Supporting Information to

Palladium-catalyzed tandem cyclization/sulfonylation of homoallenyl amides with sodium sulfinates

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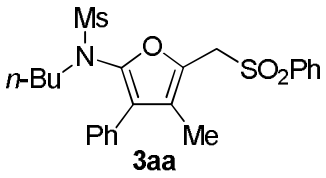

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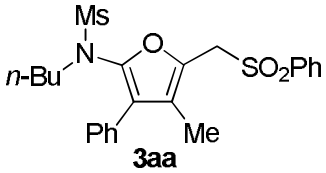

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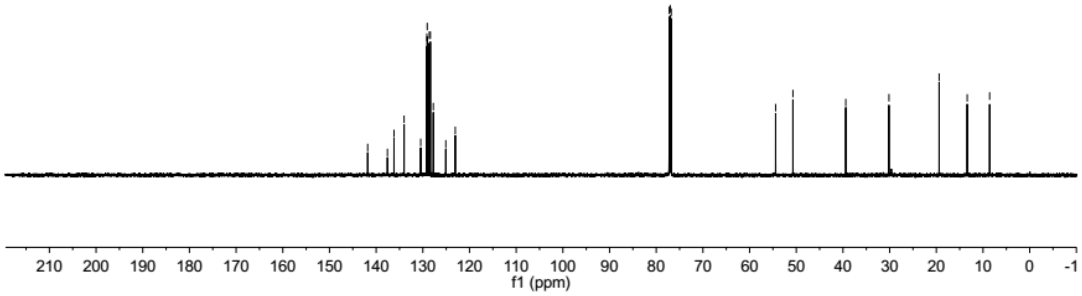


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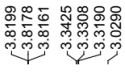
4.3917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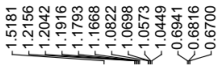
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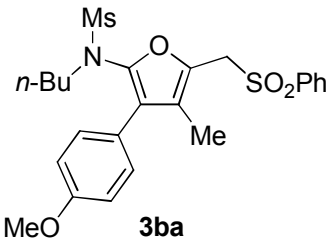
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n-Bu
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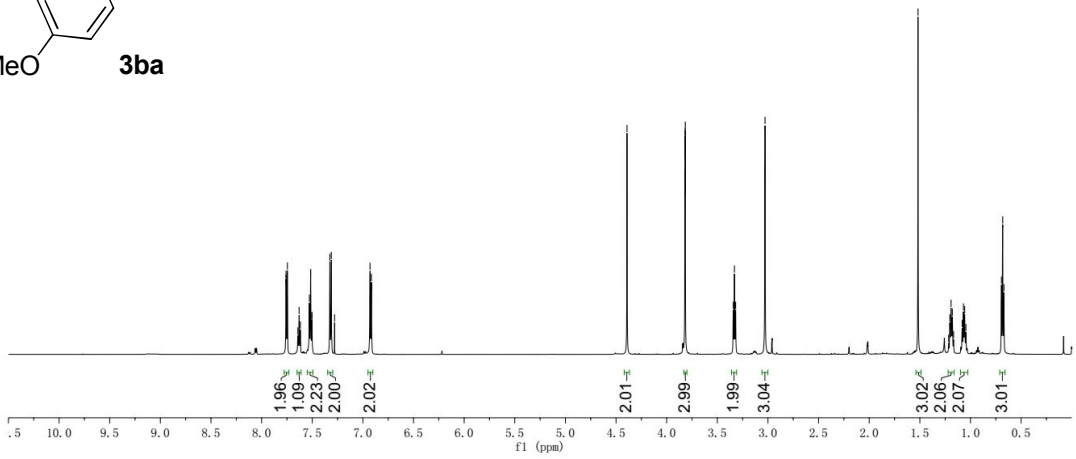
Me
MeO

3ba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f1 (ppm)


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137.5040
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122.6308
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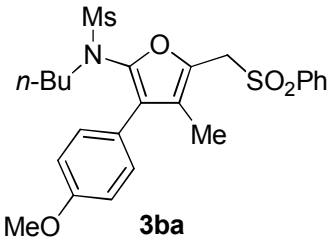
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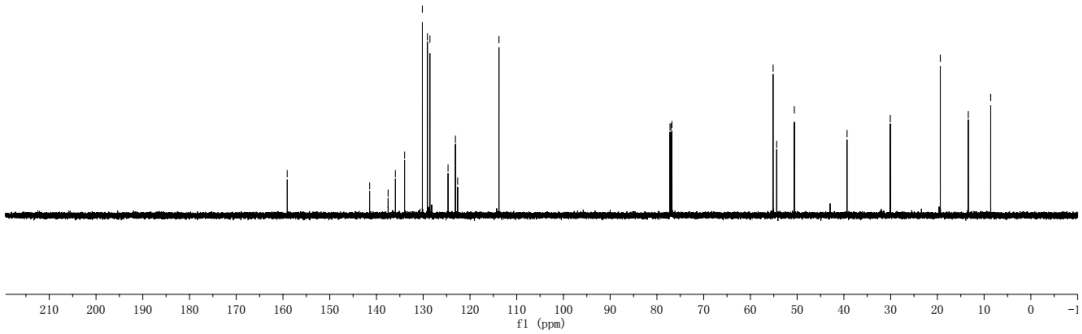
n-Bu
SO2Ph
Me
MeO

3ba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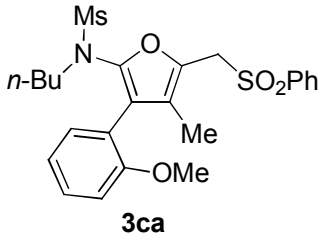
Ms
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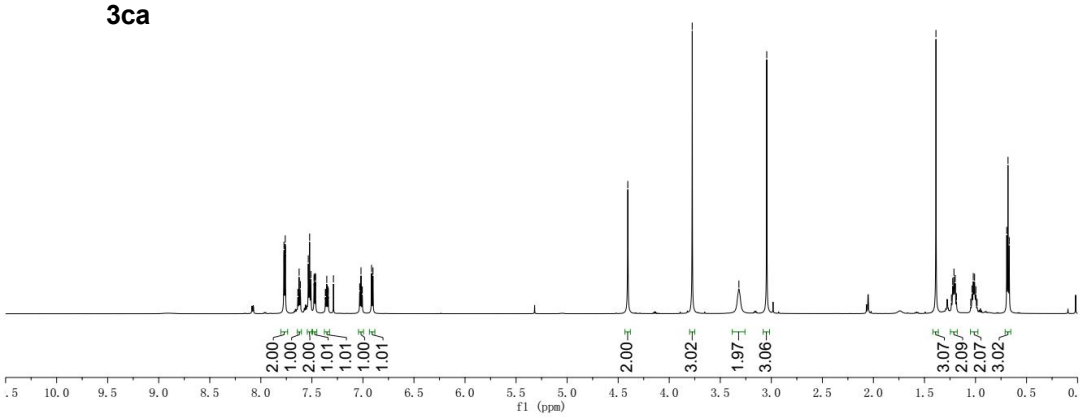
O
n-Bu
SO2Ph
Me
OMe

3ca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2.09
2.07
3.02
f1 (ppm)


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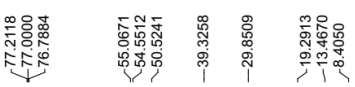
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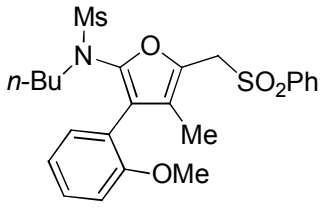
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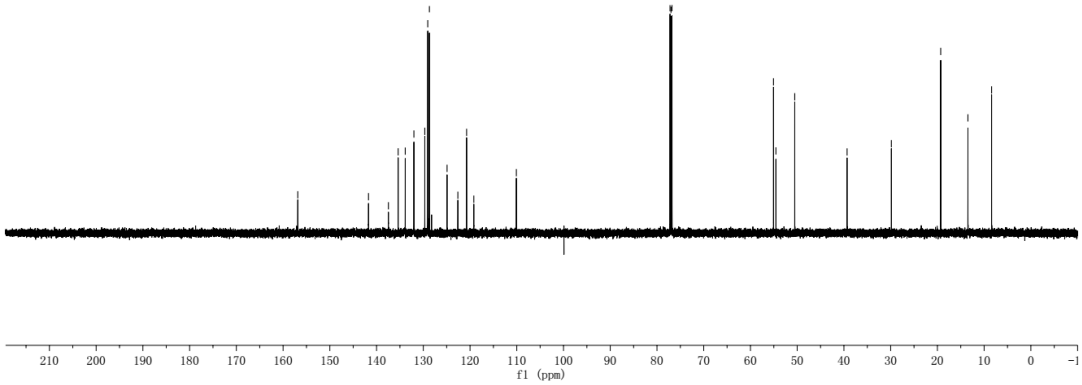
n-Bu
SO2Ph
Me
OMe

3ca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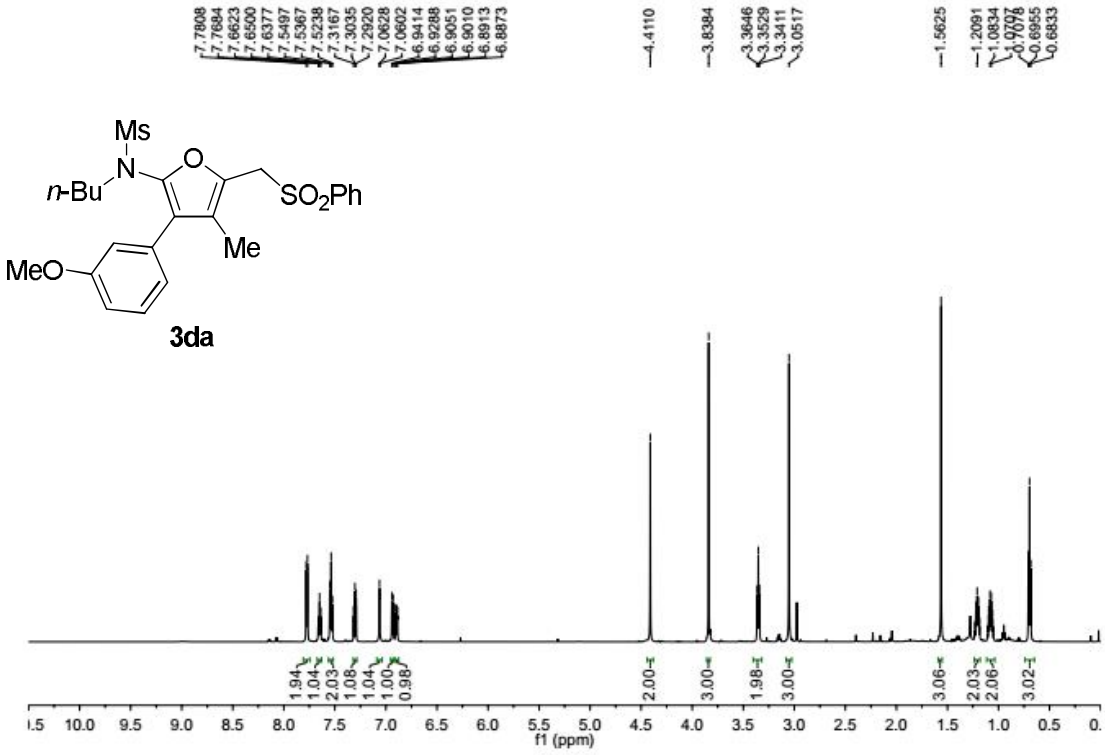
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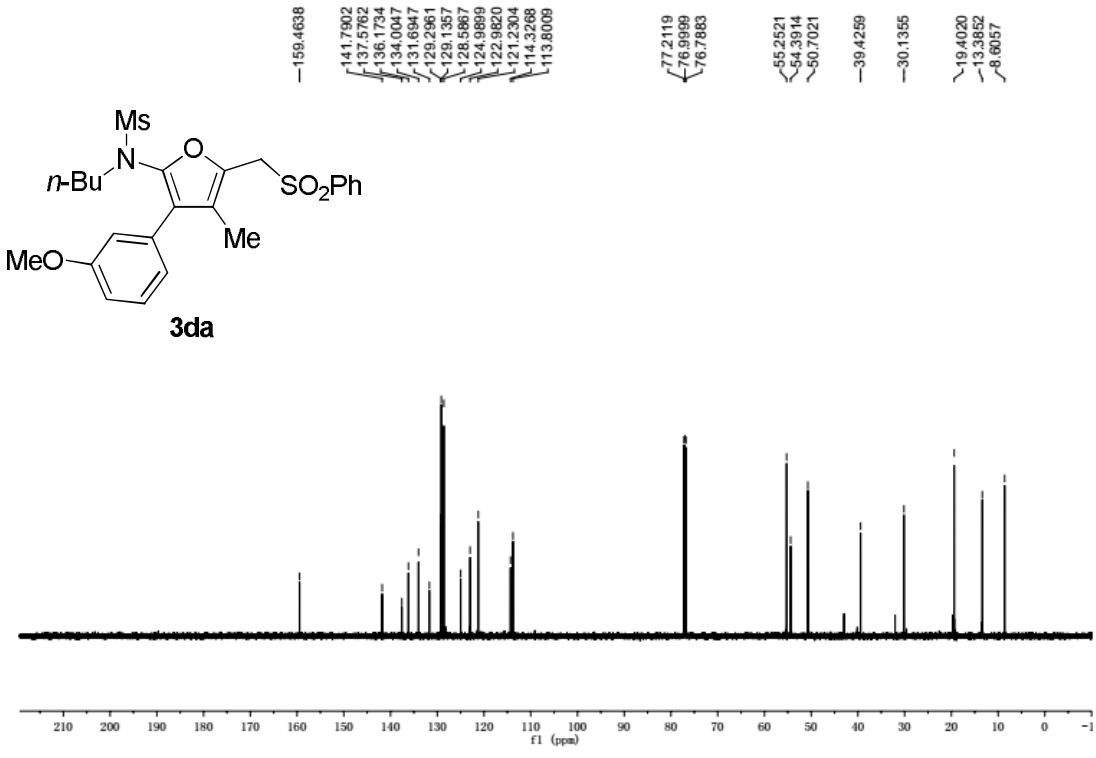
f1 (ppm)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O
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SO2Ph
Me
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3da
f1 (ppm)


