***Supporting Information* for**

Formal [4+1] Cycloaddition of o-Quinone Methides: Facile Synthesis of Dihydrobenzofurans

Xiantao Lei,[a,b] Chun-Huan Jiang,[a] Xiaoan Wen,[a] Qing-Long Xu*[a] and Hongbin Sun*[a]

[a] *Jiangsu Key Laboratory of Drug Discovery for Metabolic Diseases and State Key Laboratory of Natural Medicines, Center of Drug Discovery, China Pharmaceutical University, 24 Tongjia Xiang, Nanjing 210009, China*

[b] *State Key Laboratory of Drug Research, Shanghai Institute of Materia Medica, Chinese Academy of Science, 555 Zuchongzhi Road, Shanghai 201203, China*

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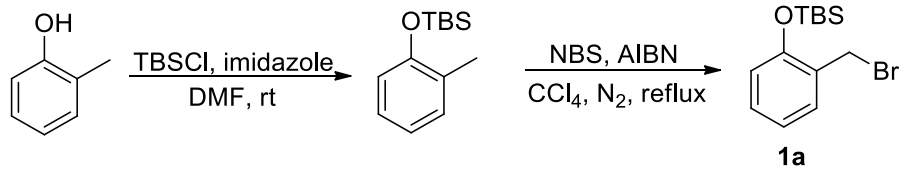
General Information

^{1}H and ^{13}C NMR spectra were recorded on an ACF* 300Q Bruker or ACF* 500Q Bruker spectrometer. Low- and high-resolution mass spectra (LRMS and HRMS) were recorded in electron impact mode. The mass analyzer type used for the HRMS measurements was TOF. Reactions were monitored by TLC on silica gel 60 F254 plates (Qingdao Ocean Chemical Company, China). Column chromatography was carried out on silica gel (200-300 mesh, Qingdao Ocean Chemical Company, China). Data for ^{1}H NMR are recorded as follows: chemical shift (δ, ppm), multiplicity (s = singlet, d = doublet, t = triplet, m = multiplet or unresolved, br s = broad singlet, coupling constant(s) in Hz, integration). Data for ^{13}C NMR are reported in terms of chemical shift (δ, ppm).

Synthesis of (2-(bromomethyl)phenoxy)(tert-butyl)dimethylsilane (1a)[1]



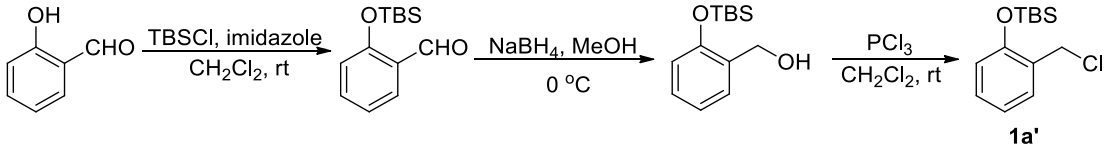
1a

To a solution of *o*-cresol (541 mg, 5 mmol) in DMF(5 mL) was added *tert*-butyldimethylsilanechloride (TMSCl) (829 mg, 5.5 mmol) followed by imidazole (749 mg, 11 mmol). Then the reaction mixture was stirred at room temperature overnight. The reaction was partitioned in water (5 mL) and EtOAc (15 mL). The organic layer was separated, washed with water (5 mL), dried over anhydrous Na_2SO_4, filtrated and concentrated under reduced pressure. The residue was purified by flash chromatography on silica gel (petroleum ether) to yield colorless oil (505 mg, 45% yield).

The silylated phenol (505 mg, 2.27 mmol) was solved in CCl_4 (10 mL), and N-bromosuccinimide (NBS) (404 mg, 2.27 mmol) and AIBN (56 mg, 0.34 mmol) were added in one portion. The solution was purged with N_2 and refluxed overnight. The reaction was allowed to cool to room temperature and filtered through a pad of SiO_2, furnished by hexane. The filtrate was concentrated under reduced pressure and

purified by flash chromatography on silica gel (hexane), giving colorless oil **1a** (343 mg, 50% yield). ^{1}H NMR (300 MHz, $CDCl_3$) δ 7.34 (dd, *J* = 1.6, 7.5 Hz, 1H), 7.19 (dt, *J* = 1.7, 8.0 Hz, 1H), 6.92 (dt, *J* = 0.9, 7.5 Hz, 1H), 6.81 (d, *J* = 8.1 Hz, 1H), 4.53 (s, 2H), 1.06 (s, 9H), 0.29 (s, 6H).

Synthesis of (2-(bromomethyl)phenoxy)(tert-butyl)dimethylsilane (1a')[1]

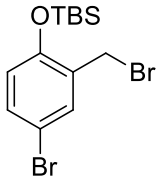


To a solution of 2-hydroxybenzaldehyde (1.22 g , 10 mmol) and imidazole (1.36 g, 20 mmol) in CH_2Cl_2 (20 mL), a solution of TBSCl (3.01 g, 20 mmol) in CH_2Cl_2 (10 mL) was added dropwise. After the addition, the reaction mixture was stirred at room temperature overnight. The reaction was partitioned in water (15 mL) and EtOAc (50 mL). The organic layer was separated, washed with water (5 mL), dried over anhydrous Na_2SO_4, filtrated and concentrated under reduced pressure. The crude oil was used without purification.

The crude oil was solved in MeOH (20 mL). $NaBH_4$ (378 mg, 10 mmol) was added in portions carefully at 0 ^{o}C. After the reaction mixture was stirred at 0 ^{o}C for 4 h, MeOH was evaporated in vacuo. A combined solution of saturated NH_4Cl (15 mL) and EtOAc (15 mL) was added, two phases were separated, and the aqueous layer was extracted with EtOAc (3 × 20 mL). The combined organic layers were washed with brine, dried over anhydrous Na_2SO_4 and concentrated in vacuo to give yellow oil. The crude oil was used without purification.

To an ice cooled solution the crude oil in dry CH_2Cl_2 (30 mL), PCl_3 (960 μL, 11 mmol) was added dropwise. After the addition, the solution was stirred at 0 ^{o}C for 4 h and was partitioned in brine (10 mL) and CH_2Cl_2 (30 mL). The organic layer was separated, dried over Na_2SO_4, filtrated and concentrated under reduce pressure. The residue was purified by flash chromatography on silica gel (petroleum ether) and yielded colorless oil **1a'** (464 mg, 18% yield over three steps). ^{1}H NMR (300 MHz,

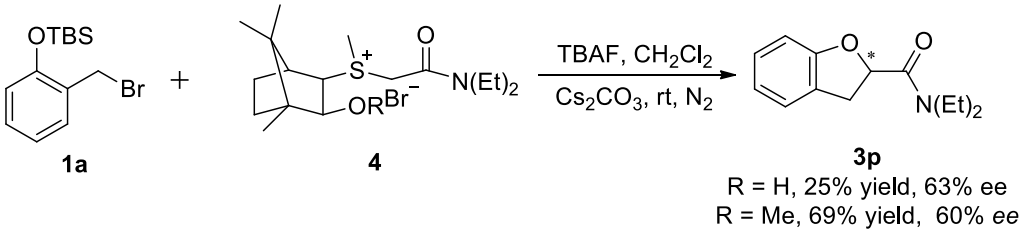
$CDCl_3$) δ 7.36 (dd, *J* = 7.5, 1.4 Hz, 1H), 7.24-7.17 (m, 1H), 6.94 (t, *J* = 7.5 Hz, 1H), 6.83 (d, *J* = 8.1 Hz, 1H), 4.63 (s, 2H), 1.05 (s, 9H), 0.28 (s, 6H).



(4-bromo-2-(bromomethyl)phenoxy)(tert-butyl)dimethylsilane

1b, colorless oil, 1.09 g, 49% yield over three steps. Prepared according to the procedure of **1a'** using 5-bromo-2-hydroxybenzaldehyde and PBr_3. ^{1}H NMR (300 MHz, $CDCl_3$) δ 7.48 (d, *J* = 2.1 Hz, 1H), 7.30 (dd, *J* = 8.7, 2.2 Hz, 1H), 6.72 (d, *J* = 8.7 Hz, 1H), 4.47 (s, 2H), 1.08 (s, 9H), 0.32 (s, 6H). ^{13}C NMR (75 MHz, $CDCl_3$) δ 153.0, 133.7, 132.6, 130.6, 120.2, 113.1, 27.8, 25.8, 18.3, -4.1.

General Procedure for Synthesis Chiral 2,3-Dihydrobenzofuran.

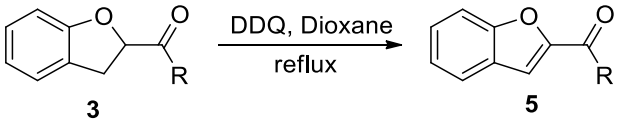


A mixture of O-silylated phenol **1a** (84.0 mg, 0.28 mmol), chiral campor sulfonium salt (**4a,** R = H, 0.42 mmol or **4b,** R = Me, 0.42 mmol) and Cs_2CO_3 (136 mg, 0.42 mmol) in dry CH_2Cl_2 (5 mL) was stirred at room temperature under N_2. Then TBAF (1.0 M in THF, 1.25 mL) was added dropwise. After the addition, the mixture was stirred at room temperature for 24 h. The reaction was concentrated under reduced pressure and purified by flash chromatography on silica gel (petroleum ether : ethyl acetate = 10:1-5:1) to afford **3p**. The absolute configuration of **3p** is not assigned.

R = H, 25% yield, 63% ee. [Daicel CHIRALPAK IC (0.46 cm x 25 cm); *n*-hexanes/*i*-propanol = 90/10; flow rate = 1.0 mL/min; detection wavelength = 230 nm; t_R = 28.05 (minor), t_R = 33.42 (major) min.]

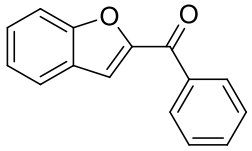
R = Me, 69% yield, 60% ee, $[\alpha]_D^{25}$ = -31.8 (c = 0.33, CH_3OH). [Daicel CHIRALPAK IC (0.46 cm x 25 cm); *n*-hexanes/*i*-propanol = 90/10; flow rate = 1.0 mL/min; detection wavelength = 230 nm; t_R = 27.36 (minor), t_R =32.54 (major) min.]

General Procedure for Synthesis of 5.

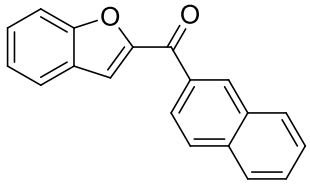


3 **5**

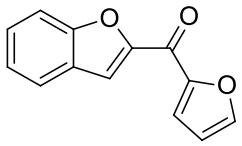
DDQ (4.0 equiv.) was added to a solution of **3** in dry dioxane. Then the reaction mixture was stirred at reflux for 24 h. Filtration and concentration in vacuo gave crude product, which was purified by flash chromatography on silica gel using petroleumether and ethyl acetate to give the product **5**.



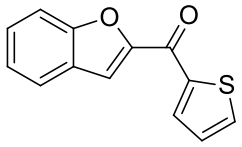
5a, [2] yellow solid, 81% yield, m.p. 83-85 ^{o}C. ^{1}H NMR (300 MHz, $CDCl_3$) δ 8.05 (d, *J* = 8.0 Hz, 2H), 7.73 (d, *J* = 7.9 Hz, 1H), 7.63 (dd, *J* = 10.1, 4.4 Hz, 2H), 7.58-7.47 (m, 4H), 7.32 (dd, *J* = 16.4, 9.1 Hz, 1H).



5k, white solid, 83% yield, m.p. 96-97.5 ^{o}C. ^{1}H NMR (300 MHz, $CDCl_3$) δ 8.62 (s, 1H), 8.10 (d, *J* = 8.5 Hz, 1H), 8.00 (t, *J* = 8.7 Hz, 2H), 7.93 (d, *J* = 7.9 Hz, 1H), 7.76 (d, *J* = 7.8 Hz, 1H), 7.68 (d, *J* = 8.5 Hz, 1H), 7.61 (q, *J* = 8.7 Hz, 3H), 7.53 (t, *J* = 7.6 Hz, 1H), 7.36 (t, *J* = 7.5 Hz, 1H).

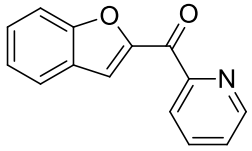


5l,[3] yellow solid, 56% yield, m.p. 66-67 ^{o}C. ^{1}H NMR (300 MHz, $CDCl_3$) δ 7.91 (s, 1H), 7.77 (d, *J* = 7.1 Hz, 2H), 7.71 (d, *J* = 3.4 Hz, 1H), 7.65 (d, *J* = 8.4 Hz, 1H), 7.51 (t, *J* = 7.8 Hz, 1H), 7.35 (t, *J* = 7.5 Hz, 1H), 6.72-6.63 (m, 1H).

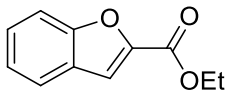


5m,[4] white solid, 81% yield, m.p. 59-61 ^{o}C. ^{1}H NMR (300 MHz, $CDCl_3$) δ 8.32 (d, *J*

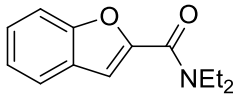
= 3.9 Hz, 1H), 7.77-7.71 (m, 3H), 7.64 (d, *J* = 8.4 Hz, 1H), 7.50 (t, *J* = 8.4 Hz, 1H), 7.34 (t, *J* = 8.1 Hz, 1H), 7.25 (d, *J* = 9.0 Hz, 1H).



5n,[5] white solid, 53% yield, m.p. 79-80.5 ^{o}C. ^{1}H NMR (300 MHz, $CDCl_3$) δ 8.79 (d, *J* = 4.6 Hz, 1H), 8.48 (s, 1H), 8.24 (d, *J* = 7.9 Hz, 1H), 7.93 (t, *J* = 7.5 Hz, 1H), 7.78 (d, *J* = 7.8 Hz, 1H), 7.66 (d, *J* = 8.6 Hz, 1H), 7.52 (dd, *J* = 16.6, 8.7 Hz, 2H), 7.37-7.29 (m, 2H).



5o,[6] colorless oil, 75% yield. ^{1}H NMR (300 MHz, $CDCl_3$) δ 7.67 (d, *J* = 7.8 Hz, 1H), 7.58 (d, *J* = 8.4 Hz, 1H), 7.52 (s, 1H), 7.43 (t, *J* = 7.2 Hz, 1H), 7.29 (t, *J* = 7.2 Hz, 1H), 4.43 (q, *J* = 7.2 Hz, 2H), 1.42 (t, *J* = 7.2Hz, 3H).



5p,[7] yellow oil, 69% yield. ^{1}H NMR (300 MHz, $CDCl_3$) δ 7.66 (d, *J* = 7.7 Hz, 1H), 7.53 (d, *J* = 8.2 Hz, 1H), 7.40 (t, *J* = 7.5 Hz, 1H), 7.33-7.25 (m, 2H), 3.62 (m, 4H), 1.32 (m, 6H).

References:

[1] Izquierdo, J.; Orue, A.; Scheidt, K. A. *J. Am. Chem. Soc.* **2013**, *135*, 10634.

[2] Carrër, A.; Brinet, D.; Florent, J. C.; Rousselle, P.; Bertounesque, E. *J. Org. Chem.* **2012**, *77*, 1316.

