Electronic Supplementary Material (ESI) for RSC Advances.

Supplementary Materials

for

Bifunctional phase-transfer catalysts for synthesis of 2-oxazolidinones from isocyanates and epoxides

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Contents

General

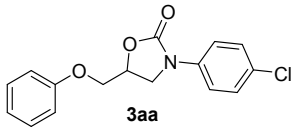
^{1}H NMR and ^{13}C NMR spectra were measured in $CDCl_3$, solution on a Bruker AV-400 spectrometer using TMS as an internal reference. Coupling constant (*J*) values are given in Hz. Multiplicities are designated by the following abbreviations: s, singlet; d, doublet; t, triplet; q, quartet; br, broad; m, multiplet. High-resolution mass spectra (HRMS) were performed on a *Bruker* microTOF-Q II Mass Spectrometer with ES ionization (ESI). All commercially available reagents were used as received. Thin-layer chromatography on silica (with GF_{254}) was used to monitor all reactions. Products were purified by flash column chromatography on silica gel purchased from Qingdao Haiyang Chemical Co., Ltd. The preparation and characterization data of all bifunctional phase-transfer catalysts (Bif-PTCs) were found in our previous report.[1]

Typical procedure for the synthesis of 2-isoxazolidinones 3

0.20 mmol of epoxide **1**, 2.7 mg of **Bif-PTC-1** (2.5 mol%), and 0.21 mmol of isocyanate **2** in 2.0 mL PhCl was stirred for 12 h at 100 ^{o}C under inert atmosphere. The solvent was evaporated under reduced pressure and the residue was purified by a flash column chromatography (petroleum ether : ethyl acetate = 2 : 1 to 1 : 3) to yield corresponding 2-oxazolidinones **3**.

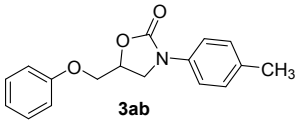
References

1. Y. Li, D. Cui, J. Zhu, P. Huang, Z. Tian, Y. Jia, P. Wang, Green Chem. 21 (2019) 5231–5237 .
2. Y. Toda, S. Gomyou, S. Tanaka, Y. Komiyama, A. Kikuchi, H. Suga, Org. Lett. 19 (2017) 5786–5789.
3. J.E. Herweh, T.A. Foglia, D. Swern, J. Org. Chem. 33 (1968) 4029–4033.
4. M. Zhou, X. Zheng, Y. Wang, D. Yuan, Y. Yao, ChemCatChem. 11 (2019) 5783-5787.



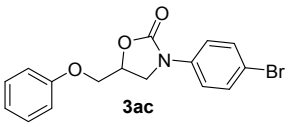
3aa

White solid,[2] ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.55 (d, *J* = 8.5 Hz, 2H), 7.42-7.29 (m, 4H), 7.03 (t, *J* = 7.2 Hz, 1H), 6.93 (d, *J* = 8.0 Hz, 2H), 5.01 (d, *J* = 3.6 Hz, 1H), 4.25 (d, *J* = 4.0 Hz, 2H), 4.20 (t, *J* = 8.8 Hz, 1H), 4.12-4.04 (m, 1H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 157.94, 154.24, 136.74, 129.68, 129.45, 129.14, 121.86, 119.42, 114.60, 70.39, 67.80, 47.34; HRMS (ESI) *m/z* calcd. for $C_{16}H_{15}ClNO_3^+$ $[M+H]^+$: 304.0735, found 304.0741.



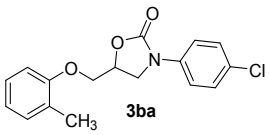
3ab

White solid,[3] ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.47 (d, *J* = 8.1 Hz, 2H), 7.34-7.30 (m, 2H), 7.21 (d, *J* = 8.0 Hz, 2H), 7.05-6.99 (m, 1H), 6.93 (d, *J* = 7.9 Hz, 2H), 4.99 (s, 1H), 4.31-4.14 (m, 3H), 4.10-4.03 (m, 1H), 2.34 (s, 3H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 158.04, 154.51, 135.61, 133.95, 129.65, 121.75, 118.46, 114.62, 70.34, 67.95, 47.63, 20.76; HRMS (ESI) *m/z* calcd. for $C_{17}H_{18}NO_3^+$ $[M+H]^+$: 284.1281, found 284.1279.



3ac

White solid,[4] ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.65 (d, *J* = 8.2 Hz, 1H), 7.51 (d, *J* = 1.4 Hz, 3H), 7.33 (t, *J* = 7.6 Hz, 2H), 7.03 (t, *J* = 7.3 Hz, 1H), 6.93 (d, *J* = 8.3 Hz, 2H), 5.01 (dd, *J* = 8.8, 4.7 Hz, 1H), 4.25 (d, *J* = 4.4 Hz, 2H), 4.19 (t, *J* = 8.8 Hz, 1H), 4.10-4.04 (m, 1H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 157.93, 154.18, 137.21, 129.69, 121.87, 119.73, 117.05, 114.60, 70.40, 67.80, 47.26; HRMS (ESI) *m/z* calcd. for $C_{16}H_{15}BrNO_3^+$ $[M+H]^+$: 348.0230, found 348.0236.



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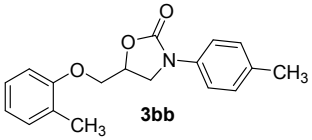
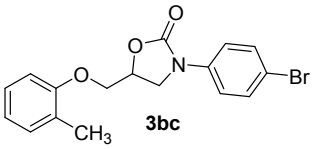
White solid, ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.56 (d, *J* = 8.7 Hz, 2H), 7.37 (d, *J* = 8.7 Hz, 2H), 7.23-7.09 (m, 2H), 6.93 (t, *J* = 7.1 Hz, 1H), 6.82 (d, *J* = 7.9 Hz, 1H), 5.03 (d, *J* = 3.9 Hz, 1H), 4.36-4.15 (m, 3H), 4.13-4.07 (m, 1H), 2.12 (s, 3H); HRMS (ESI) *m/z* calcd. for $C_{17}H_{16}ClNNaO_3^+$ $[M+Na]^+$: 340.0711, found 340.0709.



3bb

White solid, ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.49 (d, *J* = 7.5 Hz, 2H), 7.20 (dd, *J* = 15.0, 7.3 Hz, 4H), 6.95 (d, *J* = 6.7 Hz, 1H), 6.83 (d, *J* = 7.6 Hz, 1H), 4.97 (s, 1H), 4.20 (dd, *J* = 14.6, 10.4 Hz, 3H), 4.06 (s, 1H), 2.38 (s, 3H), 2.18 (s, 3H); ^{13}C NMR (101 MHz, $CDCl_3$) containing isomers, δ 156.16, 154.69, 148.97, 139.27, 135.72, 133.82, 131.24, 130.95 and 130.86, 129.97 and1 29.88, 129.63 and 129.43, 128.15, 127.03, 126.89, 121.39, 118.44, 113.20, 111.04, 70.54, 68.42 and 68.26, 47.44, 21.21 and 20.76, 16.06; HRMS (ESI) *m/z* calcd. for $C_{18}H_{20}NO_3^+$ $[M+H]^+$: 298.1438, found 298.1440.



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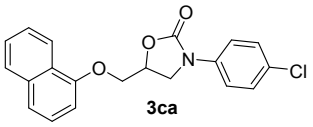
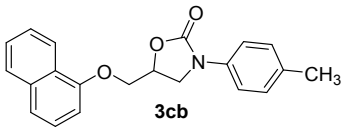


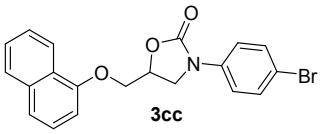
3ca

White solid, ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.07 (d, *J* = 8.4 Hz, 1H), 7.82 (d, *J* = 8.2 Hz, 1H), 7.60 (d, *J* = 8.9 Hz, 2H), 7.50 (dd, *J* = 7.6, 4.6 Hz, 2H), 7.39 (m, 4H), 6.85 (d, *J* = 7.6 Hz, 1H), 5.16 (m, 1H), 4.44 (m, 2H), 4.32 (t, *J* = 8.9 Hz, 1H), 4.20 (dd, *J* = 8.8, 5.4 Hz, 1H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 154.35, 153.61, 136.75, 134.50, 129.46, 129.17, 127.58, 126.70, 125.62, 125.60, 125.28, 121.50, 119.45, 104.94, 70.51, 68.31, 47.37; HRMS (ESI) *m/z* calcd. for $C_{20}H_{17}ClNO_3^+$ $[M+H]^+$: 354.0891, found 354.0893.



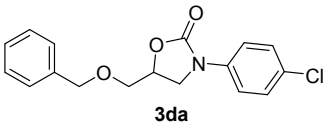
3cb

Light yellow oil, ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.37-6.27 (m, 11H), 5.32 (s, 1H), 4.29 (d, *J* = 5.1 Hz, 1H), 4.09 (d, *J* = 8.6 Hz, 1H), 3.96 (d, *J* = 8.5 Hz, 1H), 3.63-3.35 (m, 1H), 2.33 (s, 3H).



3cc

White solid, ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.07 (d, *J* = 8.3 Hz, 1H), 7.82 (d, *J* = 8.1 Hz, 1H), 7.66-7.45 (m, 5H), 7.39 (t, *J* = 7.9 Hz, 2H), 7.29 (s, 1H), 6.85 (d, *J* = 7.5 Hz, 1H), 5.16 (dd, *J* = 8.8, 4.3 Hz, 1H), 4.44 (m, 2H), 4.31 (t, *J* = 8.9 Hz, 1H), 4.19 (dd, *J* = 8.8, 5.4 Hz, 1H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 154.31, 153.60, 137.26, 134.50, 132.10, 127.58, 126.70, 125.63, 125.61, 125.27, 121.49, 119.75, 117.05, 104.95, 70.52, 68.31, 47.26; HRMS (ESI) *m/z* calcd. for $C_{20}H_{17}BrNO_3^+$ $[M+H]^+$: 398.0386, found 398.0380.



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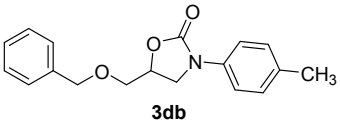
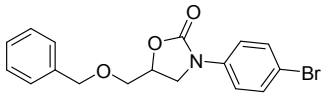
White solid, ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.44 (d, *J* = 6.2 Hz, 2H), 7.29 (s, 7H), 4.76 (s, 1H), 4.58 (s, 2H), 4.02 (s, 1H), 3.87 (s, 1H), 3.70 (d, *J* = 3.1 Hz, 2H).



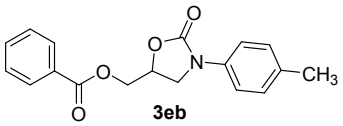
3db

White solid, ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.40 (dd, *J* = 29.5, 9.0 Hz, 6H), 7.20 (dd, *J* = 20.2, 11.9 Hz, 3H), 4.79 (s, 1H), 4.64 (d, *J* = 2.4 Hz, 2H), 4.07 (s, 1H), 3.93 (s, 1H), 3.74 (d, *J* = 4.7 Hz, 2H), 2.35 (s, 3H).



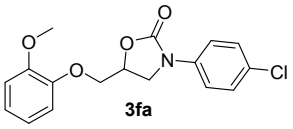
3dc

White solid, ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.54 – 7.41 (m, 4H), 7.40 – 7.31 (m, 4H), 7.28 (s, 1H), 4.80 (s, 1H), 4.64 (s, 2H), 4.05 (d, *J* = 6.3 Hz, 1H), 3.92 (d, *J* = 7.9 Hz, 1H), 3.75 (s, 2H).



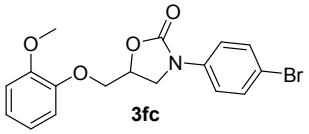
3eb

White solid, ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.01 (d, *J* = 7.1 Hz, 2H), 7.56 (d, *J* = 6.6 Hz, 1H), 7.42 (s, 4H), 7.18 (d, *J* = 7.3 Hz, 2H), 4.97 (s, 1H), 4.57 (dd, *J* = 27.9, 11.7 Hz, 2H), 4.18 (t, *J* = 8.7 Hz, 1H), 3.91 (d, *J* = 6.0 Hz, 1H), 2.34 (s, 3H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 166.11, 154.43, 135.51, 134.01, 133.47, 129.76, 129.64, 129.18, 128.52, 118.52, 70.17, 64.85, 47.35, 20.73; HRMS (ESI) *m/z* calcd. for $C_{18}H_{18}NO_4^+$ $[M+H]^+$: 312.1230, found 312.1232.



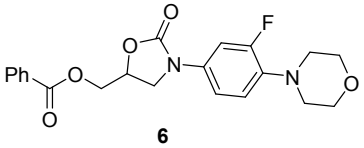
3fa

White solid, ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.56 (d, *J* = 8.8 Hz, 2H), 7.37 (d, *J* = 8.8 Hz, 2H), 6.98 (m, 4H), 5.00 (dd, *J* = 13.4, 5.2 Hz, 1H), 4.36-4.24 (m, 2H), 4.24-4.12 (m, 2H), 3.84 (s, 3H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 154.33, 150.16, 147.61, 136.86, 129.32, 129.07, 123.09, 121.03, 119.47, 115.99, 112.41, 70.67, 70.00, 55.83, 47.37; HRMS (ESI) *m/z* calcd. for $C_{17}H_{17}ClNO_4^+$ $[M+H]^+$: 334.0841, found 334.0840.



