*Supporting Information*

# Rhodium (III)-catalyzed C4-Amidation of Indole-Oximes with Dioxazolones *via* C–H Activation

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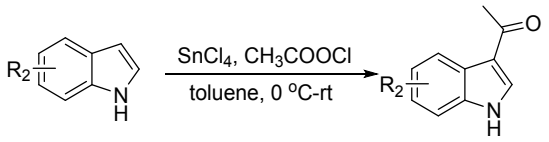
## Contents

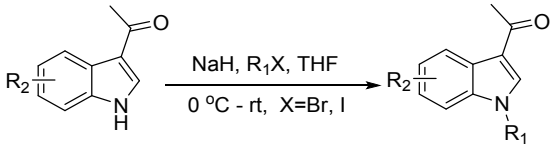
## 1. Synthetic of starting material: [1]

### 1.1 General procedure for the synthesis of 3-acetyl indole derivatives:



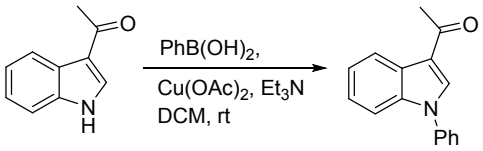

To a stirred solution of indole derivative (1 equiv) in dry toluene, acid chloride (2 equiv) was added. The reaction mixture was cooled to 0 °C and stirred for 10 min. Next, stannic chloride (2 equiv) was added drop wise to the reaction mixture and stirred for 12 h. After completion of reaction (as monitored by TLC), it was cooled to 0 °C quenched by saturated $NaHCO_3$ solution and extracted with ethyl acetate. The combined organic layers were washed with brine, dried over anhydrous $MgSO_4$ and concentrated under reduced pressure. The crude product was purified by silica gel column chromatography to provide desired product.

### 1.2. General procedure for preparation of *N*-substituted 3-acetyl indole:




To a stirred suspension of NaH (60 wt% in mineral oil, 1.5 equiv) in dry THF, solution of 3-acetyl indole derivative (1 equiv) was added at 0 °C and stirred for 15 min. Then corresponding alkyl halide (1.1 equiv) was added drop wise to the reaction mixture and stirred overnight at rt. After completion of the reaction (as monitored by TLC), it was cooled to 0 °C and quenched by addition of water and extracted with ethyl acetate. Combined organic layers were washed with water, brine, and dried over anhydrous $MgSO_4$ and concentrated under reduced pressure. The crude product was purified by silica gel column chromatography to obtain desired *N*-alkylated 3-acetyl indole derivatives.

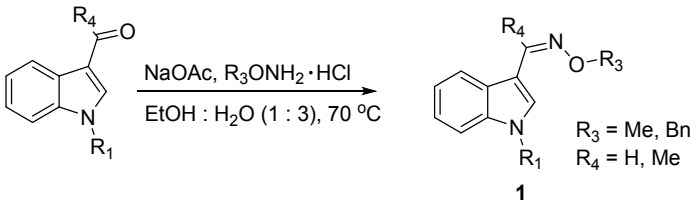
### 1.3. Procedure for synthesis of *N*-phenyl indole:




In a flame-dried sealed tube, 3-acetyl indole (1 equiv) dissolved in $CH_2Cl_2$ (6 mL), phenylboronic acid (2 equiv), anhydrous copper (II) acetate (2 equiv), and triethylamine (2 equiv) were added. The mixture was stirred at room temperature for 3 days, concentrated in *vacuo*, diluted with chloroform and water. The organic layer was separated, washed with brine and dried over anhydrous $MgSO_4$, concentrated in *vacuo*, and purified by column chromatography (EtOAc/hexane) to obtain pure

product.

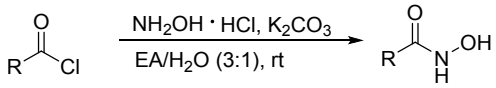
### 1.4. General procedure for preparation of ketoximes:




**1**

To a 50 mL round bottom flask equipped with a stir bar was charged with ketone (1equiv), $R_3ONH_2 \cdot HCl$ (2.7 equiv), NaOAc (4.4 equiv), and EtOH:$H_2O$ (1:3). The reaction mixture was heated at 70 °C. After completion of reaction (as monitored by TLC), it was cooled to rt and EtOH was removed under vacuum. The mixture was extracted with EtOAc. The combined organic layers were dried over anhydrous $MgSO_4$, and concentrated under reduced pressure. The crude product was purified by silica gel column chromatography to yield the desired analytically pure ketoxime **1** in moderate to good yield.

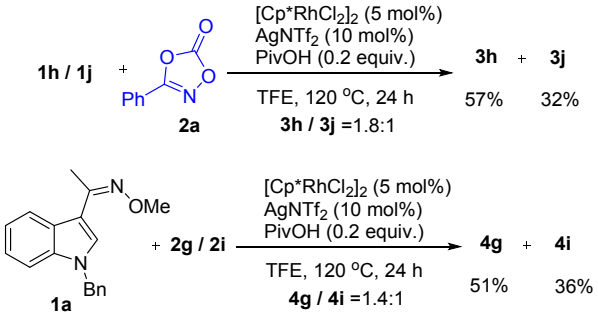
## 2. Synthetic of dioxazolones: [2]




In a 250 mL flask, hydroxylamine hydrochloride (20.0 mmol), ethyl acetate (60 mL), $H_2O$ (40 mL) and $K_2CO_3$ (20.0 mmol) were added at 0 °C. Then acyl chloride (10.0 mmol) dissolved in 20 mL ethyl acetate was added to the resulting mixture dropwise. The solution was warmed up to room temperature and stirred overnight. After that, the reaction mixture was extracted with ethyl acetate, washed with water and brine and dried over anhydrous $MgSO_4$. The solvent was evaporated under the reduced pressure to afford the desired product(s) for the next step without further purification.


To a stirred solution of hydoxamic acid (8 mmol) in freshly distilled dichloromethane (60 mL) in a 250 mL flask was added 1,1'-carbonyldiimidazole (8.4 mmol) in one portion at room temperature. After stirring for 20-30 min, the reaction mixture was quenched with 1N aqueous solution of HCl (50 mL) and extracted with dichloromethane. The combined organic layers washed with water and brine, dried over anhydrous $MgSO_4$, and then concentrated in vacuo. The resulting residue was further purified by recrystallization with ethyl acetate and hexane to give the desired 3-substituted-1,4,2-dioxazol-5-ones.

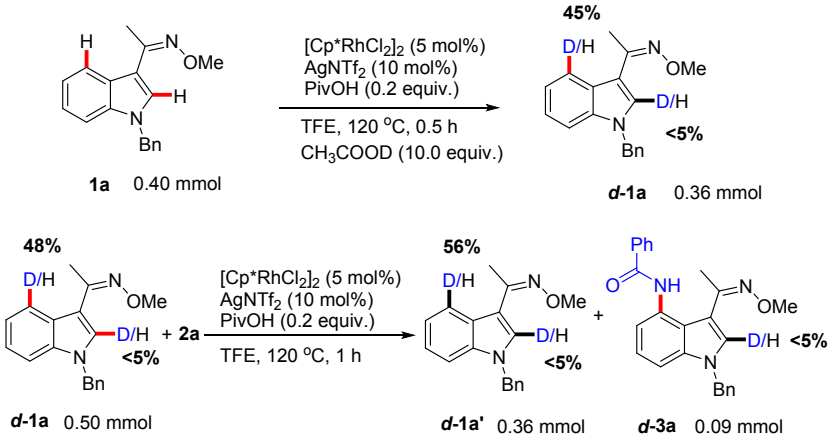
## 3. Intermolecular Competitive Reactions:




**Procedure (A):** A mixture of substrate **1h** (64.1 mg, 0.2 mmol, 0.5 equiv), **1j** (62.56 mg, 0.2 mmol, 0.5 equiv), dioxazolone **2a** (130.5 mg, 0.8mmol, 1.0 equiv), $[Cp^*RhCl_2]_2$ (12.4 mg, 5 mol%), $AgNTf_2$ (15.5 mg, 10 mol%), PivOH (8.2 mg, 0.2 equiv) in solvent (5.0 mL) was charged in a glass sealed tube and stirred under air atmosphere at 120 °C for 24 h. Upon completion of the reaction, the solution was concentrated *in vacuo* to provide a crude product, water (30 mL) and dichloromethane (15 mL) were added to the mixture, then the aqueous layer was extracted with dichloromethane (15 mL × 2). The combined organic layer was dried over anhydrous $MgSO_4$. Finally, the solution was concentrated *in vacuo* to provide a crude product, which was further purified *via* a column chromatography on silica gel to supply the product **3h** (100.2 mg, 57%) and **3j** (55.3 mg, 32%).

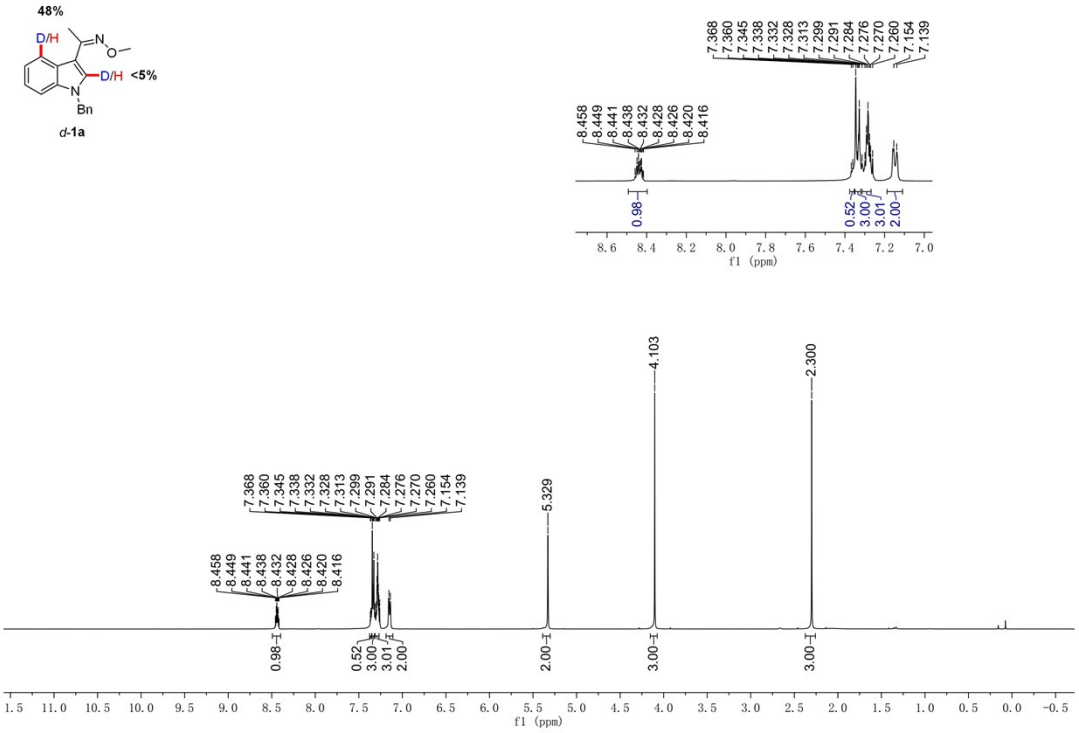
**Procedure (B):** A mixture of substrate **2g** (70.9 mg, 0.4 mmol,1.0 equiv), **2i** (72.4 mg, 0.4 mmol, 1.0 equiv), substrate **1a** (111.3 mg, 0.4 mmol, 1.0 equiv), $[Cp^*RhCl_2]_2$ (12.4 mg, 5 mol%), $AgNTf_2$ (15.5 mg, 10 mol%), PivOH (8.2 mg, 0.2 equiv) in solvent (5.0 mL) was charged in a glass sealed tube and stirred under air atmosphere at 120 °C for 24 h. Upon completion of the reaction, the solution was concentrated *in vacuo* to provide a crude product, water (30 mL) and dichloromethane (15 mL) were added to the mixture, then the aqueous layer was extracted with dichloromethane (15 mL × 2). The combined organic layer was dried over anhydrous $MgSO_4$. Finally, the solution was concentrated *in vacuo* to provide a crude product, which was further purified *via* a column chromatography on silica gel to supply the product **4g** (83.9 mg, 51%) and **4i** (59.9 mg, 36%).

## 4. Deuterium incorporation studies:

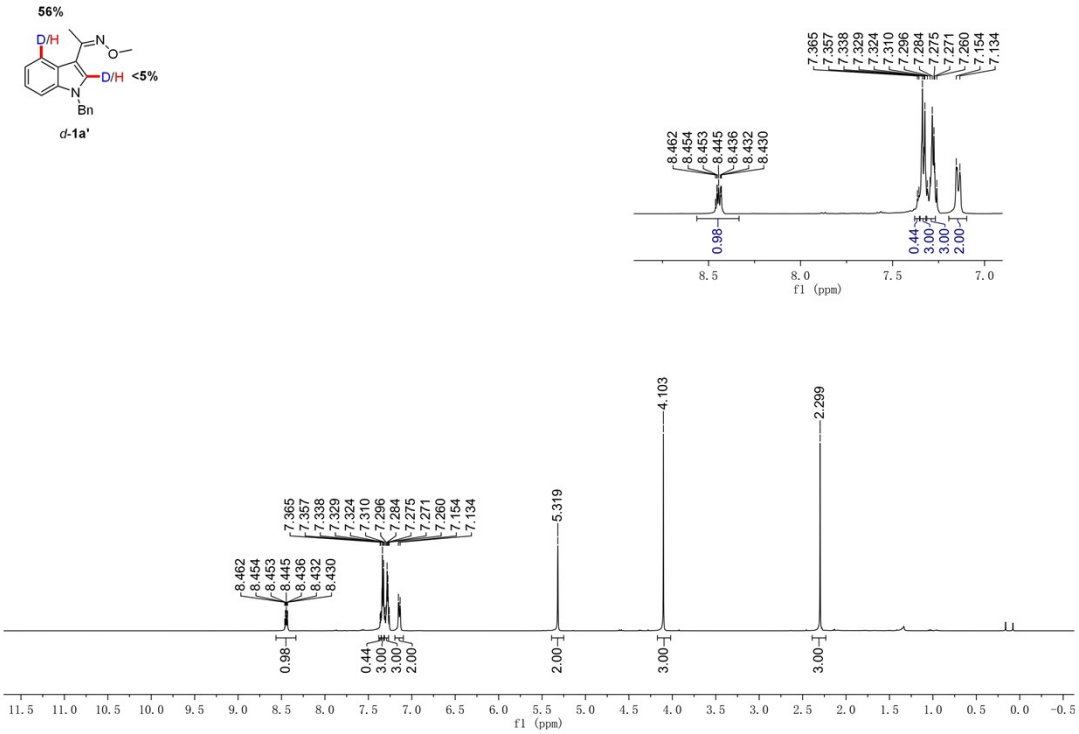



**Procedure (A) :** A mixture of substrate **1a** (167.2 mg, 0.6 mmol,1.0 equiv), $[Cp^*RhCl_2]_2$ (18.6 mg, 5 mol%), $AgNTf_2$ (23.3 mg, 10 mol%), PivOH (12.3 mg, 0.2 equiv), $CH_3COOD$ (0.38 ml, 6 mmol, 10 eq) in solvent (6.0 mL) was charged in a glass sealed tube and stirred under air atmosphere at 120 °C for 0.5 h. Upon completion of the reaction, the solution was concentrated in vacuo to provide a crude product, water (30 mL) and dichloromethane (20 mL) were added to the mixture, then the aqueous layer was extracted with dichloromethane (15 mL × 3). The combined organic layer was dried over anhydrous $MgSO_4$. Finally, the solution was concentrated in vacuo to provide a crude product, which was further purified via a column chromatography on silica gel (eluents: petroleum ether/ethyl acetate = 25:1) to supply the product *d*-**1a**. The purified product *d*-**1a** was analyzed by $^1H$ NMR which showed that 48% deuterium incorporation at C-4 position of indole **1a** was happened under above reaction conditions.

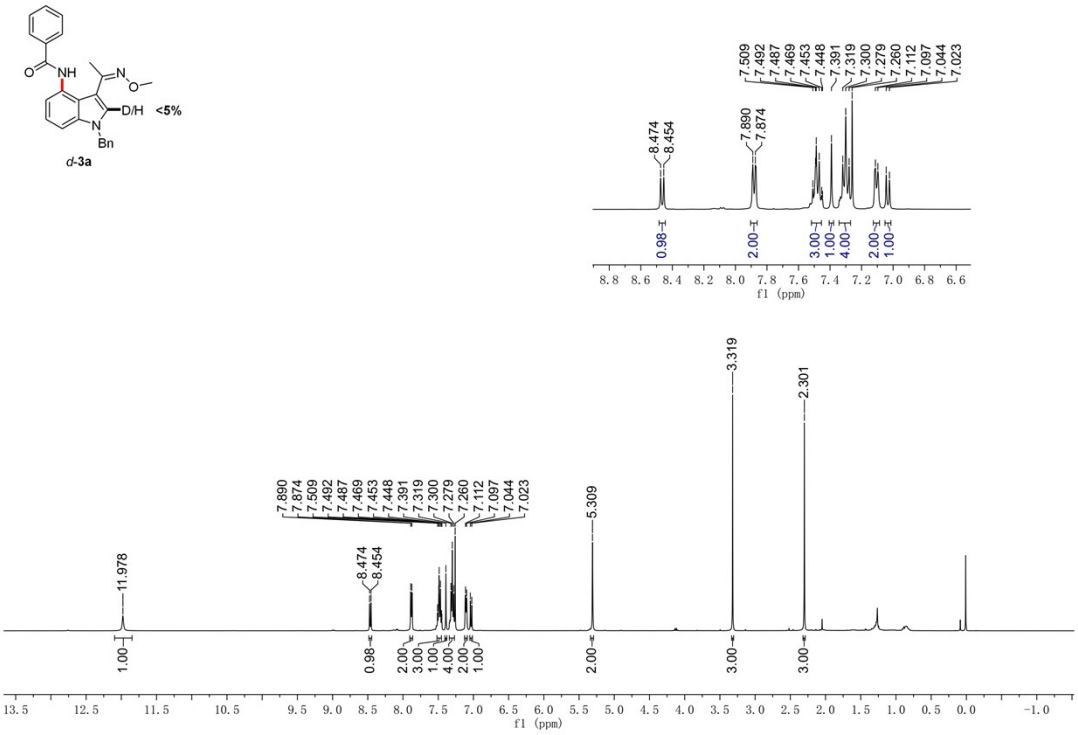
**Procedure (B):** A mixture of substrate *d*-**1a** (139.3 mg, 0.5 mmol, 1.0 equiv), $[Cp^*RhCl_2]_2$ (15.5 mg, 5 mol%), $AgNTf_2$ (19.4 mg, 10 mol%), PivOH (10.3 mg, 0.2 equiv), $CH_3COOD$ (0.31 ml, 5 mmol, 10 eq) in solvent (6.0 mL) was charged in a glass sealed tube and stirred under air atmosphere at 120 °C for 1.0 h. Upon completion of the reaction, the solution was concentrated in vacuo to provide a crude product, water (30 mL) and dichloromethane (15 mL) were added to the mixture, then the aqueous layer was extracted with dichloromethane (15 mL × 2). The combined organic layer was dried over anhydrous $MgSO_4$. Finally, the solution was concentrated in vacuo to provide a crude product, which was further purified via a column chromatography on silica gel to supply the product *d*-**1a'** and *d*-**3a**. The purified product *d*-**1a'** and *d*-**3a** was analyzed by $^1H$ NMR.




$^1$H NMR spectra of substrate *d*-**1a**



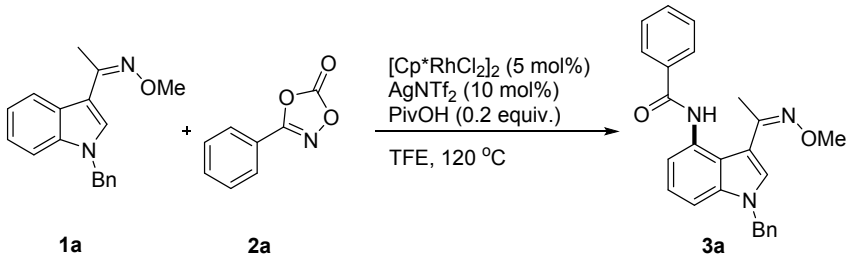

$^1$H NMR spectra of substrate *d*-**1a'**




$^{1}$H NMR spectra of substrate ***d-3*a**

## 5. Kinetic studies

The influence of concentration of indole substrate and dioxazolone were roughly explored under the standard conditions (Table 1 and Table 2). When the concentration of **2a** was decreased to 1.0 equiv., the rate was slightly reduced (Table 1, entry 1). However, unknown by-product was formed when **2a** increased to 3.0 equiv., so the generation rate of **3a** was reduced (Table 1, entry 3). Therefore, the reaction rate may be related to the concentration of **2a** within a certain range. Next, the reaction rate was not significantly changed with different concentration of **1a** (Table 2, entries 1-3). Therefore, the reaction rate may have no obvious correlation with the concentration of **1a.** In summary, these results showed that this transformation was approximate to first-order kinetic reaction.




**1a** **2a** **3a**

**Table 1** The influence of concentration of **2a**.

| **Entry** | **1a:2a** \ **T(h)** | **0.5** | **4** | **12** | **24** |
|---|---|---|---|---|---|
| | | approximate yield of **3a** based on **1a** | | | |
| 1 | 1:1 | 12 % | 50 % | 65 % | 75 % |
| 2 | 1:2 | 15 % | 65 % | 75 % | 90 % |
| 3 | 1:3 | 10 % | 45 % | 55 % | 65 % |

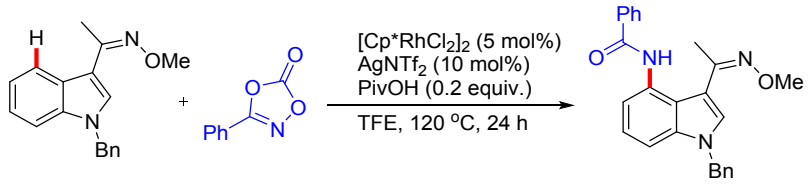
Reaction conditions: **1a** (1 equiv = 0.3 mmol), **2a** (1 equiv = 0.3 mmol), $[Cp^*RhCl_2]_2$ (0.0015 mmol), $AgNTf_2$ (0.003 mol), PivOH (0.06 mmol.), TFE (3.0 mL), 120 °C, 24 h.

**Table 2** The influence of concentration of **1a**.

| **Entry** | **1a:2a** \ **T(h)** | **0.5** | **4** | **12** | **24** |
|---|---|---|---|---|---|
| | | approximate yield of **3a** based on **2a** | | | |
| 1 | 2:1 | <15 % | 20 % | 60 % | 70 % |
| 2 | 3:1 | <15 % | 25 % | 60 % | 75 % |
| 3 | 4:1 | <15% | 25 % | 55 % | 65 % |

Reaction conditions: **1a** (1 equiv = 0.3 mmol), **2a** (1 equiv = 0.3 mmol), $[Cp^*RhCl_2]_2$ (0.0015 mmol), $AgNTf_2$ (0.003 mol), PivOH (0.06 mmol.), TFE (3.0 mL), 120 °C.

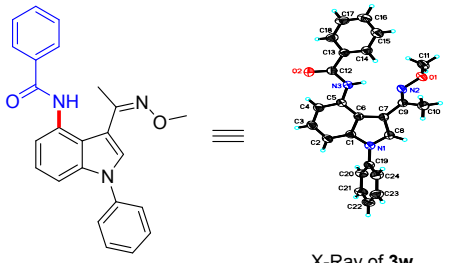
## 6. Synthetic utilities




**1a**, 1.39g, 5mmol **2a**, 2.0 equiv. **3a**, 1.57g, 79%

**Procedure :** A mixture of substrate **1a** (1.39g, 5.0 mmol, 1.0 equiv), dioxazolone **2a** (10.0 mmol, 2.0 equiv), $[Cp^*RhCl_2]_2$ (155 mg, 5 mol%), $AgNTf_2$ (194 mg, 10 mol%), PivOH (103 mg, 0.2 equiv) in TFE (50.0 mL) was charged in 100 mL round bottom flask condensate reflux and stirred under air atmosphere at 120 °C for 24 h. Upon completion of the reaction, the solution was concentrated *in vacuo* to provide a crude product, water (80 mL) and dichloromethane (250 mL) were added to the mixture, then the aqueous layer was extracted with dichloromethane (250 mL×2). The combined organic layer was dried over anhydrous $MgSO_4$. Finally, the solution was concentrated *in vacuo* to provide a crude product, which was further purified *via* a column chromatography on silica gel (eluents: petroleum ether/ethyl acetate = 8:1) to supply the product **4k** (1.57g, 79%).

