SUPPORTING INFORMATION

Vanadium-Catalyzed Oxidative C(CO)–C(CO) Bond Cleavage for C–N Bond Formation: One Pot Domino Transformation of 1,2-Diketones and Amidines into Imides and Amides

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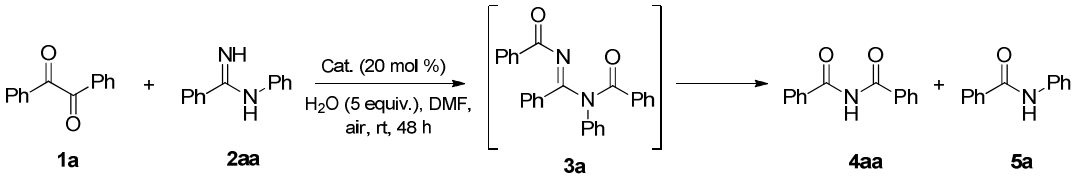
I. Table S1: The screening of metal catalyst for the reaction of benzil (**1a**) and *N*-phenylbenzimidamide (**2aa**)[a]

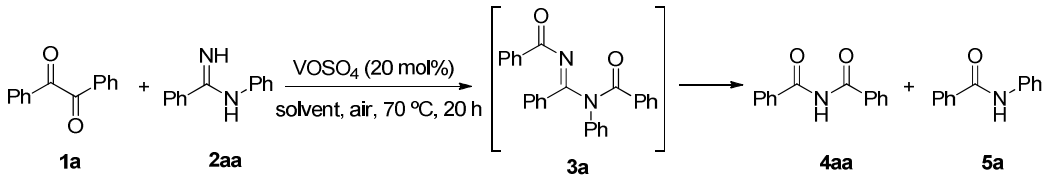


1a **2aa** **3a** **4aa** **5a**

Entry	Cat. (20 mol%)	Yield of products (%)[b]			Recovery of **1a** (%)
		3a	**4aa**	**5a**	
1	none	0	0	0	98
2	$Cu(NO_3)_2 \cdot xH_2O$	0	0	0	96
3	$CuSO_4 \cdot 5H_2O$	0	0	0	94
4	$Cu(OAc)_2 \cdot H_2O$	26	0	0	67
5	$CuCl_2 \cdot 2H_2O$	38	0	0	55
6	CuBr	47	0	0	48
7	CuI	55	0	0	40
8	$Cu(OTf)_2$	52	21	22	18
9[c]	$Cu(OTf)_2$	50	24	25	10
10[d]	$Cu(OTf)_2$	48	27	28	15
10[e]	$Cu(OTf)_2$	45	10	12	16
11	AgOTf	trace	0	0	n.d.
12	Ag_2CO_3	0	0	0	n.d.
13	$AgNO_3$	0	0	0	n.d.
14	$In(OTf)_3$	0	0	0	n.d.
15	$Zn(OTf)_2$	0	0	0	n.d.
16	$Sc(OTf)_3$	trace	0	0	n.d.
17	$FeCl_3$	trace	0	0	n.d.

[a]A mixture of **1a** (0.5 mmol), **2aa** (0.6 mmol), H_2O (45 μL) and 20 mol% catalyst in dry DMF (3 mL) was strirred at room temperature for 48 h under air. [b]Isolated yields of products based on **1a**. [c]The reaction was run for 96 h. [d]The reaction was carried out with 50 mol% of $Cu(OTf)_2$. [e]The reaction was conducted at 80 ºC. n.d.: not determined.

II. Table S2. The screening of solvent[a]

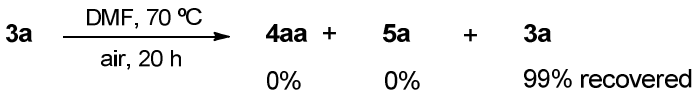


1a 2aa 3a 4aa 5a

Entry	Solvent	H_2O (equiv.)	Yield of products (%)[b]		
			3a	**4aa**	**5a**
1	n-hexane	-	0	0	0
2	toluene	-	8	0	0
3	1,4-dioxane	-	trace	0	0
4	DCM	-	0	0	0
5	DCE	-	trace	0	0
6	ethyl acetate	-	trace	0	0
7	acetone	H_2O (5)	25	trace	trace
8	ethanol	H_2O (5)	trace	0	0
9	THF	H_2O (5)	32	trace	trace
10[c]	CH_3CN	H_2O (5)	0	76	80
11[d]	DMSO	H_2O (5)	0	82	88
12[e]	DMA	H_2O (5)	0	85	84

[a]A mixture of **1a** (0.5 mmol), **2aa** (0.6 mmol) and 20 mol% $VOSO_4 \cdot xH_2O$ in solvent (3 mL) was stirred at 70 ºC for 20 h under air. [b]Isolated yields of products based on **1a**. [c]The reaction was run for 48 h. [d]The reaction was run for 36 h. [e]The reaction was run for 32 h.

III. Control experiments



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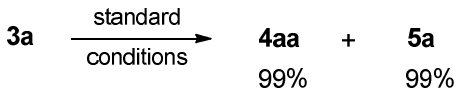

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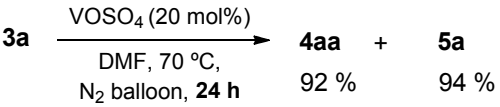

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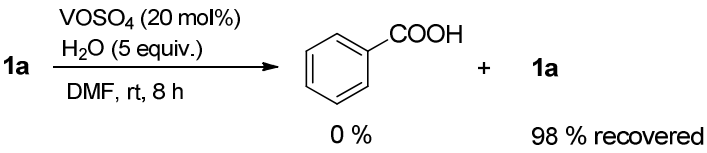

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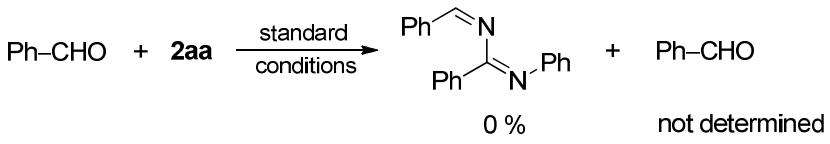

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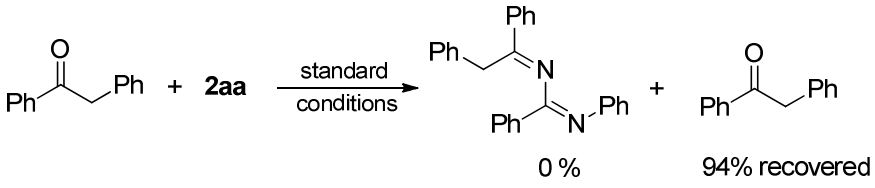
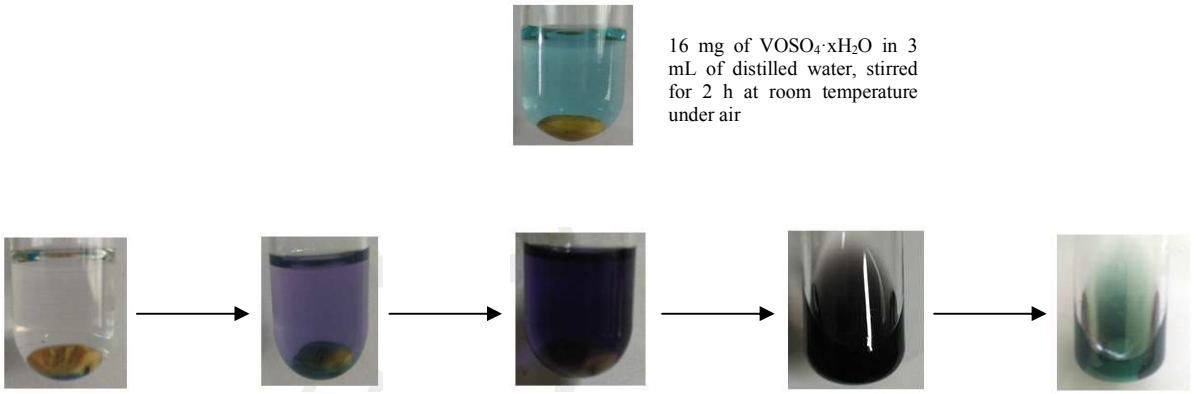


(S6)

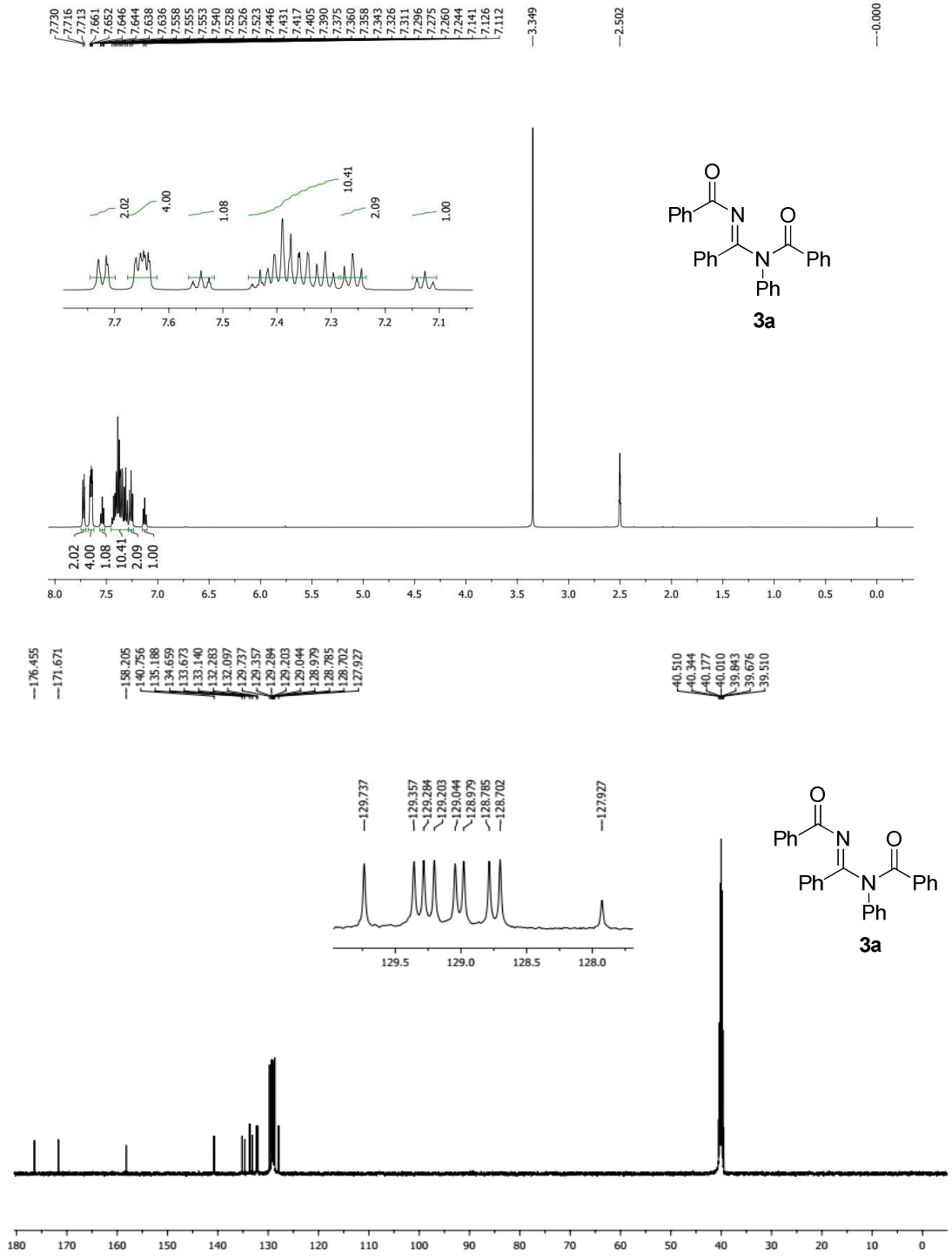
IV. Colour change during the reaction of benzil (1a) with N-phenylbenzimidamide (2aa):

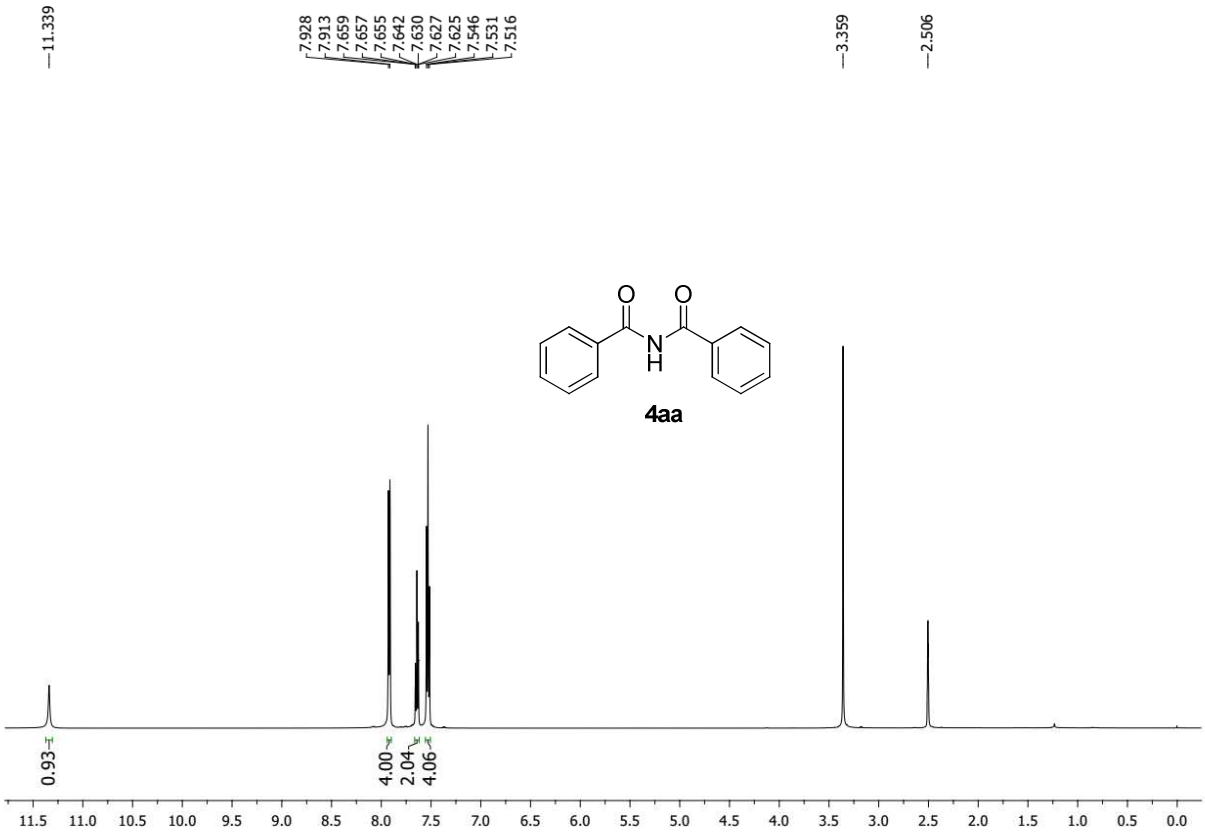


Note:

Whenever a mixture of 1,2-diketone, amidine, H_2O and 20 mol% of $VOSO_4 \cdot xH_2O$ in dry DMF was heated at 70 ºC, the color of the reaction mixture turned black within 1 h, which then turned to green in most of the cases.

v. ^{1}H- and ^{13}C-NMR spectra copies of compounds **3a**, **4**, **5** and **6**