3fc

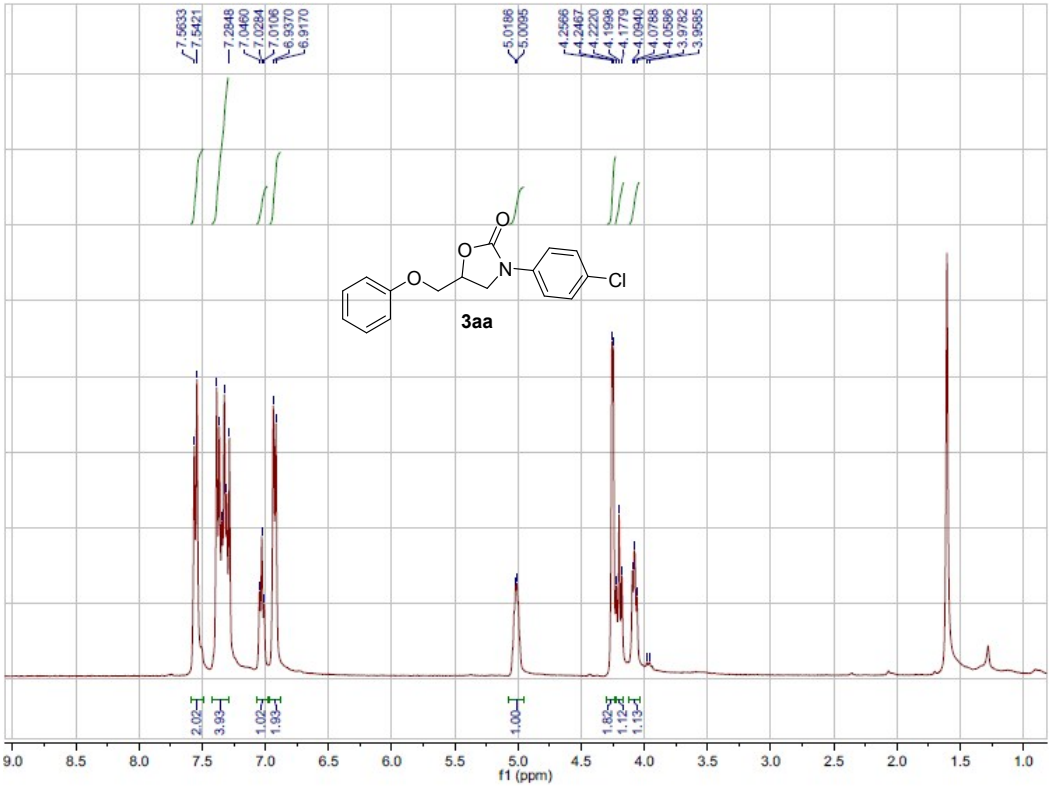
White solid, ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.64-7.40 (m, 4H), 7.09-6.85 (m, 4H), 5.05-4.97 (m, 1H), 4.34-4.23 (m, 2H), 4.23-4.12 (m, 2H), 3.80 (s, 3H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 154.27, 150.17, 147.61, 137.37, 132.01, 123.10, 121.03, 119.78, 116.93, 116.00, 112.40, 70.67, 70.00, 55.83, 47.30; HRMS (ESI) *m/z* calcd. for $C_{17}H_{17}BrNO_4^+$ $[M+H]^+$: 378.0335, found 378.0330.

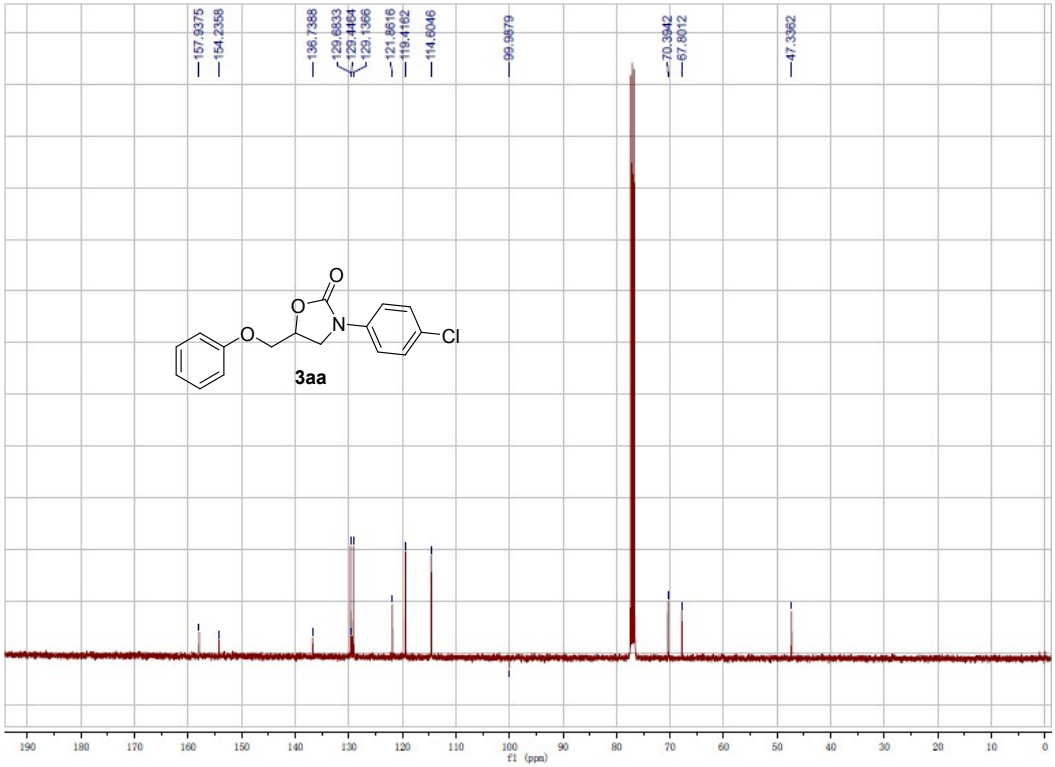


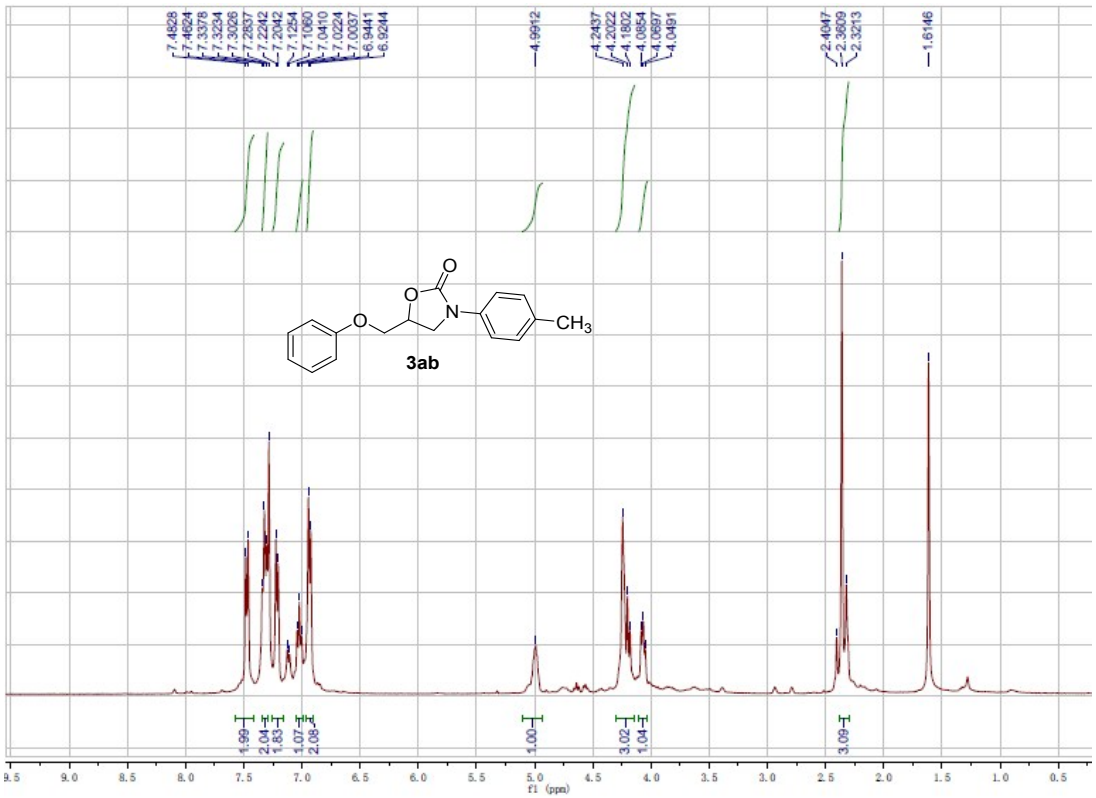
6

light yellow solid, ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.06 (d, *J* = 7.44 Hz, 2H), 7.61 (t, *J* = 8.48 Hz, 1H), 7.49 (q, J = 7.72 Hz, 2H), 6.99-6.82 (m, 2H), 6.71 (br, 1H), 5.42-5.29 (m, 1H), 4.64-4.61 (m, 2H), 4.14-4.08 (m, 1H), 3.90 (s, 4H), 3.85-3.83 (m, 1H), 3.04 (s, 4H); HRMS (ESI) *m/z* calcd. for $C_{21}H_{23}ClFN_2O_5^+$ $[M\cdot HCl+H]^+$: 437.1274, found 437.1271.