# 7. X-ray single crystal structures of product 3w



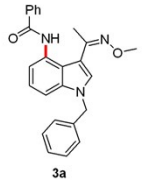

| | | |
|---|---|---|
| Identification code | mo_d8v20272_0m | |
| Empirical formula | C24 H21 N3 O2 | |
| Formula weight | 383.44 | |
| Temperature | 293(2) K | |
| Wavelength | 0.71073 Å | |
| Crystal system | Monoclinic | |
| Space group | P 21/c | |
| Unit cell dimensions | a = 9.5144(5) Å | α= 90°. |
| | b = 13.3582(7) Å | β= 102.194(2)°. |
| | c = 16.0144(10) Å | γ = 90°. |
| Volume | 1989.43(19) $Å^3$ | |
| Z | 4 | |
| Density (calculated) | 1.280 $Mg/m^3$ | |
| Absorption coefficient | 0.083 $mm^{-1}$ | |
| F(000) | 808 | |
| Crystal size | 0.200 x 0.160 x 0.130 $mm^3$ | |
| Theta range for data collection | 2.602 to 25.499°. | |
| Index ranges | -11<=h<=10, -16<=k<=14, -19<=l<=18 | |
| Reflections collected | 9340 | |
| Independent reflections | 3682 [R(int) = 0.0519] | |
| Completeness to theta = 25.242° | 99.3 % | |
| Absorption correction | Semi-empirical from equivalents | |
| Max. and min. transmission | 0.7456 and 0.5169 | |
| Refinement method | Full-matrix least-squares on $F^2$ | |
| Data / restraints / parameters | 3682 / 0 / 265 | |
| Goodness-of-fit on $F^2$ | 1.046 | |
| Final R indices [I>2sigma(I)] | R1 = 0.0487, wR2 = 0.1096 | |
| R indices (all data) | R1 = 0.0751, wR2 = 0.1292 | |
| Extinction coefficient | 0.048(5) | |
| Largest diff. peak and hole | 0.133 and -0.149 $e.Å^{-3}$ | |

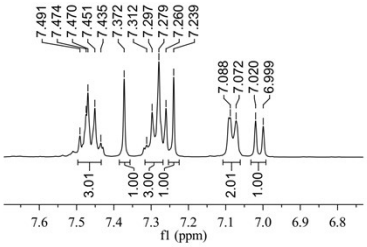
## 8. References

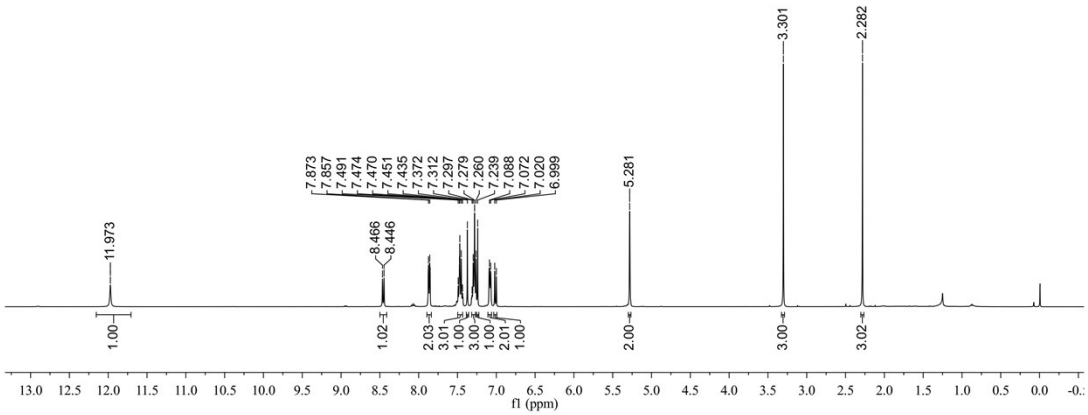
(1) (a) S. Maity, U. Karmakar and R. Samanta, *Chem. Commun,* **2017**, 53, 12197; (b) X.-P. Fu, S.-B. Tang, J.-Y. Yang, L.-L. Zhang, C.-C. Xia, Y.-F. Ji, *Eur. J. Org. Chem.* **2019**, 5974.

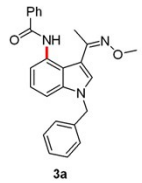
(2) J. Ding, W. Jiang, H.-Y. Bai, T.-M. Ding, D.-F. Gao, X.-G. Bao and S.-Y. Zhang, *Chem. Commun.,* **2018**, 54, 8889.

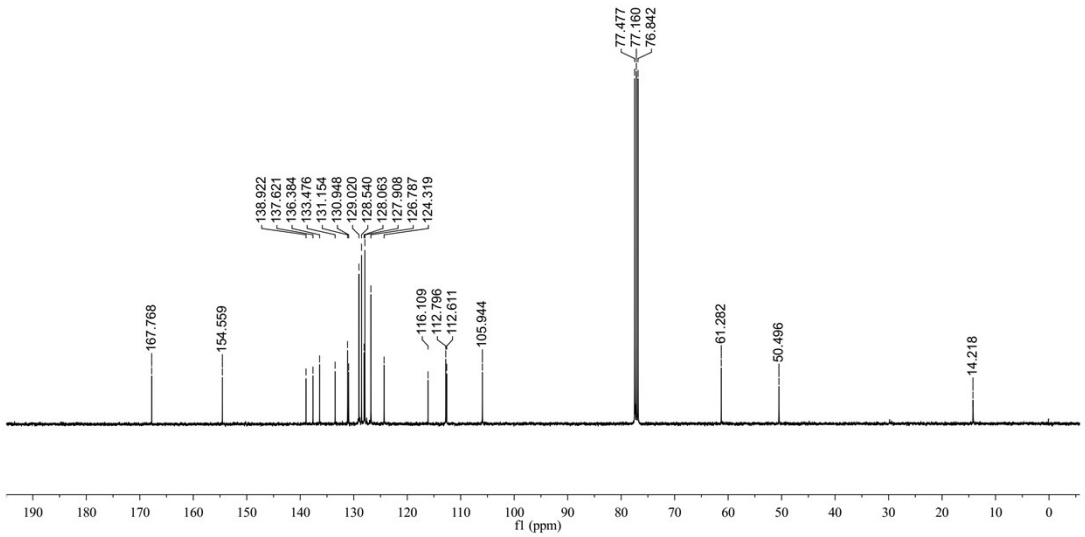
# 9. $^{1}$H NMR and $^{13}$C NMR Spectra of the products

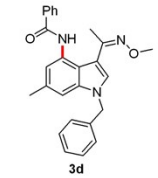
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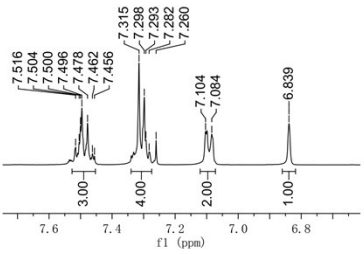
N
O
3d


7.516
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7.478
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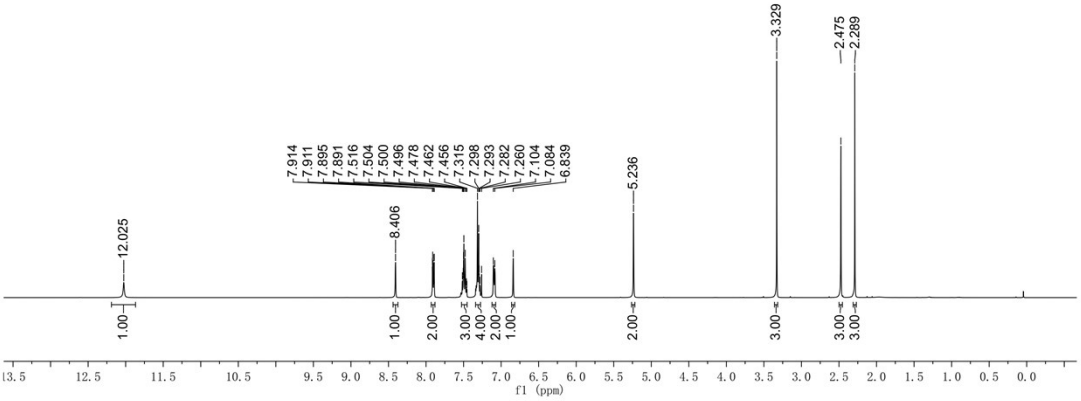
7.4
7.2
7.0
6.8
f1 (ppm)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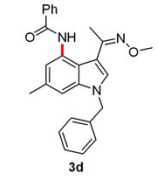
3.00
3.00
3.00
f1 (ppm)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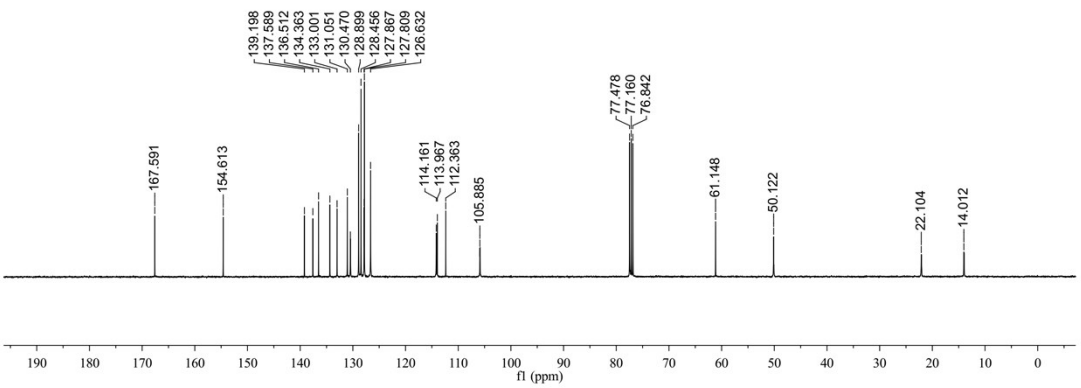
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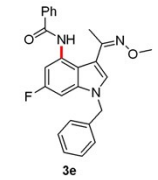
f1 (ppm)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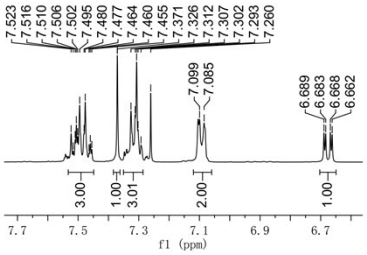
O
F
N

3e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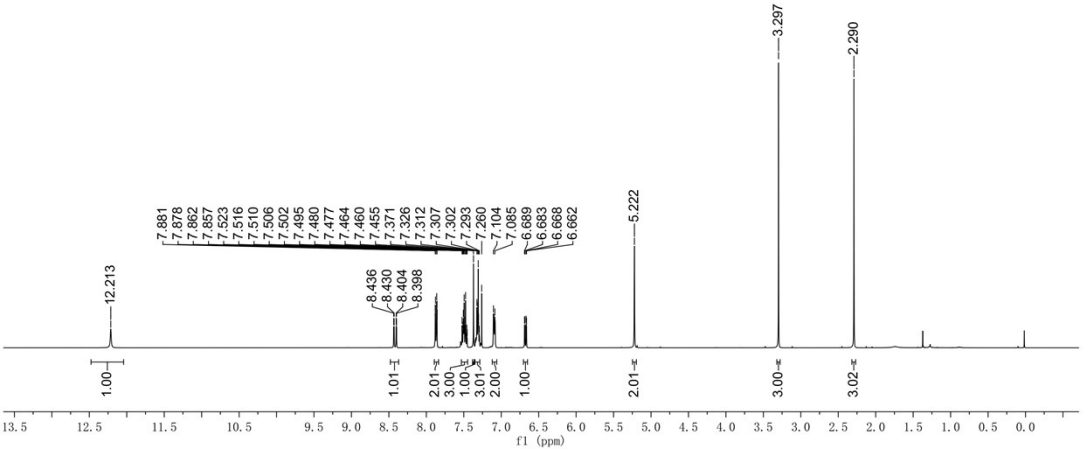
1.00
3.01
2.00
1.00
7.7
7.5
7.3
7.1
6.9
6.7
f1 (ppm)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2.290
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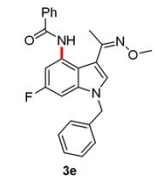
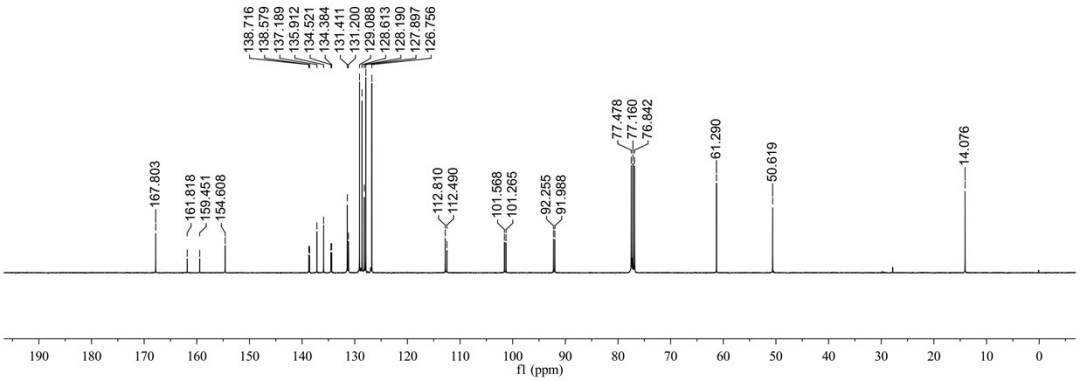
7.878
7.862
7.857
7.523
7.516
7.510
7.506
7.502
7.495
7.480
7.477
7.464
7.460
7.455
7.371
7.326
7.312
7.307
7.302
7.293
7.260
7.104
7.085
6.689
6.683
6.668
6.662
5.222
12.213
8.436
8.430
8.404
8.398
1.00
1.01
2.01
3.00
1.00
3.01
2.00
1.00
2.01
3.00
3.02
13.5
12.5
11.5
10.5
9.5
9.0
8.5
8.0
7.5
7.0
6.5
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
f1 (ppm)


Ph
NH
O
N
O
F
N

3e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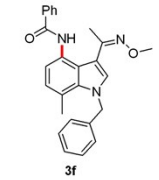
131.411
131.200
129.088
128.613
128.190
127.897
126.756
167.803
161.818
159.451
154.608
112.810
112.490
101.568
101.265
92.255
91.988
77.478
77.160
76.842
61.290
50.619
14.076
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
fl (ppm)


Ph
NH
N
O
3f


7.527
7.526
7.514
7.510
7.506
7.488
7.338
7.312
7.297
7.278
7.271
7.260
7.016
6.996
6.915
6.895
3.00
1.01
3.00
1.00
2.00
f1 (ppm)
3.401
2.478
2.322
7.925
7.922
7.906
7.902
7.527
7.526
7.519
7.514
7.510
7.506
7.488
7.476
7.472
7.466
7.338
7.312
7.297
7.278
7.271
7.260
7.016
6.996
6.915
6.895
5.547
11.890
8.362
8.342
1.00
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2.00
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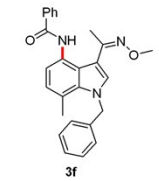
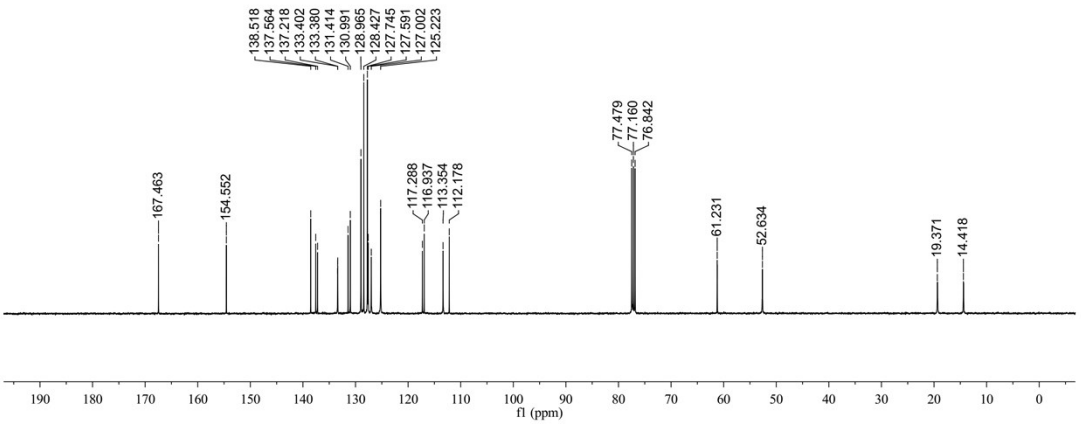
1.00
2.00
2.00
3.01
3.00
3.00
f1 (ppm)


Ph
NH
N
O
3f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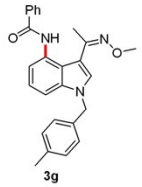
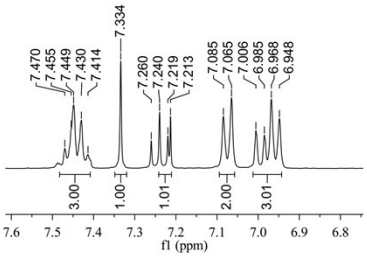
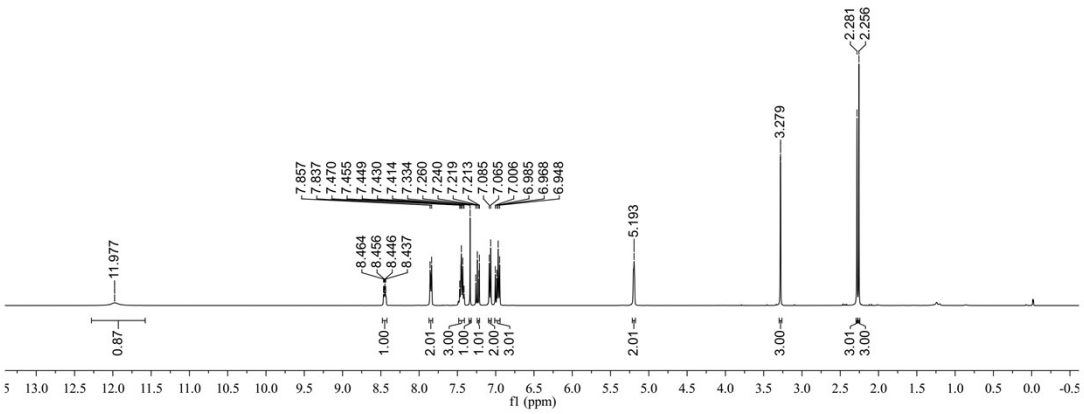
133.380
131.414
130.991
128.965
128.427
127.745
127.591
127.002
125.223
77.479
77.160
76.842
167.463
154.552
117.288
116.937
113.354
112.178
61.231
52.634
19.371
14.418
f1 (ppm)


Ph
NH
N
O
3g


7.470
7.455
7.449
7.430
7.414
7.334
7.260
7.240
7.219
7.213
7.085
7.065
7.006
6.985
6.968
6.948
3.00
1.00
1.01
2.00
3.01
7.6 7.5 7.4 7.3 7.2 7.1 7.0 6.9 6.8
f1 (ppm)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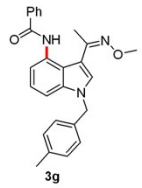
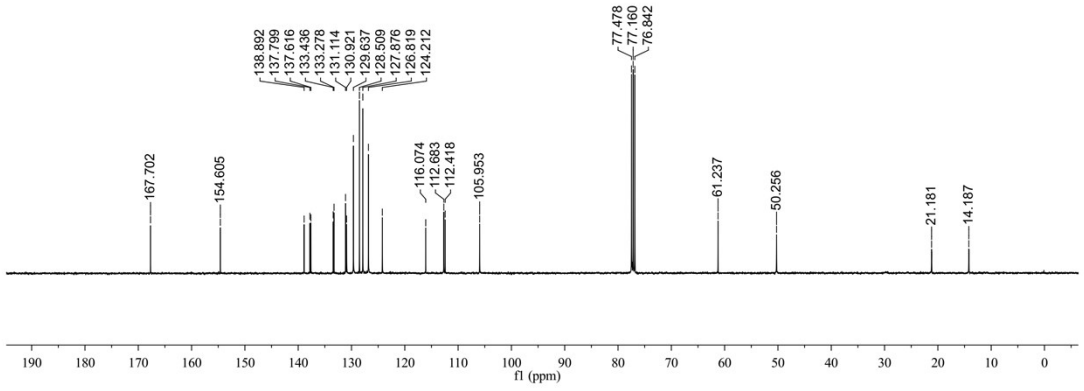
8.464
8.456
8.446
8.437
7.857
7.837
7.470
7.455
7.449
7.430
7.414
7.334
7.260
7.240
7.219
7.213
7.085
7.065
7.006
6.985
6.968
6.948
5.193
3.279
2.281
2.256
0.87
1.00
2.01
3.00
1.00
1.01
2.00
3.01
2.01
3.00
3.01
3.00
f1 (ppm)


Ph
NH
N
O
3g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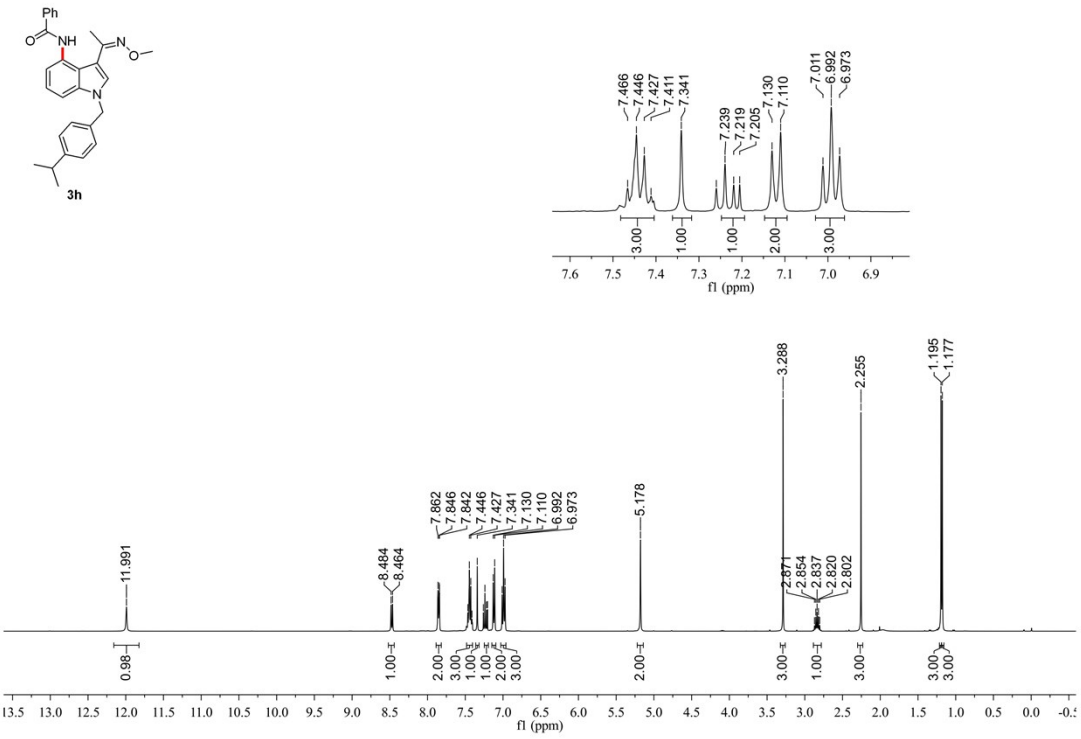
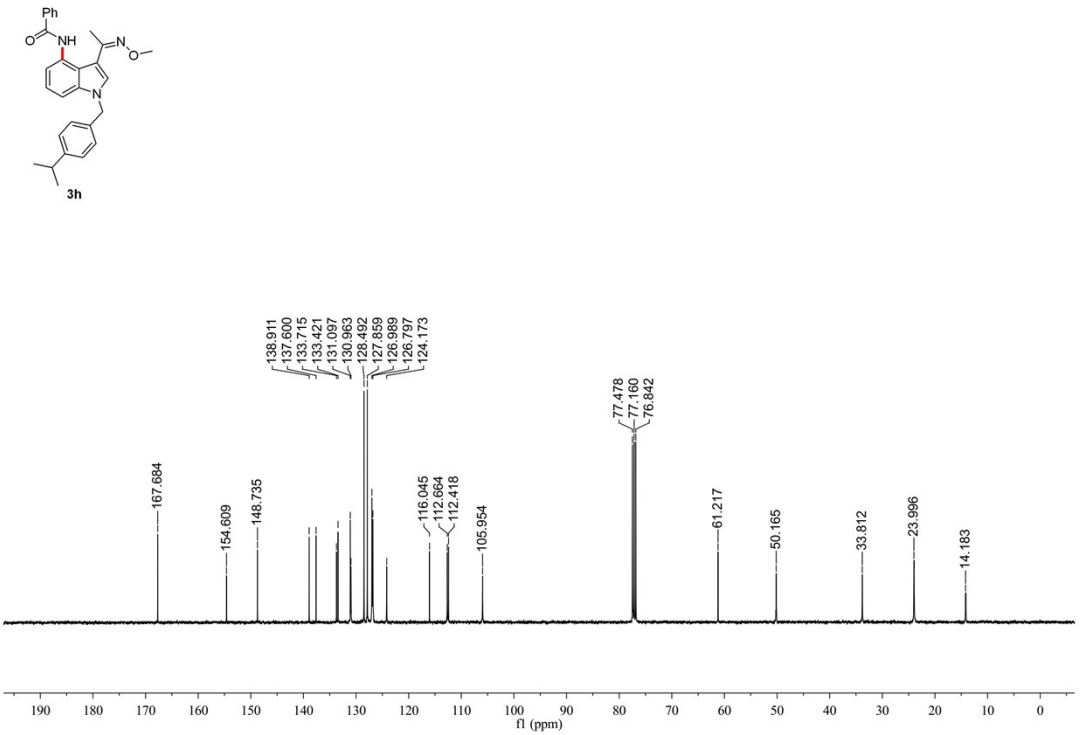
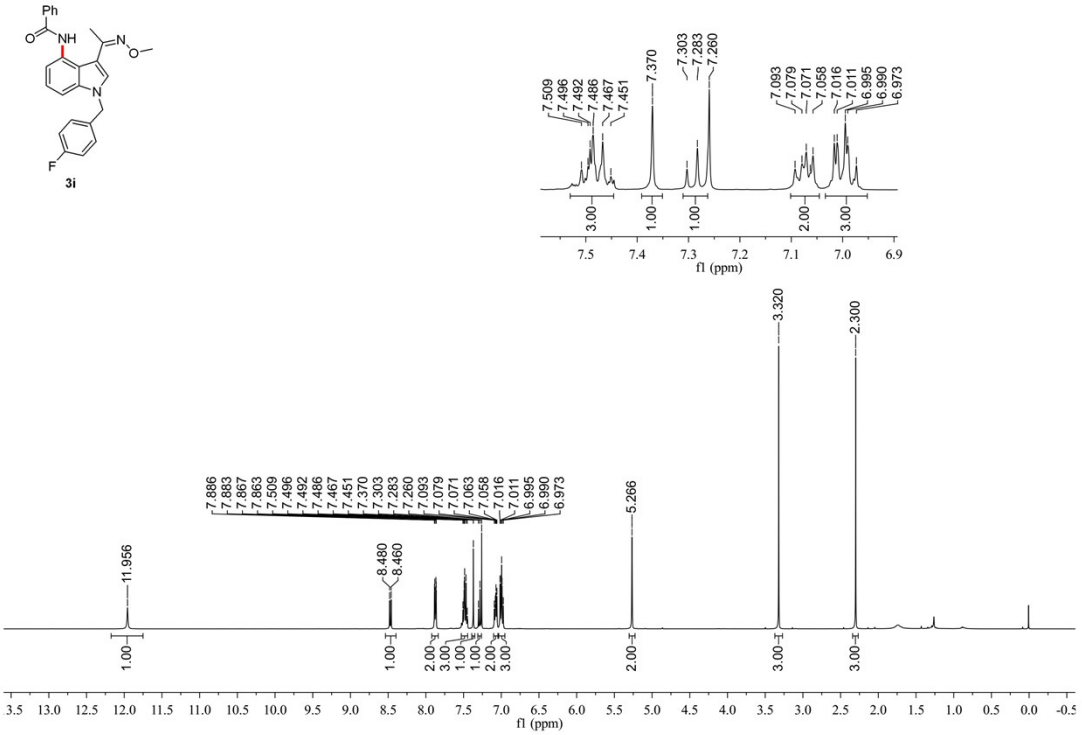
137.616
133.436
133.278
131.114
130.921
129.637
128.509
127.876
126.819
124.212
77.478
77.160
76.842
167.702
154.605
116.074
112.683
112.418
105.953
61.237
50.256
21.181
14.187
f1 (ppm)


