc
Cl
3e
9
8
7
6
5
4
3
2
1
0 ppm
0.89
0.78
1.04
1.07
0.95
3.00


168.39
134.71
129.08
127.84
124.74
122.66
121.77
77.49
77.17
76.85
24.99
NHOAc
Cl
3e
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0 ppm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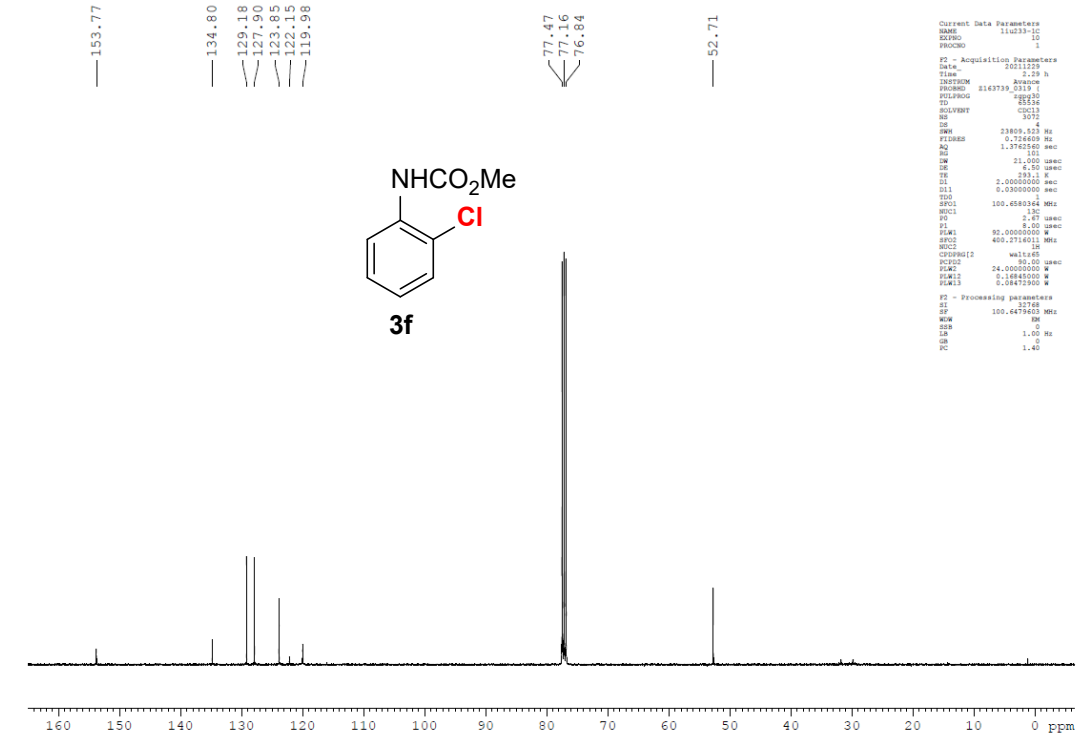
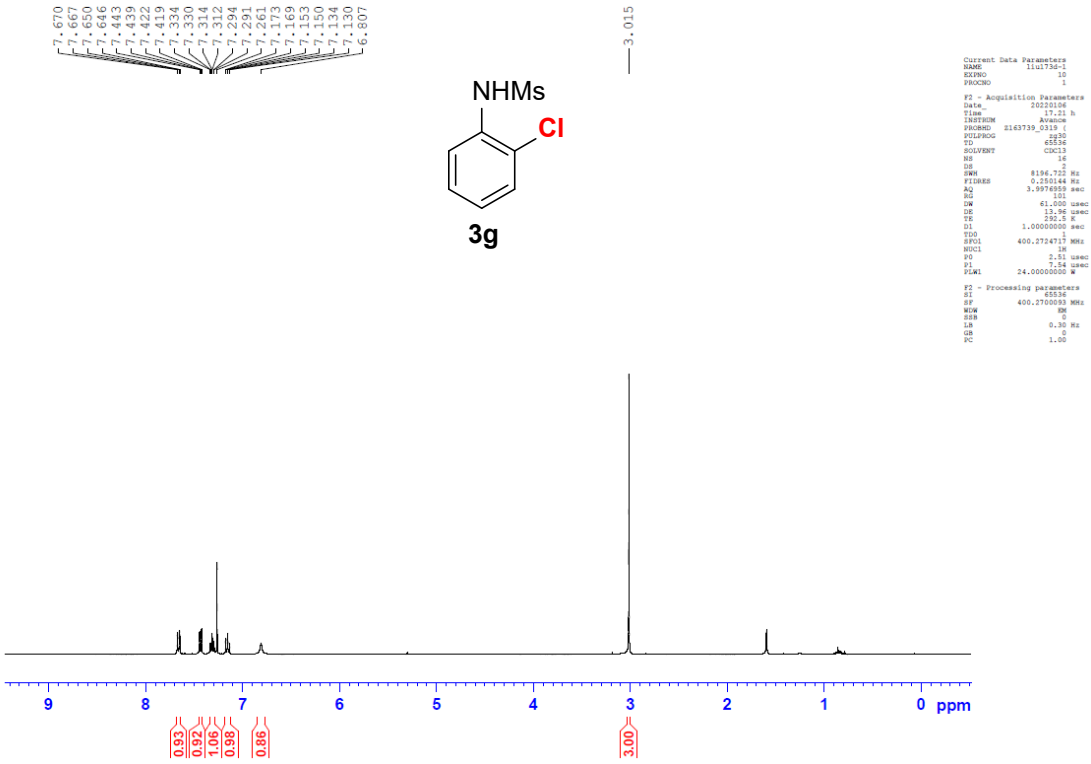
7.335
7.332
7.289
7.286
7.268
7.259
7.250
7.247
7.151
7.015
7.011
6.995
6.992
6.976
6.973
3.805
NHCO2Me
Cl
3f
9
8
7
6
5
4
3
2
1
0 ppm
0.85
1.00
0.77
0.74
1.00
3.00


153.77
134.80
129.18
127.90
123.85
122.15
119.98
77.47
77.16
76.84
52.71
NHCO2Me
Cl
3f
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0 ppm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7.667
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7.646
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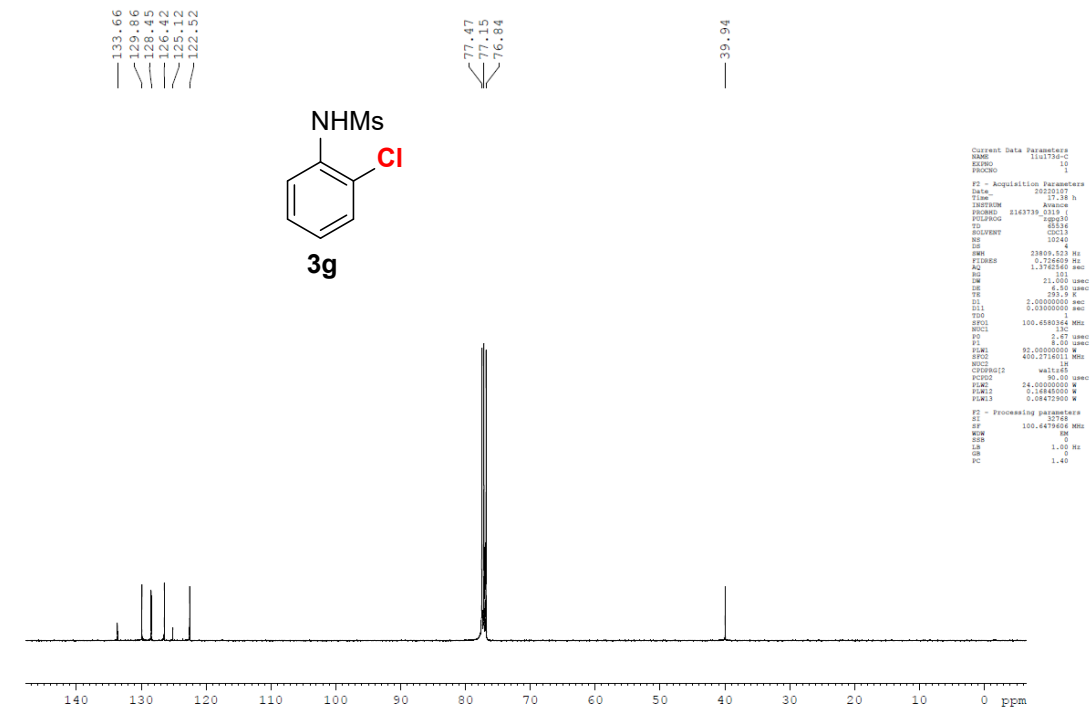
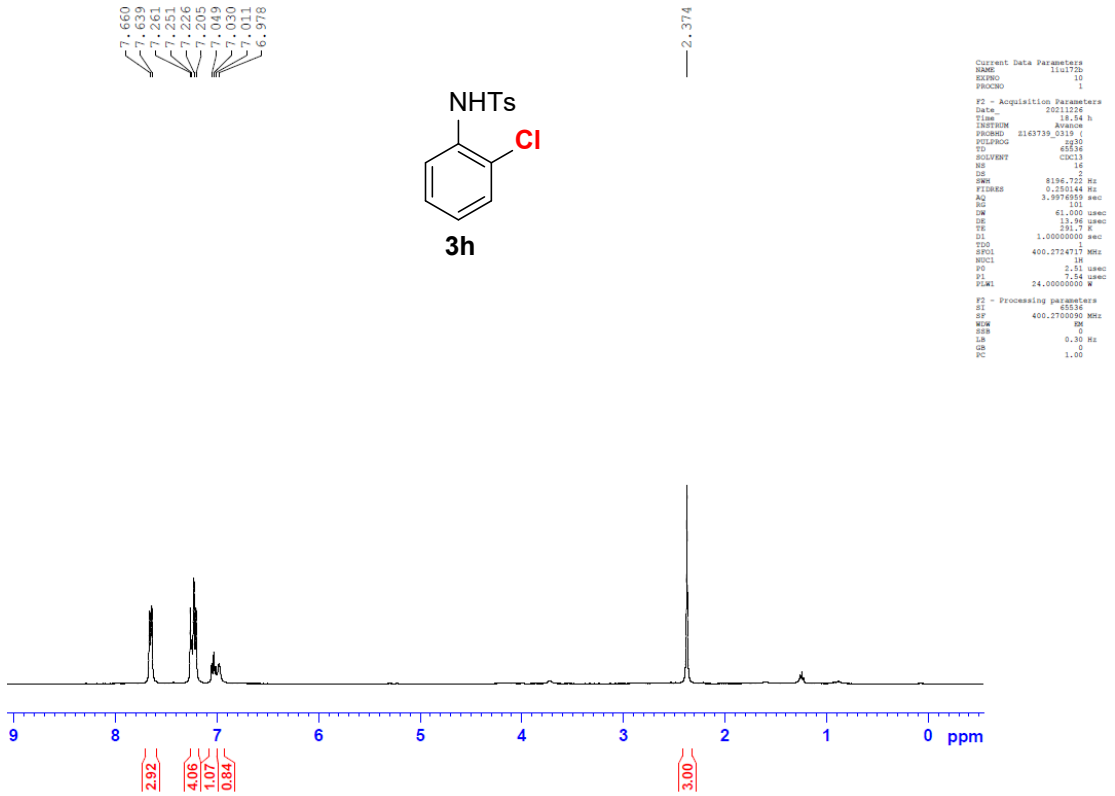
7.439
7.422
7.419
7.334
7.330
7.314
7.312
7.294
7.291
7.261
7.173
7.169
7.153
7.150
7.134
7.130
6.807
3.015
NHMs
Cl
3g
9
8
7
6
5
4
3
2
1
0
ppm
0.93
0.92
1.06
0.98
0.86
3.00


133.66
129.86
128.45
126.42
125.12
122.52
77.47
77.15
76.84
39.94
NHMs
Cl
3g
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
ppm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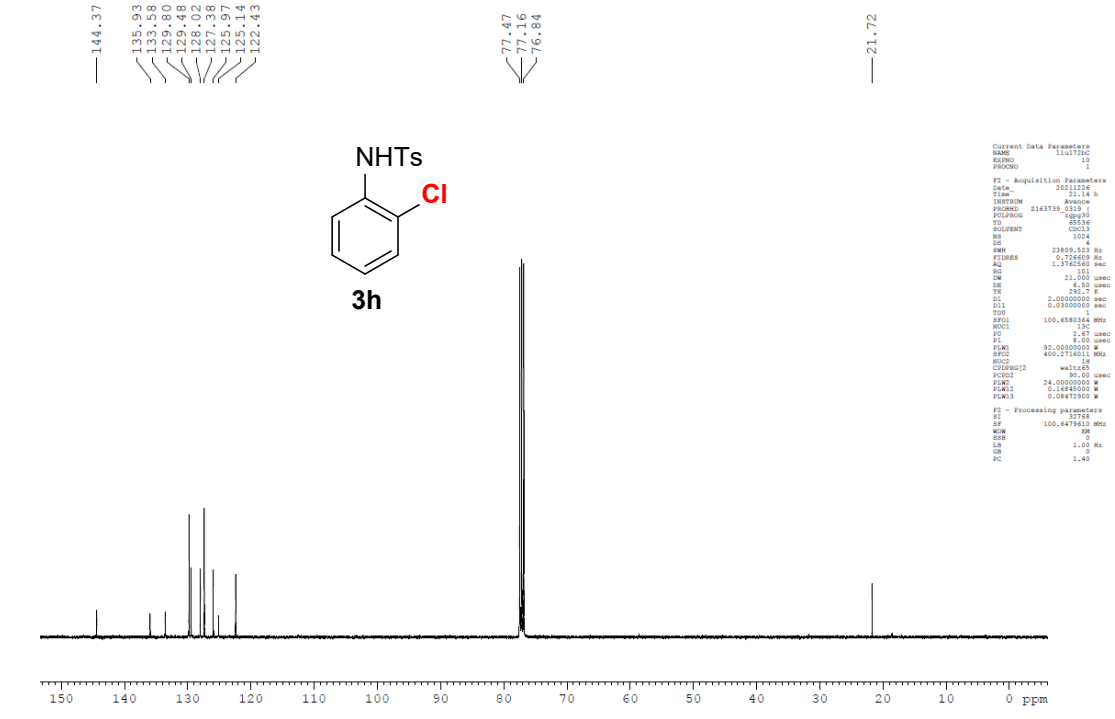
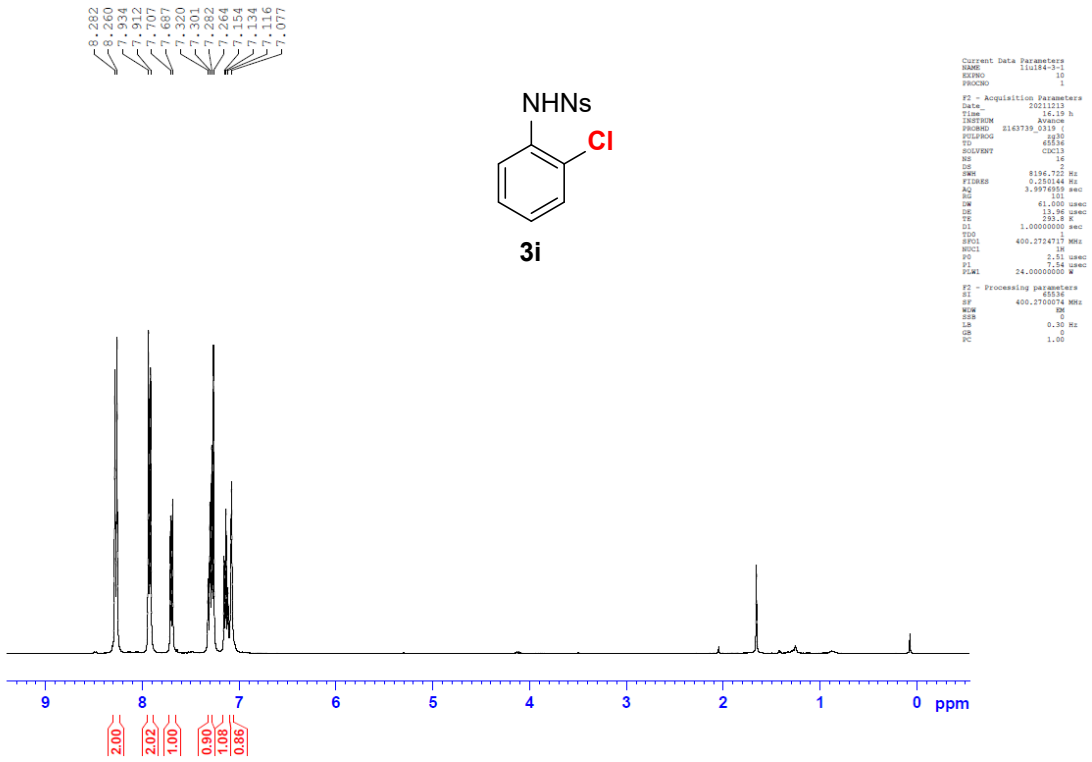
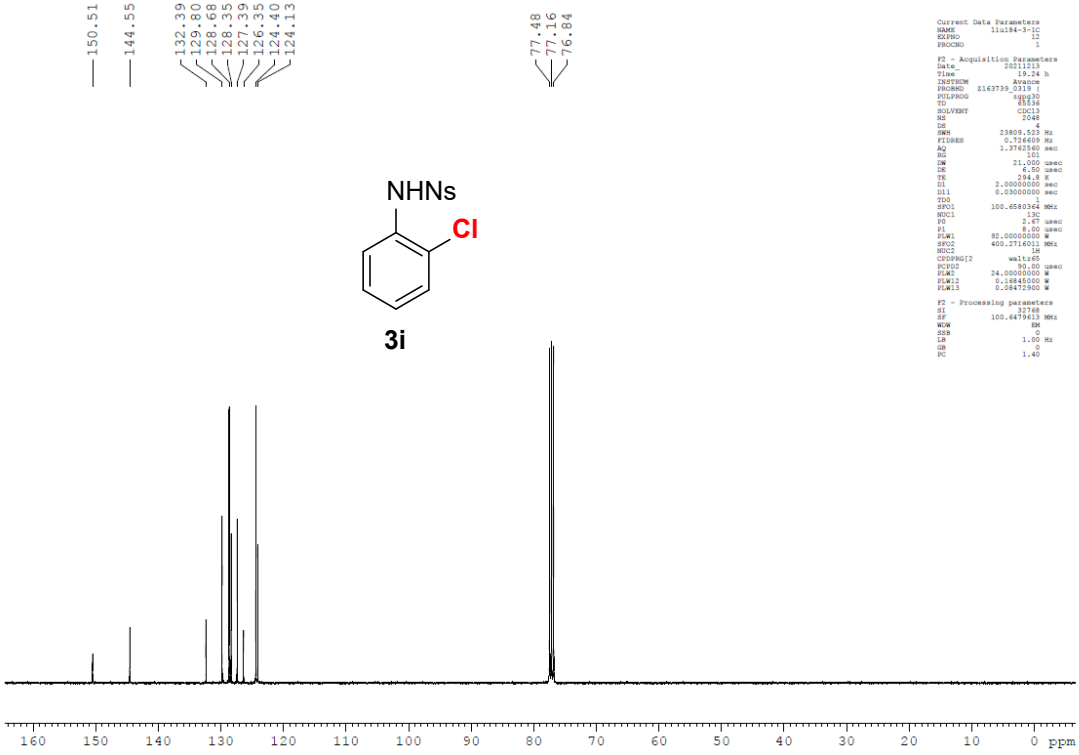
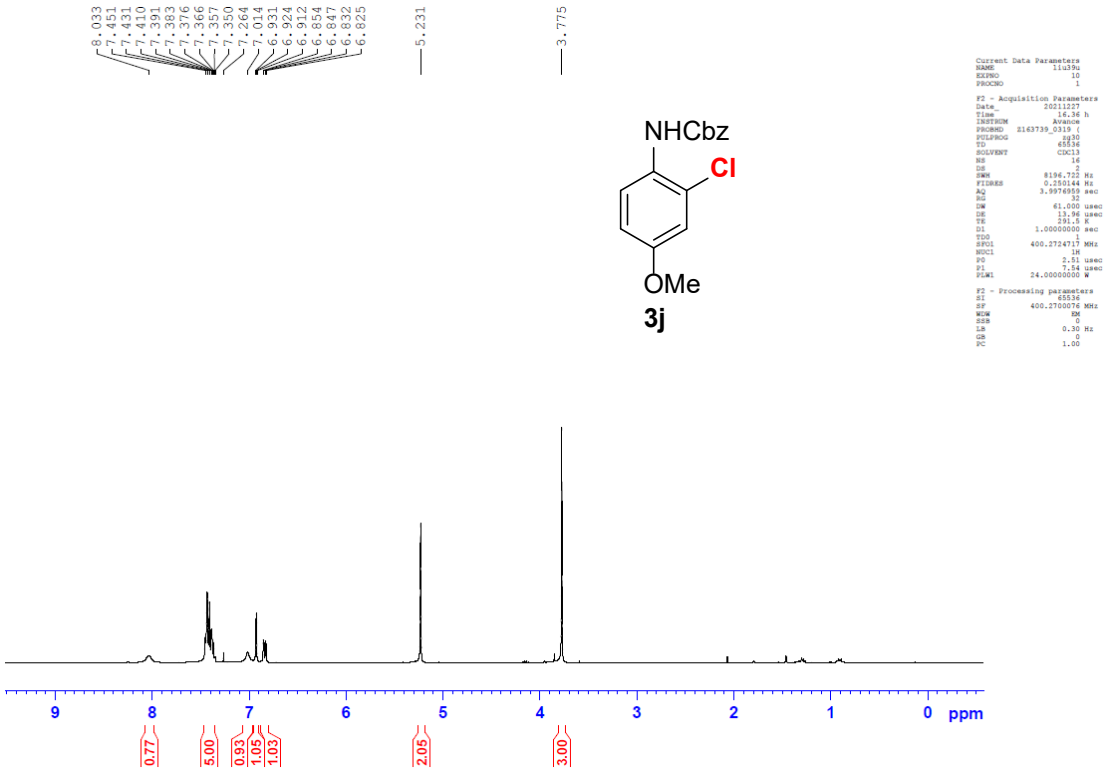
7.639
7.261
7.251
7.226
7.205
7.049
7.030
7.011
6.978
2.374
NHTs
Cl
3h
9
8
7
6
5
4
3
2
1
0
ppm
2.92
4.06
1.07
0.84
3.00


144.37
135.93
133.58
129.80
129.48
128.02
127.38
125.97
125.14
122.43
77.47
77.16
76.84
21.72
NHTs
Cl
3h
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
ppm


8.282
8.260
7.934
7.912
7.707
7.687
7.320
7.301
7.282
7.264
7.154
7.134
7.116
7.077
NHNs
Cl
3i
9
8
7
6
5
4
3
2
1
0 ppm
2.00
2.02
1.00
0.90
1.08
0.86


150.51
144.55
132.39
129.80
128.68
128.35
127.39
126.35
124.40
124.13
77.48
77.16
76.84
NHNs
Cl
3i
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0 ppm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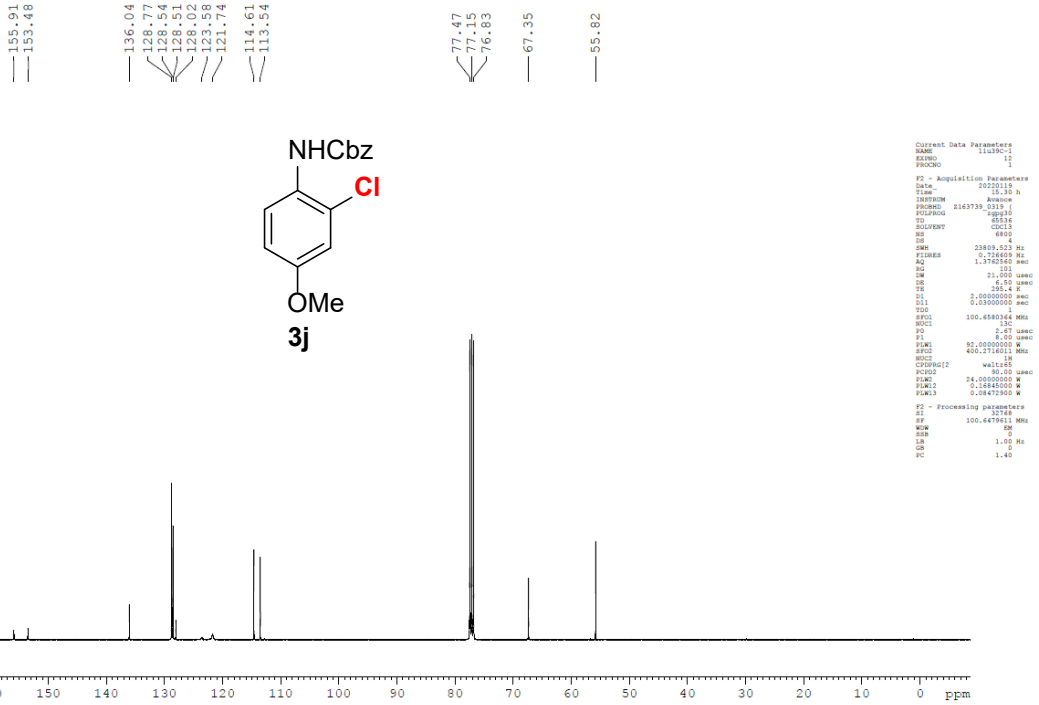
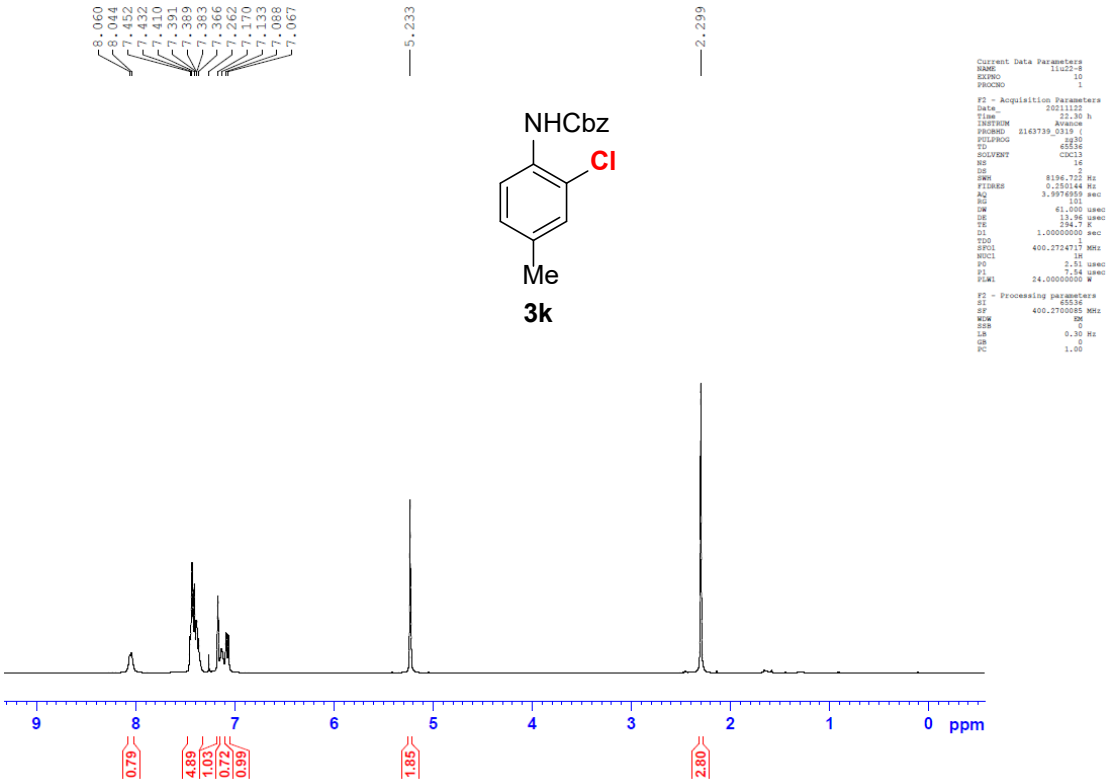
7.451
7.431
7.410
7.391
7.383
7.376
7.366
7.357
7.350
7.264
7.014
6.931
6.924
6.912
6.854
6.847
6.832
6.825
5.231
3.775
NHCbz
Cl
OMe
3j
9
8
7
6
5
4
3
2
1
0
ppm
0.77
5.00
0.93
1.05
1.03
2.05
3.00


155.91
153.48
136.04
128.77
128.54
128.51
128.02
123.58
121.74
114.61
113.54
77.47
77.15
76.83
67.35
55.82
NHCbz
Cl
OMe
3j
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
ppm


8.060
8.044
7.452
7.432
7.410
7.391
7.389
7.383
7.366
7.262
7.170
7.133
7.088
7.067
5.233
2.299
NHCbz
Cl
Me
3k
9
8
7
6
5
4
3
2
1
0
ppm
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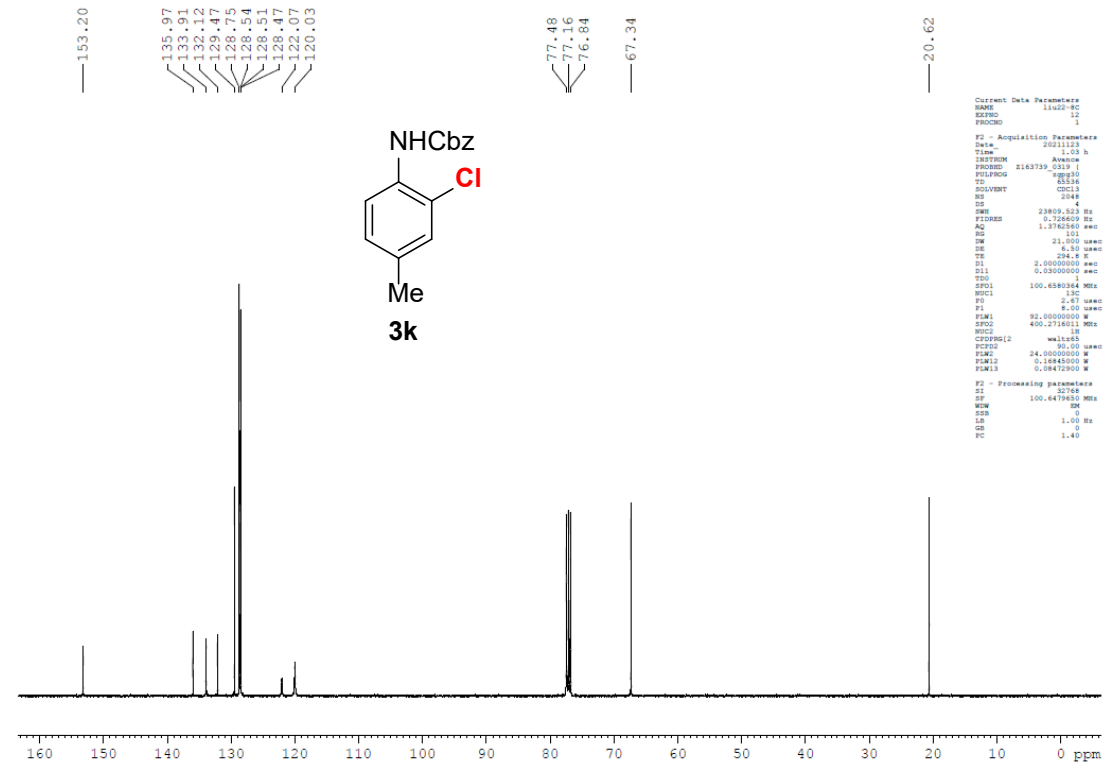
1.03
0.72
0.99
1.85
2.80