NMR copies of 2-oxazolidinoes



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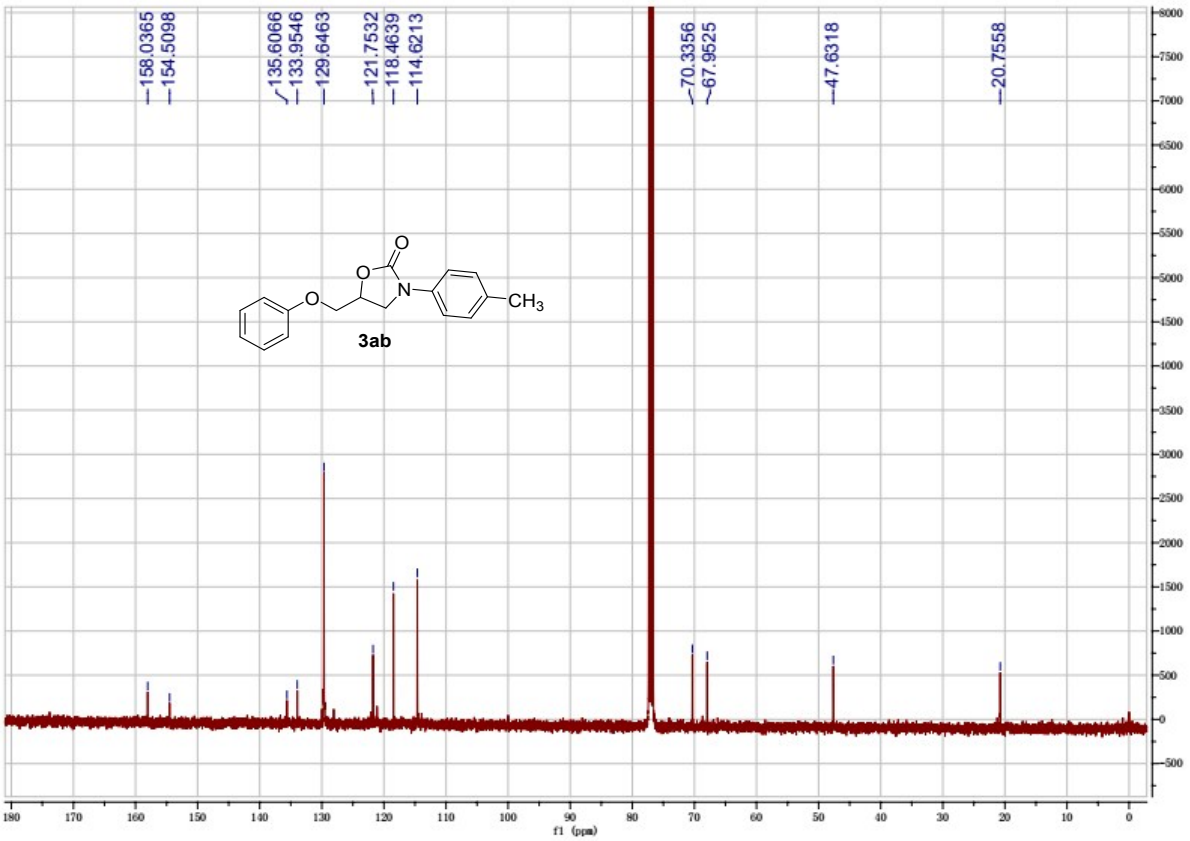
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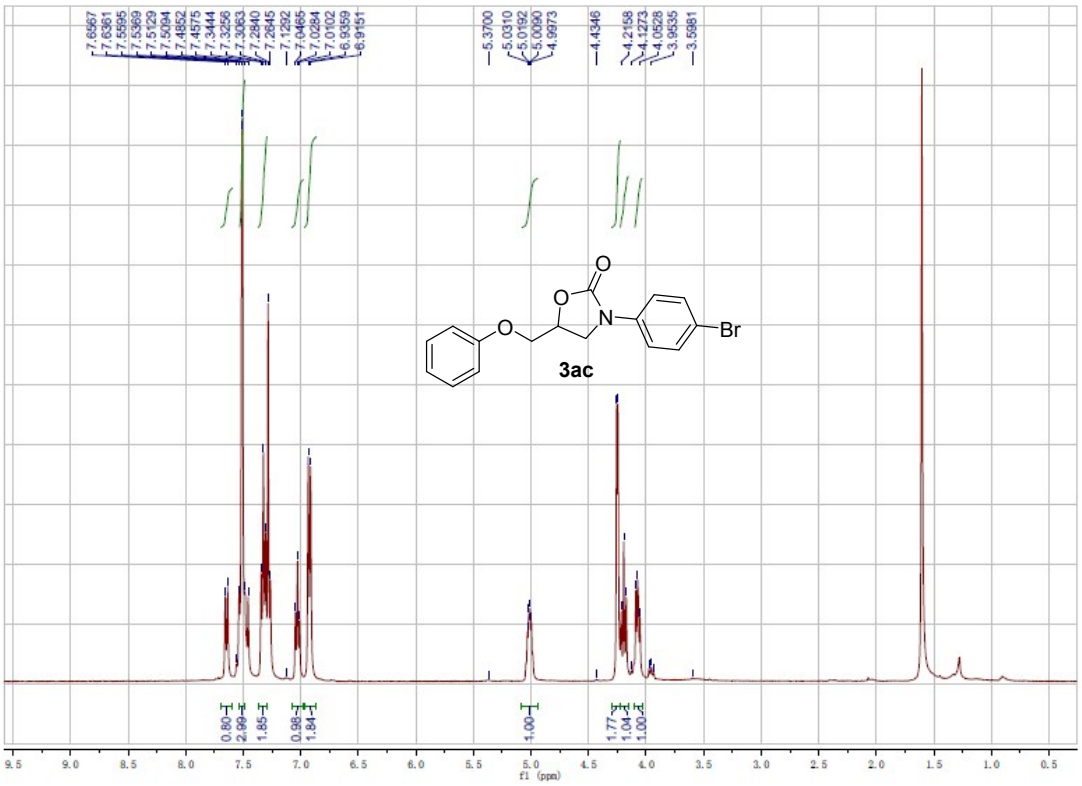
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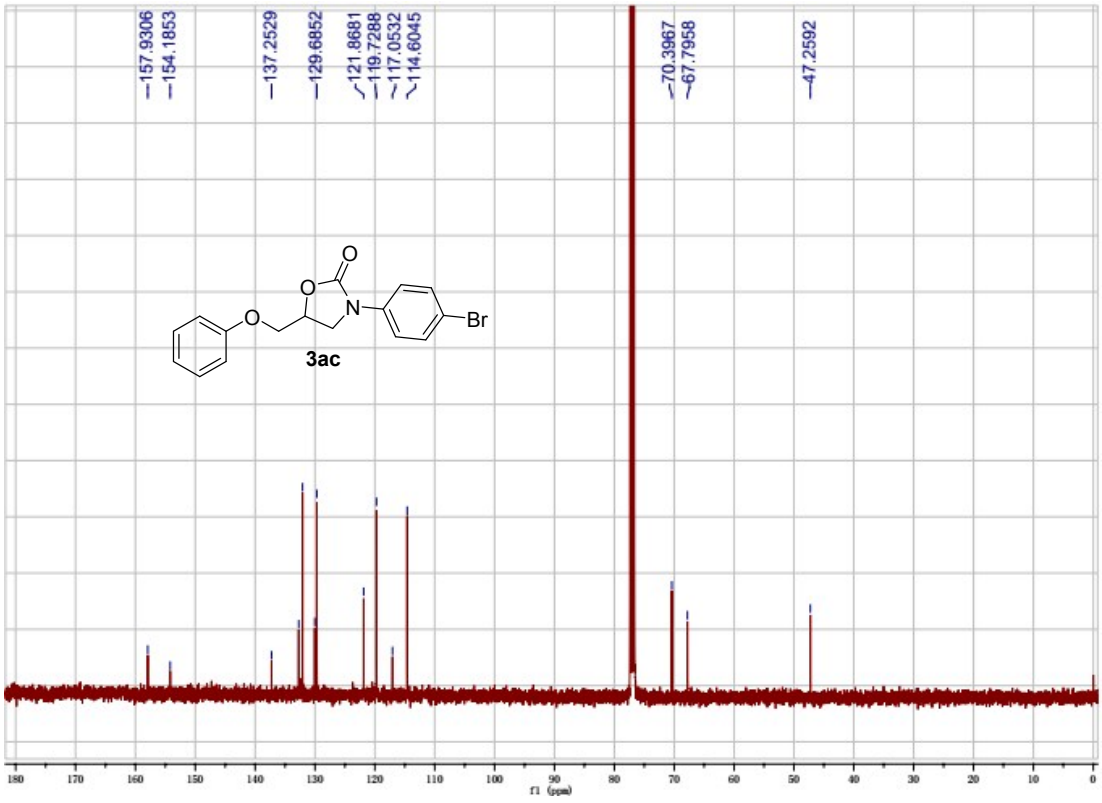
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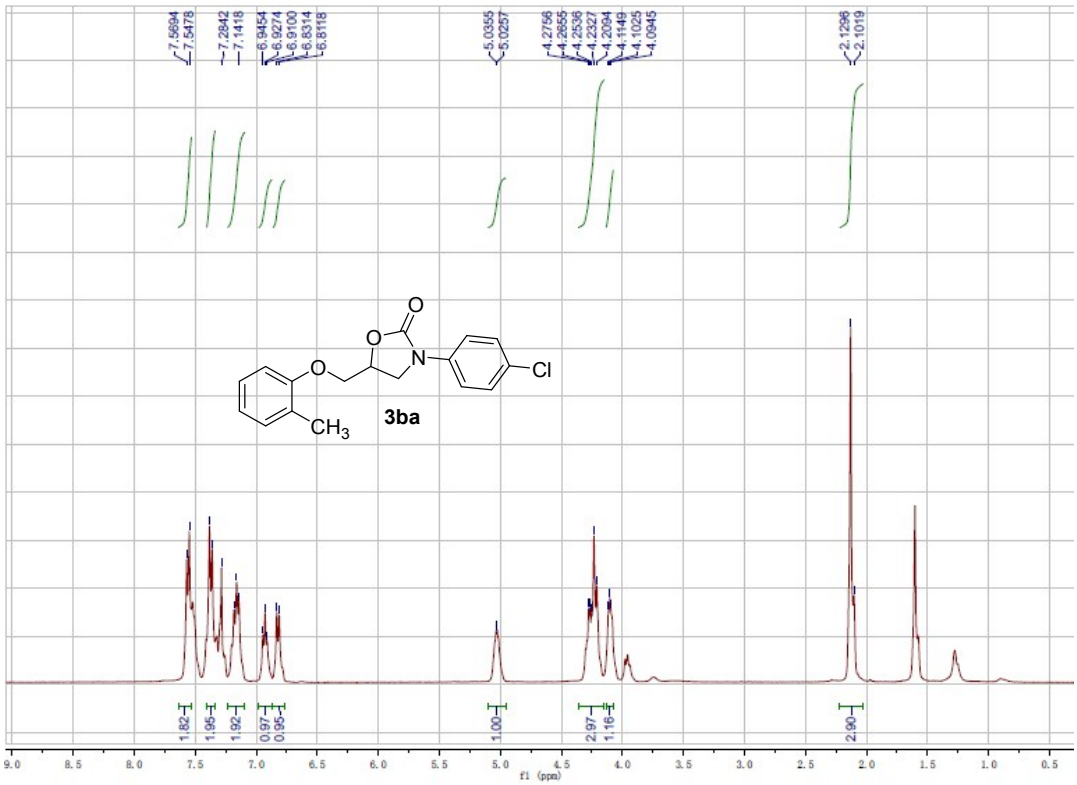
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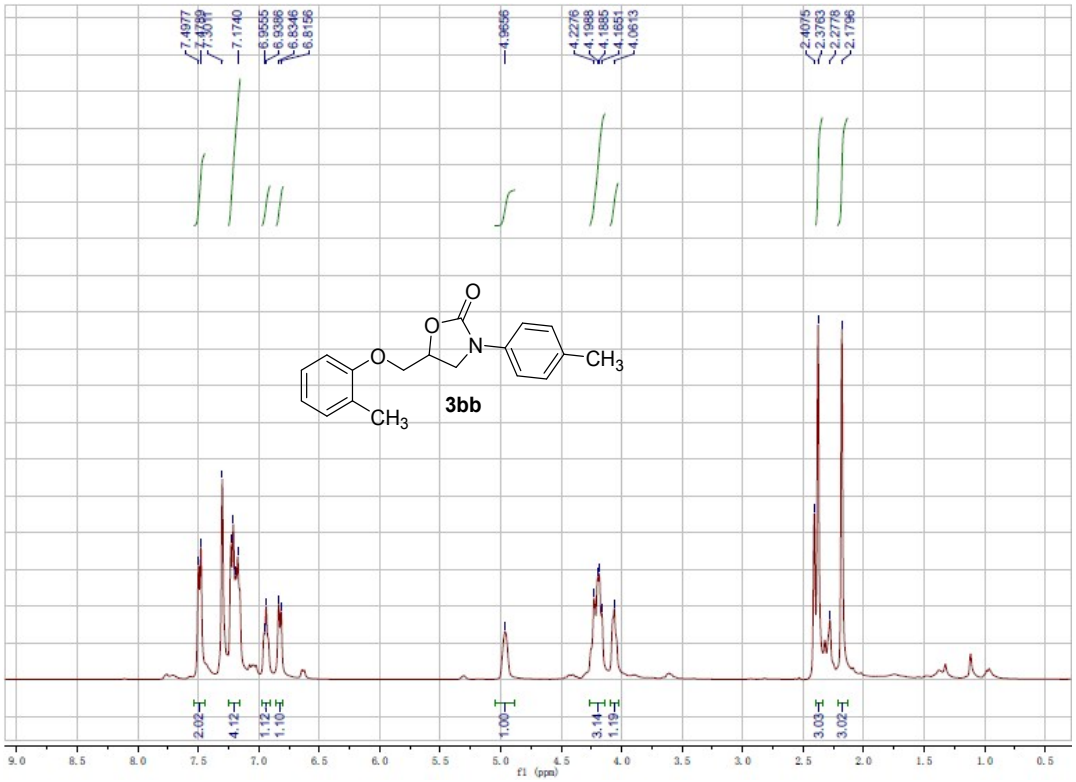
4.0945
2.1296
2.1019
O
O
N
O
Cl
CH3
3ba
1.82
1.95
1.92
0.97
0.95
1.00
2.97
1.16
2.90
f1 (ppm)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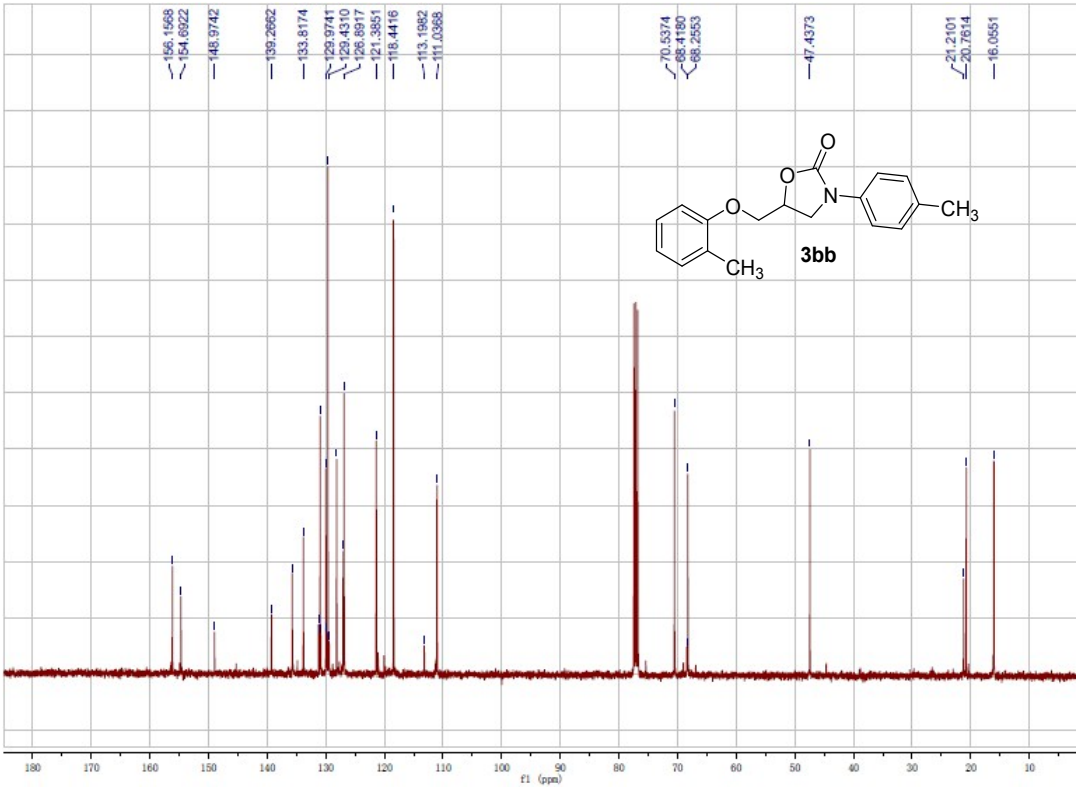
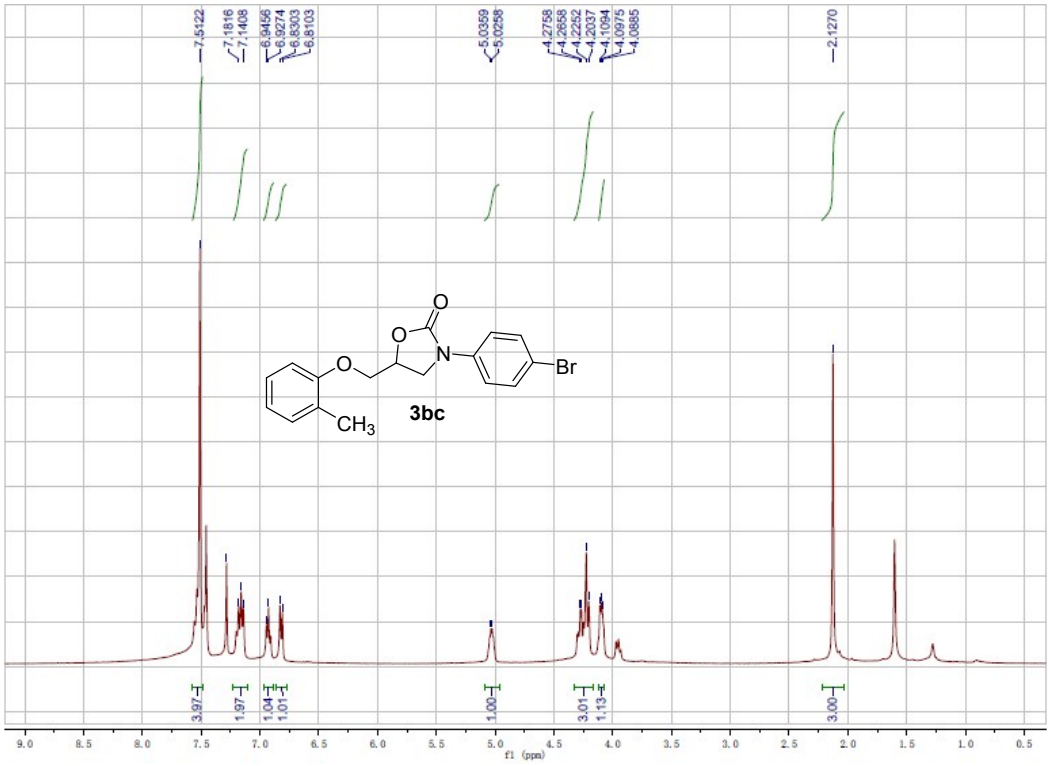
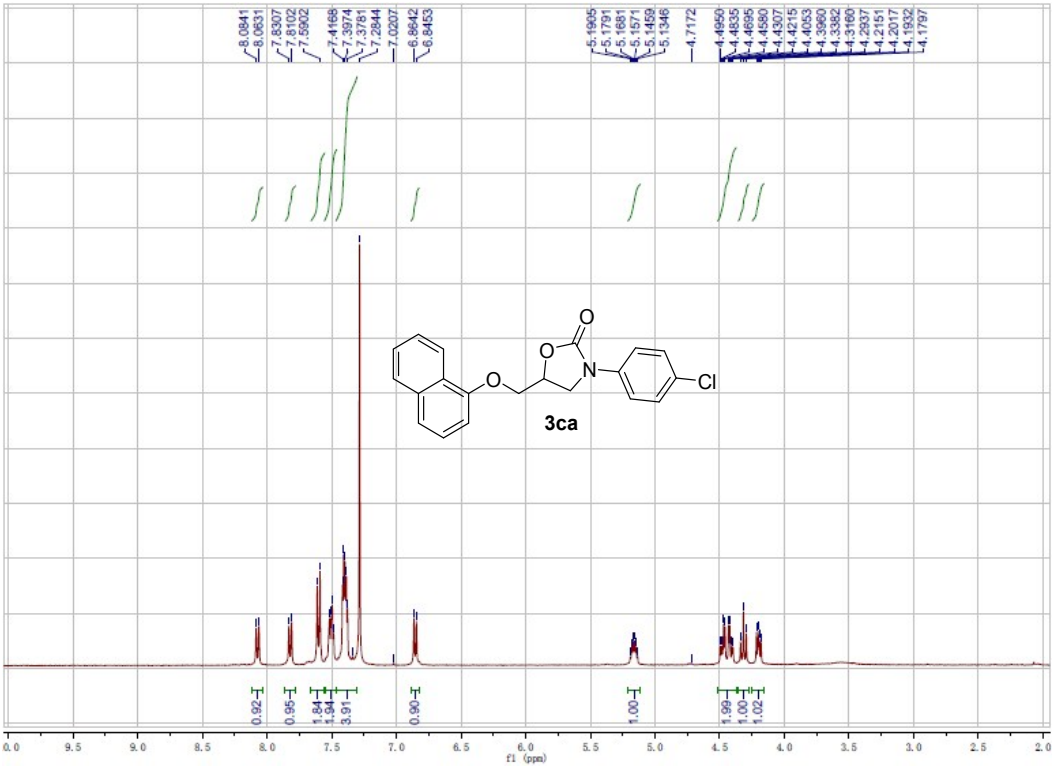
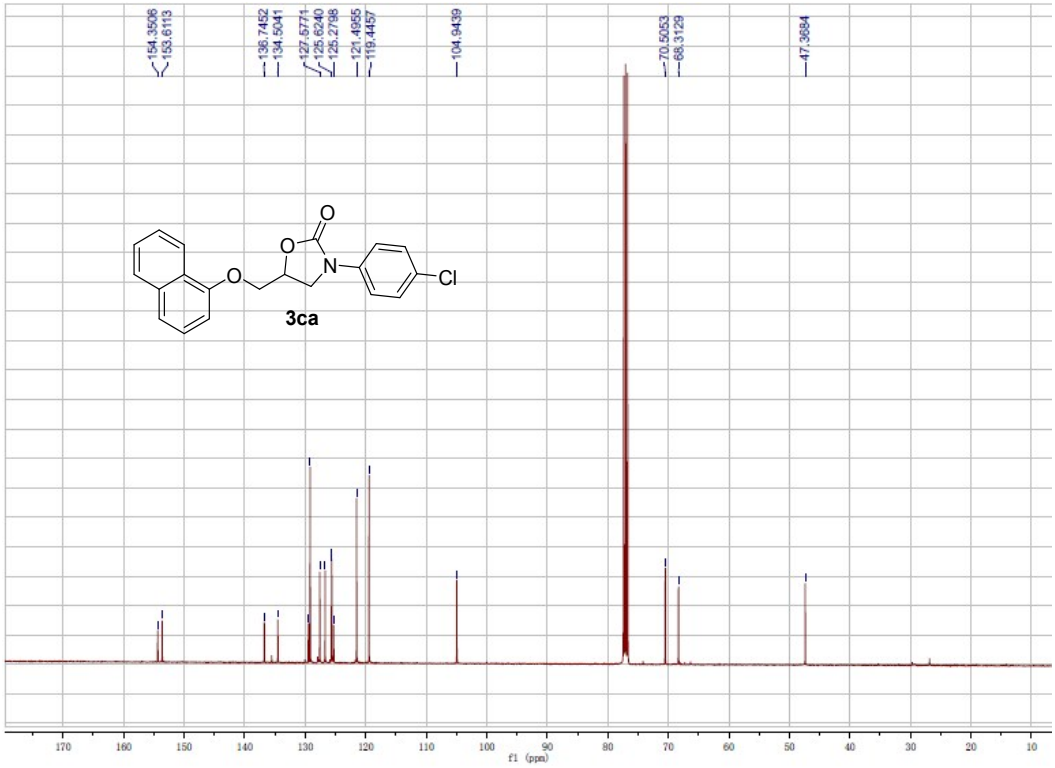
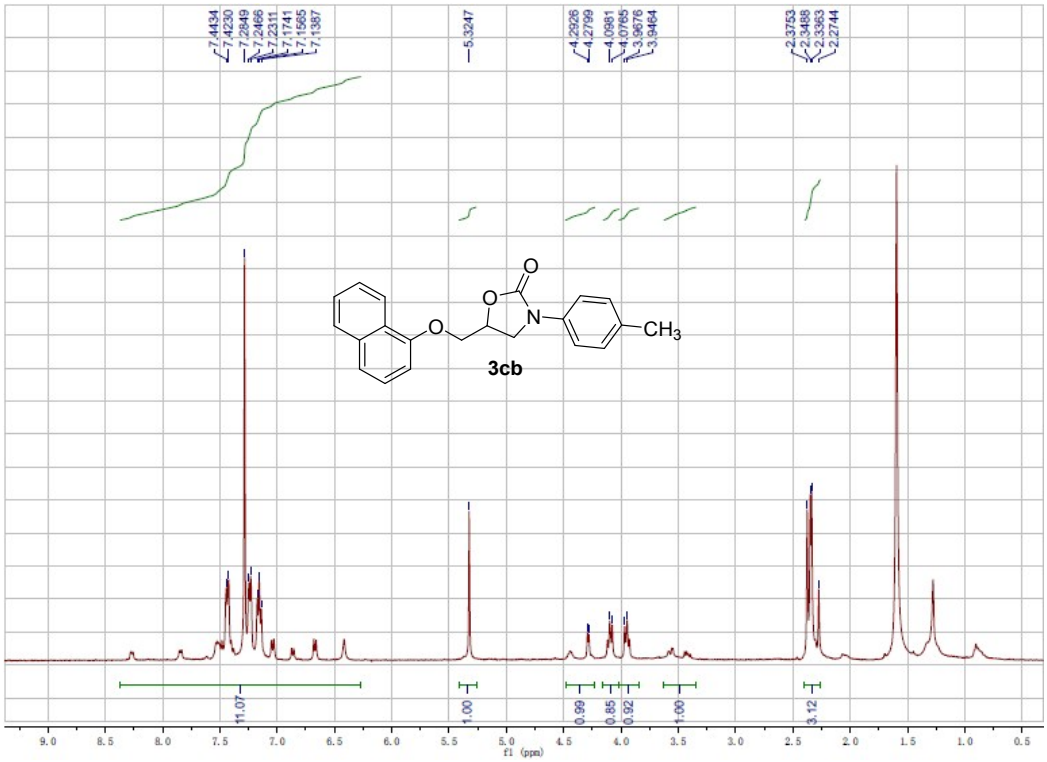
7.4789
7.3011
7.1740
6.9555
6.9386
6.8346
6.8156
4.9656
4.2276
4.1988
4.1885
4.1651
4.0613
2.4075
2.3763
2.2778
2.1796
O
O
N
O
CH3
CH3
3bb
2.02
4.12
1.12
1.10
1.00
3.14
1.19
3.03
3.02
f1 (ppm)