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7.516
3.359
2.506
4aa
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4.00
2.04
4.06
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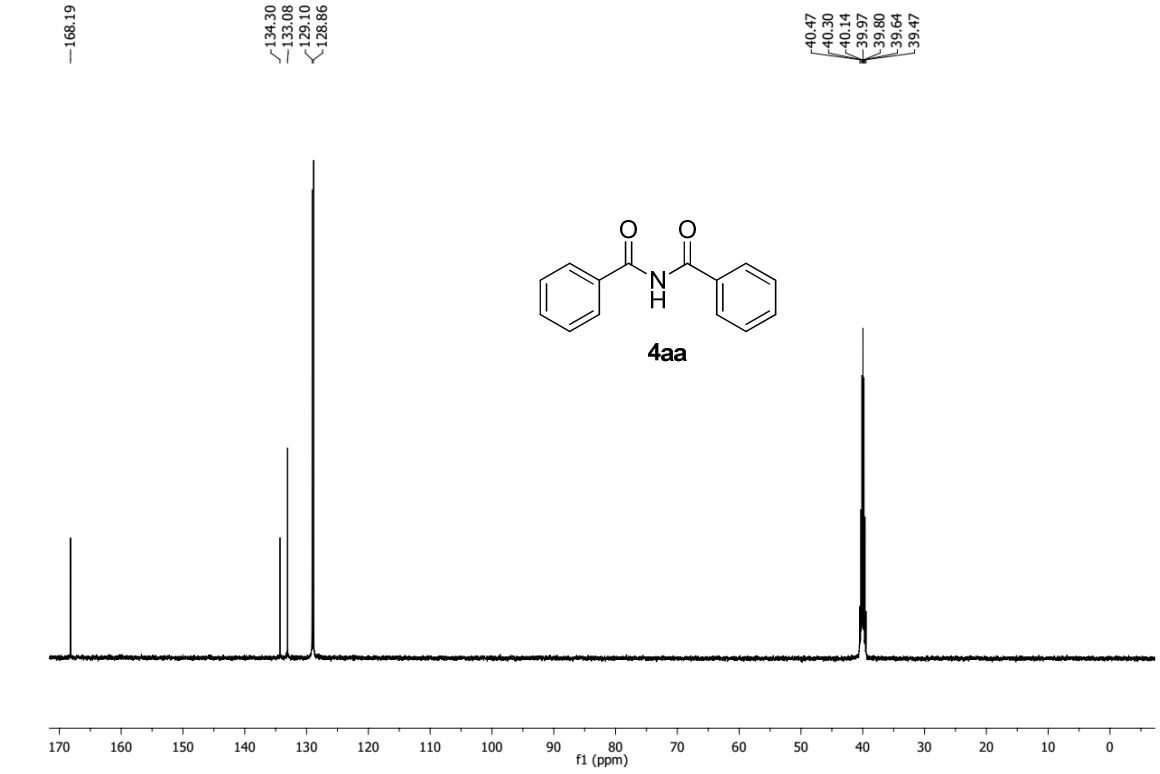
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39.47
4aa
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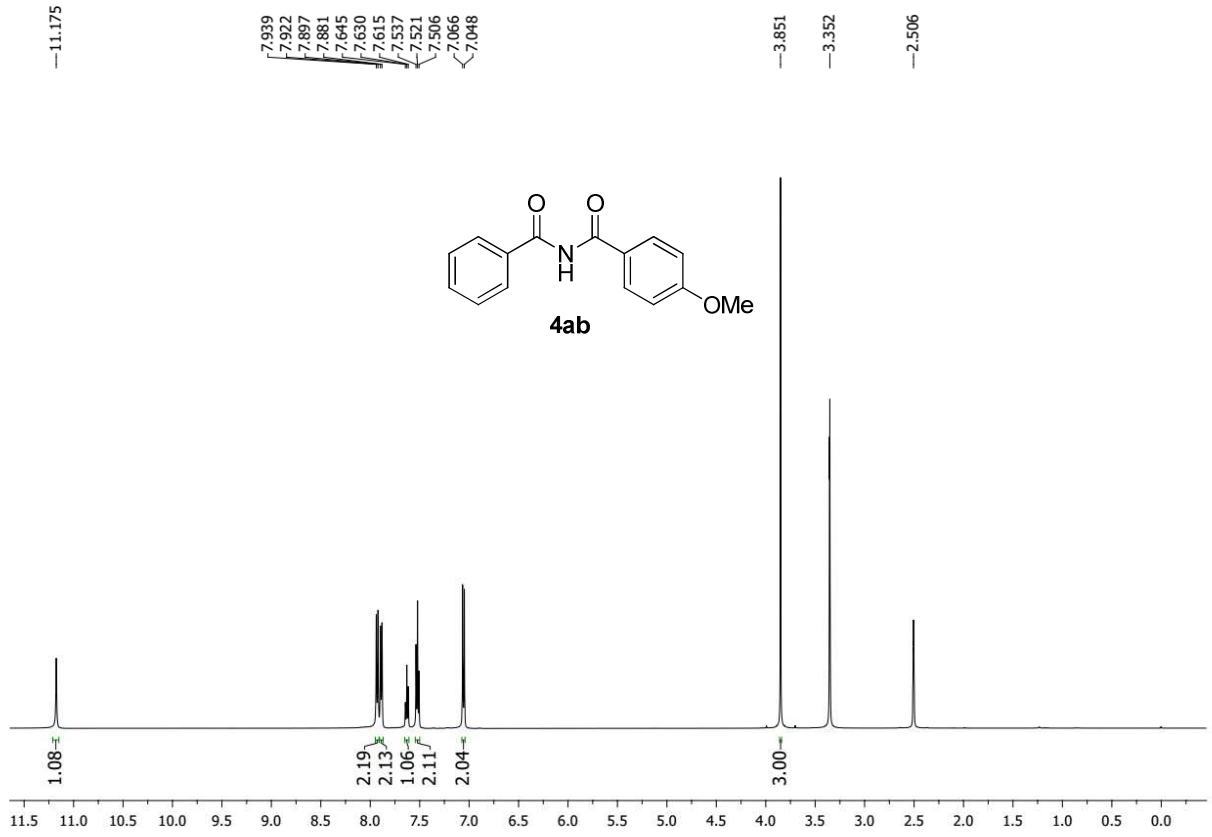
f1 (ppm)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2.13
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2.11
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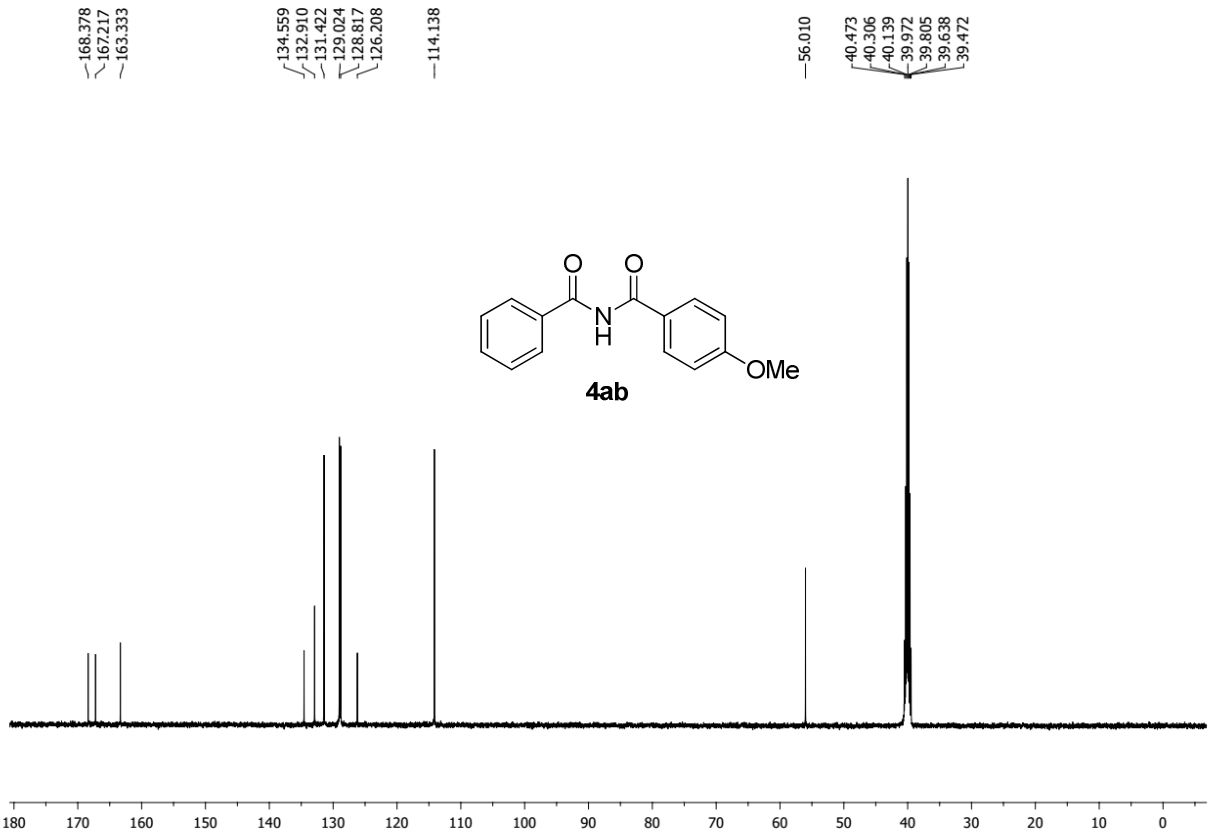
3.00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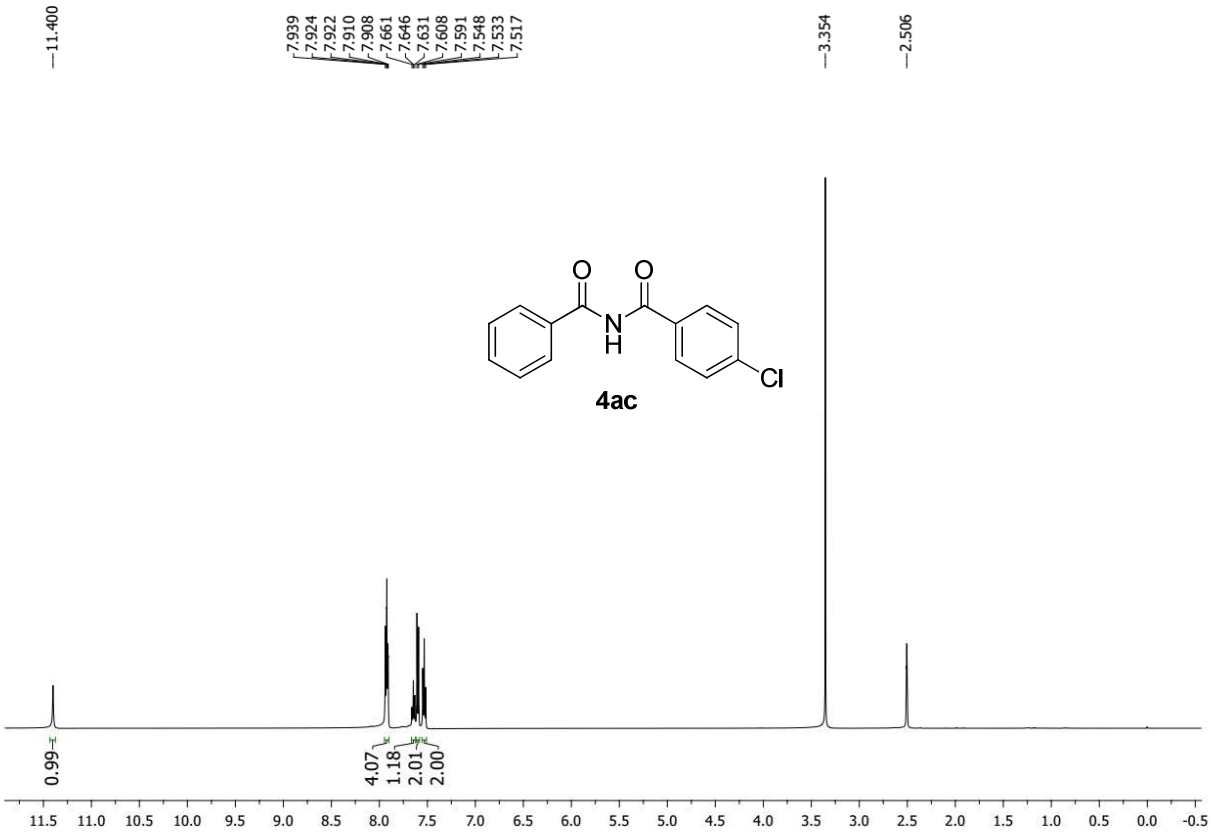
39.472
4ab
OMe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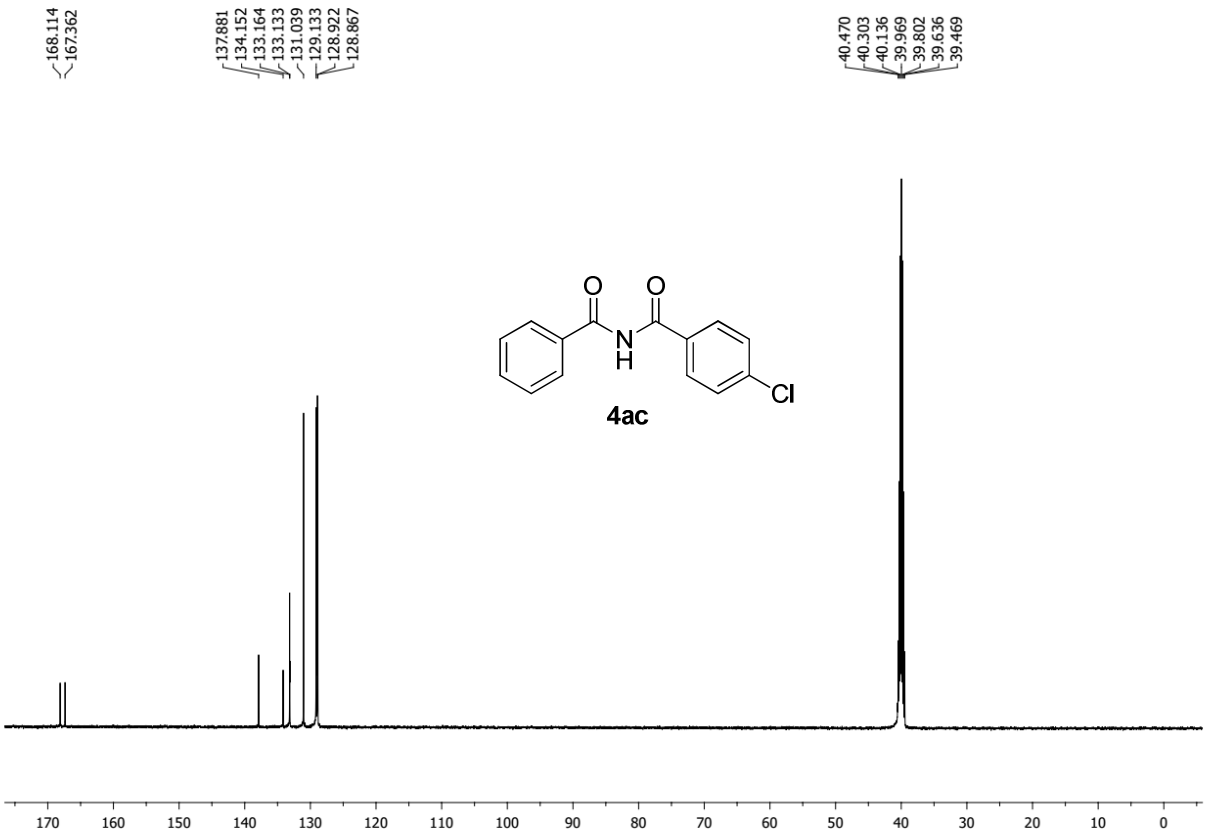
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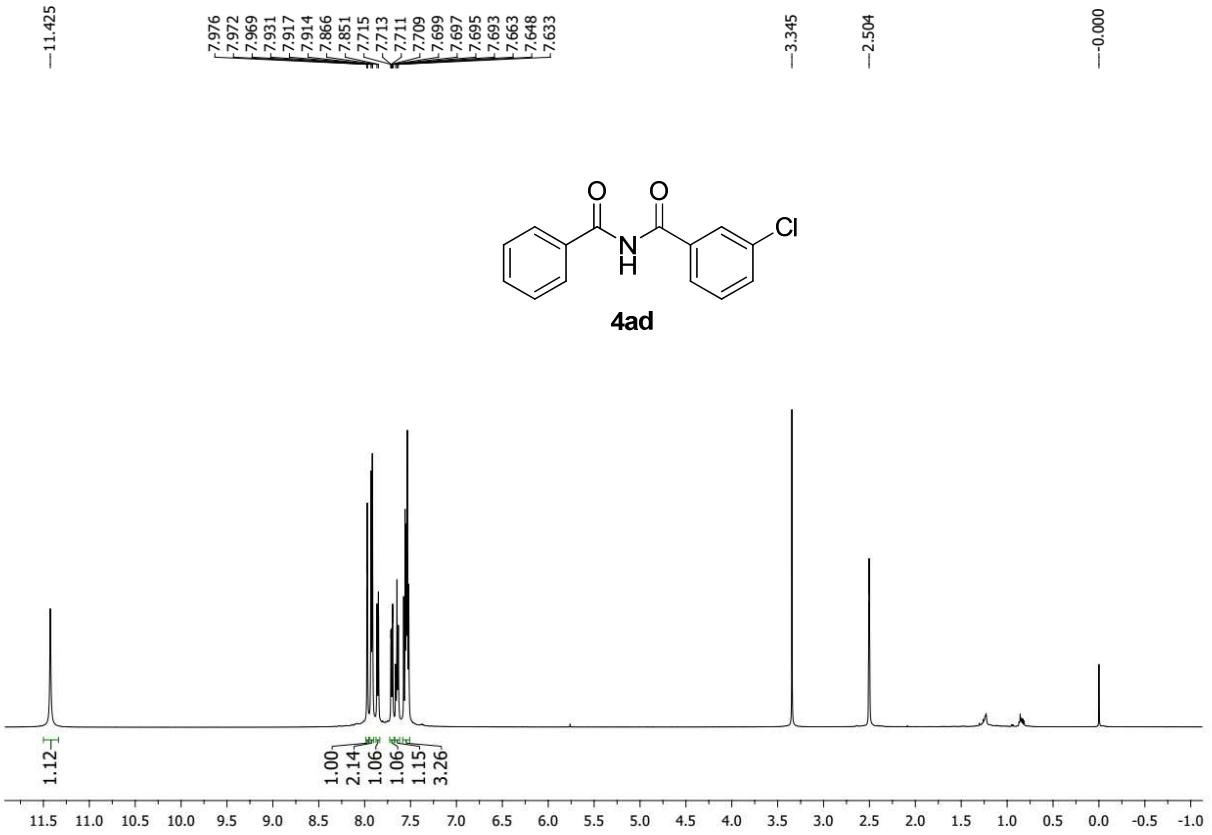
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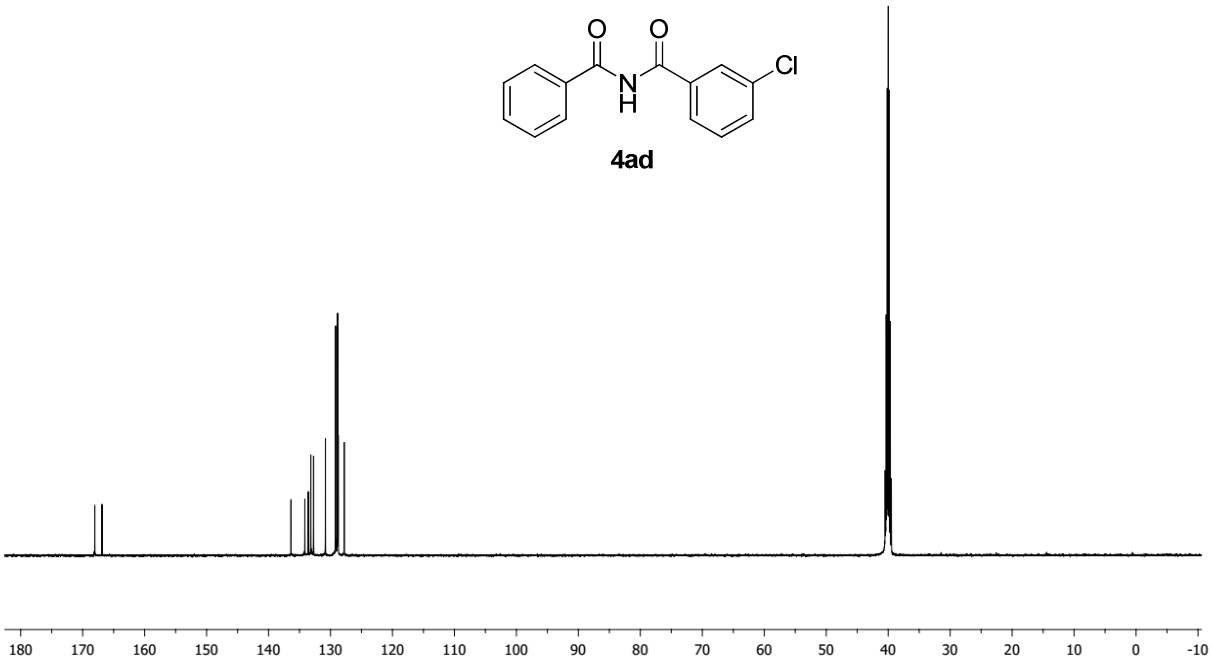
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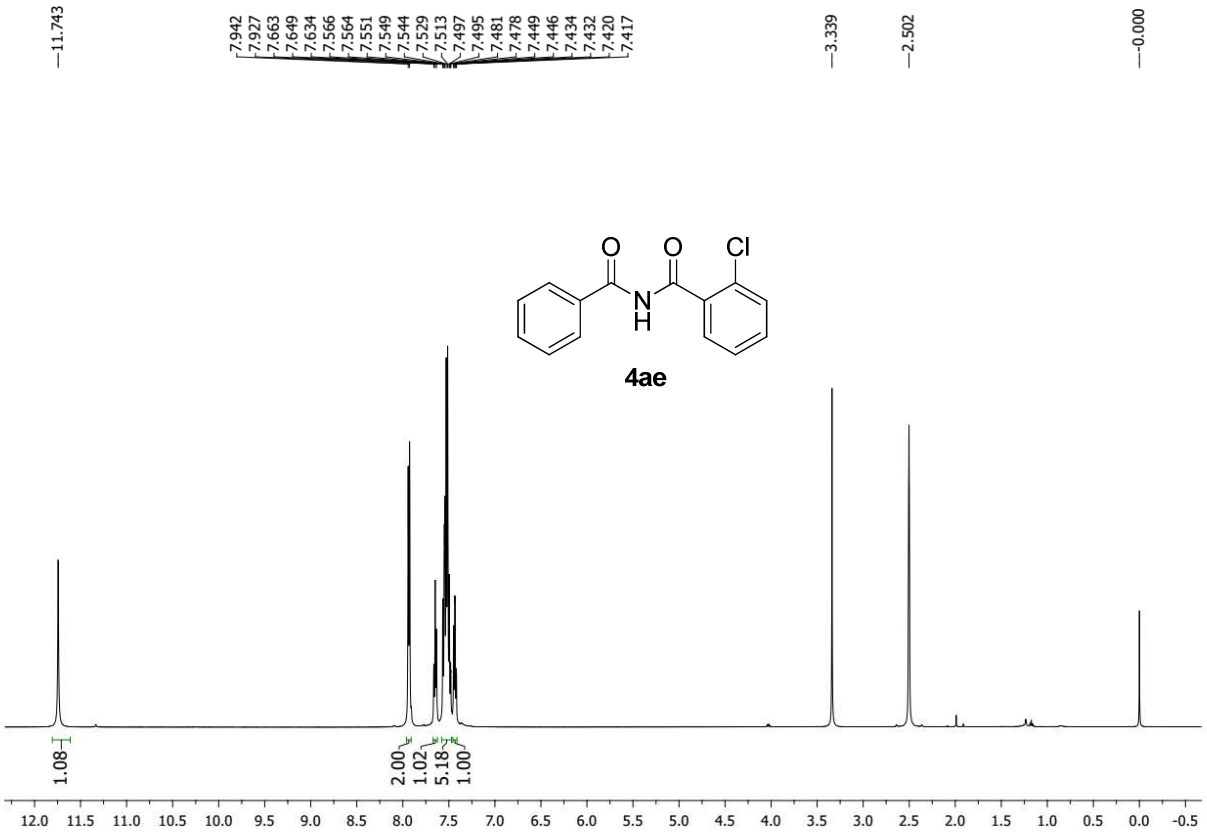
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Cl
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2.00
1.02
5.18
1.00
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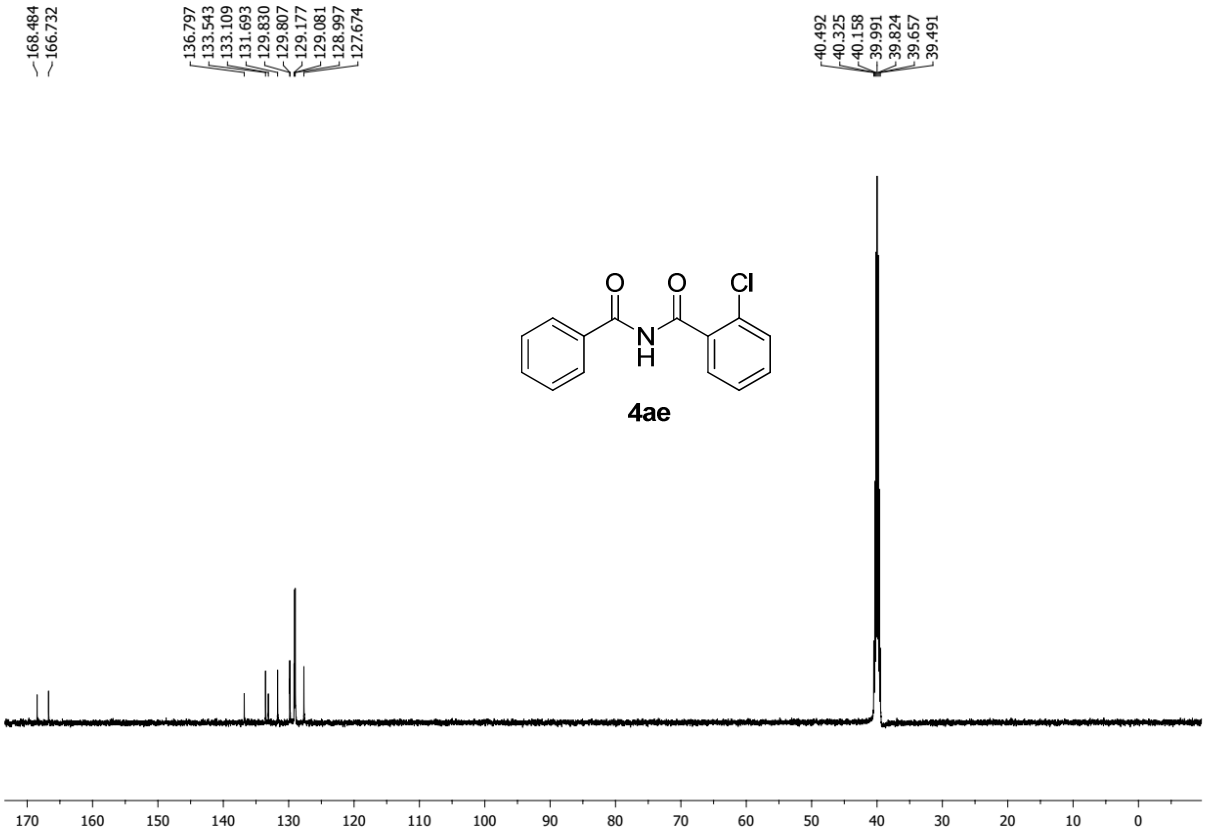
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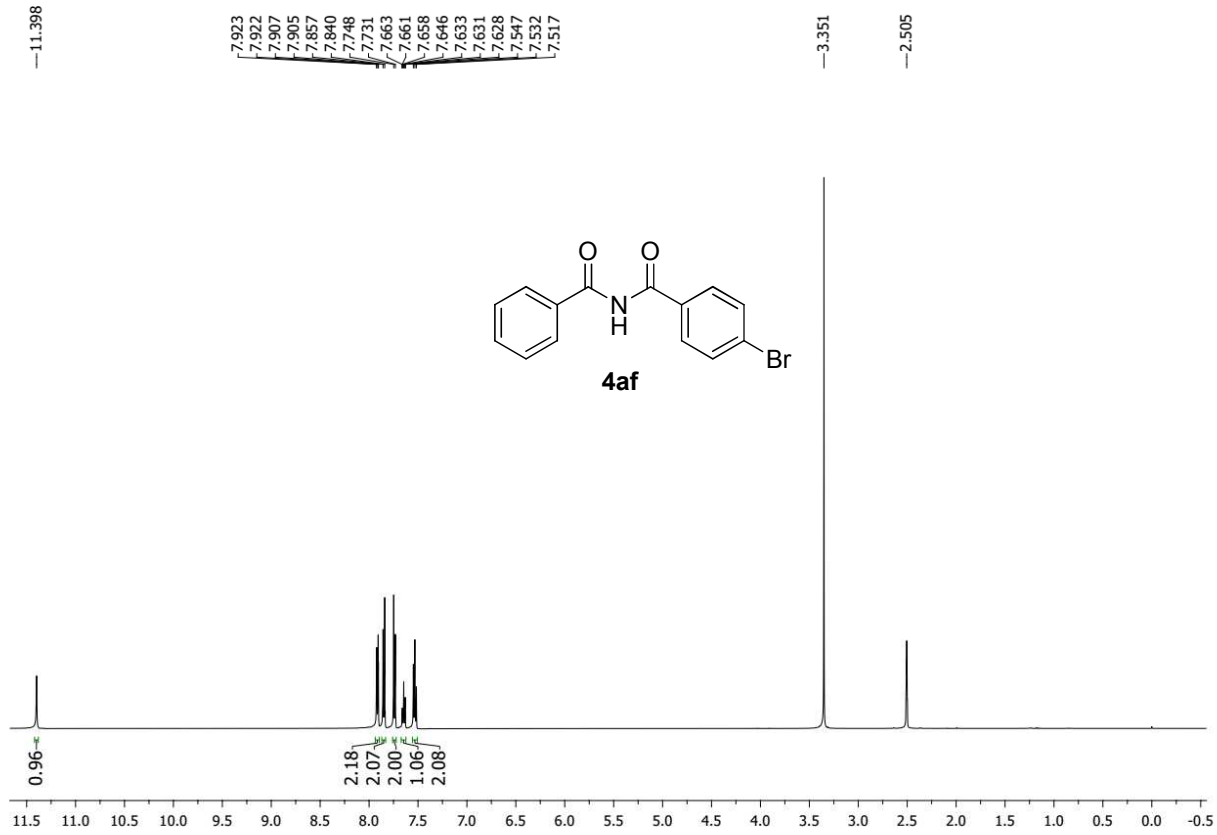
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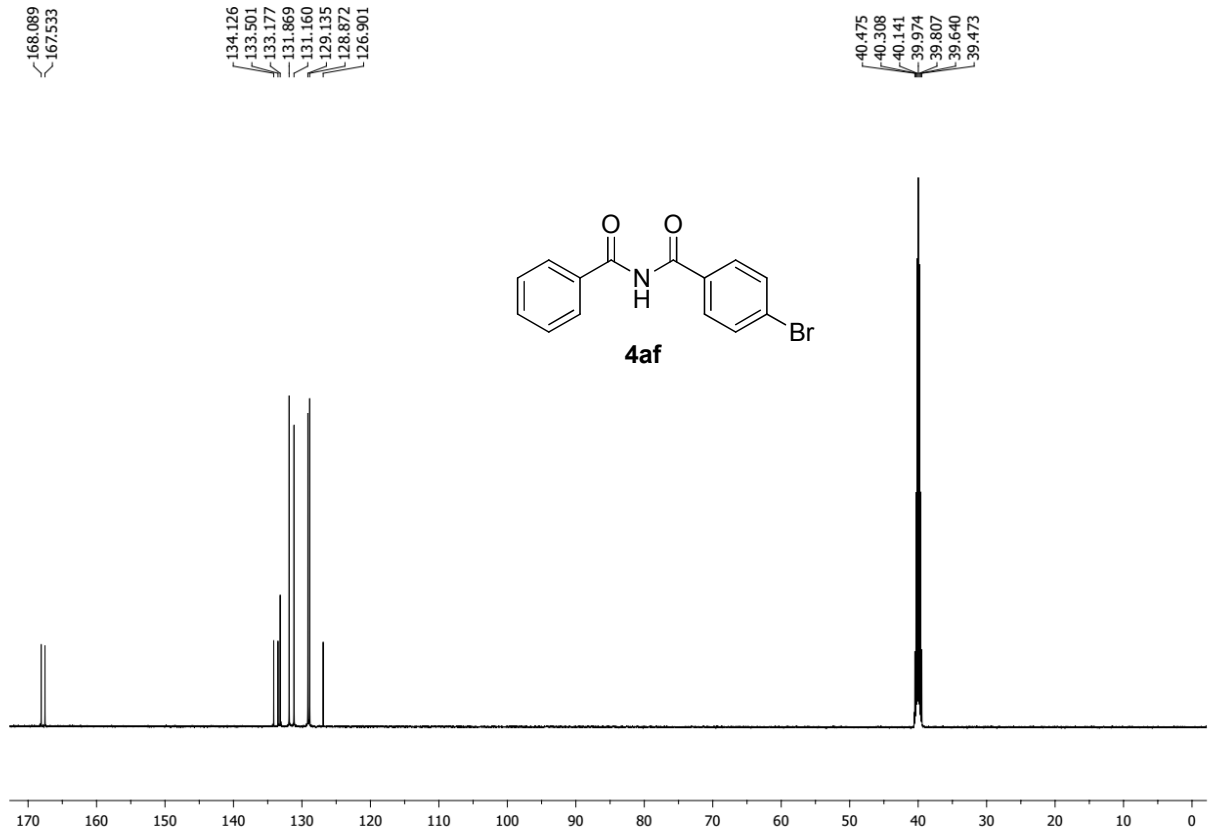
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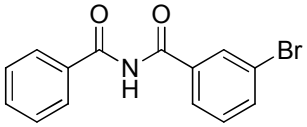
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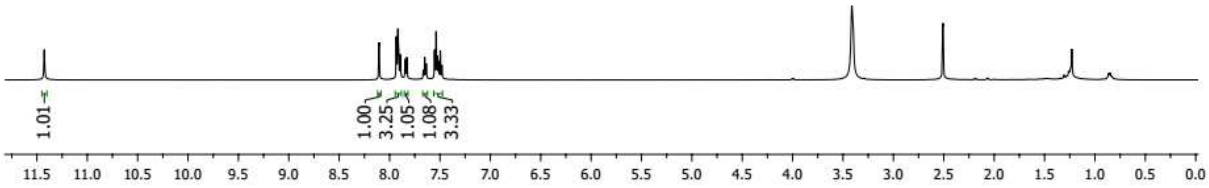
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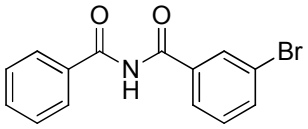
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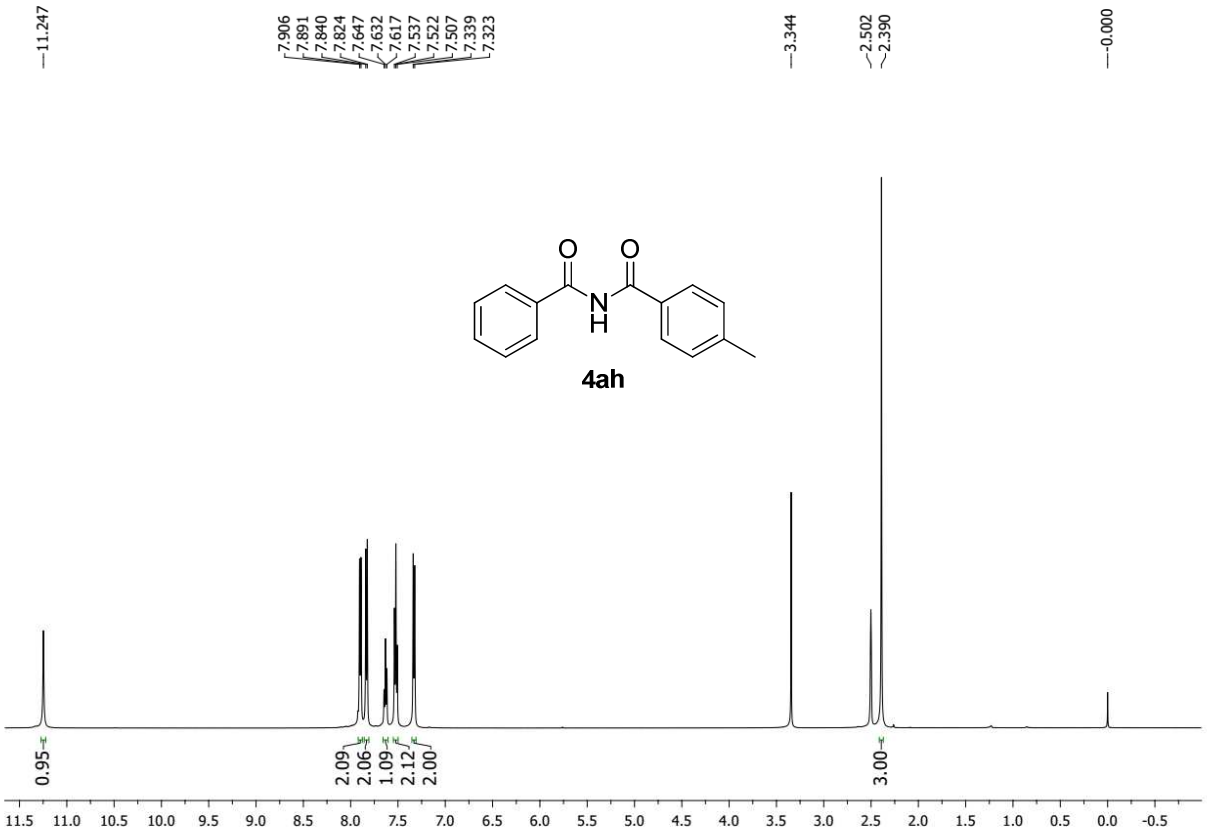
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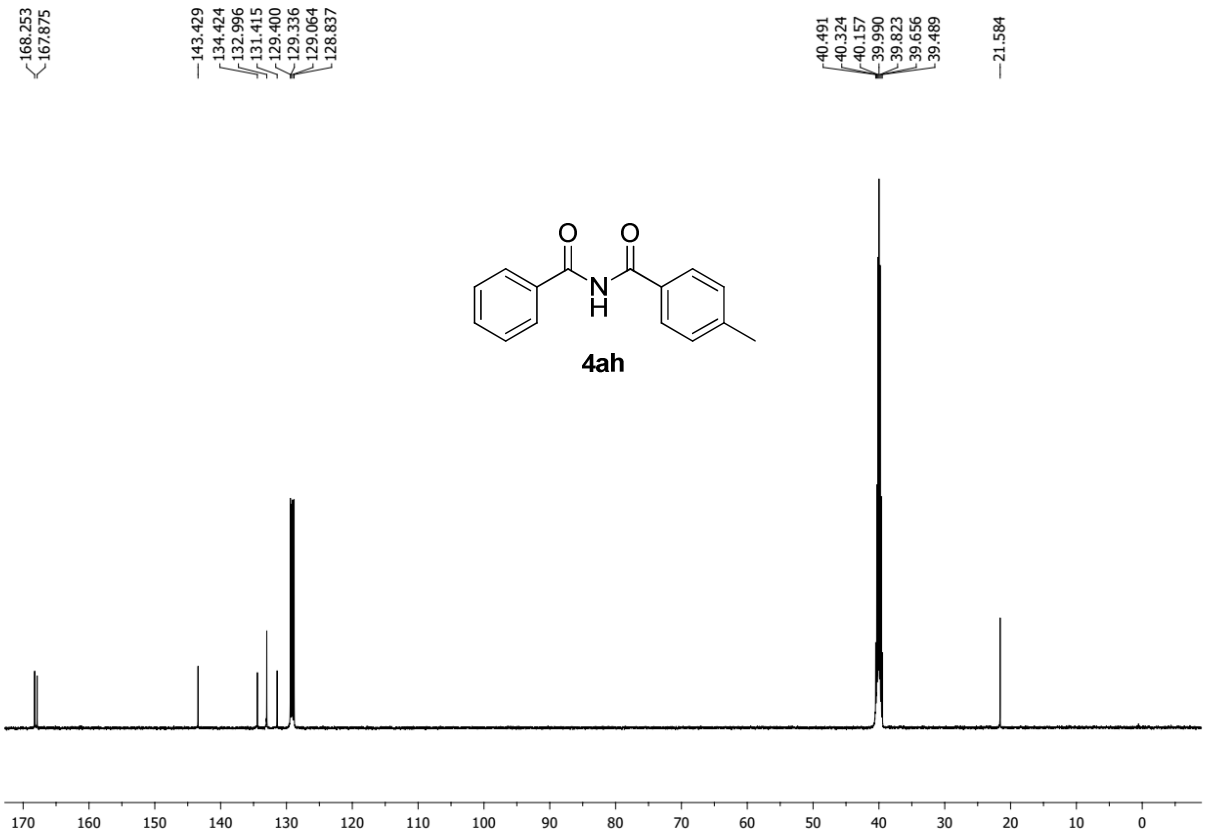
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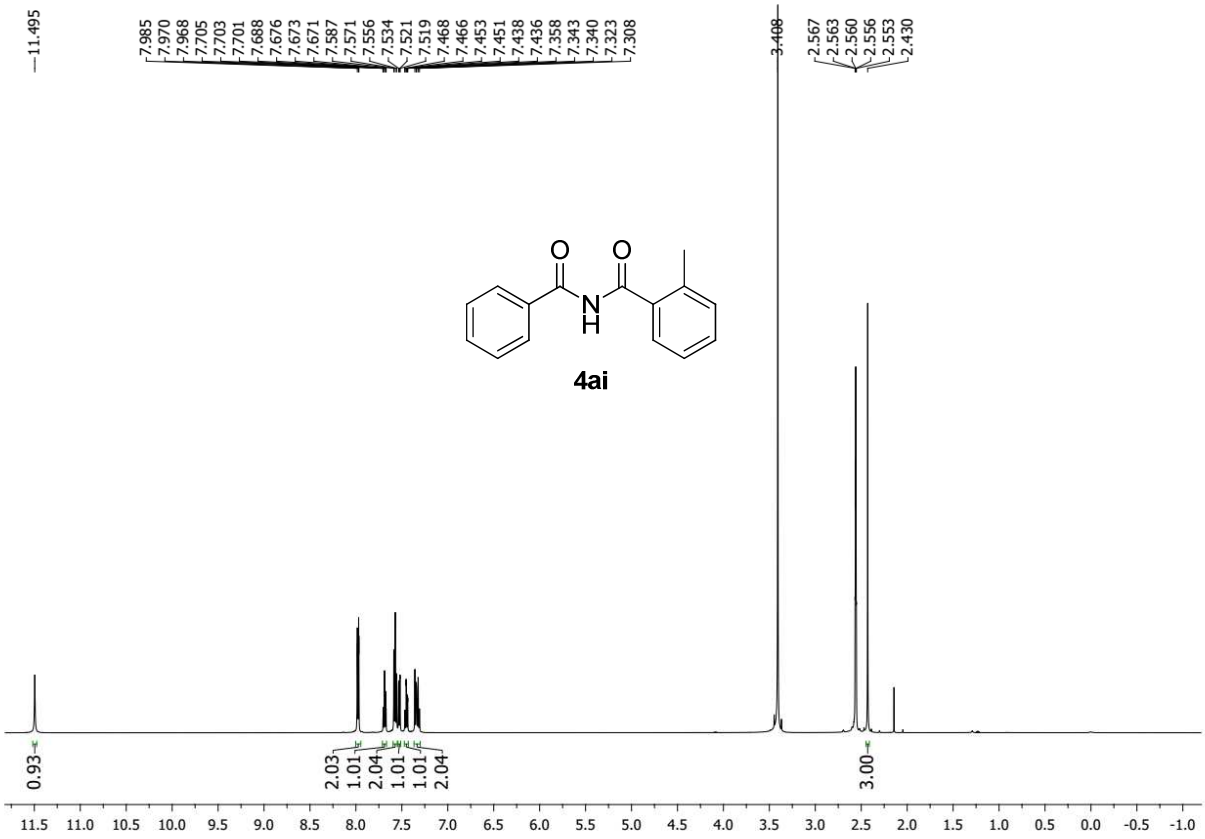
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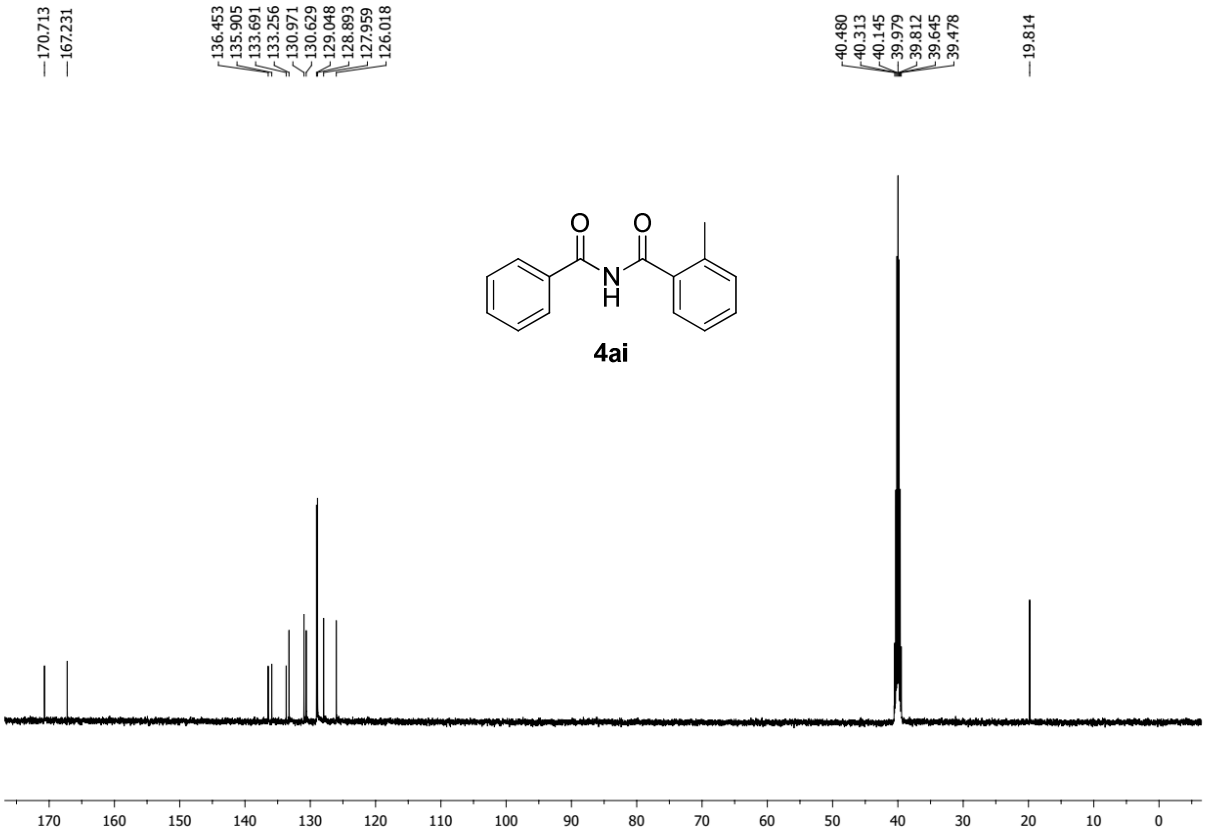
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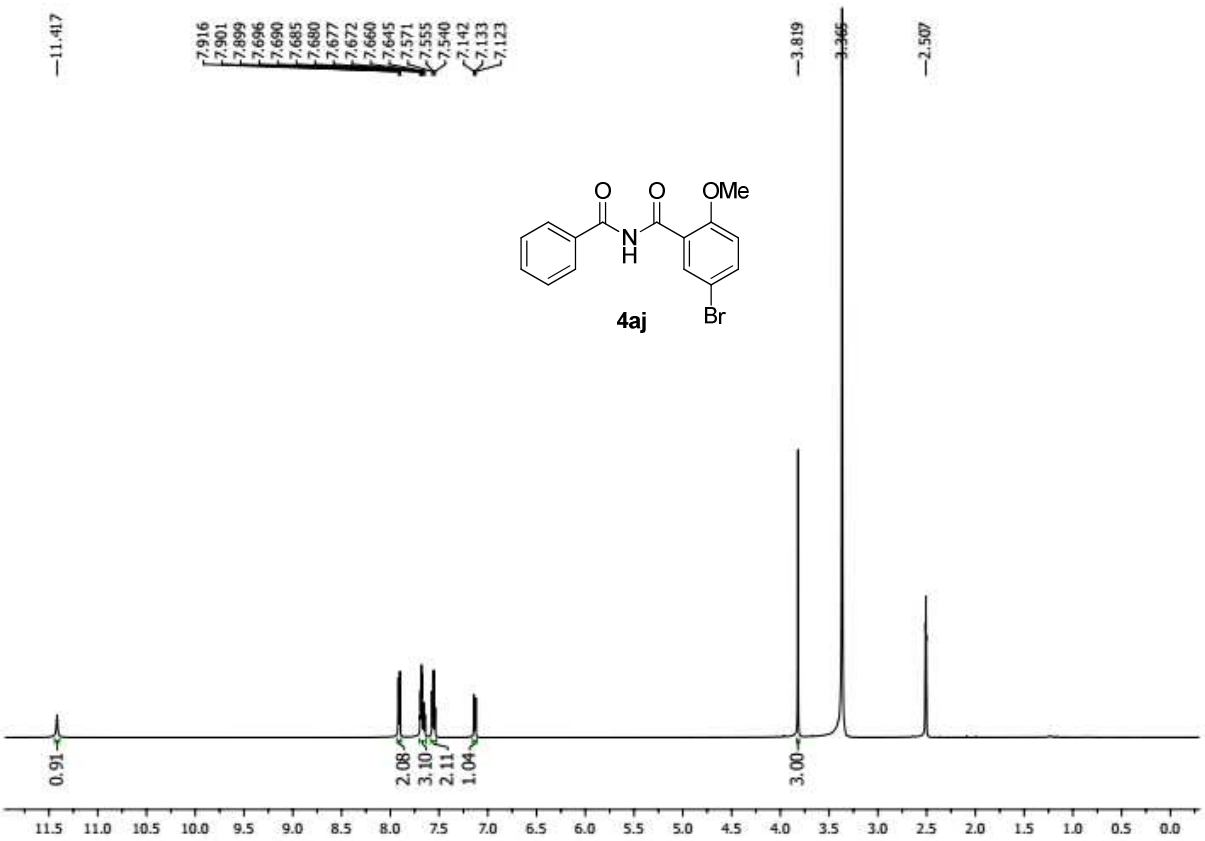
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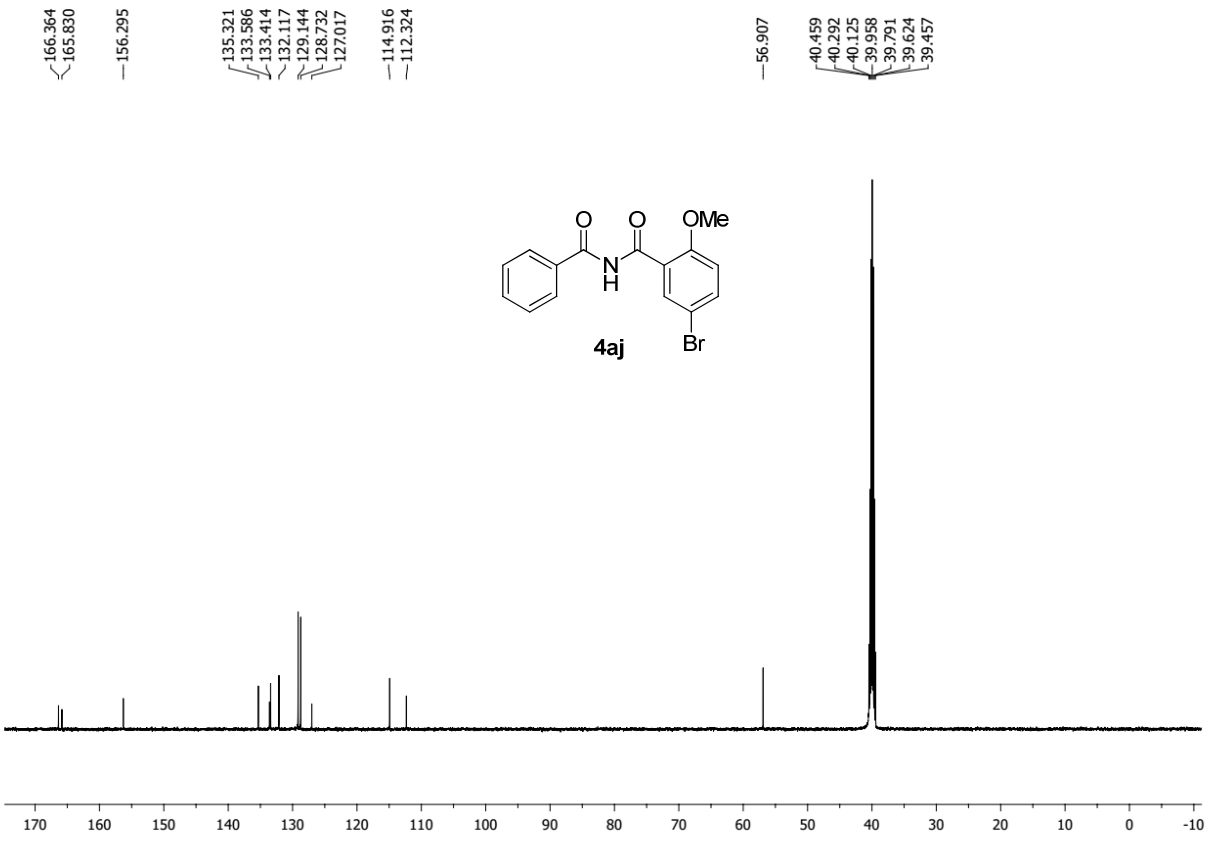
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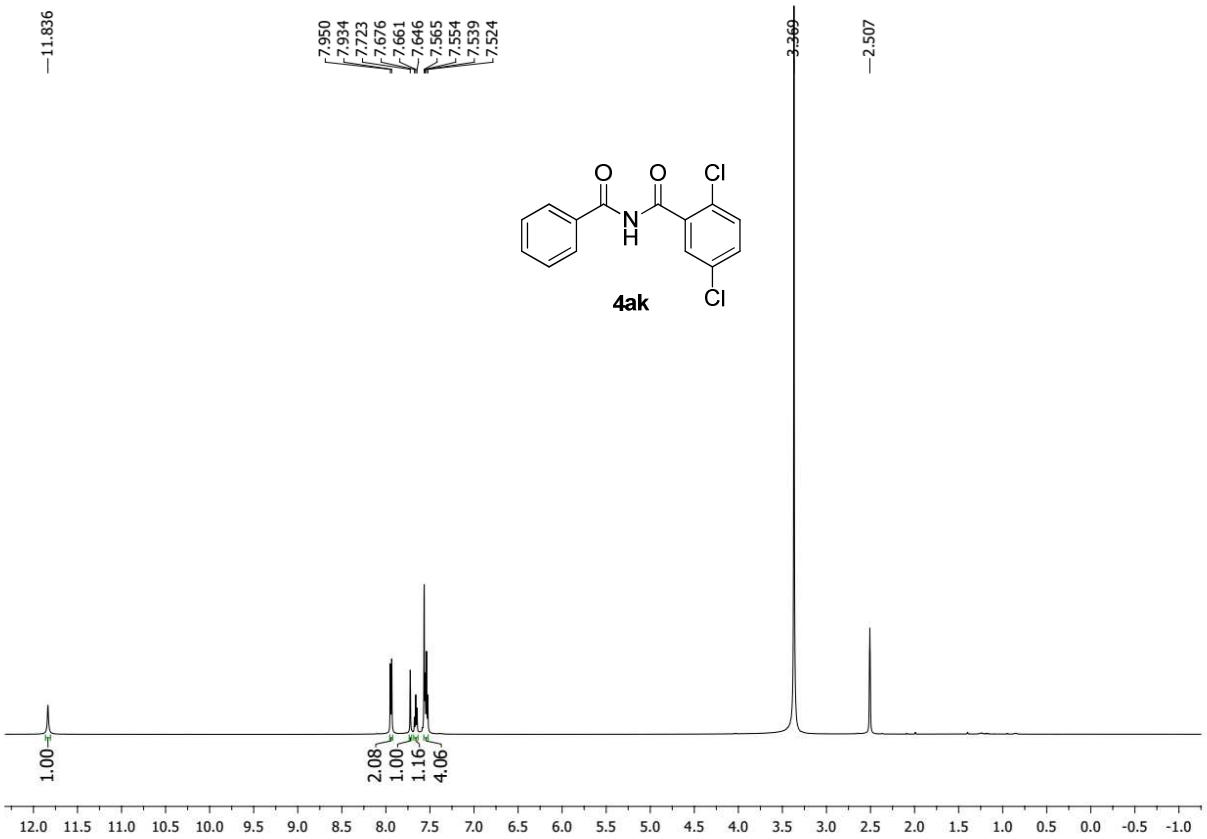
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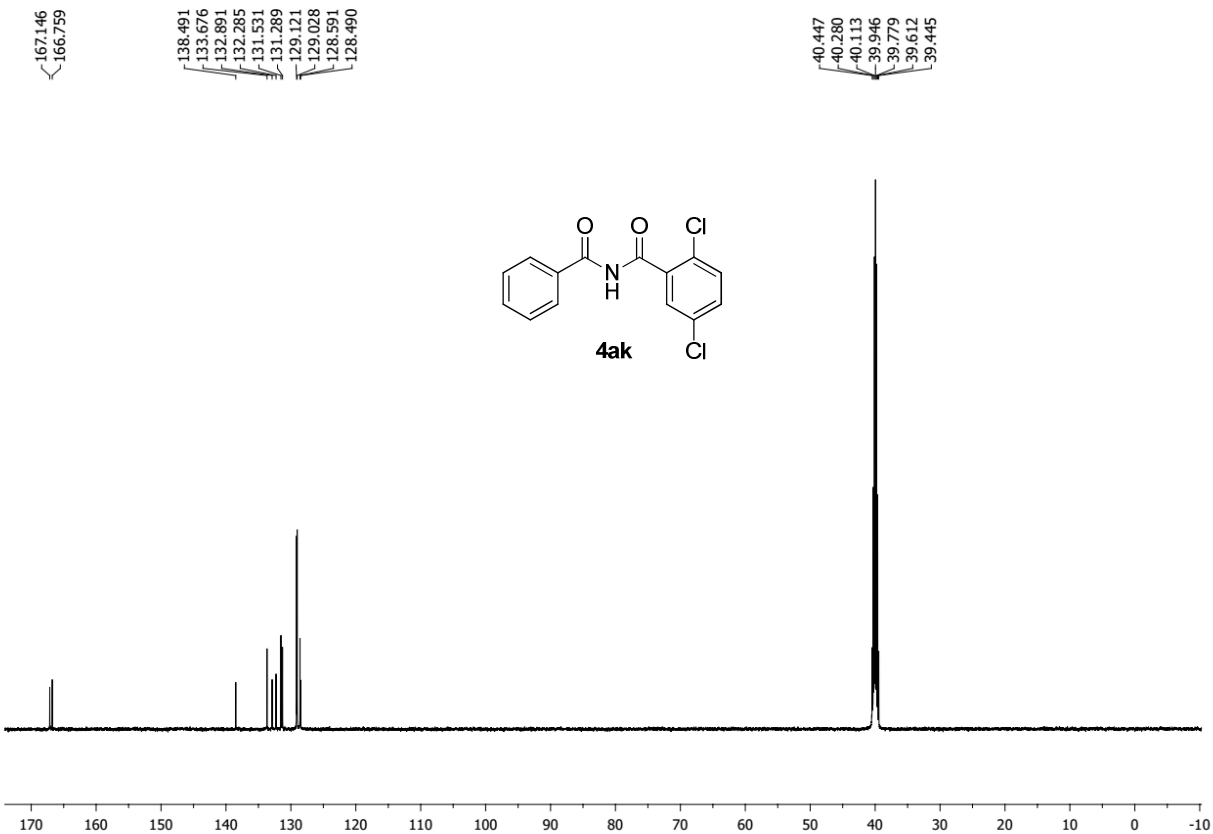
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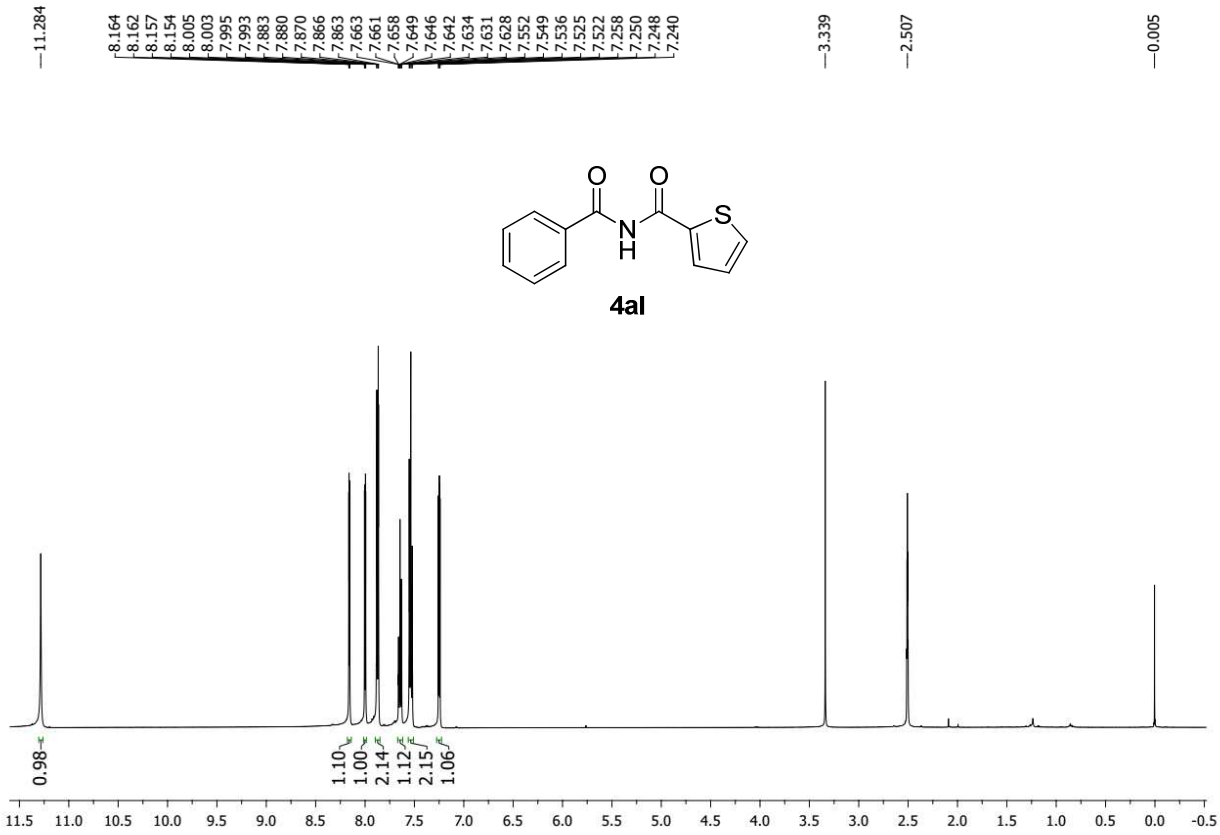
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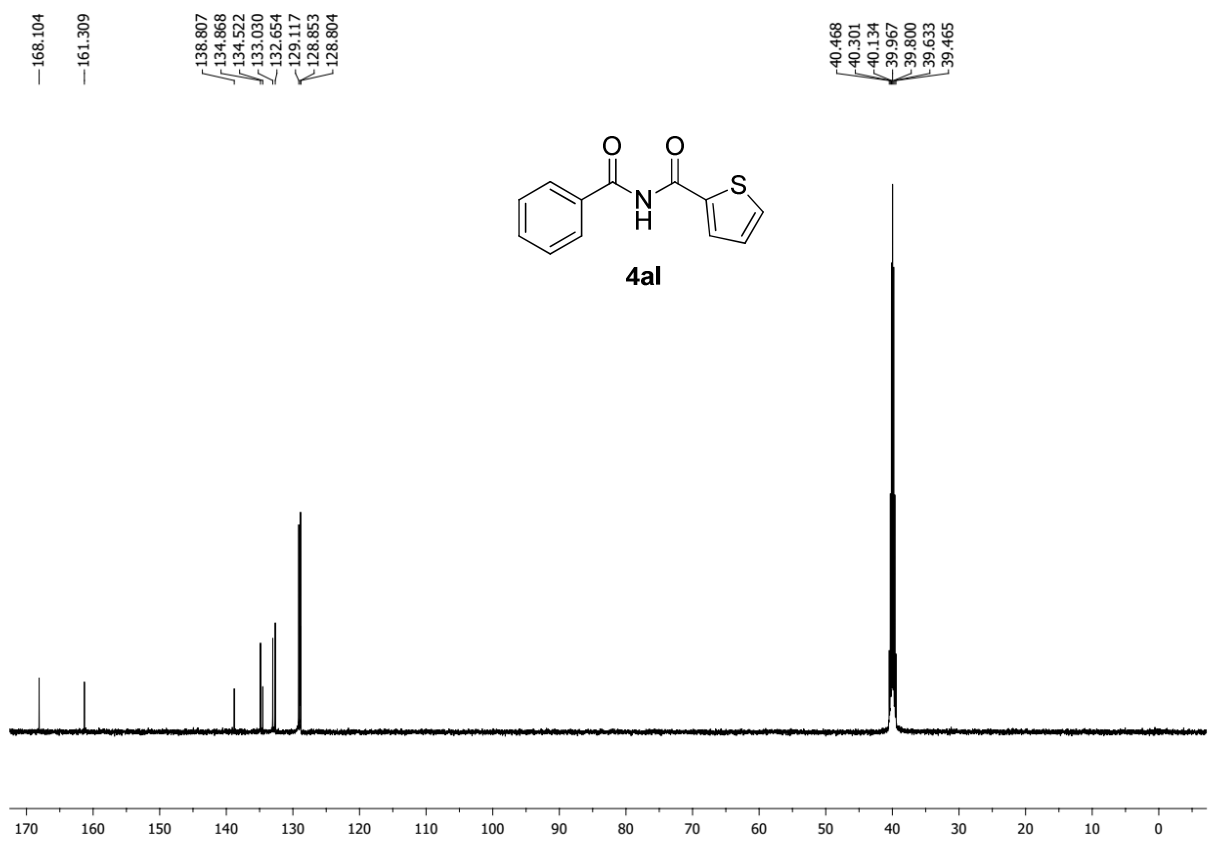
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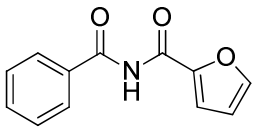

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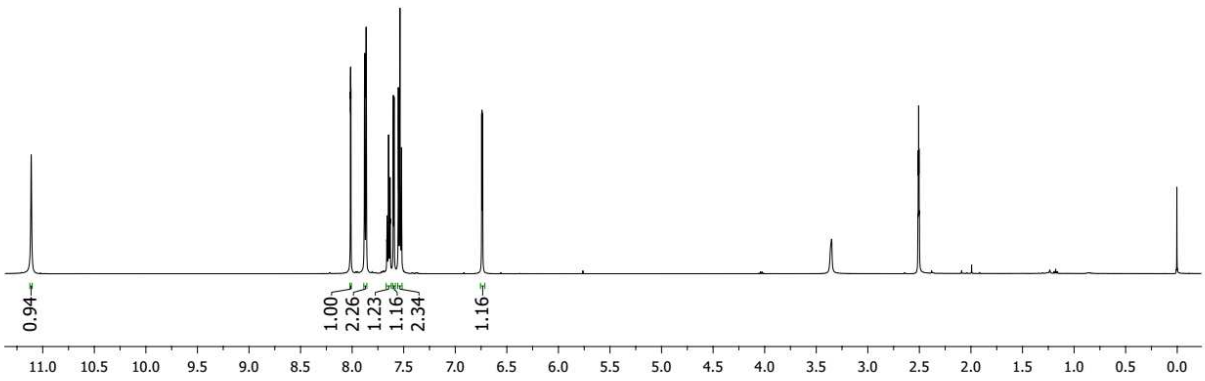
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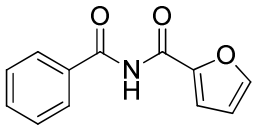