153.20
135.97
133.91
132.12
129.47
128.75
128.54
128.51
128.47
122.07
120.03
77.48
77.16
76.84
67.34
20.62
NHCbz
Cl
Me
3k
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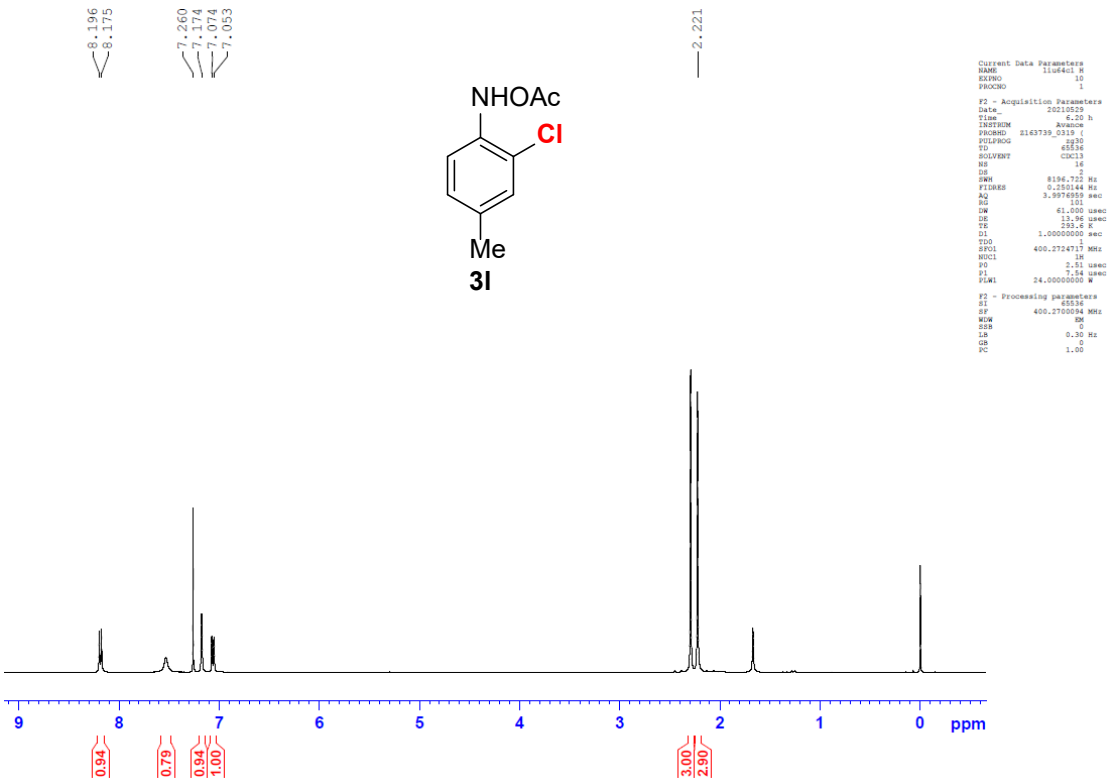
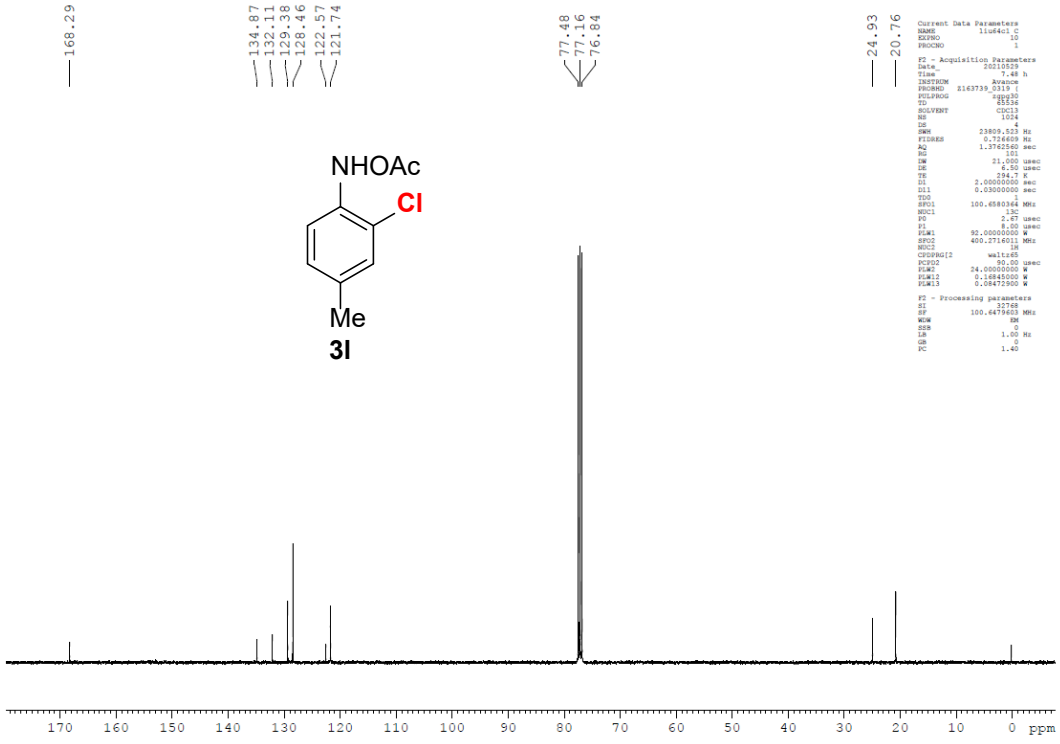
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
ppm


8.196
8.175
7.260
7.174
7.074
7.053
2.221
NHOAc
Cl
Me
3l
9
8
7
6
5
4
3
2
1
0
ppm
0.94
0.79
0.94
1.00
3.00
2.90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121.74
77.48
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76.84
24.93
20.76
NHOAc
Cl
Me
3l
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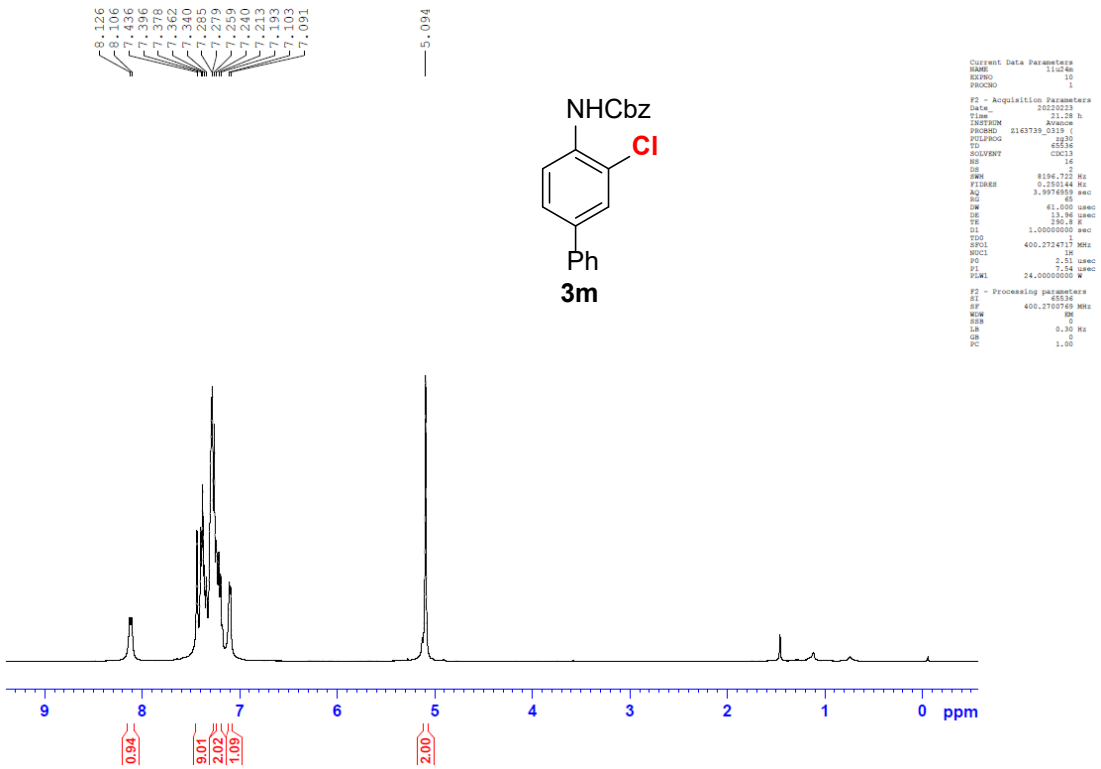
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7.285
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7.259
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7.213
7.193
7.103
7.091
5.094
NHCbz
Cl
Ph
3m
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6
5
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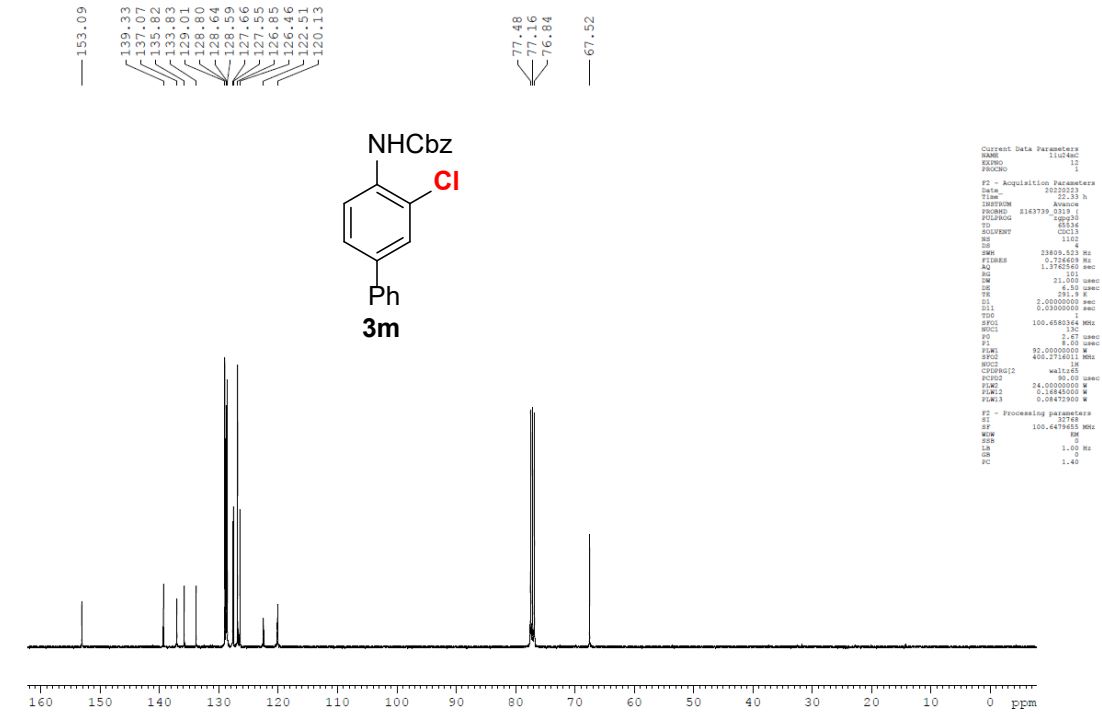
1.09
2.00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128.64
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127.55
126.85
126.46
122.51
120.13
77.48
77.16
76.84
67.52
NHCbz
Cl
Ph
3m
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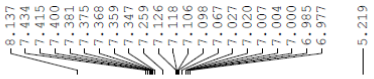
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7.359
7.347
7.259
7.126
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7.027
7.020
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7.004
7.000
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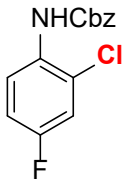
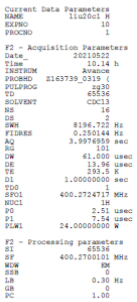
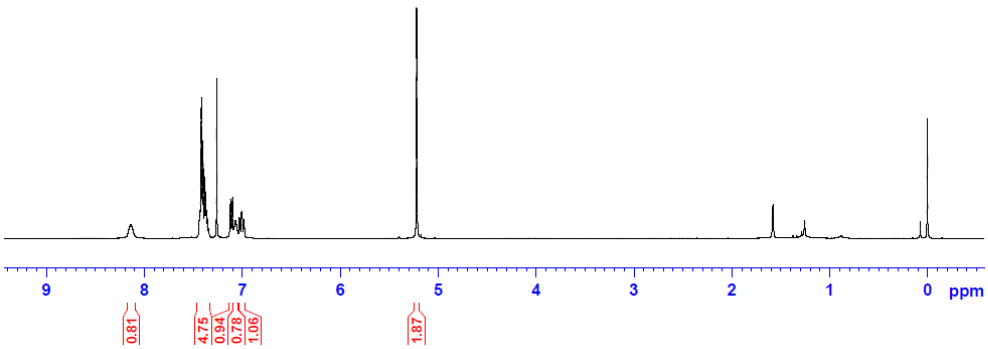
6.977
5.219


NHCbz
Cl
F

**3n**

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8
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3
2
1
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ppm
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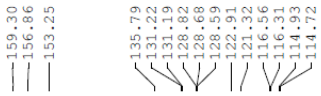
0.78
1.06
1.87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114.72
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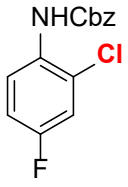
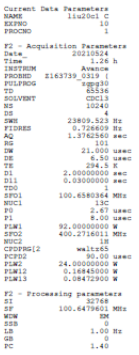
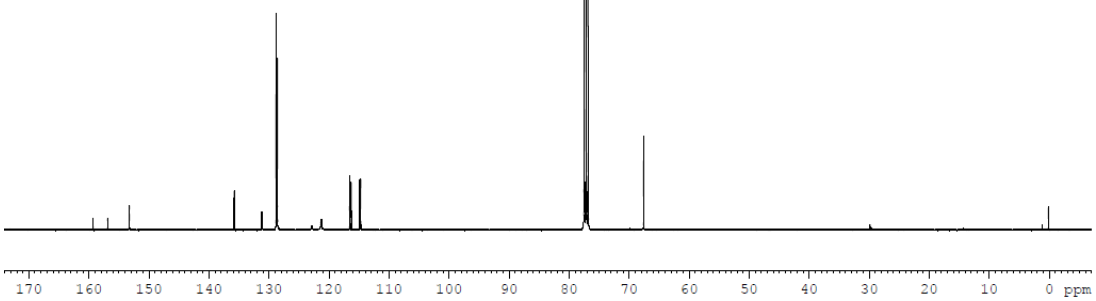
77.16
76.84
67.58