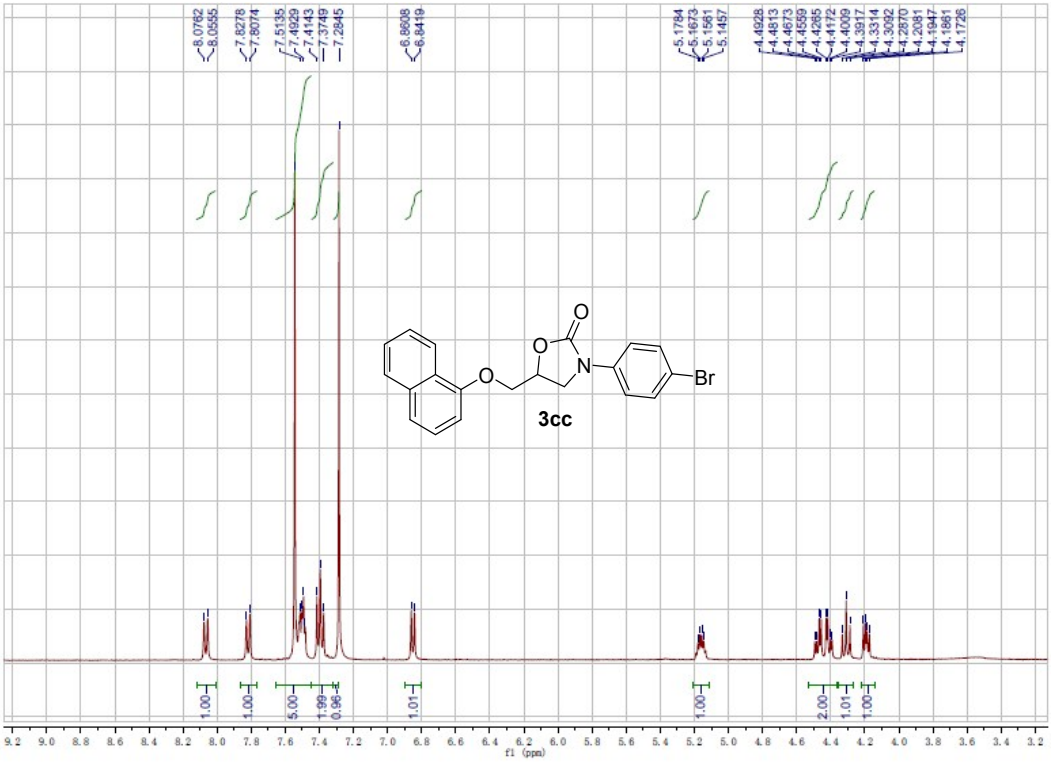

156.1568
154.6922
148.9742
139.2662
133.8174
129.9741
129.4310
126.8917
121.3851
116.4416
113.1982
111.0368
70.5374
68.4180
68.2553
47.4373
21.2101
20.7814
16.0551
O
O
N
O
CH3
CH3
3bb
f1 (ppm)

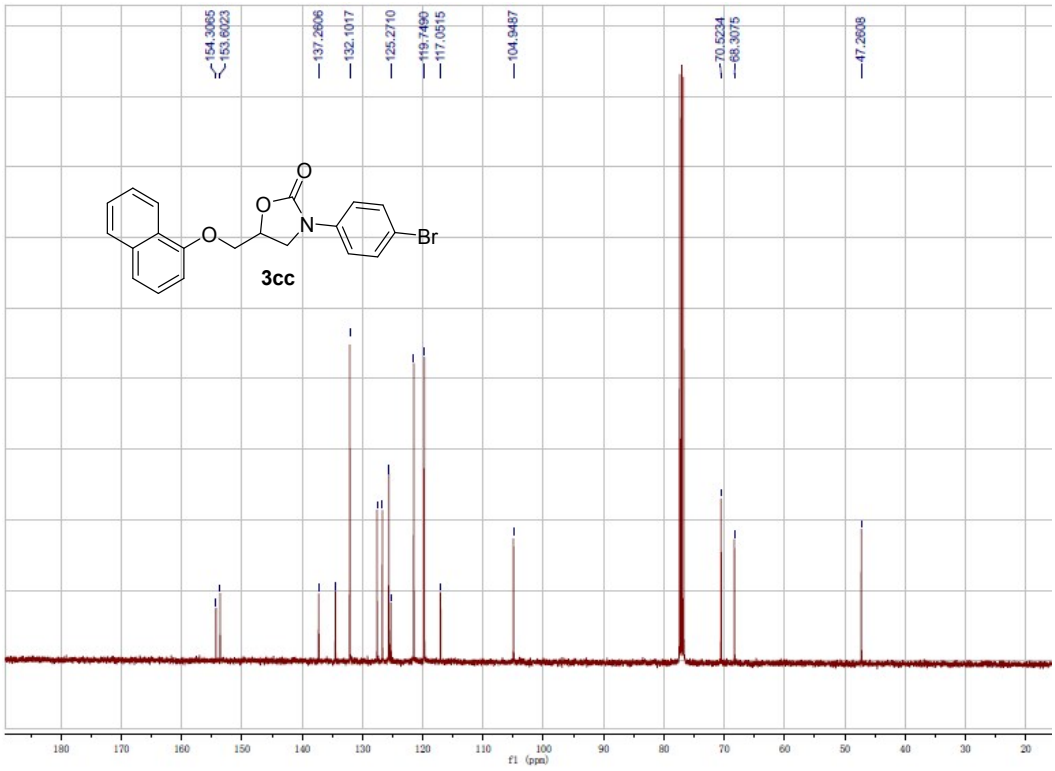

7.5122
7.1816
7.1408
6.8456
6.8274
6.8303
6.8103
5.0359
5.0258
4.2758
4.2658
4.2252
4.2037
4.1094
4.0975
4.0885
2.1270
O
O
N
O
Br
CH3
3bc
3.97
1.97
1.04
1.01
1.00
3.01
1.13
3.00
f1 (ppm)