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7.6212
7.5297
7.5168
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6.8519
6.8384
6.8361
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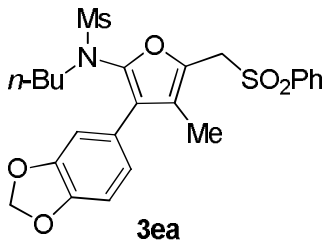
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SO2Ph
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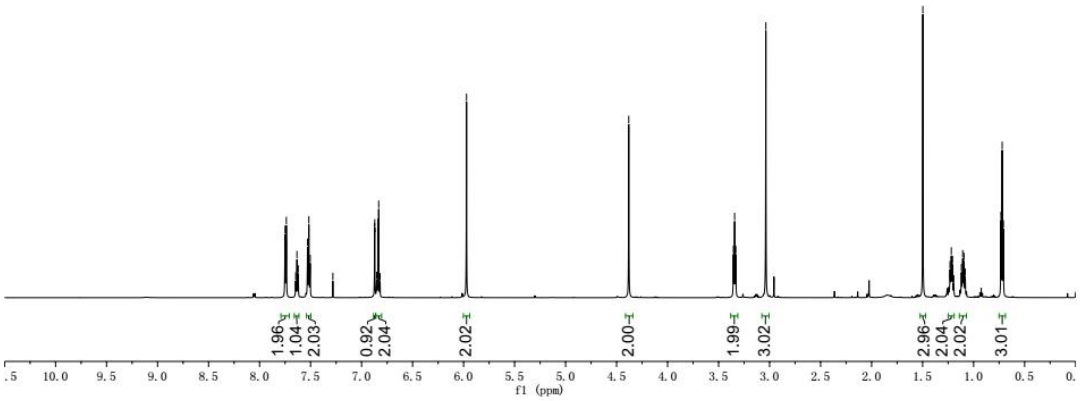
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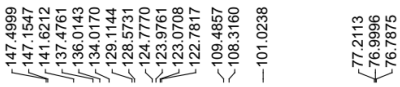
f1 (ppm)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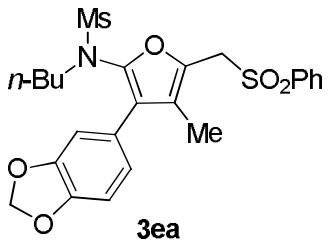
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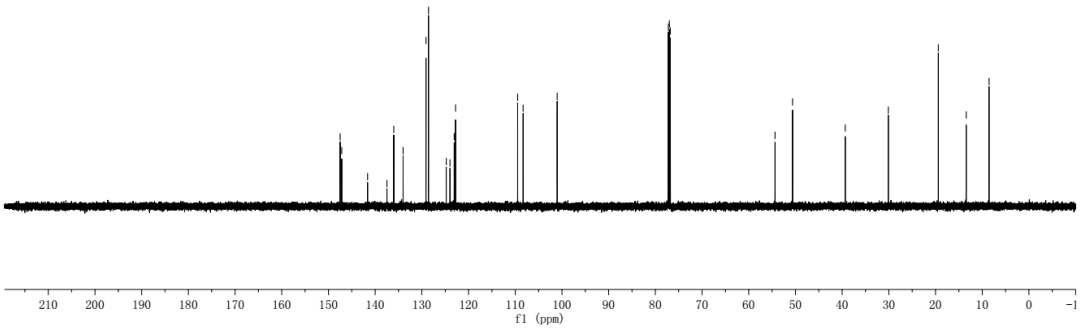
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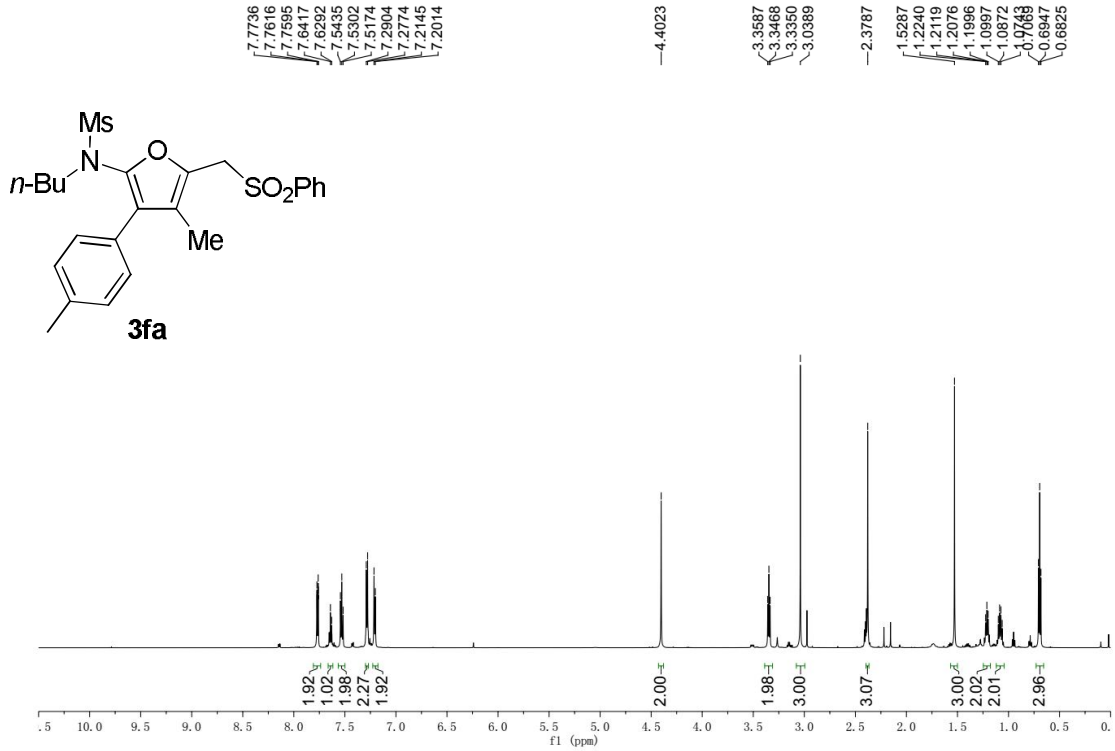
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n-Bu
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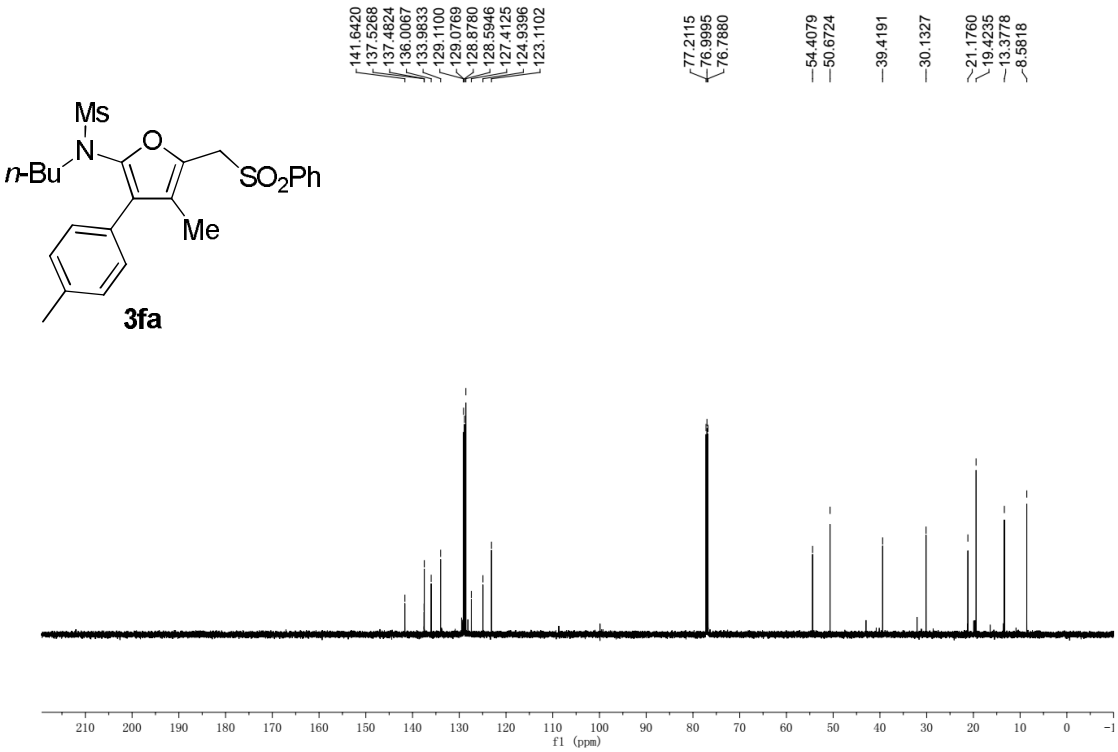
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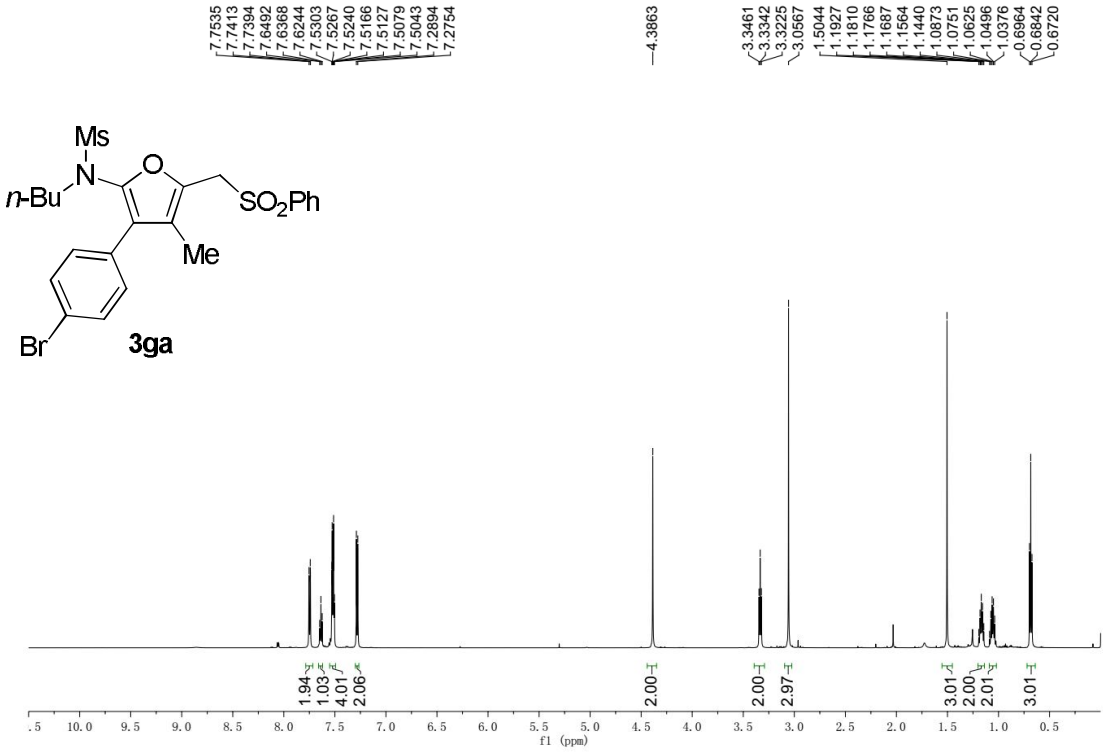
f1 (ppm)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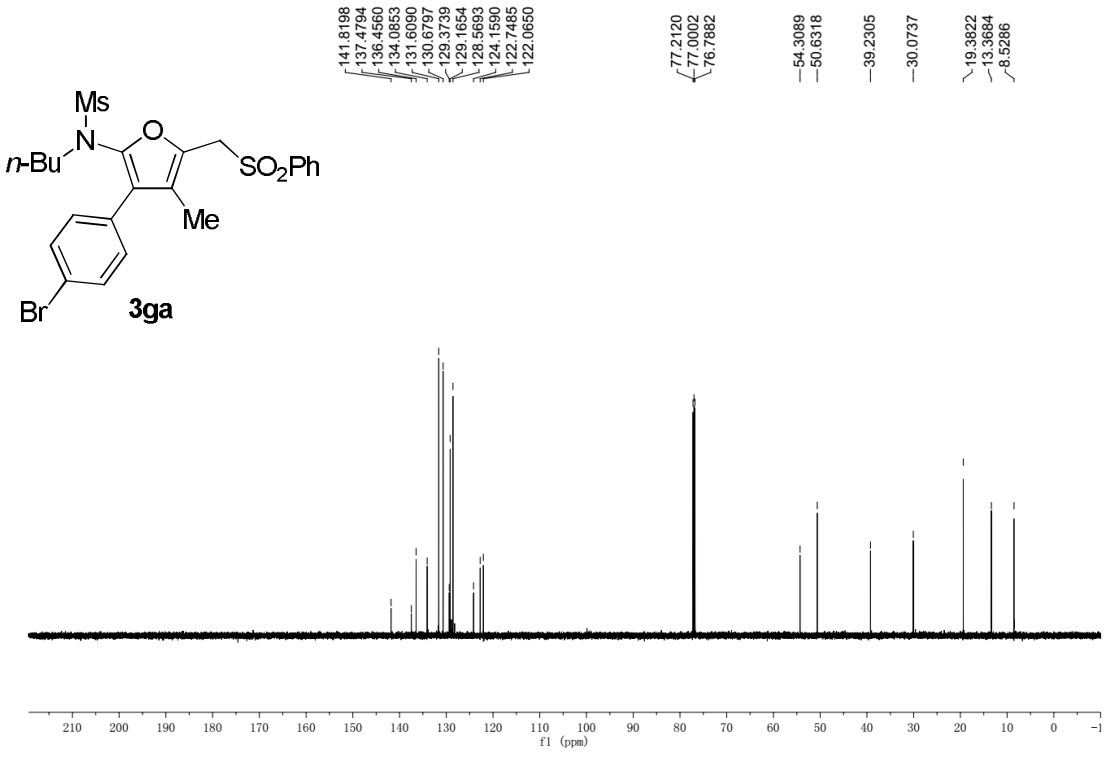
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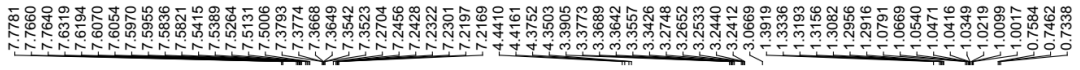

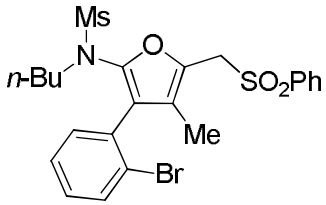
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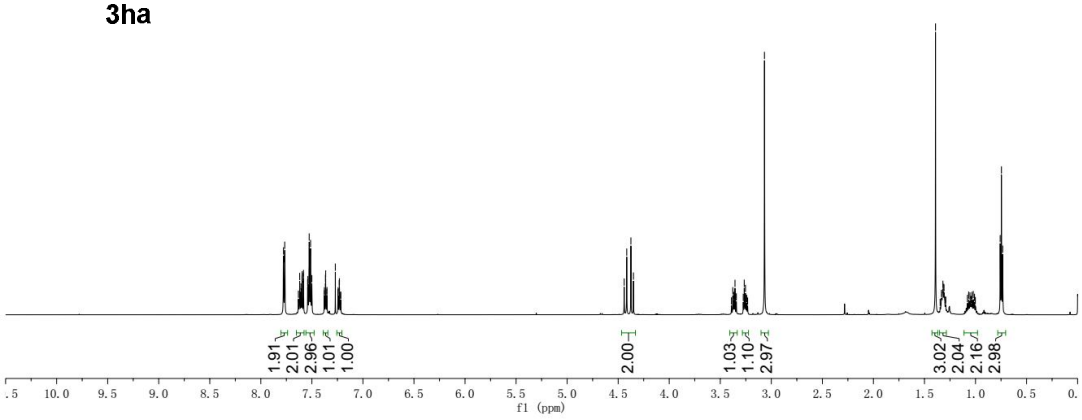
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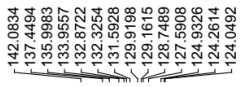