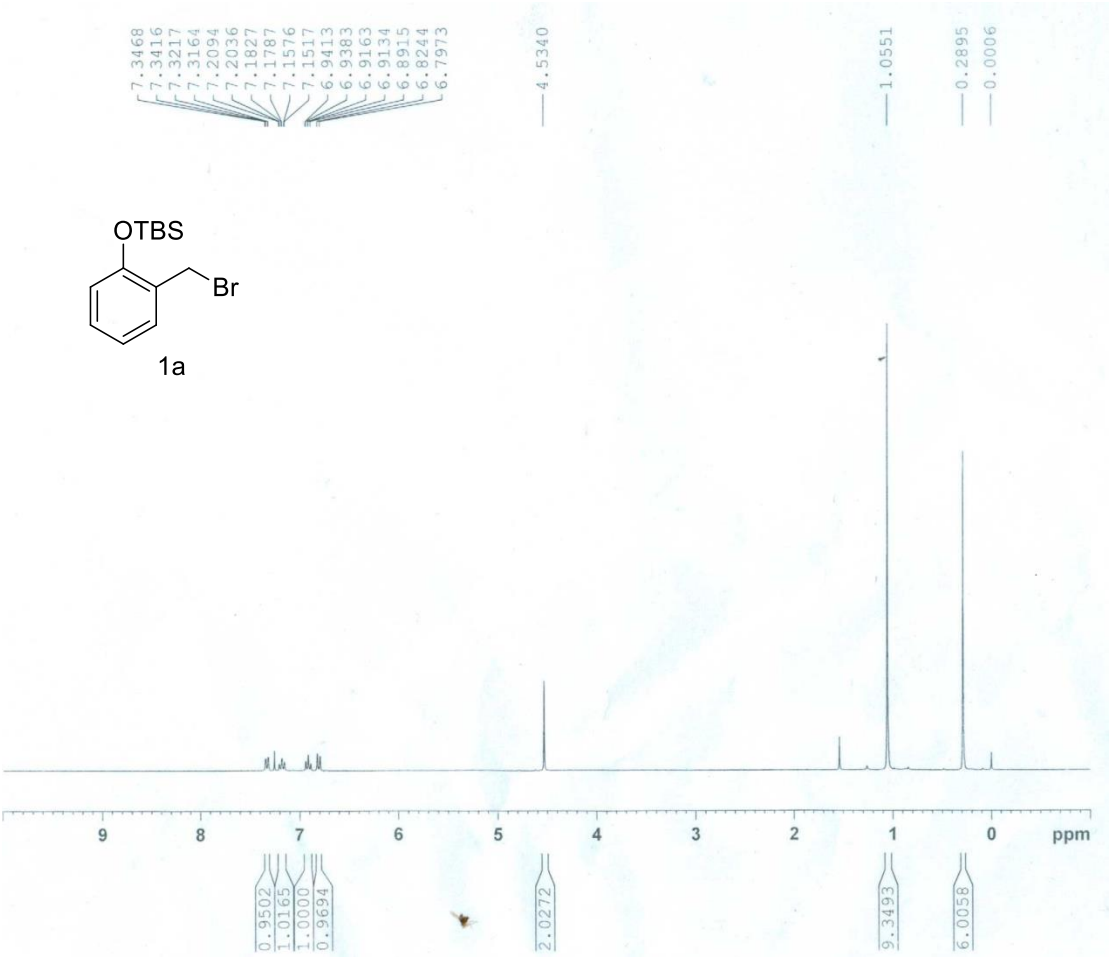
[3] Magdesieva, N. N.; Chovnikova, N. G. *Zh. Org. Khim*. **1979**, *15*, 2402.

[4] Rott, G. M.; Shevchenko, L. I.; Amoryzanova, O. A.; Savina, E. P.; Deeva, V. S.; Skvortsov, V. G.; Trofimov, F. A. Khimiko-Farmatsevticheskii Zhurnal **1998**, *32*, 28.

[5] Binon, F.; Inion, H. *Chim. Ther*. **1967**, *2*, 113.

[6] Song, W.-J.; Yang, X.-D.; Zeng, X.-H.; Xu, X.-L.; Zhang, G.-L.; Zhang, H.-B. *RSC Advances* **2012**, *2*, 4612.