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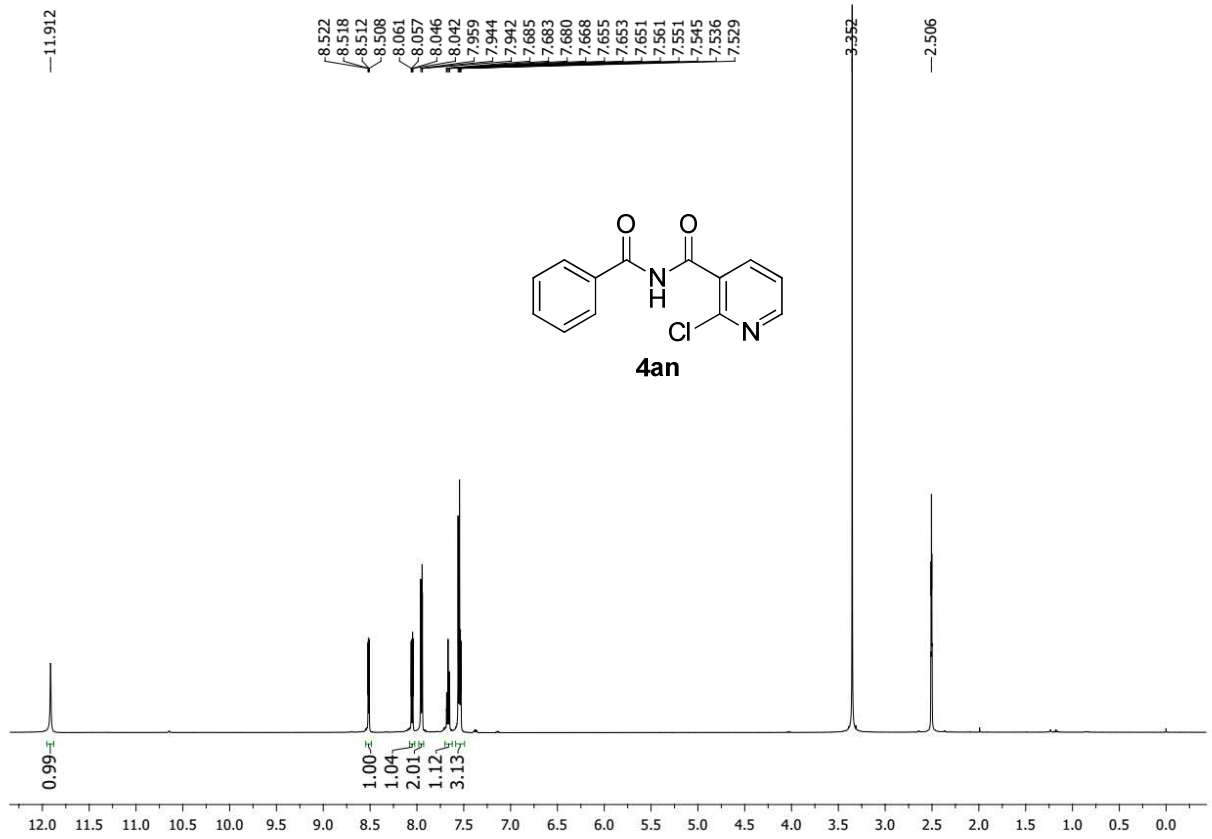
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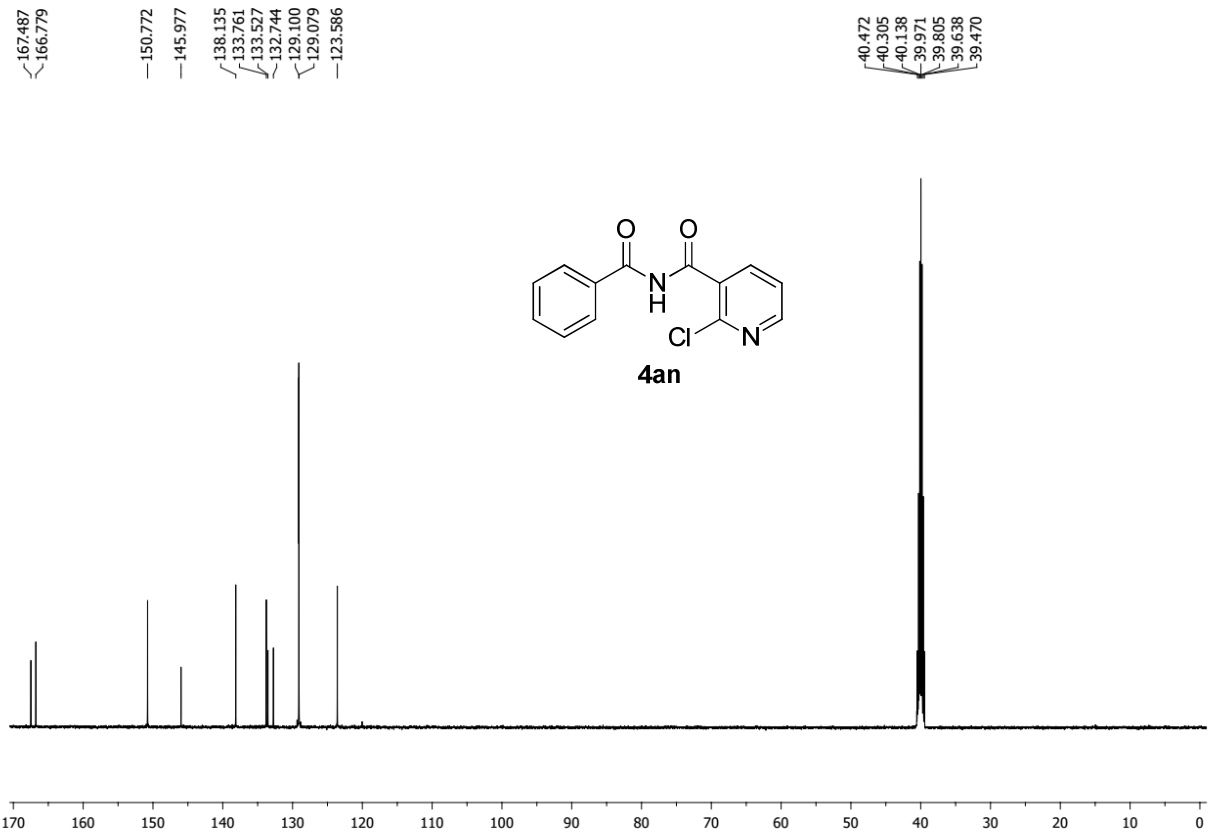
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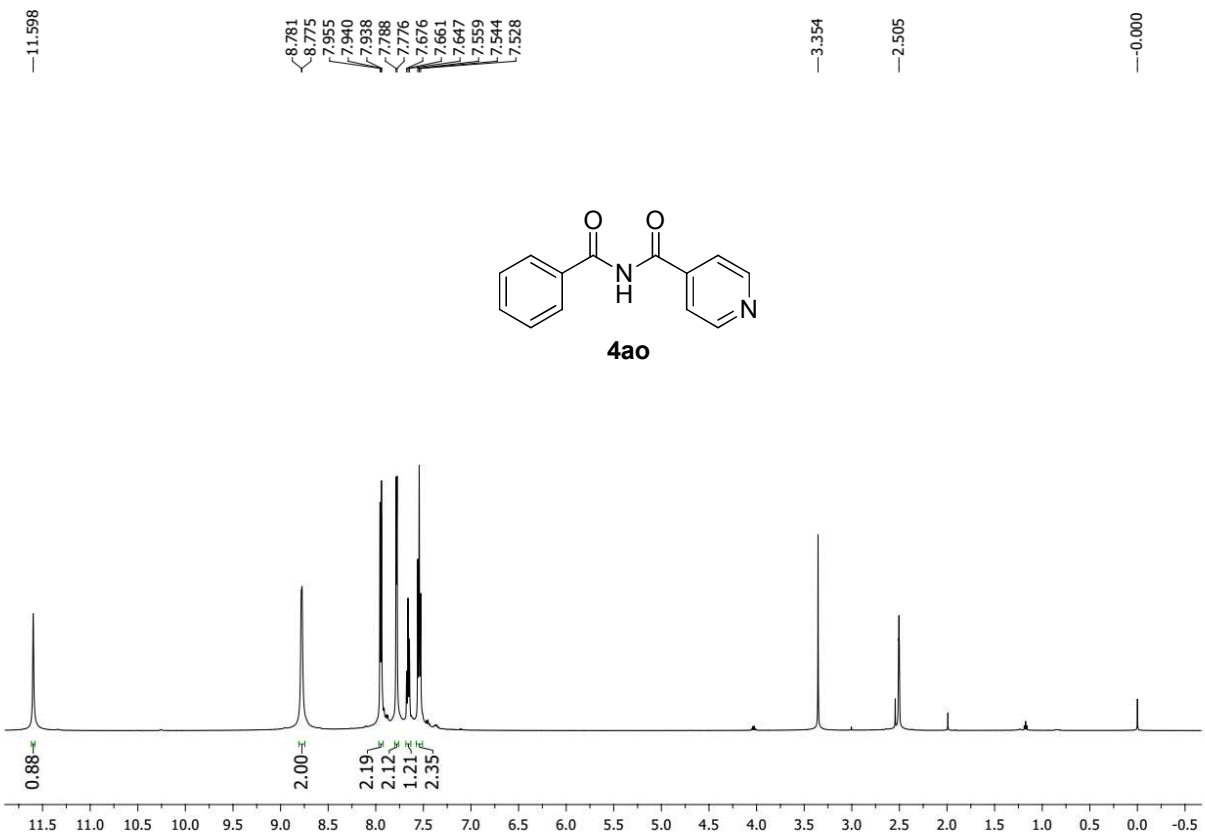
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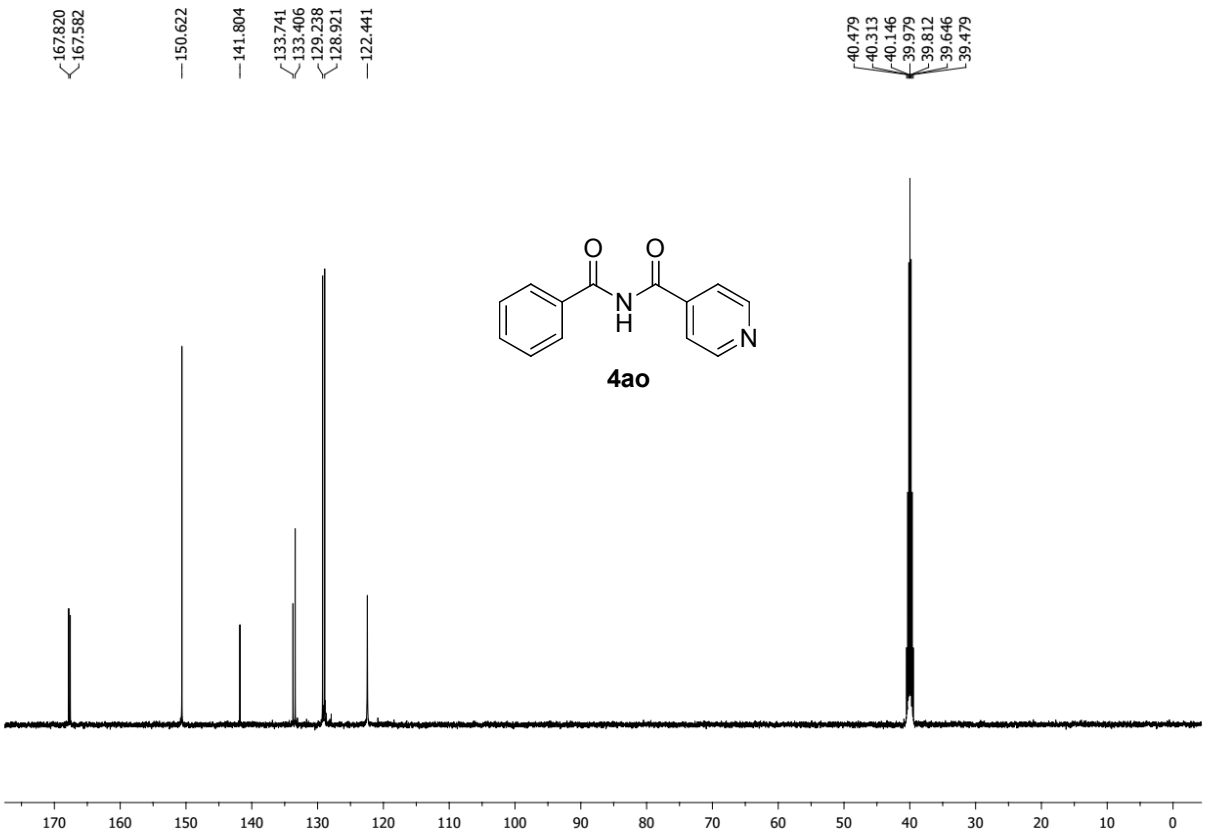
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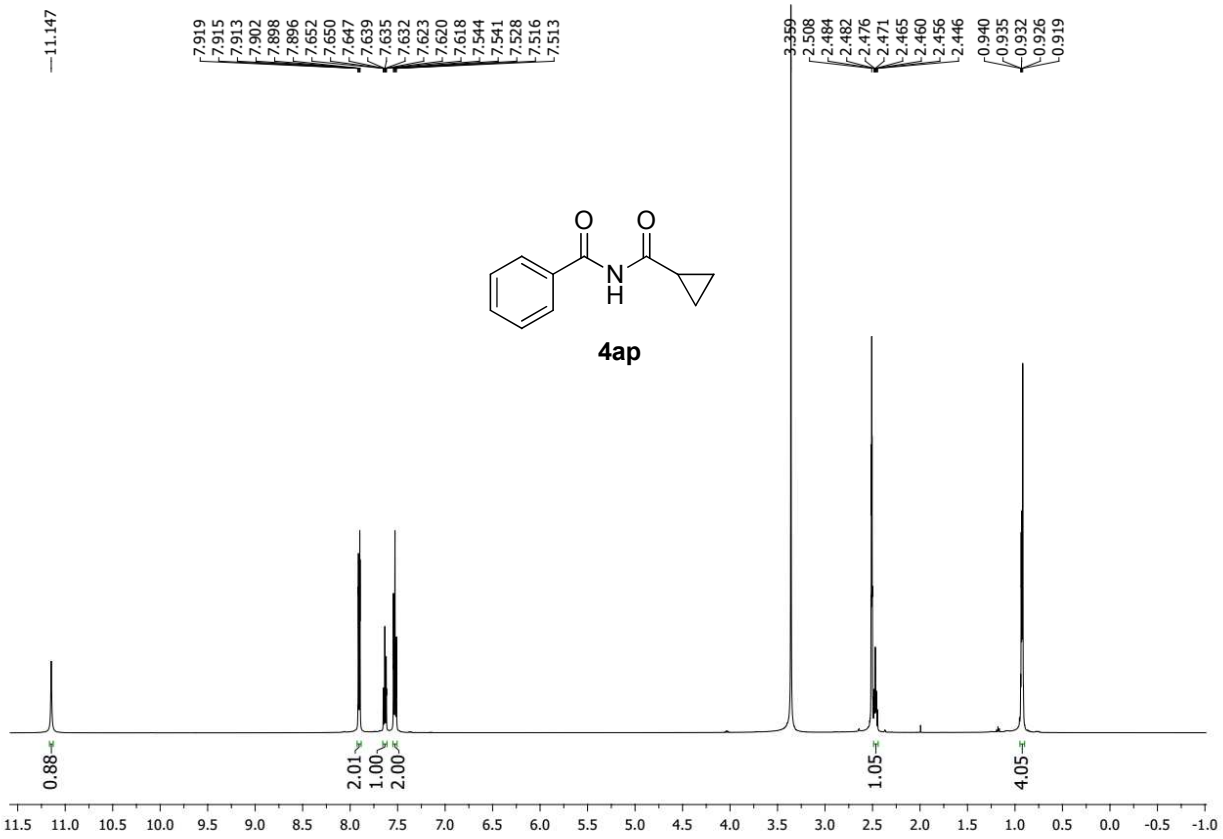
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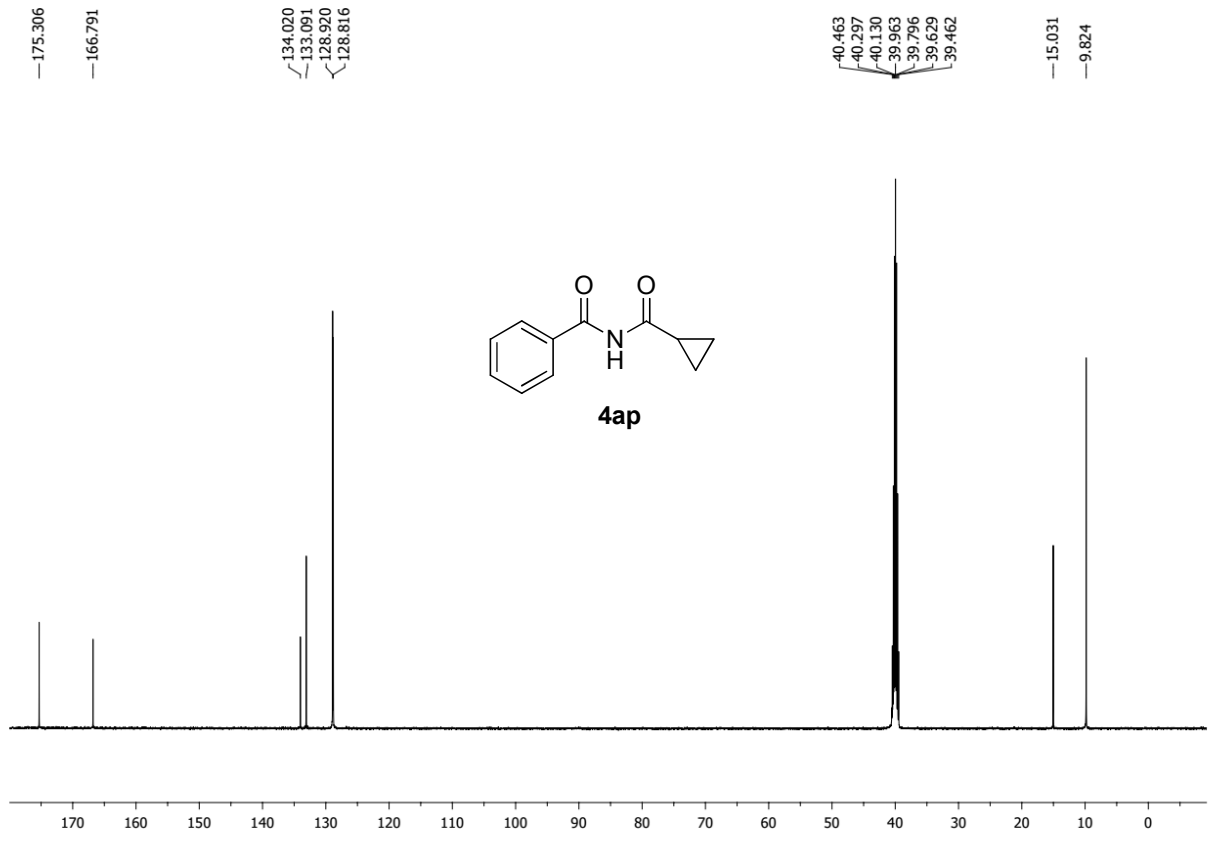
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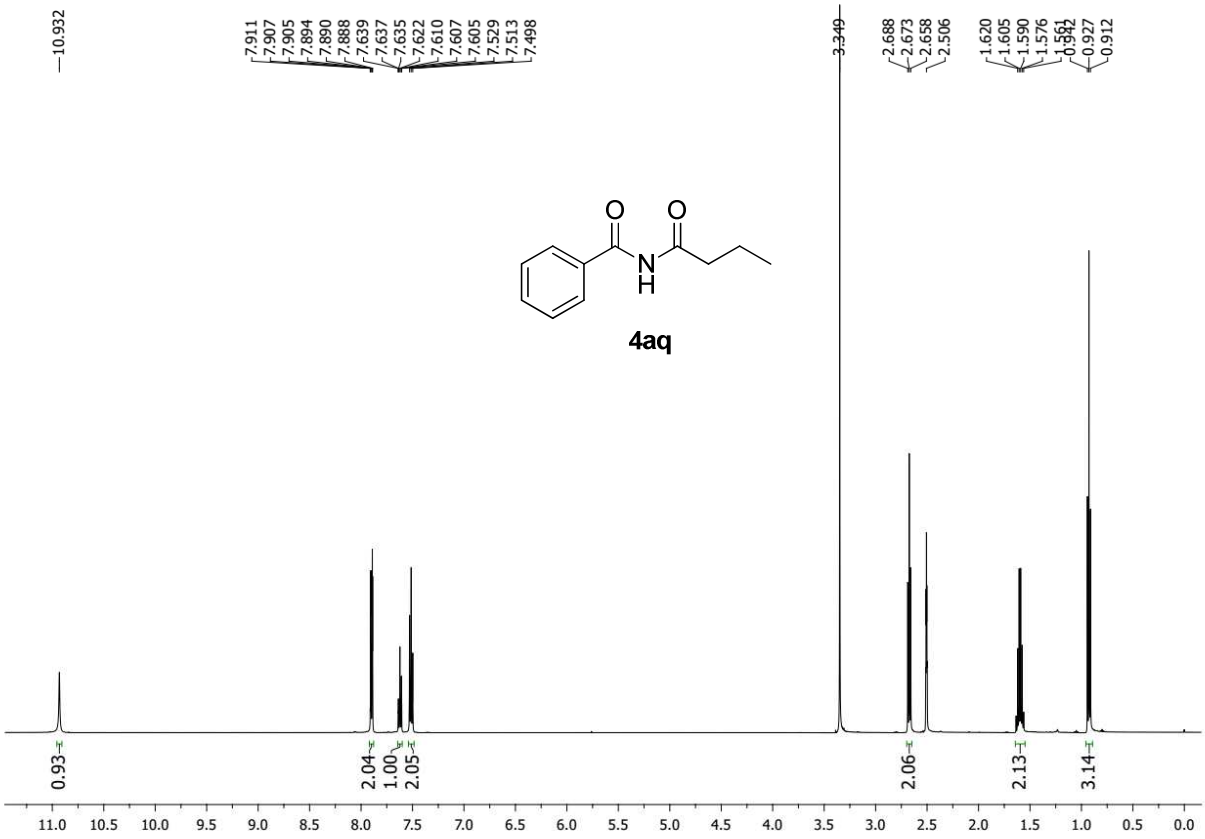
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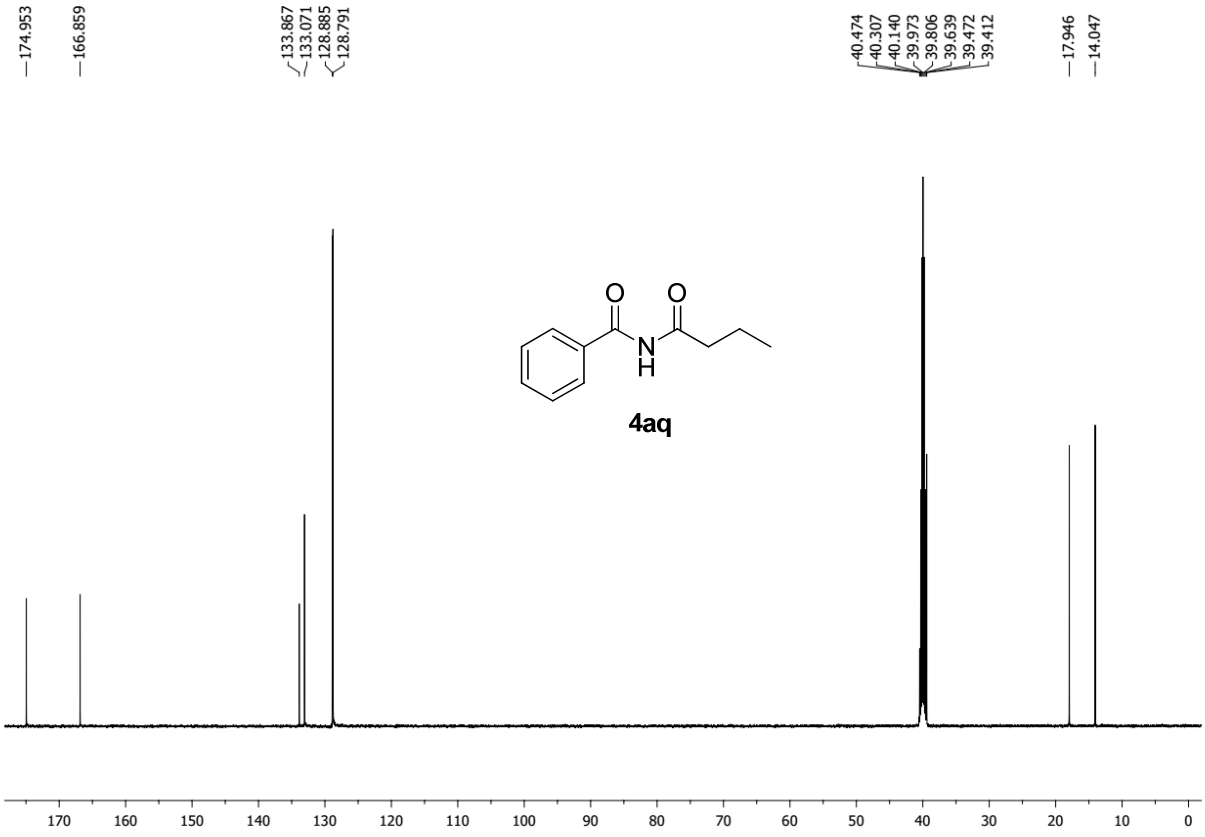
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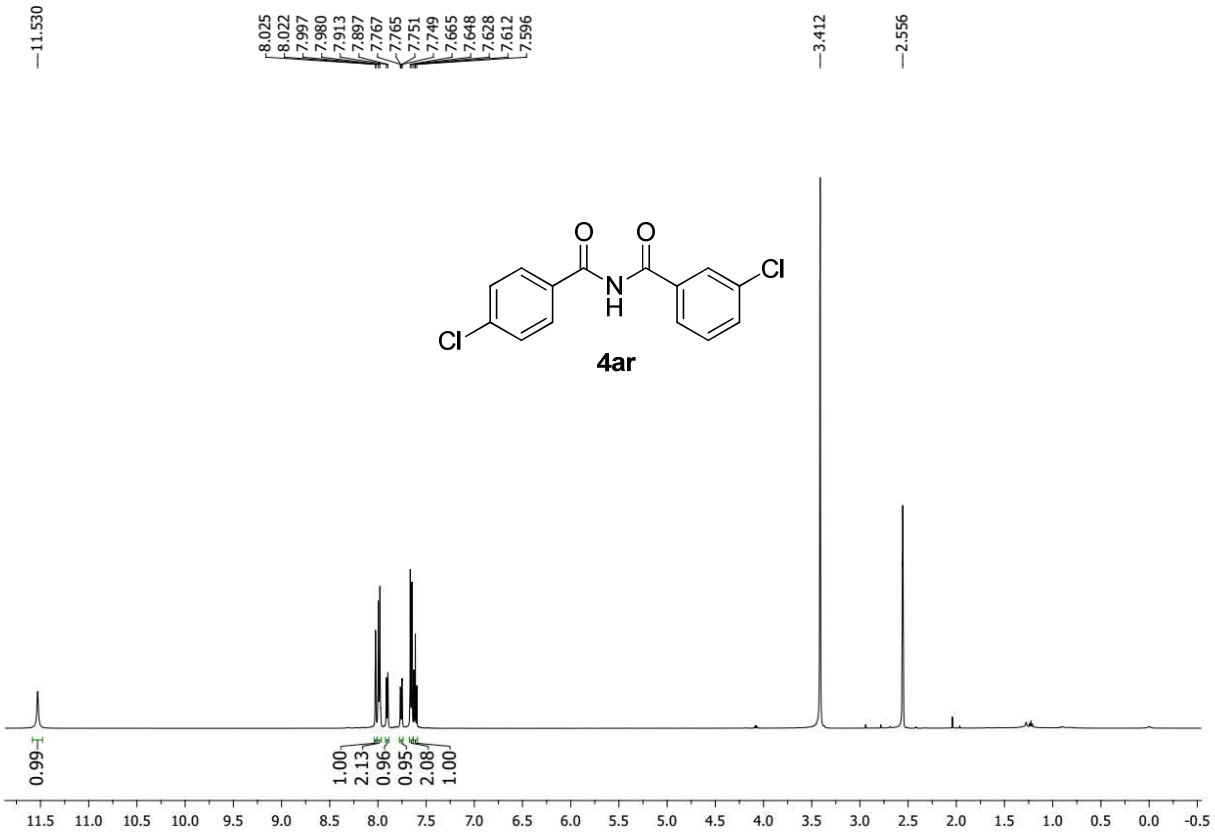
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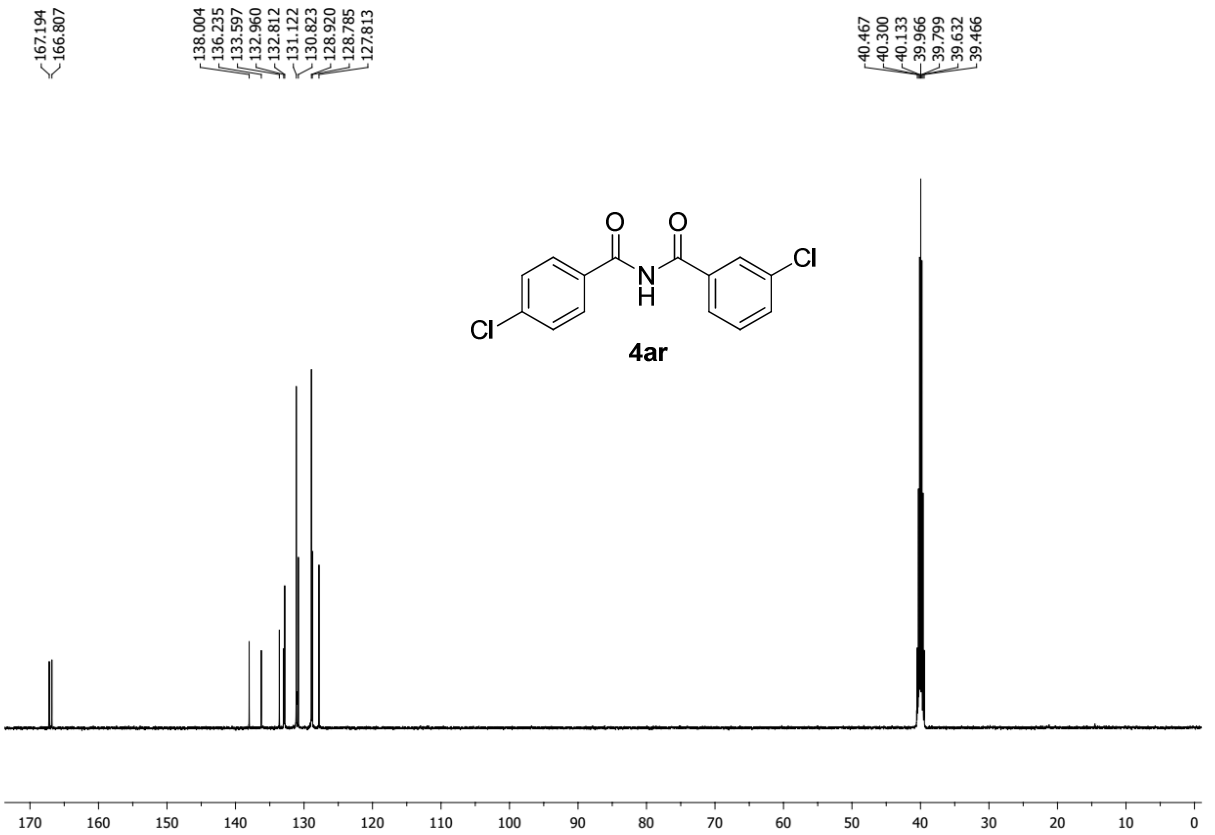
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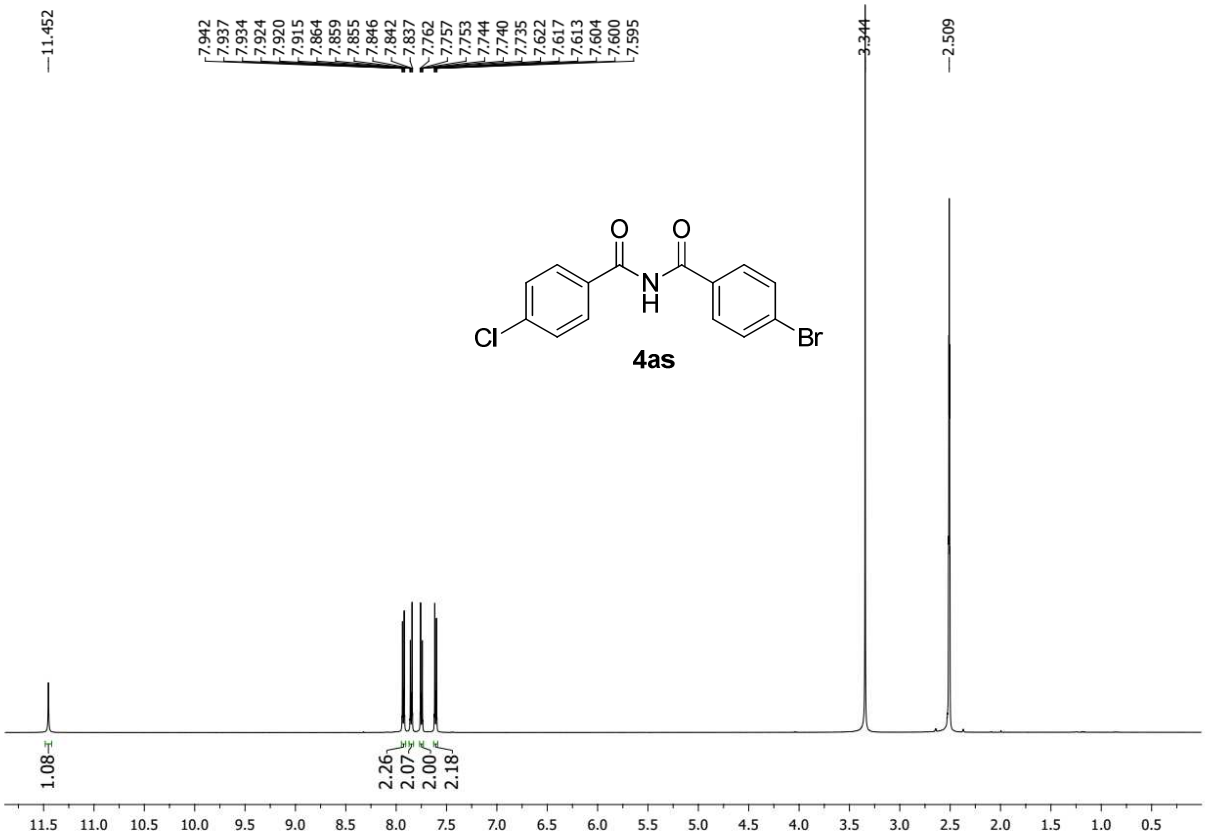
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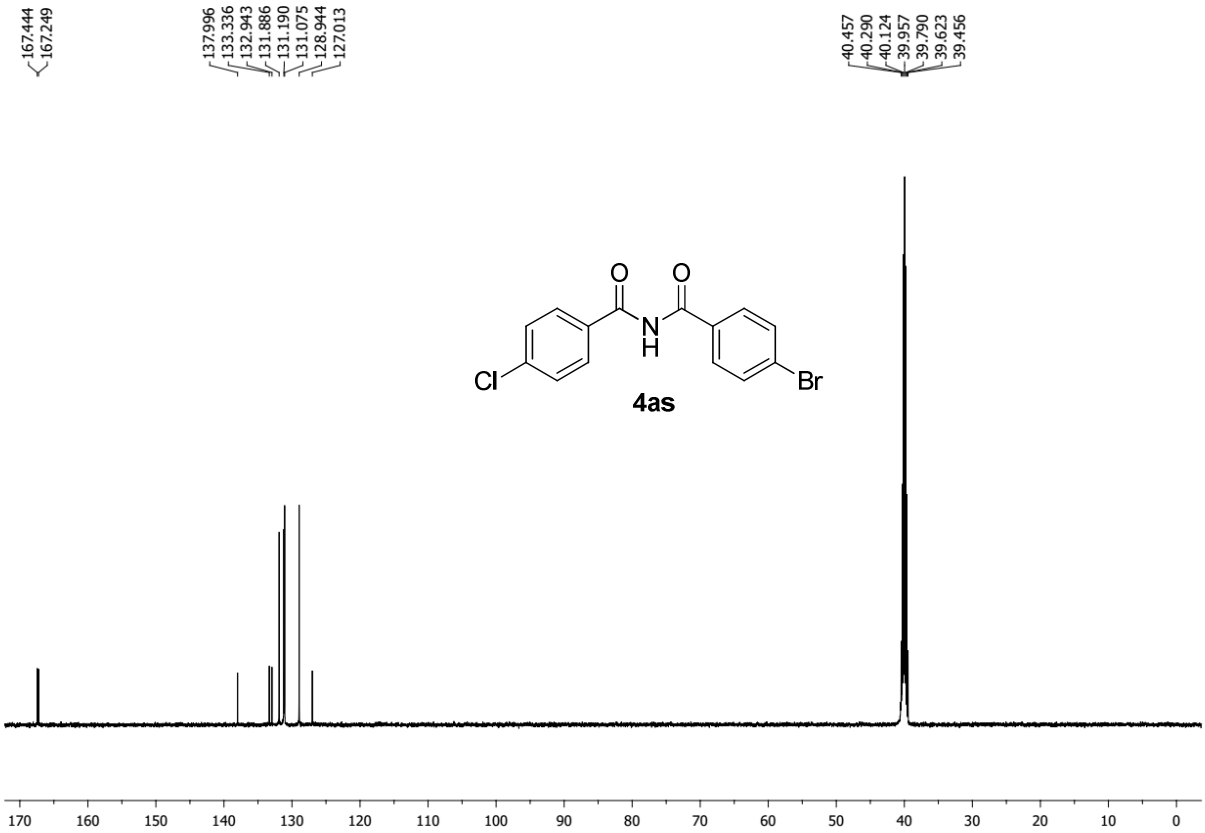
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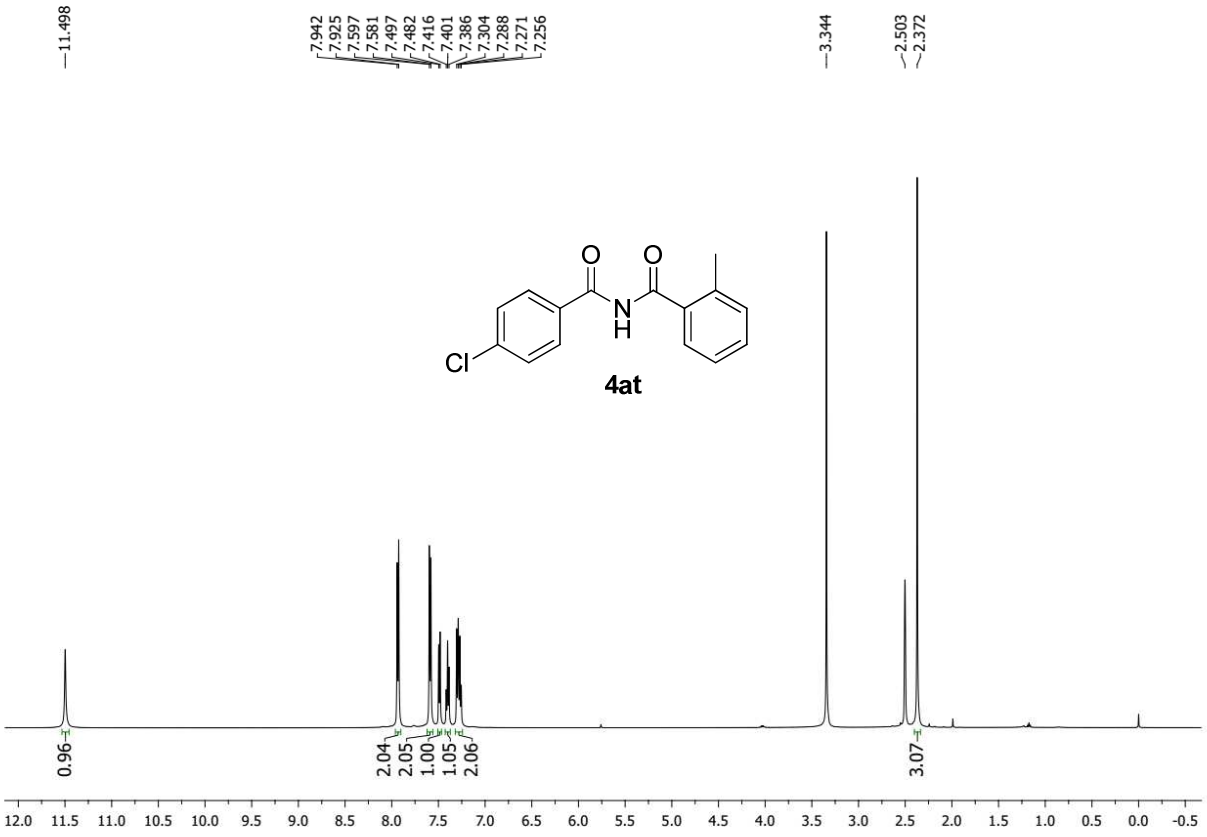
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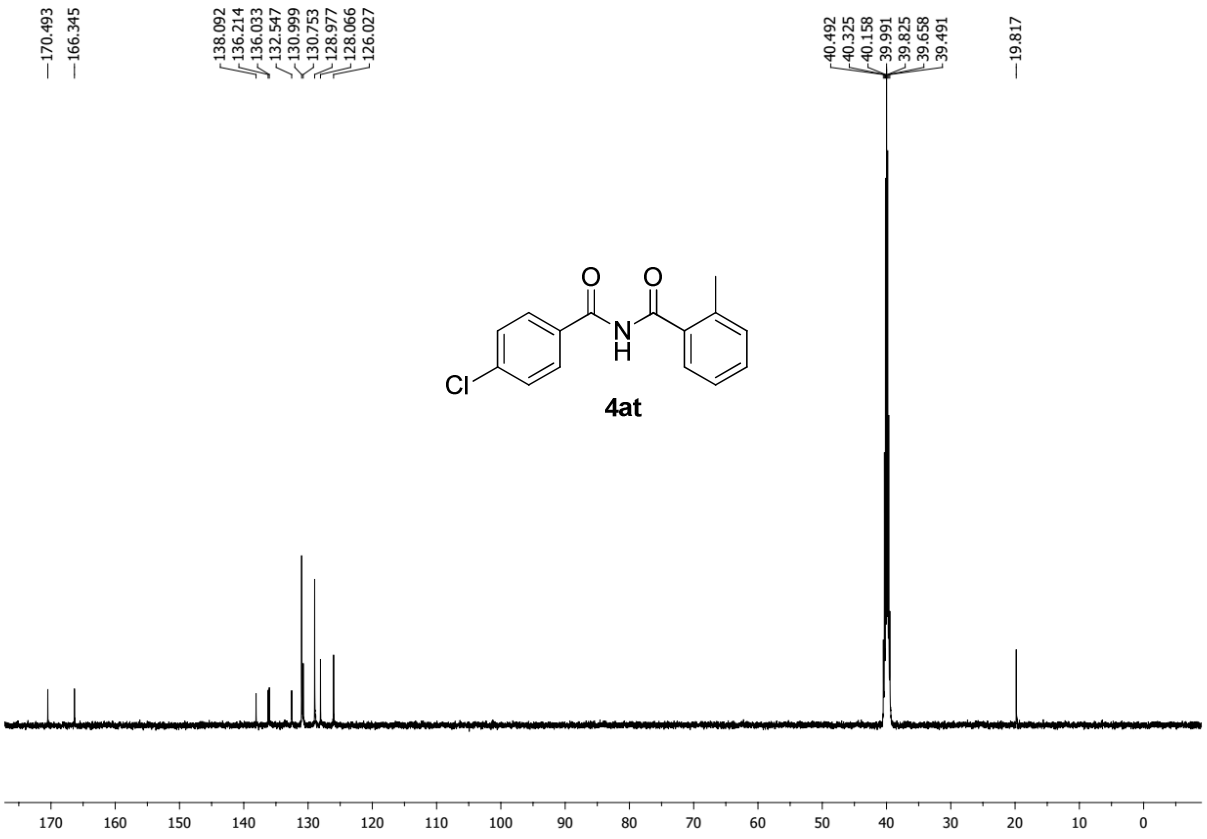
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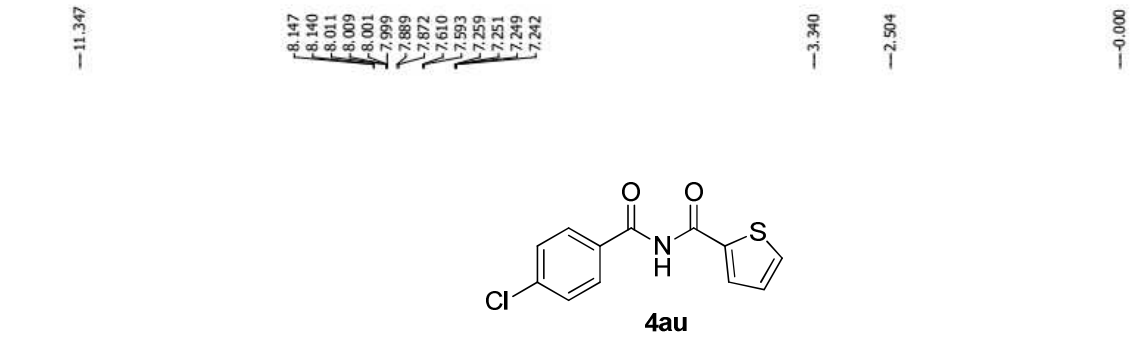
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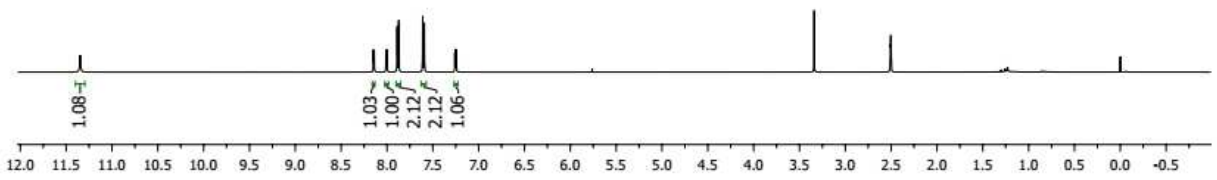
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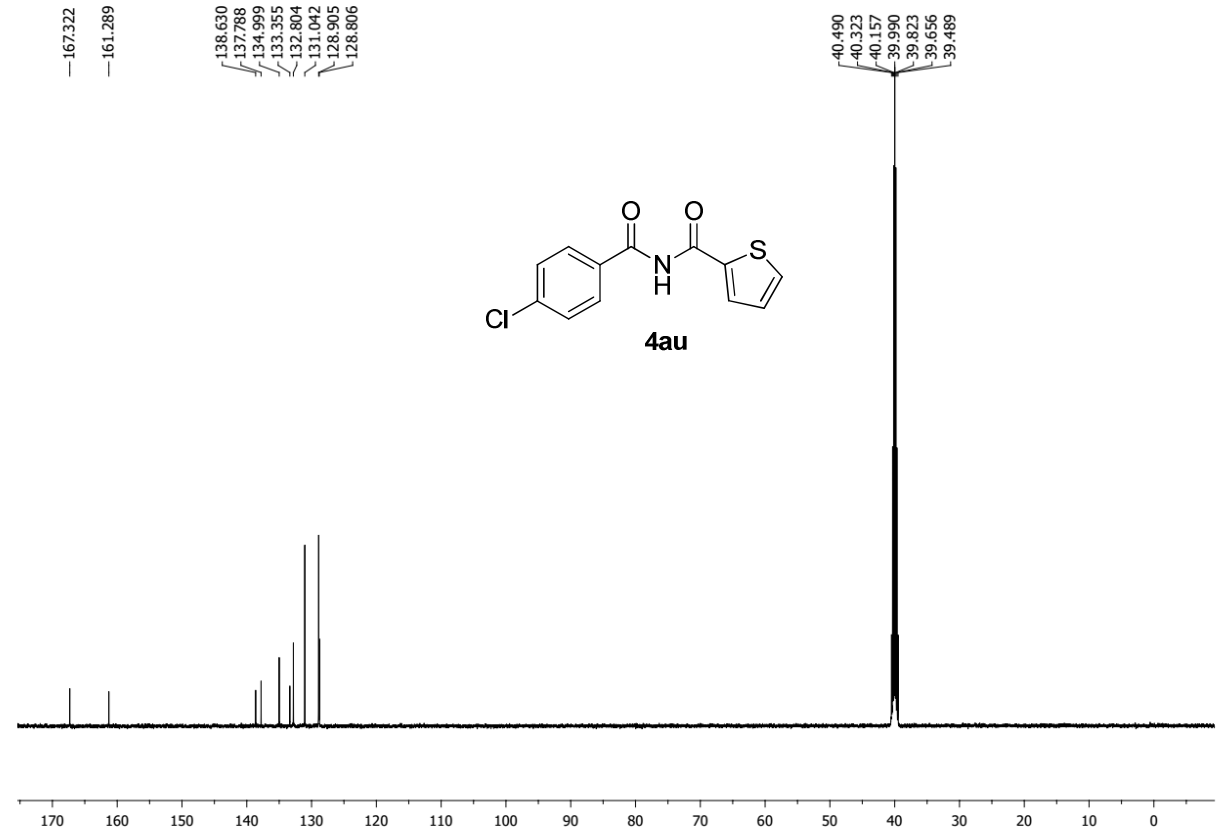
