Supporting Information

2,3-Diaroyl benzofurans from arynes: Sequential synthesis of 2-aroylbenzofurans followed by benzoylation

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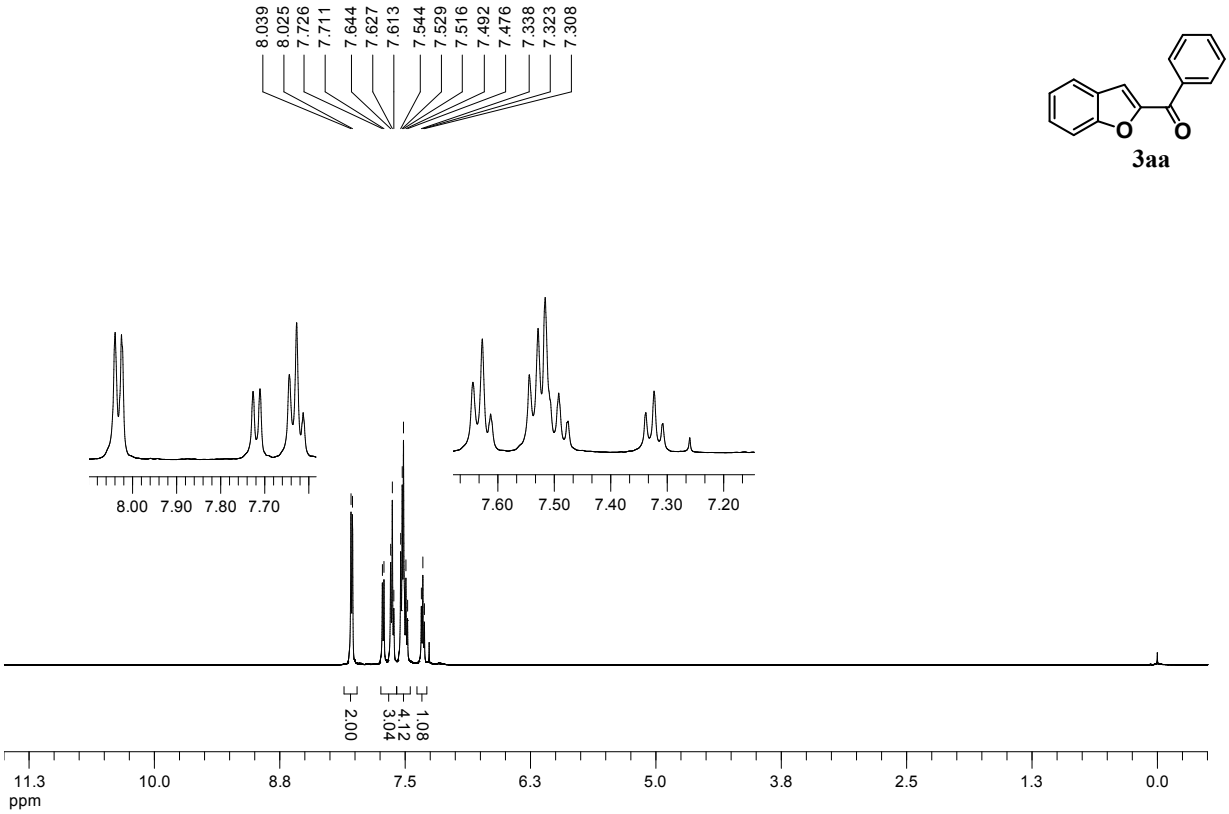
Email: gogoipranj@yahoo.co.uk; gogoipranj@gmail.com

Copies of ^{1}H , ^{13}C NMR and HRMS spectra of all products

Copies of ^{1}H and ^{13}C NMR spectra of all products



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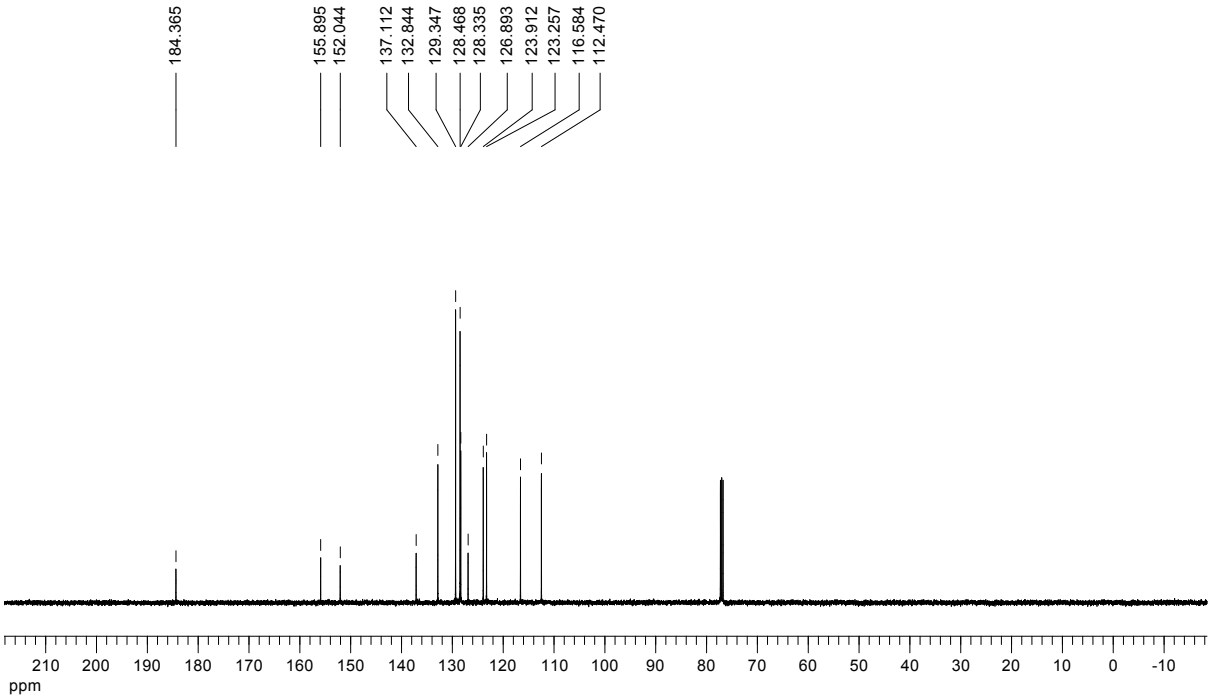

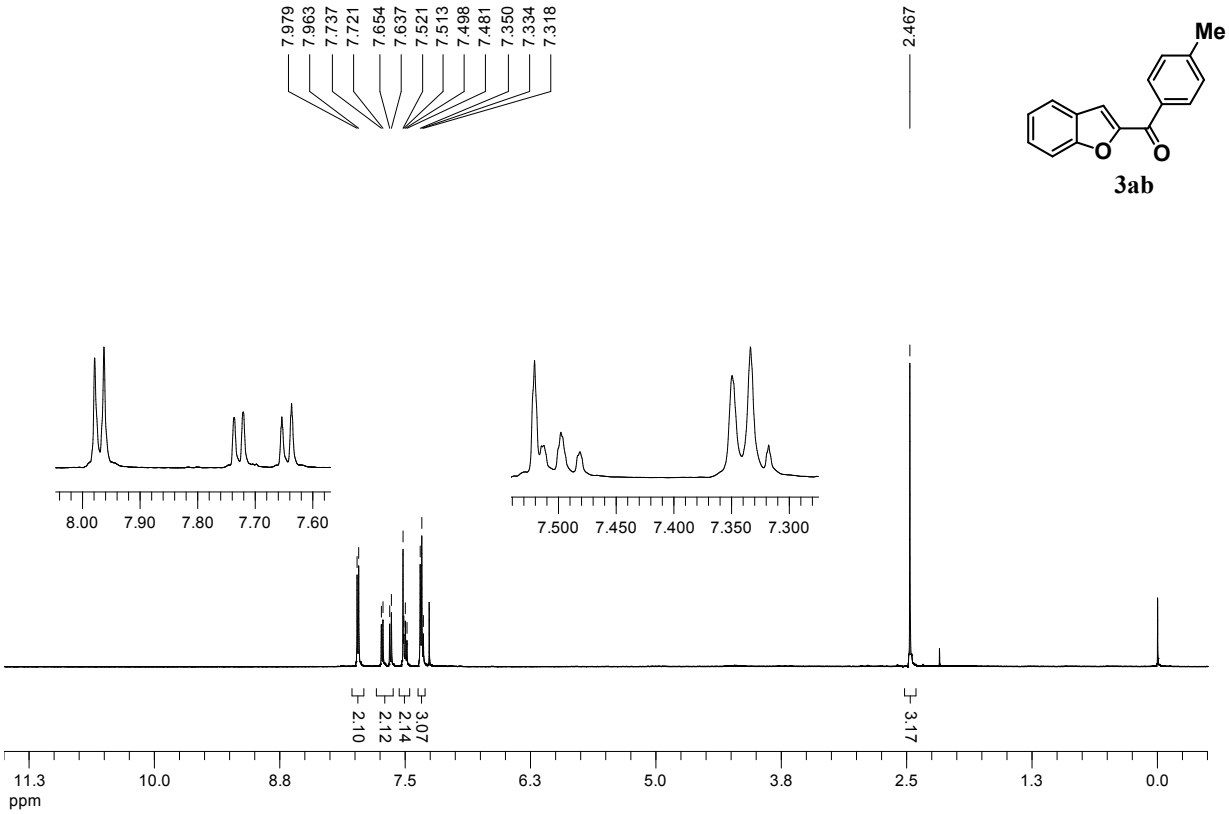
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2.467
Me
O
O
3ab
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7.500 7.450 7.400 7.350 7.300
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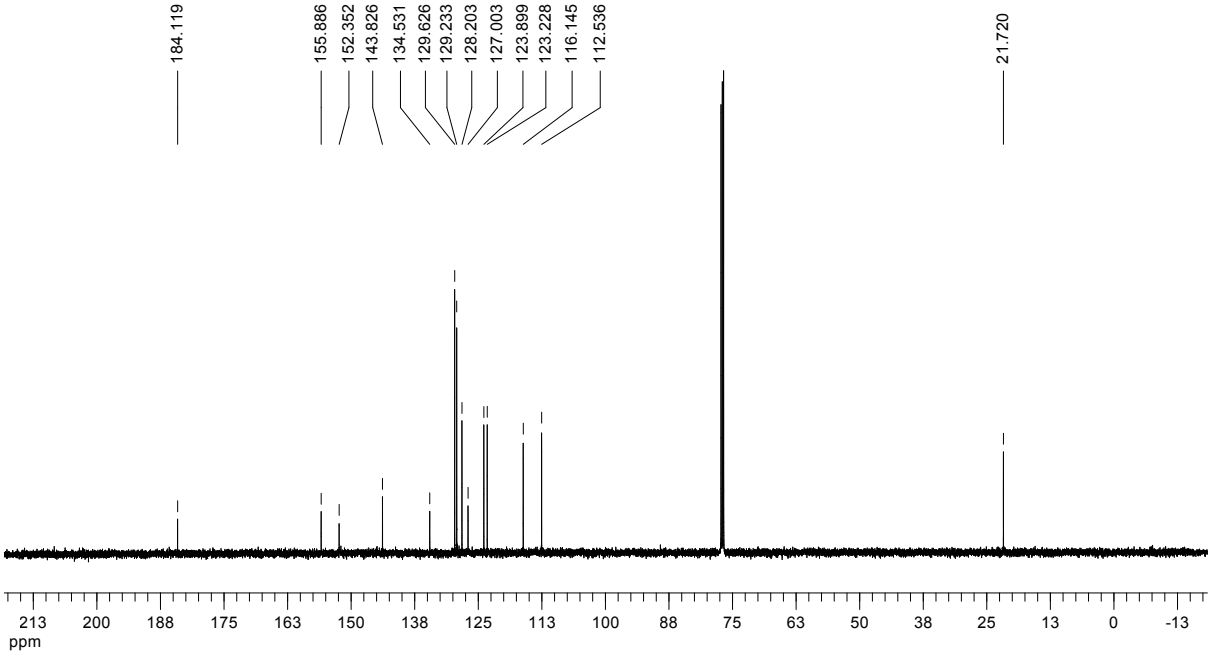
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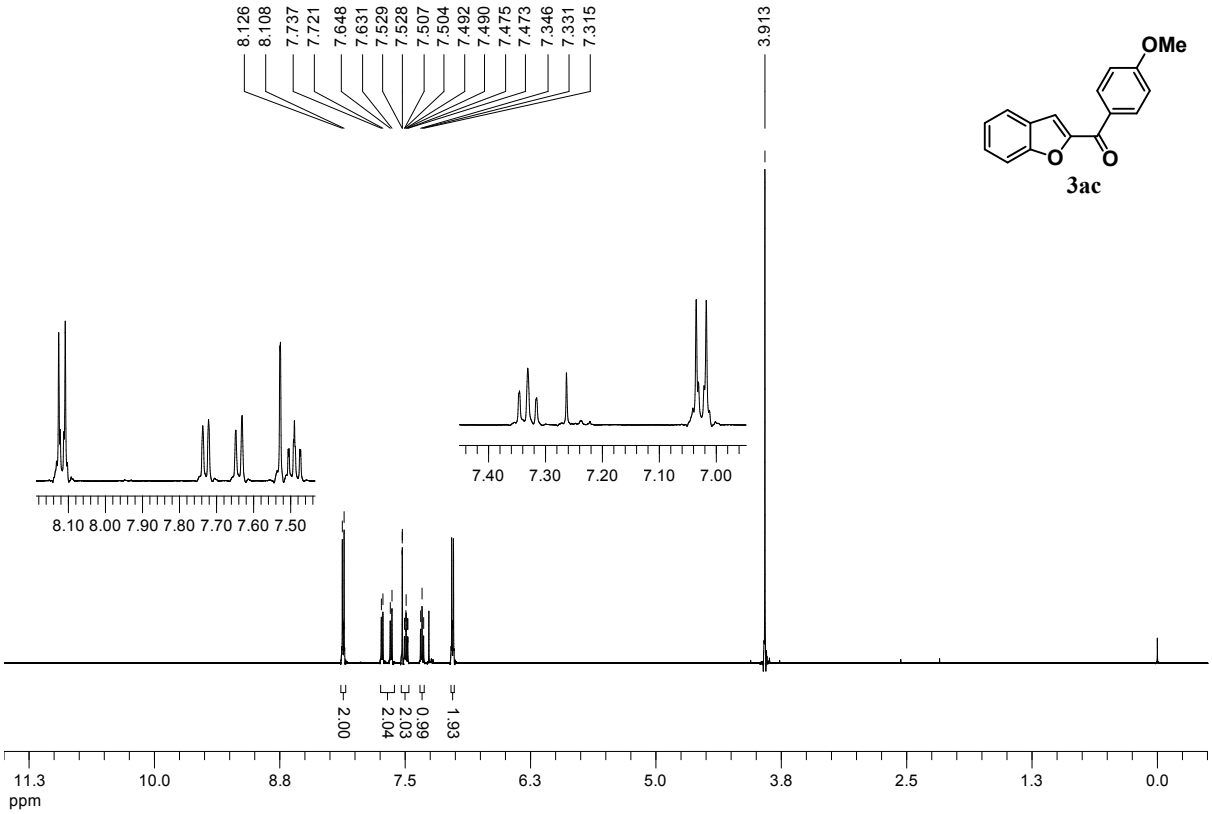
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7.331
7.315
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OMe
O
O
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2.04
2.03
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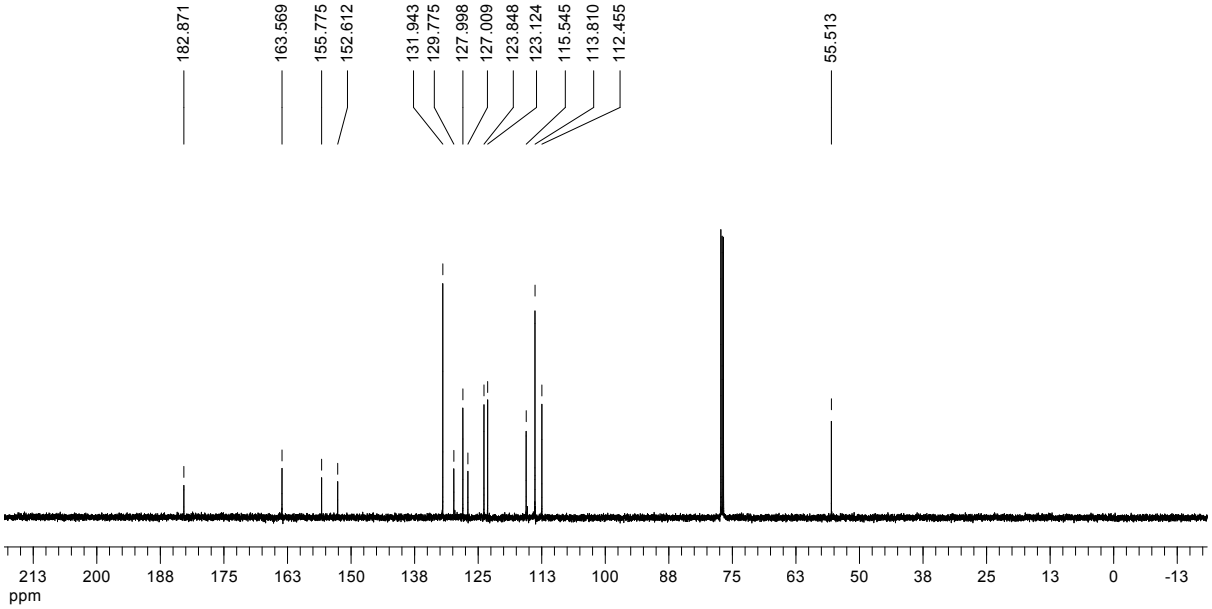
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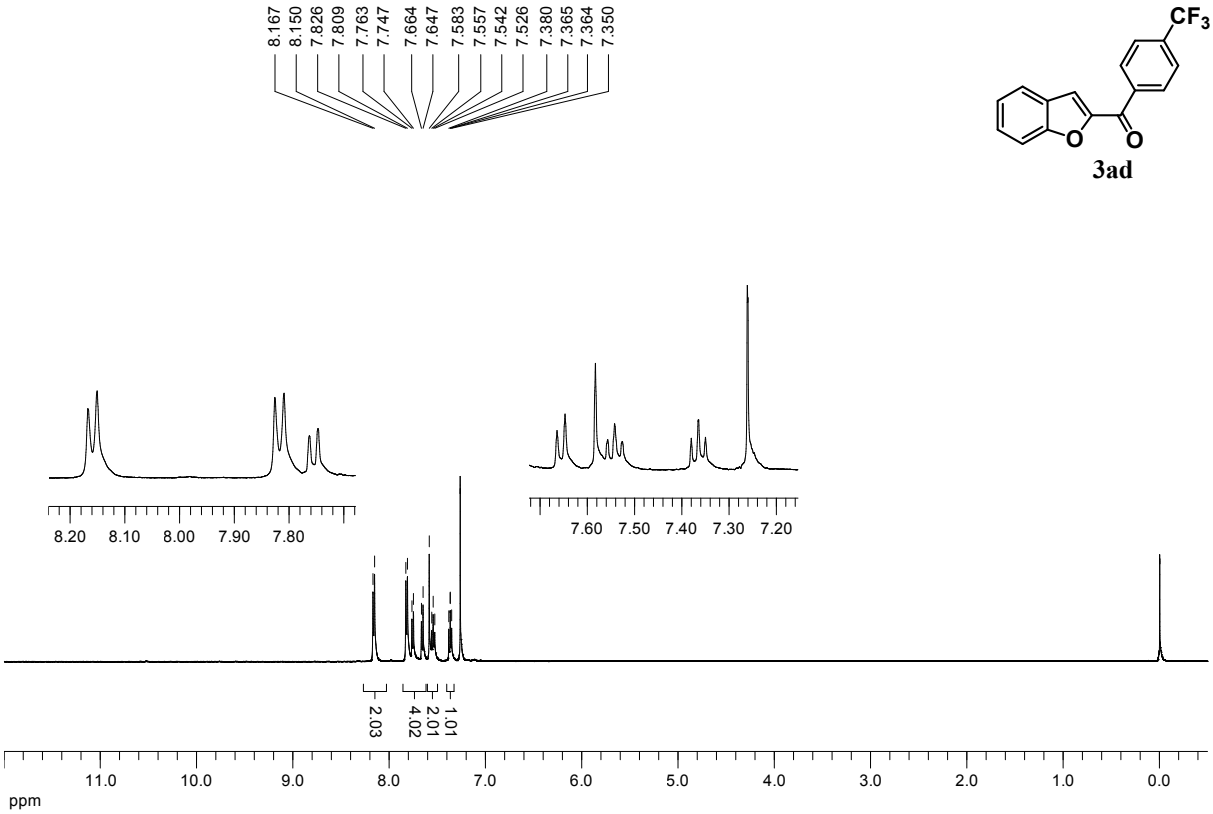
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7.380
7.365
7.364
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CF3
O
O
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8.20 8.10 8.00 7.90 7.80
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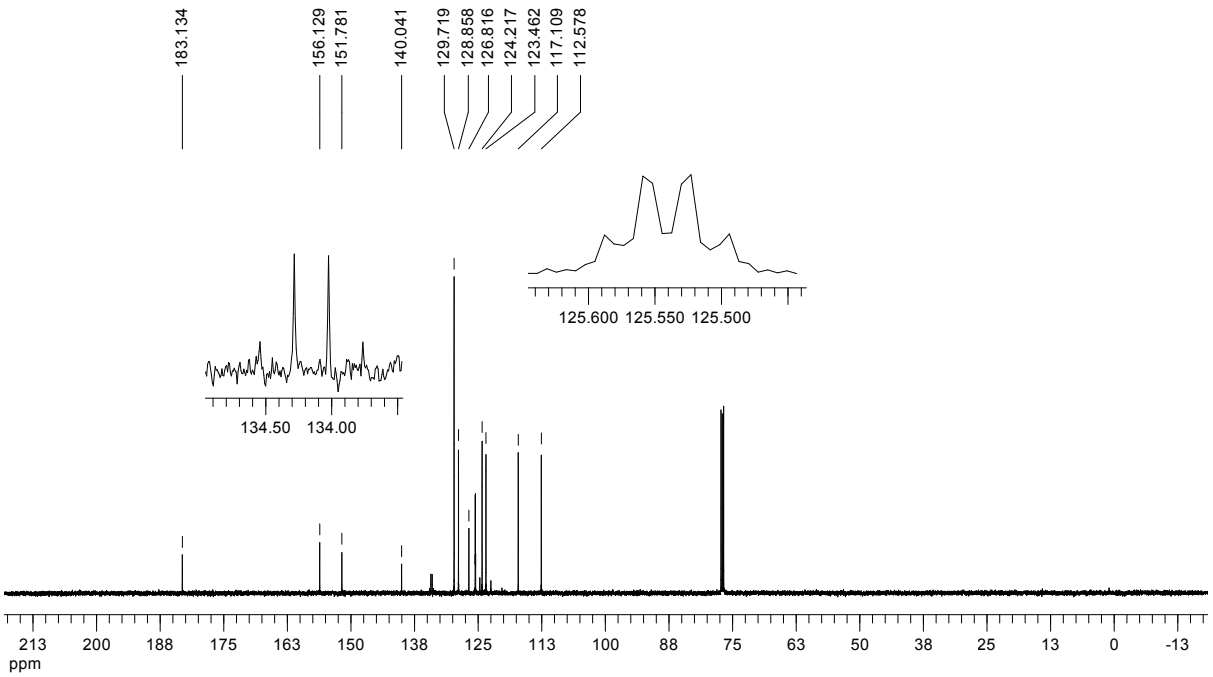
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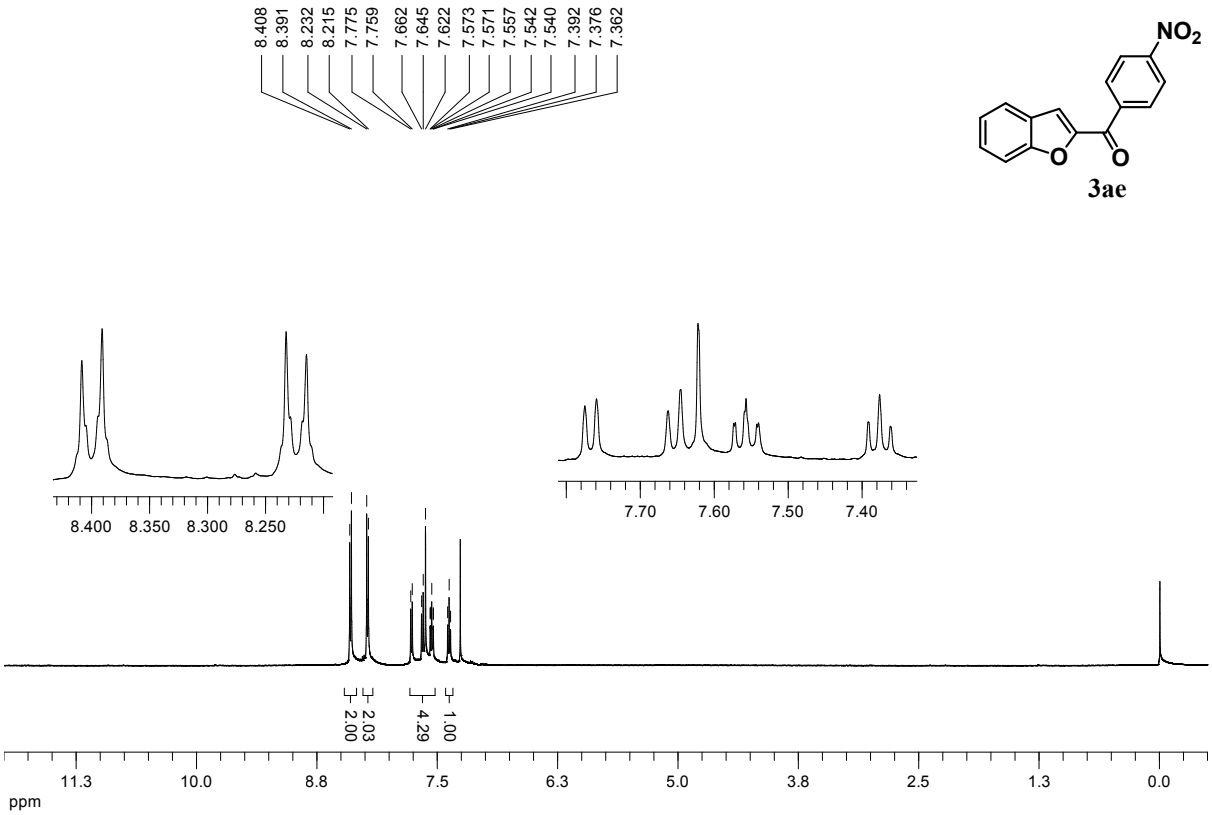
