A practical and sustainable protocol for direct amidation of unactivated esters under transition-metal-free and solvent-free conditions

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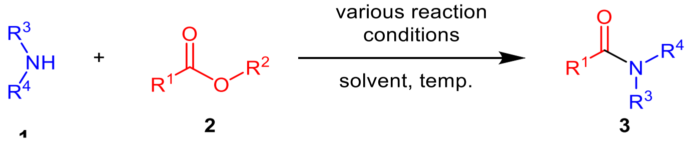
1. Comparison of representative reported methods with this work

Table S1 Comparison of representative reported methods with this work



Entry	Year	Group	Solvent	Catalyst/Reagent	Temp. (°C)	Time (h)	Yield (%)	Purification	E-factor
1[a]	2005	Porco[1]	toluene	$\mathrm{Zr(O}t\mathrm{Bu)_4}$ (10 mol%)	rt-100	2-48	75-99	Chromatography	2.2-3.2
2[a]	2011	Milstein[2]	toluene	Ruthenium-PNN complex (0.1 mol%)	reflux	18-36	52-99	Chromatography	5.7-9.9
3[a]	2014	Hong[3]	-	$\mathrm{[Cp^*IrCl_2]_2}$ (1.25 mol%)	115	24	29-99	Chromatography	2.5-11.3
4[a]	2014	Ohshima[4]	-	$\mathrm{La(OTf)_3}$ (0.05-5.0 mol%)	rt-70	24	79-99	Chromatography	0.3-0.7
5[a]	2015	Xiong[5]	toluene	Ru-MACHO (1 mol%)/ $\mathrm{KO}t\mathrm{Bu}$ (20 mol%)	reflux	48	55-94	Chromatography	6.3-10.2
6[a]	2015	Mecinović[6]	toluene	$\mathrm{ZrCp_2Cl_2}$ (10 mol%)	110	4-20	31-89	Chromatography	1.4-7.2
7[a]	2016	Shah[7]	THF	Cu–Mn (10% w/w)	80	0.5-8	50-97	Chromatography	16.4-30.6
8[a]	2016	Garg[8]	toluene	$\mathrm{Ni(cod)_2}$ (15 mol%)/ SIPr (30 mol%)	60	12	15-83	Chromatography	6.4-52.0
9[a]	2017	Hu[9]	NMP	$\mathrm{Ni(glyme)Cl_2}$ (7.5 mol%) /Phen (7.5 mol%)	90	16	41-87	Chromatography	13.3-23.0
10[a]	2018	Newman[10]	toluene	$\mathrm{Ni(cod)_2}$ (10 mol%) /IPr (20 mol%)	140	16	60-92	Chromatography	22.8-29.0
11[a]	2019	Newman[11]	toluene	$\mathrm{Ni(cod)_2}$ (10 mol%)/ NHC Ligands (10-20 mol%)	140	16	22-95	Chromatography	20.4-73.8
12[a]	2019	Zeng[12]	THF	$\mathrm{CrCl_3}$/dtbpy (10 mol%)	90	12	34-89	Chromatography	7.2-16.7

13[a]	2019	Ma[13]	DMAc	Mg (5.0 equiv.)/ TMSCl (1.0 equiv.)	120	16	41-90	Chromatography	12.5-26.4
14[a]	2021	Kobayashi[14]	diglyme	ZrO_2 (50 mg/mmol)	140	6-16	19-98	Chromatography	6.4-32.9
15[a]	2021	Niu[15]	toluene	Mn-complex (1 mol%)/ NaO*t*Bu (20 mol%)	120	18	44-96	Chromatography	7.5-12.9
16[b]	2007	Mioskowski[16]	-	TBD (30 mol%)	rt-75	12	60-94	Chromatography	0.9-2.2
17[b]	2009	Birman[17]	MeCN	1,2,4-triazole anion (10 mol%) DBU (10 mol%)	rt-95	10	62-98	Chromatography	1.0-2.0
18[b]	2009	Vaidyanathan[18]	2-Me-THF	DBU (50 mol%)	40	0.3-6.0	87-95	Chromatography	2.0-4.1
19[b]	2013	Jamieson[19]	MeCN	BEMP (10 mol%)	rt	15	40-100	Chromatography	0.4-6.5
20[b]	2015	Jamieson[20]	THF	CF_3CH_2OH (20 mol%) K_3PO_4 (1.0 equiv.)	90	22	41-95	Chromatography	2.6-8.6
21[b]	2017	Williams[21]	EtOAc	AcOH (10 mol%)	80	20	70-97	Chromatography	2.7-3.6
22[c]	2005	Movassaghi[22]	THF	IMes/LiCl (5 mol%)	23	1.5-24.0	31-100	Chromatography	4.7-17.3
23[c]	2015	Du[23]	toluene	IMes HCl (6 mol%)/ *t*BuOK (5 mol%)	60	14-42	51-87	Chromatography	13.3-20.9
24[d]	2011	Neto[24]	$[BMIM]NTf_2$	$BF_3 \bullet Et_2O$ or $SnCl_2$ or CdO in $[BMIM]NTf_2$	135	3-24	67-99	Chromatography	4.5-9.8
25[d]	2015	Wang[25]	-	$[PyPS]_3PW_{12}O_{40}$ (2 mol %)	70-140	0.17-1.0	51-97	Chromatography	1.0-1.8
26[e]	2005	Gupta[26]	THF/DMF	Zn	70	6-26	64-82	Chromatography	5.2-11.3
27[e]	2011	Verkade[27]	THF	Merrifield resin-supported $N_3@P(MeNCH_2CH_2)_3N$ (6.7 mol%)	rt	24-36	34-93	Chromatography	9.3-20.7
28[e]	2015	Shimizu[28]	-	Nb_2O_5	140	30	62-95	Chromatography	1.7-3.1
29[e]	2018	Yao[29]	-	Lanthanide–Sodium Alkoxides (0.5 mol%)	80	6	20-99	Chromatography	1.2-12.4

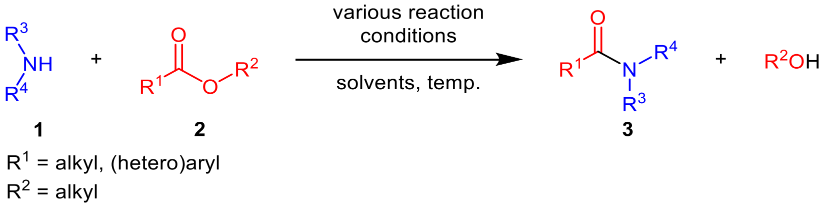
30[f]	2009	Quaedflieg[30]	THF/MTBE	Alcalase-CLEA	50	16	54-94	Extraction and trituration	21.7-49.1
31[f]	2012	Vadivel[31]	Hexane/DIPE	Immobilized *Candida antarctica*	45	2-24	41-98	Chromatography	12.8-31.6
32[f]	2017	Hernández[32]	-	Papain/Na_2CO_3•$10H_2O$ (Ball milling)	rt	2	33-98	Filtration and trituration	2.1-8.1
33[g]	1977	Weinreb[33]	DCM	Me_2AlNH_2	25-41	24-26	80-83	Recrystallization	67.5-96.6
34[g]	1992	Roskamp[34]	Hexane	$Sn[N(TMS)_2]_2$	rt	12	30-94	Chromatography	40.8-128.7
35[g]	1996	Yamamoto[35]	toluene	$Sb(OEt)_3$ (1.21 equiv.)	80	9	90	Chromatography	84.3
36[g]	1999	Varma[36]	-	KO*t*Bu	MW	0.75-7 min	55-91	Extraction and trituration	0.9-2.3
37[g]	1999	Maruoka[37]	THF	nBuLi	-78	1	80-98	Chromatography	5.9-6.7
38[g]	2001	Guo[38]	THF	MgX_2 (50-110 mol%)	rt	1-24	78-99	HPLC	20.0-24.3
39[g]	2003	Ranu[39]	-	InI_3 (20 mol%)	110-120	5.5-9.0	83-93	Recrystallization (ether/PE)	9..9-10.2
40[g]	2006	Woodward[40]	THF	DABAl-Me_3	40	19	69-99	Chromatography	43.4-76.6
41[g]	2008	Seeberger[41]	toluene/THF	$AlMe_3$	100-130	2-5 min	37-98	Chromatography	47.6-133.1
42[g]	2010	Woodward[42]	toluene	$Al_2Ph_3I_3$ (67 mol%)	80	3	56-98	Chromatography	29.0-51.0
43[g]	2011	Campbell[43]	THF	$Sm(HMDS)_3$ (1.0 equiv.)	0	16	78-99	Chromatography	16.8-21.2
44[g]	2012	Alcázar[44]	THF	*i*-PrMgCl•LiCl (3.0 equiv.)	rt	0.3	61-95	Chromatography	57.6-81.6
45[g]	2012	Ohshima[45]	toluene	NaOMe (5-10 mol%)	50	20-120	7-99	Chromatography	0.35-129.1

46[g]	2012	Yoon[46]	THF	KO*t*Bu	rt	0.17-1	53-94	Chromatography	52.3-63.4
47[g]	2013	Jamieson[47]	*i*-PrOH	K_3PO_4 (30 mol%)	60	22	42-100	Chromatography	2.9-8.8
48[g]	2019	Szostak[48]	toluene	LiHMDS	rt	15	70-98	Chromatography	22.6-48.8
49[g]	**This work**		**-**	**NaO*t*Bu (1.5 equiv.)**	**rt**	**1**	**70-99**	**Filtration and water washing**	**0.9-1.8**

[a] Transition-metal-based homogeneous catalysts. [b] Organocatalysts. [c] NHCs as catalysts. [d] Ionic liquids as catalysts. [e] Heterogeneous catalysts. [f] Enzymatic systems. [g] Metal salts or bases as promotors.

2. Green metrics of all the target compounds

Table S2 The calculated green metrics for compounds **3a-3ay**.



Ref.	No.	AE (%)	E-factor (kg/kg)	CE (%)	RME (%)	MI (kg/kg)	MP (%)
This work	**3a**	86.0	1.4	68.2	62.6	2.4	42.2
Szostak et al[48]	**3a**	86.0	30.6	79.7	74.1	31.6	3.2
Newman et al[10]	**3a**	86.0	28.3	69.4	64.6	29.3	3.4
This work	**3b**	86.8	1.3	70.5	64.8	2.3	44.3
Yoon et al[46]	**3b**	82.1	57.7	79.4	74.5	58.7	1.7
This work	**3c**	87.6	1.4	64.4	60.6	2.4	42.0
Szostak et al[48]	**3c**	87.6	25.9	81.9	76.8	26.9	3.7
Newman et al[10]	**3c**	87.6	25.6	66.7	62.5	26.6	3.8
This work	**3d**	88.7	1.0	75.3	69.8	2.0	49.6
This work	**3e**	87.0	1.5	61.0	57.5	2.5	39.5
This work	**3f**	87.8	1.4	62.6	60.3	2.4	42.0
Yoon et al[46]	**3f**	83.4	55.7	74.5	71.6	56.7	1.8
This work	**3g**	89.5	1.3	58.7	59.3	2.3	42.9
This work	**3h**	89.7	1.1	67.1	67.1	2.1	48.7
This work	**3i**	89.2	0.9	73.1	71.9	1.9	51.5
Szostak et al[48]	**3i**	89.2	22.7	80.2	75.6	23.7	4.2
This work	**3j**	87.4	1.1	72.6	67.8	2.1	46.9
This work	**3k**	86.8	1.4	65.0	59.7	2.4	40.8
This work	**3l**	86.8	1.2	71.6	65.7	2.2	44.9
Newman et al[10]	**3l**	86.8	26.8	68.3	63.9	27.8	3.6
This work	**3m**	90.0	0.9	73.6	73.9	1.9	54.0
This work	**3n**	90.0	0.9	71.2	71.5	1.9	52.2
This work	**3o**	89.5	1.3	64.2	59.3	2.3	42.8
Szostak et al[48]	**3o**	89.5	22.6	78.0	74.1	23.6	4.2
Newman et al[10]	**3o**	89.5	28.1	50.9	48.4	29.1	3.4
This work	**3p**	90.0	0.9	77.8	72.9	1.9	53.2
This work	**3q**	90.0	1.0	71.6	67.1	2.0	48.9
This work	**3r**	88.6	1.6	57.2	53.5	2.6	37.8
Szostak et al[48]	**3r**	88.6	22.6	78.0	74.1	23.6	4.2
This work	**3s**	86.1	1.6	59.7	56.1	2.6	37.8
This work	**3t**	86.1	1.6	59.7	56.1	2.6	37.8
This work	**3u**	86.1	2.0	51.7	49.9	3.0	33.7

This work	**3v**	86.8	1.3	68.3	62.7	2.3	42.9
Newman et al[10]	**3v**	86.8	29.0	63.3	59.1	30.0	3.3
Yoon et al[46]	**3v**	82.1	63.4	72.3	67.9	64.4	1.6
This work	**3w**	87.5	1.1	73.6	67.9	2.1	47.0
Newman et al[10]	**3w**	87.5	22.8	75.2	70.5	23.8	4.2
Yoon et al[46]	**3w**	83.0	52.3	82.8	77.9	53.3	1.9
This work	**3x**	86.2	1.8	56.5	53.4	2.8	36.1
This work	**3y**	86.5	1.1	73.8	68.5	2.1	46.6
Newman et al[10]	**3y**	86.5	23.4	80.3	74.8	24.4	4.1
This work	**3z**	89.2	1.7	51.7	50.8	2.7	36.4
This work	**3aa**	90.5	1.4	58.8	57.2	2.4	42.2
This work	**3ab**	88.8	1.7	54.8	52.4	2.7	37.3
This work	**3ac**	88.2	3.6	33.0	31.0	4.6	21.8
This work	**3ad**	85.5	1.5	65.6	60.8	2.5	40.6
This work	**3ae**	85.6	1.4	64.6	61.7	2.4	41.3
This work	**3af**	87.5	1.5	61.5	56.8	2.5	39.3
This work	**3ag**	86.8	7.6	18.4	17.0	8.6	11.6
This work	**3ah**	87.5	2.8	41.3	38.1	3.8	26.4
This work	**3aj**	86.8	1.3	69.8	64.4	2.3	44.4
Szostak et al[48]	**3aj**	86.8	28.8	80.2	74.9	29.8	3.4
This work	**3ak**	87.6	1.8	54.5	50.3	2.8	35.4
Szostak et al[48]	**3ak**	87.6	35.8	60.5	57.2	36.8	2.7
This work	**3al**	89.2	1.1	71.3	65.8	2.1	48.4
Szostak et al[48]	**3al**	89.2	25.6	72.1	70.0	26.6	3.8
This work	**3am**	89.6	1.7	55.0	50.4	2.7	37.4
This work	**3an**	86.8	1.4	66.0	60.9	2.4	41.9
This work	**3ao**	86.8	2.0	52.3	48.2	3.0	33.2
Szostak et al[48]	**3ao**	86.8	29.4	78.6	73.4	30.4	3.3
This work	**3ap**	86.1	1.3	71.8	65.4	2.3	44.1
This work	**3aq**	86.1	1.5	66.2	59.8	2.5	40.4
This work	**3ar**	85.4	1.4	69.7	63.0	2.4	41.7
This work	**3as**	83.4	2.3	53.7	48.0	3.3	30.1
This work	**3at**	86.4	1.8	57.9	53.1	2.8	36.1
Szostak et al[48]	**3at**	86.4	30.8	77.1	72.1	31.8	3.1
This work	**3au**	74.6	1.7	66.6	59.9	2.7	46.0
Szostak et al[48]	**3au**	74.6	48.8	61.3	58.1	49.8	2.0
This work	**3av**	88.5	1.2	68.5	63.8	2.2	46.0
Szostak et al[48]	**3av**	88.5	27.0	74.7	70.5	28.0	3.6
This work	**3aw**	89.3	1.0	71.6	68.9	2.0	50.1
This work	**3ax**	91.0	1.3	61.5	56.5	2.3	43.6
This work	**3ay**	86.3	2.0	54.6	49.8	3.0	33.7

3. Yield-time relationship with different amounts of methyl benzoate (2a)

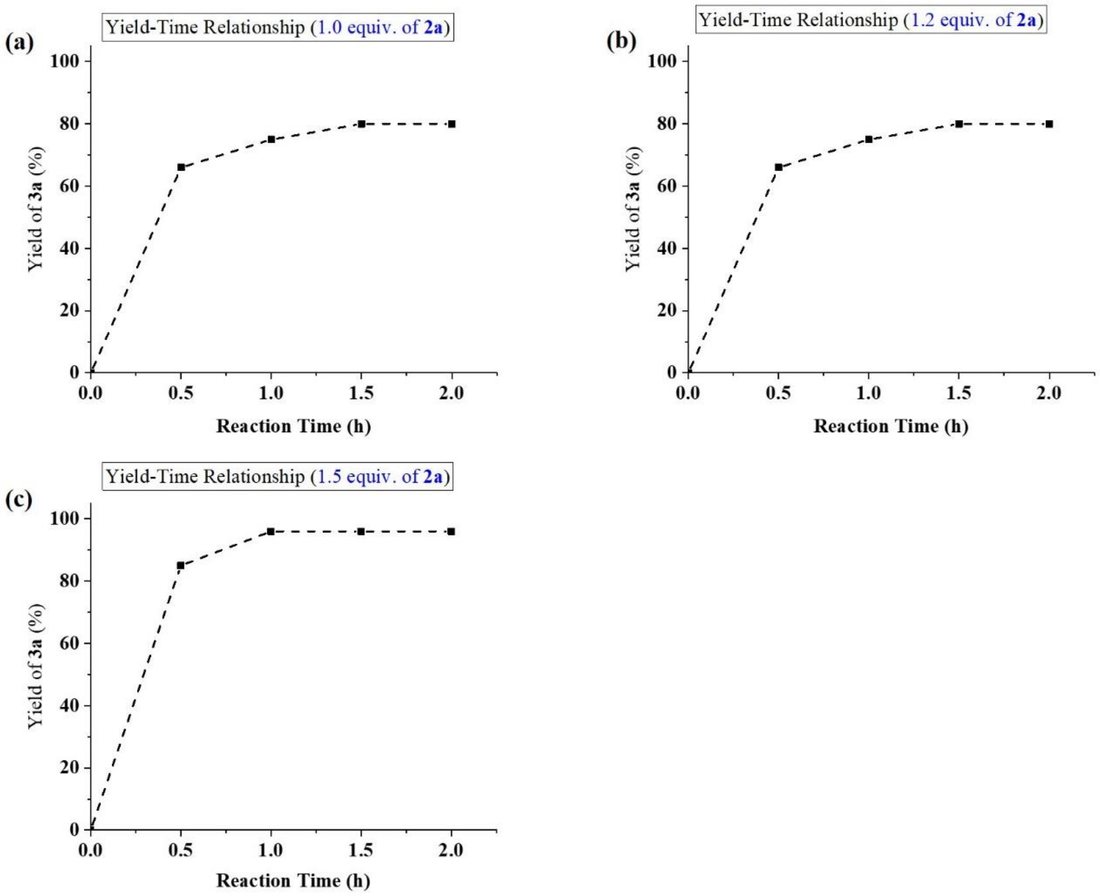


Fig. S1 Yield-time relationship of **3a** with different amounts of **2a**: (a) 1.0 equiv.; (b) 1.2 equiv.; and (c) 1.5 equiv.

4. Supplementary results for computational calculation

Cartesian coordinates of the structures

%nprocs=20

%mem=20GB

# opt b3lyp/genecp freq

Intermediate **2’**

C	-1.98129000	-0.27449900	-0.09328900
C	-1.10735900	-1.48308800	-0.16152800
O	-0.42019600	-1.89521300	0.92177900
O	-0.94905900	-2.13732000	-1.18607400
C	-0.26410200	-1.08279200	2.11547700
C	-1.39179700	0.99059300	0.04968900
C	-2.20547800	2.12395000	0.02681100
C	-3.58866300	1.99907000	-0.12575700
C	-4.16688700	0.73598600	-0.27659300
C	-3.36362000	-0.40420100	-0.27525300
H	-0.00276900	-1.78866300	2.90532400
H	-1.19682300	-0.57199400	2.36057400
H	0.55320000	-0.38568700	1.90593800
H	-0.30627000	1.05334300	0.13666700
H	-1.75485700	3.10788600	0.12401200
H	-4.21643300	2.88615500	-0.13615200
H	-5.24131200	0.63865000	-0.40504400
H	-3.80340500	-1.38799300	-0.41275500
Na	1.39180700	-1.97838700	-0.76968700
C	3.97127900	0.07714700	-0.86292200
C	2.83415600	0.78312800	-0.07266200
C	2.45089000	2.07811800	-0.83300000
O	1.73916700	-0.05225700	0.05264000
C	3.38129100	1.16729400	1.32539000
H	3.61351400	-0.19160700	-1.86864900
H	4.26885400	-0.84451200	-0.34058400
H	4.87211700	0.69365500	-0.98735700
H	1.67798000	2.62257200	-0.27618600
H	2.03647700	1.82172600	-1.81621300
H	3.30207800	2.75680600	-0.98224400
H	3.66030200	0.25973500	1.87600800
H	2.59867100	1.67940300	1.89871600
H	4.25899100	1.82685700	1.27956900

C H O 0

6-31g(d)

****

Na 0
Lanl2dz
****

Na 0
Lanl2dz

Intermediate **4**

C	-4.08350200	-0.44442700	-0.37195100
C	-4.03351500	0.94998100	-0.21875800
C	-2.78150100	1.55040000	-0.08241500
C	-1.61065100	0.78868900	-0.06754400
C	-1.63760400	-0.64070900	-0.18245900
C	-2.93200700	-1.21885600	-0.35900100
N	-0.47827700	-1.35457400	-0.06090600
H	1.03420100	-0.65459200	0.04201700
H	-0.64452000	-2.34463000	-0.23428100
H	-5.04601900	-0.93561500	-0.50520300
H	-4.94157700	1.54523200	-0.23186500
H	-2.70494900	2.63422900	-0.00890400
H	-0.64229700	1.29209700	-0.08343200
H	-3.00370800	-2.29941400	-0.47666800
Na	-0.00068500	-0.15972000	1.90810100
C	3.57701700	-1.21294400	-0.58324400
C	2.91461100	0.13423400	-0.24921800
C	2.50949200	0.87138900	-1.53638100
O	1.74824100	-0.10350900	0.54579600
C	3.85077500	1.00018500	0.60012700
H	2.89158300	-1.84280700	-1.16205000
H	3.83602200	-1.74740100	0.33773900
H	4.49165400	-1.07512400	-1.17226500
H	2.03617100	1.82967600	-1.29454800
H	1.79141300	0.27372600	-2.10903900
H	3.37905600	1.06769300	-2.17496300
H	4.11690100	0.47983400	1.52768600
H	3.36179900	1.94550700	0.86289900
H	4.77513200	1.23095100	0.05880200

C H O N 0
6-31g(d)
****
Na 0
Lanl2dz

****

Na 0
Lanl2dz

The frequency of intermediate **2’**

mode#	frequency
1	4.92
2	33.23
3	42.17
4	56.22
5	66.57
6	81.95
7	93.68
8	127.41
9	133.00
10	198.69
11	208.26
12	230.03
13	237.55
14	244.44
15	283.13
16	285.31
17	290.01
18	298.96
19	339.39
20	365.83
21	373.12
22	415.68
23	422.67
24	443.05
25	478.07
26	509.38
27	583.71
28	629.12
29	635.14
30	717.76
31	740.16
32	744.20
33	760.40
34	798.30
35	870.21
36	878.72
37	879.14
38	946.31
39	949.71
40	992.95
41	1012.18
42	1018.32

43	1024.12
44	1041.85
45	1044.25
46	1054.53
47	1063.60
48	1114.57
49	1135.62
50	1195.46
51	1198.69
52	1220.81
53	1223.28
54	1236.81
55	1240.55
56	1255.44
57	1320.96
58	1343.28
59	1381.91
60	1394.06
61	1402.99
62	1426.33
63	1477.45
64	1492.44
65	1502.85
66	1509.04
67	1510.58
68	1512.93
69	1522.92
70	1526.72
71	1537.71
72	1543.73
73	1556.73
74	1635.65
75	1662.24
76	1756.93
77	2997.12
78	3018.74
79	3027.35
80	3055.45
81	3061.13
82	3073.12
83	3083.22
84	3092.43
85	3095.32
86	3099.49

87	3144.35
88	3164.62
89	3178.24
90	3187.40
91	3197.29
92	3206.27
93	3214.59

The frequency of intermediate **4**

mode#	frequency
1	18.86
2	25.40
3	42.20
4	65.69
5	84.83
6	118.99
7	160.03
8	209.79
9	219.02
10	229.44
11	269.80
12	277.78
13	305.44
14	339.26
15	352.45
16	428.21
17	433.29
18	464.17
19	473.48
20	513.67
21	527.31
22	543.92
23	633.35
24	644.54
25	716.75
26	751.49
27	757.90
28	823.23
29	832.57
30	849.94
31	916.18
32	928.11
33	946.07
34	965.23

35	967.38
36	970.44
37	992.66
38	1042.68
39	1051.18
40	1057.88
41	1064.40
42	1099.83
43	1182.02
44	1205.44
45	1212.40
46	1252.57
47	1268.68
48	1270.33
49	1342.74
50	1363.66
51	1372.56
52	1421.94
53	1424.68
54	1448.67
55	1495.46
56	1504.25
57	1513.80
58	1515.34
59	1516.93
60	1527.83
61	1529.87
62	1544.55
63	1559.26
64	1602.31
65	1657.85
66	2630.75
67	3042.40
68	3043.37
69	3051.93
70	3110.28
71	3112.60
72	3114.33
73	3118.36
74	3122.35
75	3123.66
76	3132.47
77	3152.22
78	3166.48

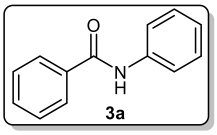
79	3173.68
80	3205.00
81	3491.67

Table S3 The ΔG values for the transformation of **1** to **4** and **2** to **2’**

A	B	C	ΔG (eV) = = (Col(C)-Col(B)-Col(A))*27.2
NaO*t*Bu	**2**	**2’**	
-233.18959	-460.01908	-693.20156	0.19323
NaO*t*Bu	**1**	**4**	
-233.18959	-287.51352	-520.70664	-0.0961

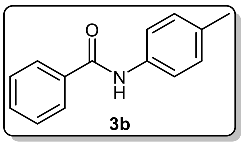
5. Characterization data for compounds 3a-3ay

N-Phenylbenzamide (3a)[41]


3a

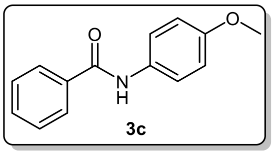
White solid, 96% yield, m.p. 162.2-163.5°C. ^{1}H-NMR (500 MHz, $CDCl_3$) δ 7.92 – 7.81 (m, 3H), 7.65 (d, *J* = 8.0 Hz, 2H), 7.55 (t, *J* = 7.4 Hz, 1H), 7.48 (t, *J* = 7.6 Hz, 2H), 7.37 (t, *J* = 7.8 Hz, 2H), 7.16 (t, *J* = 7.4 Hz, 1H). ^{13}C-NMR (126 MHz, $CDCl_3$) δ 165.8, 137.9, 135.0, 131.9, 129.1, 128.8, 127.0, 124.6, 120.2. HRMS (APCI): *m*/*z* $[M+H]^+$ calcd. for $C_{13}H_{12}NO^+$: 198.09134; found: 198.09088.

N-(*p*-Tolyl)benzamide (3b)[48]


3b

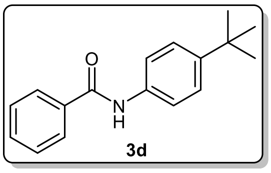
white solid, 96% yield, m.p. 159.9-161.4°C. ^{1}H-NMR (500 MHz, $CDCl_3$) δ 7.86 (d, *J* = 7.4 Hz, 2H), 7.81 (s, 1H), 7.55-7.51 (m, 3H), 7.47 (t, *J* = 7.5 Hz, 2H), 7.17 (d, *J* = 8.0 Hz, 2H), 2.34 (s, 3H). ^{13}C-NMR (126 MHz, $CDCl_3$) δ 165.7, 135.4, 135.0, 134.1, 131.6, 129.5, 128.6, 127.0, 120.4, 20.8. HRMS (APCI): *m*/*z* $[M+H]^+$ calcd. for $C_{14}H_{14}NO^+$: 212.10699; found: 212.10654.

N-(4-Methoxyphenyl)benzamide (3c)[48]


3c

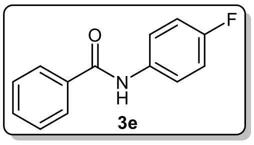
Off-white solid, 87% yield, m.p. 159.5-160.8°C. ^{1}H-NMR (500 MHz, $CDCl_3$) δ 7.87-7.80 (m, 3H), 7.55-7.50 (m, 3H), 7.46 (t, *J* = 7.5 Hz, 2H), 6.89 (d, *J* = 8.9 Hz, 2H), 3.81 (s, 3H). ^{13}C-NMR (126 MHz, $CDCl_3$) δ 165.7, 156.7, 135.1, 131.7, 131.0, 128.7, 127.0, 122.2, 114.3, 55.5. HRMS (APCI): *m*/*z* $[M+H]^+$ calcd. for $C_{14}H_{14}NO_2^+$: 228.10191; found: 228.10138.

N-(4-(*tert*-Butyl)phenyl)benzamide (3d)[49]


3d

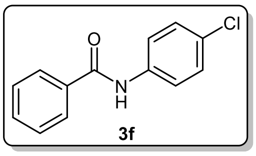
White solid, 97% yield, m.p. 141.1-141.6°C. ^{1}H-NMR (500 MHz, $CDCl_3$) δ 7.87 (d, *J* = 7.5 Hz, 2H), 7.78 (s, 1H), 7.58-7.52 (m, 3H), 7.49 (t, *J* = 7.4 Hz, 2H), 7.39 (d, *J* = 8.2 Hz, 2H), 1.33 (s, 9H). ^{13}C-NMR (126 MHz, $CDCl_3$) δ 165.6, 147.6, 135.3, 135.1, 131.7, 128.8, 127.0, 125.9, 120.0, 34.4, 31.4. HRMS (ESI): *m*/*z* $[M+H]^+$ calcd. for $C_{17}H_{20}NO^+$: 254.15394; found: 254.15341.

N-(4-Fluorophenyl)benzamide (3e)[50]



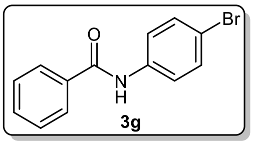
white solid, 84% yield, m.p. 187.3-188.0°C. ^{1}H-NMR (500 MHz, $CDCl_3$) δ 7.86 (d, *J* = 8.0 Hz, 2H), 7.80 (s, 1H), 7.63-7.58 (m, 2H), 7.56 (d, *J* = 6.5, 1H), 7.52-7.46 (m, 2H), 7.11-7.03 (m, 2H). ^{13}C-NMR (126 MHz, DMSO-d_6) δ 165.9, 158.8 (d, *J* = 240.7 Hz), 136.0 (d, *J* = 2.6 Hz), 135.3, 132.1, 128.9, 128.1, 122.6 (d, *J* = 7.6 Hz), 115.6 (d, *J* = 22.7 Hz). HRMS (APCI): *m*/*z* $[M+H]^+$ calcd. for $C_{13}H_{11}FNO^+$: 216.08192; found: 216.08162.

N-(4-Chlorophenyl)benzamide (3f)[51]



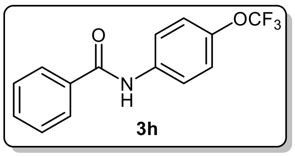
white solid, 86% yield, m.p. 195.6-197.0°C. ^{1}H-NMR (500 MHz, $CDCl_3$) δ 7.86 (d, *J* = 8.1 Hz, 2H), 7.81 (s, 1H), 7.60 (d, *J* = 7.2 Hz, 2H), 7.56 (d, *J* = 6.1 Hz, 1H), 7.50 (t, *J* = 7.8 Hz, 2H), 7.34 (d, *J* = 7.1 Hz, 2H). ^{13}C-NMR (126 MHz, DMSO-d_6) δ 166.1, 138.6, 135.2, 132.2, 129.0, 128.9, 128.2, 127.7, 122.3. HRMS (APCI): *m*/*z* $[M+H]^+$ calcd. for $C_{13}H_{11}ClNO^+$: 232.05237; found: 232.05200.

N-(4-Bromophenyl)benzamide (3g)[52]



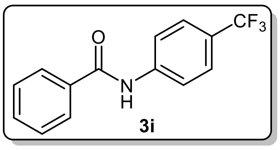
White solid, 81% yield, m.p. 206.0-206.5°C. ^{1}H-NMR (500 MHz, $CDCl_3$) δ 7.86 (d, *J* = 7.8 Hz, 2H), 7.79 (s, 1H), 7.60 – 7.53 (m, 3H), 7.52 – 7.46 (m, 4H). ^{13}C-NMR (126 MHz, $CDCl_3$) δ 165.7, 137.0, 134.6, 132.1, 128.9, 127.0, 121.7, 117.2. HRMS (APCI): *m*/*z* $[M+H]^+$ calcd. for $C_{13}H_{11}BrNO^+$: 276.00185; found: 276.00137.

N-(4-(Trifluoromethoxy)phenyl)benzamide (3h)[53]



White solid, 91% yield, m.p. 185.8-186.7°C. ^{1}H-NMR (500 MHz, $CDCl_3$) δ 7.87 (d, *J* = 7.8 Hz, 2H), 7.85 (s, 1H), 7.68 (d, *J* = 8.8 Hz, 2H), 7.58 (t, *J* = 7.7 Hz, 1H), 7.54 – 7.48 (m, 2H), 7.24 (d, *J* = 8.6 Hz, 2H). ^{13}C-NMR (126 MHz, DMSO-d_6) δ 166.2, 144.3 (q, *J* = 12.6 Hz), 138.9, 135.1, 132.2, 128.9, 128.2, 122.1, 121.9, 120.7 (q, *J* = 252.0 Hz). HRMS (APCI): *m*/*z* [M+H]$^+$ calcd. for $C_{14}H_{11}F_3NO_2^+$: 282.07364; found: 282.07300.

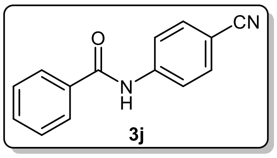
N-(4-(Trifluoromethyl)phenyl)benzamide (3i)[48]



3i

White solid, 99% yield, m.p. 203.5-204.5°C. ^{1}H-NMR (500 MHz, CDCl$_3$) δ 7.97 (s, 1H), 7.88 (d, *J* = 7.7 Hz, 2H), 7.79 (d, *J* = 8.3 Hz, 2H), 7.63 (d, *J* = 8.4 Hz, 2H), 7.59 (t, *J* = 7.4 Hz, 1H), 7.52 (t, *J* = 7.5 Hz, 2H). ^{13}C-NMR (126 MHz, DMSO-d_6) δ 166.5, 143.3, 135.0, 132.4, 128.9, 128.3, 126.3 (q, *J* = 3.8 Hz), 125.1 (q, *J* = 224.5 Hz), 123.9 (q, *J* = 15.0 Hz), 120.6. HRMS (APCI): *m*/*z* [M+H]$^+$ calcd. for $C_{14}H_{11}F_3NO^+$: 266.07873; found: 266.07806.

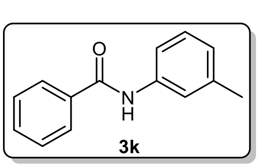
N-(4-Cyanophenyl)benzamide (3j)[54]



3j

White solid, 98% yield, m.p. 172.1-173.5°C. ^{1}H-NMR (500 MHz, CDCl$_3$) δ 8.05 (s, 1H), 7.87 (d, *J* = 7.7 Hz, 2H), 7.80 (d, *J* = 8.3 Hz, 2H), 7.66 (d, *J* = 8.3 Hz, 2H), 7.60 (t, *J* = 7.4 Hz, 1H), 7.51 (t, *J* = 7.6 Hz, 2H). ^{13}C-NMR (126 MHz, CDCl$_3$) δ 165.8, 142.0, 134.1, 133.3, 132.5, 129.0, 127.1, 119.9, 118.8, 107.4. HRMS (APCI): *m*/*z* [M+H]$^+$ calcd. for $C_{14}H_{11}N_2O^+$: 223.08659; found: 223.08603.

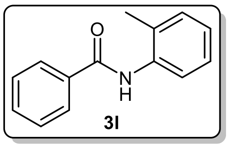
N-(*m*-Tolyl)benzamide (3k)[50]



3k

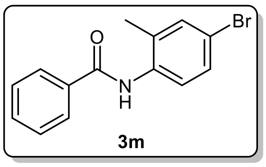
White solid, 88% yield, m.p. 126.0-127.4°C. ^{1}H-NMR (500 MHz, CDCl$_3$) δ 7.86 (d, *J* = 7.8 Hz, 2H), 7.78 (s, 1H), 7.54 (d, *J* = 6.5 Hz, 1H), 7.52-7.45 (m, 3H), 7.41 (d, *J* = 8.1 Hz, 1H), 7.27-7.24 (m, 1H), 6.97 (d, *J* = 7.6 Hz, 1H), 2.37 (s, 3H). ^{13}C-NMR (126 MHz, CDCl$_3$) δ 165.7, 139.1, 137.8, 135.1, 131.8, 128.9, 128.8, 127.0, 125.4, 120.8, 117.2, 21.5. HRMS (APCI): *m*/*z* [M+H]$^+$ calcd. for $C_{14}H_{14}NO^+$: 212.10699; found: 212.10651.

N-(*o*-Tolyl)benzamide (3l)[48]


3l

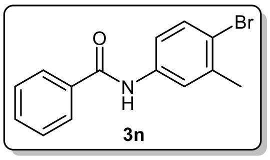
White solid, 97% yield, m.p. 143.9-144.5°C. ^{1}H-NMR (500 MHz, $CDCl_3$) δ 7.95 (d, *J* = 8.1 Hz, 1H), 7.89 (d, *J* = 7.6 Hz, 2H), 7.68 (s, 1H), 7.57 (t, *J* = 7.3 Hz, 1H), 7.50 (t, *J* = 7.5 Hz, 2H), 7.30 – 7.21 (m, 2H), 7.13 (t, *J* = 7.5 Hz, 1H), 2.34 (s, 3H). ^{13}C-NMR (126 MHz, $CDCl_3$) δ 165.7, 135.8, 135.1, 131.9, 130.6, 129.2, 128.9, 127.1, 127.0, 125.4, 123.1, 17.9. HRMS (APCI): *m*/*z* $[M+H]^+$ calcd. for $C_{14}H_{14}NO^+$: 212.10699; found: 212.10649.

N-(4-Bromo-2-methylphenyl)benzamide (3m)


3m

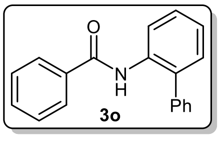
off-white solid, 99% yield, m.p. 177.8-178.2°C. ^{1}H-NMR (500 MHz, $CDCl_3$) δ 7.93-7.85 (m, 3H), 7.60 (d, *J* = 6.6 Hz, 1H), 7.57 (d, *J* = 6.6 Hz, 1H), 7.54 – 7.48 (m, 2H), 7.39 (d, *J* = 6.1 Hz, 2H), 2.32 (s, 3H). ^{13}C-NMR (126 MHz, $CDCl_3$) δ 165.6, 134.9, 134.6, 133.2, 132.1, 131.4, 129.9, 128.9, 127.1, 124.6, 118.2, 17.7. HRMS (APCI): *m*/*z* $[M+H]^+$ calcd. for $C_{14}H_{13}BrNO^+$: 290.01750; found: 290.01688.

N-(4-Bromo-3-methylphenyl)benzamide (3n)[54]


3n

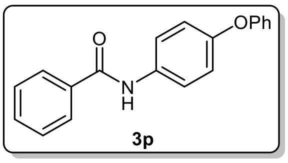
off-white solid, 96% yield, m.p. 120.7-122.1°C. ^{1}H-NMR (500 MHz, $CDCl_3$) δ 7.86 (d, *J* = 7.9 Hz, 2H), 7.75 (s, 1H), 7.59 (s, 1H), 7.58 – 7.54 (m, 1H), 7.52-7.45 (m, 3H), 7.34 (d, *J* = 8.1 Hz, 1H), 2.41 (s, 3H). ^{13}C-NMR (126 MHz, $CDCl_3$) δ 165.6, 138.7, 137.1, 134.7, 132.8, 132.0, 128.9, 127.0, 122.3, 119.8, 119.1, 23.1. HRMS (APCI): *m*/*z* $[M+H]^+$ calcd. for $C_{14}H_{13}BrNO^+$: 290.01750; found: 290.01697.

N-([1,1'-Biphenyl]-2-yl)benzamide (3o)[48]


3o

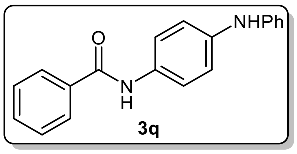
Yellow solid, 81% yield, m.p. 80.2-81.4°C. ^{1}H-NMR (500 MHz, $CDCl_3$) δ 8.53 (d, *J* = 8.3 Hz, 1H), 8.00 (s, 1H), 7.59 (d, *J* = 7.7 Hz, 2H), 7.51 (t, *J* = 7.5 Hz, 2H), 7.48 – 7.41 (m, 5H), 7.37 (t, *J* = 7.6 Hz, 2H), 7.30 (d, *J* = 7.5 Hz, 1H), 7.21 (t, *J* = 7.5 Hz, 1H). ^{13}C-NMR (126 MHz, $CDCl_3$) δ 164.9, 138.0, 134.9, 134.8, 132.4, 131.7, 129.9, 129.3, 129.2, 128.7, 128.6, 128.1, 126.8, 124.3, 121.1. HRMS (APCI): *m*/*z* $[M+H]^+$ calcd. for $C_{19}H_{16}NO^+$: 274.12264; found: 274.12195.

N-(4-Phenoxyphenyl)benzamide (3p)[50]


3p

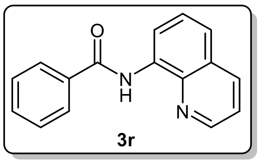
white solid, 98% yield, m.p. 161.4-162.9°C. ^{1}H-NMR (500 MHz, $CDCl_3$) δ 10.28 (s, 1H), 7.95 (d, *J* = 8.0 Hz, 2H), 7.80 (d, *J* = 9.4 Hz, 2H), 7.63 – 7.56 (m, 1H), 7.53 (t, *J* = 7.7 Hz, 2H), 7.41 – 7.34 (m, 2H), 7.11 (t, *J* = 7.4 Hz, 1H), 7.05-6.99 (m, 4H). ^{13}C-NMR (126 MHz, DMSO-d_6) δ 165.9, 157.8, 152.6, 135.5, 135.4, 132.0, 130.4, 128.8, 128.1, 123.5, 122.6, 119.7, 118.4. HRMS (APCI): *m*/*z* $[M+H]^+$ calcd. for $C_{19}H_{16}NO_2^+$: 290.11756; found: 290.11703.

N-(4-(Phenylamino)phenyl)benzamide (3q)[55]


3q

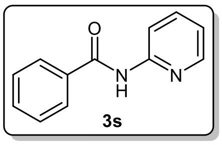
Brown solid, 90% yield, m.p. 167.3-167.7°C. ^{1}H-NMR (500 MHz, DMSO-d_6) δ 10.11 (s, 1H), 8.09 (s, 1H), 7.98 – 7.91 (m, 2H), 7.64 (d, *J* = 7.3 Hz, 2H), 7.58 (t, *J* = 6.5 Hz, 1H), 7.55 – 7.49 (m, 2H), 7.25 – 7.18 (m, 2H), 7.10-7.05 (m, 2H), 7.04 (d, *J* = 7.9 Hz, 2H), 6.78 (t, *J* = 7.3 Hz, 1H). ^{13}C-NMR (126 MHz, DMSO-d_6) δ 165.5, 144.5, 139.8, 135.6, 132.4, 131.8, 129.6, 128.8, 128.0, 122.3, 119.6, 118.0, 116.5. HRMS (APCI): *m*/*z* $[M+H]^+$ calcd. for $C_{19}H_{17}N_2O^+$: 289.13354; found: 289.13287.

N-(Quinolin-8-yl)benzamide (3r)[50]


3r

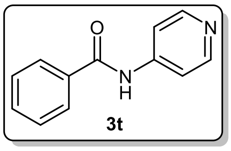
Yellow solid, 75% yield, m.p. 90.6-91.1°C. ^{1}H-NMR (500 MHz, $CDCl_3$) δ 10.74 (s, 1H), 8.94 (d, *J* = 7.6 Hz, 1H), 8.83 (d, *J* = 4.2 Hz, 1H), 8.16 (d, *J* = 8.2 Hz, 1H), 8.09 (d, *J* = 7.4 Hz, 2H), 7.60-7.50 (m, 5H), 7.46 (dd, *J* = 8.3, 4.2 Hz, 1H). ^{13}C-NMR (126 MHz, $CDCl_3$) δ 165.4, 148.2, 138.7, 136.3, 135.1, 134.5, 131.8, 128.7, 127.9, 127.4, 127.2, 121.6, 116.5. HRMS (APCI): *m*/*z* $[M+H]^+$ calcd. for $C_{16}H_{13}N_2O^+$: 249.10224; found: 249.10167.

N-(Pyridin-2-yl)benzamide (3s)[48]


3s

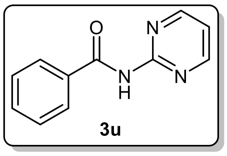
White solid, 85% yield, m.p. 84.3-85.1°C. ^{1}H-NMR (500 MHz, $CDCl_3$) δ 8.62 (s, 1H), 8.40 (d, *J* = 8.4 Hz, 1H), 8.30 (d, *J* = 4.9 Hz, 1H), 7.93 (d, *J* = 7.9 Hz, 2H), 7.77 (t, *J* = 7.9 Hz, 1H), 7.58 (t, *J* = 6.7 Hz, 1H), 7.54 – 7.47 (m, 2H), 7.08 (dd, *J* = 7.3, 5.0 Hz, 1H). ^{13}C-NMR (126 MHz, $CDCl_3$) δ 165.7, 151.5, 147.9, 138.5, 134.3, 132.3, 128.9, 127.2, 120.0, 114.2. HRMS (APCI): *m*/*z* $[M+H]^+$ calcd. for $C_{12}H_{11}N_2O^+$: 199.08659; found:199.08627.

N-(Pyridin-4-yl)benzamide (3t)[56]


3t

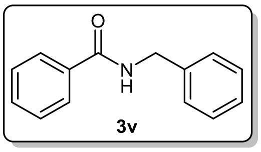
White solid, 85% yield, m.p. 210.3-211.6°C. ^{1}H-NMR (500 MHz, DMSO-d_6) δ 10.59 (s, 1H), 8.48 (d, *J* = 5.2 Hz, 2H), 7.96 (d, *J* = 7.6 Hz, 2H), 7.79 (d, *J* = 5.3 Hz, 2H), 7.63 (t, *J* = 7.2 Hz, 1H), 7.56 (t, *J* = 7.5 Hz, 2H). ^{13}C-NMR (126 MHz, $CDCl_3$) δ 166.1, 150.8, 145.1, 134.1, 132.6, 129.0, 127.2, 113.8. HRMS (APCI): *m*/*z* $[M+H]^+$ calcd. for $C_{12}H_{11}N_2O^+$: 199.08659; found:199.08623.

N-(Pyrimidin-2-yl)benzamide (3u)[57]


3u

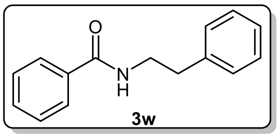
White solid, 75% yield, m.p. 138.8-139.1°C. ^{1}H-NMR (500 MHz, $CDCl_3$) δ 8.88 (s, 1H), 8.63 (d, *J* = 4.7 Hz, 2H), 7.95 (d, *J* = 7.7 Hz, 2H), 7.58 (t, *J* = 7.3 Hz, 1H), 7.50 (t, *J* = 7.5 Hz, 2H), 7.05 (t, *J* = 4.7 Hz, 1H). ^{13}C-NMR (126 MHz, $CDCl_3$) δ 165.1, 158.3, 157.7, 134.3, 132.3, 128.7, 127.5, 116.7. HRMS (APCI): *m*/*z* $[M+H]^+$ calcd. for $C_{11}H_{10}N_3O^+$: 200.08184; found: 200.08150.

N-Benzylbenzamide (3v)[58]


3v

White solid, 93% yield, m.p. 105.7-107.1°C. ^{1}H-NMR (500 MHz, $CDCl_3$) δ 7.79 (d, *J* = 7.6 Hz, 2H), 7.49 (t, *J* = 7.3 Hz, 1H), 7.42 (t, *J* = 7.5 Hz, 2H), 7.35 (d, *J* = 4.3 Hz, 4H), 7.32 – 7.27 (m, 1H), 6.46 (s, 1H), 4.64 (d, *J* = 5.6 Hz, 2H). ^{13}C-NMR (126 MHz, $CDCl_3$) δ 167.4, 138.3, 134.4, 131.5, 128.8, 128.6, 127.9, 127.6, 127.0, 44.1. HRMS (APCI): *m/z* $[M+H]^+$ calcd. for $C_{14}H_{14}NO^+$: 212.10699; found: 212.10661.

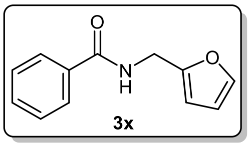
N-Phenethylbenzamide (3w)[59]



3w

White solid, 98% yield, m.p. 116.9-117.6°C. ^{1}H-NMR (500 MHz, $CDCl_3$) δ 7.69 (d, *J* = 8.0 Hz, 2H), 7.50 – 7.45 (m, 1H), 7.39 (t, *J* = 7.5 Hz, 2H), 7.32 (t, *J* = 7.4 Hz, 2H), 7.25-7.20 (m, 3H), 6.24 (s, 1H), 3.71 (q, *J* = 6.6 Hz, 2H), 2.93 (t, *J* = 7.0 Hz, 2H). ^{13}C-NMR (126 MHz, $CDCl_3$) δ 167.5, 138.9, 134.7, 131.4, 128.8, 128.7, 128.6, 126.8, 126.6, 41.2, 35.7. HRMS (APCI): *m/z* $[M+H]^+$ calcd. for $C_{15}H_{16}NO^+$: 226.12264; found: 226.12224.

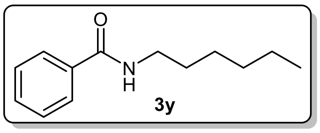
N-(Furan-2-ylmethyl)benzamide (3x)[60]



3x

White solid, 80% yield, m.p. 103.8-105.1°C. ^{1}H-NMR (500 MHz, $CDCl_3$) δ 7.78 (d, *J* = 7.6 Hz, 2H), 7.50 (t, *J* = 7.6 Hz, 1H), 7.43 (t, *J* = 7.5 Hz, 2H), 7.38 (s, 1H), 6.42 (s, 1H), 6.36-6.33 (m, 1H), 6.30 (d, *J* = 3.2 Hz, 1H), 4.65 (d, *J* = 5.5 Hz, 2H). ^{13}C-NMR (126 MHz, $CDCl_3$) δ 167.2, 151.2, 142.3, 134.2, 131.6, 128.6, 127.0, 110.5, 107.7, 37.0. HRMS (APCI): m/z $[M+H]^+$ calcd. for $C_{12}H_{12}NO_2$+: 202.08626; found: 202.08586.

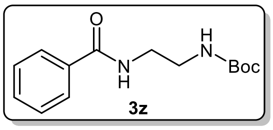
N-Hexylbenzamide (3y)[61]



3y

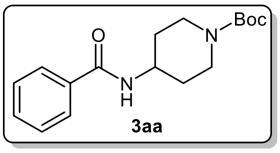
White solid, 95% yield, m.p. 42.2-43.6°C. ^{1}H-NMR (500 MHz, $CDCl_3$) δ 7.75 (d, *J* = 7.6 Hz, 2H), 7.47 (t, *J* = 7.3 Hz, 1H), 7.41 (t, *J* = 7.5 Hz, 2H), 6.26 (s, 1H), 3.43 (q, *J* = 6.8 Hz, 2H), 1.59 (q, *J* = 7.4 Hz, 2H), 1.40 – 1.26 (m, 6H), 0.94 – 0.83 (m, 3H). ^{13}C-NMR (126 MHz, $CDCl_3$) δ 167.5, 134.9, 131.2, 128.5, 126.8, 40.1, 31.5, 29.6, 26.6, 22.5, 13.9. HRMS (APCI): *m/z* $[M+H]^+$ calcd. for $C_{13}H_{20}NO^+$: 206.15394; found: 206.15349.

tert-Butyl (2-benzamidoethyl)carbamate (3z)[62]


3z

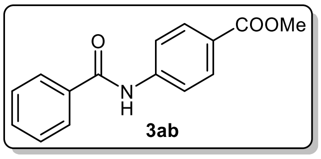
White solid, 70% yield, m.p. 129.8-131.2°C. ^{1}H-NMR (500 MHz, $CDCl_3$) δ 7.82 (d, *J* = 7.6 Hz, 2H), 7.48 (t, *J* = 7.3 Hz, 1H), 7.41 (t, *J* = 7.5 Hz, 2H), 7.26 (s, 1H), 5.12 (s, 1H), 3.55 (q, *J* = 5.4 Hz, 2H), 3.40 (q, *J* = 5.9 Hz, 2H), 1.42 (s, 9H). ^{13}C-NMR (126 MHz, $CDCl_3$) δ 167.9, 157.5, 134.1, 131.4, 128.4, 127.0, 79.9, 41.9, 39.9, 28.3. HRMS (APCI): *m*/*z* $[M+H]^+$ calcd. for $C_{14}H_{21}N_2O_3^+$: 265.15467; found: 265.15411.

tert-Butyl 4-benzamidopiperidine-1-carboxylate (3aa)[63]


3aa

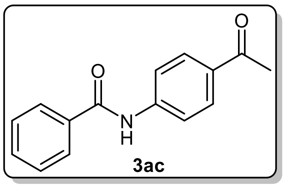
White solid, 76% yield, m.p. 172.3-173.6°C. ^{1}H-NMR (500 MHz, $CDCl_3$) δ 7.75 (d, *J* = 7.6 Hz, 2H), 7.53 – 7.46 (m, 1H), 7.44 (d, *J* = 7.6 Hz, 2H), 6.06 – 5.92 (m, 1H), 4.18 – 4.04 (m, 3H), 2.97-2.84 (m, 2H), 2.05-1.97 (m, 2H), 1.47 (s, 9H), 1.43-1.30 (m, 2H). ^{13}C-NMR (126 MHz, $CDCl_3$) δ 166.8, 154.7, 134.6, 131.5, 128.6, 126.8, 79.7, 47.3, 42.8, 32.2, 28.4. HRMS (APCI): *m*/*z* $[M-H]^-$ calcd. for $C_{17}H_{23}N_2O_3^-$: 303.17142; found: 303.17145.

Methyl 4-benzamidobenzoate (3ab)[64]


3ab

White solid, 73% yield, m.p. 160.0-161.3°C. ^{1}H NMR (500 MHz, $CDCl_3$) δ 8.06 (d, *J* = 7.5 Hz, 2H), 8.01 (s, 1H), 7.88 (d, *J* = 6.7 Hz, 2H), 7.75 (d, *J* = 7.5 Hz, 2H), 7.57 (d, *J* = 6.5 Hz, 1H), 7.51 (d, *J* = 6.6 Hz, 2H), 3.92 (s, 3H). ^{13}C NMR (126 MHz, $CDCl_3$) δ 166.6, 165.7, 142.1, 134.5, 132.2, 130.9, 128.9, 127.0, 125.9, 119.2, 52.0. HRMS (APCI): *m*/*z* $[M+H]^+$ calcd. for $C_{15}H_{14}NO_3^+$: 256.09682; found: 256.09647.