3h
7.466
7.446
7.427
7.411
7.341
7.239
7.219
7.205
7.130
7.110
7.011
6.992
6.973
3.00
1.00
1.00
2.00
3.00
f1 (ppm)
11.991
8.484
8.464
7.862
7.846
7.842
7.446
7.427
7.341
7.130
7.110
6.992
6.973
5.178
3.288
2.871
2.854
2.837
2.820
2.802
2.255
1.195
1.177
f1 (ppm)


3h
138.911
137.600
133.715
133.421
131.097
130.963
128.492
127.859
126.989
126.797
124.173
167.684
154.609
148.735
116.045
112.664
112.418
105.954
77.478
77.160
76.842
61.217
50.165
33.812
23.996
14.183
f1 (ppm)


3i
7.509
7.496
7.492
7.486
7.467
7.451
7.370
7.303
7.283
7.260
7.093
7.079
7.071
7.058
7.016
7.011
6.995
6.990
6.973
3.00
1.00
1.00
2.00
3.00
7.5
7.4
7.3
7.2
7.1
7.0
6.9
f1 (ppm)
3.320
2.300
7.886
7.883
7.867
7.863
7.509
7.496
7.492
7.486
7.467
7.451
7.370
7.303
7.283
7.260
7.093
7.079
7.071
7.063
7.058
7.016
7.011
6.995
6.990
6.973
5.266
11.956
8.480
8.460
1.00
1.00
2.00
3.00
1.00
1.00
2.00
3.00
2.00
3.00
3.00
3.5
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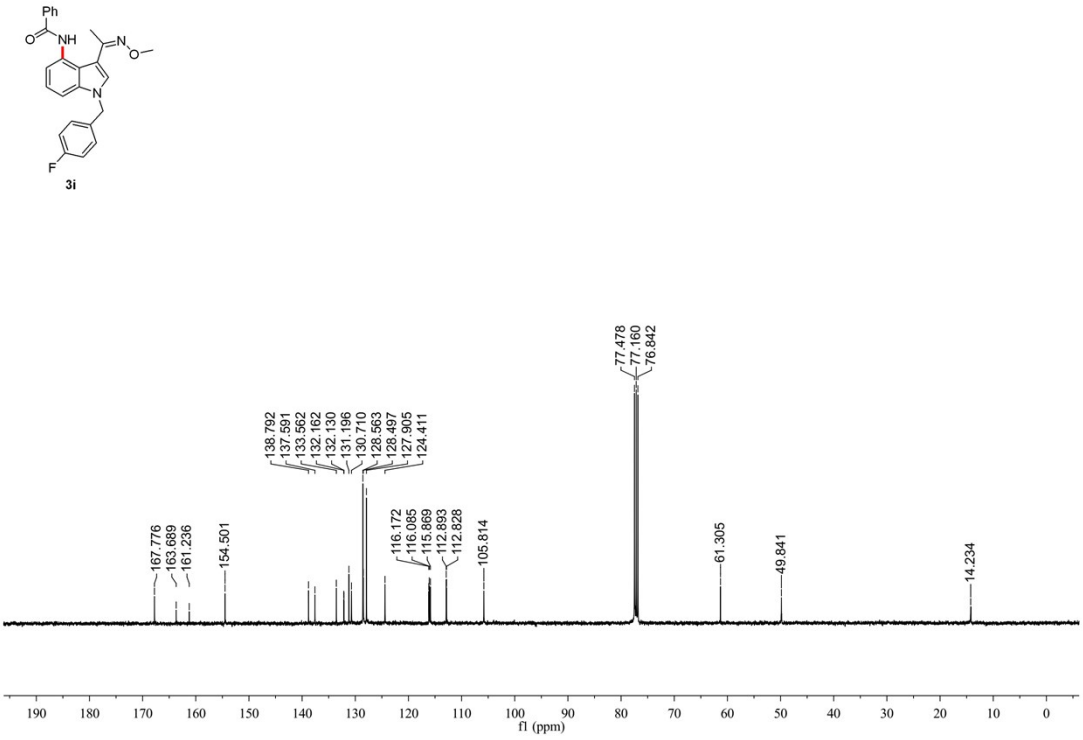
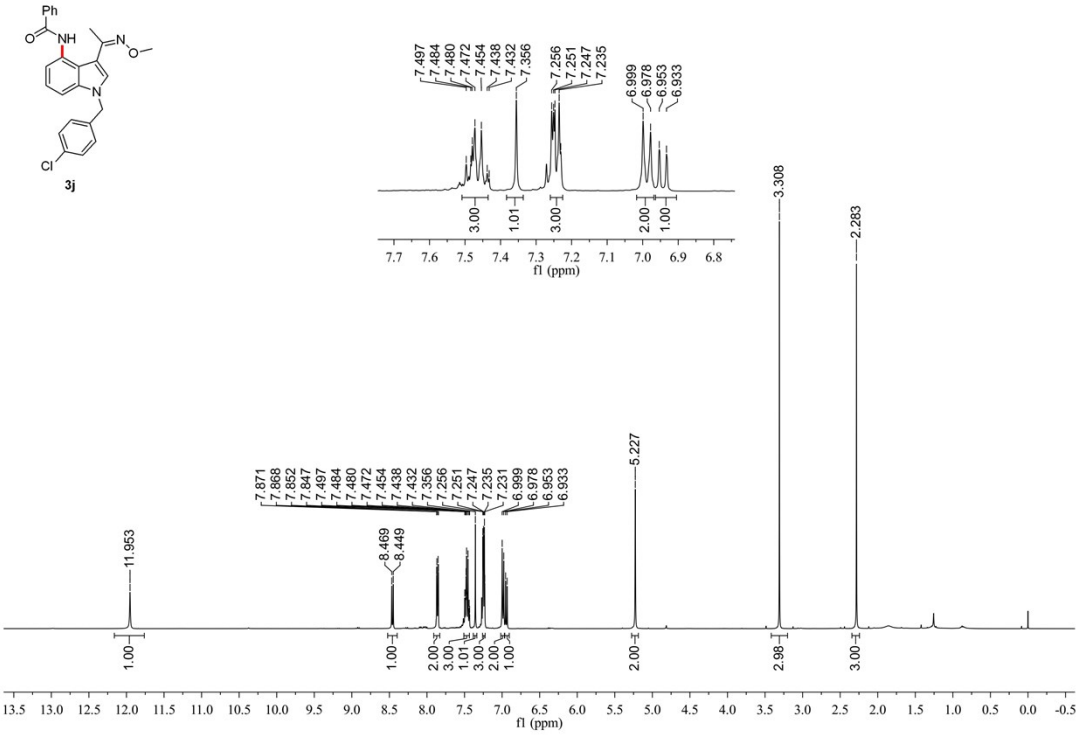
12.5
12.0
11.5
11.0
10.5
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
-0.5
f1 (ppm)


3i
77.478
77.160
76.842
138.792
137.591
133.562
132.162
132.130
131.196
130.710
128.563
128.497
127.905
124.411
116.172
116.085
115.869
112.893
112.828
105.814
167.776
163.689
161.236
154.501
61.305
49.841
14.234
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)


Ph
NH
O
N
O
Cl
3j
7.497
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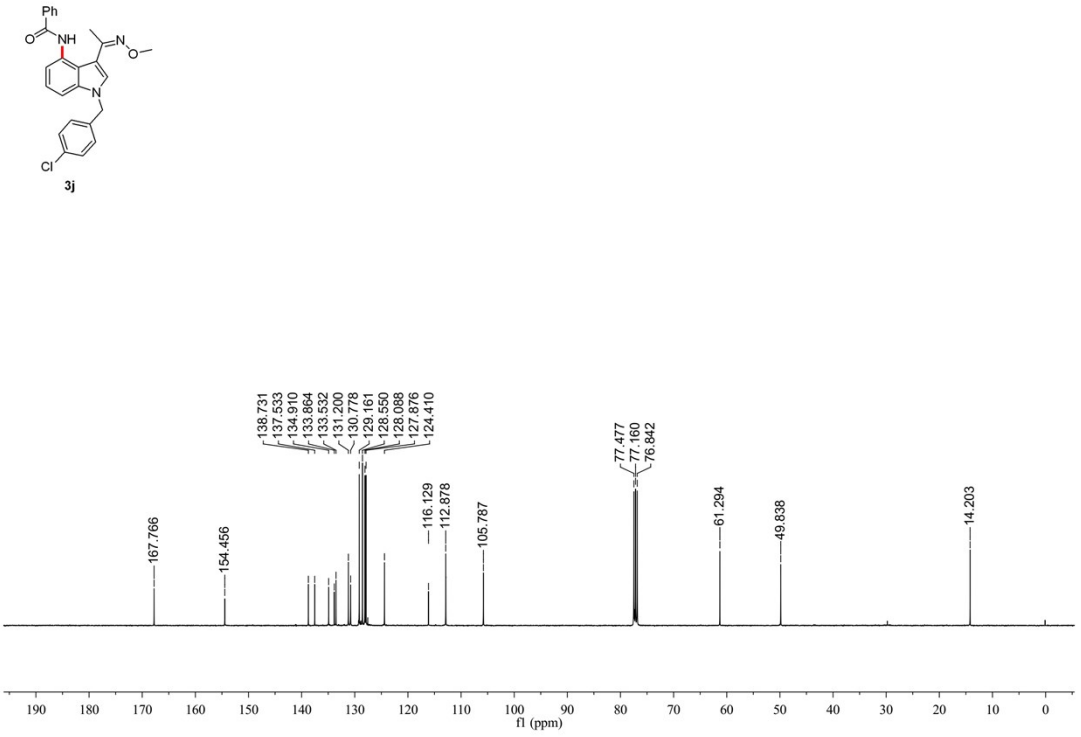
7.480
7.472
7.454
7.438
7.432
7.356
7.256
7.251
7.247
7.235
6.999
6.978
6.953
6.933
3.00
1.01
3.00
2.00
1.00
3.308
2.283
5.227
11.953
8.469
8.449
2.00
2.98
3.00
fl (ppm)


Ph
NH
O
N
O
Cl
3j
138.731
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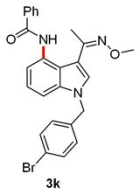
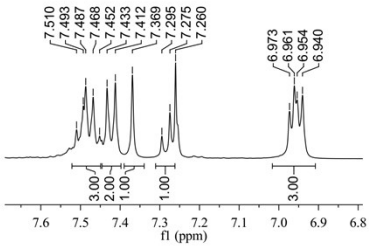
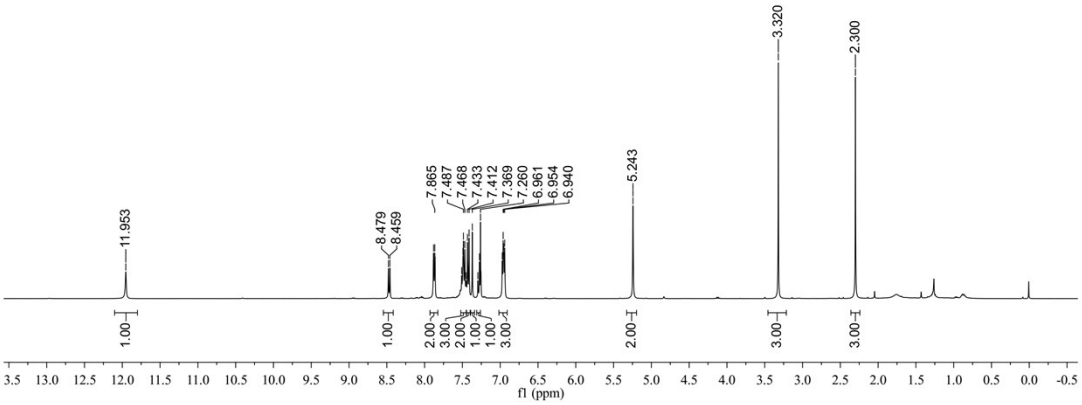
134.910
133.864
133.532
131.200
130.778
129.161
128.550
128.088
127.876
124.410
77.477
77.160
76.842
116.129
112.878
105.787
61.294
49.838
14.203
167.766
154.456
fl (ppm)


Ph
NH
N
O
Br

3k


7.510
7.493
7.487
7.468
7.452
7.433
7.412
7.369
7.295
7.275
7.260
6.973
6.961
6.954
6.940
3.00
2.00
1.00
1.00
3.00
7.6 7.5 7.4 7.3 7.2 7.1 7.0 6.9 6.8
f1 (ppm)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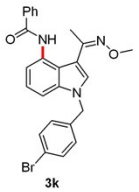
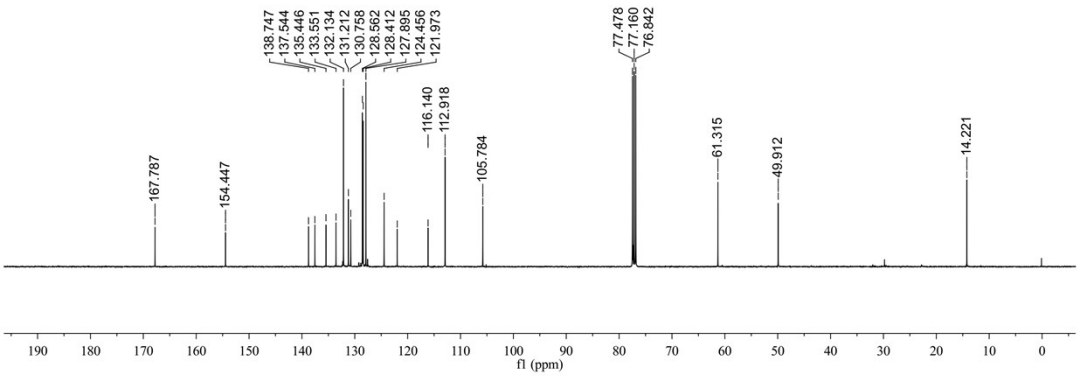
7.487
7.468
7.433
7.412
7.369
7.260
6.961
6.954
6.940
5.243
3.320
2.300
1.00
1.00
2.00
3.00
2.00
1.00
3.00
2.00
3.00
3.00
3.5 13.0 12.5 12.0 11.5 11.0 10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5
f1 (ppm)


Ph
NH
N
O
Br

3k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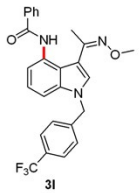
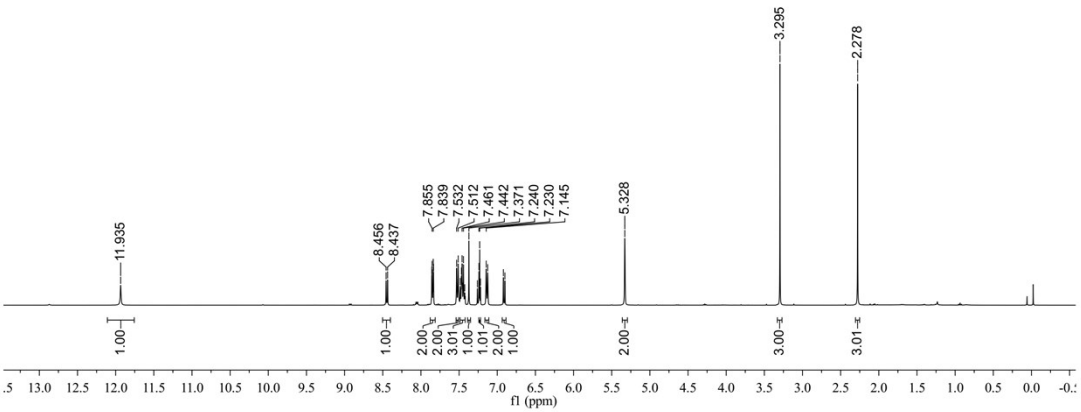
128.412
127.895
124.456
121.973
116.140
112.918
105.784
77.478
77.160
76.842
61.315
49.912
14.221
167.787
154.447
190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)


Ph
NH
N
O
F3C

3l


7.532
7.512
7.486
7.469
7.461
7.442
7.426
7.371
7.260
7.240
7.230
7.220
7.145
7.125
6.919
6.900
2.00
3.01
1.00
1.01
2.00
1.00
7.6 7.5 7.4 7.3 7.2 7.1 7.0 6.9 6.8
f1 (ppm)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7.839
7.532
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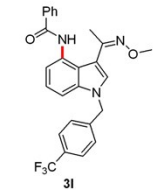
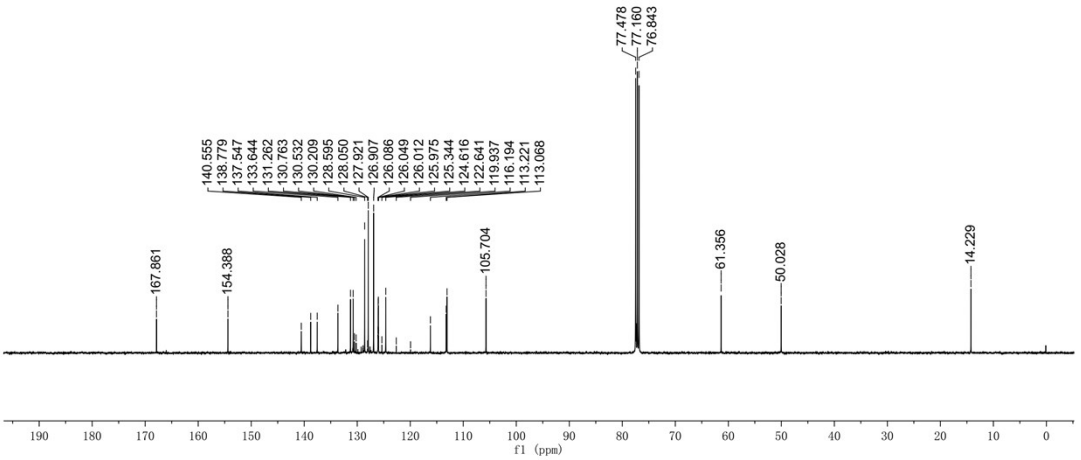
7.461
7.442
7.371
7.240
7.230
7.145
5.328
3.295
2.278
1.00
1.00
2.00
2.00
3.01
1.00
1.01
2.00
1.00
2.00
3.00
3.01
f1 (ppm)


Ph
NH
N
O
F3C

3l


77.478
77.160
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137.547
133.644
131.262
130.763
130.532
130.209
128.595
128.050
127.921
126.907
126.086
126.049
126.012
125.975
125.344
124.616
122.641
119.937
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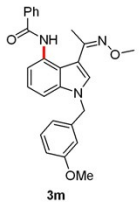
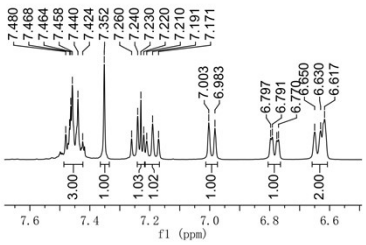
113.221
113.068
167.861
154.388
105.704
61.356
50.028
14.229
f1 (ppm)


Ph
NH
N
O
OMe

**3m**


7.480
7.468
7.464
7.458
7.440
7.424
7.352
7.260
7.240
7.230
7.220
7.210
7.191
7.171
7.003
6.983
6.797
6.791
6.650
6.630
6.617
3.00
1.00
1.03
1.02
1.00
1.00
2.00
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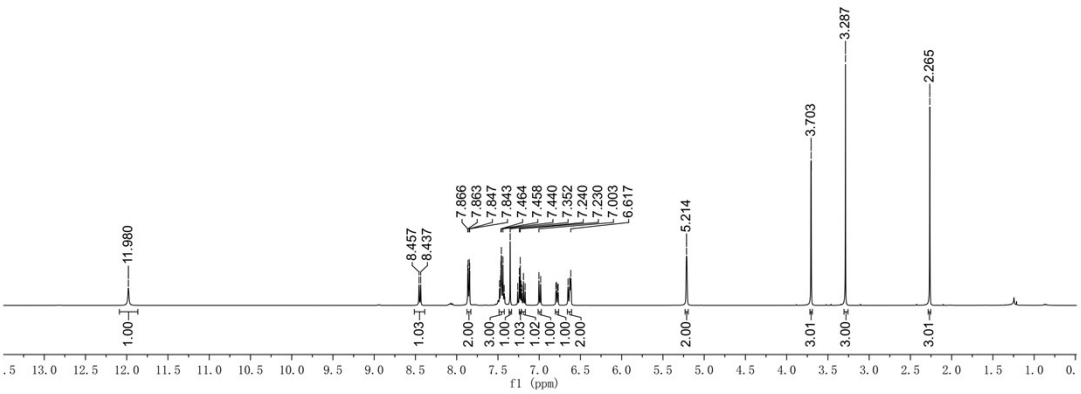
7.2
7.0
6.8
6.6
f1 (ppm)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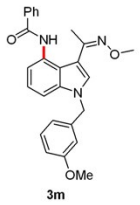
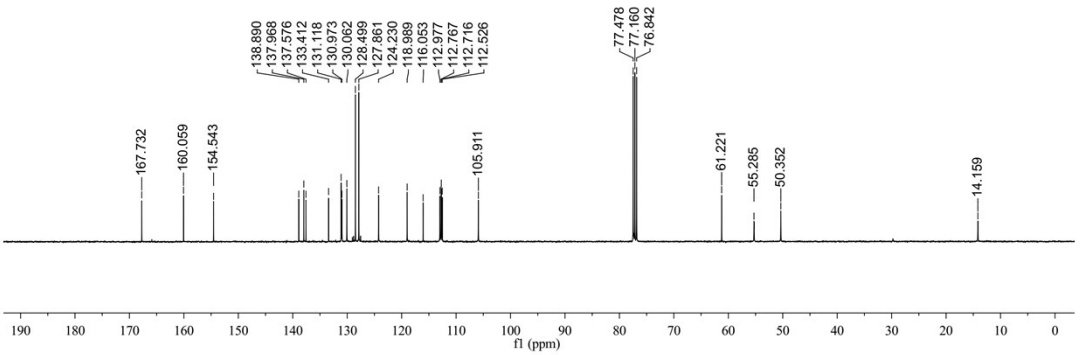
8.457
8.437
7.866
7.863
7.847
7.843
7.464
7.458
7.440
7.352
7.240
7.230
7.003
6.617
5.214
3.703
3.287
2.265
1.00
1.03
2.00
3.00
1.00
1.03
1.02
1.00
2.00
2.00
3.01
3.00
3.01
f1 (ppm)


Ph
NH
N
O
OMe

**3m**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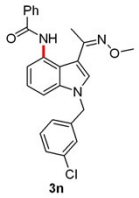
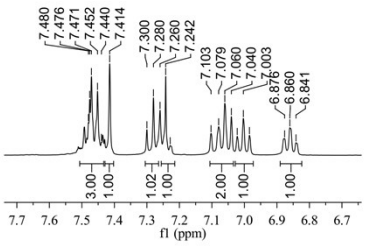
137.576
133.412
131.118
130.973
130.062
128.499
127.861
124.230
118.989
116.053
112.977
112.767
112.716
112.526
77.478
77.160
76.842
167.732
160.059
154.543
105.911
61.221
55.285
50.352
14.159
f1 (ppm)