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7.540
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7.362
NO2
O
O
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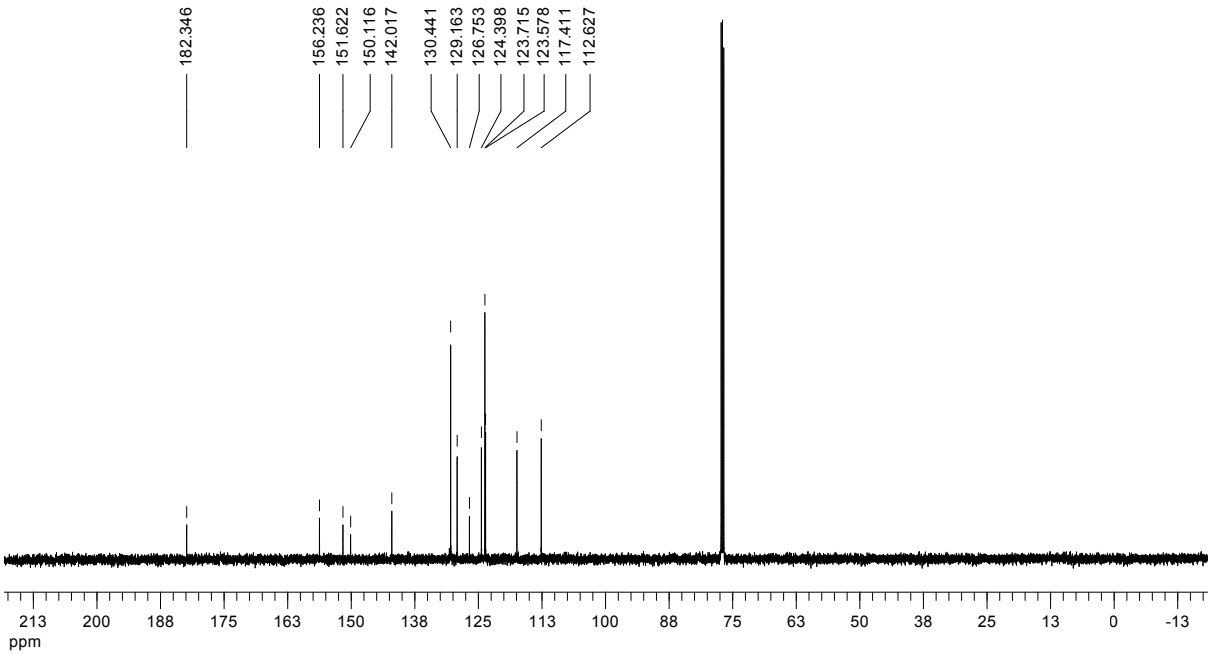
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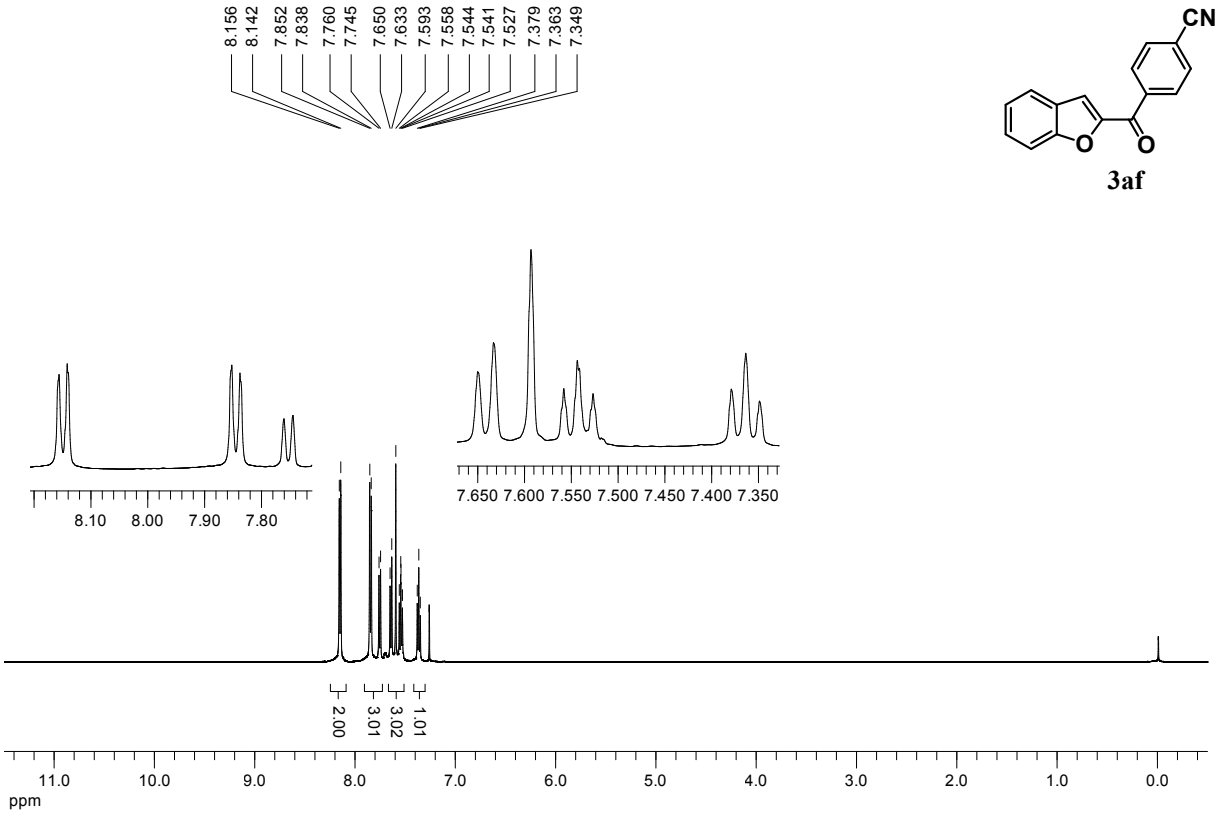
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7.379
7.363
7.349
CN
O
O
3af
8.10 8.00 7.90 7.80
7.650 7.600 7.550 7.500 7.450 7.400 7.350
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3.02
1.01
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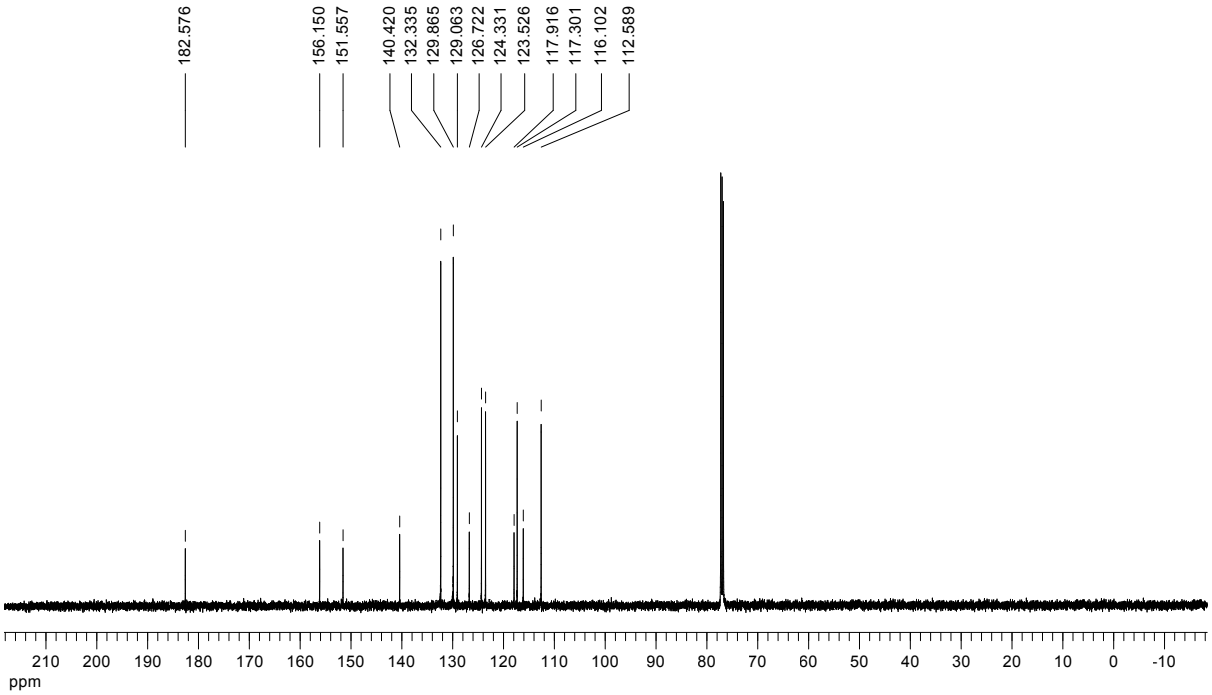
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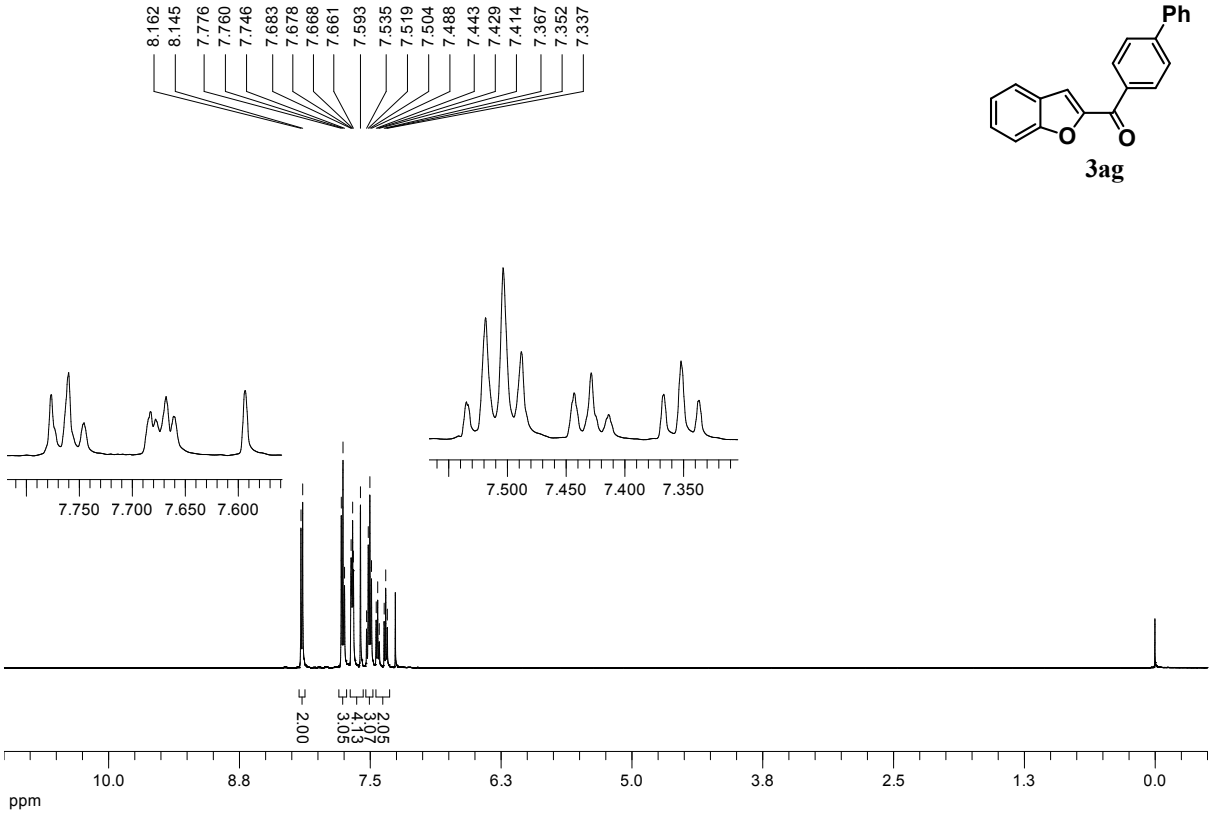
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7.488
7.443
7.429
7.414
7.367
7.352
7.337
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O
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7.500 7.450 7.400 7.350
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3.05
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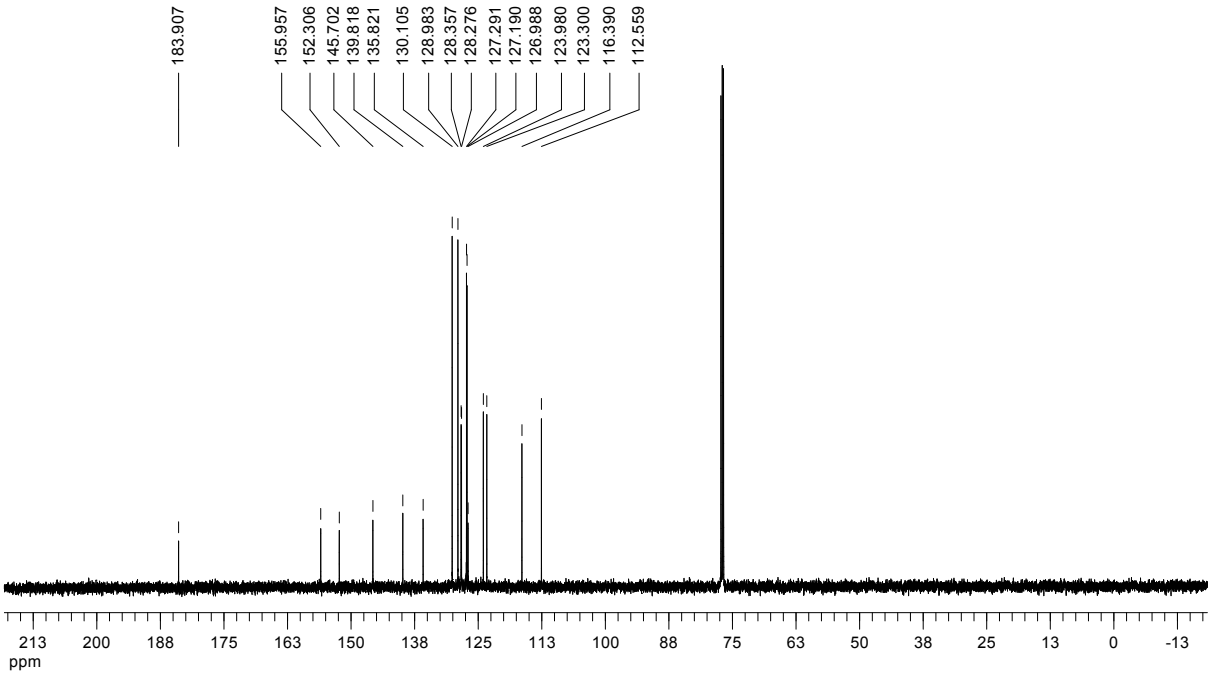
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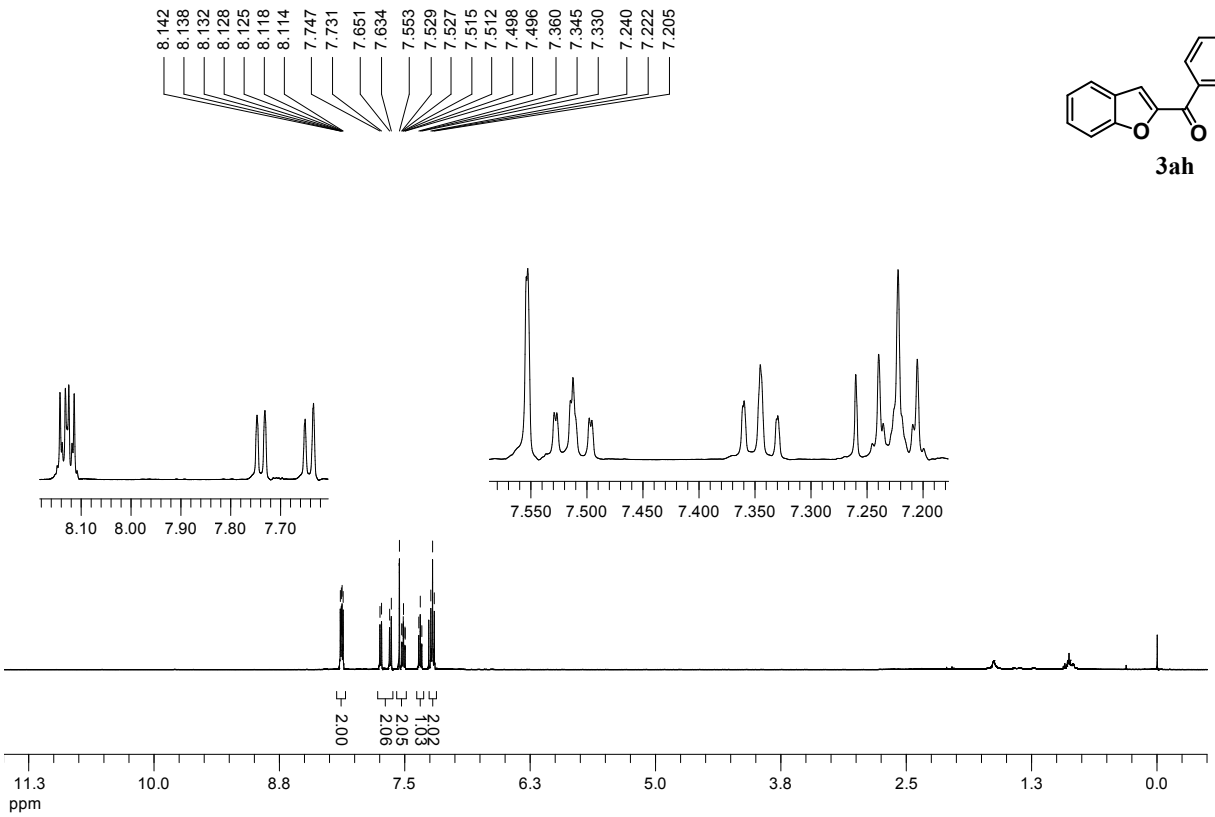
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O
O
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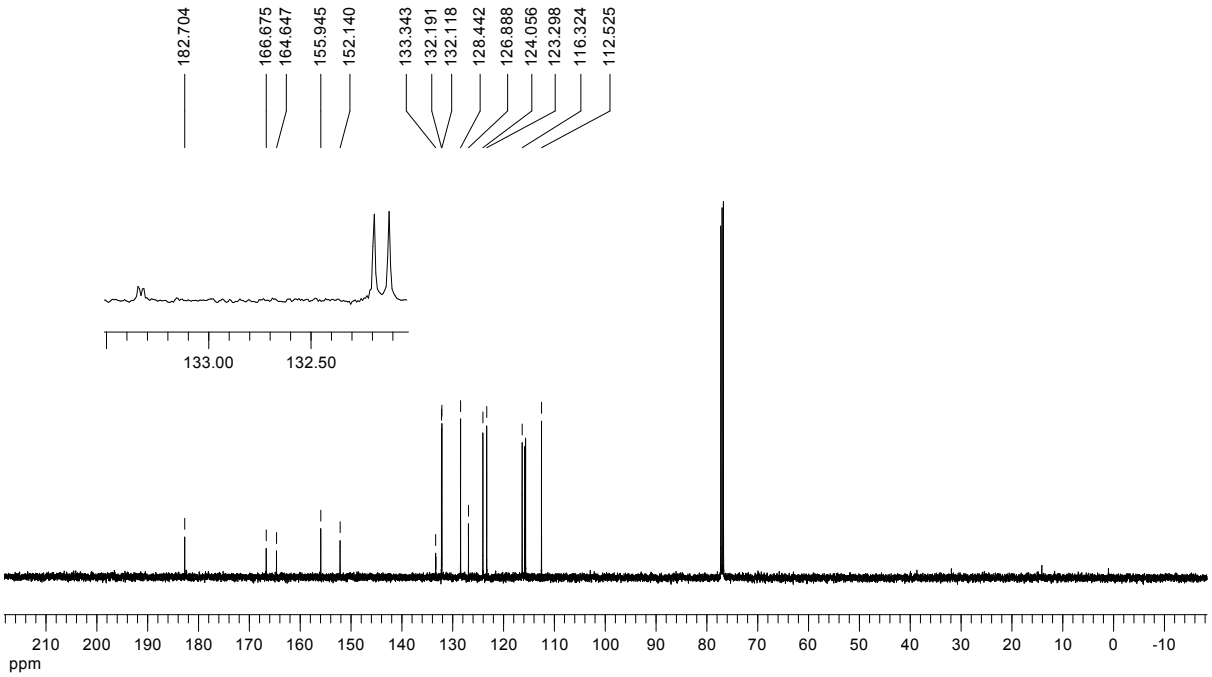
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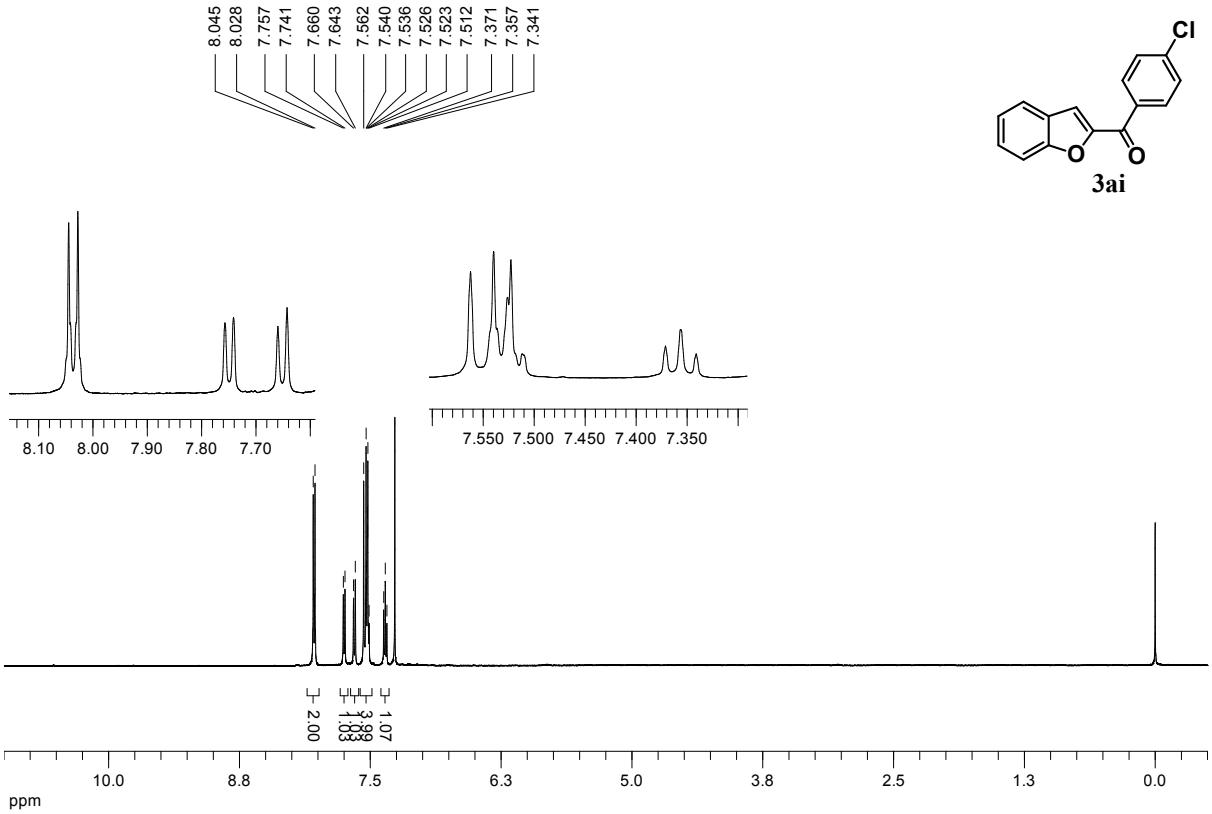
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O
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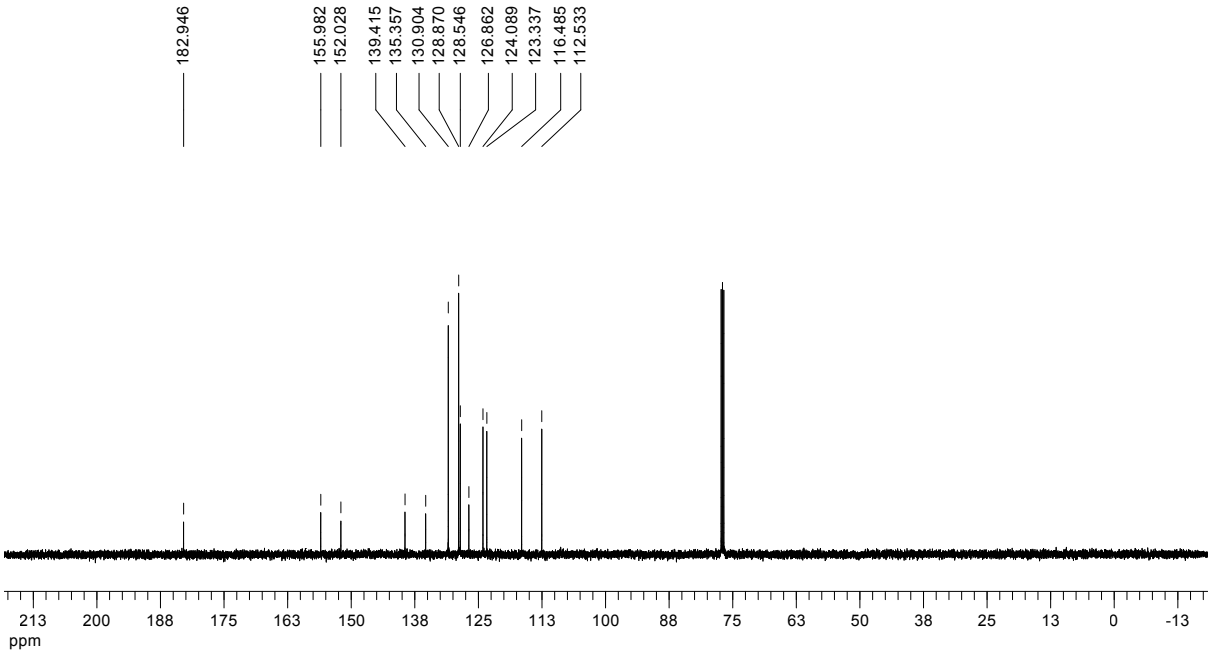
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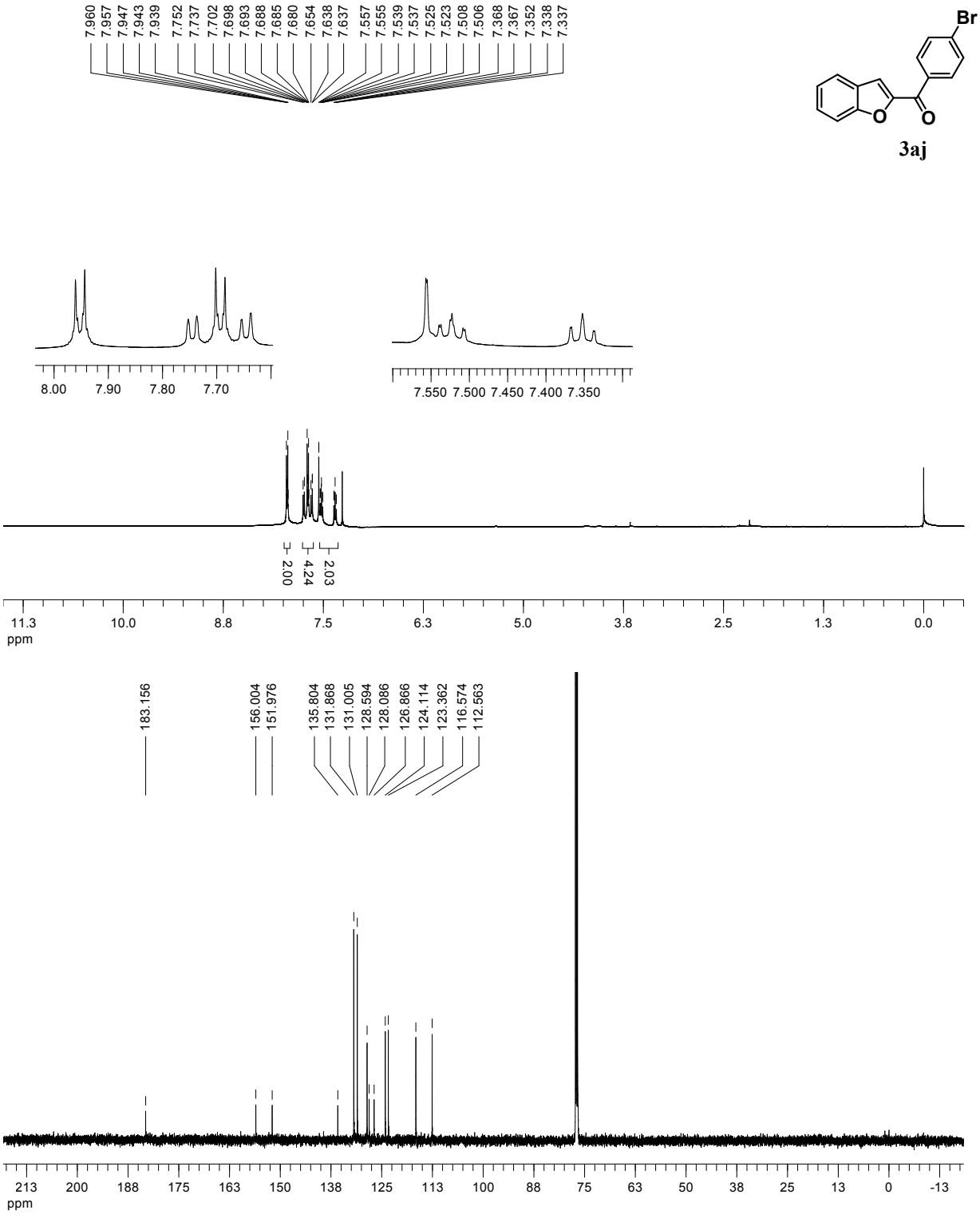