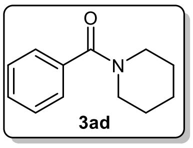
N-(4-(3-oxo-3-phenylpropanoyl)phenyl)benzamide (3ac)[65]


3ac

White solid, 44% yield, m.p. 199.5-201.0°C. ^{1}H NMR (500 MHz, $CDCl_3$) δ 8.00 (d, *J* = 7.8 Hz, 3H), 7.89 (d, *J* = 7.3 Hz, 2H), 7.77 (d, *J* = 8.2 Hz, 2H), 7.61 – 7.56 (m, 1H), 7.52 (t, *J* = 7.3 Hz, 2H), 2.60 (s, 3H). ^{13}C NMR (126 MHz, $CDCl_3$) δ 196.9, 165.7, 142.2, 134.5, 133.2, 132.3, 129.8, 128.9, 127.1, 119.2, 26.5. HRMS (APCI): *m*/*z*

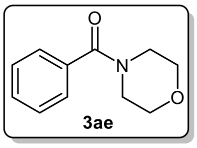
$[M+H]^+$ calcd. for $C_{15}H_{14}NO_2^+$: 240.10191; found: 240.10165.

Phenyl(piperidin-1-yl)methanone (3ad)[60]


3ad

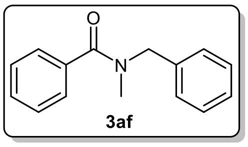
White solid, 93% yield, m.p. 46.5-48.0°C. ^{1}H-NMR (500 MHz, $CDCl_3$) δ 7.38 (s, 5H), 3.71 (s, 2H), 3.33 (s, 2H), 1.70 – 1.48 (m, 6H). ^{13}C-NMR (126 MHz, $CDCl_3$) δ 170.2, 136.5, 129.3, 128.3, 126.7, 48.7, 43.0, 26.5, 25.6, 24.5.

Morpholino(phenyl)methanone (3ae)[60]


3ae

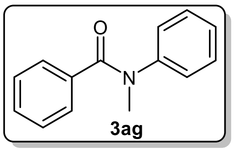
Colorless solid, 94% yield, m.p. 73.6-74.9°C. ^{1}H-NMR (500 MHz, $CDCl_3$) δ 7.43 – 7.32 (m, 5H), 3.82 – 3.31 (m, 8H). ^{13}C-NMR (126 MHz, $CDCl_3$) δ 170.4, 135.3, 129.9, 128.6, 127.1, 66.9, 48.2, 42.6.

***N*-benzyl-*N*-methylbenzamide (3af)[60]**


3af

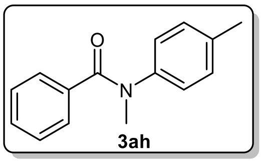
White solid, 82% yield, m.p. 163.7-165.1°C. ^{1}H-NMR (500 MHz, $CDCl_3$) δ 7.48 – 7.43 (m, 2H), 7.42 – 7.32 (m, 6H), 7.31 – 7.26 (m, 1H), 7.17 (s, 1H), 4.82 – 4.41 (m, 2H), 3.12 – 2.77 (m, 3H). ^{13}C-NMR (126 MHz, $CDCl_3$) δ 172.3, 171.6, 137.0, 136.6, 136.2, 129.6, 128.8, 128.4, 128.2, 127.5, 127.0, 126.8, 55.2, 50.8, 37.0, 33.1.

***N*-Methyl-*N*-phenylbenzamide (3ag)[66]**


3ag

Colorless oil, 25% yield. ^{1}H-NMR (500 MHz, $CDCl_3$) δ 7.29 (d, *J* = 7.7 Hz, 2H), 7.26 – 7.19 (m, 3H), 7.19 – 7.11 (m, 3H), 7.03 (d, *J* = 7.8 Hz, 2H), 3.50 (s, 3H). ^{13}C NMR (126 MHz, $CDCl_3$) δ 170.6, 144.9, 135.9, 129.5, 129.1, 128.7, 127.7, 126.9, 126.4, 38.4. HRMS (APCI): *m*/*z* $[M+H]^+$ calcd. for $C_{14}H_{14}NO^+$: 212.10699; found: 212.10667.

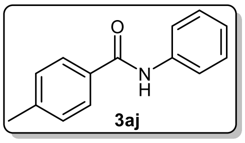
N-Methyl-*N*-(*p*-tolyl)benzamide (3ah)[67]



3ah

Colorless oil, 55% yield. ^{1}H-NMR (500 MHz, $CDCl_3$) δ 7.30 (d, *J* = 7.6 Hz, 2H), 7.22 (t, *J* = 7.4 Hz, 1H), 7.16 (t, *J* = 7.5 Hz, 2H), 7.01 (d, *J* = 7.8 Hz, 2H), 6.91 (d, *J* = 7.8 Hz, 2H), 3.46 (s, 3H), 2.26 (s, 3H). ^{13}C NMR (126 MHz, $CDCl_3$) δ 170.6, 142.3, 136.2, 136.0, 129.7, 129.4, 128.6, 127.6, 126.6, 38.4, 20.9. HRMS (APCI): *m*/*z* $[M+H]^+$ calcd. for $C_{15}H_{16}NO^+$: 226.12264; found: 226.12129.

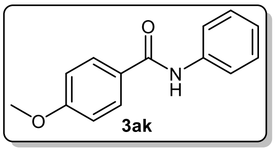
4-Methyl-*N*-phenylbenzamide (3aj)[52]



3aj

White solid, 97% yield, m.p. 145.5-145.6°C. ^{1}H-NMR (500 MHz, $CDCl_3$) δ 7.80 (s, 1H), 7.77 (d, *J* = 7.1 Hz, 2H), 7.64 (d, *J* = 7.9 Hz, 2H), 7.37 (t, *J* = 7.2 Hz, 2H), 7.29 (d, *J* = 7.8 Hz, 2H), 7.15 (t, *J* = 6.9 Hz, 1H), 2.43 (s, 3H). ^{13}C-NMR (126 MHz, $CDCl_3$) δ 165.6, 142.4, 138.0, 132.1, 129.4, 129.1, 127.0, 124.4, 120.1, 21.5. HRMS (APCI): *m*/*z* $[M+H]^+$ calcd. for $C_{14}H_{14}NO^+$: 212.10699; found: 212.10651.

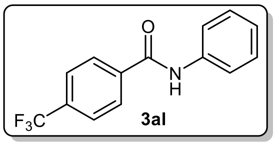
4-Methoxy-*N*-phenylbenzamide (3ak)[52]



3ak

White solid, 76% yield, m.p. 172.4-173.0°C. ^{1}H-NMR (500 MHz, $CDCl_3$) δ 7.84 (d, *J* = 7.2 Hz, 2H), 7.74 (s, 1H), 7.63 (d, *J* = 8.0 Hz, 2H), 7.40 – 7.33 (m, 2H), 7.14 (t, *J* = 7.5 Hz, 1H), 6.98 (d, *J* = 7.2 Hz, 2H), 3.87 (s, 3H). ^{13}C-NMR (126 MHz, $CDCl_3$) δ 165.3, 162.5, 138.1, 129.1, 128.9, 127.2, 124.4, 120.2, 114.0, 55.5. HRMS (APCI): *m*/*z* $[M+H]^+$ calcd. for $C_{14}H_{14}NO_2^+$: 228.10191; found: 228.10135.

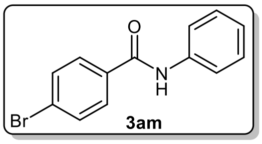
N-Phenyl-4-(trifluoromethyl)benzamide (3al)[48]



3al

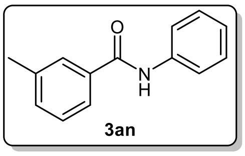
White solid, 99% yield, m.p. 207.5-208.2°C. ^{1}H-NMR (500 MHz, $CDCl_3$) δ 7.99 (d, *J* = 7.9 Hz, 2H), 7.80 (s, 1H), 7.76 (d, *J* = 8.1 Hz, 2H), 7.64 (d, *J* = 7.9 Hz, 2H), 7.40 (t, *J* = 7.8 Hz, 2H), 7.19 (t, *J* = 7.5 Hz, 1H). ^{13}C-NMR (126 MHz, DMSO-*d*$_6$) δ 164.9, 139.3, 139.2, 131.9 (q, *J* = 31.8 Hz), 129.1, 129.0, 125.8 (q, *J* = 3.7 Hz), 124.5 (q, *J* = 274.9 Hz), 124.4, 120.9. HRMS (APCI): *m/z* $[M+H]^+$ calcd. for $C_{14}H_{11}F_3NO^+$: 266.07873; found: 266.07803.

4-Bromo-*N*-phenylbenzamide (3am)[68]


3am

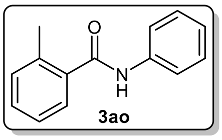
White solid, 76% yield, m.p. 207.5-208.2°C. ^{1}H-NMR (500 MHz, DMSO-d_6) δ 10.31 (s, 1H), 7.92 (d, *J* = 7.7 Hz, 2H), 7.80-7.72 (m, 4H), 7.36 (t, *J* = 7.6 Hz, 2H), 7.12 (t, *J* = 7.4 Hz, 1H). ^{13}C-NMR (126 MHz, DMSO-d_6) δ 165.0, 139.4, 134.5, 131.9, 130.3, 129.1, 125.8, 124.3, 120.9. HRMS (APCI): *m/z* $[M+H]^+$ calcd. for $C_{13}H_{11}BrNO^+$: 276.00185; found: 276.00140.

3-Methyl-*N*-phenylbenzamide (3an)[52]


3an

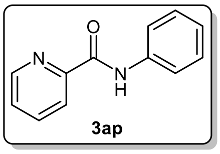
White solid, 92% yield, m.p. 129.2-129.5°C. ^{1}H-NMR (500 MHz, $CDCl_3$) δ 7.78 (s, 1H), 7.69 (s, 1H), 7.64 (d, *J* = 7.7 Hz, 3H), 7.40-7.34 (m, 4H), 7.21 – 7.15 (m, 1H), 2.44 (s, 3H). ^{13}C-NMR (126 MHz, $CDCl_3$) δ 166.0, 138.6, 138.0, 134.9, 132.5, 129.0, 128.5, 127.8, 124.4, 123.9, 120.2, 21.3. HRMS (APCI): *m/z* $[M+H]^+$ calcd. for $C_{14}H_{14}NO^+$: 212.10699; found: 212.10658.

2-Methyl-*N*-phenylbenzamide (3ao)[48]


3ao

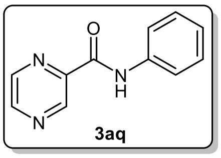
White solid, 73% yield, m.p. 127.3-127.6°C. ^{1}H-NMR (500 MHz, $CDCl_3$) δ 7.77 (s, 1H), 7.59 (d, *J* = 7.9 Hz, 2H), 7.39 (d, *J* = 6.8 Hz, 1H), 7.37-7.30 (m, 3H), 7.27-7.17 (m, 2H), 7.13 (t, *J* = 7.5 Hz, 1H), 2.44 (s, 3H). ^{13}C-NMR (126 MHz, $CDCl_3$) δ 168.1, 138.0, 136.4, 136.3, 131.1, 130.1, 129.0, 126.6, 125.7, 124.4, 119.9, 19.7. HRMS (APCI): *m/z* $[M+H]^+$ calcd. for $C_{14}H_{14}NO^+$: 212.10699; found: 212.10655.

N-Phenylpicolinamide (3ap)[69]


3ap

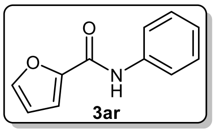
White solid, 98% yield, m.p. 76.7-77.8°C. ^{1}H-NMR (500 MHz, $CDCl_3$) δ 10.03 (s, 1H), 8.62 (d, *J* = 4.7 Hz, 1H), 8.31 (d, *J* = 7.8 Hz, 1H), 7.91 (t, *J* = 7.7 Hz, 1H), 7.79 (d, *J* = 8.0 Hz, 2H), 7.52 – 7.45 (m, 1H), 7.39 (t, *J* = 7.3 Hz, 2H), 7.19 – 7.12 (m, 1H). ^{13}C-NMR (126 MHz, $CDCl_3$) δ 162.0, 149.9, 148.0, 137.8, 137.7, 129.1, 126.5, 124.3, 122.4, 119.7. HRMS (APCI): *m/z* $[M+H]^+$ calcd. for $C_{12}H_{11}N_2O^+$: 199.08659; found: 199.08618.

N-Phenylpyrazine-2-carboxamide (3aq)[70]


3aq

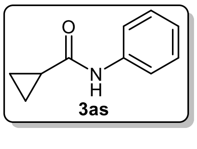
White solid, 90% yield, m.p. 126.8-128.1°C. ^{1}H-NMR (500 MHz, $CDCl_3$) δ 9.67 (s, 1H), 9.52 (s, 1H), 8.81 (s, 1H), 8.59 (s, 1H), 7.76 (d, *J* = 7.9 Hz, 2H), 7.40 (t, *J* = 7.8 Hz, 2H), 7.18 (t, *J* = 7.4 Hz, 1H). ^{13}C-NMR (126 MHz, $CDCl_3$) δ 160.6, 147.5, 144.7, 144.4, 142.4, 137.2, 129.2, 124.9, 119.8. HRMS (APCI): *m/z* $[M+H]^+$ calcd. for $C_{11}H_{10}N_3O^+$: 200.08184; found: 200.08160.

N-Phenylfuran-2-carboxamide (3ar)[69]


3ar

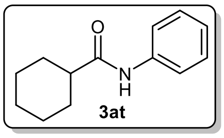
White solid, 95% yield, m.p. 121.8-122.6°C. ^{1}H-NMR (500 MHz, $CDCl_3$) δ 8.06 (s, 1H), 7.65 (d, *J* = 8.0 Hz, 2H), 7.52 (s, 1H), 7.37 (t, *J* = 7.7 Hz, 2H), 7.25 (d, *J* = 3.5 Hz, 1H), 7.15 (t, *J* = 7.4 Hz, 1H), 6.57 (dd, *J* = 3.4, 1.7 Hz, 1H). ^{13}C-NMR (126 MHz, $CDCl_3$) δ 156.1, 147.8, 144.2, 137.4, 129.1, 124.5, 119.9, 115.3, 112.7. HRMS (APCI): *m/z* $[M+H]^+$ calcd. for $C_{11}H_{10}NO_2^+$: 188.07060; found: 188.07018.

N-Phenylcyclopropanecarboxamide (3as)[71]


3as

White solid, 73% yield, m.p. 113.9-114.1°C. ^{1}H-NMR (500 MHz, $CDCl_3$) δ 7.51 (d, *J* = 7.9 Hz, 2H), 7.36 (s, 1H), 7.31 (t, *J* = 7.7 Hz, 2H), 7.09 (t, *J* = 7.6 Hz, 1H), 1.49 (s, 1H), 1.09 (dq, *J* = 7.8, 4.0 Hz, 2H), 0.85 (dq, *J* = 7.4, 4.2 Hz, 2H). ^{13}C-NMR (126 MHz, $CDCl_3$) δ 172.1, 138.1, 128.9, 124.0, 119.8, 15.7, 7.9. HRMS (APCI): *m/z* [M+H]$^+$ calcd. for $C_{10}H_{12}NO^+$: 162.09134; found: 162.09102.

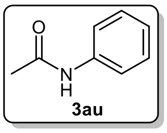
_N_-Phenylcyclohexanecarboxamide (3at)[72]



3at

White solid, 80% yield, m.p. 147.0-148.4°C. ^{1}H-NMR (500 MHz, CDCl$_3$) δ 7.52 (d, *J* = 8.0 Hz, 2H), 7.31 (t, *J* = 7.1 Hz, 2H), 7.13 (s, 1H), 7.09 (t, *J* = 7.4 Hz, 1H), 2.27 – 2.17 (m, 1H), 2.00 – 1.92 (m, 2H), 1.87 – 1.79 (m, 2H), 1.74 – 1.66 (m, 1H), 1.56 – 1.49 (m, 2H), 1.36 – 1.22 (m, 3H). ^{13}C-NMR (126 MHz, CDCl$_3$) δ 174.3, 138.1, 129.0, 124.1, 119.7, 46.6, 29.7, 25.7. HRMS (APCI): *m/z* [M+H]$^+$ calcd. for $C_{13}H_{18}NO^+$: 204.13829; found: 204.13791.

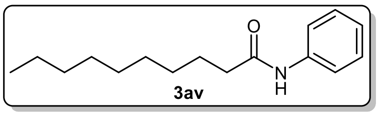
_N_-Phenylacetamide (3au)[71]



3au

White solid, 95% yield, m.p. 114.8-116.0°C. ^{1}H-NMR (500 MHz, CDCl$_3$) δ 7.62 – 7.45 (m, 3H), 7.30 (t, *J* = 7.4 Hz, 2H), 7.10 (t, *J* = 7.4 Hz, 1H), 2.16 (s, 3H). ^{13}C-NMR (126 MHz, CDCl$_3$) δ 168.5, 137.9, 129.0, 124.3, 120.0, 24.6. HRMS (APCI): *m/z* [M+H]$^+$ calcd. for $C_8H_{10}NO^+$: 136.07569; found: 136.07558.

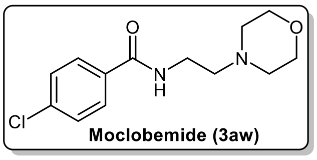
_N_-Phenyldecanamide (3av)[73]



3av

White solid, 96% yield, m.p. 67.7-67.8°C. ^{1}H-NMR (500 MHz, CDCl$_3$) δ 7.51 (d, *J* = 8.0 Hz, 2H), 7.30 (t, *J* = 7.7 Hz, 2H), 7.26 (s, 1H), 7.09 (t, *J* = 7.5 Hz, 1H), 2.34 (t, *J* = 7.6 Hz, 2H), 1.72 (q, *J* = 7.4 Hz, 2H), 1.40 – 1.21 (m, 12H), 0.87 (t, *J* = 6.8 Hz, 3H). ^{13}C-NMR (126 MHz, CDCl$_3$) δ 171.5, 138.0, 129.0, 124.2, 119.8, 37.9, 31.9, 29.5, 29.4, 29.3, 25.7, 22.7, 14.1. HRMS (APCI): *m/z* [M+H]$^+$ calcd. for $C_{16}H_{26}NO^+$: 248.20089; found: 248.20047.

4-Chloro-_N_-(2-morpholinoethyl)benzamide (Moclobemide, 3aw)[48]

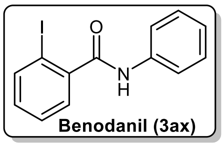


Moclobemide (3aw)

White solid, 99% yield, m.p. 139.5-140.4°C. ^{1}H-NMR (500 MHz, CDCl$_3$) δ 7.71 (d, *J* = 8.1 Hz, 2H), 7.41 (d, *J* = 8.1 Hz, 2H), 6.77 (s, 1H), 3.72 (t, *J* = 4.6 Hz, 4H), 3.53 (q, *J* = 5.6

Hz, 2H), 2.59 (t, J = 6.0 Hz, 2H), 2.50 (t, J = 4.8 Hz, 4H). ^{13}C-NMR (126 MHz, CDCl$_3$) δ 166.3, 137.6, 133.0, 128.8, 128.4, 67.0, 56.8, 53.3, 36.1. HRMS (APCI): *m/z* [M+H]$^+$ calcd. for $C_{13}H_{18}ClN_2O_2{}^+$: 269.10513; found: 269.10458.

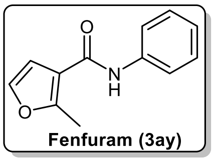
2-Iodo-*N*-phenylbenzamide (Benodanil, 3ax)^{74}



Benodanil (3ax)

White solid, 85% yield, m.p. 141.8-143.1°C. ^{1}H-NMR (500 MHz, CDCl$_3$) δ 7.88 (d, J = 8.0 Hz, 1H), 7.63 (d, J = 8.3 Hz, 3H), 7.49 (d, J = 7.6 Hz, 1H), 7.41-7.31 (m, 3H), 7.17 (t, J = 7.4 Hz, 1H), 7.12 (t, J = 7.7 Hz, 1H). ^{13}C-NMR (126 MHz, CDCl$_3$) δ 167.2, 142.1, 140.0, 137.5, 131.4, 129.1, 128.5, 128.3, 124.9, 120.1, 92.3. HRMS (APCI): *m/z* [M+H]$^+$ calcd. for $C_{13}H_{11}INO^+$: 323.98798; found: 323.98734.

2-Methyl-*N*-phenylfuran-3-carboxamide (Fenfuram, 3ay)^{10}



Fenfuram (3ay)

White solid, 75% yield, m.p. 112.0-113.4°C. ^{1}H-NMR (500 MHz, CDCl$_3$) δ 7.57 (d, J = 7.9 Hz, 2H), 7.48 – 7.38 (m, 1H), 7.38 – 7.32 (m, 2H), 7.30 (t, J = 2.7 Hz, 1H), 7.13 (t, J = 7.4 Hz, 1H), 6.54 (s, 1H), 2.64 (s, 3H). ^{13}C-NMR (126 MHz, CDCl$_3$) δ 162.0, 158.0, 140.6, 137.8, 129.0, 124.4, 120.2, 120.2, 115.8, 108.2, 108.1, 13.6. HRMS (APCI): *m/z* [M+H]$^+$ calcd. for $C_{12}H_{12}NO_2{}^+$: 202.08626; found: 202.08583.

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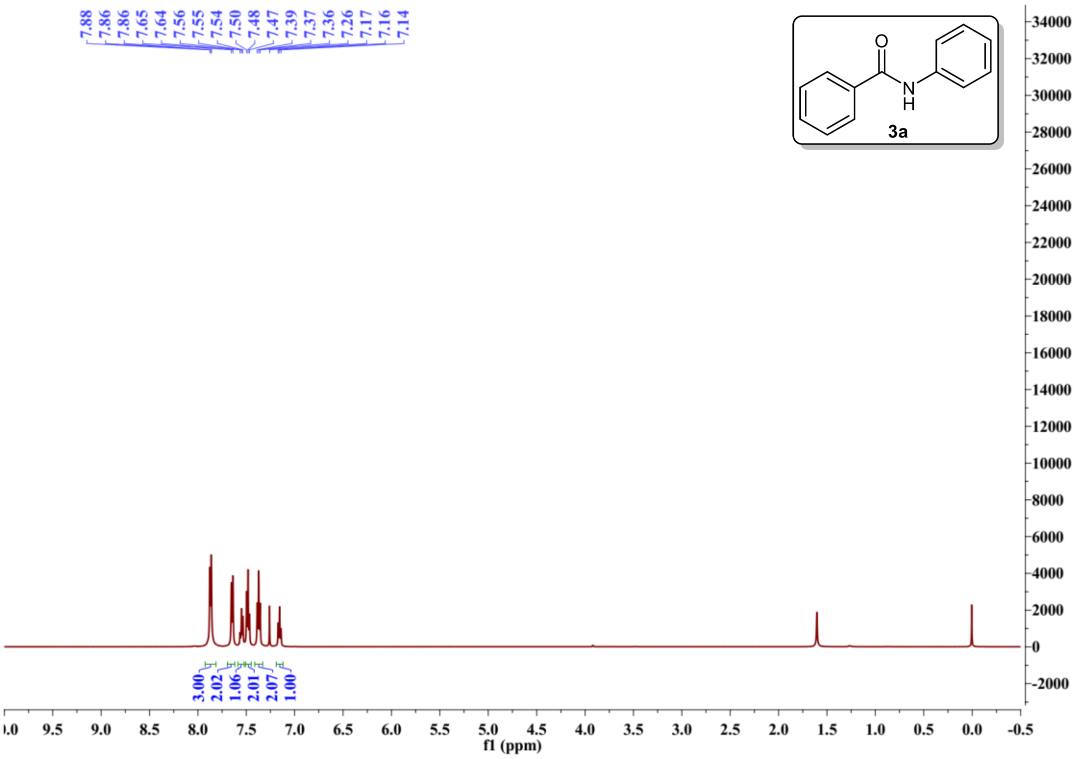
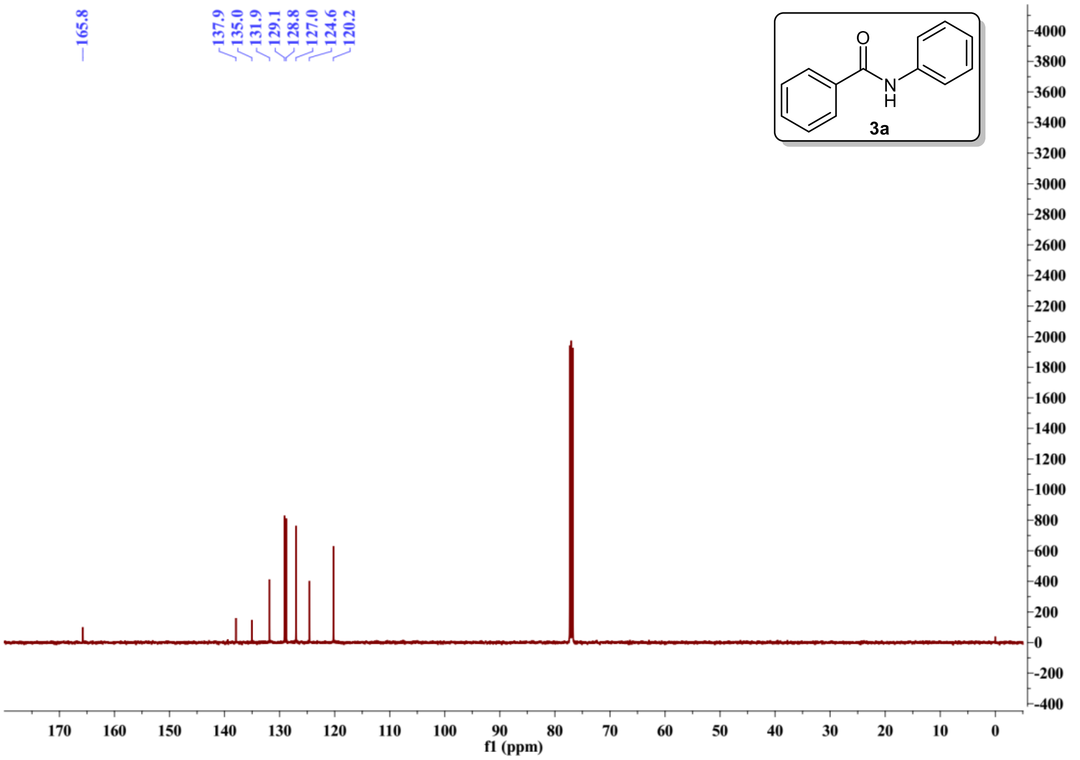
6. Original ^{1}H-NMR, ^{13}C-NMR and HR-MS spectra for 3a-3ay