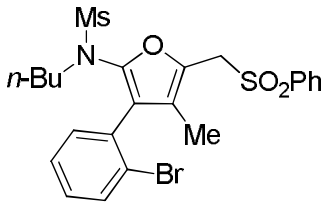
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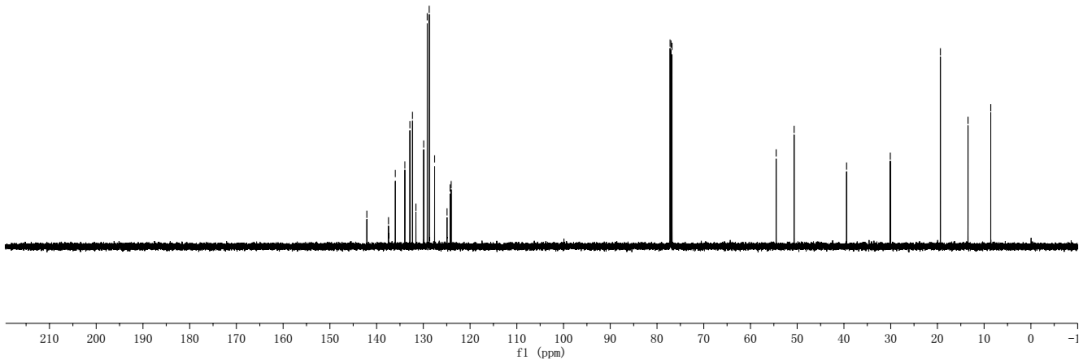
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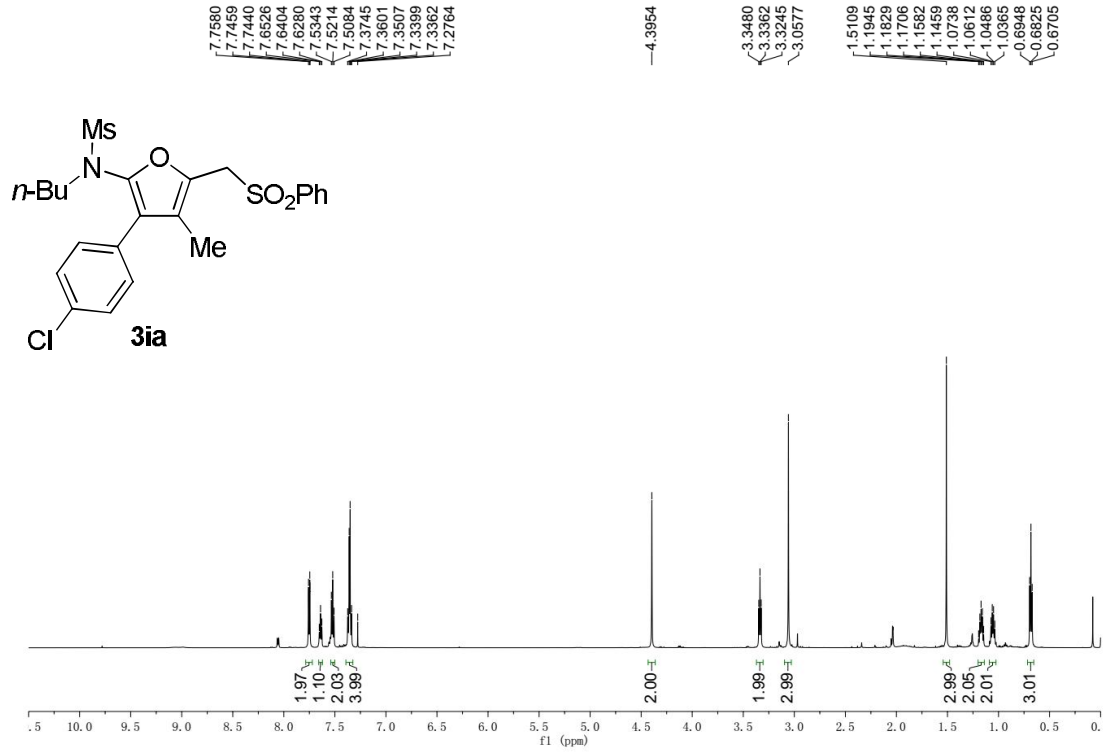
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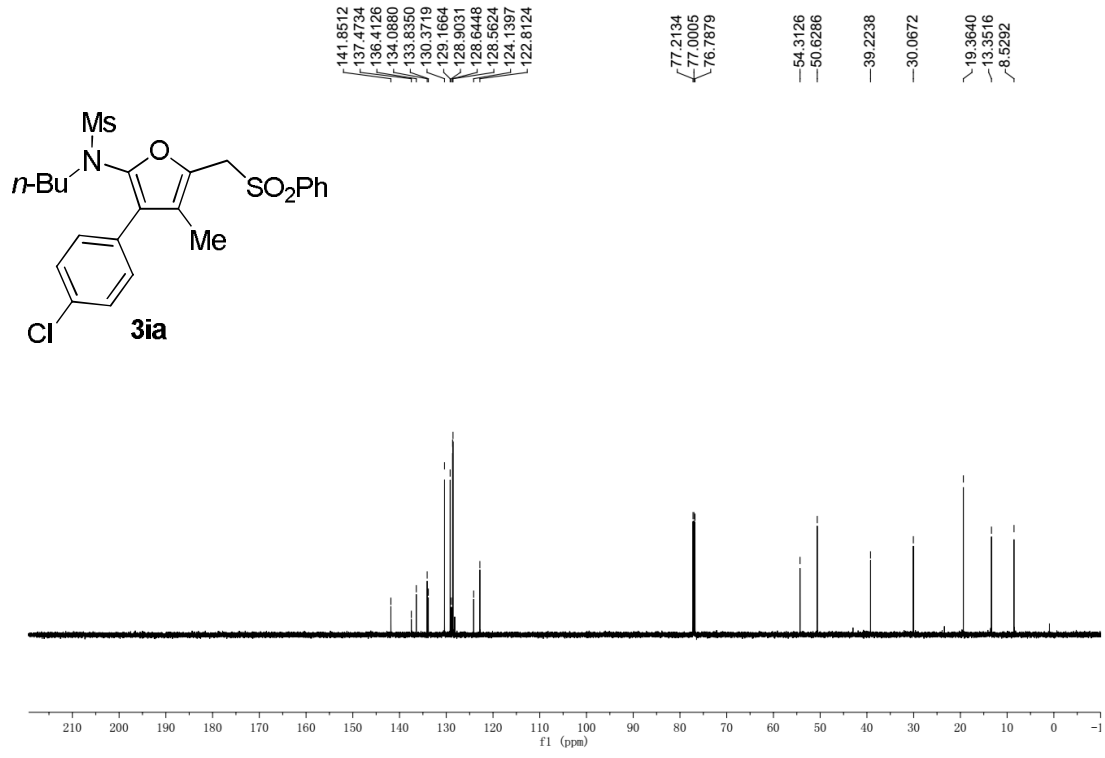
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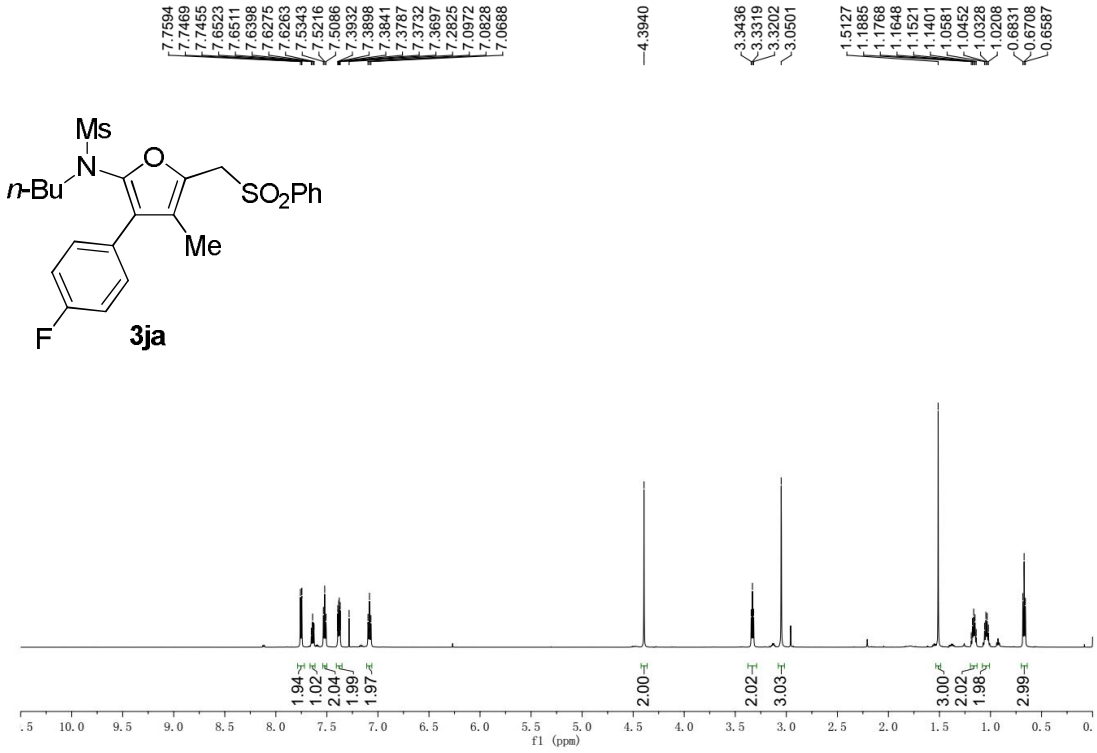
f1 (ppm)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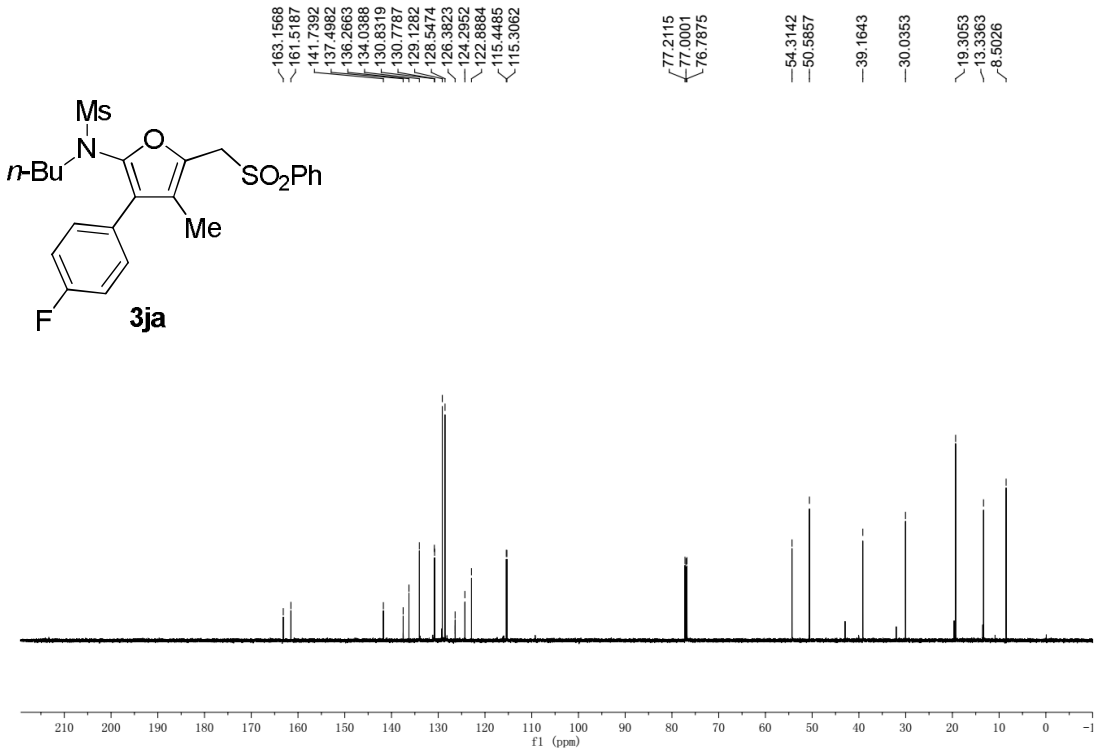
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129.1282
128.5474
126.3823
124.2952
122.8884
115.4485
115.3062
77.2115
77.0001
76.7875
54.3142
50.5857
39.1643
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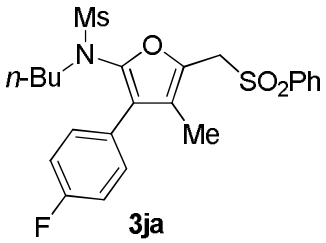
Ms
N
O
n-Bu
SO2Ph
Me
F
3ja
f1 (ppm)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N
O
n-Bu
SO2Ph
Me
F

3ja

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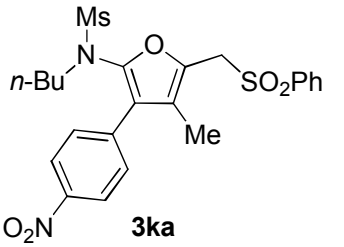
f1 (ppm)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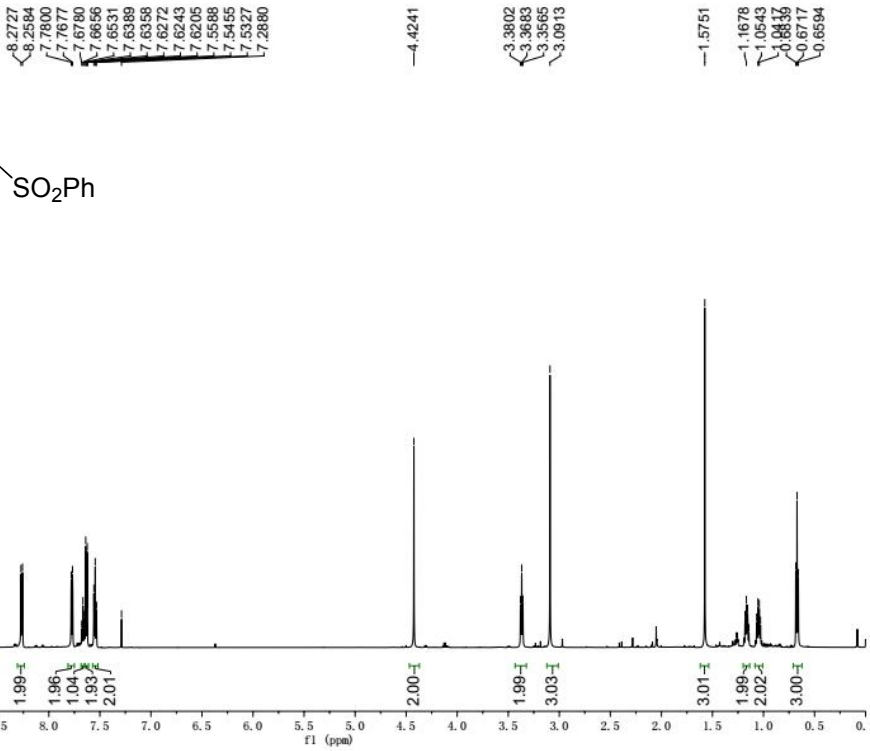
N
O
n-Bu
SO2Ph
Me
O2N