[7] Papa, D.; Schwenk, E.; Villani, F.; Klingsberg, E. *J. Am. Chem. Soc*. **1950**, *72*, 3885.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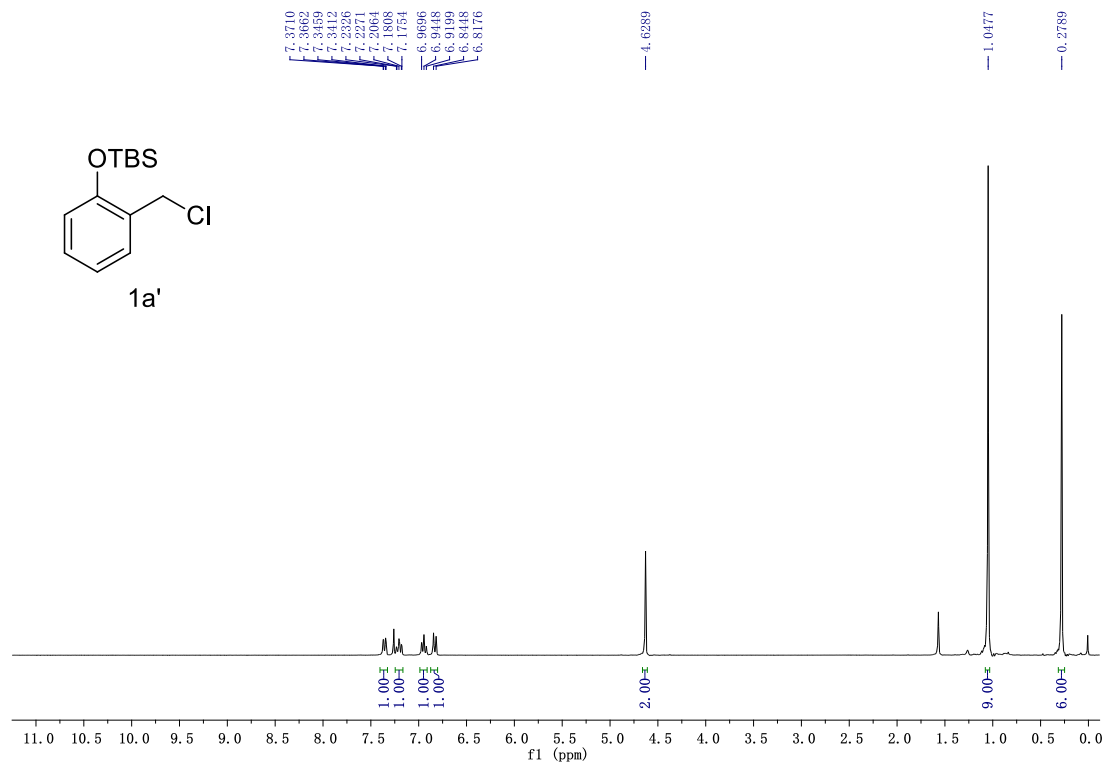
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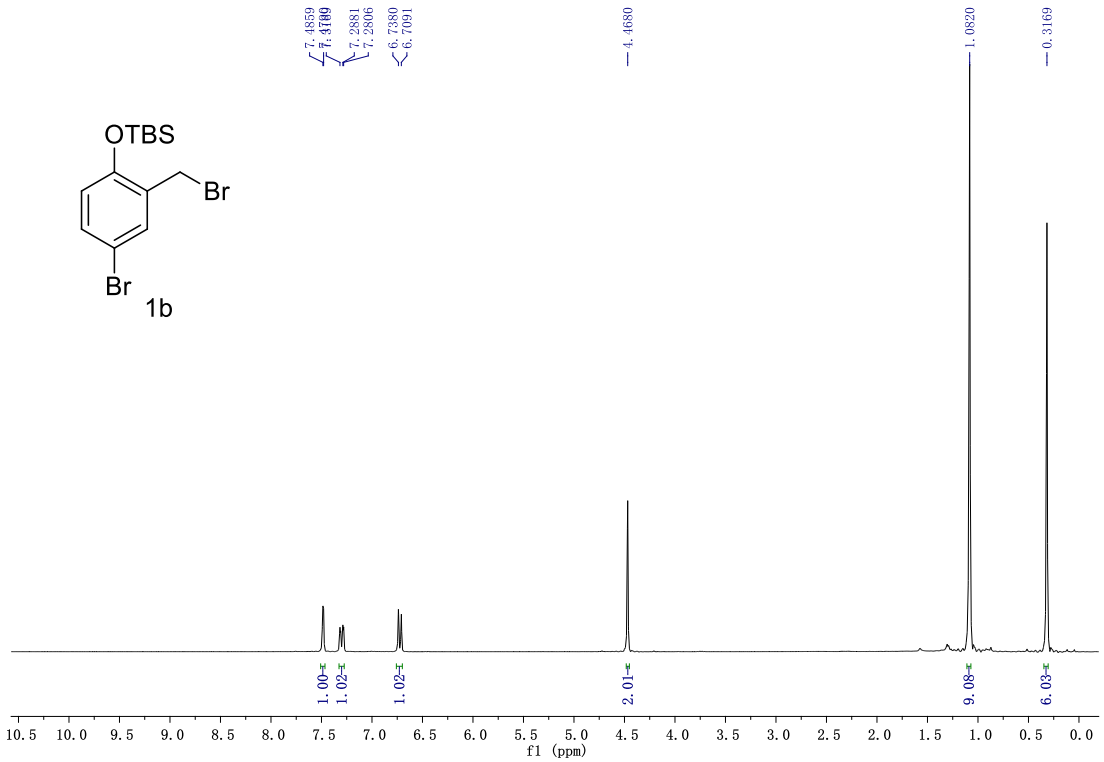
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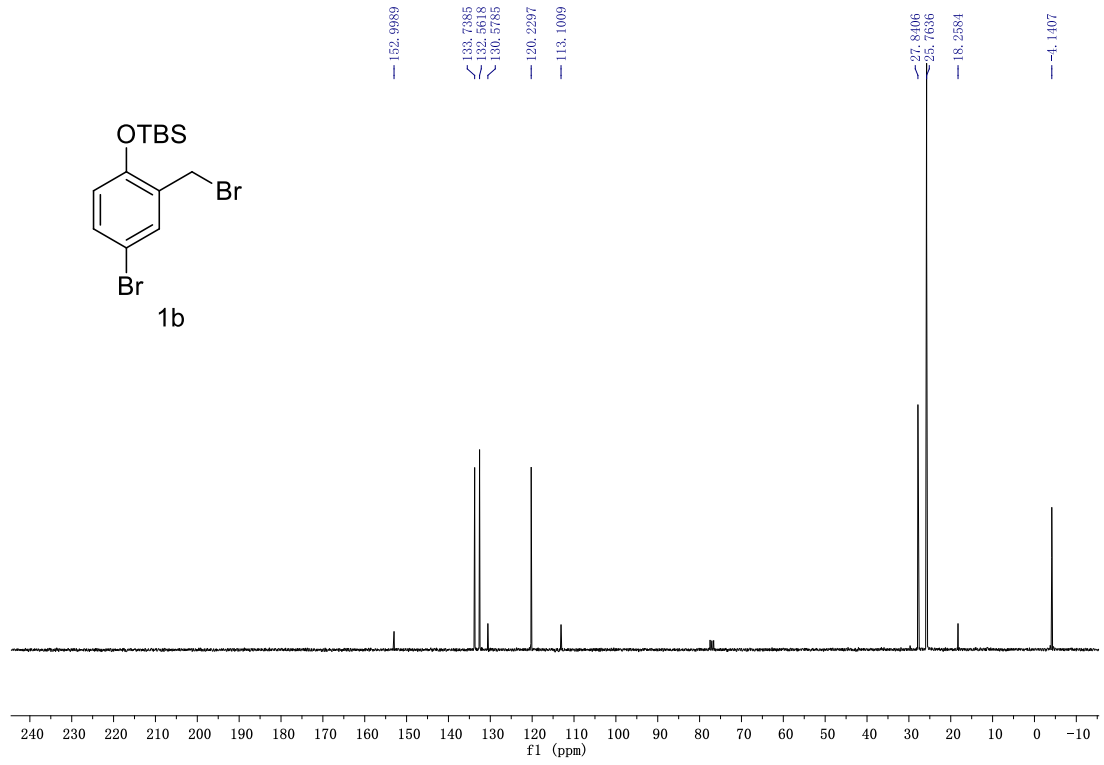
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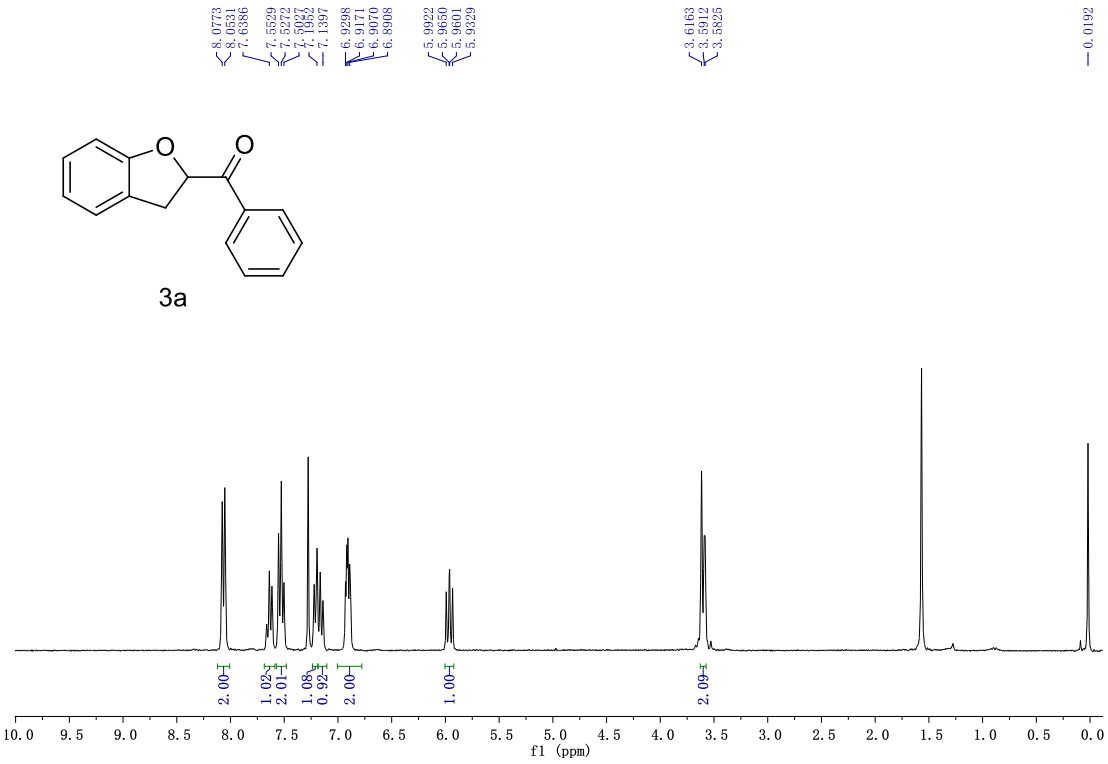
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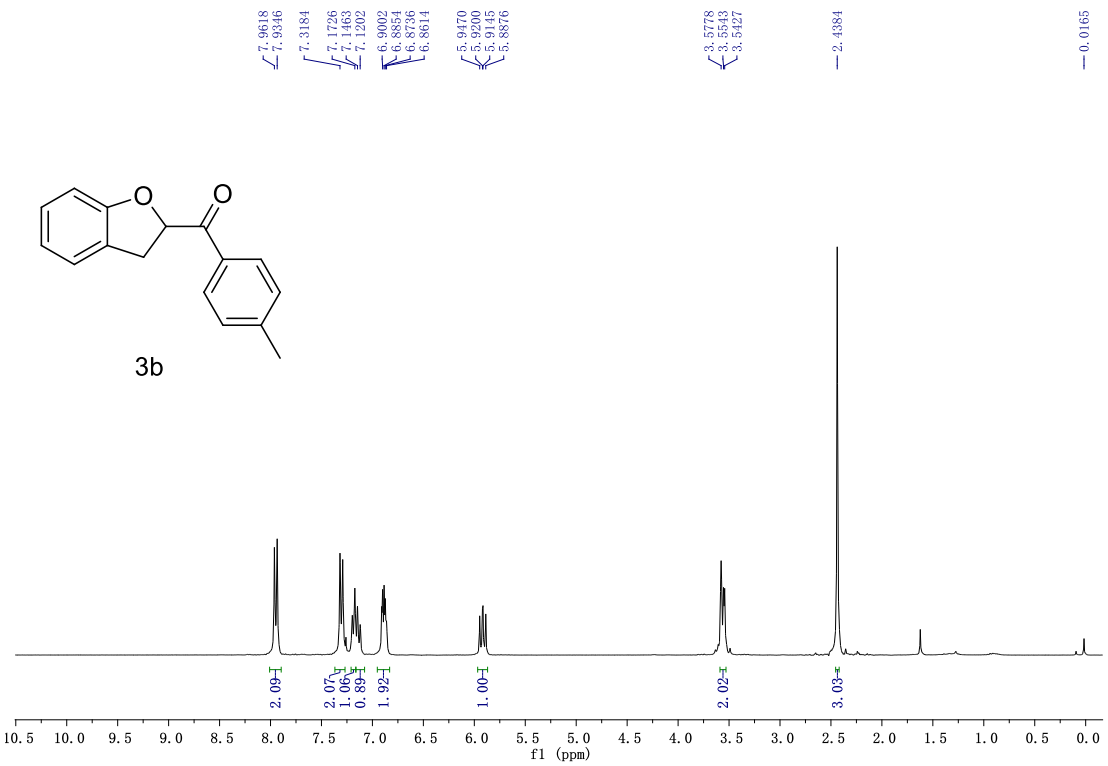
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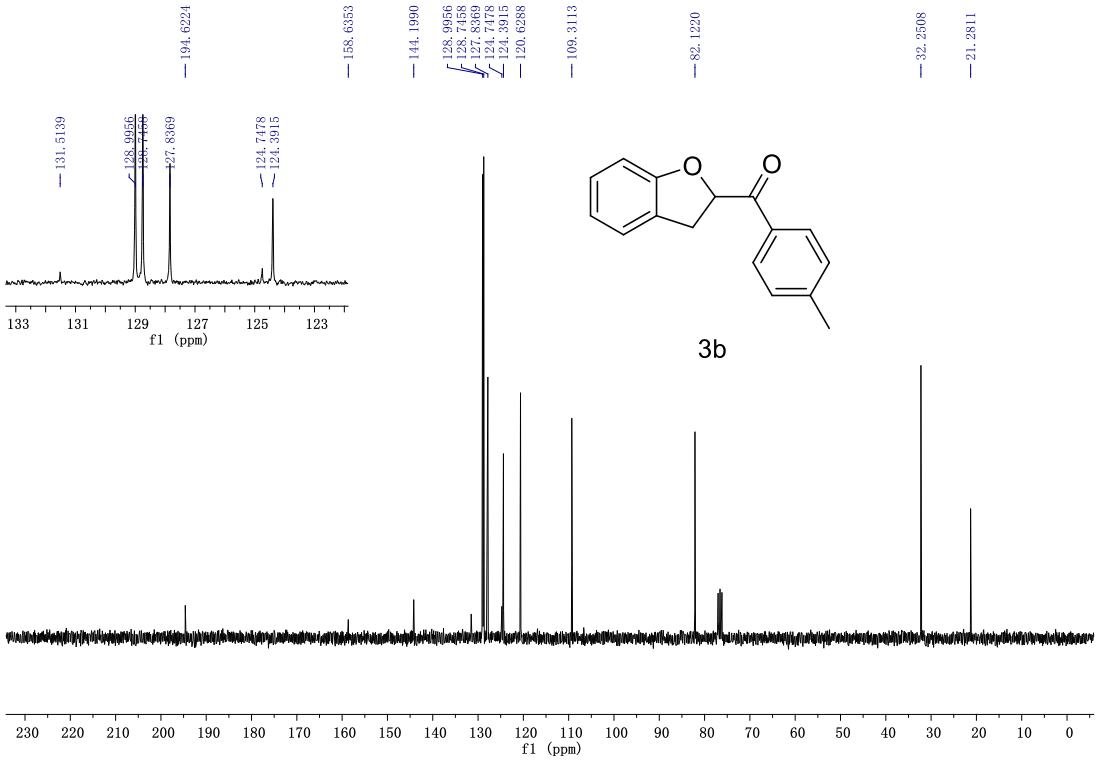
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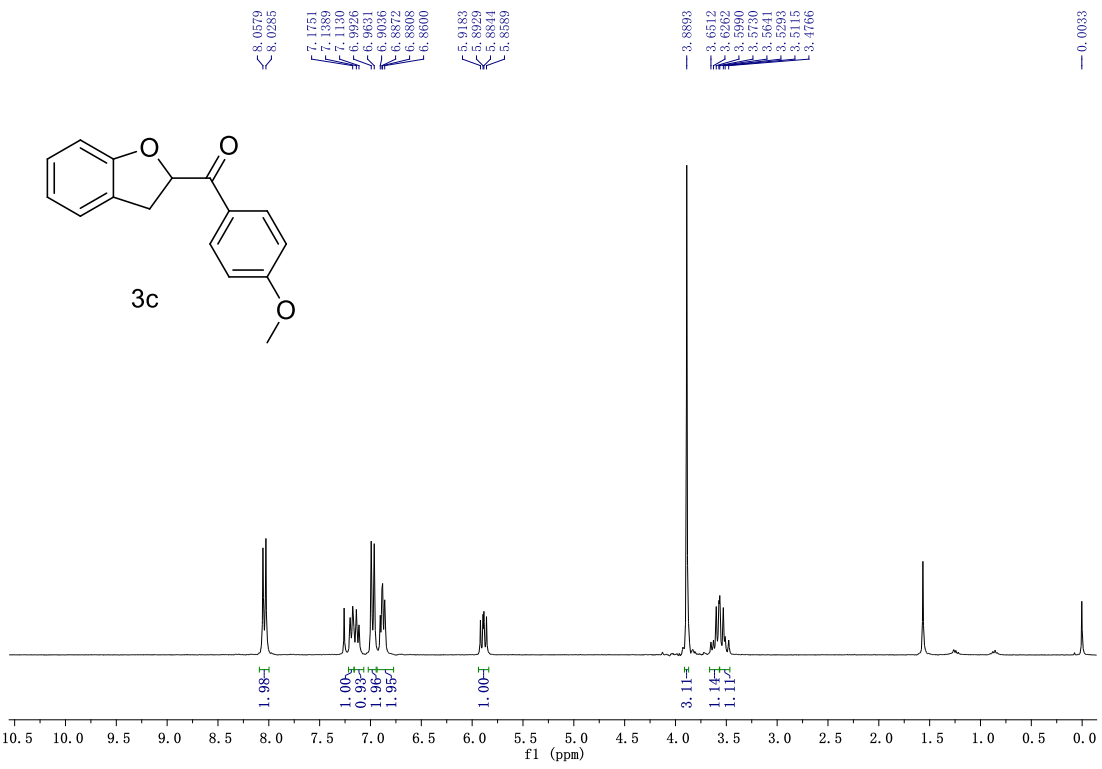
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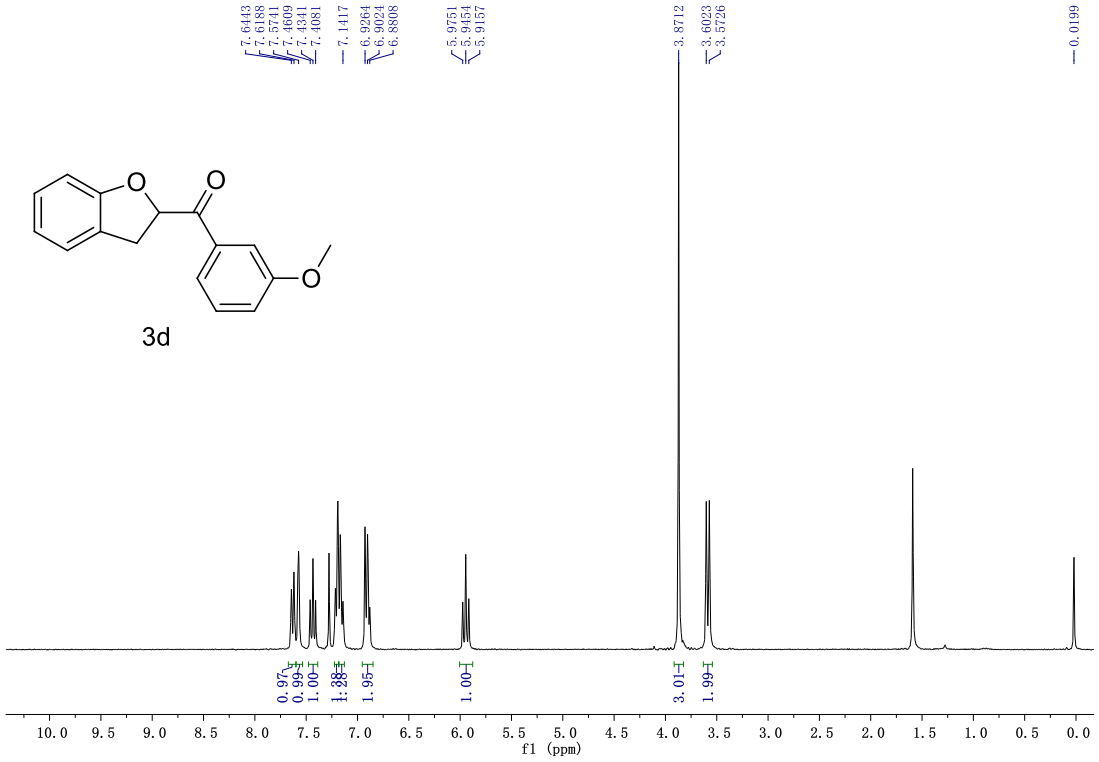
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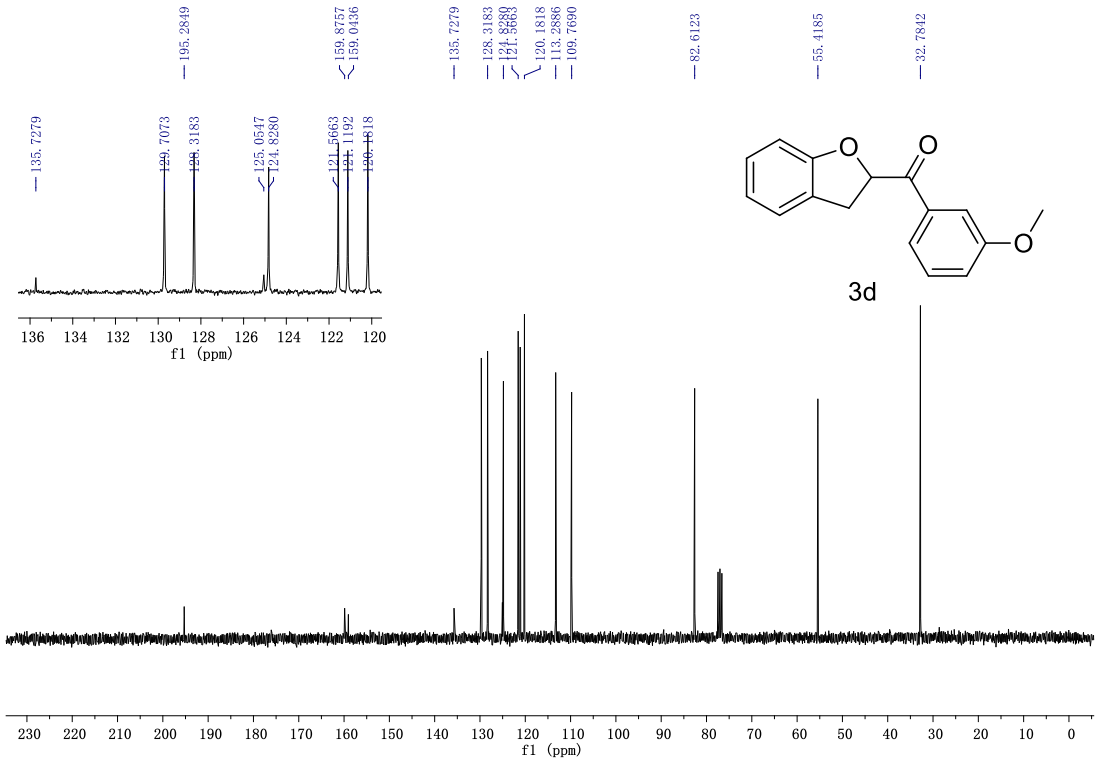
1.00
1.88
1.95
1.00
3.01
1.99
10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)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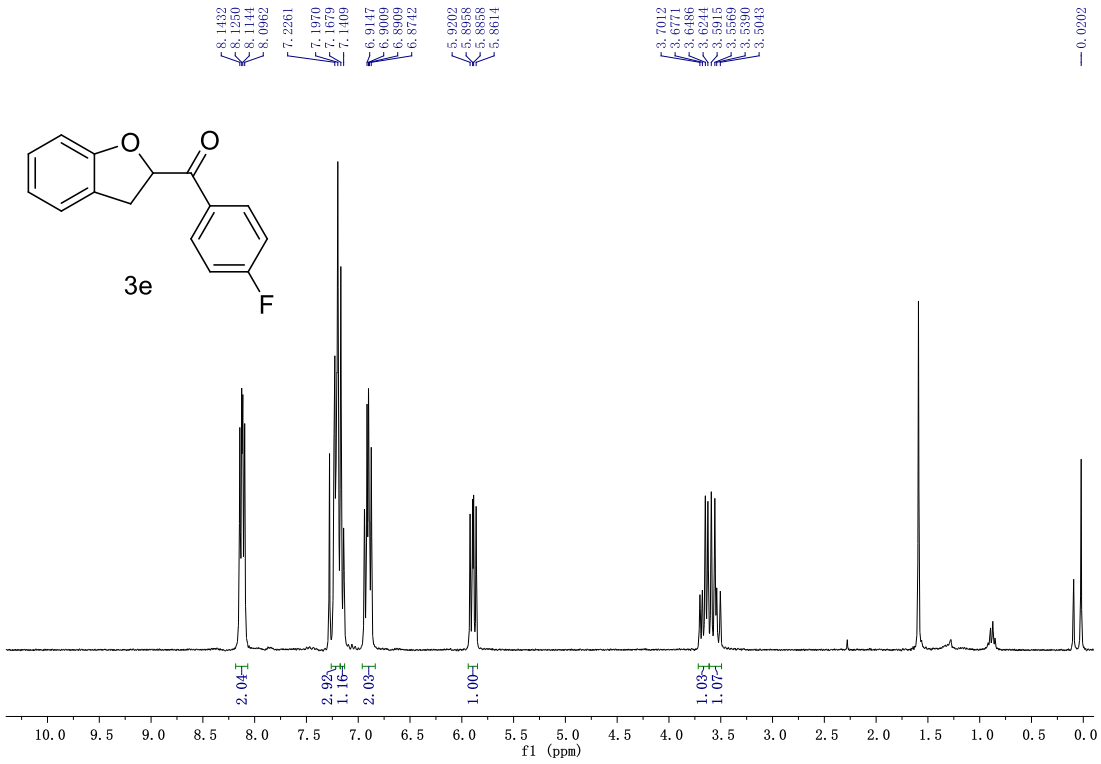
159.8757
159.0436
135.7279
128.3183
121.5663
121.1192
120.1818
113.2886
109.7690
82.6123
55.4185
32.7842
135.7279
129.7073
128.3183
125.0547
124.8280
121.5663
121.1192
120.1818
136 134 132 130 128 126 124 122 120
f1 (ppm)
O
O
O
3d
230 220 210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)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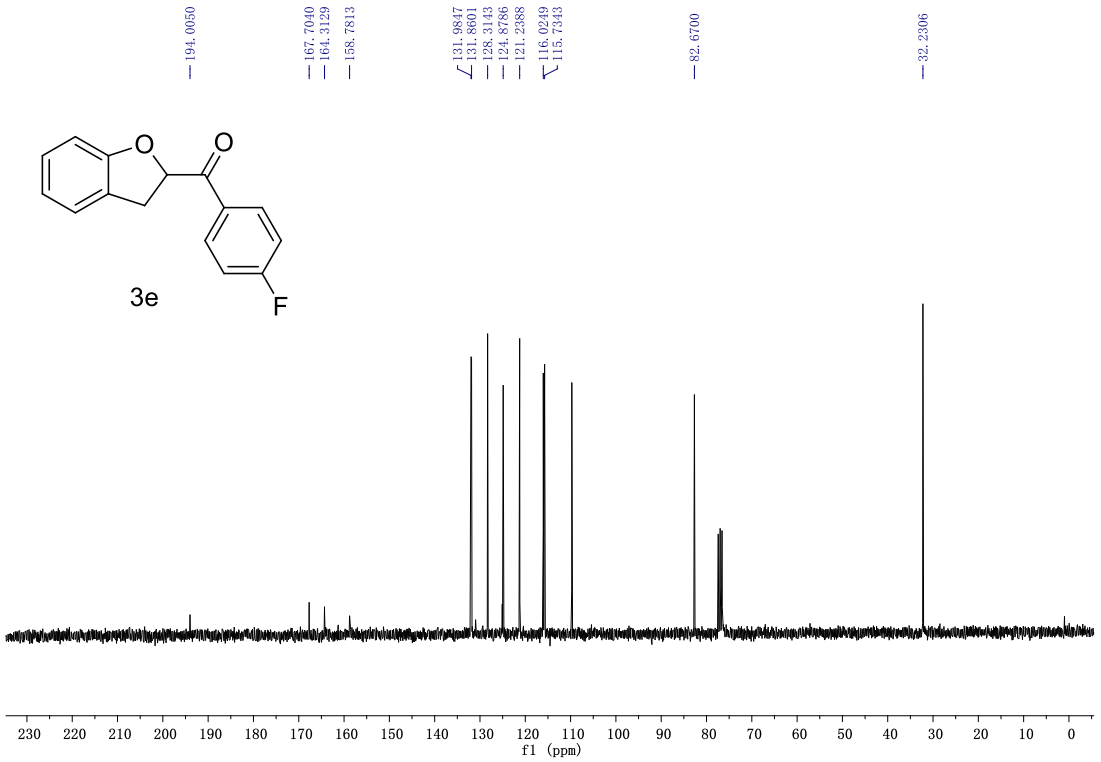
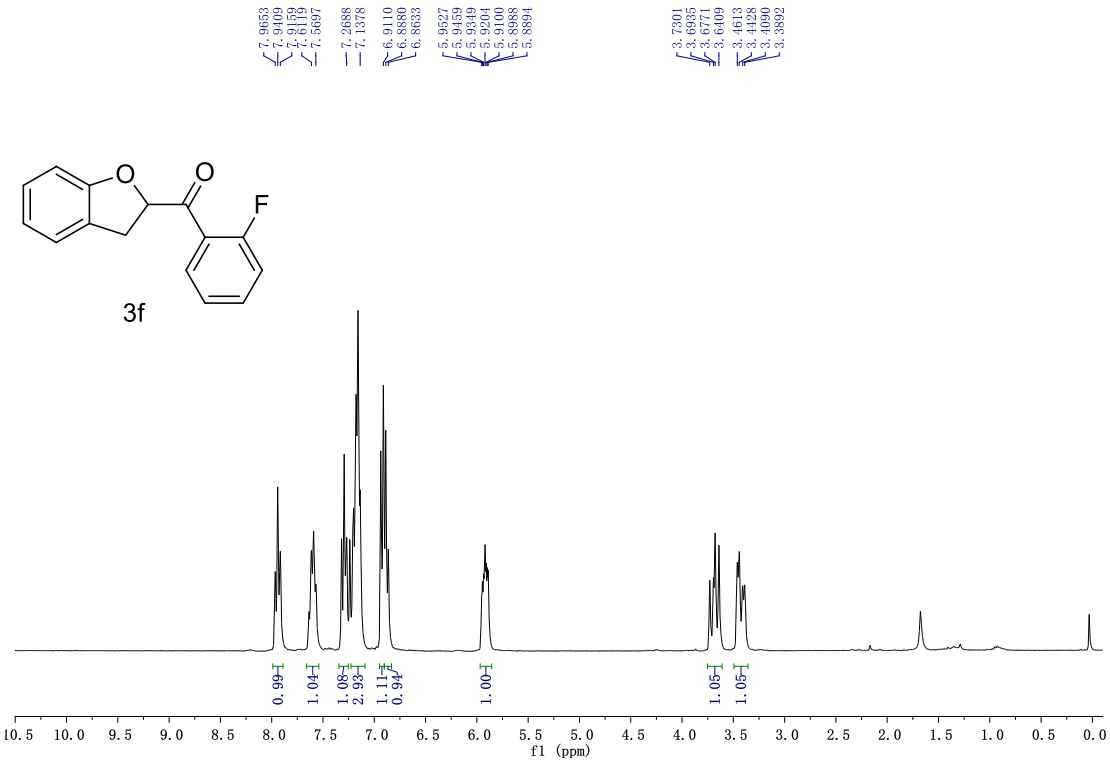
8.1250
8.1144
8.0962
7.2261
7.1970
7.1679
7.1409
6.9147
6.9009
6.8909
6.8742
5.9202
5.8958
5.8858
5.8614
3.7012
3.6771
3.6486
3.6244
3.5915
3.5569
3.5390
3.5043
0.0202
3e
F
2.04
2.92
1.16
2.03
1.00
1.03
1.07
10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)