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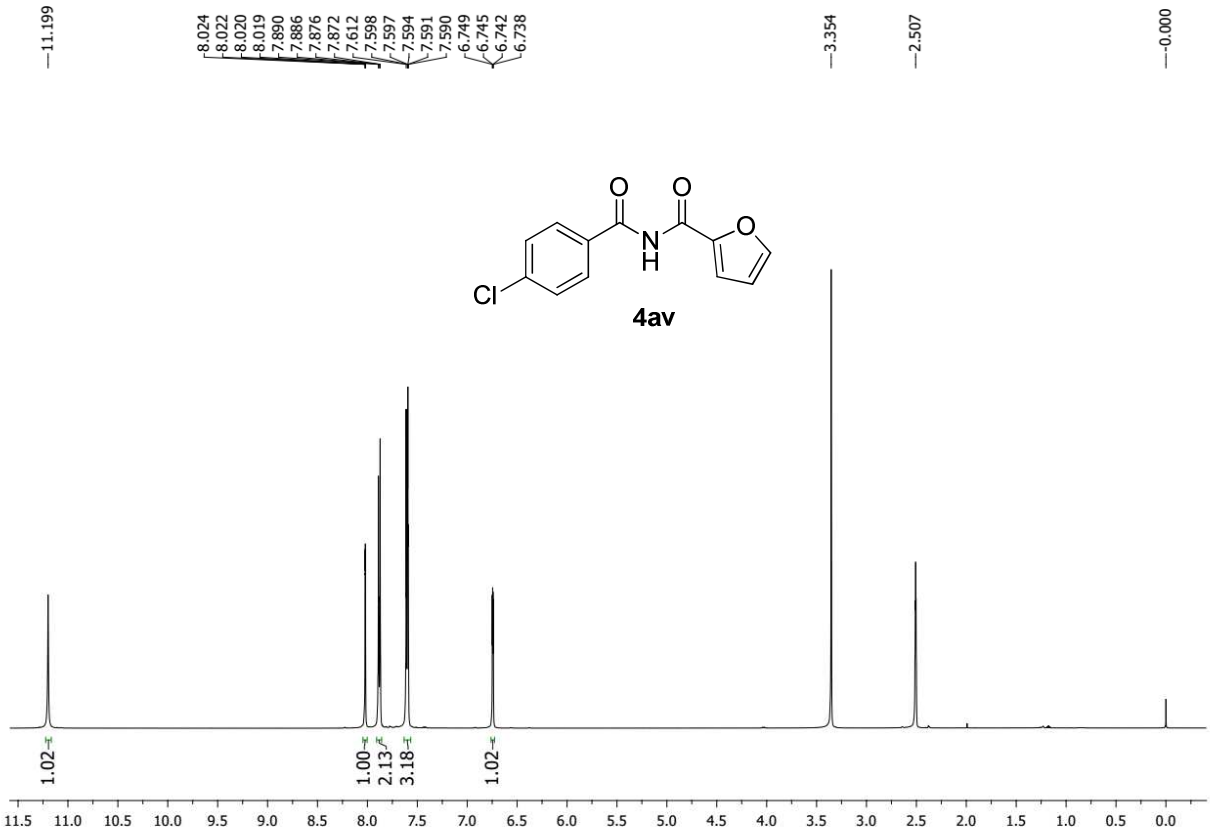
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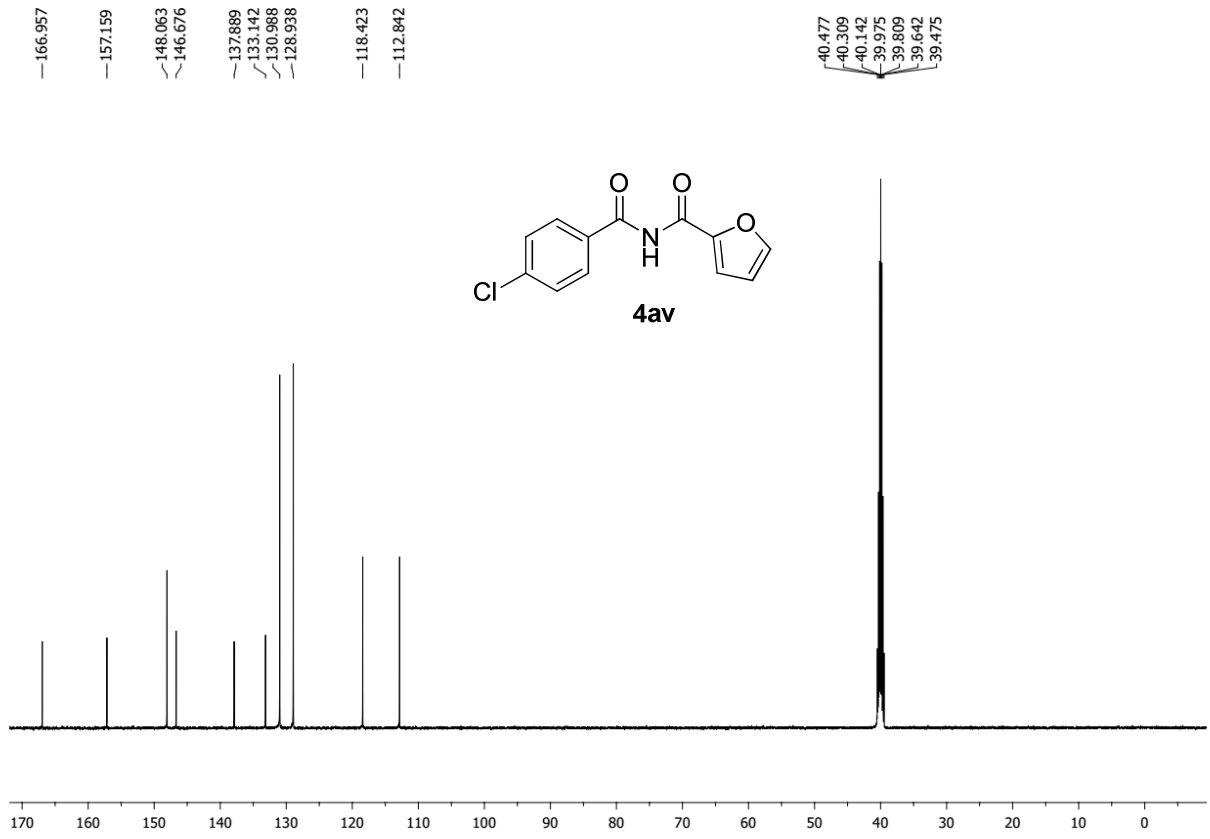
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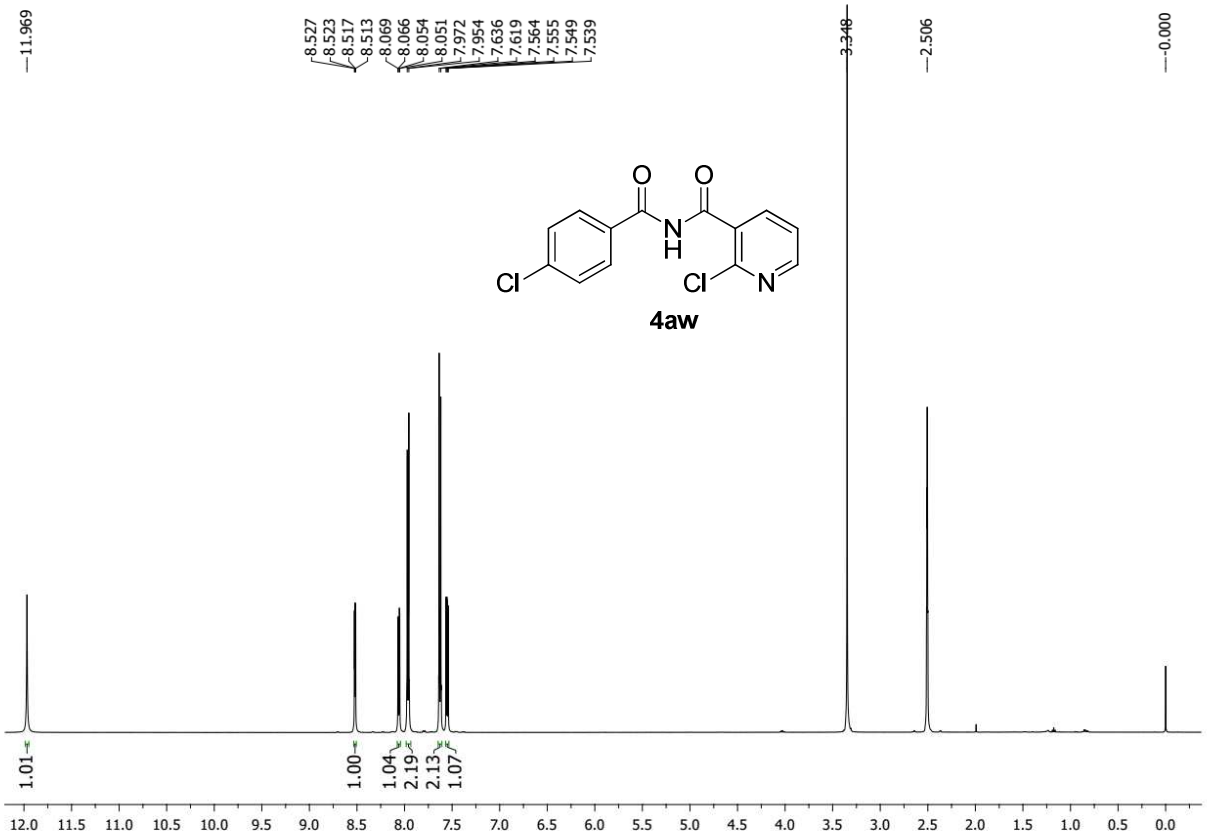
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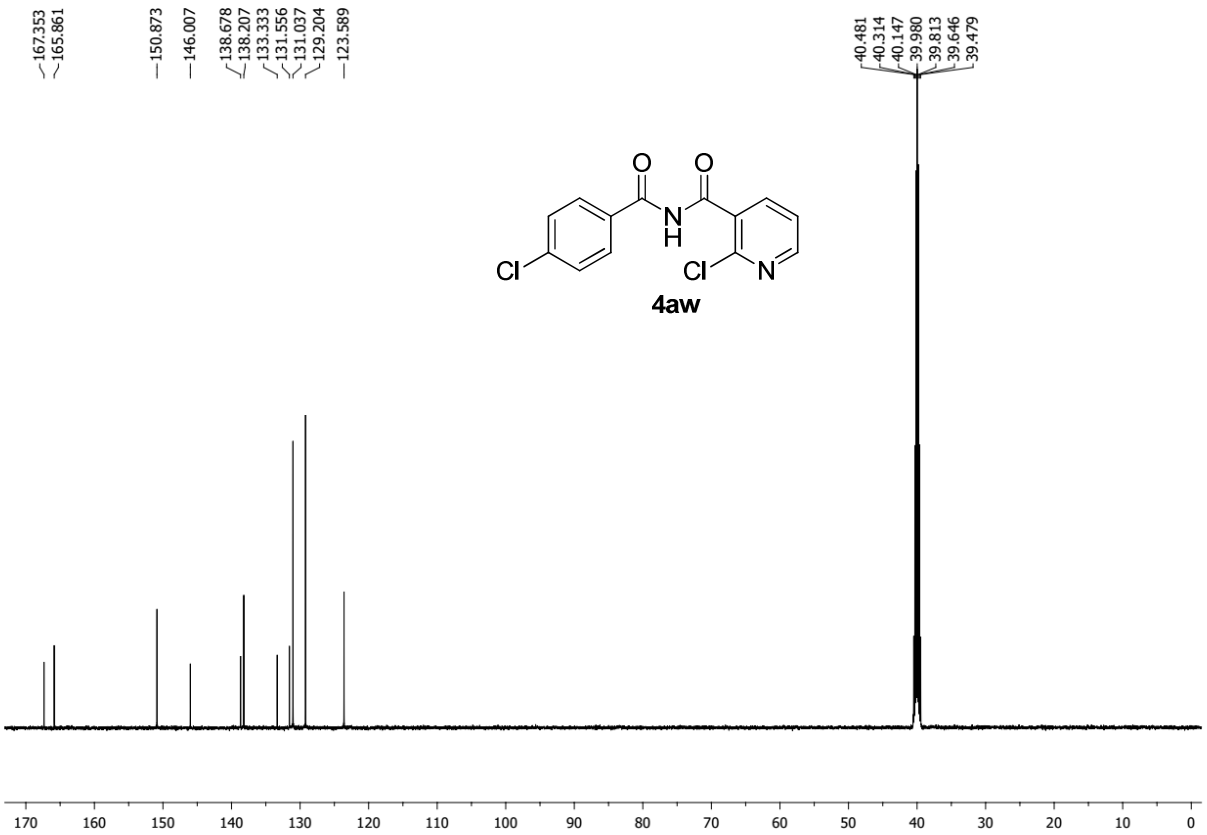
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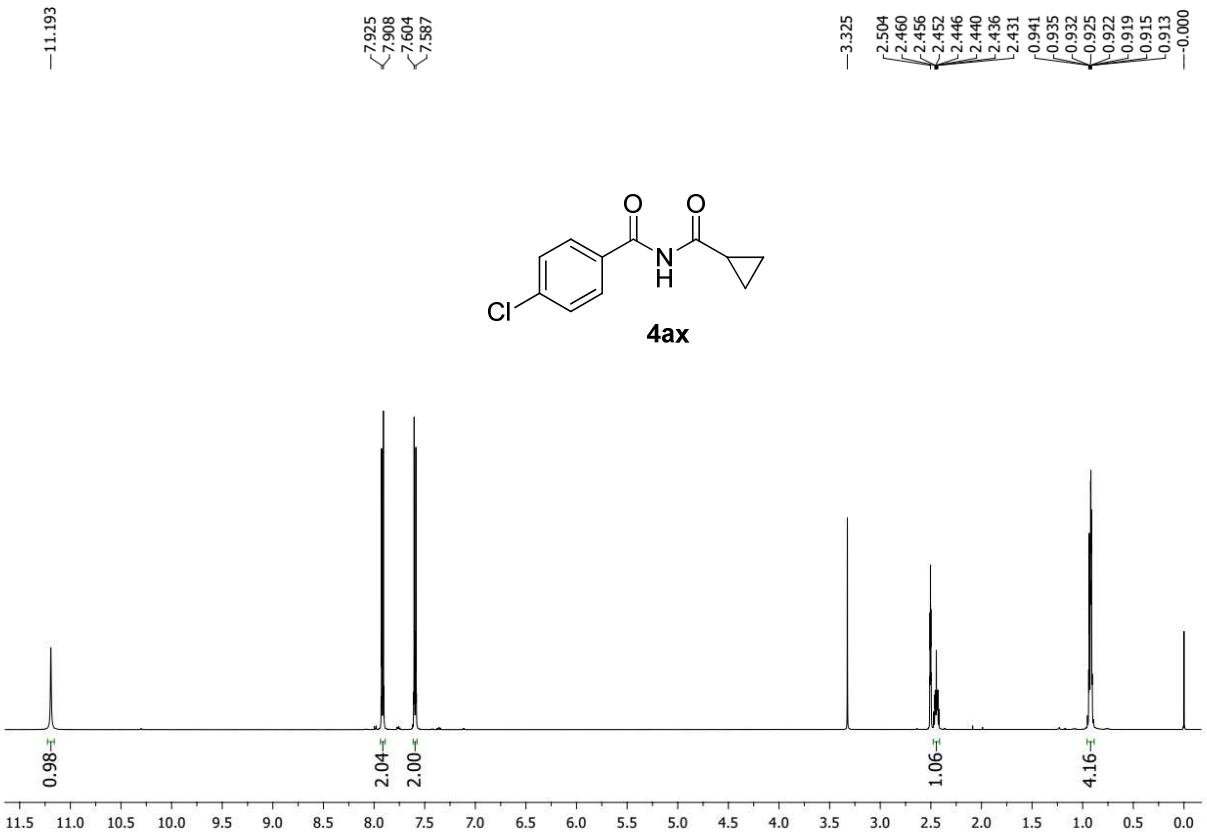
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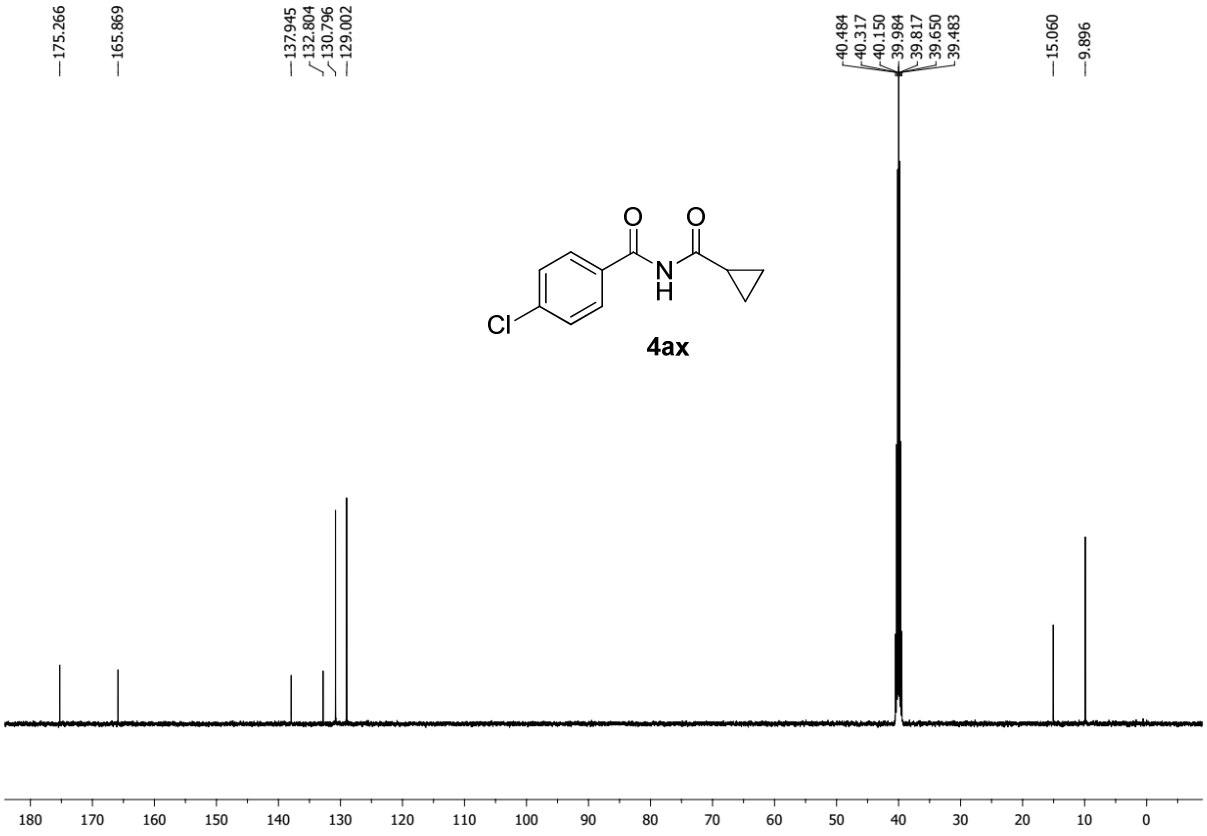
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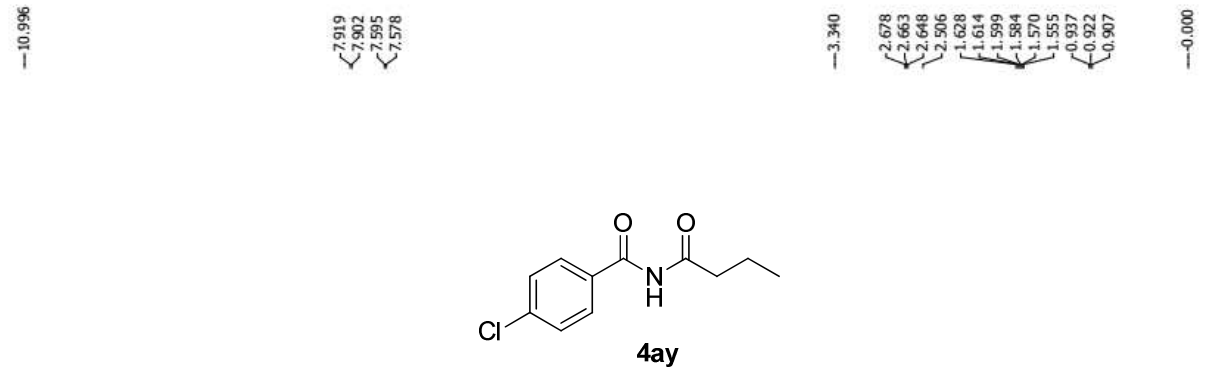
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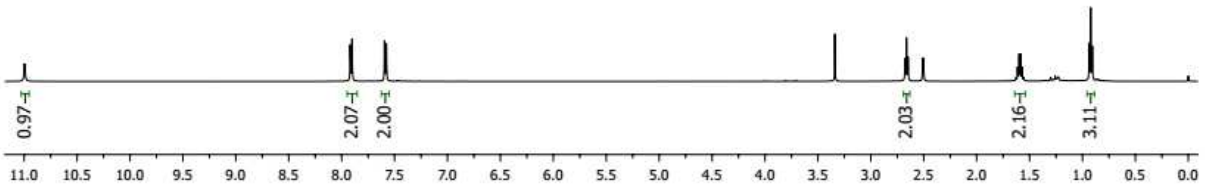
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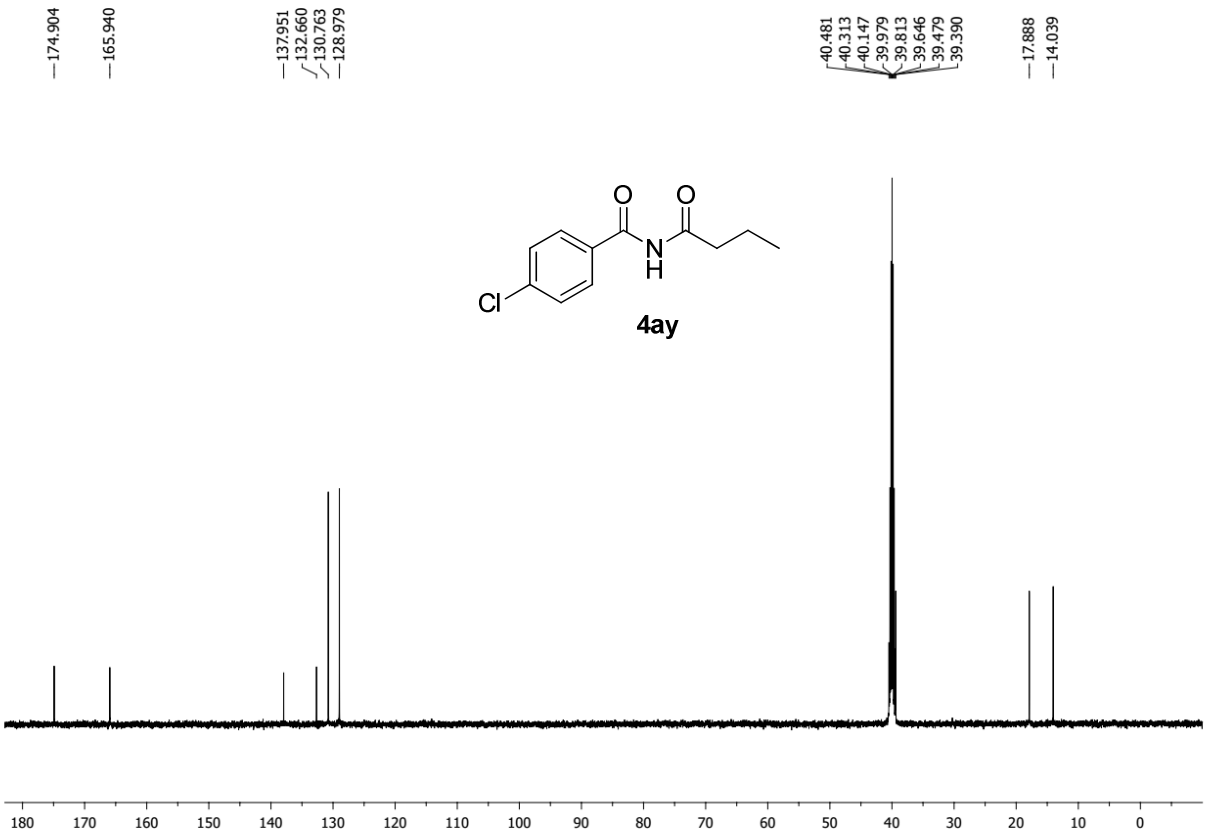
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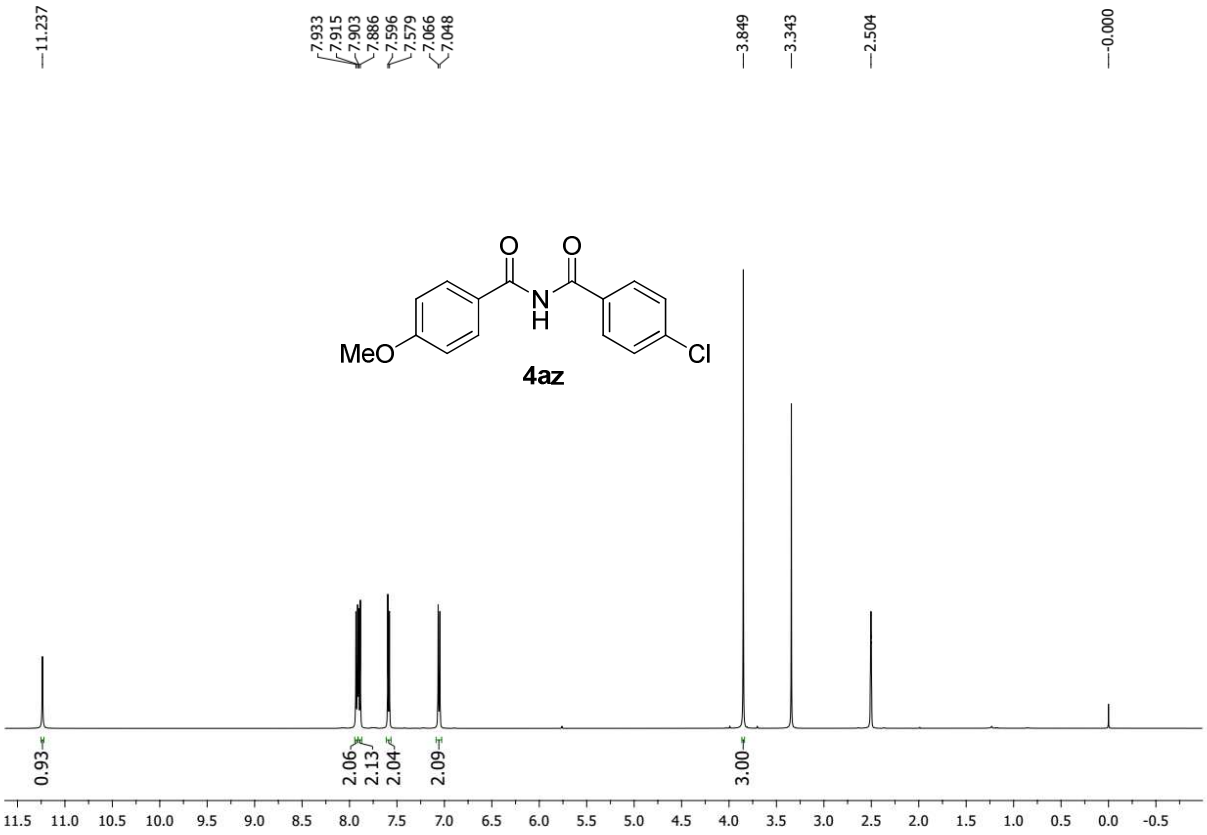
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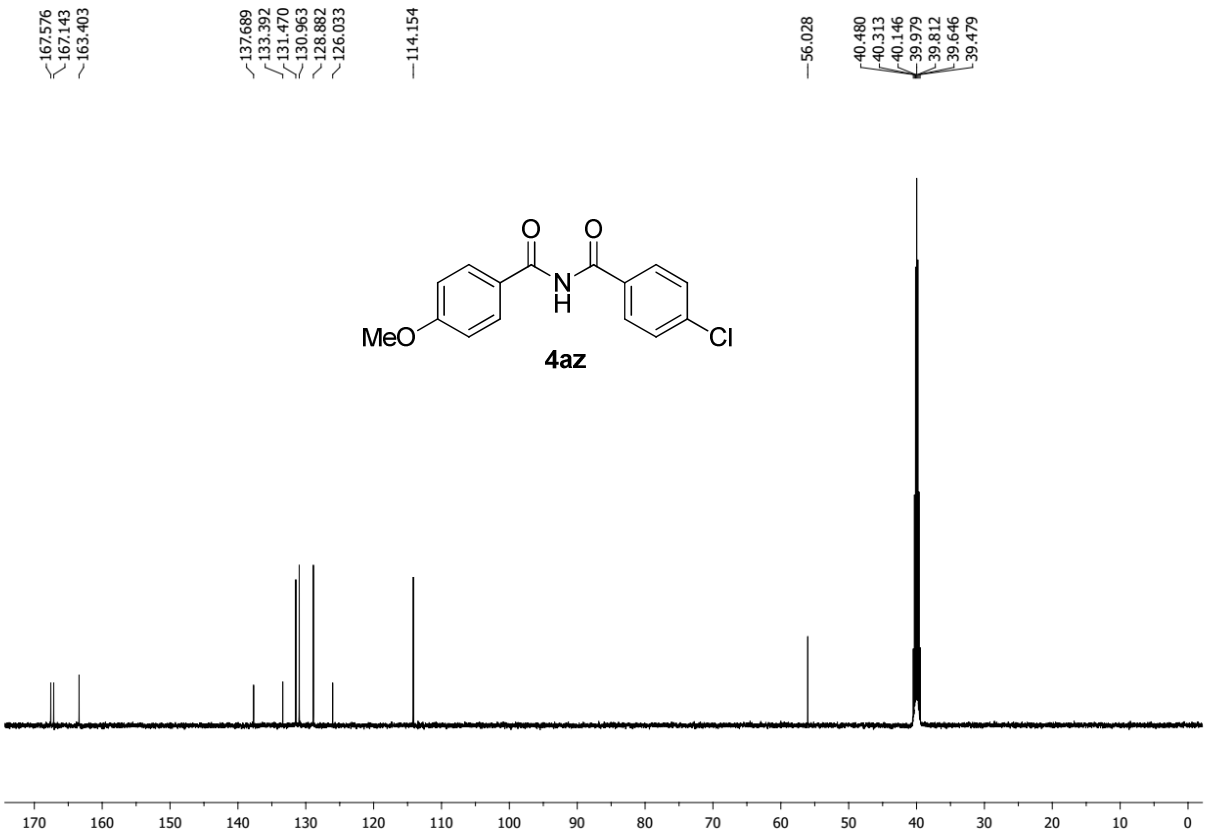
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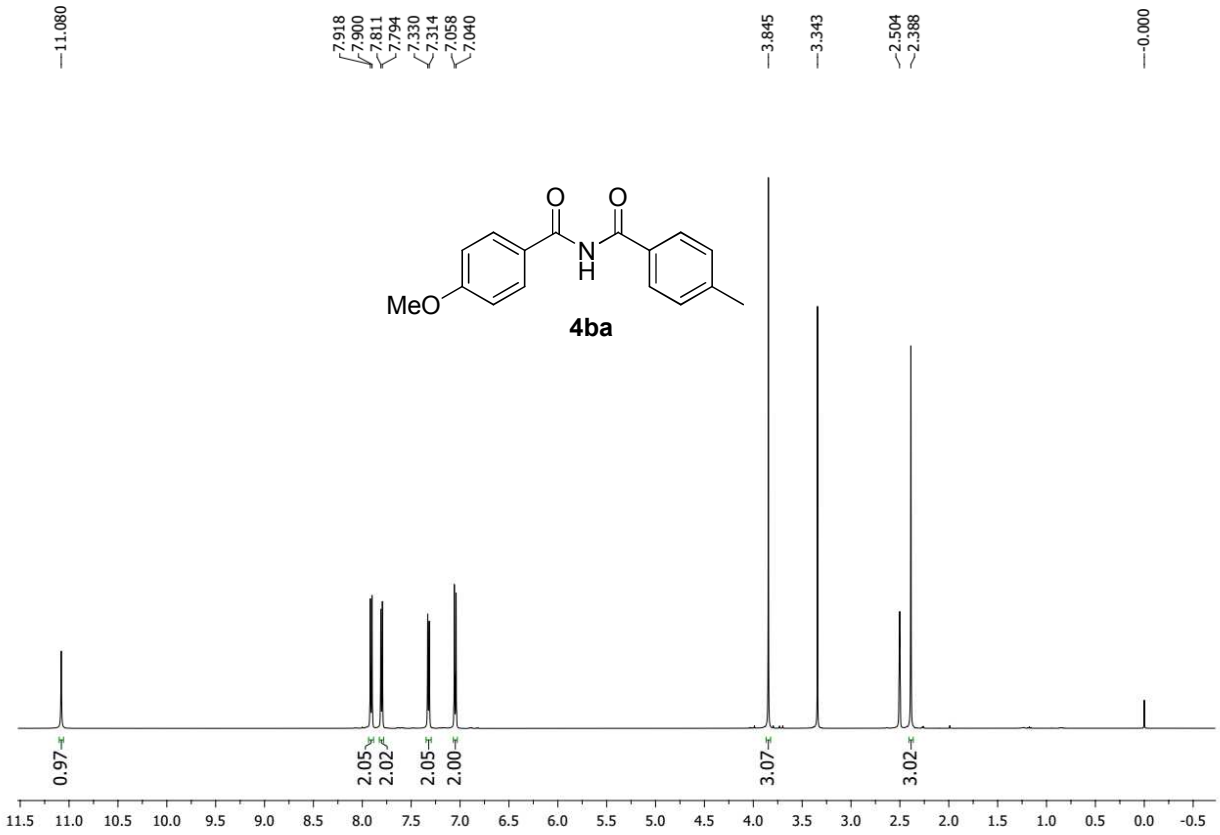
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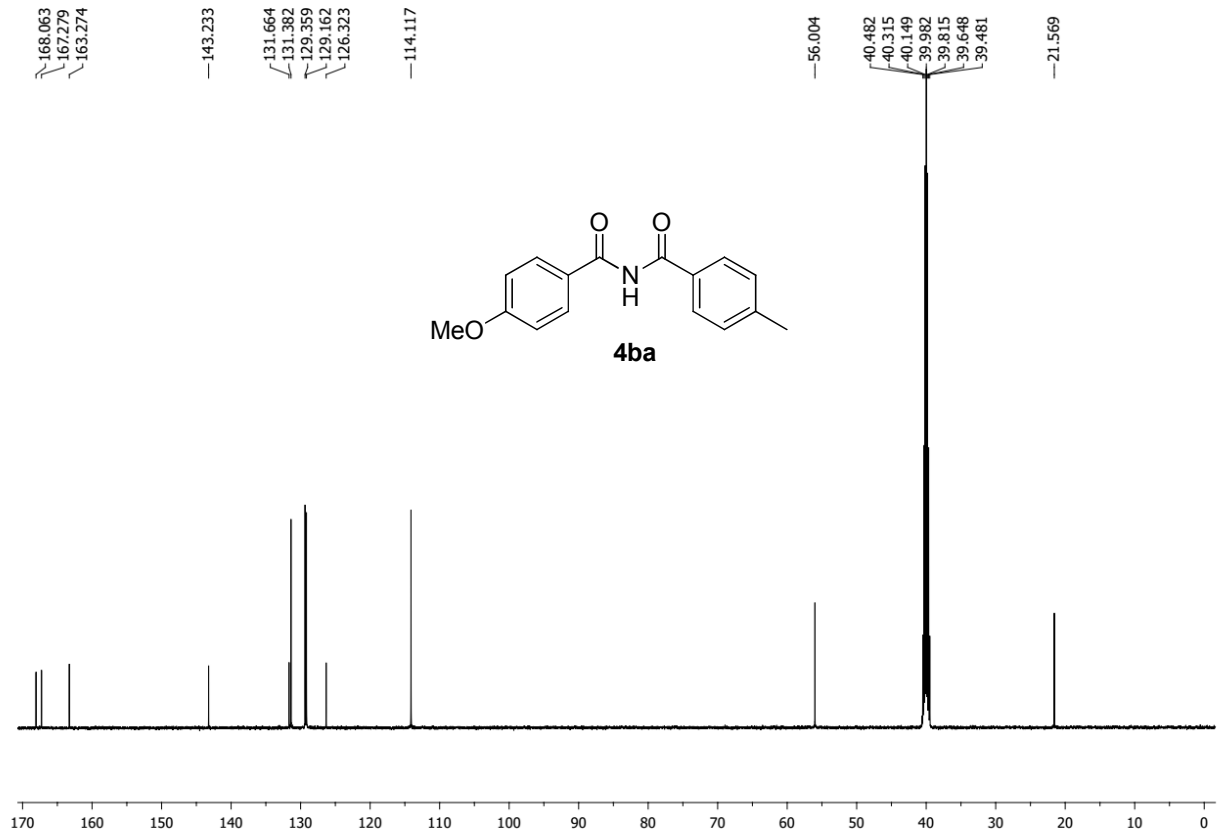
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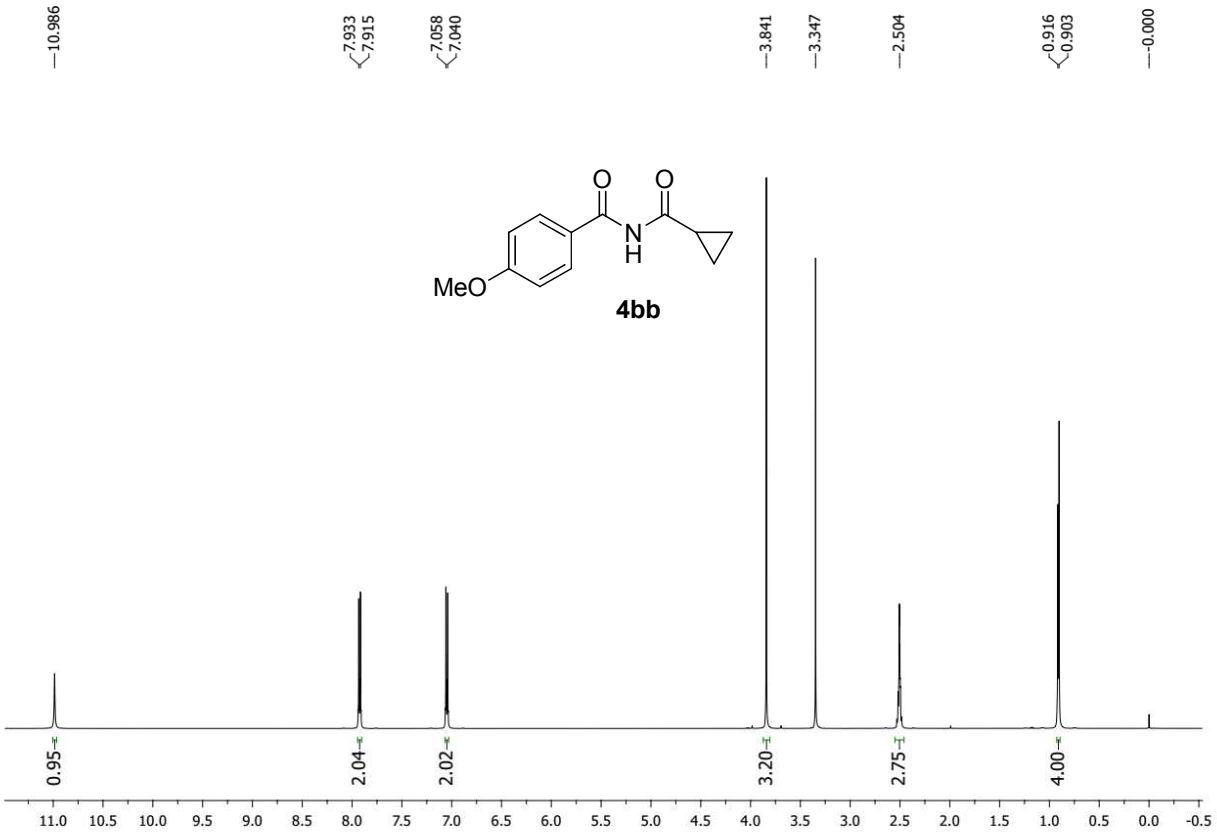
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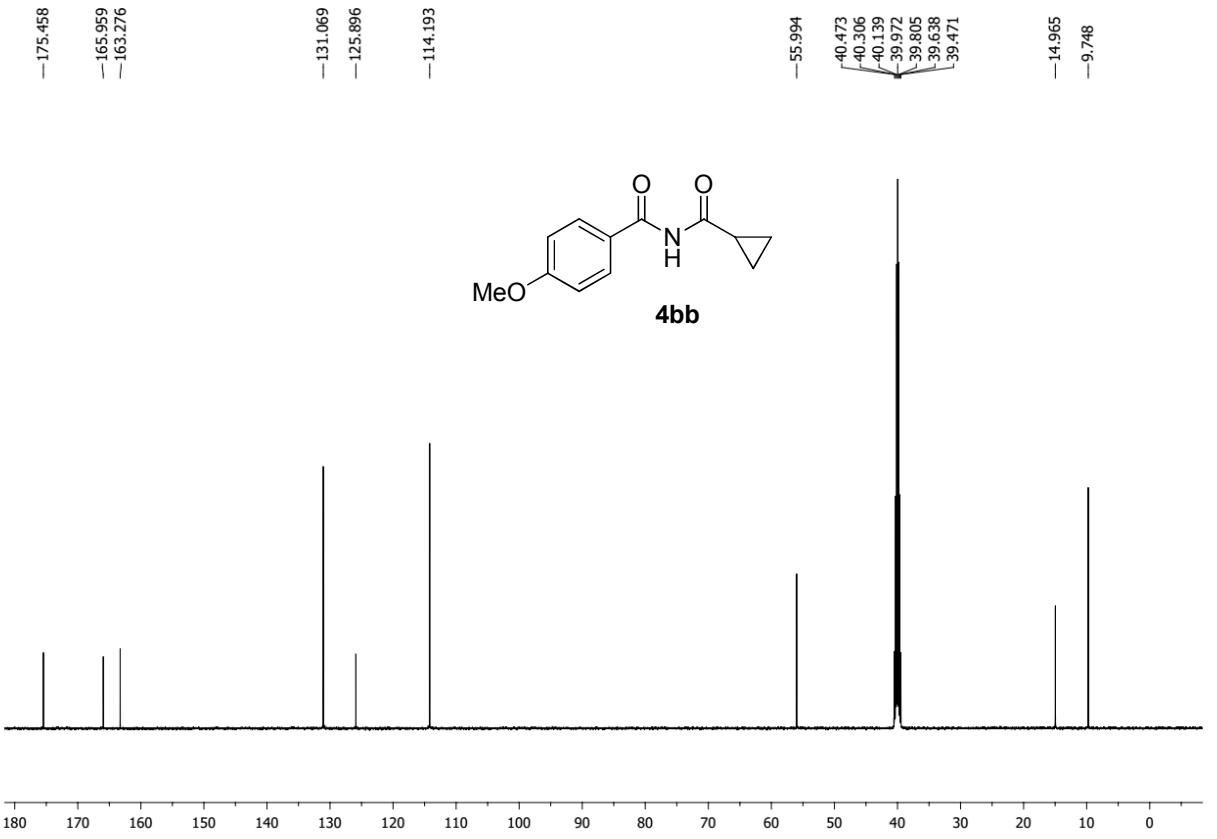
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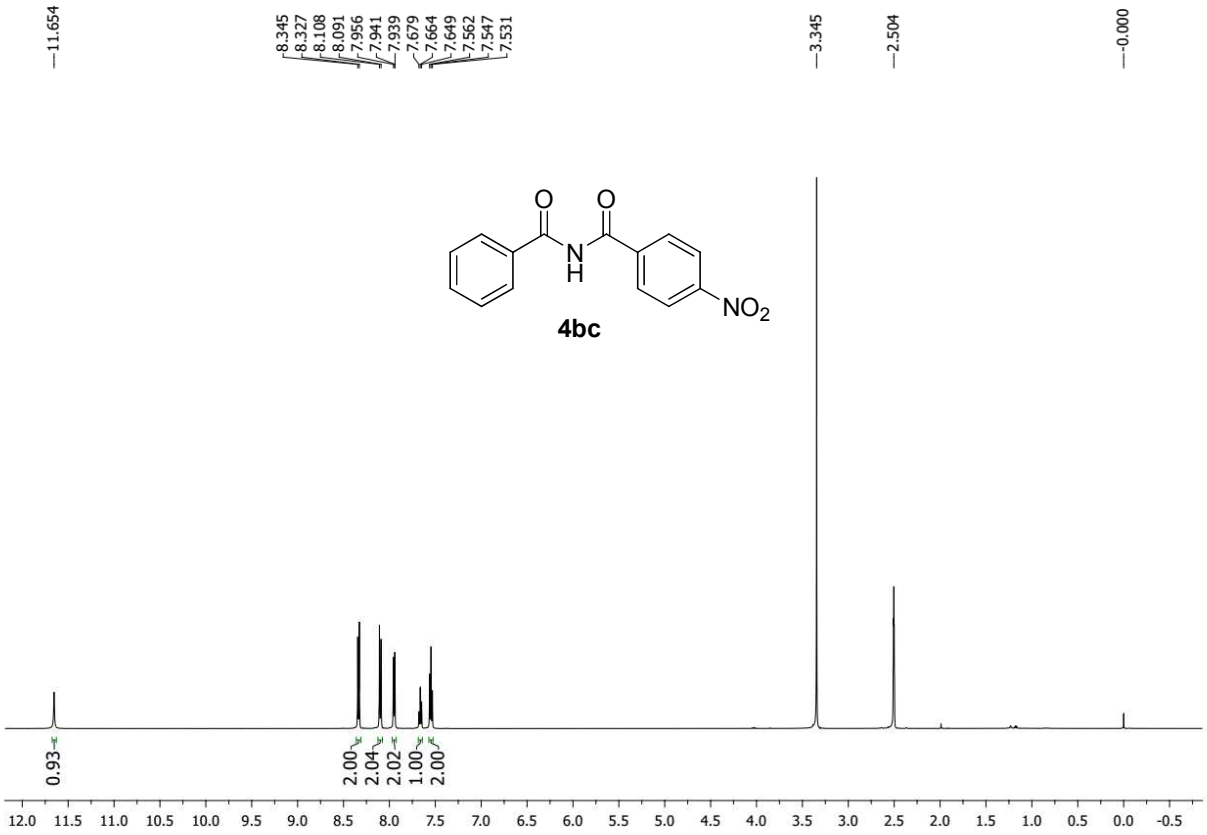
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1.00
2.00
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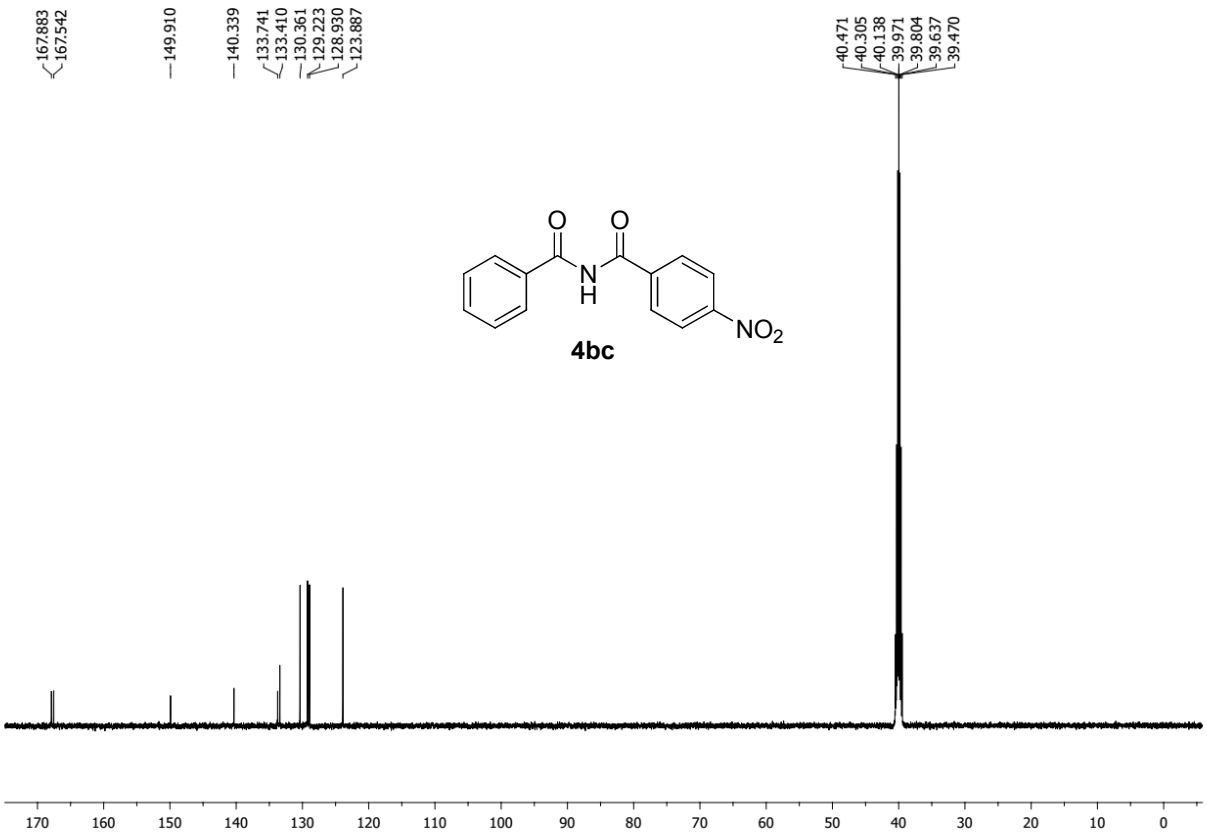