3ka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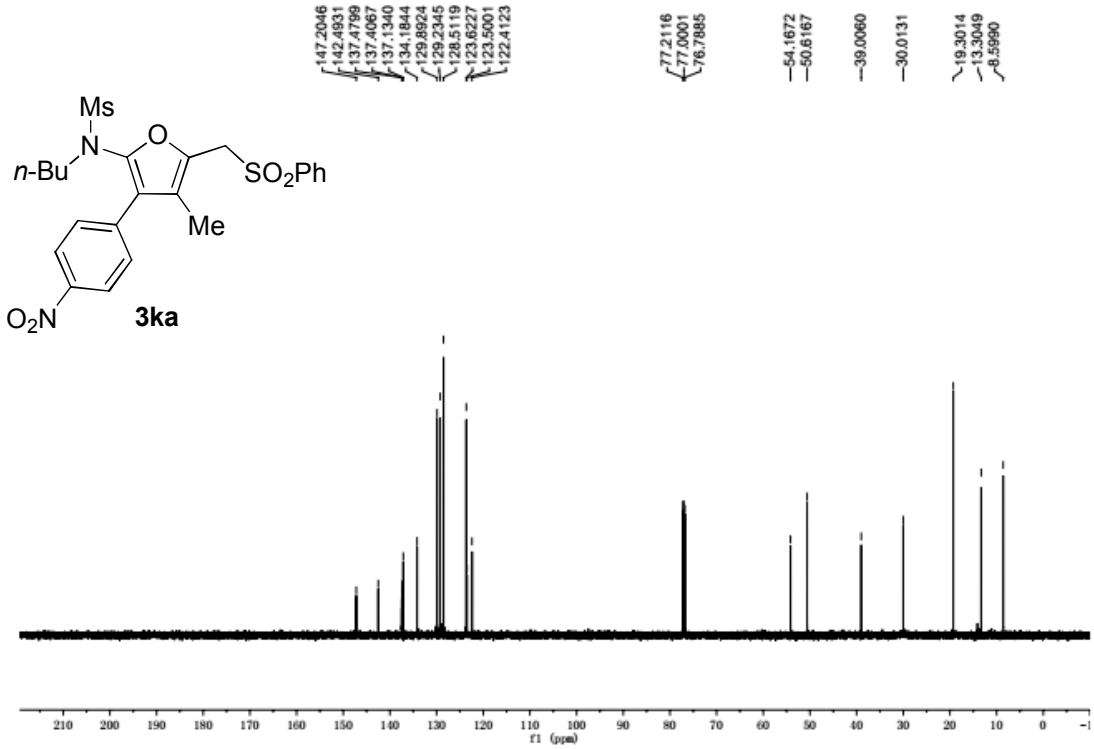
7.6243
7.6205
7.5588
7.5455
7.5327
7.2880
4.4241
3.3802
3.3683
3.3565
3.0913
1.5751
1.1678
1.0543
0.6717
0.6594
1.99
1.96
1.04
1.93
2.01
2.00
1.99
3.03
3.01
1.99
2.02
3.00
f1 (ppm)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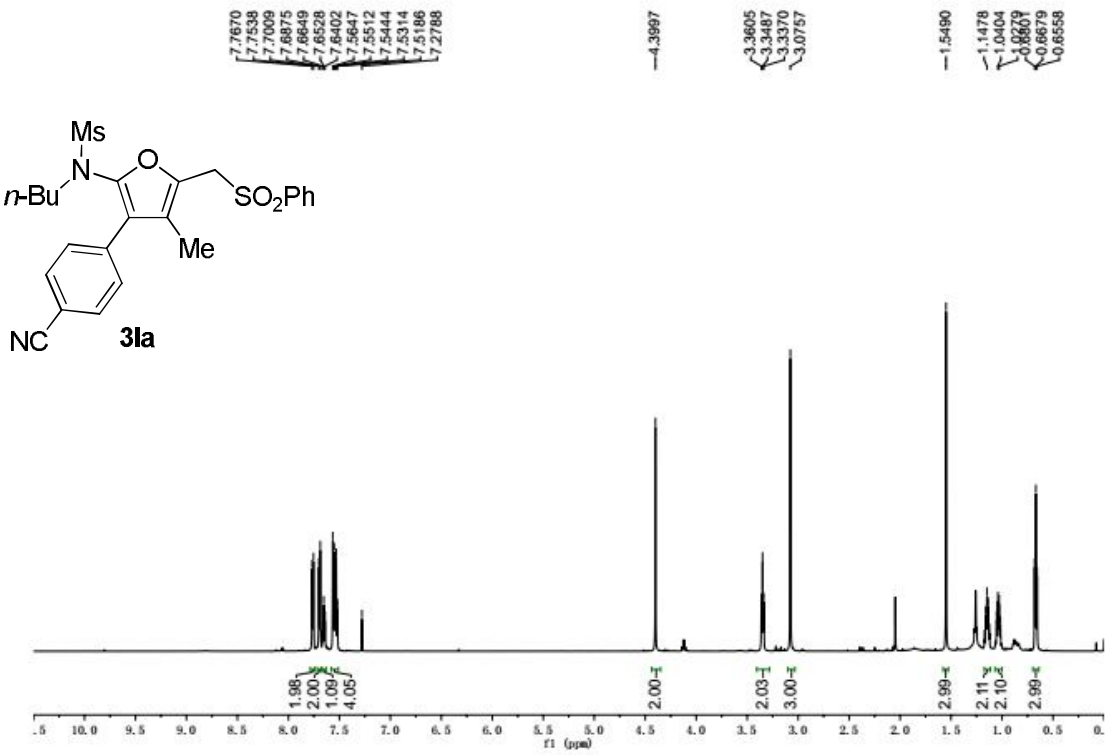
137.1340
134.1844
129.8924
129.2345
128.5119
123.6227
123.5001
122.4123
77.2116
77.0001
76.7885
54.1672
50.6167
39.0060
30.0131
19.3014
13.3049
8.5990
Ms
N
O
n-Bu
SO2Ph
Me
O2N
3ka
f1 (ppm)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7.7009
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7.6849
7.6528
7.6402
7.5647
7.5512
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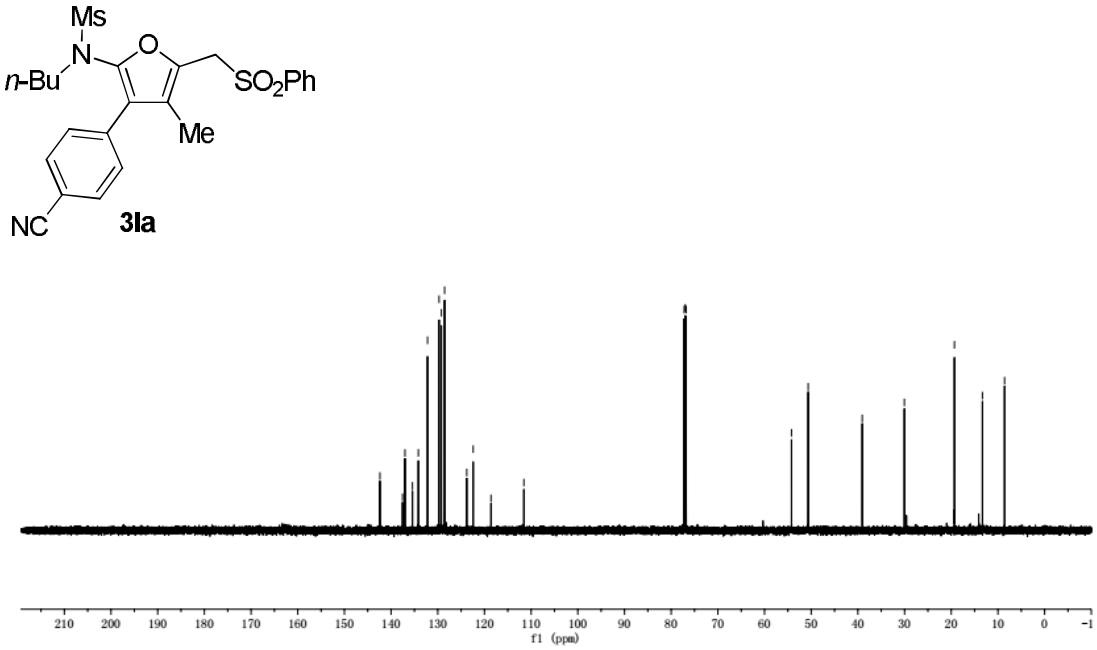
7.5314
7.5186
7.2788
4.3997
3.3605
3.3487
3.3370
3.0757
1.5490
1.1478
1.0404
0.8801
0.6679
0.6558
Ms
N
O
n-Bu
SO2Ph
Me
NC
3la
1.98
2.00
1.09
4.05
2.00
2.03
3.00
2.99
2.11
2.10
2.99
f1 (ppm)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137.0275
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129.7221
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123.7913
122.4155
118.5923
111.5465
77.2123
77.0001
76.7885
54.2211
50.6527
39.0725
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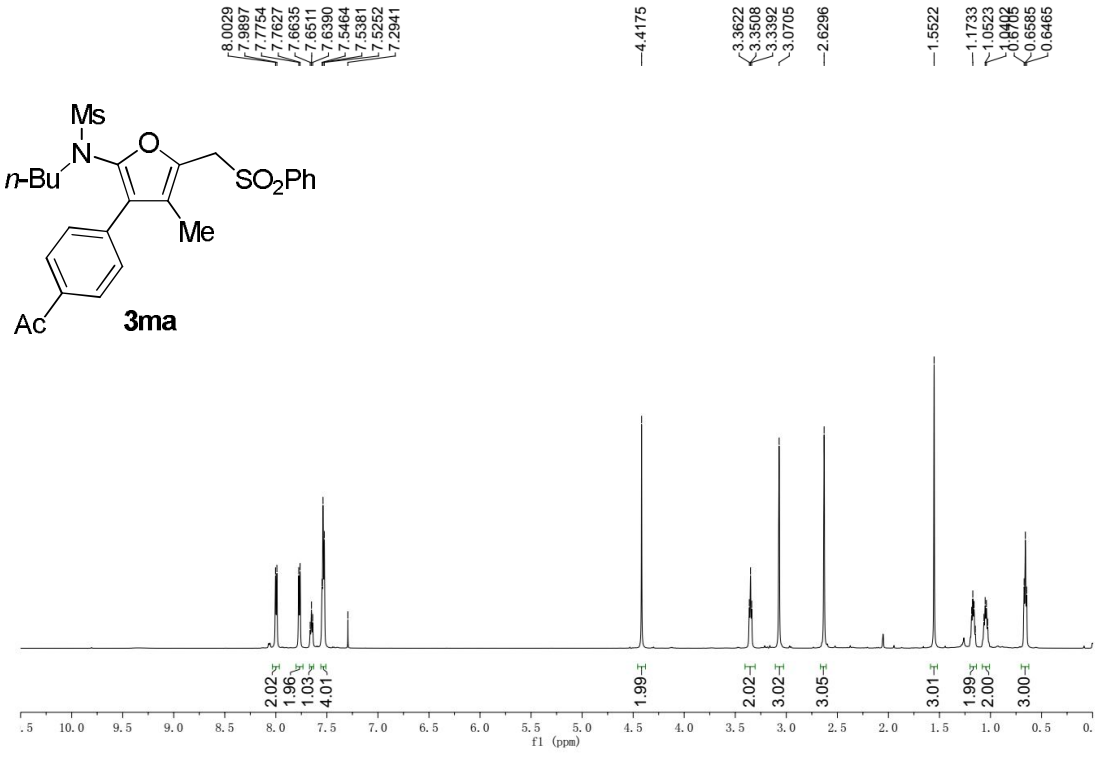
13.3212
8.5771
Ms
N
O
n-Bu
SO2Ph
Me
NC
3la
f1 (ppm)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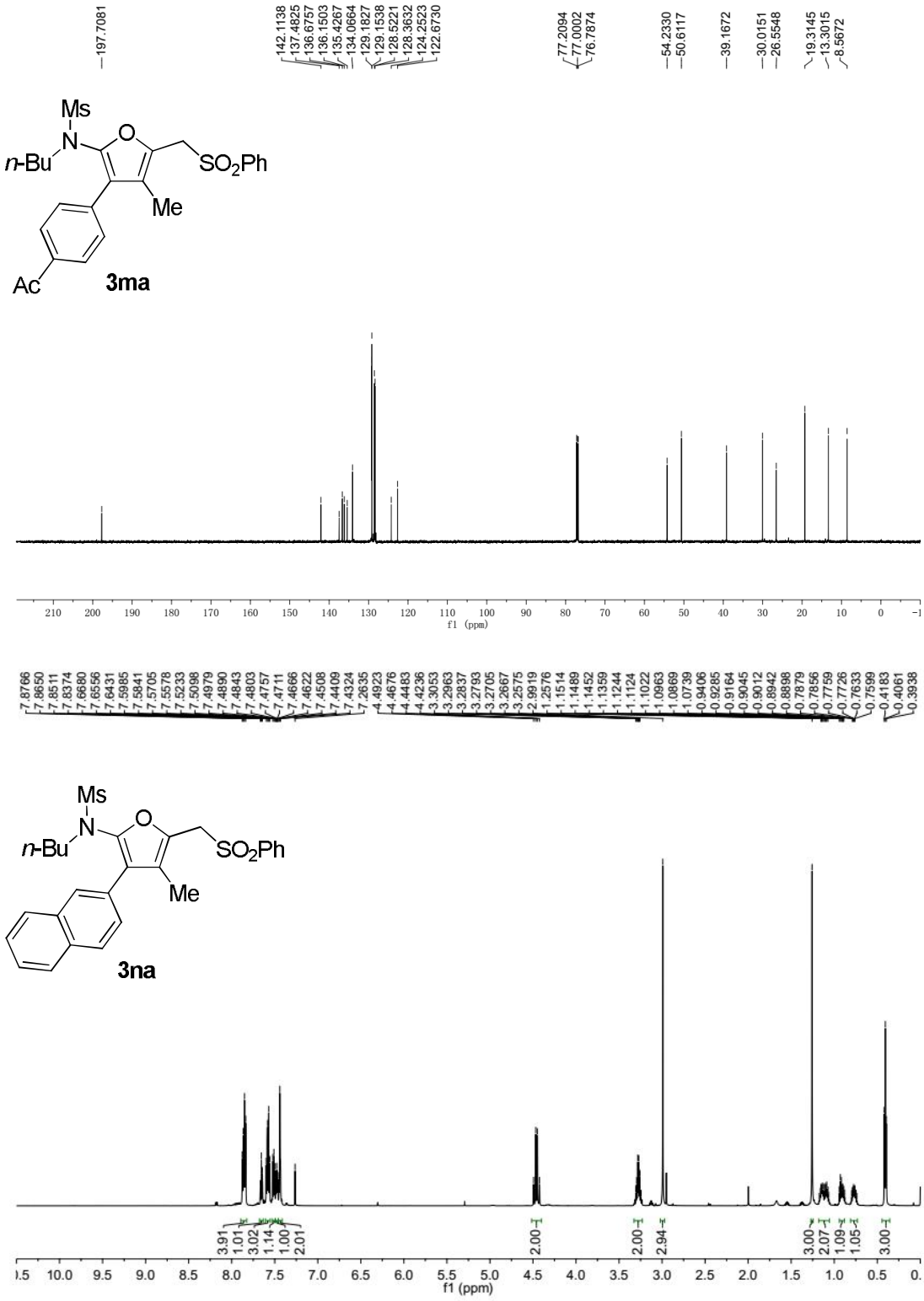
7.6511
7.6390
7.5464
7.5381
7.5252
7.2941
4.4175
3.3622
3.3508
3.3392
3.0705
2.6296
1.5522
1.1733
1.0523
0.6585
0.6465
Ms
N
O
n-Bu
SO2Ph
Me
Ac
3ma
2.02
1.96
1.03
4.01
1.99
2.02
3.02
3.05
3.01
1.99
2.00
3.00
f1 (ppm)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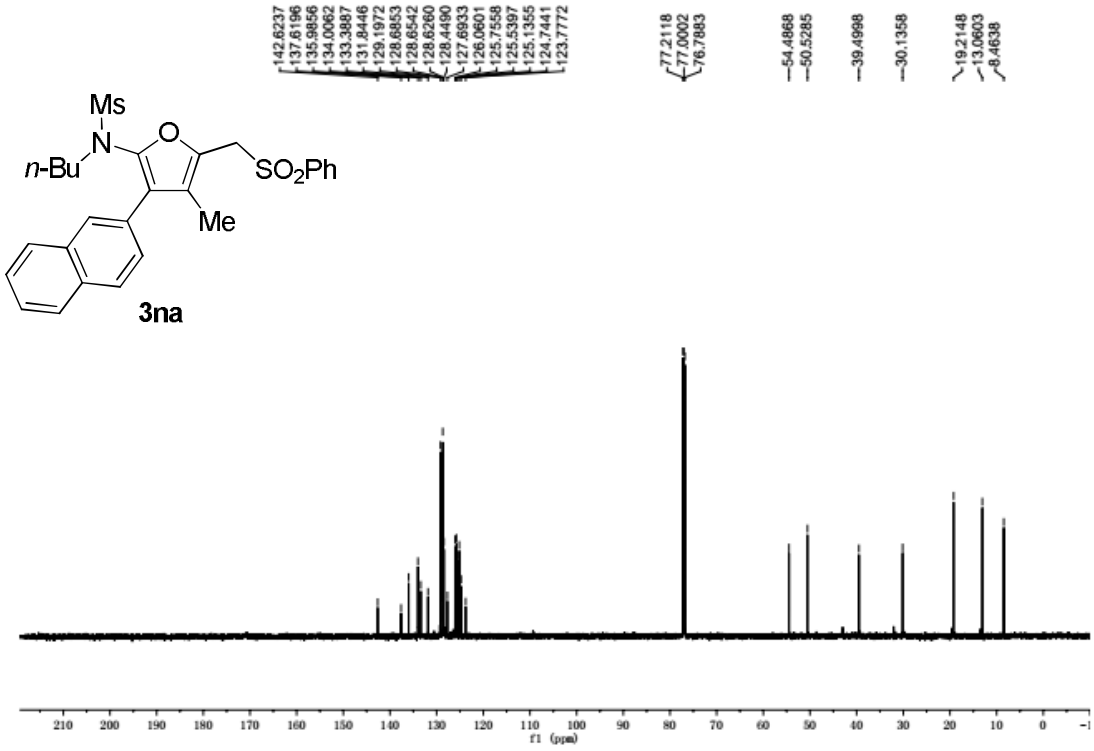
136.1503
135.4267
134.0664
129.1827
129.1538
128.5221
128.3632
124.2523
122.6730
77.2094
77.0002
76.7874
54.2330
50.6117
39.1672
30.0151
26.5548
19.3145
13.3015
8.5672
Ms
N
O
n-Bu
SO2Ph
Me
Ac
3ma
f1 (ppm)
Ms
N
O
n-Bu
SO2Ph
Me
3na
3.91
1.01
3.02
1.14
1.00
2.01
2.00
2.00
2.94
3.00
2.07
1.09
1.05
3.00
f1 (ppm)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133.3887
131.8446
129.1972
128.6853
128.6542
128.6260
128.4490
127.6933
126.0601
125.7558
125.5397
125.1355
124.7441
123.7772
77.2118
77.0002
76.7883
54.4868
50.5285
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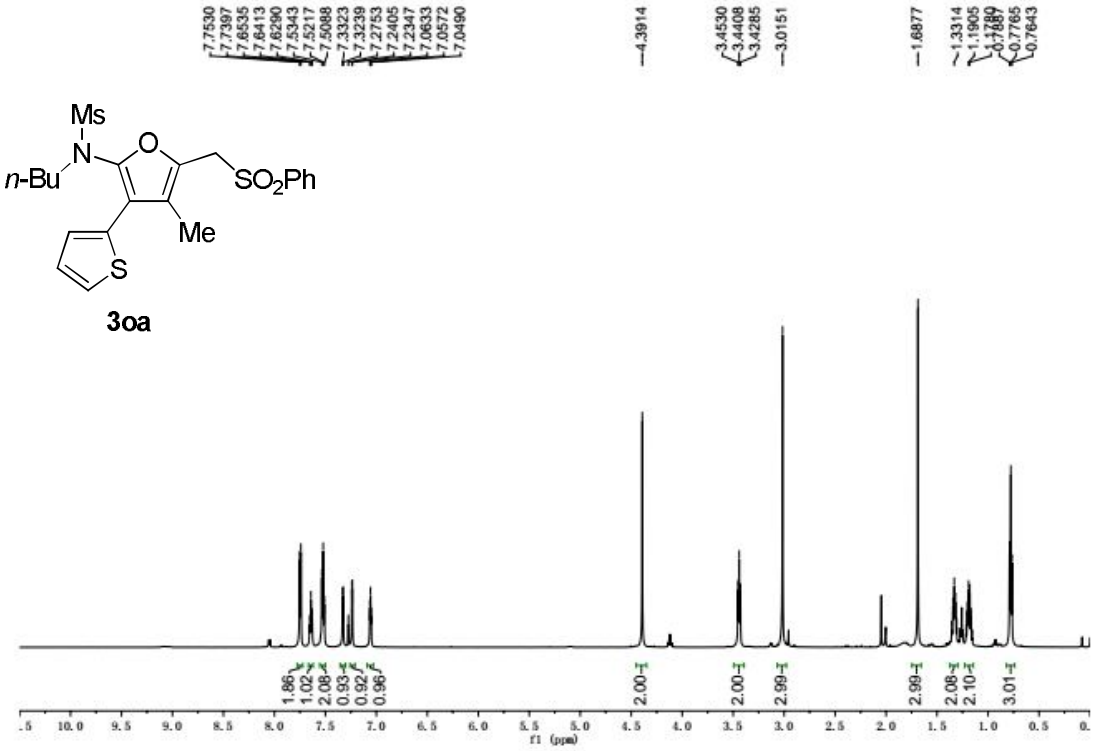
13.0603
8.4638
Ms
N
O
n-Bu
SO2Ph
Me
3na
f1 (ppm)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7.5343
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7.3323
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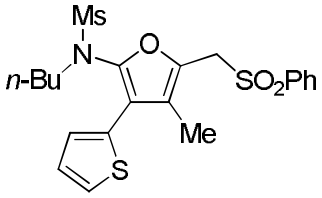
7.2753
7.2405
7.2347
7.0633
7.0572
7.0490
4.3914
3.4530
3.4408
3.4285
3.0151
1.6877
1.3314
1.1905
1.1780
0.7887
0.7785
0.7643
Ms
N
O
n-Bu
SO2Ph
Me
S
3oa
1.86
1.02
2.08
0.93
0.92
0.96
2.00
2.00
2.99
2.99
2.08
2.10
3.01
f1 (ppm)


Ms
N
O
n-Bu
SO2Ph
Me
S

3oa

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134.0476
131.0366
129.2209
128.5288
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118.9655
77.2125
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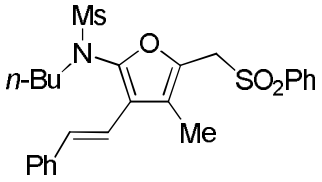
54.2337
50.6094
39.2520
30.1653
19.6005
13.4763
9.3039
f1 (ppm)


Ms
N
O
n-Bu
SO2Ph
Me
Ph

3pa

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7.6443
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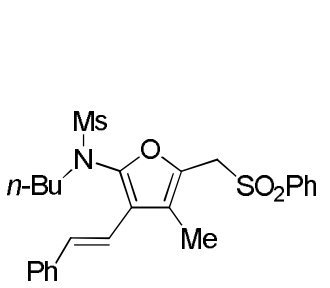
7.5393
7.5264
7.5135
7.4482
7.4356
7.3468
7.3343
7.3215
7.2622
7.2504
7.2382
6.9769
6.9490
6.8384
6.8105
4.3687
3.5046
3.4928
3.4807
2.9916
1.7836
1.4316
1.3639
1.3512
0.8836
0.8715
0.8595
1.95
1.00
2.01
1.99
2.01
1.08
0.99
0.99
2.00
1.99
2.98
2.99
2.00
2.08
2.98
f1 (ppm)


Ms
N
O
n-Bu
SO2Ph
Me
Ph

3pa

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137.0920
136.6047
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131.0741
129.2377
128.5576
128.4788
127.7670
126.3130
122.0112
121.5330
117.2396
77.2126
77.0004
76.7882
54.0632
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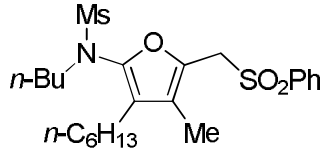
19.5973
13.5105
9.7710
f1 (ppm)


Ms
N
O
n-Bu
SO2Ph
n-C6H13
Me

3qa

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7.6740
7.6547
7.6422
7.6298
7.5184
7.5055
7.4923
7.2894
4.3159
3.4448
3.4331
3.4209
2.9590
2.2752
2.2621
2.2482
1.4901
1.4103
1.3595
1.3072
0.9143
0.9024
0.8915
0.8798
1.92
0.99
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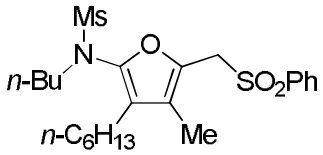
2.00
1.99
2.99
2.03
3.01
4.11
8.02
6.03
f1 (ppm)


Ms
N
O
n-Bu
SO2Ph
n-C6H13
Me

3qa

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129.0380
128.4575
124.5450
123.4319
77.2120
77.0000
76.7877
54.2476
50.0392
38.3123
31.4284
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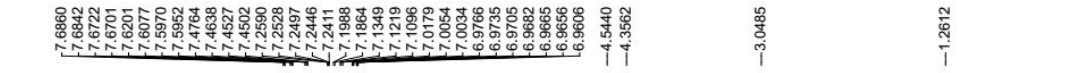
28.8983
23.2988
22.4570
19.5318
13.9470
13.5198
8.0799
f1 (ppm)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7.6201
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7.4527
7.4502
7.2590
7.2528
7.2497
7.2446
7.2411
7.1988
7.1864
7.1349
7.1219
7.1096
7.0179
7.0054
7.0034
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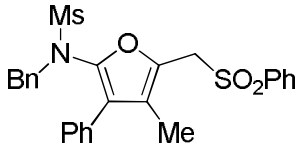
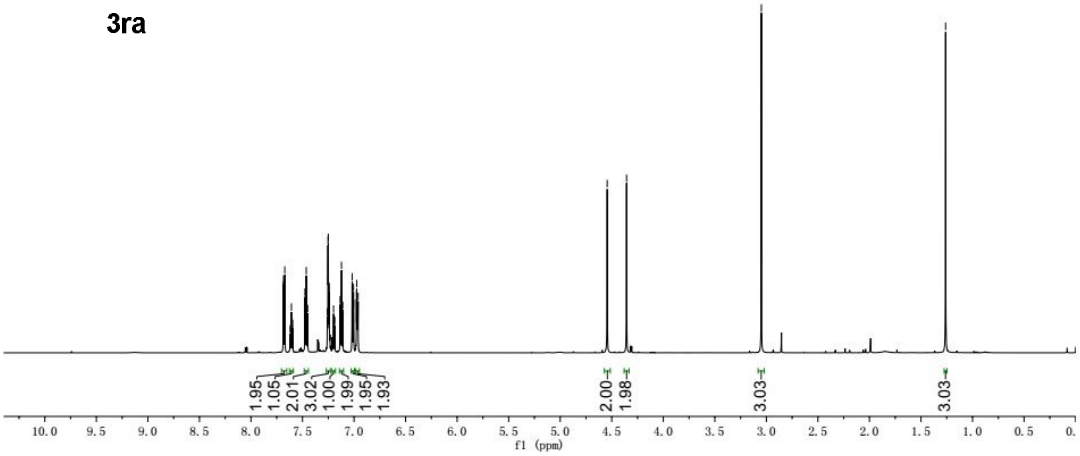
4.5440
4.3562
3.0485
1.2612