NHCbz
Cl
F

**3n**

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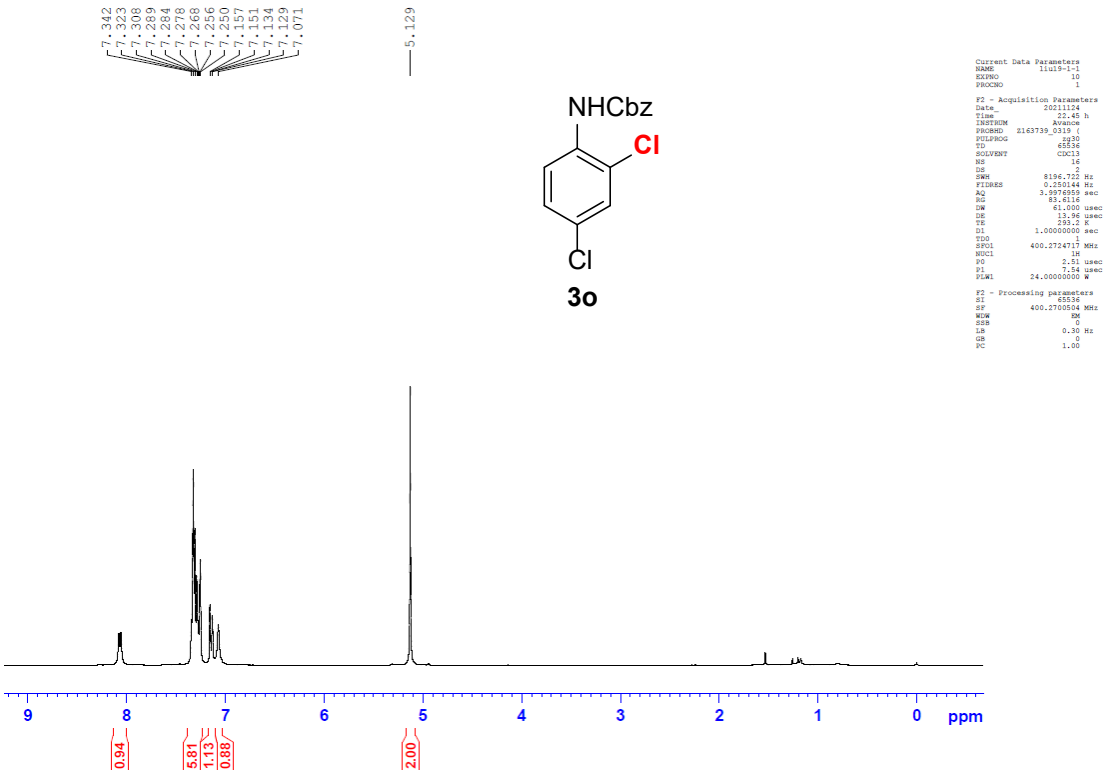
20
10
0
ppm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7.308
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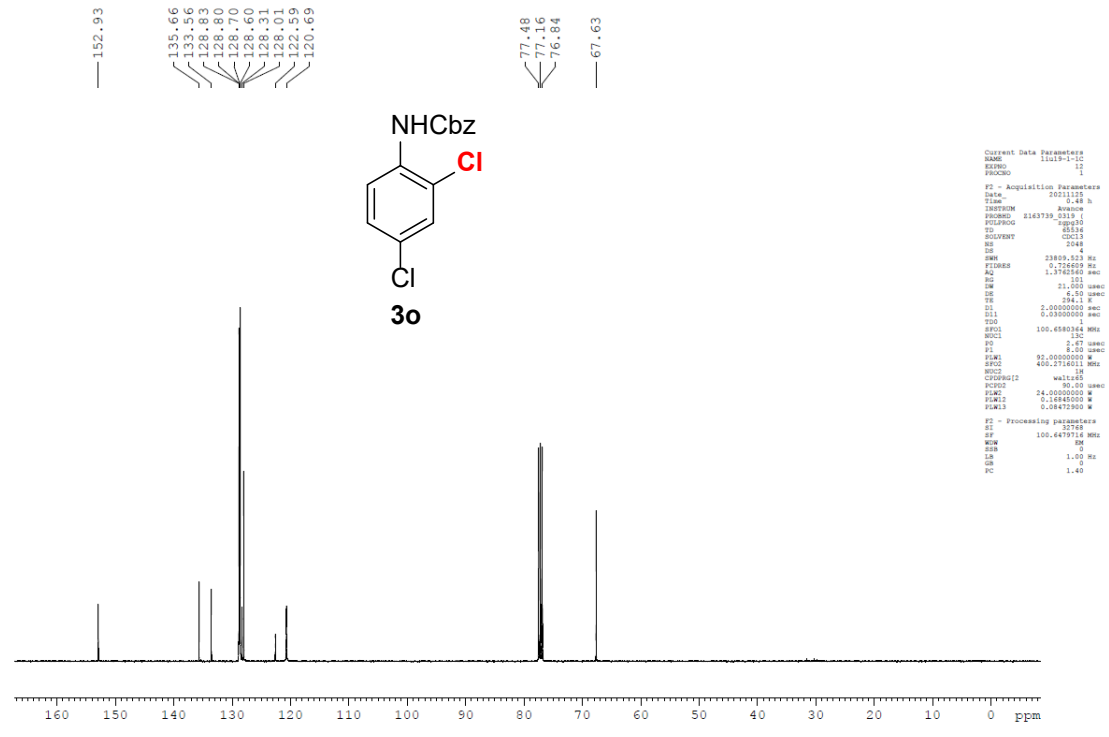
7.284
7.278
7.268
7.256
7.250
7.157
7.151
7.134
7.129
7.071
5.129
NHCbz
Cl
Cl
3o
9
8
7
6
5
4
3
2
1
0
ppm
0.94
5.81
1.13
0.88
2.00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120.69
77.48
77.16
76.84
67.63
NHCbz
Cl
Cl
3o
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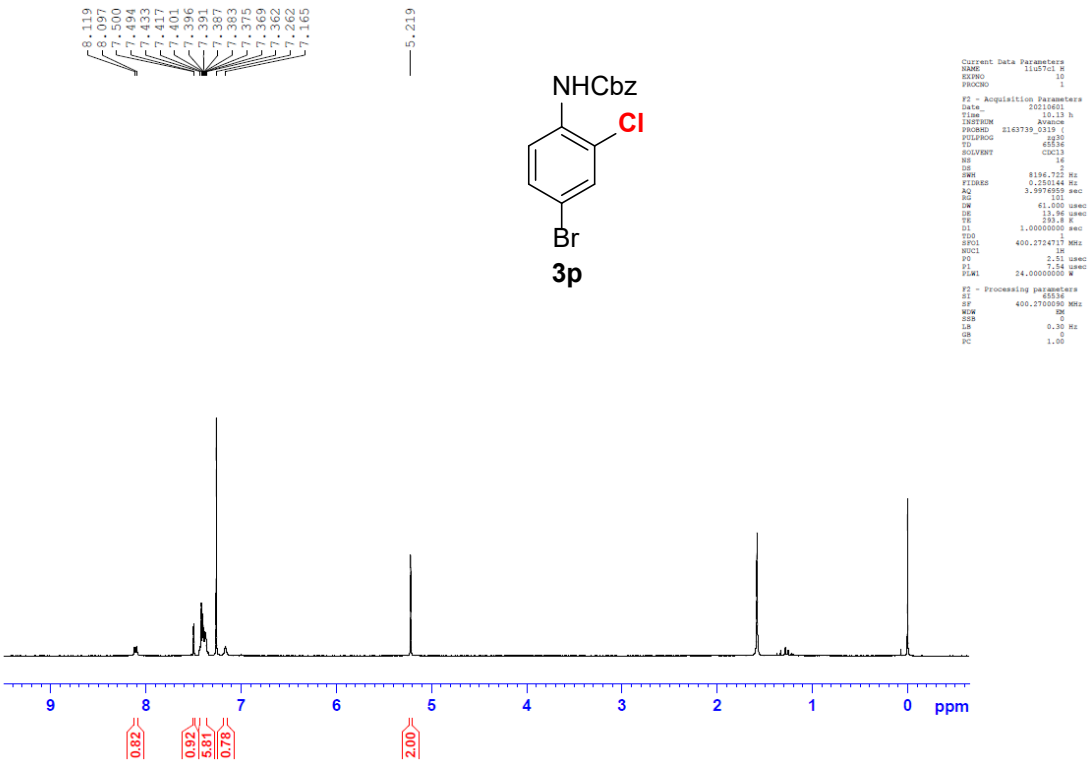
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
ppm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7.401
7.396
7.391
7.387
7.383
7.375
7.369
7.362
7.262
7.165
5.219
NHCbz
Cl
Br
3p
9
8
7
6
5
4
3
2
1
0
ppm
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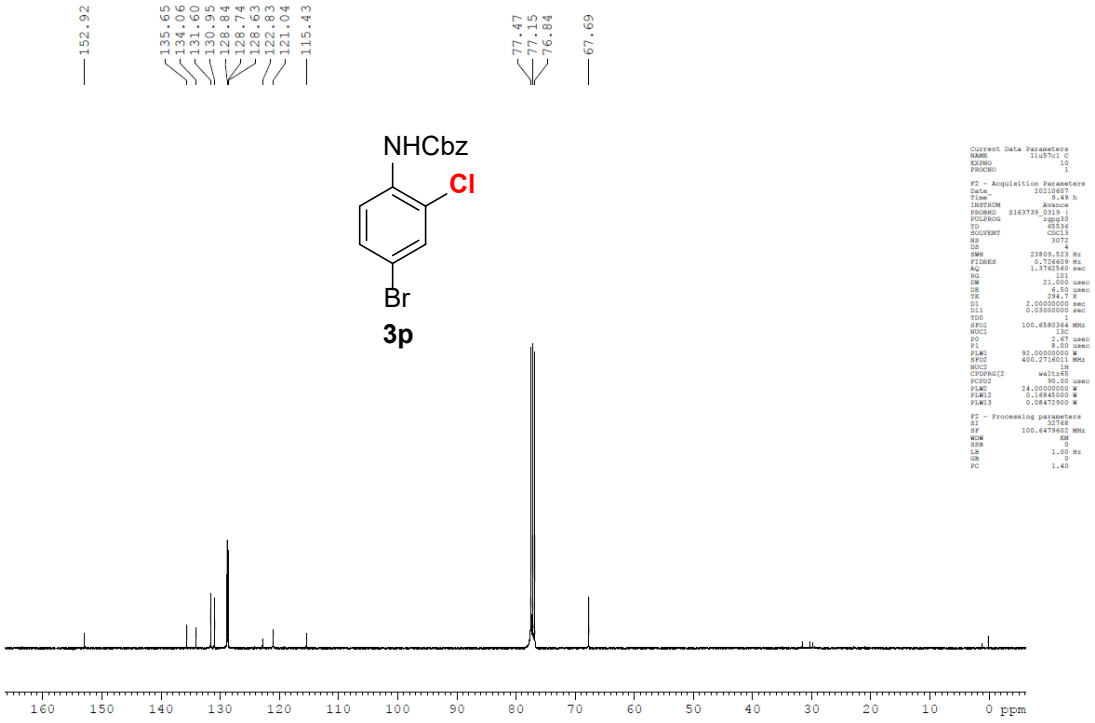
0.92
5.81
0.78
2.00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128.74
128.63
122.83
121.04
115.43
77.47
77.15
76.84
67.69
NHCbz
Cl
Br
3p
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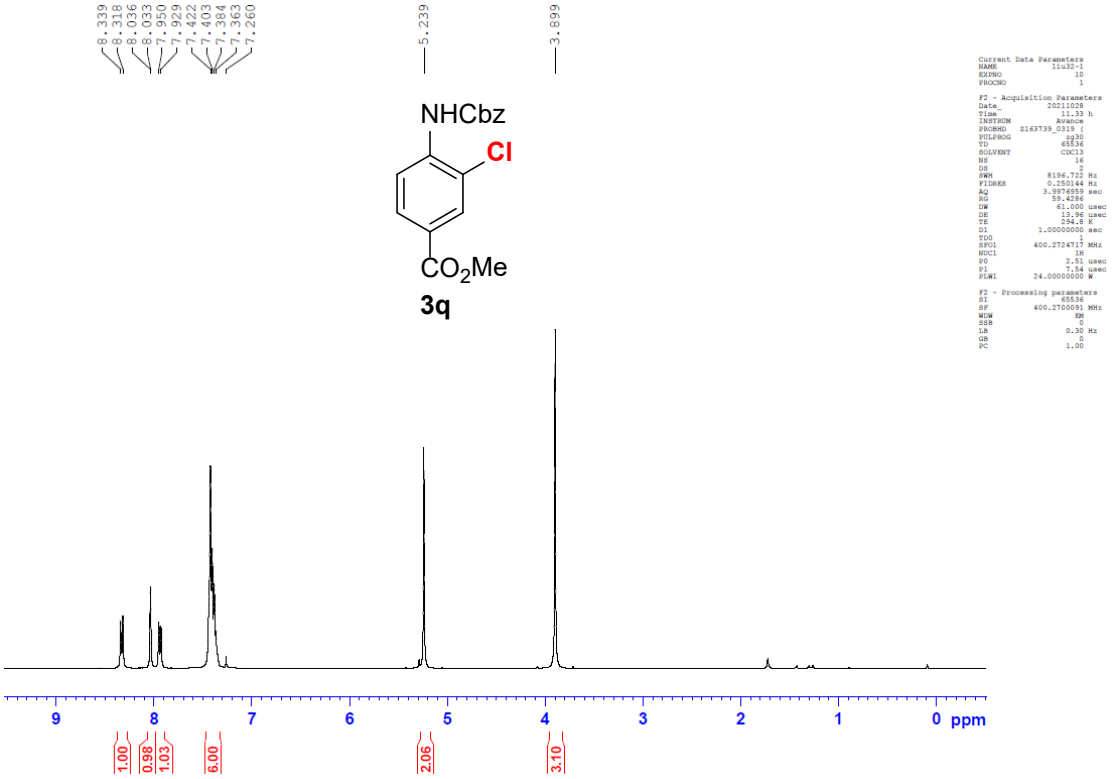
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0 ppm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7.403
7.384
7.363
7.260
5.239
3.899
NHCbz
Cl
CO2Me
3q
9
8
7
6
5
4
3
2
1
0 ppm
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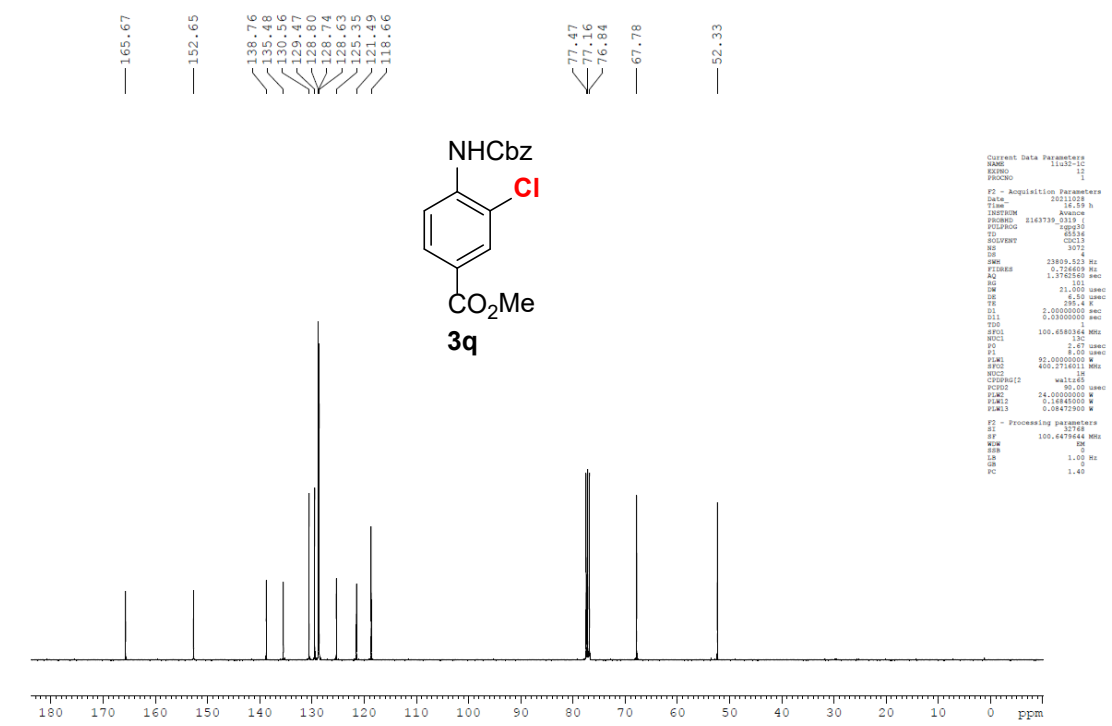
0.98
1.03
6.00
2.06
3.10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128.74
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125.35
121.49
118.66
77.47
77.16
76.84
67.78
52.33
NHCbz
Cl
CO2Me
3q
180
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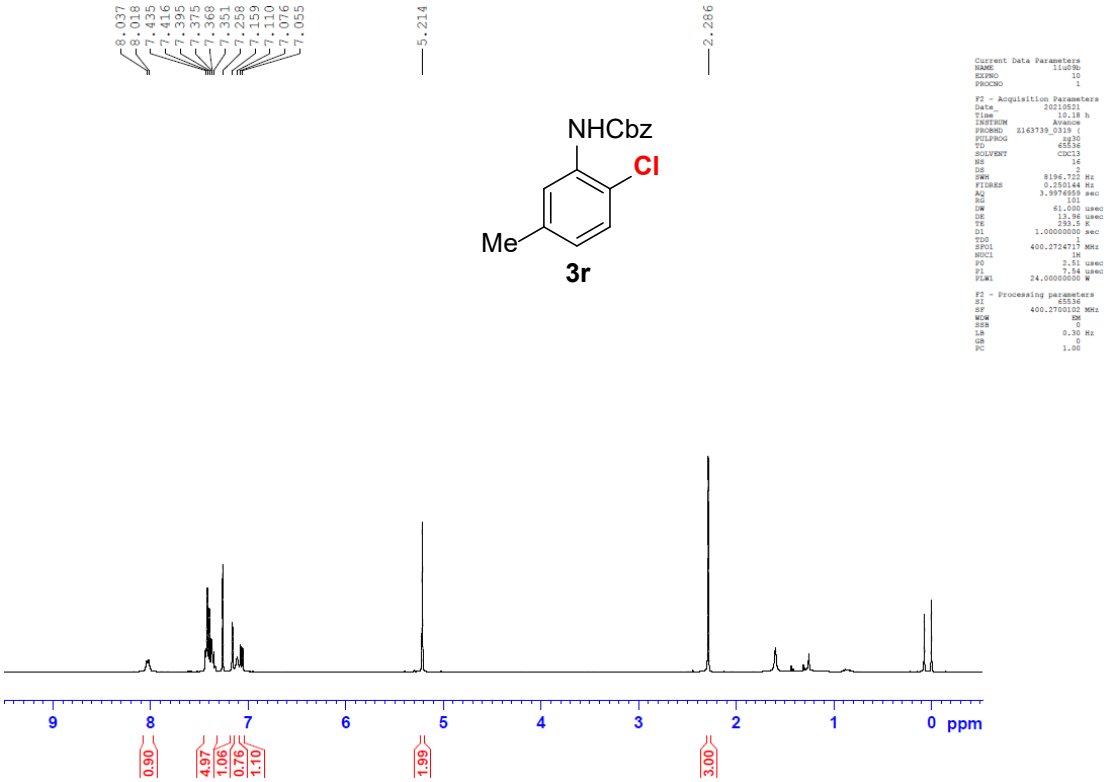
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0 ppm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7.159
7.110
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7.055
5.214
2.286
NHCbz
Cl
Me
3r
9
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6
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3
2
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1.06
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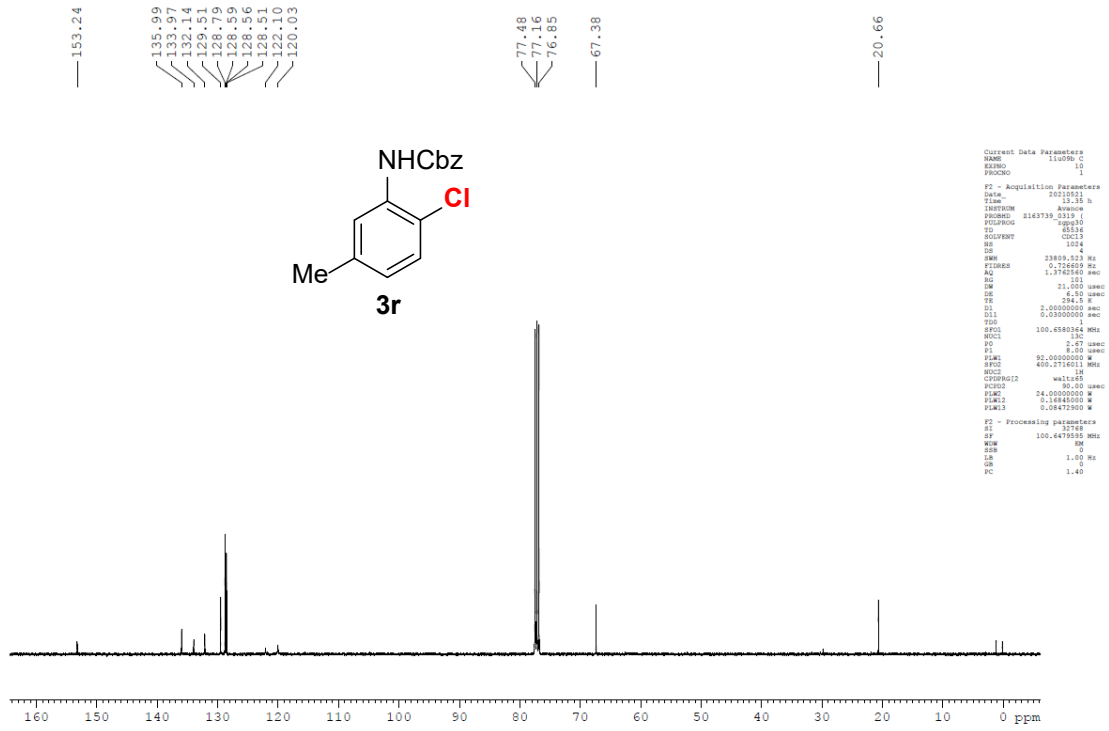
1.10
1.99
3.00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128.56
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122.10
120.03
77.48
77.16
76.85
67.38
20.66
NHCbz
Cl
Me
3r
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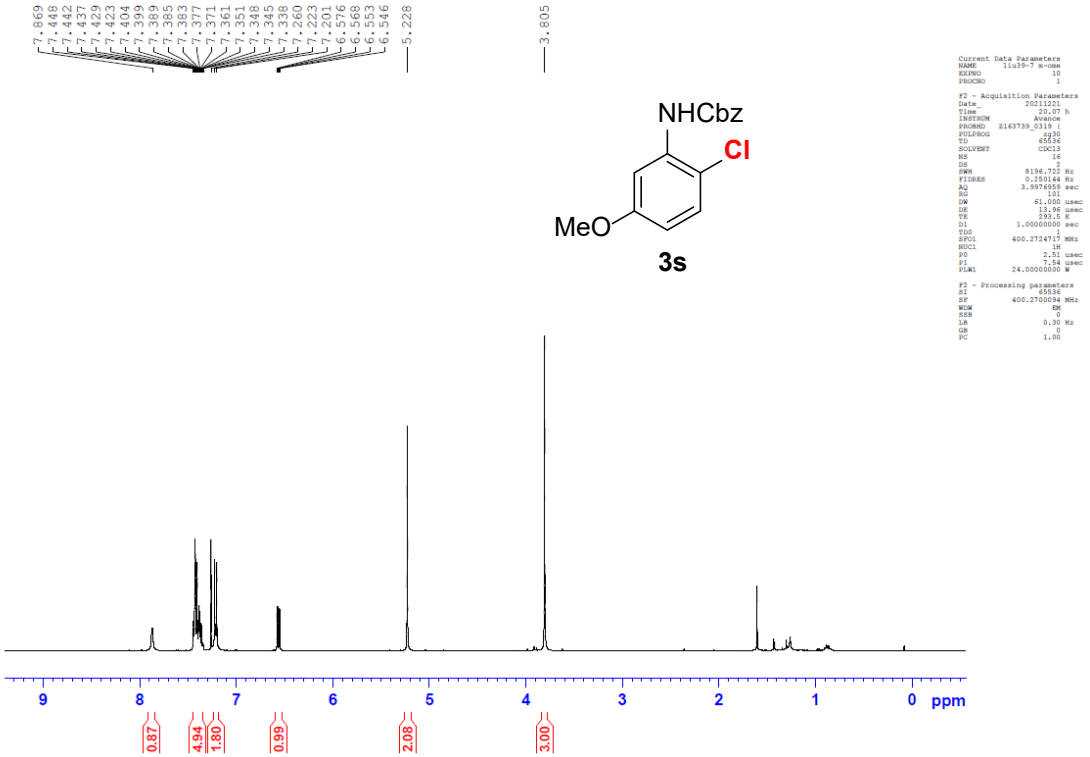
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0 ppm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7.371
7.361
7.351
7.348
7.345
7.338
7.260
7.223
7.201
6.576
6.568
6.553
6.546
5.228
3.805
NHCbz
Cl
MeO
3s
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4
3
2
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0
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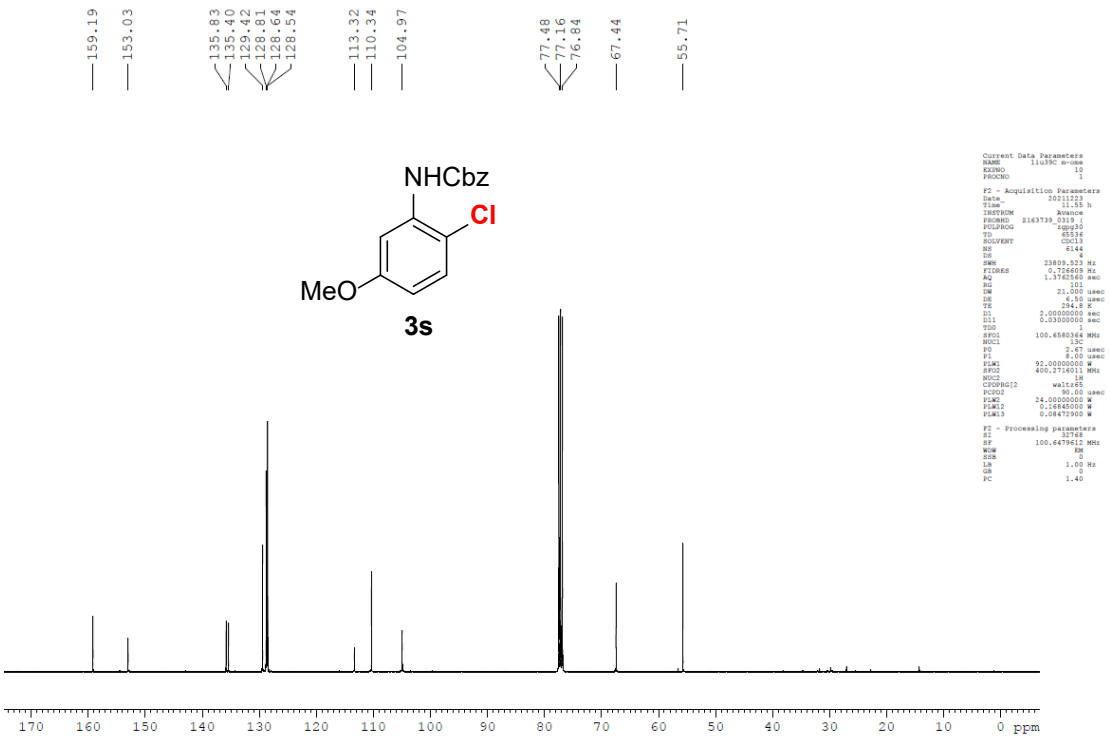
3.00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128.54
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110.34
104.97
77.48
77.16
76.84
67.44
55.71
NHCbz
Cl
MeO
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140
130
120
110
100
90
80
70
60
50
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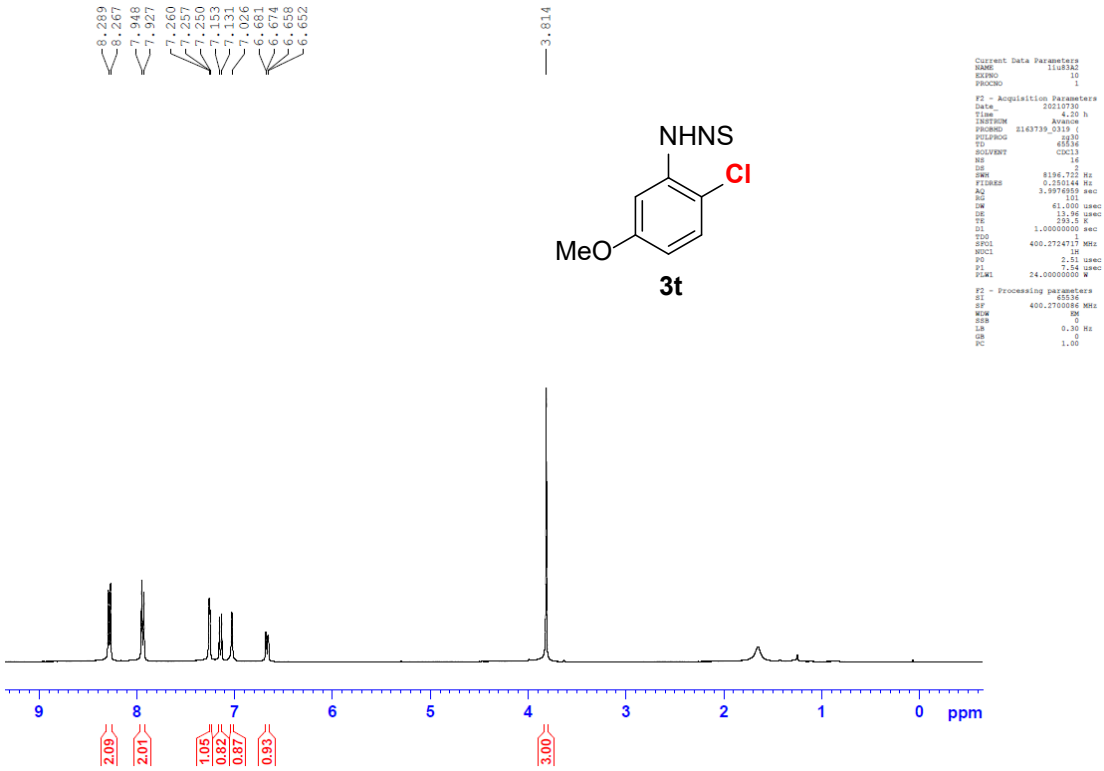
20
10
0
ppm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7.153
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6.674
6.658
6.652
3.814
NHNS
Cl
MeO
3t
9
8
7
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5
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1.05
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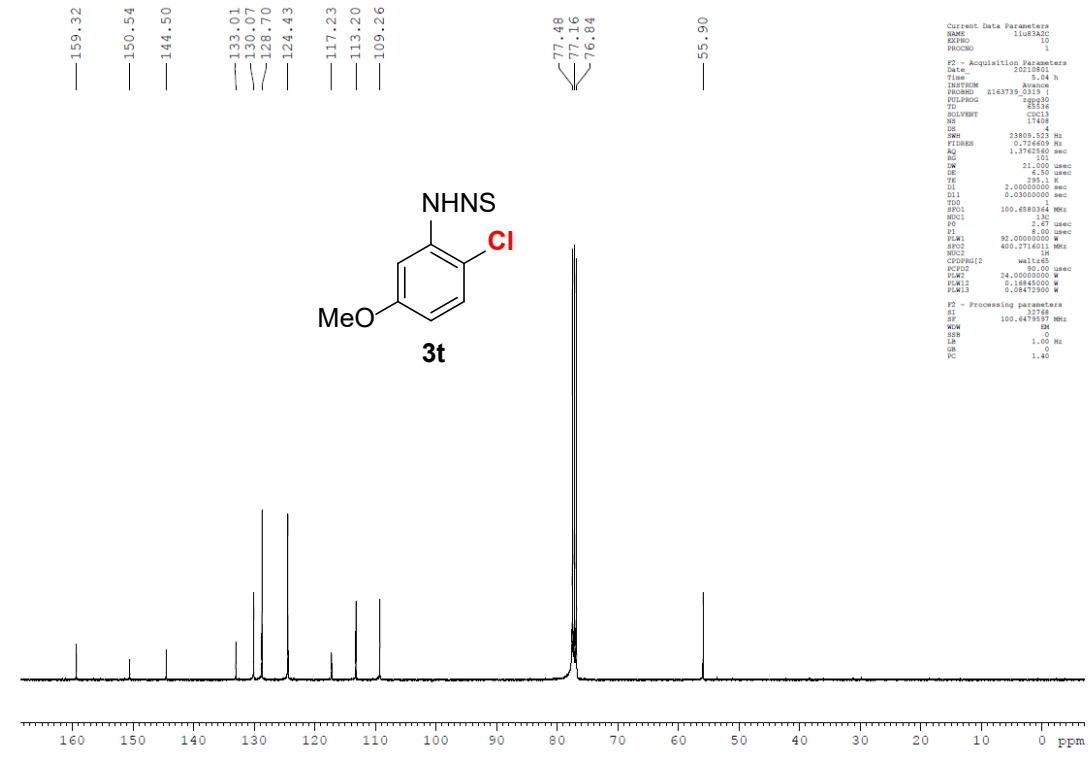
3.00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128.70
124.43
117.23
113.20
109.26
77.48
77.16
76.84
55.90
NHNS
Cl
MeO
3t
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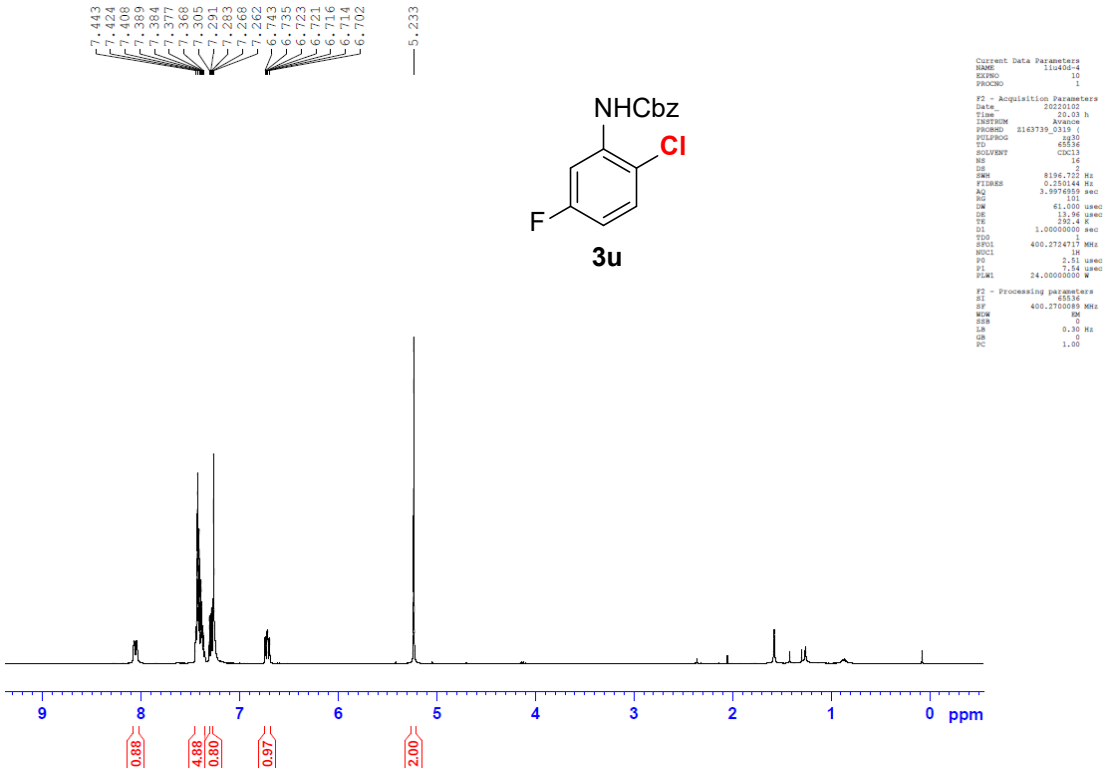
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
ppm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7.291
7.283
7.268
7.262
6.743
6.735
6.723
6.721
6.716
6.714
6.702
5.233
NHCbz
Cl
F
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5
4
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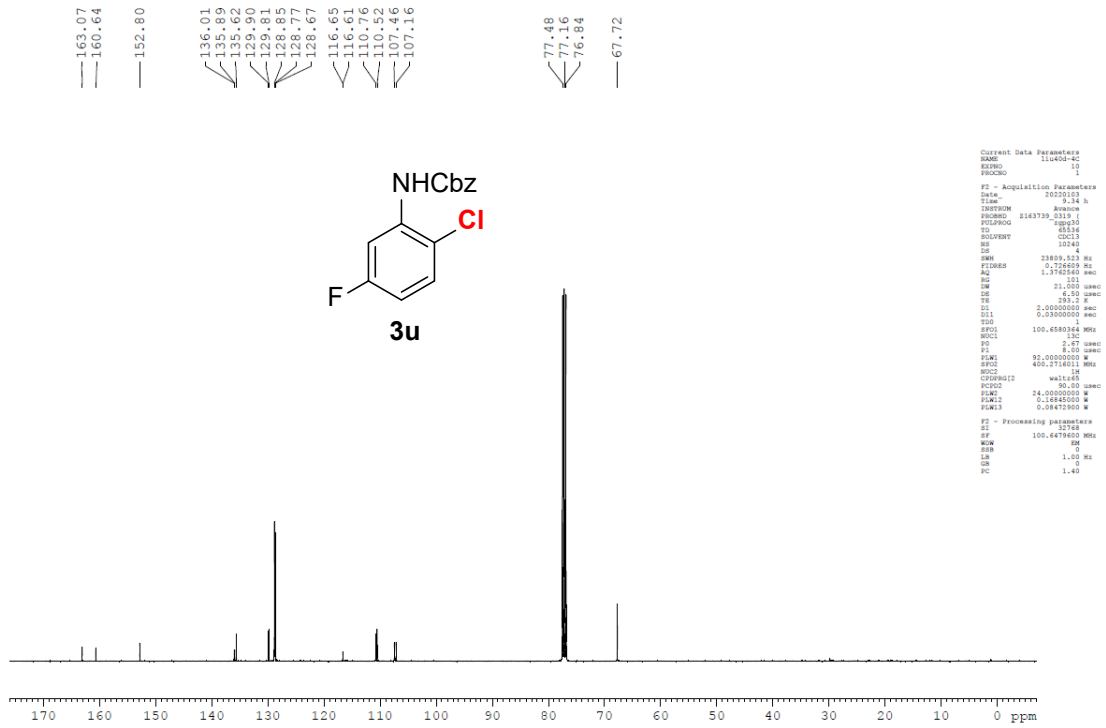
0.97
2.00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128.77
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116.65
116.61
110.76
110.52
107.46
107.16
77.48
77.16
76.84
67.72
NHCbz
Cl
F
3u
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140
130
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100
90
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70
60
50
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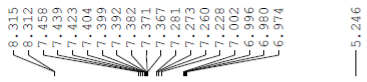
20
10
0
ppm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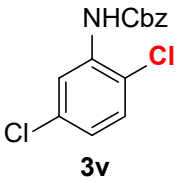
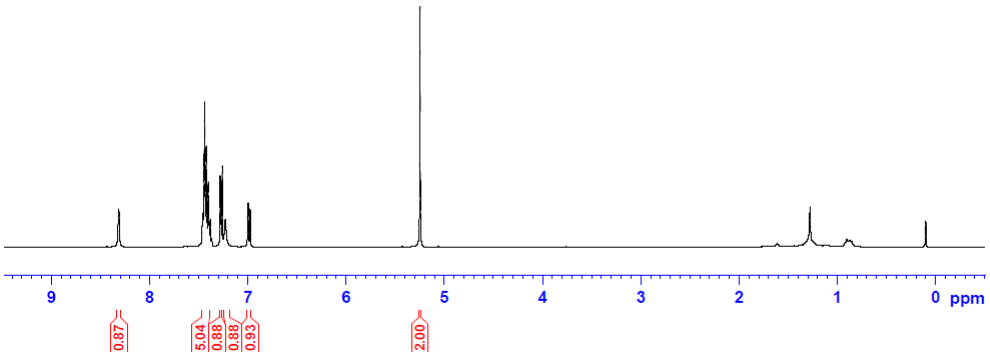
7.228
7.002
6.996
6.980
6.974


NHCbz
Cl
Cl

3v


9
8
7
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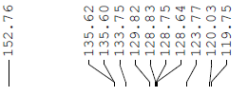
5
4
3
2
1
0 ppm
0.87
5.04
0.88
0.88
0.93
2.00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77.16
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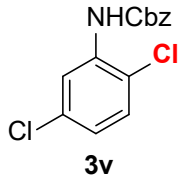
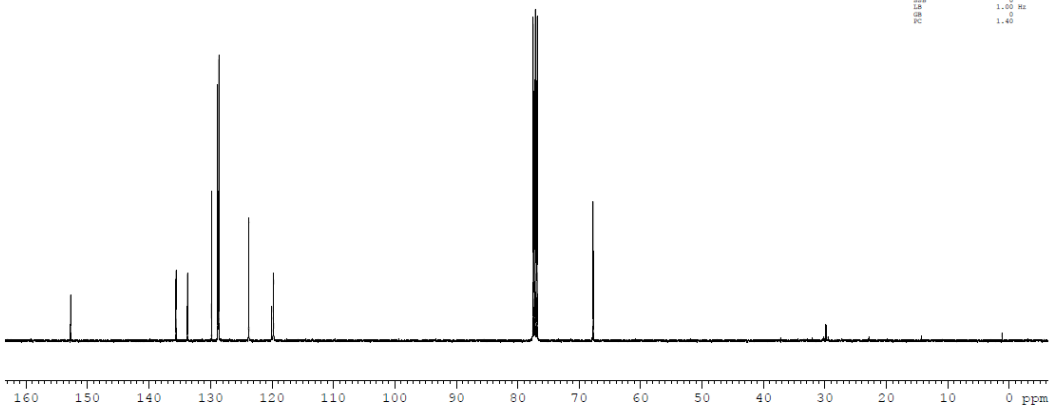
67.72