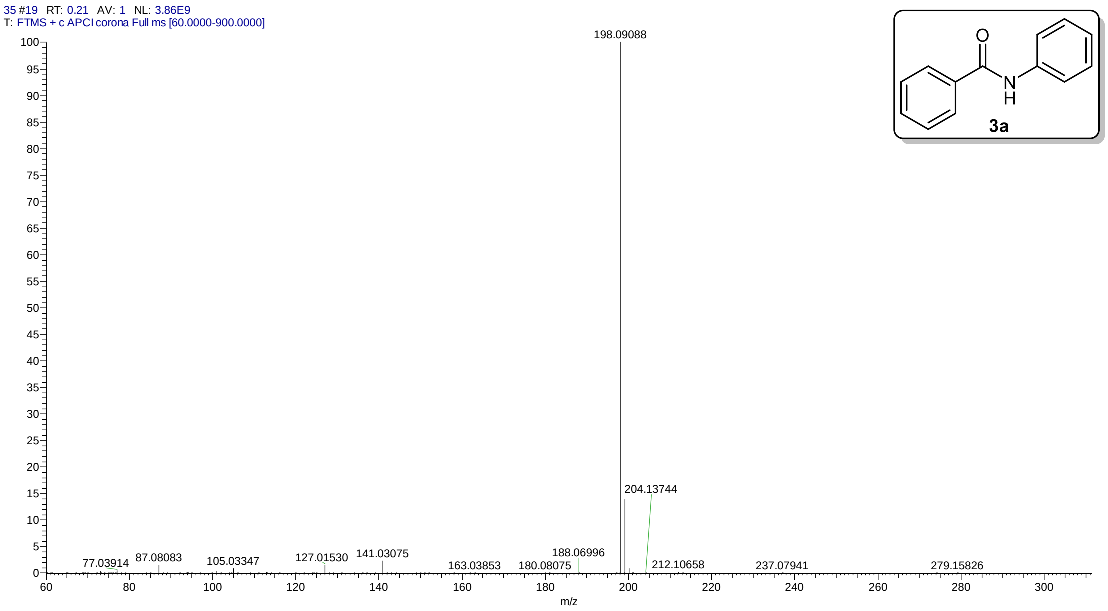
- ^{1}H-NMR spectrum for **3a**



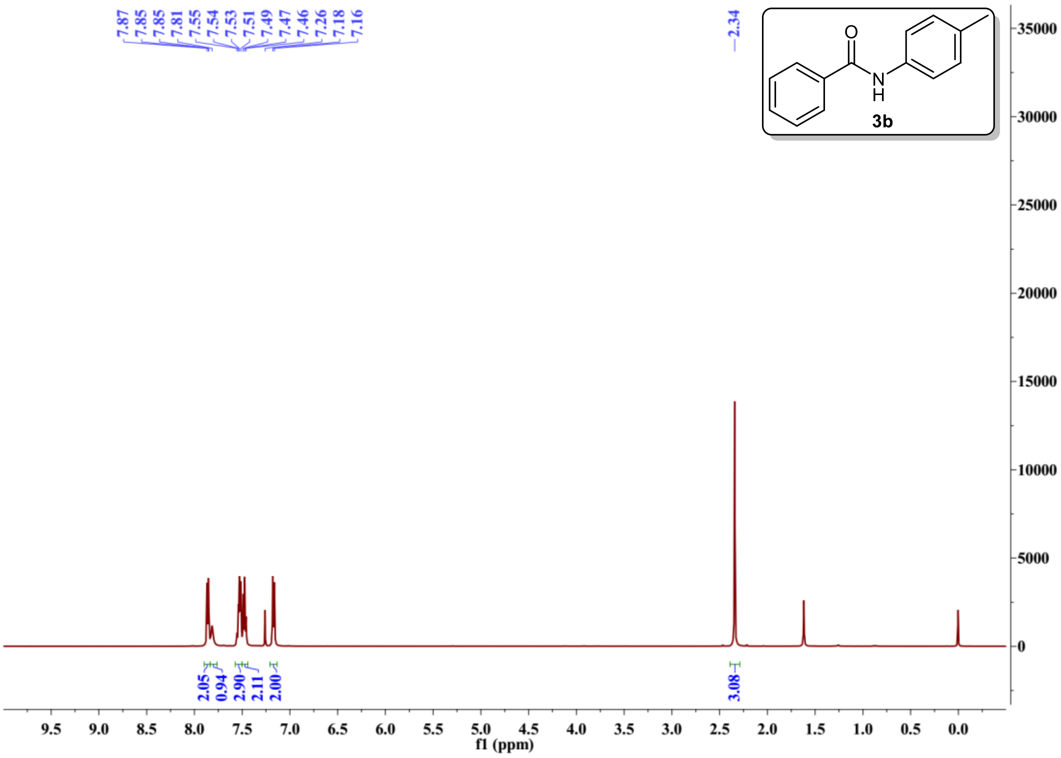
- ^{13}C-NMR spectrum for **3a**



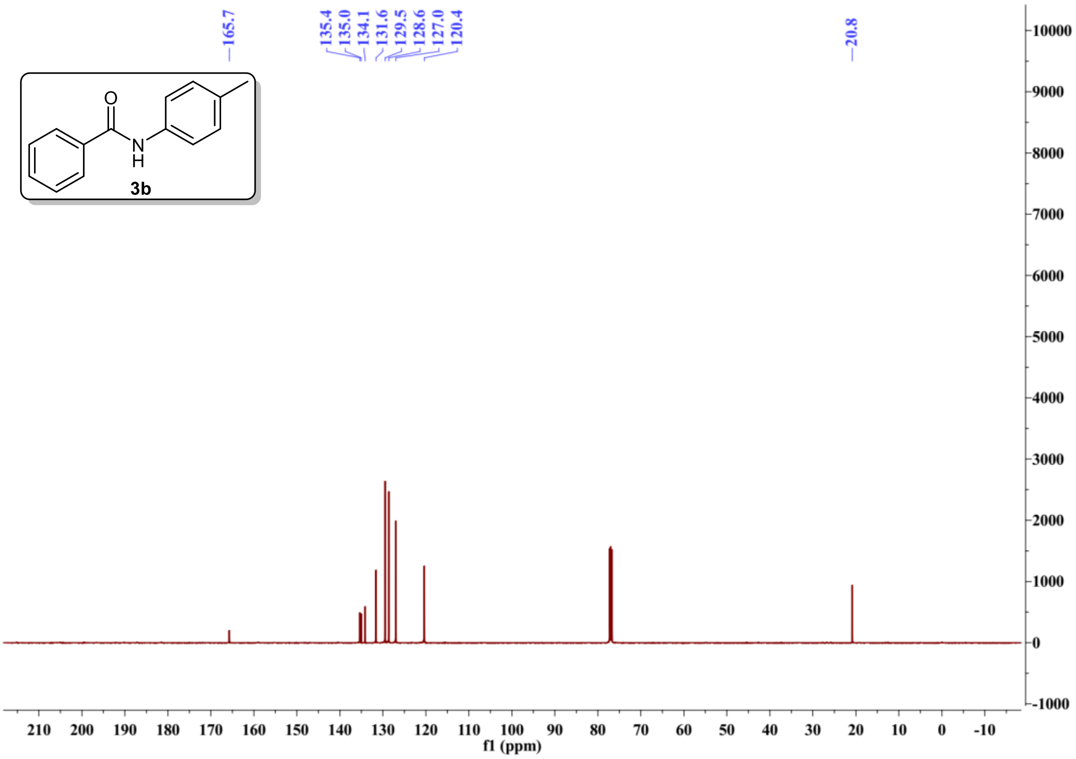
- HRMS spectrum for **3a**



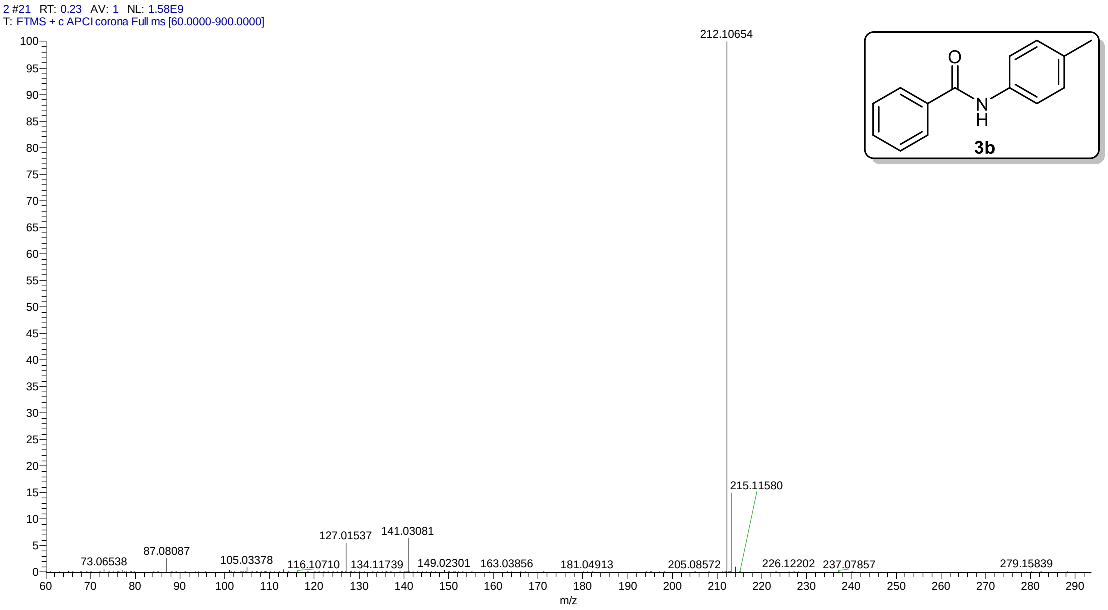
- ^{1}H-NMR spectrum for **3b**



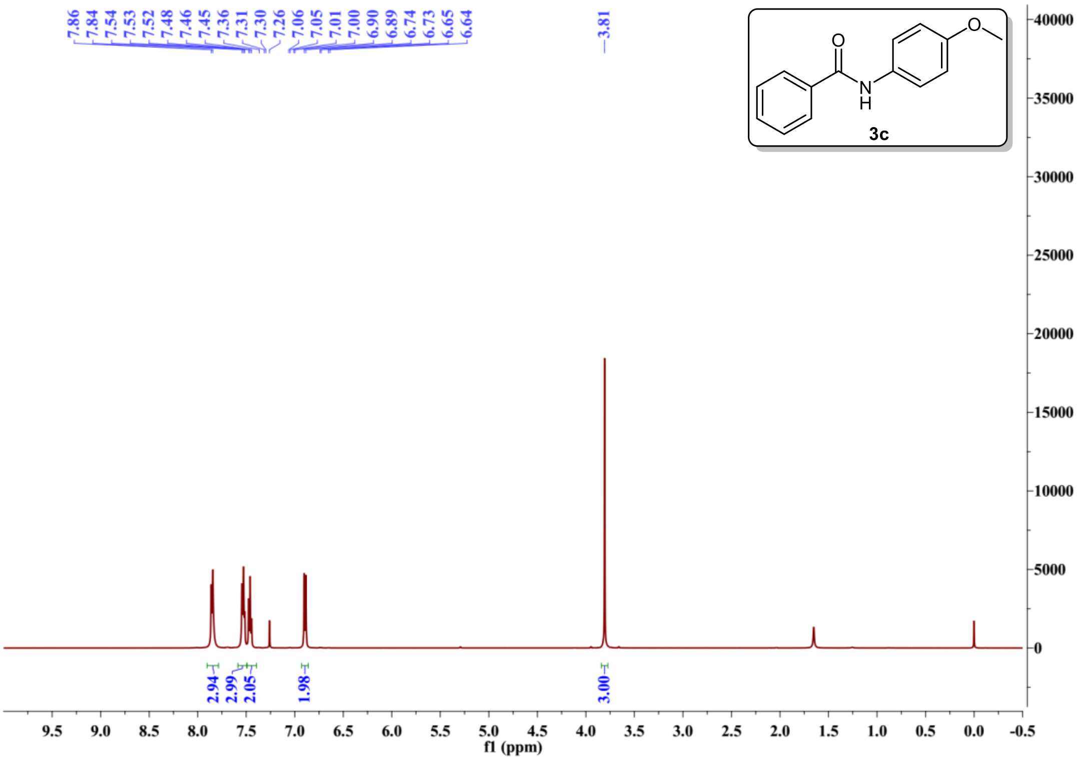
- ^{13}C-NMR spectrum for **3b**



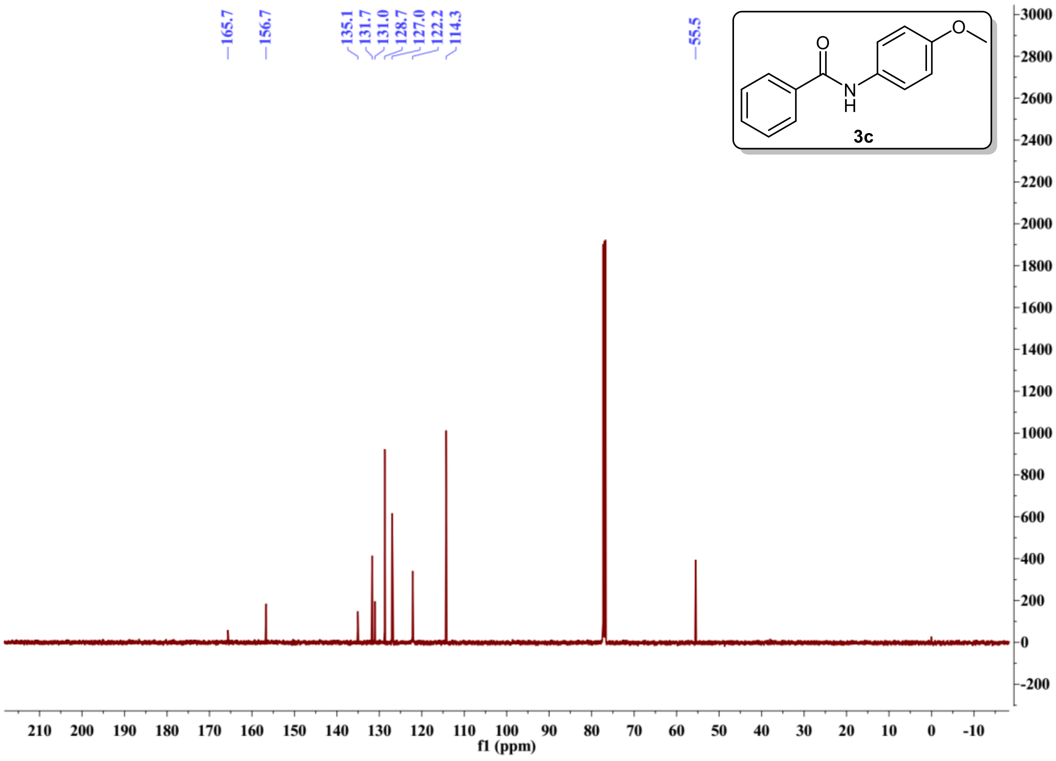
➢ HRMS spectrum for **3b**



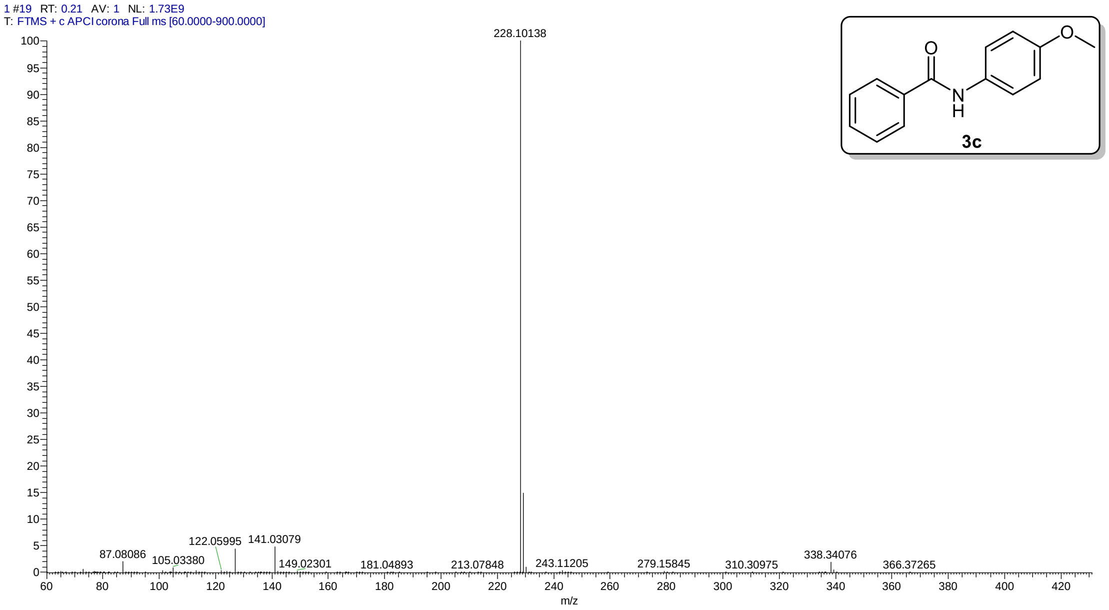
➢ ^{1}H-NMR spectrum for **3c**



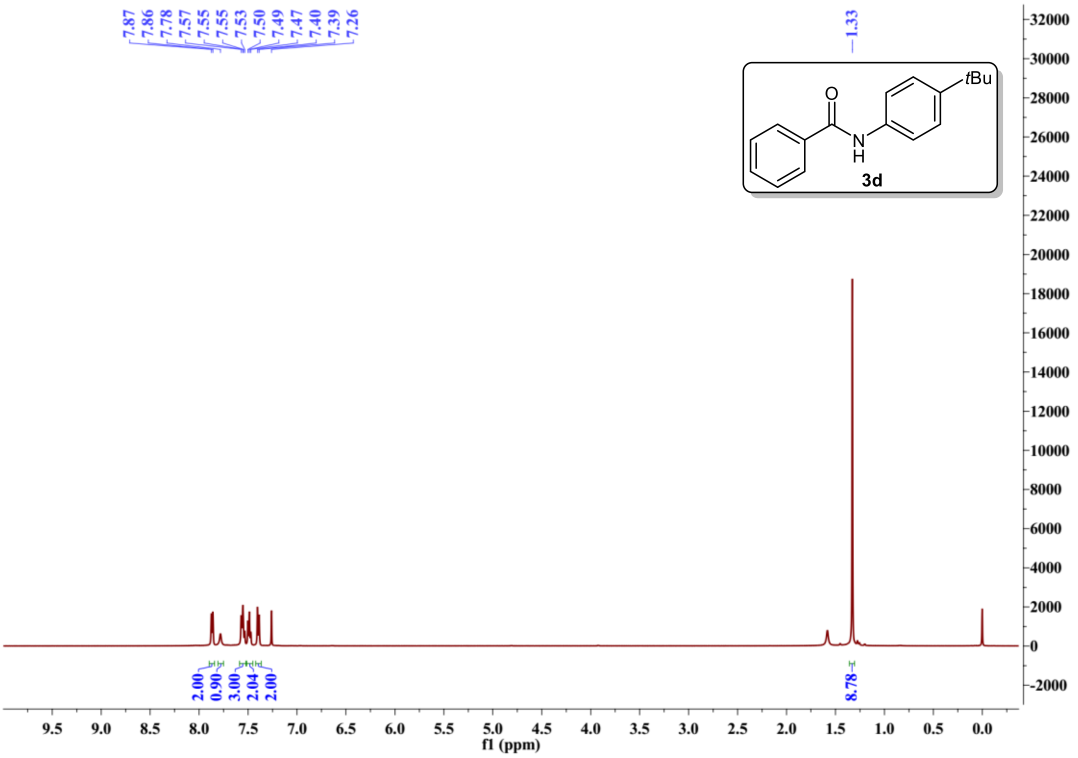
➢ ^{13}C-NMR spectrum for **3c**



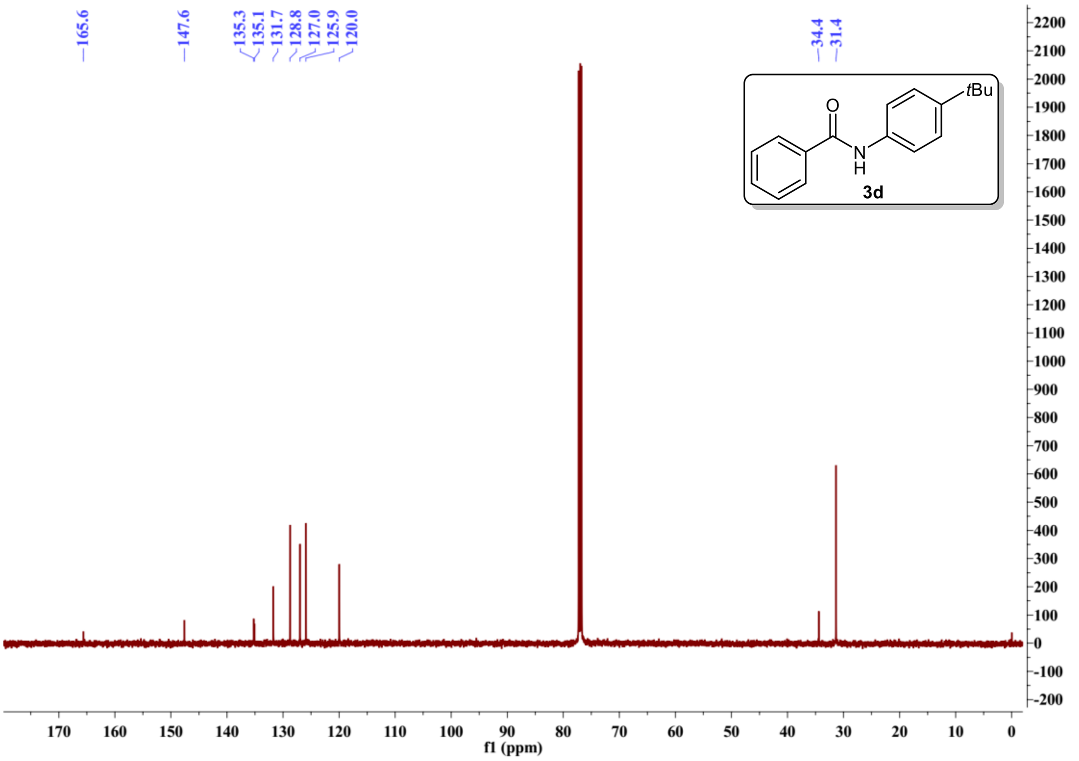
➢ HRMS spectrum for **3c**



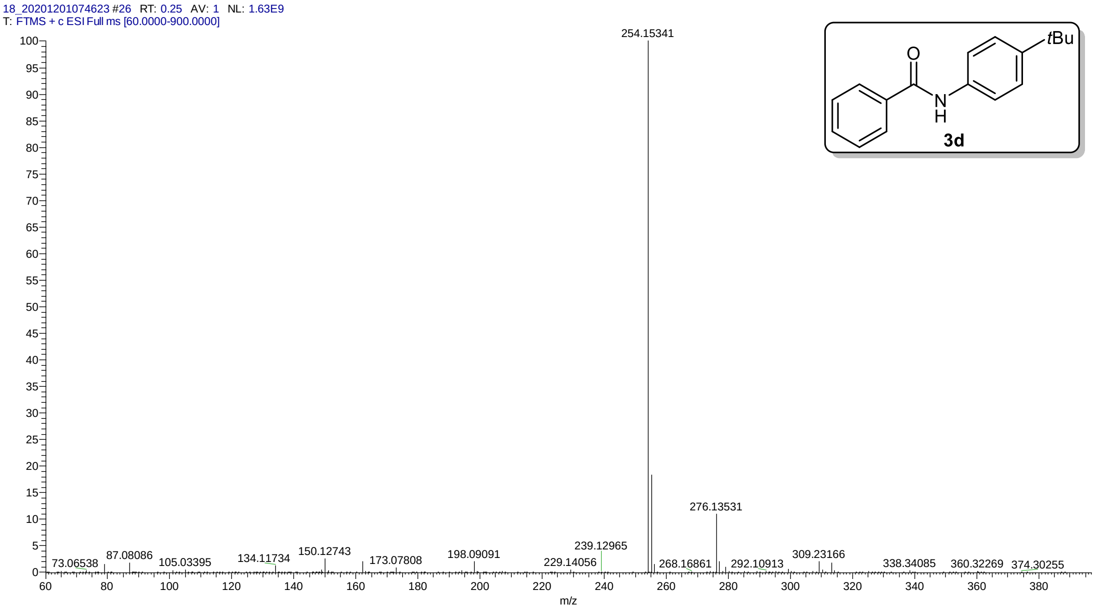
➢ ^{1}H-NMR spectrum for **3d**



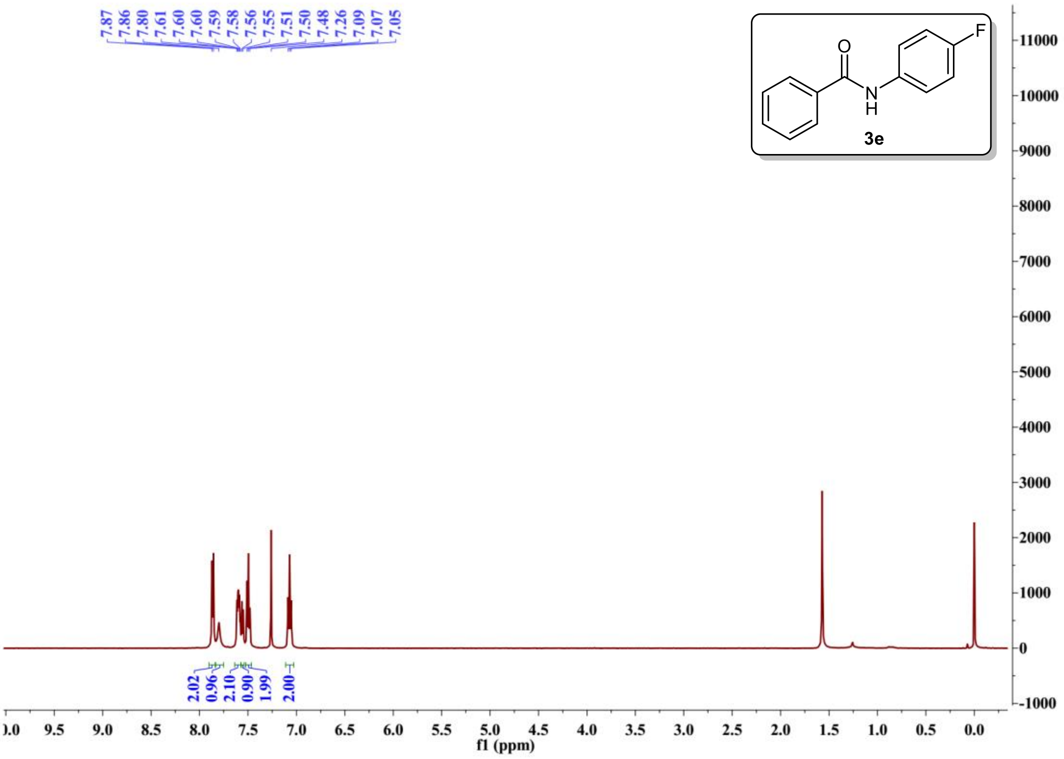
➢ ^{13}C-NMR spectrum for **3d**



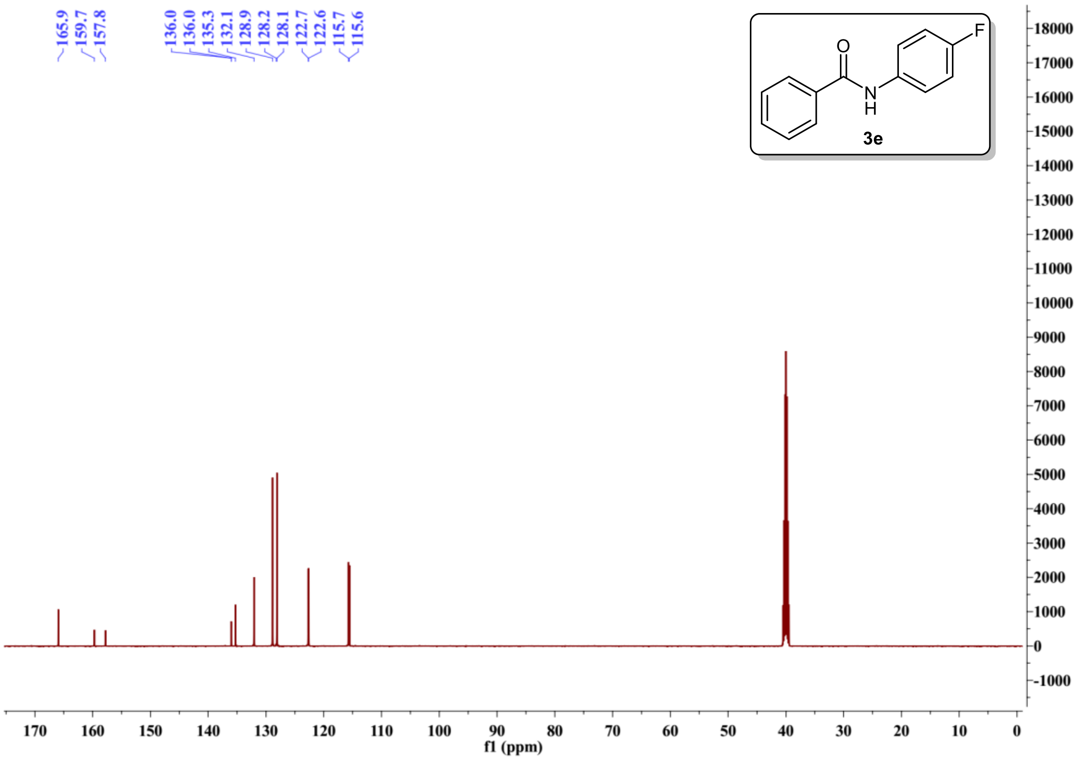
➢ HRMS spectrum for **3d**



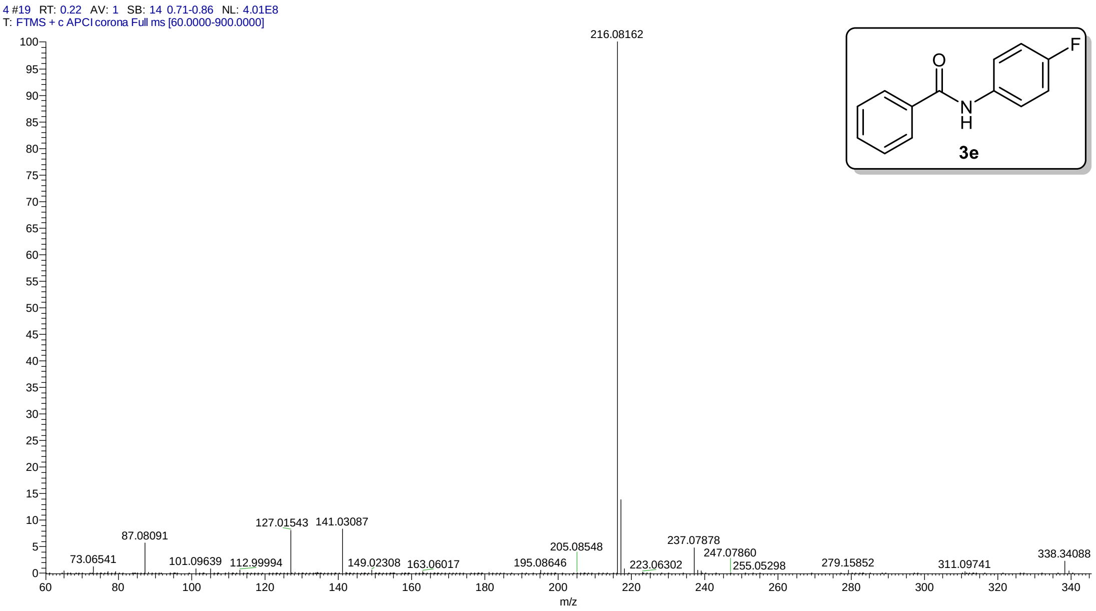
➢ ^{1}H-NMR spectrum for **3e**



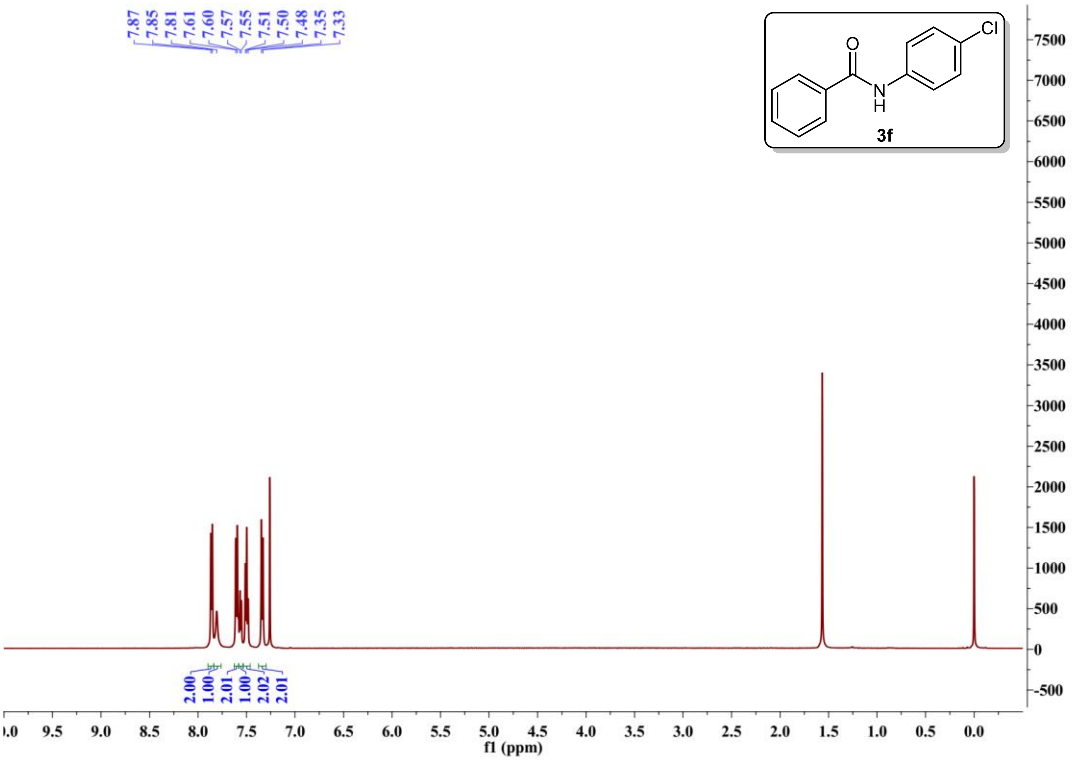
➢ ^{13}C-NMR spectrum for **3e**



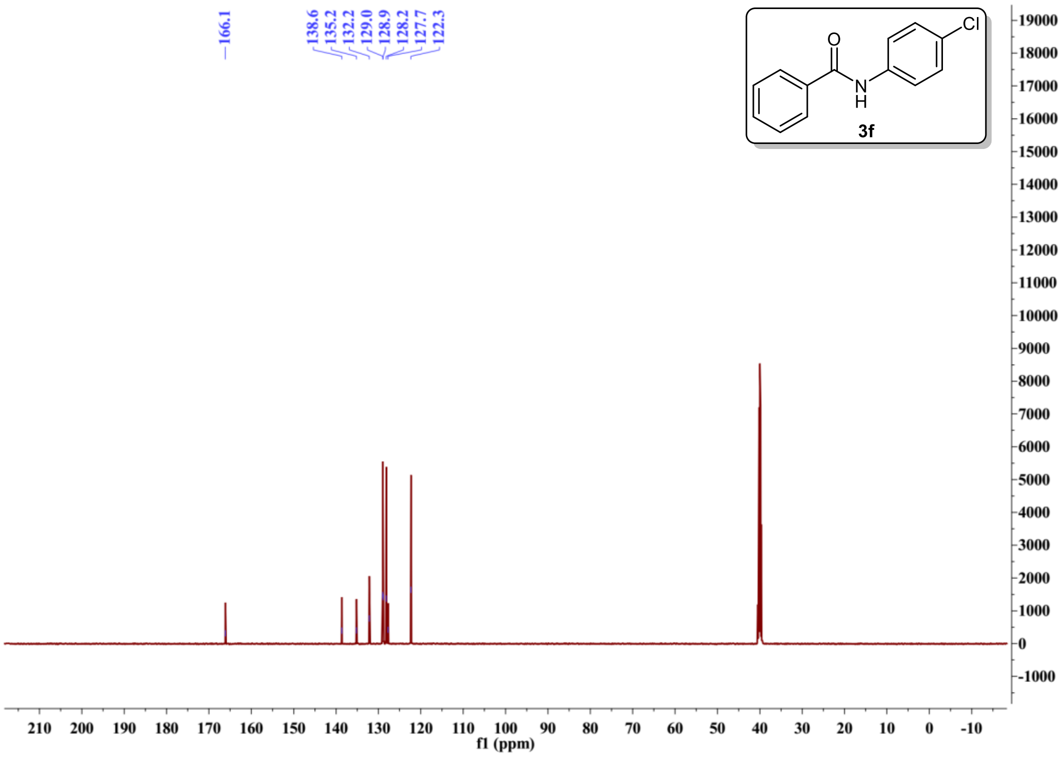
➢ HRMS spectrum for **3e**



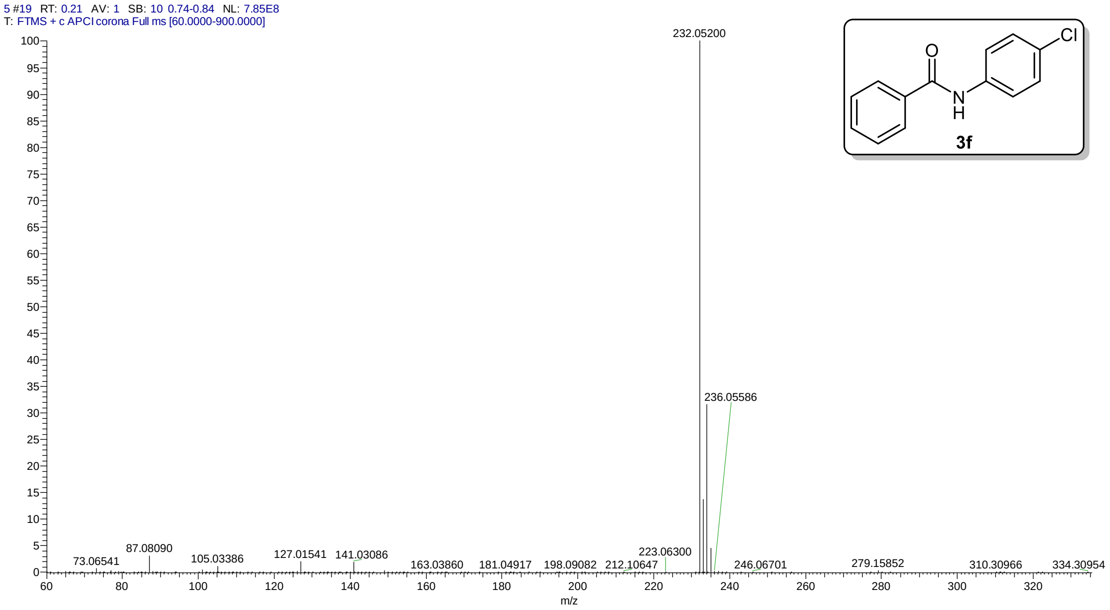
➢ ^{1}H-NMR spectrum for **3f**



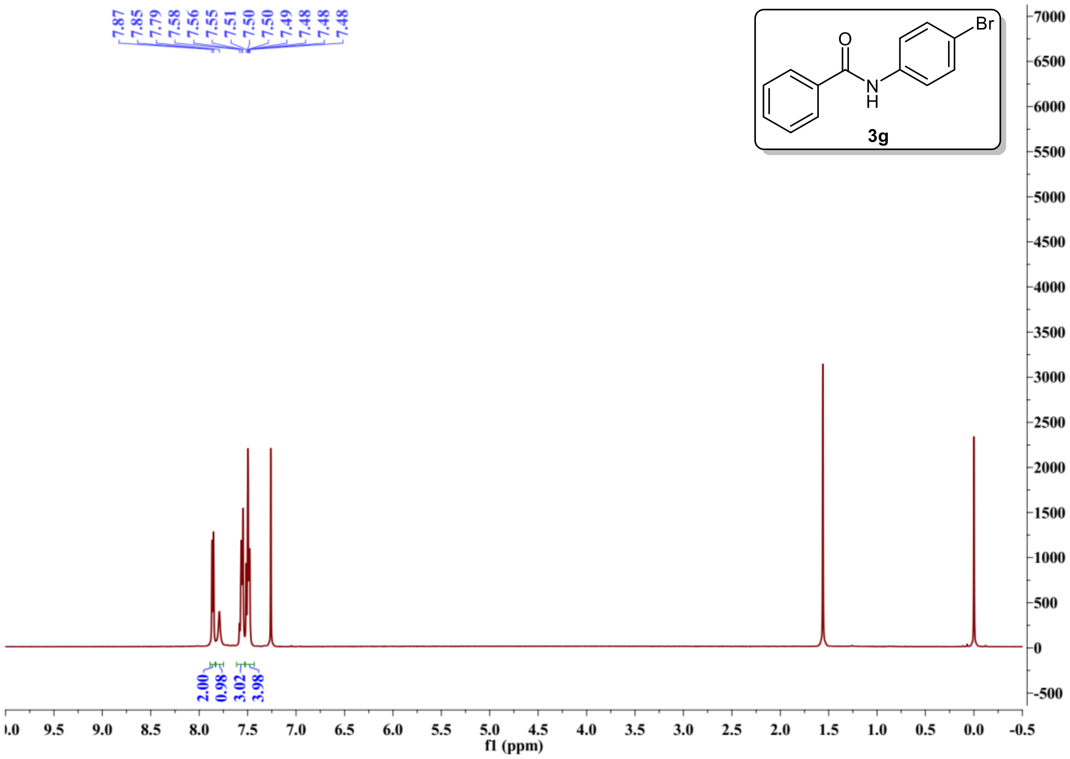
➢ ^{13}C-NMR spectrum for **3f**



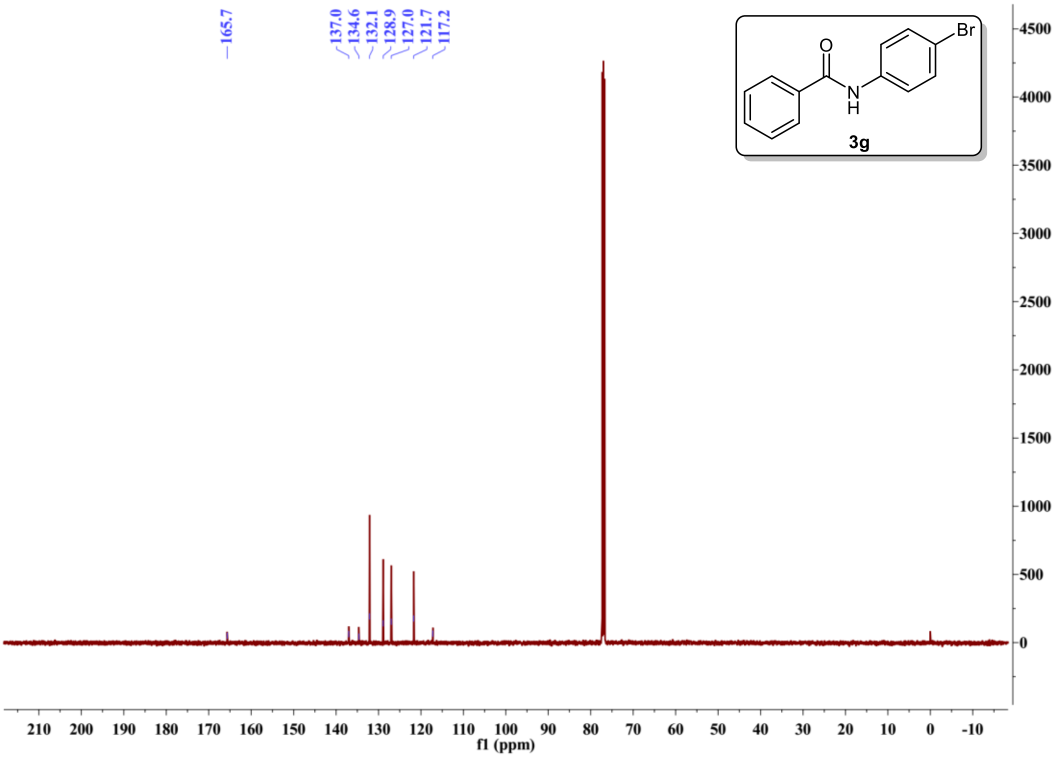
➢ HRMS spectrum for **3f**



- ^{1}H-NMR spectrum for **3g**



- ^{13}C-NMR spectrum for **3g**



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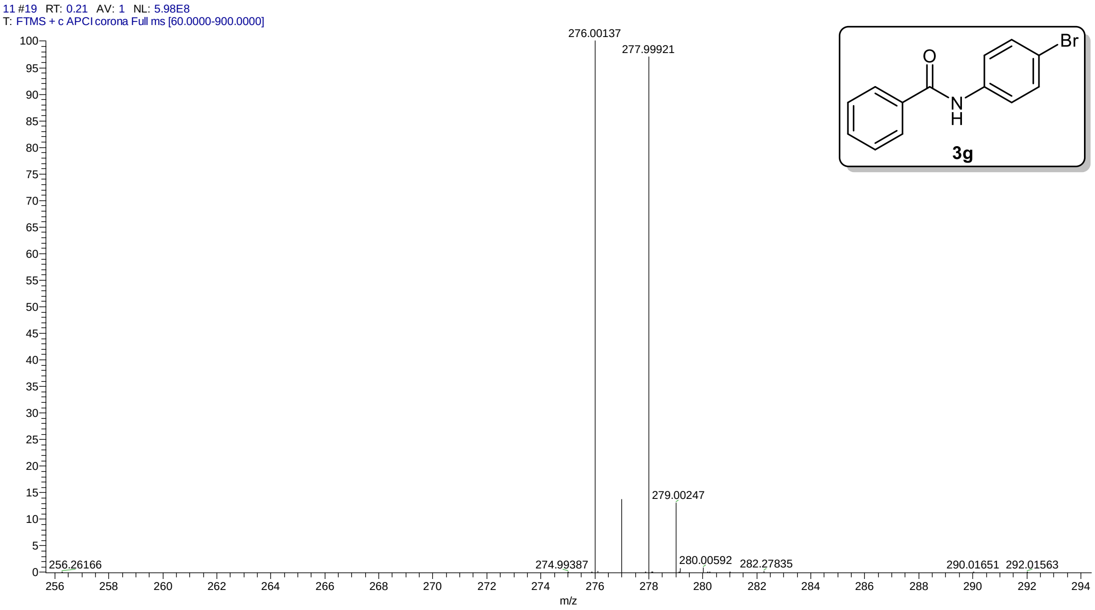
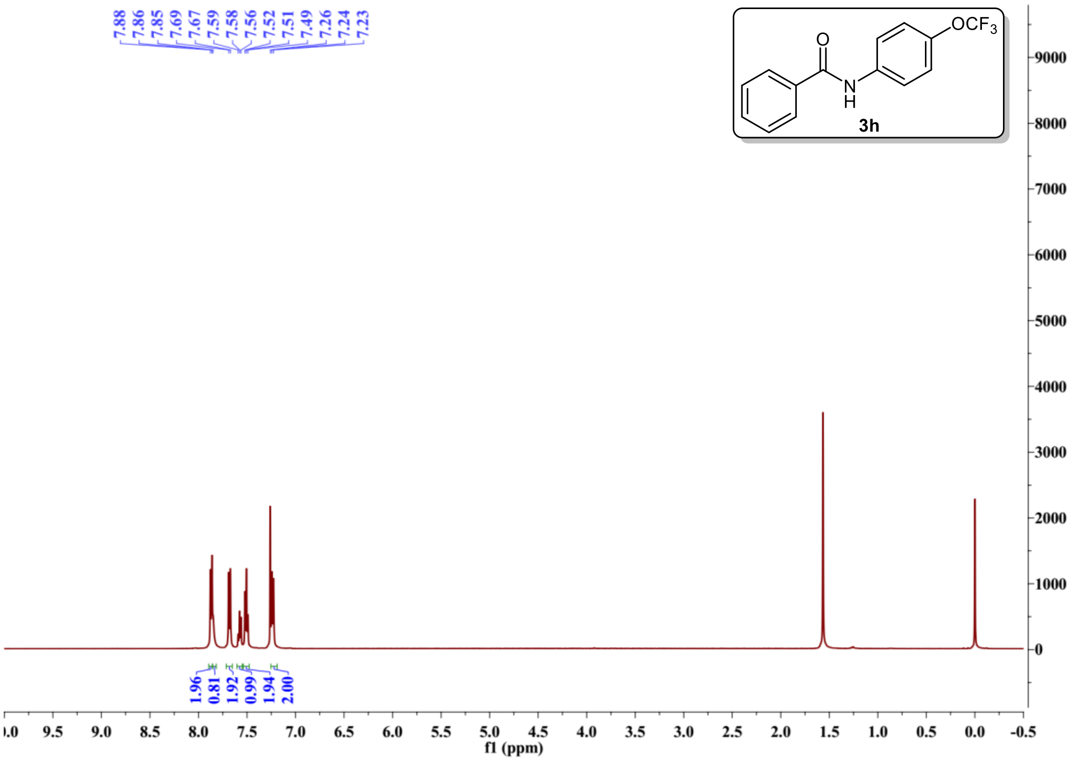
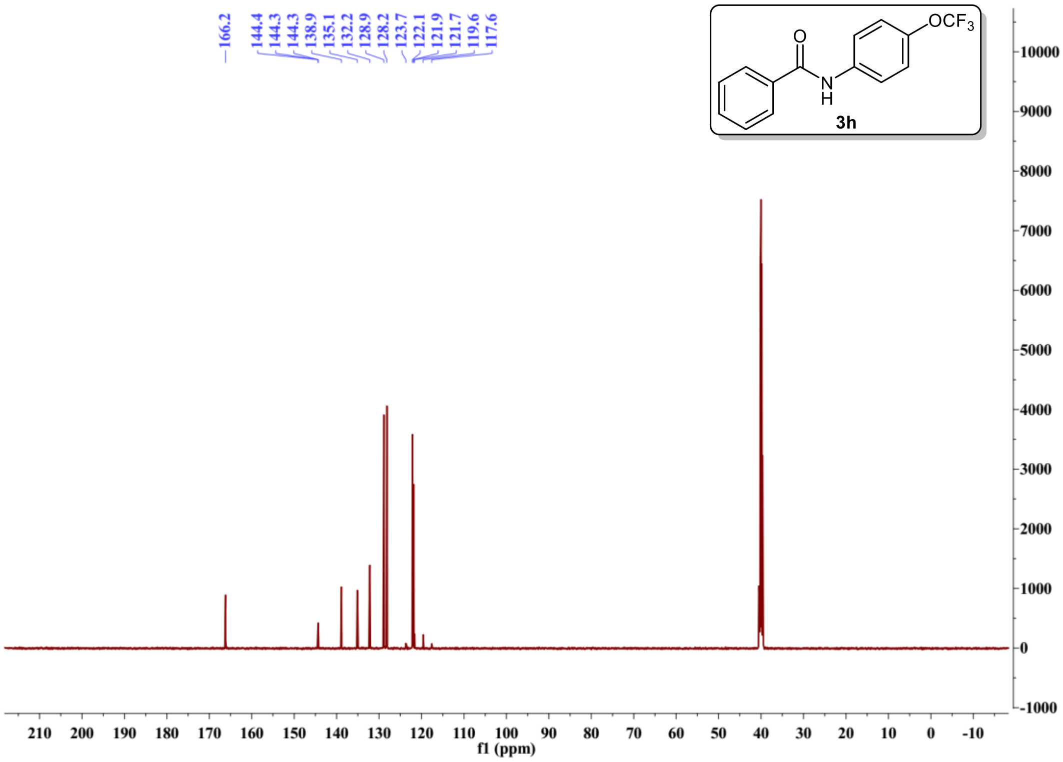