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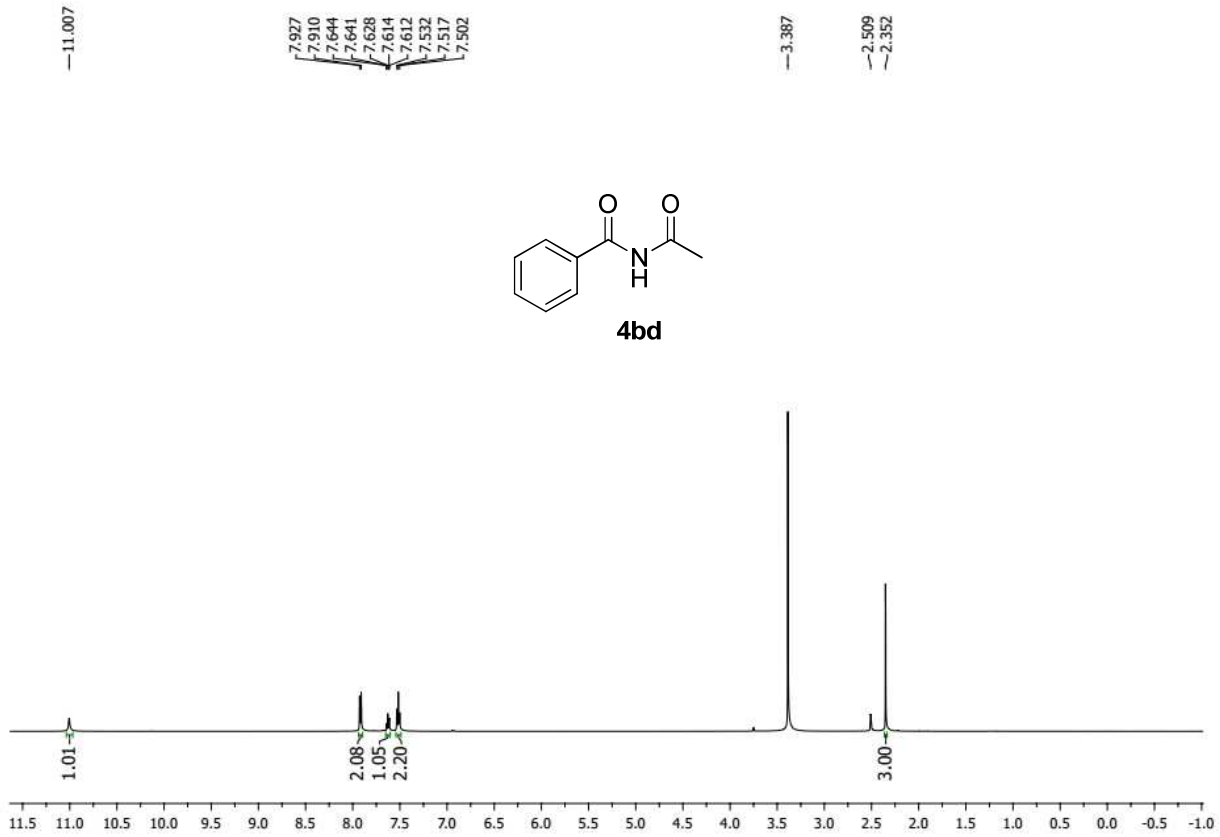
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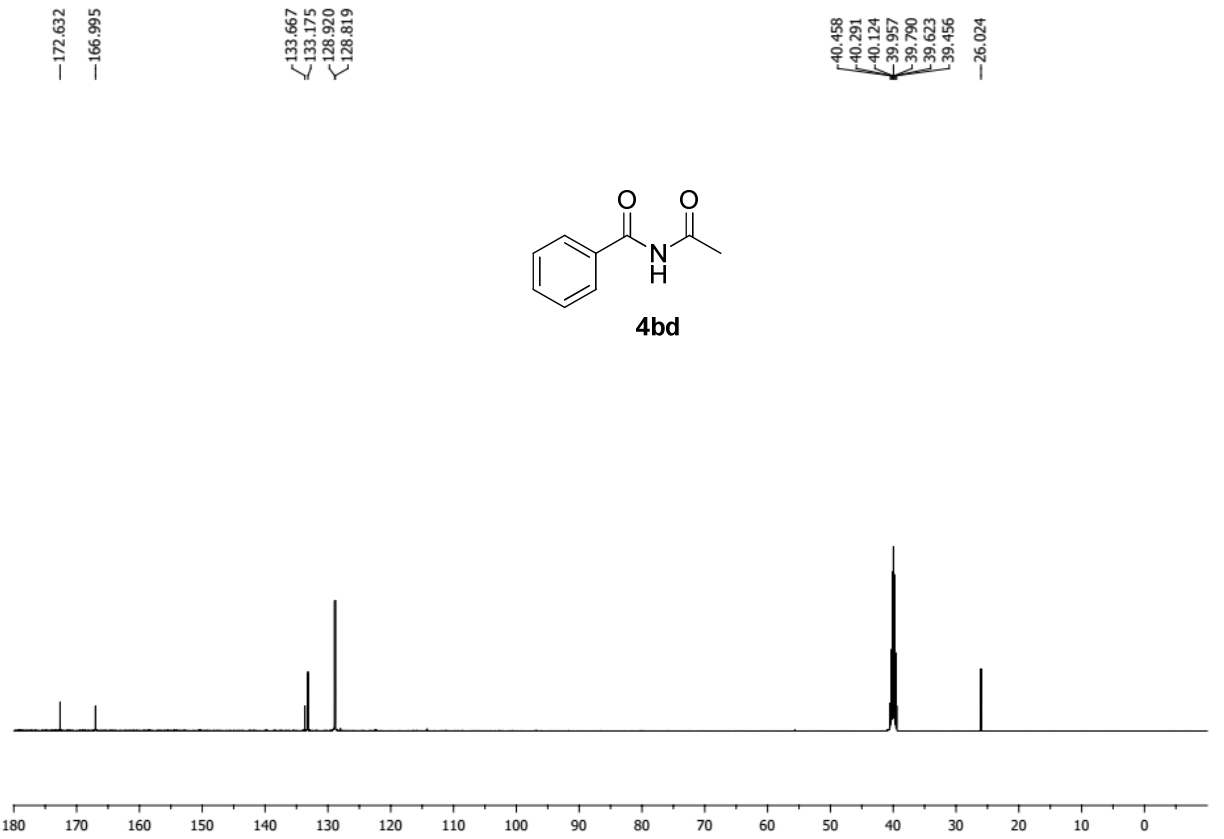
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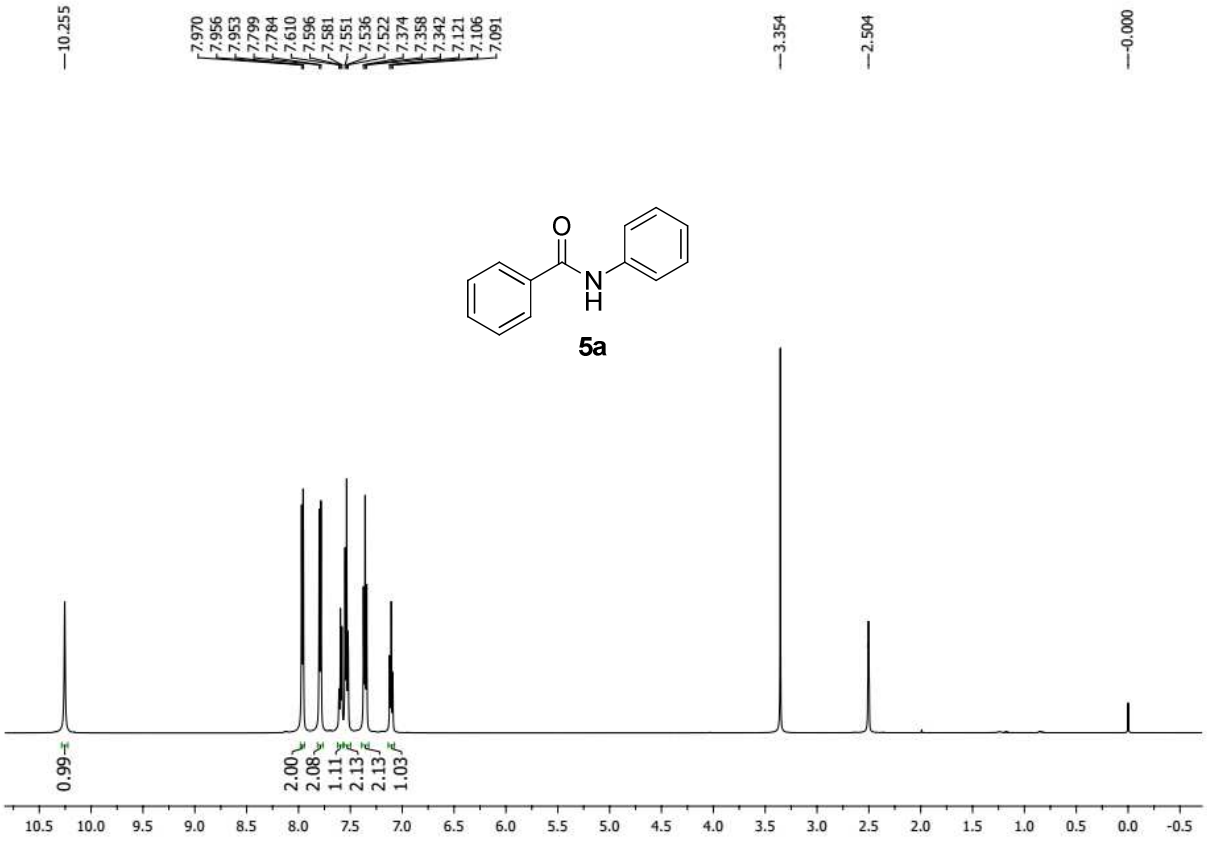
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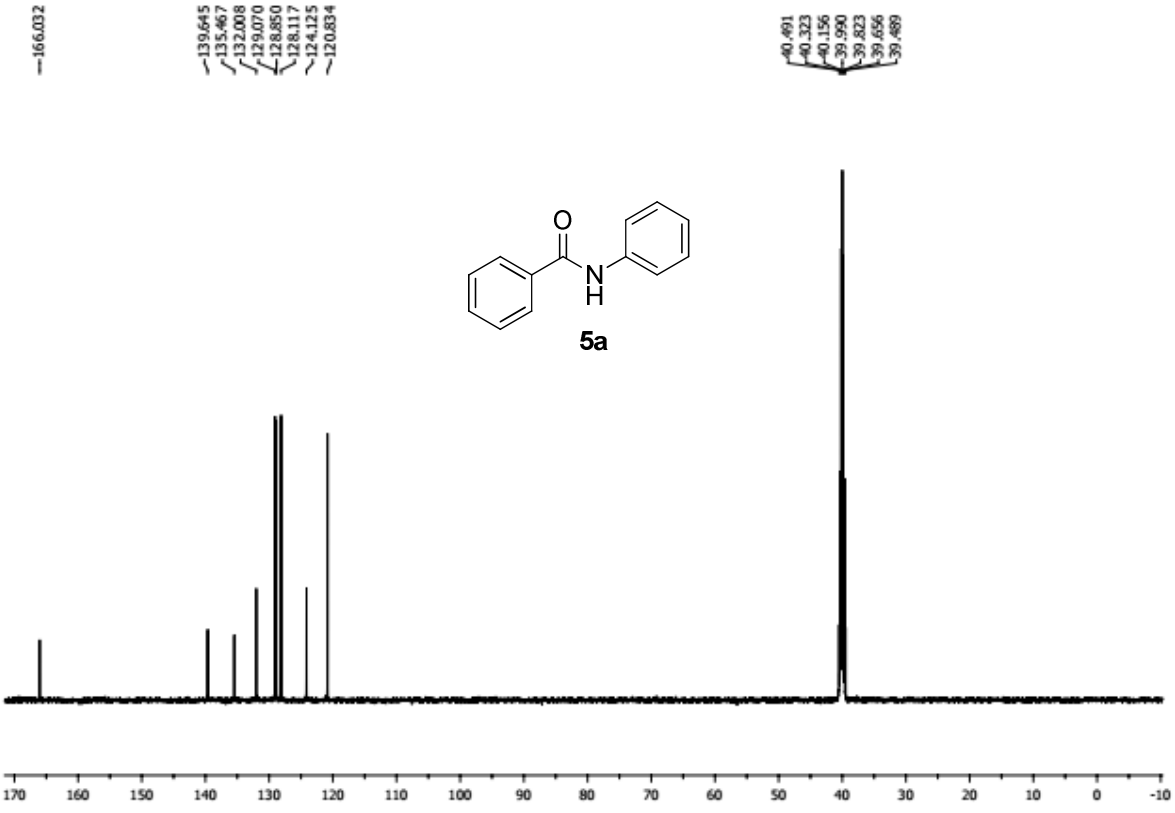
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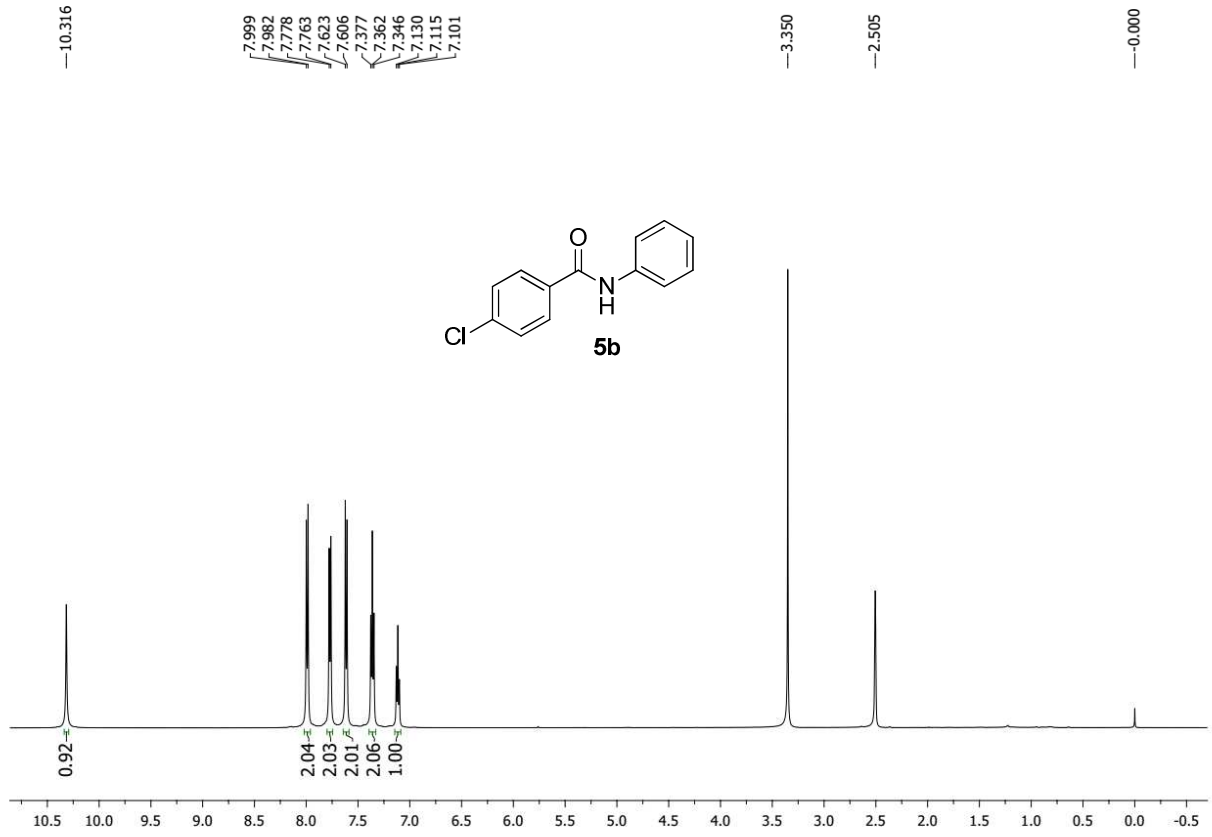
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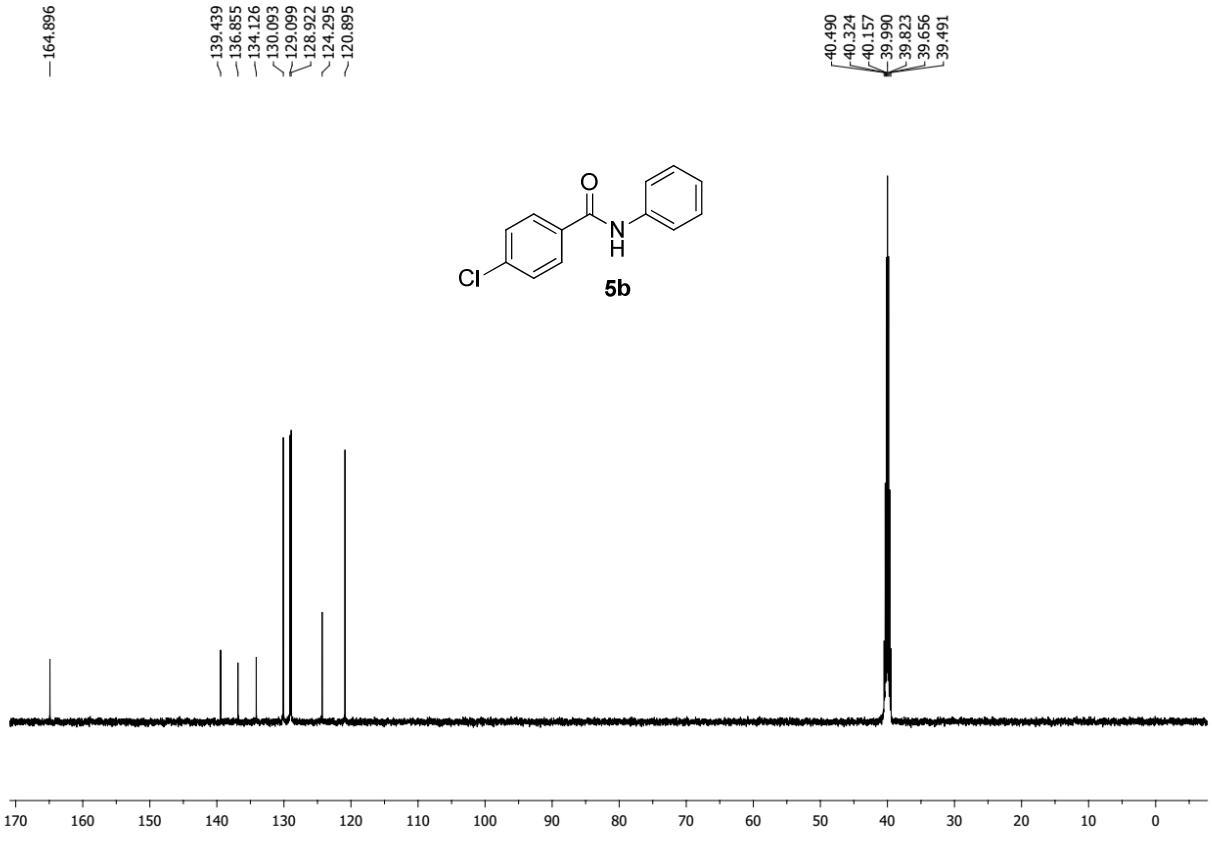
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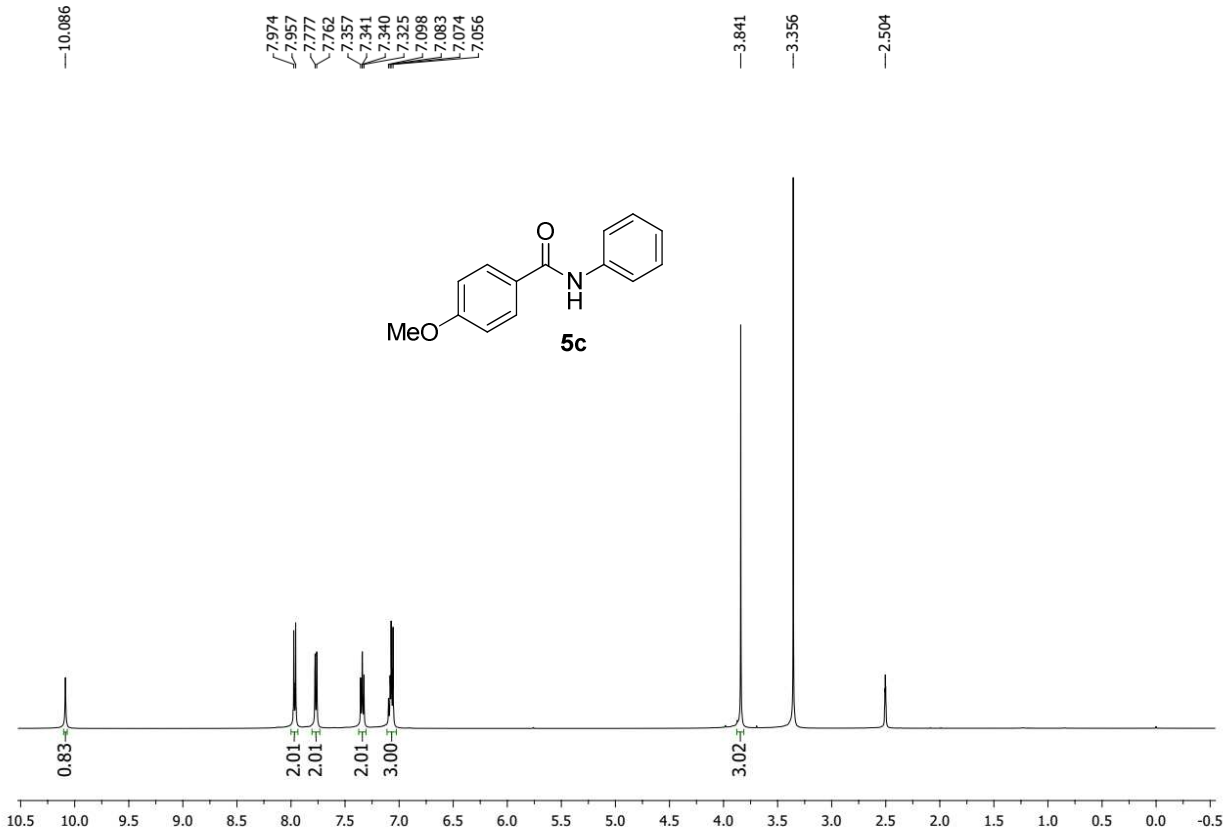
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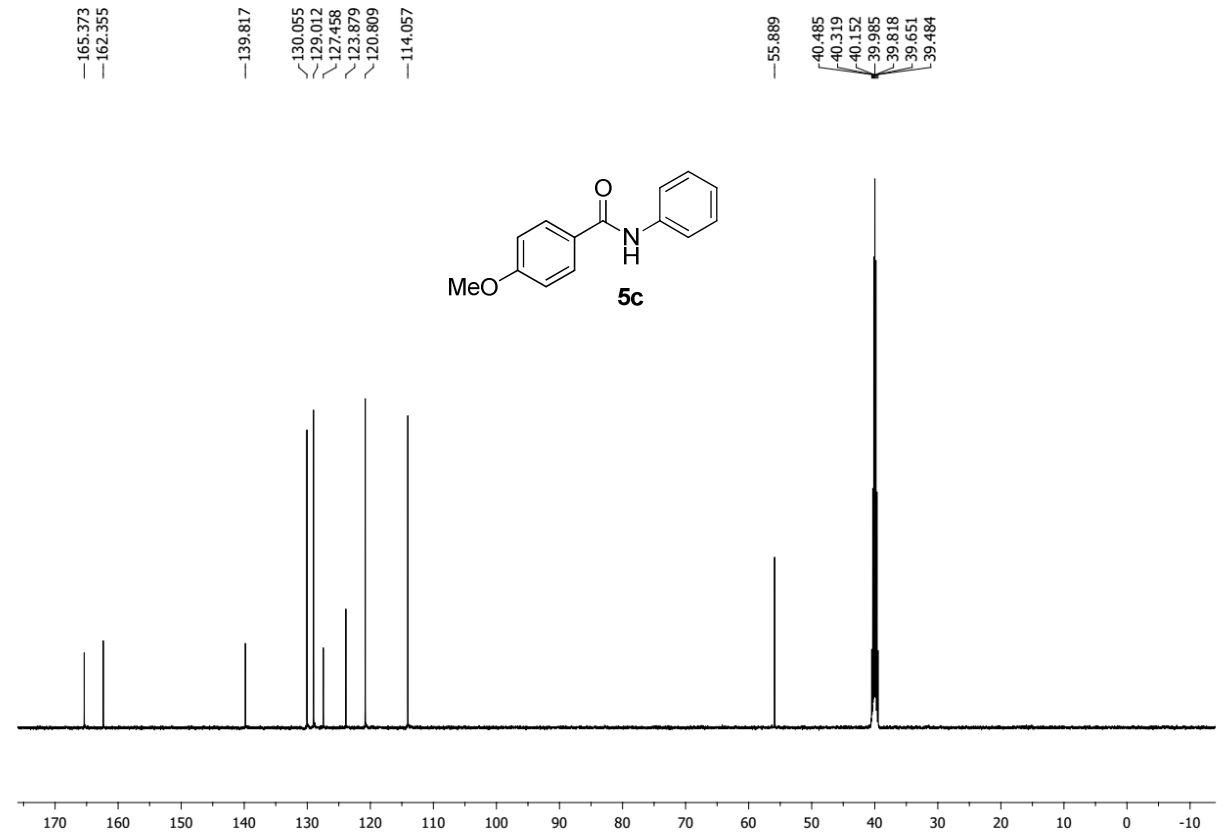
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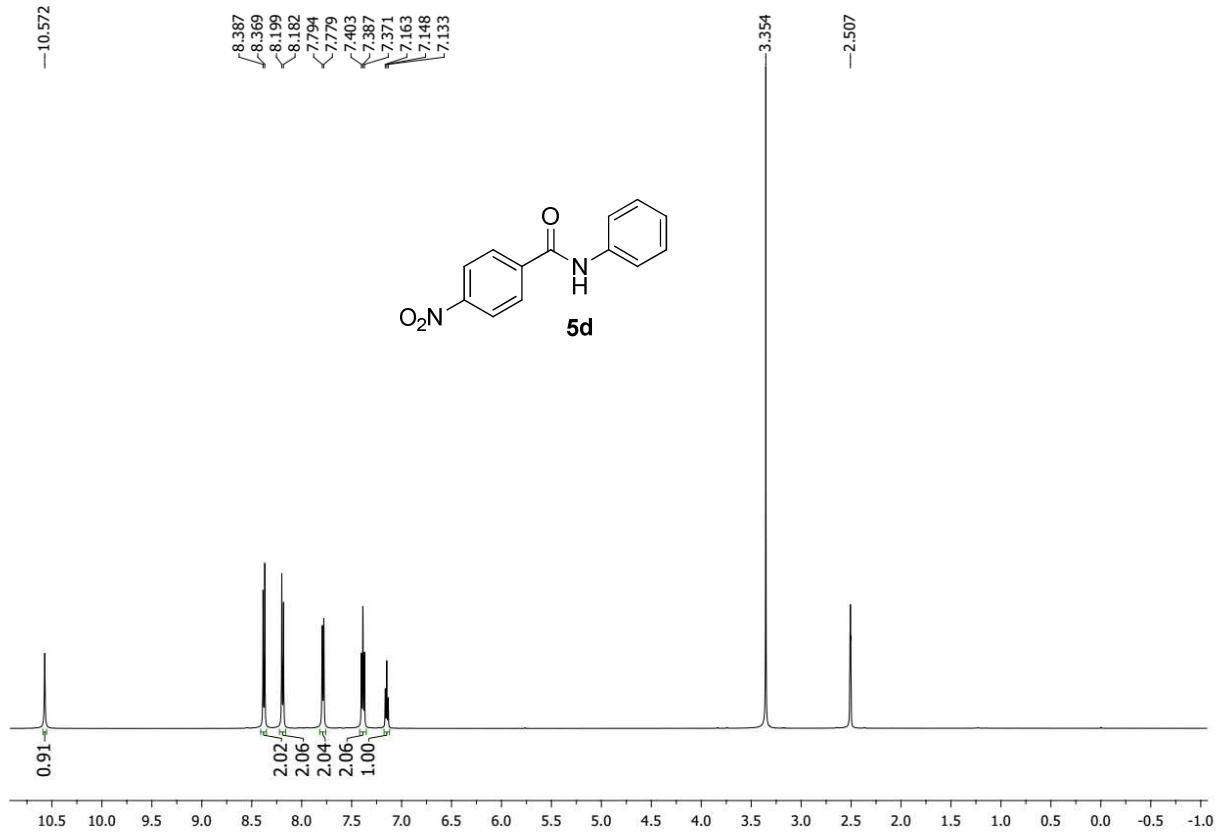
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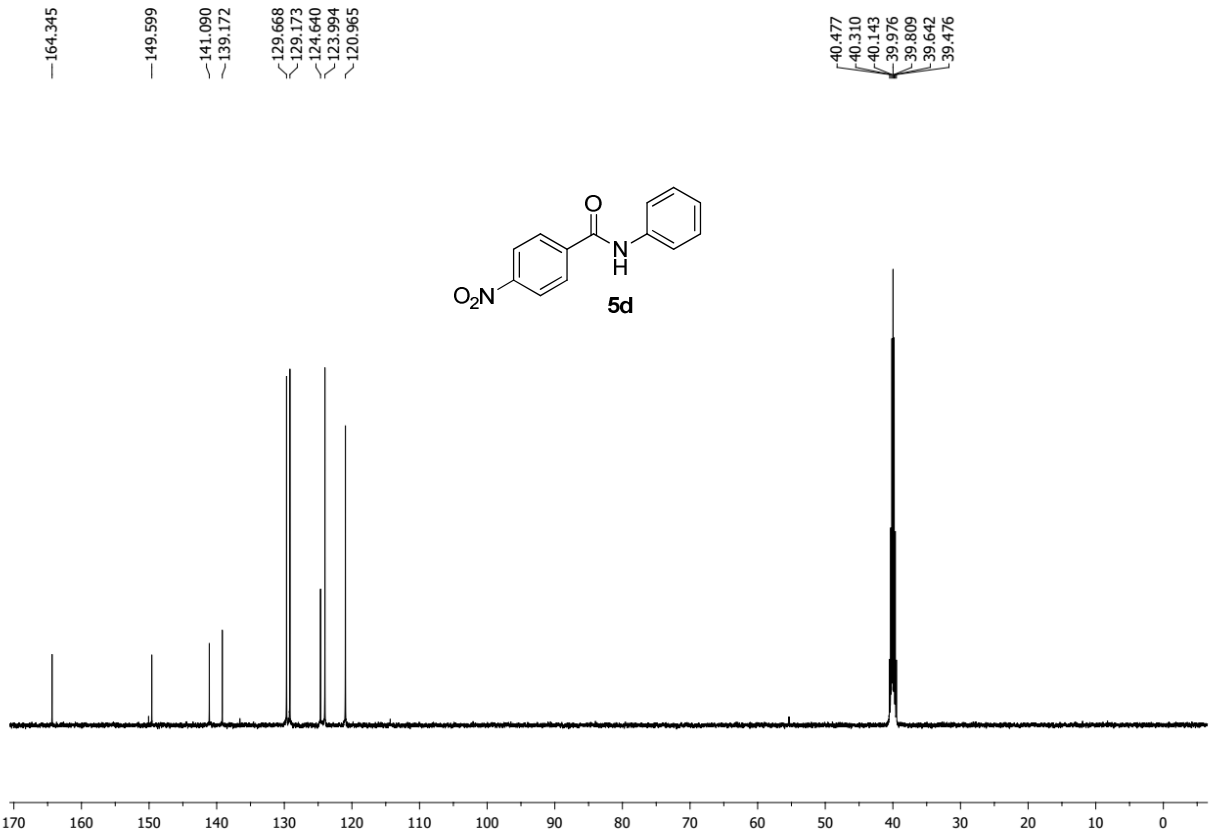
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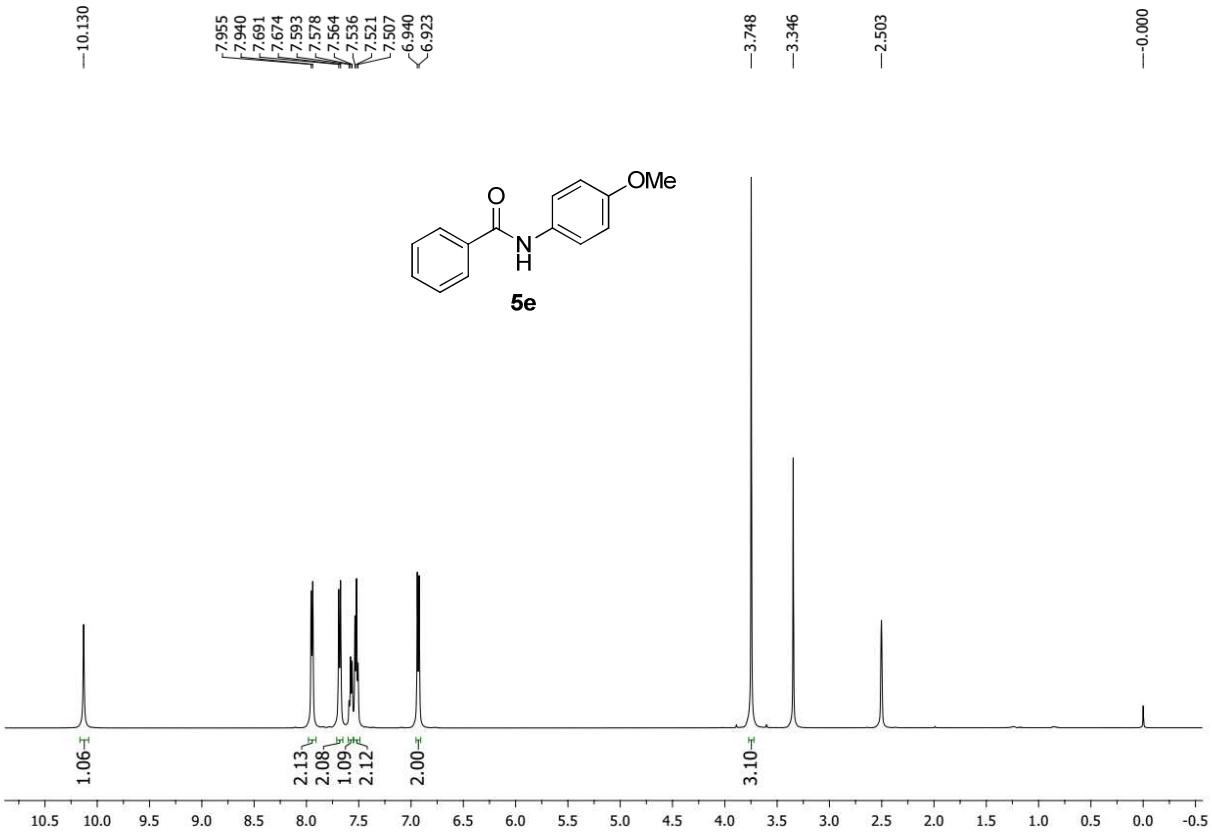
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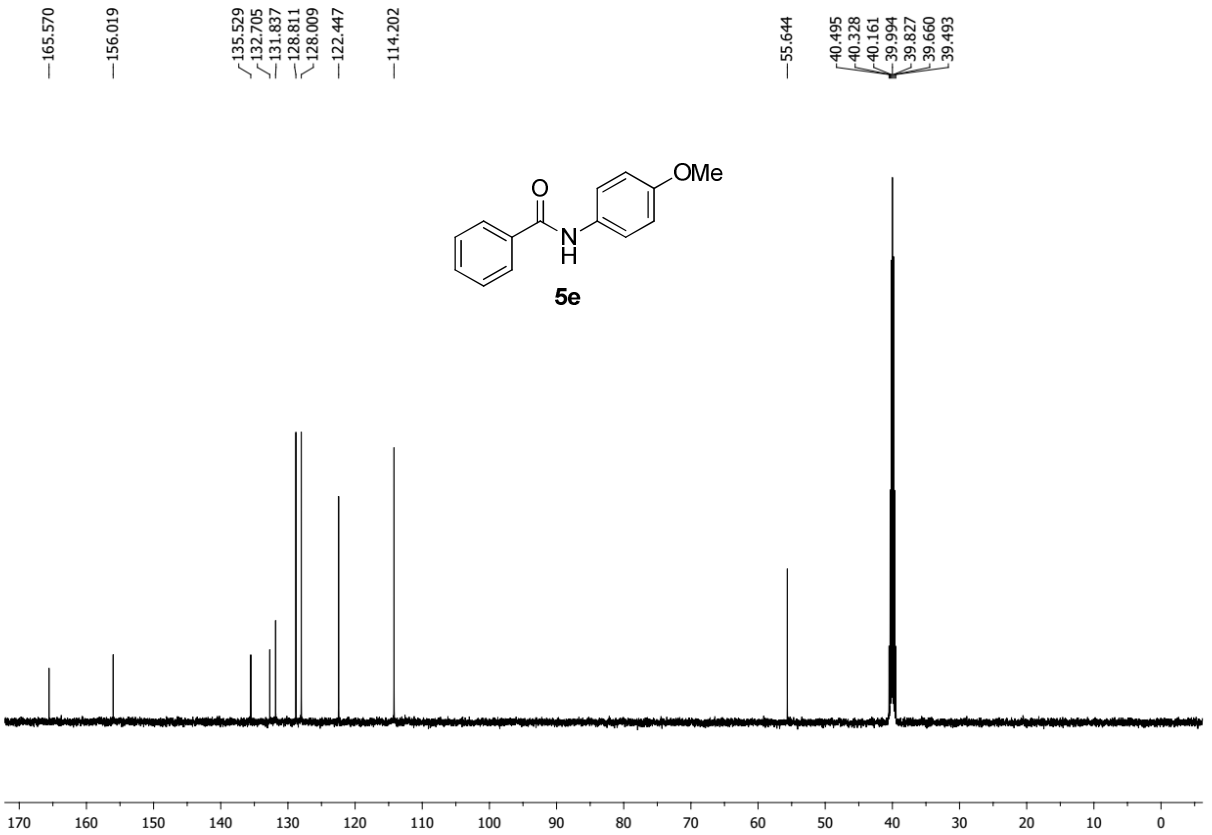
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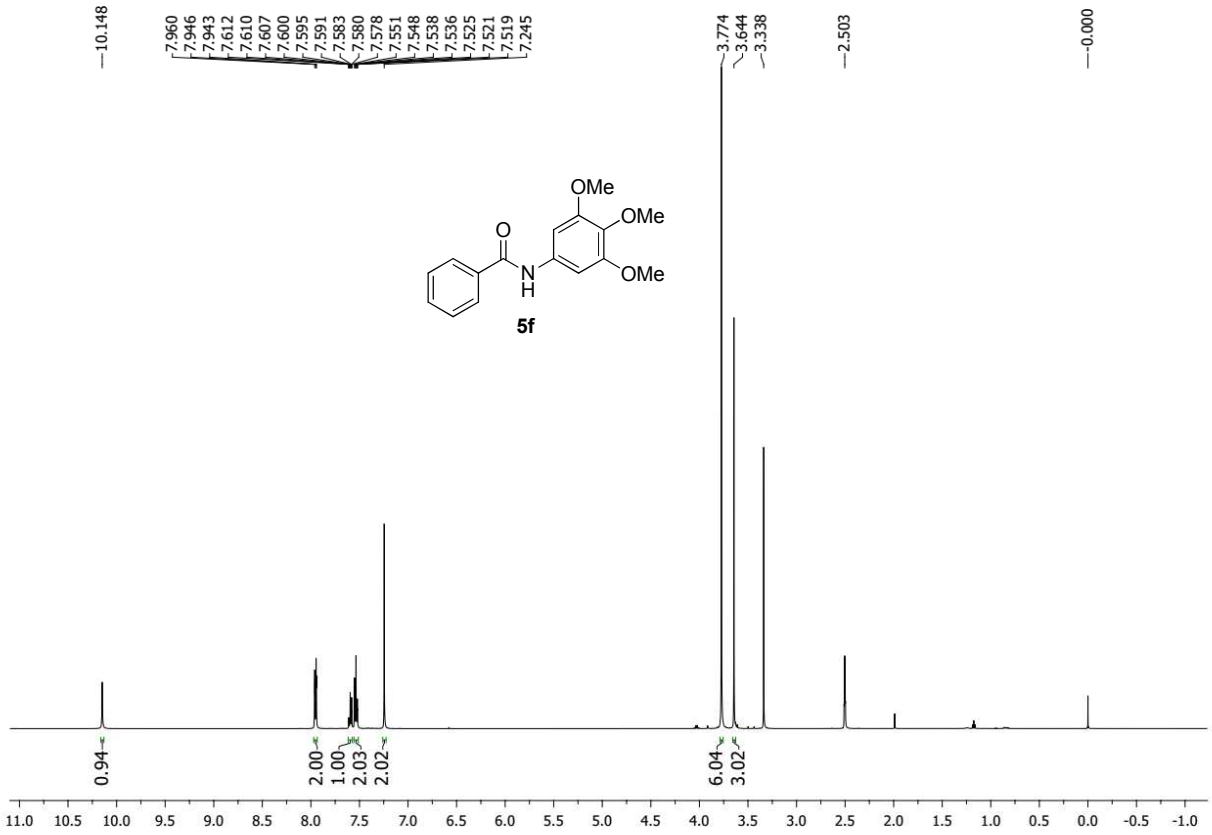
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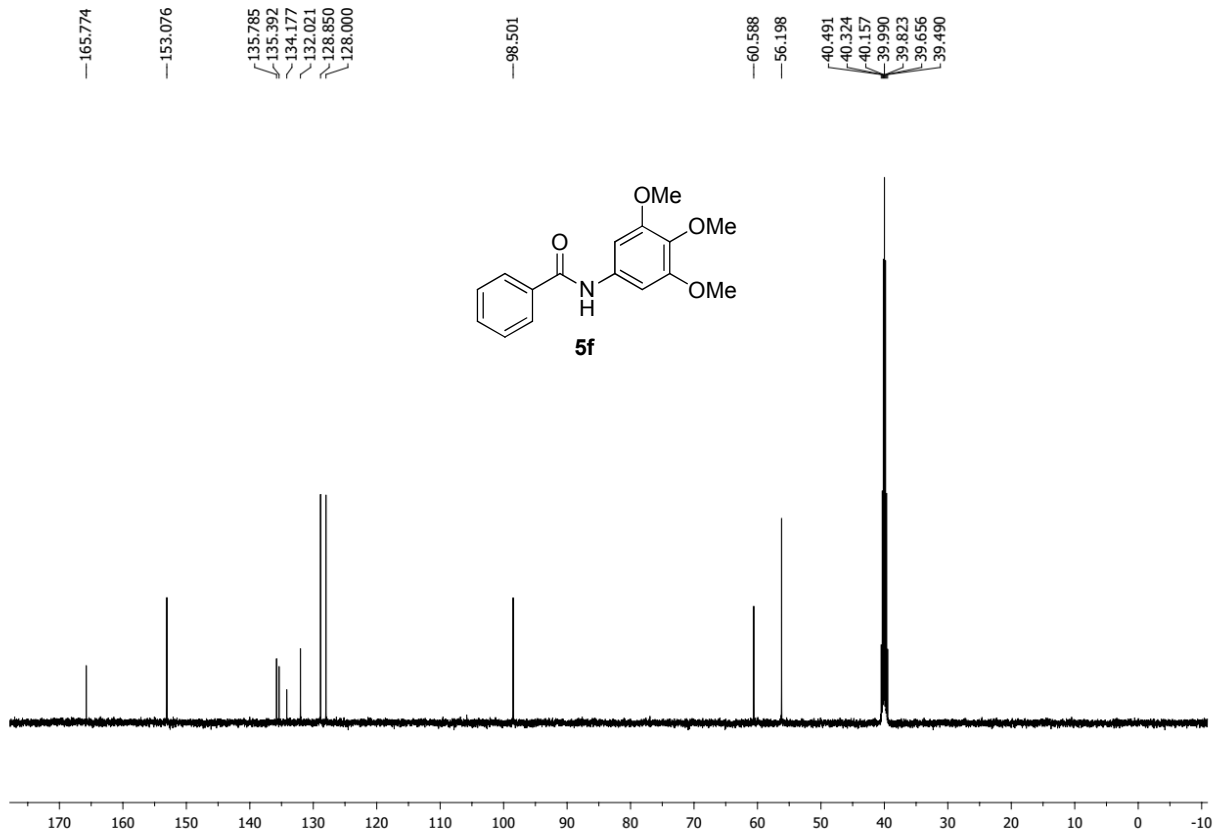
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OMe
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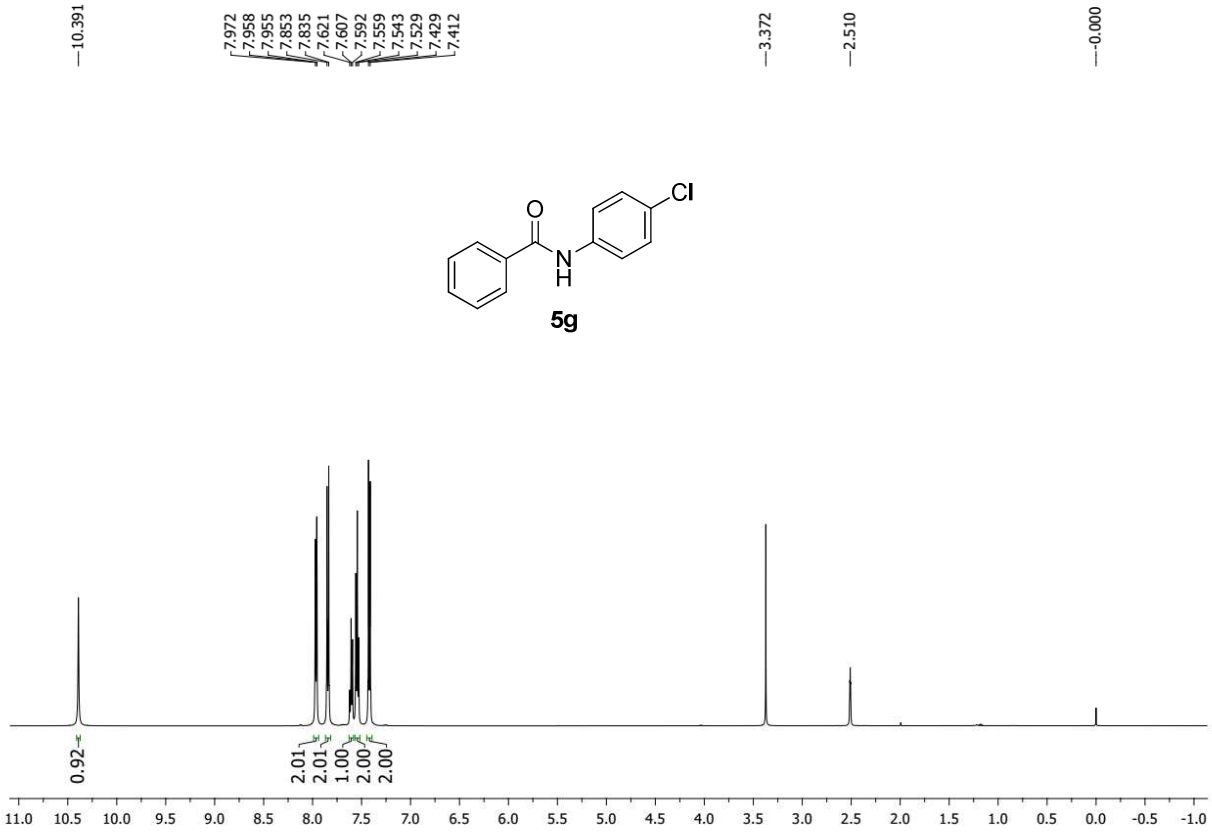
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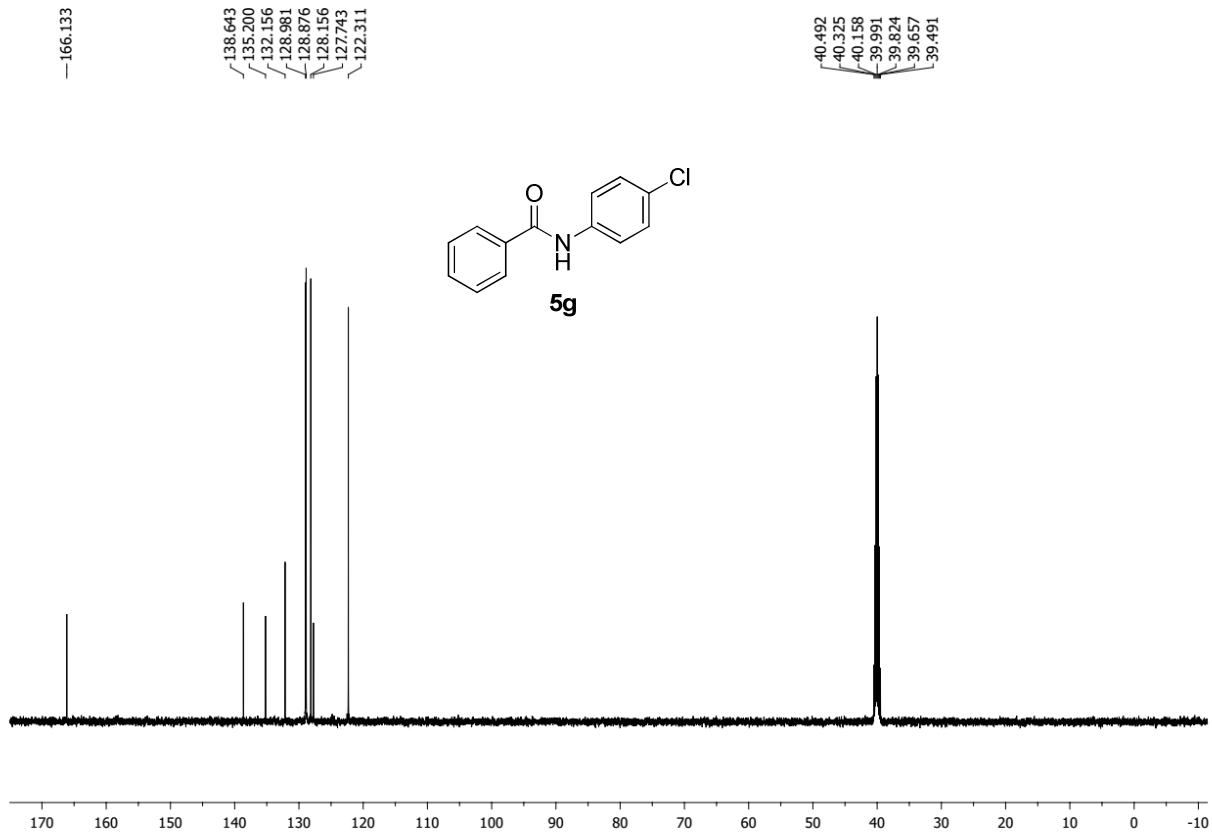
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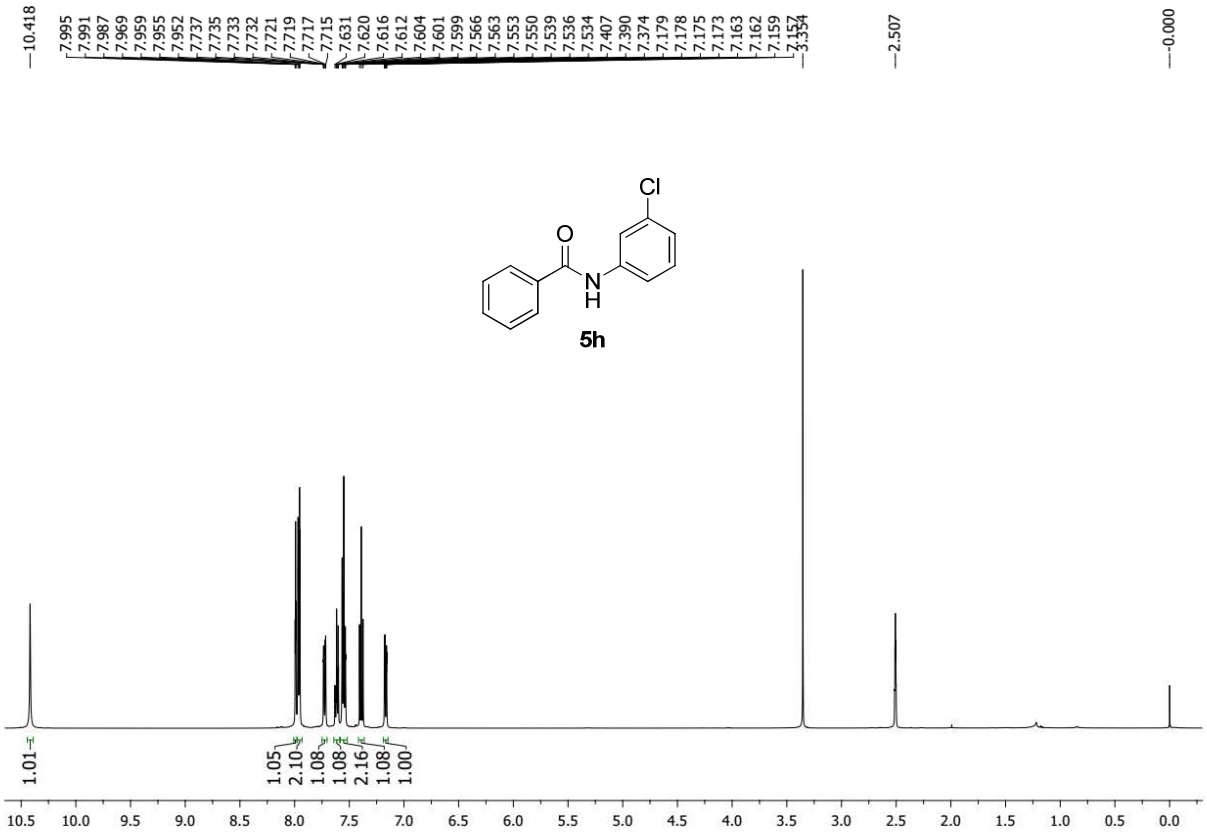