NHCbz
Cl
Cl

3v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100
90
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70
60
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30
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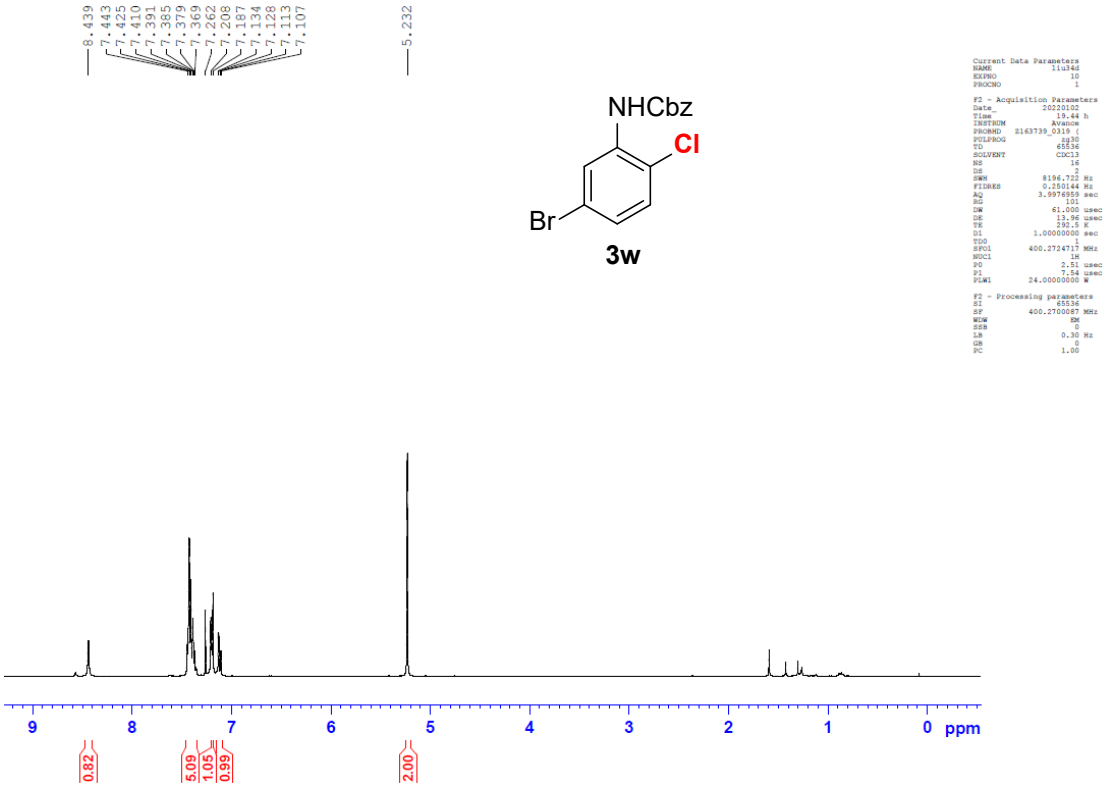
10
0 ppm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7.113
7.107
5.232
NHCbz
Cl
Br
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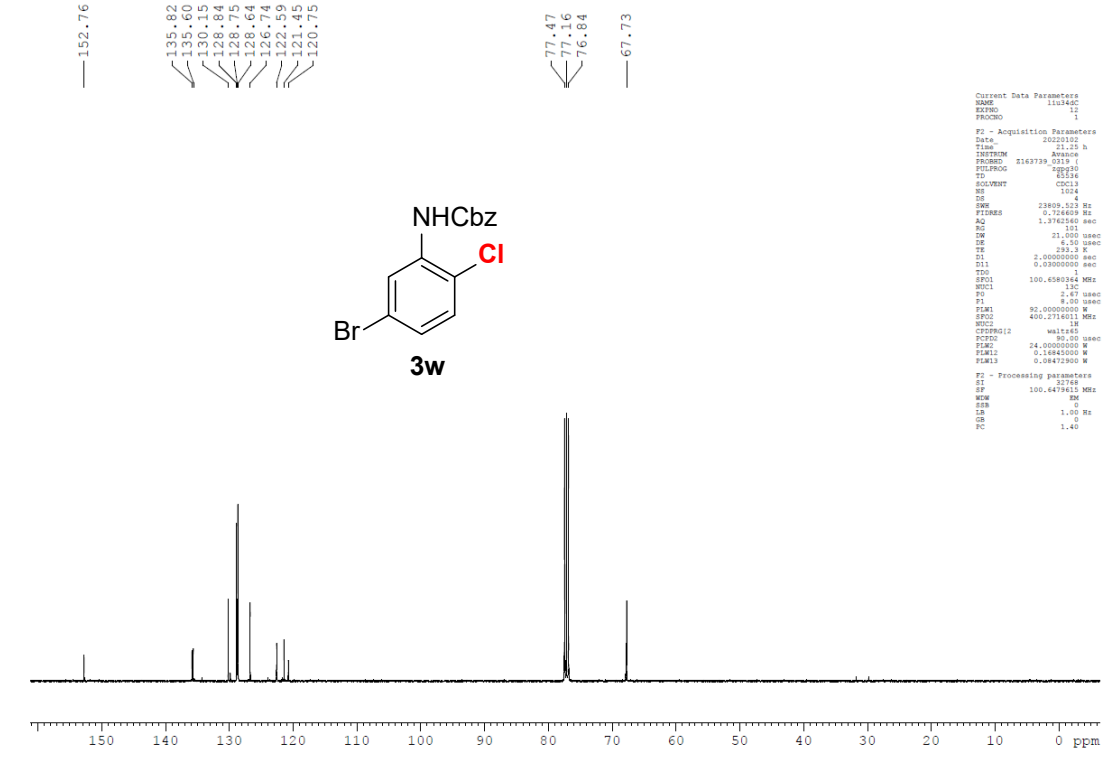
2.00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126.74
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121.45
120.75
77.47
77.16
76.84
67.73
NHCbz
Cl
Br
3w
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120
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100
90
80
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60
50
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20
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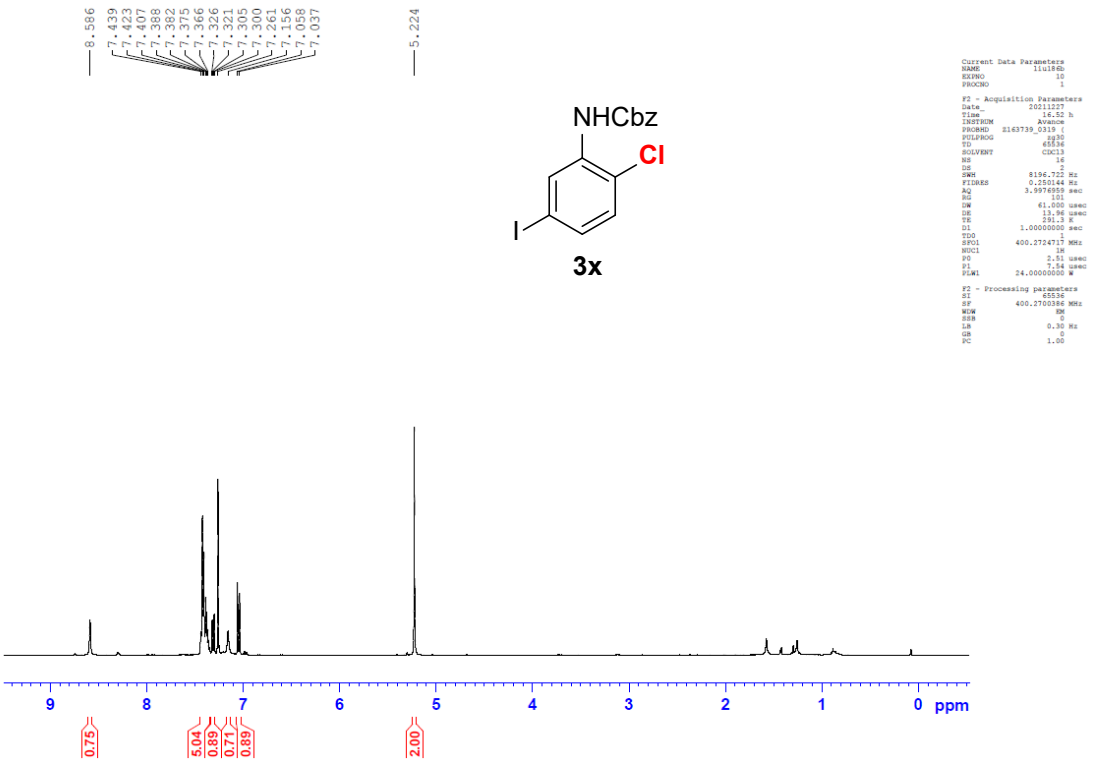
0
ppm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7.382
7.375
7.366
7.326
7.321
7.305
7.300
7.261
7.156
7.058
7.037
5.224
NHCbz
Cl
I
3x
9
8
7
6
5
4
3
2
1
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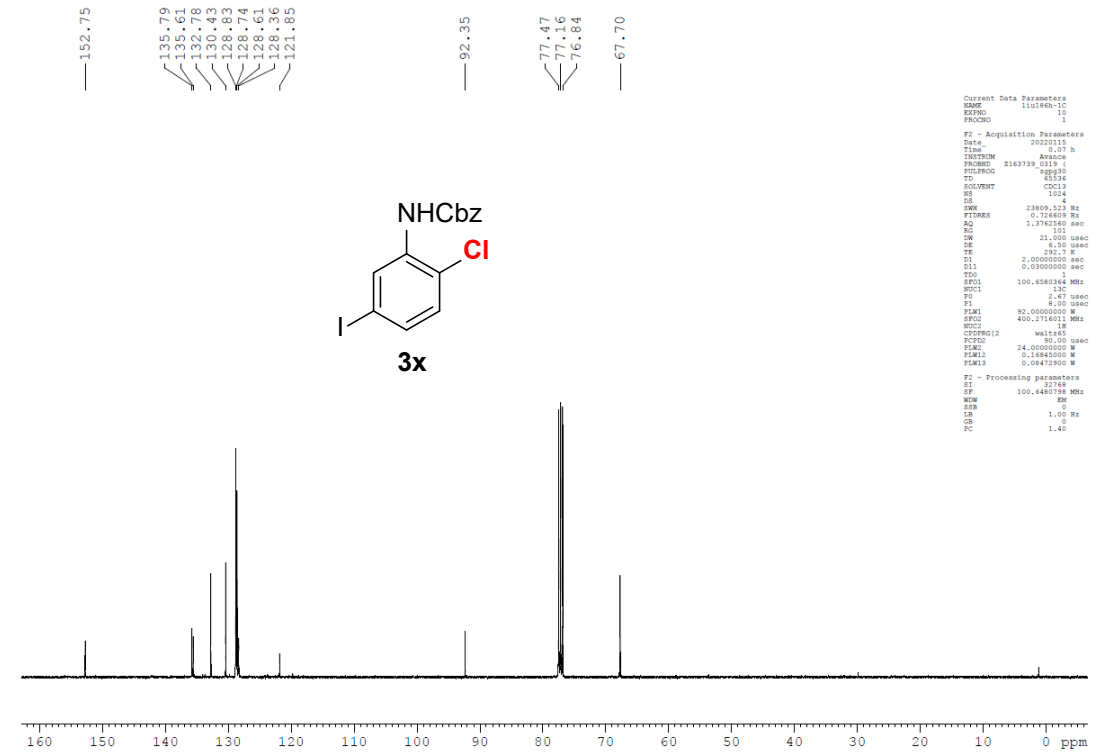
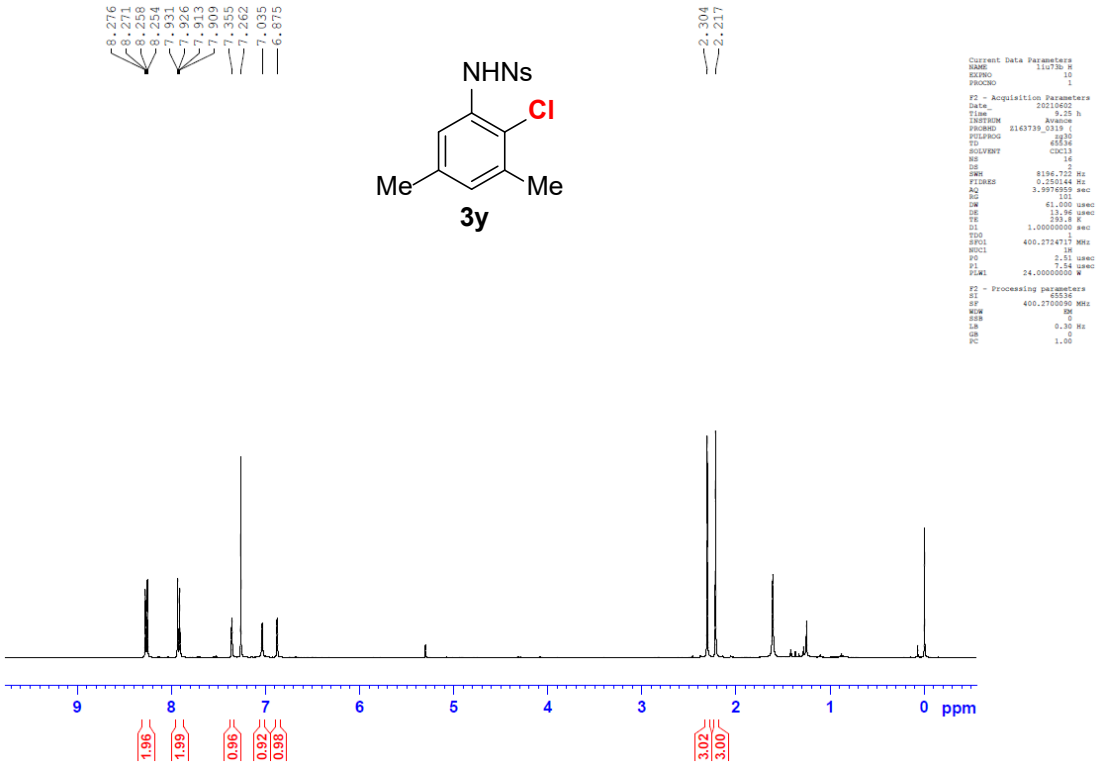
0.75
5.04
0.89
0.71
0.89
2.00


152.75
135.79
135.61
132.78
130.43
128.83
128.74
128.61
128.36
121.85
92.35
77.47
77.16
76.84
67.70
NHCbz
Cl
I
3x
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0 ppm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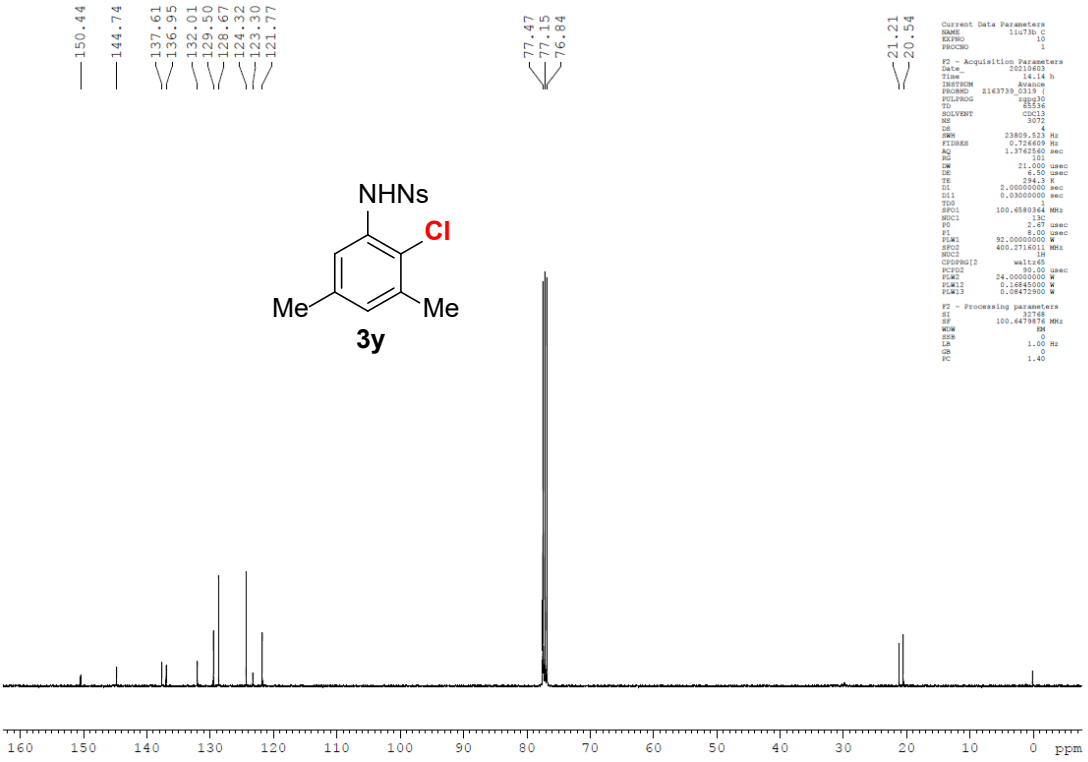
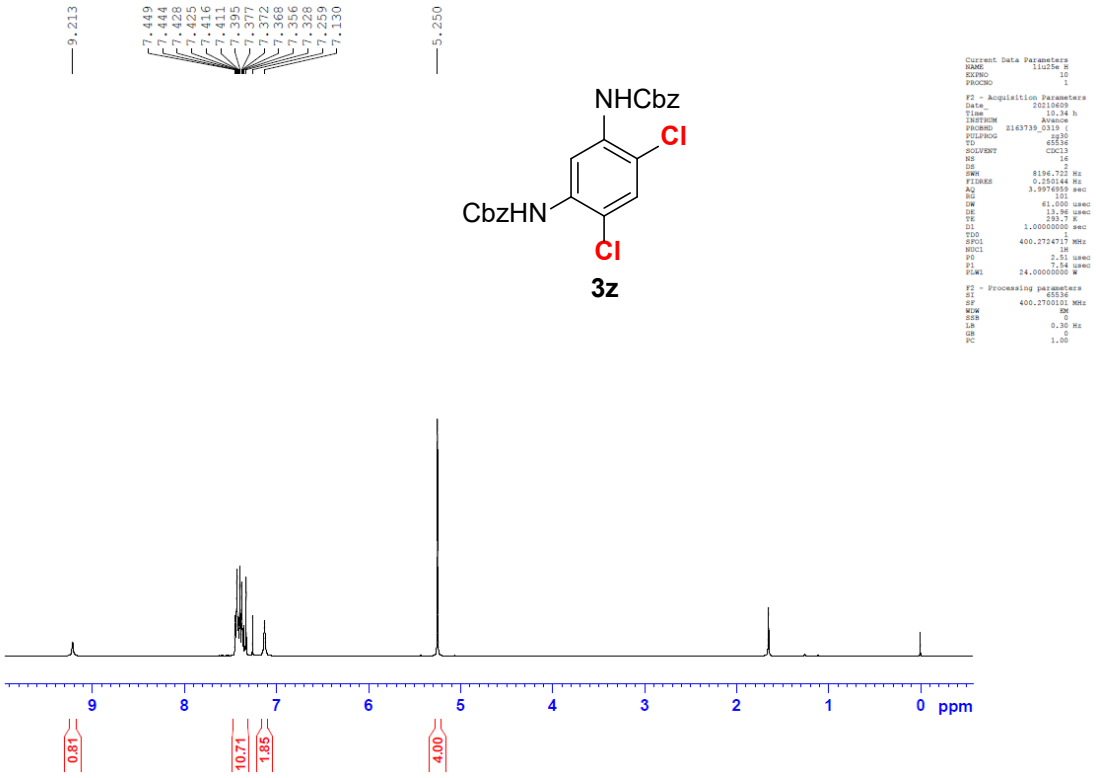
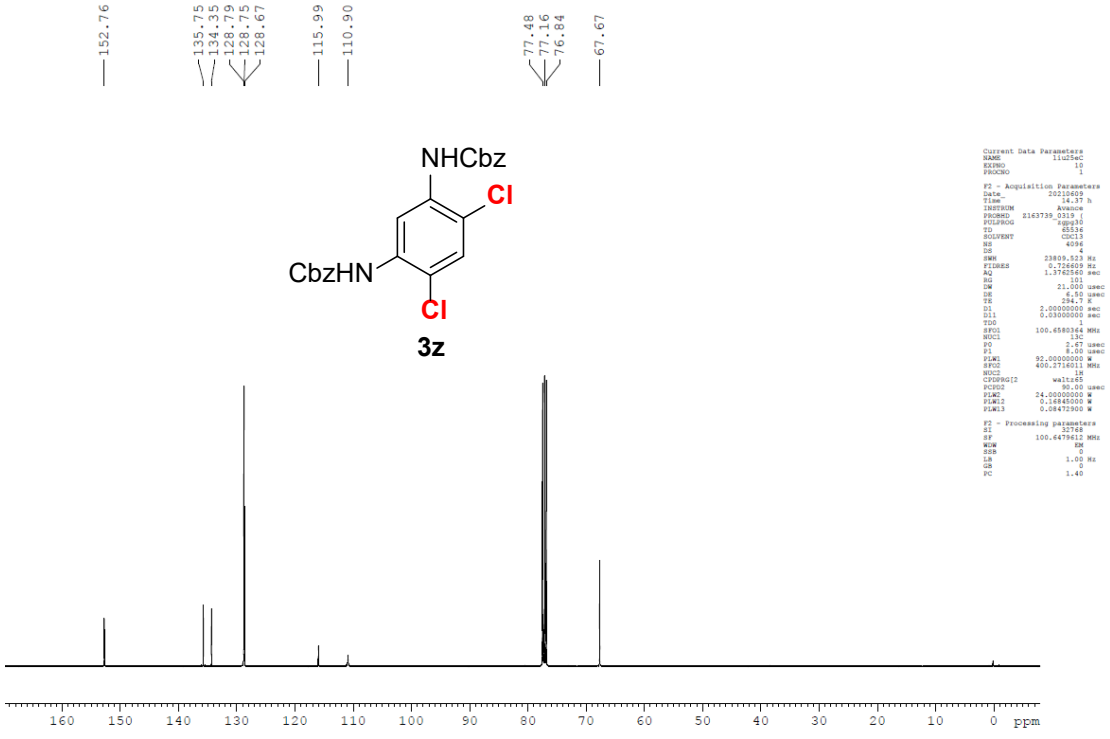
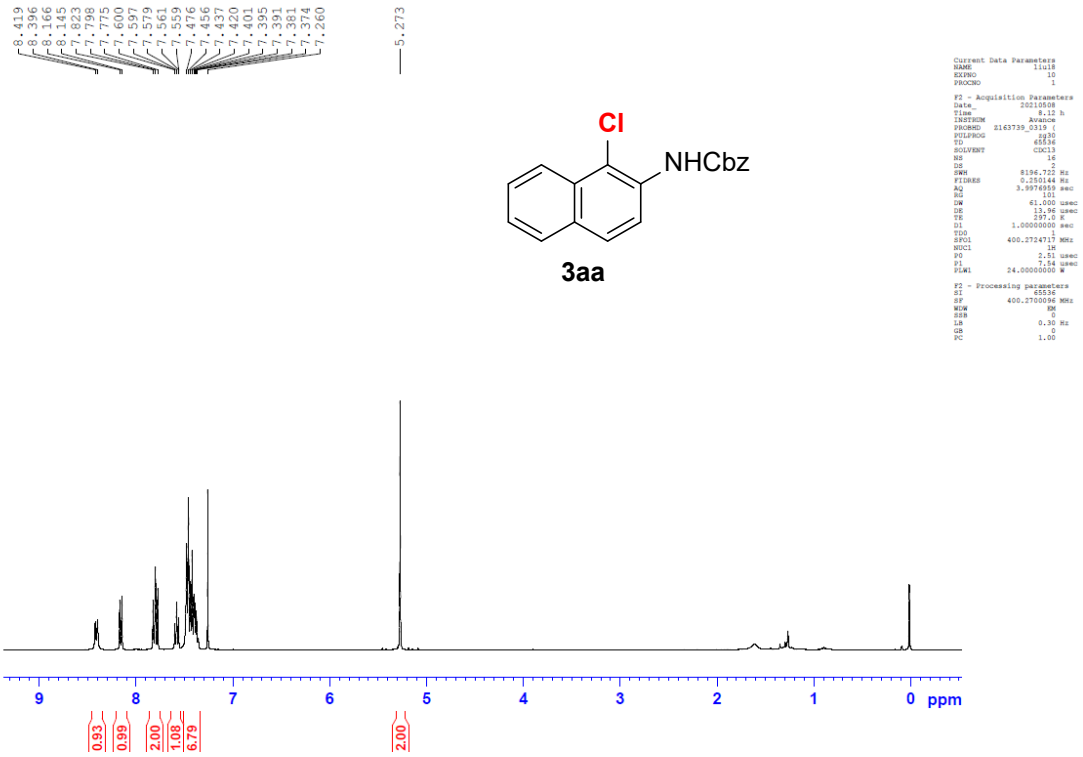
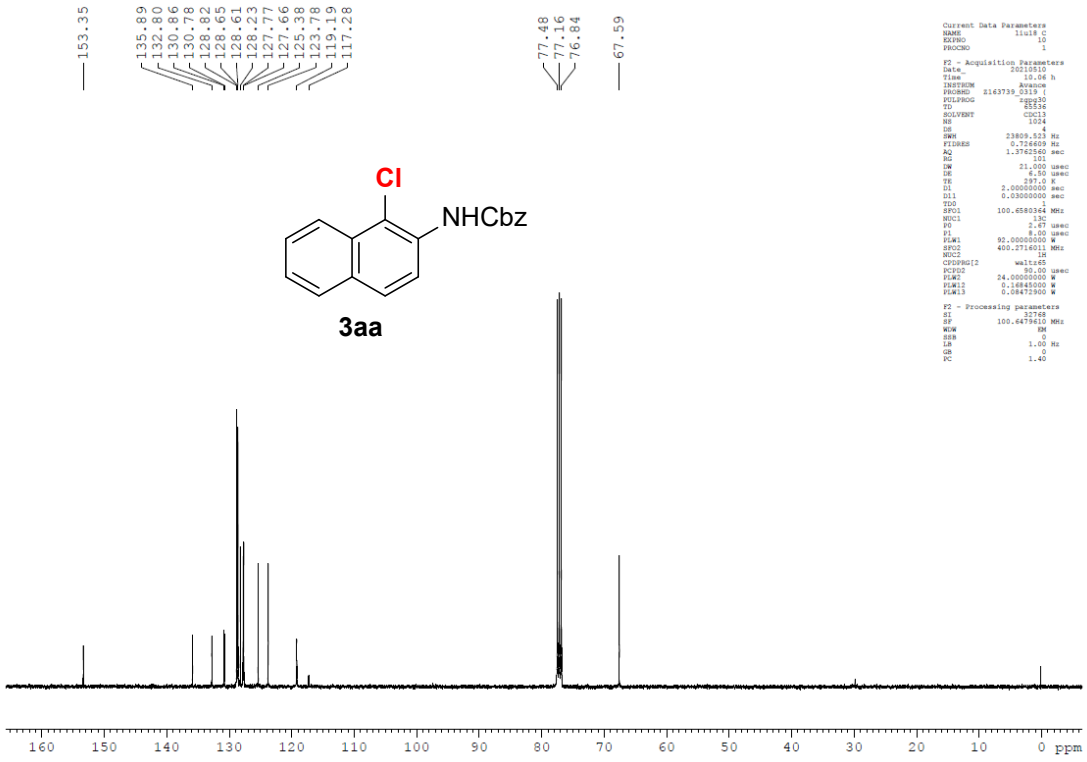
8.271
8.258
8.254
7.931
7.926
7.913
7.909
7.355
7.262
7.035
6.875
2.304
2.217
NHNs
Cl
Me
Me
3y
9
8
7
6
5
4
3
2
1
0
ppm
1.96
1.99
0.96
0.92
0.98
3.02
3.00

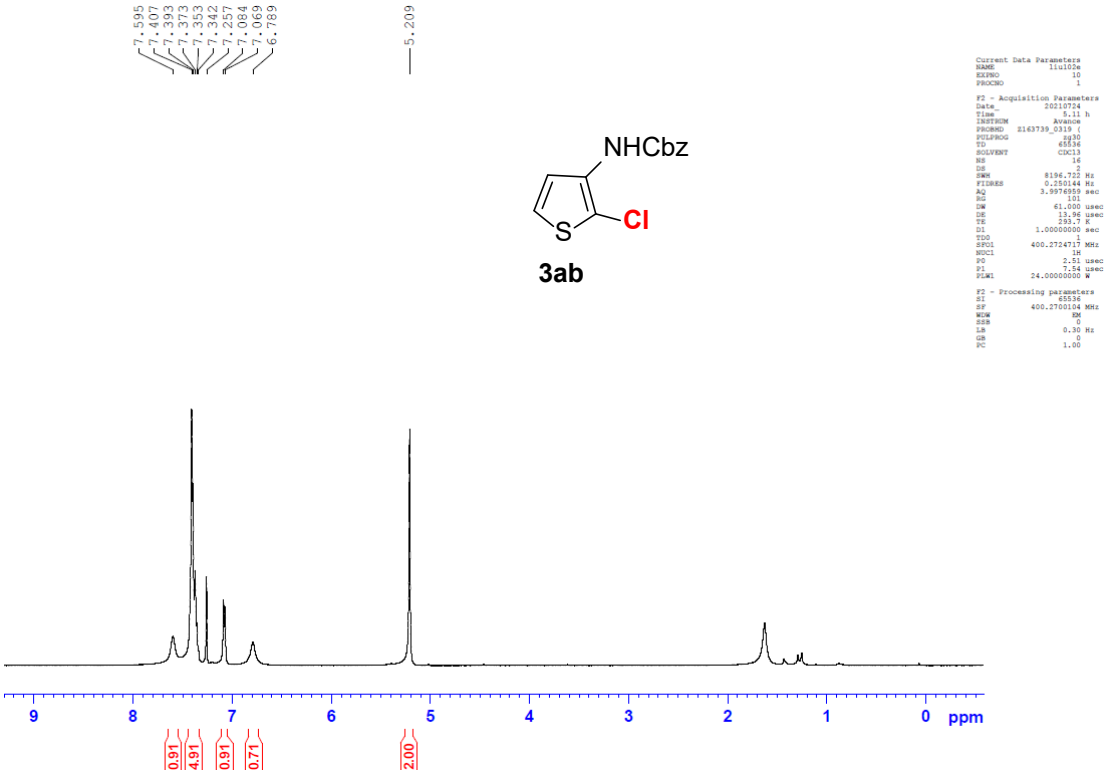

150.44
144.74
137.61
136.95
132.01
129.50
128.67
124.32
123.30
121.77
77.47
77.15
76.84
21.21
20.54
NHNs
Cl
Me
Me
3y
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
ppm

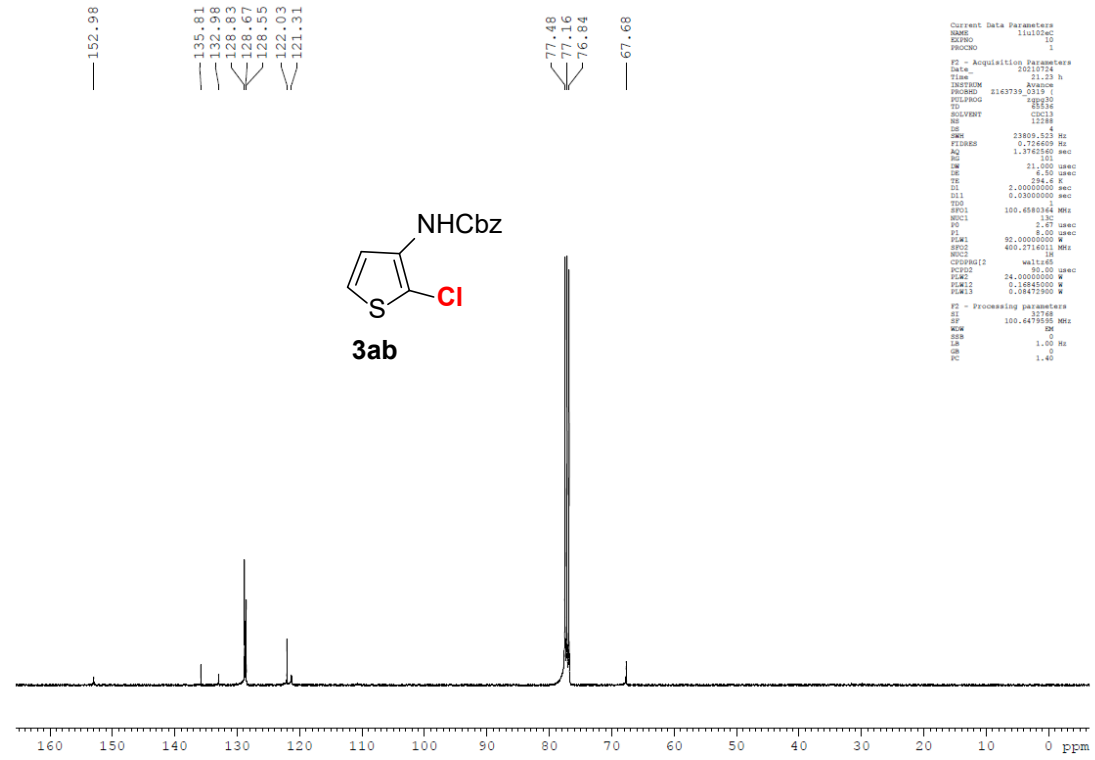

9.213
7.449
7.444
7.428
7.425
7.416
7.411
7.395
7.377
7.372
7.368
7.356
7.328
7.259
7.130
5.250
NHCbz
Cl
CbzHN
Cl
3z
9
8
7
6
5
4
3
2
1
0
ppm
0.81
10.71
1.85
4.00