194.0050
167.7040
164.3129
158.7813
131.9847
131.8601
128.3143
124.8786
121.2388
116.0249
115.7343
82.6700
32.2306
3e
F
230 220 210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)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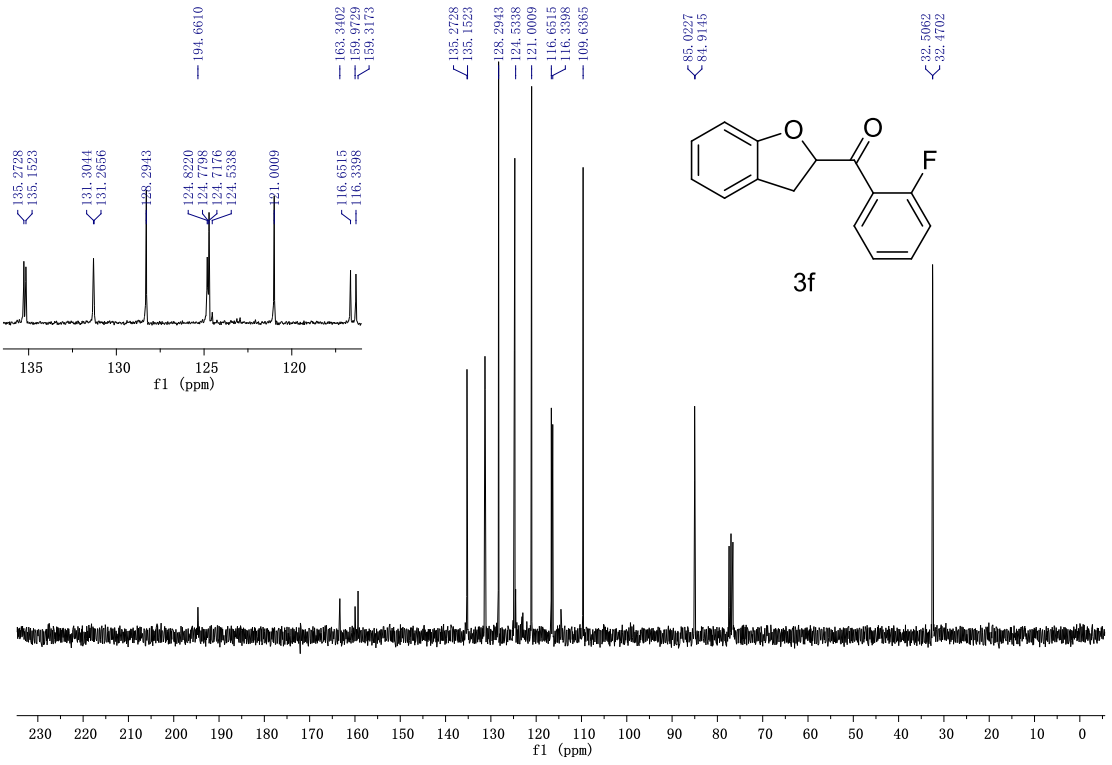
7.9409
7.9159
7.6119
7.5697
7.2688
7.1378
6.9110
6.8880
6.8633
5.9527
5.9459
5.9349
5.9204
5.9100
5.8988
5.8894
3.7301
3.6935
3.6771
3.6409
3.4613
3.4428
3.4090
3.3892
O
O
F
3f
0.99
1.04
1.08
2.93
1.11
0.94
1.00
1.05
1.05
f1 (ppm)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159.9729
159.3173
135.2728
135.1523
128.2943
124.5338
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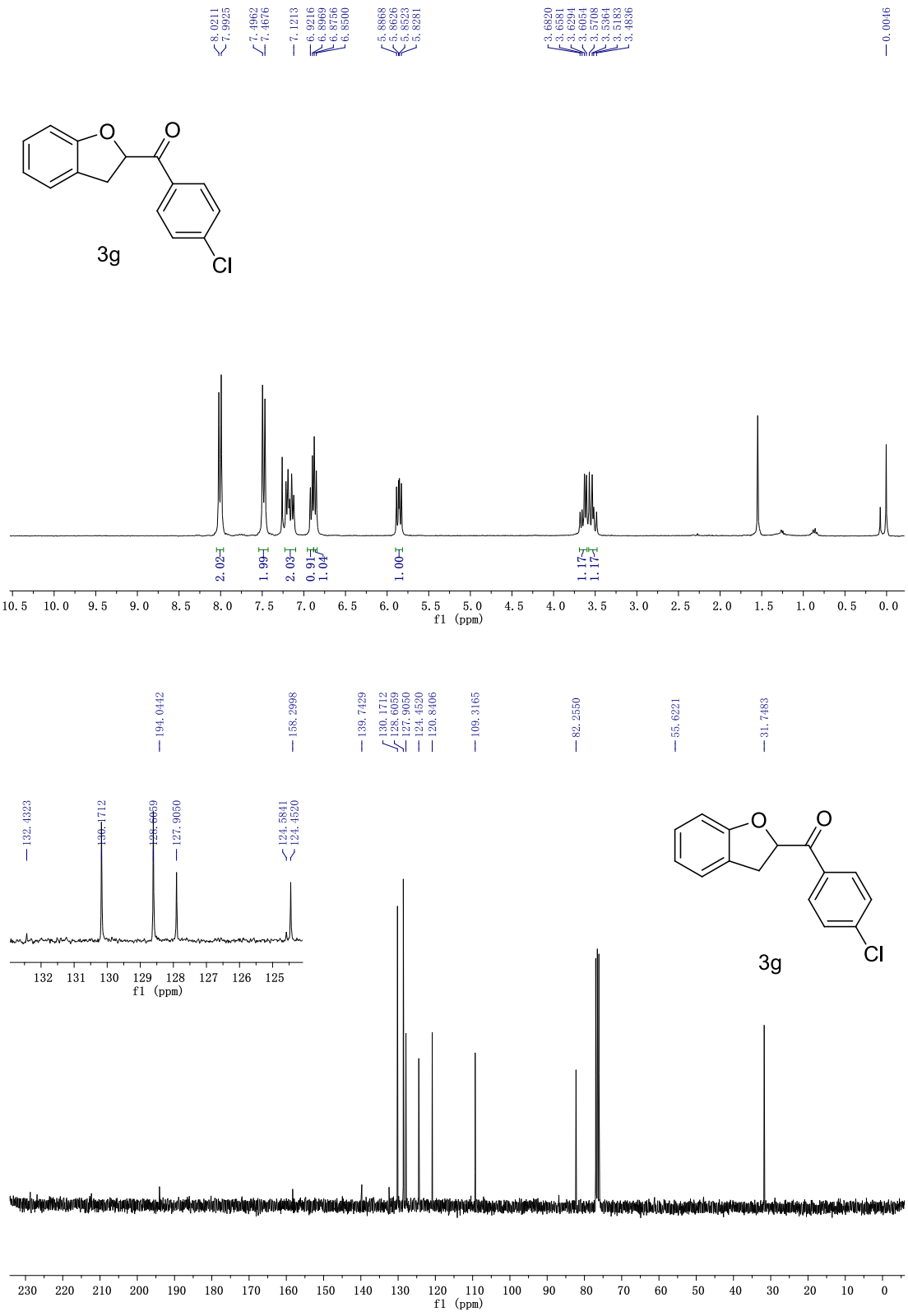
116.6515
116.3398
109.6365
85.0227
84.9145
32.5062
32.4702
135.2728
135.1523
131.3044
131.2656
128.2943
124.8220
124.7798
124.7176
124.5338
121.0009
116.6515
116.3398
O
O
F
3f
f1 (ppm)
f1 (ppm)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7.4962
7.4676
7.1213
6.9216
6.8969
6.8756
6.8500
5.8868
5.8626
5.8523
5.8281
3.6820
3.6581
3.6294
3.6054
3.5708
3.5364
3.5183
3.4836
0.0046
O
O
Cl
3g
2.02
1.99
2.03
0.91
1.04
1.00
1.17
1.17
f1 (ppm)
194.0442
158.2998
139.7429
130.1712
128.6059
127.9050
124.4520
120.8406
109.3165
82.2550
55.6221
31.7483
132.4323
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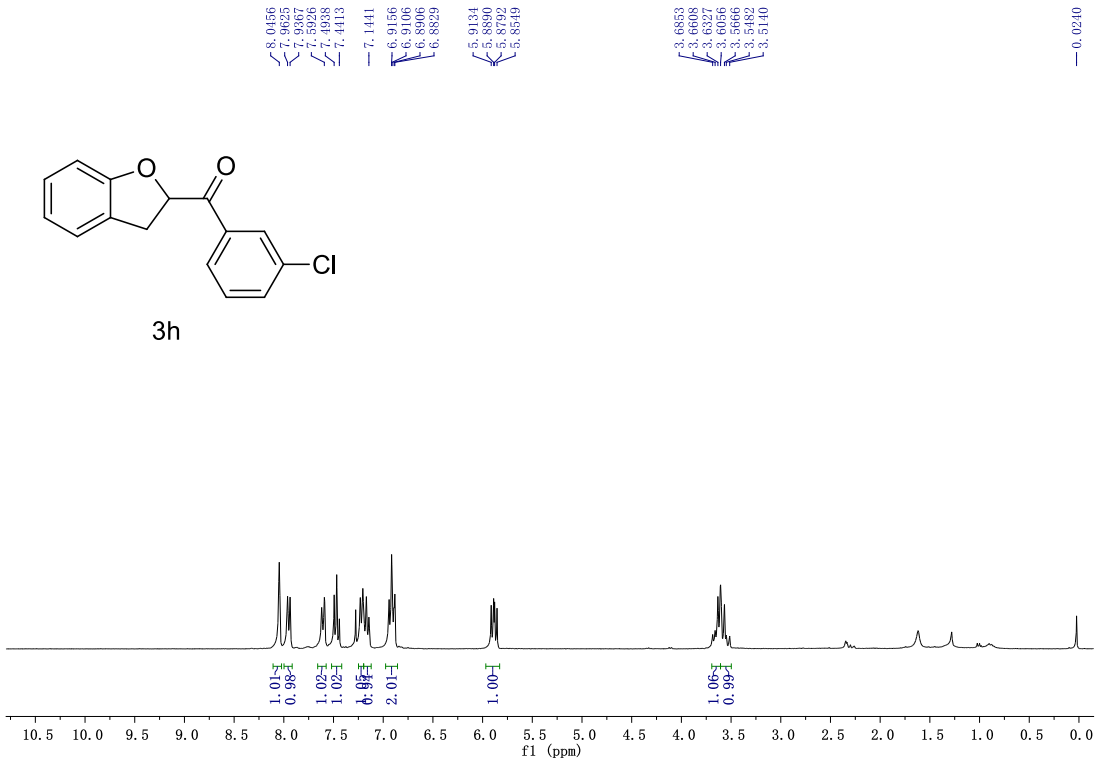
128.6059
127.9050
124.5841
124.4520
f1 (ppm)
O
O
Cl
3g
f1 (ppm)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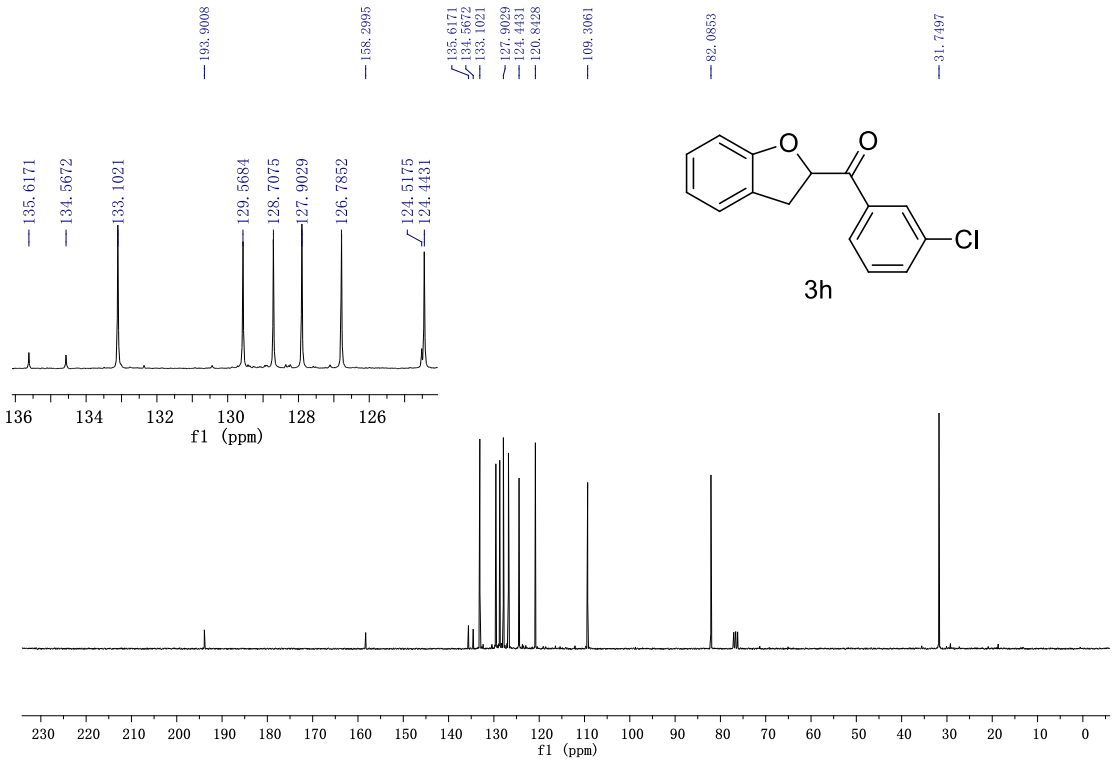
7.9625
7.9367
7.5926
7.4938
7.4413
7.1441
6.9156
6.9106
6.8906
6.8829
5.9134
5.8890
5.8792
5.8549
3.6853
3.6608
3.6327
3.6056
3.5666
3.5482
3.5140
0.0240
O
O
Cl
3h
1.01
0.98
1.02
1.02
2.01
1.00
1.06
0.99
10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)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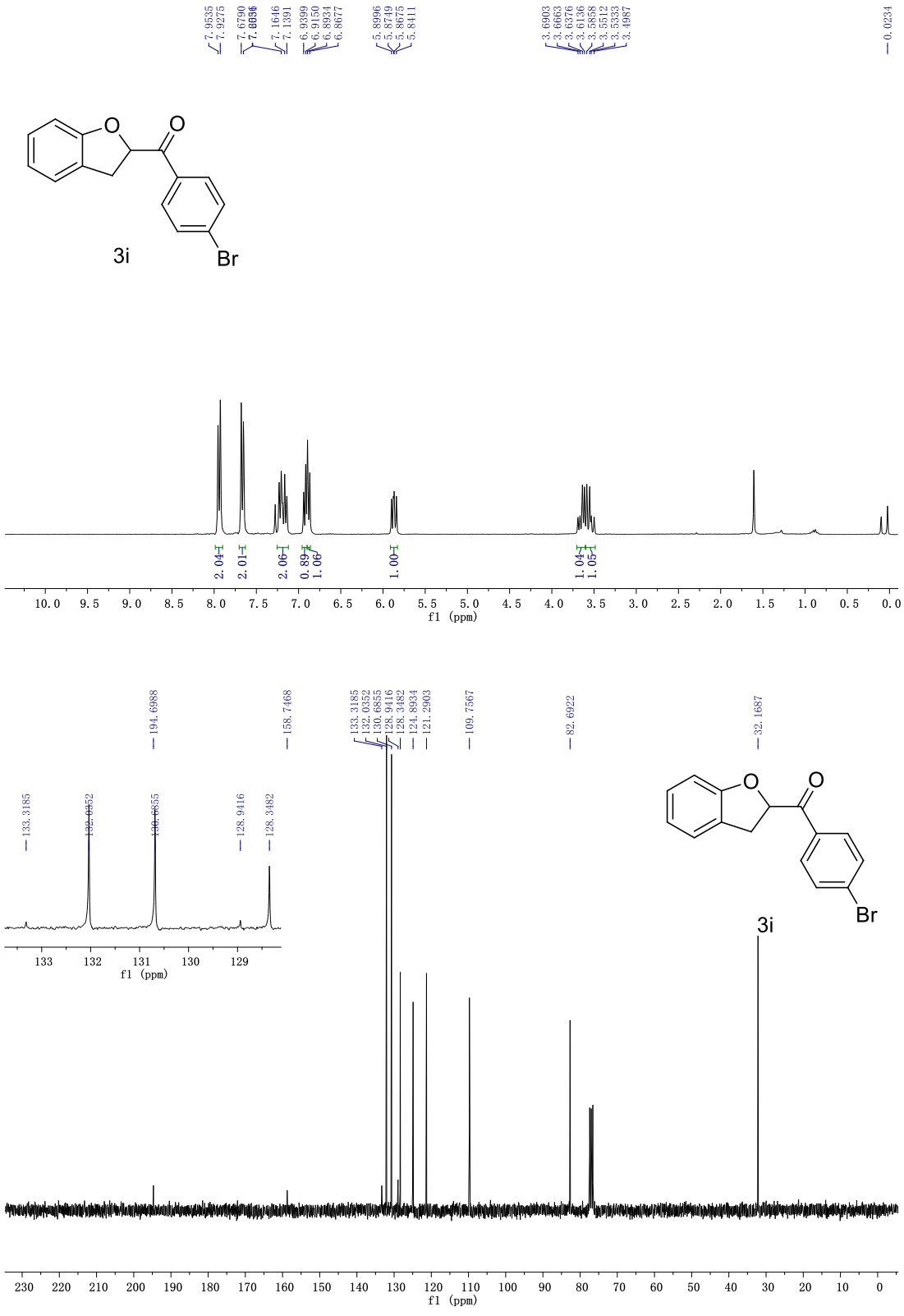
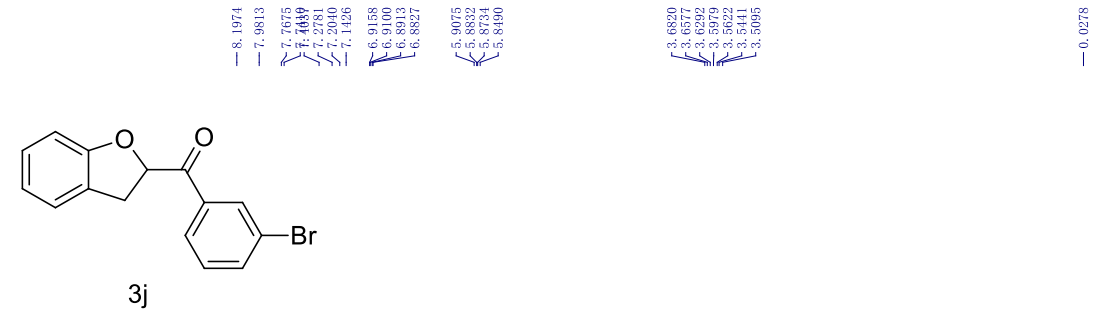
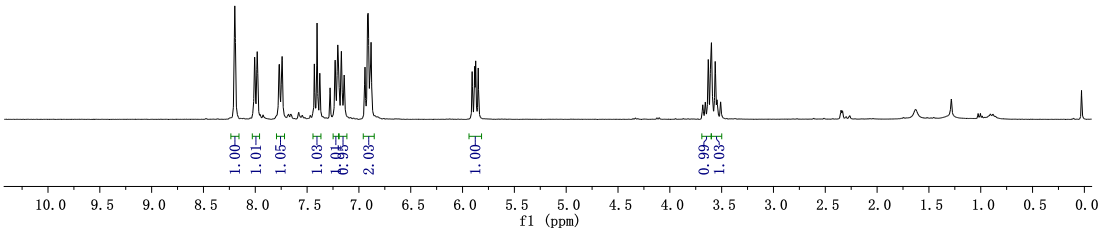
158.2995
135.6171
134.5672
133.1021
127.9029
124.4431
120.8428
109.3061
82.0853
31.7497
135.6171
134.5672
133.1021
129.5684
128.7075
127.9029
126.7852
124.5175
124.4431
O
O
Cl
3h
136 134 132 130 128 126
f1 (ppm)
230 220 210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)