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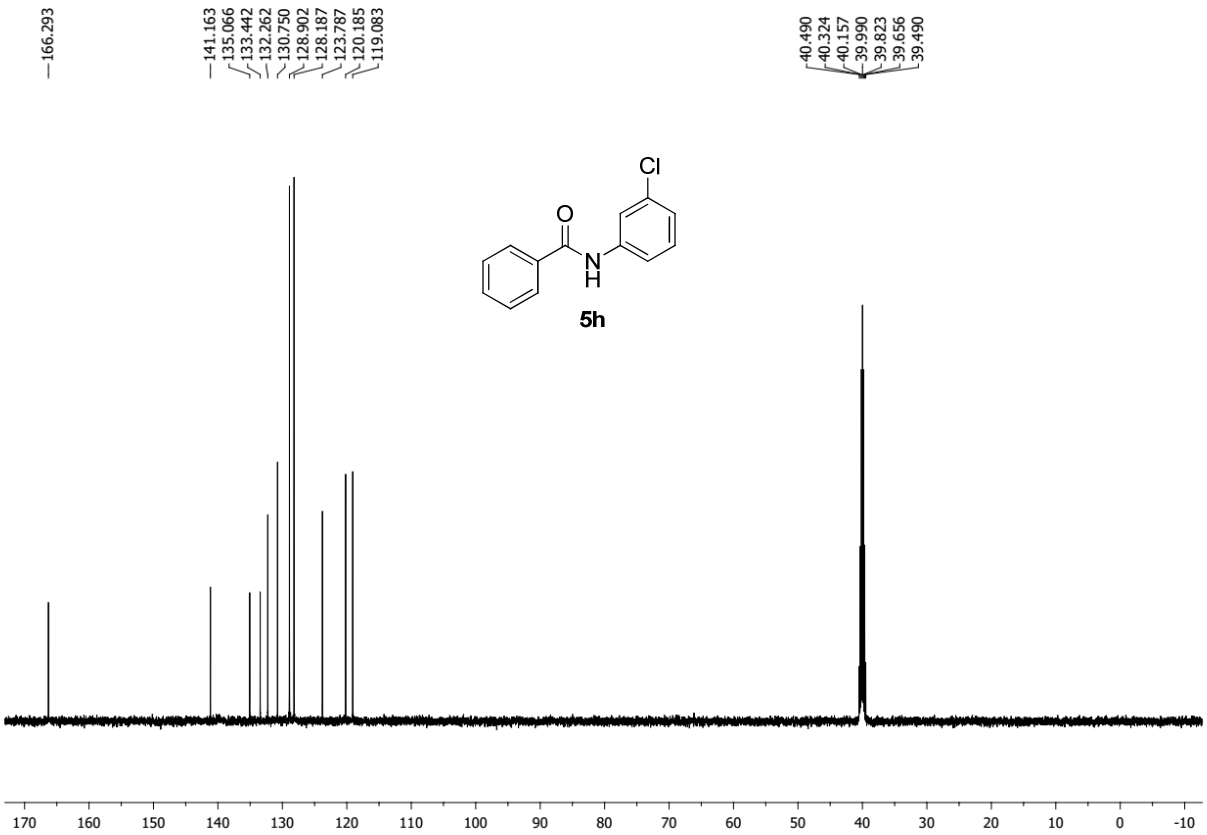
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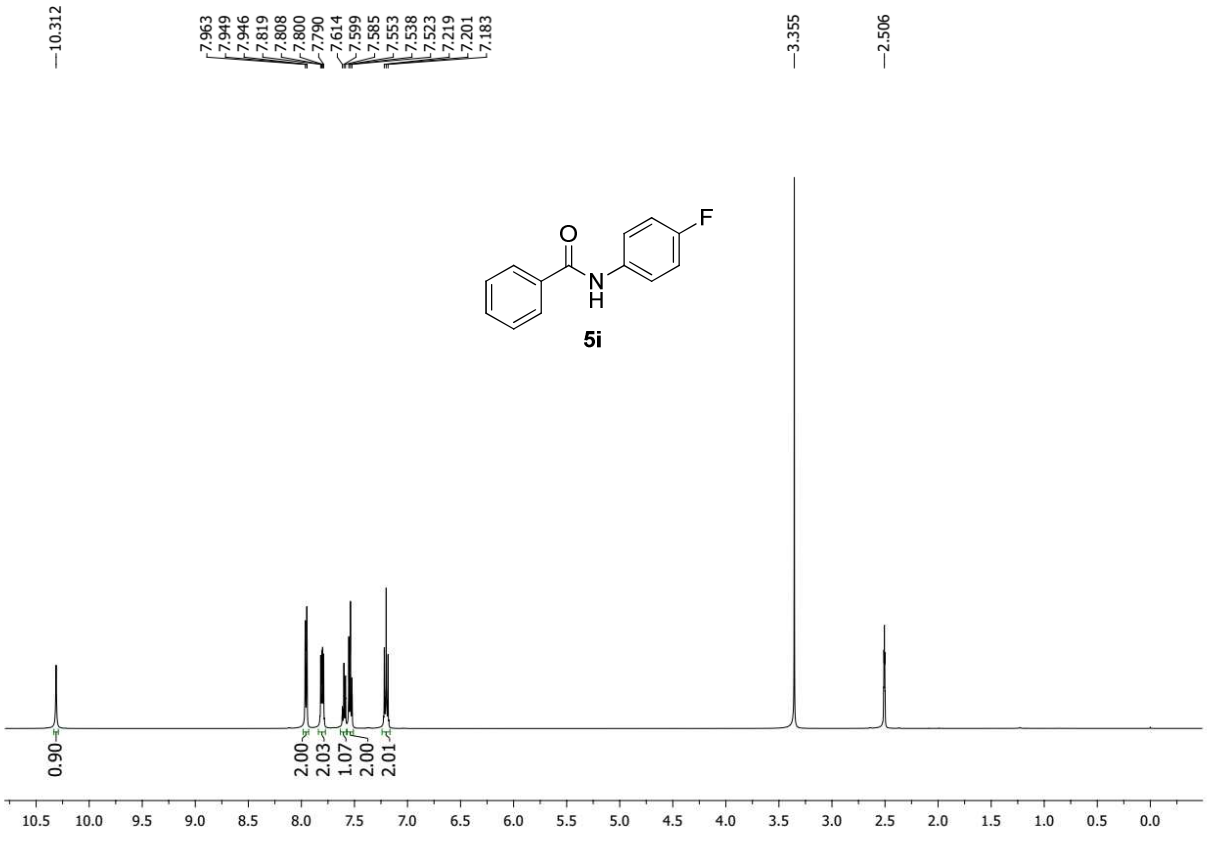
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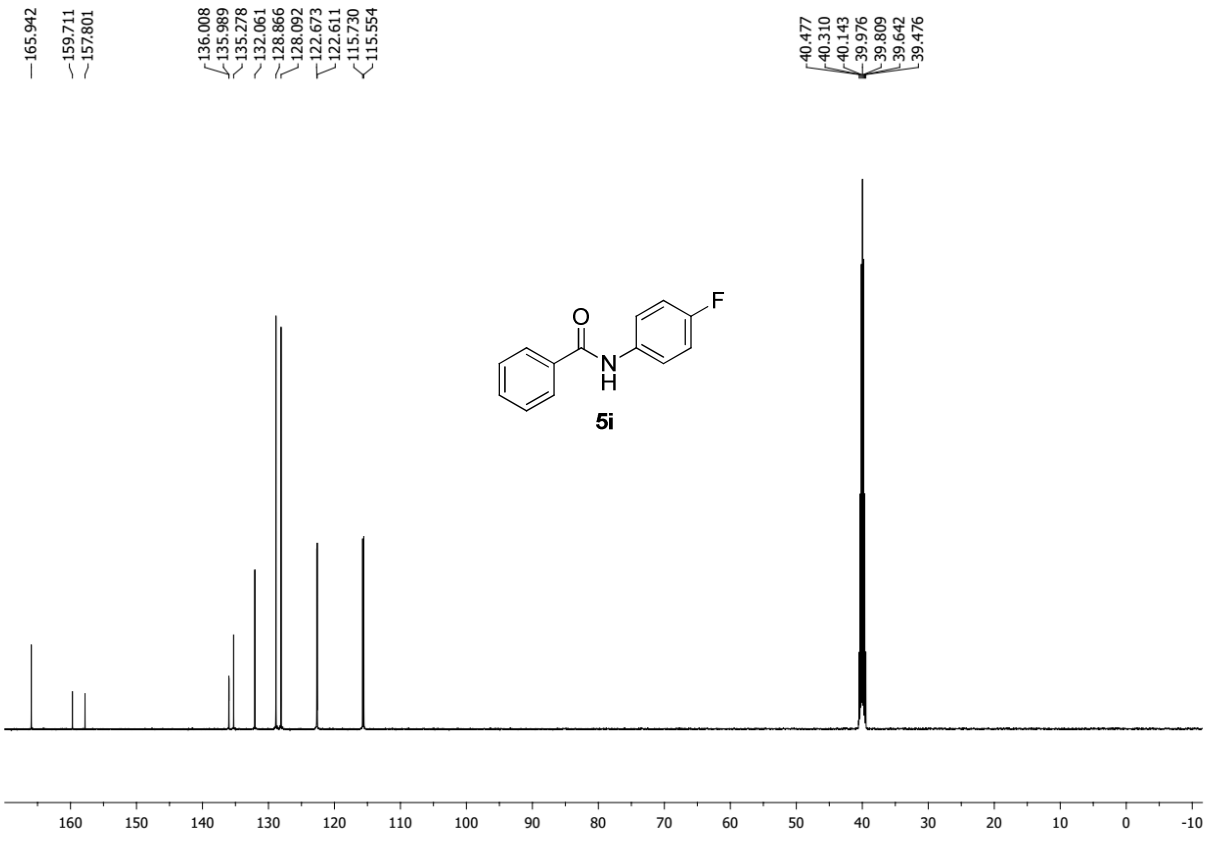
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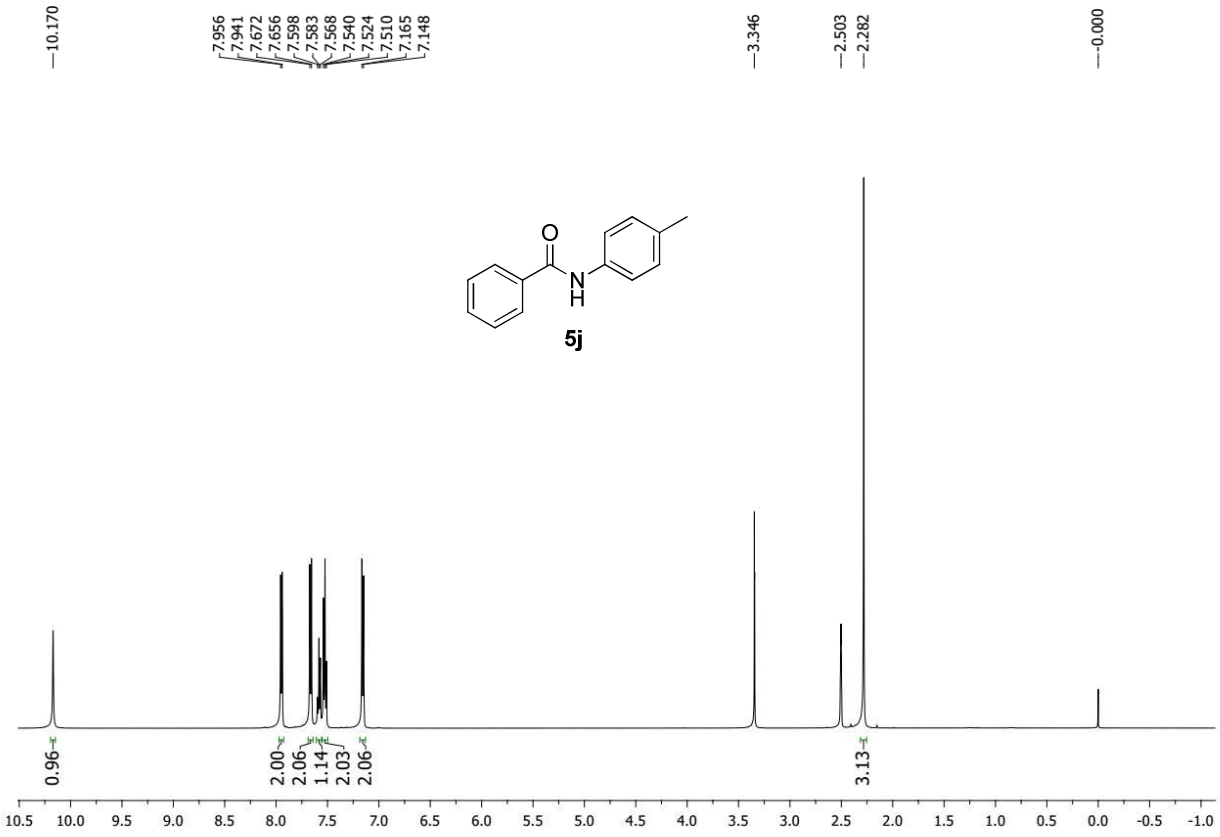
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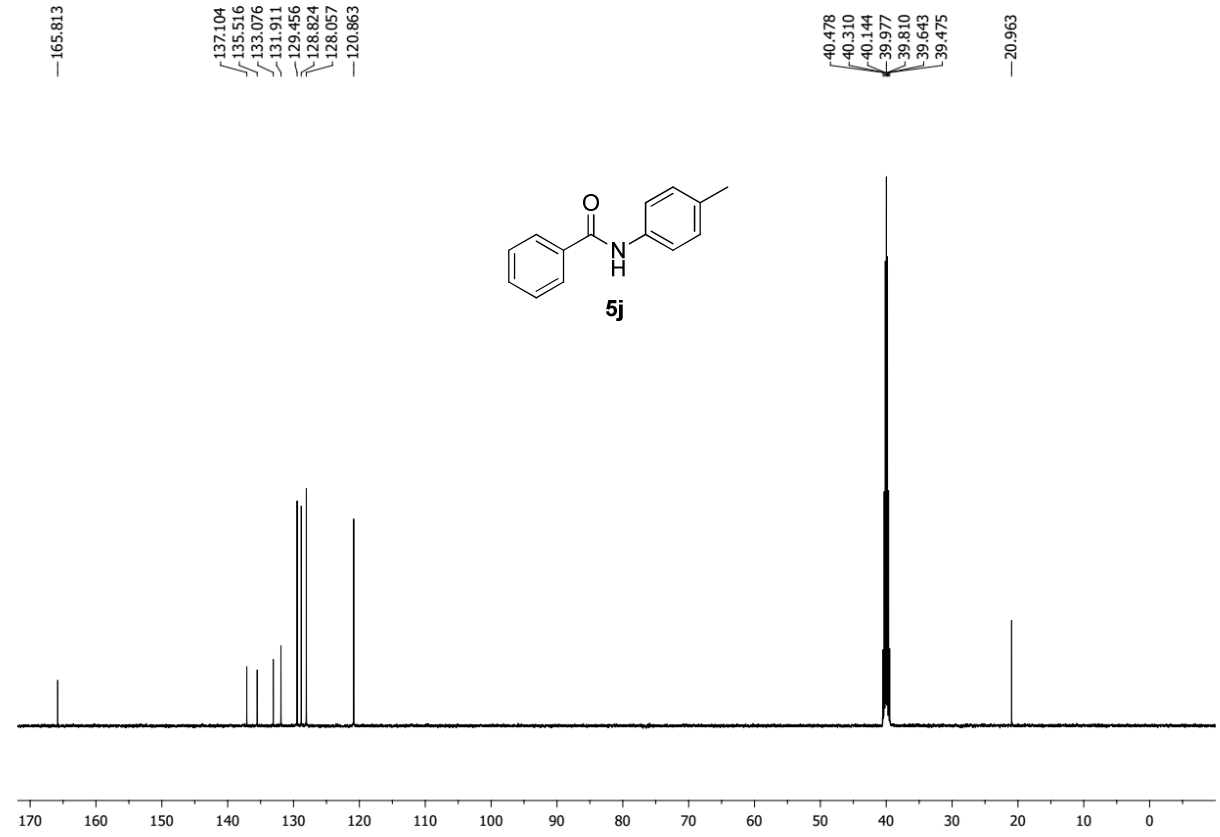
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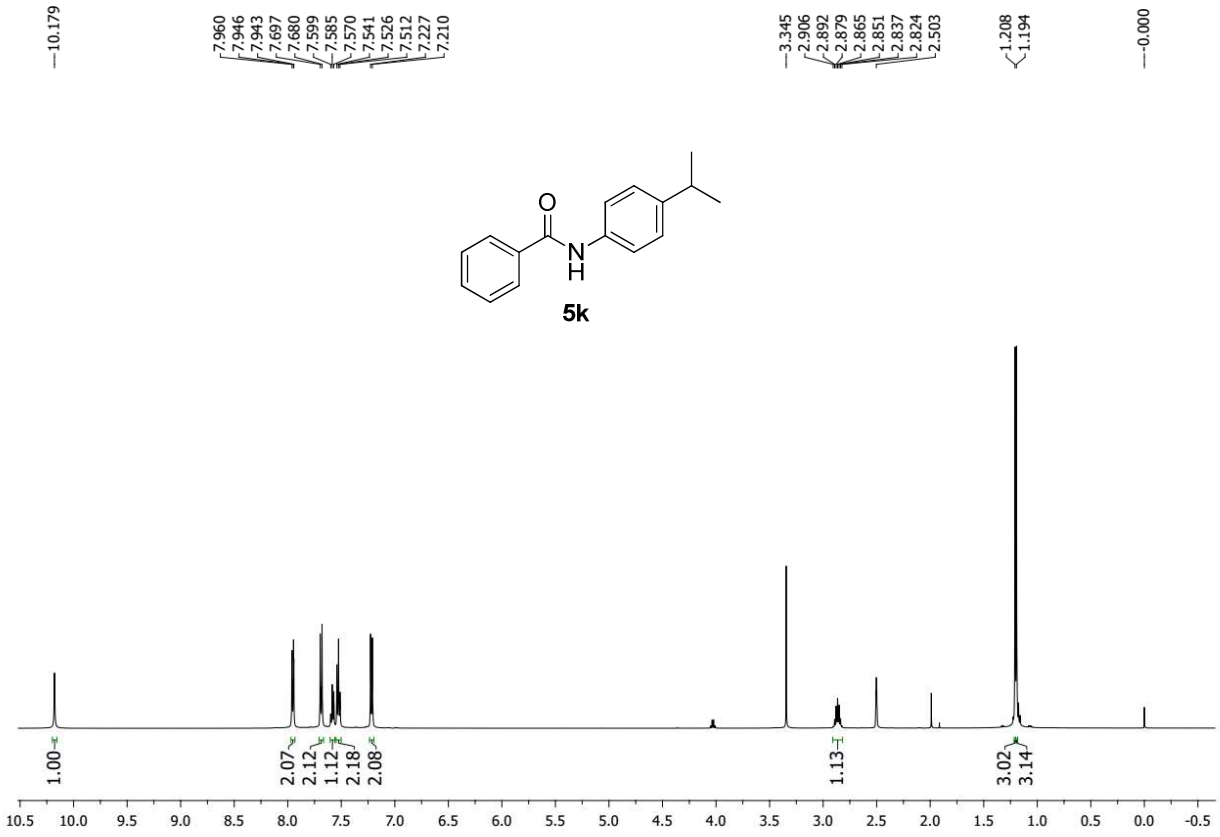
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3.02
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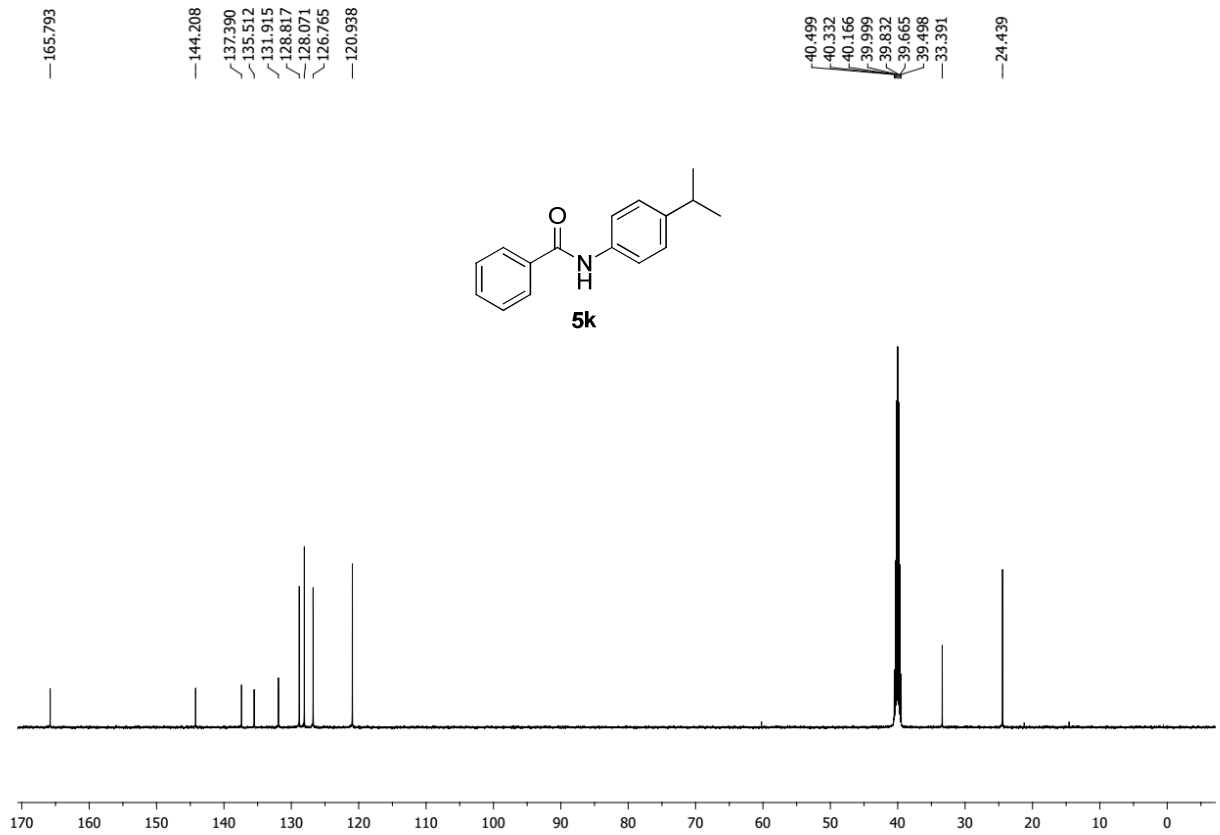
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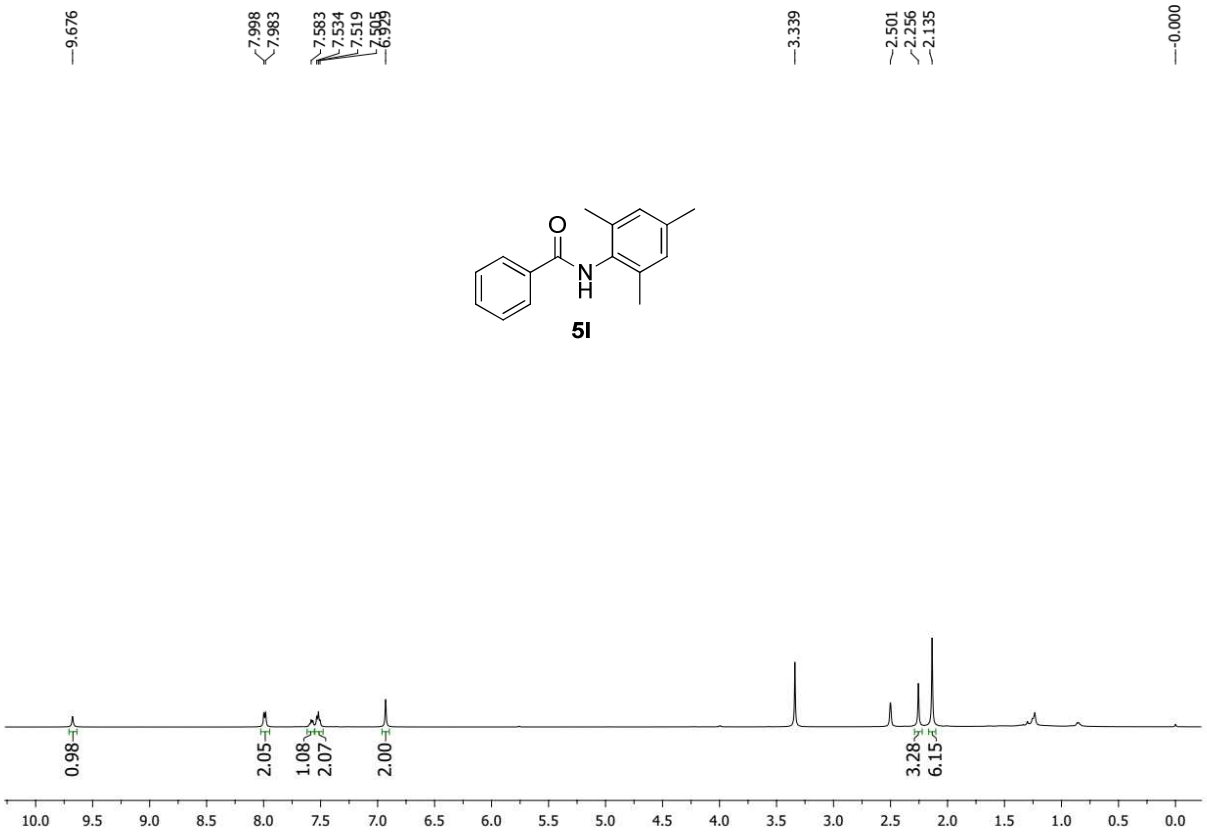
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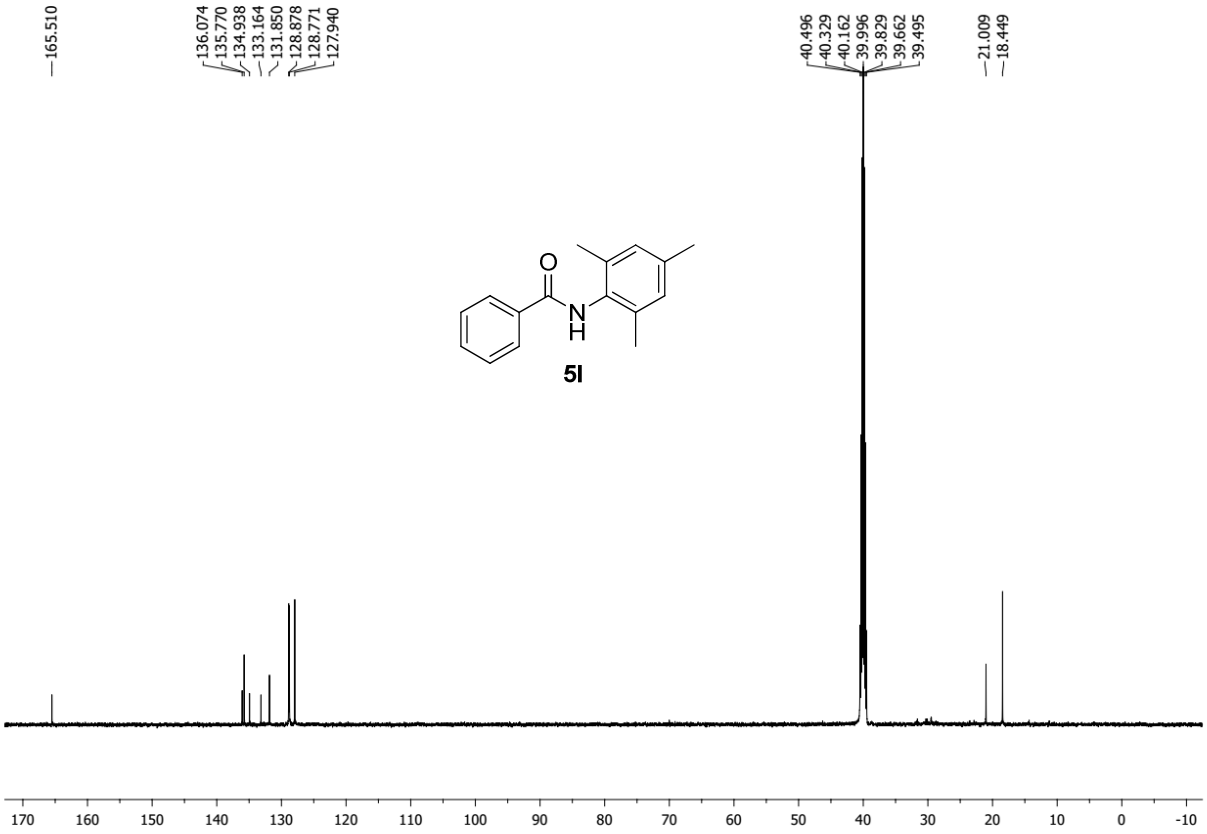
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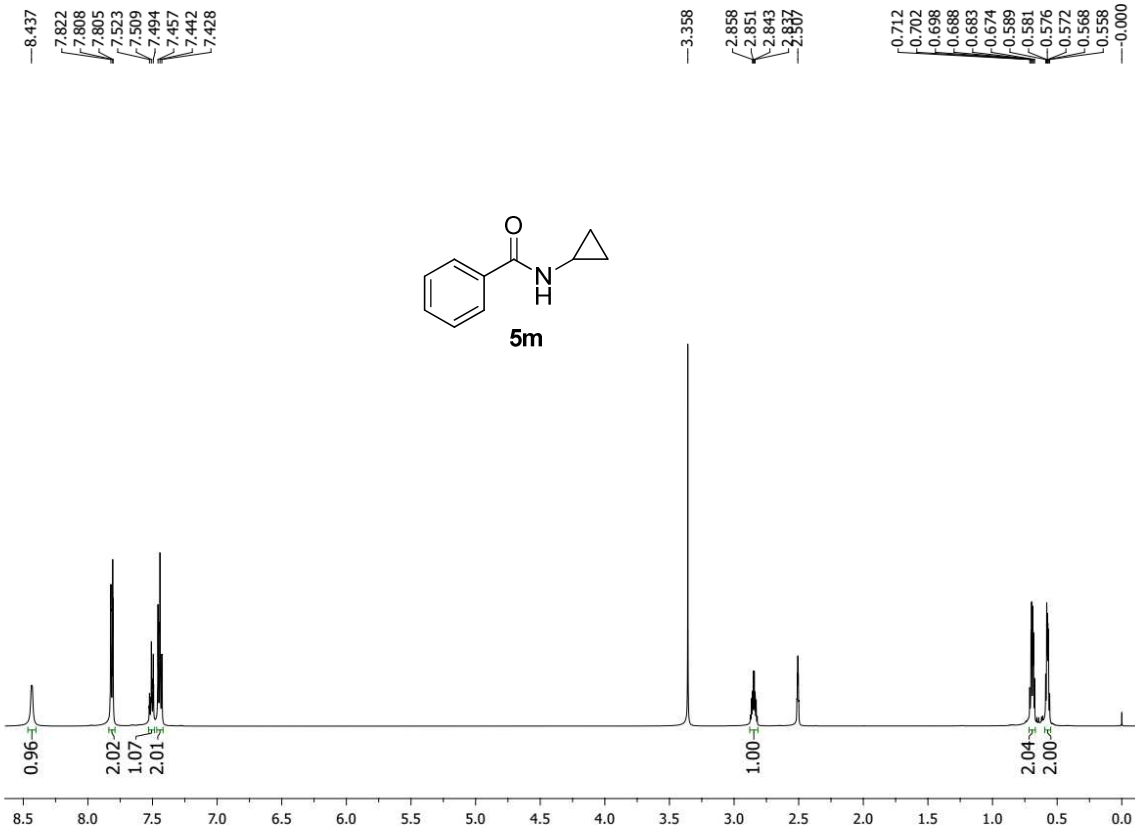
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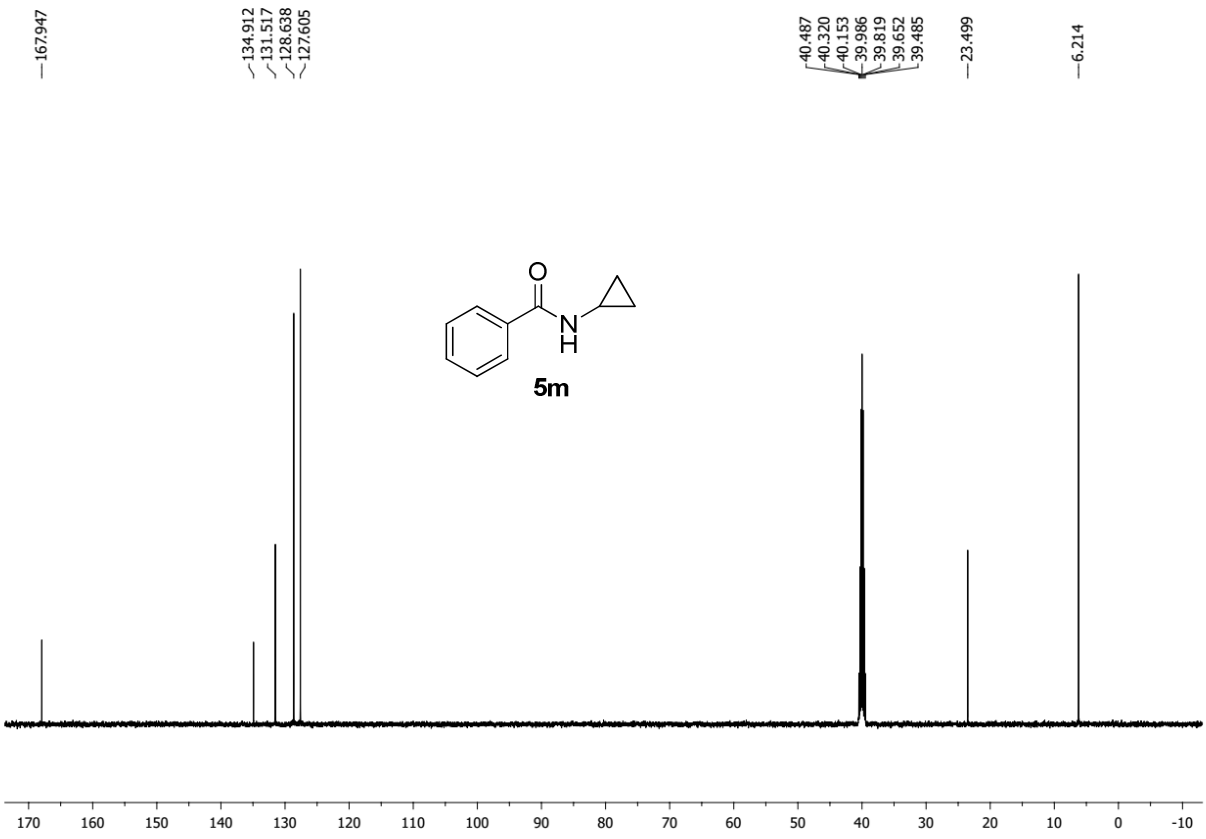
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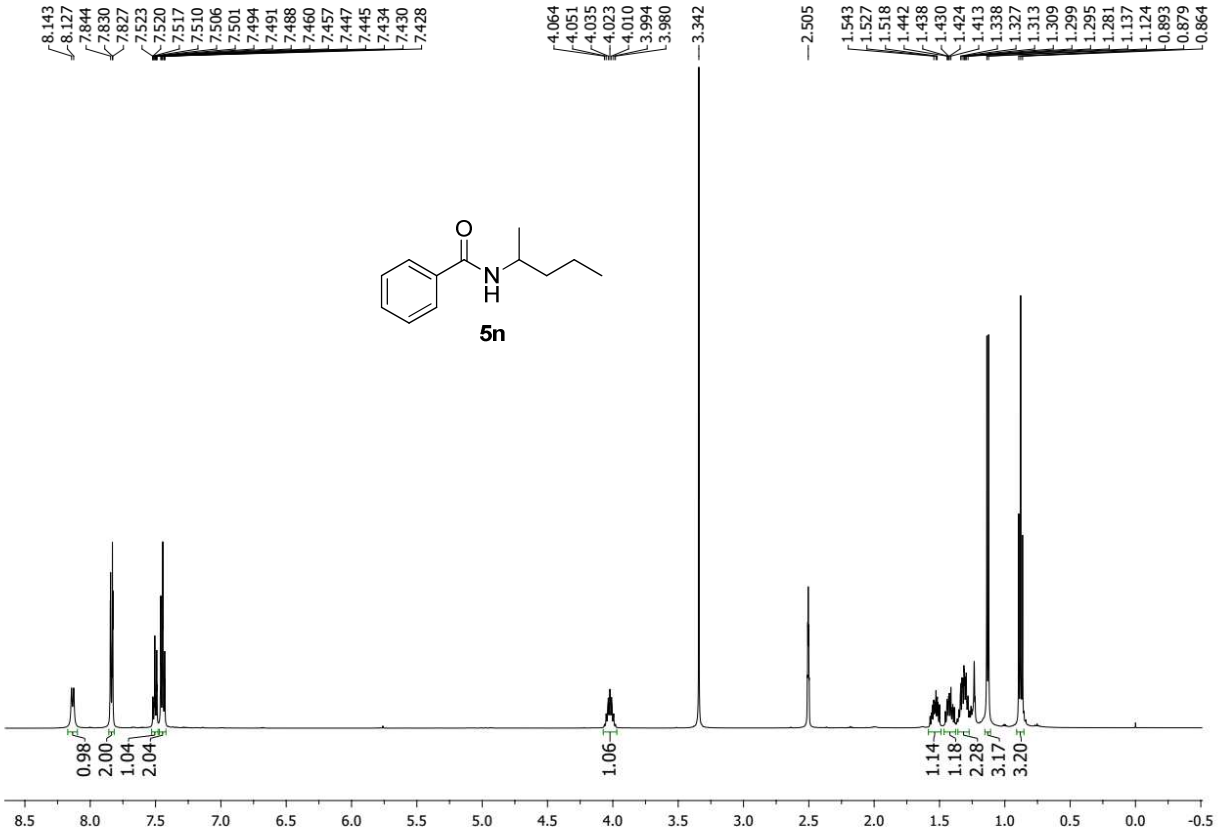
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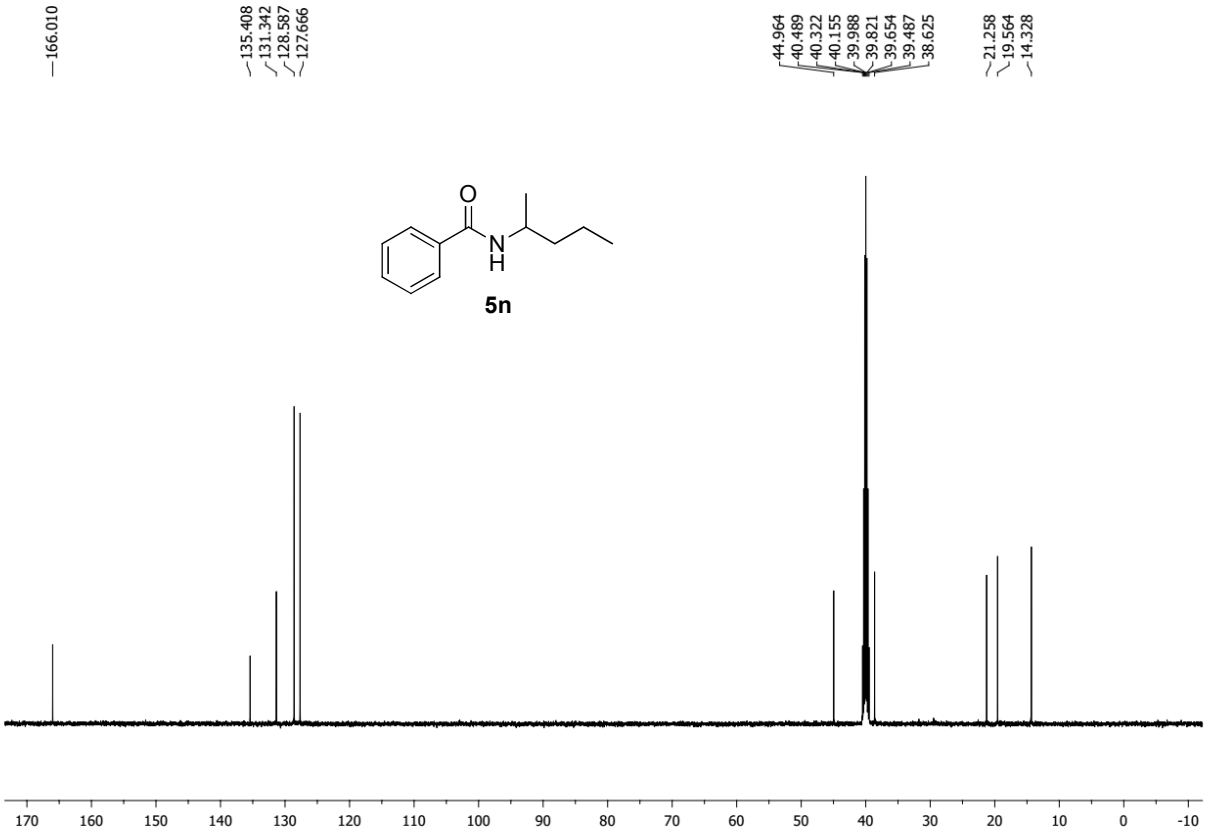
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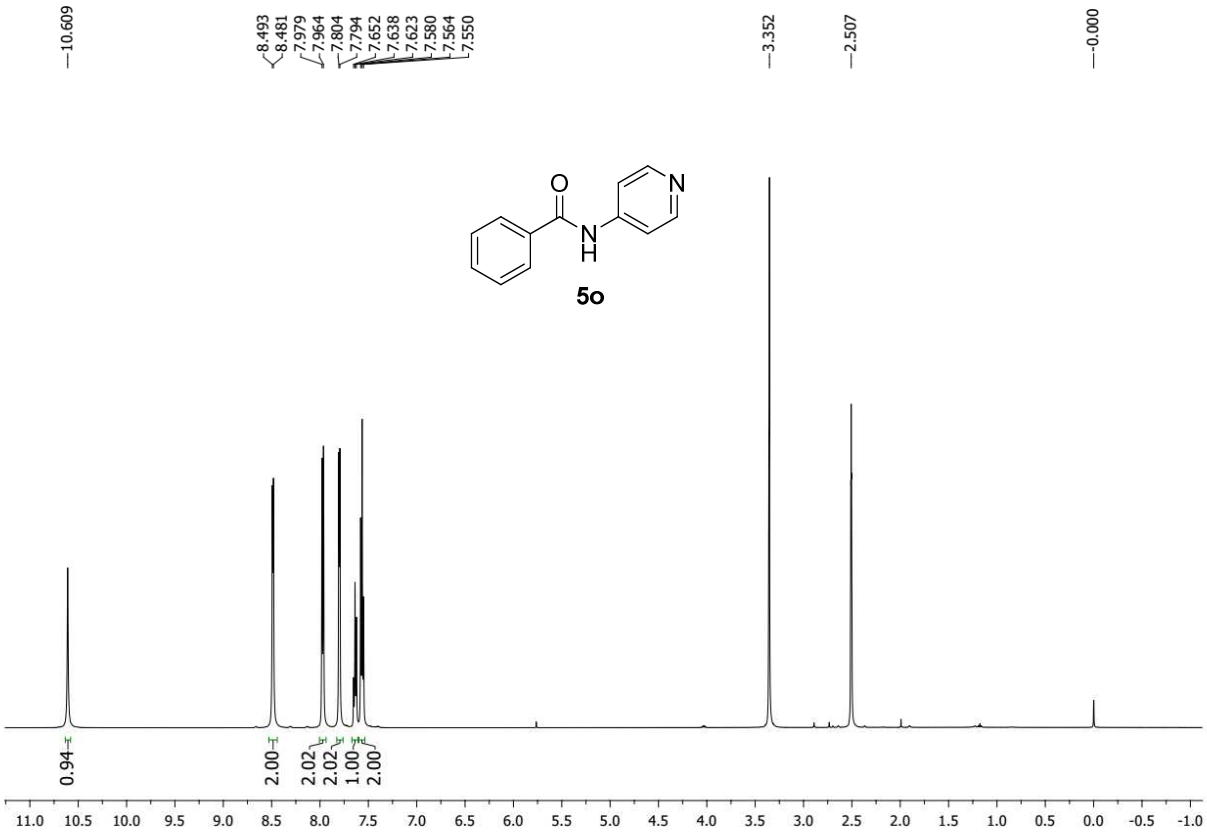
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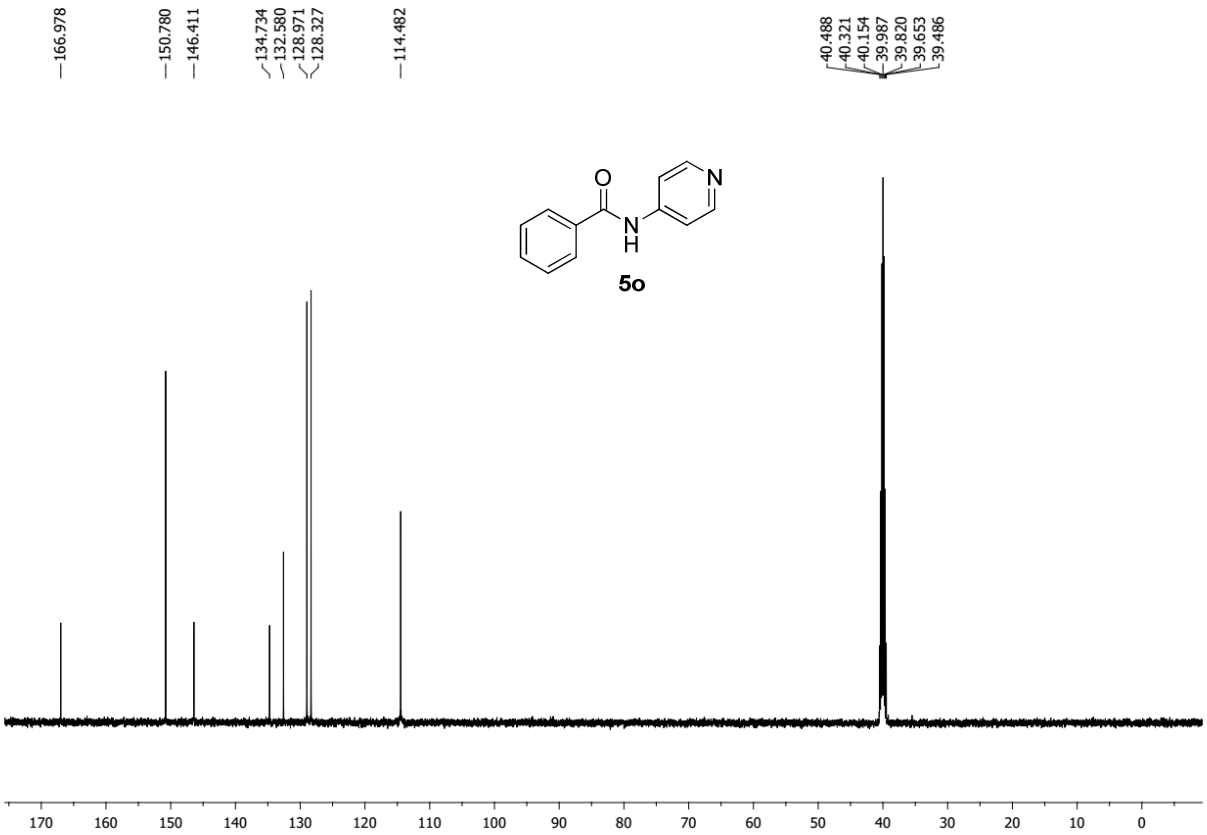
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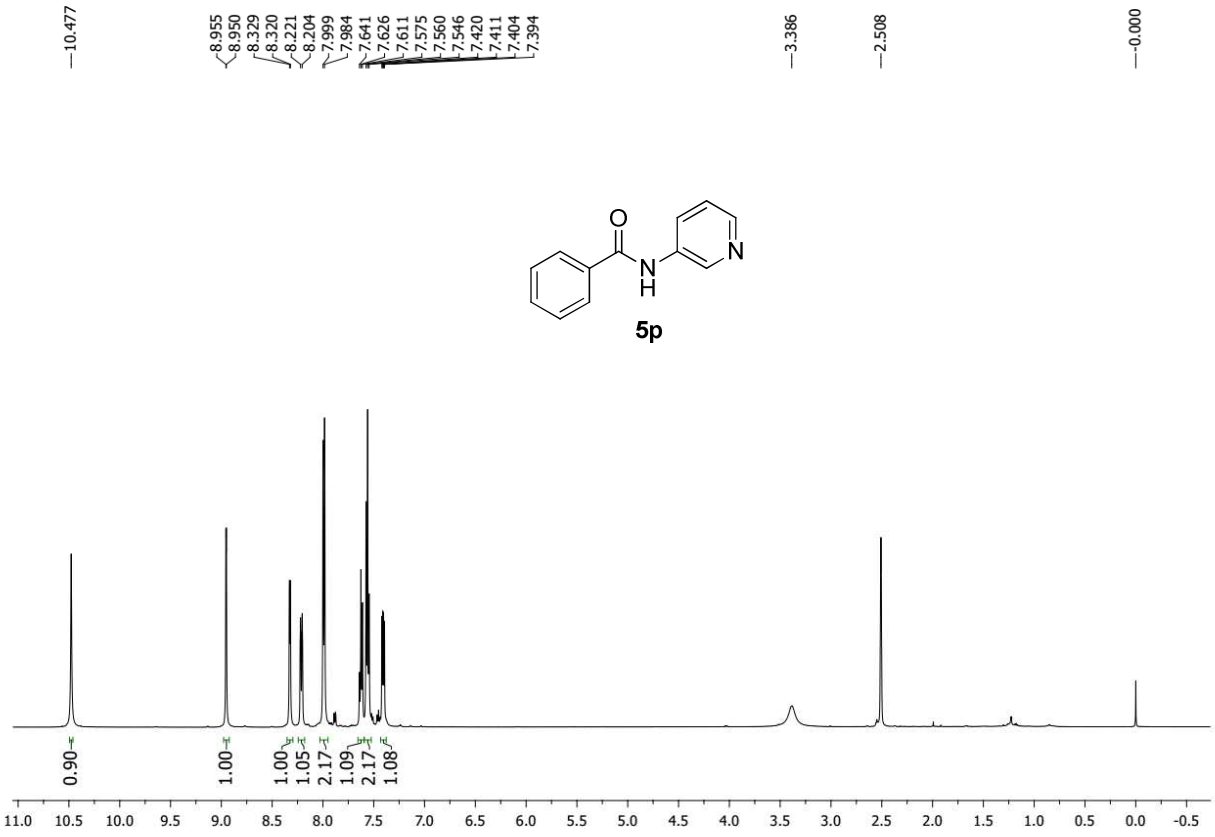
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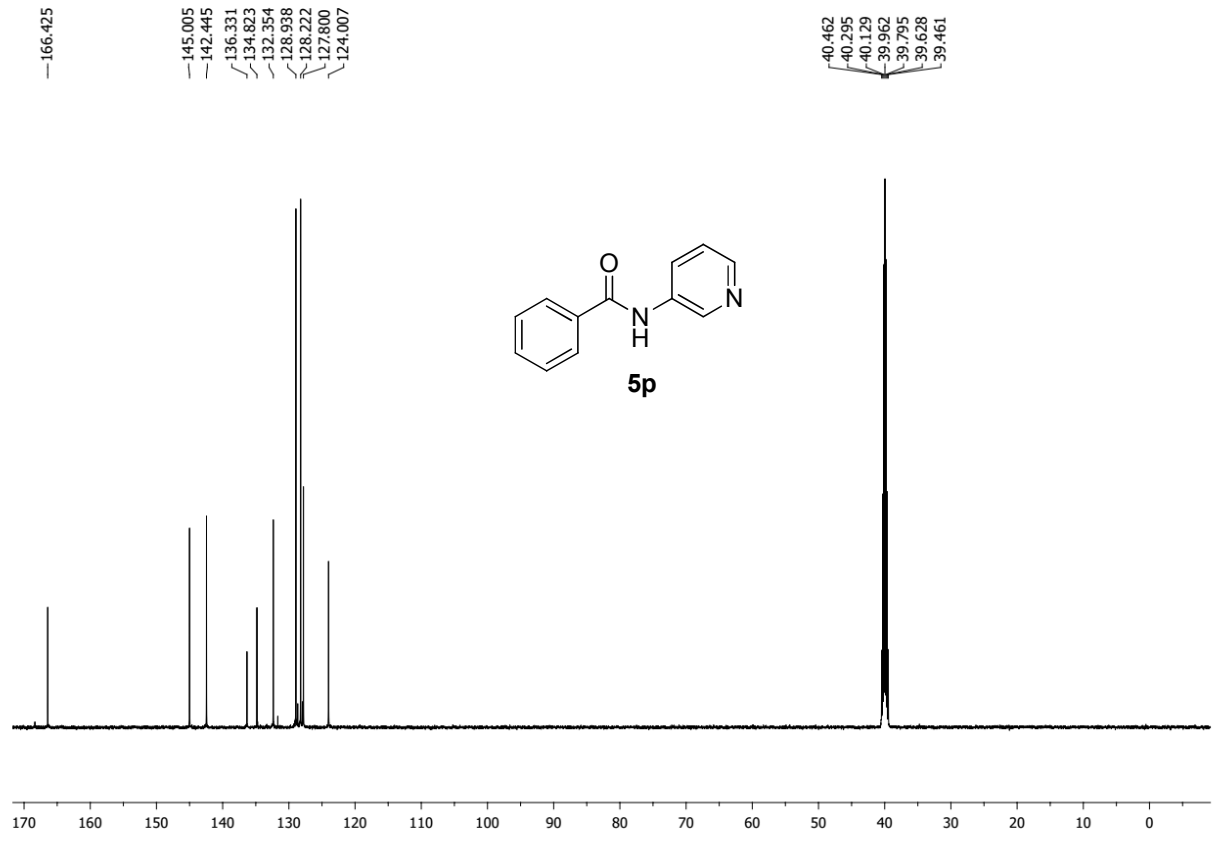