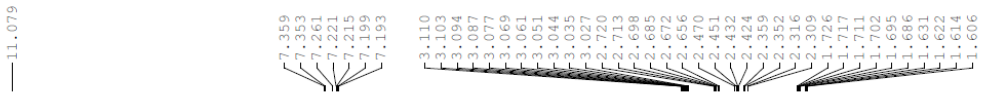

152.76
135.75
134.35
128.79
128.75
128.67
115.99
110.90
77.48
77.16
76.84
67.67
NHCbz
Cl
CbzHN
Cl
3z
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
ppm

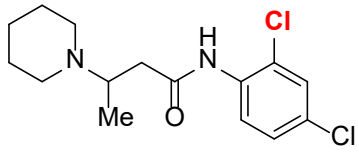

8.419
8.396
8.166
8.145
7.823
7.798
7.775
7.600
7.597
7.579
7.561
7.559
7.476
7.456
7.437
7.420
7.401
7.395
7.391
7.381
7.374
7.260
5.273
Cl
NHCbz
3aa
9
8
7
6
5
4
3
2
1
0
ppm
0.93
0.99
2.00
1.08
6.79
2.00


153.35
135.89
132.80
130.86
130.78
128.82
128.65
128.61
128.23
127.77
127.66
125.38
123.78
119.19
117.28
77.48
77.16
76.84
67.59
Cl
NHCbz
3aa
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
ppm

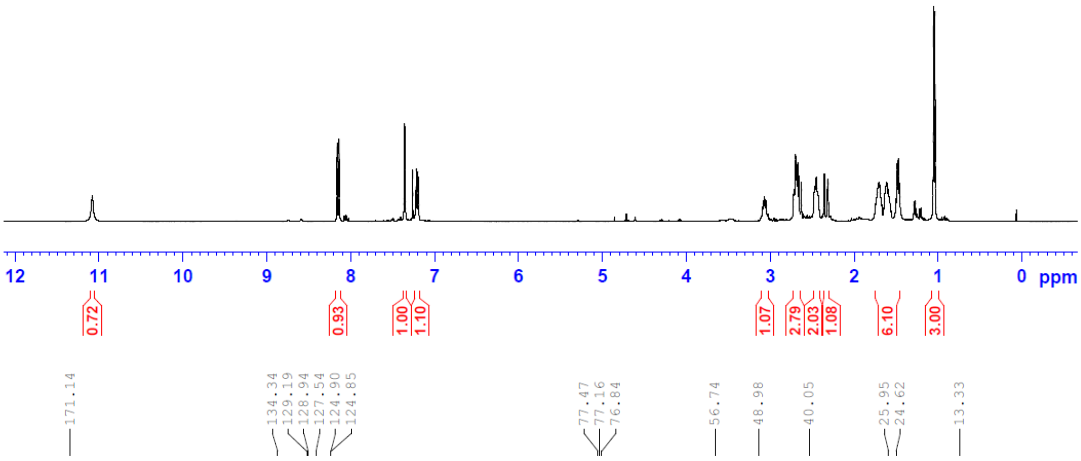

7.595
7.407
7.393
7.373
7.353
7.342
7.257
7.084
7.069
6.789
5.209
NHCbz
Cl
S
3ab
9
8
7
6
5
4
3
2
1
0
ppm
0.91
4.91
0.91
0.71
2.00


152.98
135.81
132.98
128.83
128.67
128.55
122.03
121.31
77.48
77.16
76.84
67.68
NHCbz
Cl
S
3ab
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
ppm

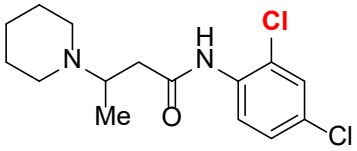

11.079
7.359
7.353
7.261
7.221
7.215
7.199
7.193
3.110
3.103
3.094
3.087
3.077
3.069
3.061
3.051
3.044
3.035
3.027
2.720
2.713
2.698
2.685
2.672
2.656
2.470
2.451
2.432
2.424
2.359
2.352
2.316
2.309
1.726
1.717
1.711
1.702
1.695
1.686
1.631
1.622
1.614
1.606


Cl
H
N
N
Me
O
Cl

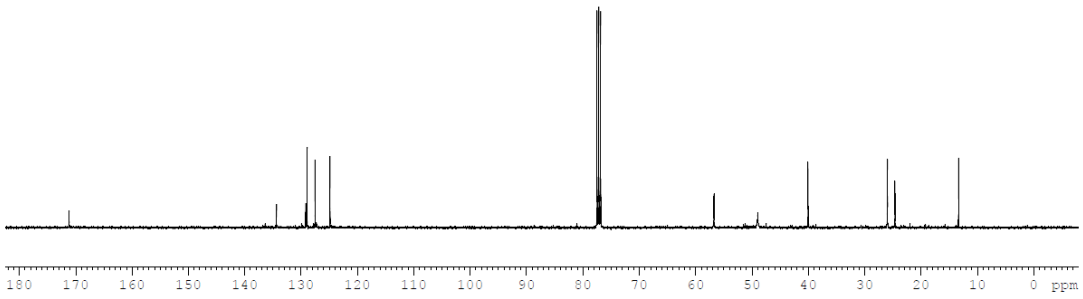
**4a**

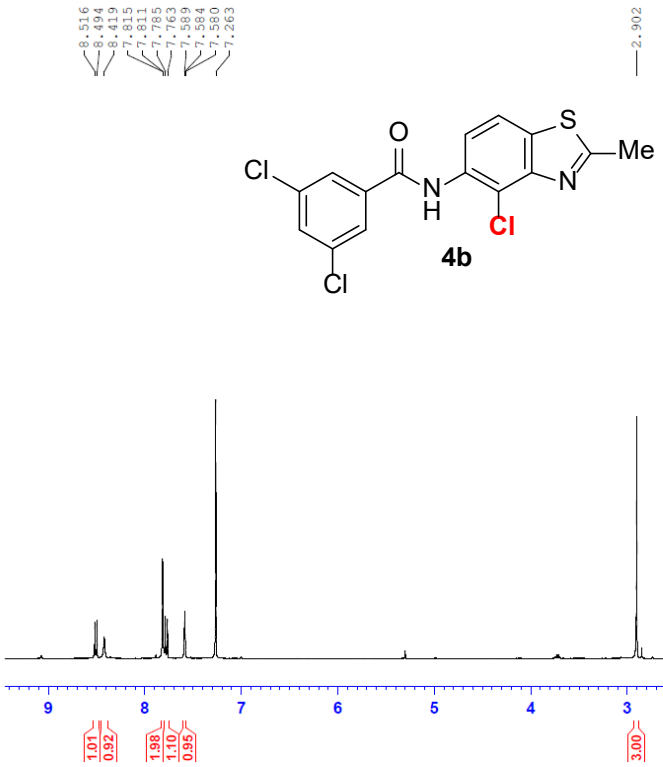

12
11
10
9
8
7
6
5
4
3
2
1
0 ppm
0.72
0.93
1.00
1.10
1.07
2.79
2.03
1.08
6.10
3.00

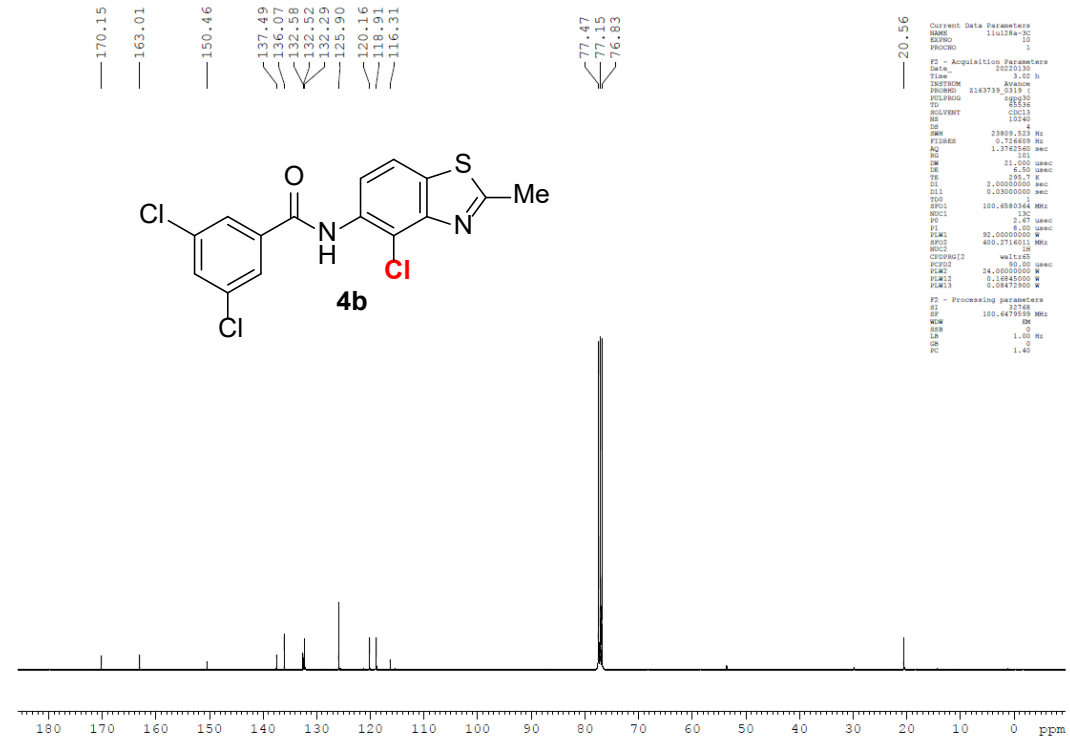

171.14
134.34
129.19
128.94
127.54
124.90
124.85
77.47
77.16
76.84
56.74
48.98
40.05
25.95
24.62
13.33

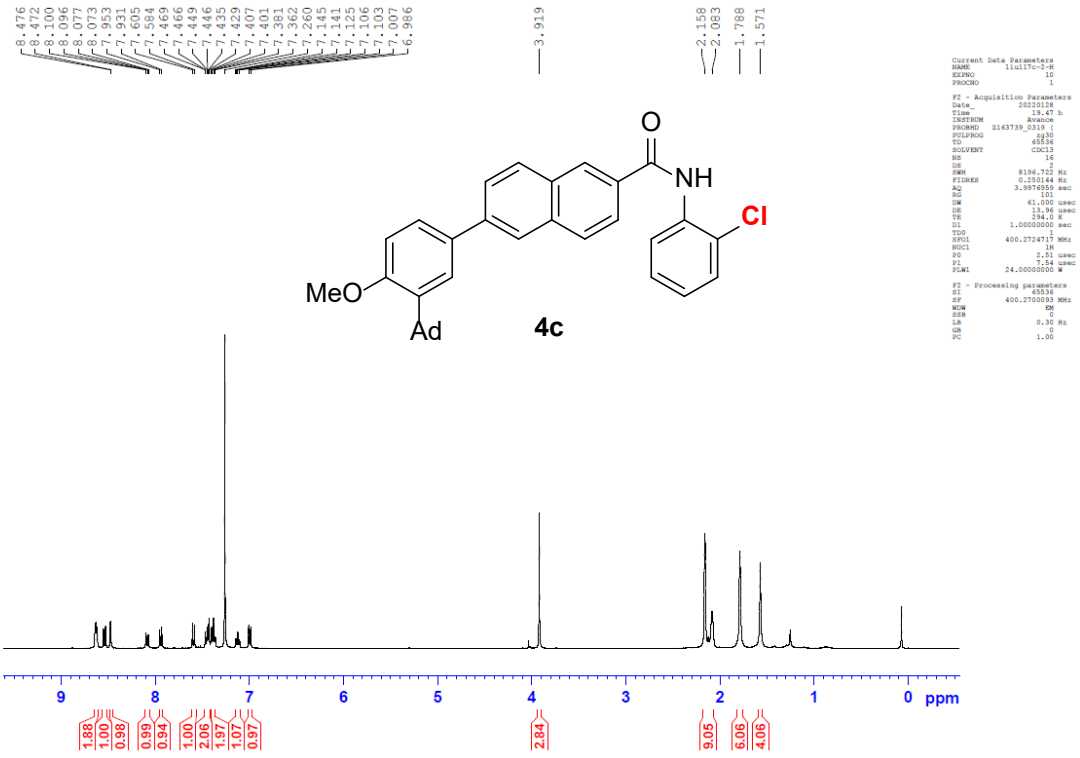

Cl
H
N
N
Me
O
Cl

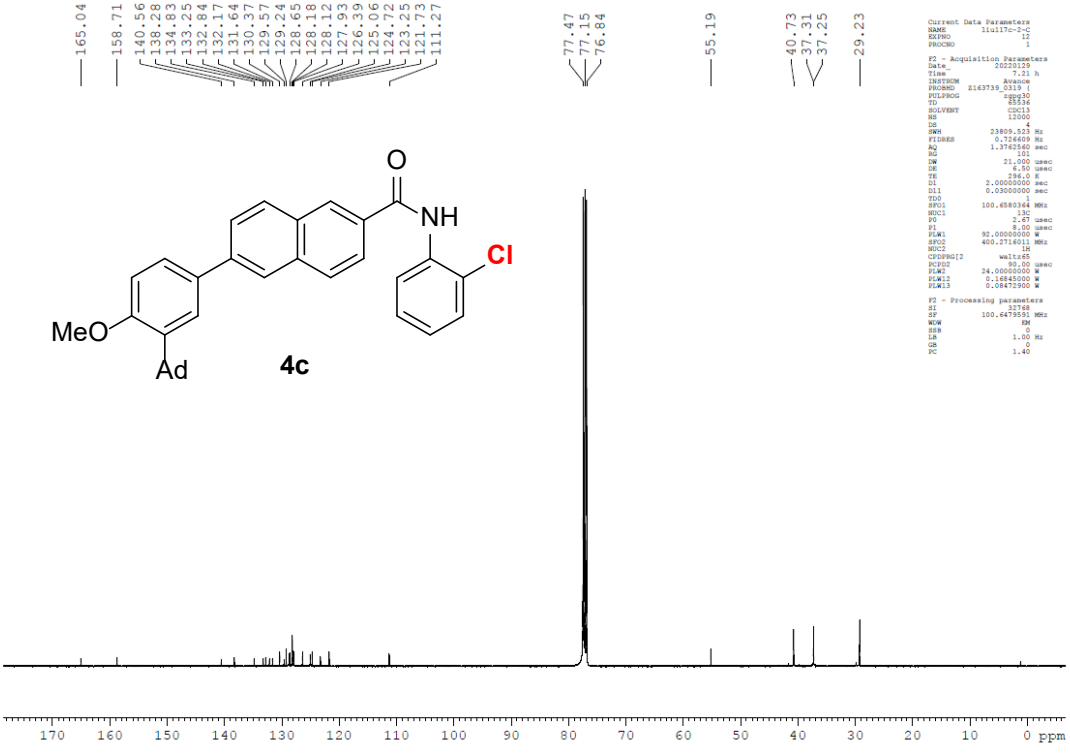
**4a**

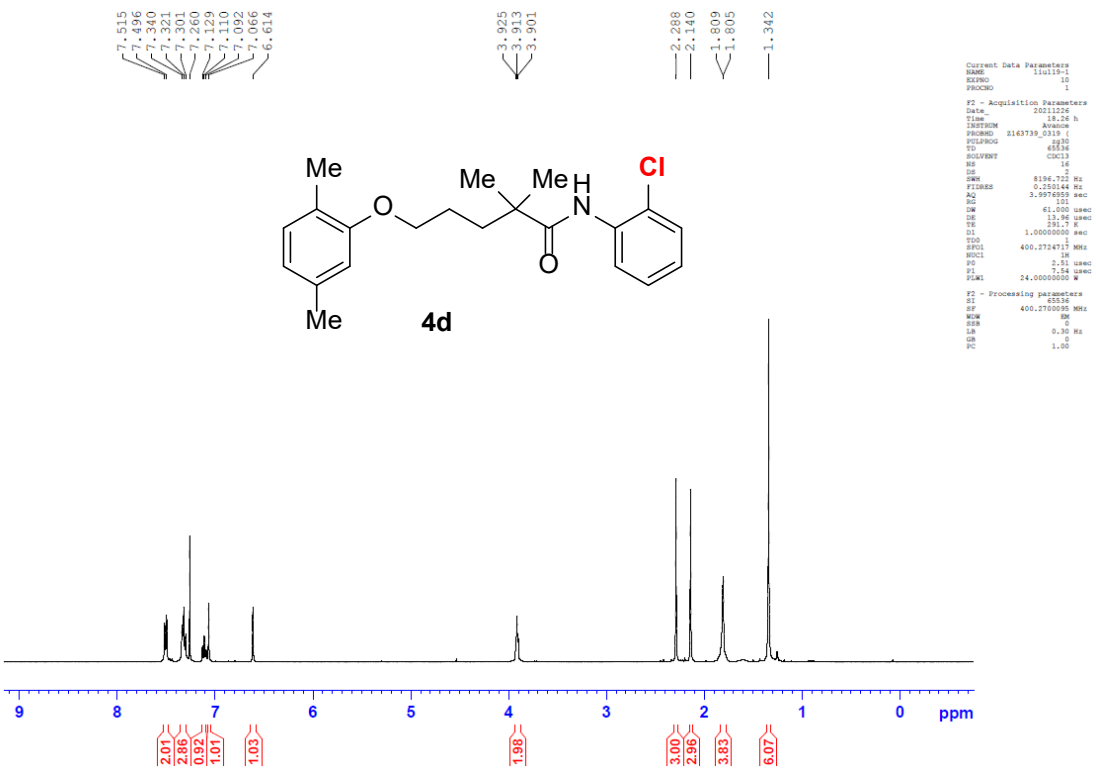

180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0 ppm

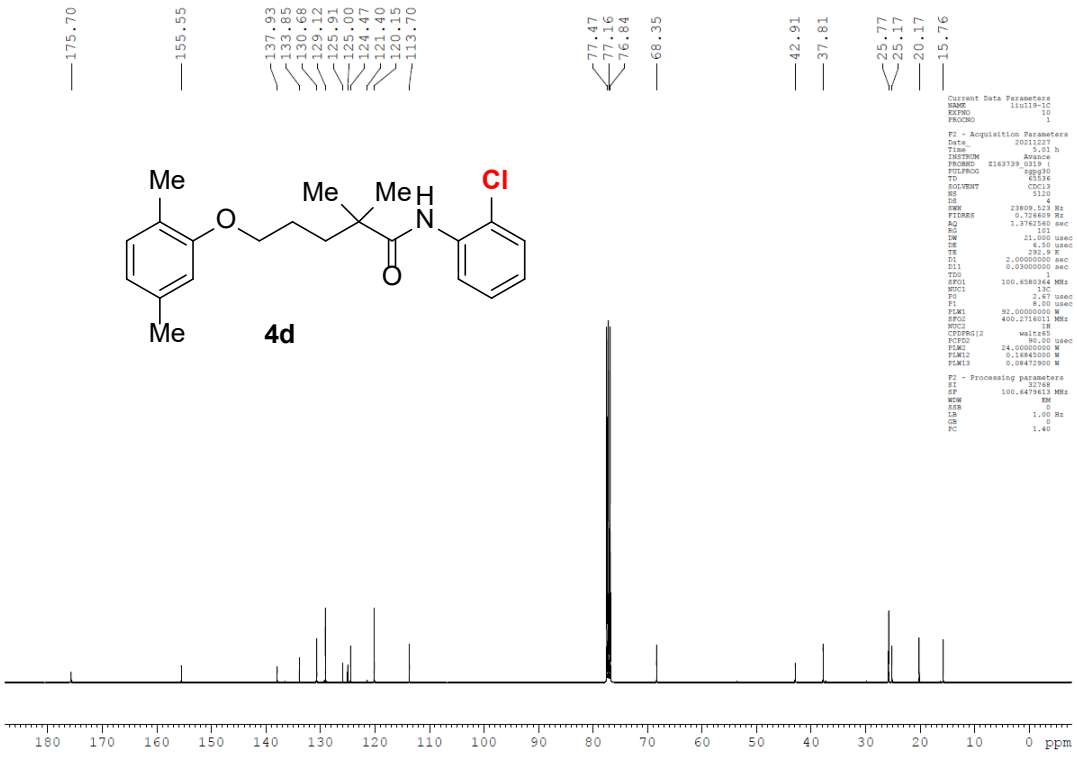

8.516
8.494
8.419
8.415
7.811
7.785
7.763
7.589
7.584
7.580
7.263
2.902
Cl
O
N
H
S
N
Me
Cl
Cl
4b
9
8
7
6
5
4
3
2
1
0
ppm
1.01
0.92
1.98
1.10
0.95
3.00

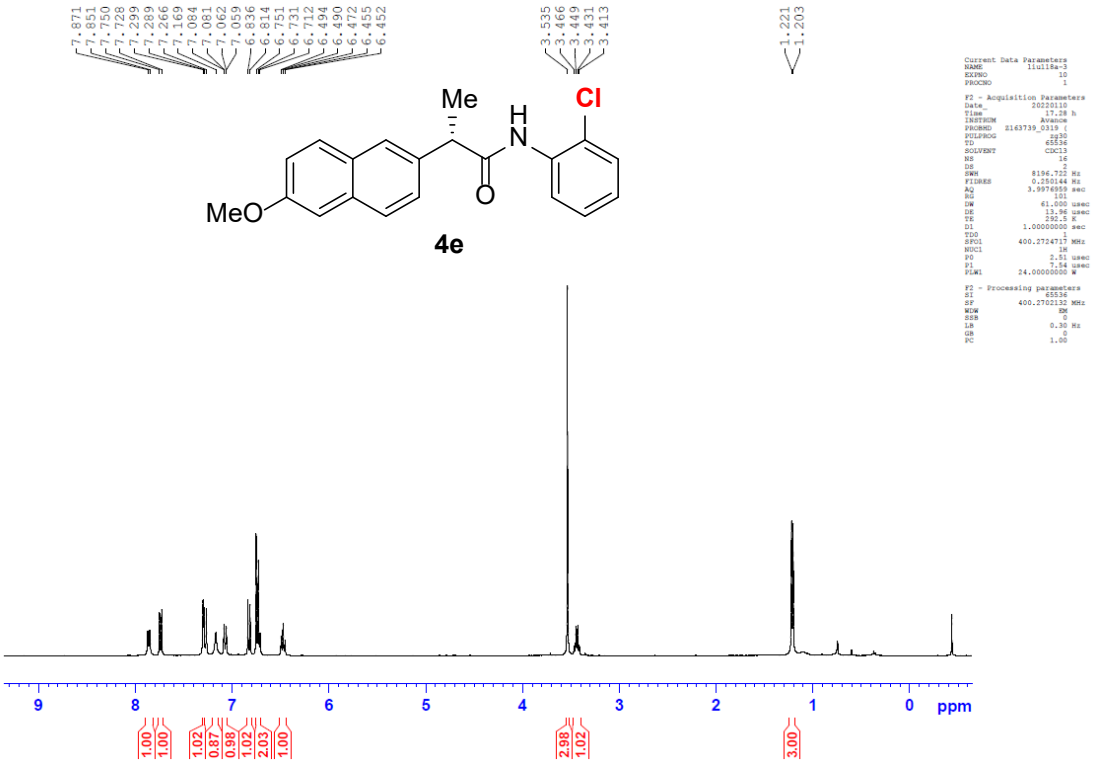

170.15
163.01
150.46
137.49
136.07
132.58
132.52
132.29
125.90
120.16
118.91
116.31
77.47
77.15
76.83
20.56
Cl
O
N
H
S
N
Me
Cl
Cl
4b
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
ppm


8.476
8.472
8.100
8.096
8.077
8.073
7.953
7.931
7.605
7.584
7.469
7.466
7.449
7.446
7.435
7.429
7.407
7.401
7.381
7.362
7.260
7.145
7.141
7.125
7.106
7.103
7.007
6.986
3.919
2.158
2.083
1.788
1.571
O
NH
Cl
MeO
Ad
4c
9
8
7
6
5
4
3
2
1
0 ppm
1.88
1.00
0.98
0.99
0.94
1.00
2.06
1.97
1.07
0.97
2.84
9.05
6.06
4.06


165.04
158.71
140.56
138.28
134.83
133.25
132.84
132.17
131.64
130.37
129.57
129.24
128.65
128.18
128.12
127.93
126.39
125.06
124.72
123.25
121.73
111.27
77.47
77.15
76.84
55.19
40.73
37.31
37.25
29.23
O
NH
Cl
MeO
Ad
4c
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0 ppm


7.515
7.496
7.340
7.321
7.301
7.260
7.129
7.110
7.092
7.066
6.614
3.925
3.913
3.901
2.288
2.140
1.809
1.805
1.342
Me
Me
Me
H
N
O
O
Cl
Me
4d
9
8
7
6
5
4
3
2
1
0
ppm
2.01
2.86
0.92
1.01
1.03
1.98
3.00
2.96
3.83
6.07


175.70
155.55
137.93
133.85
130.68
129.12
125.91
125.00
124.47
121.40
120.15
113.70
77.47
77.16
76.84
68.35
42.91
37.81
25.77
25.17
20.17
15.76
Me
Me
Me
H
N
O
O
Cl
Me
4d
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
ppm


7.871
7.851
7.750
7.728
7.299
7.289
7.266
7.169
7.084
7.081
7.062
7.059
6.836
6.814
6.751
6.731
6.712
6.494
6.490
6.472
6.455
6.452
3.535
3.466
3.449
3.431
3.413
1.221
1.203
Me
H
N
Cl
O
MeO
4e
9
8
7
6
5
4
3
2
1
0
ppm
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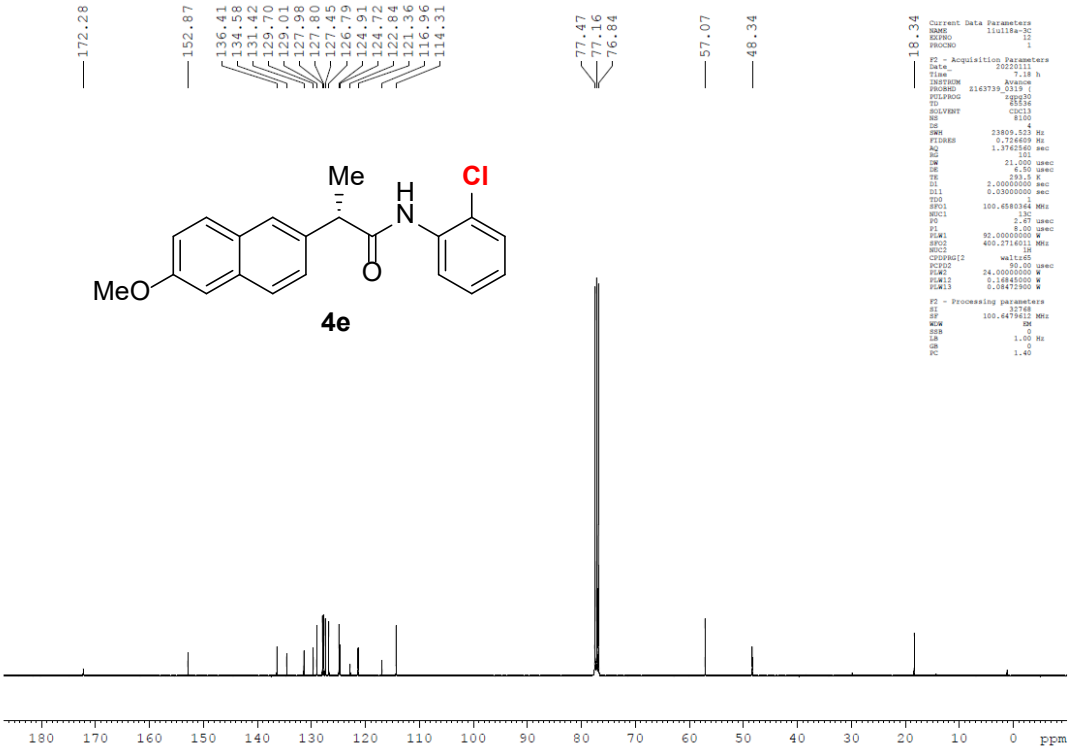
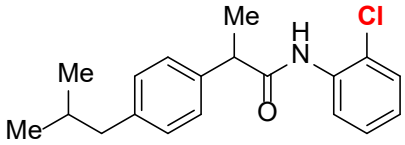
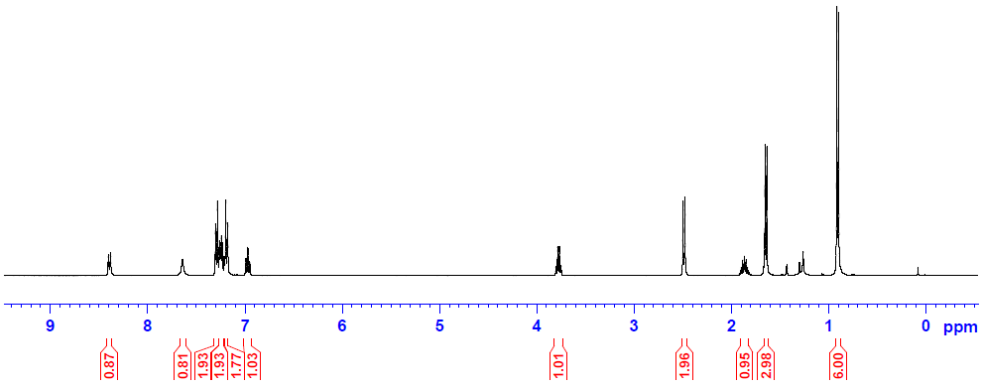
1.00
1.02
0.87
0.98
1.02
2.03
1.00
2.98
1.02
3.00