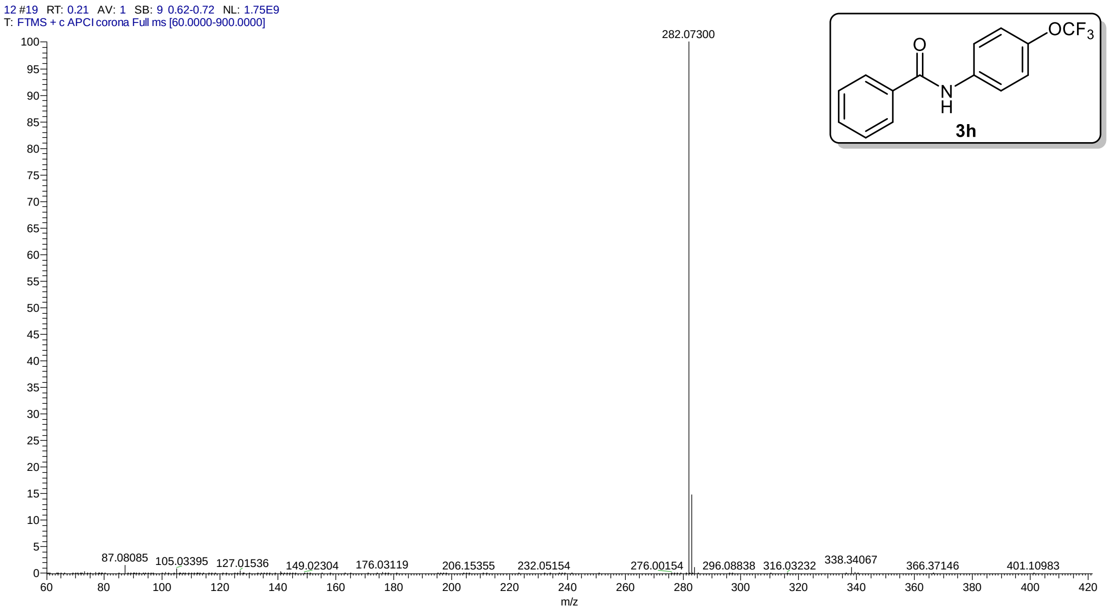
- ^{1}H-NMR spectrum for **3h**



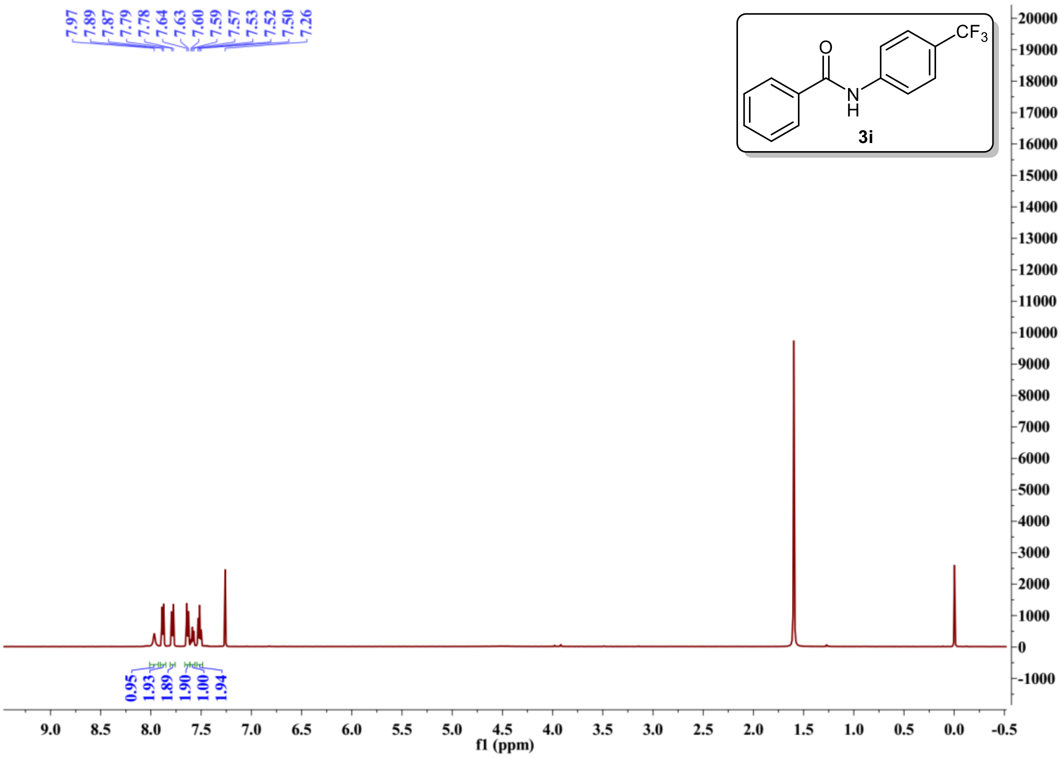
- ^{13}C-NMR spectrum for **3h**



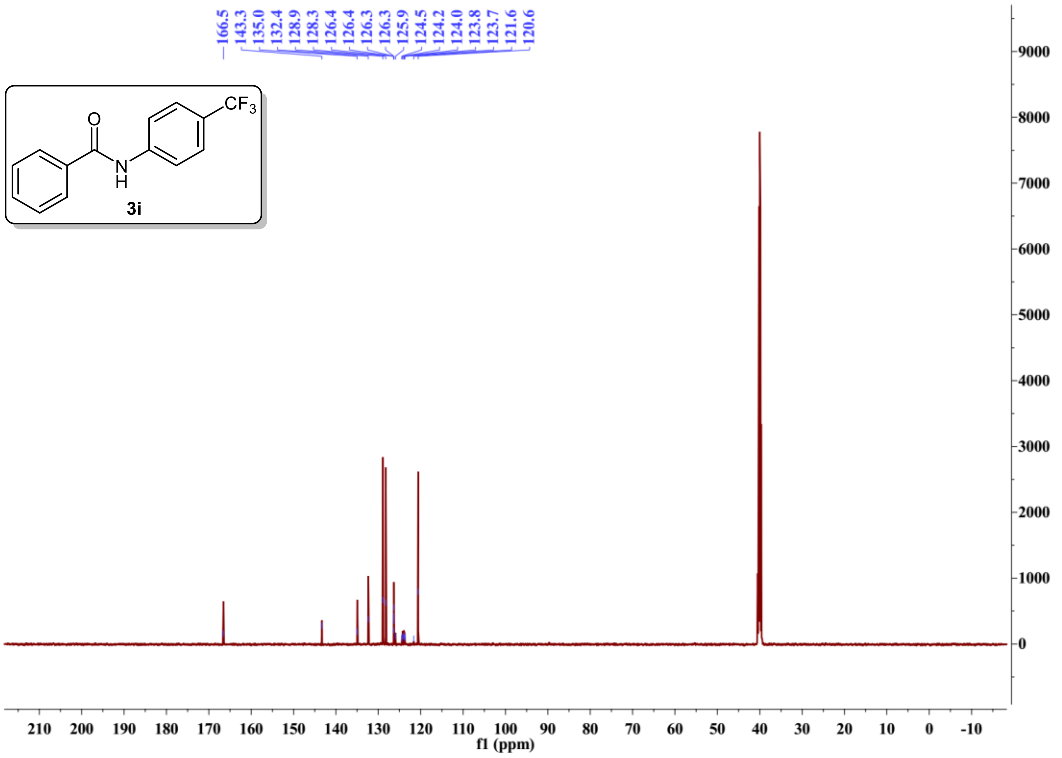
➢ HRMS spectrum for **3h**



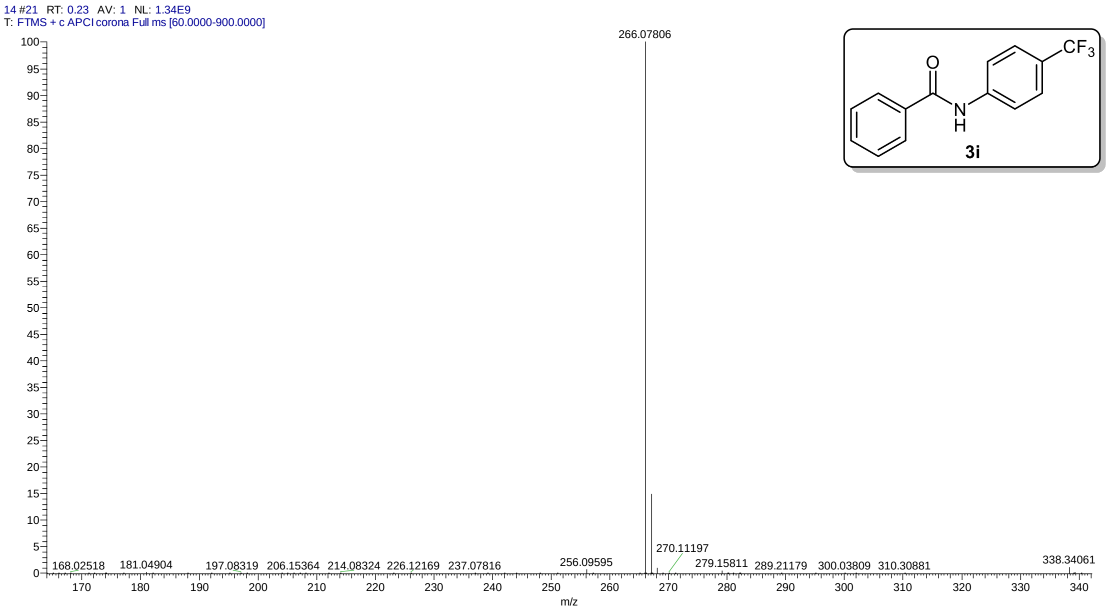
- ^{1}H-NMR spectrum for **3i**



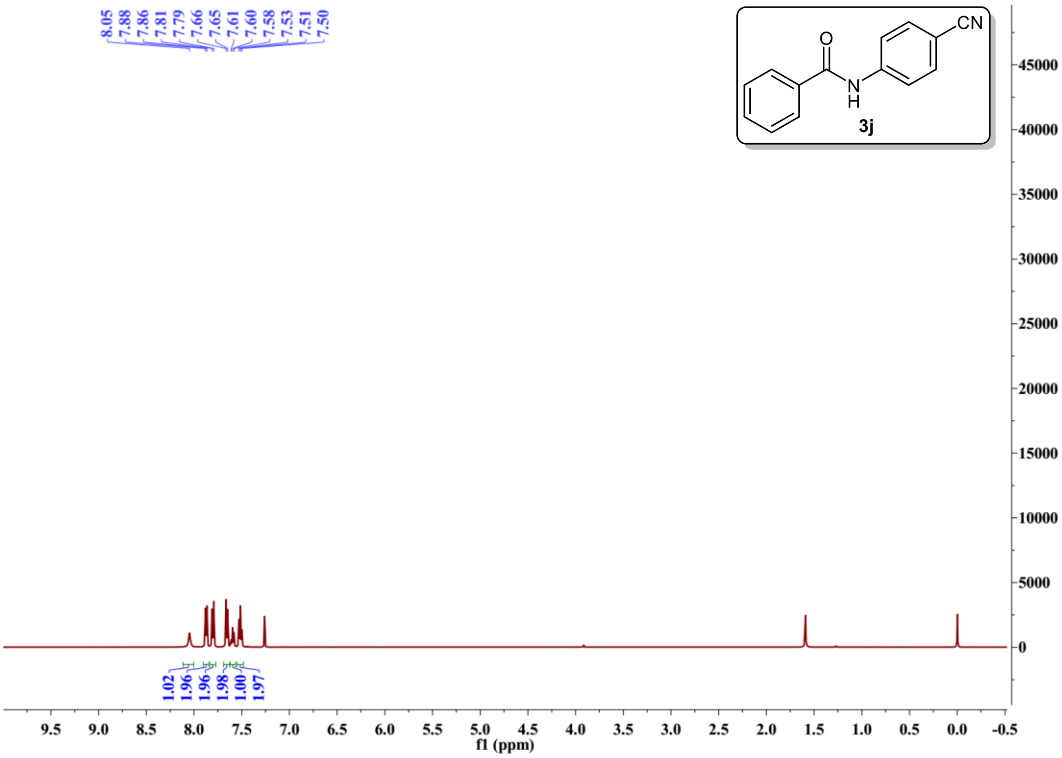
- ^{13}C-NMR spectrum for **3i**



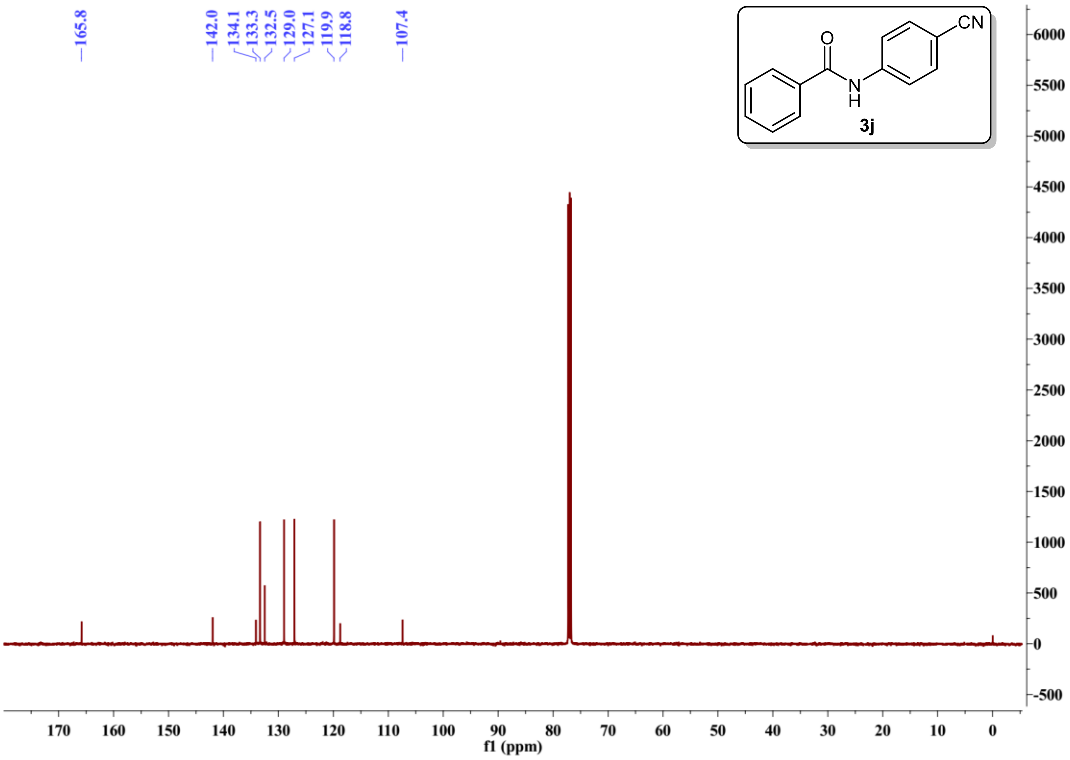
➢ HRMS spectrum for **3i**



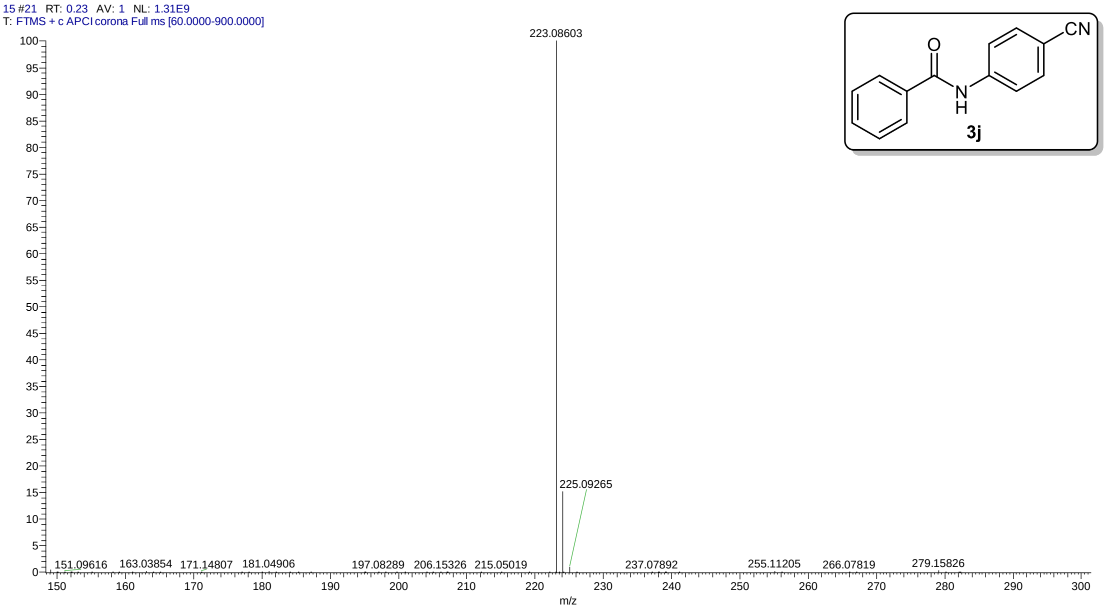
➤ ^{1}H-NMR spectrum for **3j**



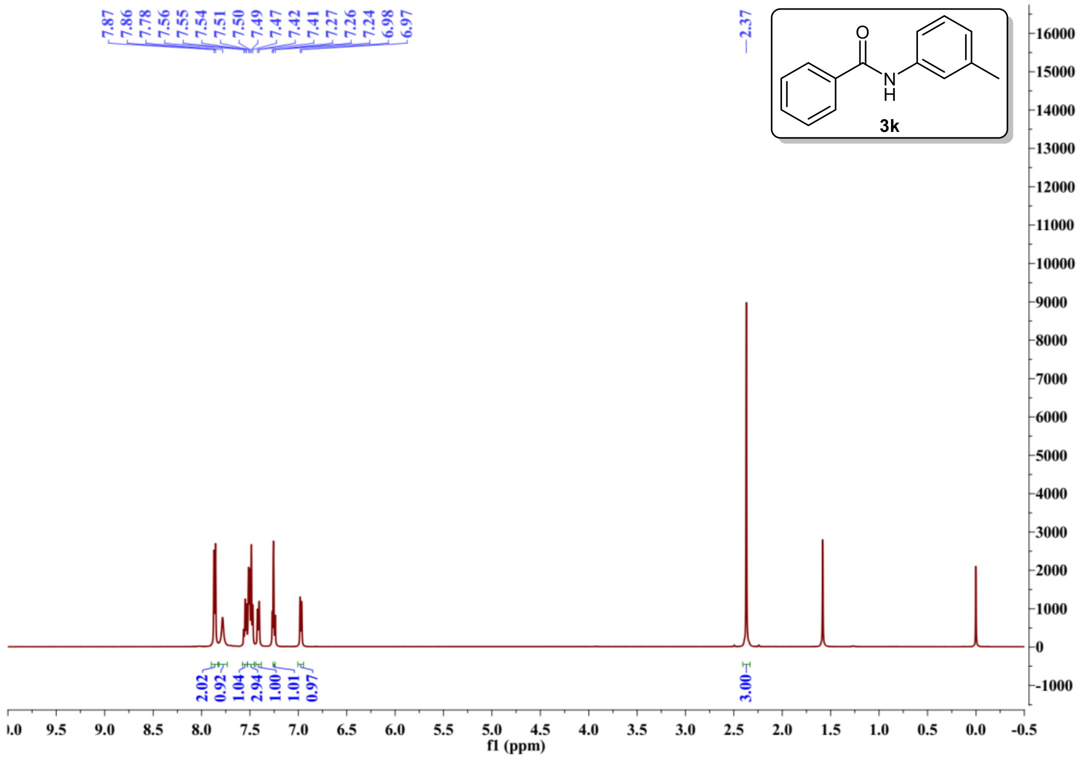
➤ ^{13}C-NMR spectrum for **3j**



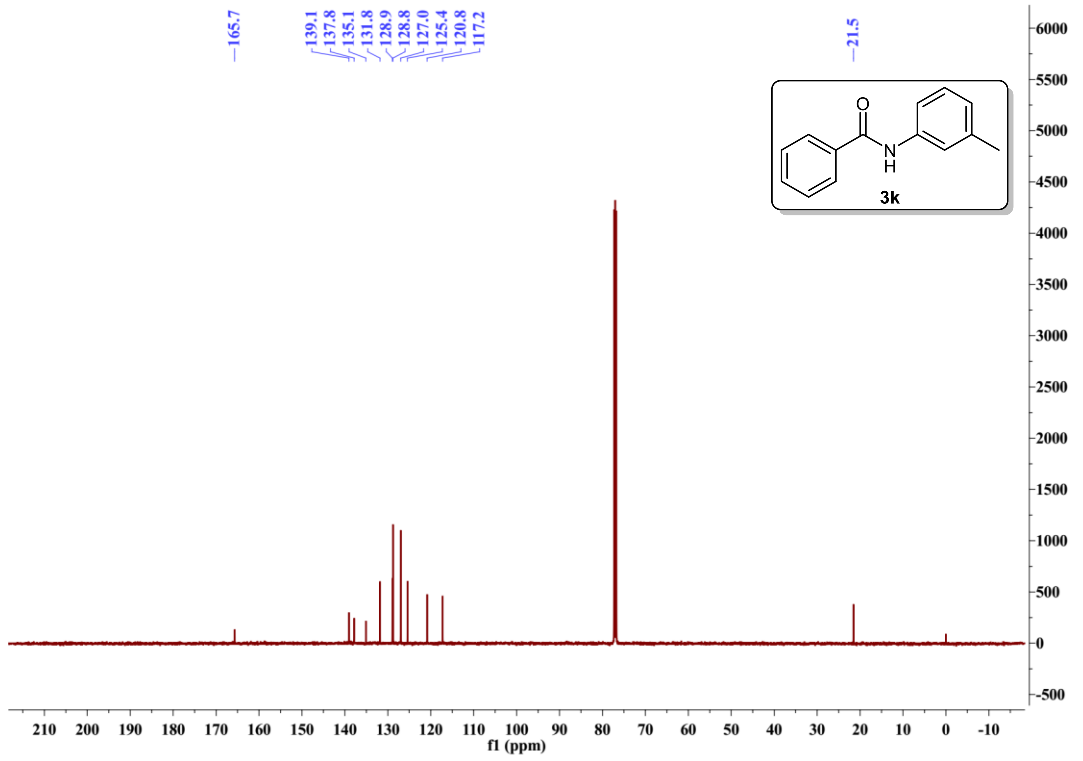
➢ HRMS spectrum for **3j**



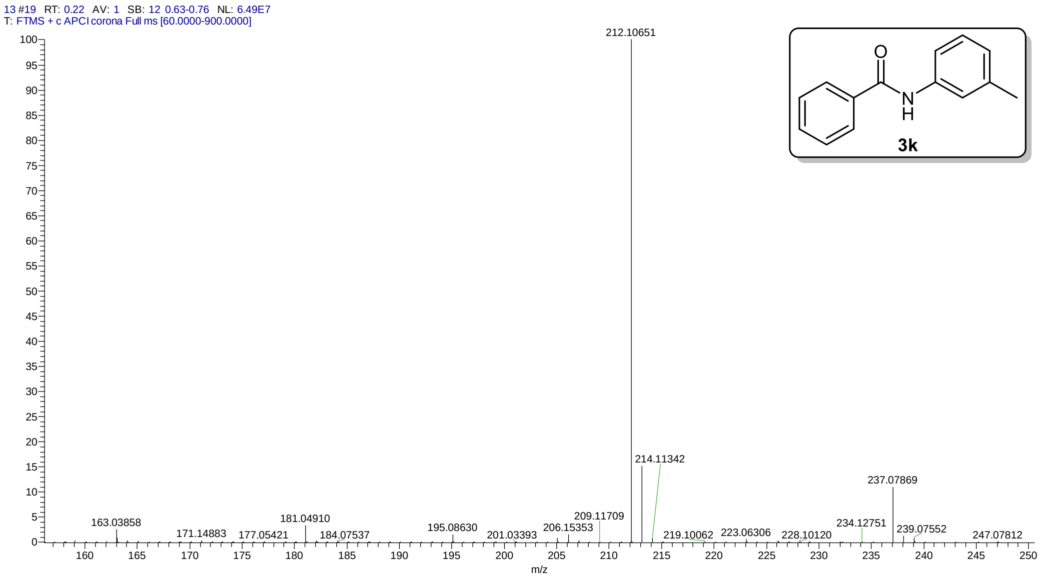
➢ ^{1}H-NMR spectrum for **3k**



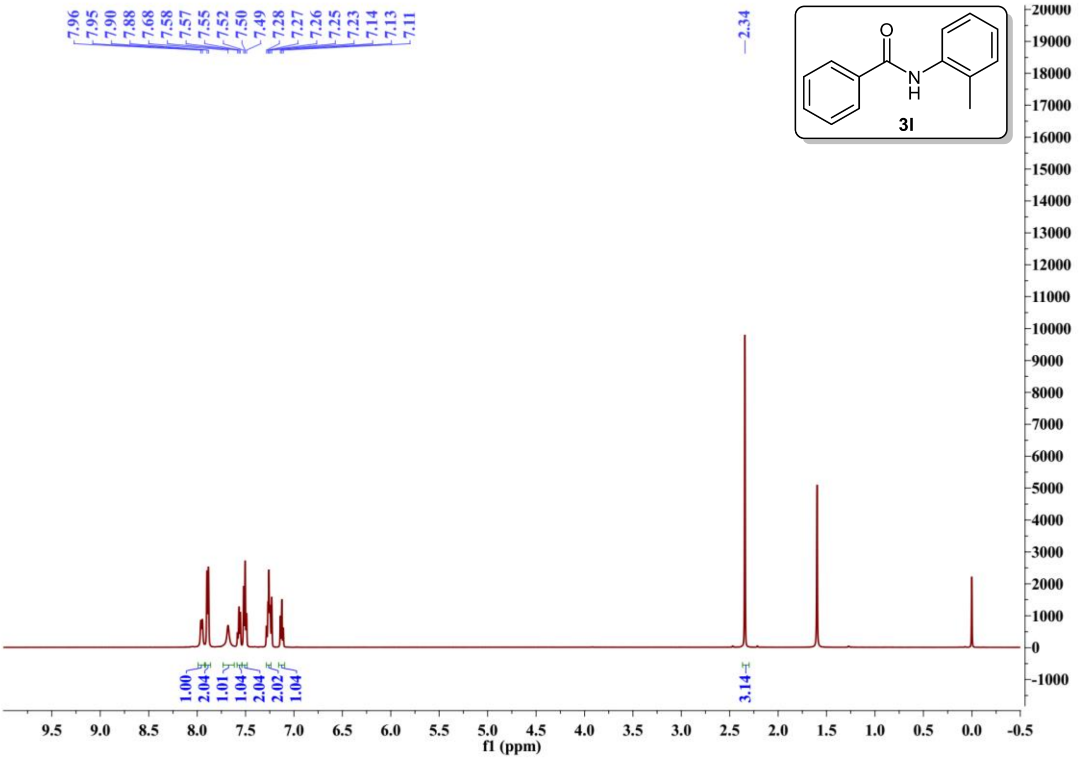
➢ ^{13}C-NMR spectrum for **3k**



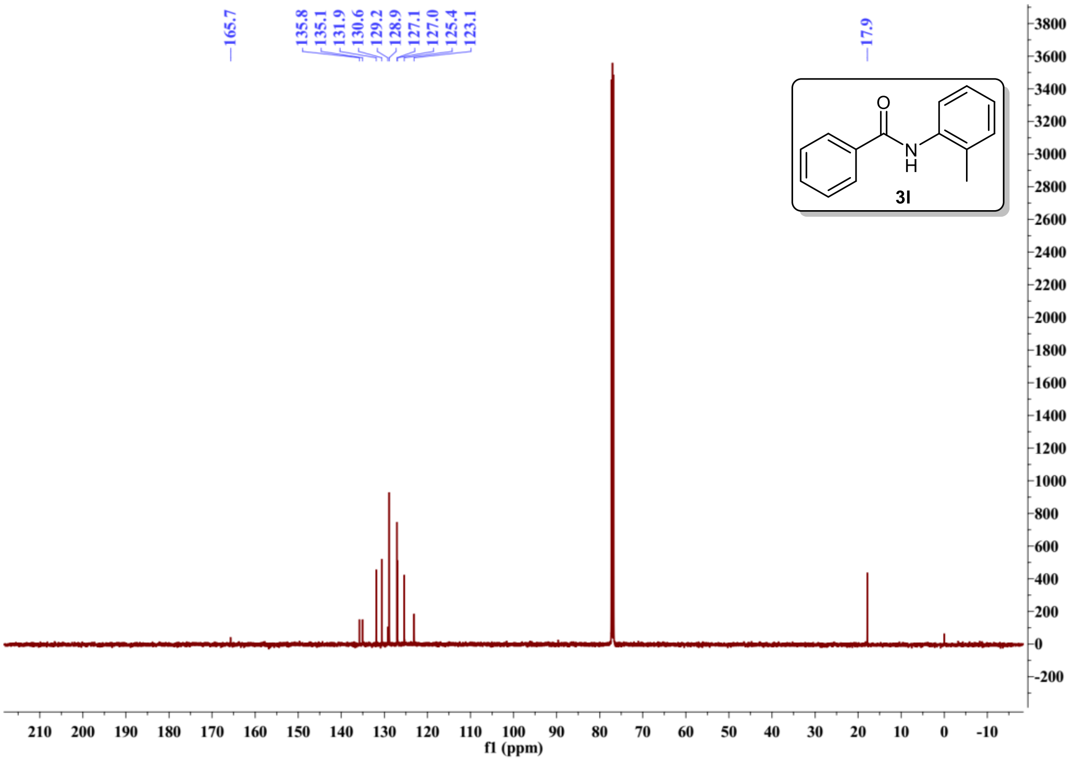
➢ HRMS spectrum for **3k**



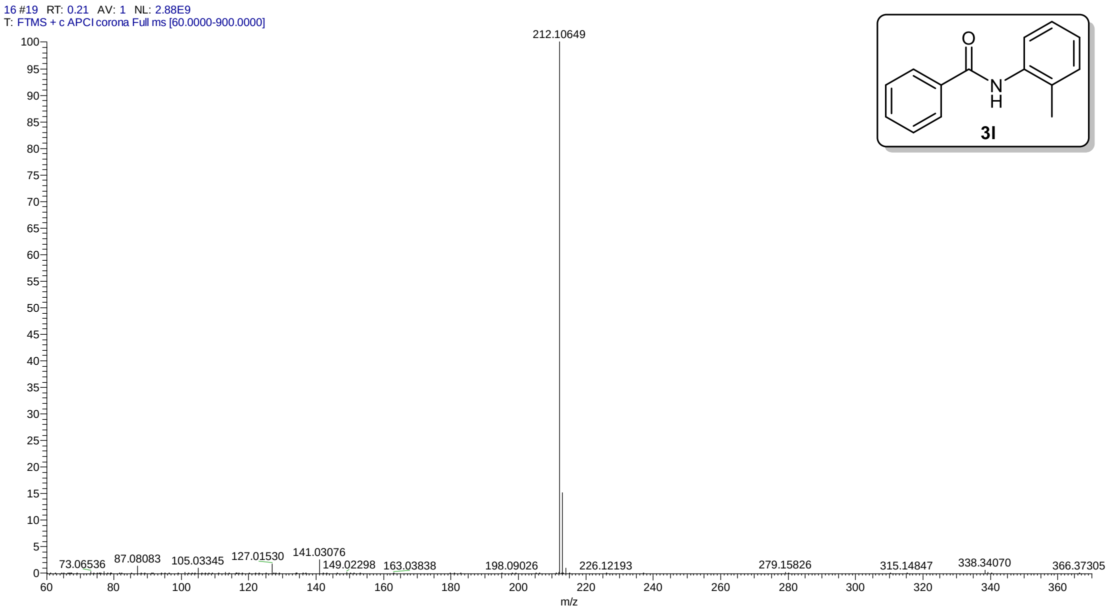
- ^{1}H-NMR spectrum for **3l**



- ^{13}C-NMR spectrum for **3l**

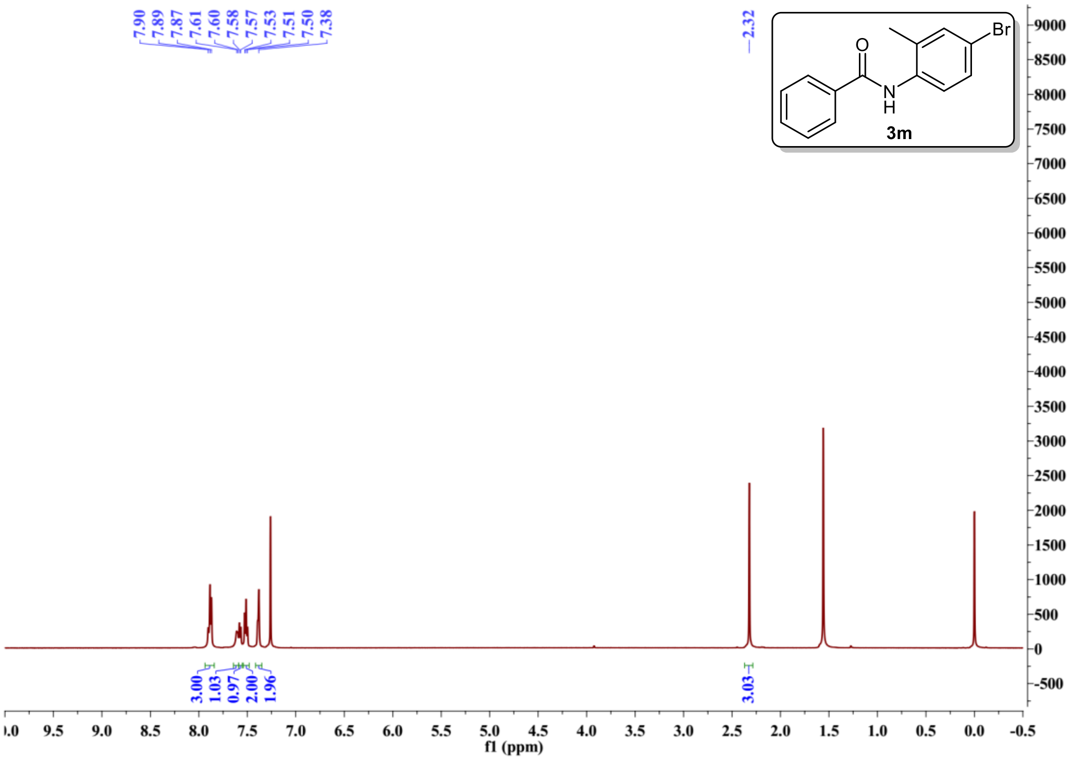


➢ HRMS spectrum for **3l**

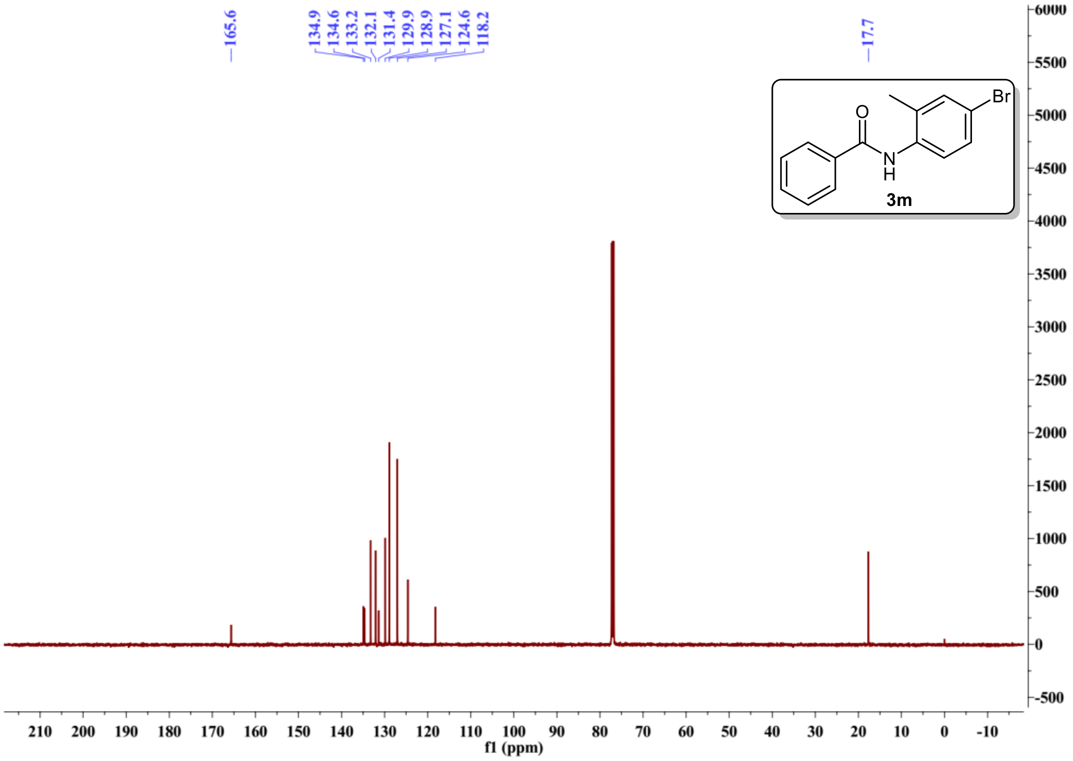


3l

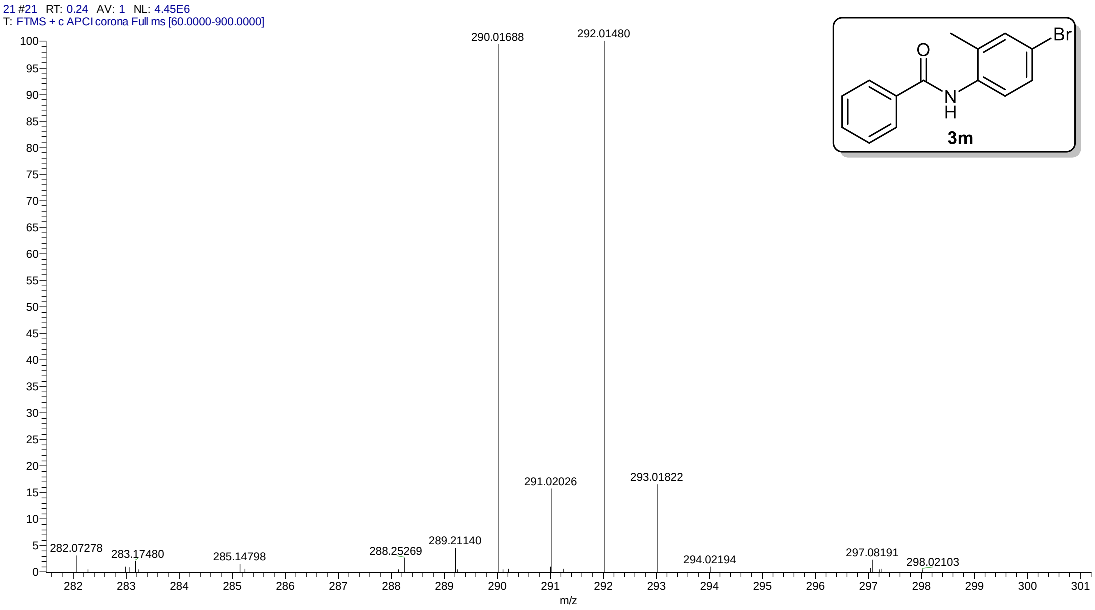
➢ ^{1}H-NMR spectrum for **3m**



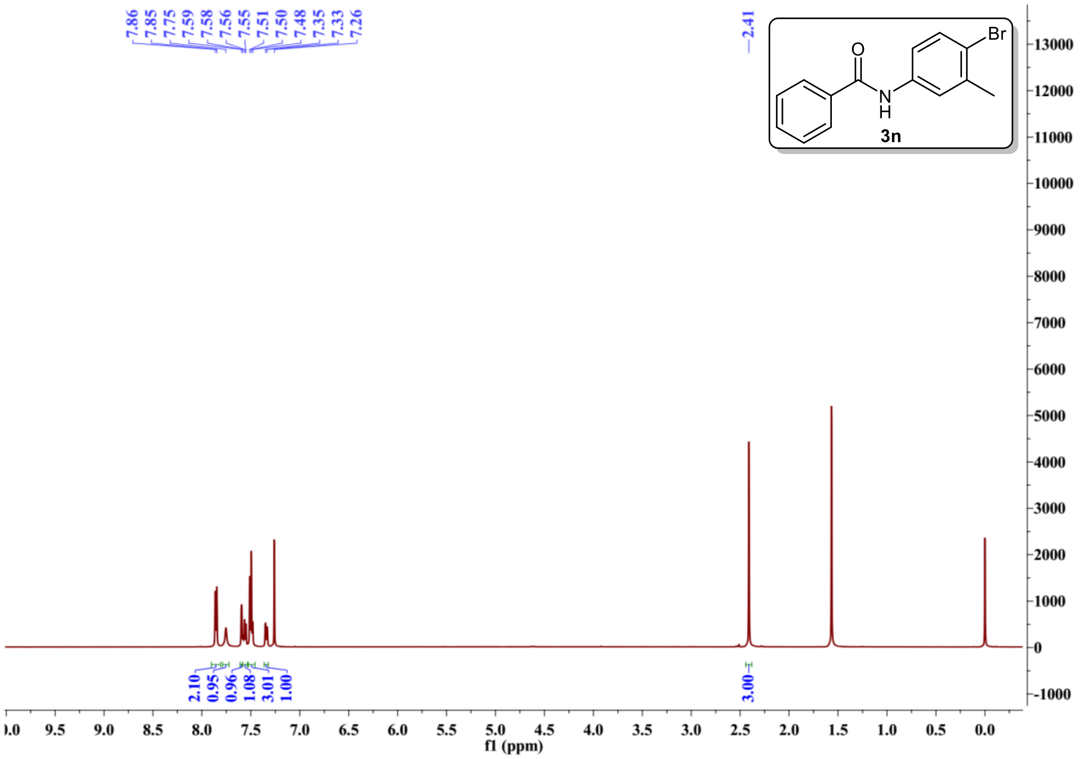
➢ ^{13}C-NMR spectrum for **3m**



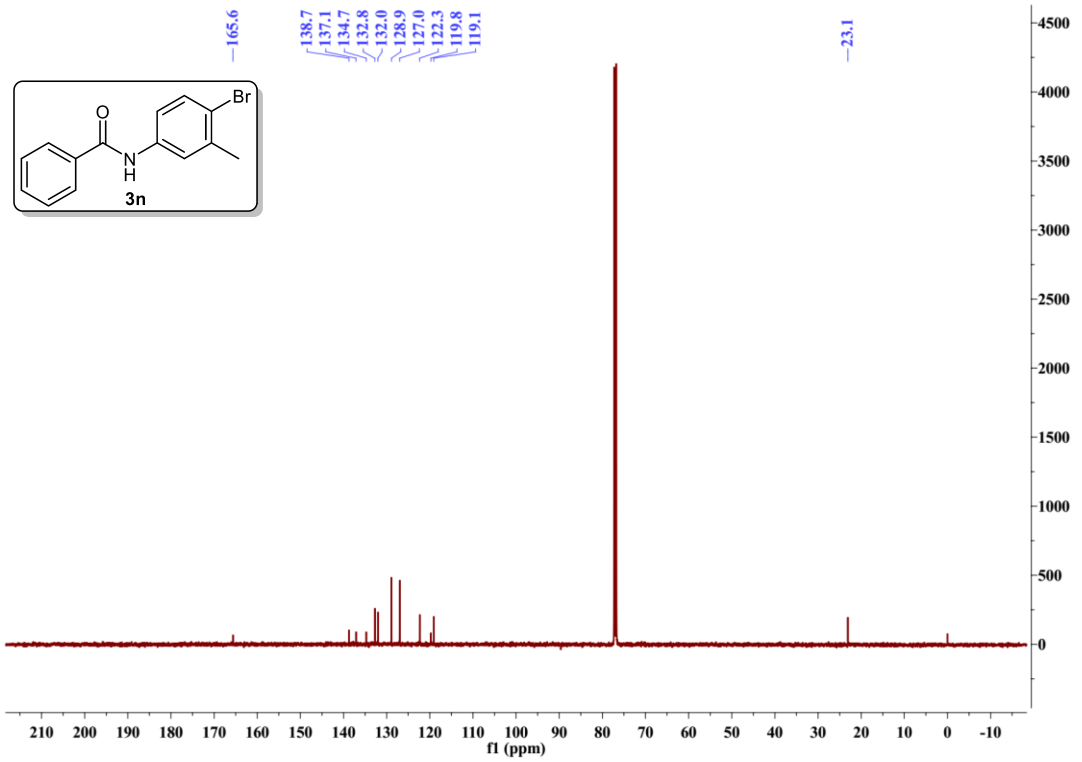
➢ HRMS spectrum for **3m**



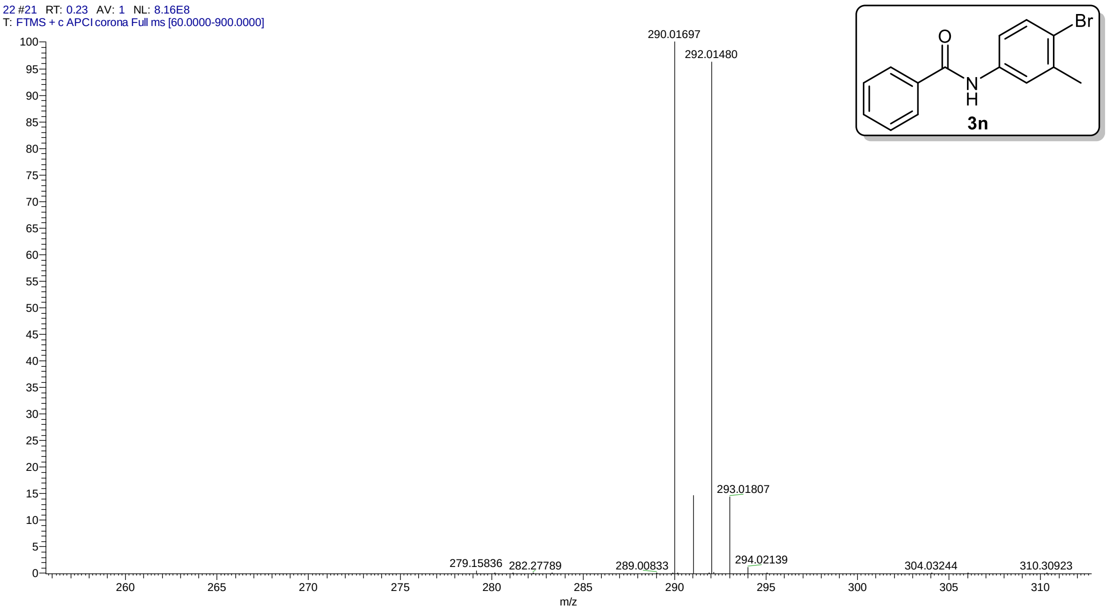
➢ ^{1}H-NMR spectrum for **3n**



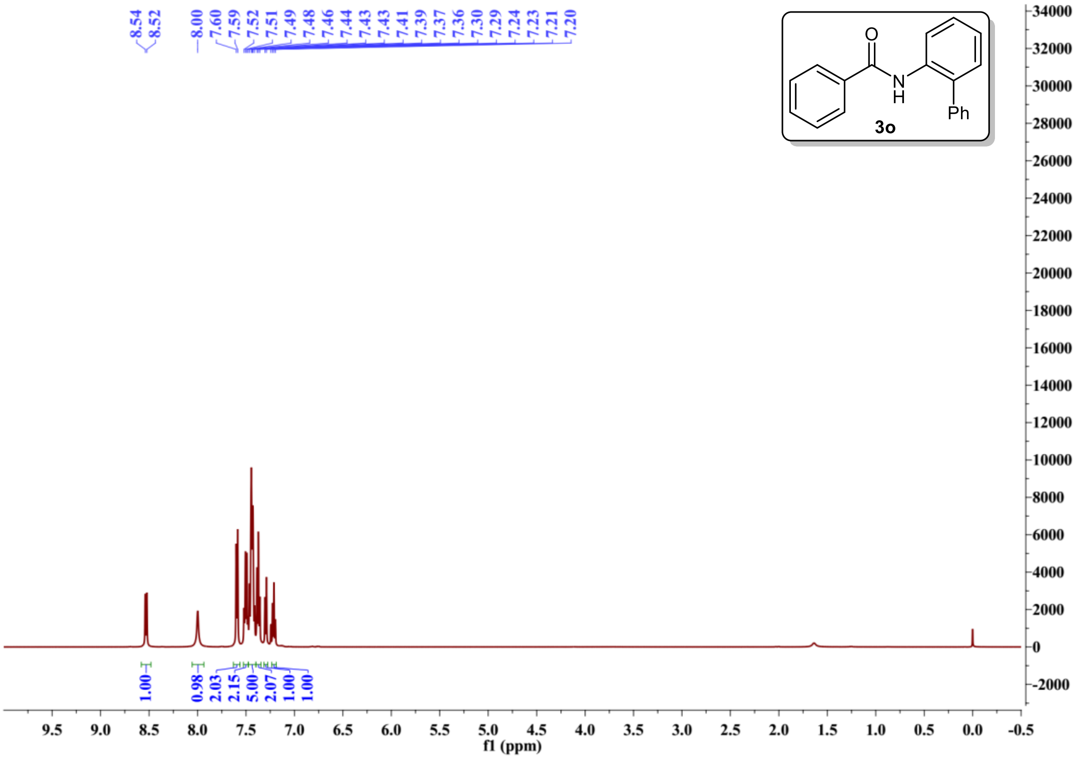
➢ ^{13}C-NMR spectrum for **3n**



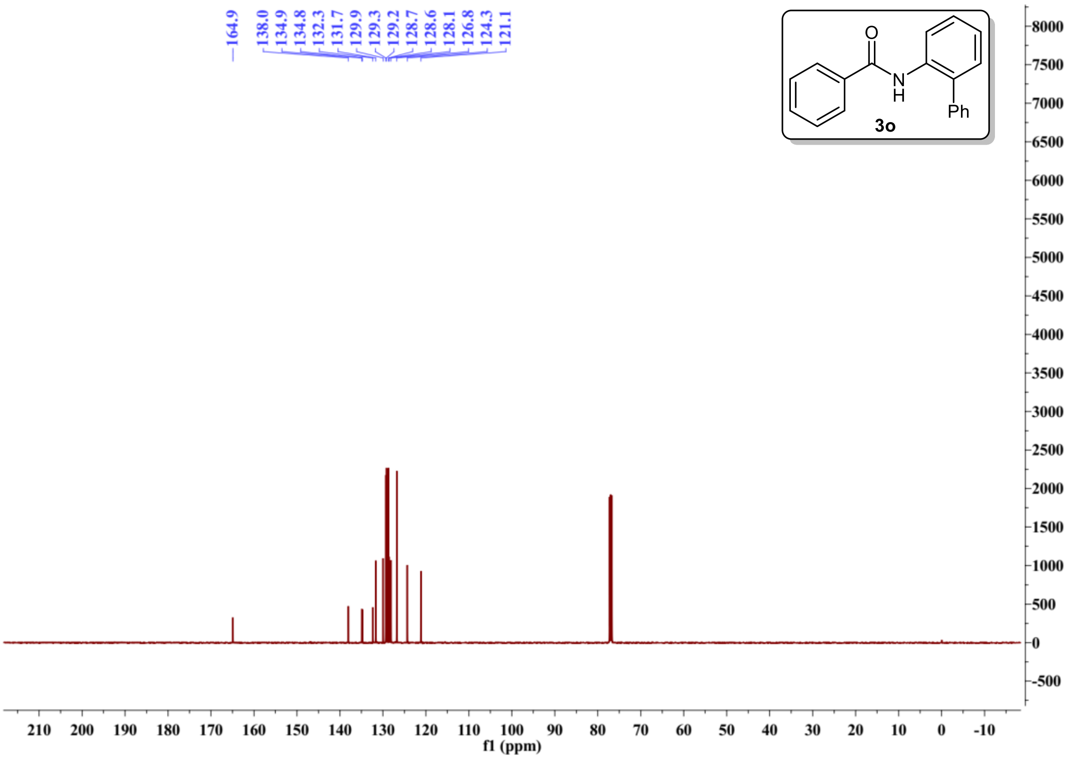
- HRMS spectrum for **3n**



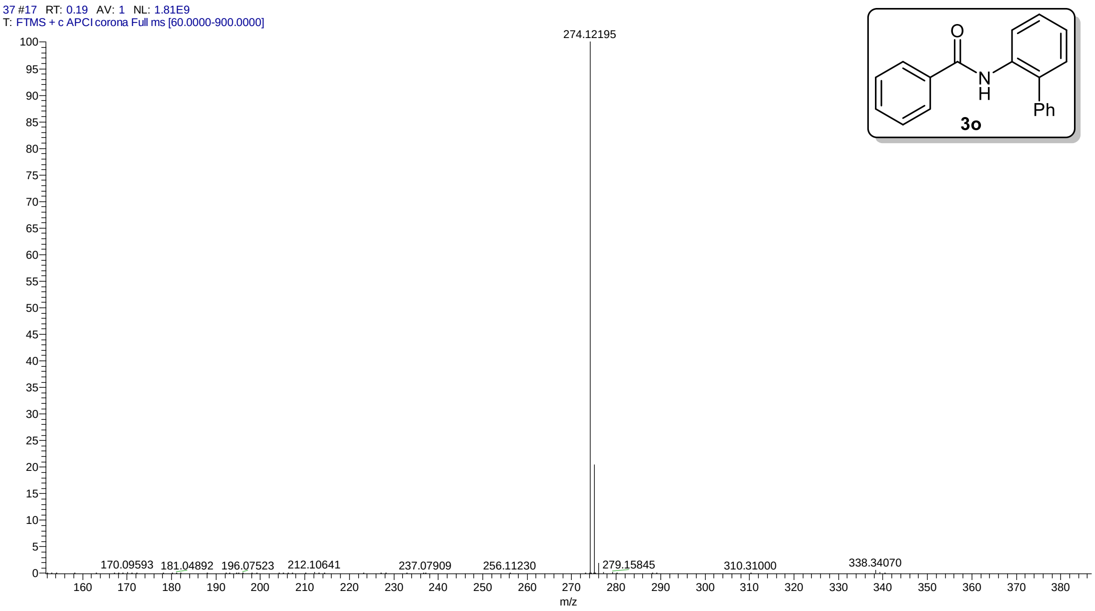
➢ ^{1}H-NMR spectrum for **3o**



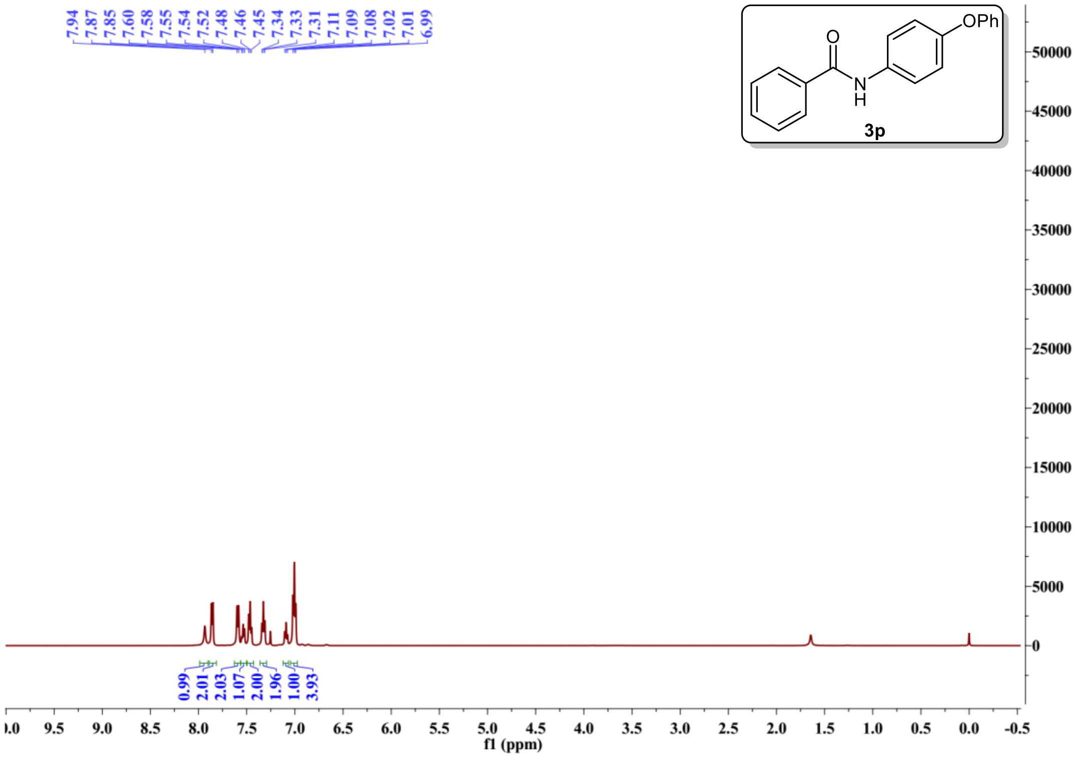
➢ ^{13}C-NMR spectrum for **3o**



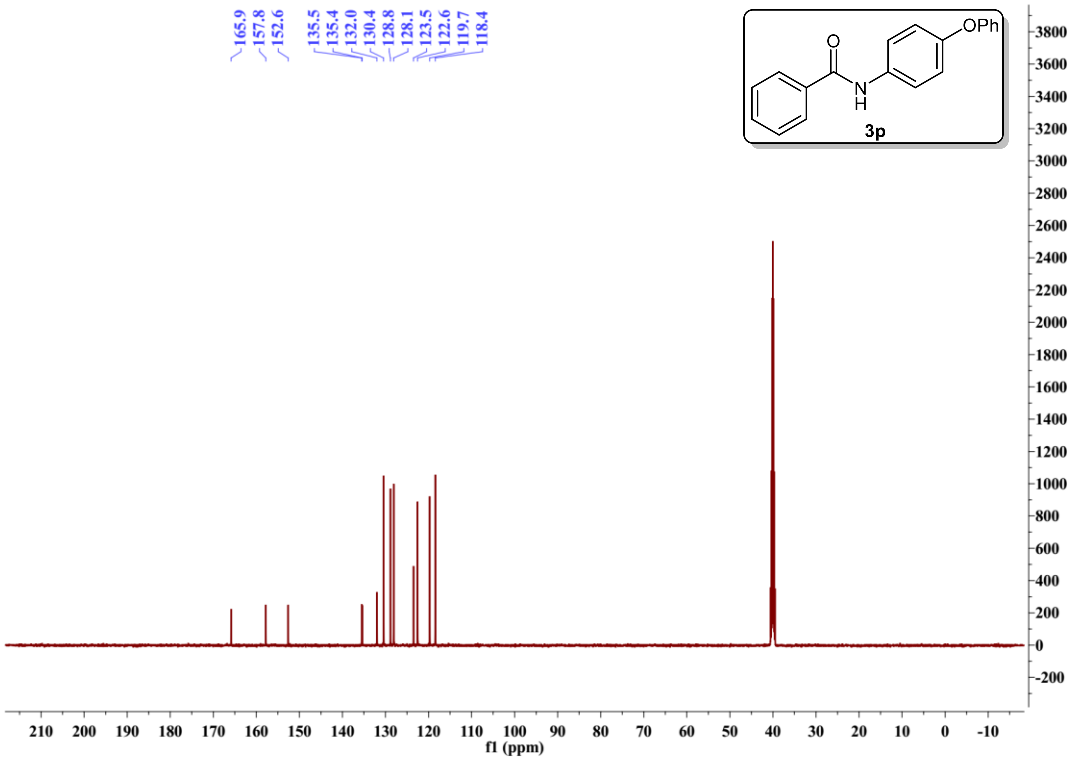
➢ HRMS spectrum for **3o**



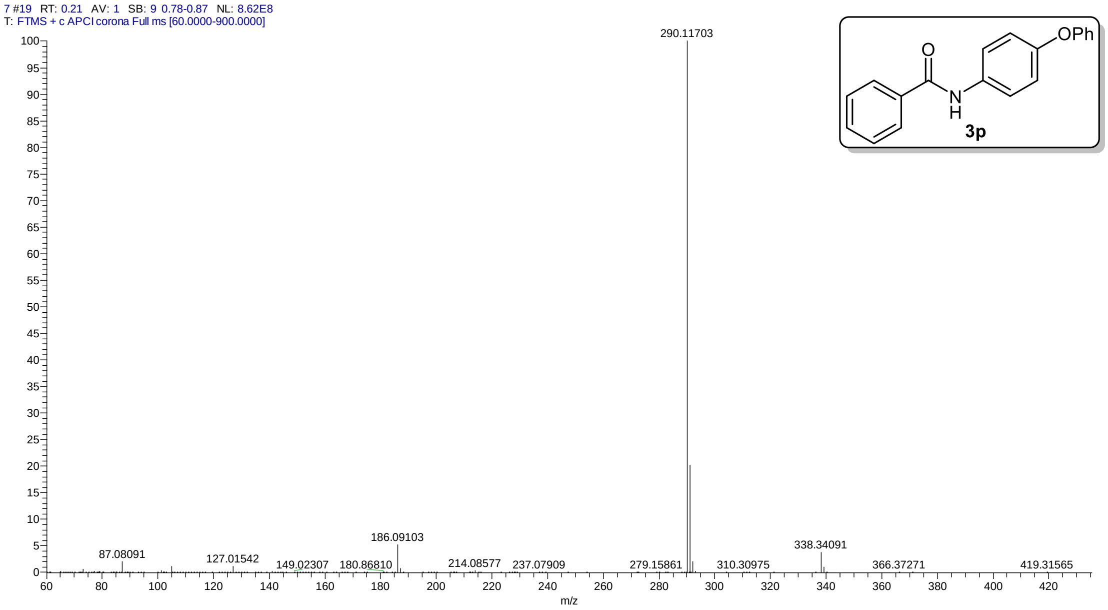
- ^{1}H-NMR spectrum for **3p**



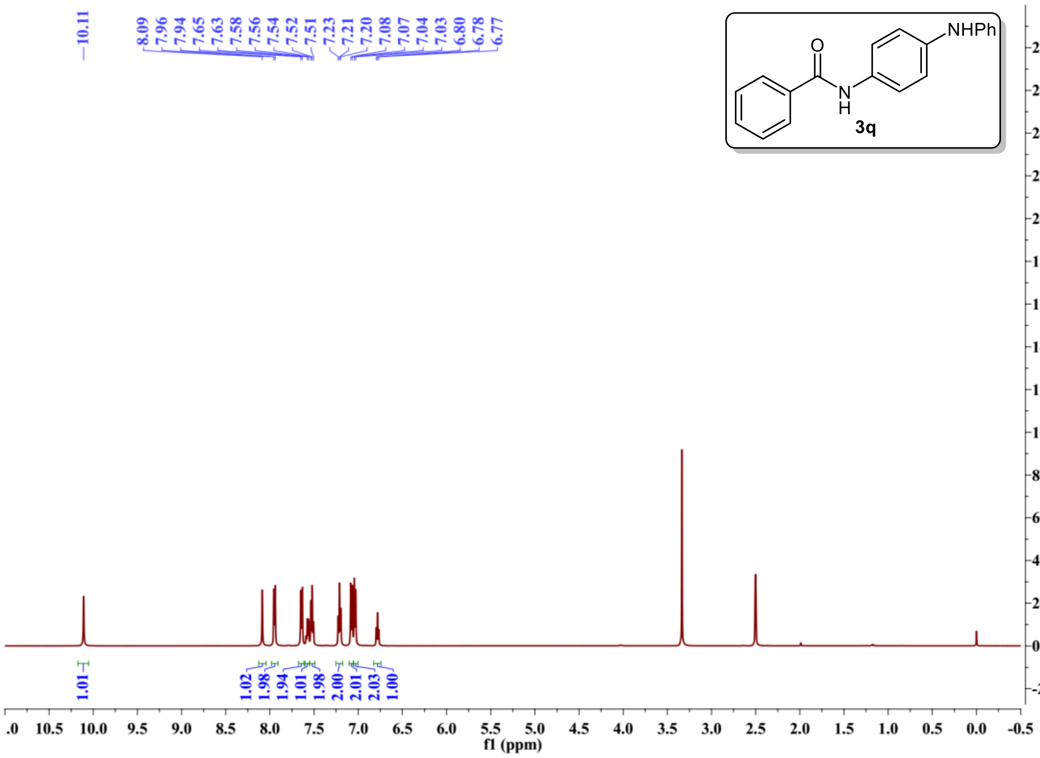
- ^{13}C-NMR spectrum for **3p**



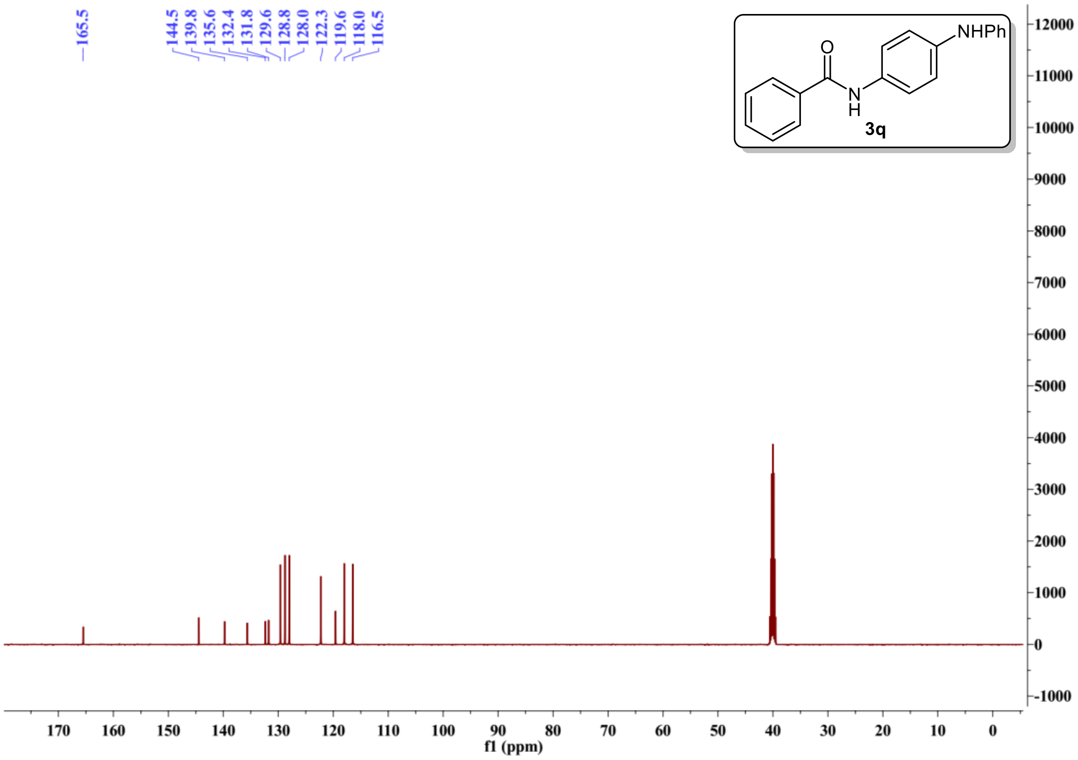
➢ HRMS spectrum for **3p**