Ph
NH
N
O
N
Cl
3n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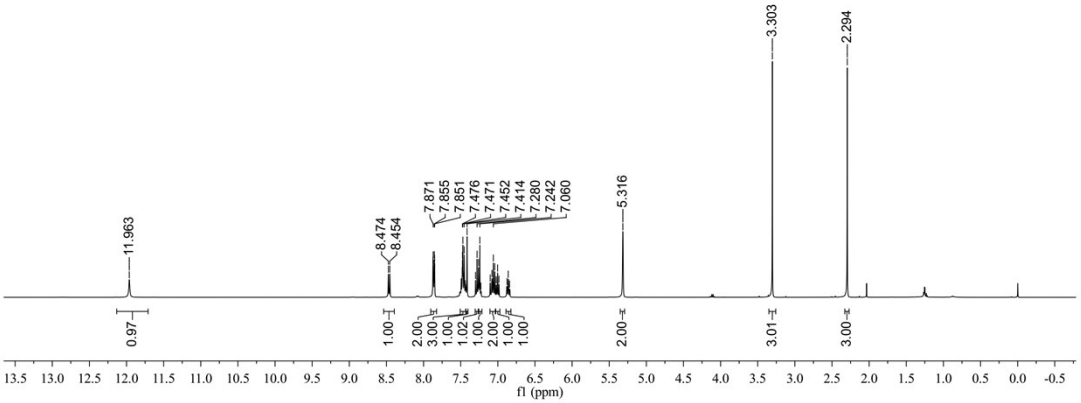
7.476
7.471
7.452
7.440
7.414
7.300
7.280
7.260
7.242
7.103
7.079
7.060
7.040
7.003
6.876
6.860
6.841
3.00
1.00
1.02
1.00
2.00
1.00
1.00
7.7 7.6 7.5 7.4 7.3 7.2 7.1 7.0 6.9 6.8 6.7
f1 (ppm)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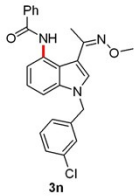
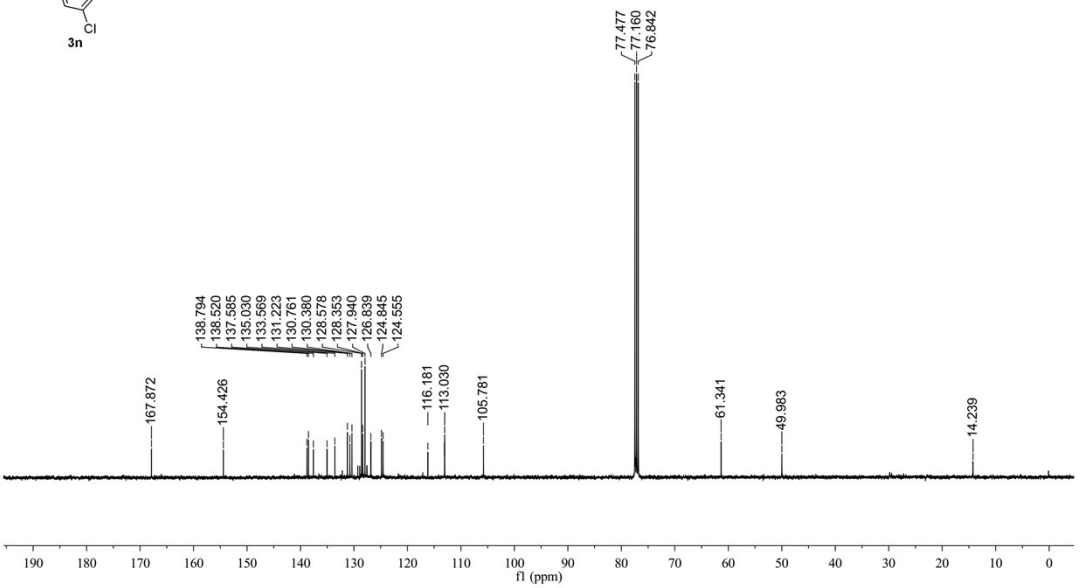
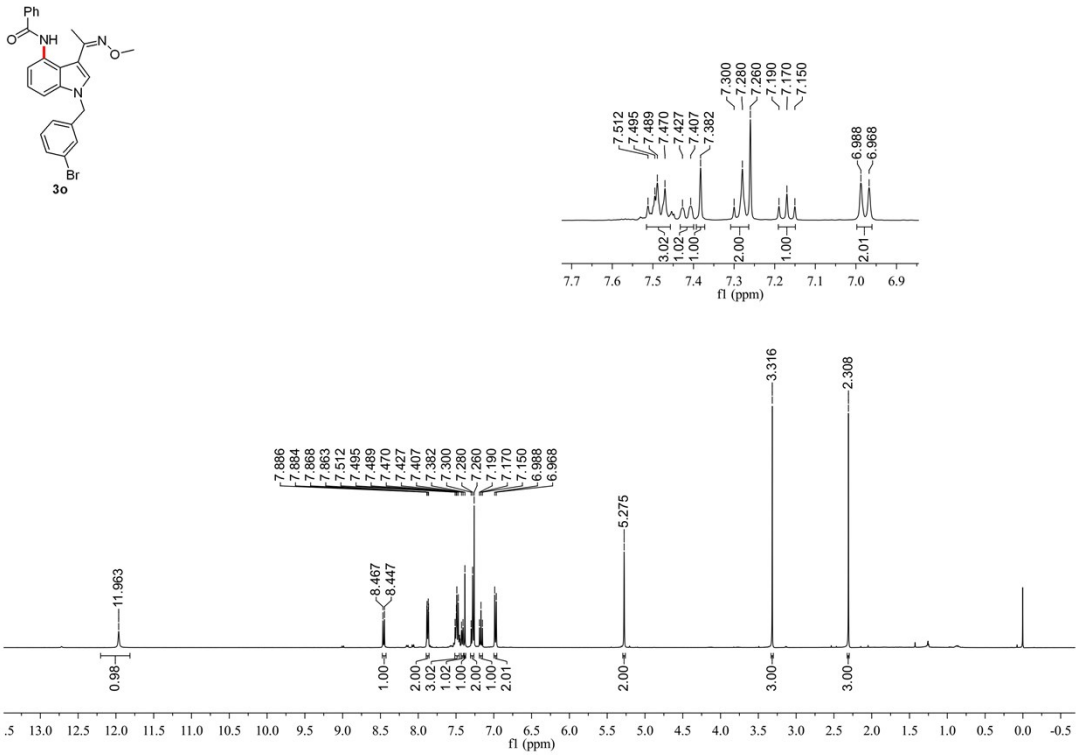
8.454
7.871
7.855
7.851
7.476
7.471
7.452
7.414
7.280
7.242
7.060
5.316
3.303
2.294
0.97
1.00
2.00
3.00
1.00
1.02
1.00
2.00
1.00
1.00
2.00
3.01
3.00
13.5 13.0 12.5 12.0 11.5 11.0 10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5
f1 (ppm)


Ph
NH
N
O
N
Cl
3n


77.477
77.160
76.842
138.794
138.520
137.585
135.030
133.569
131.223
130.761
130.380
128.578
128.353
127.940
126.839
124.845
124.555
167.872
154.426
116.181
113.030
105.781
61.341
49.983
14.239
190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)


Ph
NH
N
O
Br
3o
7.512
7.495
7.489
7.470
7.427
7.407
7.382
7.300
7.280
7.260
7.190
7.170
7.150
6.988
6.968
3.02
1.02
1.00
2.00
1.00
2.01
f1 (ppm)
11.963
8.467
8.447
7.886
7.884
7.868
7.863
5.275
3.316
2.308
0.98
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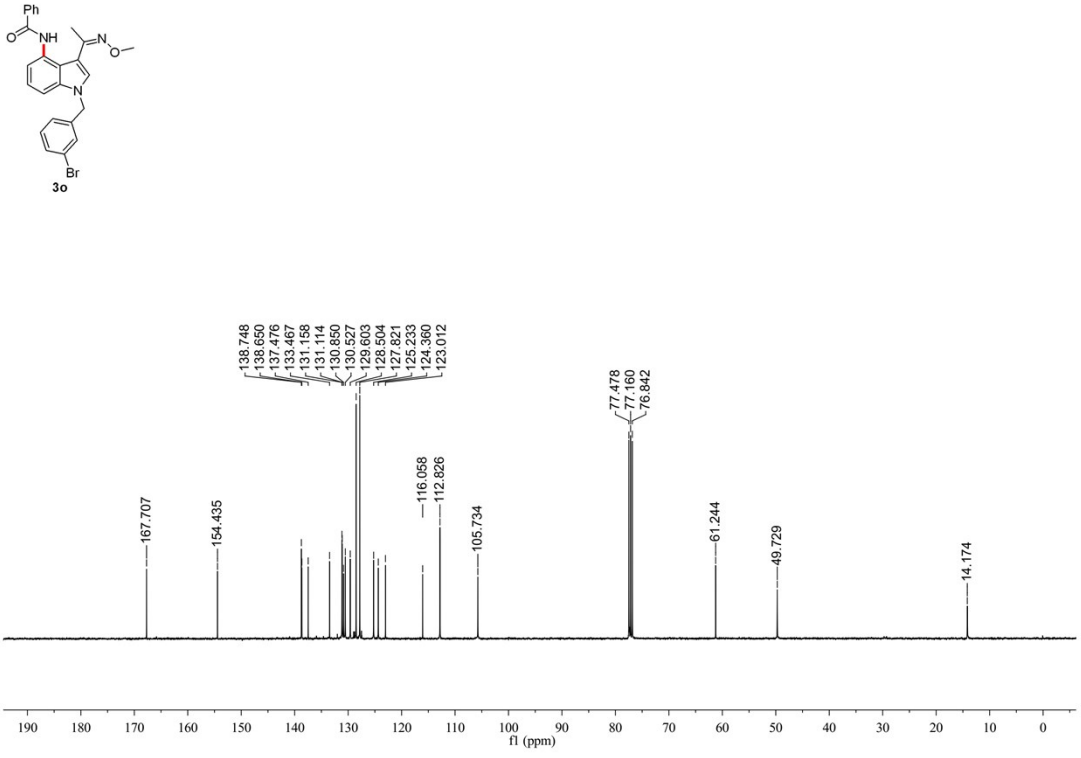
2.00
3.02
1.02
1.00
2.00
1.00
2.01
2.00
3.00
3.00
f1 (ppm)


Ph
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N
O
Br
3o
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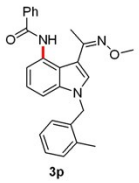
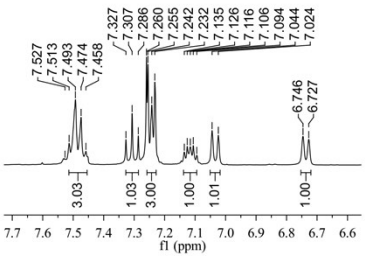
138.650
137.476
133.467
131.158
131.114
130.850
130.527
129.603
128.504
127.821
125.233
124.360
123.012
116.058
112.826
105.734
77.478
77.160
76.842
167.707
154.435
61.244
49.729
14.174
f1 (ppm)


Ph
NH
N
O
3p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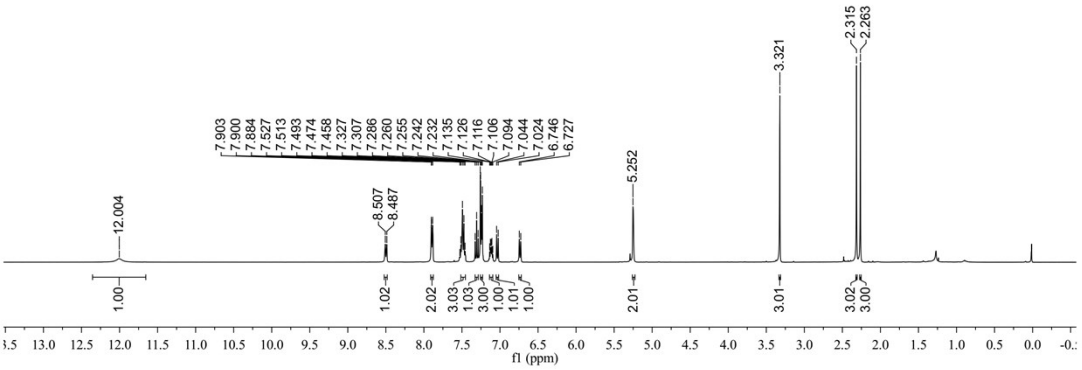
7.493
7.474
7.458
7.327
7.307
7.286
7.260
7.255
7.242
7.232
7.135
7.126
7.116
7.106
7.094
7.044
7.024
6.746
6.727
3.03
1.03
3.00
1.00
1.01
1.00
7.7 7.6 7.5 7.4 7.3 7.2 7.1 7.0 6.9 6.8 6.7 6.6
f1 (ppm)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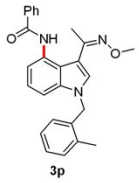
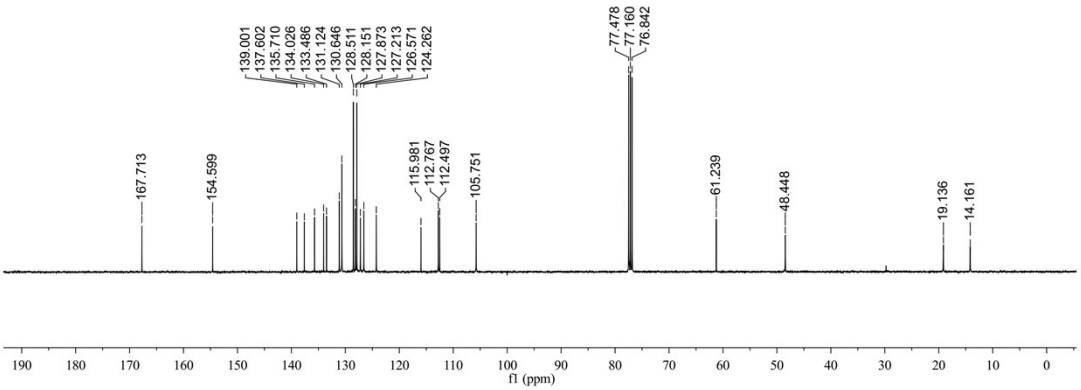
8.507
8.487
7.903
7.900
7.884
7.527
7.513
7.493
7.474
7.458
7.327
7.307
7.286
7.260
7.255
7.242
7.232
7.135
7.126
7.116
7.106
7.094
7.044
7.024
6.746
6.727
5.252
3.321
2.315
2.263
1.00
1.02
2.02
3.03
1.03
3.00
1.00
1.01
1.00
2.01
3.01
3.02
3.00
f1 (ppm)


Ph
NH
N
O
3p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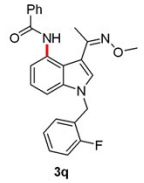
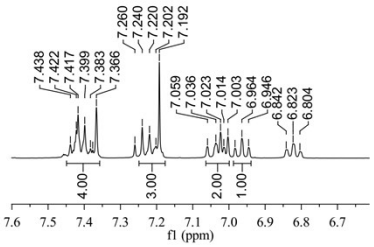
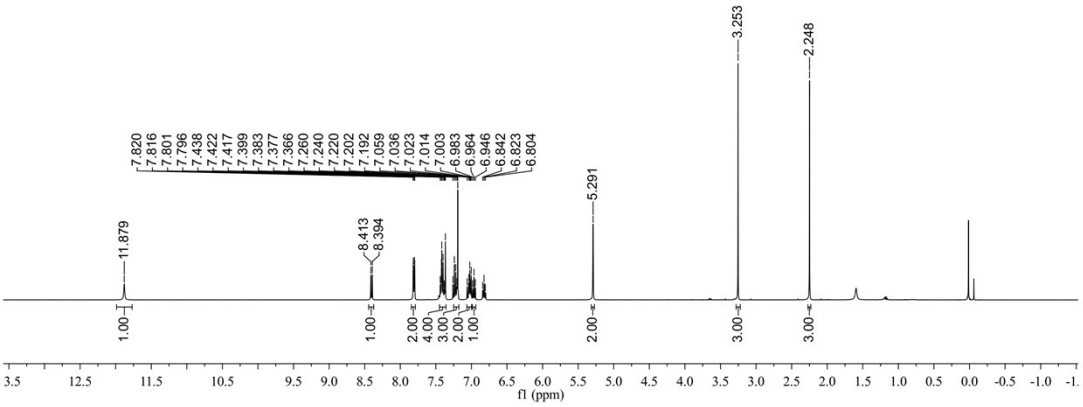
137.602
135.710
134.026
133.486
131.124
130.646
128.511
128.151
127.873
127.213
126.571
124.262
77.478
77.160
76.842
167.713
154.599
115.981
112.767
112.497
105.751
61.239
48.448
19.136
14.161
f1 (ppm)


Ph
NH
N
O
N
F

3q


7.438
7.422
7.417
7.399
7.383
7.366
7.260
7.240
7.220
7.202
7.192
7.059
7.036
7.023
7.014
7.003
6.964
6.946
6.842
6.823
6.804
4.00
3.00
2.00
1.00
7.6 7.5 7.4 7.3 7.2 7.1 7.0 6.9 6.8 6.7
f1 (ppm)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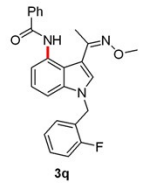
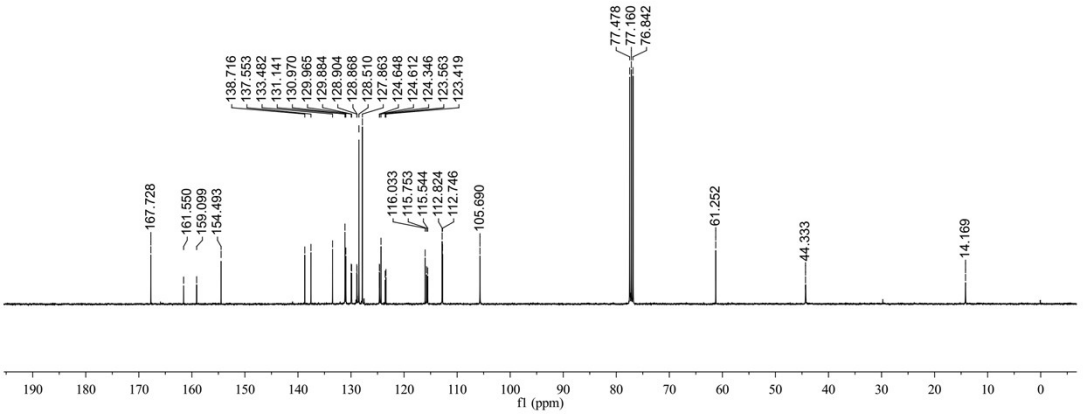
7.820
7.816
7.801
7.796
7.438
7.422
7.417
7.399
7.383
7.377
7.366
7.260
7.240
7.220
7.202
7.192
7.059
7.036
7.023
7.014
7.003
6.983
6.964
6.946
6.842
6.823
6.804
5.291
3.253
2.248
1.00
1.00
2.00
4.00
3.00
2.00
1.00
2.00
3.00
3.00
f1 (ppm)


Ph
NH
N
O
N
F

3q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131.141
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129.965
129.884
128.904
128.868
128.510
127.863
124.648
124.612
124.346
123.563
123.419
116.033
115.753
115.544
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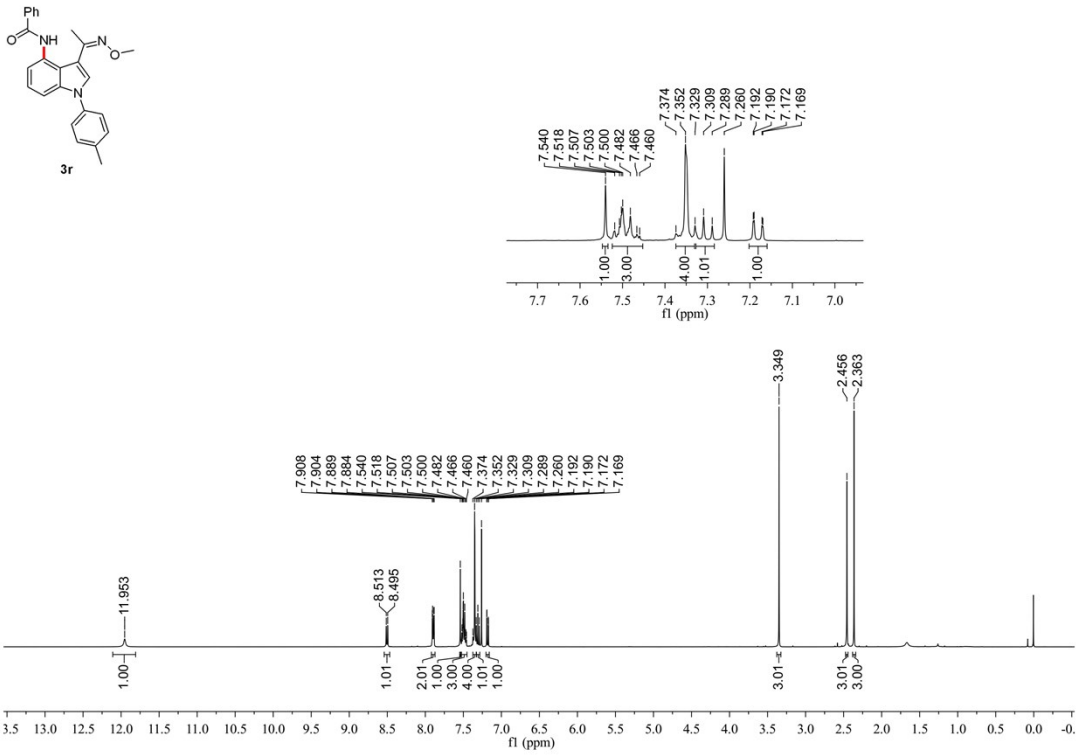
112.746
105.690
77.478
77.160
76.842
61.252
44.333
14.169
f1 (ppm)


Ph
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O
N
O
3r
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7.503
7.500
7.482
7.466
7.460
7.374
7.352
7.329
7.309
7.289
7.260
7.192
7.190
7.172
7.169
1.00
3.00
4.00
1.01
1.00
f1 (ppm)
11.953
8.513
8.495
7.908
7.904
7.889
7.884
3.349
2.456
2.363
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1.00
3.00
4.00
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3.01
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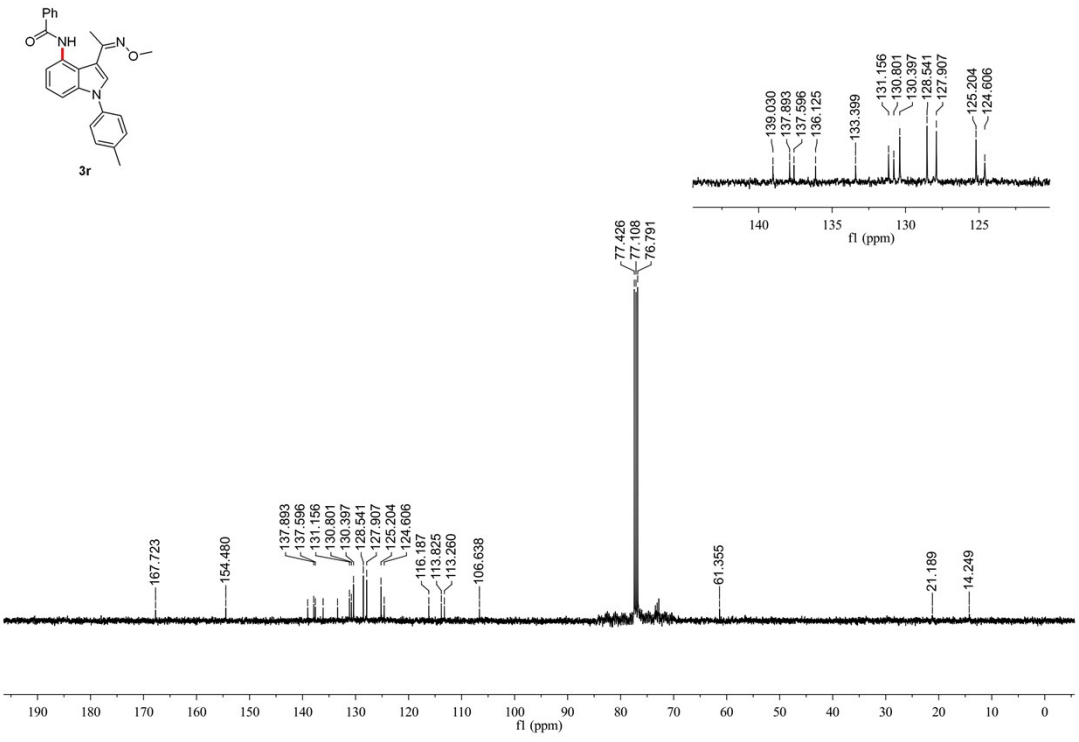
3.00
f1 (ppm)


Ph
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O
N
O
3r
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137.893
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130.801
130.397
128.541
127.907
125.204
124.606
f1 (ppm)
77.426
77.108
76.791
167.723
154.480
137.893
137.596
131.156
130.801
130.397
128.541
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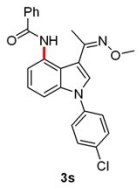
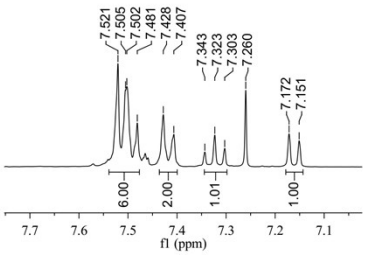
f1 (ppm)


Ph
NH
N
O
Cl

3s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7.481
7.428
7.407
7.343
7.323
7.303
7.260
7.172
7.151
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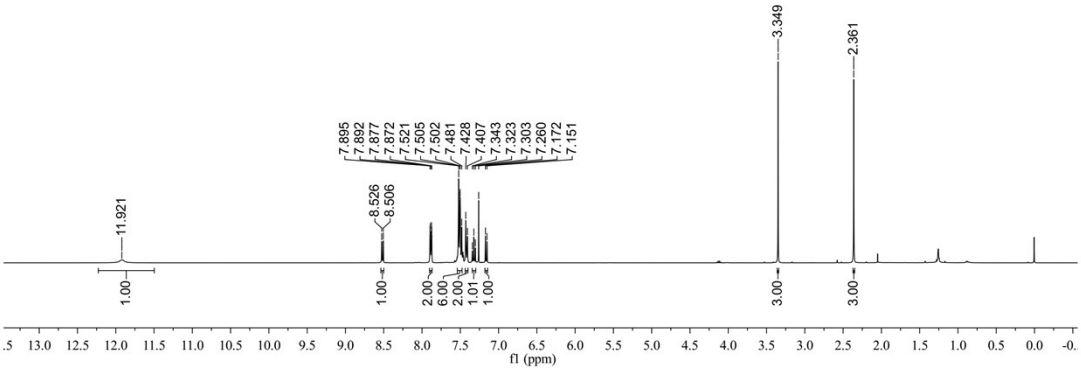
2.00
1.01
1.00
7.7
7.6
7.5
7.4
7.3
7.2
7.1
f1 (ppm)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7.872
7.521
7.505
7.502
7.481
7.428
7.407
7.343
7.323
7.303
7.260
7.172
7.151
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1.00
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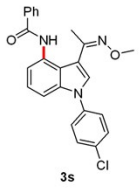
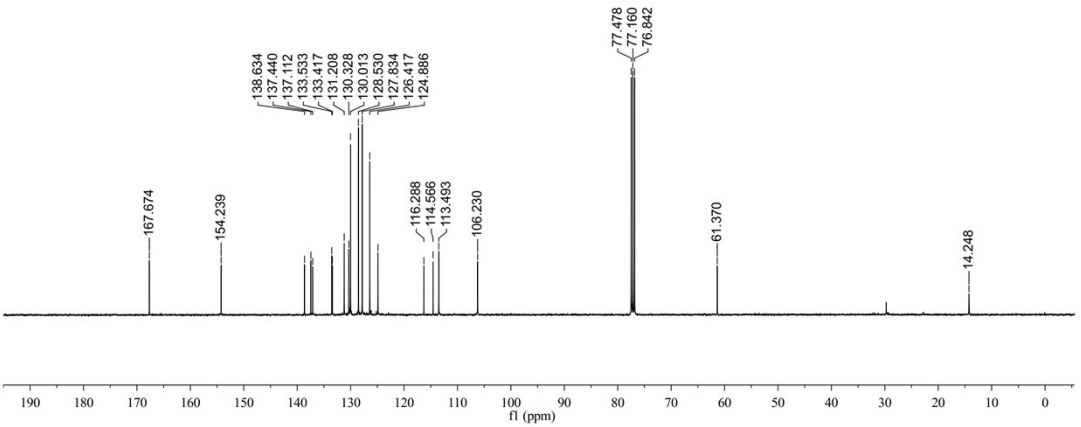
6.00
2.00
1.01
1.00
3.00
3.00
f1 (ppm)