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7.506
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7.367
7.352
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7.337
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O
O
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7.80
7.70
7.550 7.500 7.450 7.400 7.350
2.00
4.24
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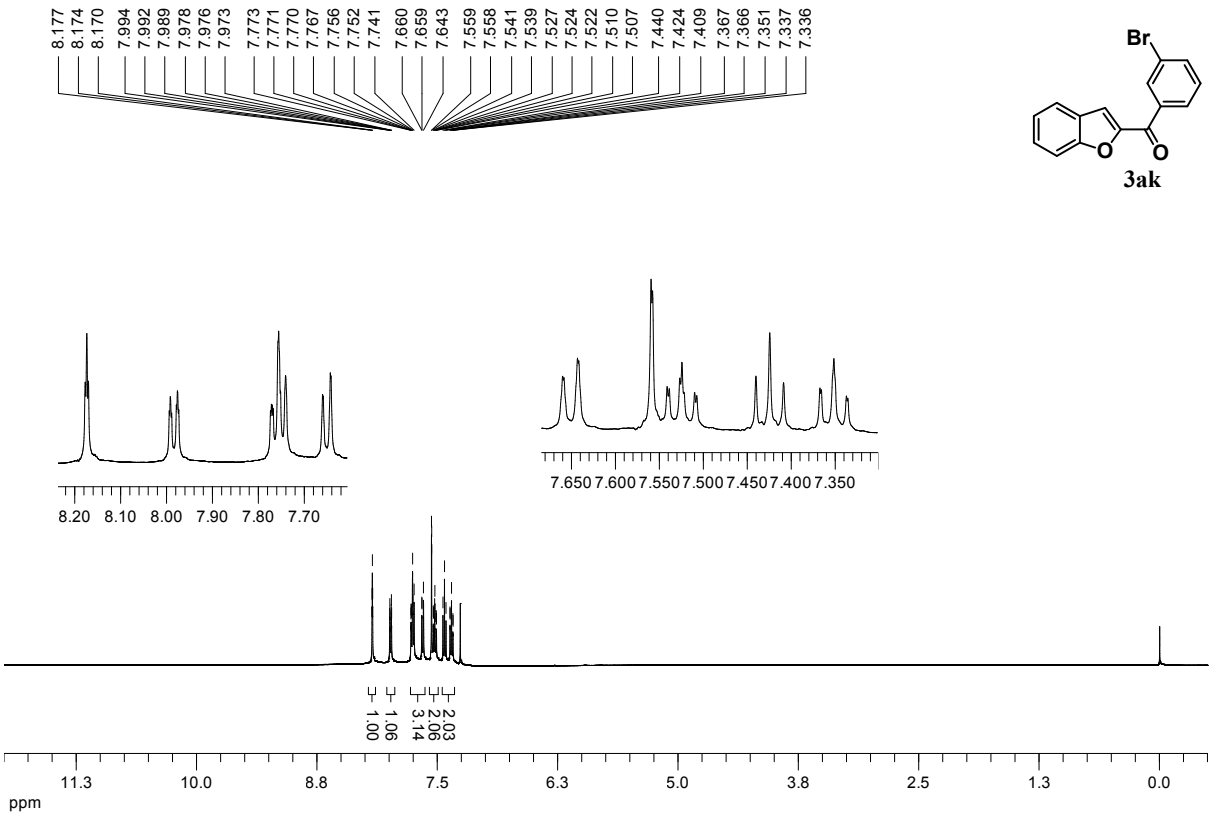
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7.337
7.336
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O
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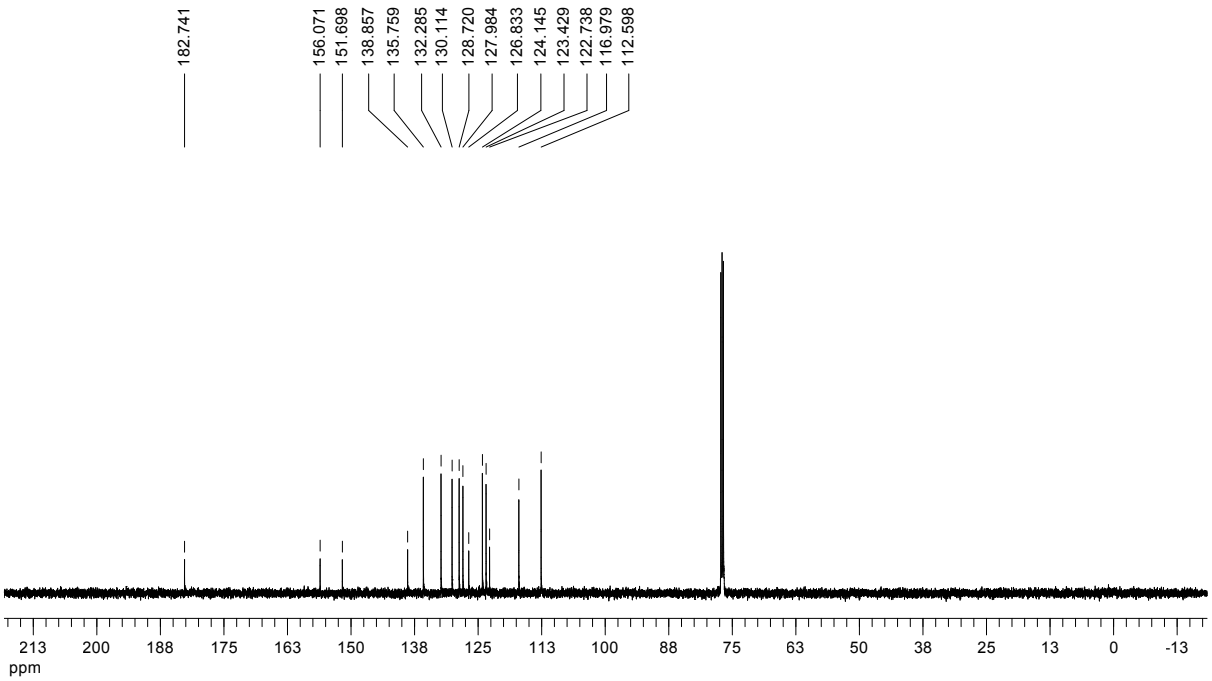
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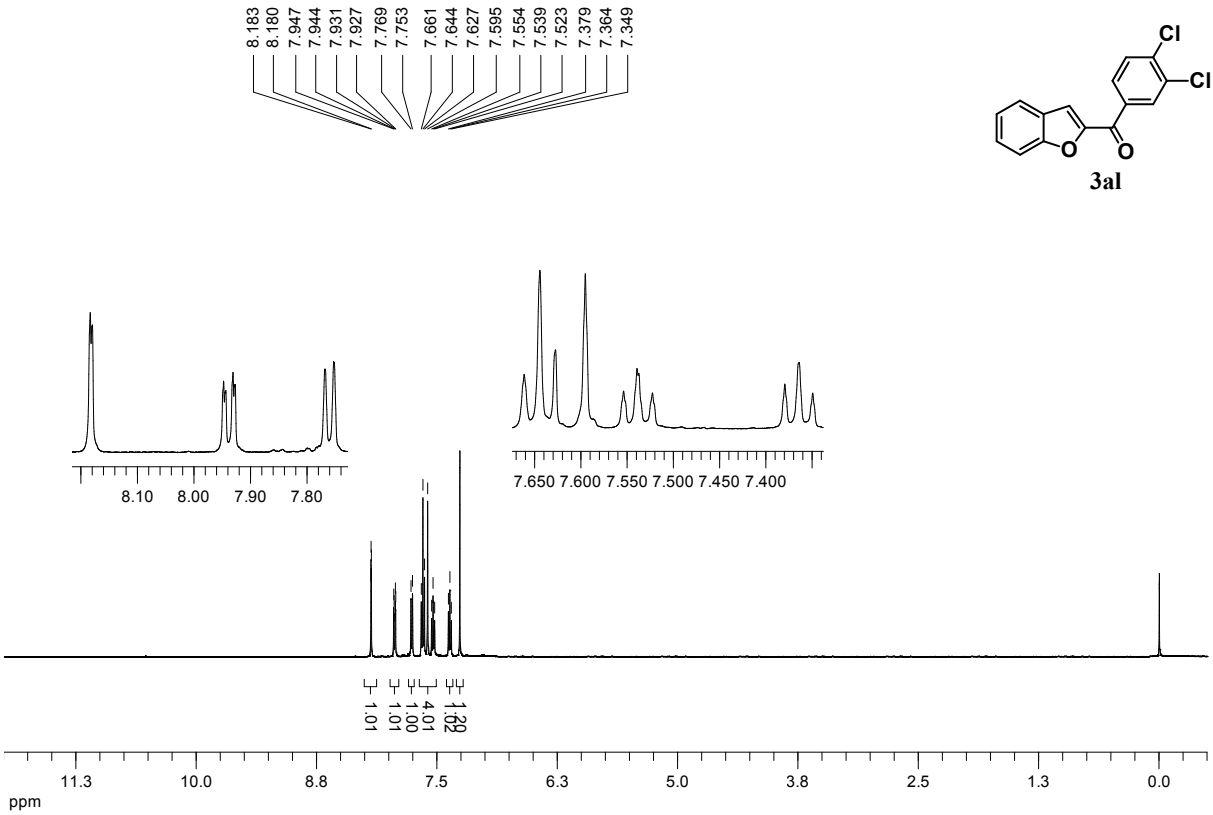
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7.554
7.539
7.523
7.379
7.364
7.349
Cl
Cl
O
O
3al
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7.650 7.600 7.550 7.500 7.450 7.400
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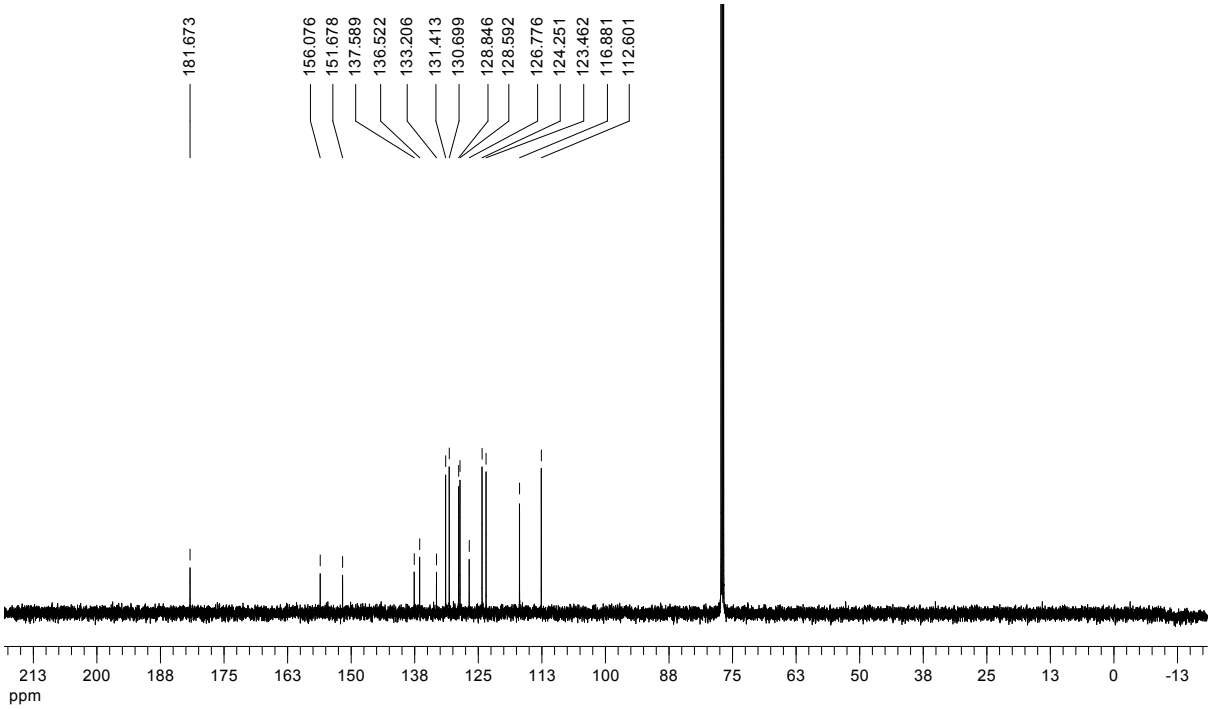
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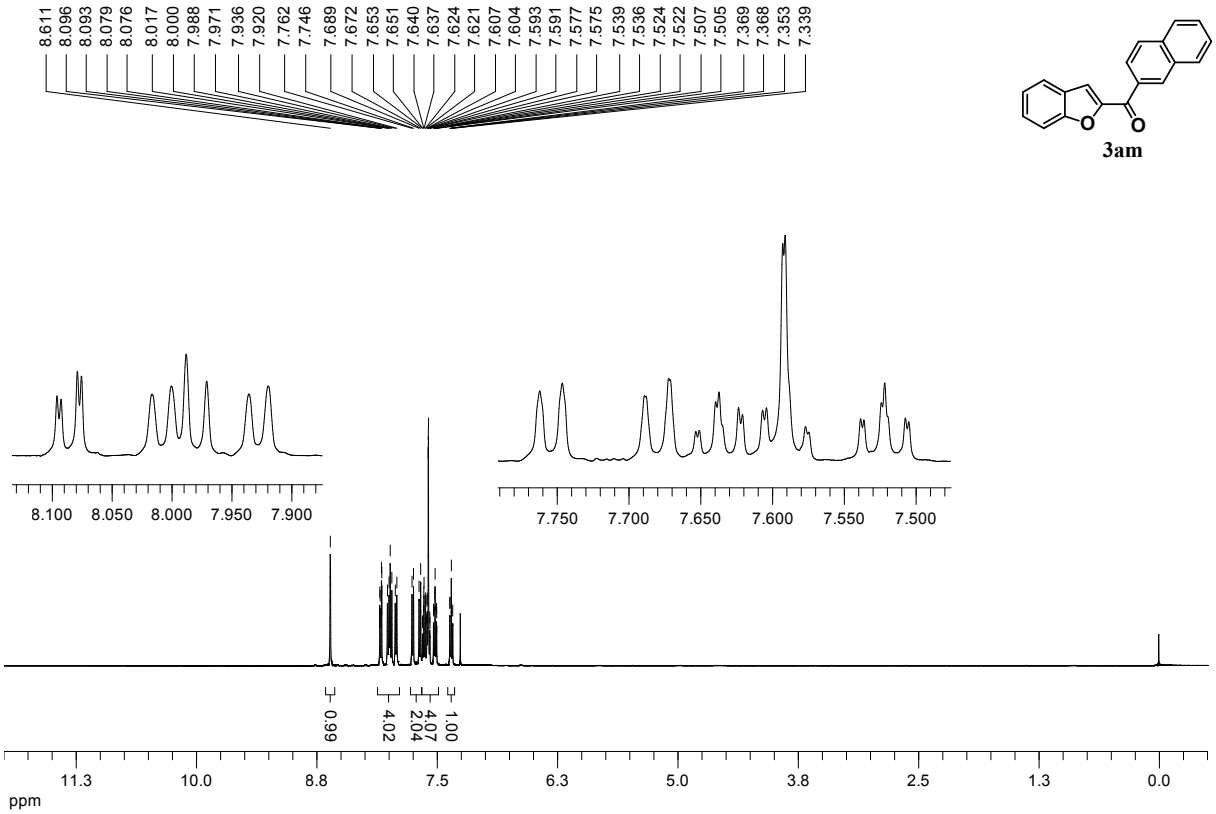
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7.369
7.368
7.353
7.339
3am
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7.750 7.700 7.650 7.600 7.550 7.500
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4.07
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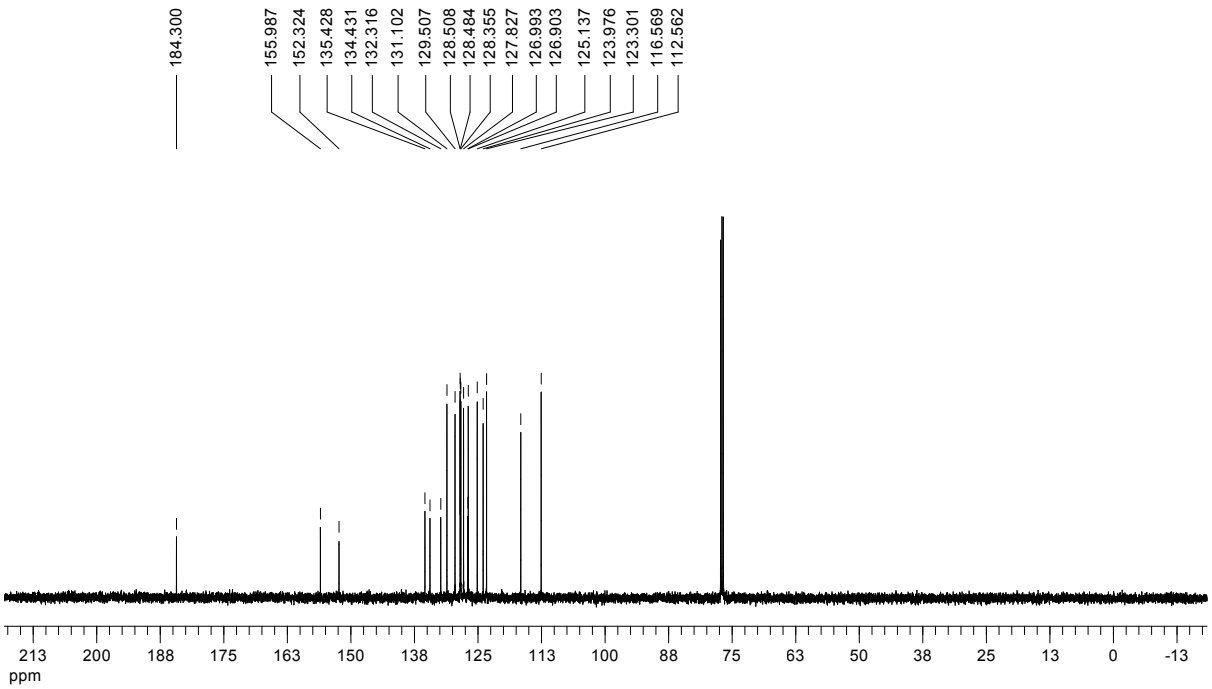
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116.569
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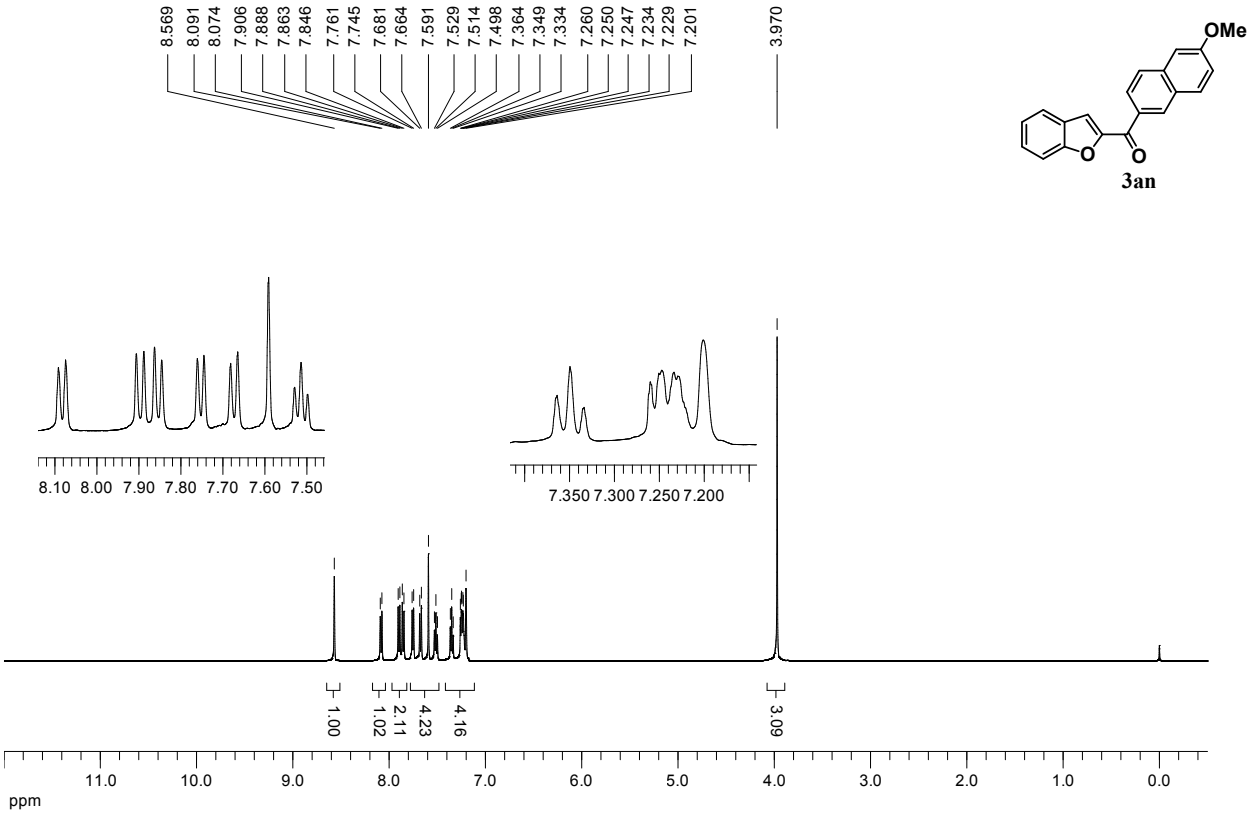