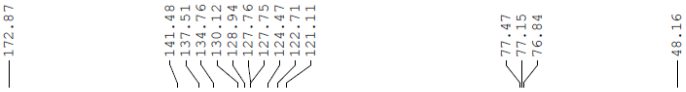

172.28
152.87
136.41
134.58
131.42
129.70
129.01
127.98
127.80
127.45
126.79
124.91
124.72
122.84
121.36
116.96
114.31
77.47
77.16
76.84
57.07
48.34
18.34
Me
H
N
Cl
O
MeO
4e
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
ppm

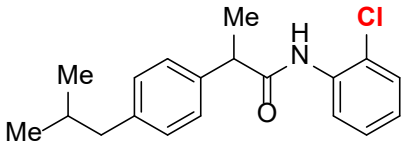

8.403
8.383
7.642
7.303
7.283
7.265
7.262
7.257
7.252
7.244
7.242
7.233
7.213
7.210
7.197
7.177
6.991
6.988
6.972
6.969
6.953
6.949
3.804
3.786
3.768
3.750
2.496
2.478
1.900
1.883
1.866
1.849
1.832
1.654
1.636
0.915
0.899


Me
H
N
Cl
Me
Me
O

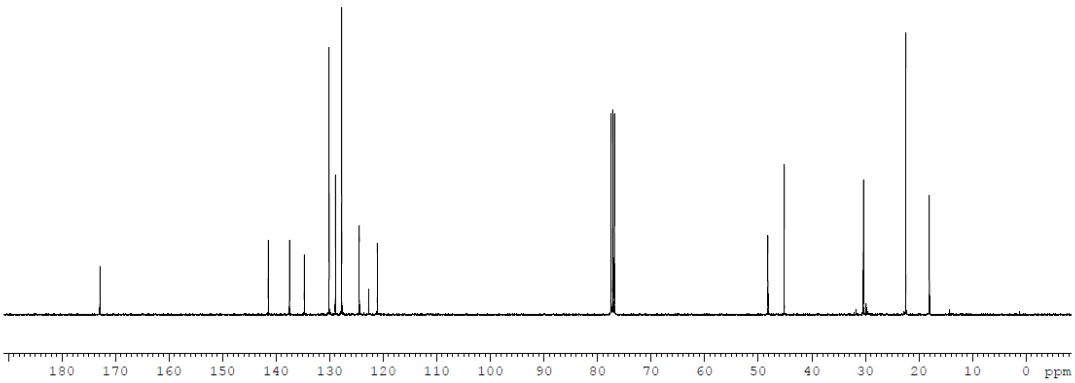
4f

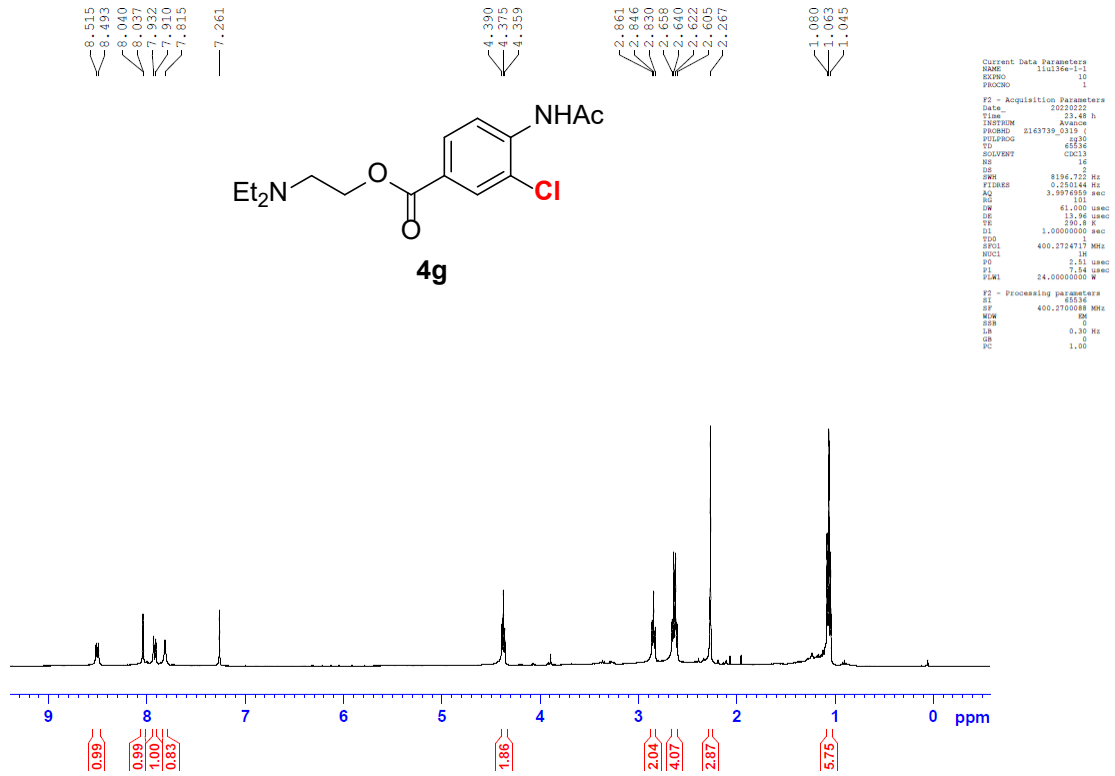

9
8
7
6
5
4
3
2
1
0
ppm
0.87
0.81
1.93
1.93
1.77
1.03
1.01
1.96
0.95
2.98
6.00

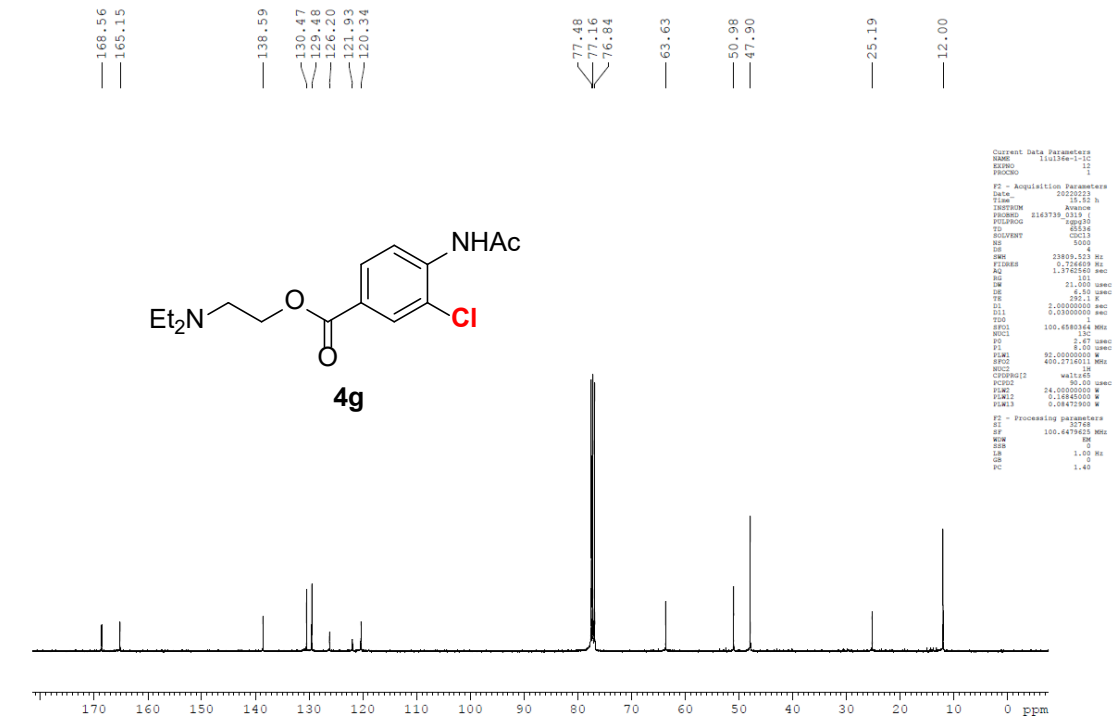

172.87
141.48
137.51
134.76
130.12
128.94
127.76
127.75
124.47
122.71
121.11
77.47
77.15
76.84
48.16
45.11
30.35
22.42
18.02


Me
H
N
Cl
Me
Me
O

4f


180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
ppm


8.515
8.493
8.040
8.037
7.932
7.910
7.815
7.261
4.390
4.375
4.359
2.861
2.846
2.830
2.658
2.640
2.622
2.605
2.267
1.080
1.063
1.045
NHAc
Et2N
O
Cl
4g
9
8
7
6
5
4
3
2
1
0
ppm
0.99
0.99
1.00
0.83
1.86
2.04
4.07
2.87
5.75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138.59
130.47
129.48
126.20
121.93
120.34
77.48
77.16
76.84
63.63
50.98
47.90
25.19
12.00
NHAc
Et2N
O
Cl
4g
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140
130
120
110
100
90
80
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60
50
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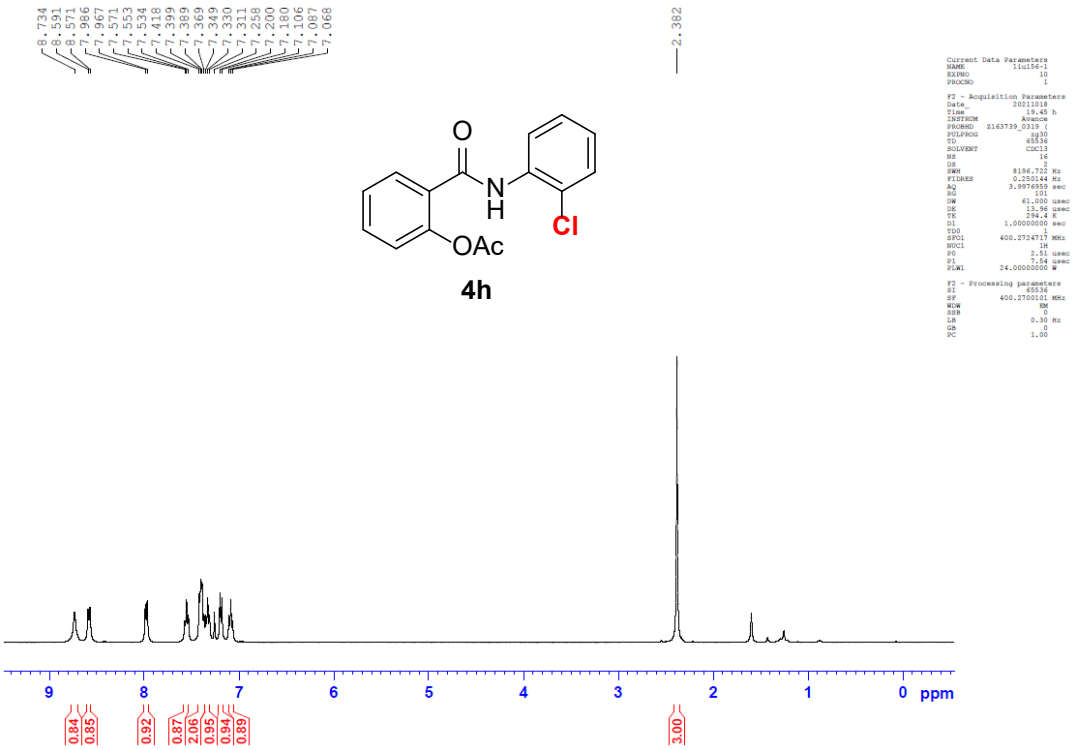
30
20
10
0
ppm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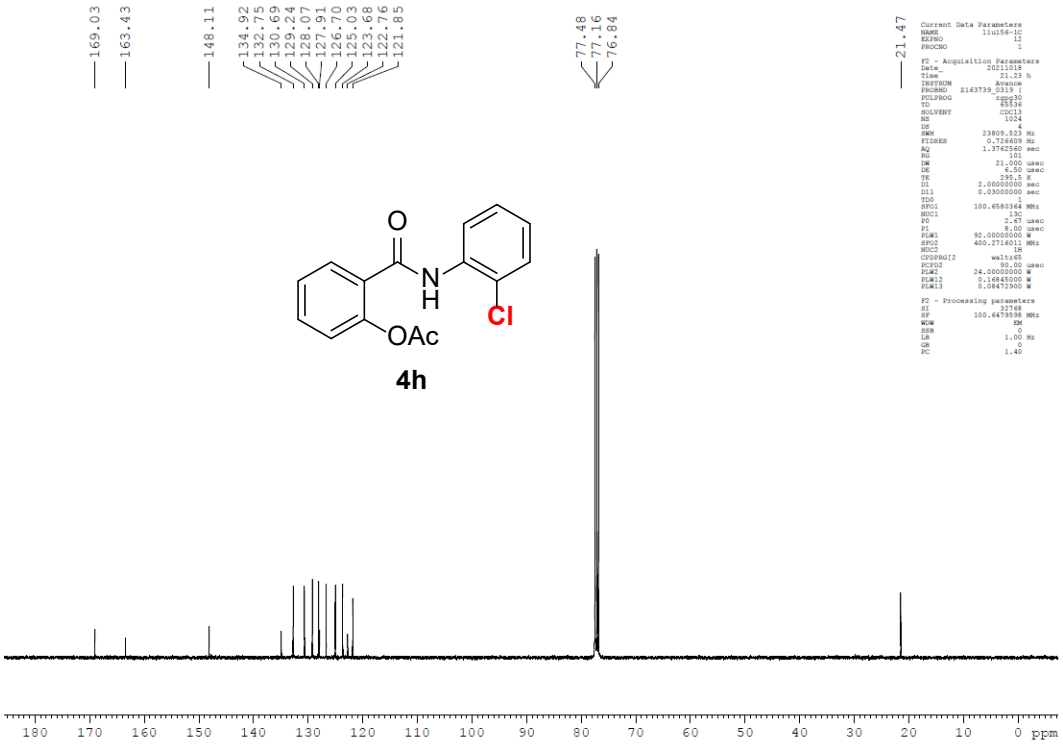
8.571
7.986
7.967
7.571
7.553
7.534
7.418
7.399
7.389
7.369
7.349
7.330
7.311
7.258
7.200
7.180
7.106
7.087
7.068
2.382
O
N
H
Cl
OAc
4h
9
8
7
6
5
4
3
2
1
0 ppm
0.84
0.85
0.92
0.87
2.06
0.95
0.94
0.89
3.00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132.75
130.69
129.24
128.07
127.91
126.70
125.03
123.68
122.76
121.85
77.48
77.16
76.84
21.47
O
N
H
Cl
OAc
4h
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170
160
150
140
130
120
110
100
90
80
70
60
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30
20
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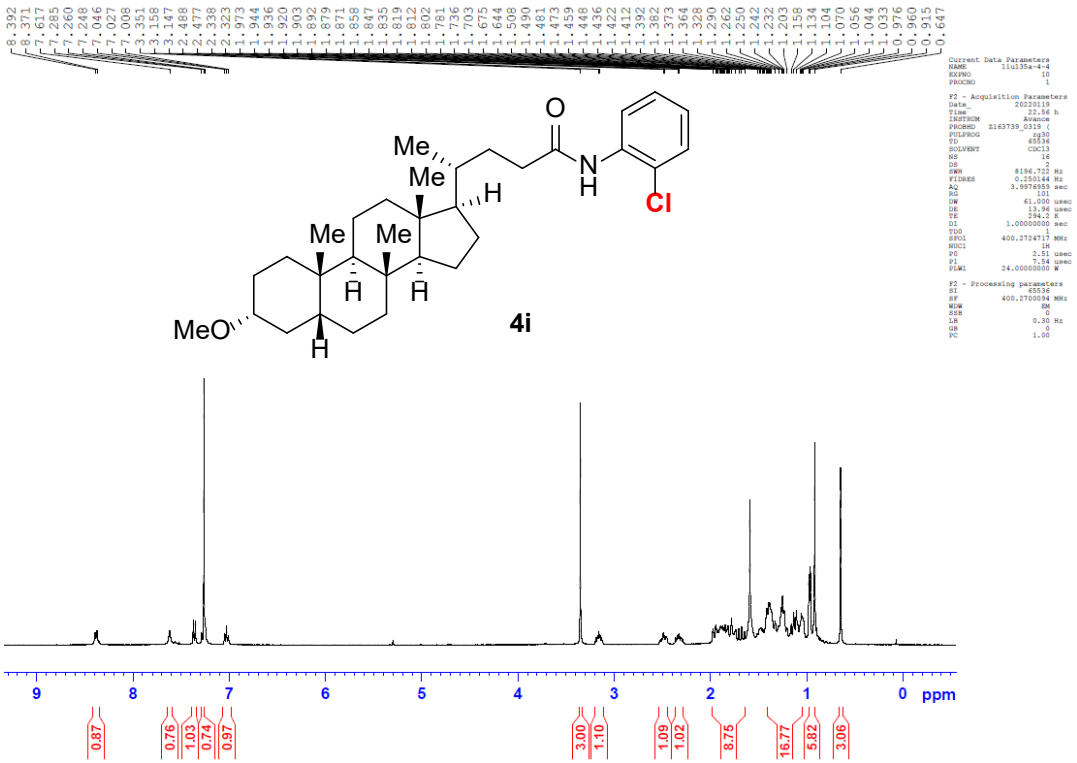
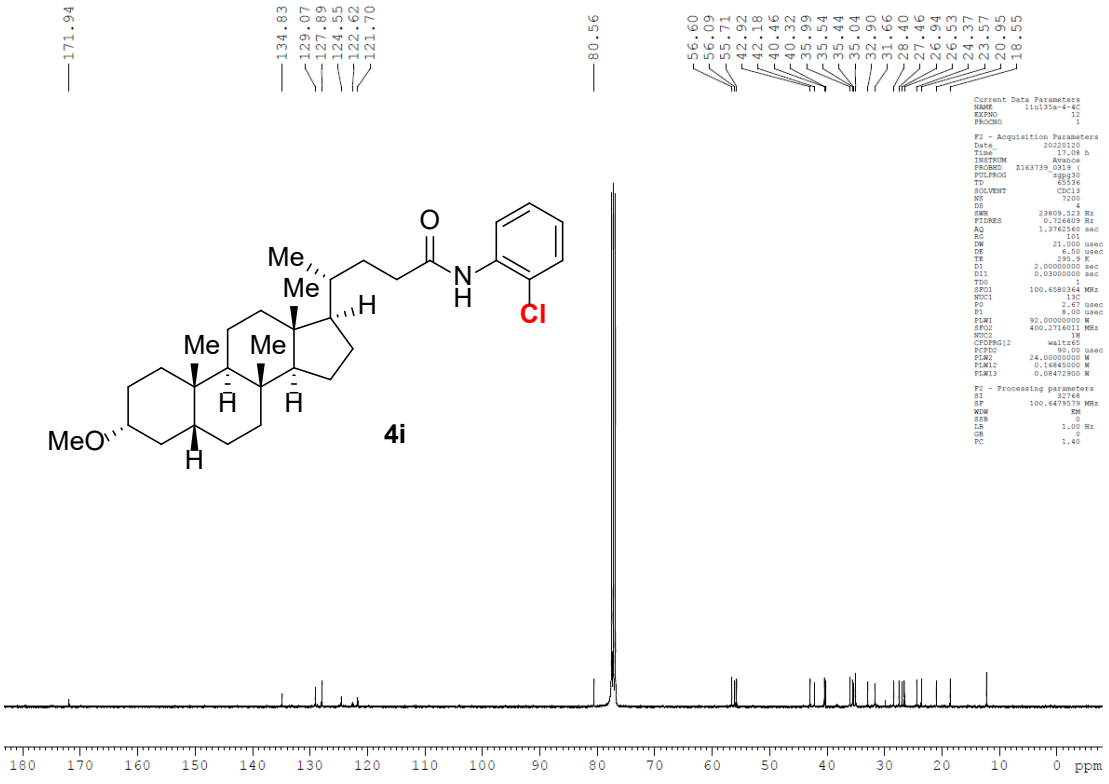
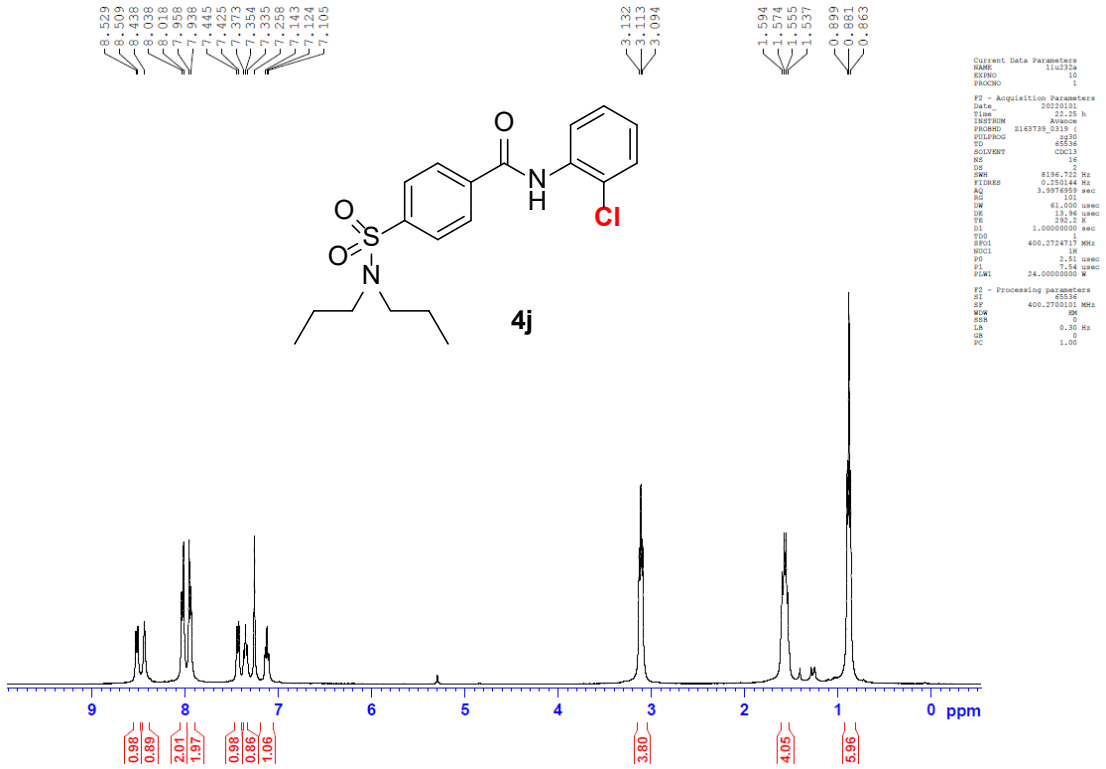
0 ppm


4i
ppm


4i
ppm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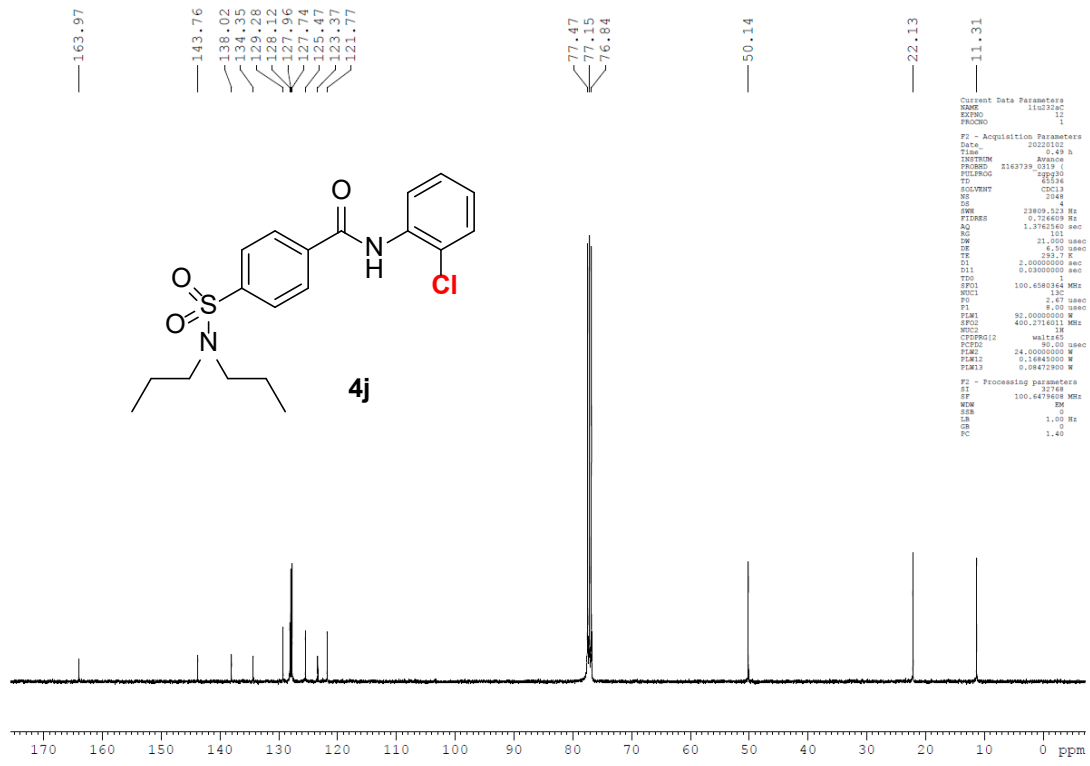
8.509
8.438
8.038
8.018
7.958
7.938
7.445
7.425
7.373
7.354
7.335
7.258
7.143
7.124
7.105
3.132
3.113
3.094
1.594
1.574
1.555
1.537
0.899
0.881
0.863
O
N
H
Cl
O
S
O
N
4j
9
8
7
6
5
4
3
2
1
0 ppm
0.98
0.89
2.01
1.97
0.98
0.86
1.06
3.80
4.05
5.96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138.02
134.35
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128.12
127.96
127.74
125.47
123.37
121.77
77.47
77.15
76.84
50.14
22.13
11.31
O
N
H
Cl
O
S
O
N
4j
170
160
150
140
130
120
110
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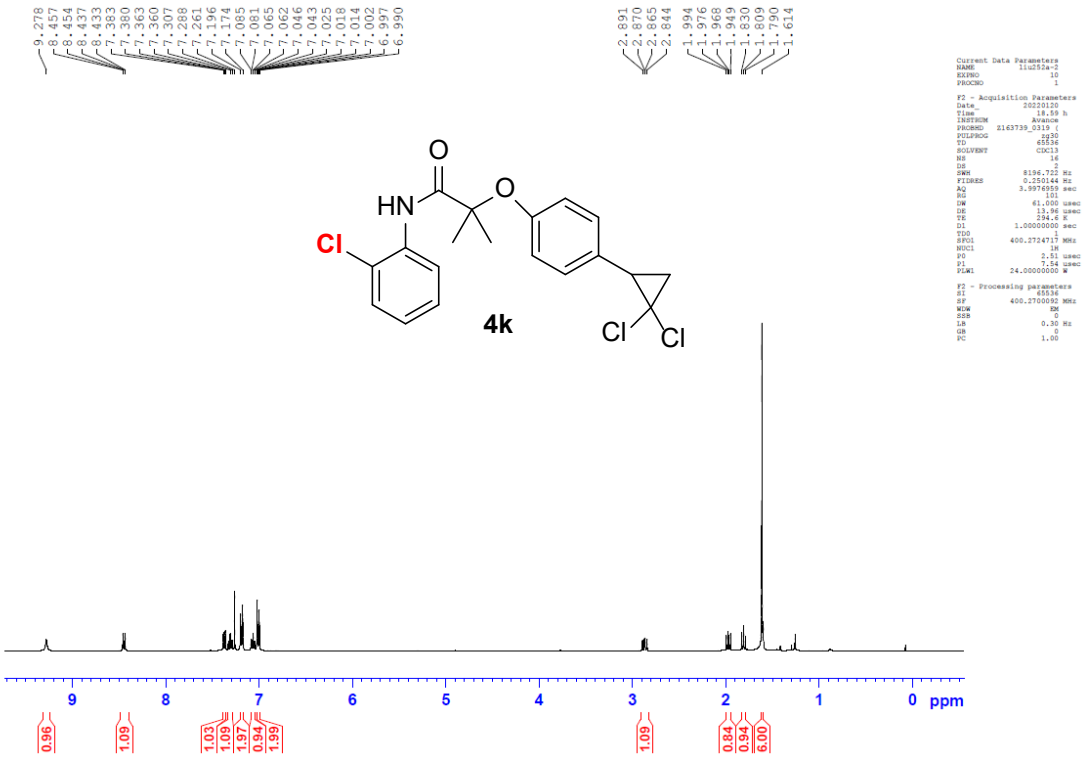
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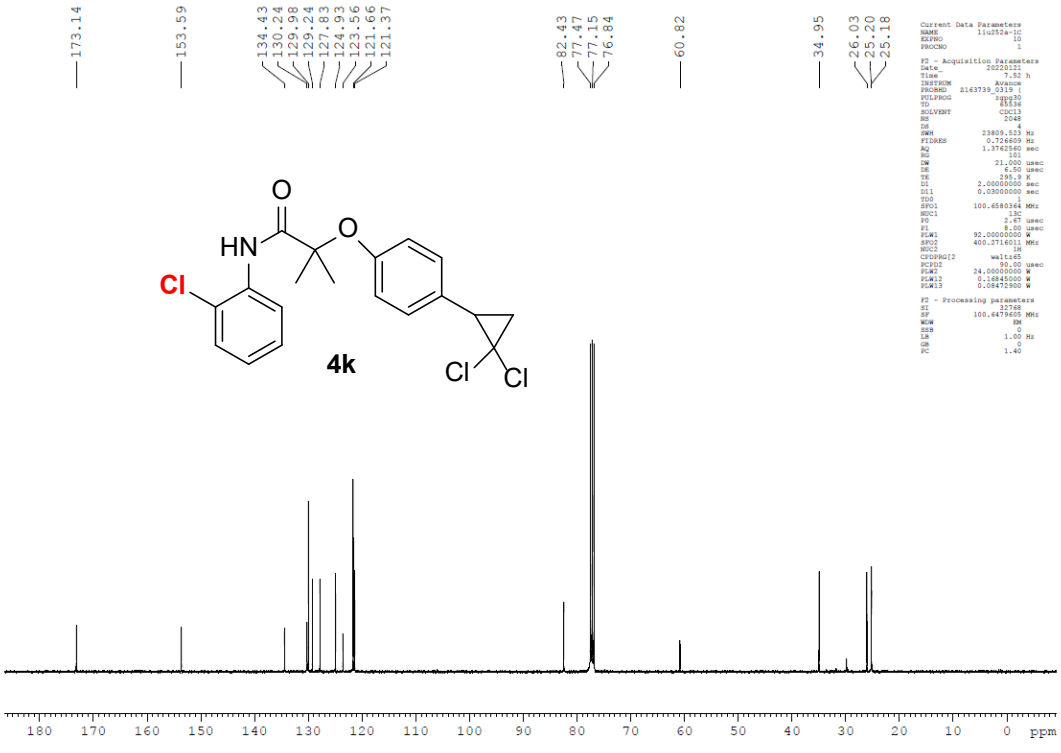
8.454
8.437
8.433
7.383
7.380
7.363
7.360
7.307
7.288
7.261
7.196
7.174
7.085
7.081
7.065
7.062
7.046
7.043
7.025
7.018
7.014
7.002
6.997
6.990
2.891
2.870
2.865
2.844
1.994
1.976
1.968
1.949
1.830
1.809
1.790
1.614
HN
O
O
Cl
Cl
Cl
4k
9
8
7
6
5
4
3
2
1
0 ppm
0.96
1.09
1.03
1.09
1.97
0.84
1.99
1.09
0.84
0.94
6.00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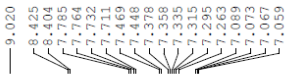
153.59
134.43
130.24
129.98
129.24
127.83
124.93
123.56
121.66
121.37
82.43
77.47
77.15
76.84
60.82
34.95
26.03
25.20
25.18
HN
O
O
Cl
Cl
Cl
4k
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0 ppm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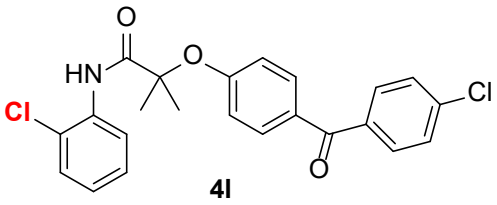
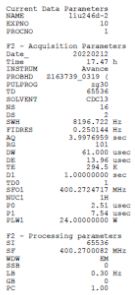
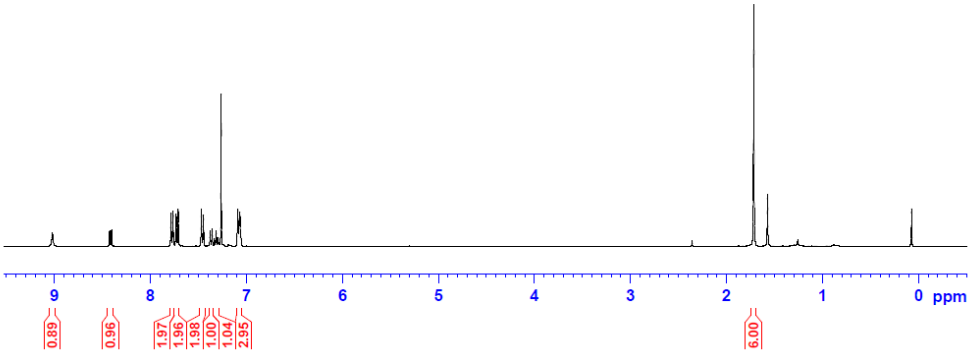
8.425
8.404
7.785
7.764
7.732
7.711
7.469
7.448
7.378
7.358
7.335
7.315
7.295
7.263
7.089
7.073
7.067
7.059