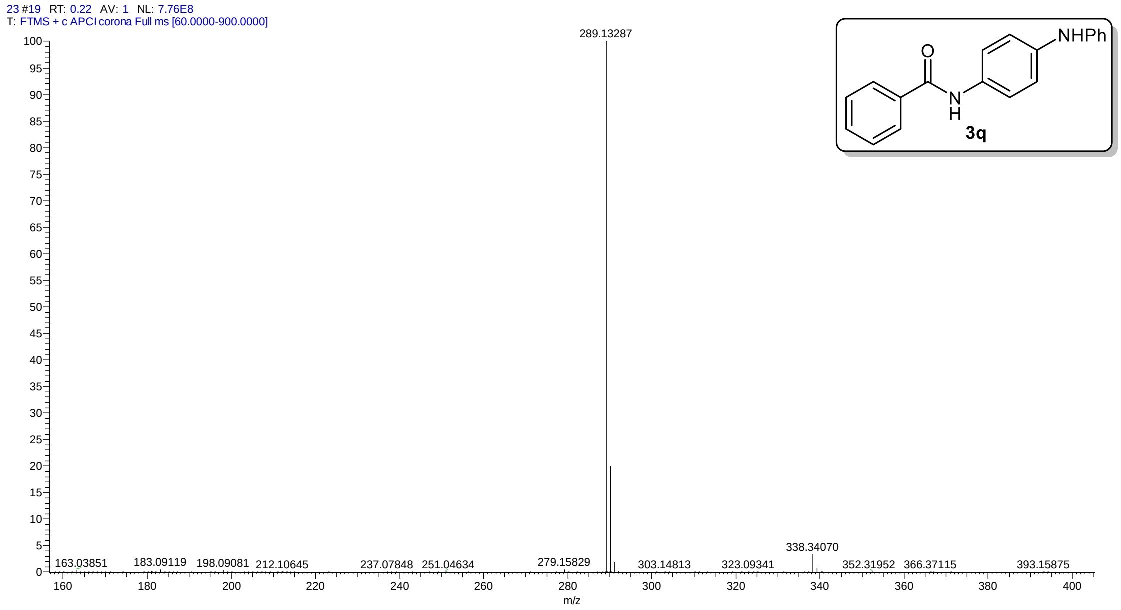
- ^{1}H-NMR spectrum for **3q**



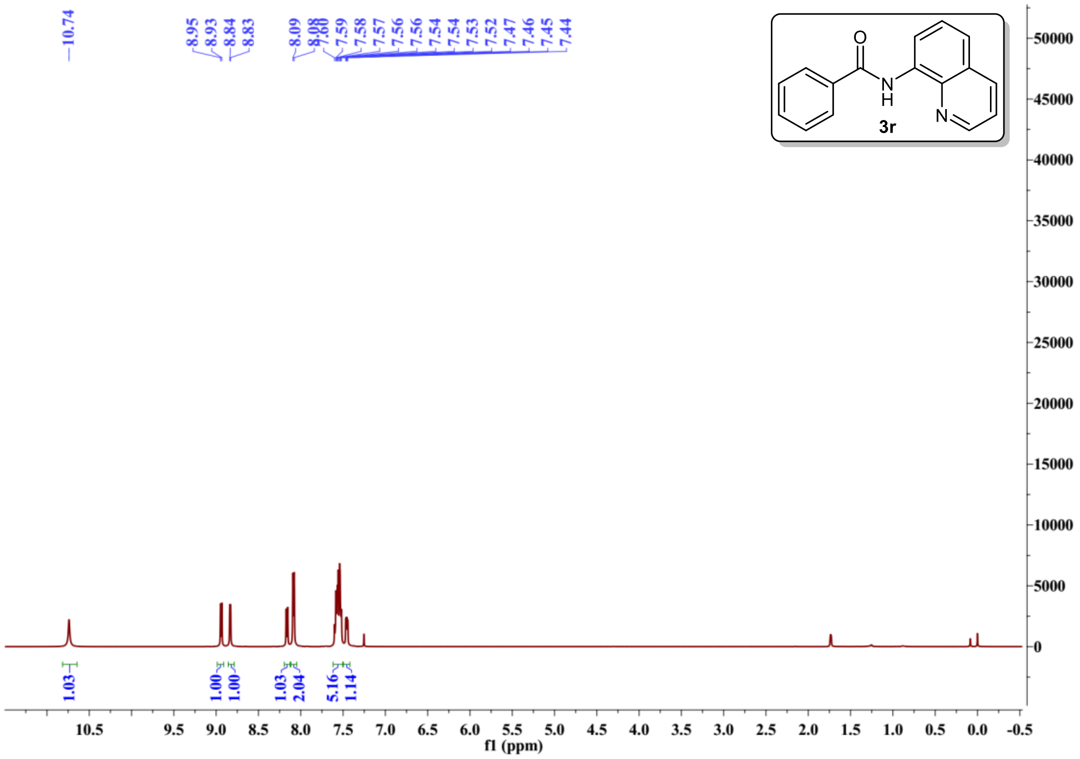
- ^{13}C-NMR spectrum for **3q**



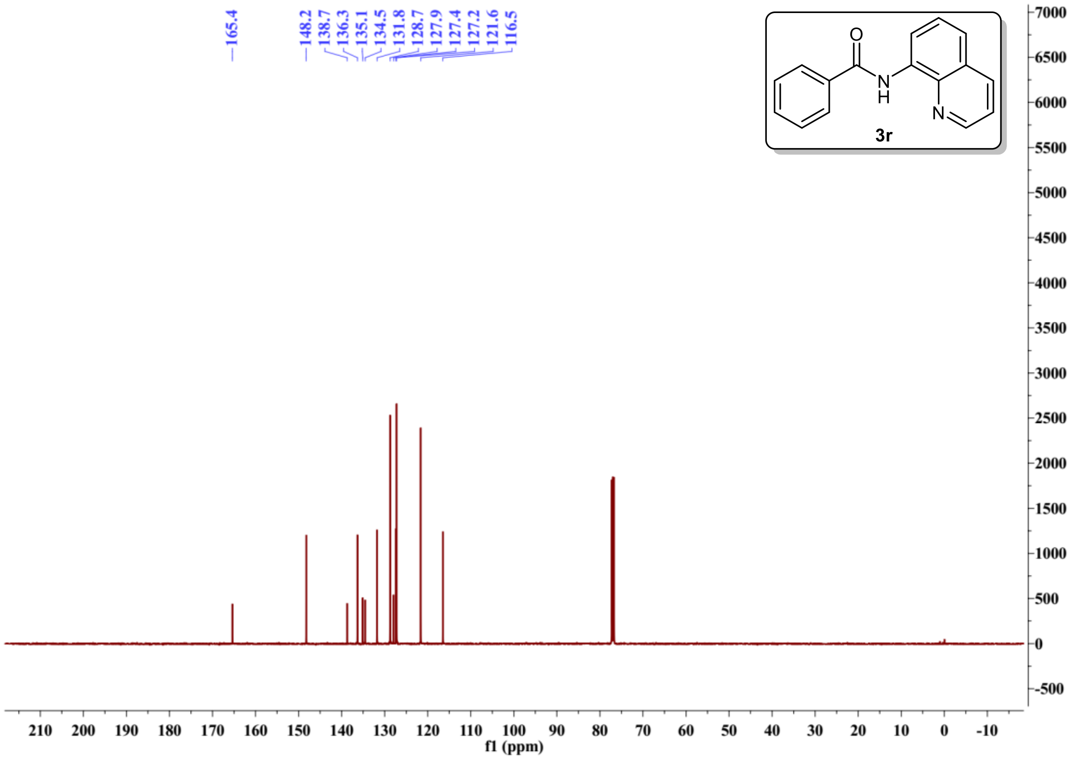
➢ HRMS spectrum for **3q**



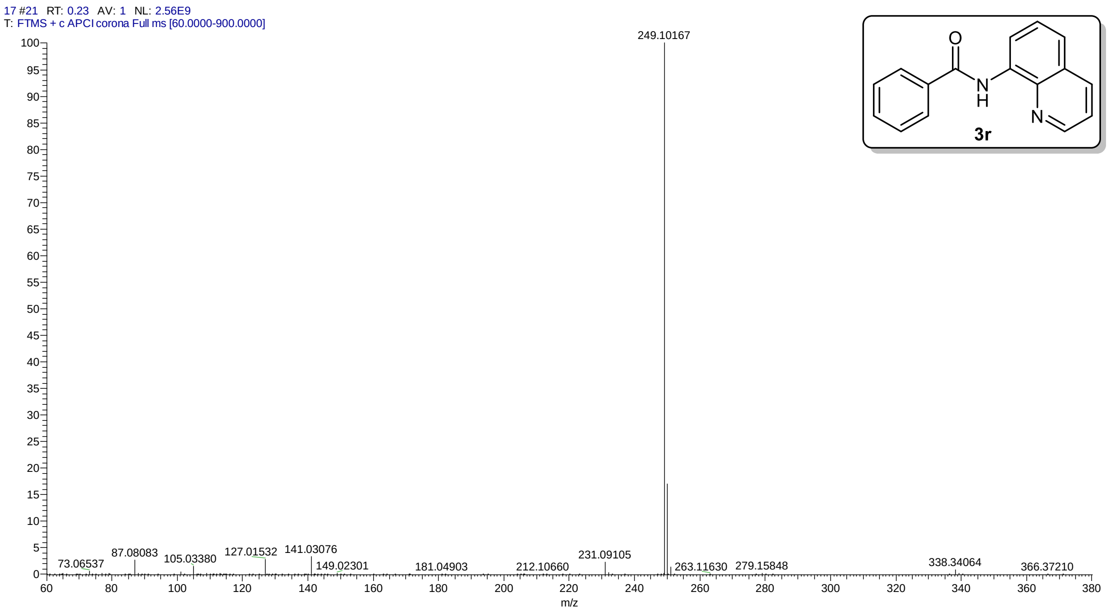
- ^{1}H-NMR spectrum for **3r**



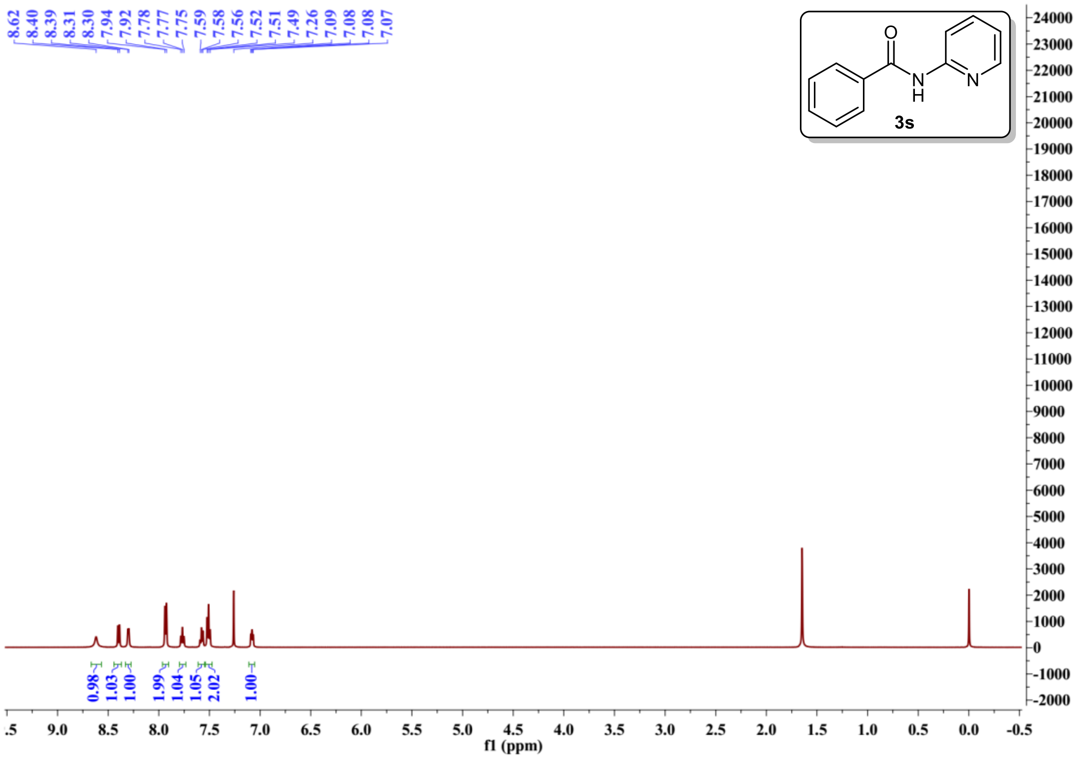
- ^{13}C-NMR spectrum for **3r**



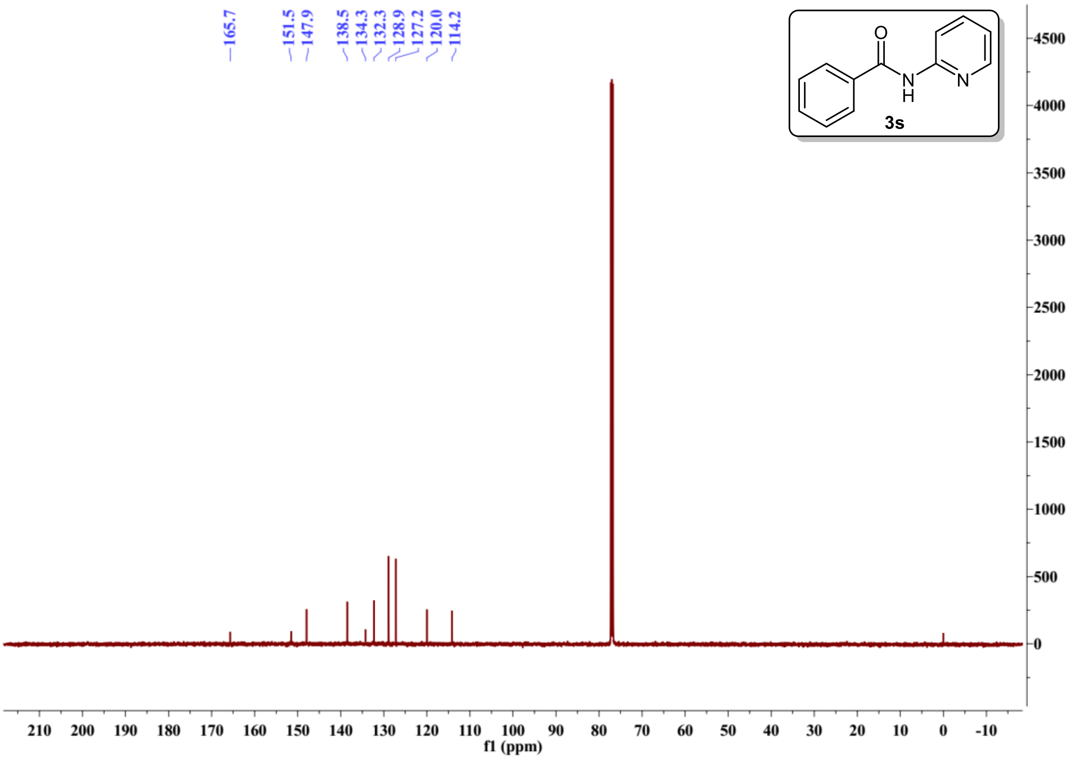
➢ HRMS spectrum for **3r**



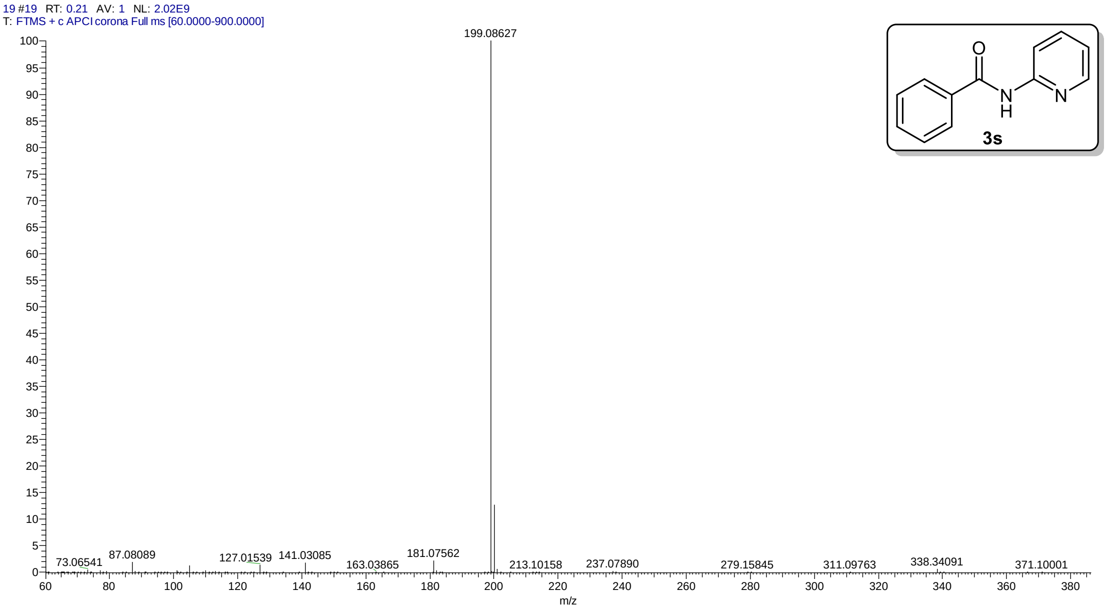
- ^{1}H-NMR spectrum for **3s**



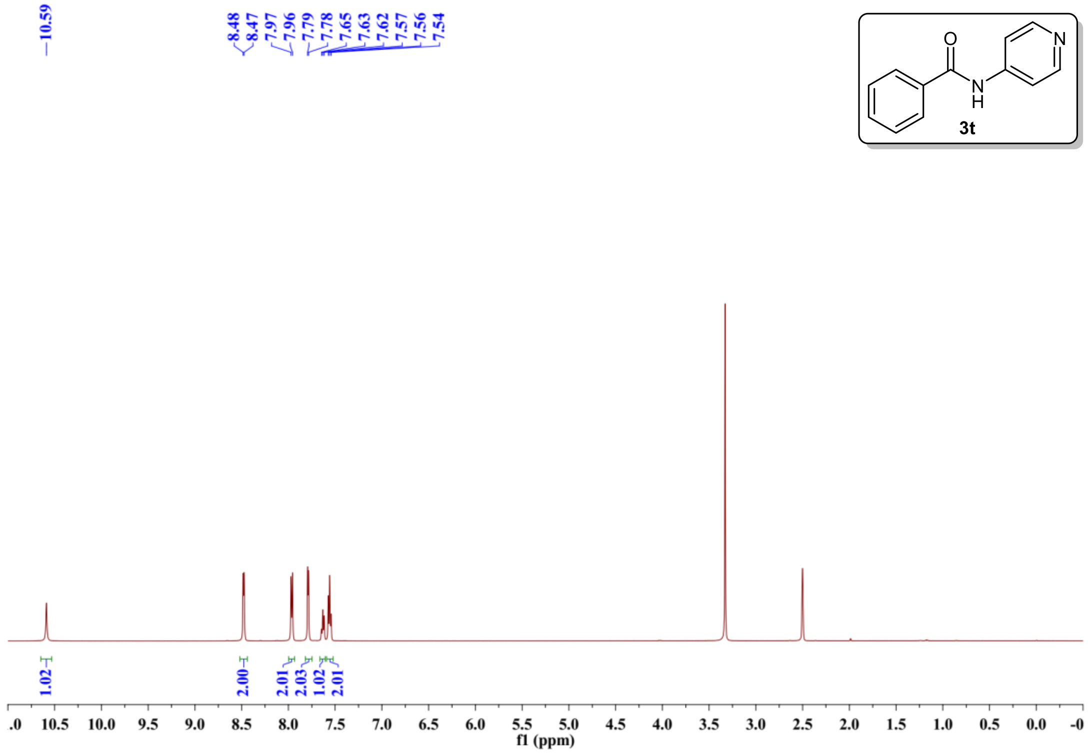
- ^{13}C-NMR spectrum for **3s**



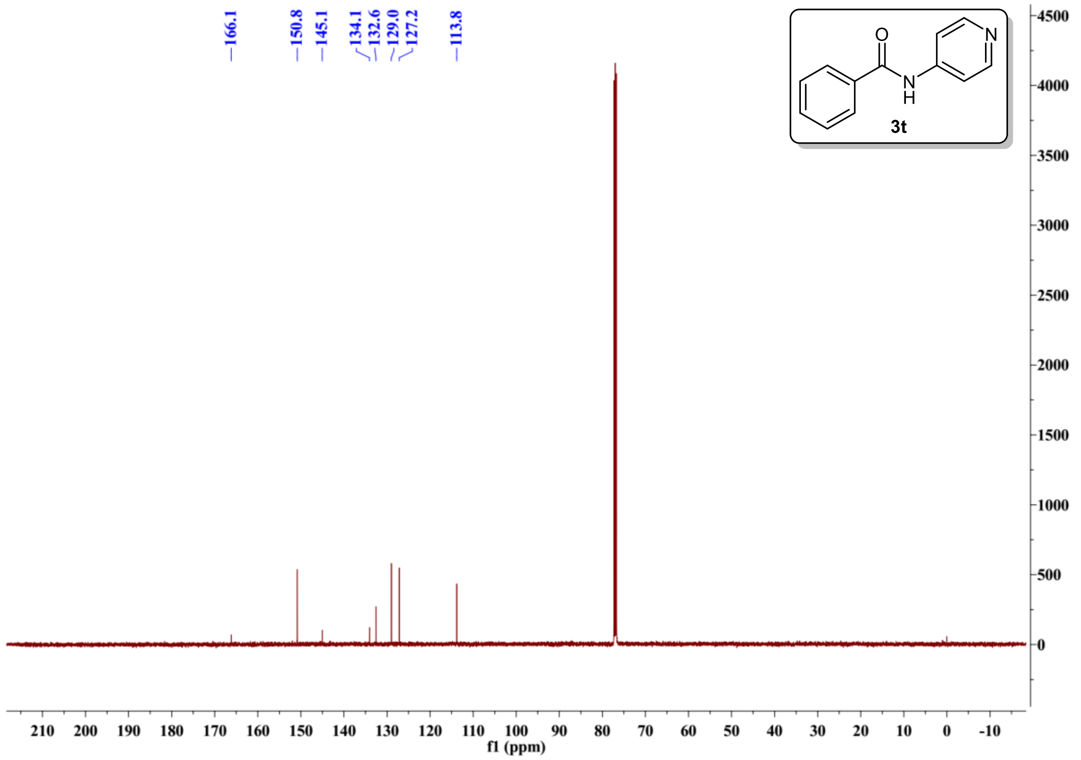
➢ HRMS spectrum for **3s**



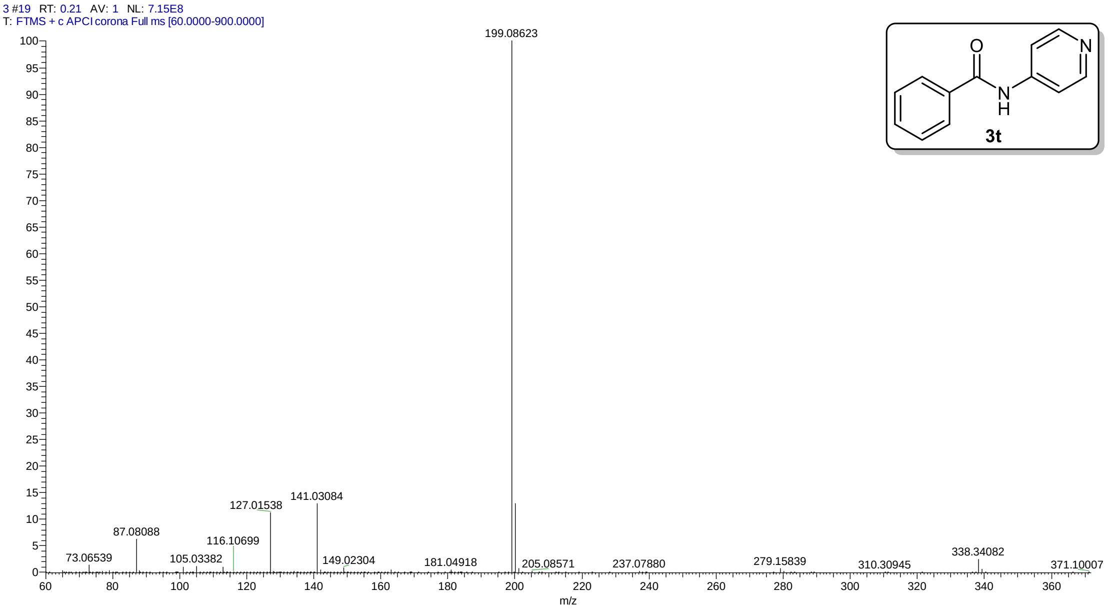
➢ ^{1}H-NMR spectrum for **3t**



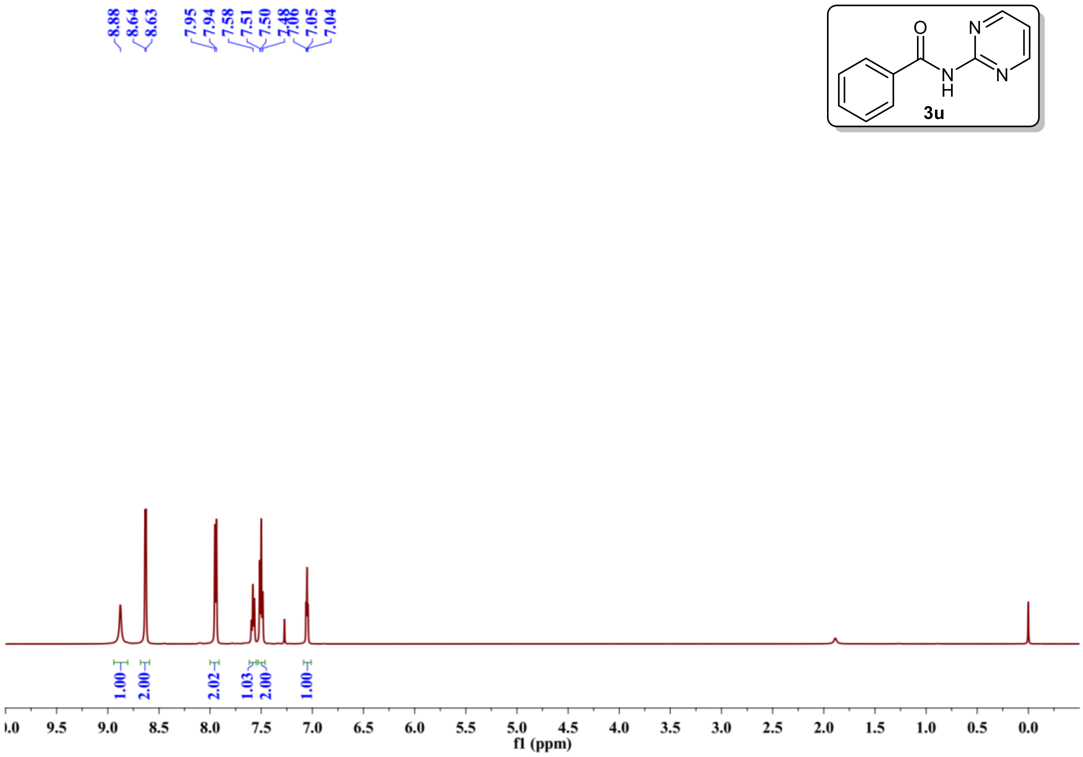
➢ ^{13}C-NMR spectrum for **3t**



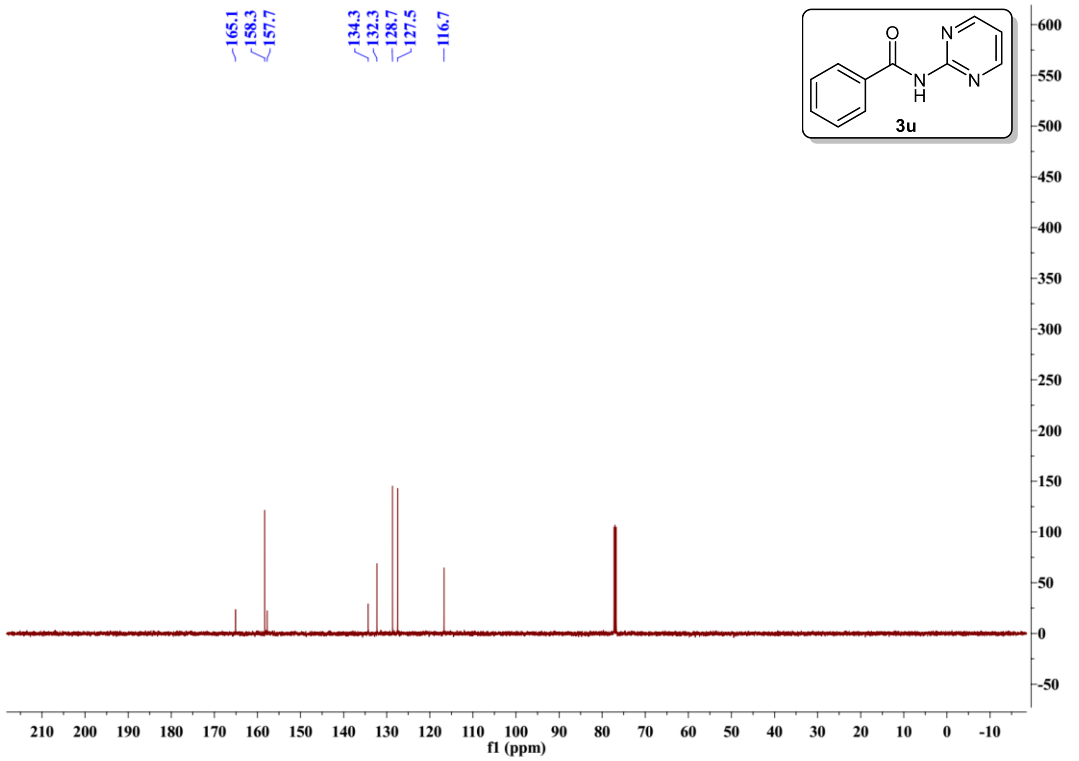
➢ HRMS spectrum for **3t**



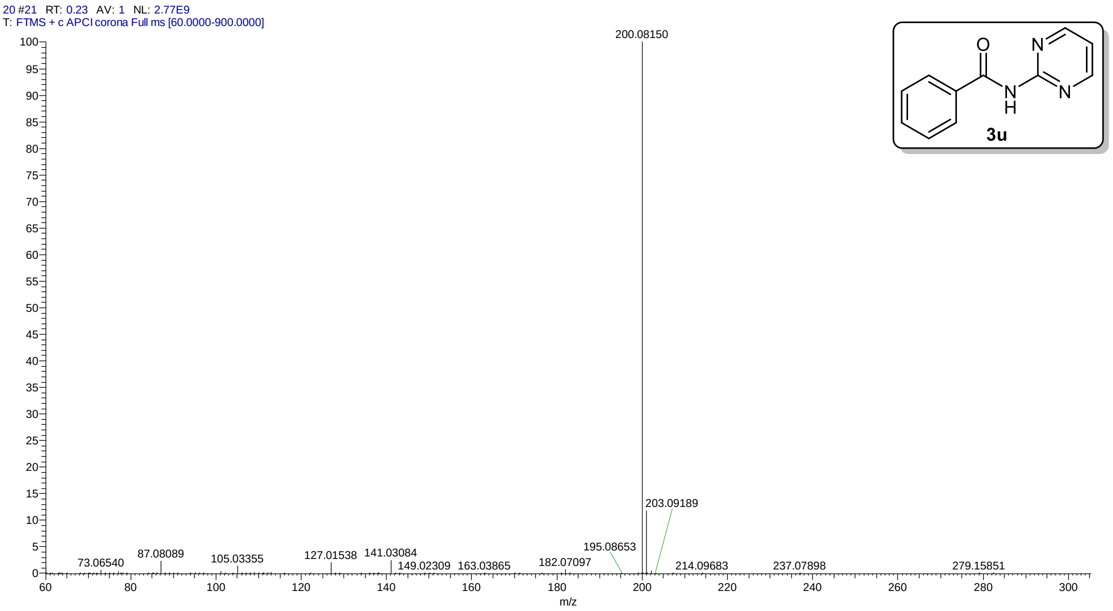
- ^{1}H-NMR spectrum for **3u**



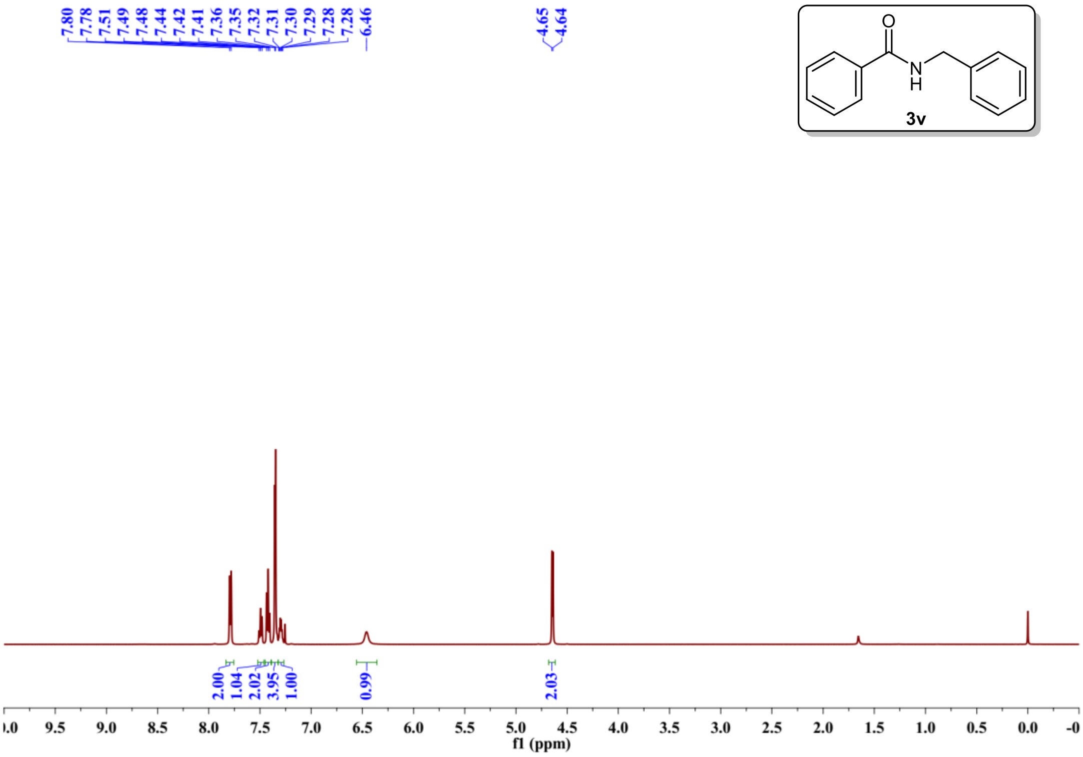
- ^{13}C-NMR spectrum for **3u**



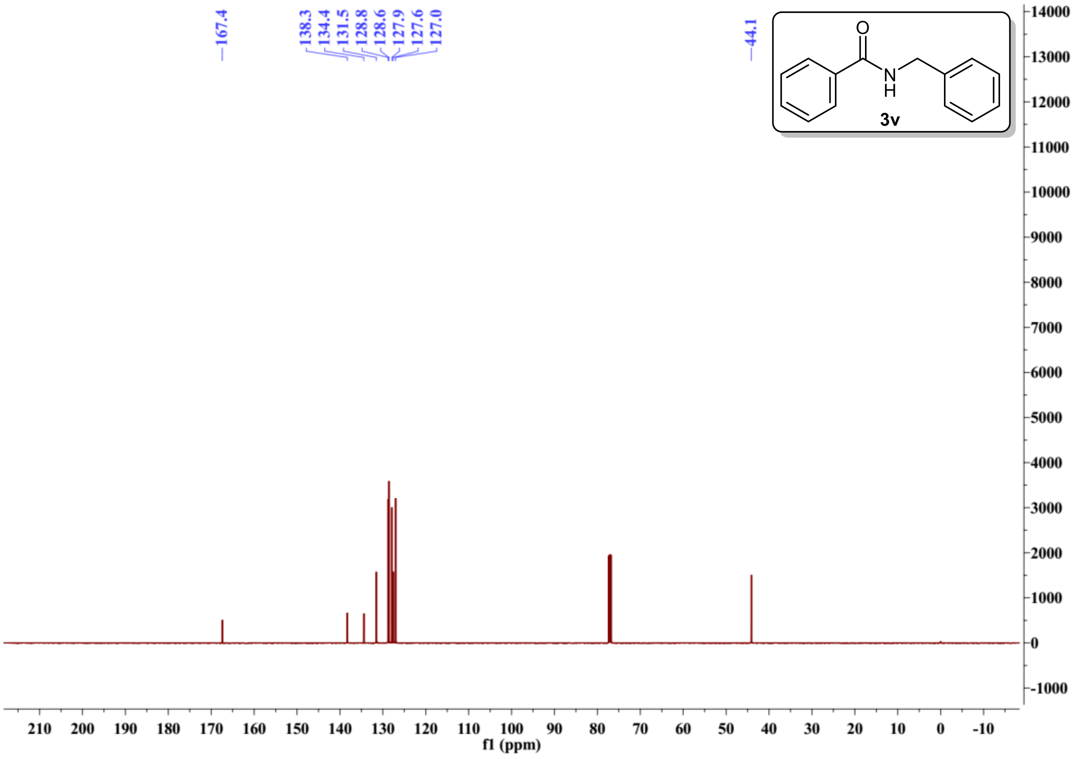
➢ HRMS spectrum for **3u**



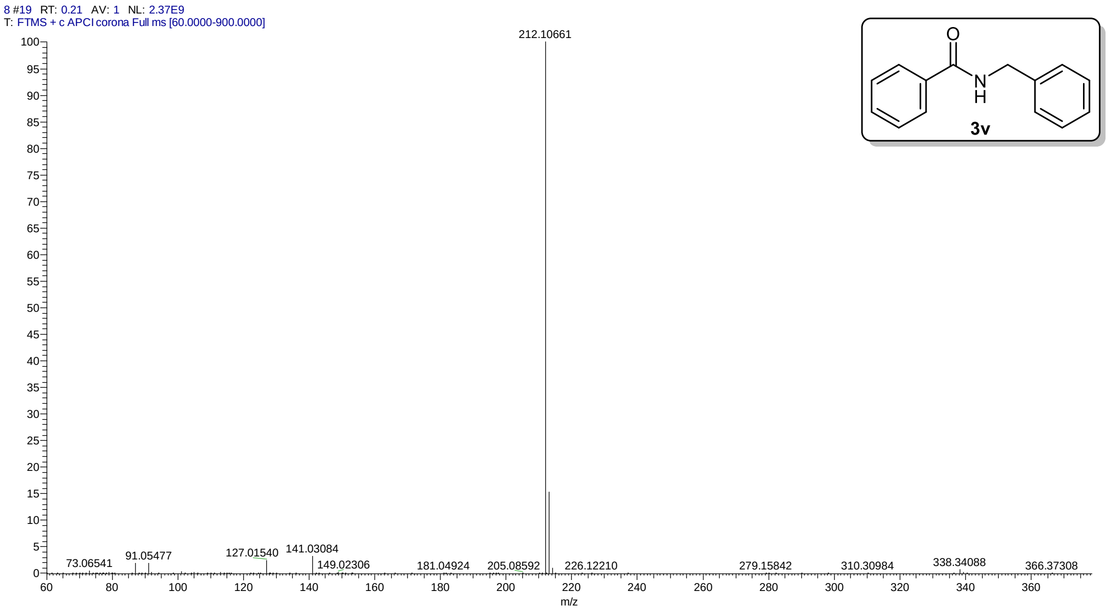
➢ ^{1}H-NMR spectrum for **3v**



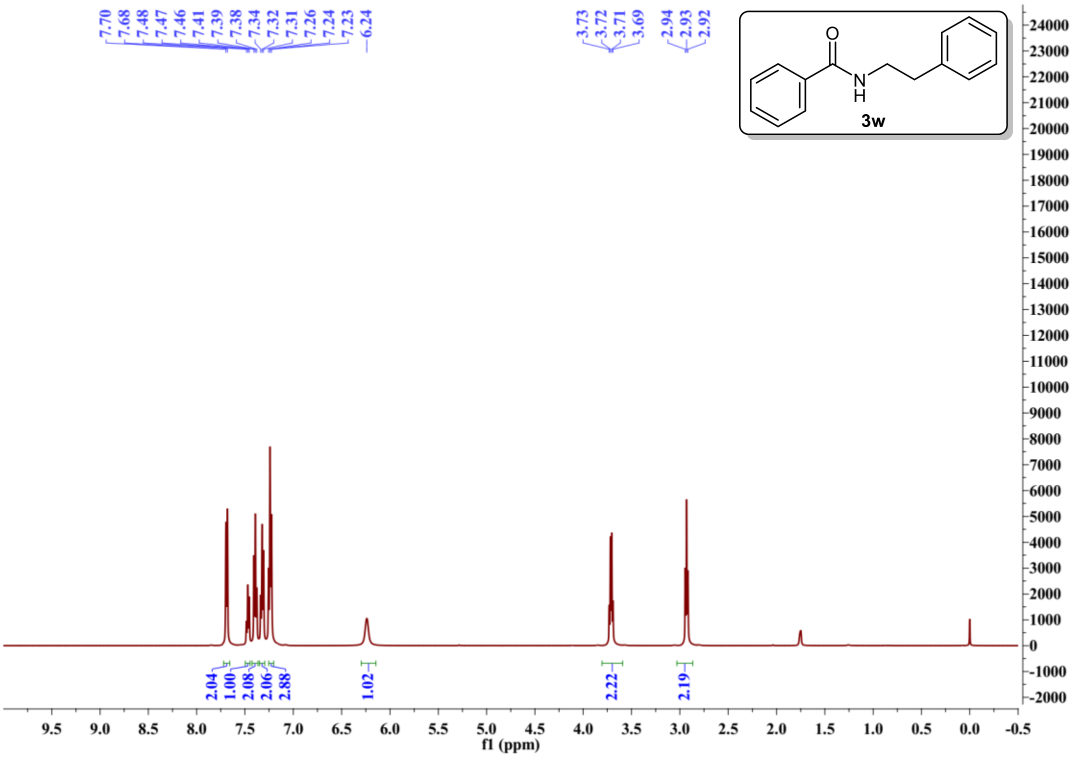
➢ ^{13}C-NMR spectrum for **3v**



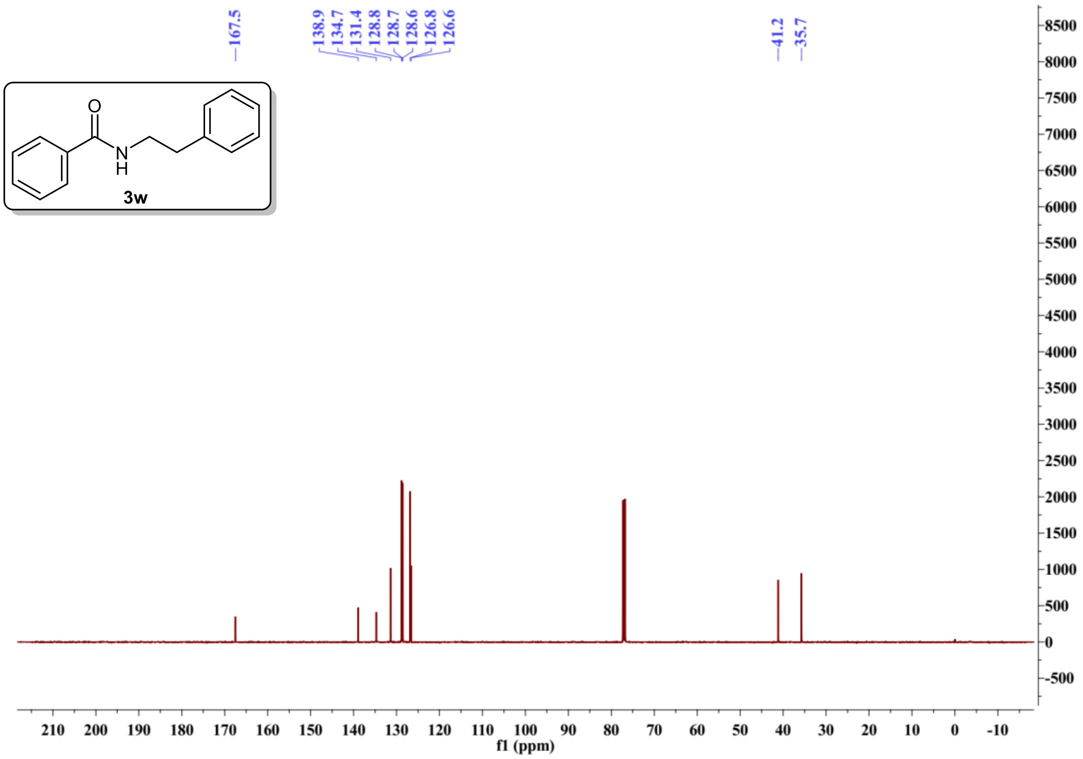
➢ HRMS spectrum for **3v**



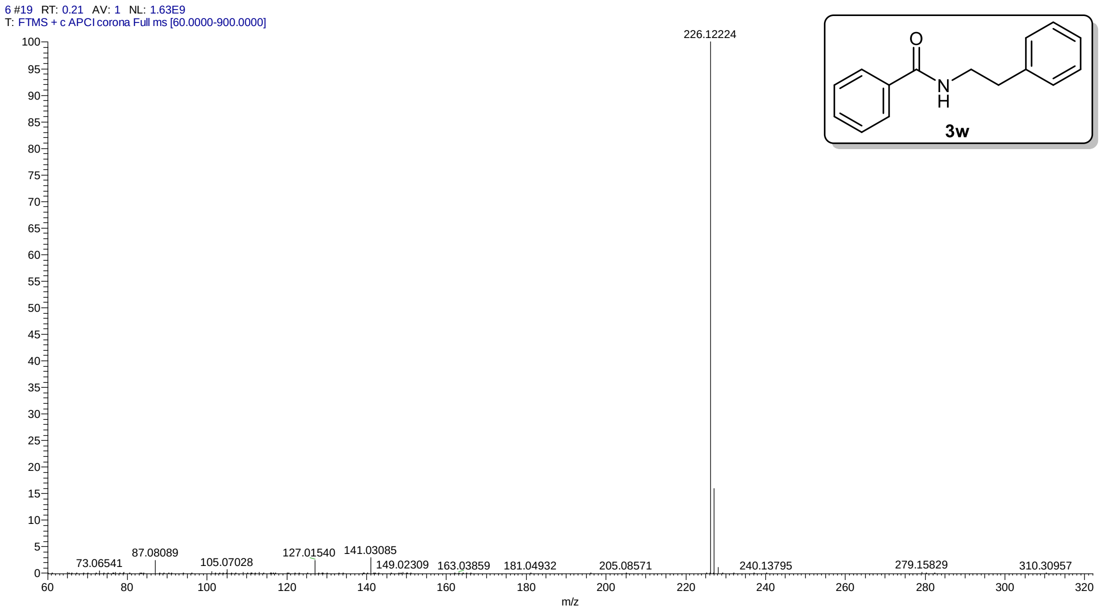
- ^{1}H-NMR spectrum for **3w**



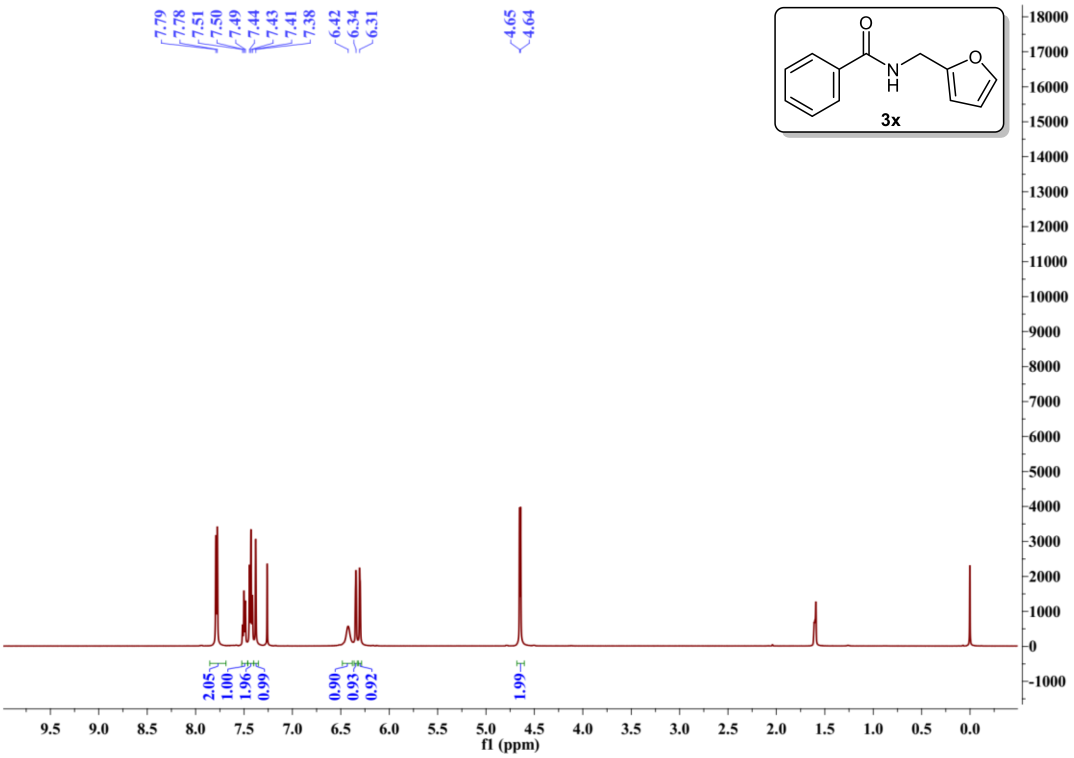
- ^{13}C-NMR spectrum for **3w**



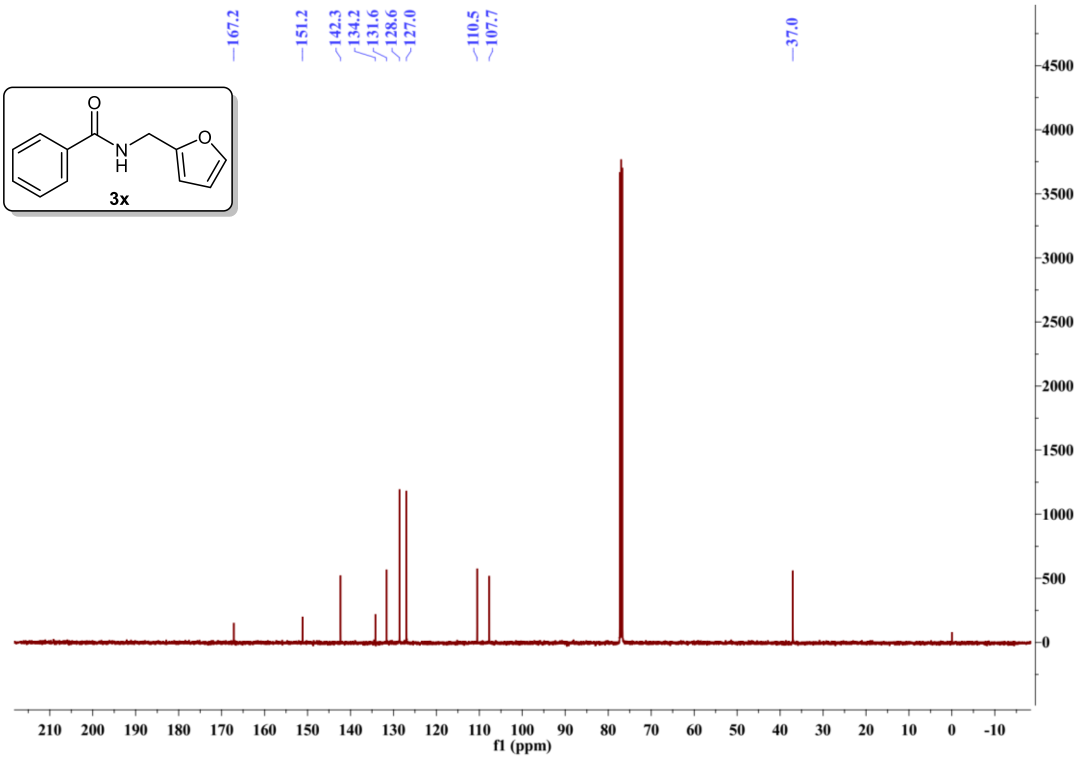
➢ HRMS spectrum for **3w**



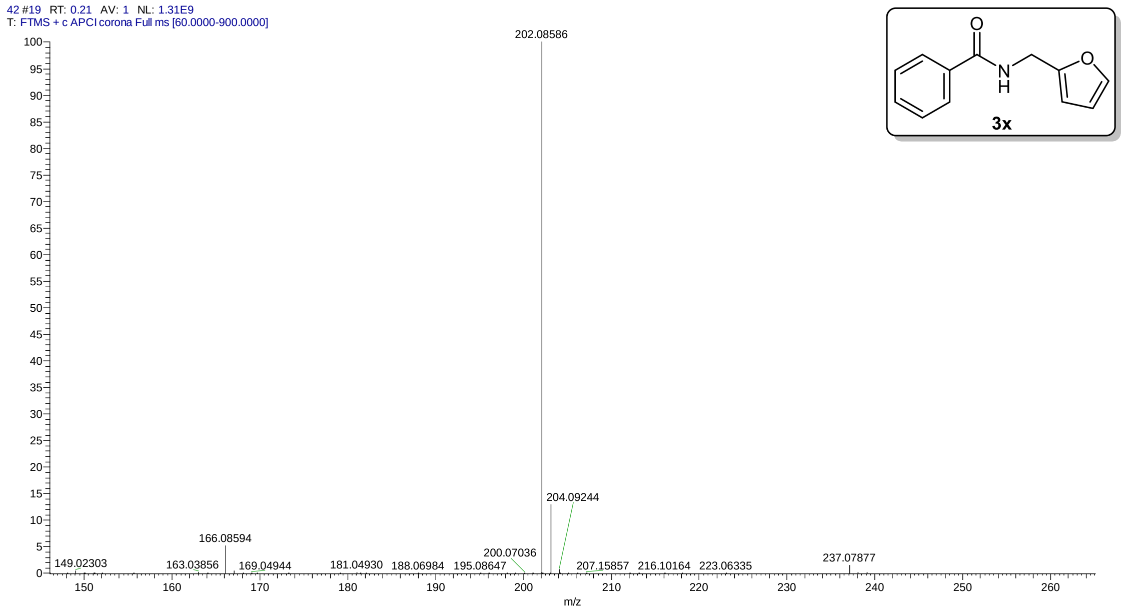
➢ ^{1}H-NMR spectrum for **3x**



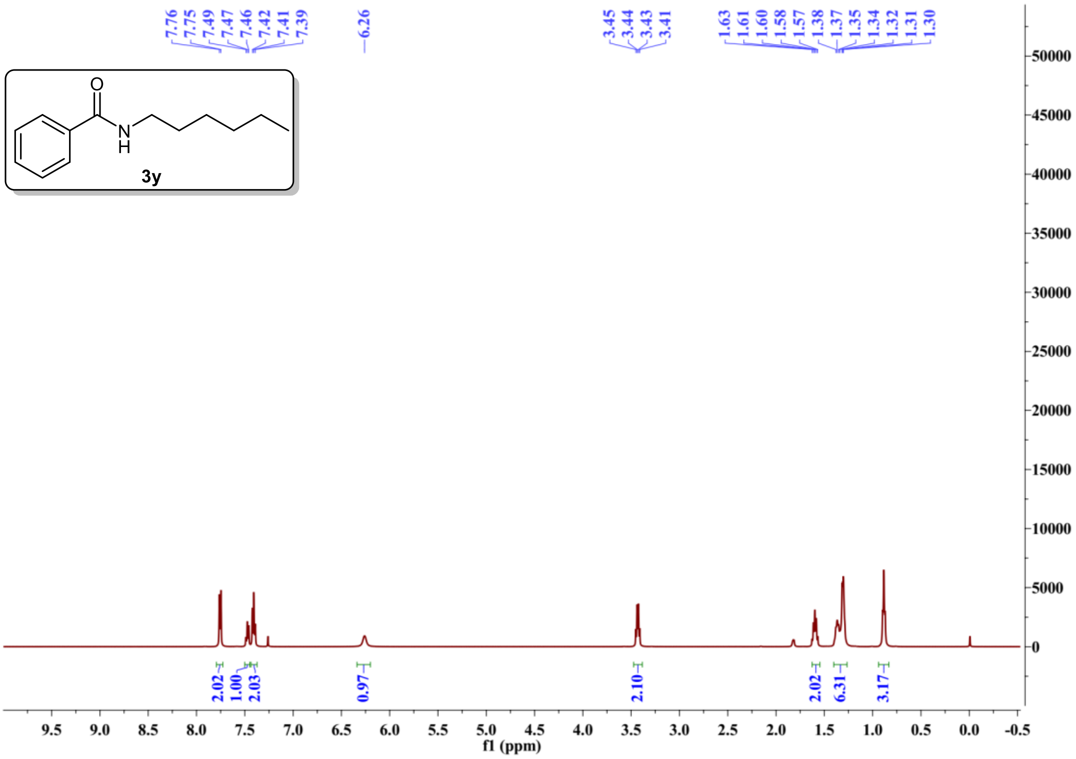
➢ ^{13}C-NMR spectrum for **3x**



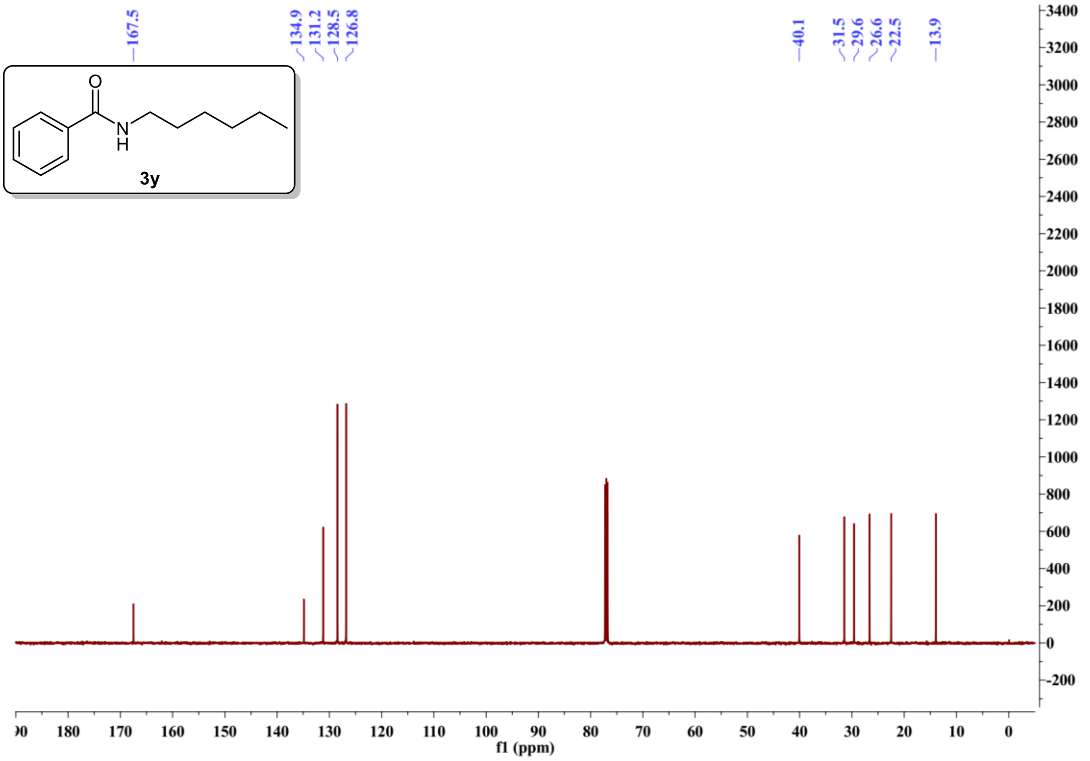
➢ HRMS spectrum for **3x**



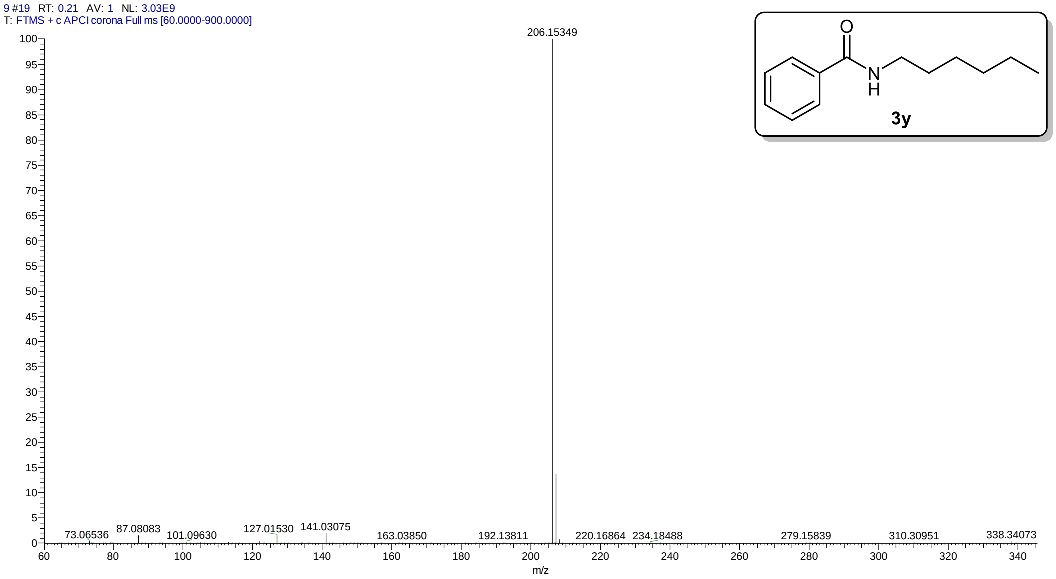
➢ ^{1}H-NMR spectrum for **3y**



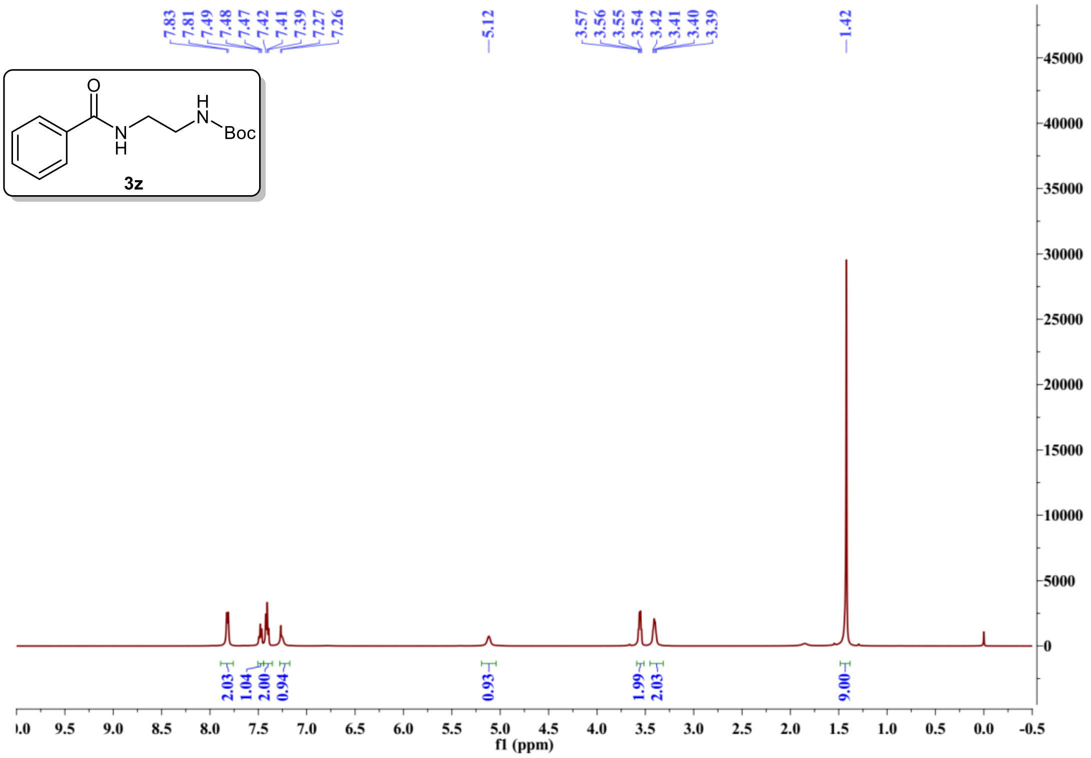
➢ ^{13}C-NMR spectrum for **3y**



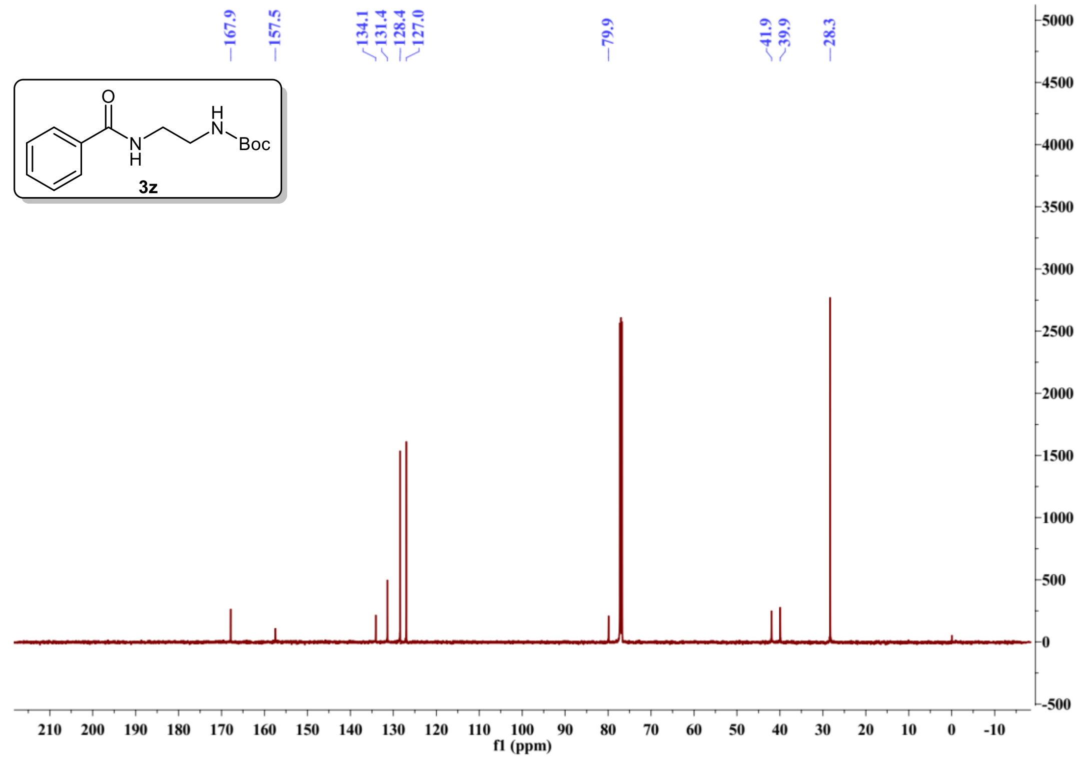
➢ HRMS spectrum for **3y**