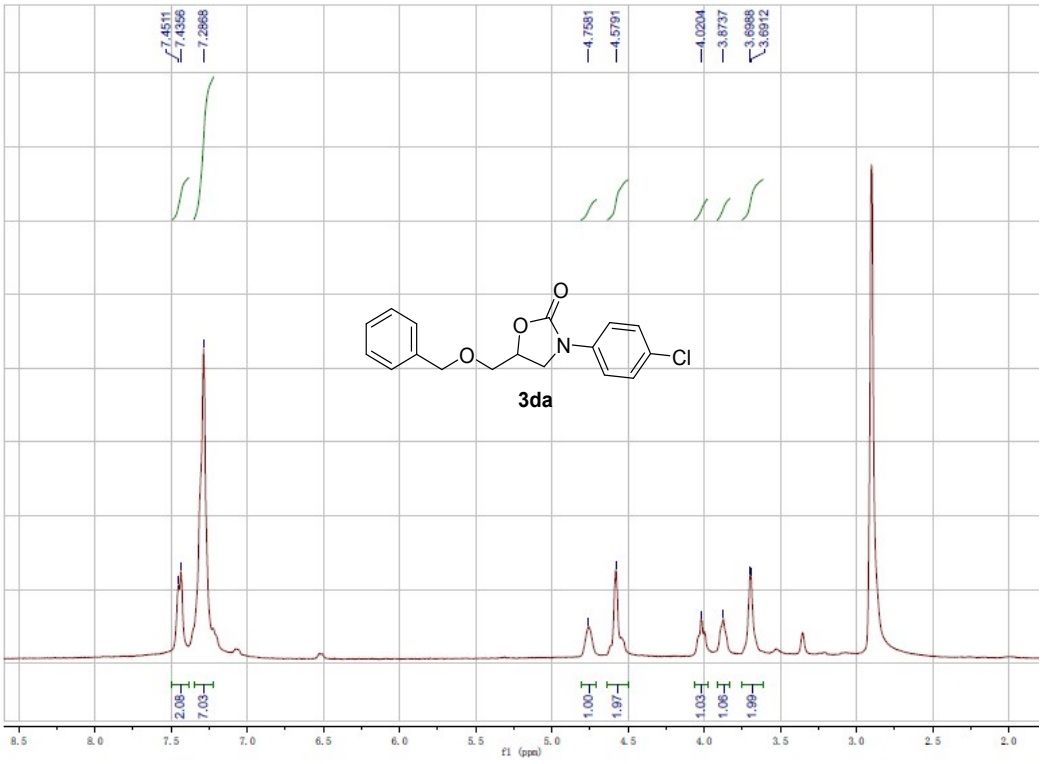

8.0841
8.0631
7.8307
7.8102
7.5902
7.4168
7.3974
7.3781
7.2844
7.0207
6.8642
6.8453
5.1905
5.1791
5.1681
5.1571
5.1459
5.1346
4.7172
4.4950
4.4835
4.4695
4.4580
4.4307
4.4215
4.4053
4.3960
4.3382
4.3160
4.2937
4.2151
4.2017
4.1932
4.1797
0.92
0.95
1.84
1.94
3.91
0.90
1.00
1.99
1.00
1.02
f1 (ppm)
O
O
N
O
Cl
3ca

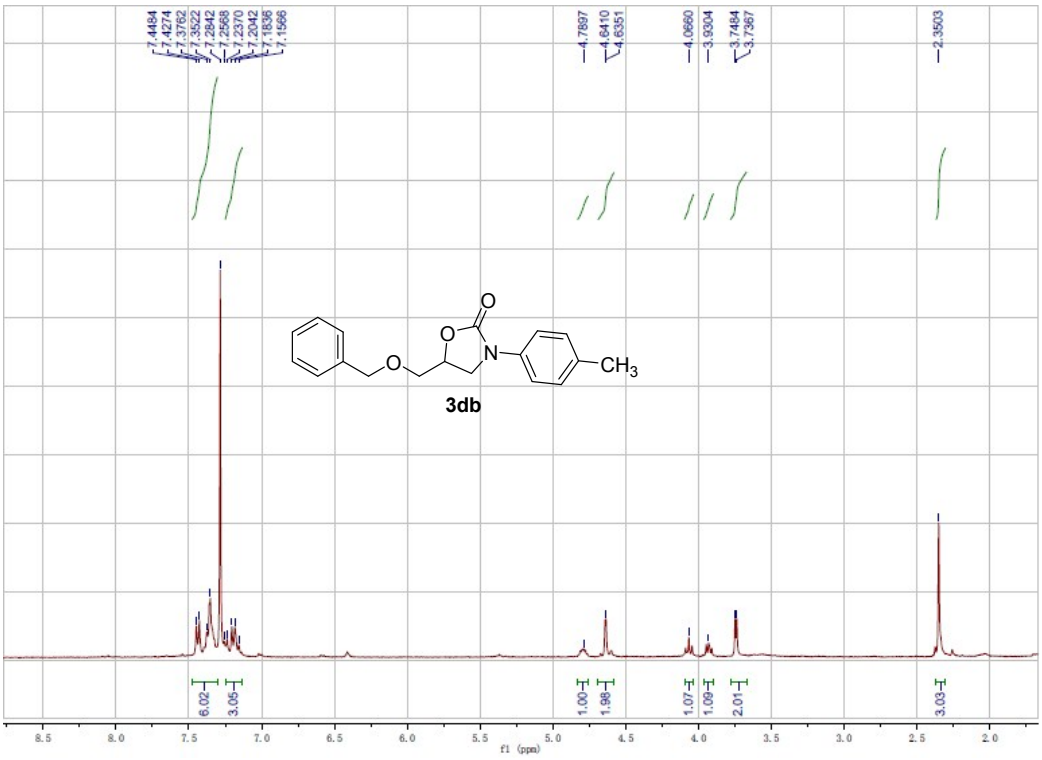

154.3506
153.6113
136.7452
134.5041
127.5771
125.6240
125.2798
121.4955
119.4457
104.9439
70.5053
68.3129
47.3684
f1 (ppm)
O
O
N
O
Cl
3ca


7.4434
7.4230
7.2849
7.2466
7.2311
7.1741
7.1565
7.1387
5.3247
4.2926
4.2799
4.0981
4.0765
3.9676
3.9464
2.3753
2.3488
2.3363
2.2744
O
O
N
O
CH3
3cb
11.07
1.00
0.99
0.85
0.92
1.00
3.12
f1 (ppm)

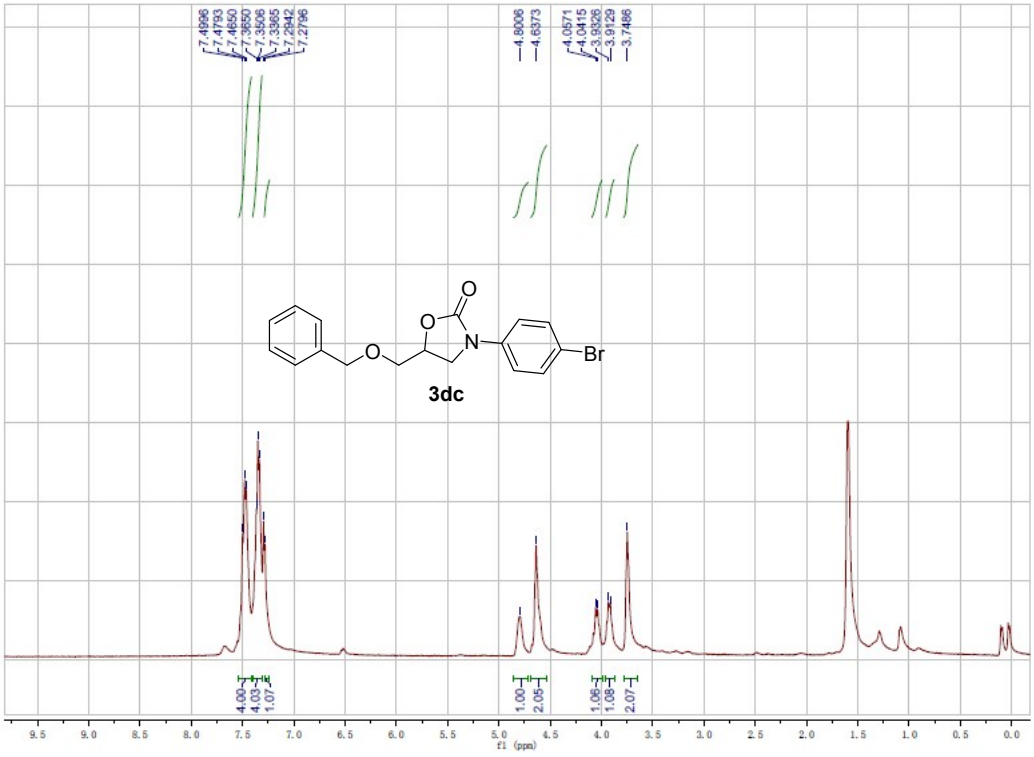

8.0762
8.0555
7.8278
7.8074
7.5135
7.4929
7.4143
7.3749
7.2845
6.8608
6.8419
5.1784
5.1673
5.1581
5.1457
4.4928
4.4813
4.4673
4.4559
4.4285
4.4172
4.4009
4.3917
4.3314
4.3092
4.2870
4.2081
4.1947
4.1861
4.1726
O
O
N
O
Br
3cc
1.00
1.00
5.00
1.99
0.96
1.01
1.00
2.00
1.01
1.00
f1 (ppm)


154.3065
153.6023
137.2606
132.1017
125.2710
119.7490
117.0515
104.9487
70.5234
68.3075
47.2608
O
O
N
O
Br
3cc
f1 (ppm)

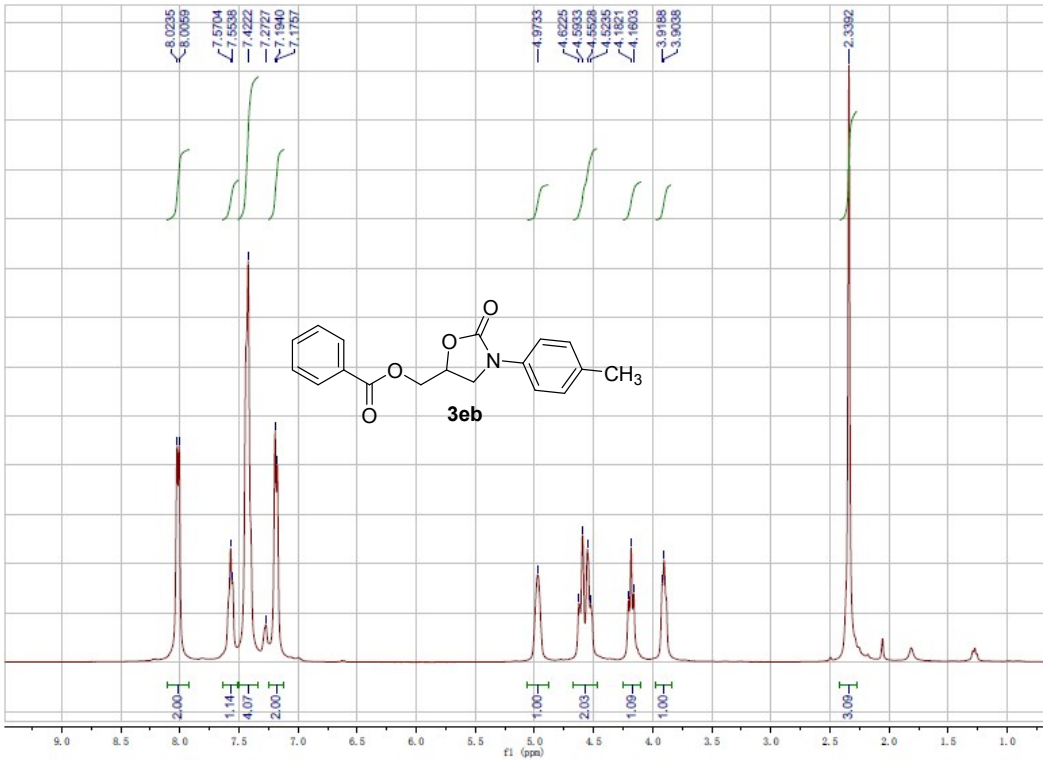

7.4511
7.4366
7.2868
4.7581
4.5791
4.0204
3.8737
3.6988
3.6912
O
O
N
O
Cl
3da
2.08
7.03
1.00
1.97
1.03
1.06
1.99
f1 (ppm)

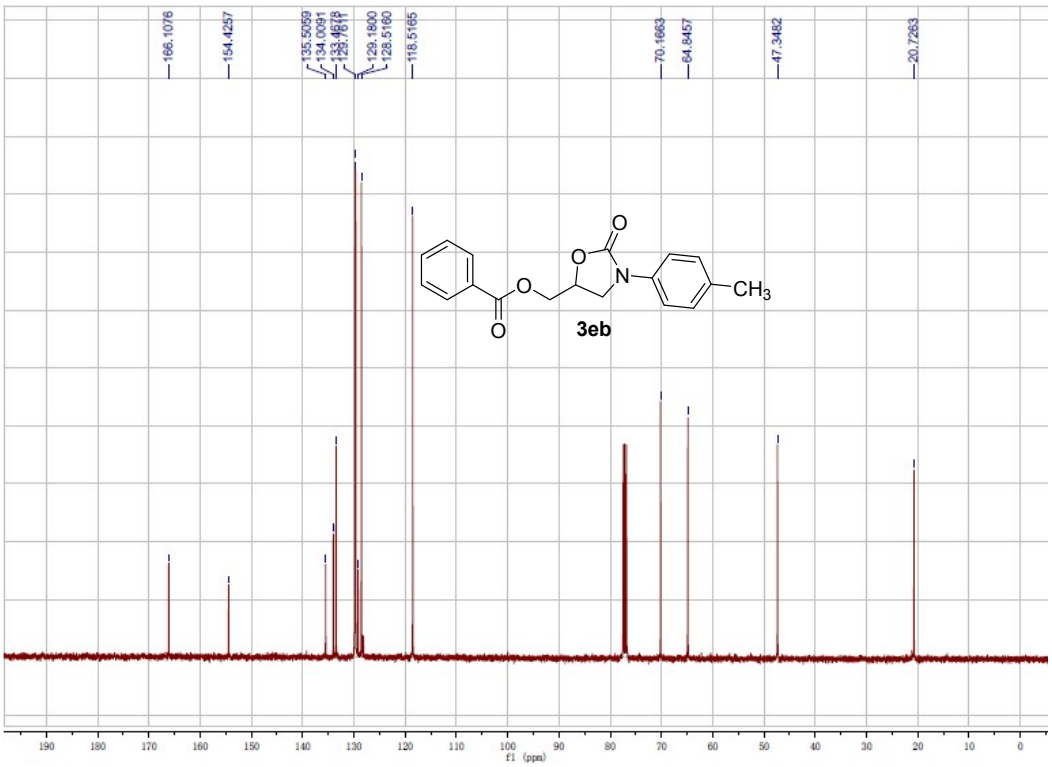

7.4484
7.4274
7.3762
7.3522
7.2842
7.2568
7.2370
7.2042
7.1836
7.1566
4.7897
4.6410
4.6351
4.0660
3.9304
3.7484
3.7367
2.3503
O
O
N
O
CH3
6.02
3.05
1.00
1.98
1.07
1.09
2.01
3.03
f1 (ppm)