Ph
NH
N
O
Cl

3s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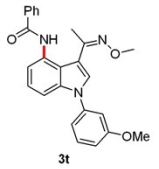
137.112
133.533
133.417
131.208
130.328
130.013
128.530
127.834
126.417
124.886
77.478
77.160
76.842
167.674
154.239
116.288
114.566
113.493
106.230
61.370
14.248
f1 (ppm)


Ph
NH
N
O
OMe
3t


7.566
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7.504
7.500
7.482
7.466
7.445
7.425
7.324
7.304
7.269
7.266
7.260
7.248
7.083
7.080
7.079
7.061
7.024
7.018
7.013
6.990
1.01
3.01
1.01
1.00
1.02
1.02
1.00
1.00
7.6
7.5
7.4
7.3
7.2
7.1
7.0
6.9
f1 (ppm)
3.872
3.353
2.368
7.907
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7.888
7.884
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7.504
7.500
7.482
7.466
7.460
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7.425
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8.502
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1.00
1.02
1.02
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1.00
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3.00
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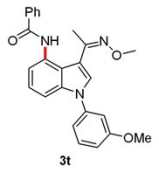
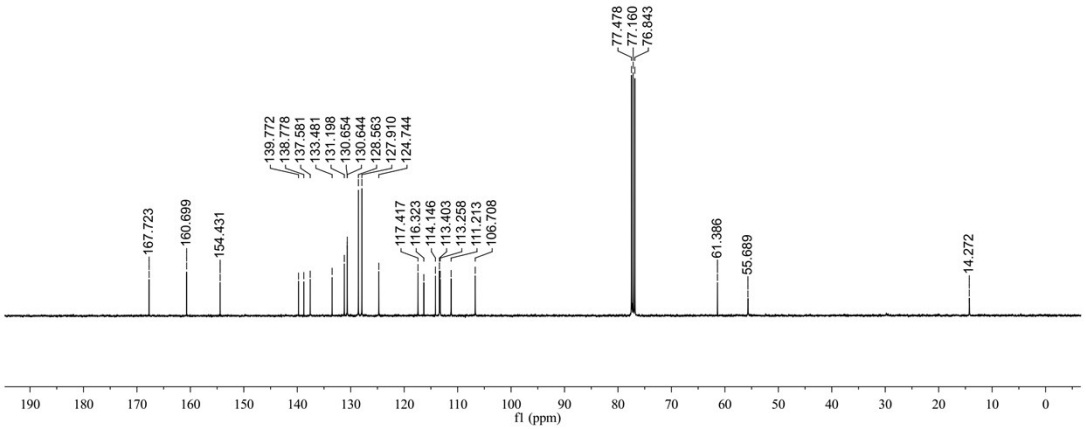
-0
f1 (ppm)


Ph
NH
N
O
OMe
3t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131.198
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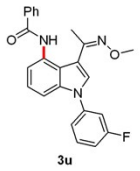
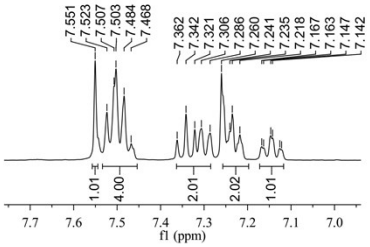
130.644
128.563
127.910
124.744
167.723
160.699
154.431
117.417
116.323
114.146
113.403
113.258
111.213
106.708
61.386
55.689
14.272
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)


Ph
NH
N
O
N
F

3u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7.523
7.507
7.503
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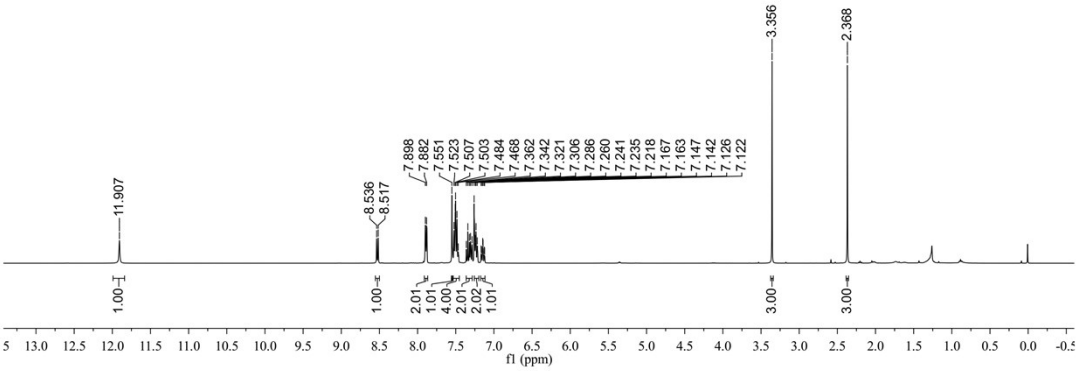
7.468
7.362
7.342
7.321
7.306
7.286
7.260
7.241
7.235
7.218
7.167
7.163
7.147
7.142
1.01
4.00
2.01
2.02
1.01
7.7
7.6
7.5
7.4
7.3
7.2
7.1
7.0
f1 (ppm)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8.517
7.898
7.882
7.551
7.523
7.507
7.503
7.484
7.468
7.362
7.342
7.321
7.306
7.286
7.260
7.241
7.235
7.218
7.167
7.163
7.147
7.142
7.126
7.122
3.356
2.368
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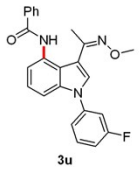
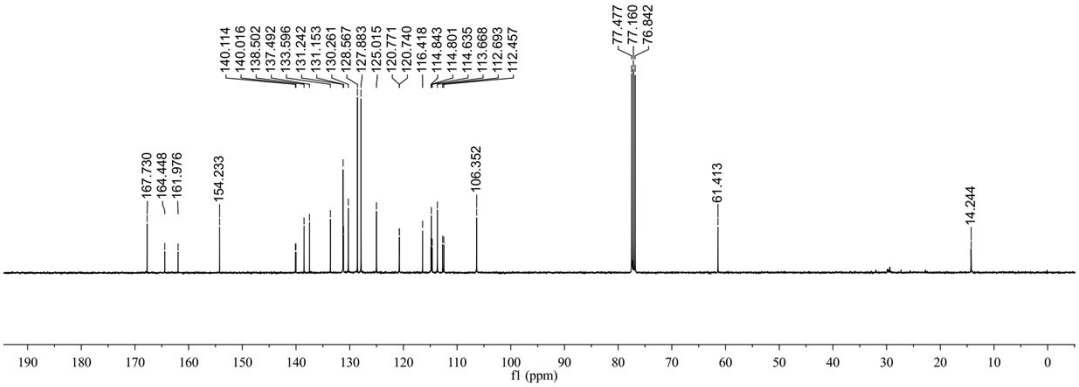
1.00
2.01
1.01
4.00
2.01
2.02
1.01
3.00
3.00
f1 (ppm)


Ph
NH
N
O
N
F

3u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131.242
131.153
130.261
128.567
127.883
123.015
120.771
120.740
116.418
114.843
114.801
114.635
113.668
112.693
112.457
77.477
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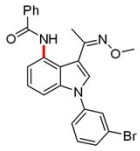
76.842
167.730
164.448
161.976
154.233
106.352
61.413
14.244
f1 (ppm)


Ph
NH
N
O
N
Br

3v


7.562
7.544
7.539
7.529
7.504
7.498
7.480
7.426
7.422
7.416
7.397
7.329
7.309
7.260
7.210
7.208
7.189
7.188
7.642
7.638
7.634
1.01
1.00
1.01
3.00
2.00
1.00
1.00
7.7
7.6
7.5
7.4
7.3
7.2
7.1
f1 (ppm)
3.353
2.363
7.898
7.895
7.879
7.875
7.642
7.638
7.634
7.566
7.562
7.557
7.548
7.544
7.539
7.529
7.521
7.504
7.498
7.480
7.464
7.442
7.426
7.422
7.416
7.397
7.377
7.350
7.329
7.309
7.260
7.210
7.208
7.189
7.188
11.914
8.539
8.520
1.00
1.00
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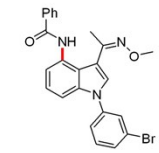
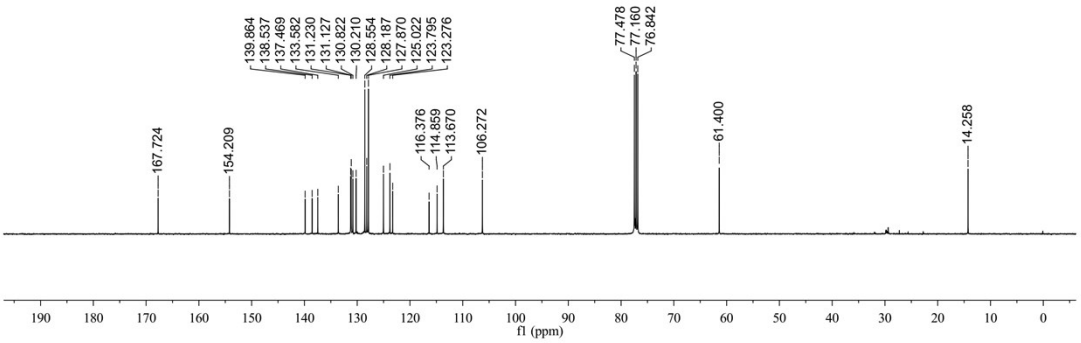
1.01
1.00
1.01
3.00
2.00
1.00
1.00
3.00
3.00
f1 (ppm)


Ph
NH
N
O
N
Br

3v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138.537
137.469
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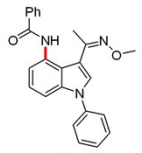
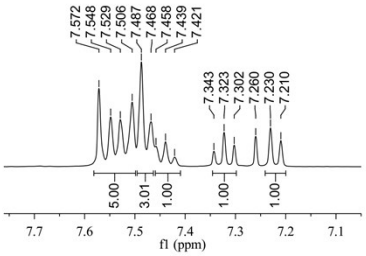
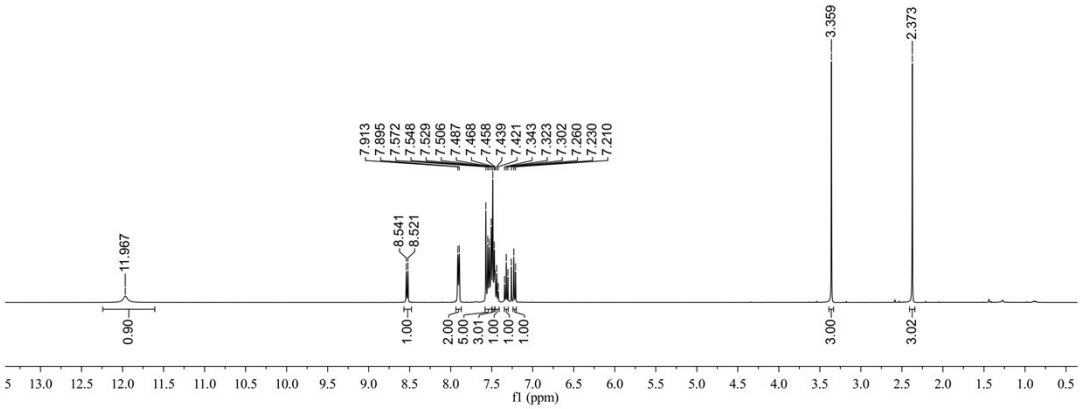
131.230
131.127
130.822
130.210
128.554
128.187
127.870
125.022
123.795
123.276
116.376
114.859
113.670
106.272
77.478
77.160
76.842
61.400
14.258
167.724
154.209
f1 (ppm)


Ph
NH
N
O
3w


7.572
7.548
7.529
7.506
7.487
7.468
7.458
7.439
7.421
7.343
7.323
7.302
7.260
7.230
7.210
5.00
3.01
1.00
1.00
1.00
7.7
7.6
7.5
7.4
7.3
7.2
7.1
f1 (ppm)


11.967
8.541
8.521
7.913
7.895
7.572
7.548
7.529
7.506
7.487
7.468
7.458
7.439
7.421
7.343
7.323
7.302
7.260
7.230
7.210
3.359
2.373
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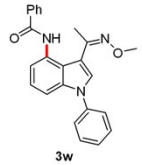
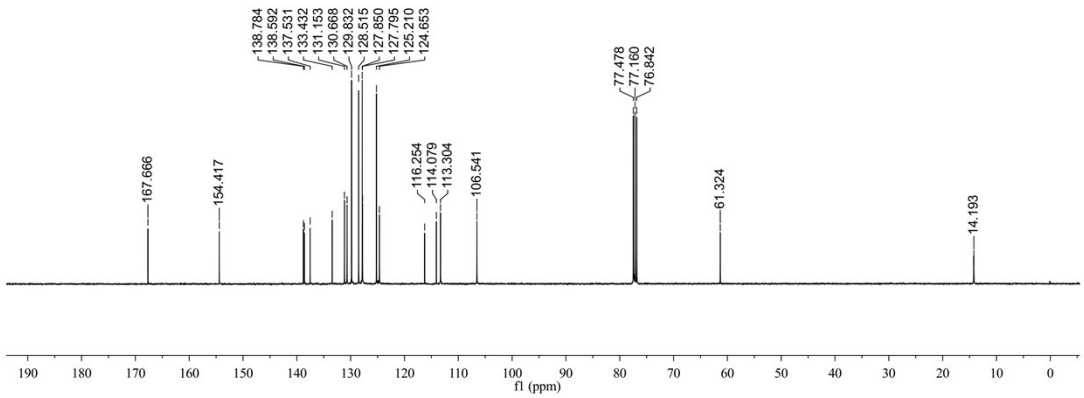
2.00
5.00
3.01
1.00
1.00
1.00
3.00
3.02
f1 (ppm)


Ph
NH
N
O
3w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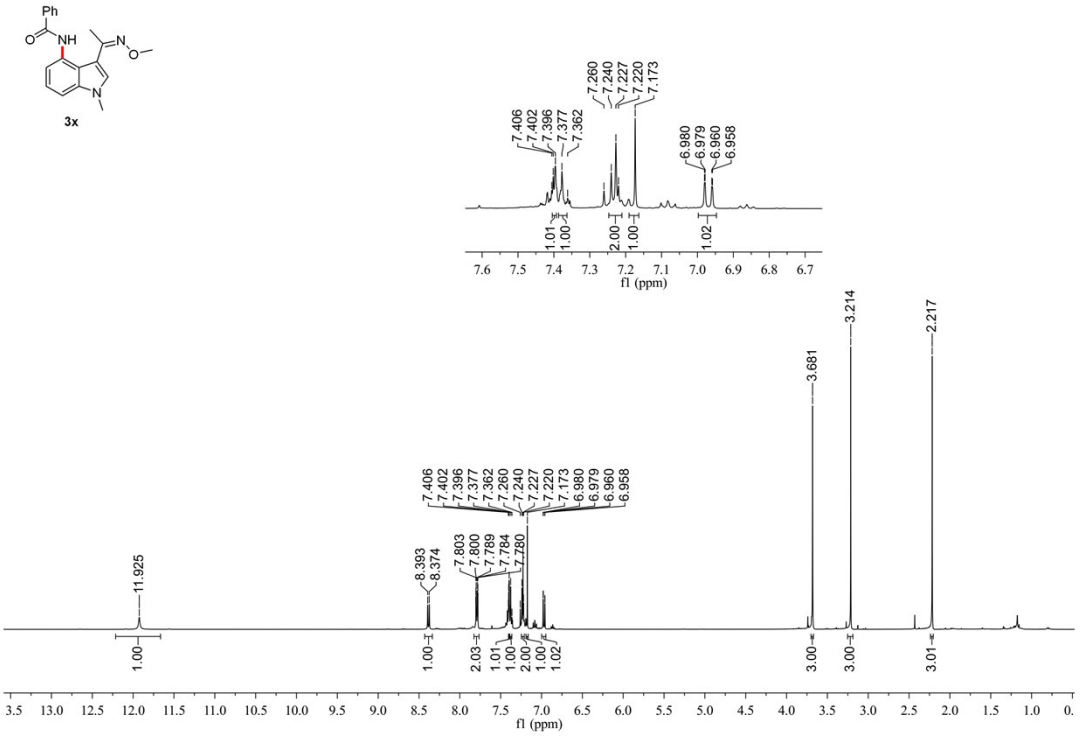
138.592
137.531
133.432
131.153
130.668
129.832
128.515
127.850
127.795
125.210
124.653
167.666
154.417
116.254
114.079
113.304
106.541
77.478
77.160
76.842
61.324
14.193
f1 (ppm)


Ph
NH
N
O
3x
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7.402
7.396
7.377
7.362
7.260
7.240
7.227
7.220
7.173
6.980
6.979
6.960
6.958
1.01
1.00
2.00
1.00
1.02
f1 (ppm)
3.214
2.217
3.681
11.925
8.393
8.374
7.803
7.800
7.789
7.784
7.780
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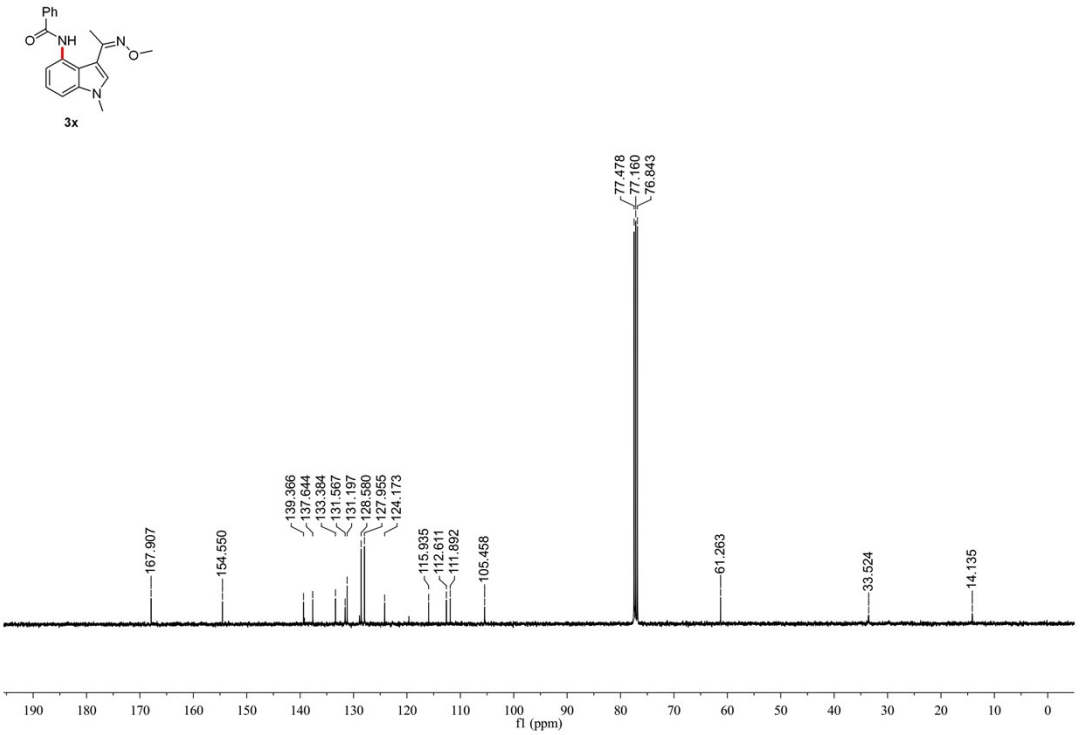
1.00
2.03
1.01
1.00
2.00
1.00
1.02
3.00
3.00
3.01
f1 (ppm)


Ph
NH
N
O
3x
77.478
77.160
76.843
139.366
137.644
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131.567
131.197
128.580
127.955
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154.550
115.935
112.611
111.892
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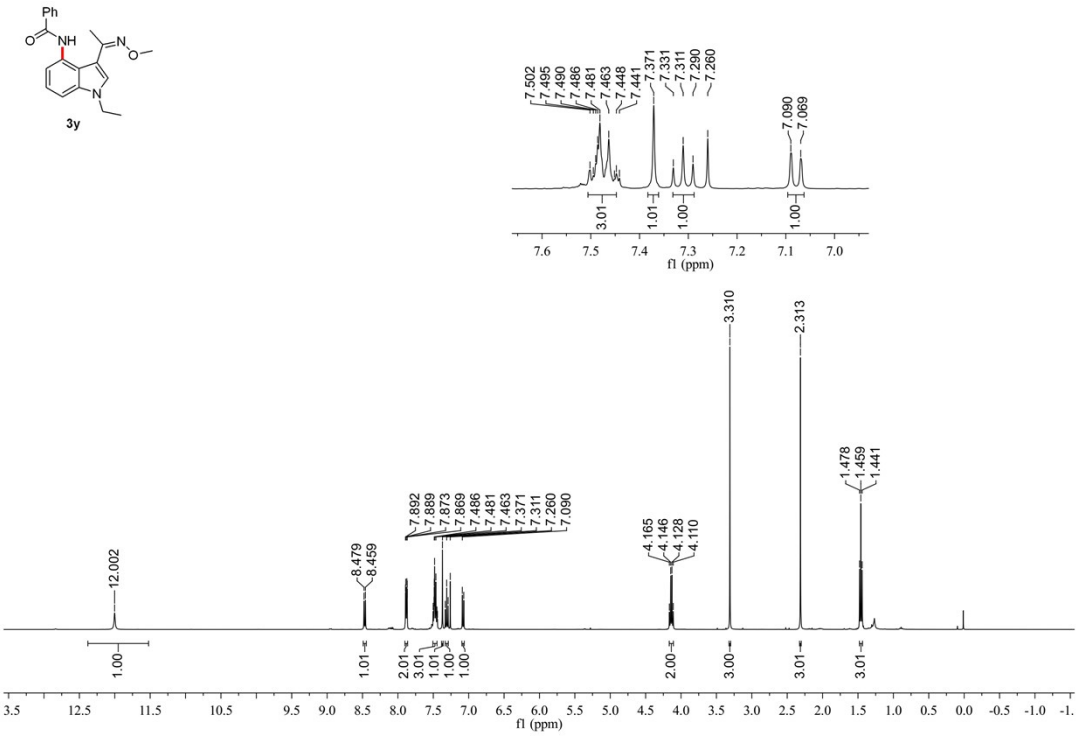
61.263
33.524
14.135
f1 (ppm)


Ph
NH
N
O
3y
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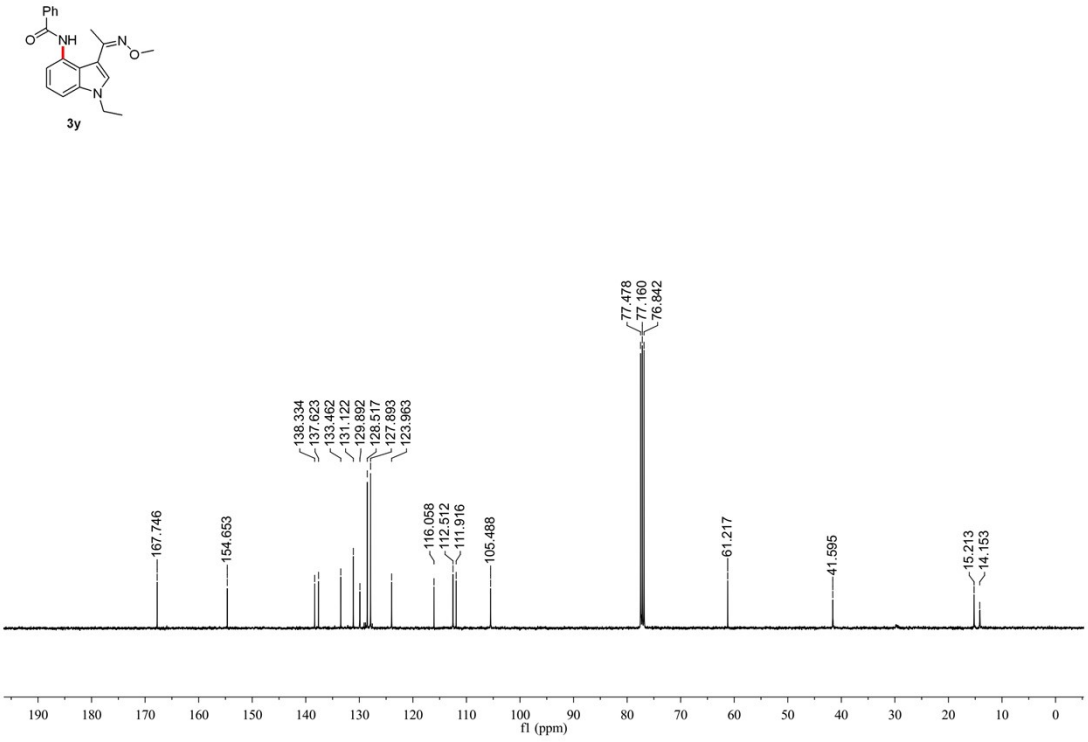
7.490
7.486
7.481
7.463
7.448
7.441
7.371
7.331
7.311
7.290
7.260
7.090
7.069
3.01
1.01
1.00
1.00
f1 (ppm)
12.002
8.479
8.459
7.892
7.889
7.873
7.869
7.486
7.481
7.463
7.371
7.311
7.260
7.090
4.165
4.146
4.128
4.110
3.310
2.313
1.478
1.459
1.441
1.00
1.01
2.01
3.01
1.01
1.00
1.00
2.00
3.00
3.01
3.01
f1 (ppm)