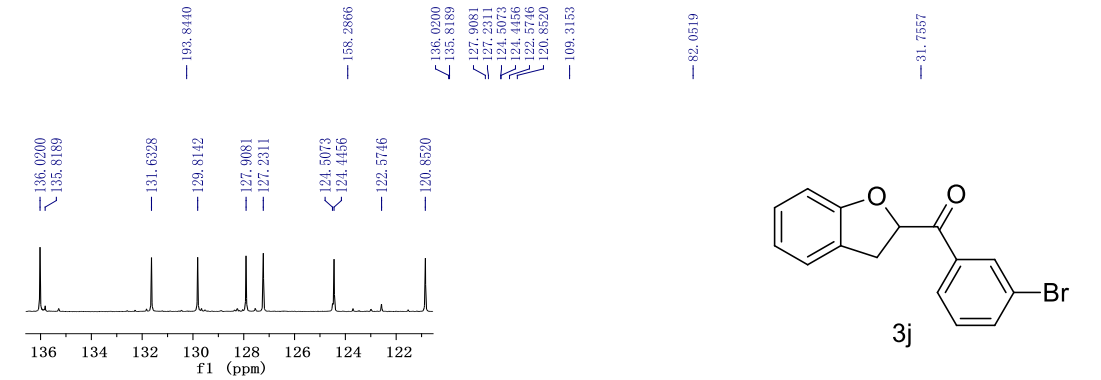

7.9535
7.9275
7.6790
7.6636
7.1646
7.1391
6.9399
6.9150
6.8934
6.8677
5.8996
5.8749
5.8675
5.8411
3.6903
3.6663
3.6376
3.6136
3.5858
3.5512
3.5333
3.4987
0.0234
O
O
Br
3i
2.04
2.01
2.06
0.89
1.06
1.00
1.04
1.05
10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)
194.6988
158.7468
133.3185
132.0352
130.6855
128.9416
128.3482
124.8934
121.2903
109.7567
82.6922
32.1687
133
132
131
130
129
f1 (ppm)
230 220 210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)


8.1974
7.9813
7.7675
7.4439
7.4281
7.2781
7.2040
7.1426
6.9158
6.9100
6.8913
6.8827
5.9075
5.8832
5.8734
5.8490
3.6820
3.6577
3.6292
3.5979
3.5622
3.5441
3.5095
0.0278