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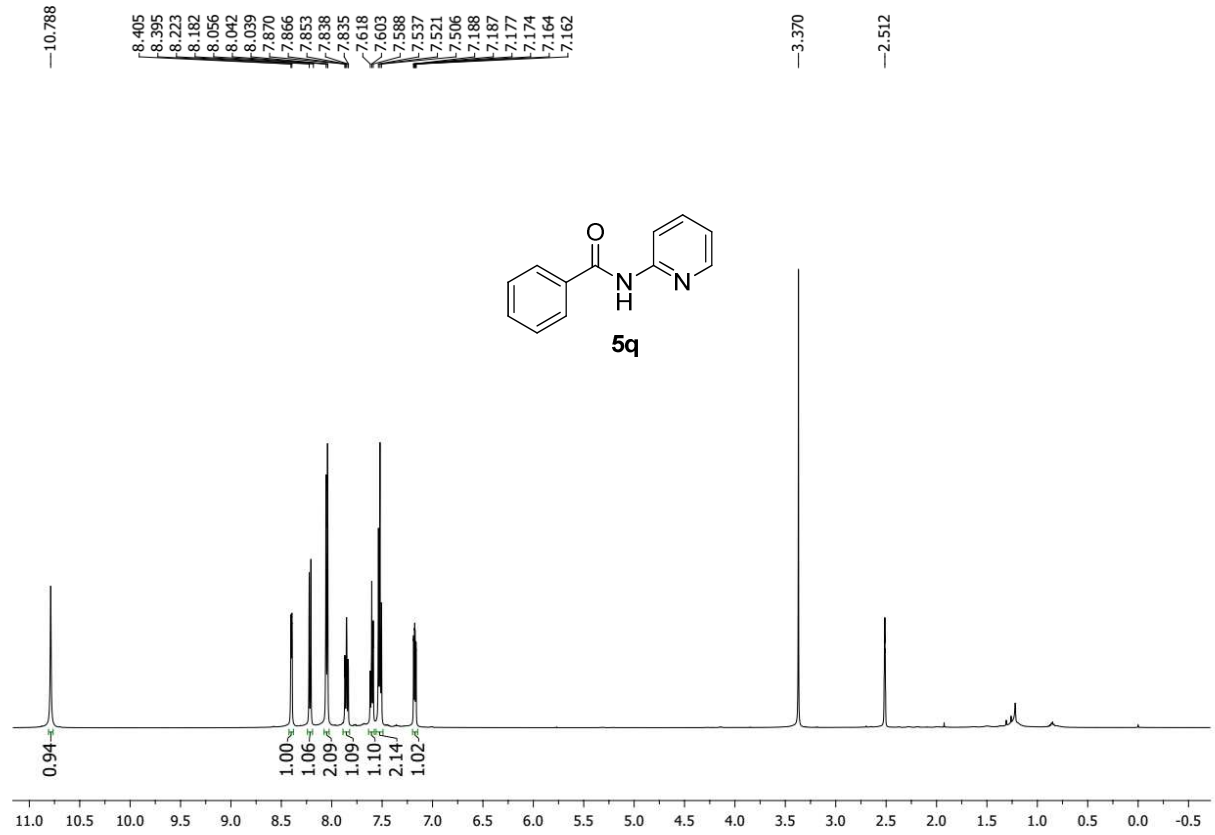
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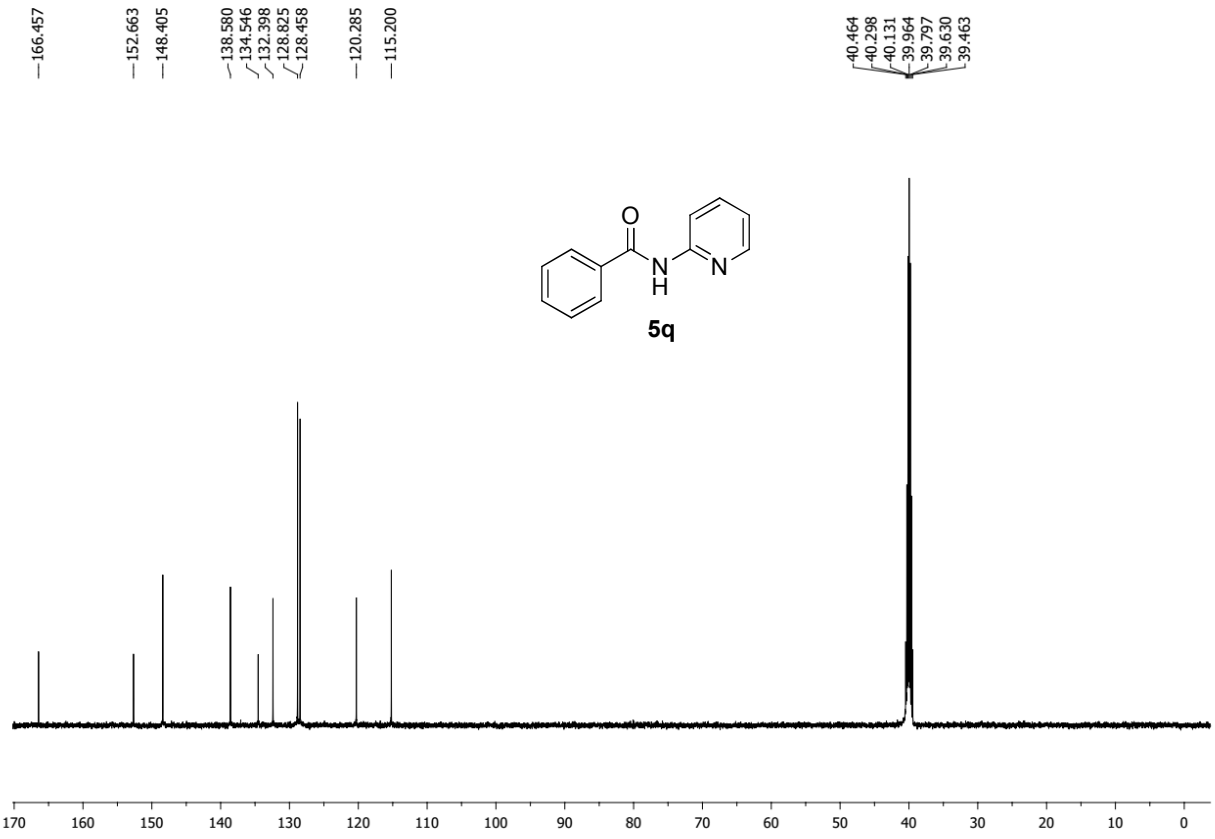
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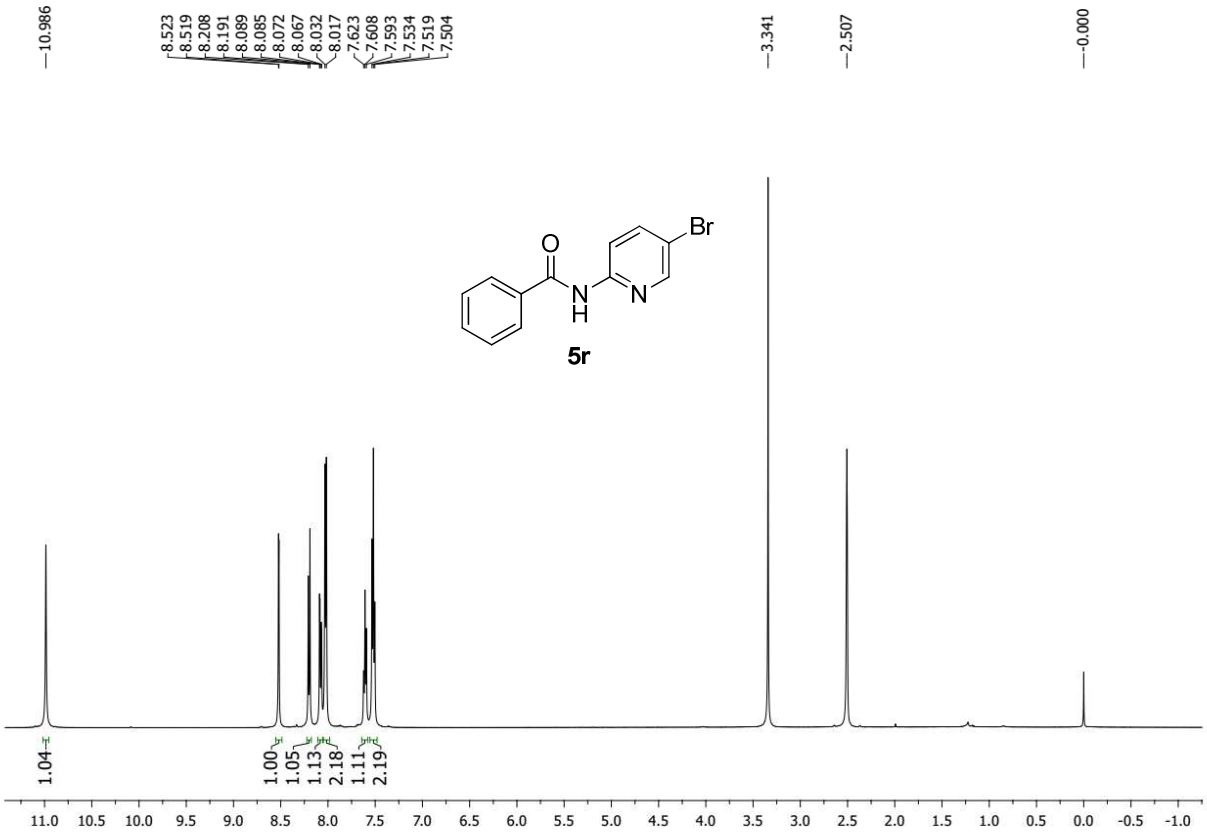
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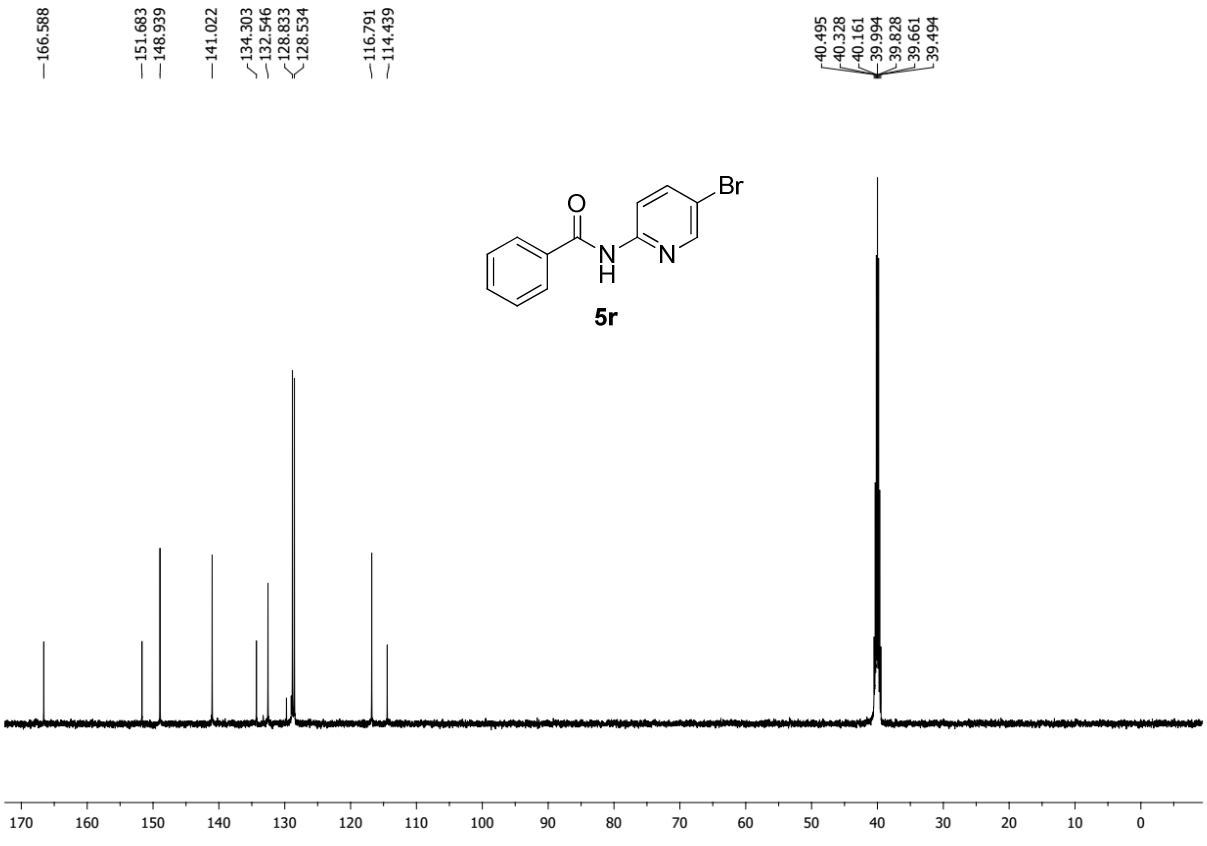
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H
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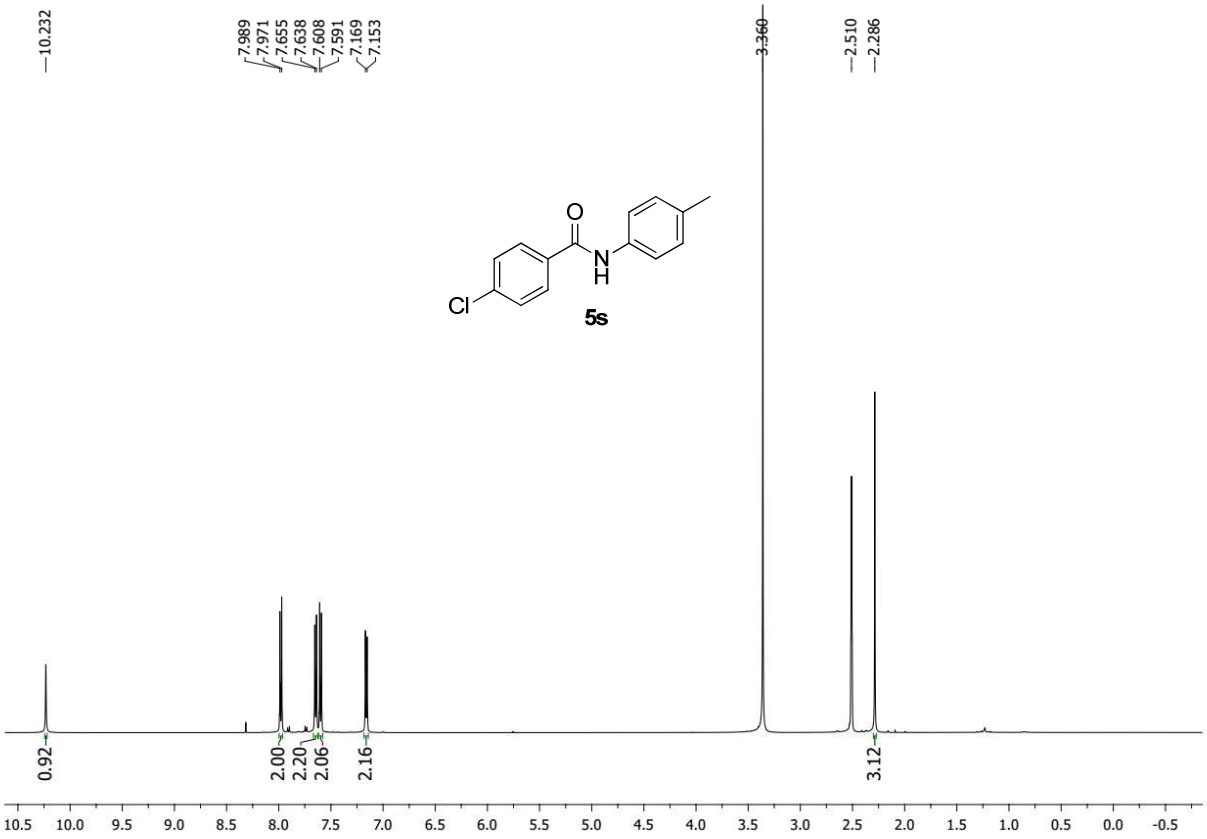
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H
Cl
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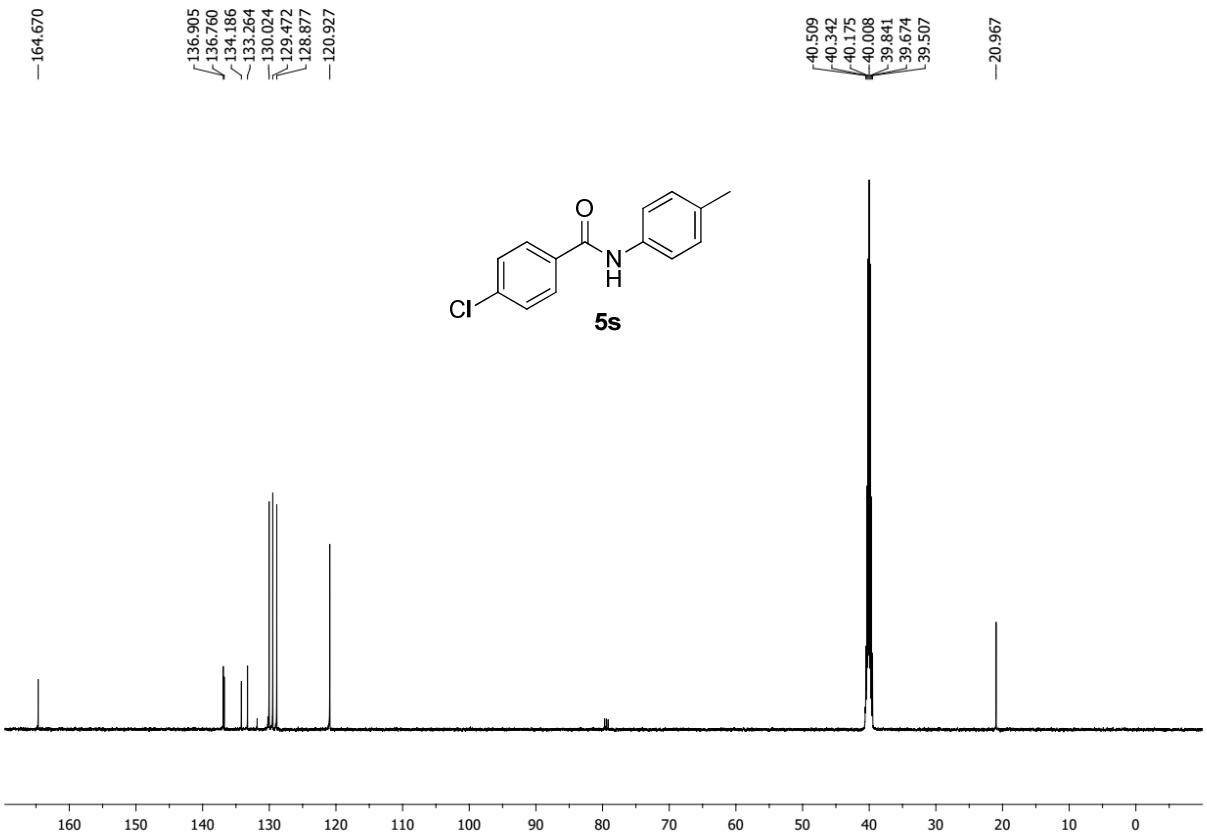
2.20
2.06
2.16
3.12
10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5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Cl
5s
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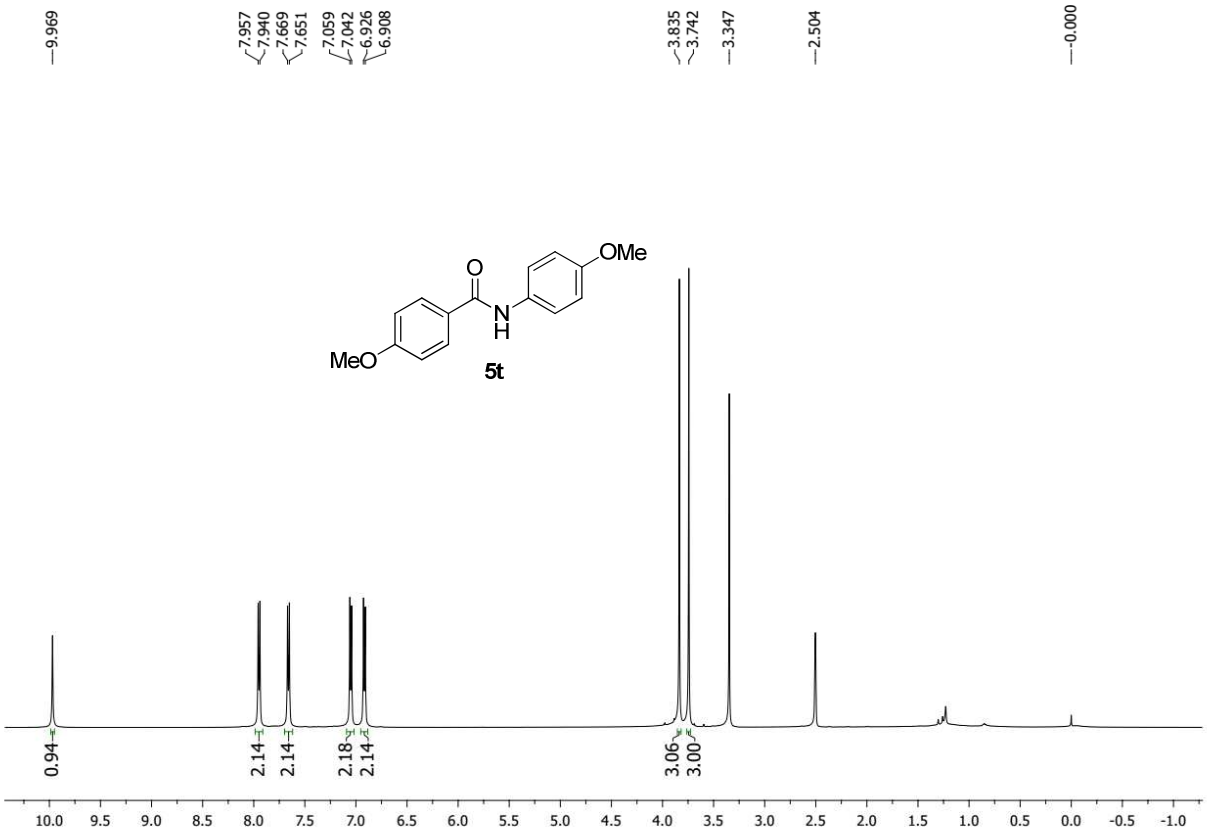
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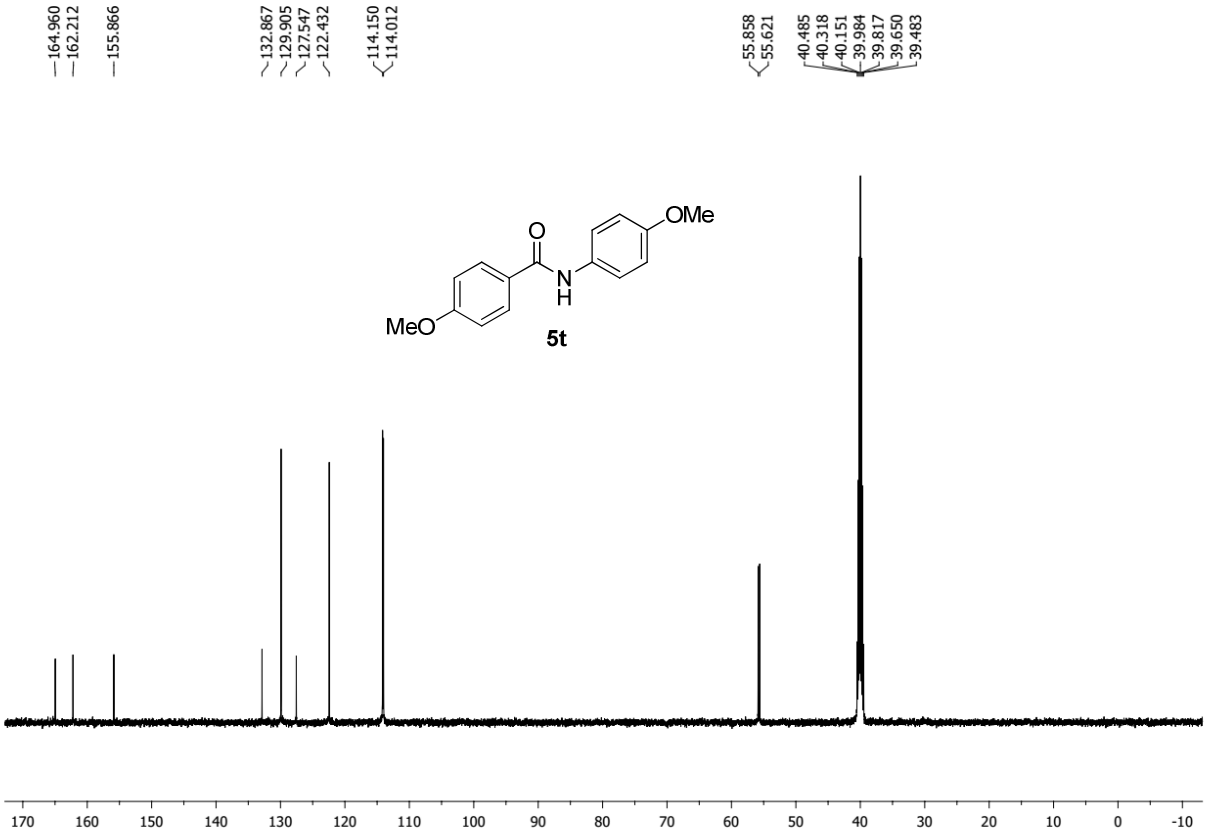
3.347
2.504
0.000
OMe
O
N
H
MeO
5t
0.94
2.14
2.14
2.18
2.14
3.06
3.00
10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5 -1.0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40.318
40.151
39.984
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N
H
MeO
5t
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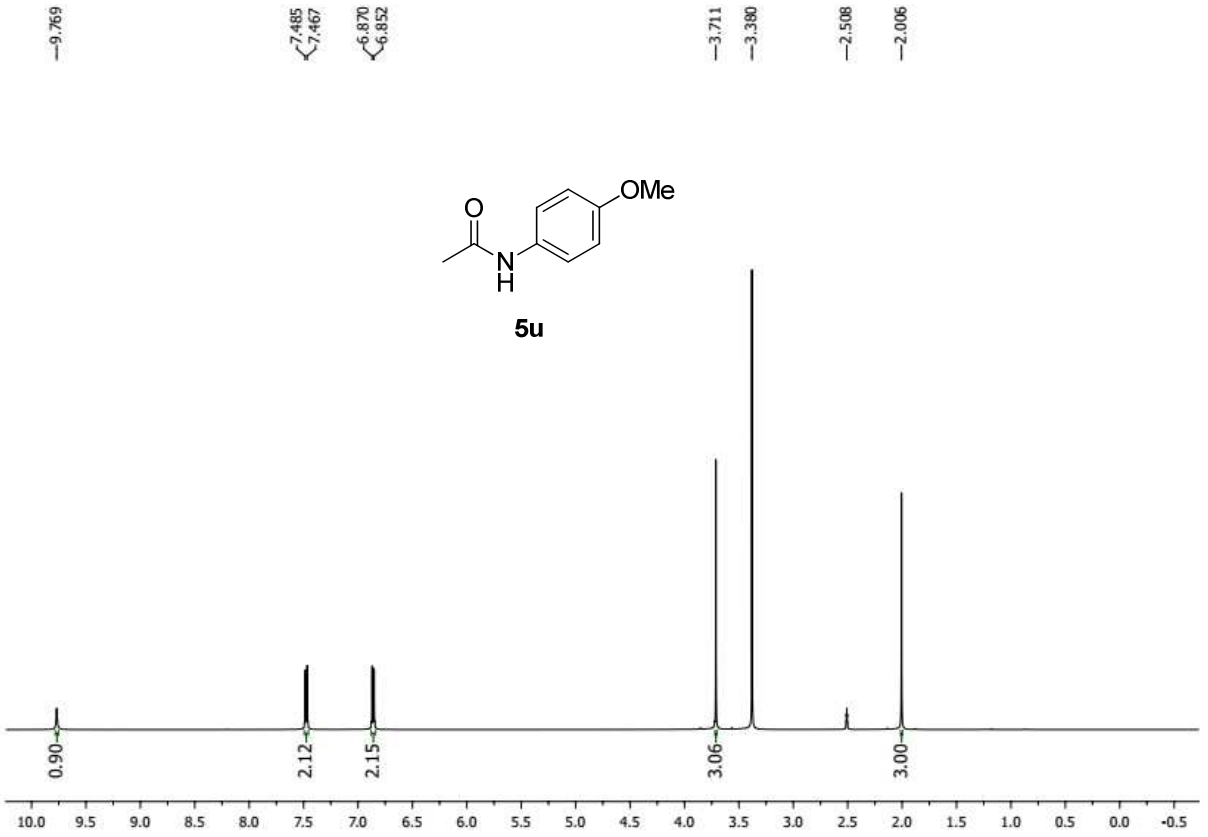
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H
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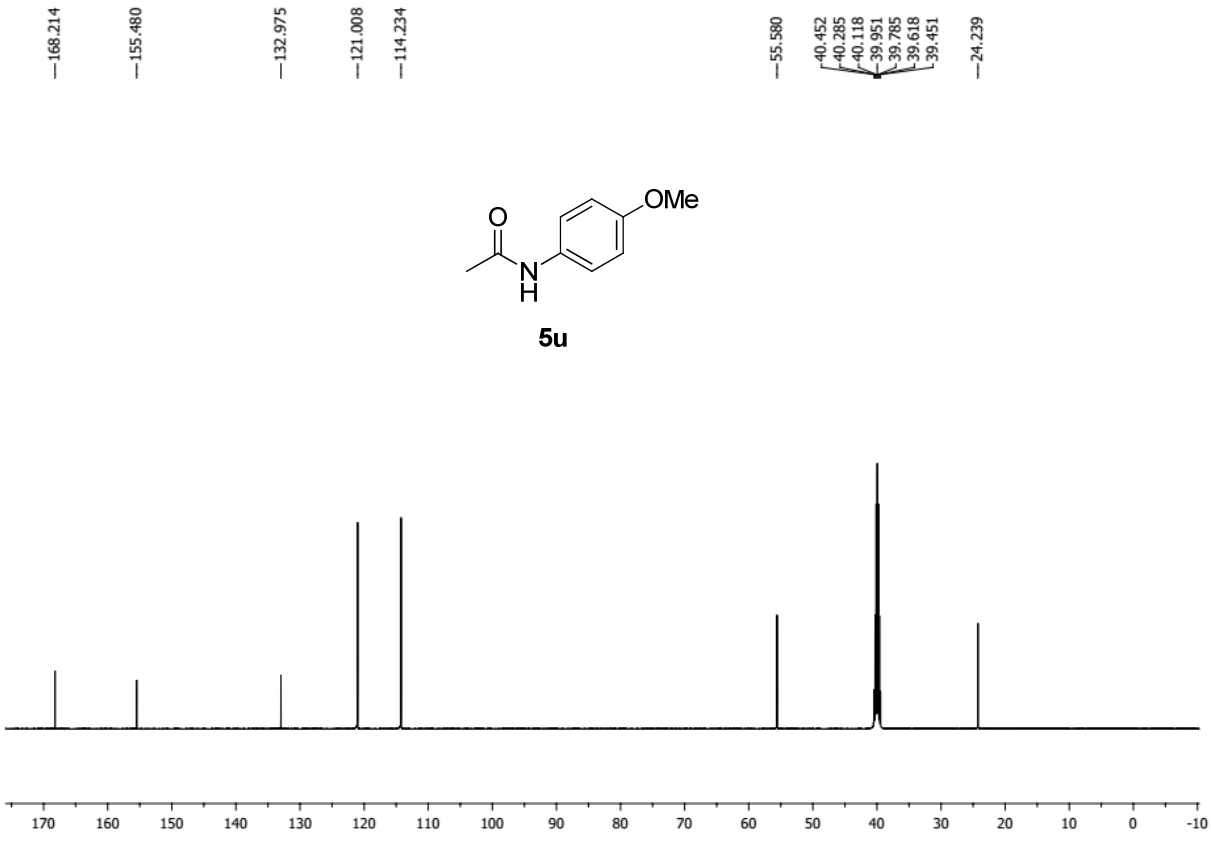
2.12
2.15
3.06
3.00
10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5