ppm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7.761
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7.681
7.664
7.591
7.529
7.514
7.498
7.364
7.349
7.334
7.260
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7.247
7.234
7.229
7.201
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OMe
O
O
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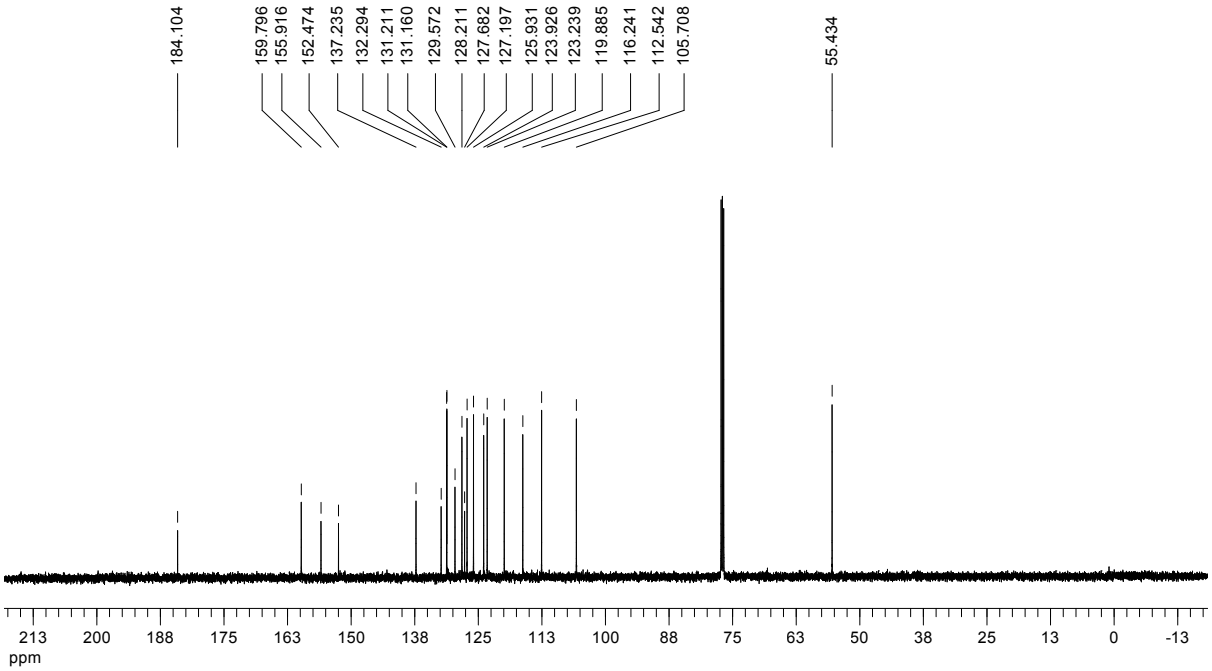
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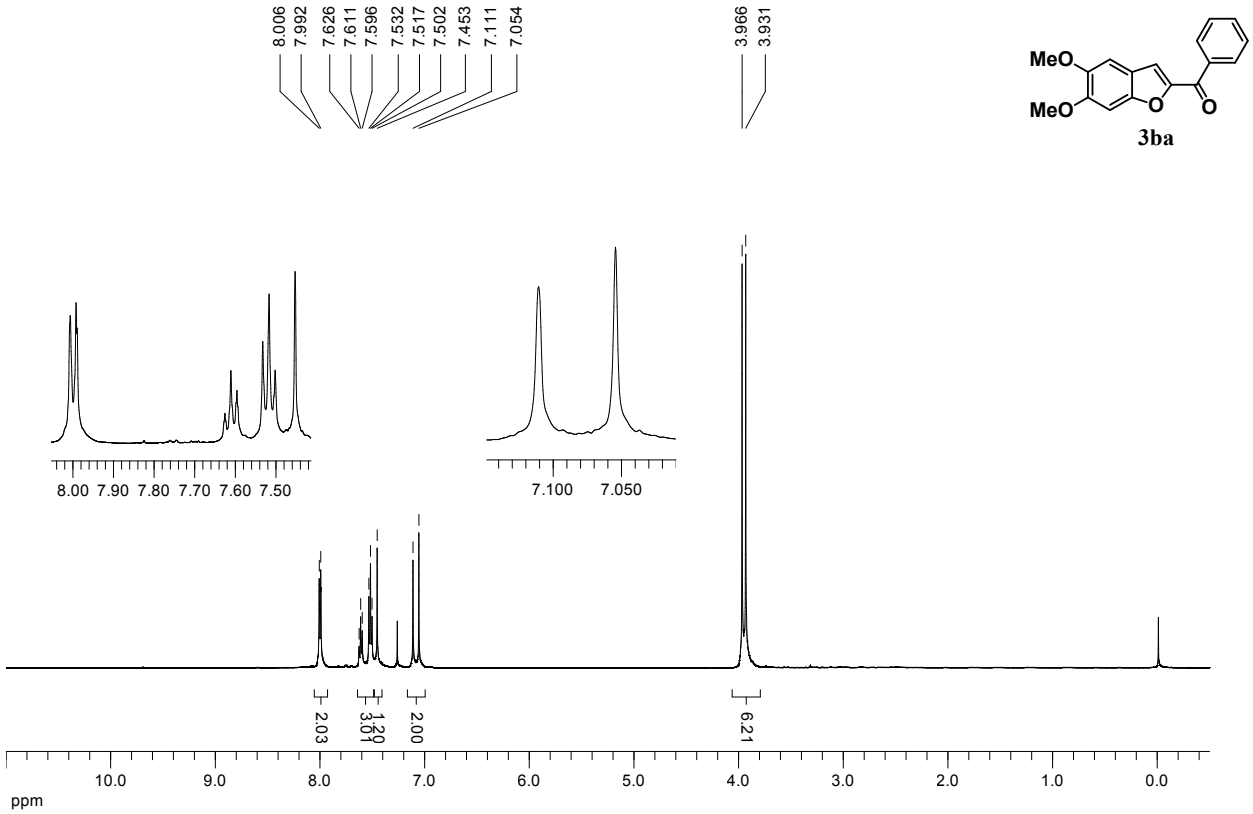
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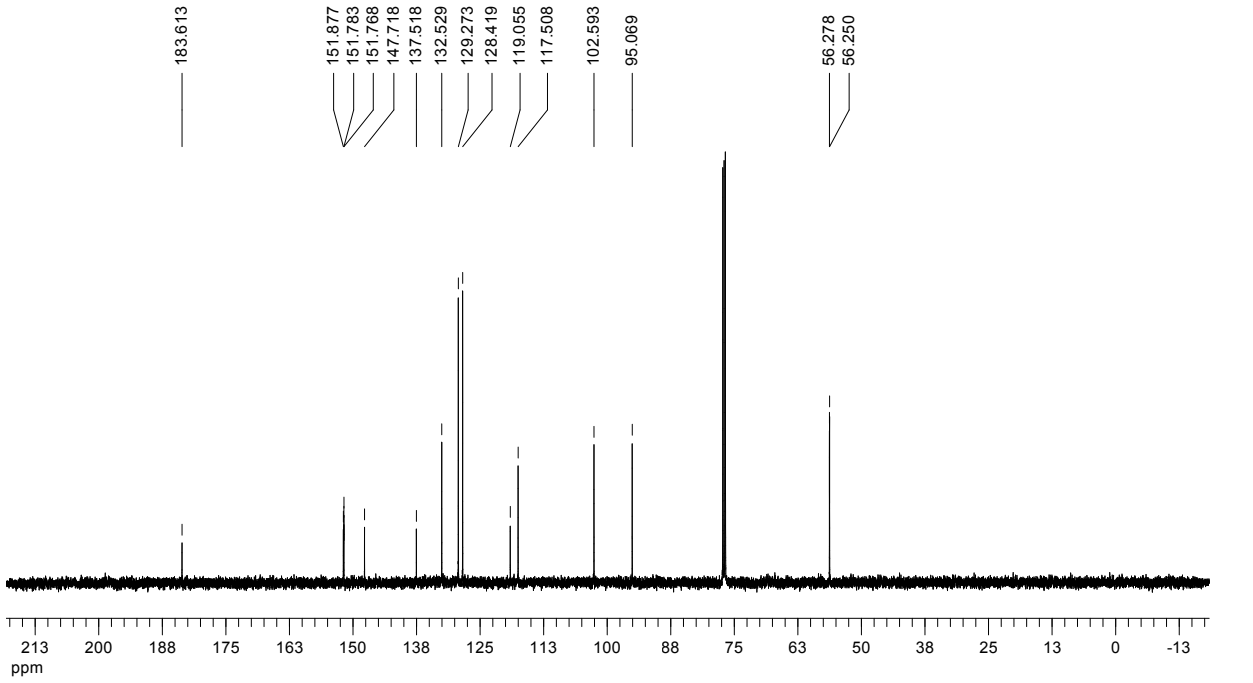
7.532
7.517
7.502
7.453
7.111
7.054
3.966
3.931
MeO
MeO
O
O
3ba
8.00 7.90 7.80 7.70 7.60 7.50
7.100 7.050
2.03
3.01
1.20
2.00
6.21
10.0 9.0 8.0 7.0 6.0 5.0 4.0 3.0 2.0 1.0 0.0
ppm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129.273
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56.278
56.250
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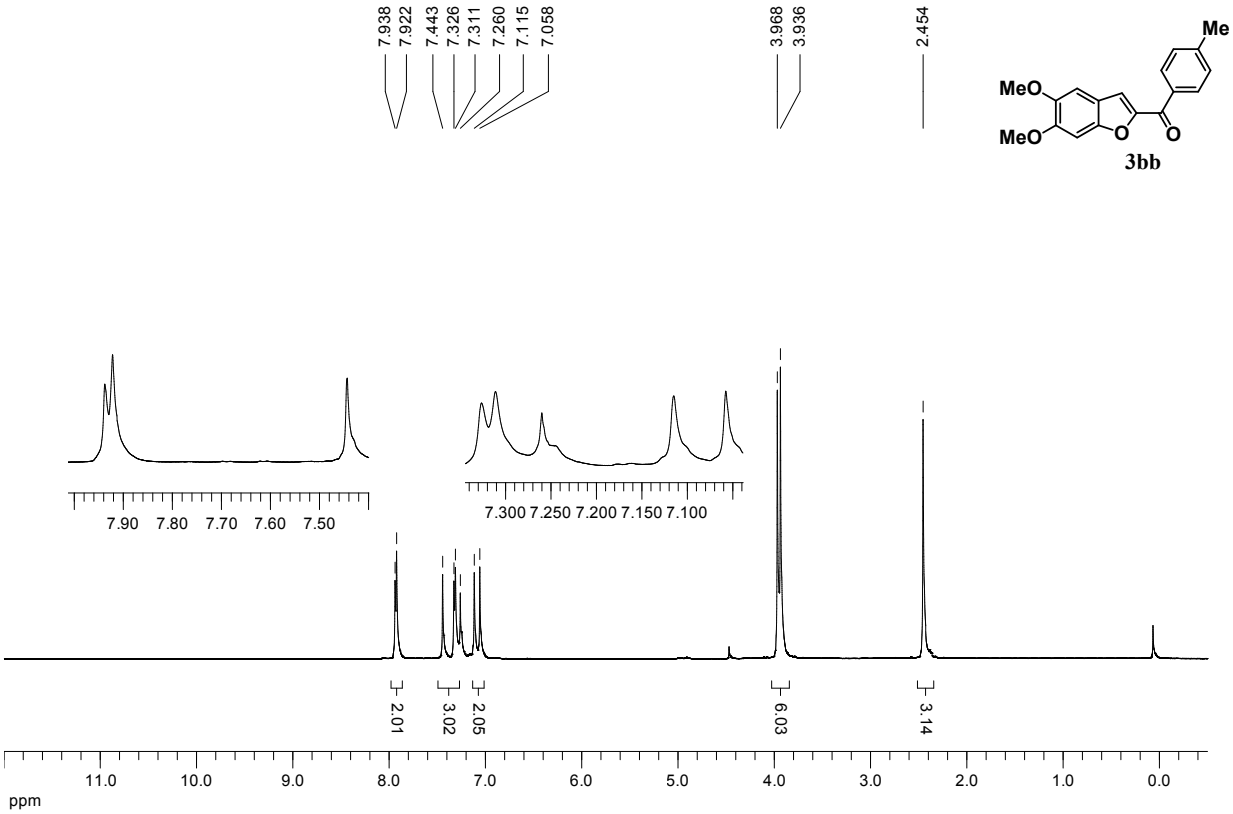
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7.326
7.311
7.260
7.115
7.058
3.968
3.936
2.454
Me
MeO
MeO
O
O
3bb
7.90 7.80 7.70 7.60 7.50
7.300 7.250 7.200 7.150 7.100
2.01
3.02
2.05
6.03
3.14
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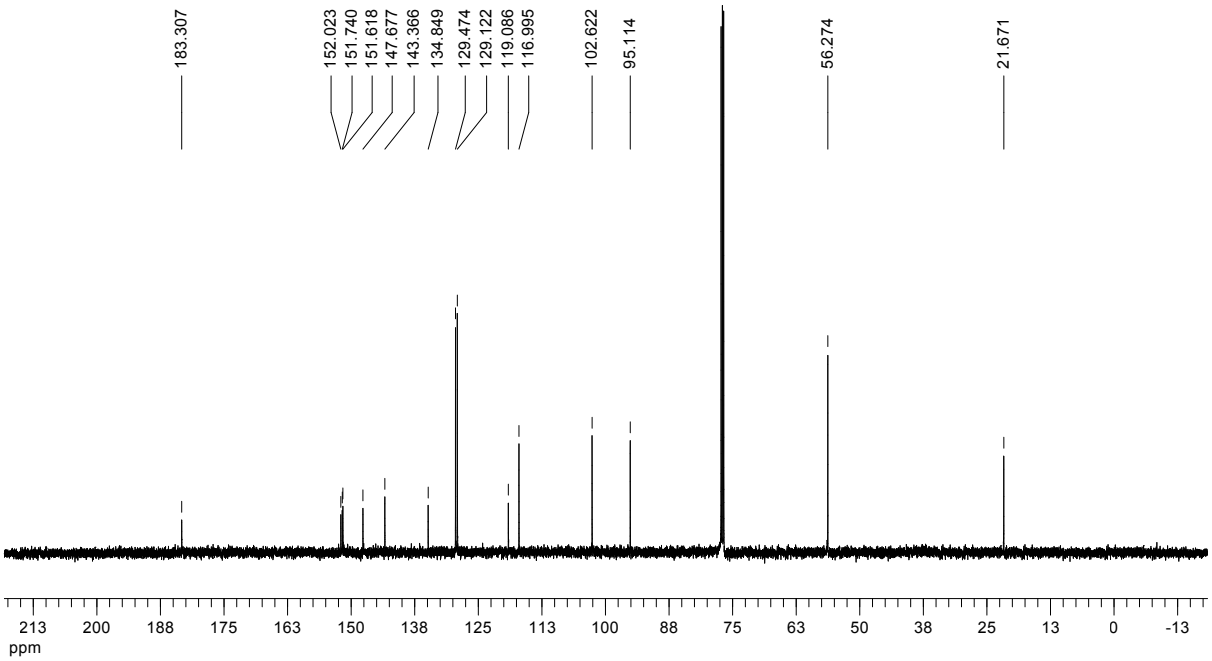
ppm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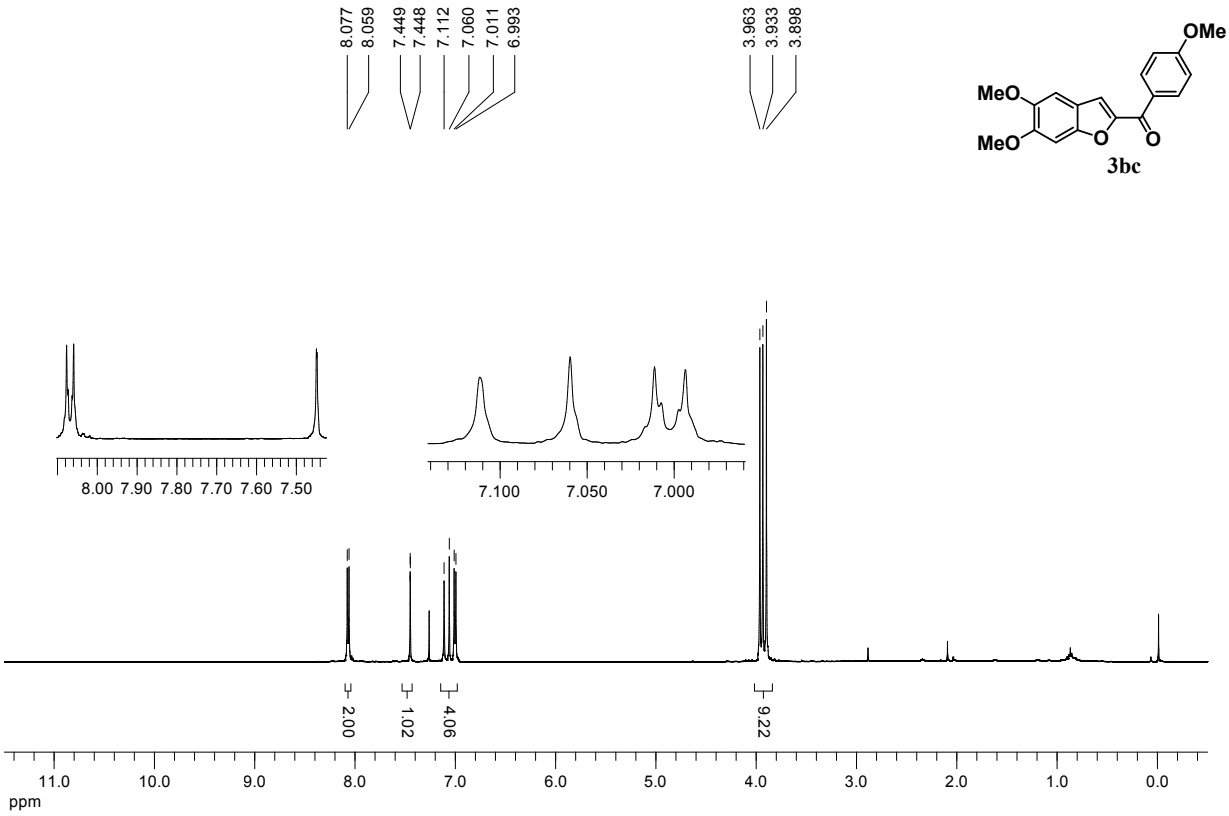
134.849
129.474
129.122
119.086
116.995
102.622
95.114
56.274
21.671
213 200 188 175 163 150 138 125 113 100 88 75 63 50 38 25 13 0 -13
ppm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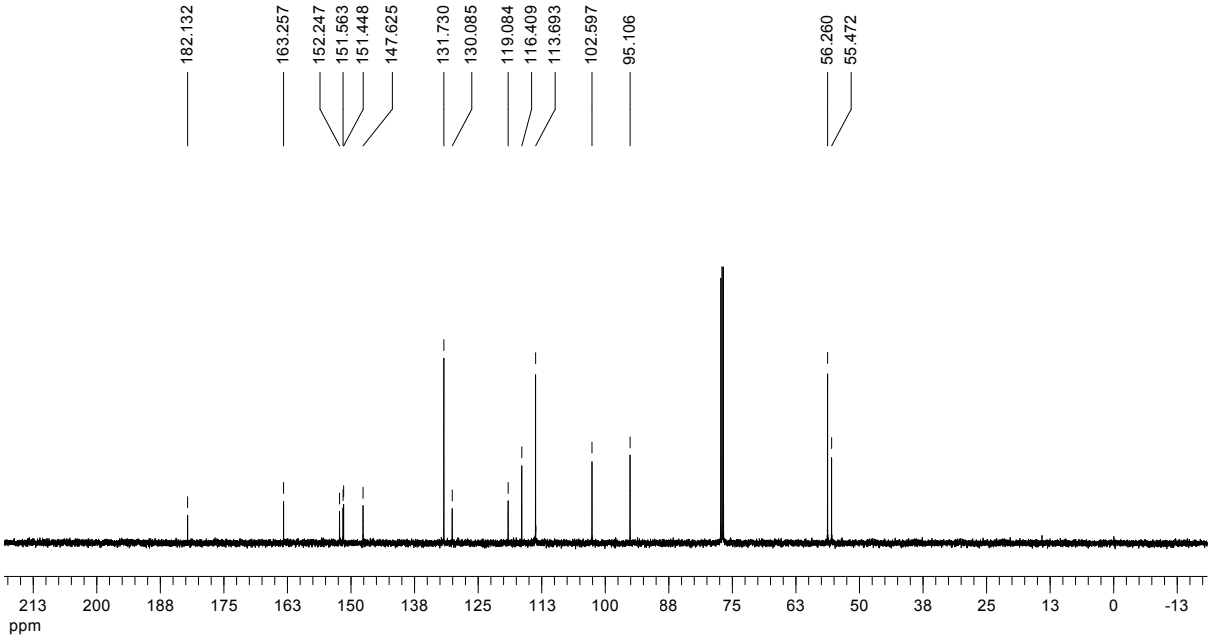
7.449
7.448
7.112
7.060
7.011
6.993
3.963
3.933
3.898
OMe