Ms
N
O
Bn
SO2Ph
Ph
Me

3ra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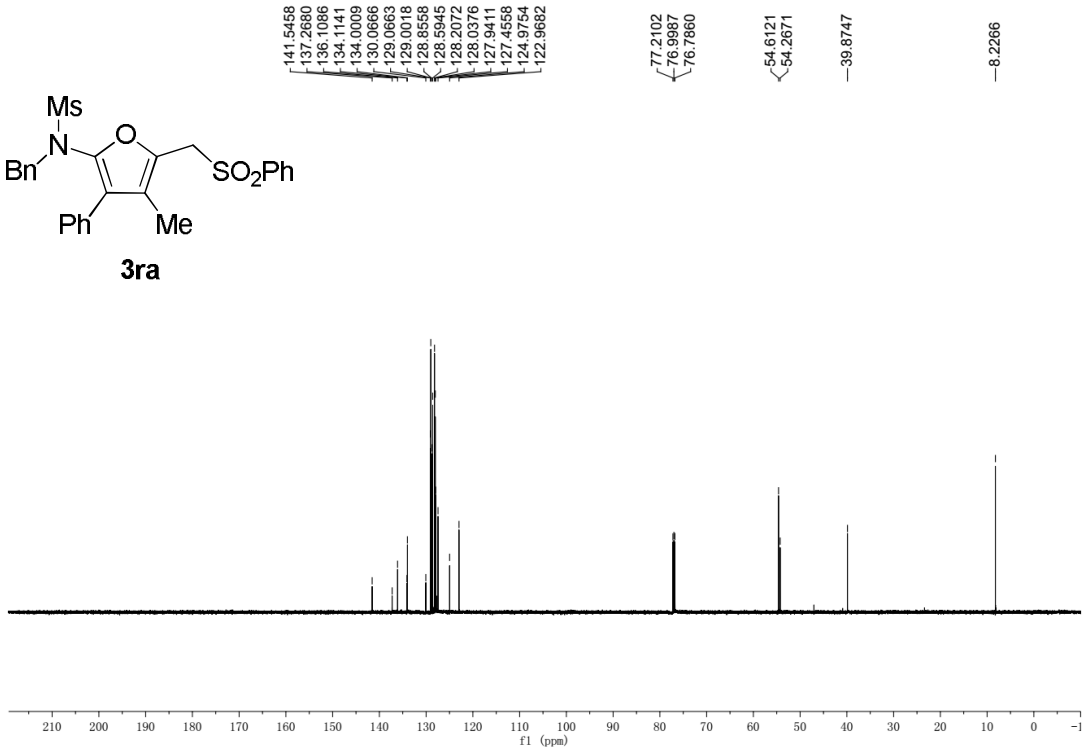
1.99
1.95
1.93
2.00
1.98
3.03
3.03
f1 (ppm)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127.9411
127.4558
124.9754
122.9682
77.2102
76.9987
76.7860
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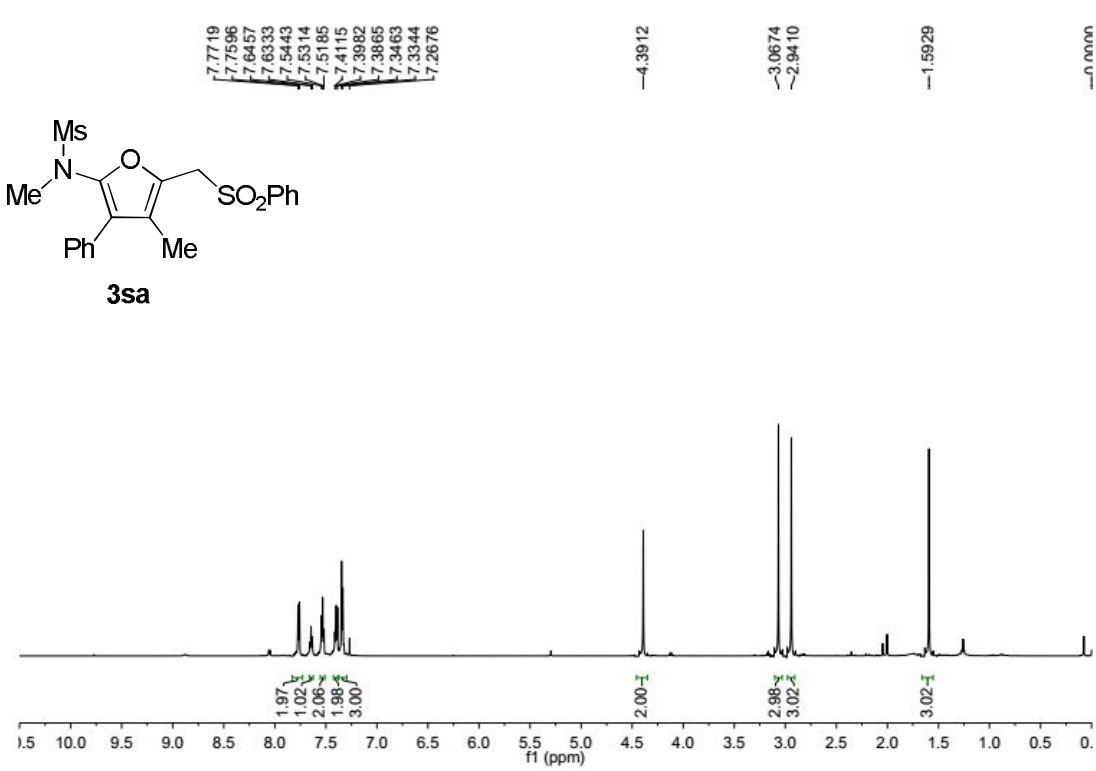
Ms
N
Bn
O
SO2Ph
Ph
Me
f1 (ppm)

3ra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7.3982
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7.3344
7.2676
4.3912
3.0674
2.9410
1.5929
0.0000
Ms
N
Me
O
SO2Ph
Ph
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1.97
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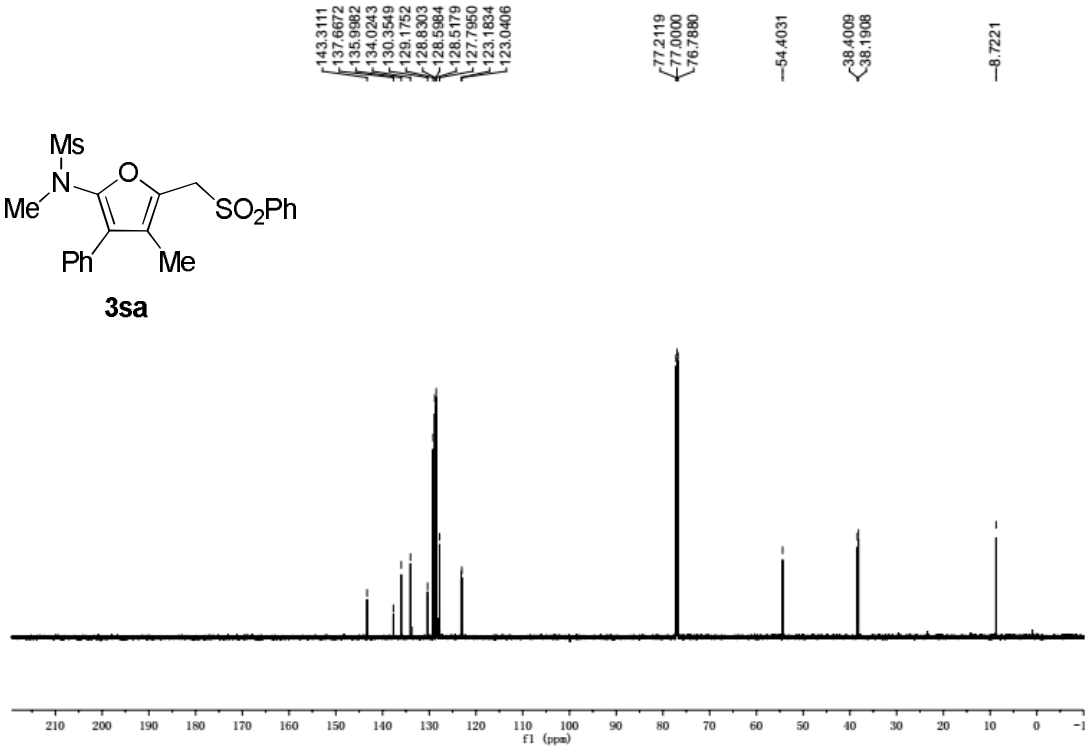
2.06
1.98
3.00
2.00
2.98
3.02
3.02
f1 (ppm)

3sa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128.5984
128.5179
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77.0000
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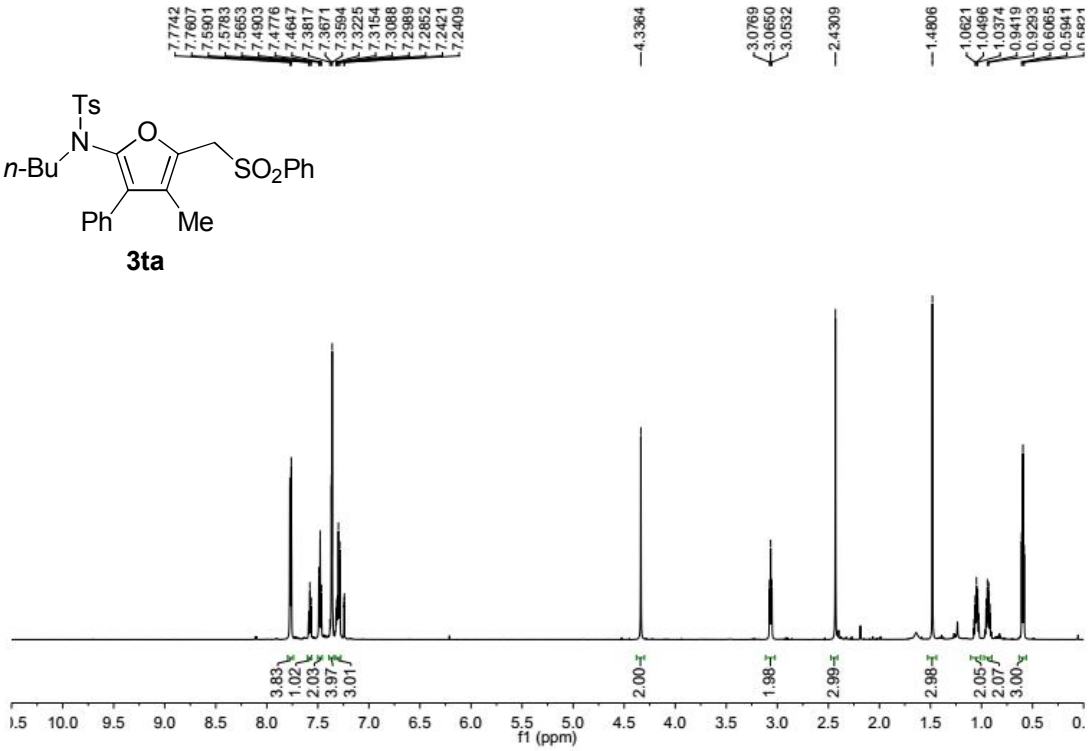
Me
O
SO2Ph
Ph
Me
f1 (ppm)

3sa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7.3594
7.3225
7.3154
7.3088
7.2989
7.2852
7.2421
7.2409
4.3364
3.0769
3.0650
3.0532
2.4309
1.4806
1.0621
1.0496
1.0374
0.9419
0.9293
0.6065
0.5941
Ts
N
n-Bu
O
SO2Ph
Ph
Me
3.83
1.02
2.03
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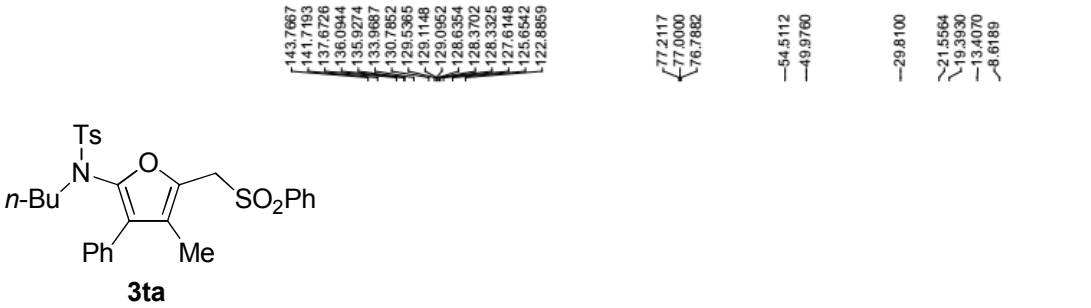
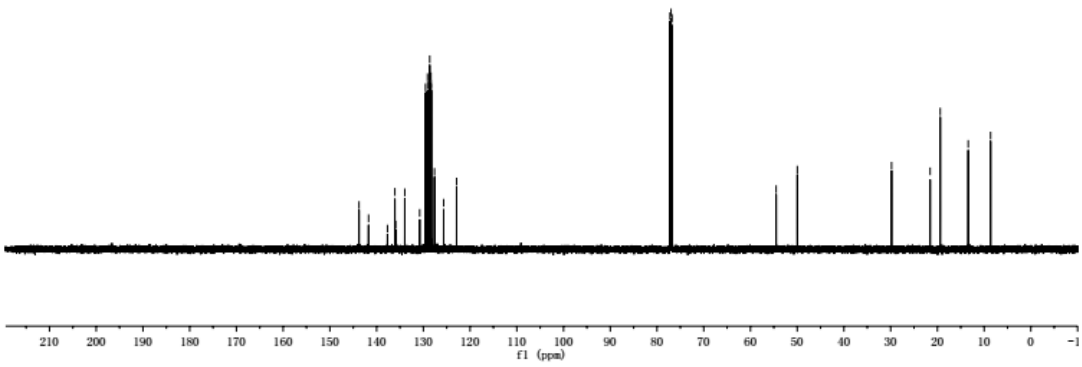
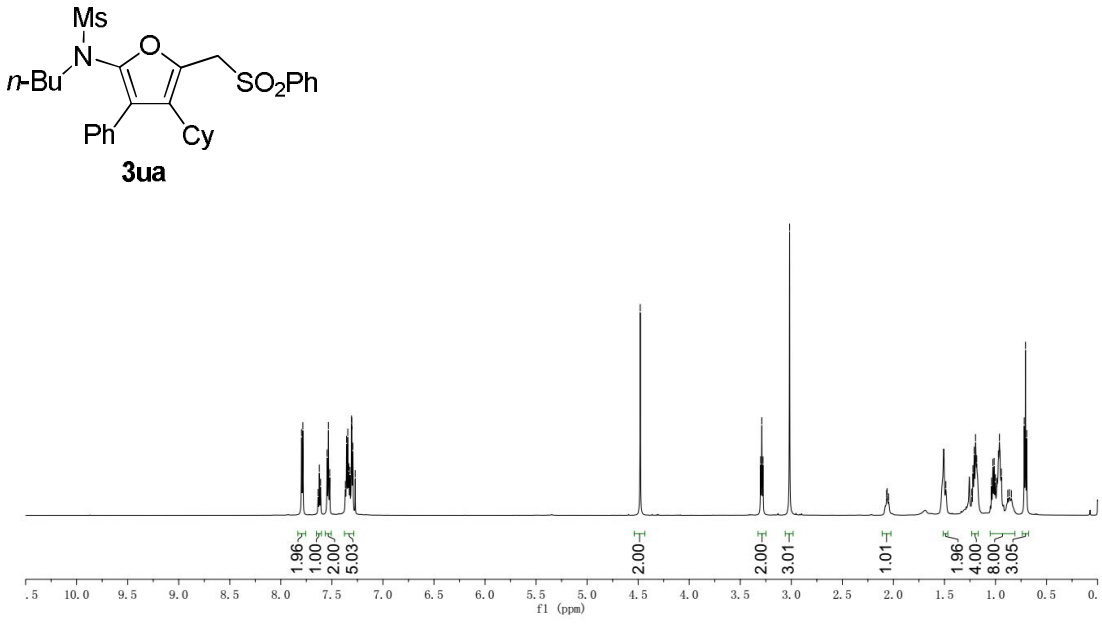
2.00
1.98
2.99
2.98
2.05
2.07
3.00
f1 (ppm)