Ph
NH
N
O
3y
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77.160
76.842
138.334
137.623
133.462
131.122
129.892
128.517
127.893
123.963
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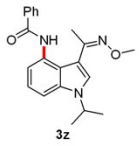
116.058
112.512
111.916
105.488
61.217
41.595
15.213
14.153
f1 (ppm)


Ph
NH
N
O
N
3z


7.505
7.498
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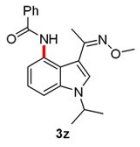
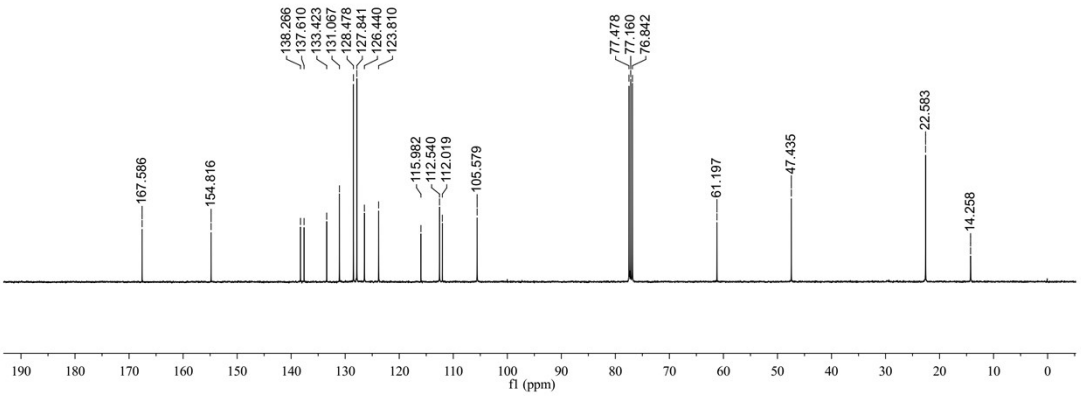
7.481
7.469
7.454
7.348
7.328
7.308
7.260
7.149
7.129
4.00
1.01
1.00
7.6
7.5
7.4
7.3
7.2
7.1
7.0
f1 (ppm)
3.326
2.353
1.543
1.526
12.013
8.499
8.479
7.901
7.897
7.882
7.878
4.697
4.681
4.664
4.647
4.630
1.00
1.04
2.08
4.00
1.01
1.00
1.03
3.01
3.00
3.00
3.00
13.0
12.5
12.0
11.5
11.0
10.5
10.0
9.5
9.0
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
f1 (ppm)


Ph
NH
N
O
N
3z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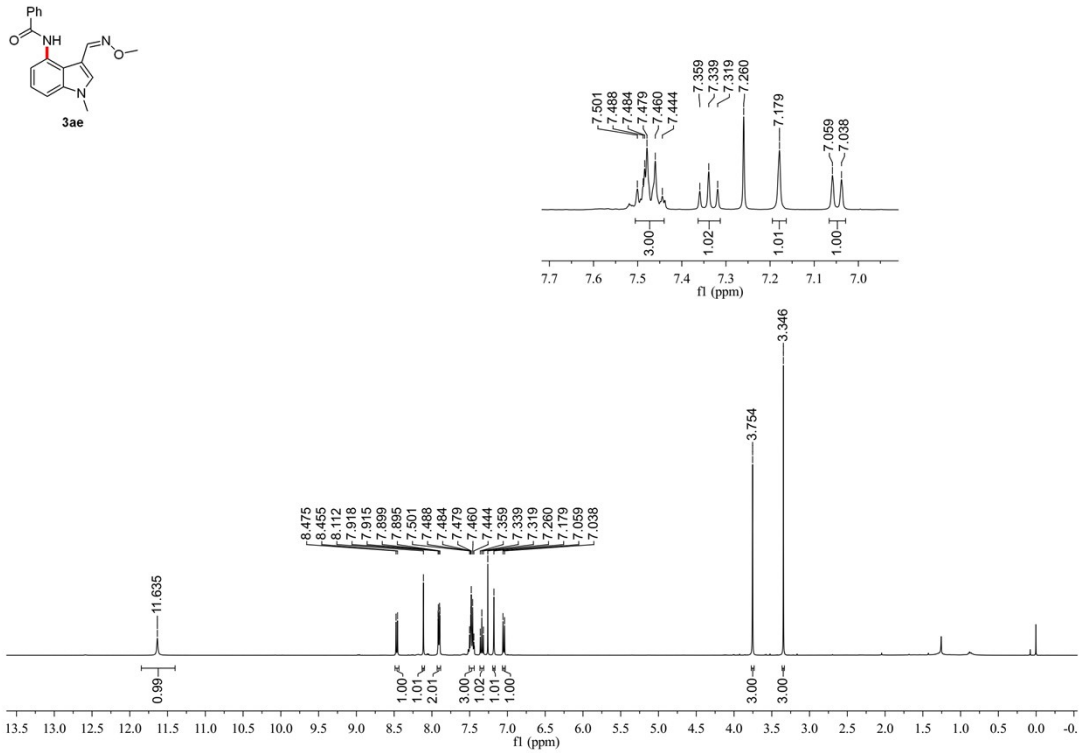
123.810
115.982
112.540
112.019
105.579
77.478
77.160
76.842
167.586
154.816
61.197
47.435
22.583
14.258
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)


Ph
NH
N
O
3ae
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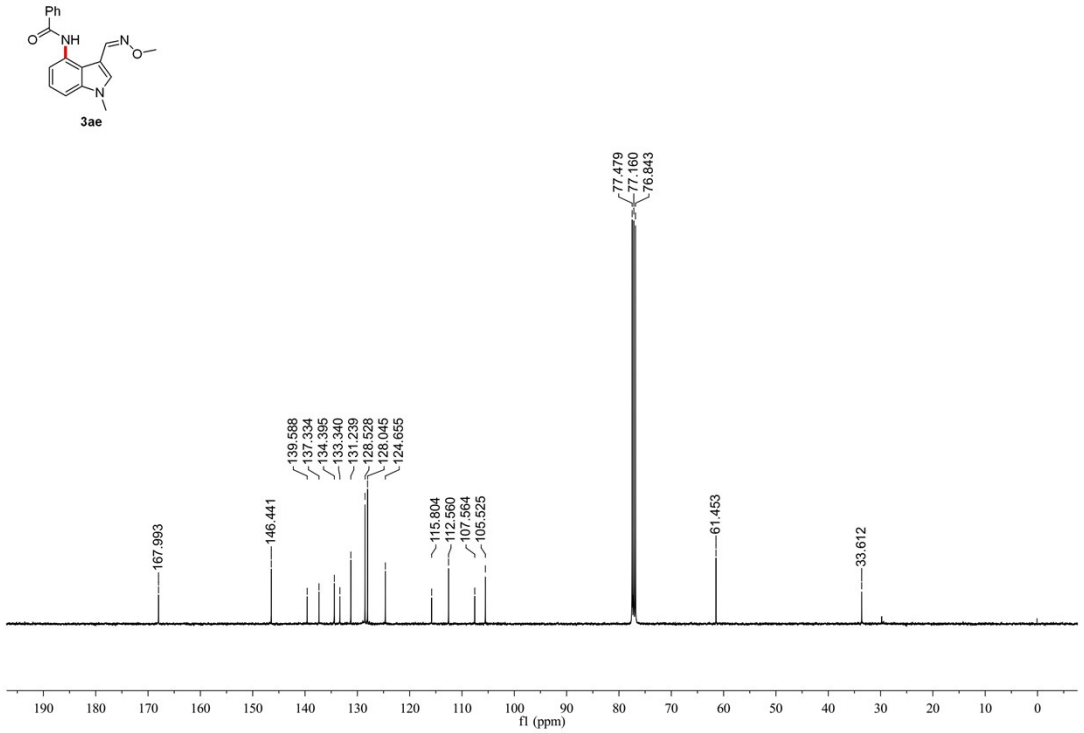
7.488
7.484
7.479
7.460
7.444
7.359
7.339
7.319
7.260
7.179
7.059
7.038
3.00
1.02
1.01
1.00
fl (ppm)
3.346
3.754
8.475
8.455
8.112
7.918
7.915
7.899
7.895
11.635
0.99
1.00
1.01
2.01
3.00
1.02
1.01
1.00
3.00
3.00
fl (ppm)


Ph
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N
O
3ae
77.479
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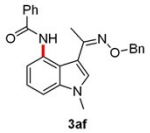
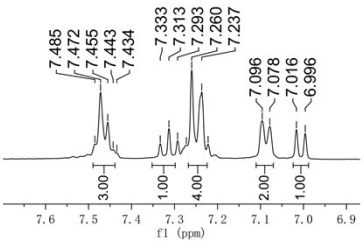
76.843
139.588
137.334
134.395
133.340
131.239
128.528
128.045
124.655
115.804
112.560
107.564
105.525
167.993
146.441
61.453
33.612
fl (ppm)


Ph
NH
N
O-Bn
3af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7.434
7.333
7.313
7.293
7.260
7.237
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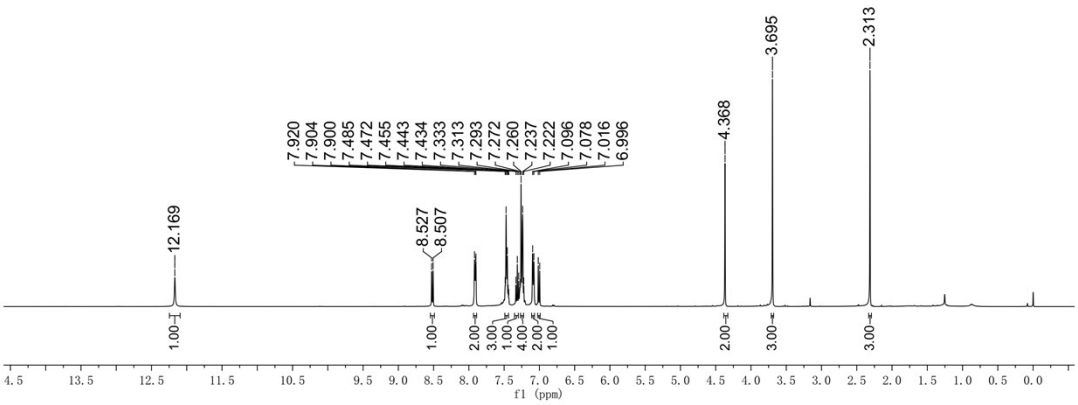
7.078
7.016
6.996
3.00
1.00
4.00
2.00
1.00
f1 (ppm)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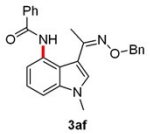
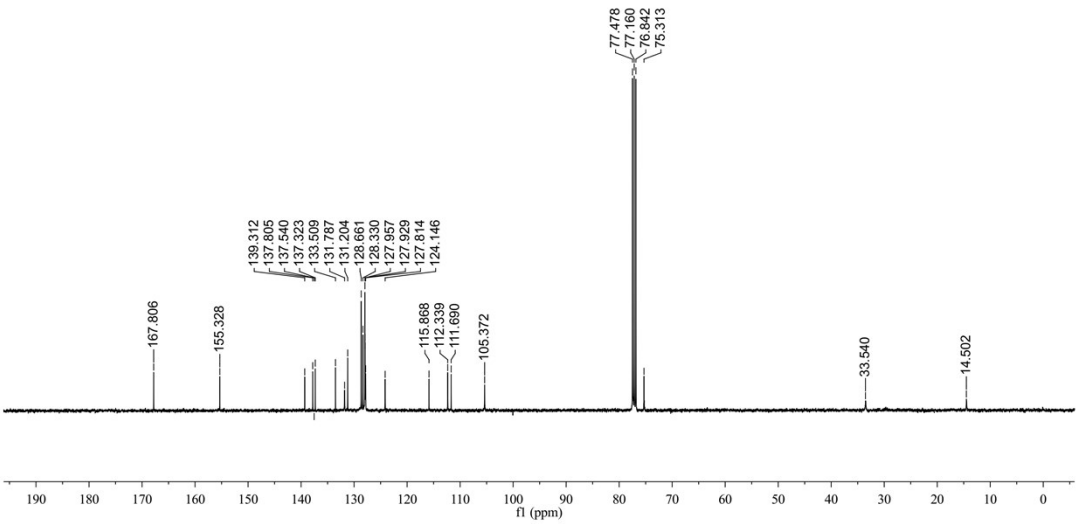
7.904
7.900
7.485
7.472
7.455
7.443
7.434
7.333
7.313
7.293
7.272
7.260
7.237
7.222
7.096
7.078
7.016
6.996
4.368
3.695
2.313
f1 (ppm)


Ph
NH
N
O-Bn
3af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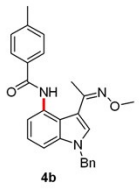
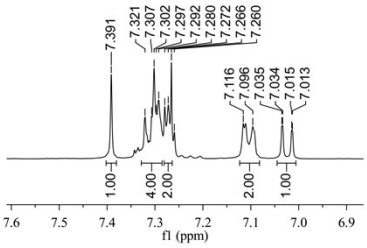
137.323
133.509
131.787
131.204
128.661
128.330
127.957
127.929
127.814
124.146
115.868
112.339
111.690
105.372
77.478
77.160
76.842
75.313
33.540
14.502
f1 (ppm)


NH
N
O
N
Bn

4b


7.391
7.321
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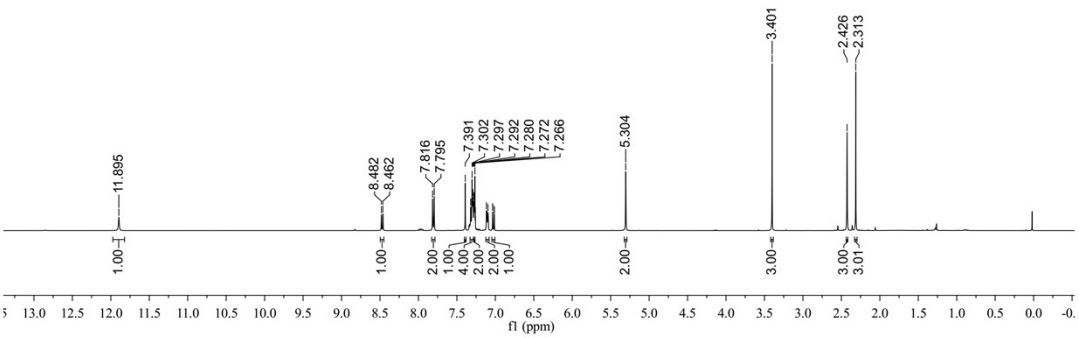
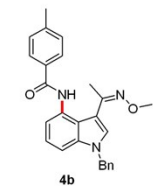
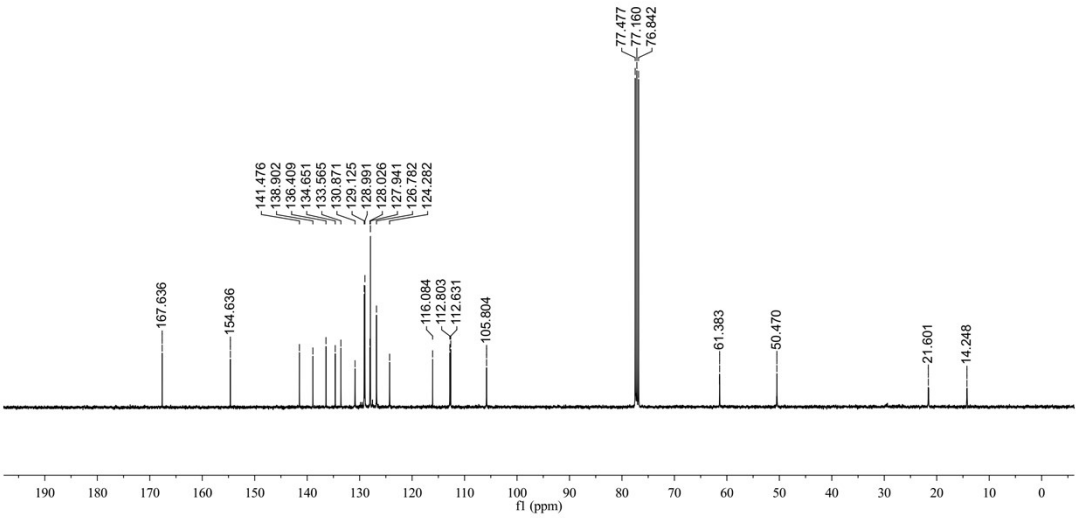
7.302
7.297
7.292
7.280
7.272
7.266
7.260
7.116
7.096
7.035
7.034
7.015
7.013
1.00
4.00
2.00
2.00
1.00
7.6
7.5
7.4
7.3
7.2
7.1
7.0
6.9
f1 (ppm)


11.895
8.482
8.462
7.816
7.795
7.391
7.302
7.297
7.292
7.280
7.272
7.266
5.304
3.401
2.426
2.313
1.00
1.00
2.00
1.00
4.00
2.00
2.00
1.00
2.00
3.00
3.00
3.01
f1 (ppm)


NH
N
O
N
Bn

4b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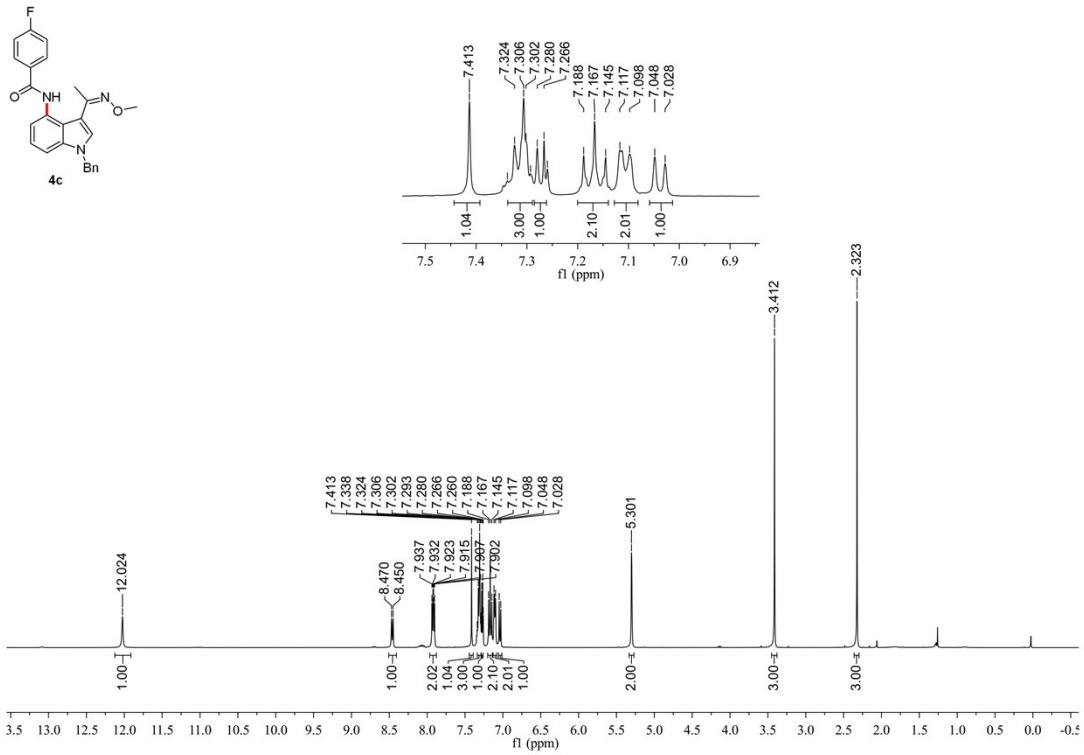
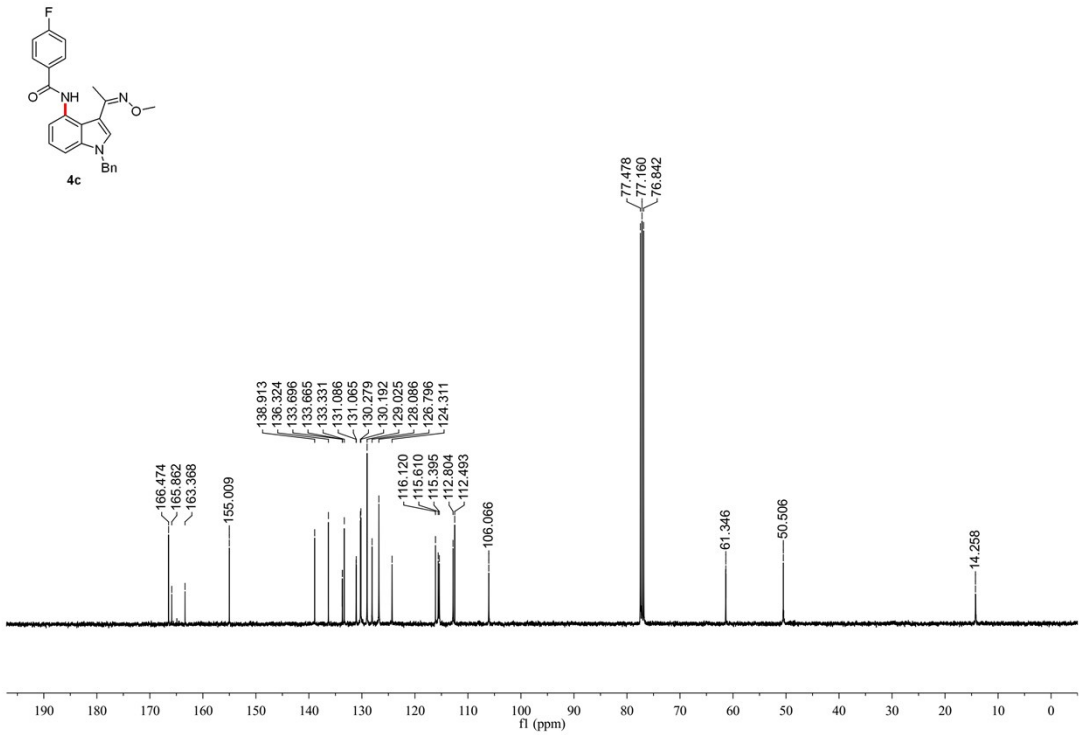
77.160
76.842
141.476
138.902
136.409
134.651
133.565
130.871
129.125
128.991
128.026
127.941
126.782
124.282
167.636
154.636
116.084
112.803
112.631
105.804
61.383
50.470
21.601
14.248
f1 (ppm)


4c
7.413
7.324
7.306
7.302
7.280
7.266
7.188
7.167
7.145
7.117
7.098
7.048
7.028
1.04
3.00
1.00
2.10
2.01
1.00
f1 (ppm)
3.412
2.323
5.301
12.024
8.470
8.450
7.937
7.932
7.923
7.915
7.907
7.902
1.00
2.02
1.04
3.00
1.00
2.10
2.01
1.00
2.00
3.00
3.00
f1 (ppm)


4c
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76.842
138.913
136.324
133.696
133.665
133.331
131.086
131.065
130.279
130.192
129.025
128.086
126.796
124.311
116.120
115.610
115.395
112.804
112.493
166.474
165.862
163.368
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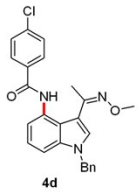
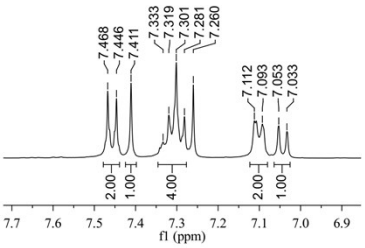
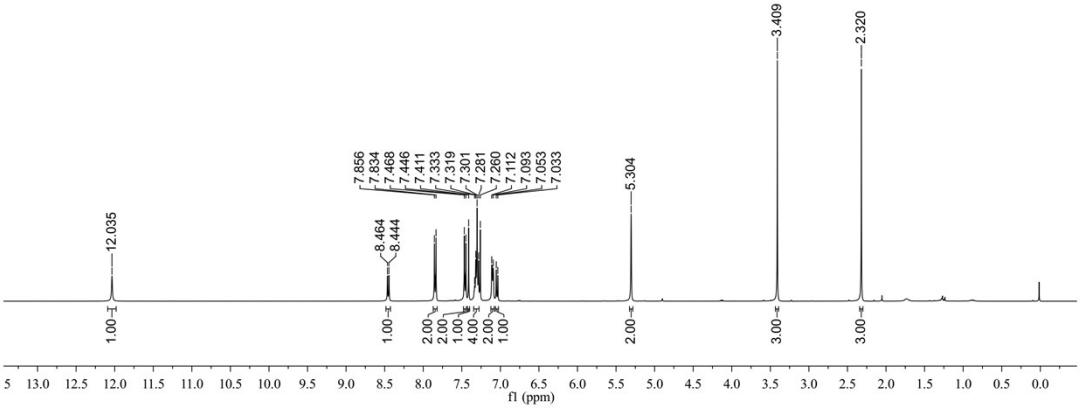
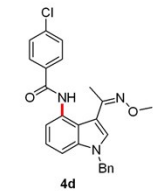
106.066
61.346
50.506
14.258
f1 (ppm)