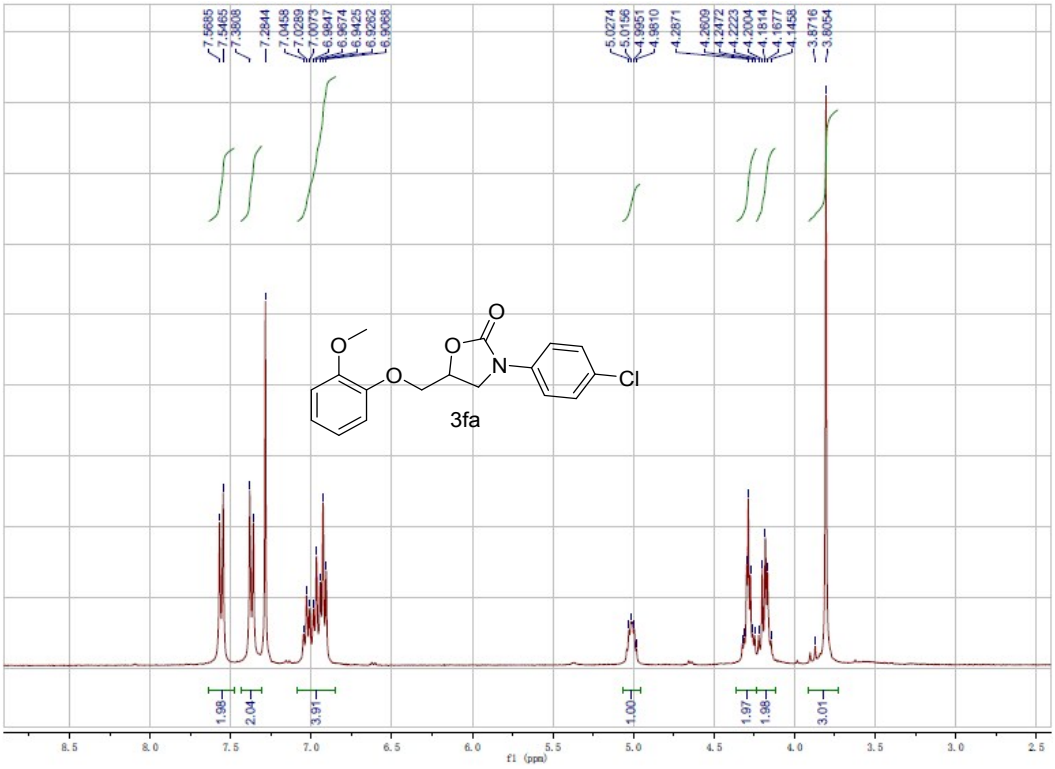
3db

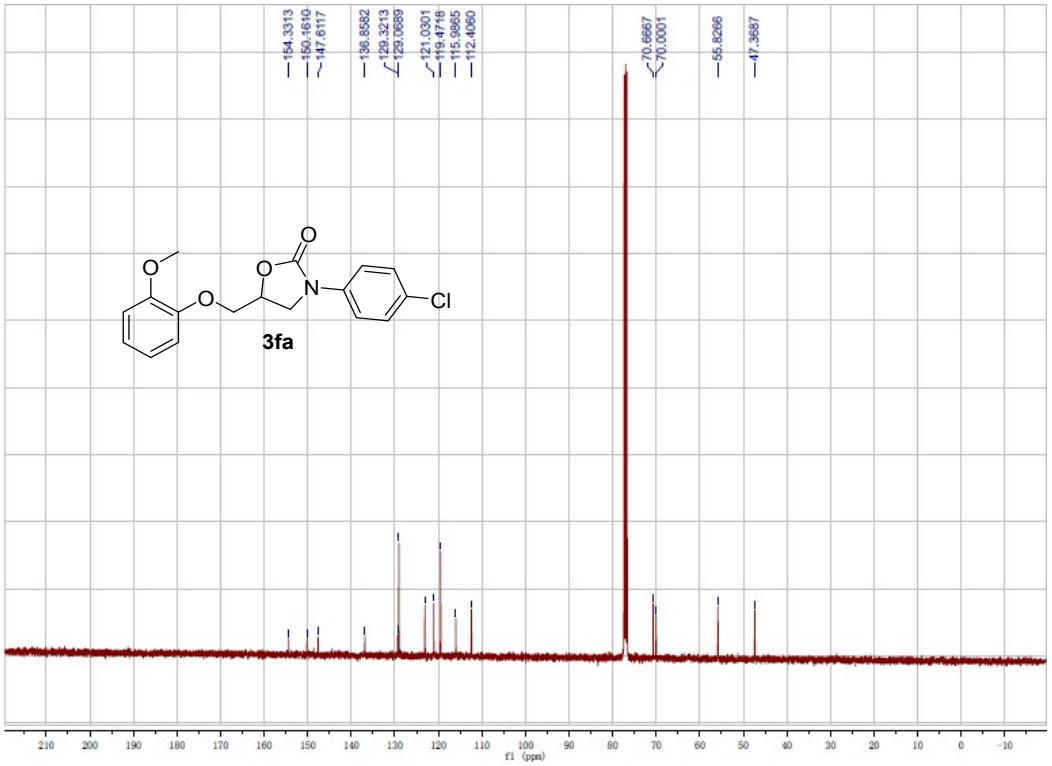

7.4996
7.4793
7.4650
7.3650
7.3506
7.3365
7.2942
7.2796
4.8006
4.6373
4.0571
4.0415
3.9326
3.9129
3.7486
O
O
N
O
Br
4.00
4.03
1.07
1.00
2.05
1.06
1.08
2.07
f1 (ppm)

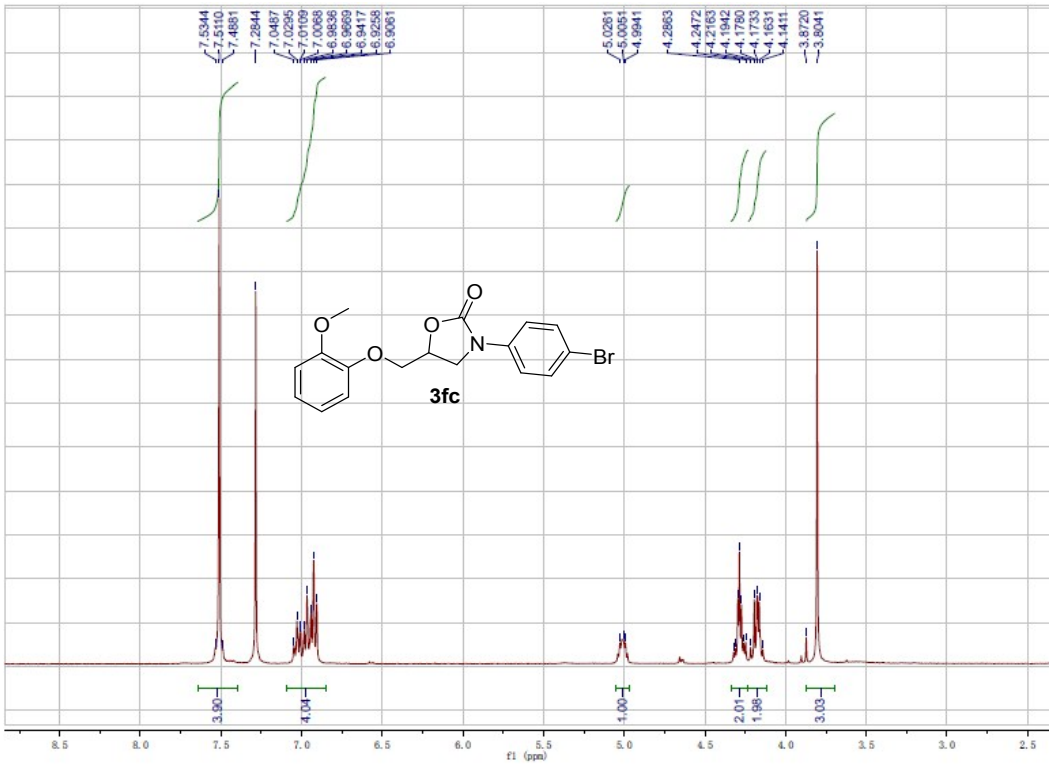
3dc

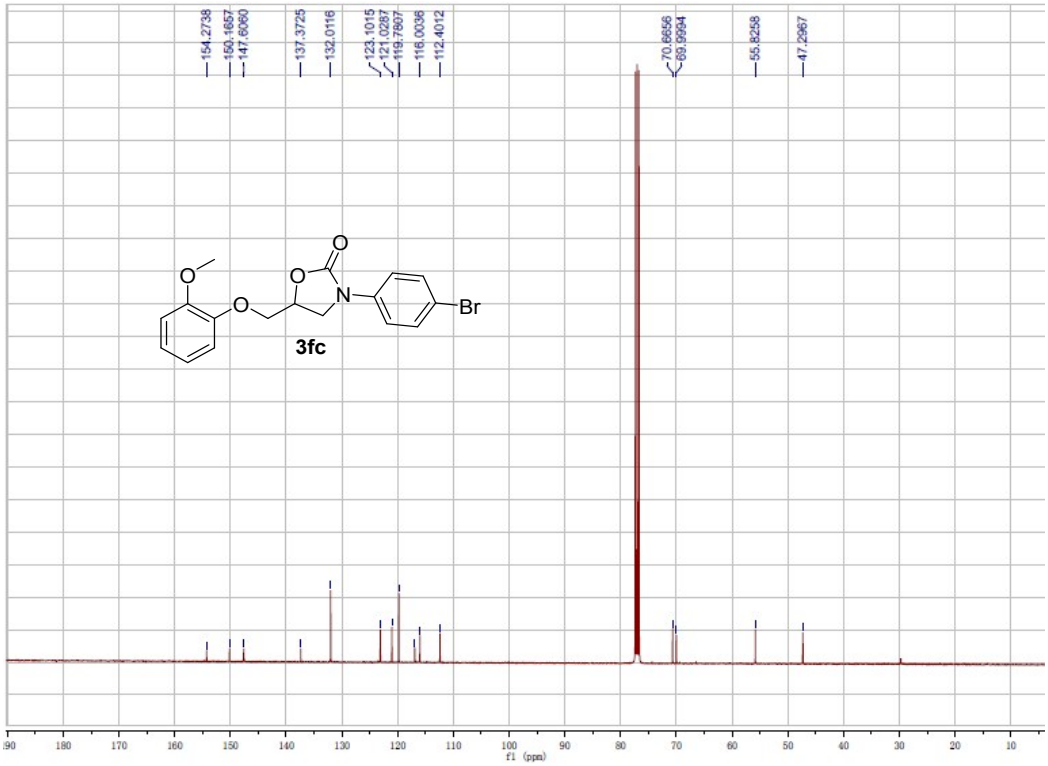

8.0235
8.0069
7.5704
7.5538
7.4222
7.2727
7.1940
7.1757
4.9733
4.6225
4.5933
4.5528
4.5235
4.1821
4.1603
3.9188
3.9038
2.3392
2.00
1.14
4.07
2.00
1.00
2.03
1.09
1.00
3.09
f1 (ppm)
O
O
O
N
CH3
O
3eb

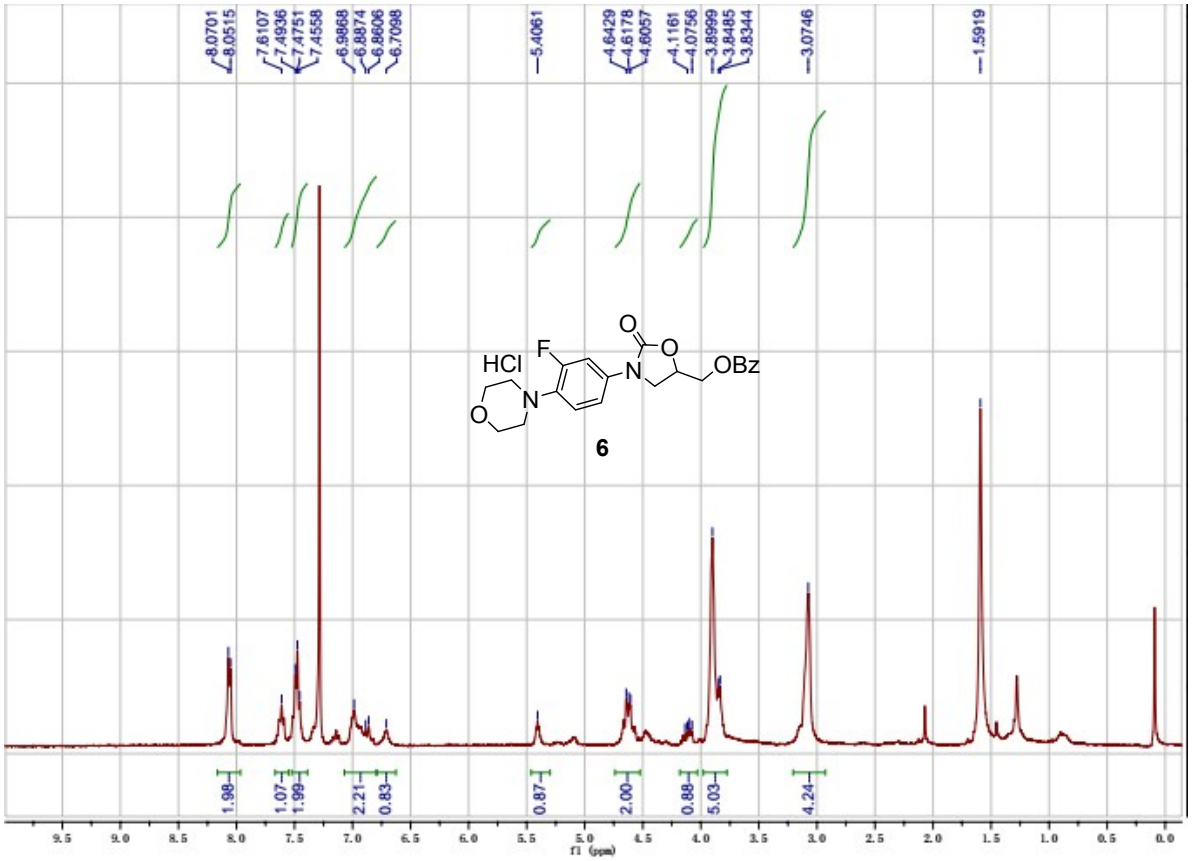

166.1076
154.4257
135.5089
134.0091
129.1800
128.5180
116.5165
70.1663
64.8457
47.3482
20.7263
f1 (ppm)
O
O
O
N
CH3
O
3eb