MeO
MeO
O
O
3bc
8.00 7.90 7.80 7.70 7.60 7.50
7.100 7.050 7.000
2.00
1.02
4.06
9.22
11.0 10.0 9.0 8.0 7.0 6.0 5.0 4.0 3.0 2.0 1.0 0.0
ppm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163.257
152.247
151.563
151.448
147.625
131.730
130.085
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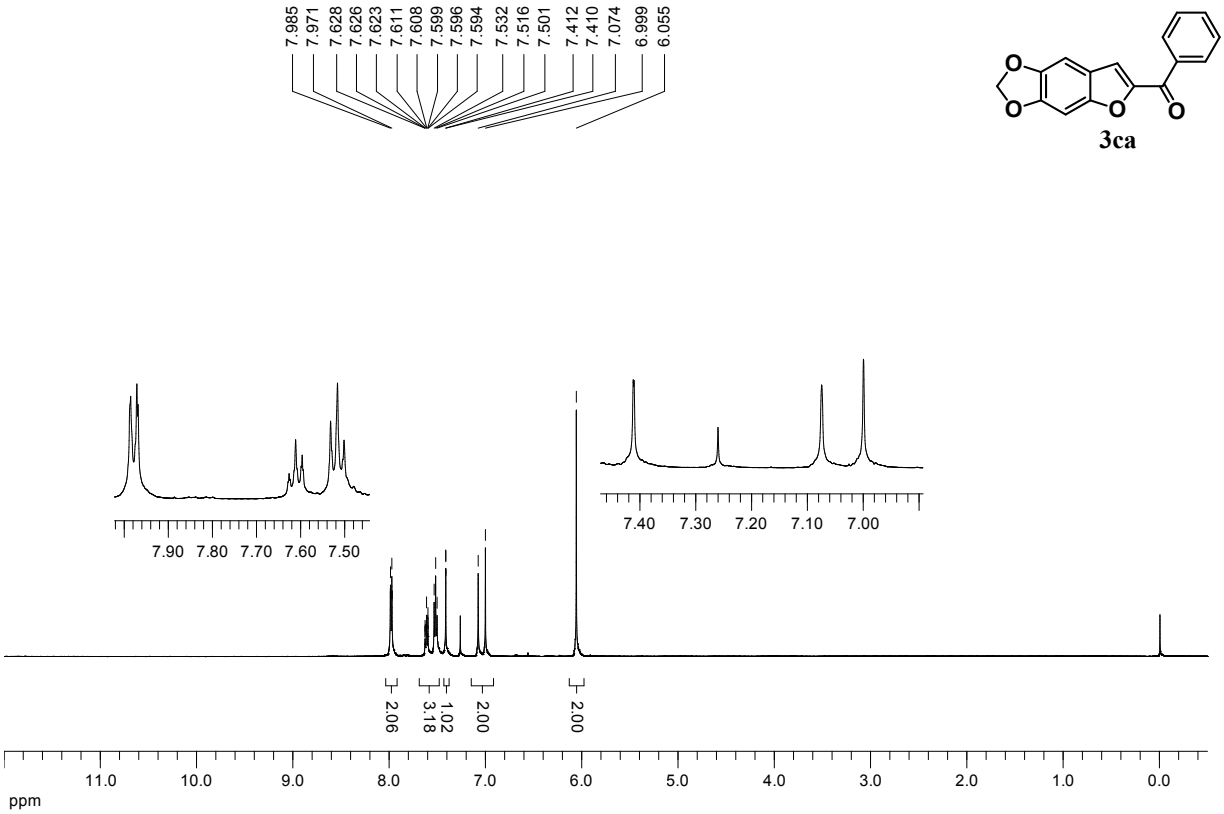
102.597
95.106
56.260
55.472
213 200 188 175 163 150 138 125 113 100 88 75 63 50 38 25 13 0 -13
ppm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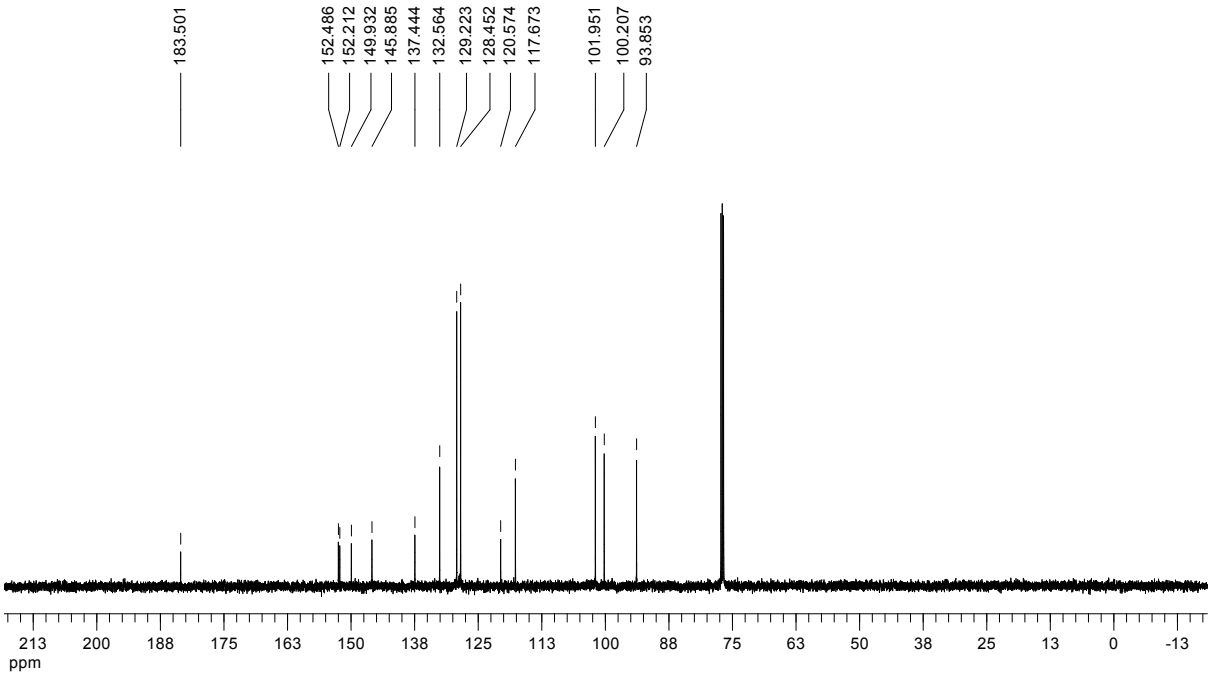
7.971
7.628
7.626
7.623
7.611
7.608
7.599
7.596
7.594
7.532
7.516
7.501
7.412
7.410
7.074
6.999
6.055
7.90 7.80 7.70 7.60 7.50
7.40 7.30 7.20 7.10 7.00
2.06
3.18
1.02
2.00
2.00
11.0 10.0 9.0 8.0 7.0 6.0 5.0 4.0 3.0 2.0 1.0 0.0
ppm

3ca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152.212
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137.444
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128.452
120.574
117.673
101.951
100.207
93.853
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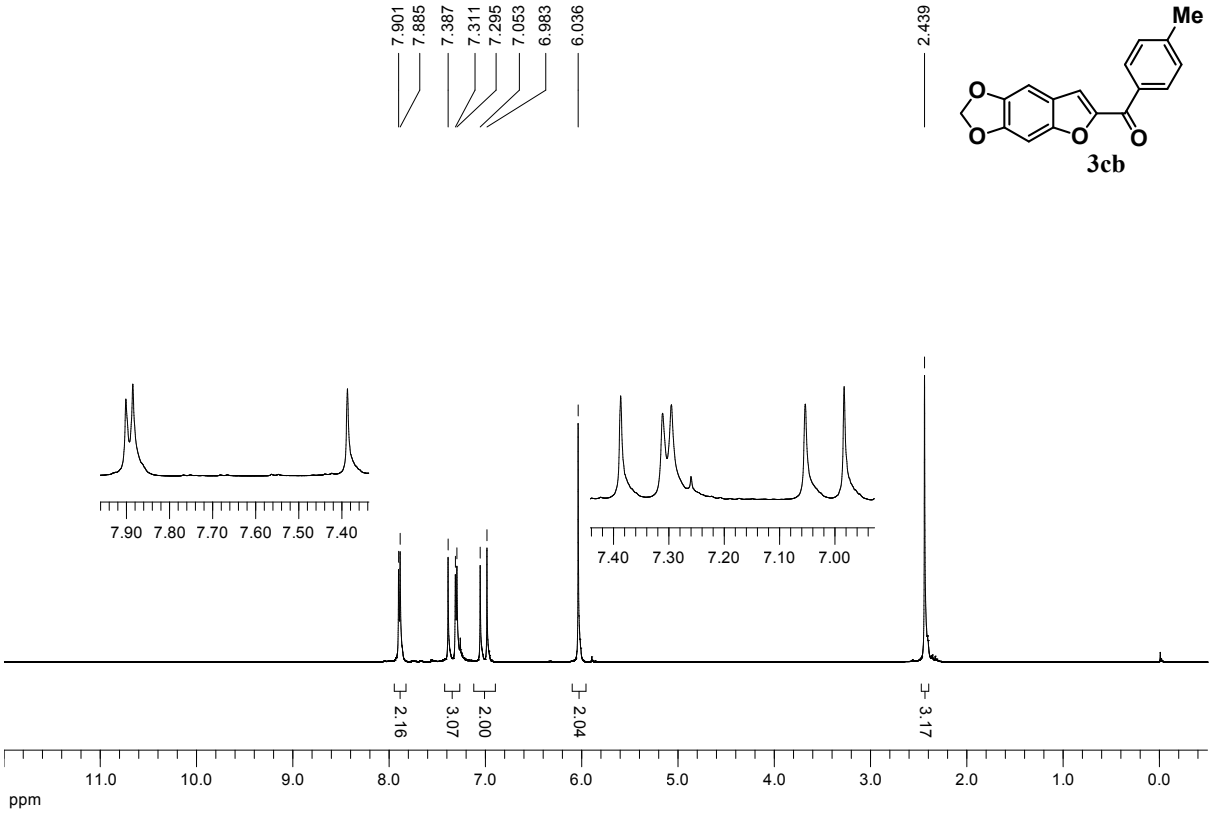
ppm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7.885
7.387
7.311
7.295
7.053
6.983
6.036
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Me
O
O
O
O
3cb
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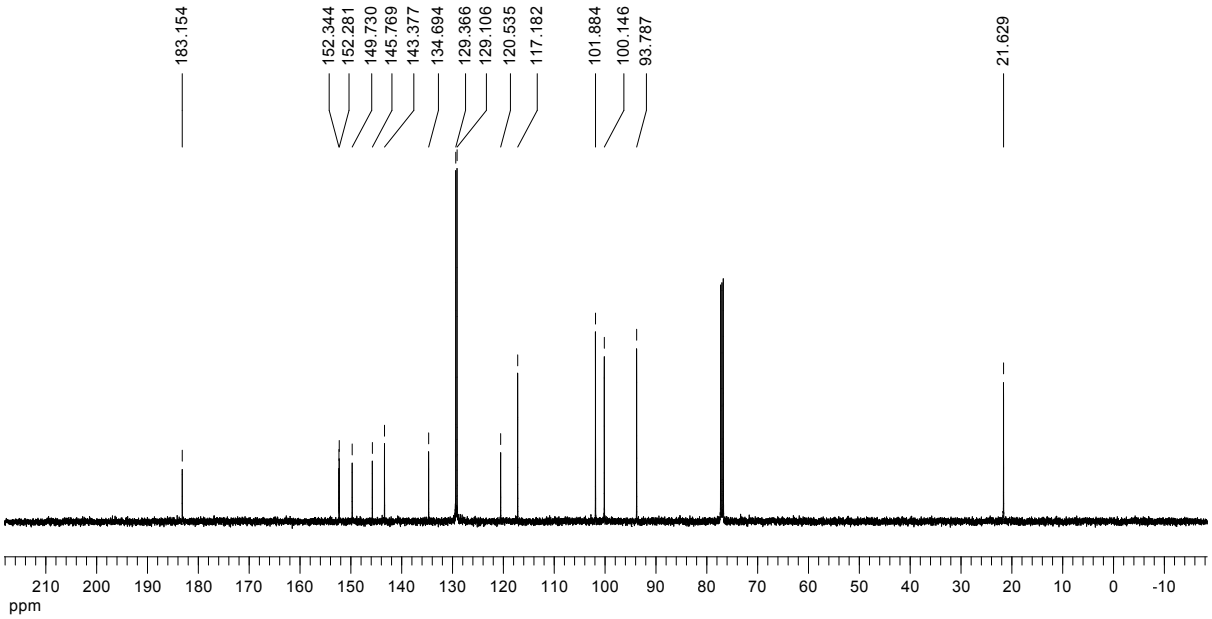
3.07
2.00
2.04
3.17
ppm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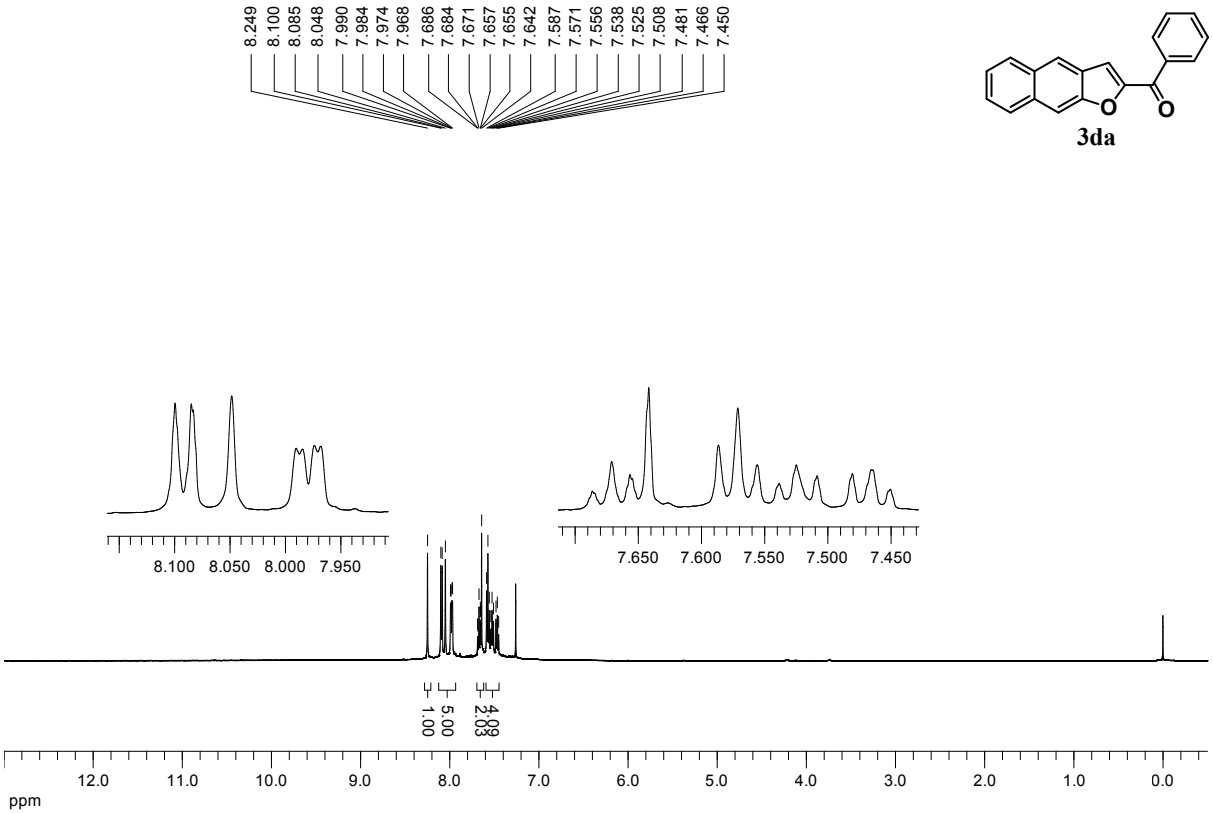
152.344
152.281
149.730
145.769
143.377
134.694
129.366
129.106
120.535
117.182
101.884
100.146
93.787
21.629
ppm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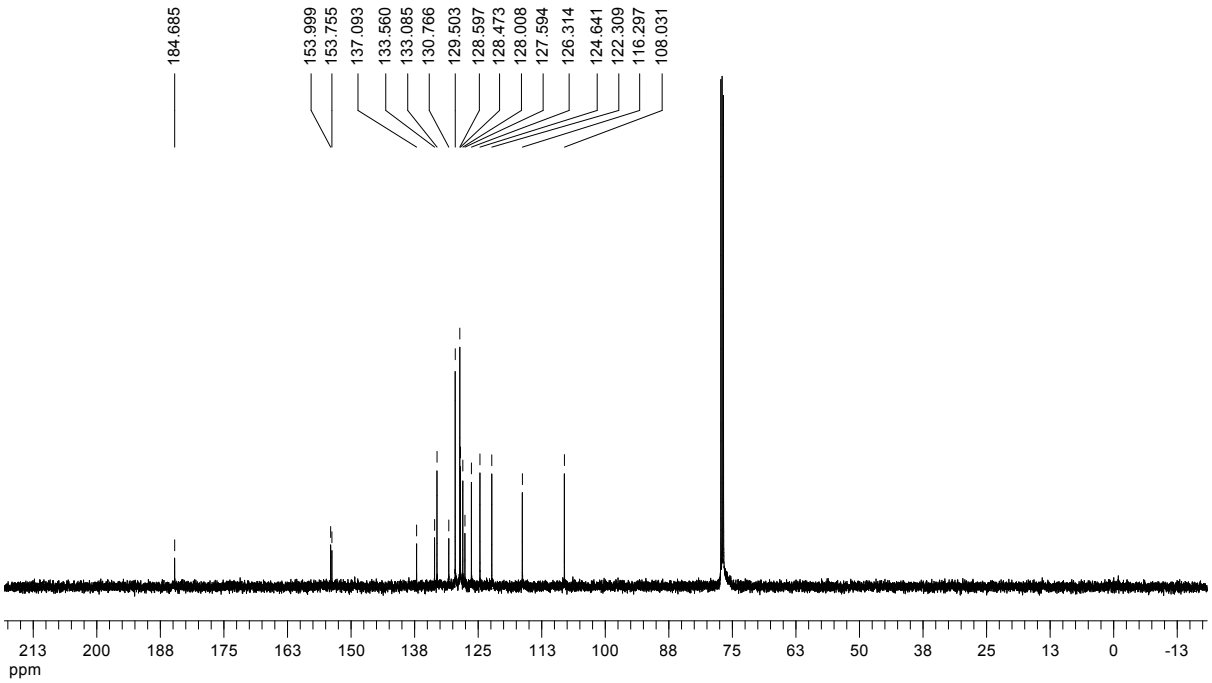