Cl
NH
N
O
Bn

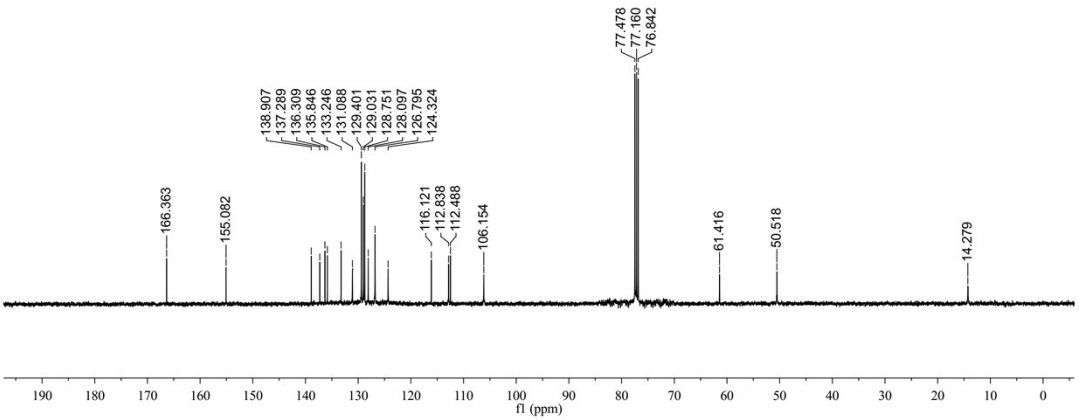
4d


7.468
7.446
7.411
7.333
7.319
7.301
7.281
7.260
7.112
7.093
7.053
7.033
2.00
1.00
4.00
2.00
1.00
f1 (ppm)


12.035
8.464
8.444
7.856
7.834
7.468
7.446
7.411
7.333
7.319
7.301
7.281
7.260
7.112
7.093
7.053
7.033
5.304
3.409
2.320
f1 (ppm)


Cl
NH
N
O
Bn

4d


166.363
155.082
138.907
137.289
136.309
135.846
133.246
131.088
129.401
129.031
128.751
128.097
126.795
124.324
116.121
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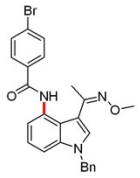
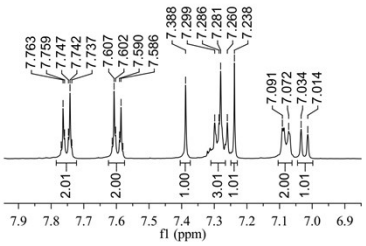
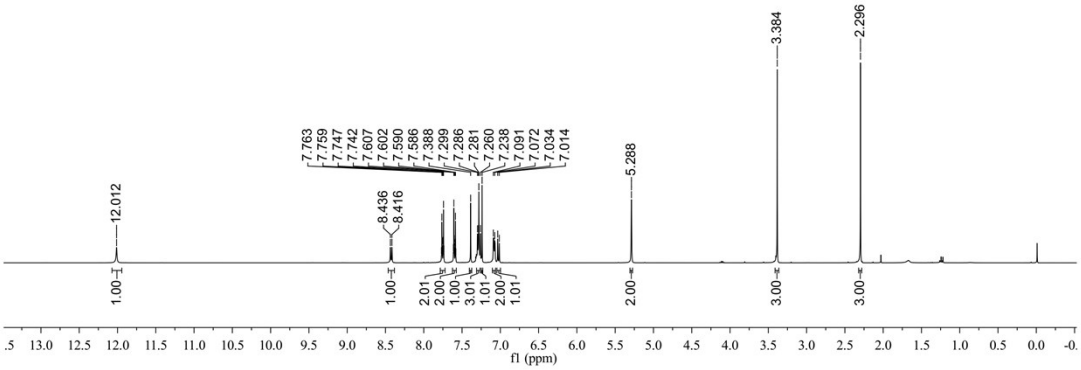
112.488
106.154
77.478
77.160
76.842
61.416
50.518
14.279
f1 (ppm)


Br
NH
N
O
Bn

4e


7.763
7.759
7.747
7.742
7.737
7.607
7.602
7.590
7.586
7.388
7.299
7.286
7.281
7.260
7.238
7.091
7.072
7.034
7.014
2.01
2.00
1.00
3.01
1.01
2.00
1.01
7.9 7.8 7.7 7.6 7.5 7.4 7.3 7.2 7.1 7.0 6.9
f1 (ppm)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8.436
8.416
7.763
7.759
7.747
7.742
7.607
7.602
7.590
7.586
7.388
7.299
7.286
7.281
7.260
7.238
7.091
7.072
7.034
7.014
5.288
3.384
2.296
1.00
1.00
2.01
2.00
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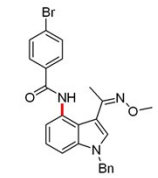
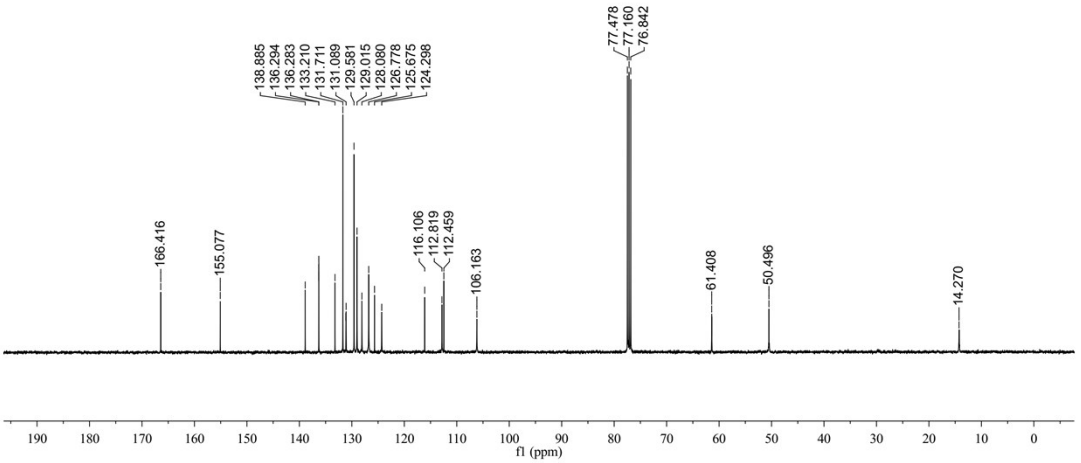
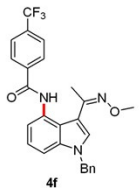
1.01
2.00
3.00
3.00
f1 (ppm)

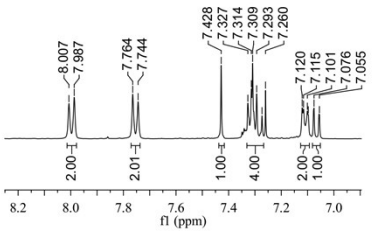

Br
NH
N
O
Bn

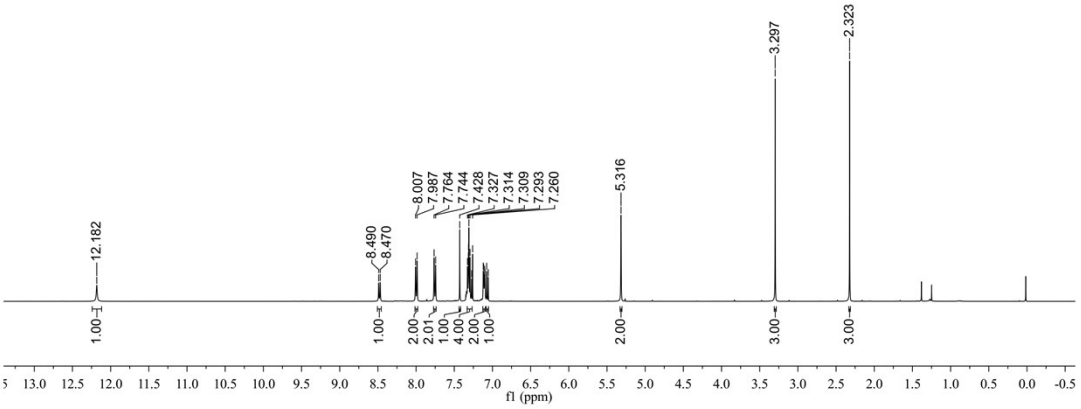
4e

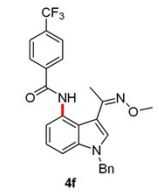

166.416
155.077
138.885
136.294
136.283
133.210
131.711
131.089
129.581
129.015
128.080
126.778
125.675
124.298
116.106
112.819
112.459
106.163
77.478
77.160
76.842
61.408
50.496
14.270
f1 (ppm)


CF3
NH
O
N
O
Bn

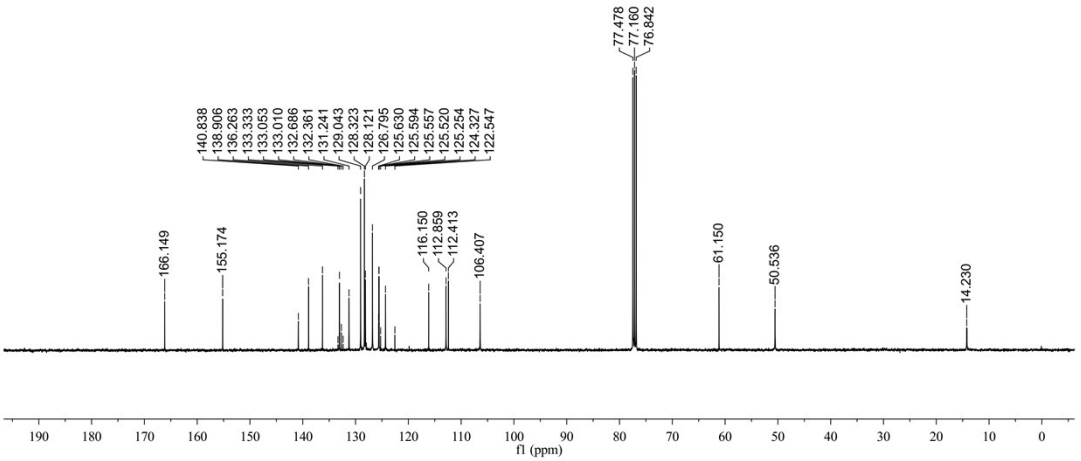
4f

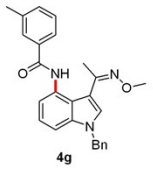

8.007
7.987
7.764
7.744
7.428
7.327
7.314
7.309
7.293
7.260
7.120
7.115
7.101
7.076
7.055
2.00
2.01
1.00
4.00
2.00
1.00
8.2
8.0
7.8
7.6
7.4
7.2
7.0
f1 (ppm)


12.182
8.490
8.470
8.007
7.987
7.764
7.744
7.428
7.327
7.314
7.309
7.293
7.260
5.316
3.297
2.323
1.00
1.00
2.00
2.01
1.00
4.00
2.00
1.00
2.00
3.00
3.00
f1 (ppm)

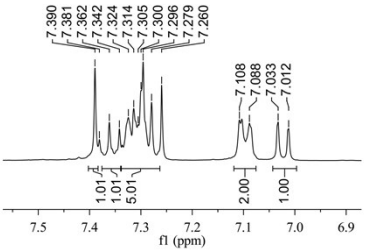

CF3
NH
O
N
O
Bn

4f


77.478
77.160
76.842
140.838
138.906
136.263
133.333
133.053
133.010
132.686
132.361
131.241
129.043
128.323
128.121
126.795
125.630
125.594
125.557
125.520
125.254
124.327
122.547
166.149
155.174
116.150
112.859
112.413
106.407
61.150
50.536
14.230
f1 (ppm)


NH
N
O
Bn

4g


7.390
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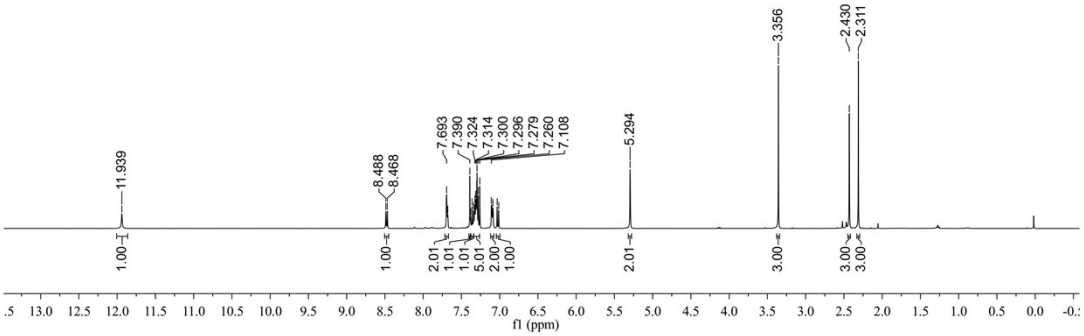
7.362
7.342
7.324
7.314
7.305
7.300
7.296
7.279
7.260
7.108
7.088
7.033
7.012
1.01
1.01
5.01
2.00
1.00
7.5
7.4
7.3
7.2
7.1
7.0
6.9
f1 (ppm)


11.939
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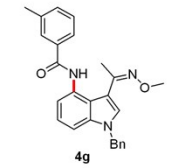
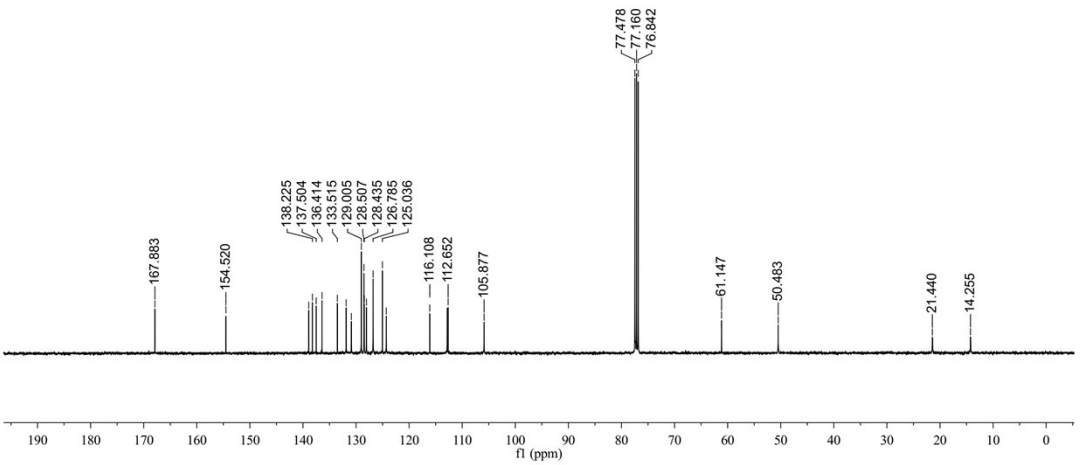
8.468
7.693
7.390
7.324
7.314
7.300
7.296
7.279
7.260
7.108
5.294
3.356
2.430
2.311
1.00
1.00
2.01
1.01
1.01
5.01
2.00
1.00
2.01
3.00
3.00
3.00
f1 (ppm)


NH
N
O
Bn

4g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77.160
76.842
138.225
137.504
136.414
133.515
129.005
128.507
128.435
126.785
125.036
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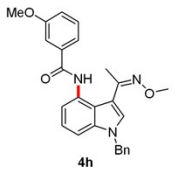
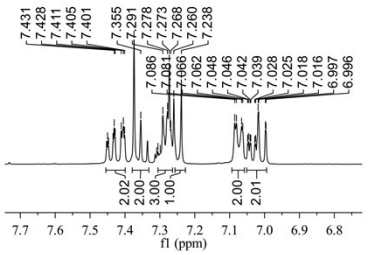
61.147
50.483
21.440
14.255
f1 (ppm)


MeO
NH
N
O
Bn

4h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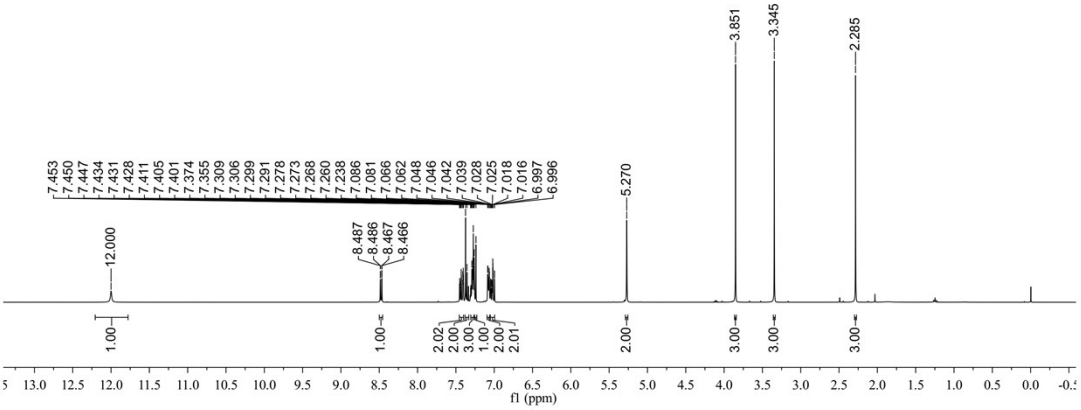
7.428
7.411
7.405
7.401
7.355
7.291
7.278
7.273
7.268
7.260
7.238
7.086
7.081
7.066
7.062
7.048
7.046
7.042
7.039
7.028
7.025
7.018
7.016
6.997
6.996
2.02
2.00
3.00
1.00
2.00
2.01
7.7 7.6 7.5 7.4 7.3 7.2 7.1 7.0 6.9 6.8
f1 (ppm)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7.447
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7.431
7.428
7.411
7.405
7.401
7.374
7.355
7.309
7.306
7.299
7.291
7.278
7.273
7.268
7.260
7.238
7.086
7.081
7.066
7.062
7.048
7.046
7.042
7.039
7.028
7.025
7.018
7.016
6.997
6.996
5.270
12.000
8.487
8.486
8.467
8.466
1.00
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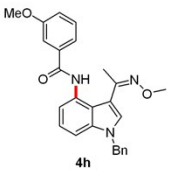
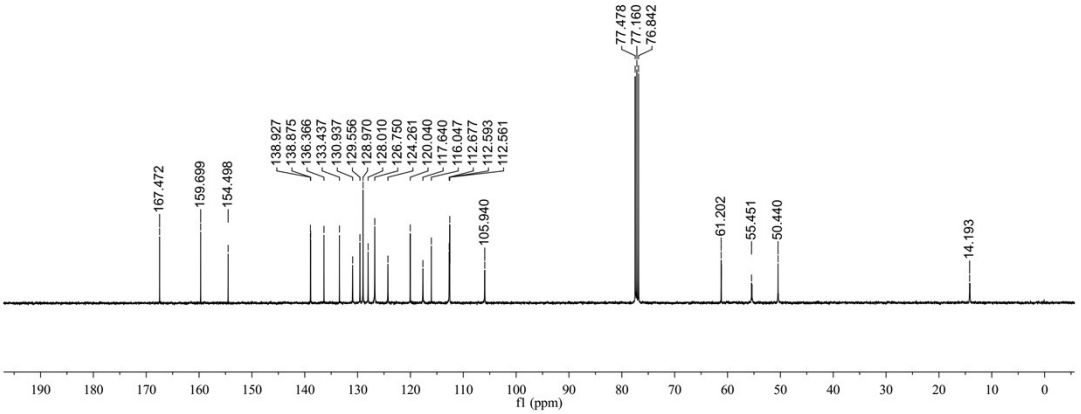
2.00
3.00
3.00
3.00
fl (ppm)


MeO
NH
N
O
Bn

4h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76.842
138.927
138.875
136.366
133.437
130.937
129.556
128.970
128.010
126.750
124.261
120.040
117.640
116.047
112.677
112.593
112.561
167.472
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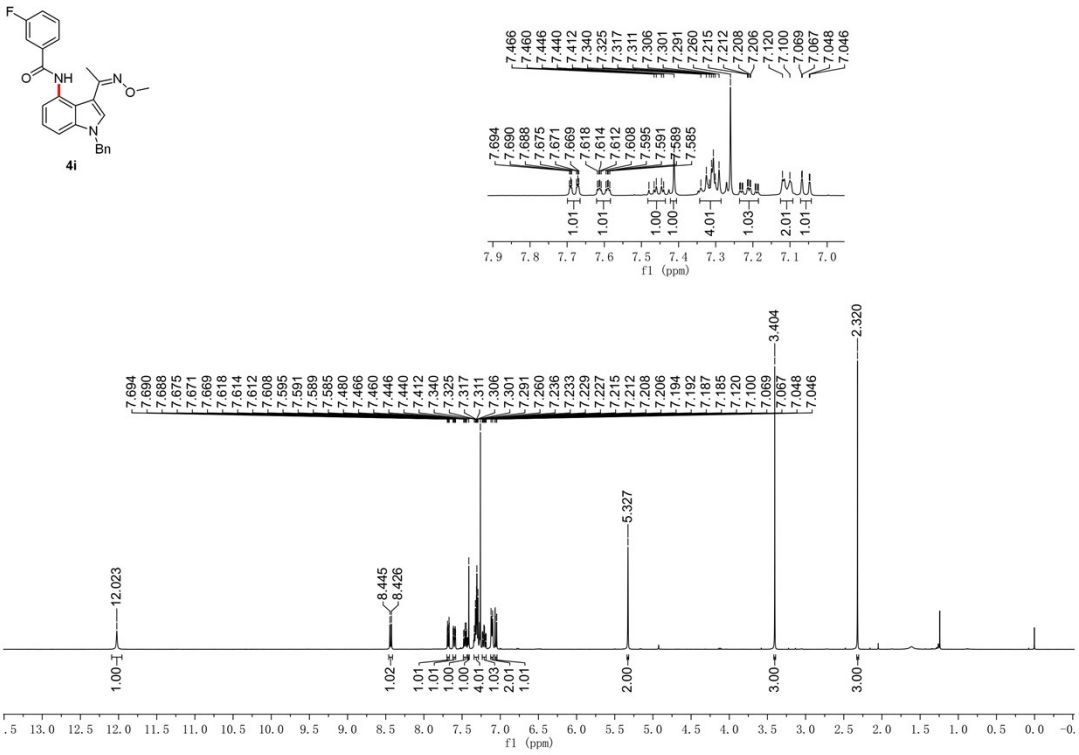
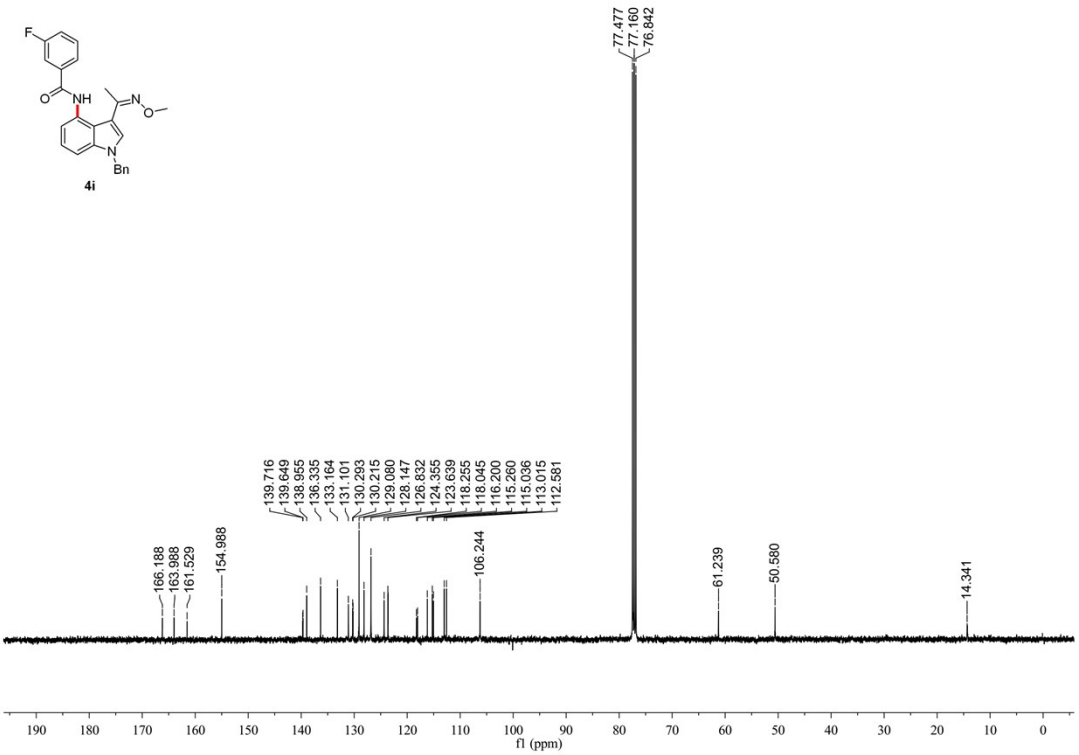
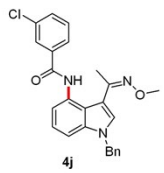
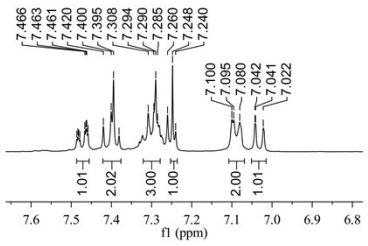
154.498
105.940
61.202
55.451
50.440
14.193
fl (ppm)


4i
7.9 7.8 7.7 7.6 7.5 7.4 7.3 7.2 7.1 7.0
f1 (ppm)
12.023
8.445
8.426
5.327
3.404
2.320
f1 (ppm)


4i
77.477
77.160
76.842
166.188
163.988
161.529
154.988
139.716
139.649
138.955
136.335
133.164
131.101
130.293
130.215
129.080
128.147
126.832
124.355
123.639
118.255
118.045
116.200
115.260
115.036
113.015
112.581
106.244
61.239
50.580
14.341
190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)