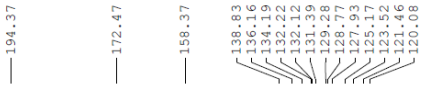

O
HN
O
Cl
Cl
O

4l


1.715

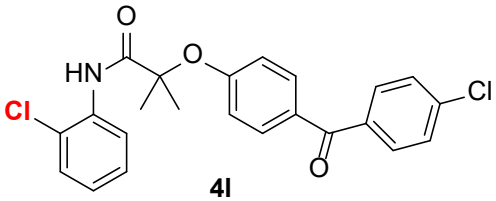



9
8
7
6
5
4
3
2
1
0 ppm
0.89
0.96
1.97
1.96
1.98
1.00
1.04
2.95
6.00

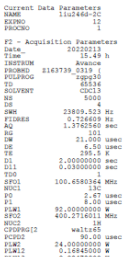

194.37
172.47
158.37
138.83
136.16
134.19
132.22
132.12
131.39
129.28
129.27
127.93
125.17
123.52
121.46
120.08


82.71
77.47
77.16
76.84

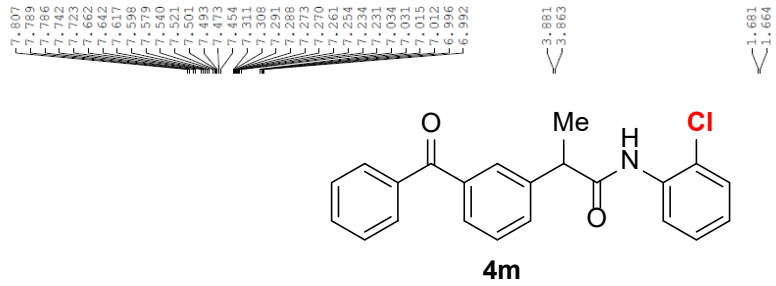

25.28


O
HN
O
Cl
Cl
O

4l




190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0 ppm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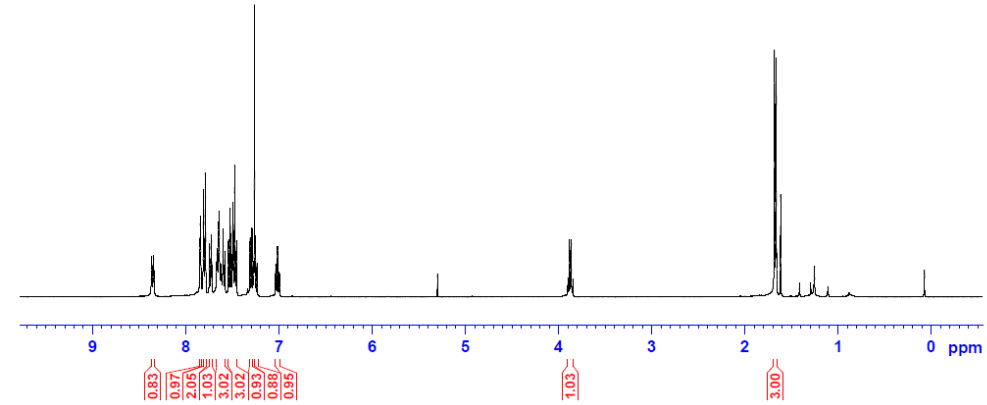
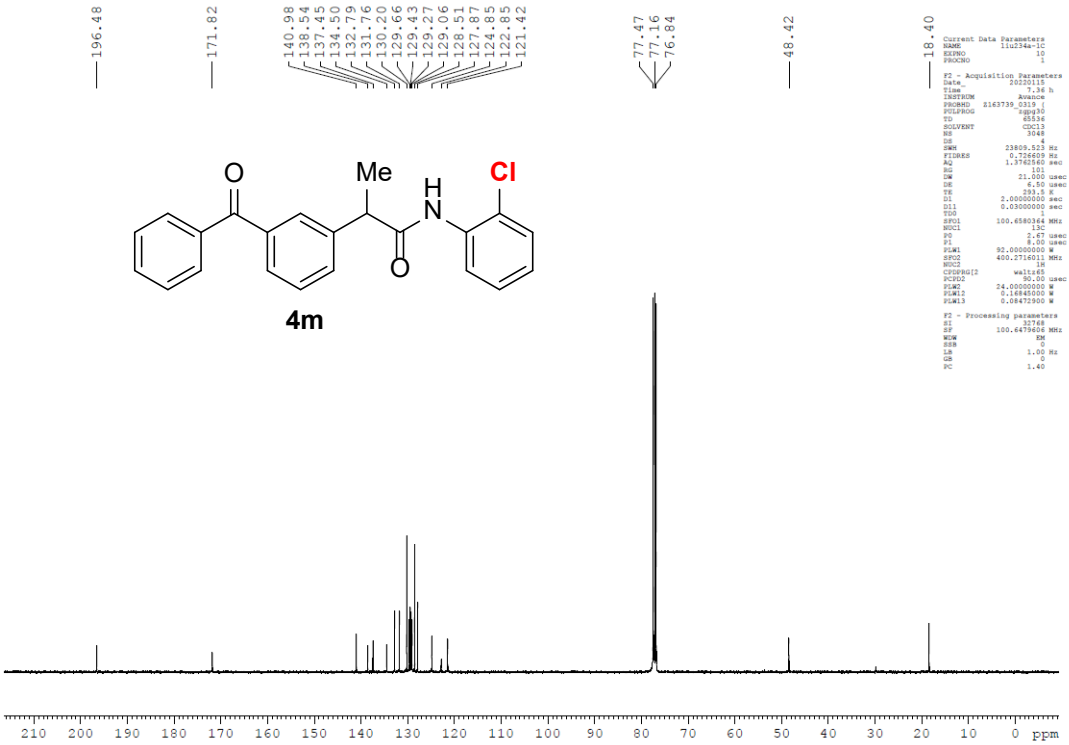
7.789
7.786
7.742
7.723
7.662
7.642
7.617
7.598
7.579
7.540
7.521
7.501
7.493
7.473
7.454
7.311
7.308
7.291
7.288
7.273
7.270
7.261
7.254
7.234
7.231
7.034
7.031
7.015
7.012
6.996
6.992
3.881
3.863
1.681
1.664
O
Me
H
N
Cl
O

**4m**


9
8
7
6
5
4
3
2
1
0
ppm
0.83
0.97
2.05
1.03
3.02
3.02
0.93
0.88
0.95
1.03
3.00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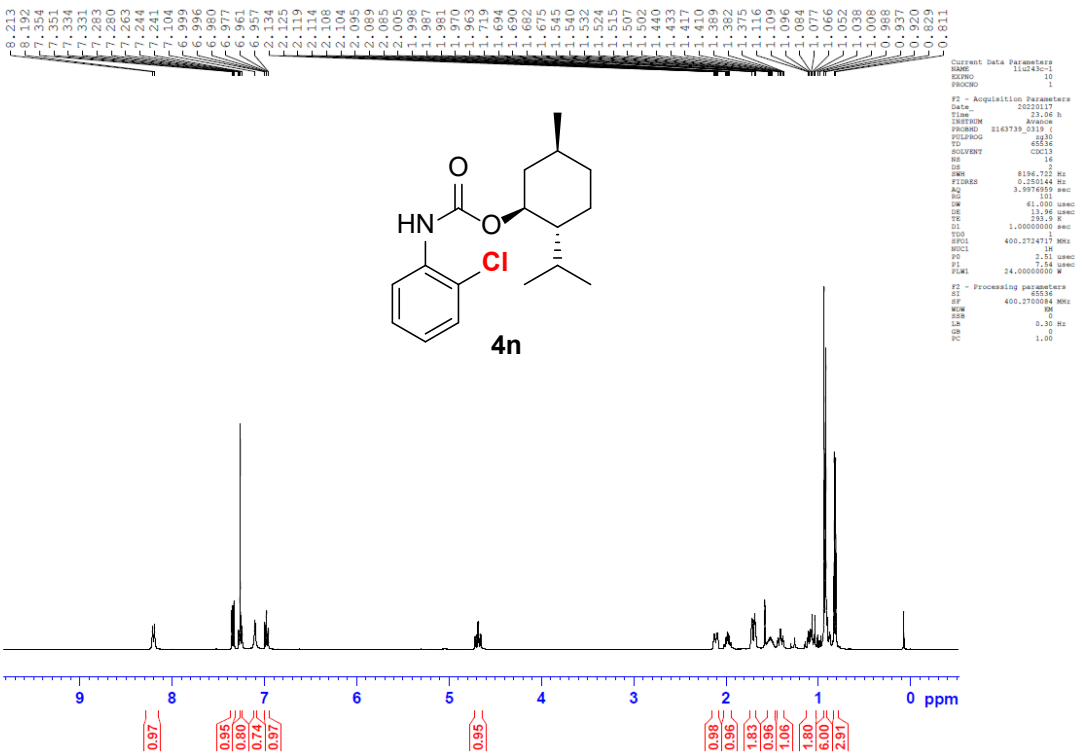
171.82
140.98
138.54
137.45
134.50
132.79
131.76
130.20
129.66
129.43
129.27
129.06
128.51
127.87
124.85
122.85
121.42
77.47
77.16
76.84
48.42
18.40
O
Me
H
N
Cl
O
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
ppm

**4m**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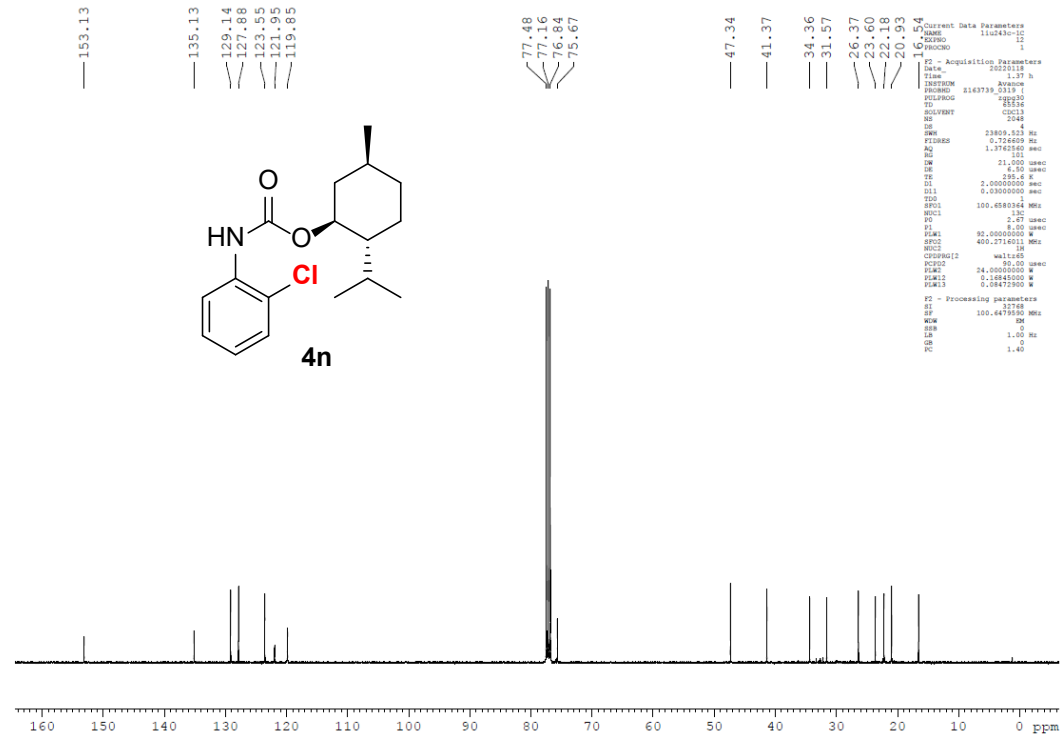
7.280
7.263
7.244
7.241
7.104
6.999
6.996
6.980
6.977
6.961
6.957
2.134
2.125
2.119
2.114
2.108
2.104
2.095
2.089
2.085
2.005
1.998
1.987
1.981
1.970
1.963
1.719
1.694
1.690
1.682
1.675
1.545
1.540
1.532
1.524
1.515
1.507
1.502
1.440
1.433
1.417
1.410
1.389
1.382
1.375
1.116
1.109
1.096
1.084
1.077
1.066
1.052
1.038
1.008
0.988
0.937
0.920
0.829
0.811
O
HN
O
Cl
4n
9
8
7
6
5
4
3
2
1
0 ppm
0.97
0.95
0.80
0.74
0.97
0.95
0.98
0.96
1.83
0.96
1.06
1.80
6.00
2.91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129.14
127.88
123.55
121.95
119.85
77.48
77.16
76.84
75.67
47.34
41.37
34.36
31.57
26.37
23.60
22.18
20.93
16.54
O
HN
O
Cl
4n
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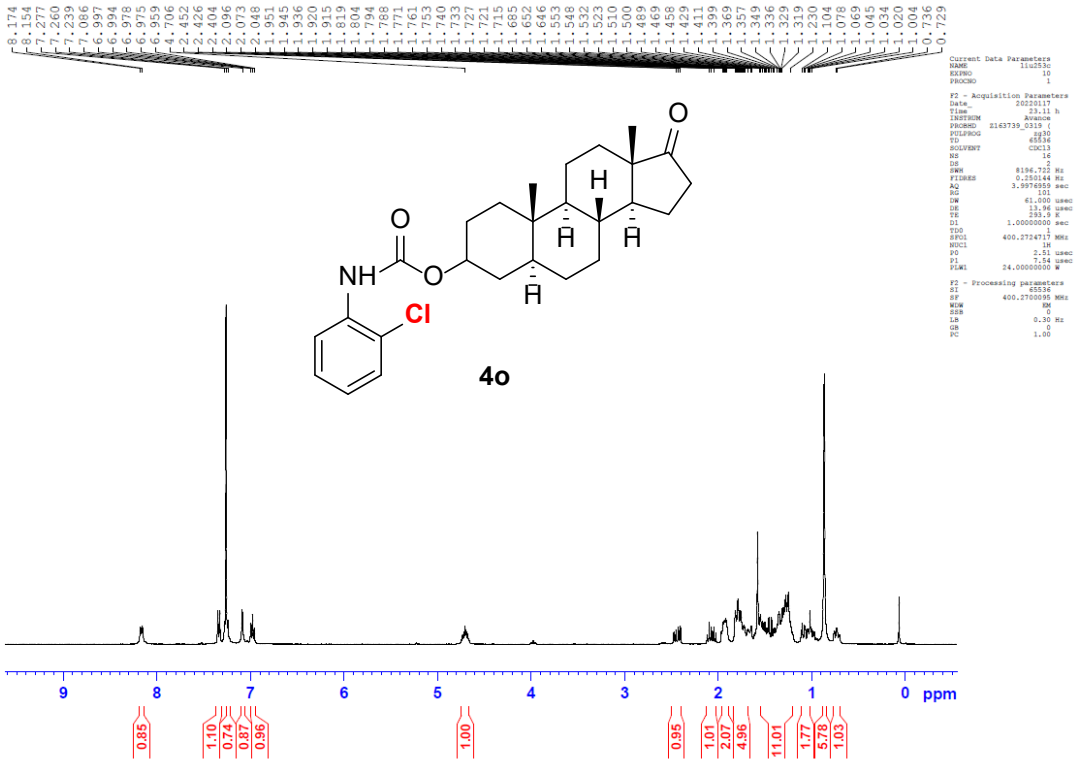
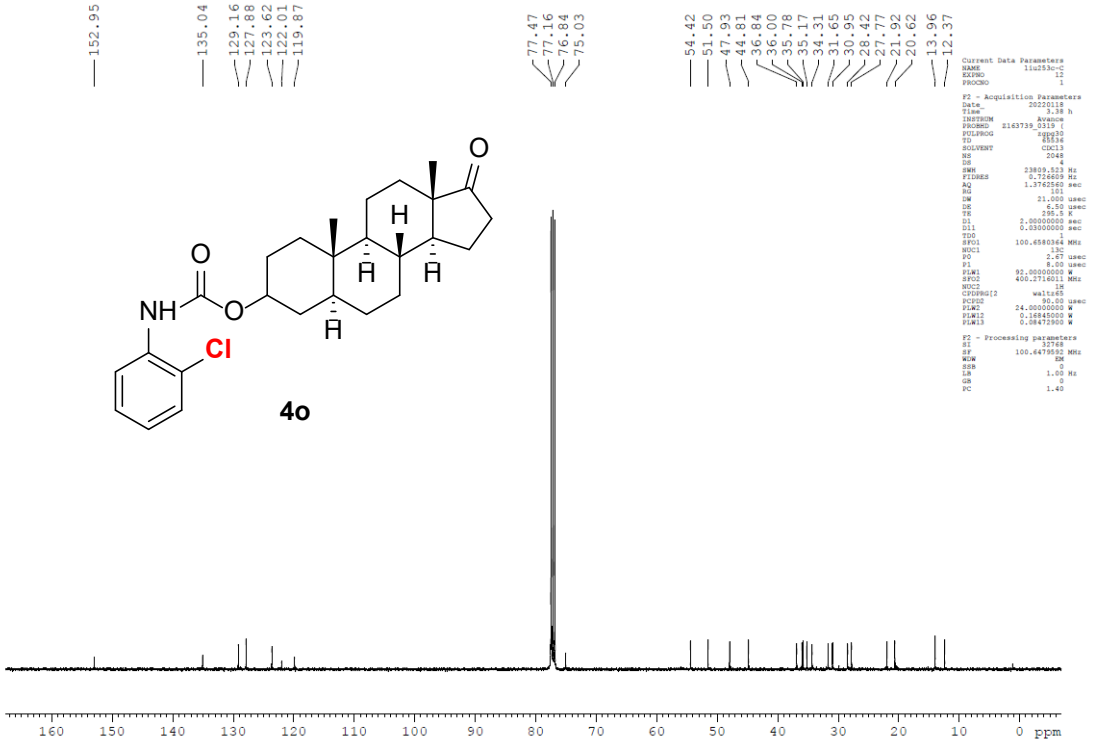
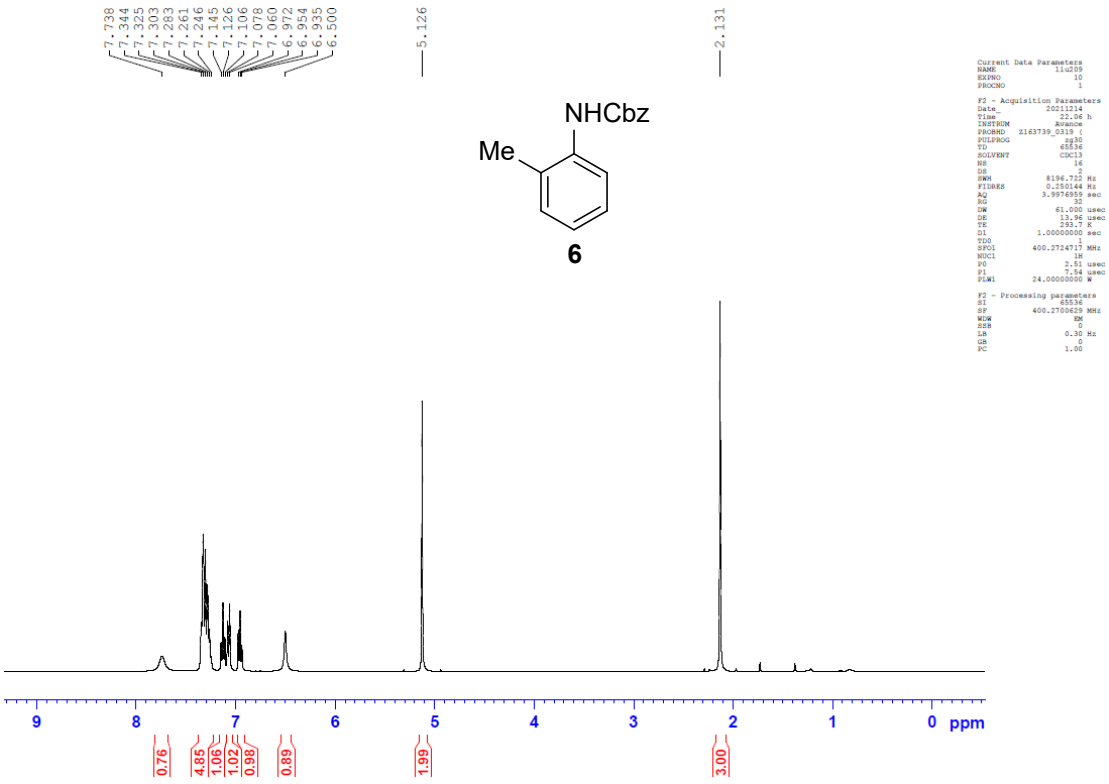
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0 ppm


4o
ppm


4o
ppm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7.303
7.283
7.261
7.246
7.145
7.126
7.106
7.078
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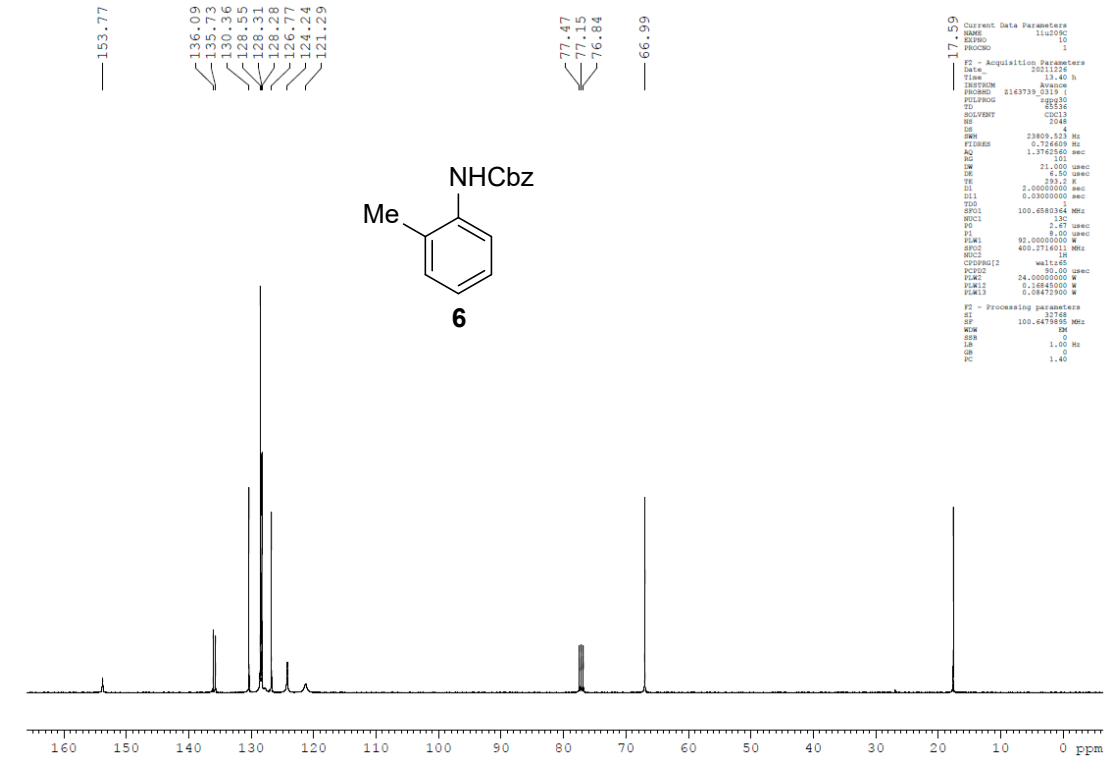
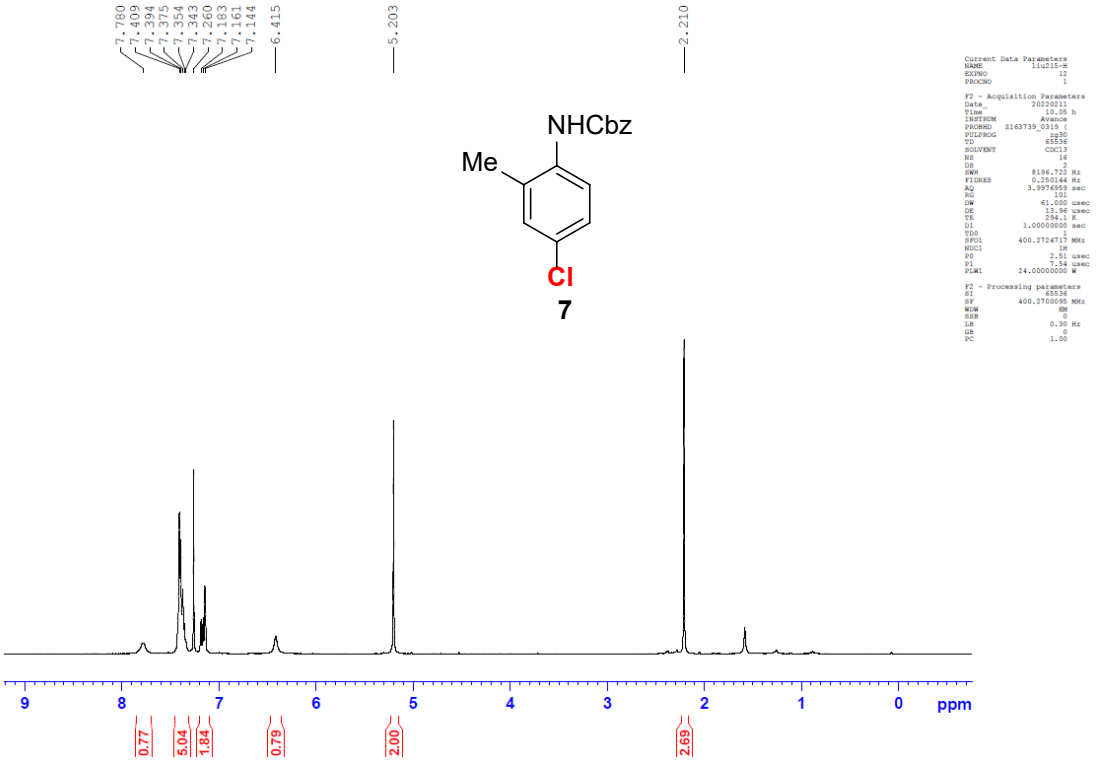
6.972
6.954
6.935
6.500
5.126
2.131
NHCbz
Me
6
9
8
7
6
5
4
3
2
1
0 ppm
0.76
4.85
1.06
1.02
0.98
0.89
1.99
3.00