8.100
8.085
8.048
7.990
7.984
7.974
7.968
7.686
7.684
7.671
7.657
7.655
7.642
7.587
7.571
7.556
7.538
7.525
7.508
7.481
7.466
7.450
8.100 8.050 8.000 7.950
7.650 7.600 7.550 7.500 7.450
1.00
5.00
2.03
4.08
12.0 11.0 10.0 9.0 8.0 7.0 6.0 5.0 4.0 3.0 2.0 1.0 0.0
ppm

3da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133.560
133.085
130.766
129.503
128.597
128.473
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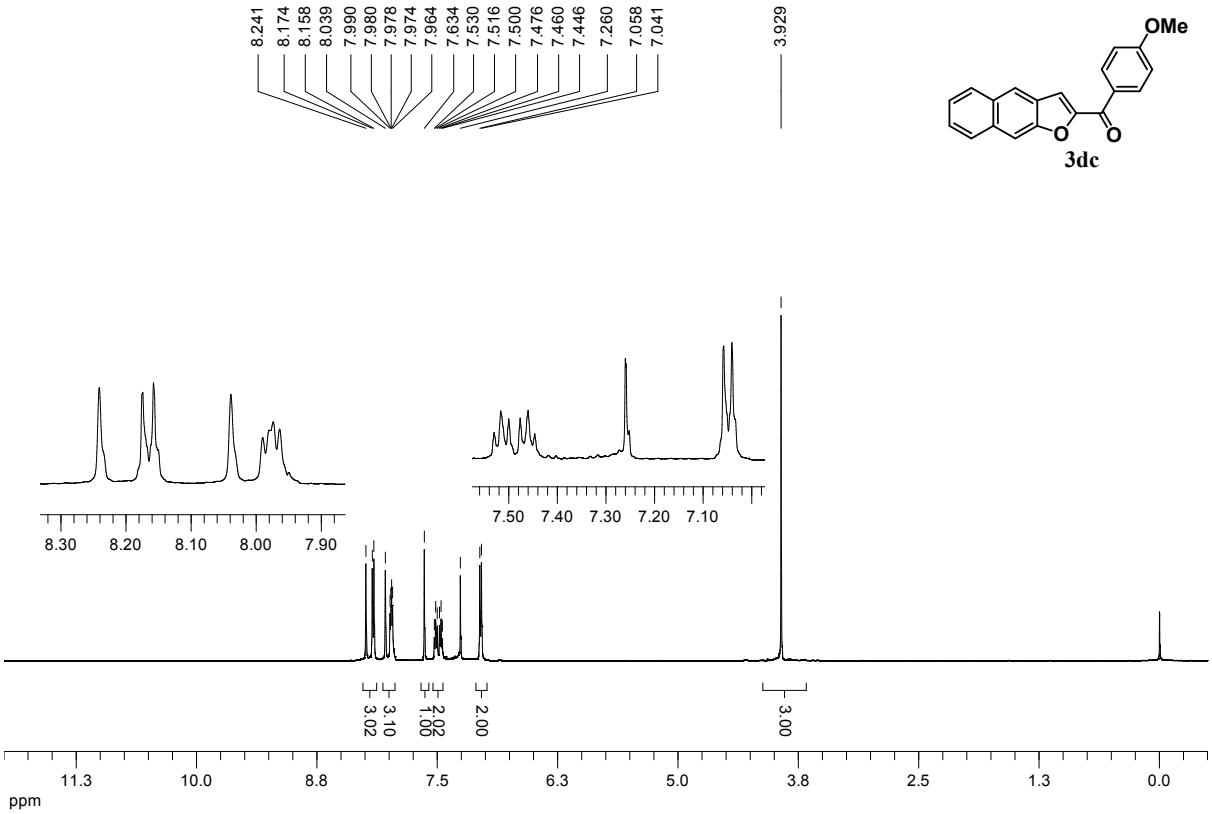
126.314
124.641
122.309
116.297
108.031
213 200 188 175 163 150 138 125 113 100 88 75 63 50 38 25 13 0 -13
ppm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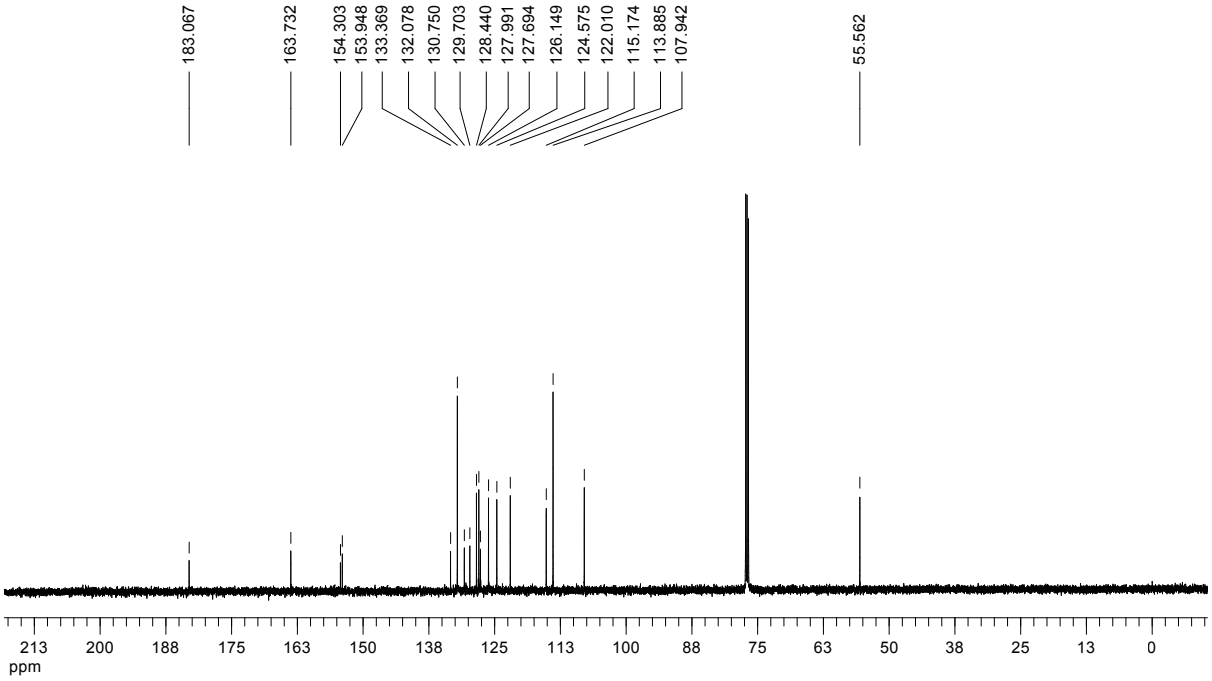
8.174
8.158
8.039
7.990
7.980
7.978
7.974
7.964
7.634
7.530
7.516
7.500
7.476
7.460
7.446
7.260
7.058
7.041
3.929
OMe
O
O
3dc
8.30 8.20 8.10 8.00 7.90
7.50 7.40 7.30 7.20 7.10
3.02
3.10
2.02
1.00
2.00
3.00
11.3 10.0 8.8 7.5 6.3 5.0 3.8 2.5 1.3 0.0
ppm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129.703
128.440
127.991
127.694
126.149
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122.010
115.174
113.885
107.942
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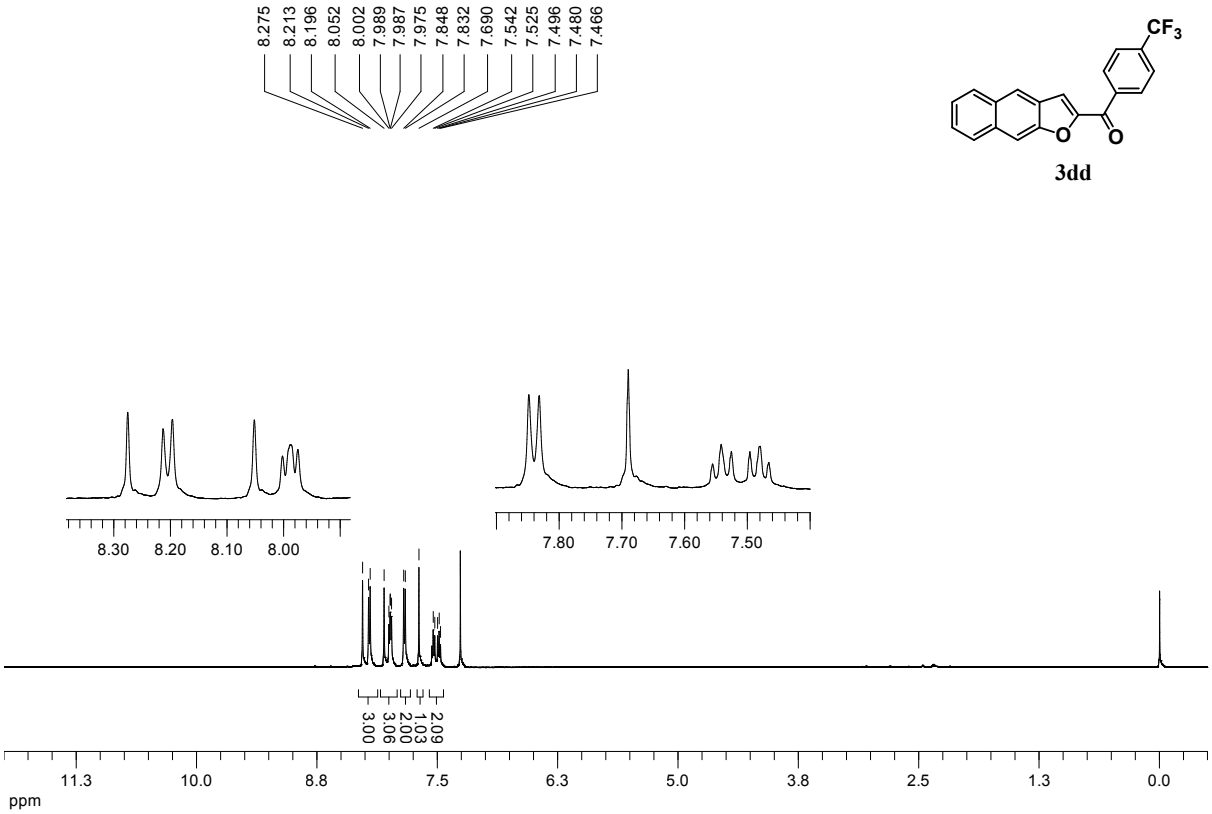
213 200 188 175 163 150 138 125 113 100 88 75 63 50 38 25 13 0
ppm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8.213
8.196
8.052
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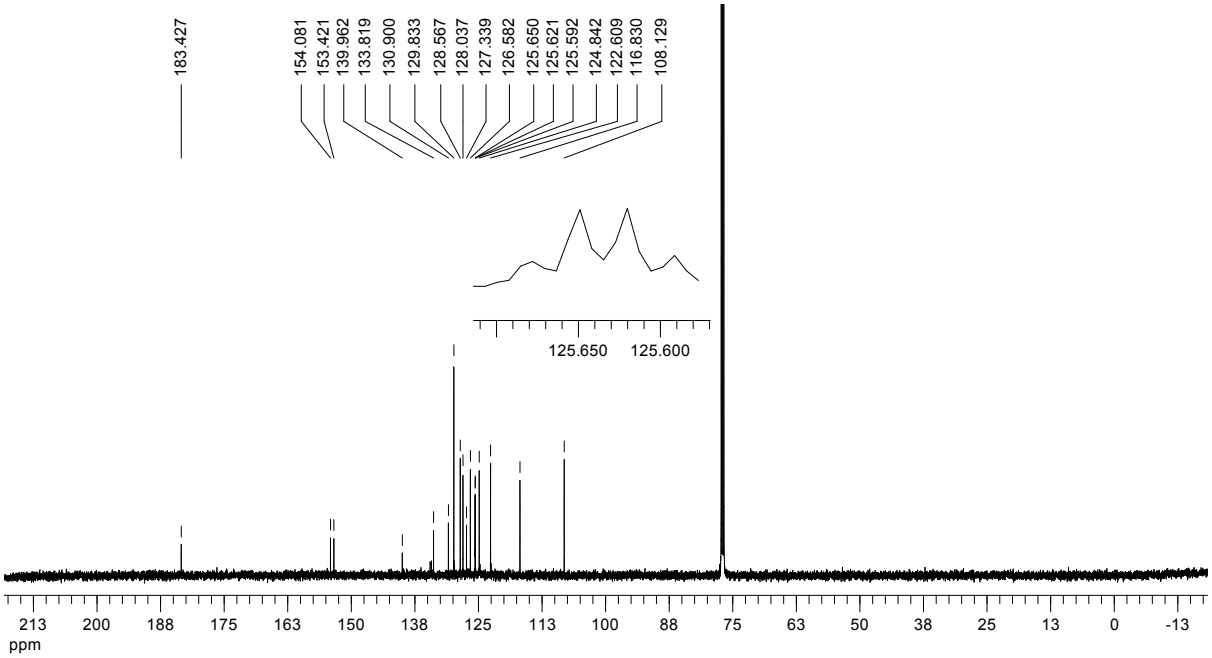
7.989
7.987
7.975
7.848
7.832
7.690
7.542
7.525
7.496
7.480
7.466
CF3
O
O
3dd
8.30 8.20 8.10 8.00
7.80 7.70 7.60 7.50
3.00
3.06
2.00
1.03
2.09
11.3 10.0 8.8 7.5 6.3 5.0 3.8 2.5 1.3 0.0