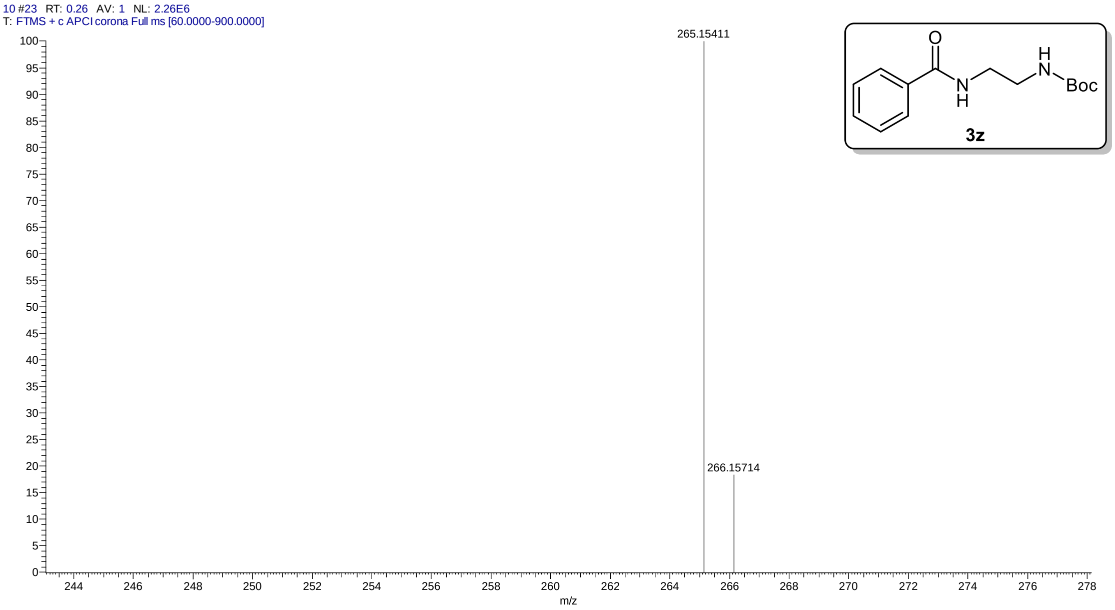
➢ ^{1}H-NMR spectrum for **3z**



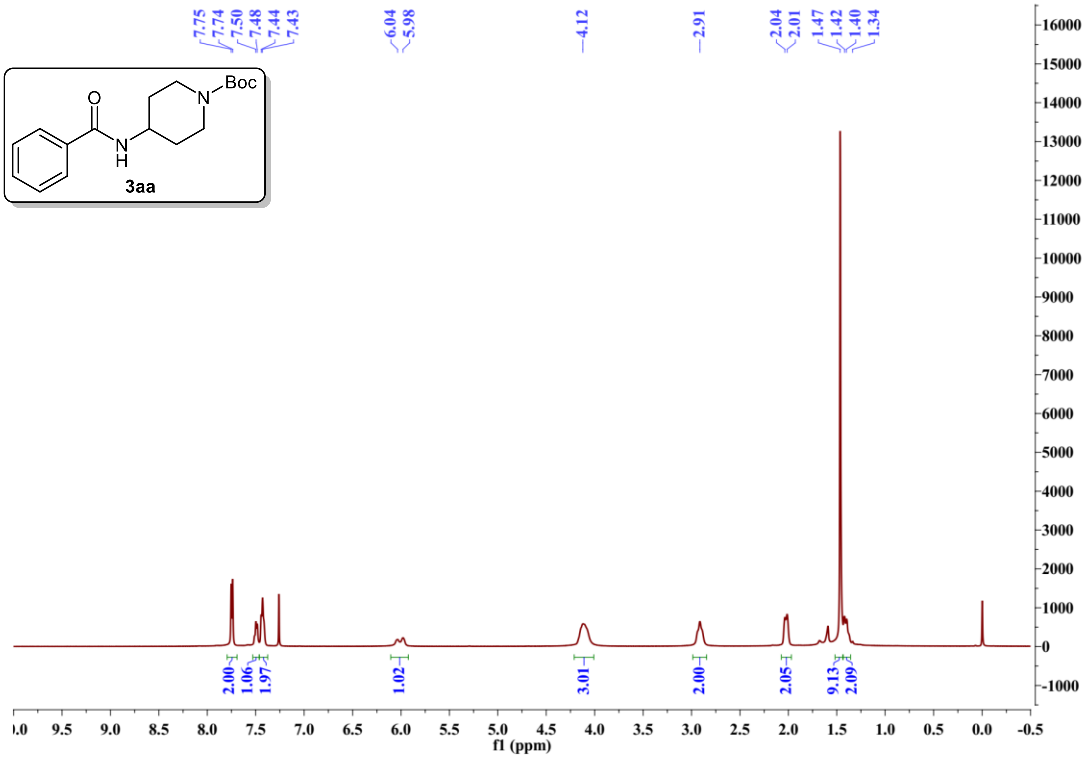
➢ ^{13}C-NMR spectrum for **3z**



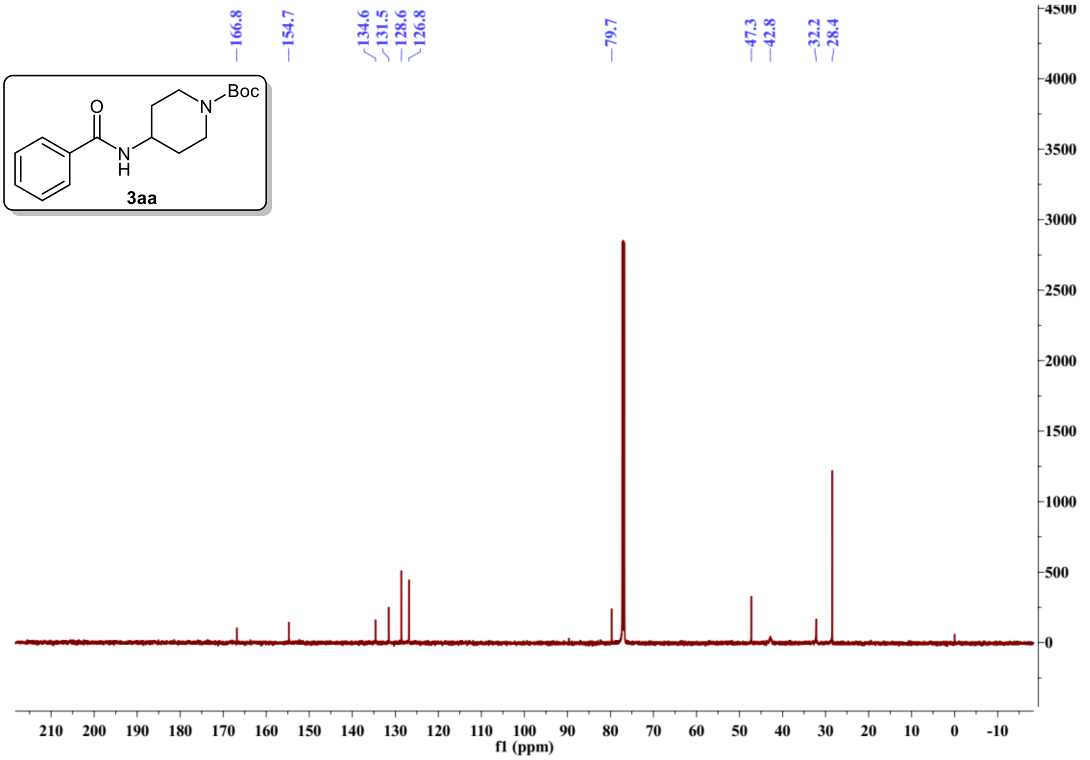
➢ HRMS spectrum for **3z**



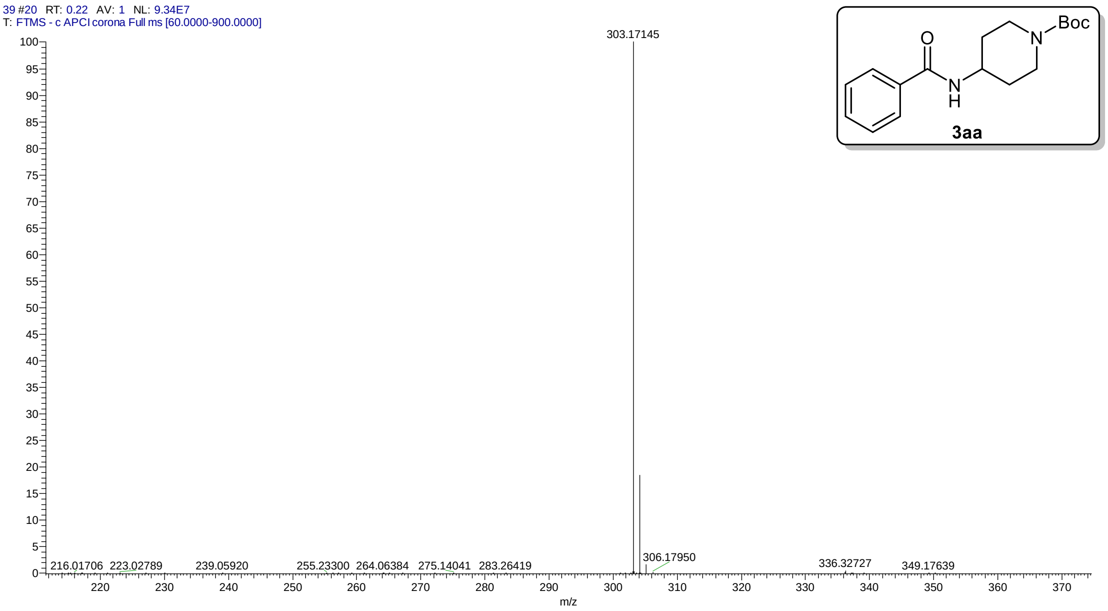
➢ ^{1}H-NMR spectrum for **3aa**



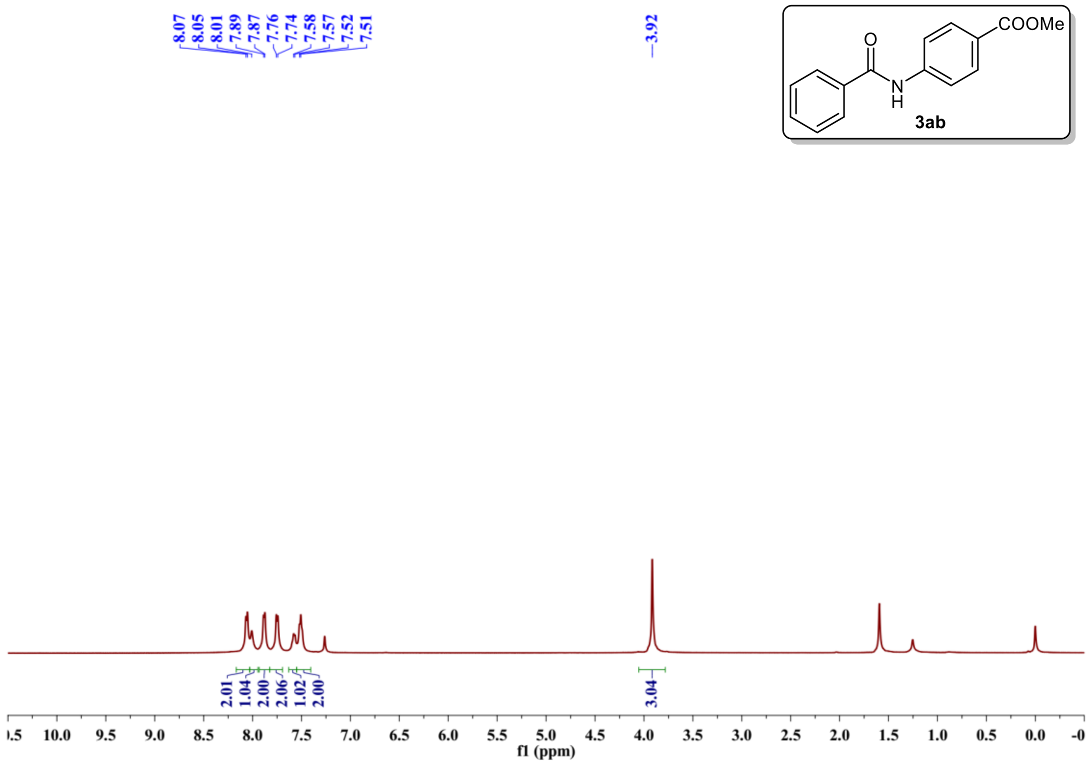
➢ ^{13}C-NMR spectrum for **3aa**



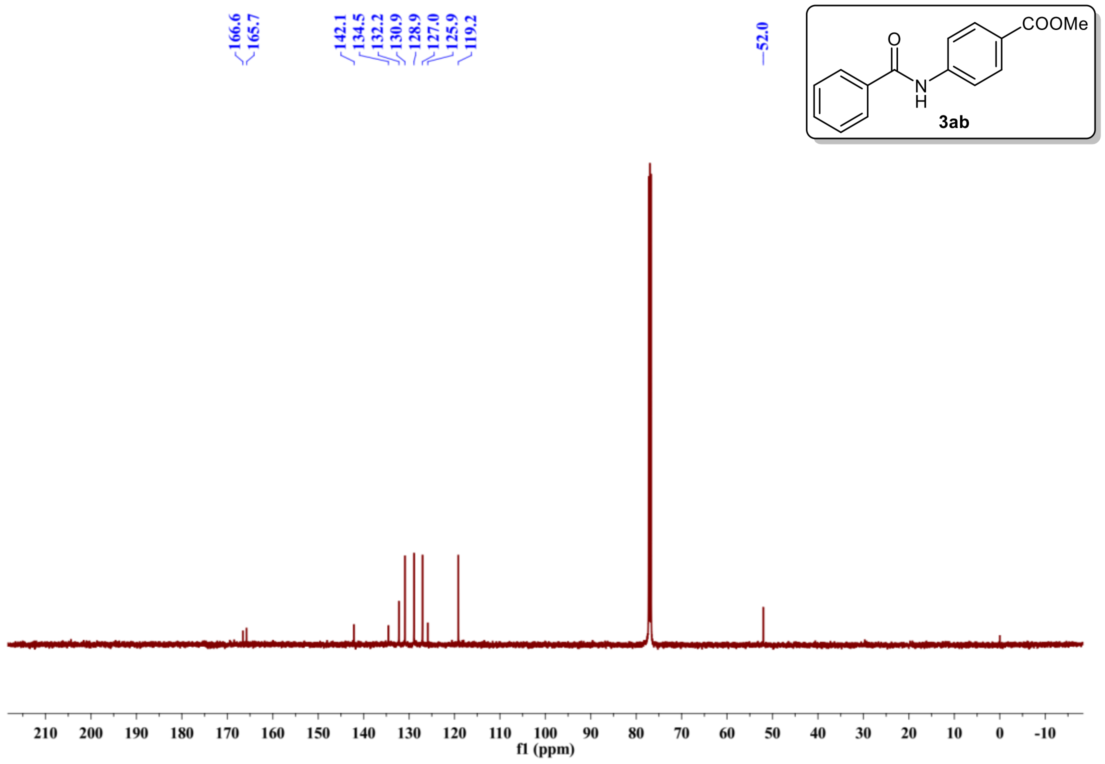
➢ HRMS spectrum for **3aa**



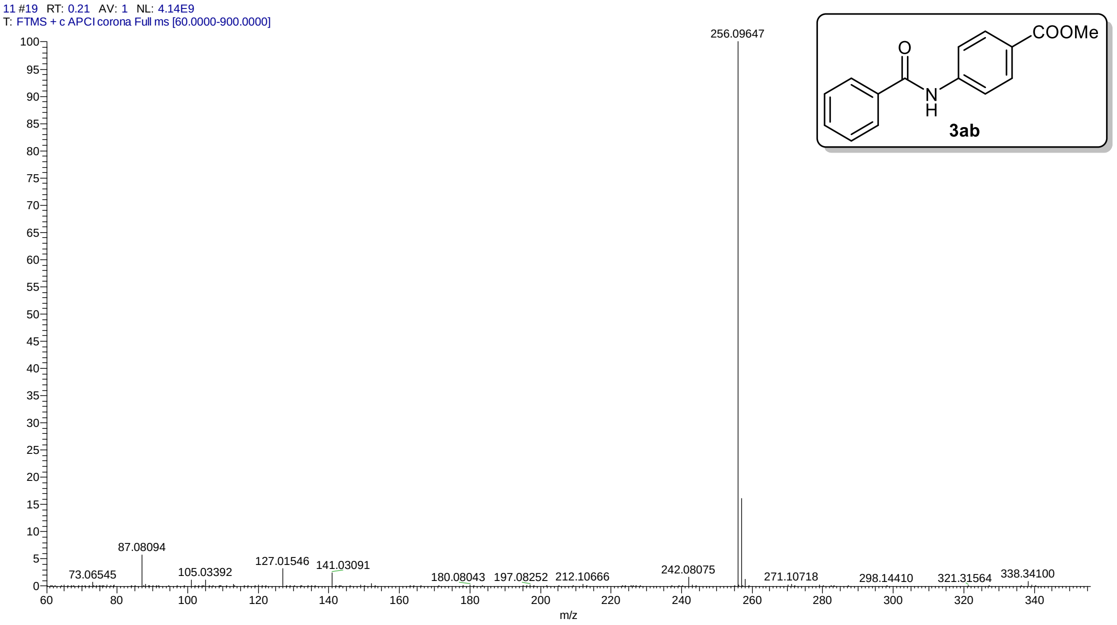
➢ ^{1}H-NMR spectrum for **3ab**



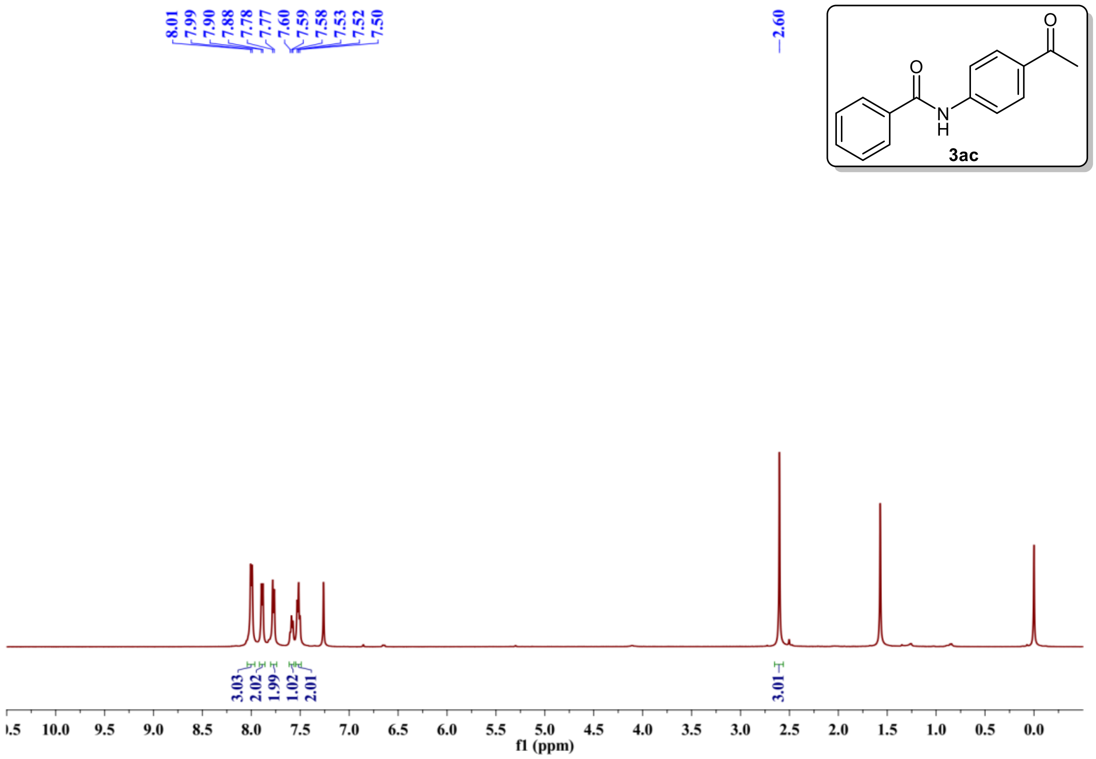
➢ ^{13}C-NMR spectrum for **3ab**



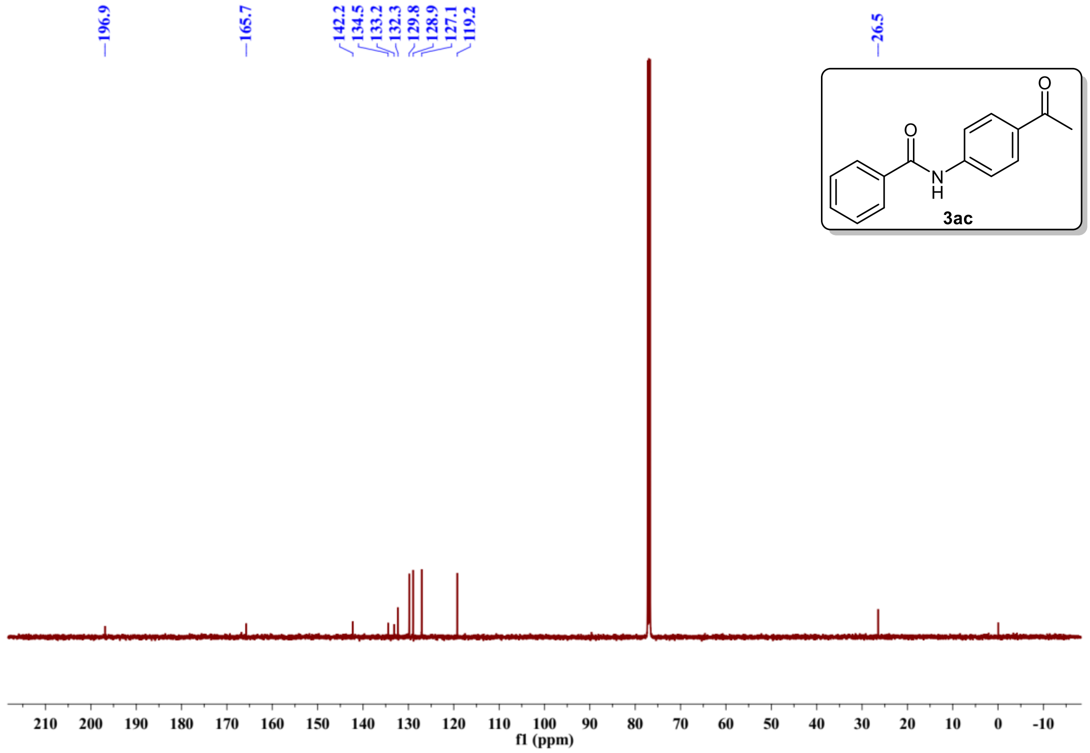
➢ HRMS spectrum for **3ab**



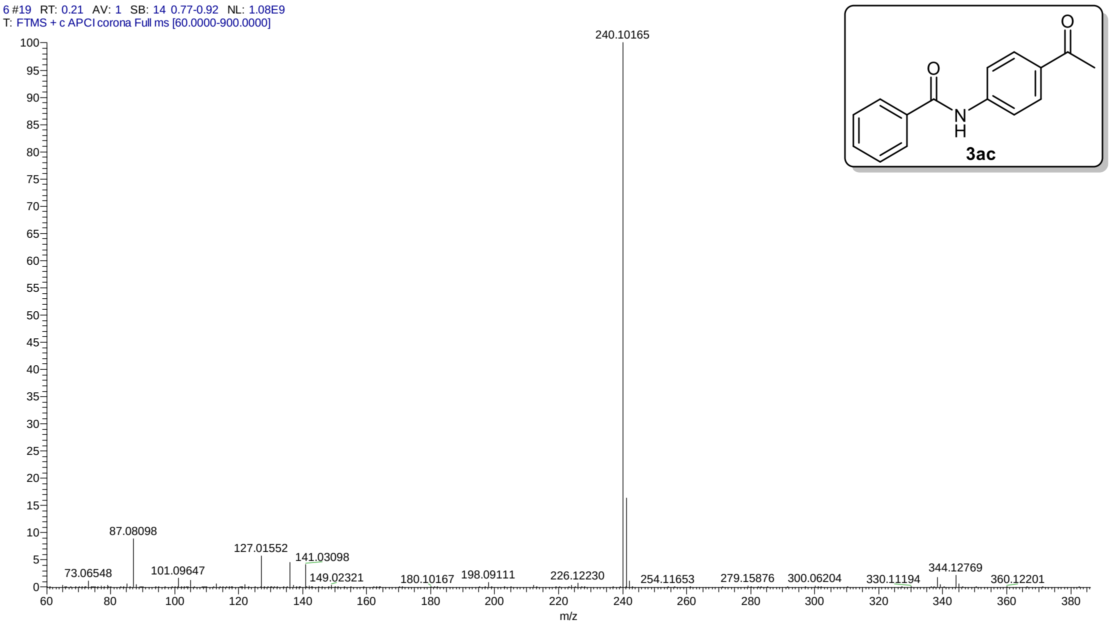
➢ ^{1}H-NMR spectrum for **3ac**



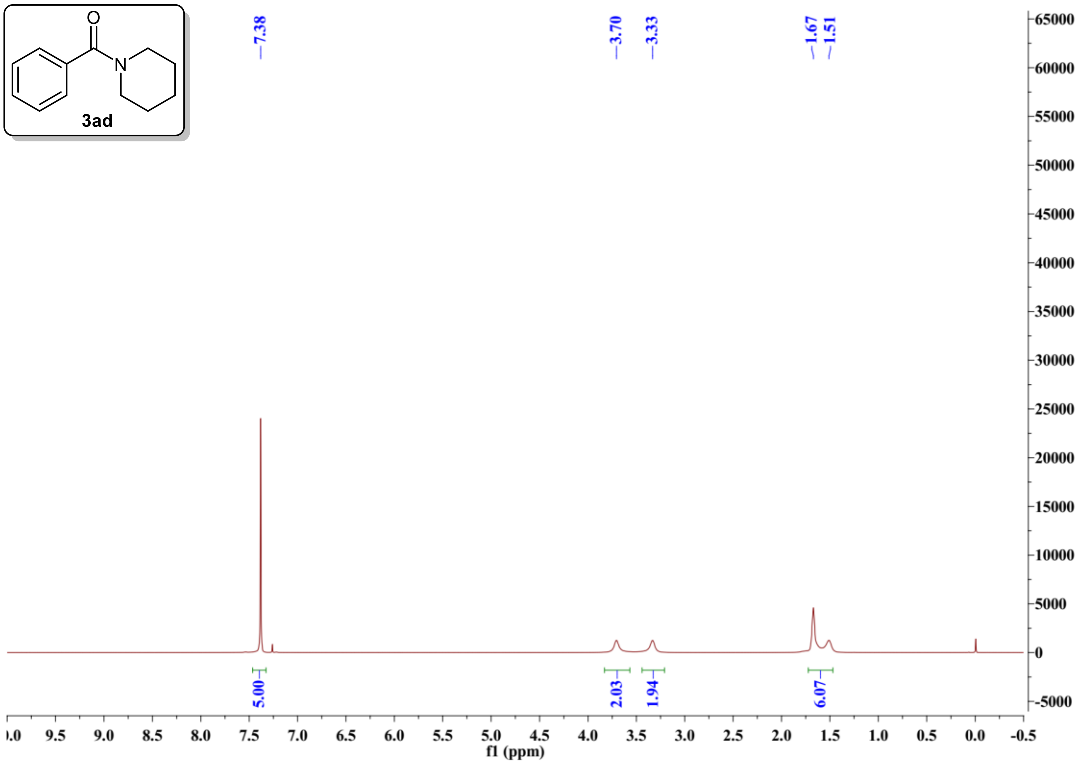
➢ ^{13}C-NMR spectrum for **3ac**



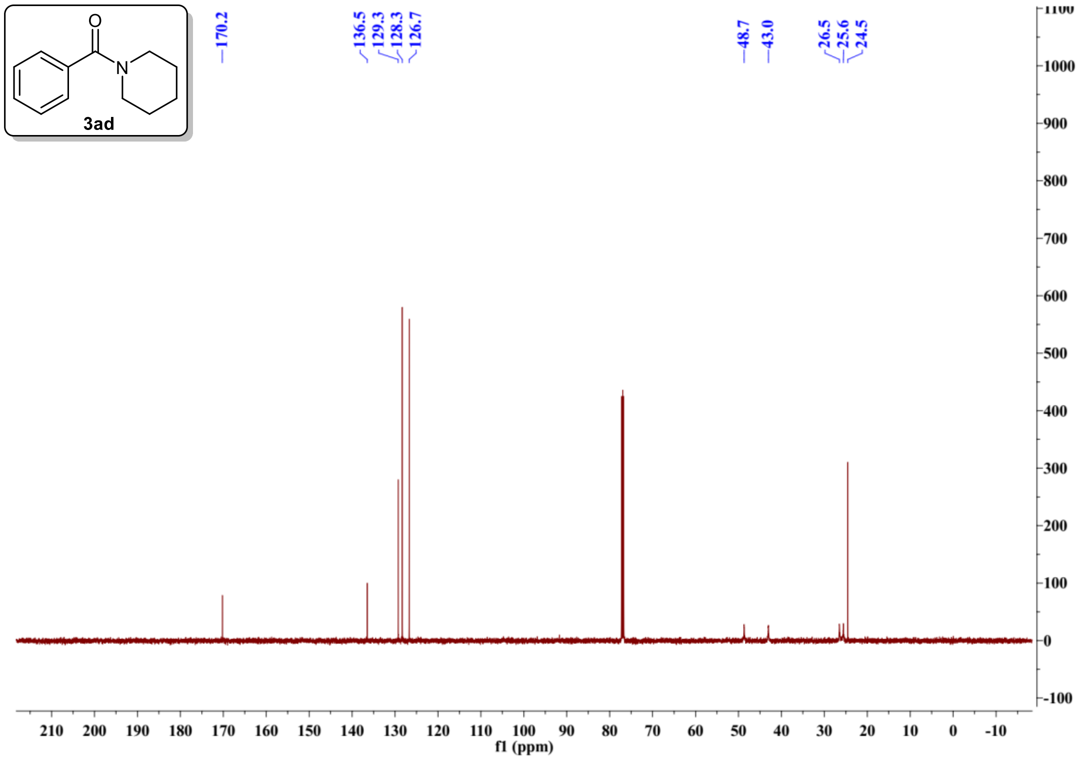
➢ HRMS spectrum for **3ac**



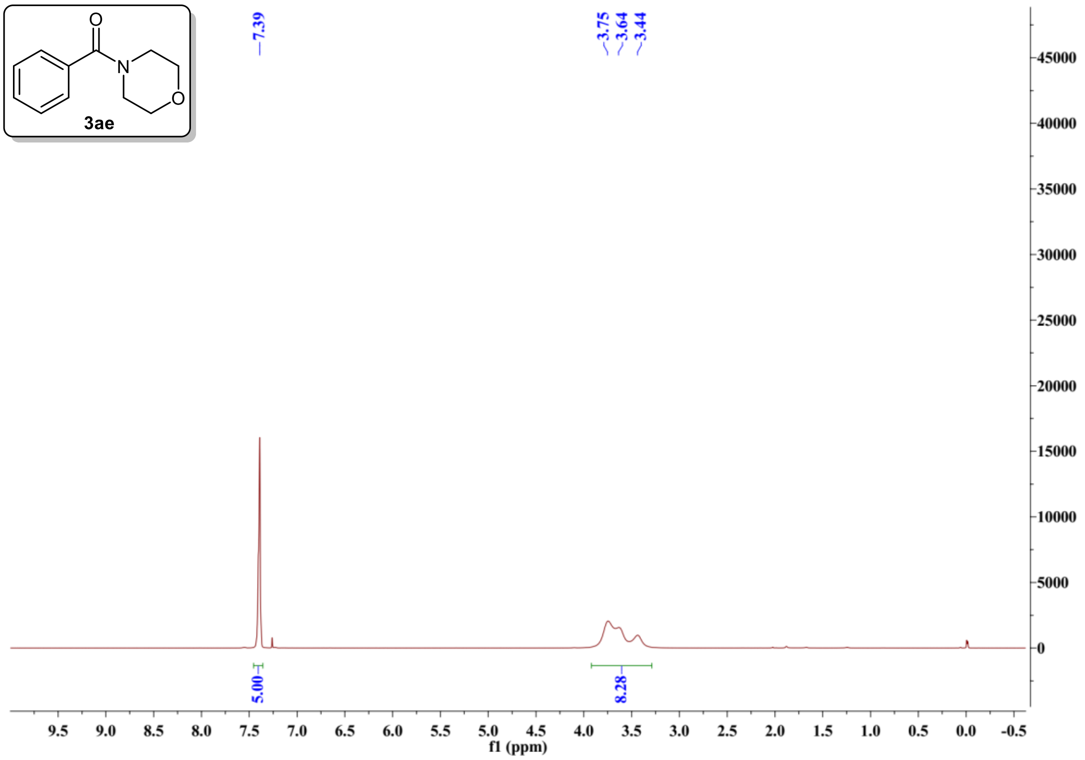
➢ ^{1}H-NMR spectrum for **3ad**



➢ ^{13}C-NMR spectrum for **3ad**



➢ ^{1}H-NMR spectrum for **3ae**



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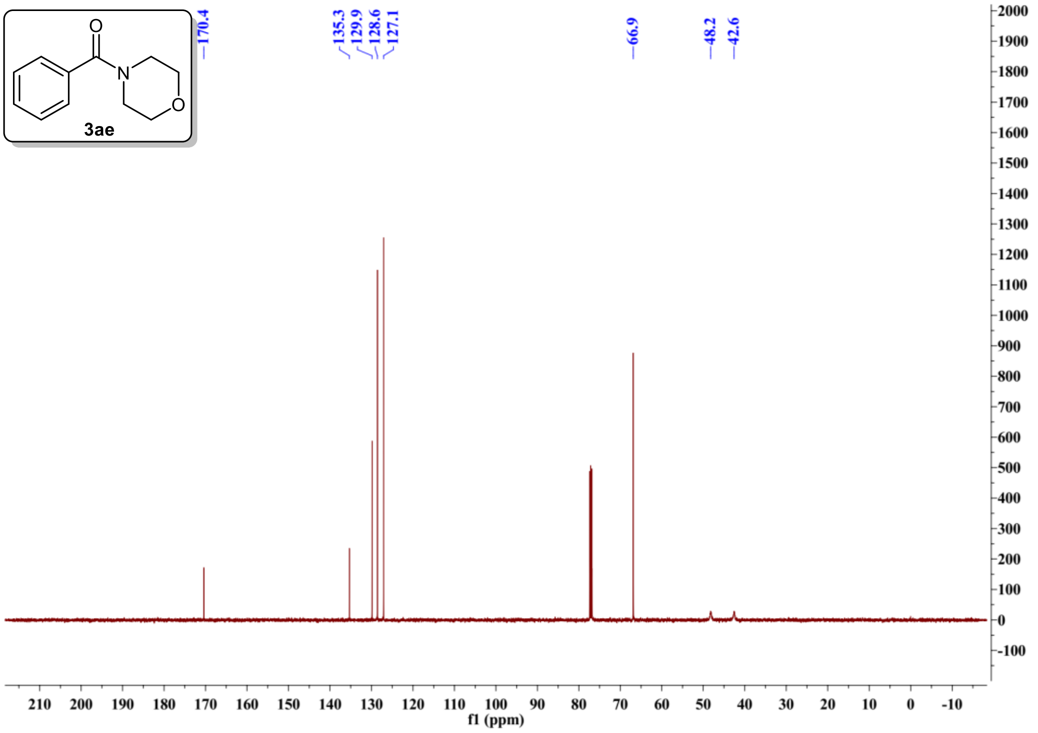

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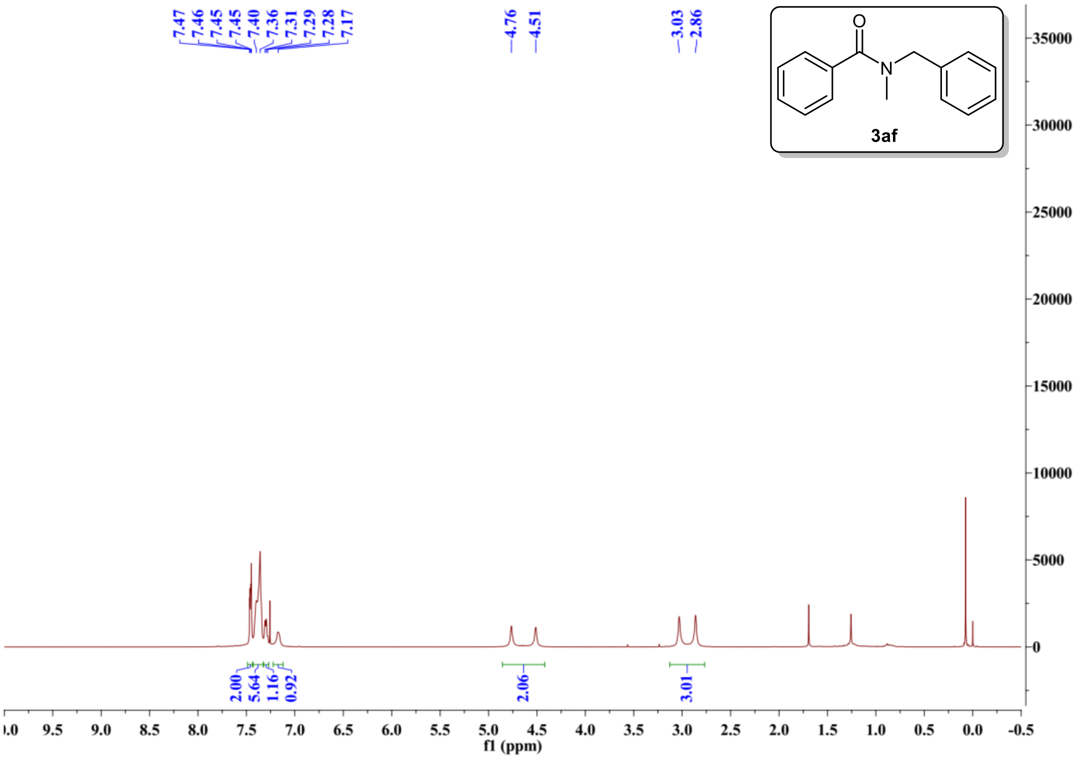

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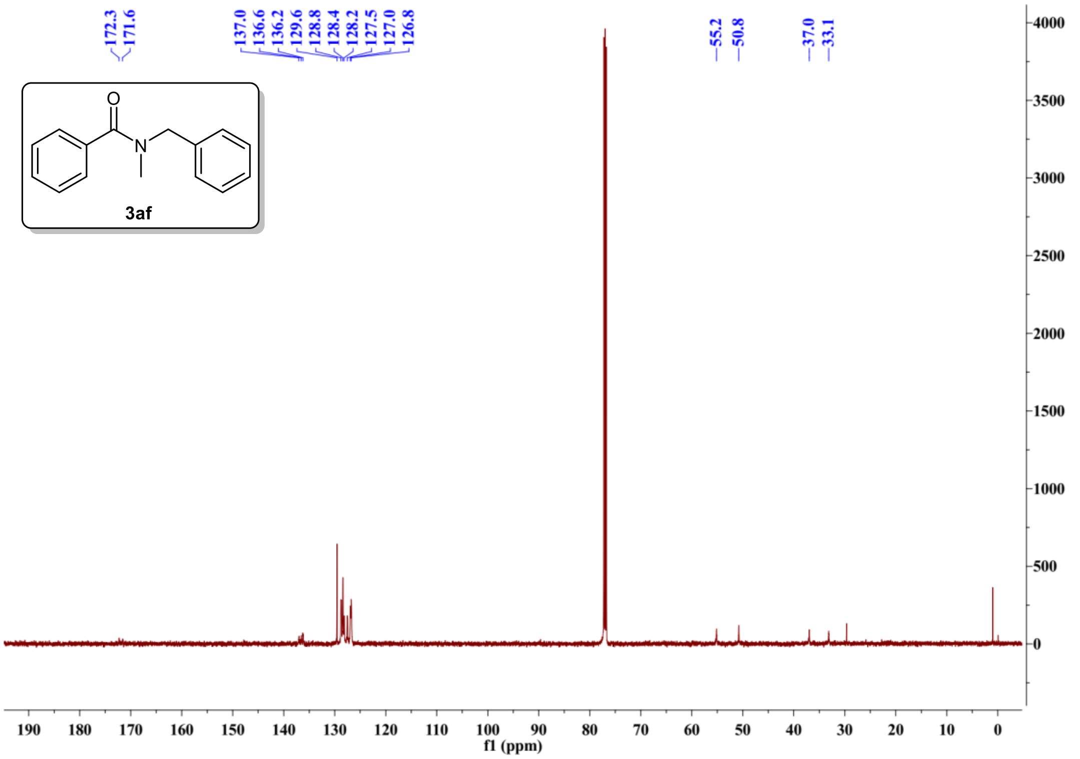
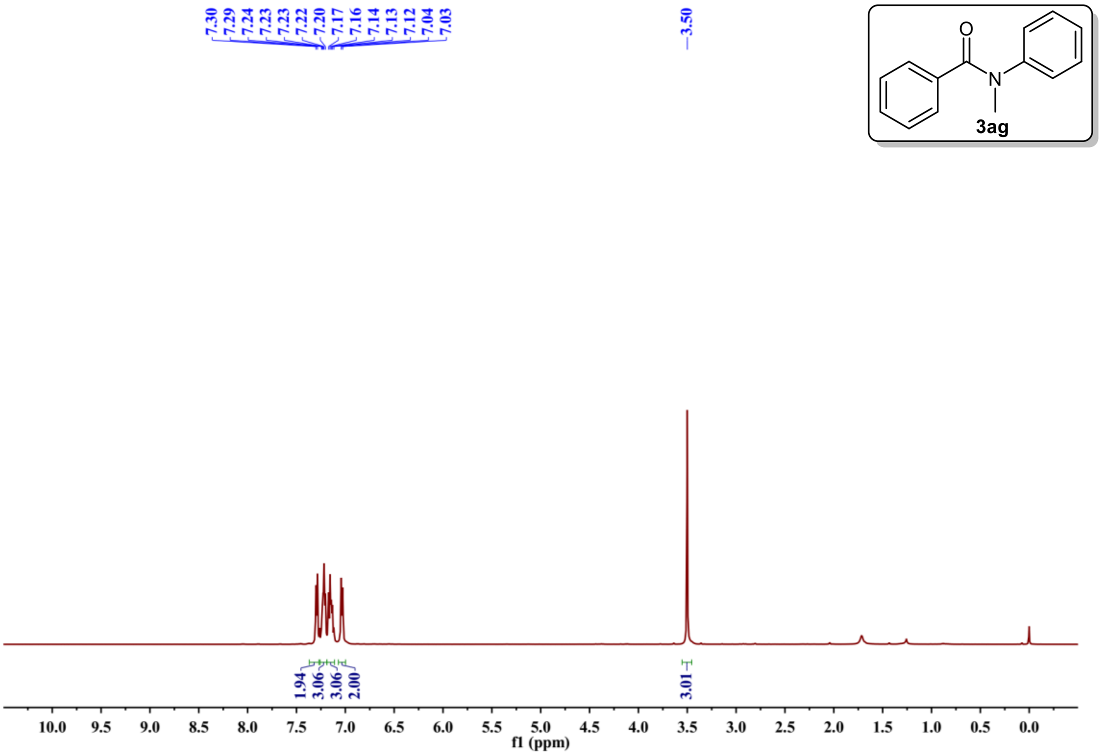
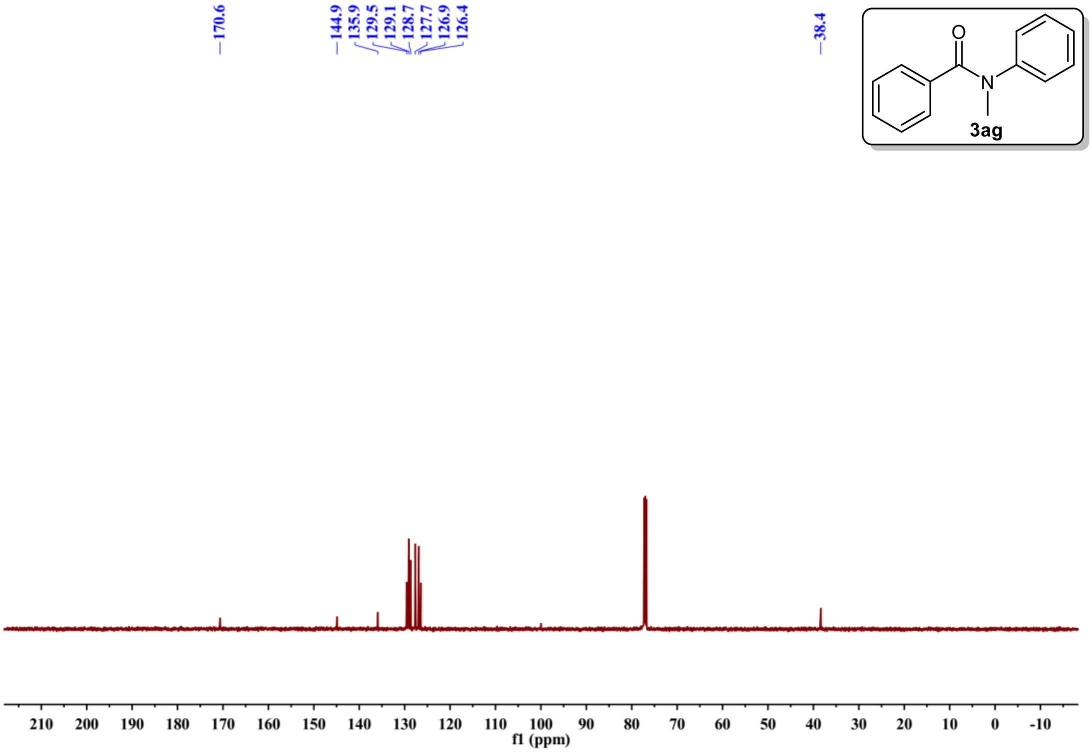


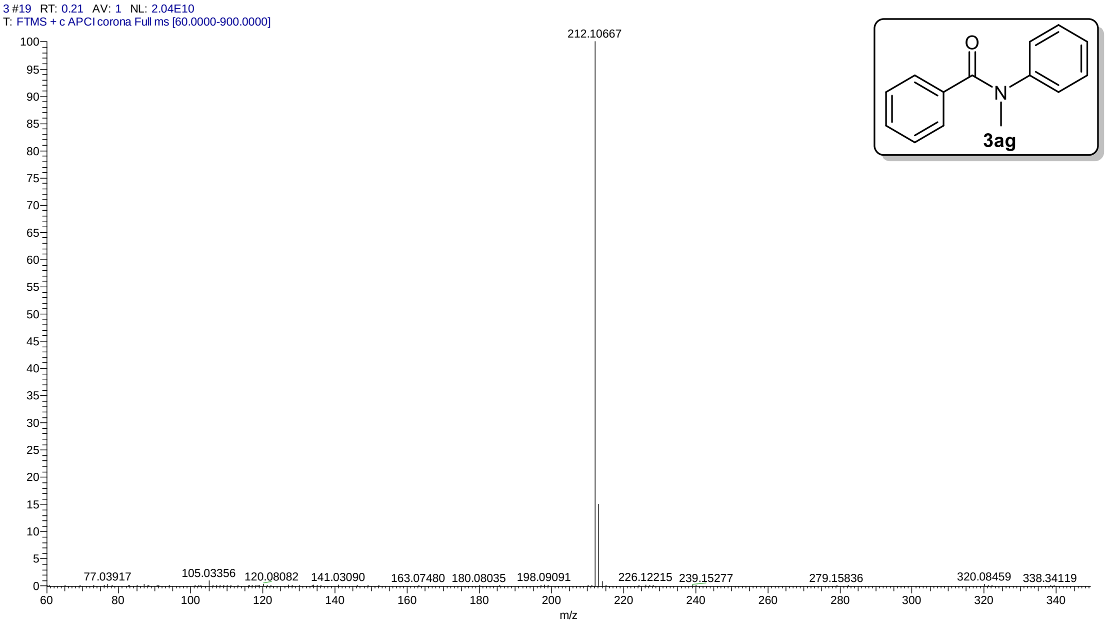
- ^{1}H-NMR spectrum for **3ag**



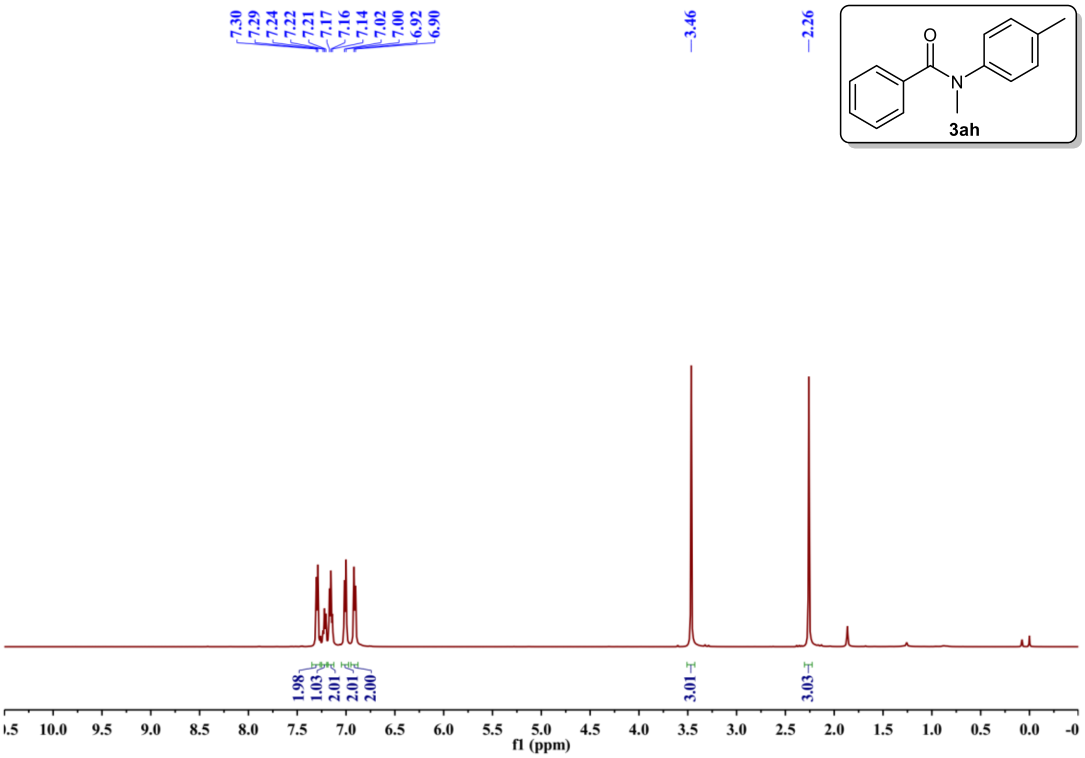
- ^{13}C-NMR spectrum for **3ag**



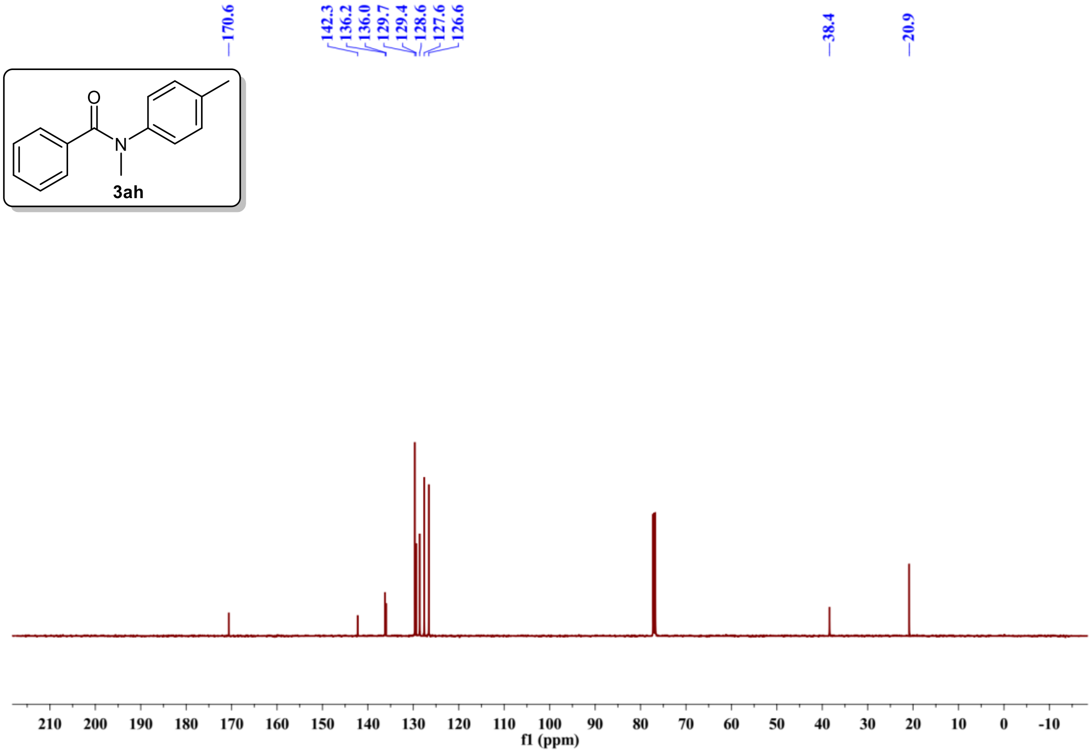
➢ HRMS spectrum for **3ag**



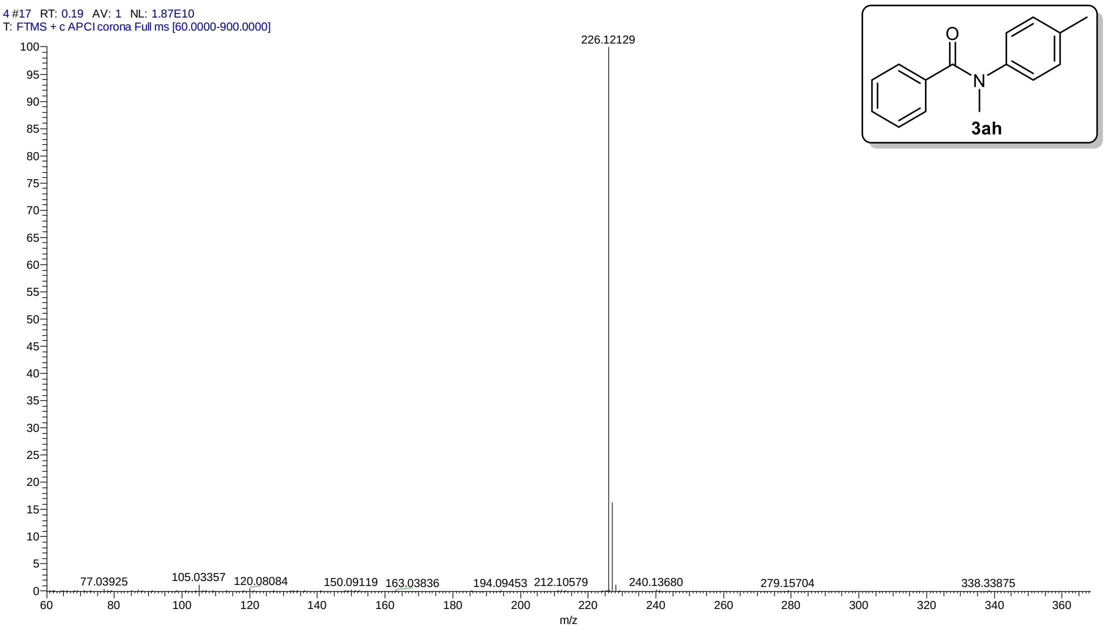
^{1}H-NMR spectrum for **3ah**



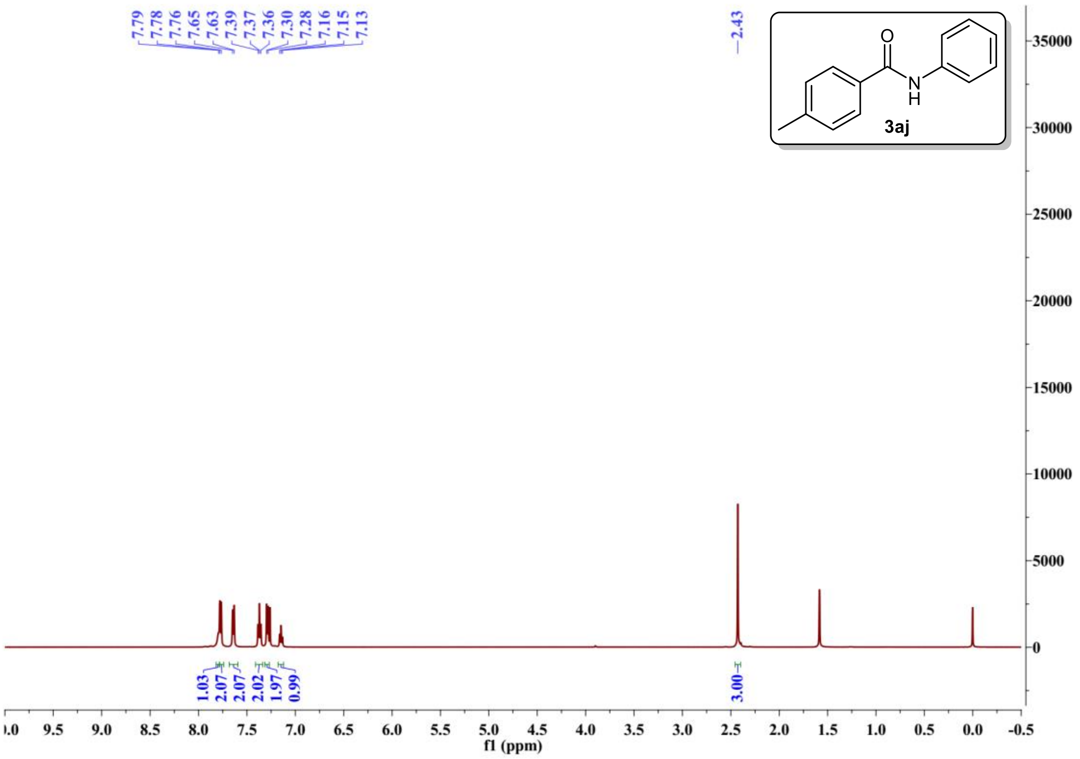
^{13}C-NMR spectrum for **3ah**



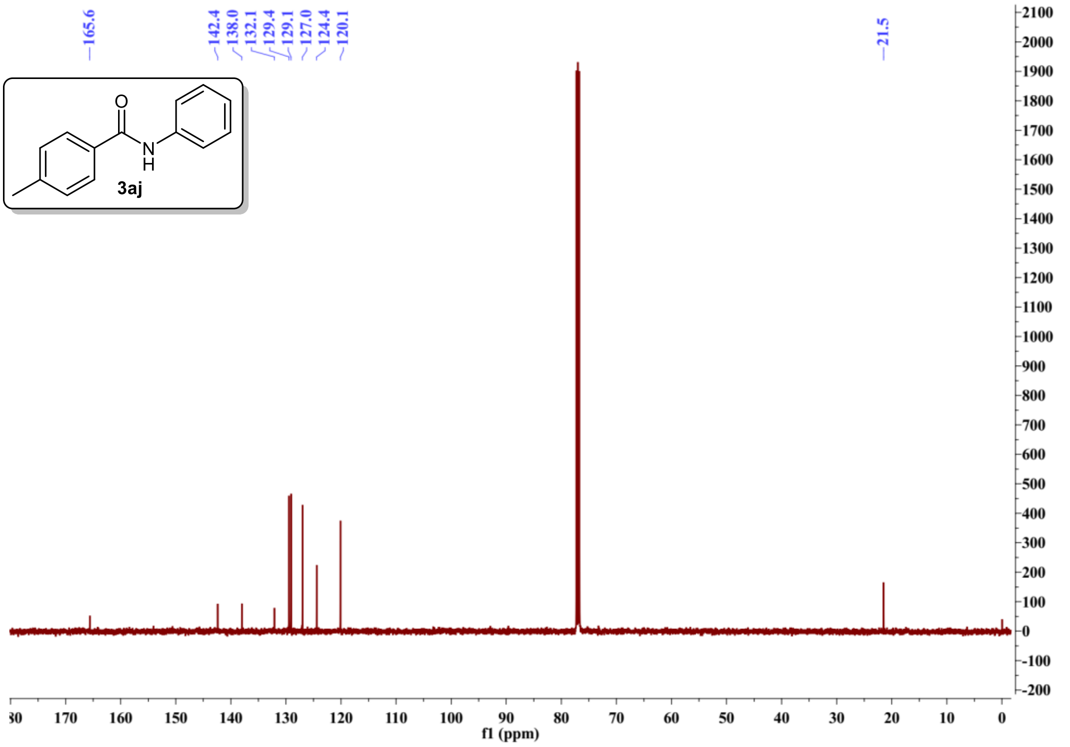
➢ HRMS spectrum for **3ah**



- ^{1}H-NMR spectrum for **3aj**



- ^{13}C-NMR spectrum for **3aj**



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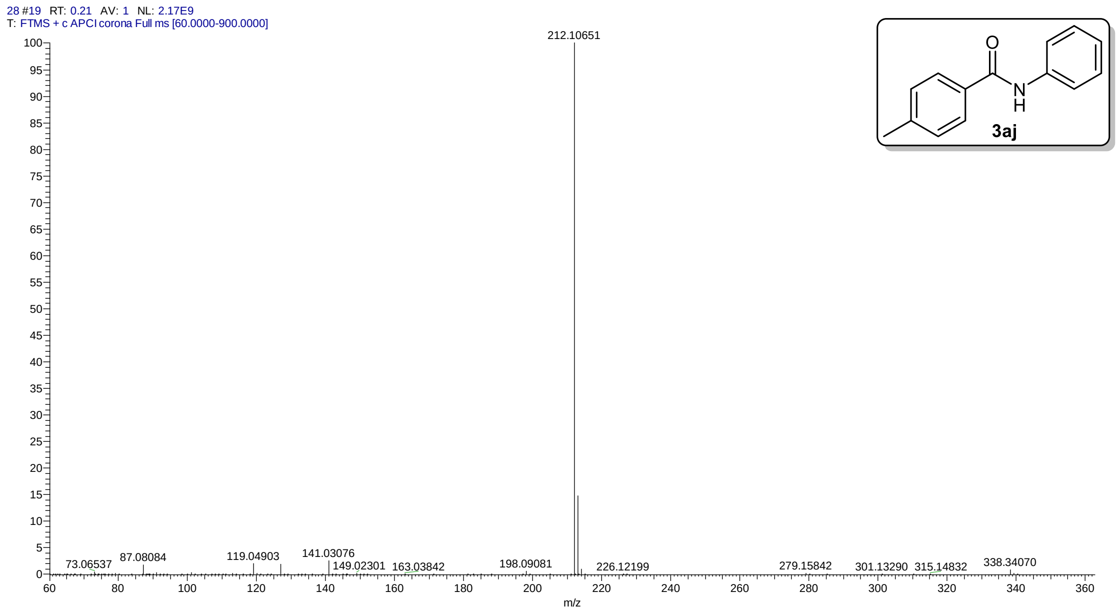