5u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O
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H
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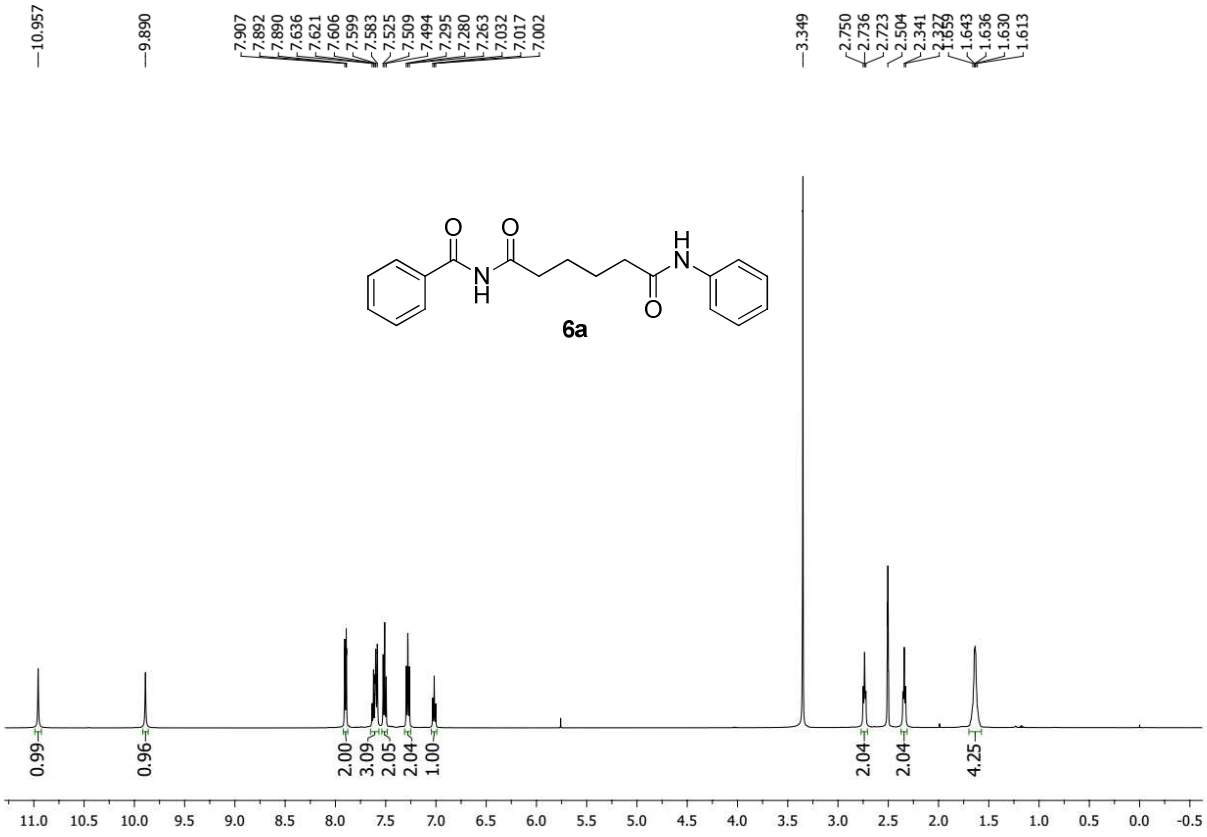
5u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7.509
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7.017
7.002
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2.723
2.504
2.341
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1.636
1.630
1.613
6a
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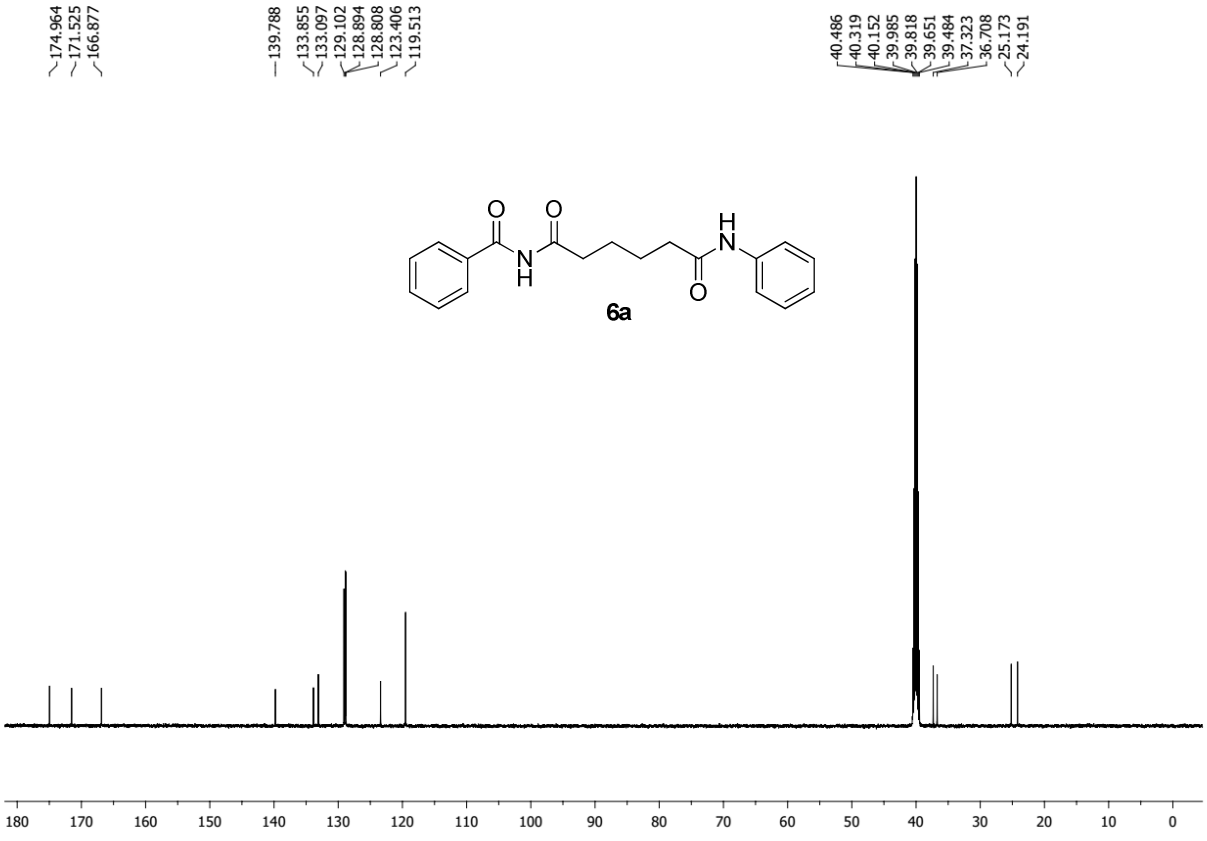
0.96
2.00
3.09
2.05
2.04
1.00
2.04
2.04
4.25
11.0 10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5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6a
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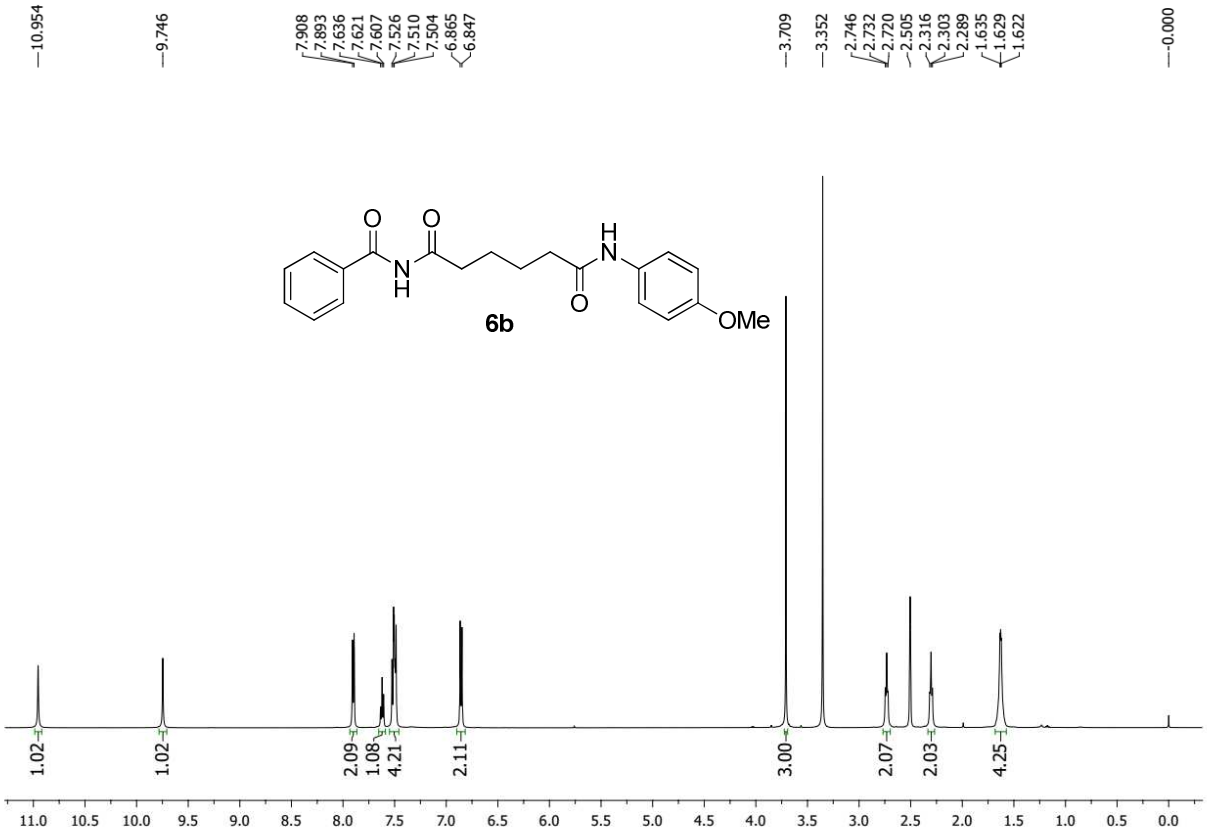
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7.504
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3.709
3.352
2.746
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2.720
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2.303
2.289
1.635
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1.02
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1.08
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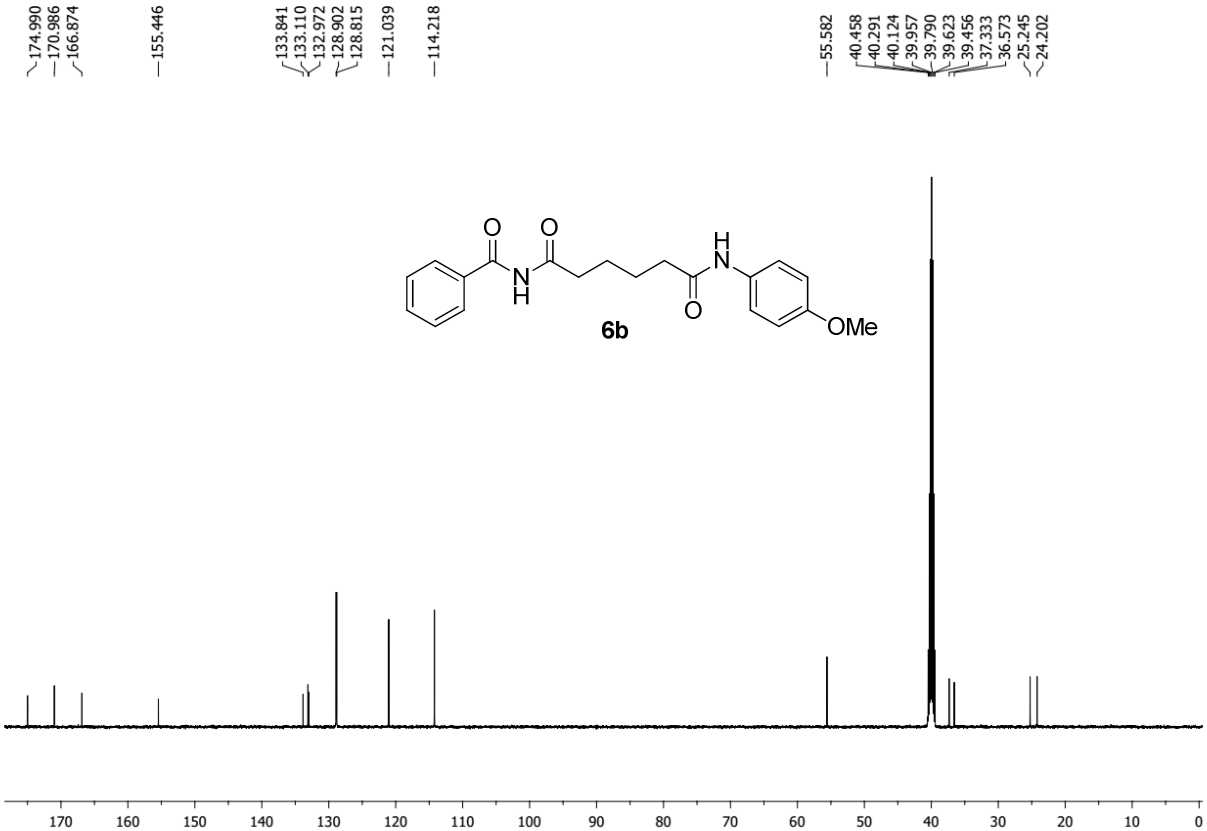
2.07
2.03
4.25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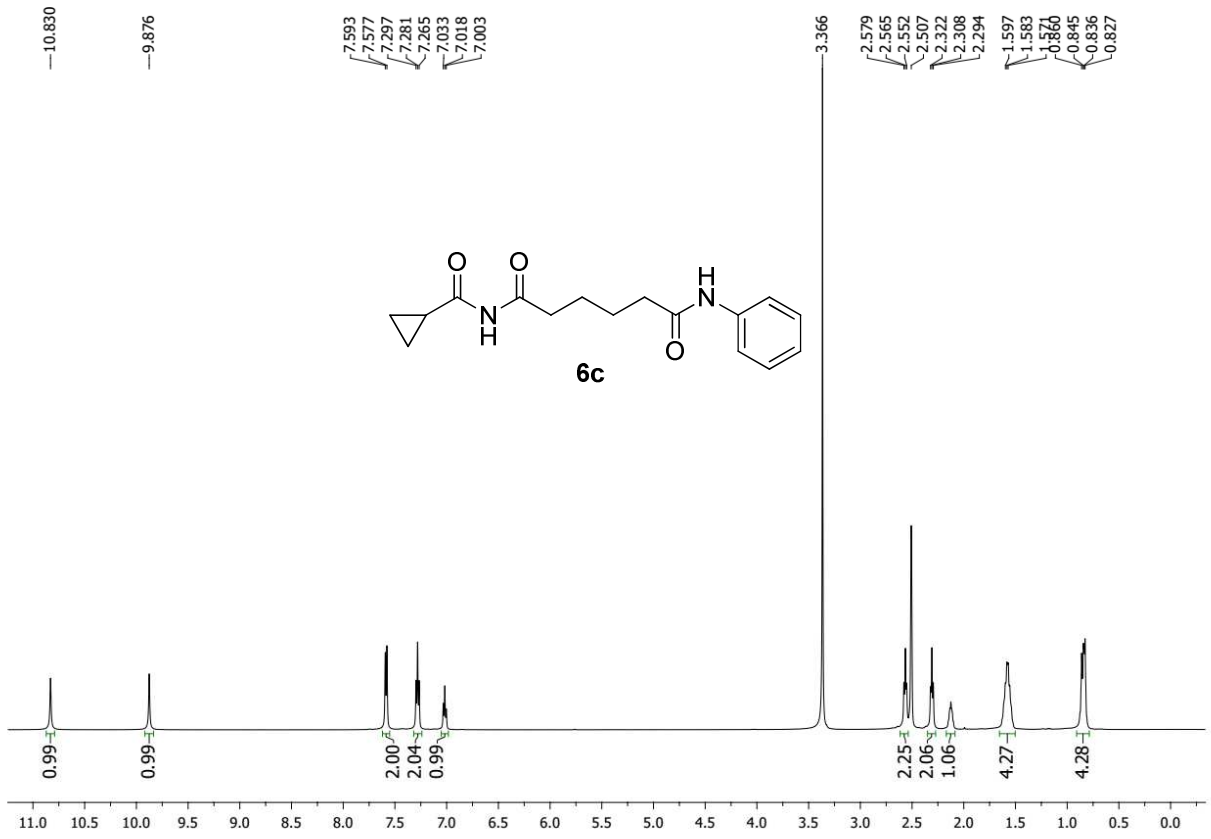
6b
OMe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0.836
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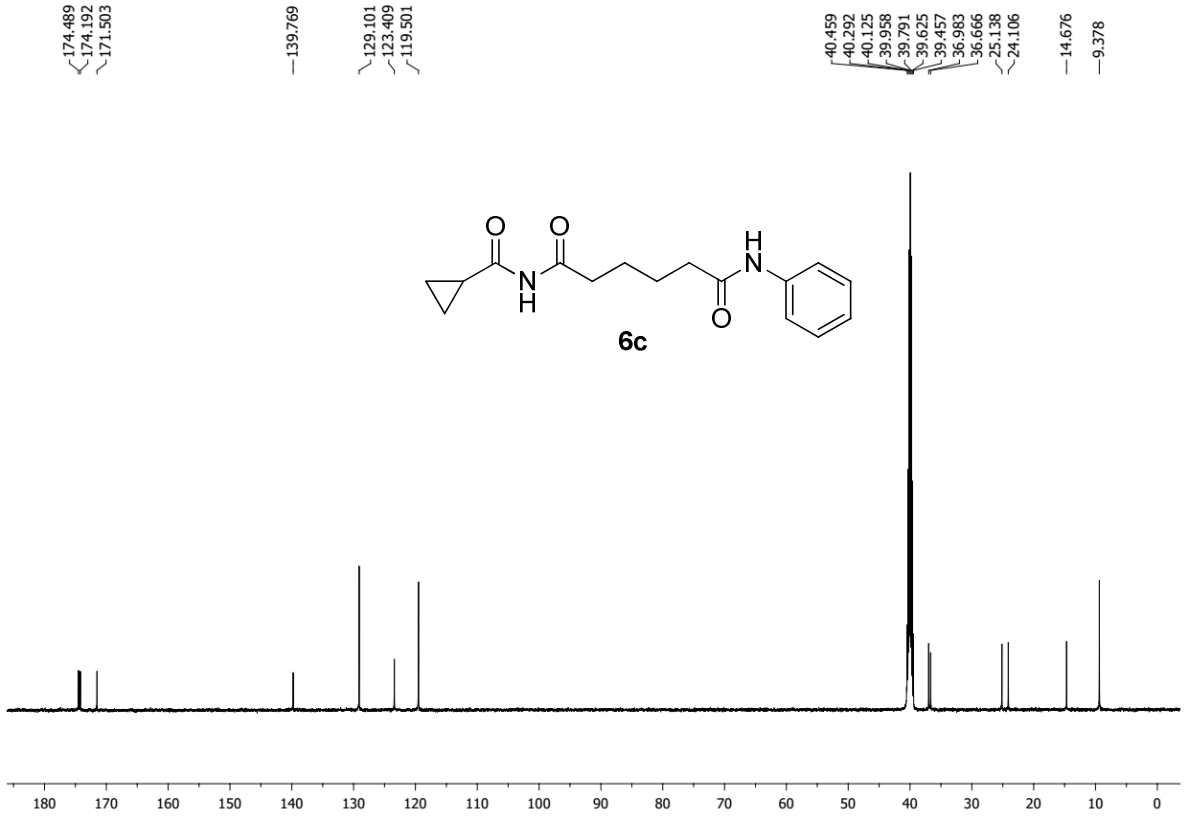
4.28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