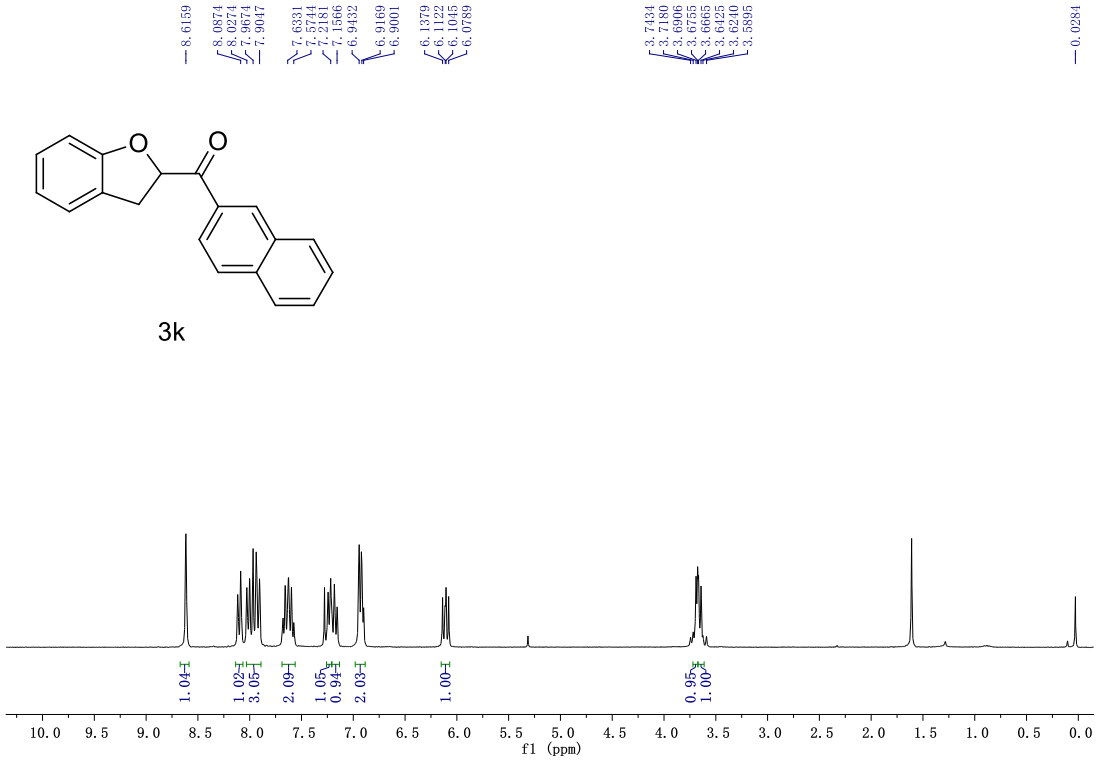
O
O
Br

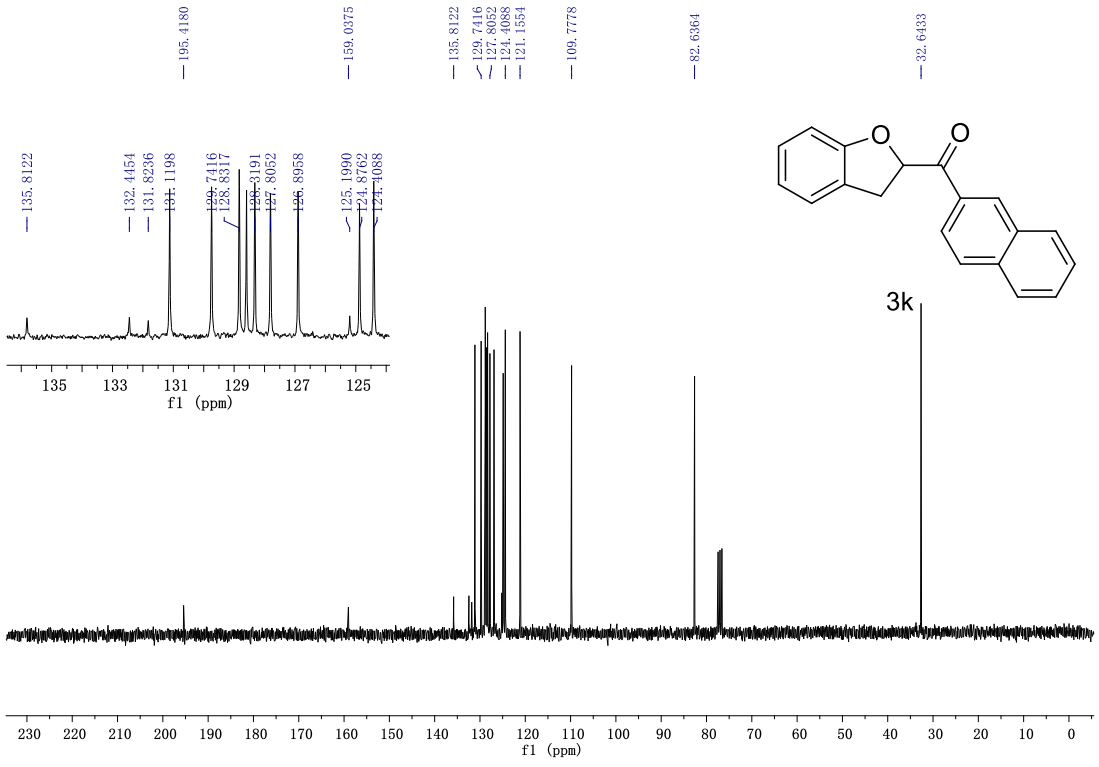
3j

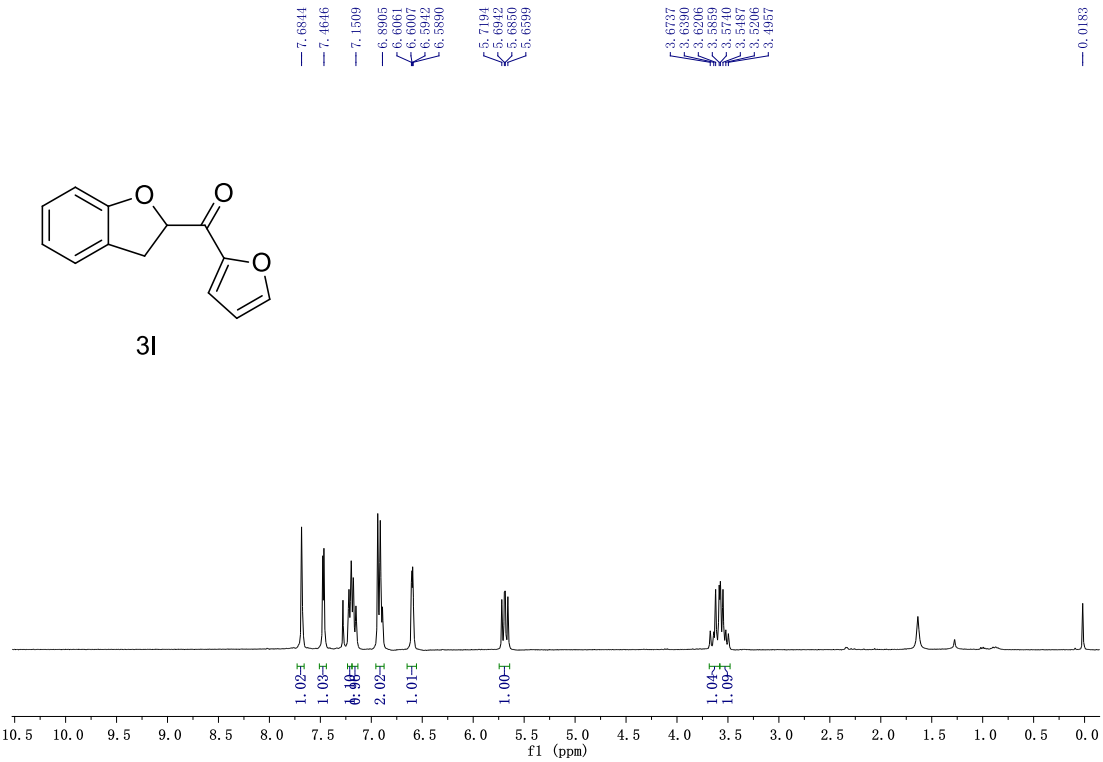

1.00
1.01
1.05
1.03
0.95
2.03
1.00
0.99
1.03
10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)


193.8440
158.2866
136.0200
135.8189
127.9081
127.2311
124.5073
124.4456
122.5746
120.8520
109.3153
82.0519
31.7557
136.0200
135.8189
131.6328
129.8142
127.9081
127.2311
124.5073
124.4456
122.5746
120.8520
136 134 132 130 128 126 124 122
f1 (ppm)
O
O
Br
230 220 210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)

3j


8.6159
8.0874
8.0274
7.9674
7.9047
7.6331
7.5744
7.2181
7.1566
6.9432
6.9169
6.9001
6.1379
6.1122
6.1045
6.0789
3.7434
3.7180
3.6906
3.6755
3.6665
3.6425
3.6240
3.5895
0.0284
O
O
3k
1.04
1.02
3.05
2.09
1.05
0.94
2.03
1.00
0.95
1.00
10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)


195.4180
159.0375
135.8122
129.7416
127.8052
124.4088
121.1554
109.7778
82.6364
32.6433
135.8122
132.4454
131.8236
131.1198
129.7416
128.8317
128.3191
127.8052
126.8958
125.1990
124.8762
124.4088
135 133 131 129 127 125
f1 (ppm)
O
O
3k
230 220 210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)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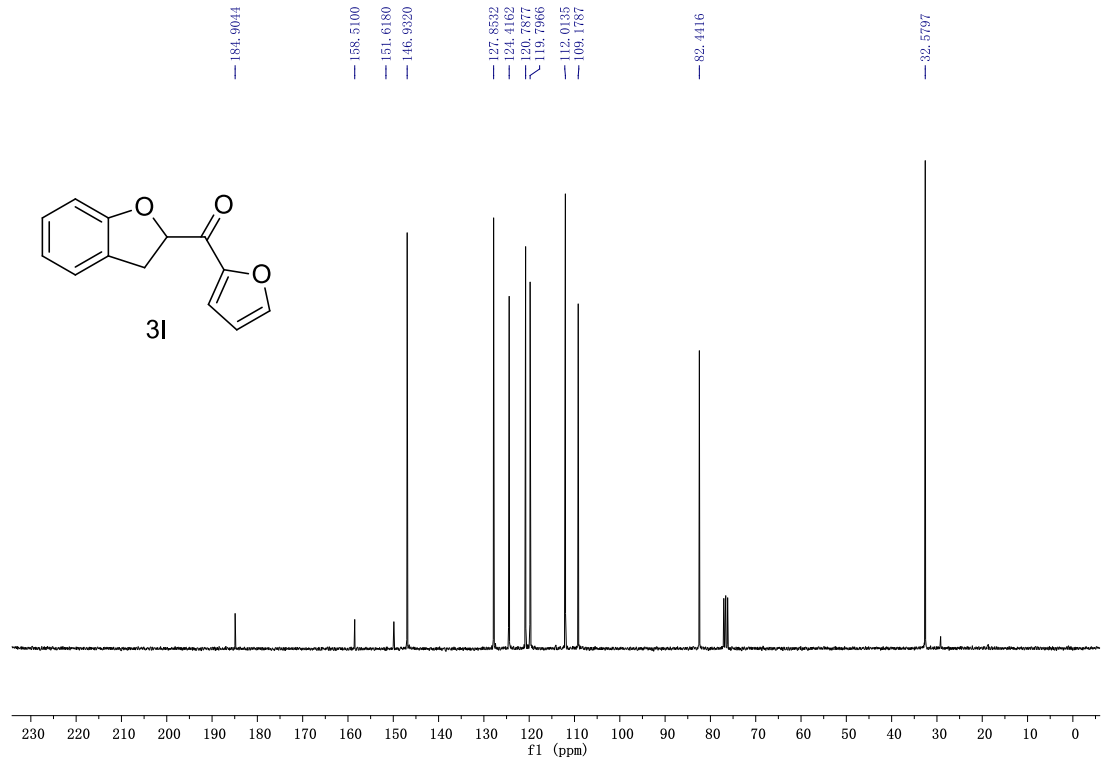
7.1509
6.8905
6.6061
6.6007
6.5942
6.5890
5.7194
5.6942
5.6850
5.6599
3.6737
3.6390
3.6206
3.5859
3.5740
3.5487
3.5206
3.4957
0.0183
3I
1.02
1.03
2.02
1.01
1.00
1.04
1.09
f1 (ppm)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146.9320
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120.7877
119.7966
112.0135
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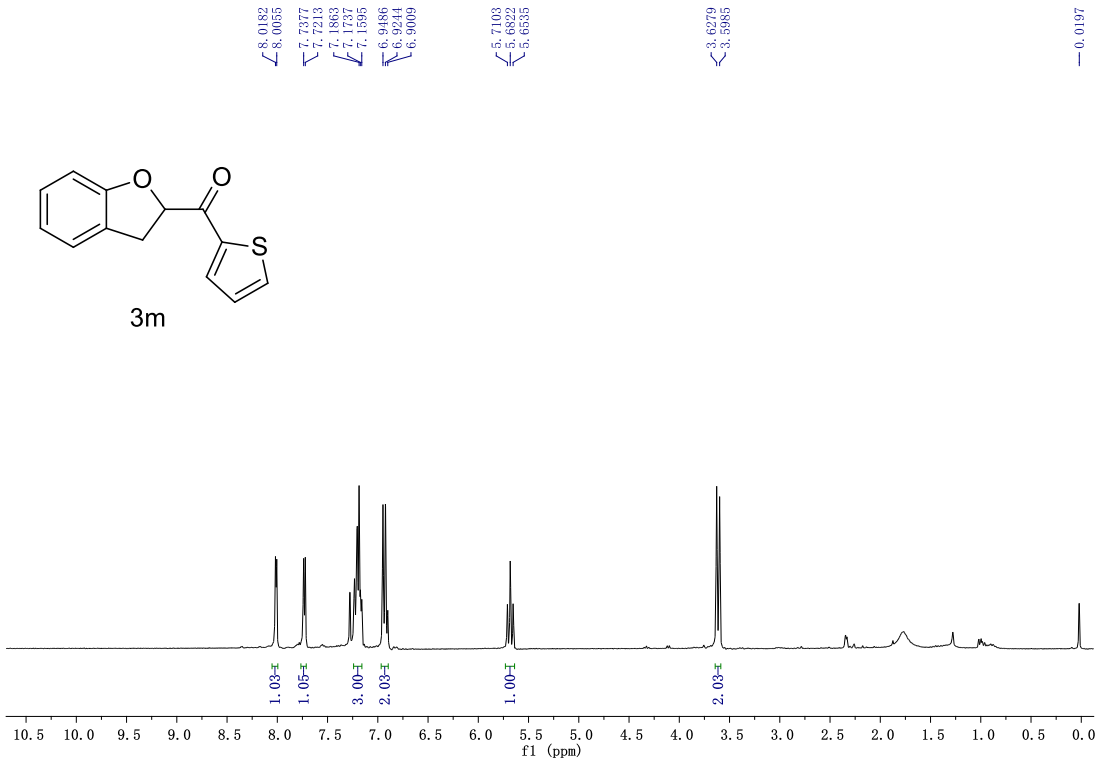
82.4416
32.5797
3I
f1 (ppm)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8.0055
7.7377
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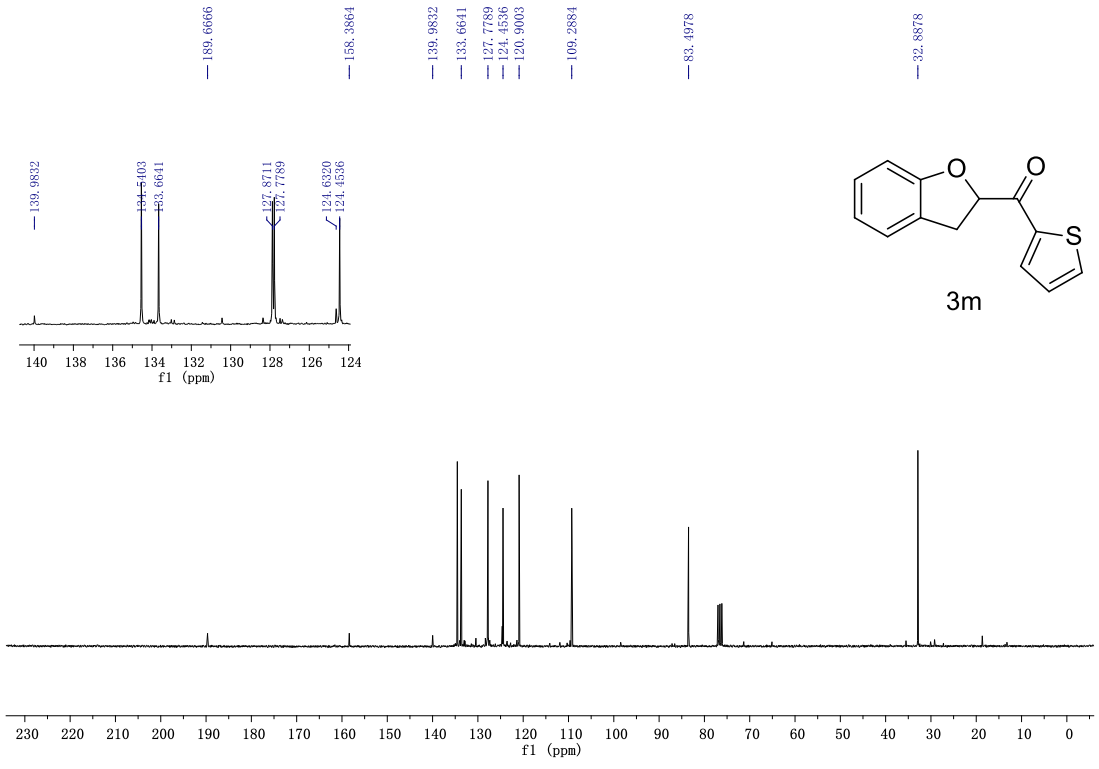
7.1863
7.1737
7.1595
6.9486
6.9244
6.9009
5.7103
5.6822
5.6535
3.6279
3.5985
0.0197
O
O
S
3m
1.03
1.05
3.00
2.03
1.00
2.03
10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)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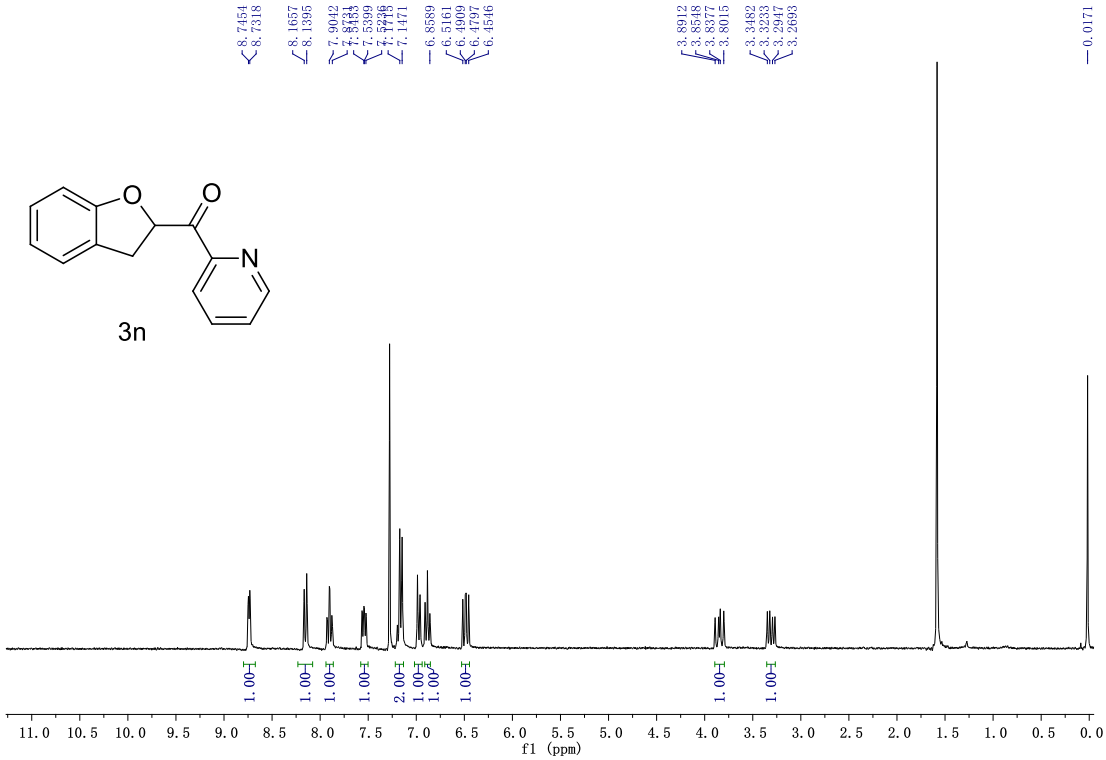
32.8878
139.9832
134.5403
133.6641
127.8711
127.7789
124.6320
124.4536
140 138 136 134 132 130 128 126 124
f1 (ppm)
O
O
S
3m
230 220 210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)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8.1657
8.1395
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7.5399
7.5236
7.1718
7.1471
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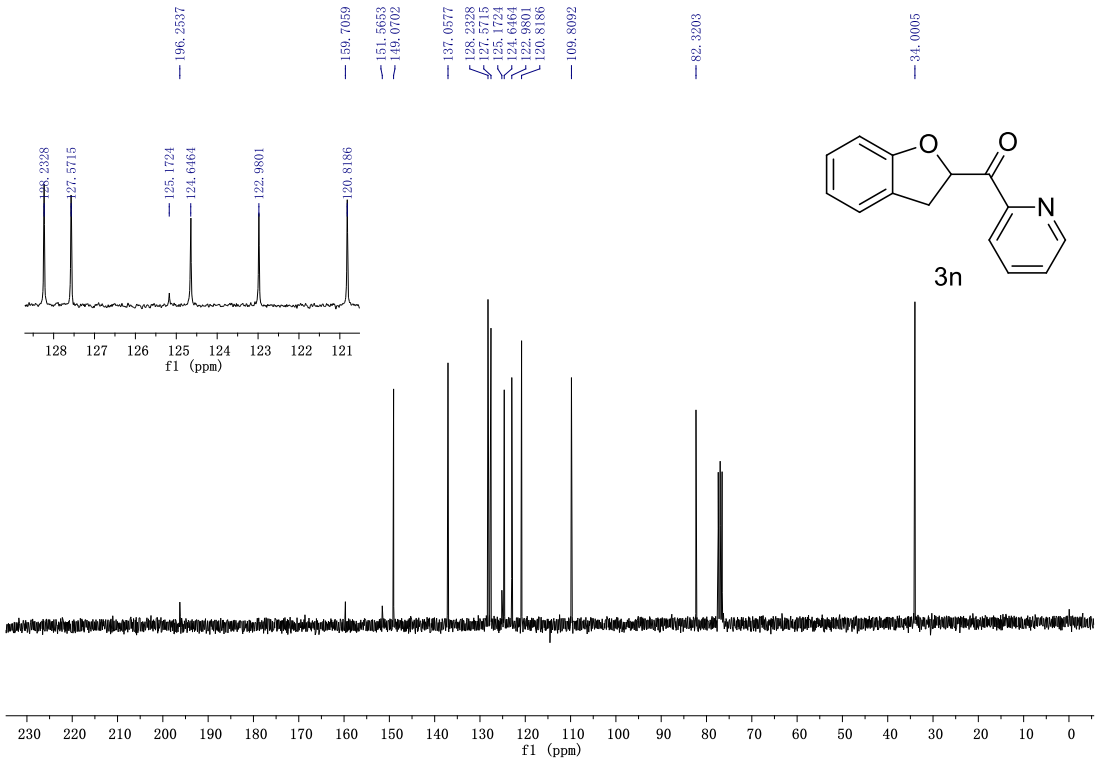
6.5161
6.4909
6.4797
6.4546
3.8912
3.8548
3.8377
3.8015
3.3482
3.3233
3.2947
3.2693
0.0171
O
O
N
3n
1.00
1.00
1.00
1.00
2.00
1.00
1.00
1.00
1.00
1.00
11.0 10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)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151.5653
149.0702
137.0577
128.2328
127.5715
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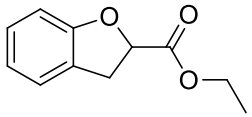
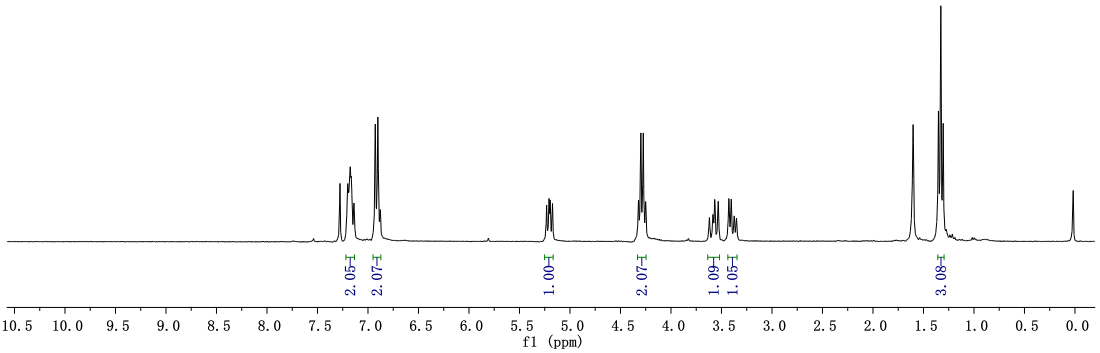
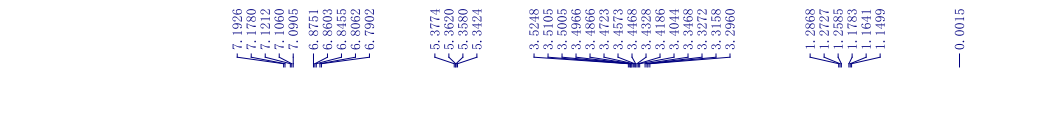
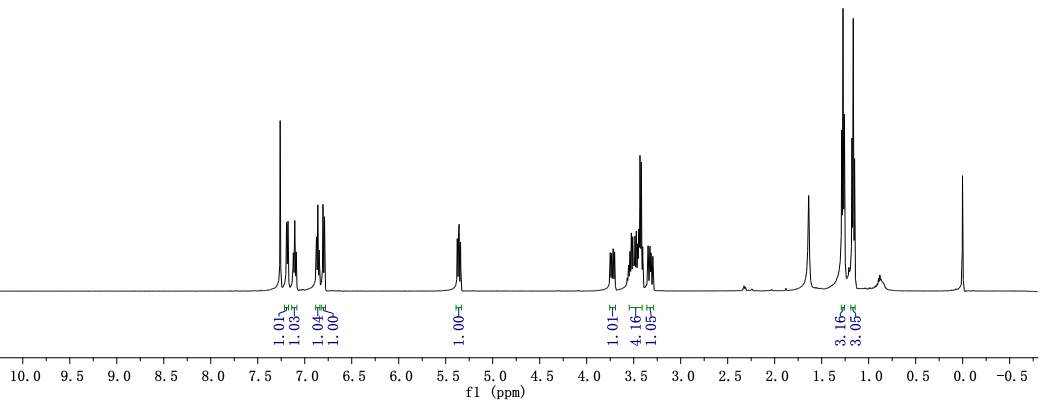
124.6464
122.9801
120.8186
109.8092
82.3203
34.0005
O
O
N
3n
128 127 126 125 124 123 122 121
f1 (ppm)
230 220 210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)