3ta

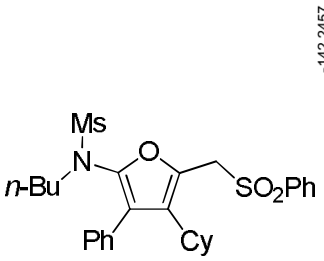


3ta





3ua


Ms
N
O
n-Bu
SO2Ph
Ph
Cy

3ua

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131.2770
130.1963
129.1006
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127.9851
127.7482
124.7466
77.2116
76.9998
76.7879
54.8798
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35.8696
32.3588
30.2420
26.6031
25.5669
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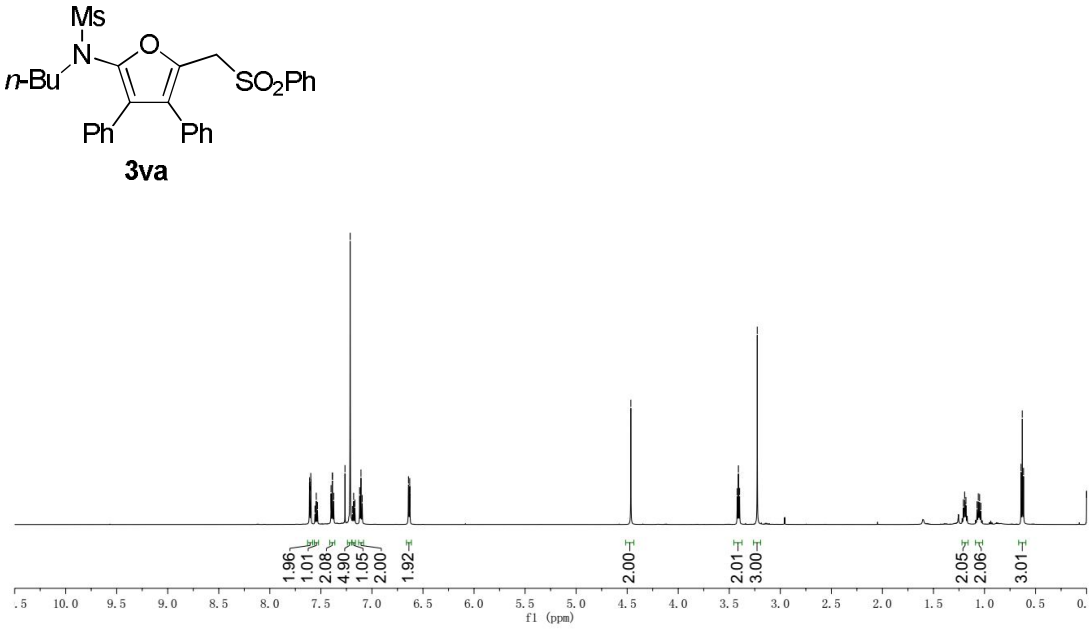
13.4568
f1 (ppm)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7.2131
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6.6298
6.6278
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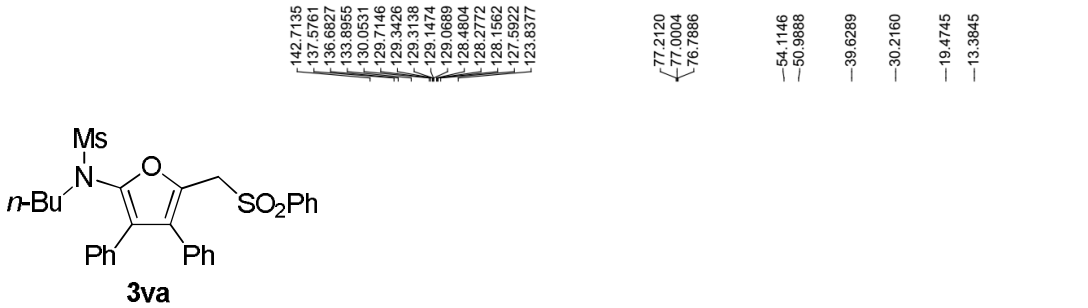
1.1820
1.0734
1.0608
1.0481
1.0358
0.6422
0.6300
0.6177
f1 (ppm)

Ms
N
O
n-Bu
SO2Ph
Ph
Ph

3va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137.5761
136.6827
133.8955
130.0531
129.7146
129.3426
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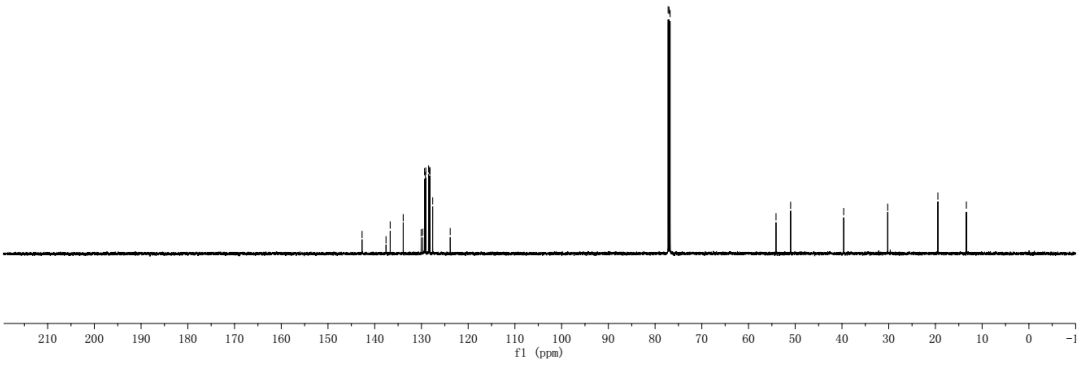
129.0689
128.4804
128.2772
128.1562
127.5922
123.8377
77.2120
77.0004
76.7886
54.1146
50.9888
39.6289
30.2160
19.4745
13.3845
Ms
N
O
n-Bu
SO2Ph
Ph
Ph

3va


f1 (ppm)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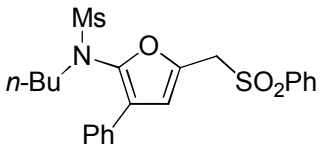
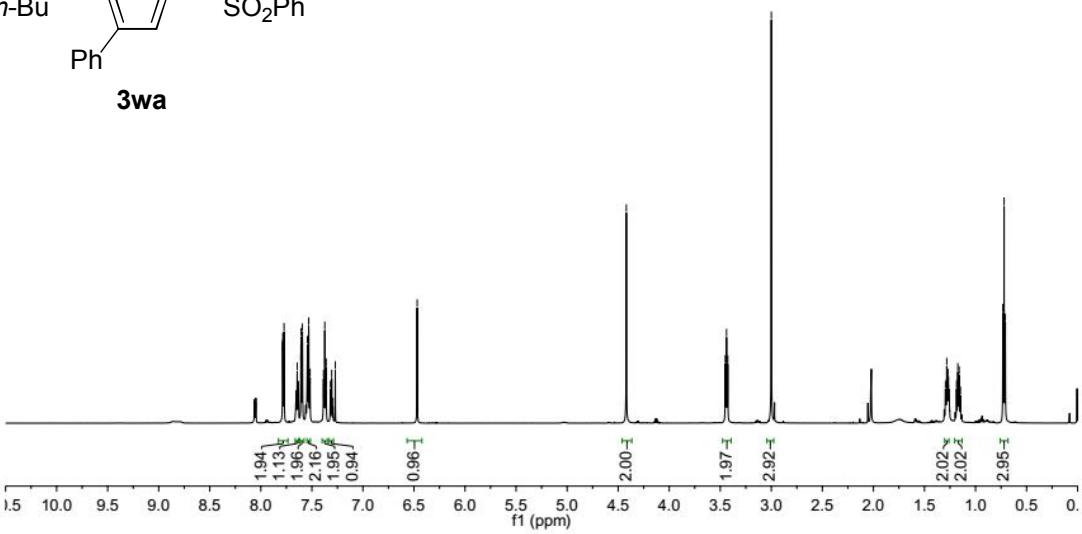
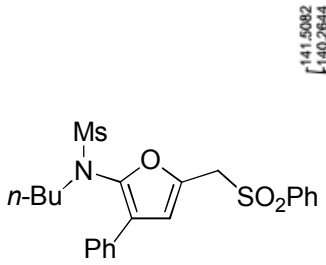
7.7847
7.7726
7.7705
7.6558
7.6539
7.6434
7.6327
7.6309
7.6073
7.6052
7.5933
7.5439
7.5311
7.5177
7.3856
7.3734
7.3605
7.3178
7.3056
7.2931
7.2704
6.4685
4.4199
3.4507
3.4386
3.4263
2.9996
1.2942
1.2815
1.2767
1.2694
1.2646
1.2567
1.1855
1.1730
1.1602
1.1481
0.7322
0.7199
0.7077


Ms
N
O
n-Bu
SO2Ph
Ph

3wa


1.94
1.13
1.96
2.16
1.95
0.94
0.96
2.00
1.97
2.92
2.02
2.02
2.95
f1 (ppm)


Ms
N
O
n-Bu
SO2Ph
Ph

3wa

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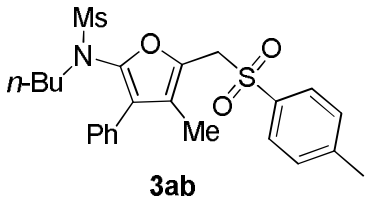
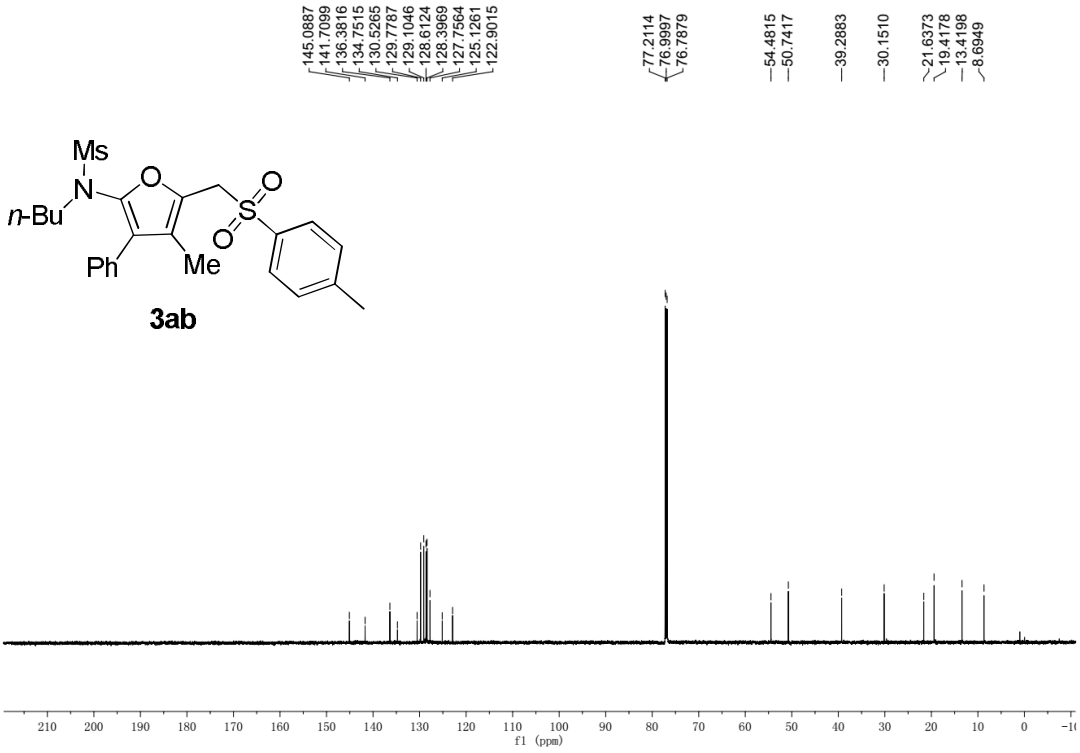
140.2644
137.6086
134.0920
130.3332
129.2109
128.9506
128.6052
128.5680
127.9236
127.1574
124.0336
113.8460
77.2120
77.0005
76.7885
55.9675
50.8819
39.3332
30.1026
19.6112
13.3953
f1 (ppm)


Ms
N
O
n-Bu
S
O
O
Ph
Me

3ab

7.6316
7.6179
7.3958
7.3884
7.3122
7.2986
7.2660
4.3657
3.3436
3.3319
3.3202
3.0145
2.4139
1.5634
1.1769
1.0429
1.0302
0.6546
0.6423
1.88
3.89
0.96
1.95
2.00
2.00
3.01
2.95
2.98
2.05
2.00
3.00
f1 (ppm)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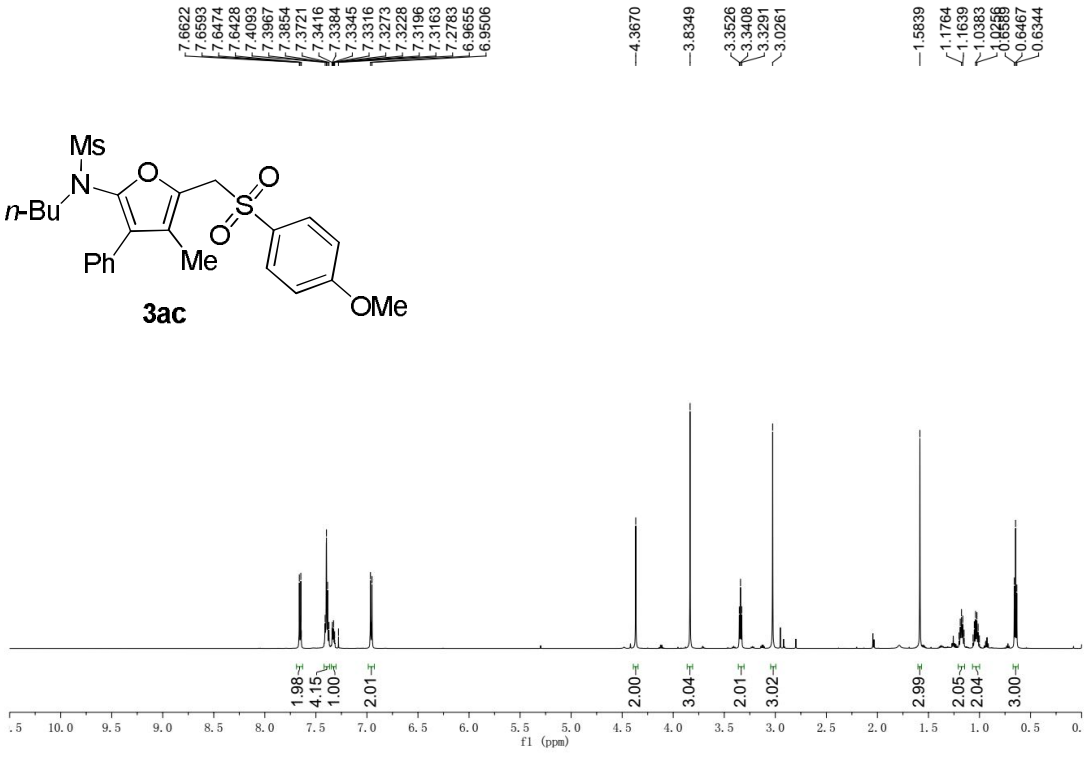
141.7099
136.3816
134.7515
130.5265
129.7787
129.1046
128.6124
128.3969
127.7564
125.1261
122.9015
77.2114
76.9997
76.7879
54.4815
50.7417
39.2883
30.1510
21.6373
19.4178
13.4198
8.6949
Ms
N
n-Bu
O
S
O
O
Ph
Me
3ab
f1 (ppm)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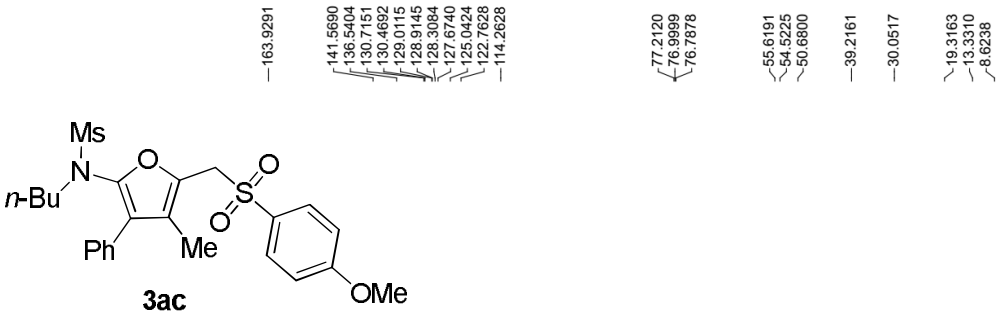
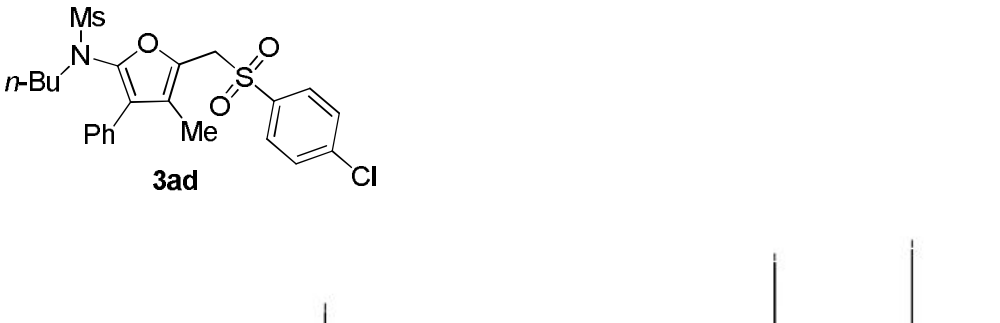
7.6474
7.6428
7.4093
7.3967
7.3854
7.3721
7.3416
7.3384
7.3345
7.3316
7.3273
7.3228
7.3196
7.3163
7.2783
6.9655
6.9506
4.3670
3.8349
3.3526
3.3408
3.3291
3.0261
1.5839
1.1764
1.1639
1.0383
1.0256
0.6467
0.6344
Ms
N
n-Bu
O
S
O
O
Ph
Me
OMe
3ac
1.98
4.15
1.00
2.01
2.00
3.04
2.01
3.02
2.99
2.05
2.04
3.00
f1 (ppm)

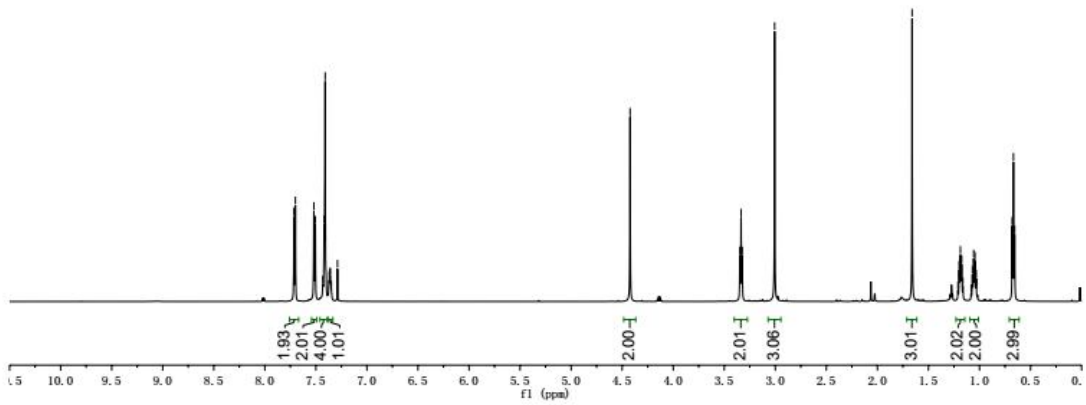

Ms
N
O
n-Bu
S
O
O
Ph
Me
OMe

3ac

163.9291
141.5690
136.5404
130.7151
130.4692
129.0115
128.9145
128.3084
127.6740
125.0424
122.7628
114.2628
77.2120
76.9999
76.7878
55.6191
54.5225
50.6800
39.2161
30.0517
19.3163
13.3310
8.6238
f1 (ppm)