ppm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128.037
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125.650
125.621
125.592
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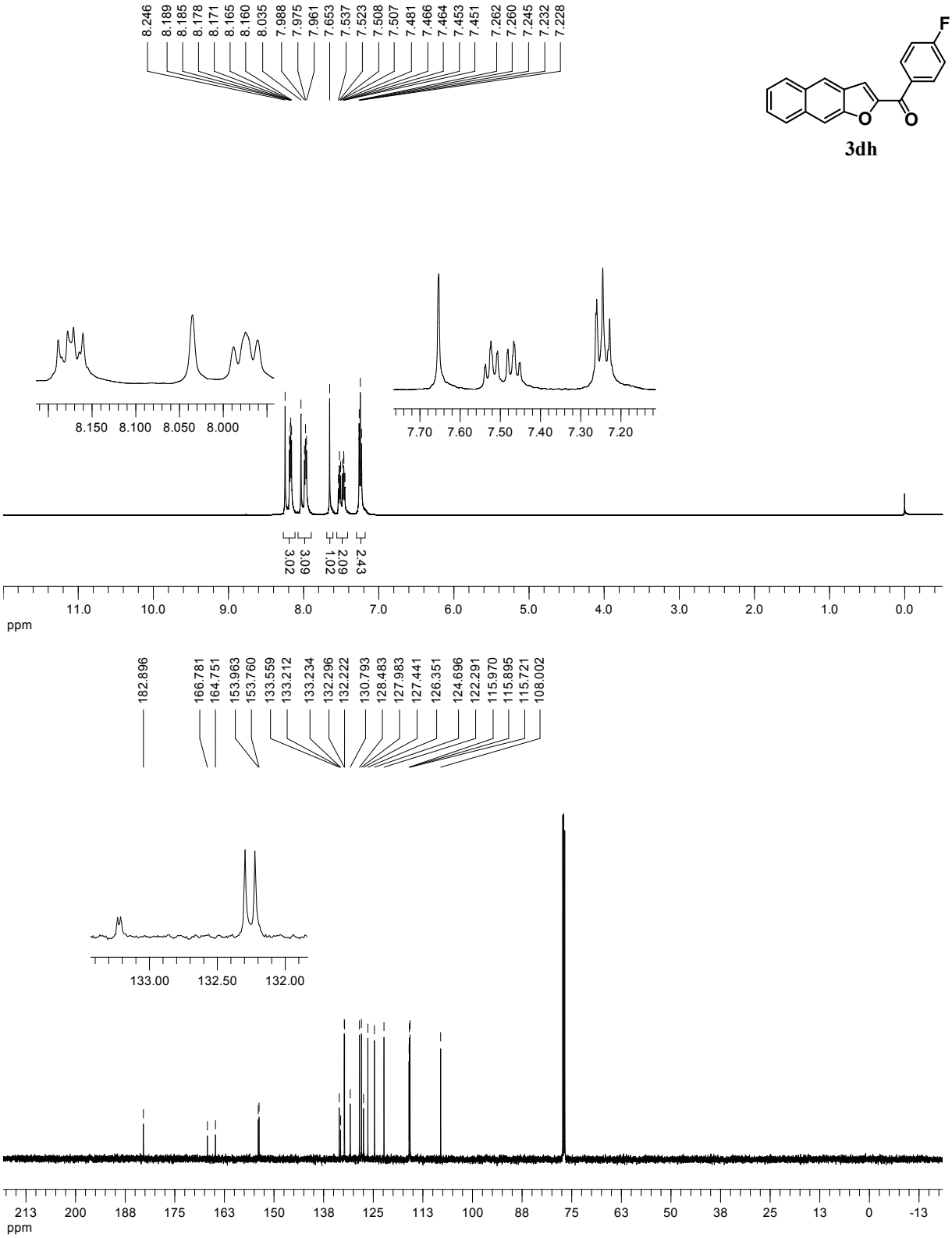
122.609
116.830
108.129
125.650 125.600
213 200 188 175 163 150 138 125 113 100 88 75 63 50 38 25 13 0 -13
ppm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8.160
8.035
7.988
7.975
7.961
7.653
7.537
7.523
7.508
7.507
7.481
7.466
7.464
7.453
7.451
7.262
7.260
7.245
7.232
7.228
F
O
O
3dh
8.150 8.100 8.050 8.000
7.70 7.60 7.50 7.40 7.30 7.20
3.02
3.09
1.02
2.09
2.43
11.0 10.0 9.0 8.0 7.0 6.0 5.0 4.0 3.0 2.0 1.0 0.0
ppm
182.896
166.781
164.751
153.963
153.760
133.559
133.212
133.234
132.296
132.222
130.793
128.483
127.983
127.441
126.351
124.696
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115.721
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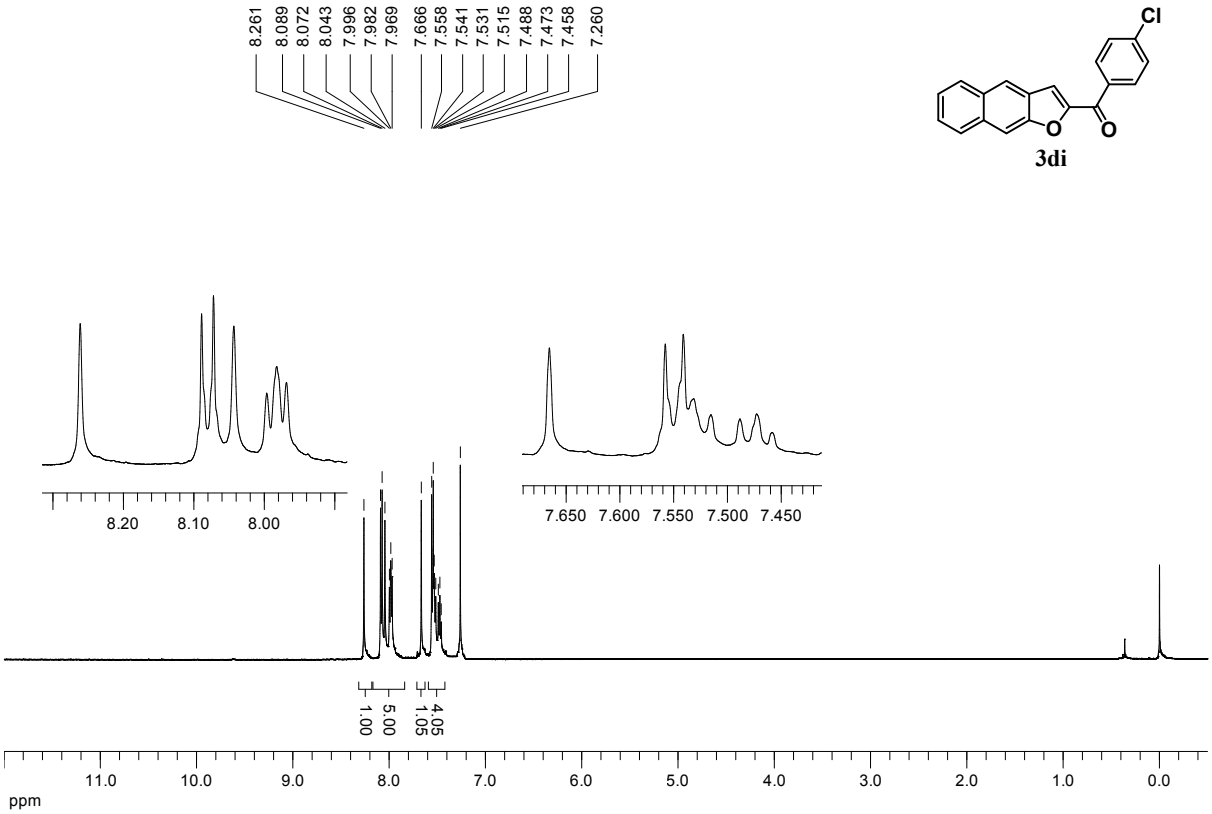
133.00 132.50 132.00
213 200 188 175 163 150 138 125 113 100 88 75 63 50 38 25 13 0 -13
ppm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7.541
7.531
7.515
7.488
7.473
7.458
7.260
Cl
O
O
3di
8.20
8.10
8.00
7.650
7.600
7.550
7.500
7.450
1.00
5.00
1.05
4.05
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9.0
8.0
7.0
6.0
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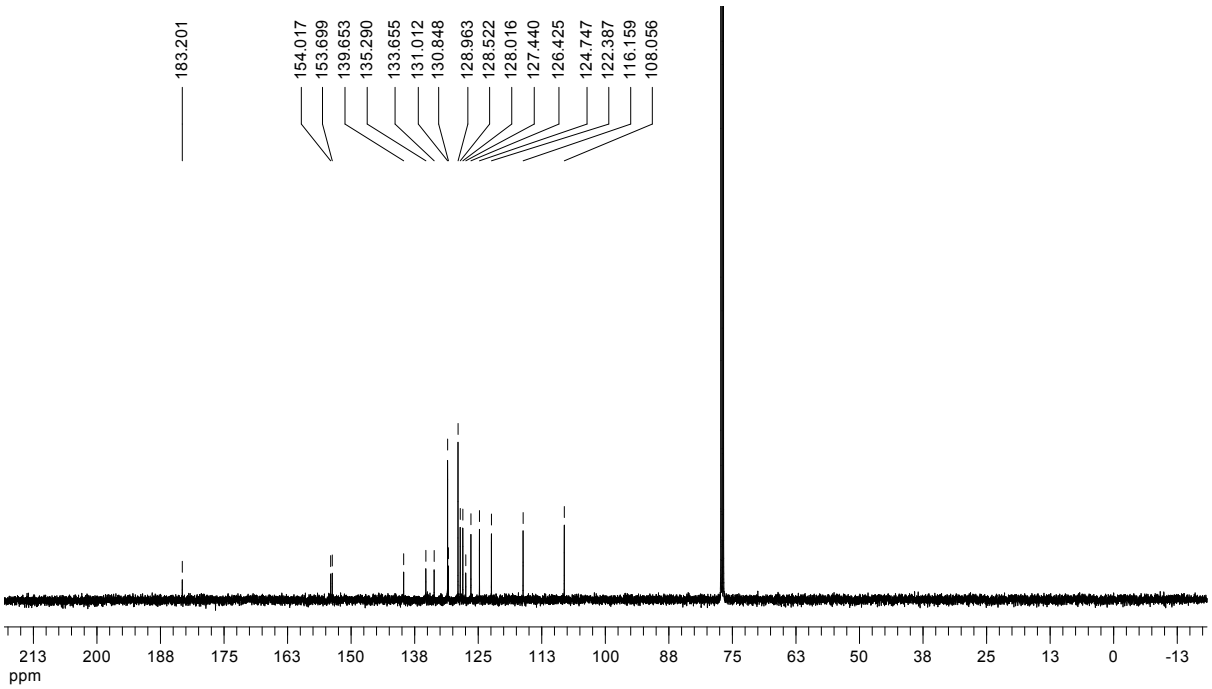
4.0
3.0
2.0
1.0
0.0
ppm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130.848
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128.522
128.016
127.440
126.425
124.747
122.387
116.159
108.056
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200
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175