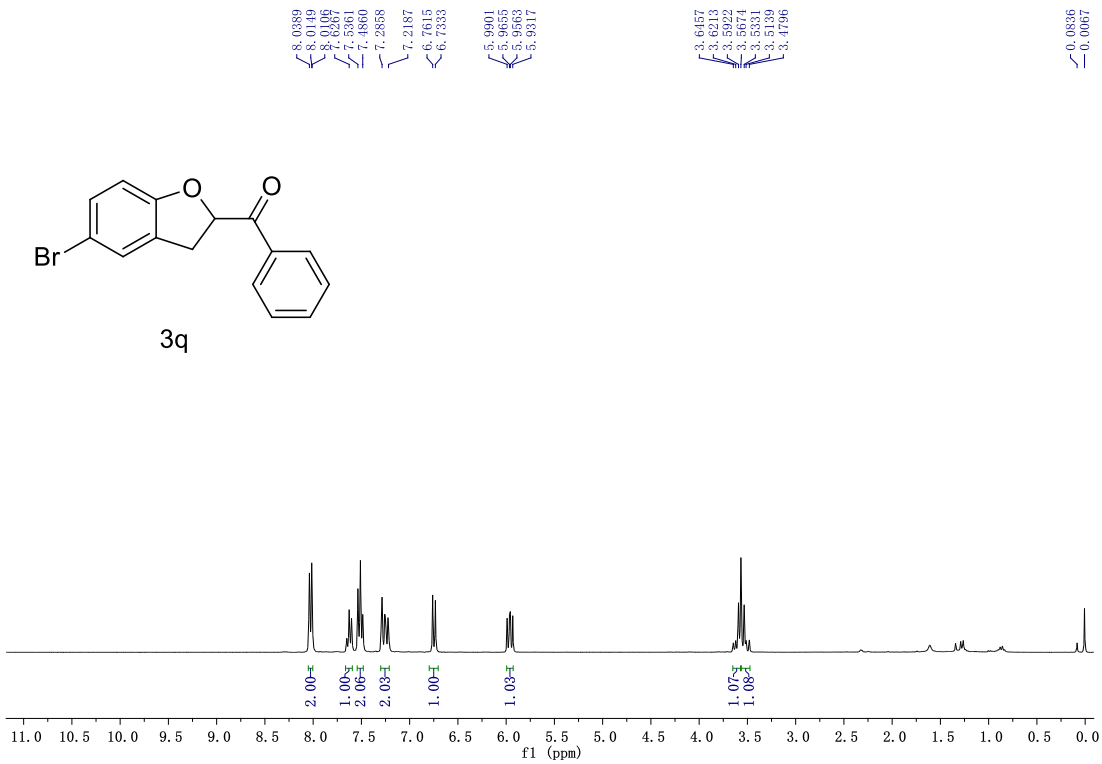
3o







3p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6.7333
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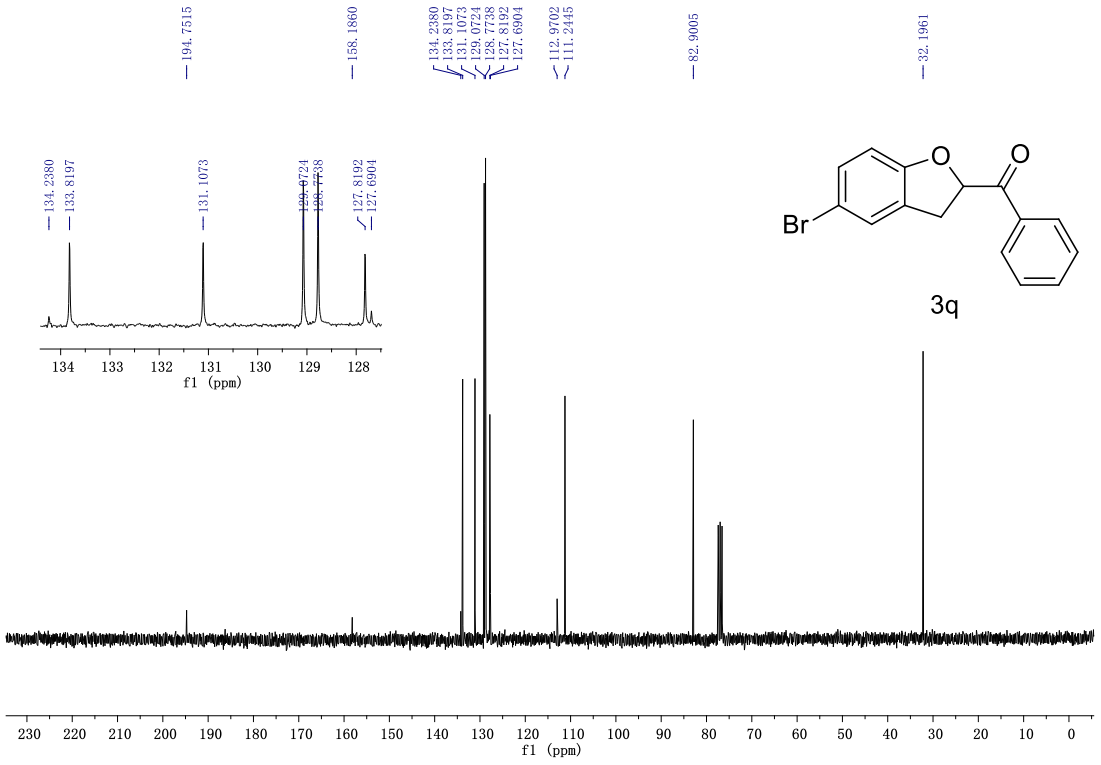
5.9655
5.9563
5.9317
3.6457
3.6213
3.5922
3.5674
3.5331
3.5139
3.4796
0.0836
0.0067
Br
O
O
3q
2.00
1.00
2.06
2.03
1.00
1.03
1.07
1.08
11.0 10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)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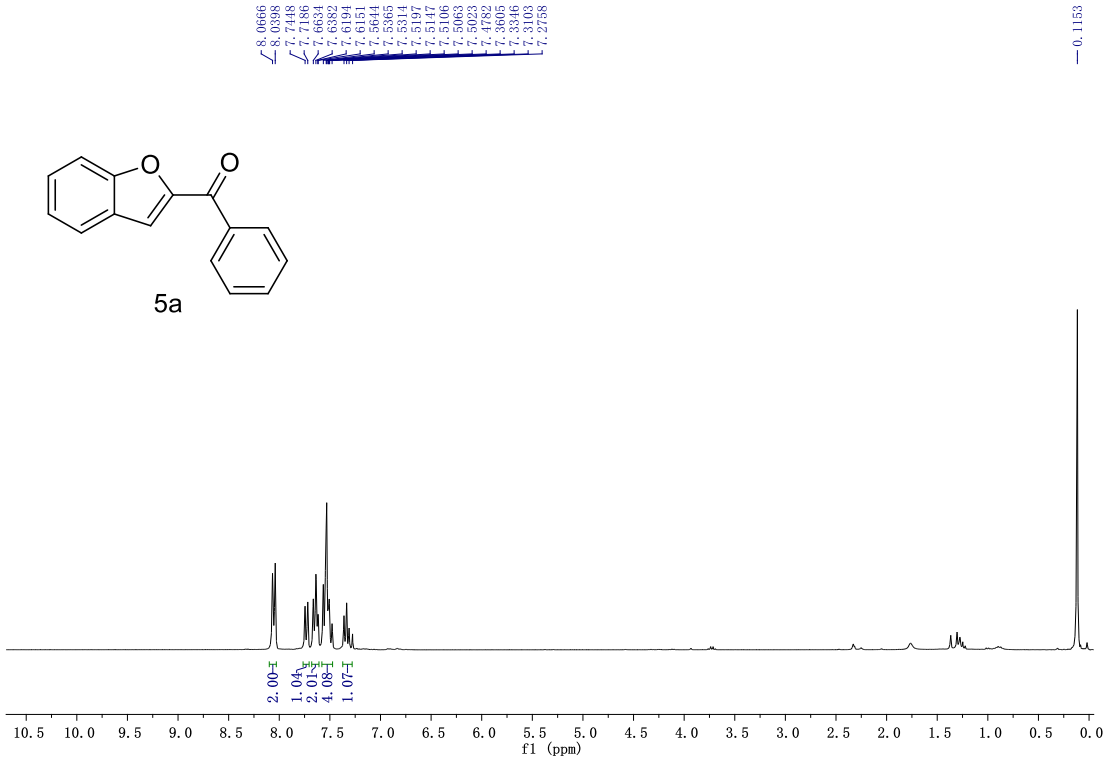
129.0724
128.7738
127.8192
127.6904
112.9702
111.2445
82.9005
32.1961
Br
O
O
3q
230 220 210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)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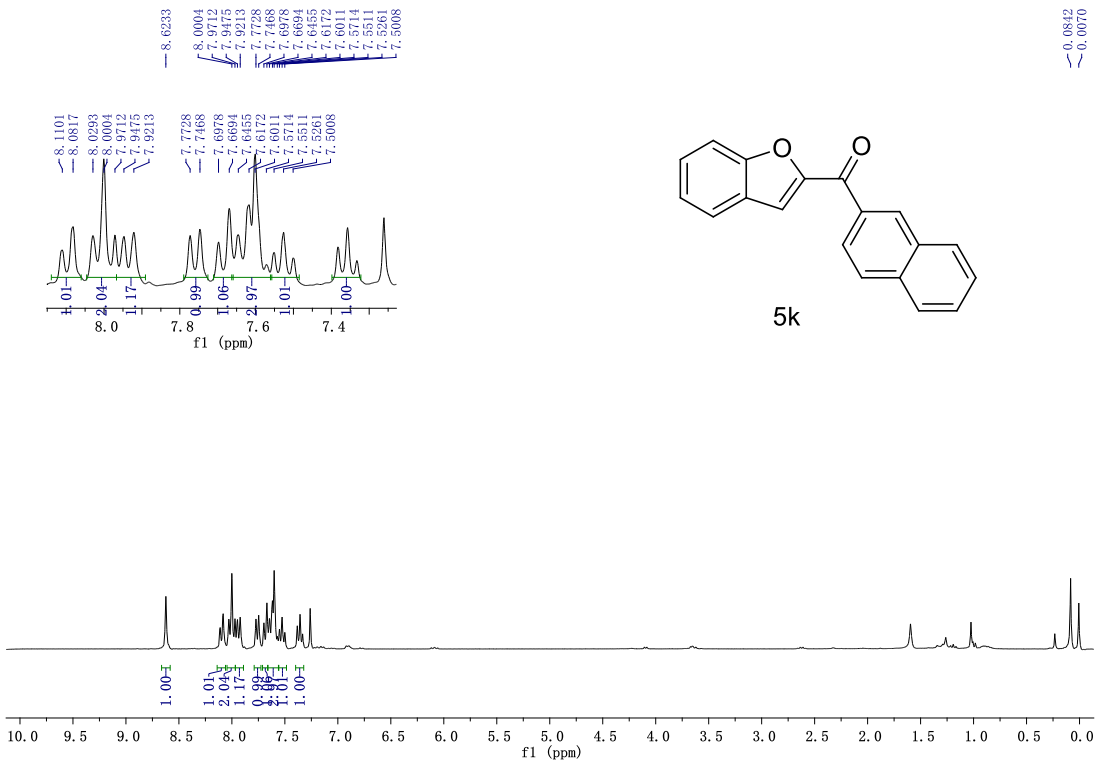
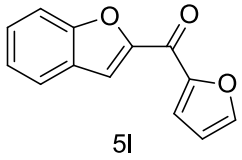
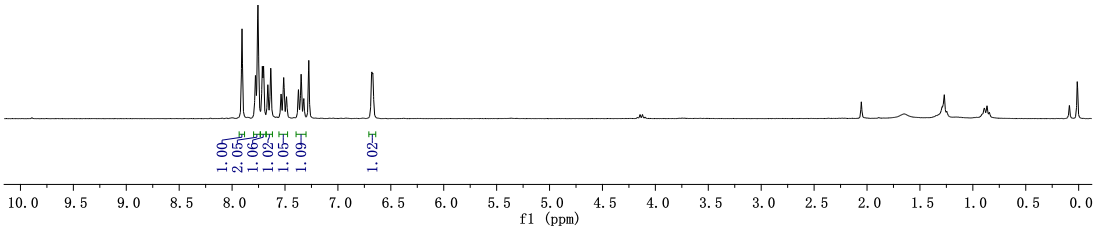
7.5197
7.5147
7.5106
7.5063
7.5023
7.4782
7.3605
7.3346
7.3103
7.2758
0.1153
O
O
5a
2.00
1.04
2.01
4.08
1.07
10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)