Cl
O
NH
N
O
N
Bn

4j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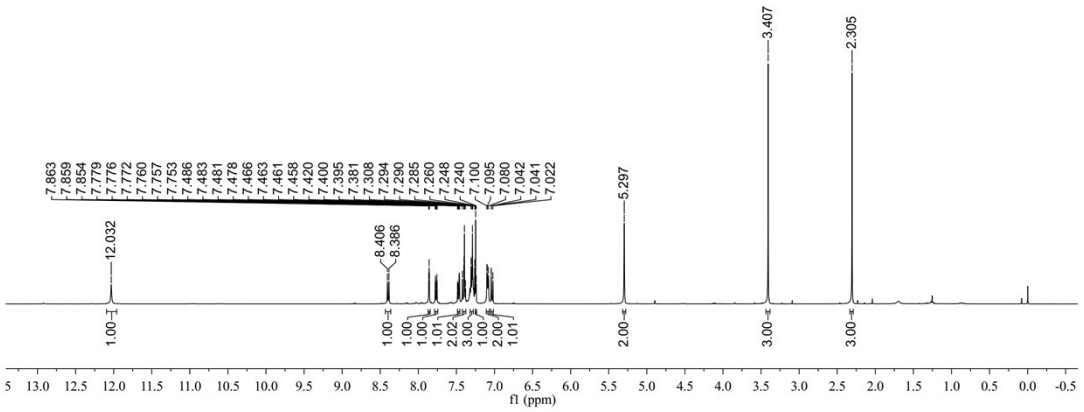
7.461
7.420
7.400
7.395
7.308
7.294
7.290
7.285
7.260
7.248
7.240
7.100
7.095
7.080
7.042
7.041
7.022
1.01
2.02
3.00
1.00
2.00
1.01
7.6 7.5 7.4 7.3 7.2 7.1 7.0 6.9 6.8
f1 (ppm)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7.854
7.779
7.776
7.772
7.760
7.757
7.753
7.486
7.483
7.481
7.478
7.466
7.463
7.461
7.458
7.420
7.400
7.395
7.381
7.308
7.294
7.290
7.285
7.260
7.248
7.240
7.100
7.095
7.080
7.042
7.041
7.022
5.297
12.032
8.406
8.386
1.00
1.00
1.00
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2.02
3.00
1.00
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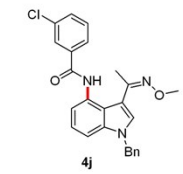
2.00
3.00
3.00
f1 (ppm)


Cl
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NH
N
O
N
Bn

4j


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76.842
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131.101
129.964
129.102
128.166
126.847
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113.130
112.615
106.295
166.181
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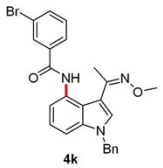
61.301
50.617
14.338
f1 (ppm)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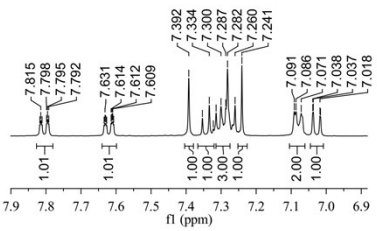
N
Bn
4k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7.631
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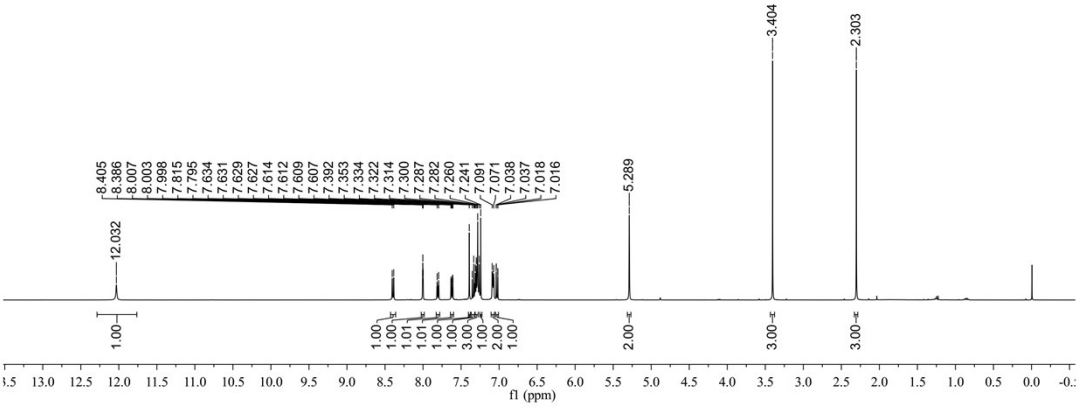
7.612
7.609
7.392
7.334
7.300
7.287
7.282
7.260
7.241
7.091
7.086
7.071
7.038
7.037
7.018
1.01
1.01
1.00
1.00
3.00
1.00
2.00
1.00
7.9 7.8 7.7 7.6 7.5 7.4 7.3 7.2 7.1 7.0 6.9
f1 (ppm)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8.007
8.003
7.998
7.815
7.795
7.634
7.631
7.629
7.627
7.614
7.612
7.609
7.607
7.392
7.353
7.334
7.322
7.314
7.300
7.287
7.282
7.260
7.241
7.091
7.071
7.038
7.037
7.018
7.016
12.032
5.289
3.404
2.303
1.00
1.00
1.00
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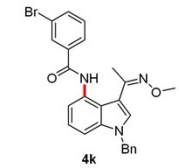
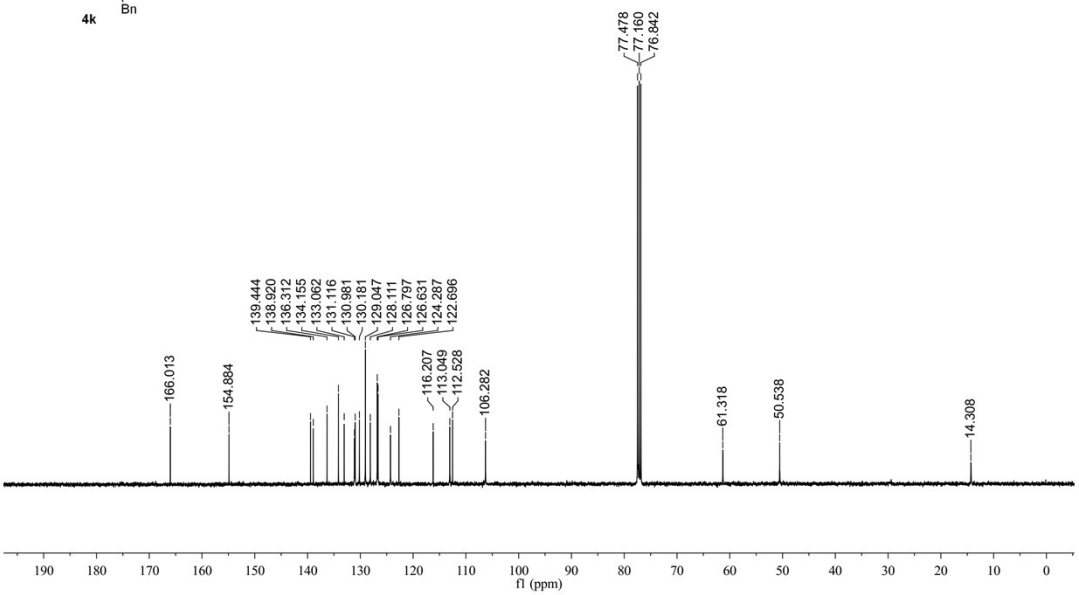
2.00
3.00
3.00
f1 (ppm)


Br
NH
O
N
O
N
Bn
4k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76.842
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134.155
133.062
131.116
130.981
130.181
129.047
128.111
126.797
126.631
124.287
122.696
166.013
154.884
116.207
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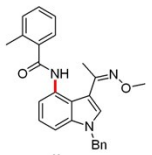
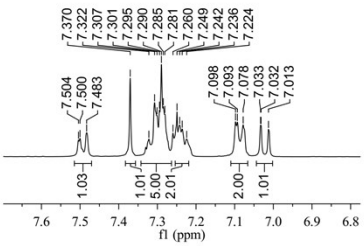
106.282
61.318
50.538
14.308
190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)



**4l**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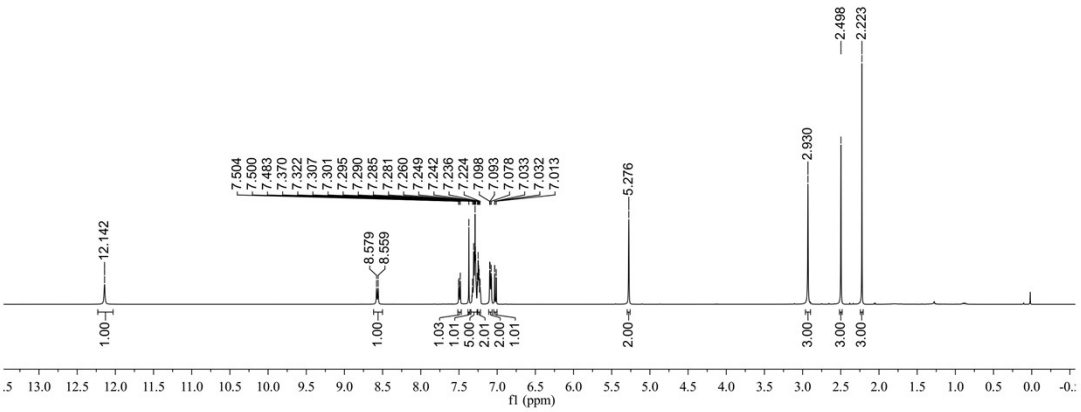
7.307
7.301
7.295
7.290
7.285
7.281
7.260
7.249
7.242
7.236
7.224
7.504
7.500
7.483
7.098
7.093
7.078
7.033
7.032
7.013
1.03
1.01
5.00
2.01
2.00
1.01
f1 (ppm)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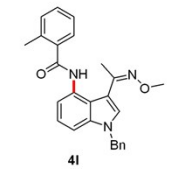
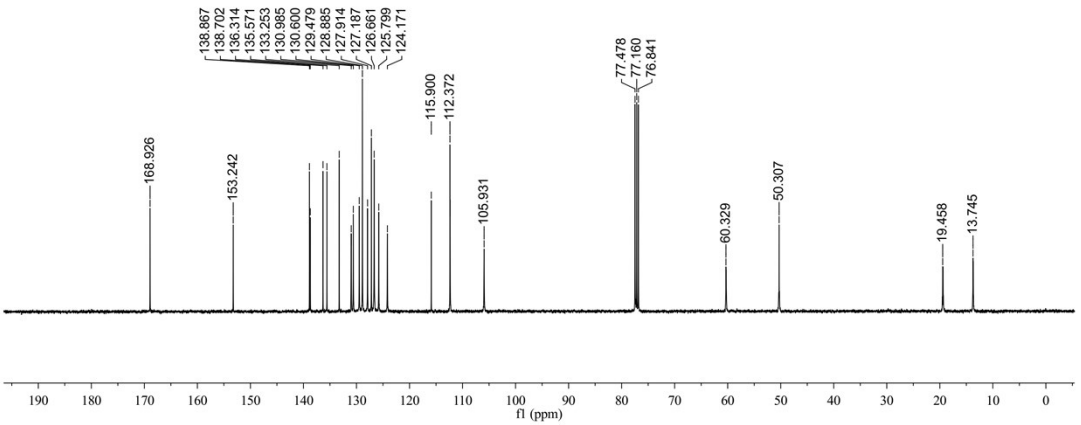
8.559
7.504
7.500
7.483
7.370
7.322
7.307
7.301
7.295
7.290
7.285
7.281
7.260
7.249
7.242
7.236
7.224
7.098
7.093
7.078
7.033
7.032
7.013
5.276
2.930
2.498
2.223
1.00
1.00
1.03
1.01
5.00
2.01
2.00
1.01
2.00
3.00
3.00
3.00
f1 (ppm)



**4l**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138.702
136.314
135.571
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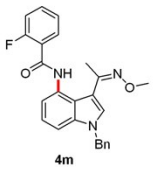
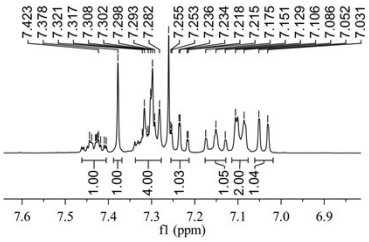
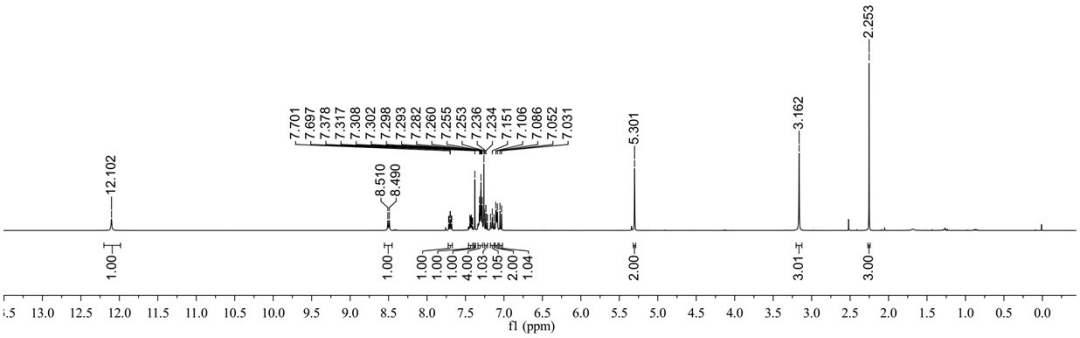
130.985
130.600
129.479
128.885
127.914
127.187
126.661
125.799
124.171
115.900
112.372
105.931
77.478
77.160
76.841
60.329
50.307
19.458
13.745
f1 (ppm)


F
O
NH
N
O
N
Bn

4m


7.423
7.378
7.321
7.317
7.308
7.302
7.298
7.293
7.282
7.255
7.253
7.236
7.234
7.218
7.215
7.175
7.151
7.129
7.106
7.086
7.052
7.031
1.00
1.00
4.00
1.03
1.05
2.00
1.04
7.6 7.5 7.4 7.3 7.2 7.1 7.0 6.9
f1 (ppm)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8.490
7.701
7.697
7.378
7.317
7.308
7.302
7.298
7.293
7.282
7.260
7.255
7.253
7.236
7.234
7.151
7.106
7.086
7.052
7.031
5.301
3.162
2.253
1.00
1.00
1.00
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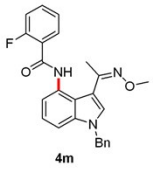
1.04
2.00
3.01
3.00
f1 (ppm)


F
O
NH
N
O
N
Bn

4m


77.477
77.160
76.842
138.983
136.395
133.007
132.004
131.925
131.008
130.249
129.082
128.128
126.824
124.491
124.369
116.476
112.948
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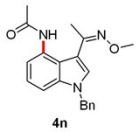
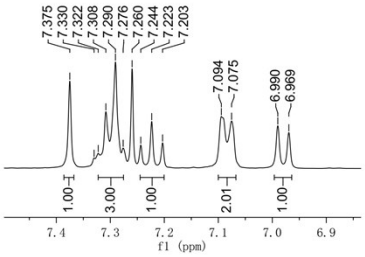
106.280
163.615
161.025
158.529
153.737
60.770
50.575
14.065
f1 (ppm)


NH
N
O
Bn

4n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7.322
7.308
7.290
7.276
7.260
7.244
7.223
7.203
7.094
7.075
6.990
6.969
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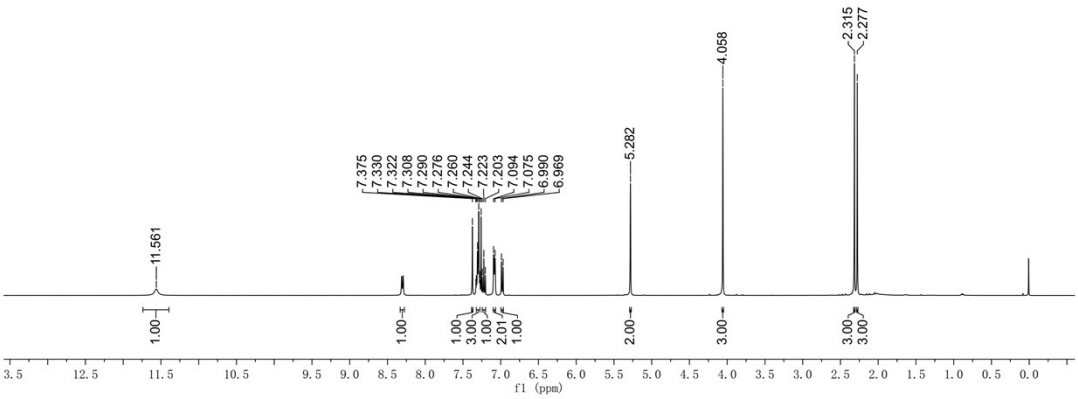
3.00
1.00
2.01
1.00
7.4
7.3
7.2
7.1
7.0
6.9
f1 (ppm)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7.322
7.308
7.290
7.276
7.260
7.244
7.223
7.203
7.094
7.075
6.990
6.969
5.282
4.058
2.315
2.277
1.00
1.00
1.00
3.00
1.00
2.01
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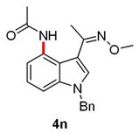
2.00
3.00
3.00
3.00
f1 (ppm)


NH
N
O
Bn

4n


77.478
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76.843
154.421
138.909
136.383
133.175
131.107
129.070
128.120
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115.825
112.740
112.413
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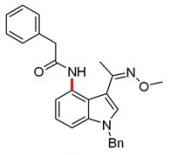
50.583
25.564
14.279
f1 (ppm)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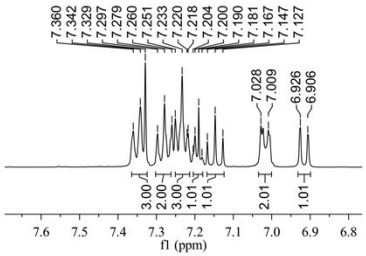
N
O
Bn

4o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7.297
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7.260
7.251
7.233
7.220
7.218
7.204
7.200
7.190
7.181
7.167
7.147
7.127
7.028
7.009
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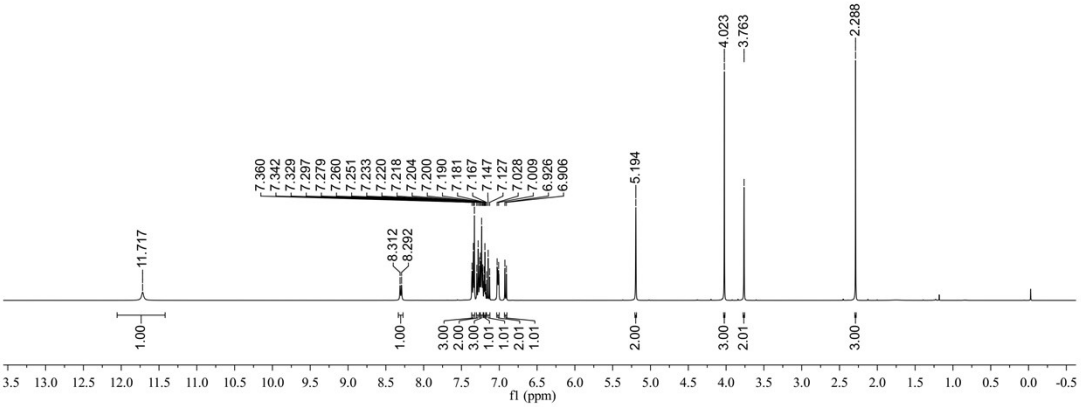
6.906
3.00
2.00
3.00
1.01
1.01
2.01
1.01
f1 (ppm)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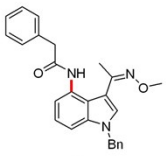
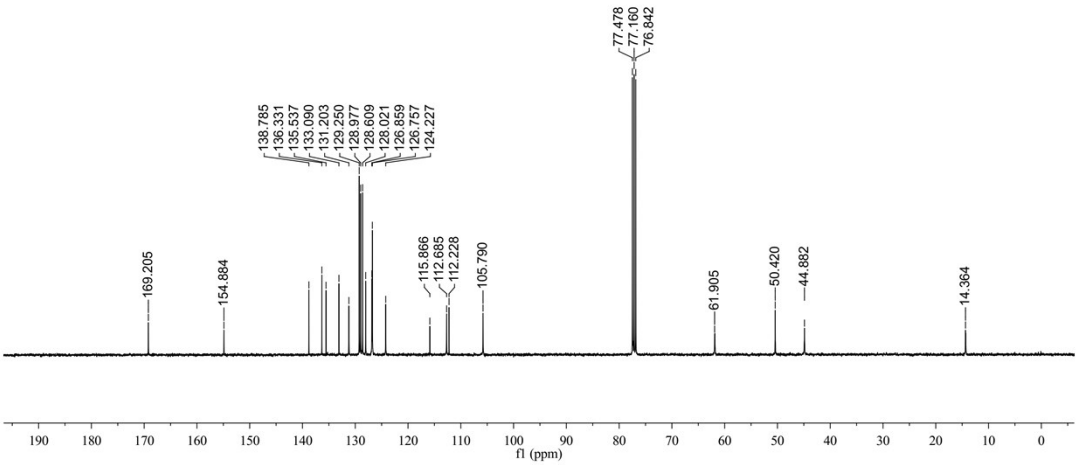
8.292
7.360
7.342
7.329
7.297
7.279
7.260
7.251
7.233
7.220
7.218
7.204
7.200
7.190
7.181
7.167
7.147
7.127
7.028
7.009
6.926
6.906
5.194
4.023
3.763
2.288
1.00
1.00
3.00
2.00
3.00
1.01
1.01
2.01
1.01
2.00
3.00
2.01
3.00
f1 (ppm)


NH
N
O
Bn

4o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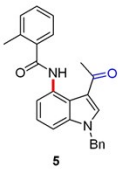
138.785
136.331
135.537
133.090
131.203
129.250
128.977
128.609
128.021
126.859
126.757
124.227
115.866
112.685
112.228
105.790
77.478
77.160
76.842
61.905
50.420
44.882
14.364
f1 (ppm)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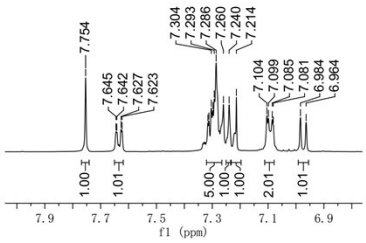
O
O
N
Bn

5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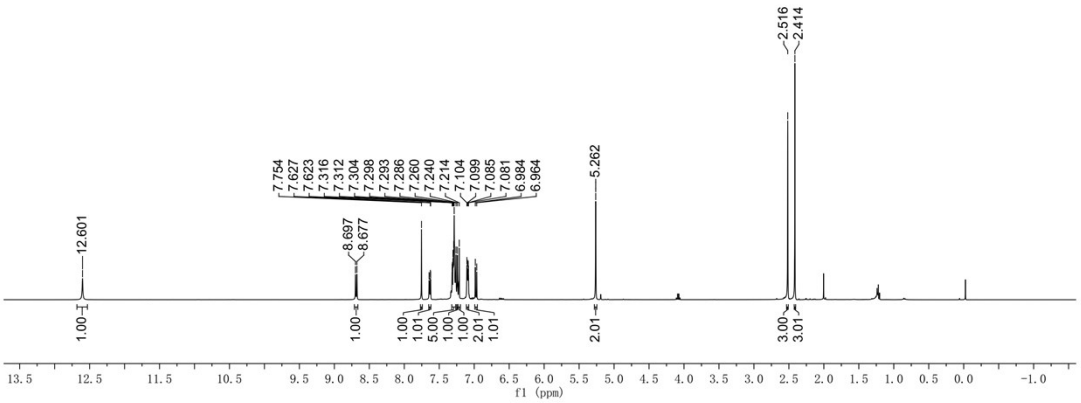
7.293
7.286
7.260
7.240
7.214
7.104
7.099
7.085
7.081
6.984
6.964
1.00
1.01
5.00
1.00
1.00
2.01
1.01
7.9
7.7
7.5
7.3
7.1
6.9
f1 (ppm)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7.627
7.623
7.316
7.312
7.304
7.298
7.293
7.286
7.260
7.240
7.214
7.104
7.099
7.085
7.081
6.984
6.964
5.262
2.516
2.414
1.00
1.00
1.01
5.00
1.00
1.00
2.01
1.01
2.01
3.00
3.01
13.5
12.5
11.5
10.5
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
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3.0
2.5
2.0
1.5
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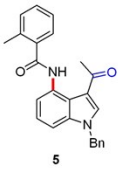
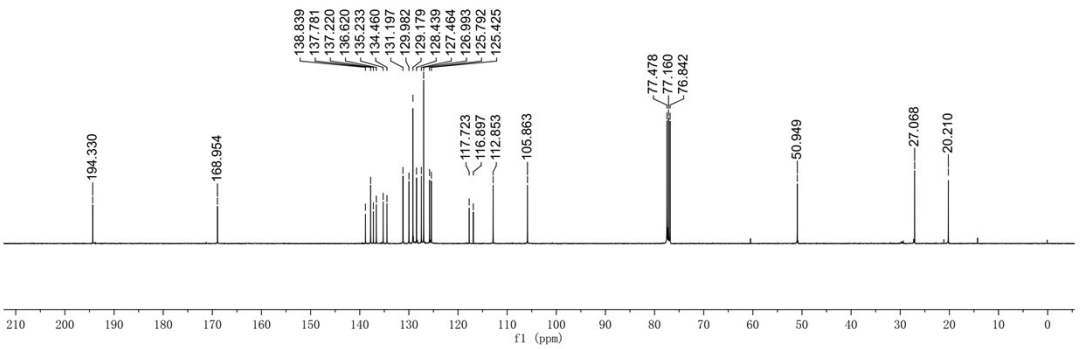
0.5
0.0
-1.0
f1 (ppm)


NH
O
O
N
Bn

5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137.781
137.220
136.620
135.233
134.460
131.197
129.982
129.179
128.439
127.464
126.993
125.792
125.425
117.723
116.897
112.853
105.863
77.478
77.160
76.842
50.949
27.068
20.210
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)