7.5685
7.5465
7.3808
7.2844
7.0458
7.0289
7.0073
6.9847
6.9674
6.9425
6.9262
6.9068
5.0274
5.0156
4.9951
4.9810
4.2871
4.2609
4.2472
4.2223
4.2004
4.1814
4.1677
4.1458
3.8716
3.8054
1.98
2.04
3.91
1.00
1.97
1.98
3.01
O
O
O
N
Cl
3fa
f1 (ppm)


154.3313
150.1610
147.6117
136.8582
129.3213
129.0689
121.0301
119.4716
115.9865
112.4060
70.6667
70.0001
55.8266
47.3687
O
O
O
N
Cl
3fa
f1 (ppm)

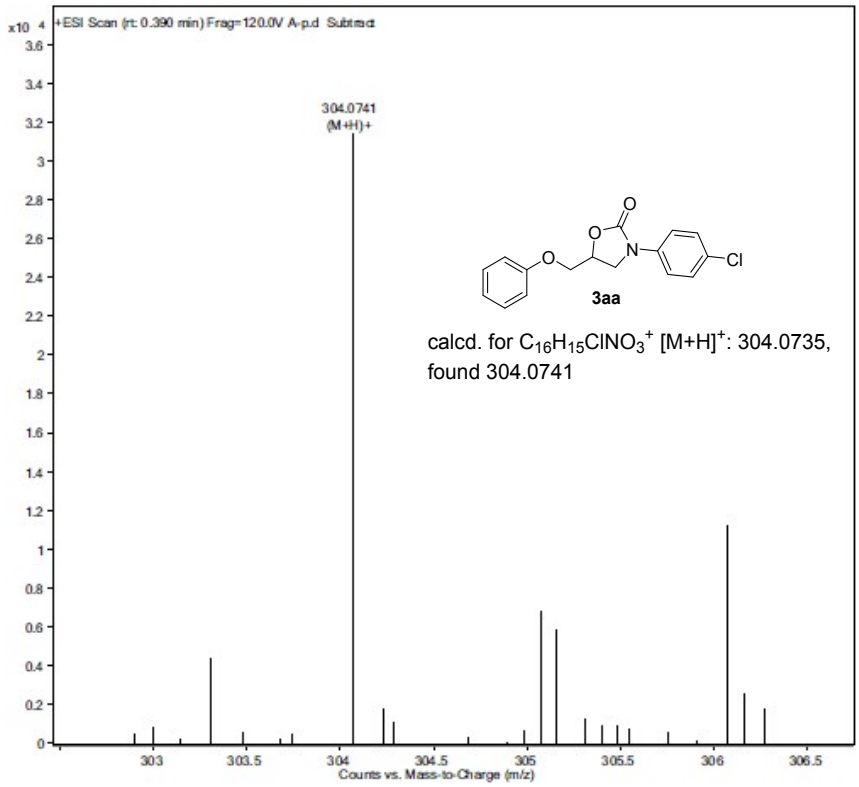

7.5344
7.5110
7.4881
7.2844
7.0457
7.0295
7.0109
7.0068
6.9836
6.9669
6.9417
6.9258
6.9061
5.0261
5.0051
4.9941
4.2863
4.2472
4.2163
4.1942
4.1780
4.1733
4.1631
4.1411
3.8720
3.8041
3.90
4.04
1.00
2.01
1.98
3.03
O
O
O
N
Br
3fc
f1 (ppm)

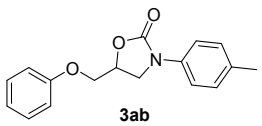

154.2738
150.1657
147.6060
137.3725
132.0116
123.1015
121.0287
119.7807
116.0036
112.4012
70.6656
69.9994
55.8258
47.2967
O
O
O
N
Br
3fc
f1 (ppm)


8.0701
8.0515
7.6107
7.4936
7.4751
7.4558
6.9868
6.8874
6.8606
6.7098
5.4061
4.6429
4.6178
4.6057
4.1161
4.0756
3.8999
3.8485
3.8344
3.0746
1.5919
1.98
1.07
1.99
2.21
0.83
0.87
2.00
0.88
5.03
4.24
f1 (ppm)
HCl
F
O
O
N
OBz
N
O