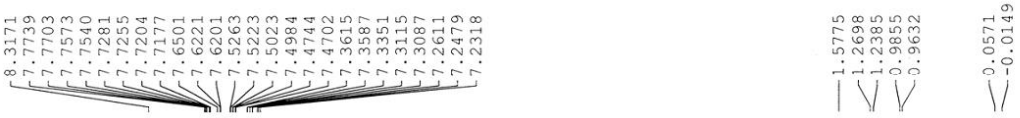

8.6233
8.0004
7.9712
7.9475
7.9213
7.7728
7.7468
7.6978
7.6694
7.6455
7.6172
7.6011
7.5714
7.5511
7.5261
7.5008
0.0842
0.0070
8.1101
8.0817
8.0293
8.0004
7.9712
7.9475
7.9213
7.7728
7.7468
7.6978
7.6694
7.6455
7.6172
7.6011
7.5714
7.5511
7.5261
7.5008
1.01
2.04
1.17
0.99
1.06
2.97
1.01
1.00
8.0
7.8
7.6
7.4
f1 (ppm)
O
O
5k
1.00
1.01
2.04
1.17
0.99
1.06
2.97
1.01
1.00
10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)

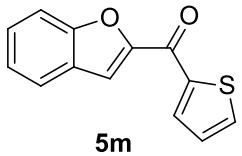


5l

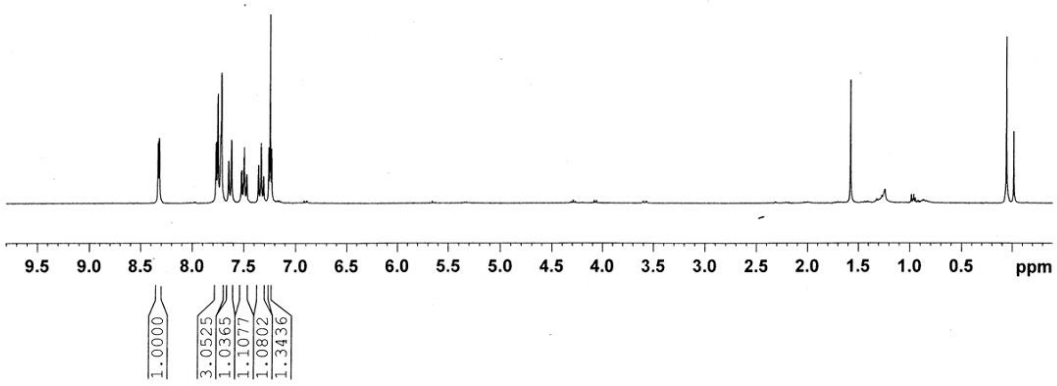


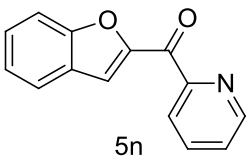
LXT-C-283 CDCL3 1HNMR AV300





5m





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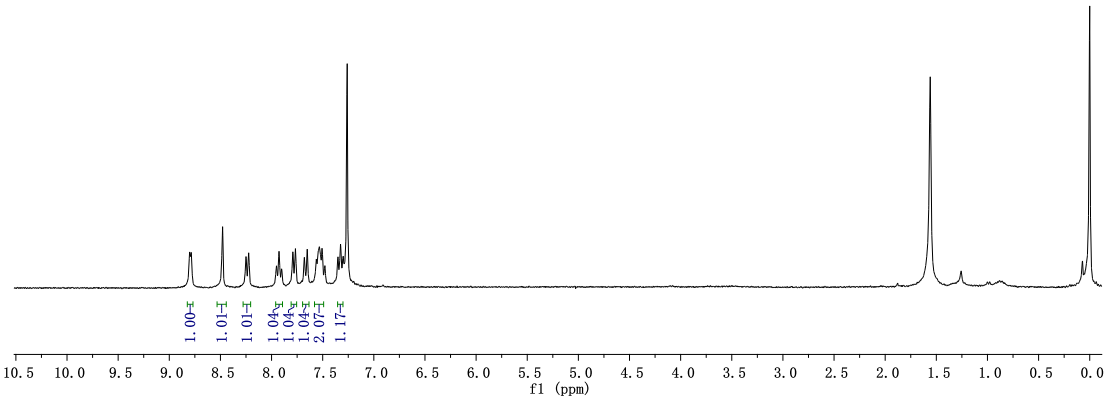
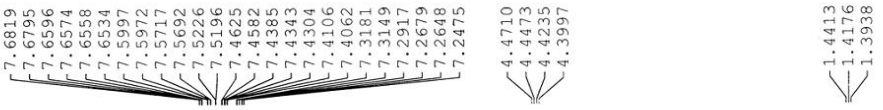
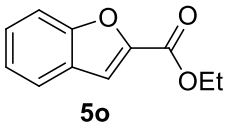


LXT-C-286 CDCL3 1HNMR AV300





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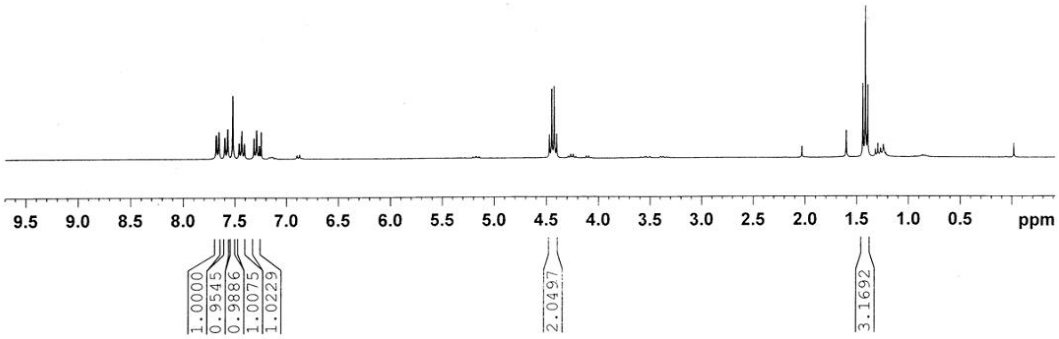

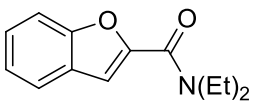

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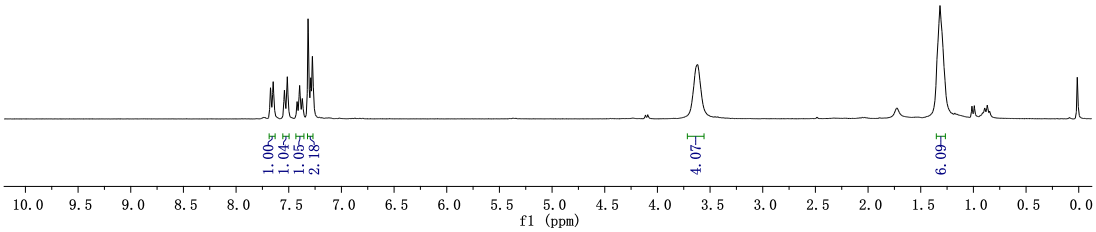

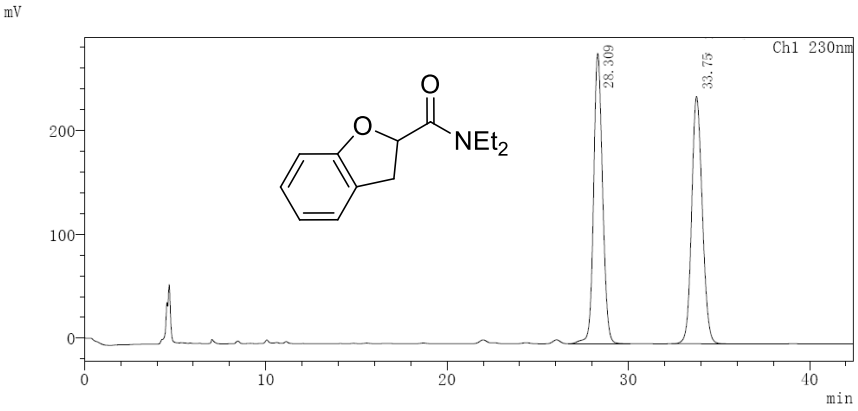

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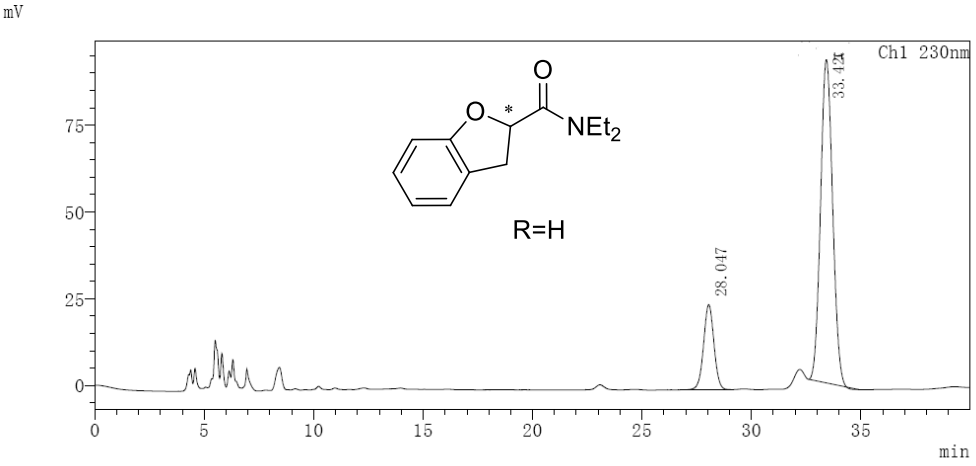
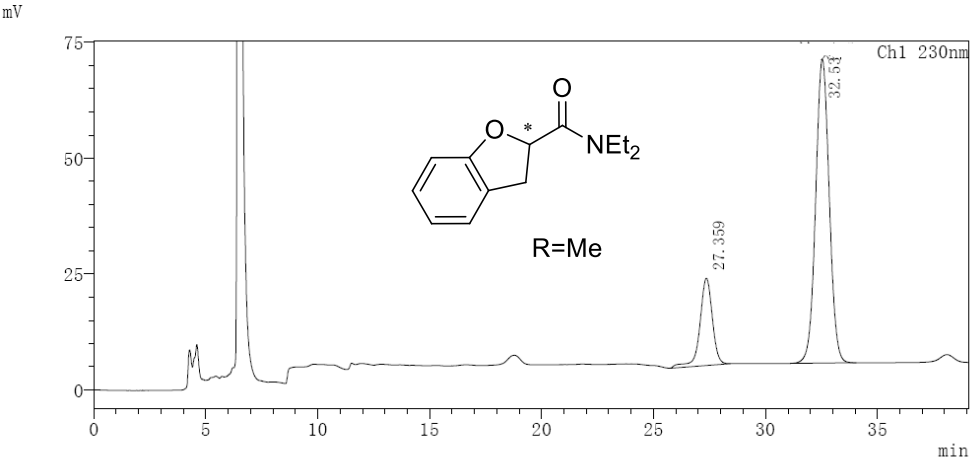
2	33.756	9711257	50.219



	save time(min)	area	area(%)
1	28.047	809252	18.5
2	33.420	3565134	81.5



	save time(min)	area	area(%)
1	27.359	727887	20.796
2	32.537	2772229	79.204