Ms
N
O
n-Bu
S
O
O
Ph
Me
Cl

3ad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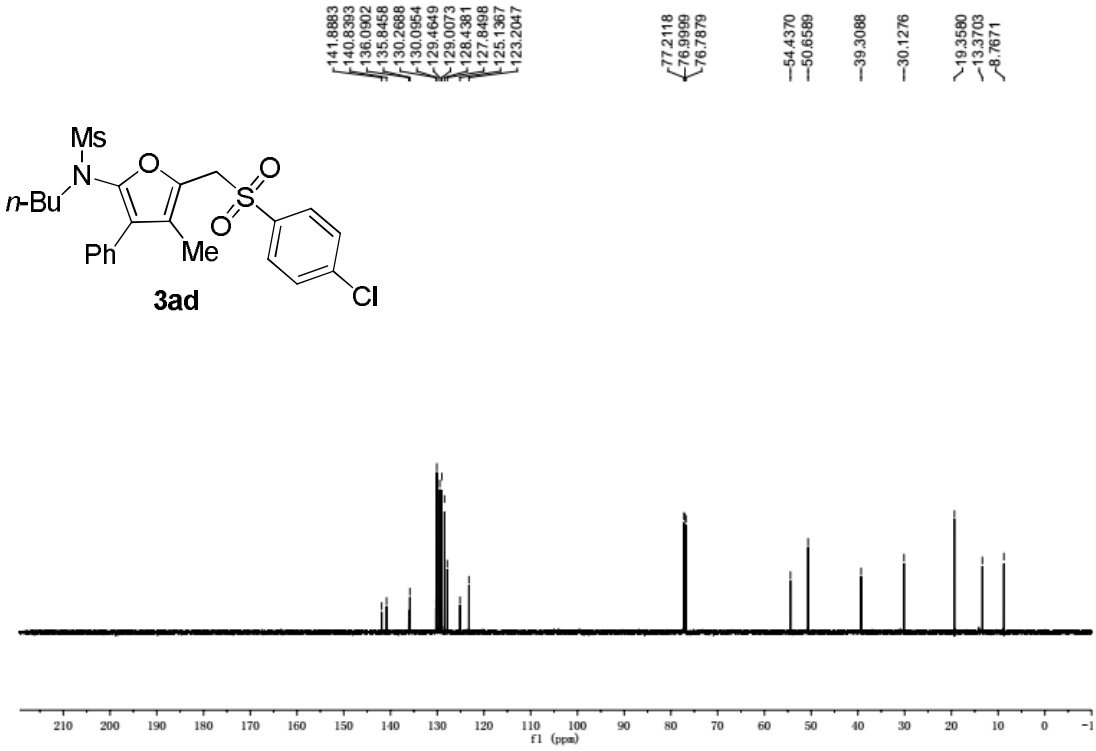
7.7006
7.5197
7.5056
7.4321
7.4189
7.4090
7.3687
7.3623
7.3588
7.3485
7.2886
4.4226
3.3470
3.3353
3.3236
3.0066
1.6603
1.1870
1.1746
1.0569
0.6677
0.6555
1.93
2.01
4.00
1.01
2.00
2.01
3.06
3.01
2.02
2.00
2.99
f1 (ppm)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140.8393
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128.4381
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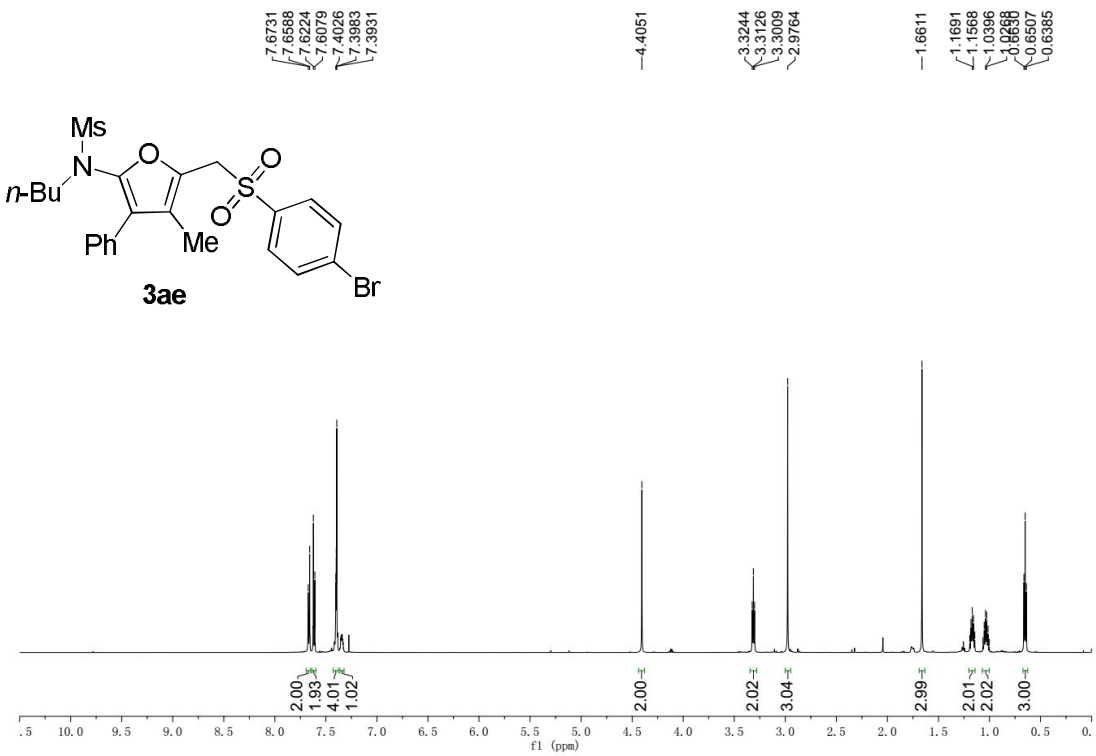
125.1367
123.2047
77.2118
76.9999
76.7879
54.4370
50.6589
39.3088
30.1276
19.3580
13.3703
8.7671
Ms
N
n-Bu
O
S
O
O
Ph
Me
Cl
3ad
f1 (ppm)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7.6588
7.6224
7.6079
7.4026
7.3983
7.3931
4.4051
3.3244
3.3126
3.3009
2.9764
1.6611
1.1691
1.1568
1.0396
1.0268
0.8630
0.6507
0.6385
Ms
N
n-Bu
O
S
O
O
Ph
Me
Br
3ae
2.00
1.93
4.01
1.02
2.00
2.02
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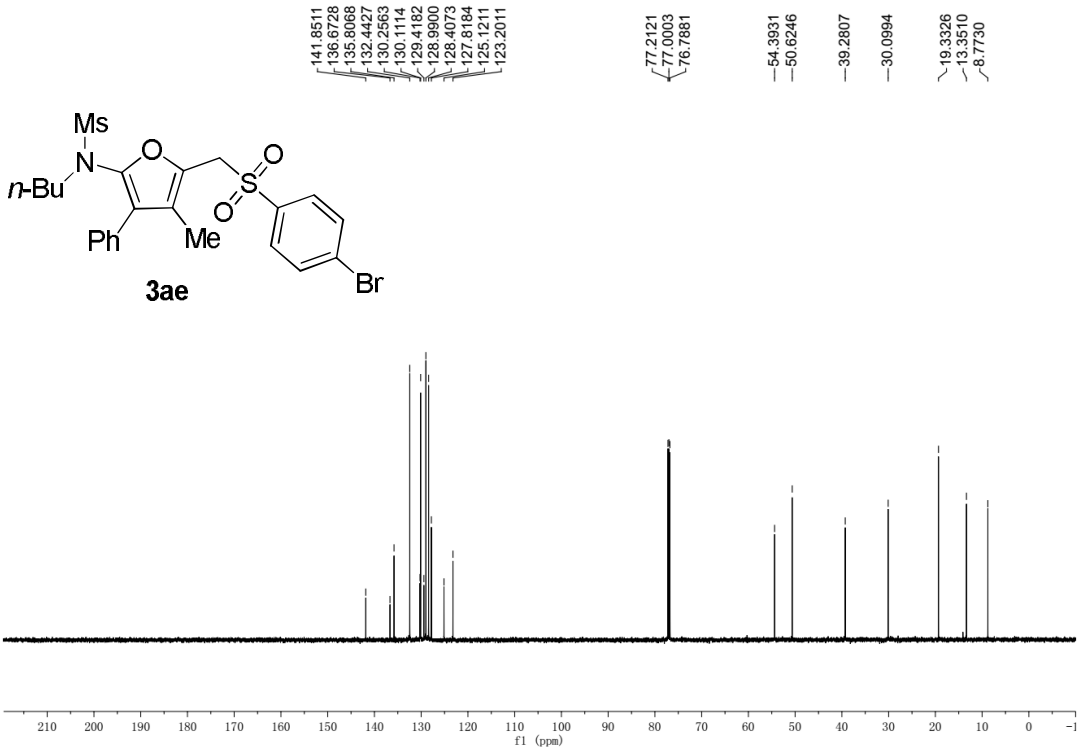
2.99
2.01
2.02
3.00
f1 (ppm)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132.4427
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130.1114
129.4182
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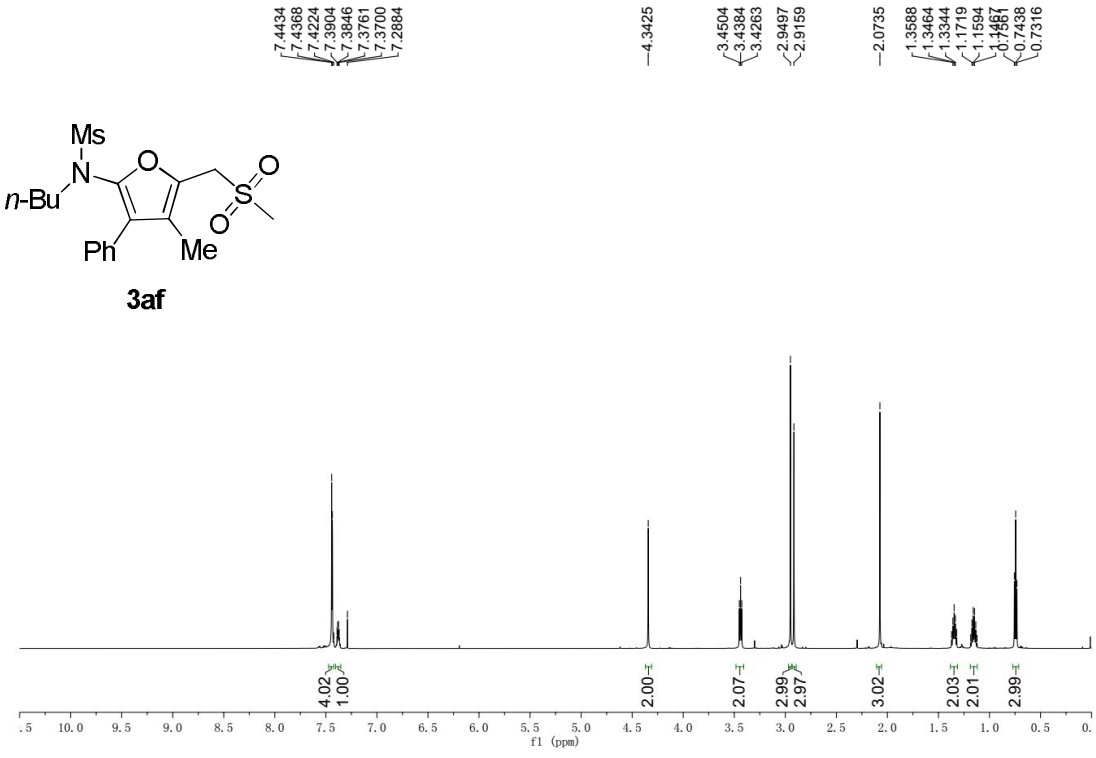
128.4073
127.8184
125.1211
123.2011
77.2121
77.0003
76.7881
54.3931
50.6246
39.2807
30.0994
19.3326
13.3510
8.7730
Ms
N
n-Bu
O
S
O
O
Ph
Me
Br
3ae
f1 (ppm)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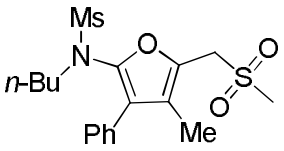
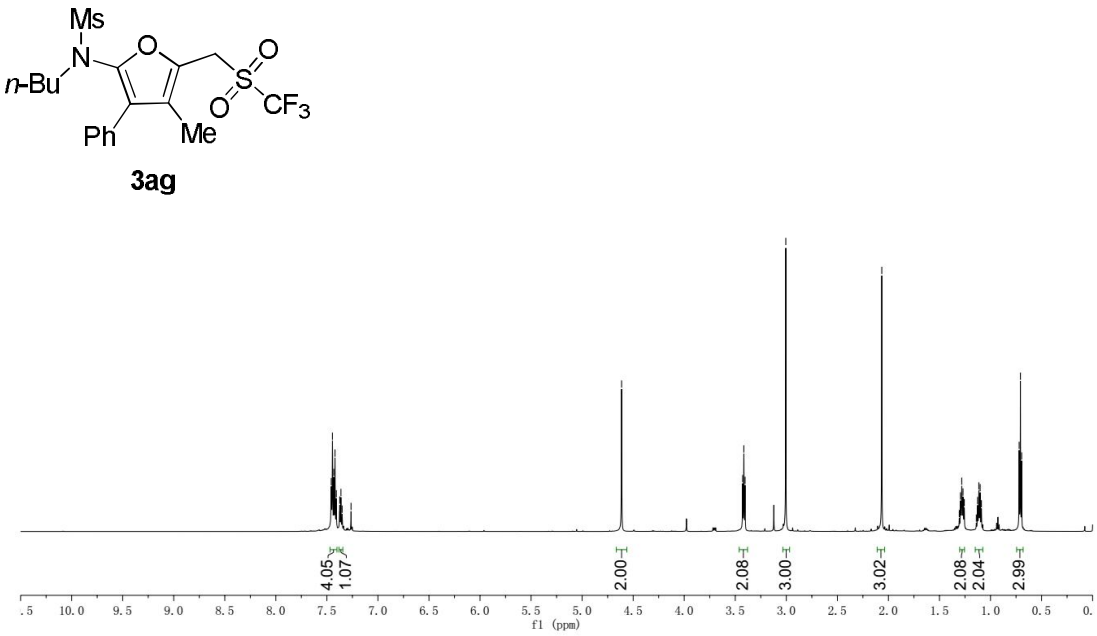
7.4224
7.3904
7.3846
7.3761
7.3700
7.2884
4.3425
3.4504
3.4384
3.4263
2.9497
2.9159
2.0735
1.3588
1.3464
1.3344
1.1719
1.1594
0.7438
0.7316
Ms
N
n-Bu
O
S
O
O
Ph
Me
3af
4.02
1.00
2.00
2.07
2.99
2.97
3.02
2.03
2.01
2.99
f1 (ppm)


Ms
N
O
n-Bu
S
O
O
Ph
Me

3af

141.8304
136.2994
130.3896
129.0296
128.5224
127.9611
124.9825
122.9918
77.2120
77.0002
76.7882
52.8453
50.8909
39.9496
39.7714
30.4458
19.4557
13.4150
9.4044
f1 (ppm)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7.3503
7.2632
4.6134
3.4279
3.4159
3.4039
3.0050
2.0649
1.2939
1.2815
1.2693
1.1267
1.1141
0.7194
0.7072
0.6949
f1 (ppm)