6

HRMS copies of 2-oxazolidinoes



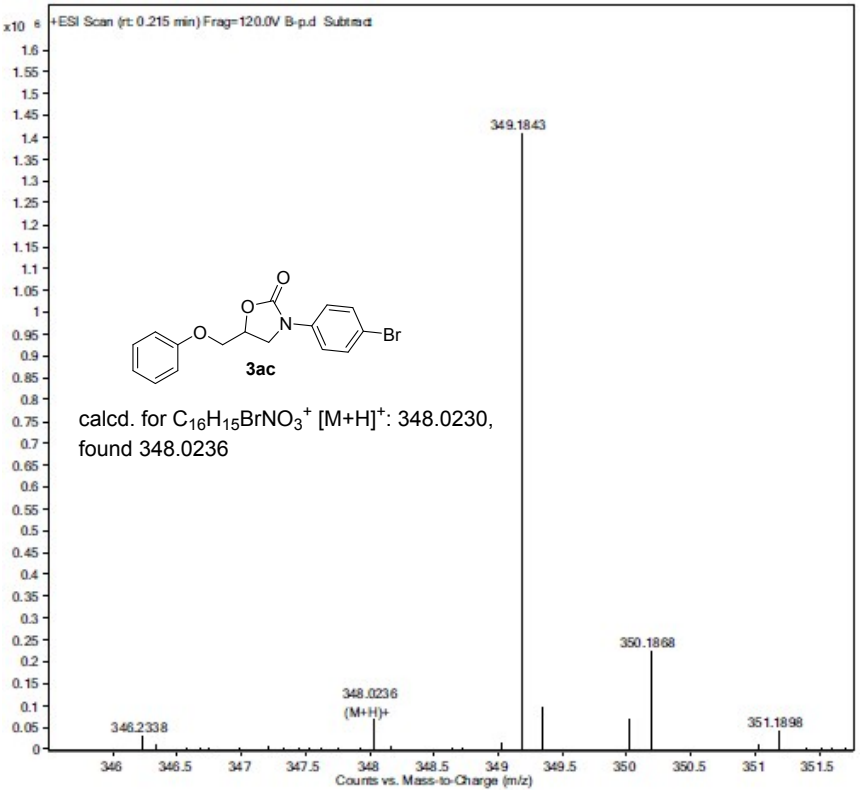


3aa

calcd. for $C_{16}H_{15}ClNO_3^+$ [M+H]$^+$: 304.0735, found 304.0741

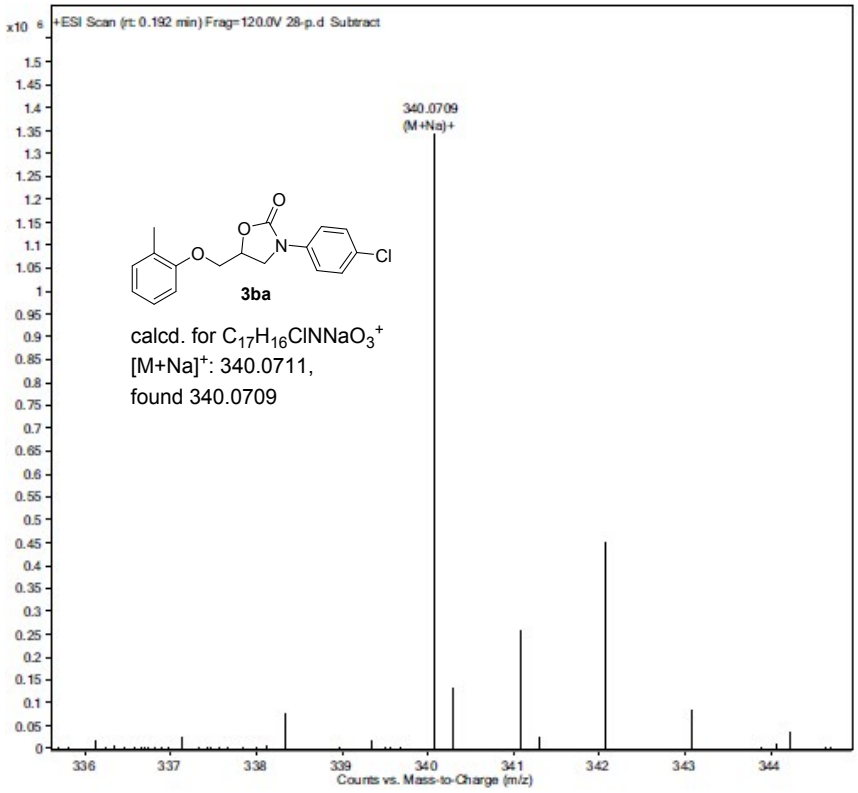
3ab

calcd. for $C_{17}H_{18}NO_3^+$ [M+H]$^+$: 284.1281, found 284.1279



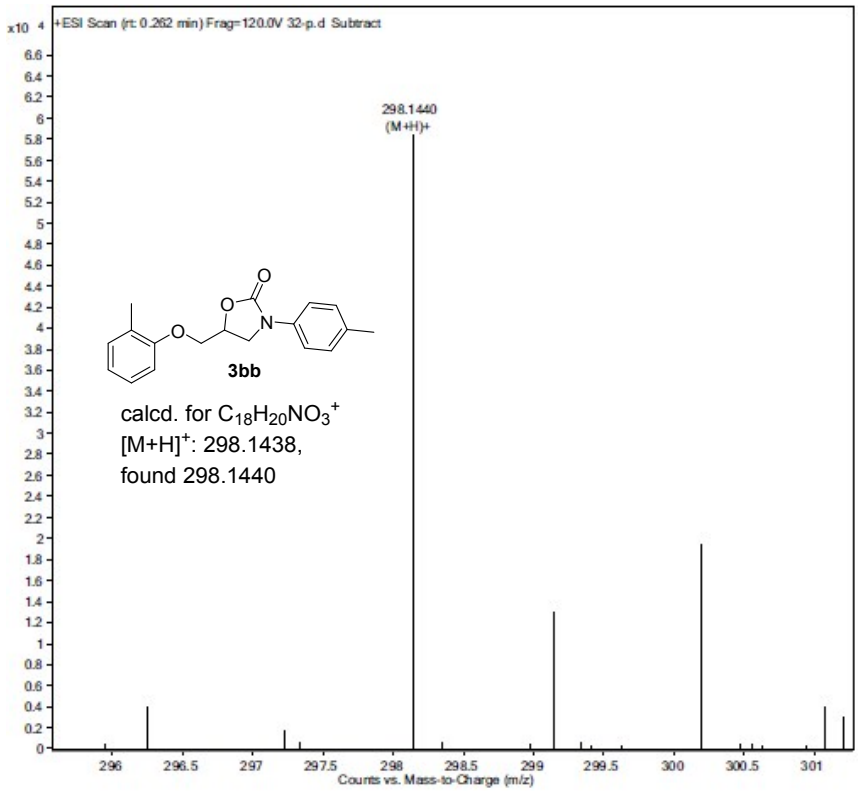
3ac

calcd. for $C_{16}H_{15}BrNO_3^+$ $[M+H]^+$: 348.0230,
found 348.0236



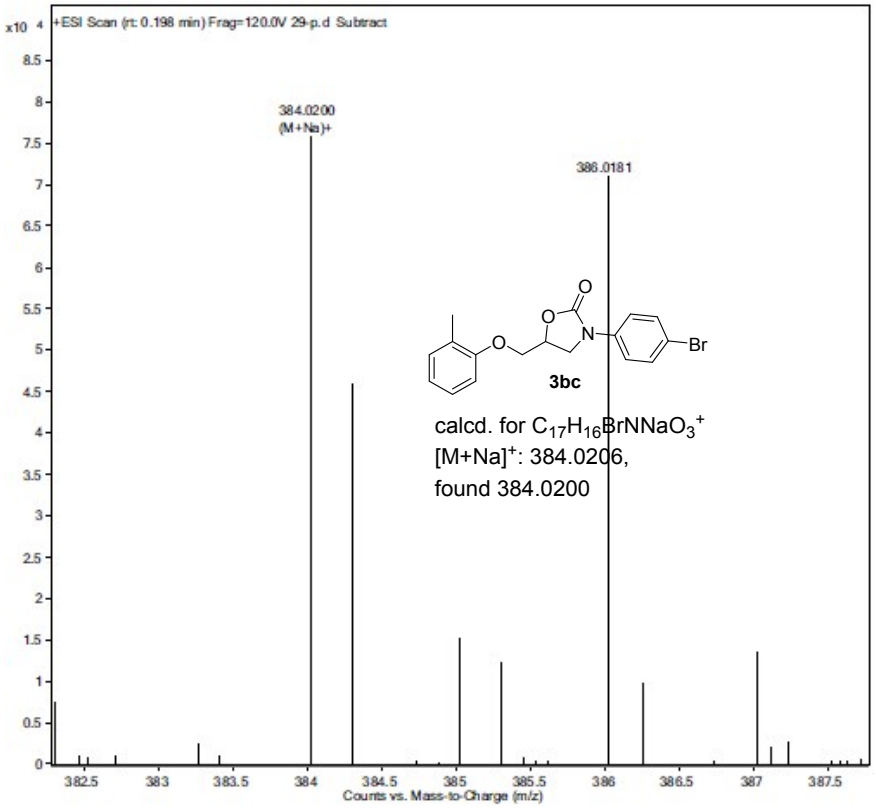
3ba

calcd. for $C_{17}H_{16}ClNNaO_3^+$
$[M+Na]^+$: 340.0711,
found 340.0709



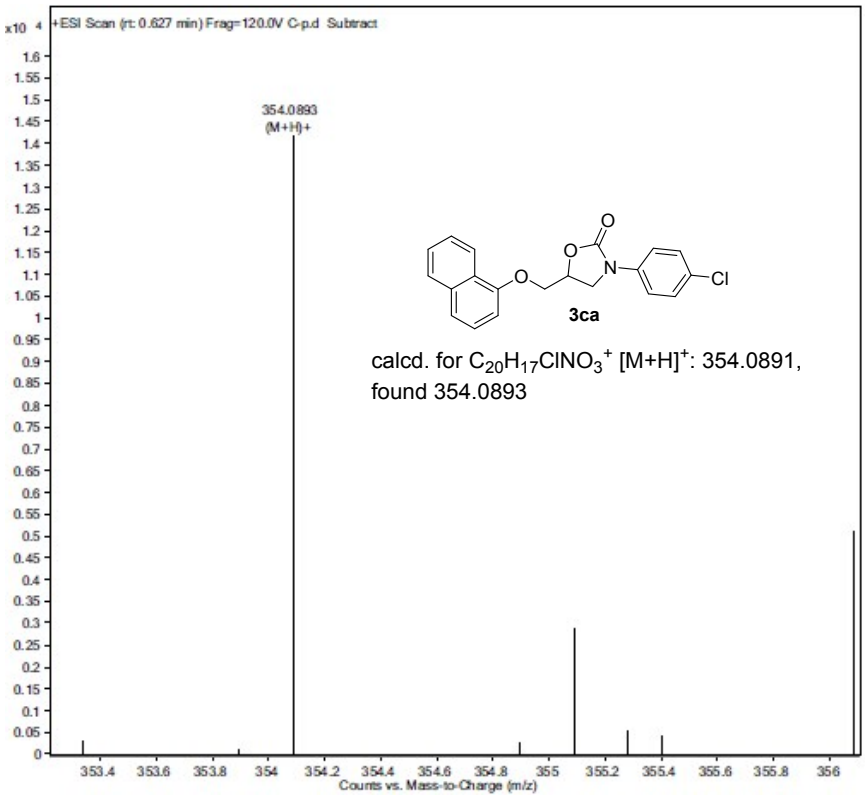
3bb

calcd. for $C_{18}H_{20}NO_3^+$
$[M+H]^+$: 298.1438,
found 298.1440



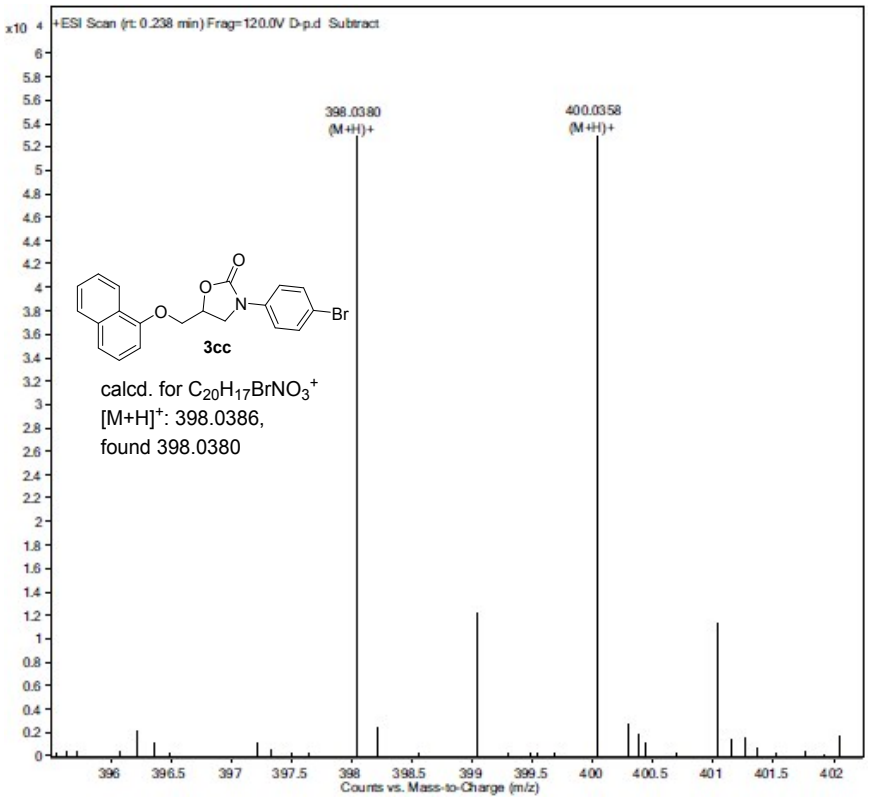
3bc

calcd. for $C_{17}H_{16}BrNNaO_3^+$
$[M+Na]^+$: 384.0206,
found 384.0200



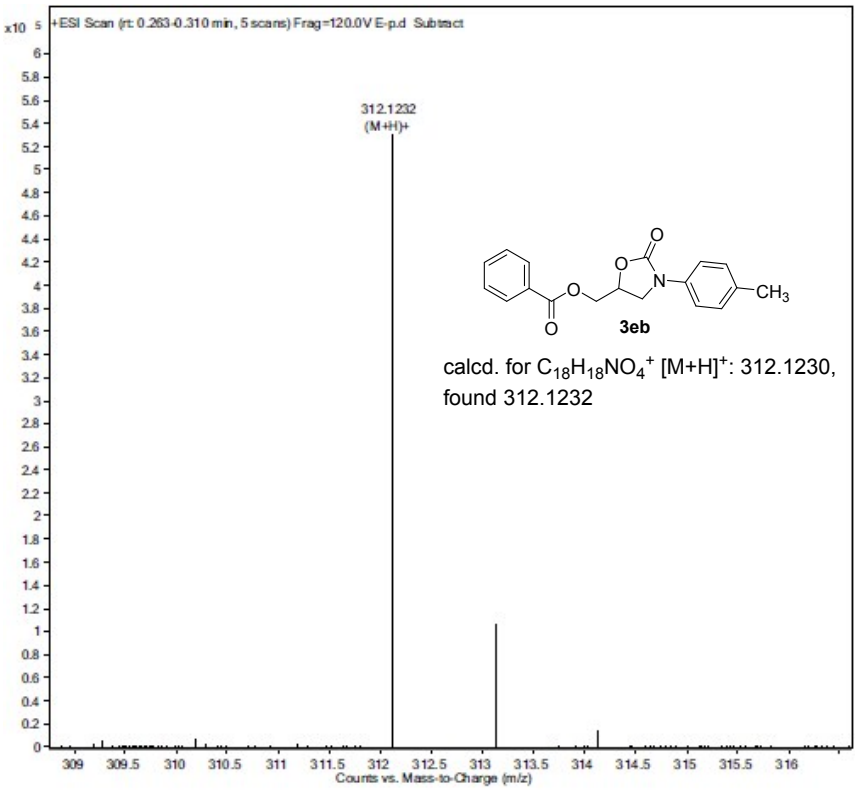
3ca

calcd. for $C_{20}H_{17}ClNO_3^+$ $[M+H]^+$: 354.0891,
found 354.0893



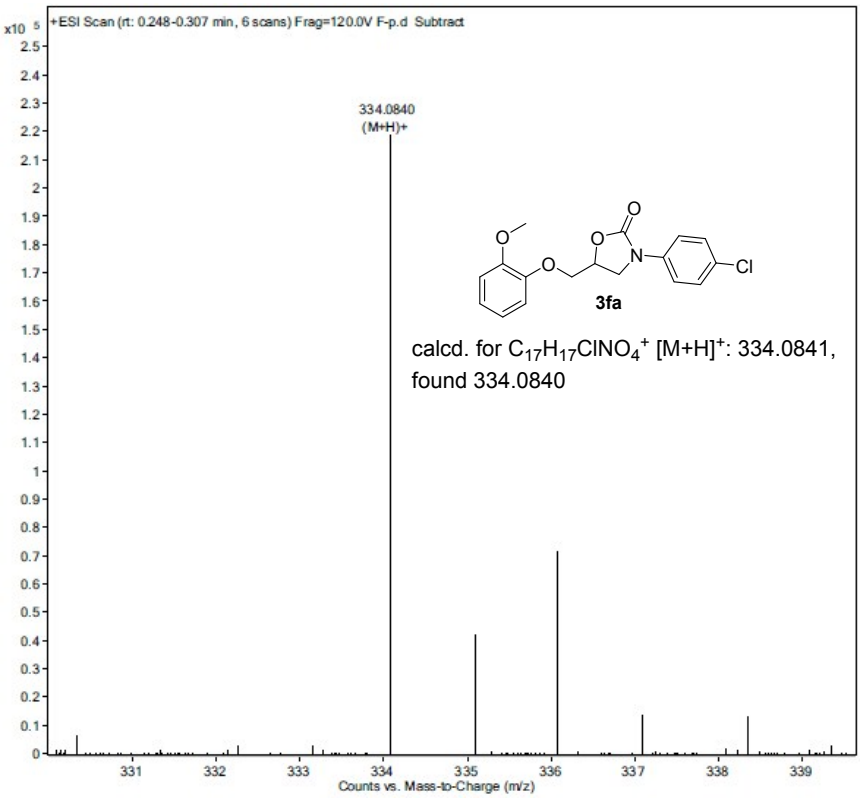
3cc

calcd. for $C_{20}H_{17}BrNO_3^+$
$[M+H]^+$: 398.0386,
found 398.0380



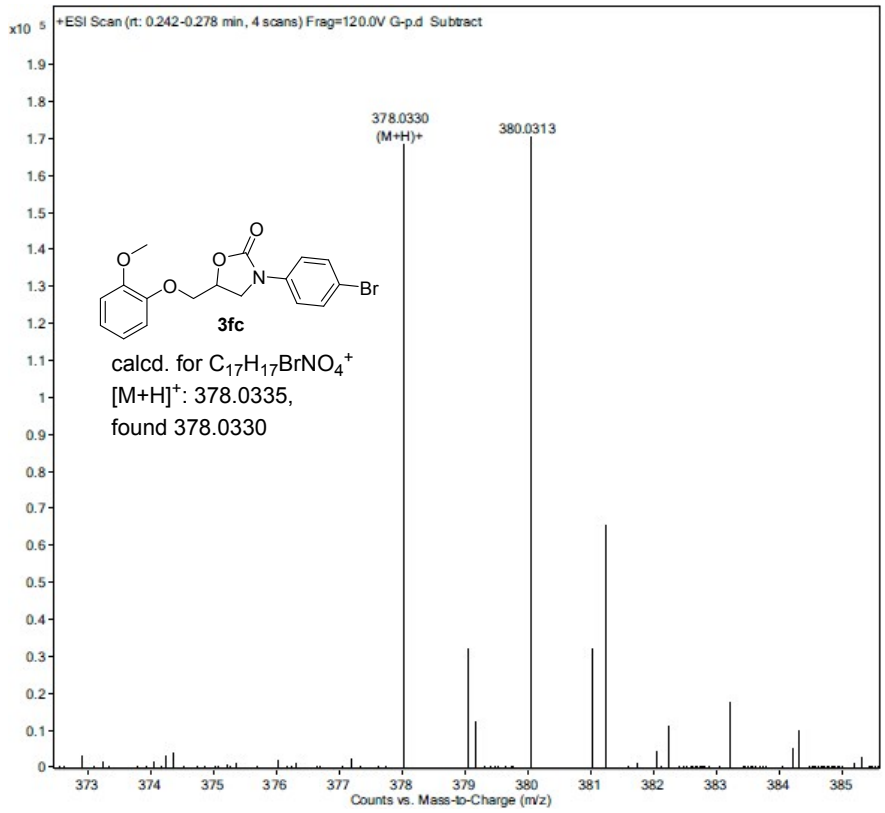
3eb

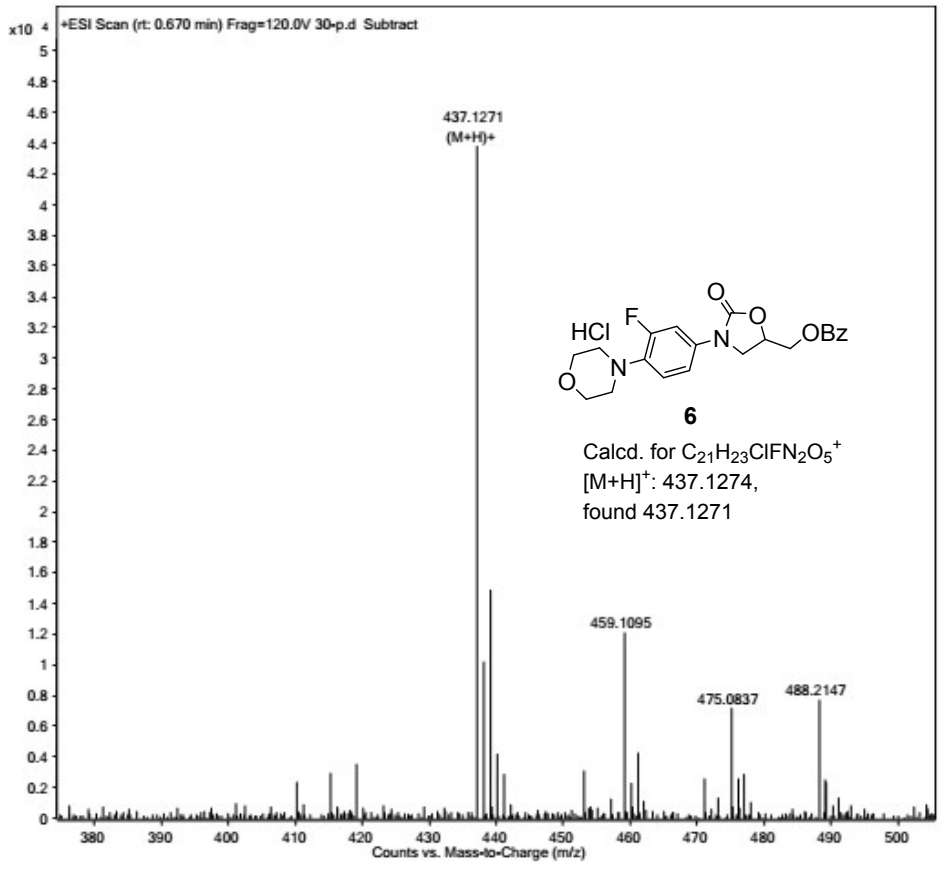
calcd. for $C_{18}H_{18}NO_4^+$ [M+H]$^+$: 312.1230, found 312.1232



3fa

calcd. for $C_{17}H_{17}ClNO_4^+$ [M+H]$^+$: 334.0841, found 334.0840


+ESI Scan (rt: 0.242-0.278 min, 4 scans) Frag=120.0V G-p.d Subtract
x10 5
378.0330
(M+H)+
380.0313
Br
3fc
calcd. for C17H17BrNO4+
[M+H]+: 378.0335,
found 378.0330
Counts vs. Mass-to-Charge (m/z)


+ESI Scan (rt: 0.670 min) Frag=120.0V 30-p.d Subtract
x10 4
437.1271
(M+H)+
HCl
F
OBz
6
Calcd. for C21H23ClFN2O5+
[M+H]+: 437.1274,
found 437.1271
459.1095
475.0837
488.2147
Counts vs. Mass-to-Charge (m/z)