153.77
136.09
135.73
130.36
128.55
128.31
128.28
126.77
124.24
121.29
77.47
77.15
76.84
66.99
17.59
NHCbz
Me
6
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0 ppm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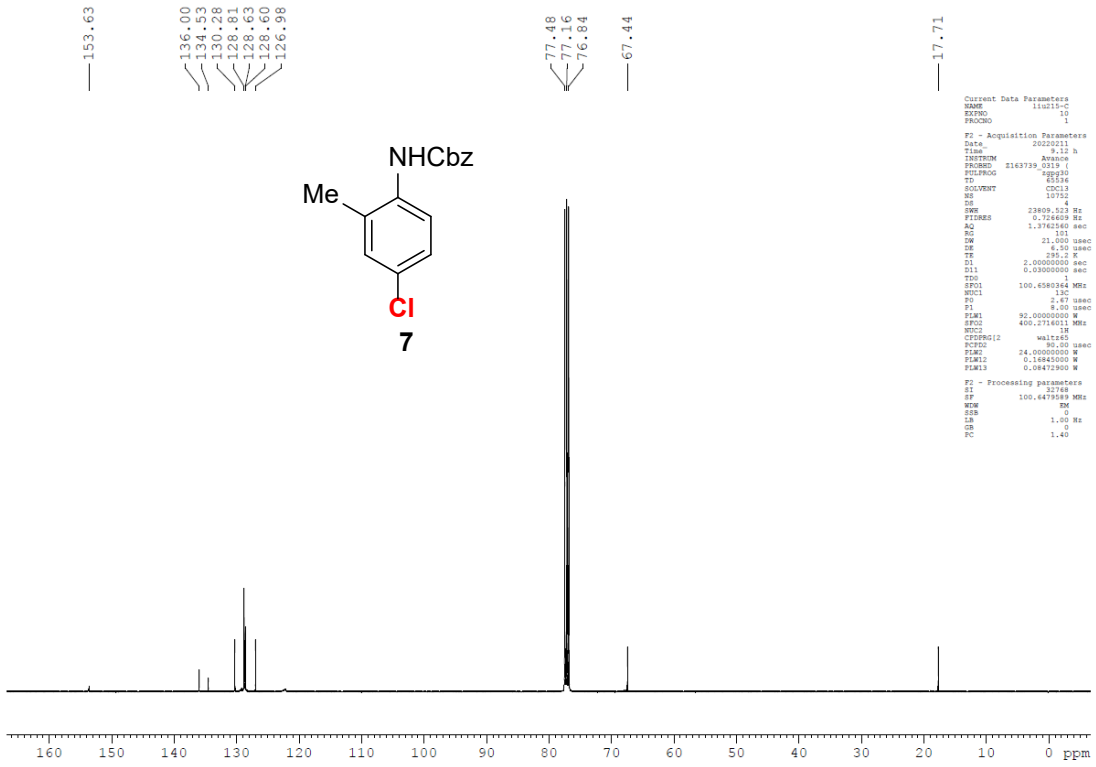
7.409
7.394
7.375
7.354
7.343
7.260
7.183
7.161
7.144
6.415
5.203
2.210
NHCbz
Me
Cl
7
ppm
0.77
5.04
1.84
0.79
2.00
2.69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134.53
130.28
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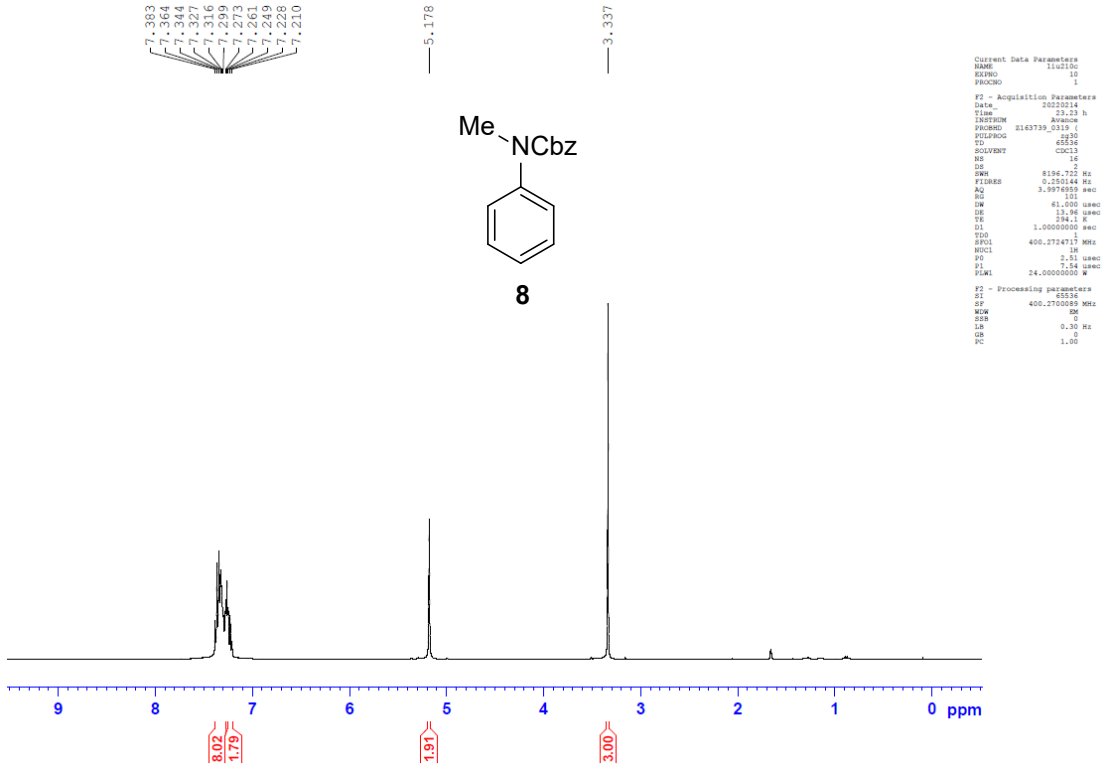
126.98
77.48
77.16
76.84
67.44
17.71
NHCbz
Me
Cl
7
ppm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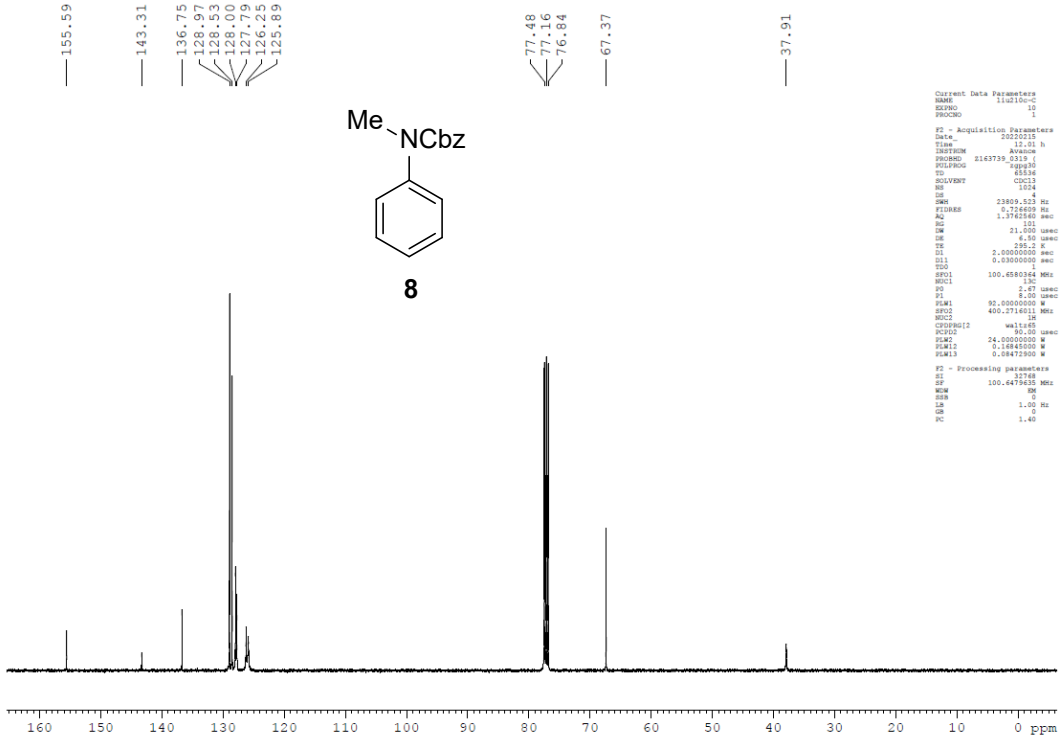
7.364
7.344
7.327
7.316
7.299
7.273
7.261
7.249
7.228
7.210
5.178
3.337
Me
NCbz
8
9
8
7
6
5
4
3
2
1
0 ppm
8.02
1.79
1.91
3.00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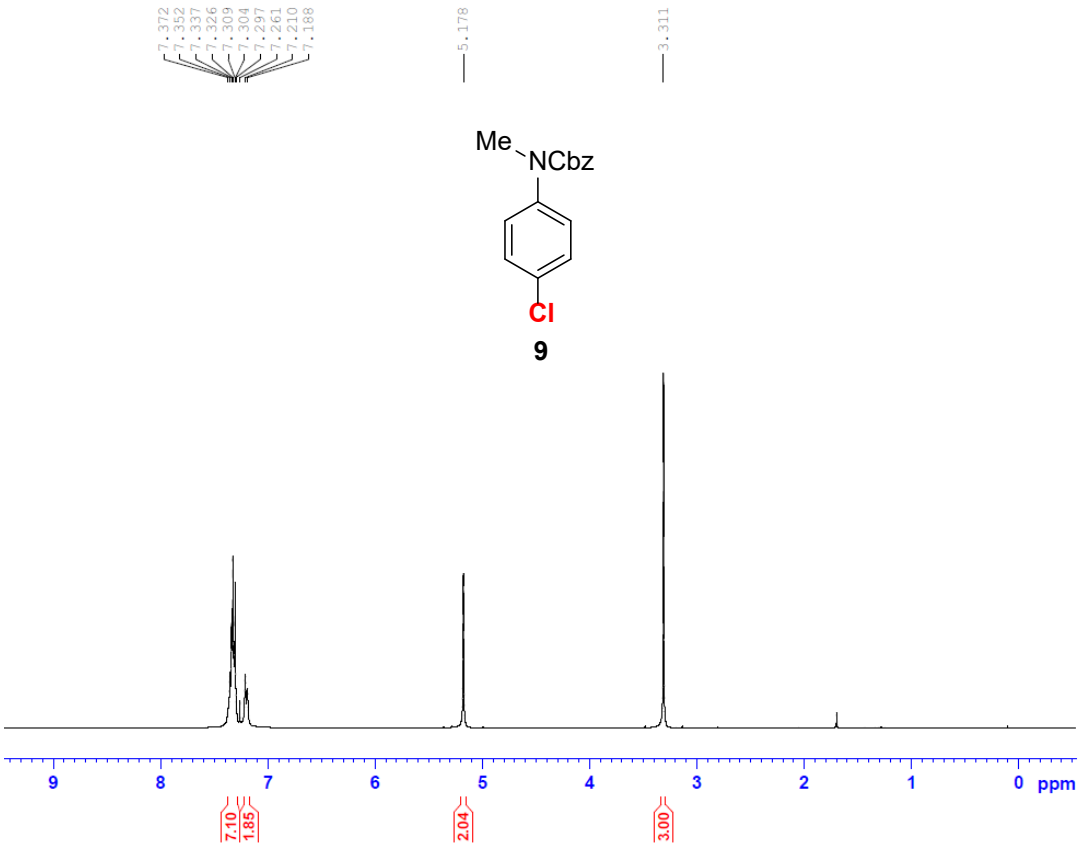
143.31
136.75
128.97
128.53
128.00
127.79
126.25
125.89
77.48
77.16
76.84
67.37
37.91
Me
NCbz
8
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0 ppm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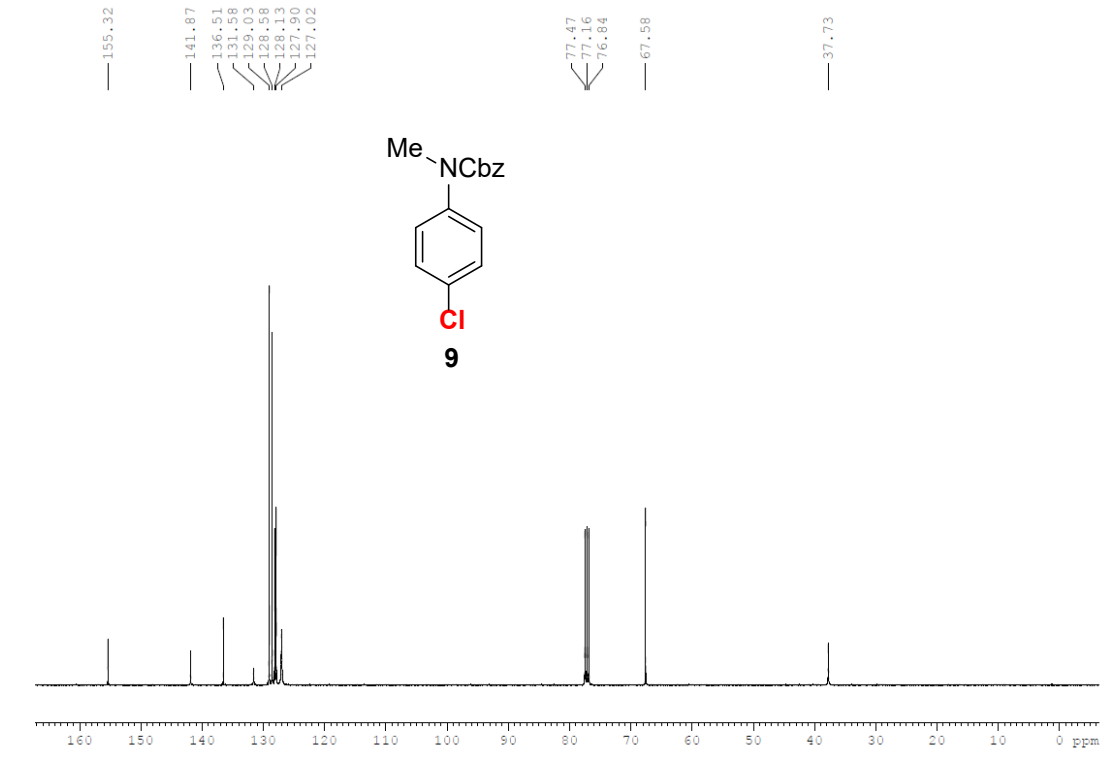
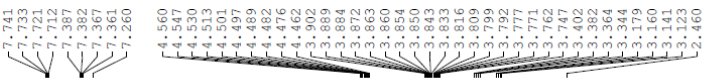
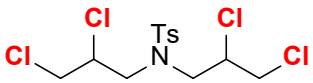
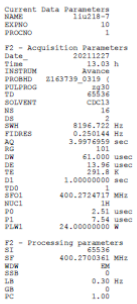
7.352
7.337
7.326
7.309
7.304
7.297
7.261
7.210
7.188
5.178
3.311
Me
NCbz
Cl
9
9
8
7
6
5
4
3
2
1
0 ppm
7.10
1.85
2.04
3.00

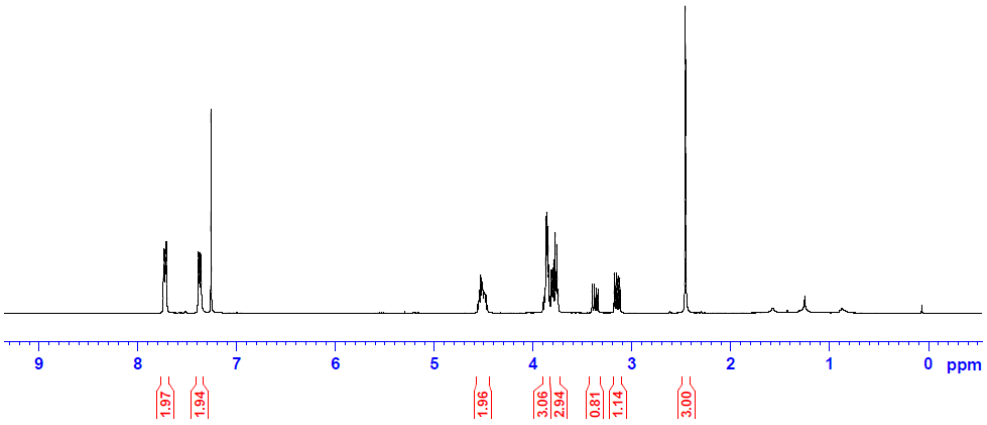

155.32
141.87
136.51
131.58
129.03
128.58
128.13
127.90
127.02
77.47
77.16
76.84
67.58
37.73
Me
NCbz
Cl
9
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0 ppm


7.741
7.733
7.721
7.712
7.387
7.382
7.367
7.361
7.260
4.560
4.547
4.530
4.513
4.501
4.497
4.489
4.482
4.476
4.462
3.902
3.889
3.884
3.872
3.863
3.860
3.854
3.850
3.843
3.833
3.816
3.809
3.799
3.792
3.777
3.771
3.762
3.747
3.402
3.382
3.364
3.344
3.179
3.160
3.141
3.123
2.460

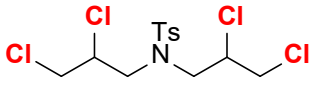

Cl
Cl
Ts
N
Cl
Cl

**11**

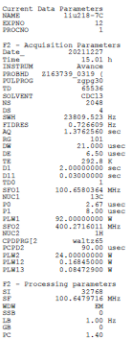


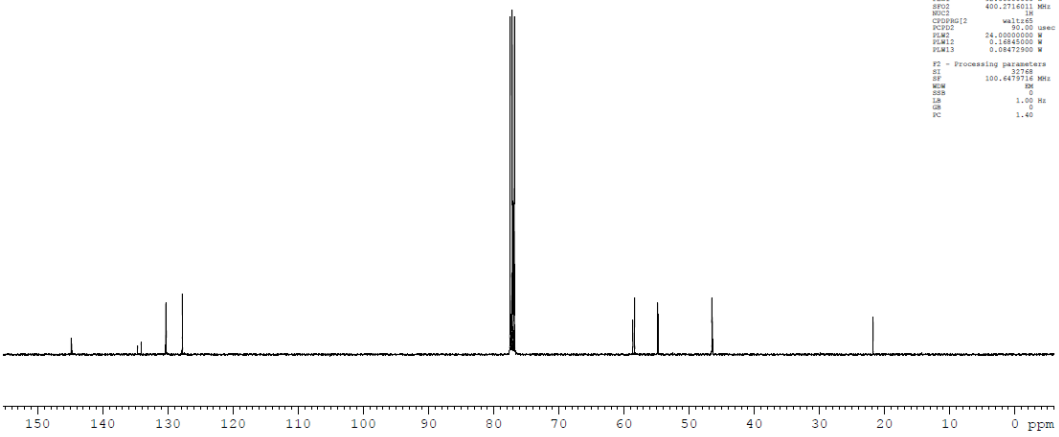

9
8
7
6
5
4
3
2
1
0 ppm
1.97
1.94
1.96
3.06
2.94
0.81
1.14
3.00

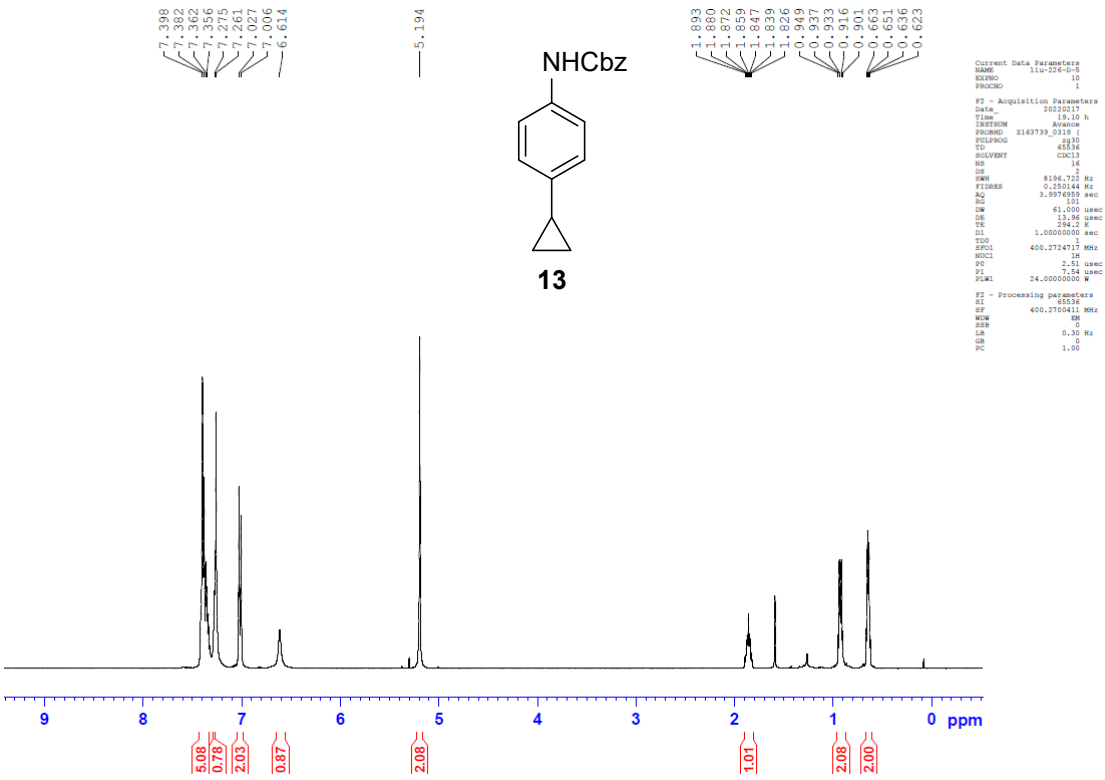

144.86
144.75
134.64
134.10
130.31
130.25
127.79
127.76
77.48
77.16
76.84
58.64
58.36
54.83
54.75
46.53
46.43
21.77

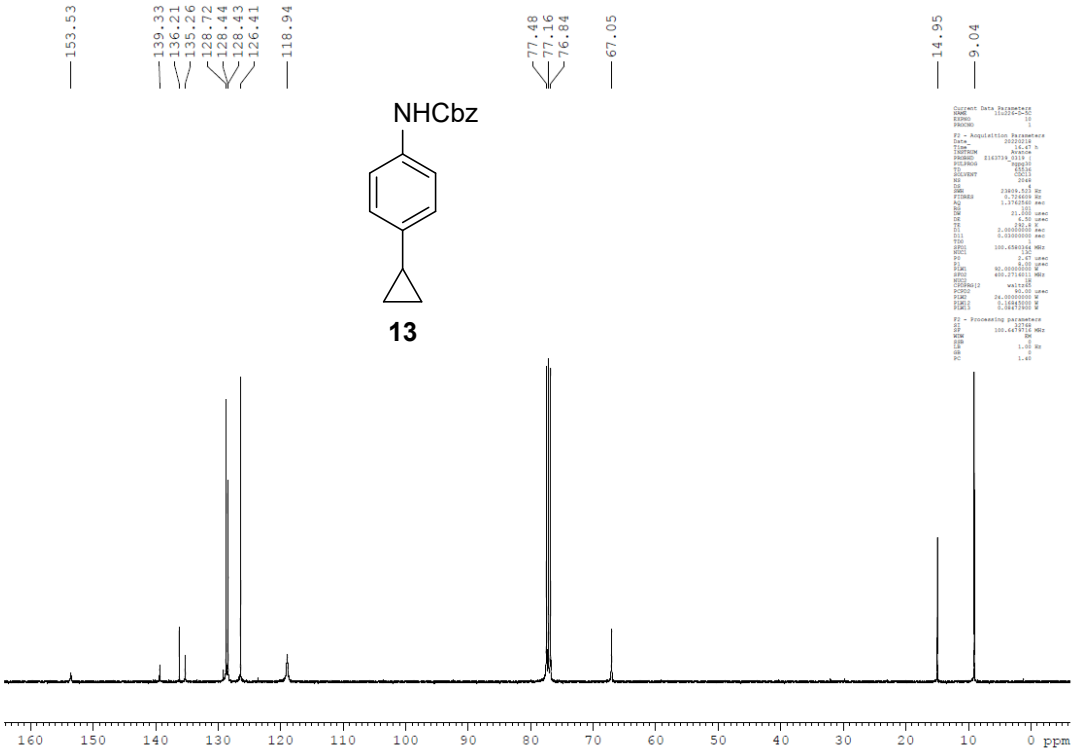

Cl
Cl
Ts
N
Cl
Cl

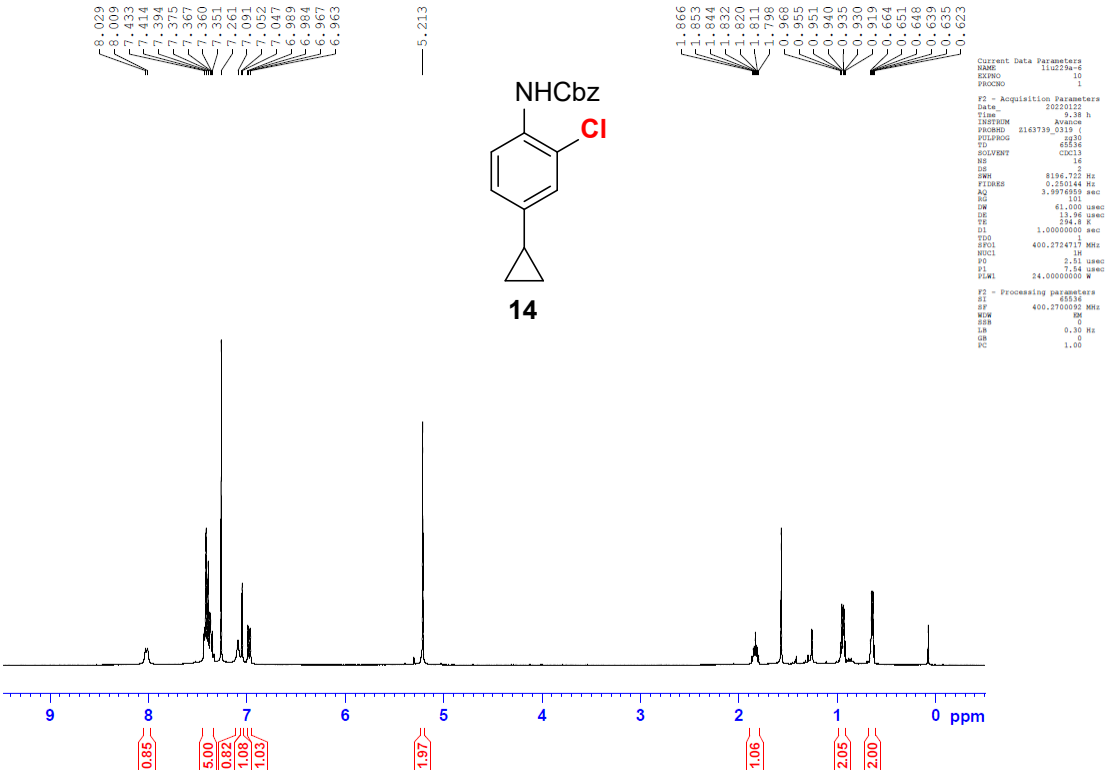
**11**

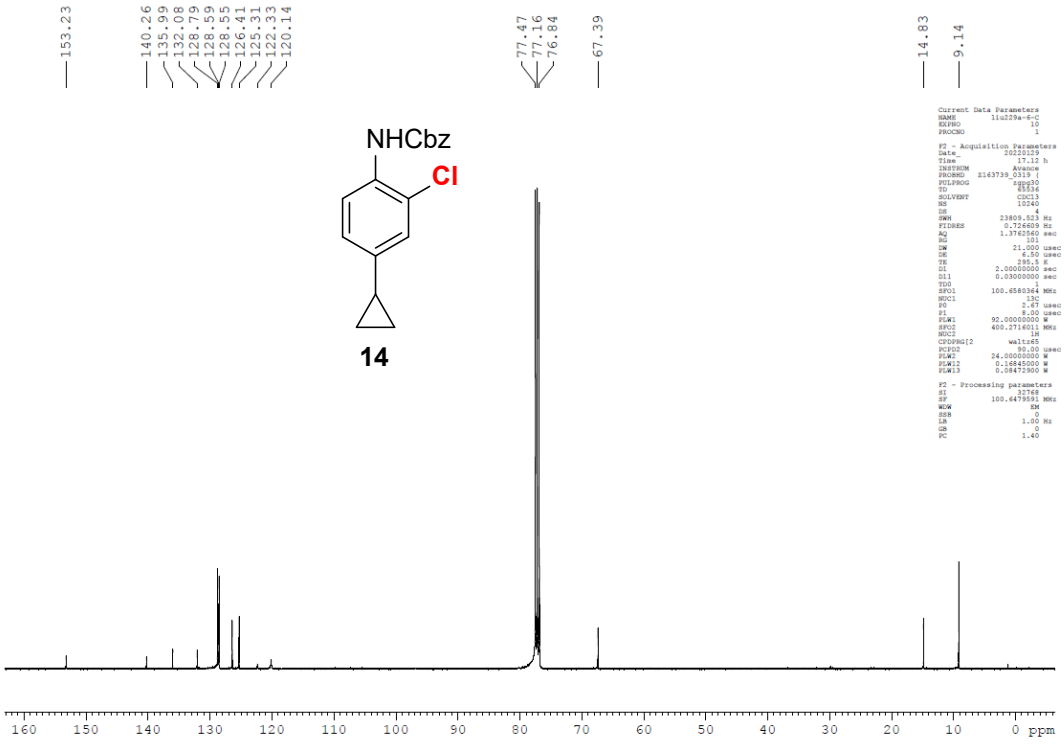



150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0 ppm


7.398
7.382
7.362
7.356
7.275
7.261
7.027
7.006
6.614
5.194
1.893
1.880
1.872
1.859
1.847
1.839
1.826
0.949
0.937
0.933
0.916
0.901
0.663
0.651
0.636
0.623
NHCbz
13
9
8
7
6
5
4
3
2
1
0 ppm
5.08
0.78
2.03
0.87
2.08
1.01
2.08
2.00


153.53
139.33
136.21
135.26
128.72
128.44
128.43
126.41
118.94
77.48
77.16
76.84
67.05
14.95
9.04
NHCbz
13
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0 ppm


8.029
8.009
7.433
7.414
7.394
7.375
7.367
7.360
7.351
7.261
7.091
7.052
7.047
6.989
6.984
6.967
6.963
5.213
1.866
1.853
1.844
1.832
1.820
1.811
1.798
0.968
0.955
0.951
0.940
0.935
0.930
0.919
0.664
0.651
0.648
0.639
0.635
0.623
NHCbz
Cl
14
9 8 7 6 5 4 3 2 1 0 ppm
0.85
5.00
0.82
1.08
1.03
1.97
1.06
2.05
2.00


153.23
140.26
135.99
132.08
128.79
128.59
128.55
126.41
125.31
122.33
120.14
77.47
77.16
76.84
67.39
14.83
9.14
NHCbz
Cl
14
160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 ppm