Ms
N
O
n-Bu
S
O
O
CF3
Ph
Me

3ag

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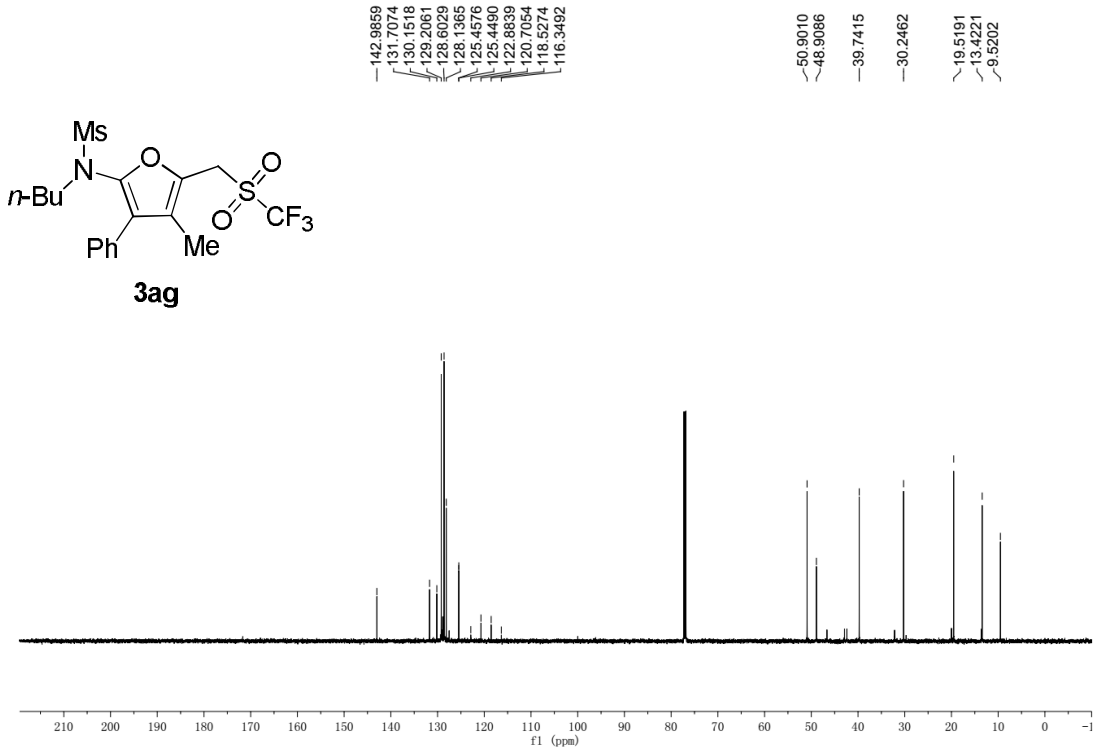
1.07
2.00
2.08
3.00
3.02
2.08
2.04
2.99
f1 (ppm)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128.1365
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125.4490
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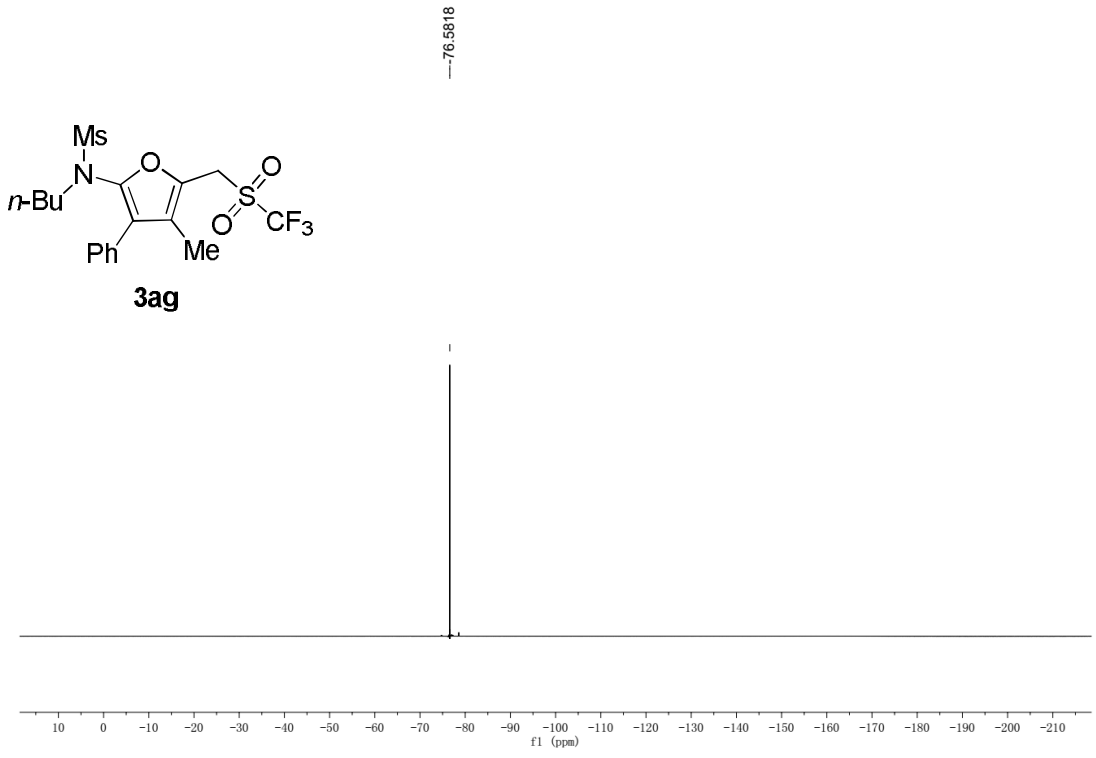
120.7054
118.5274
116.3492
50.9010
48.9086
39.7415
30.2462
19.5191
13.4221
9.5202
Ms
N
n-Bu
O
S
O
O
CF3
Ph
Me
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -1
f1 (ppm)

3ag


-76.5818
Ms
N
n-Bu
O
S
O
O
CF3
Ph
Me
10 0 -10 -20 -30 -40 -50 -60 -70 -80 -90 -100 -110 -120 -130 -140 -150 -160 -170 -180 -190 -200 -210
f1 (ppm)

3ag


8.1314
8.1187
7.6706
7.6088
7.5958
7.5831
7.4997
7.4871
7.4705
7.4572
7.2719
6.2602
3.1503
3.1391
3.1280
3.1169
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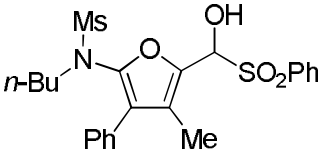
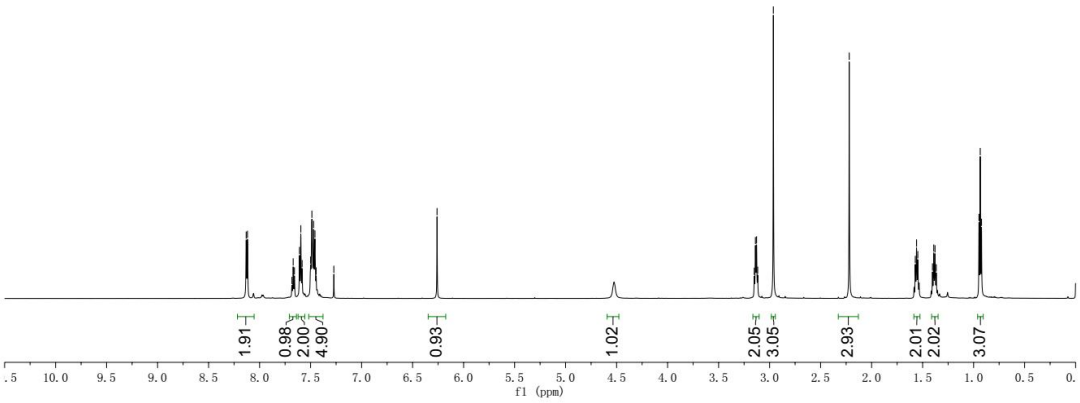
0.9228


Ms
N
O
OH
n-Bu
SO2Ph
Ph
Me

4a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2.00
4.90
0.93
1.02
2.05
3.05
2.93
2.01
2.02
3.07
f1 (ppm)


165.9979
155.7333
145.6681
141.1783
133.9739
131.0388
130.1362
129.3241
129.1834
128.8776
128.2589
128.1250
109.1399
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77.0844
76.8725
43.0709
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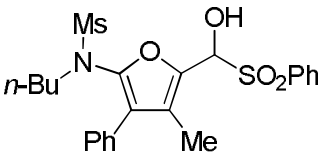
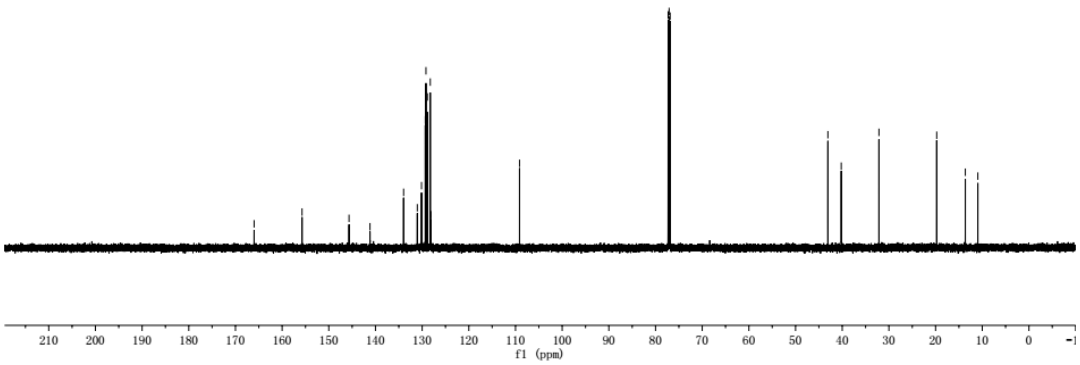
32.1315
19.7573
13.6274
10.9498


Ms
N
O
OH
n-Bu
SO2Ph
Ph
Me

4a


f1 (ppm)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7.4922
7.4837
7.4819
7.4262
7.4231
7.4137
7.4033
7.4006
7.3473
7.3452
7.3430
7.3359
7.3329
7.3205
7.2883
3.4404
3.4285
3.4166
3.0308
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2.2674
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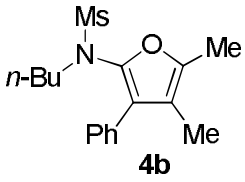
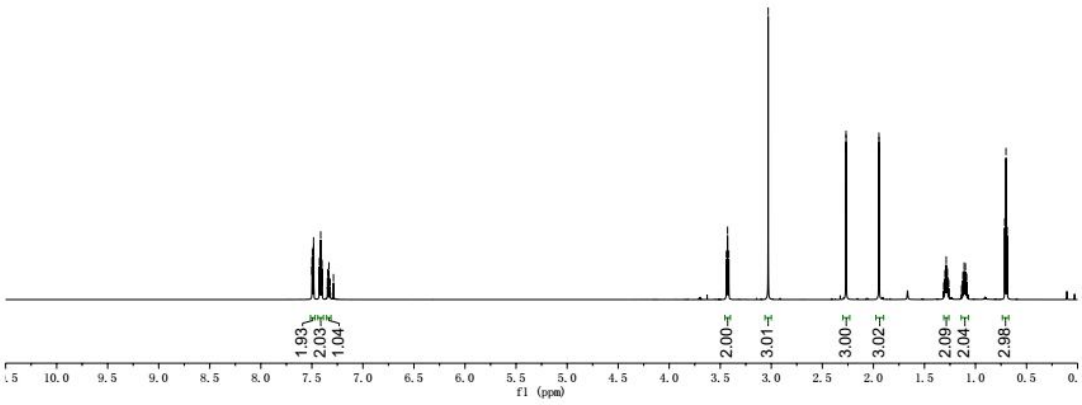
1.2746
1.1114
0.7016
0.6893


Ms
N
O
Me
n-Bu
Ph
Me

4b


1.93
2.03
1.04
2.00
3.01
3.00
3.02
2.09
2.04
2.98
f1 (ppm)


145.5830
138.4063
131.7785
129.0807
128.2386
127.2394
124.5953
115.2170
77.2114
76.9997
76.7878
50.9623
39.4098
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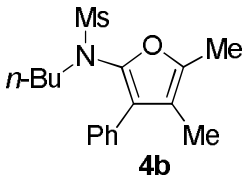
19.4838
13.4412
11.6474
9.2123


Ms
N
O
Me
n-Bu
Ph
Me

4b

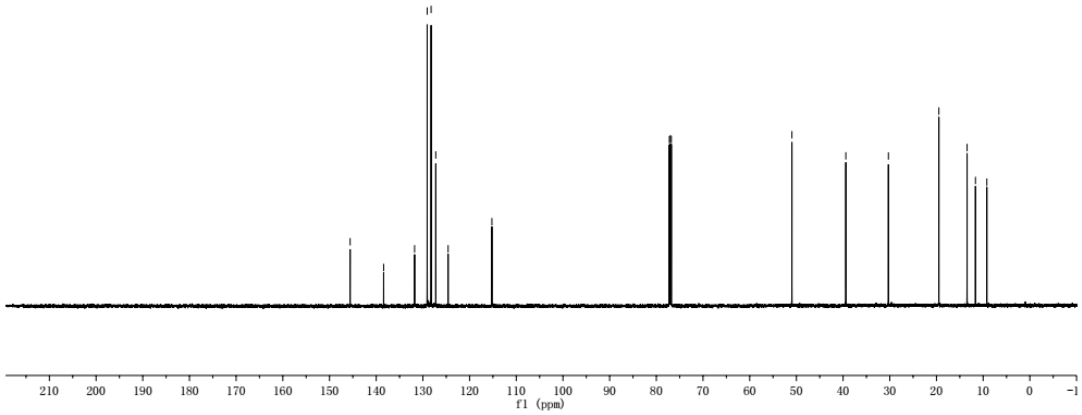
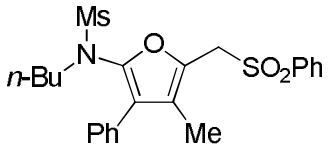
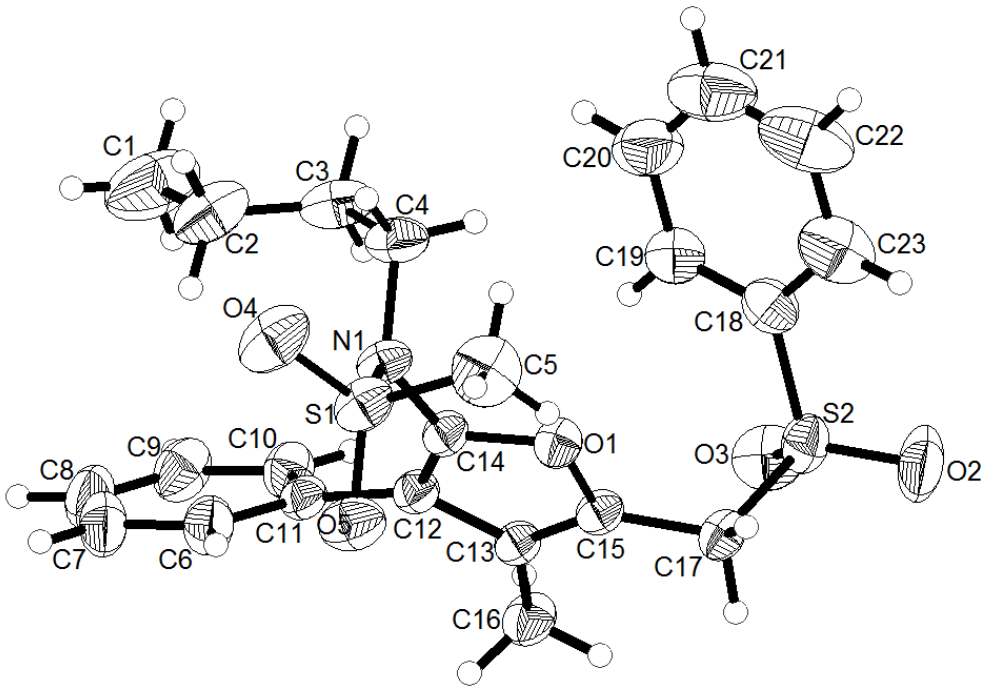

f1 (ppm)

Figure S1. ORTEP drawing of 3aa showing the atom-labeling scheme and displacement ellipsoids drawn at the 50% probability level



3aa



Checkcif Report of 3aa

checkCIF/PLATON report

You have not supplied any structure factors. As a result the full set of tests cannot be run.

THIS REPORT IS FOR GUIDANCE ONLY. IF USED AS PART OF A REVIEW PROCEDURE FOR PUBLICATION, IT SHOULD NOT REPLACE THE EXPERTISE OF AN EXPERIENCED CRYSTALLOGRAPHIC REFEREE.

No syntax errors found. CIF dictionary Interpreting this report

Datablock: 1

```
Bond precision:  C-C = 0.0035 A          Wavelength=0.71073

Cell:           a=11.6931(6)    b=12.6204(6)        c=16.4696(8)
                alpha=90        beta=104.241(3)     gamma=90
Temperature:    296 K

                Calculated                Reported
Volume          2355.8(2)                 2355.8(2)
Space group     P 21/c                    P2(1)/c
Hall group      -P 2ybc                   ?
Moiety formula  C23 H27 N O5 S2           ?
Sum formula     C23 H27 N O5 S2           C23 H27 N O5 S2
Mr              461.58                    461.58
Dx,g cm-3       1.301                     1.301
Z               4                         4
Mu (mm-1)       0.259                     0.259
F000            976.0                     976.0
F000'           977.42
h,k,lmax        15,16,21                  15,16,21
Nref            5517                      5493
Tmin,Tmax       0.940,0.974               0.940,0.974
Tmin'           0.902

Correction method= # Reported T Limits: Tmin=0.940 Tmax=0.974
AbsCorr = EMPIRICAL

Data completeness= 0.996          Theta(max)= 27.680

R(reflections)= 0.0482( 3813)     wR2(reflections)= 0.1209( 5493)

S = 1.020                 Npar= 283
```

The following ALERTS were generated. Each ALERT has the format
test-name_ALERT_alert-type_alert-level.
Click on the hyperlinks for more details of the test.

Alert level C

PLAT220_ALERT_2_C Non-Solvent Resd 1 C Ueq(max)/Ueq(min) Range 3.3 Ratio
PLAT790_ALERT_4_C Centre of Gravity not Within Unit Cell: Resd. # 1 Note
C23 H27 N O5 S2

Alert level G

PLAT005_ALERT_5_G No Embedded Refinement Details found in the CIF Please Do !
PLAT066_ALERT_1_G Predicted and Reported Tmin&Tmax Range Identical ? Check
PLAT093_ALERT_1_G No s.u.'s on H-positions, Refinement Reported as mixed Check
PLAT398_ALERT_2_G Deviating C-O-C Angle from 120 Deg for O1 105.5 Degree
PLAT899_ALERT_4_G SHELXL97 is Deprecated and Succeeded by SHELXL 2014 Note

0 **ALERT level A** = Most likely a serious problem - resolve or explain
0 **ALERT level B** = A potentially serious problem, consider carefully
2 **ALERT level C** = Check. Ensure it is not caused by an omission or oversight
5 **ALERT level G** = General information/check it is not something unexpected

2 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
2 ALERT type 2 Indicator that the structure model may be wrong or deficient
0 ALERT type 3 Indicator that the structure quality may be low
2 ALERT type 4 Improvement, methodology, query or suggestion
1 ALERT type 5 Informative message, check

It is advisable to attempt to resolve as many as possible of the alerts in all categories. Often the minor alerts point to easily fixed oversights, errors and omissions in your CIF or refinement strategy, so attention to these fine details can be worthwhile. In order to resolve some of the more serious problems it may be necessary to carry out additional measurements or structure refinements. However, the purpose of your study may justify the reported deviations and the more serious of these should normally be commented upon in the discussion or experimental section of a paper or in the "special_details" fields of the CIF. checkCIF was carefully designed to identify outliers and unusual parameters, but every test has its limitations and alerts that are not important in a particular case may appear. Conversely, the absence of alerts does not guarantee there are no aspects of the results needing attention. It is up to the individual to critically assess their own results and, if necessary, seek expert advice.

Publication of your CIF in IUCr journals

A basic structural check has been run on your CIF. These basic checks will be run on all CIFs submitted for publication in IUCr journals (*Acta Crystallographica*, *Journal of Applied Crystallography*, *Journal of Synchrotron Radiation*); however, if you intend to submit to *Acta Crystallographica Section C* or *E* or *IUCrData*, you should make sure that full publication checks are run on the final version of your CIF prior to submission.

Publication of your CIF in other journals

Please refer to the *Notes for Authors* of the relevant journal for any special instructions relating to CIF submission.

PLATON version of 27/03/2017; check.def file version of 24/03/2017

Datablock 1 - ellipsoid plot