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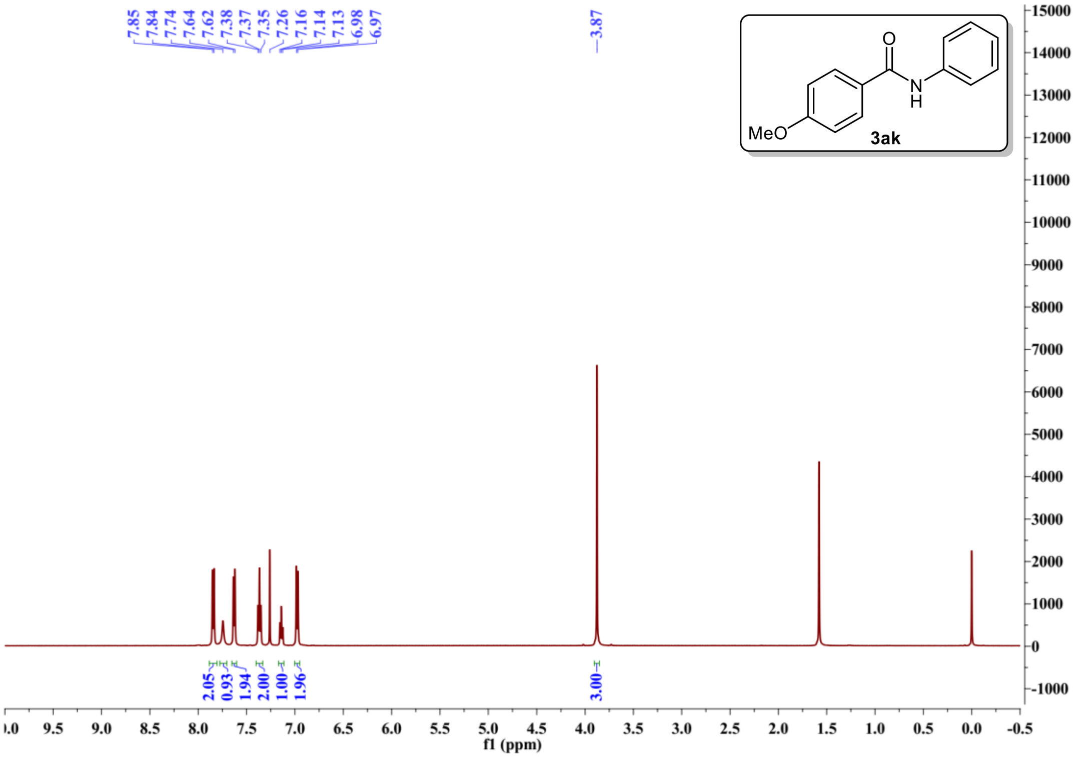
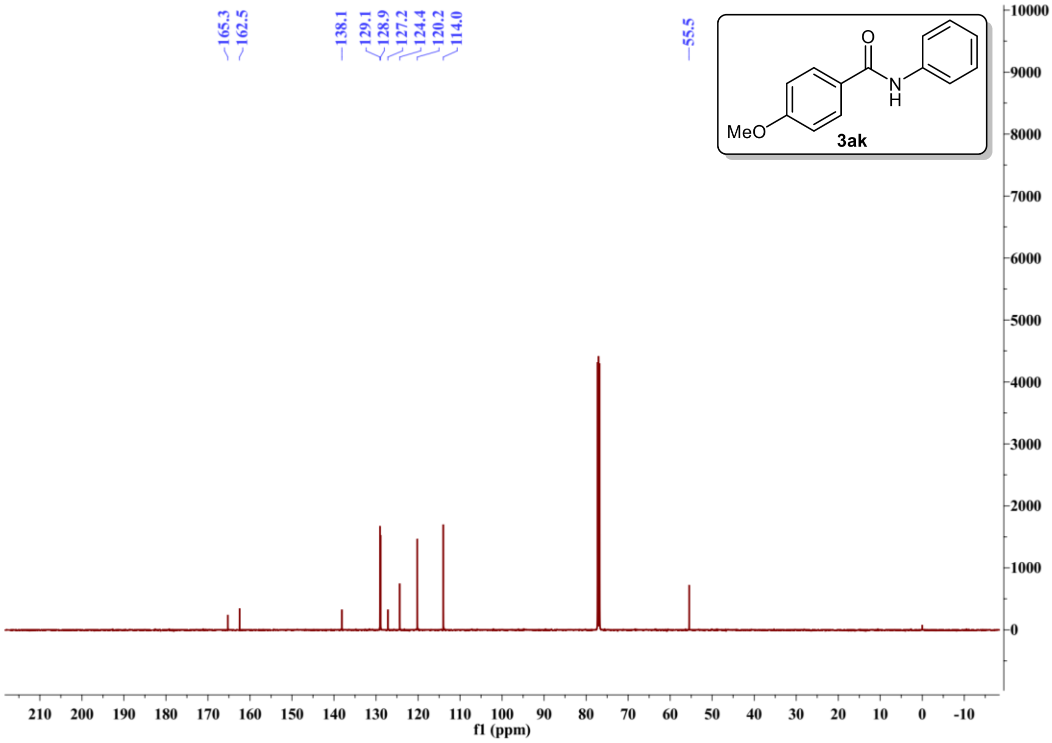
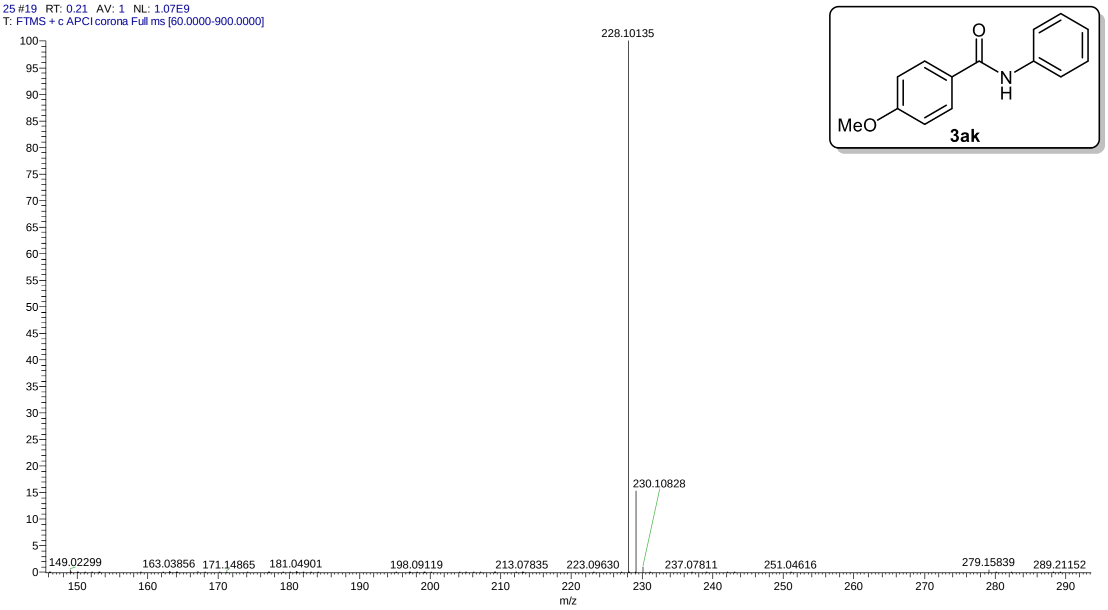


➢ ^{13}C-NMR spectrum for **3ak**



- HRMS spectrum for **3ak**



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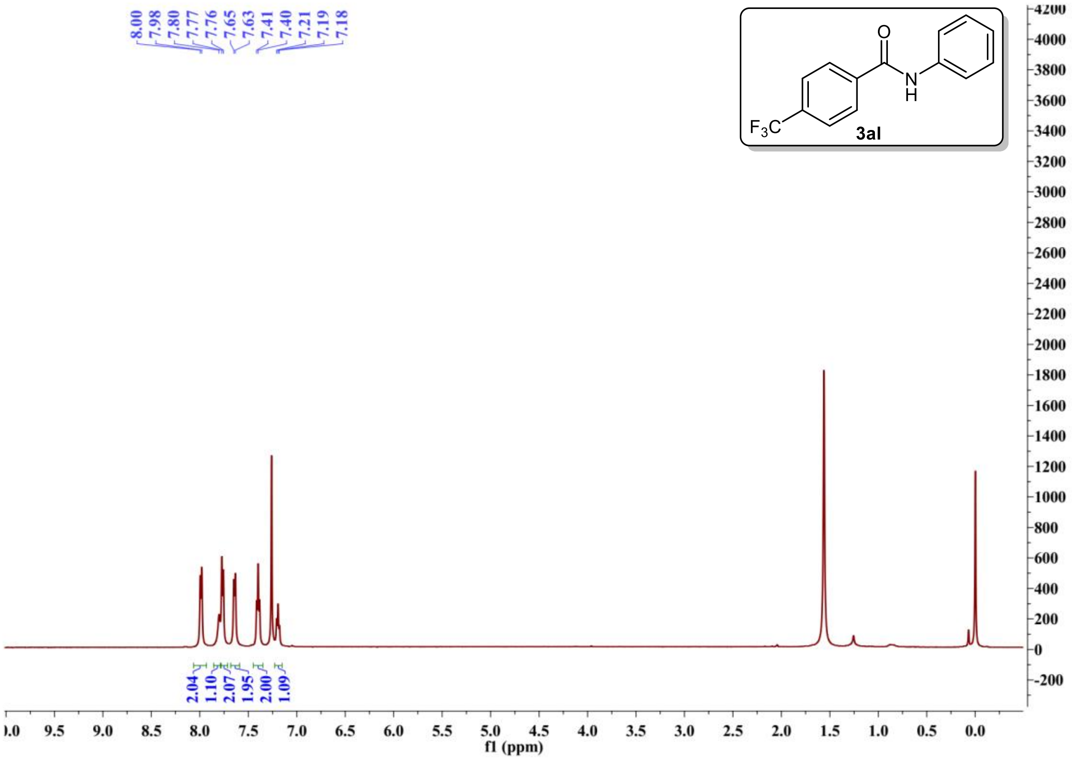

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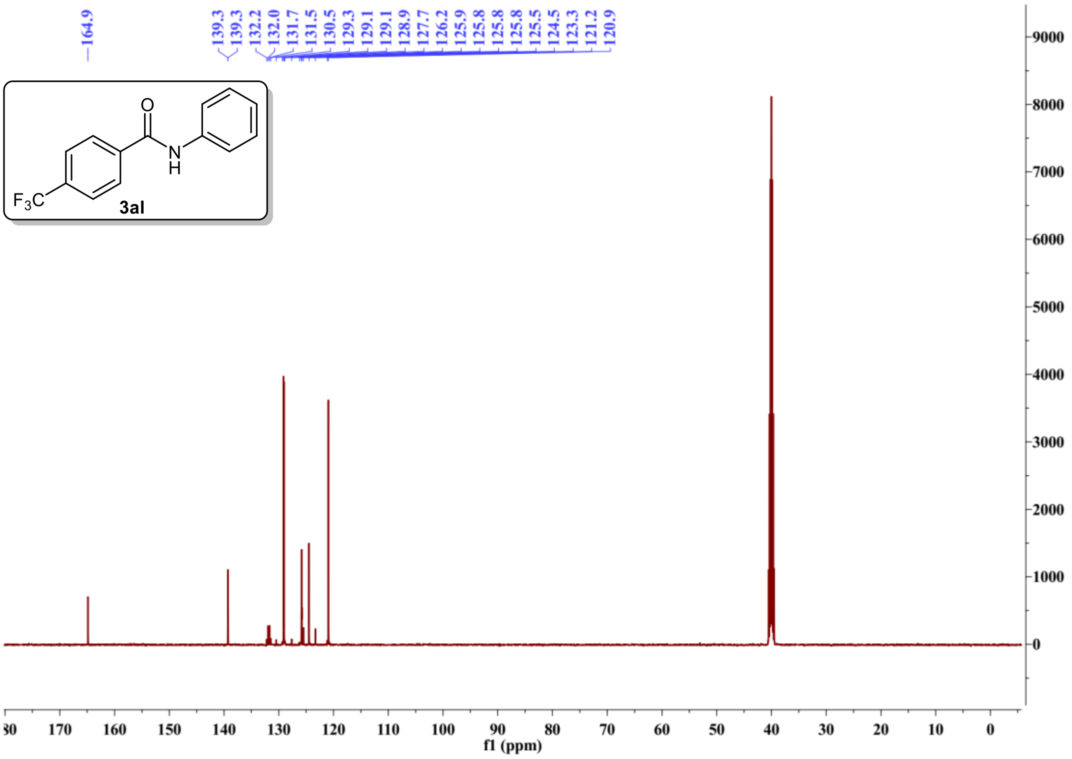

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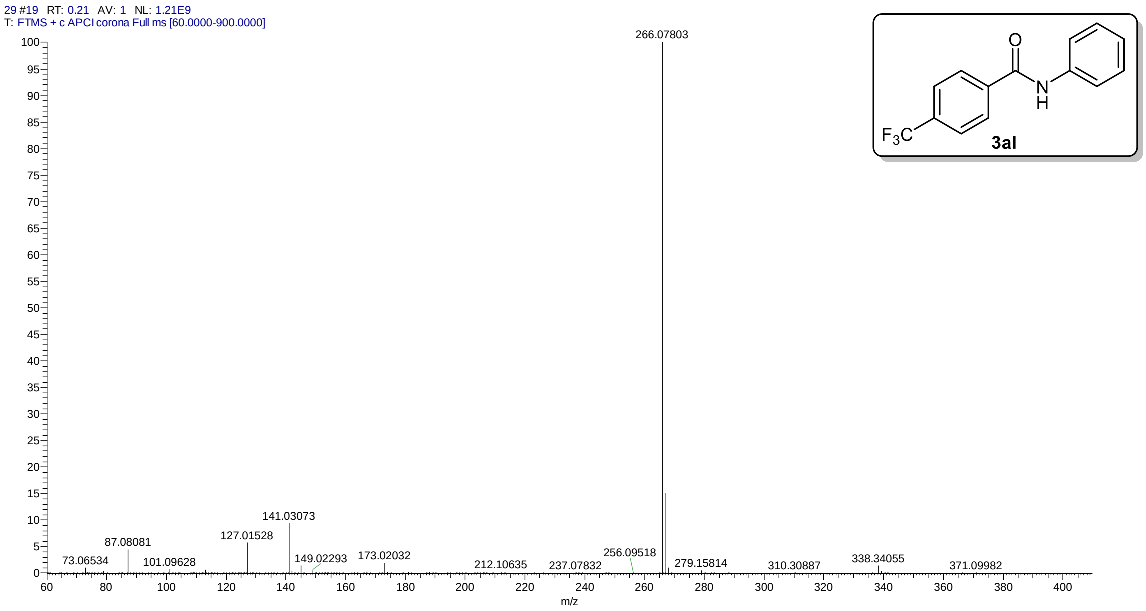

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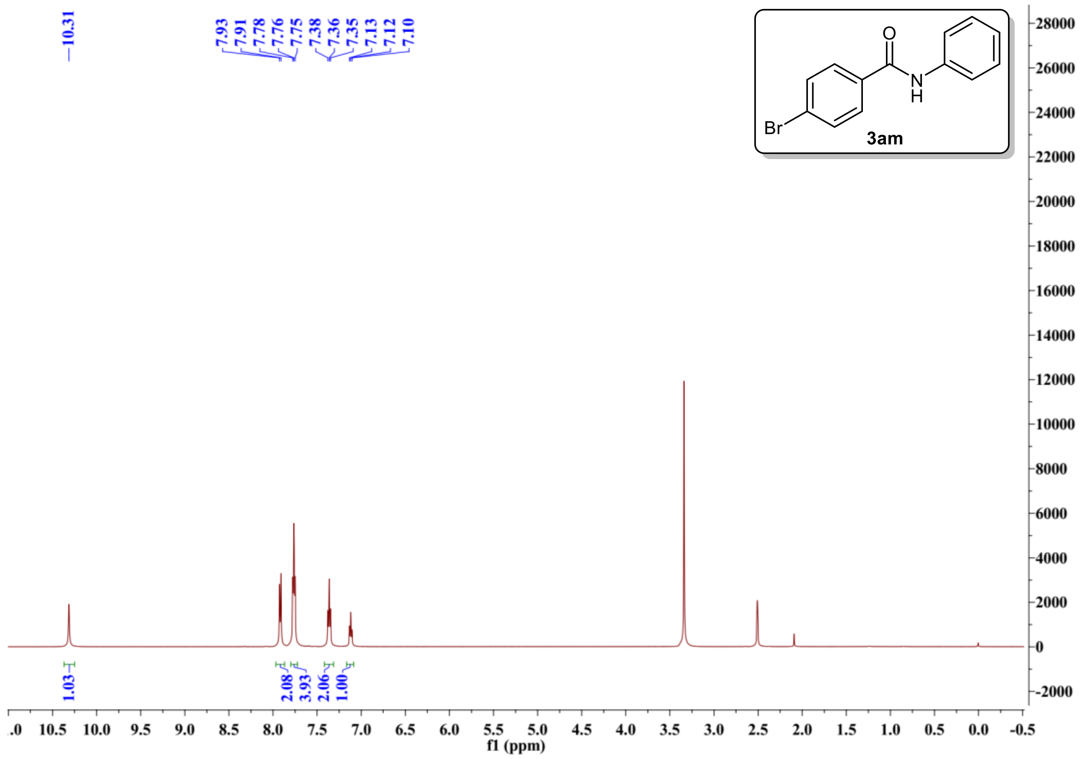

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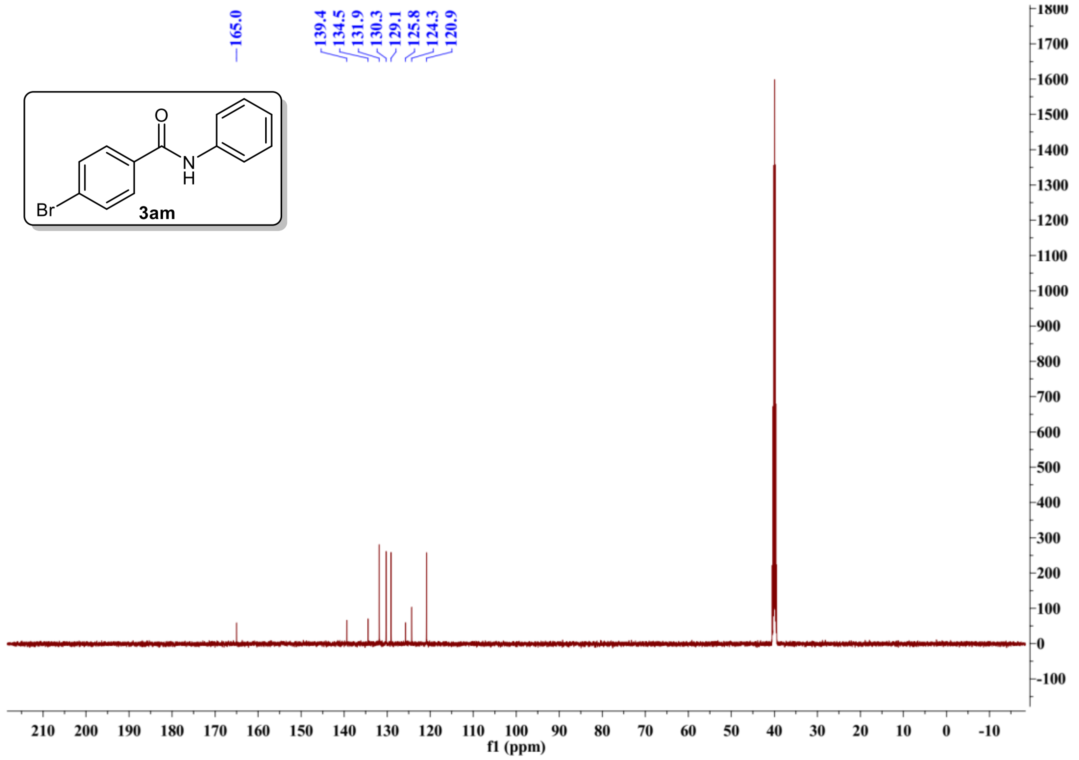
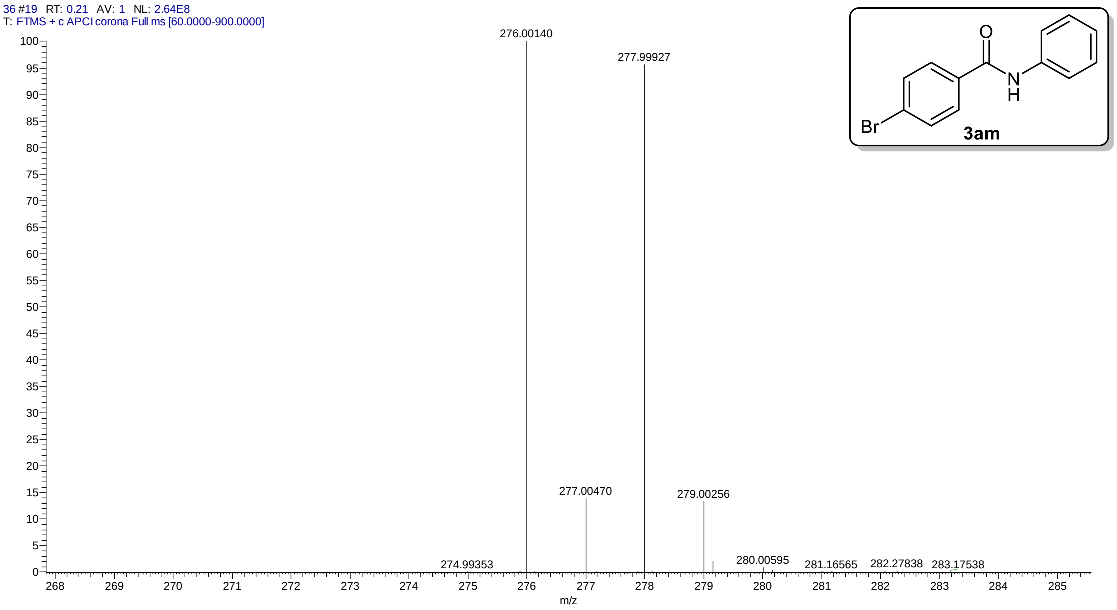


➢ HRMS spectrum for **3am**



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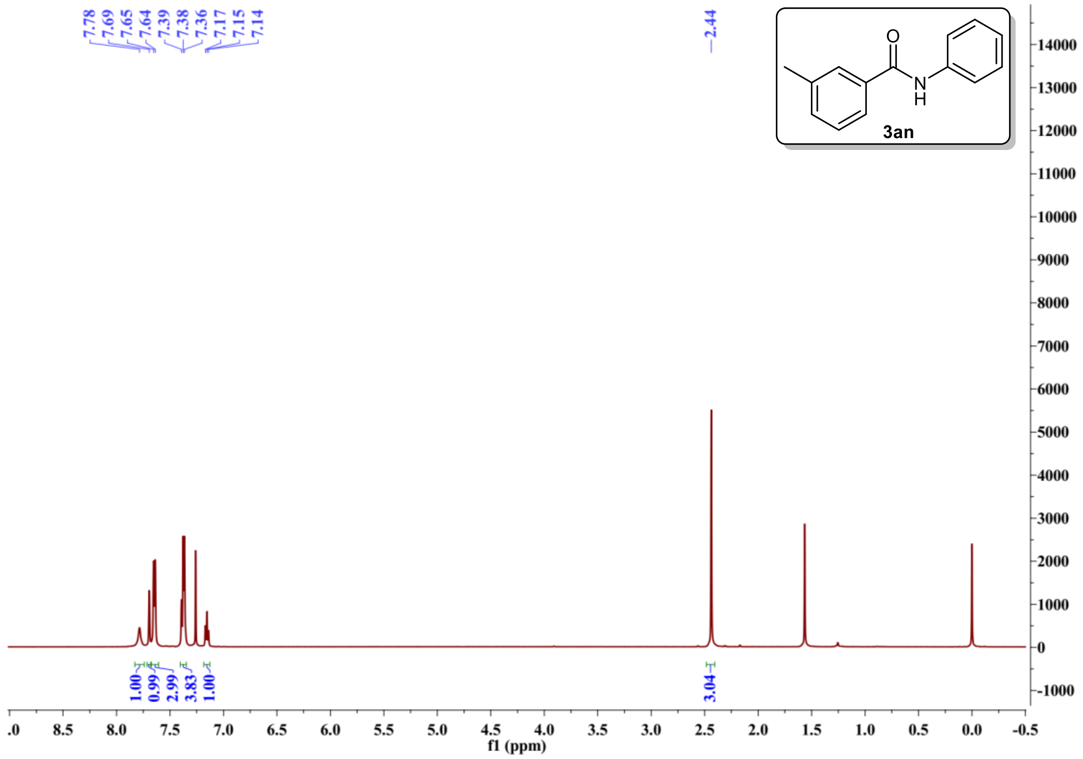

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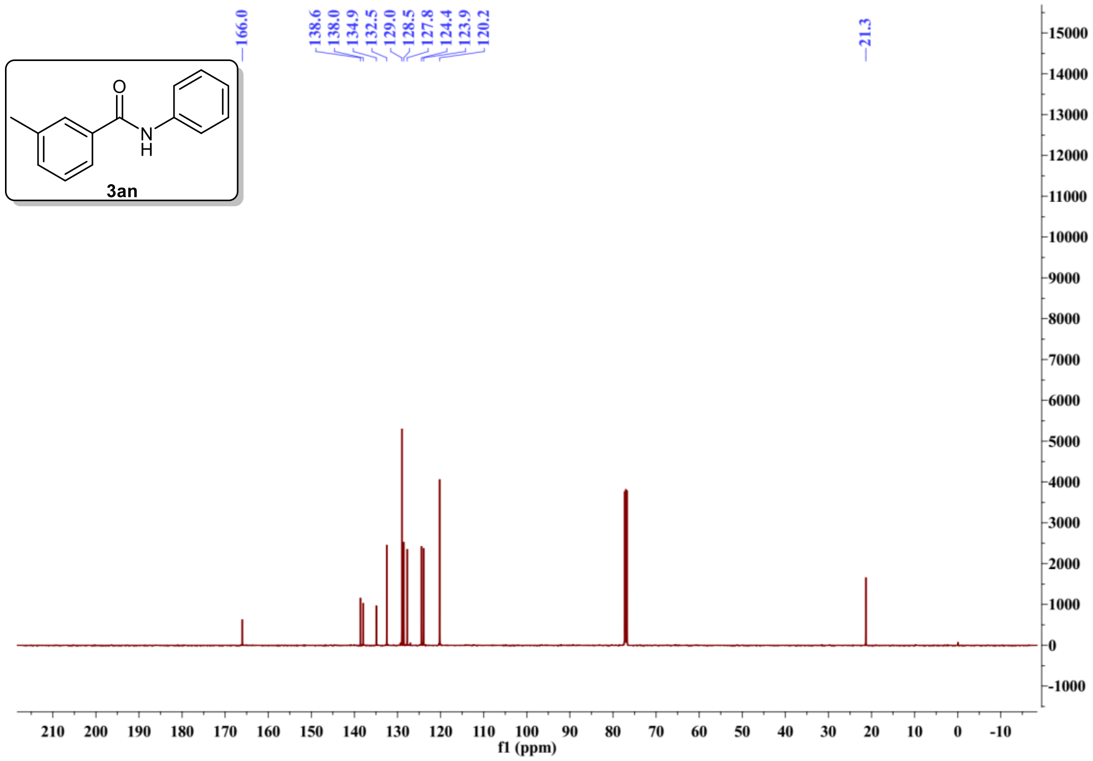

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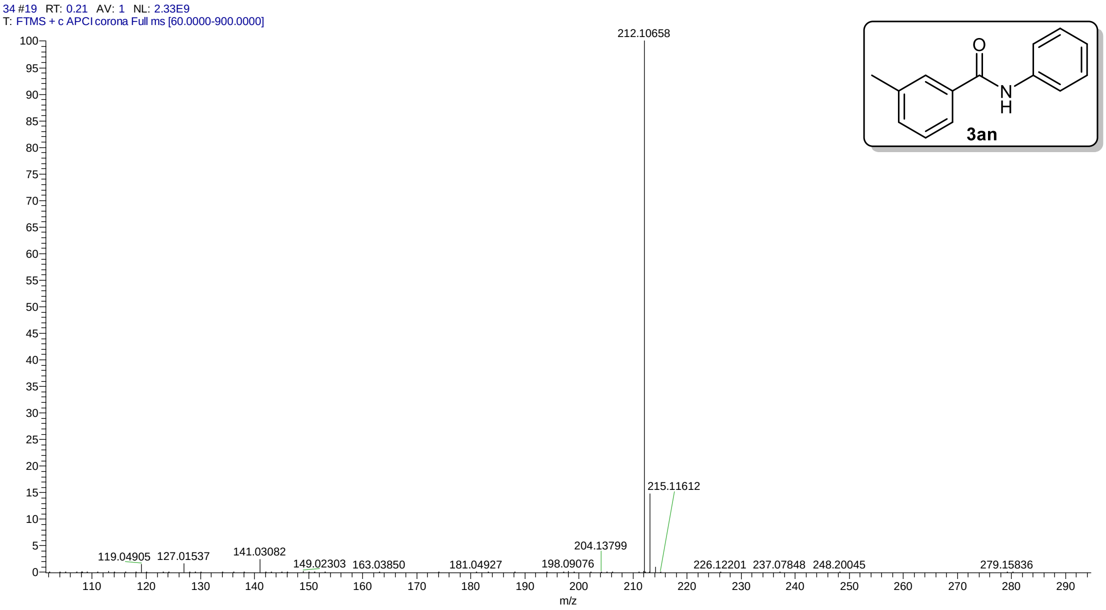
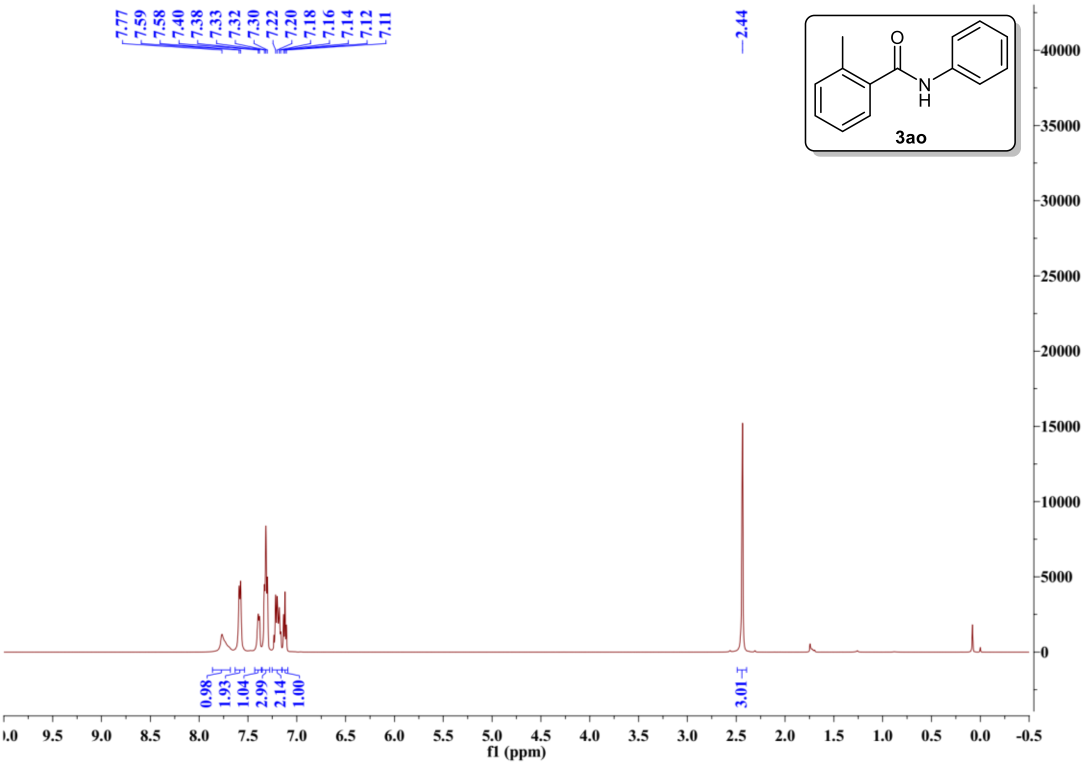
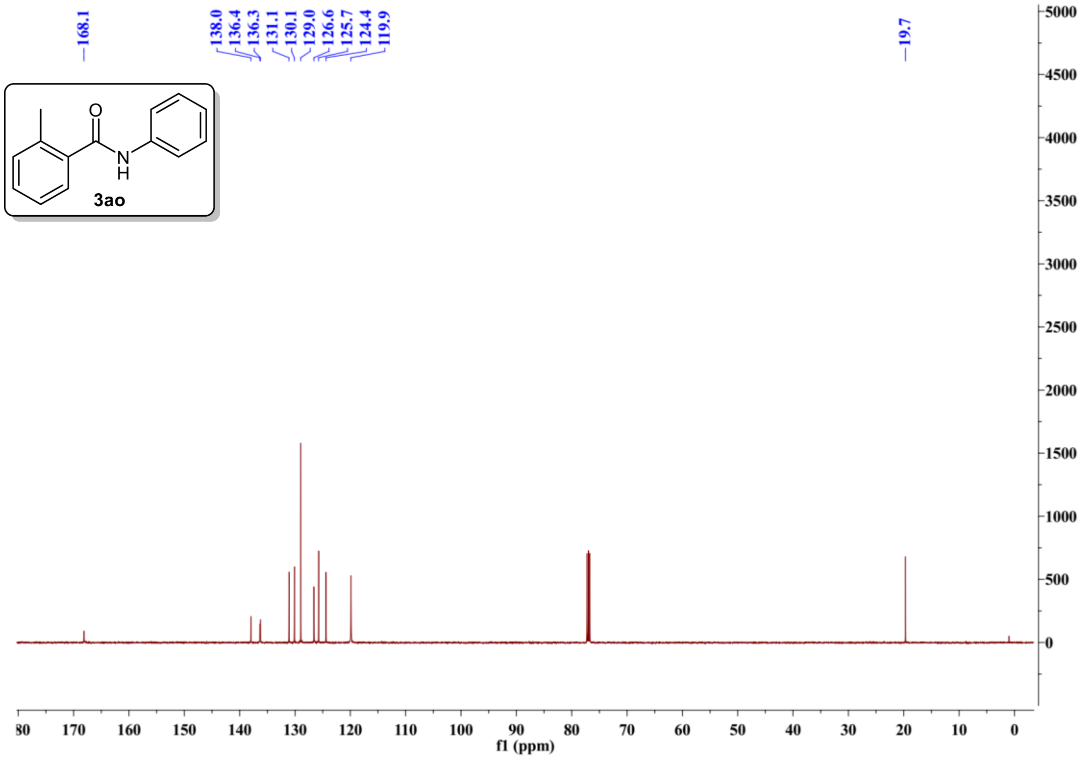


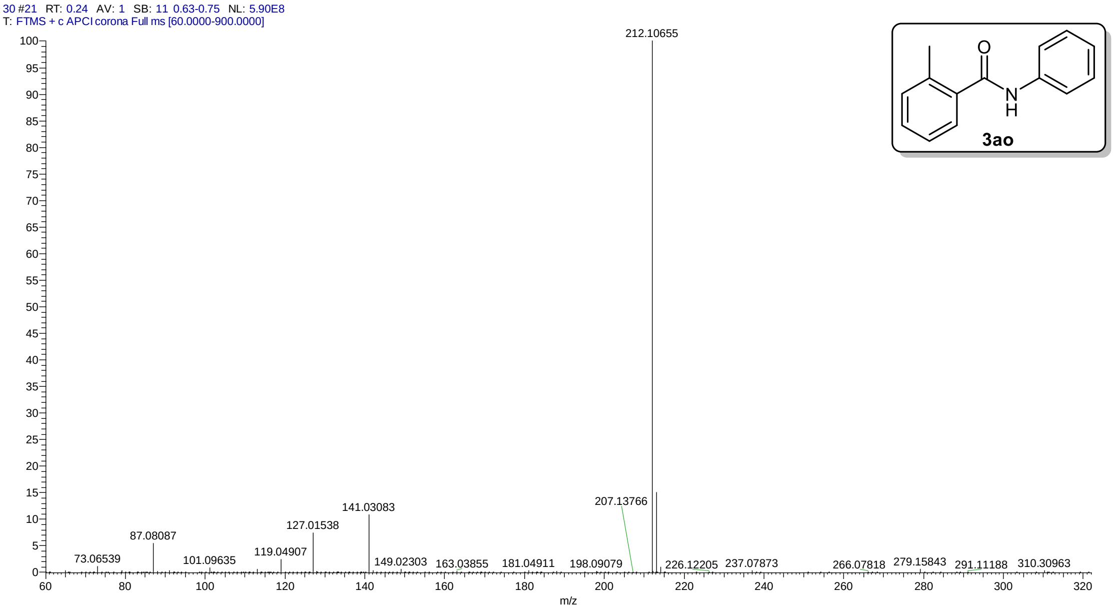
➢ ^{1}H-NMR spectrum for **3ao**



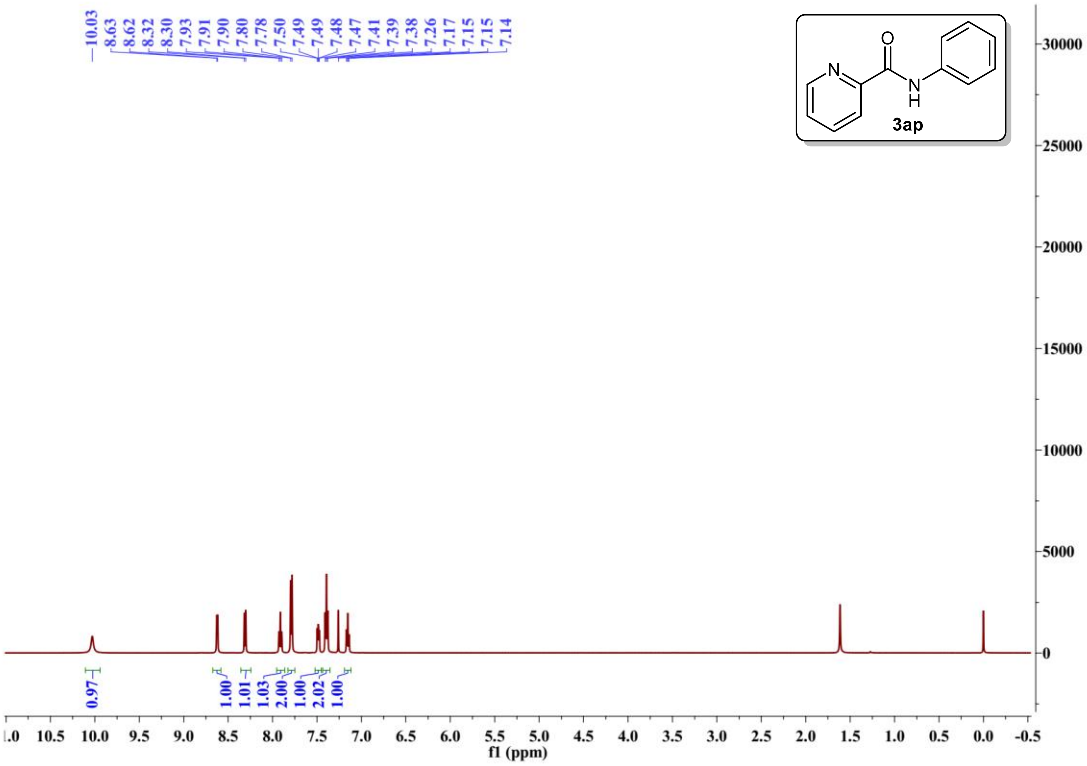
➢ ^{13}C-NMR spectrum for **3ao**



➢ HRMS spectrum for **3ao**



➢ ^{1}H-NMR spectrum for **3ap**



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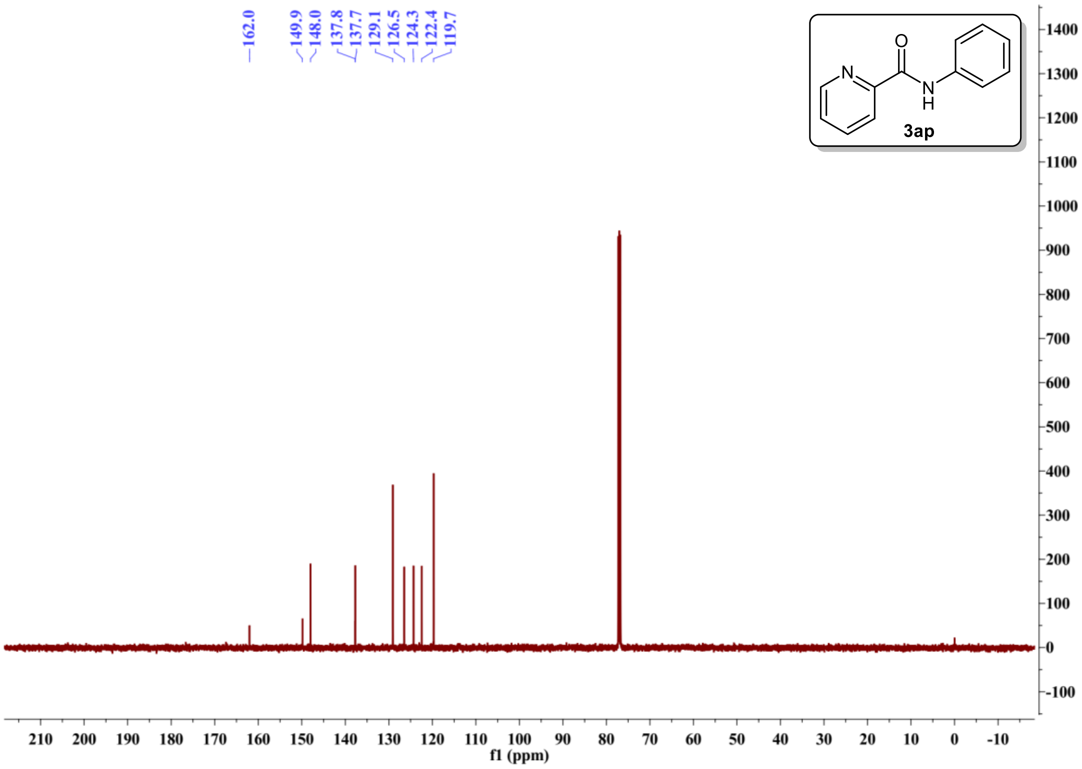
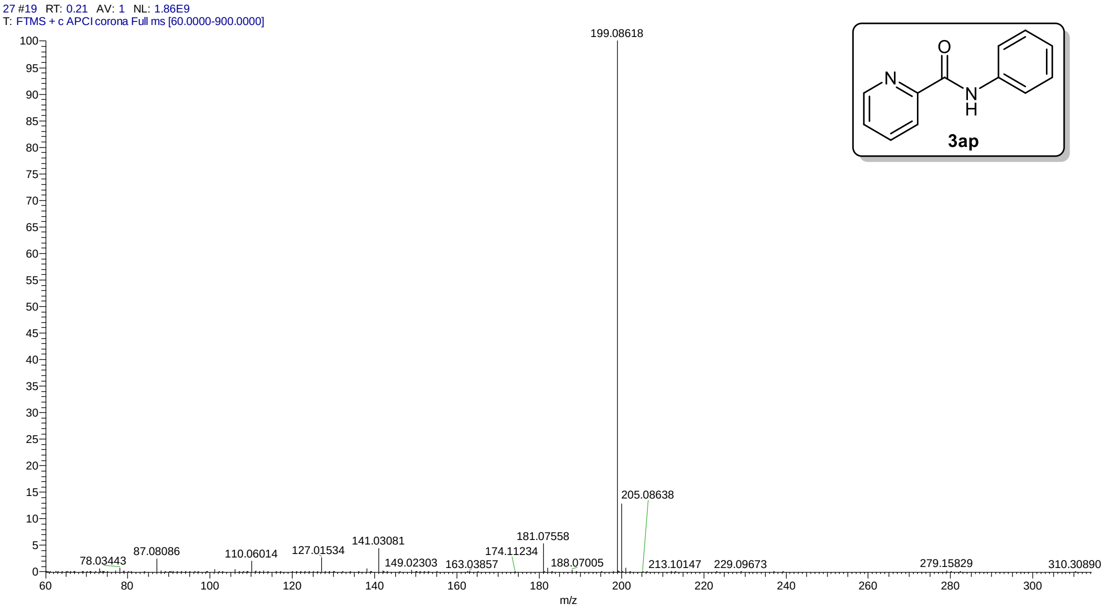
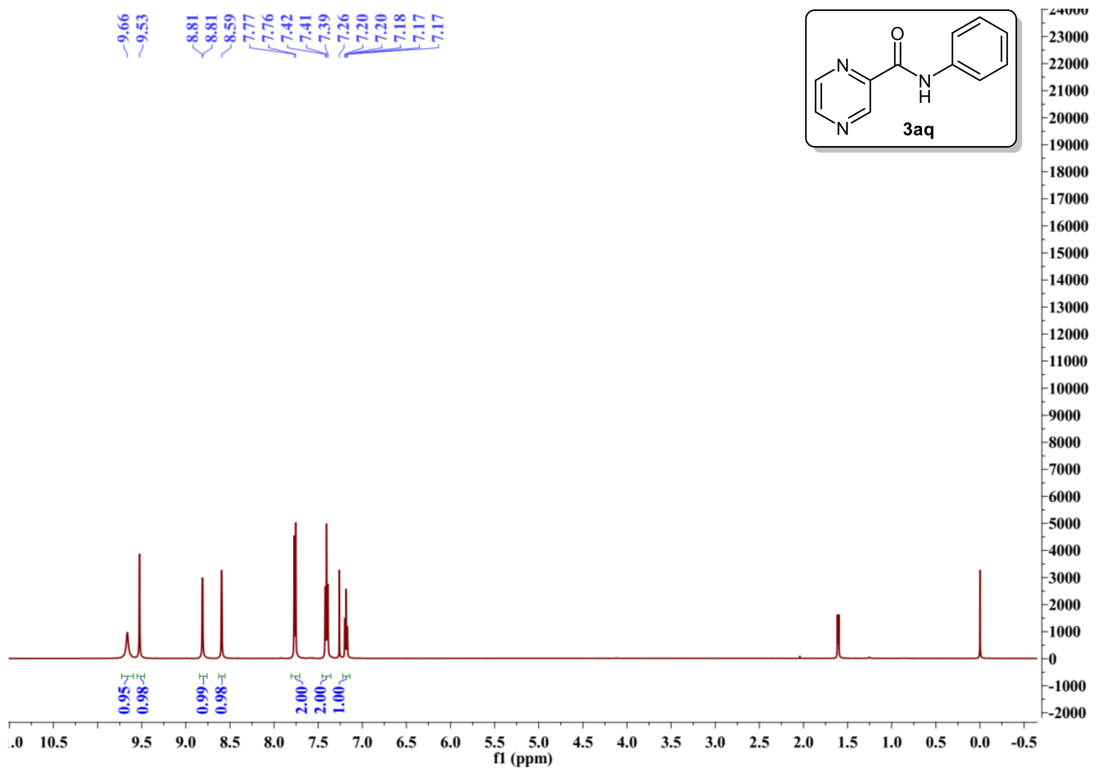


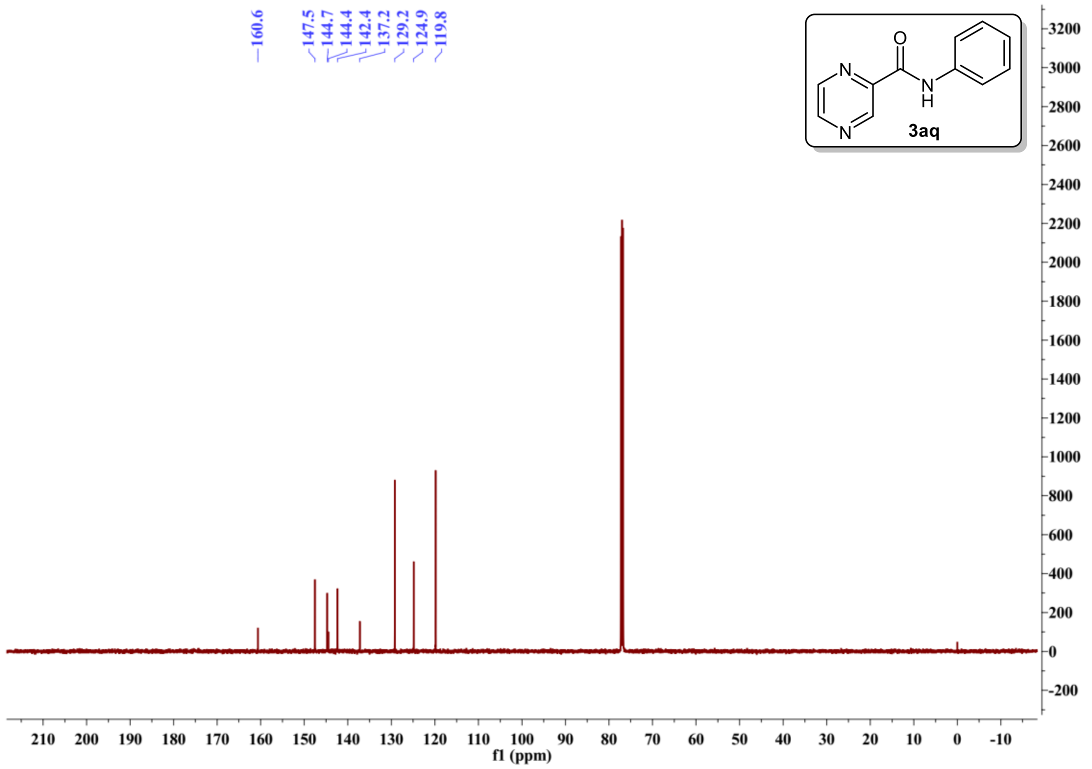
➢ HRMS spectrum for **3ap**



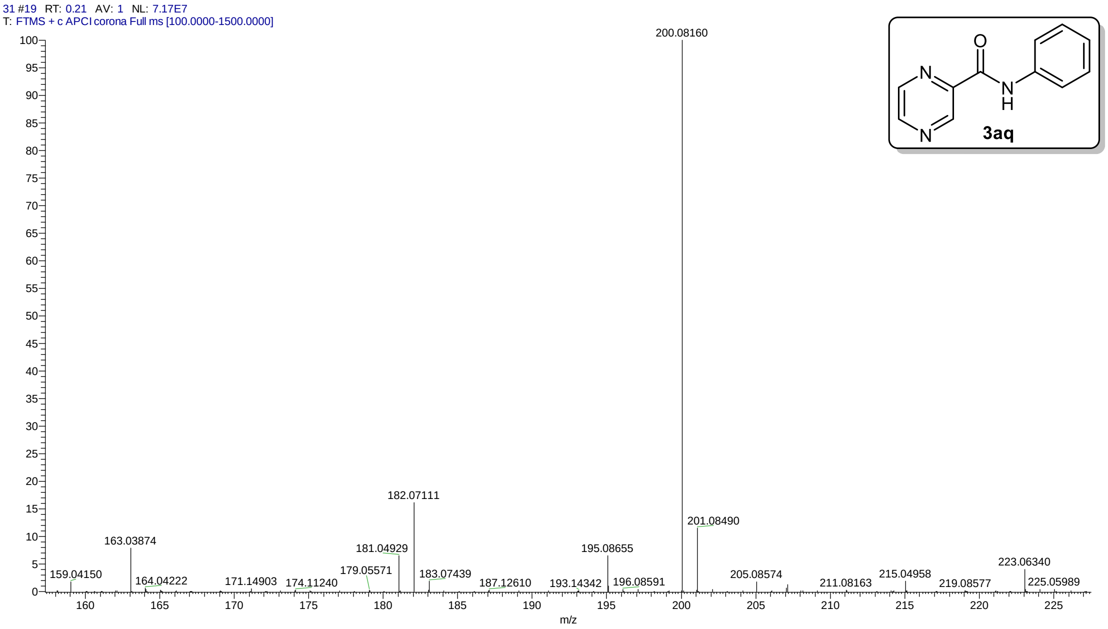
➢ ^{1}H-NMR spectrum for **3aq**



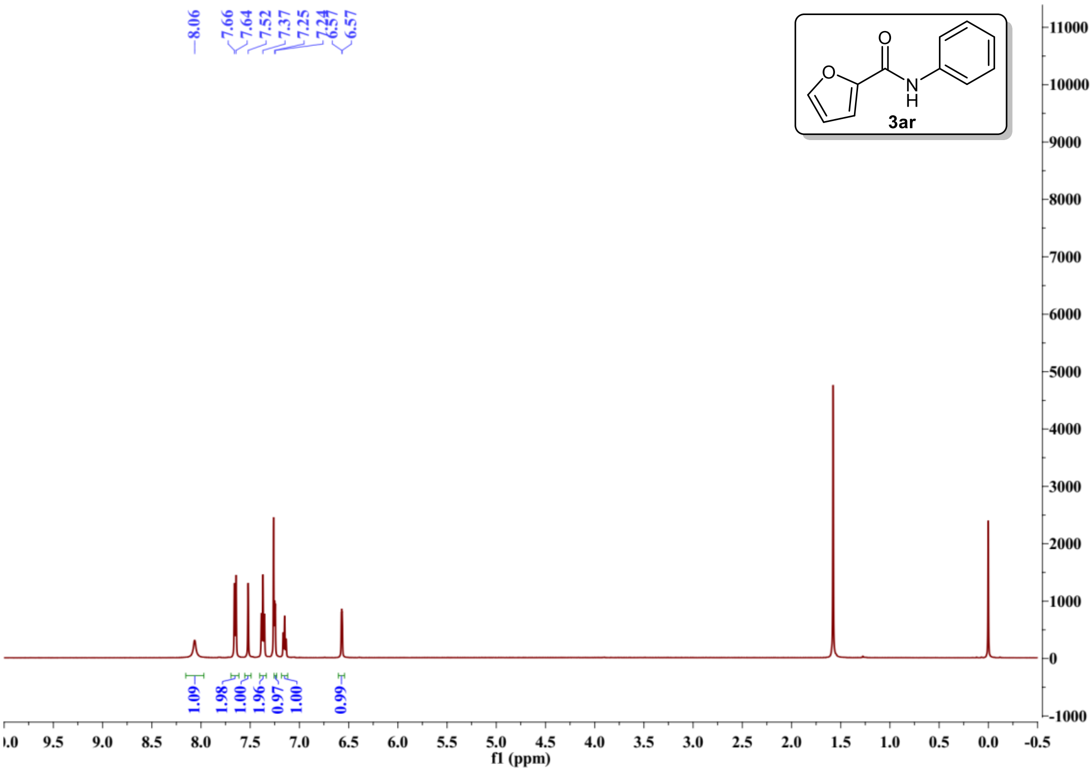
➢ ^{13}C-NMR spectrum for **3aq**



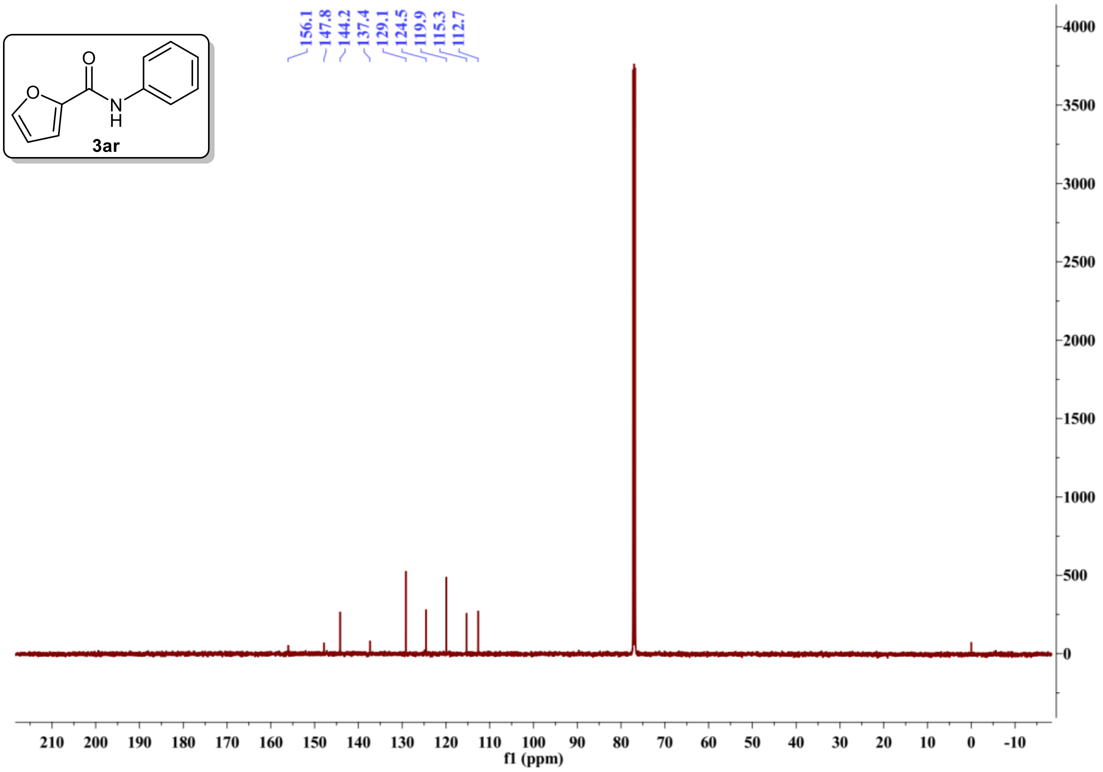
➢ HRMS spectrum for **3aq**



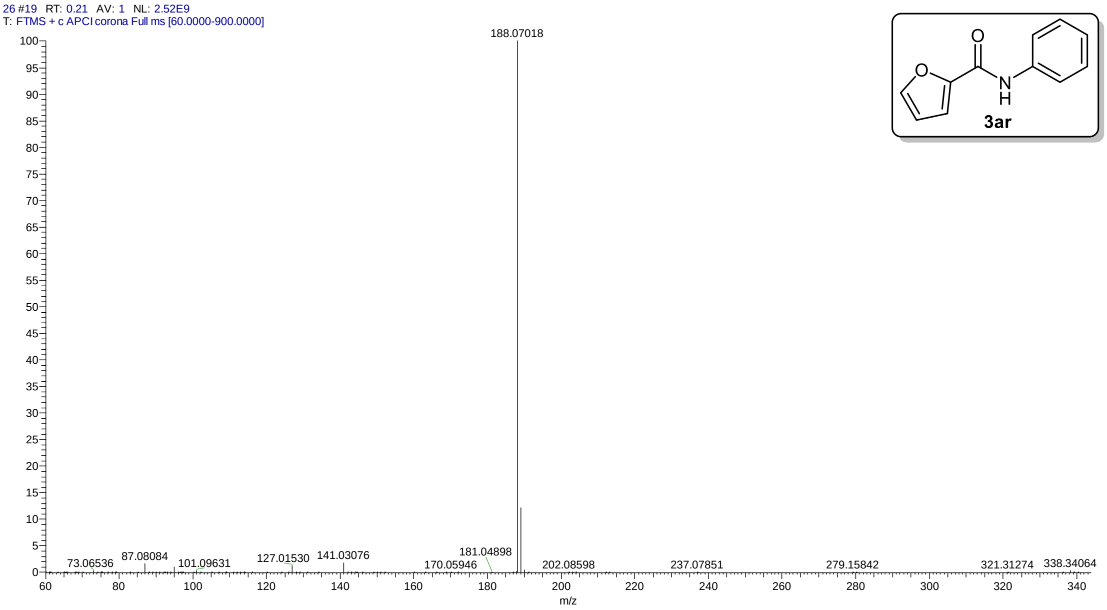
- ^{1}H-NMR spectrum for **3ar**



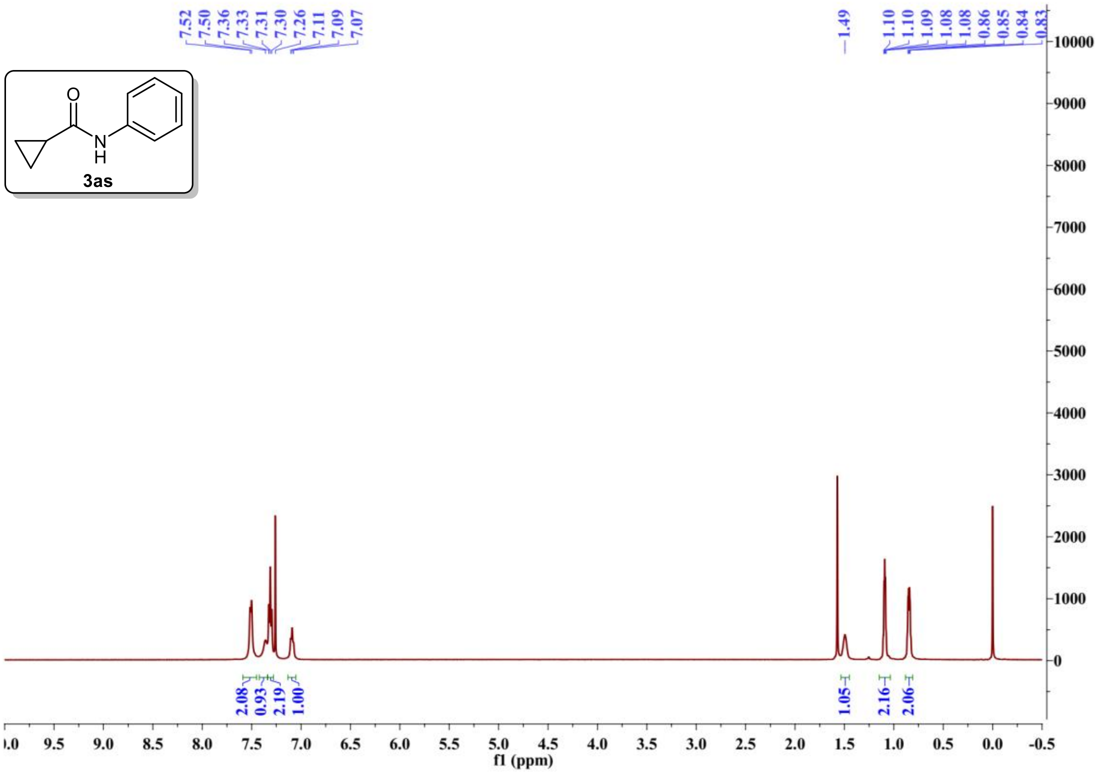
- ^{13}C-NMR spectrum for **3ar**



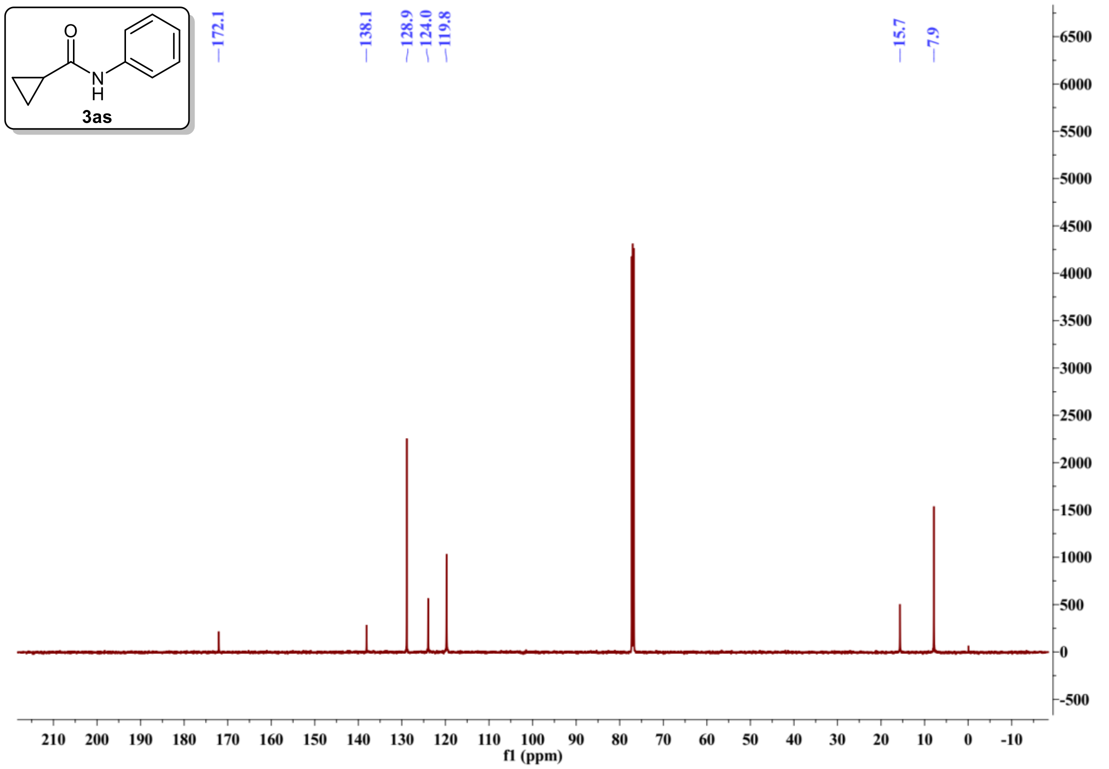
➢ HRMS spectrum for **3ar**



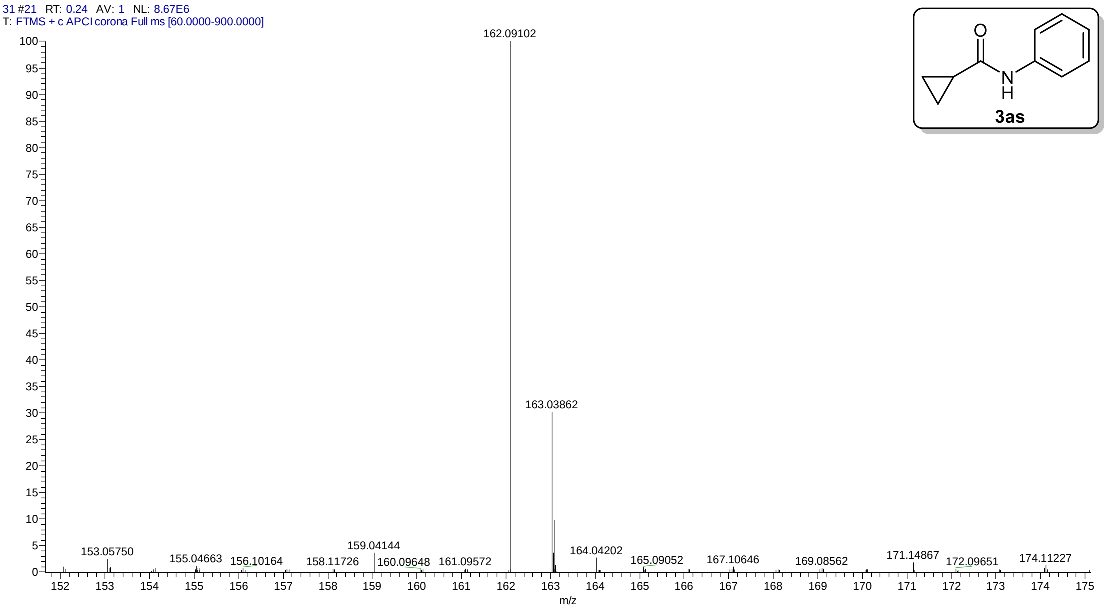
- ^{1}H-NMR spectrum for **3as**



- ^{13}C-NMR spectrum for **3as**

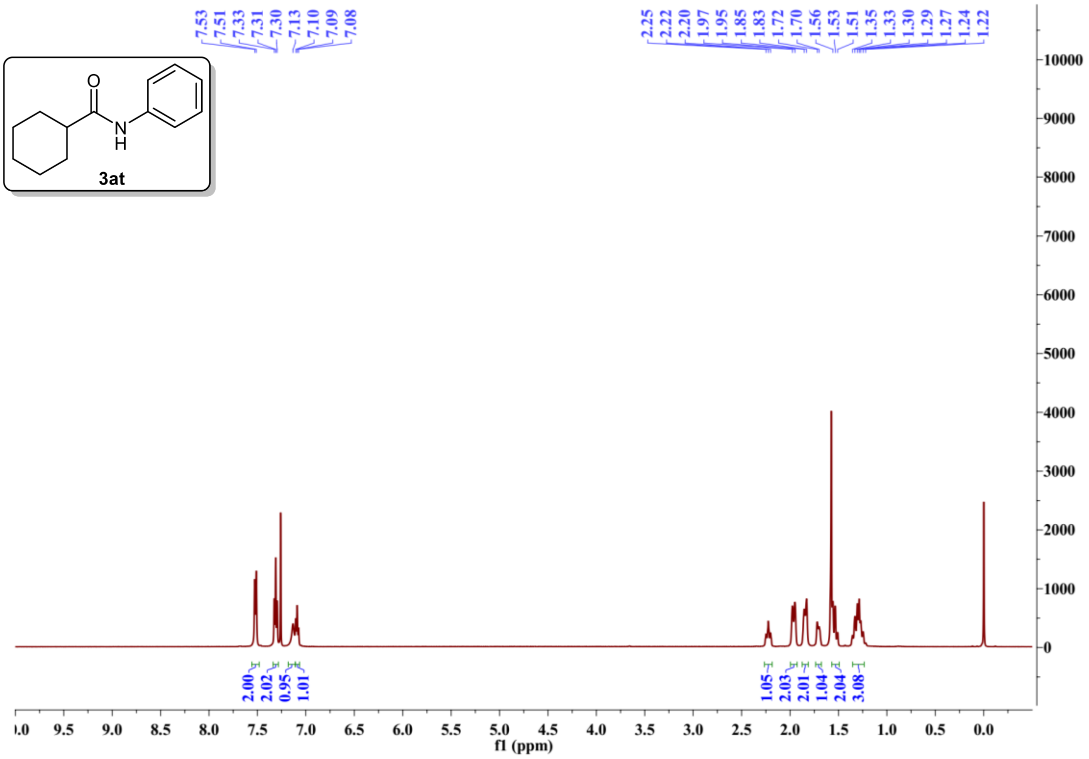


➢ HRMS spectrum for **3as**

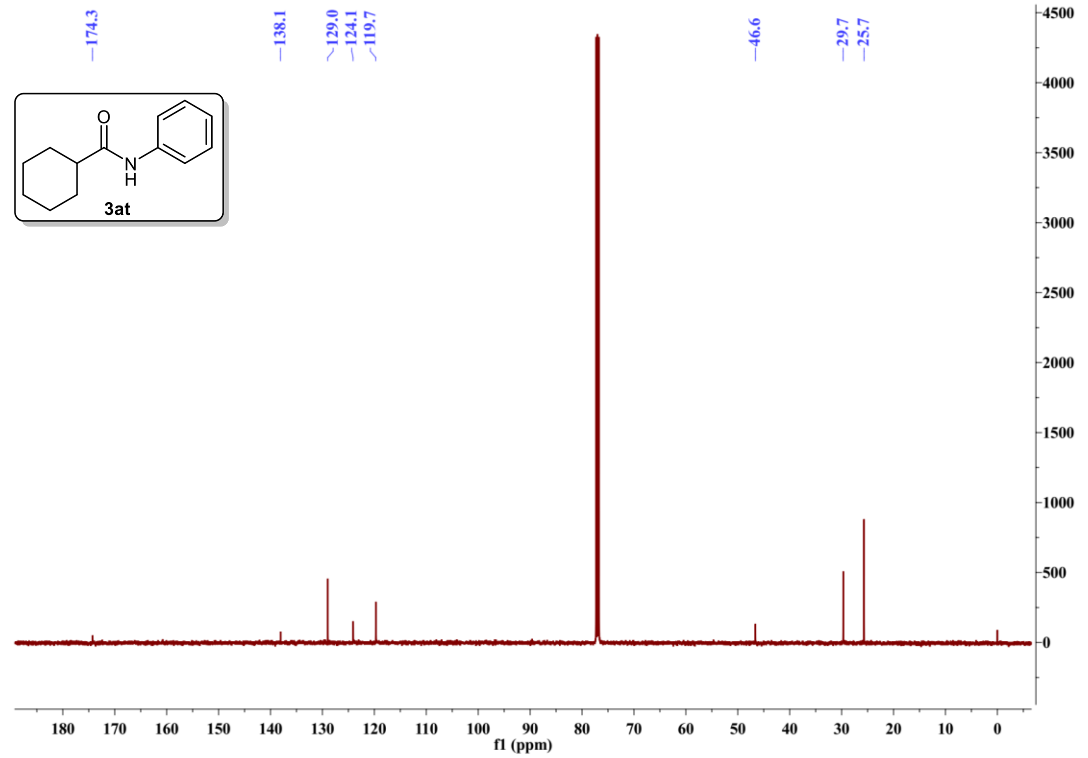


3as

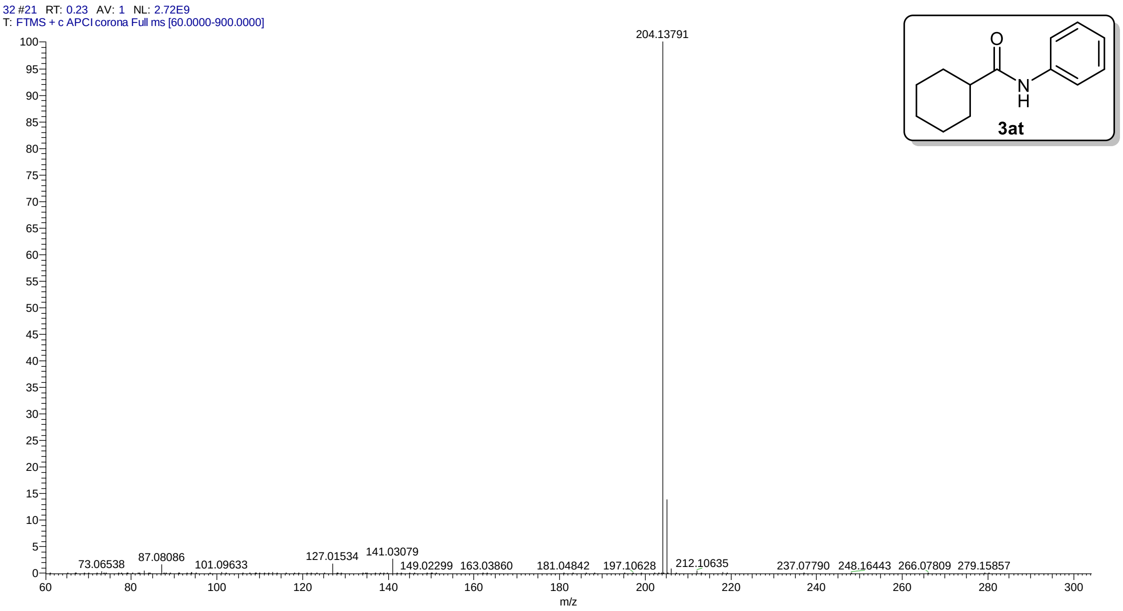
➢ ^{1}H-NMR spectrum for **3at**



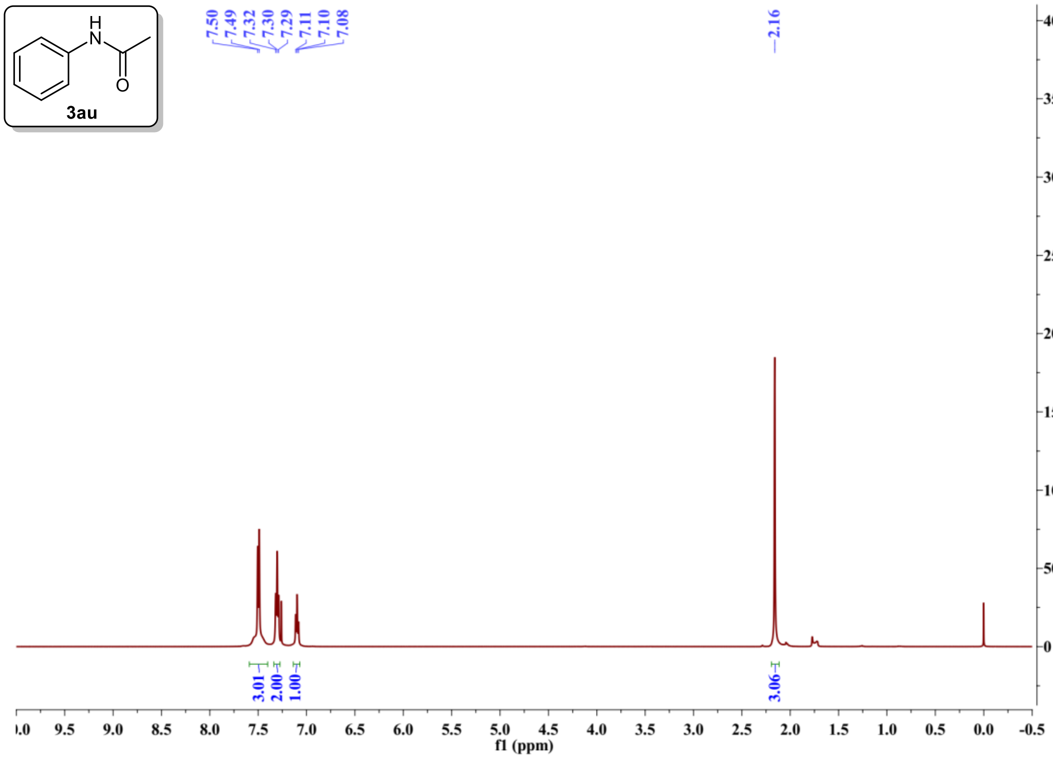
➢ ^{13}C-NMR spectrum for **3at**



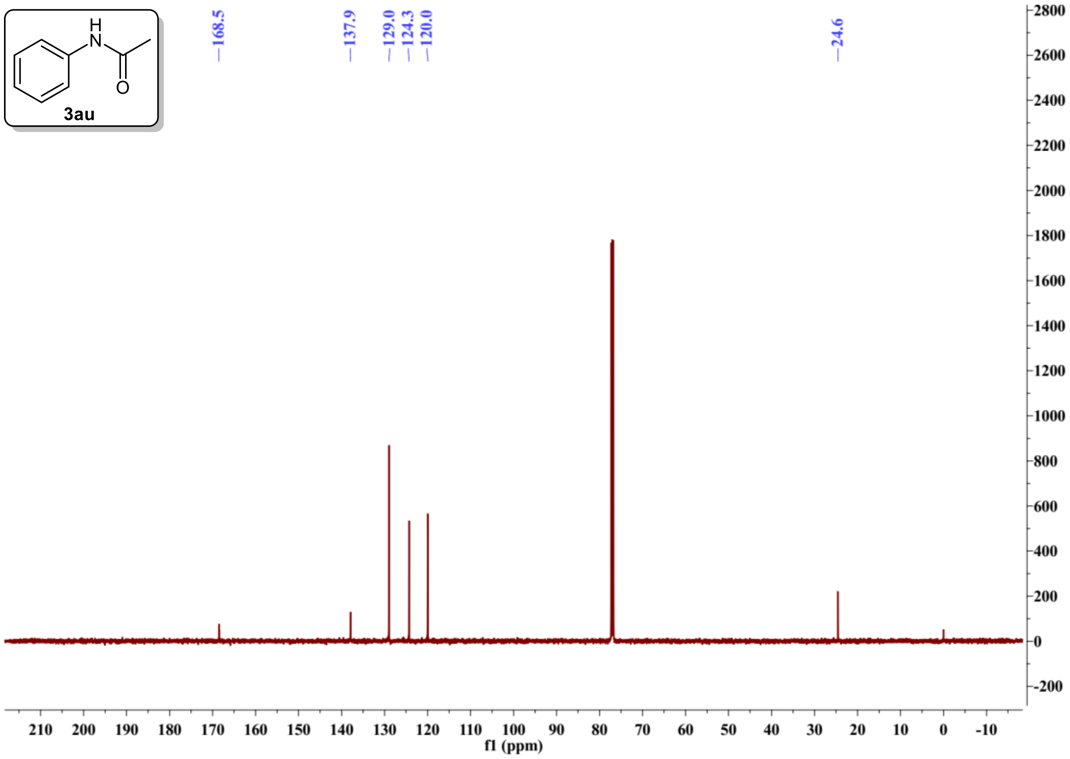
➢ HRMS spectrum for **3at**



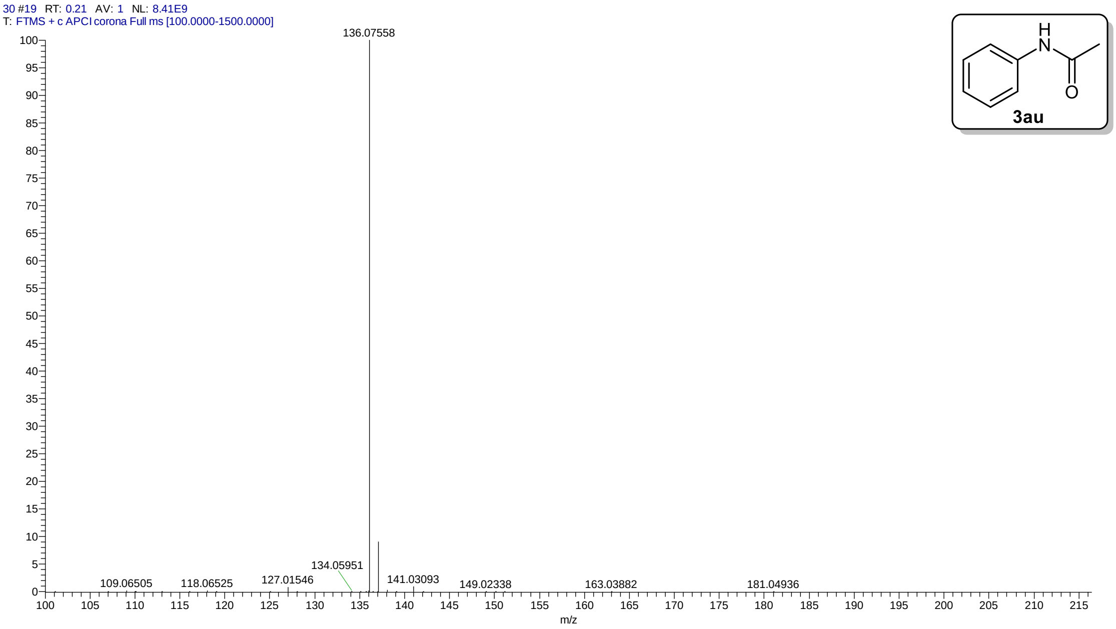
➢ ^{1}H-NMR spectrum for **3au**



➢ ^{13}C-NMR spectrum for **3au**

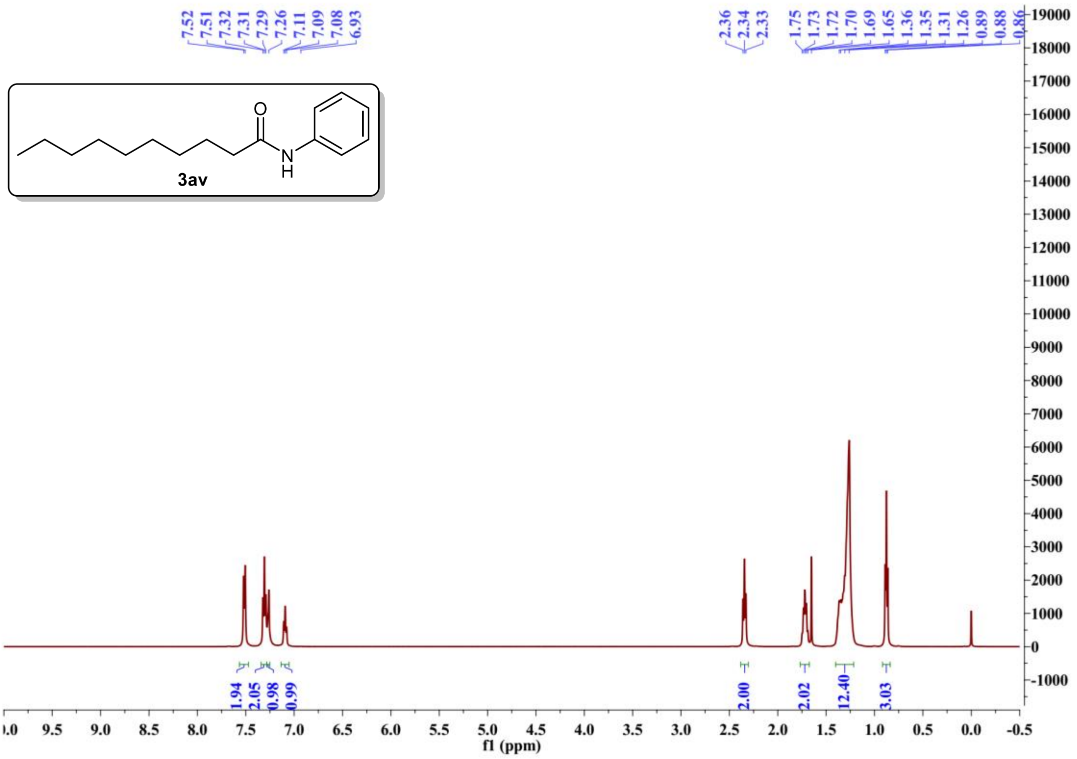


➢ HRMS spectrum for **3au**

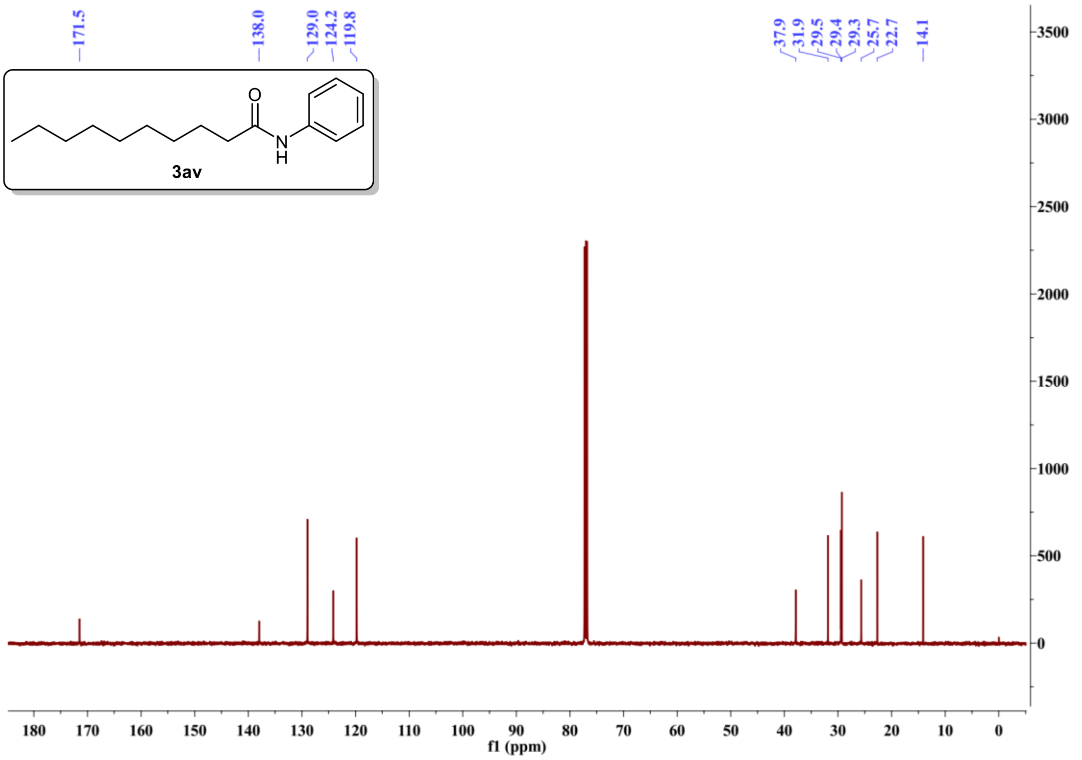


3au

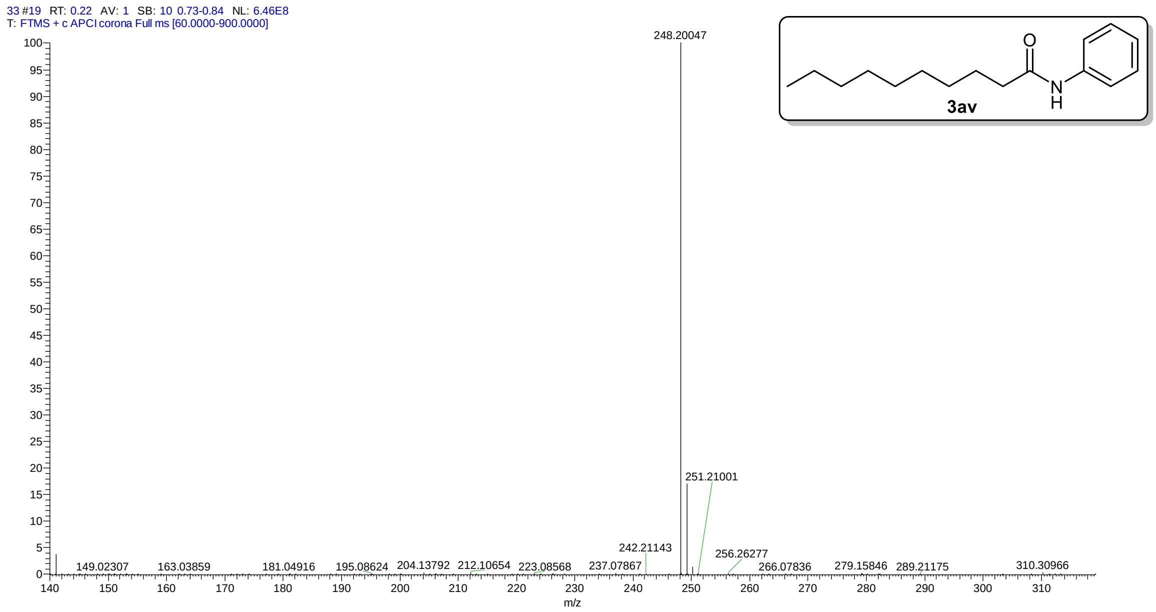
- ^{1}H-NMR spectrum for **3av**



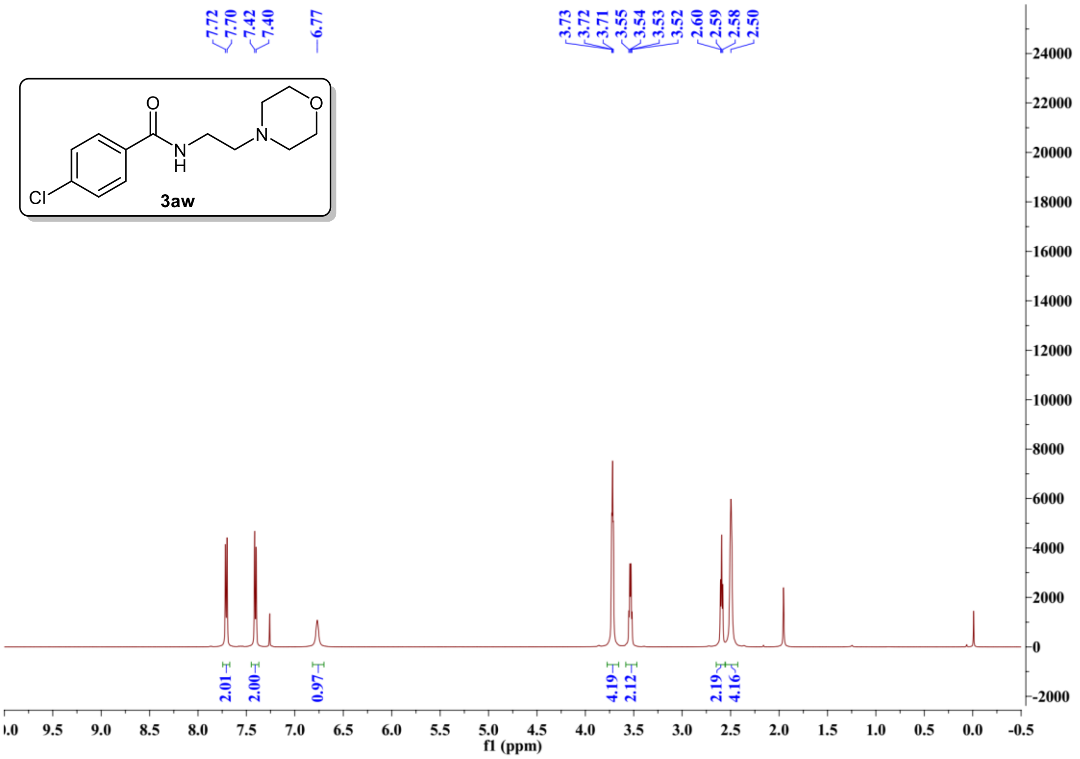
- ^{13}C-NMR spectrum for **3av**



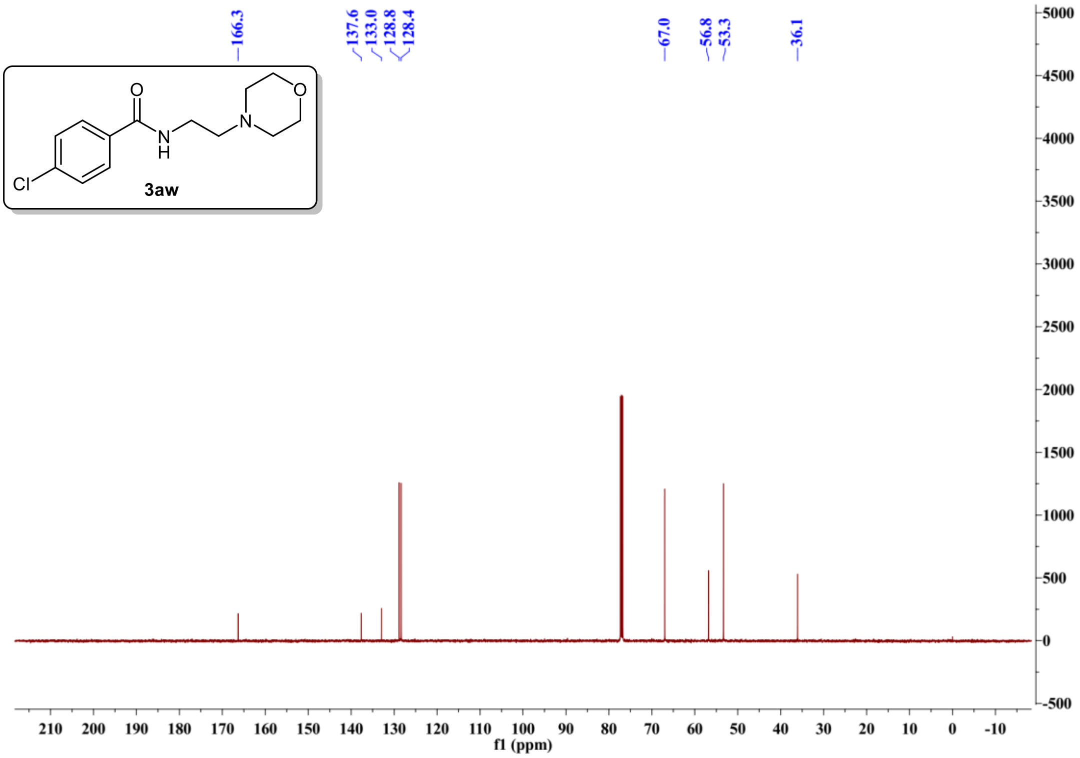
➢ HRMS spectrum for **3av**



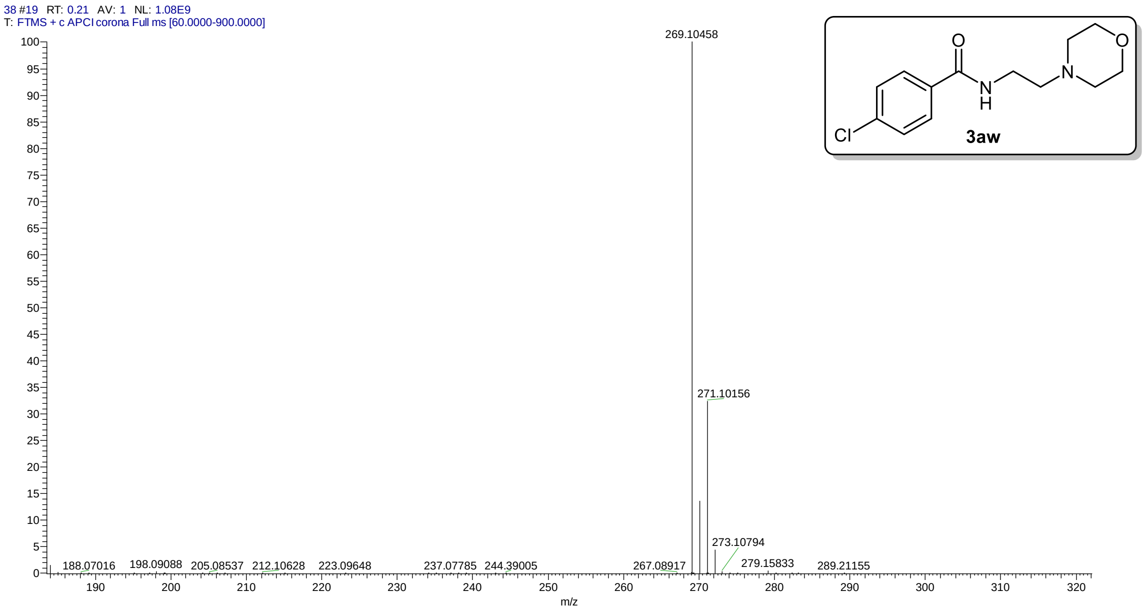
➢ ^{1}H-NMR spectrum for **3aw**



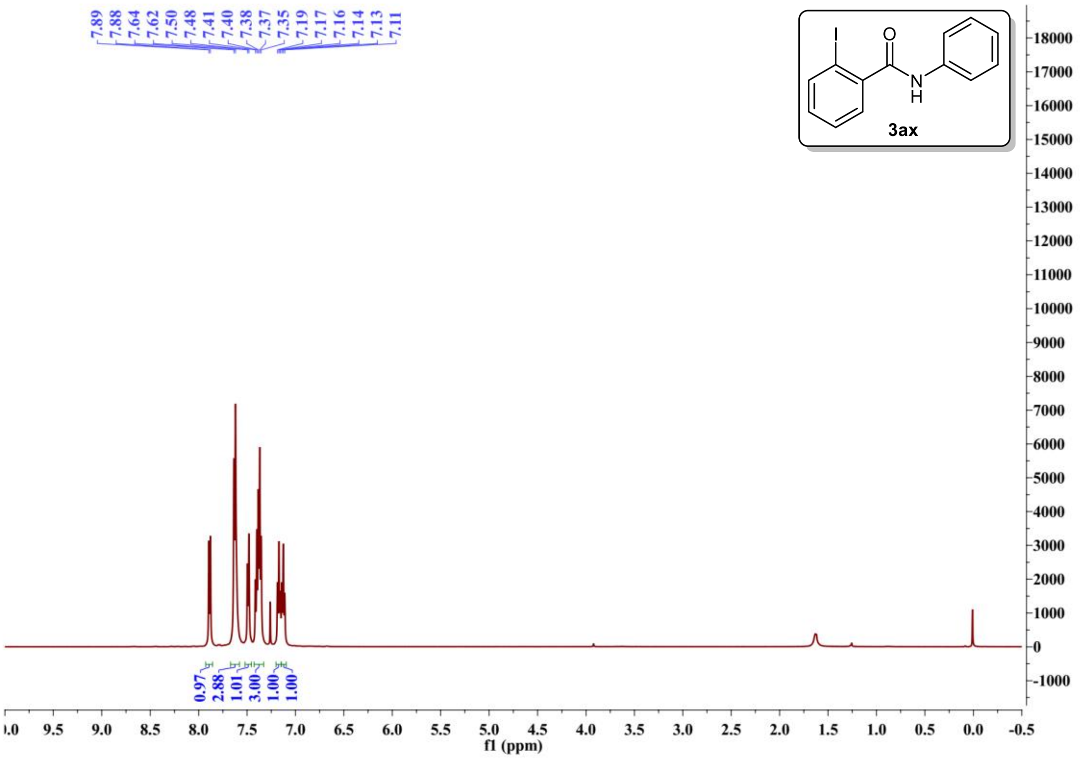
➢ ^{13}C-NMR spectrum for **3aw**



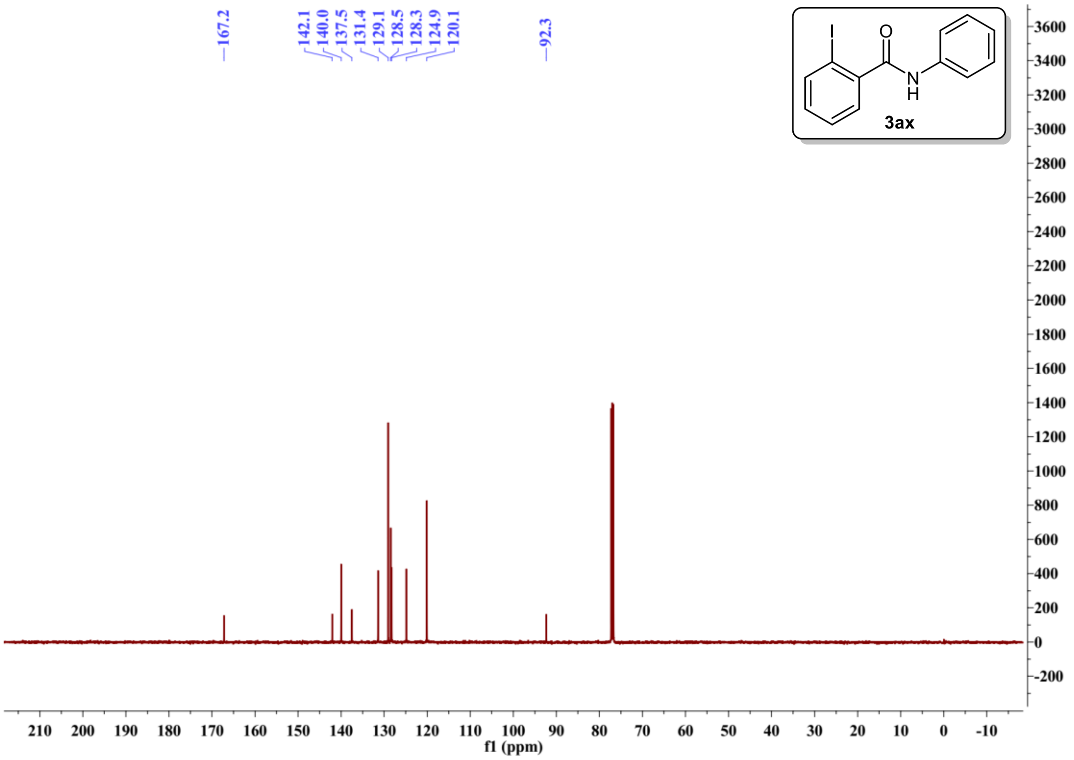
➢ HRMS spectrum for **3aw**



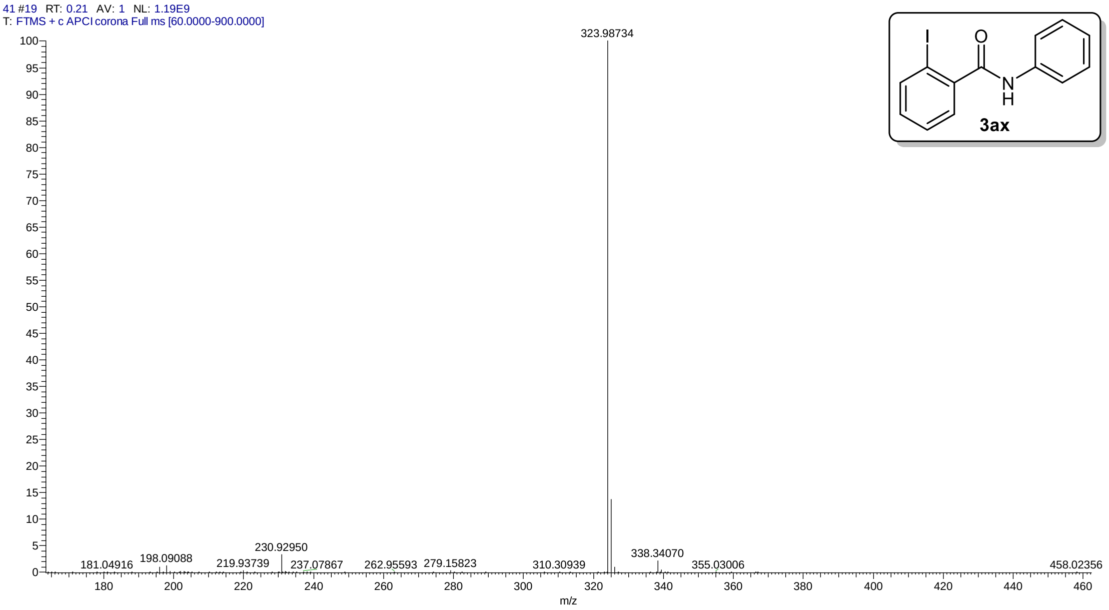
➢ ^{1}H-NMR spectrum for **3ax**



➢ ^{13}C-NMR spectrum for **3ax**

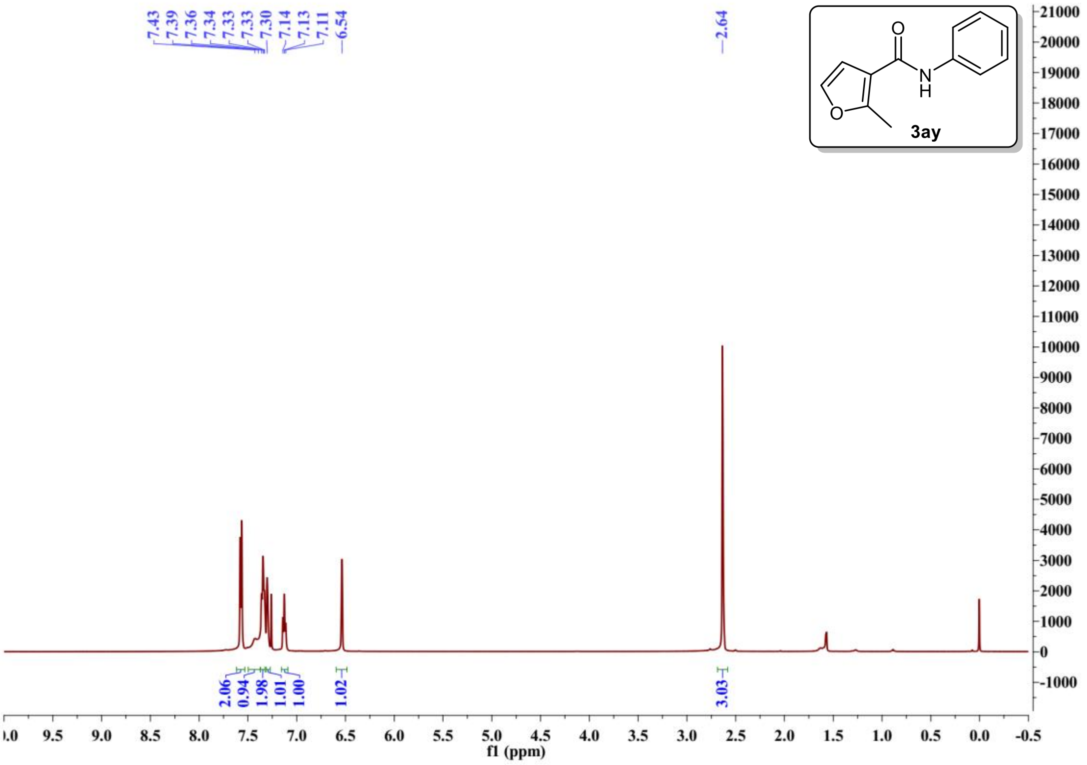


- HRMS spectrum for **3ax**

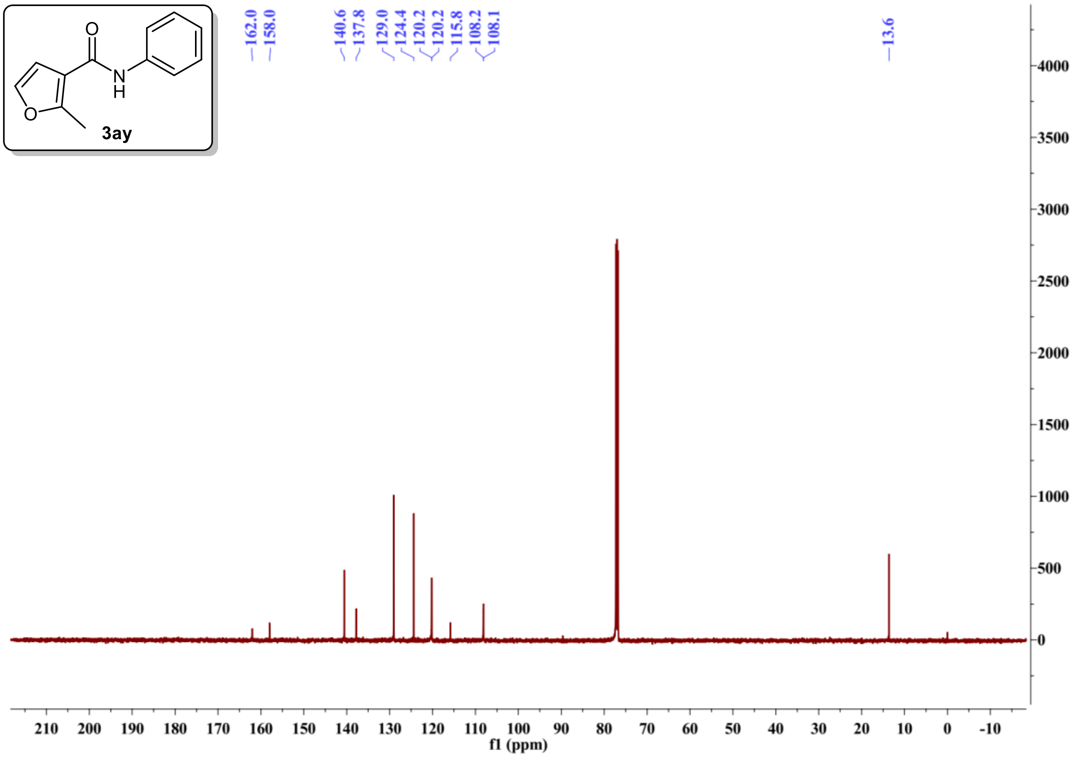


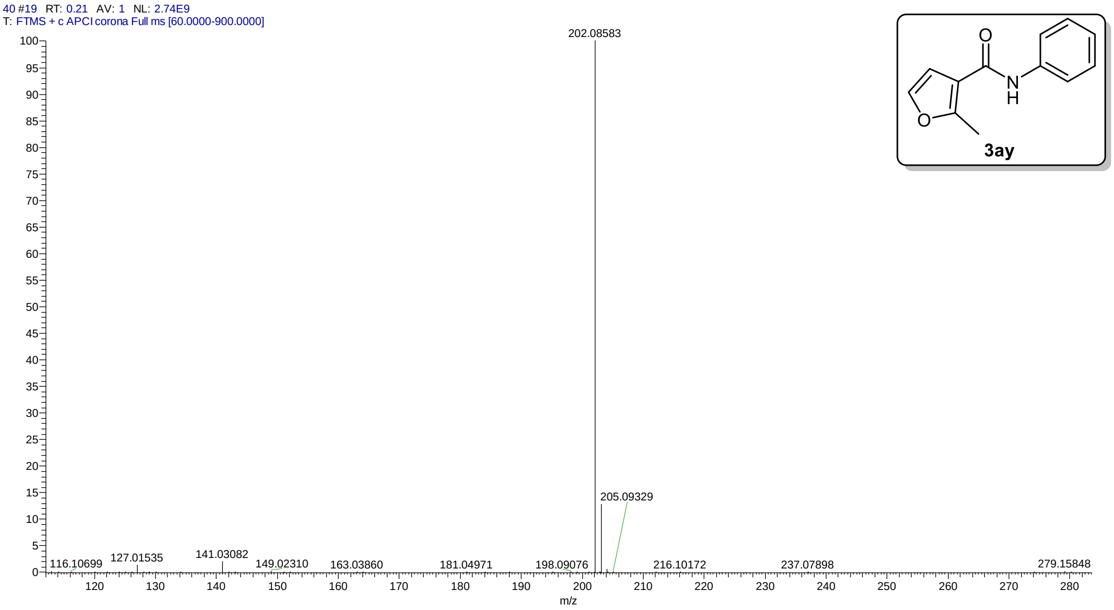
3ax

➢ ^{1}H-NMR spectrum for **3ay**



➢ ^{13}C-NMR spectrum for **3ay**



➢ HRMS spectrum for **3ay**