163
150
138
125
113
100
88
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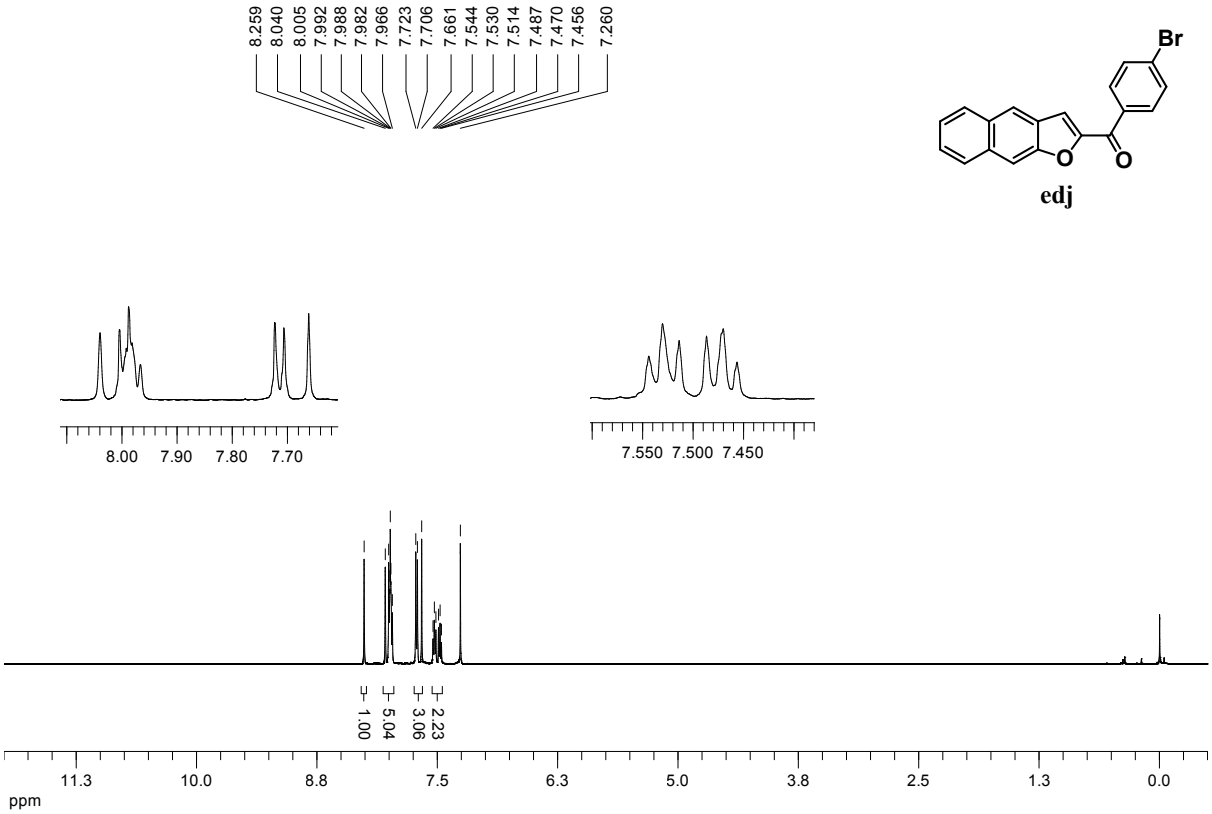
63
50
38
25
13
0
-13
ppm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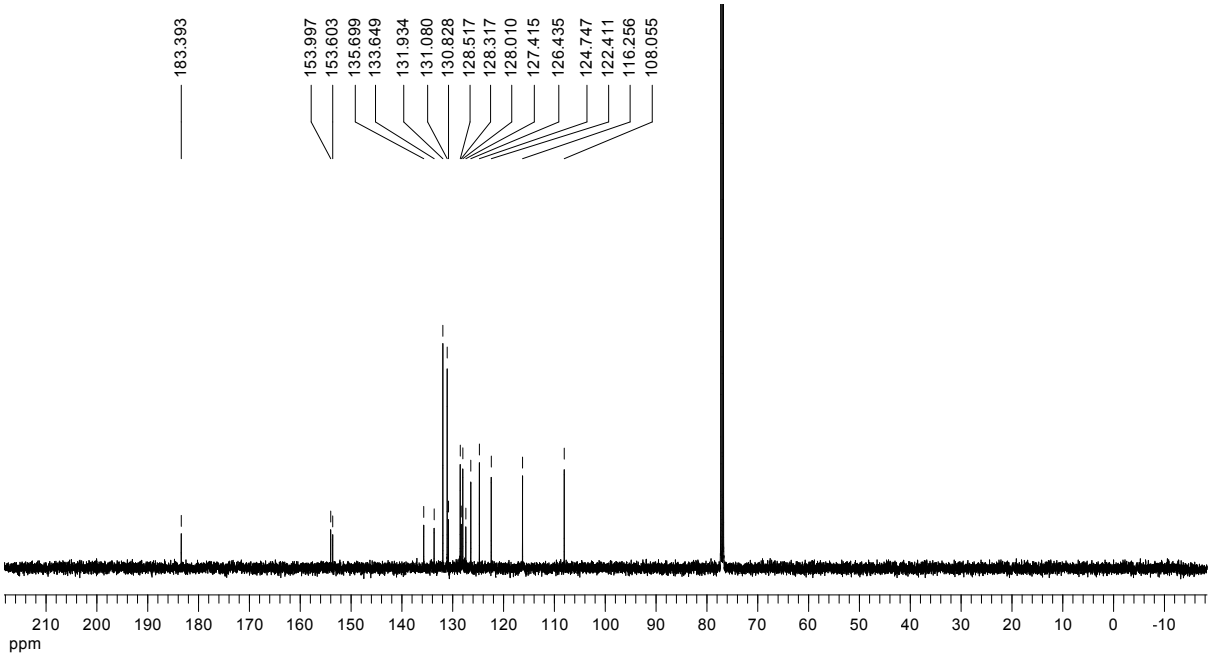
8.005
7.992
7.988
7.982
7.966
7.723
7.706
7.661
7.544
7.530
7.514
7.487
7.470
7.456
7.260
Br
O
O
edj
8.00 7.90 7.80 7.70
7.550 7.500 7.450
1.00
5.04
3.06
2.23
11.3 10.0 8.8 7.5 6.3 5.0 3.8 2.5 1.3 0.0
ppm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130.828
128.517
128.317
128.010
127.415
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122.411
116.256
108.055
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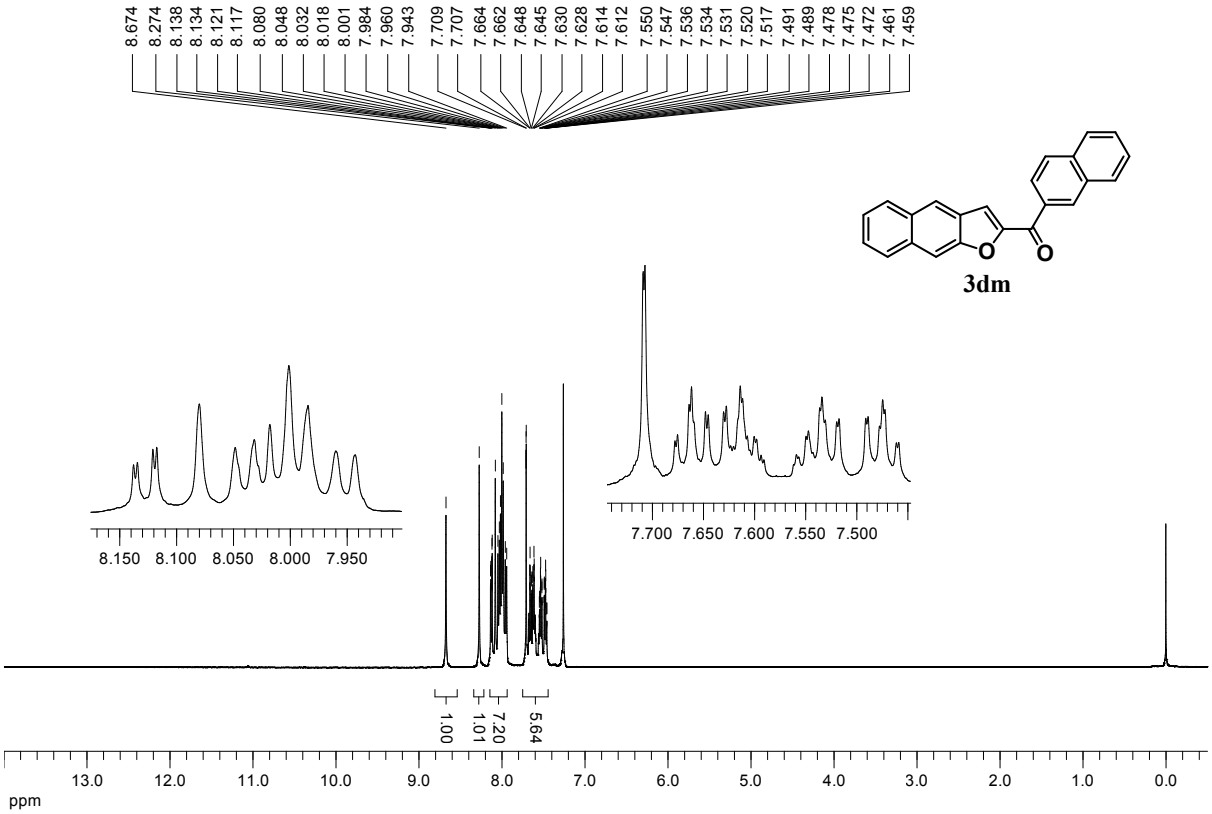
ppm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8.032
8.018
8.001
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7.709
7.707
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7.662
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7.628
7.614
7.612
7.550
7.547
7.536
7.534
7.531
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7.517
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7.489
7.478
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7.472
7.461
7.459
3dm
8.150 8.100 8.050 8.000 7.950
7.700 7.650 7.600 7.550 7.500
1.00
1.01
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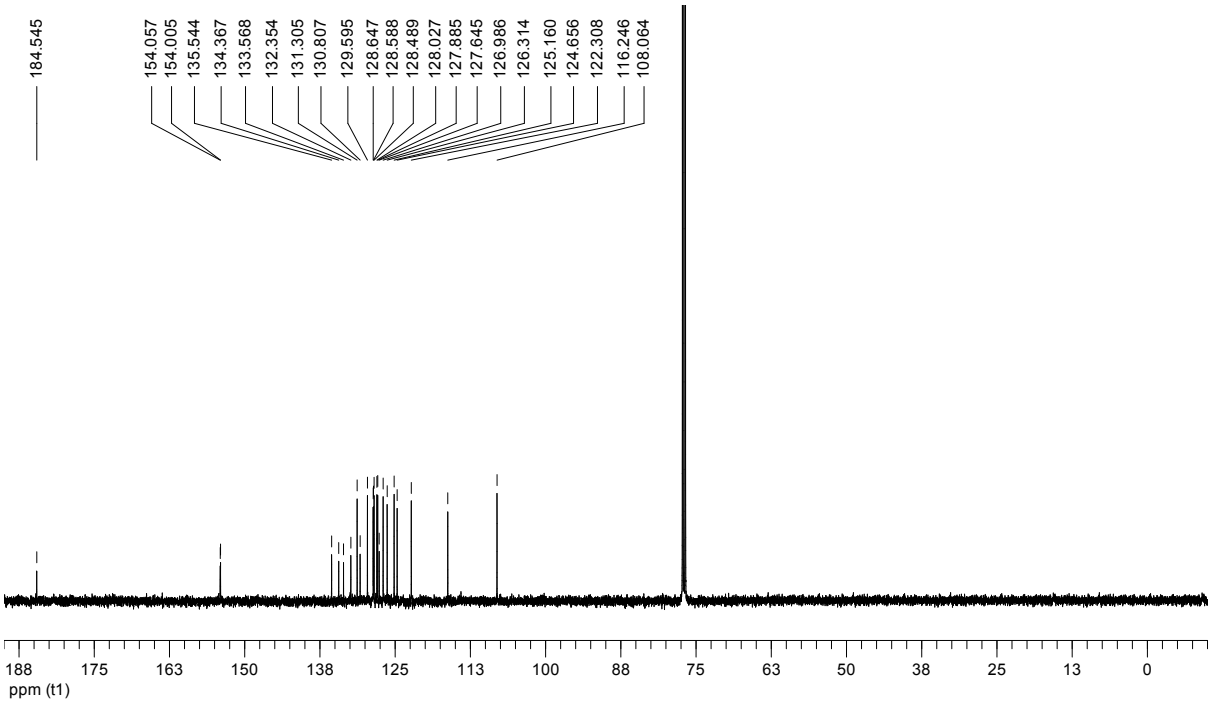
ppm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128.588
128.489
128.027
127.885
127.645
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124.656
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116.246
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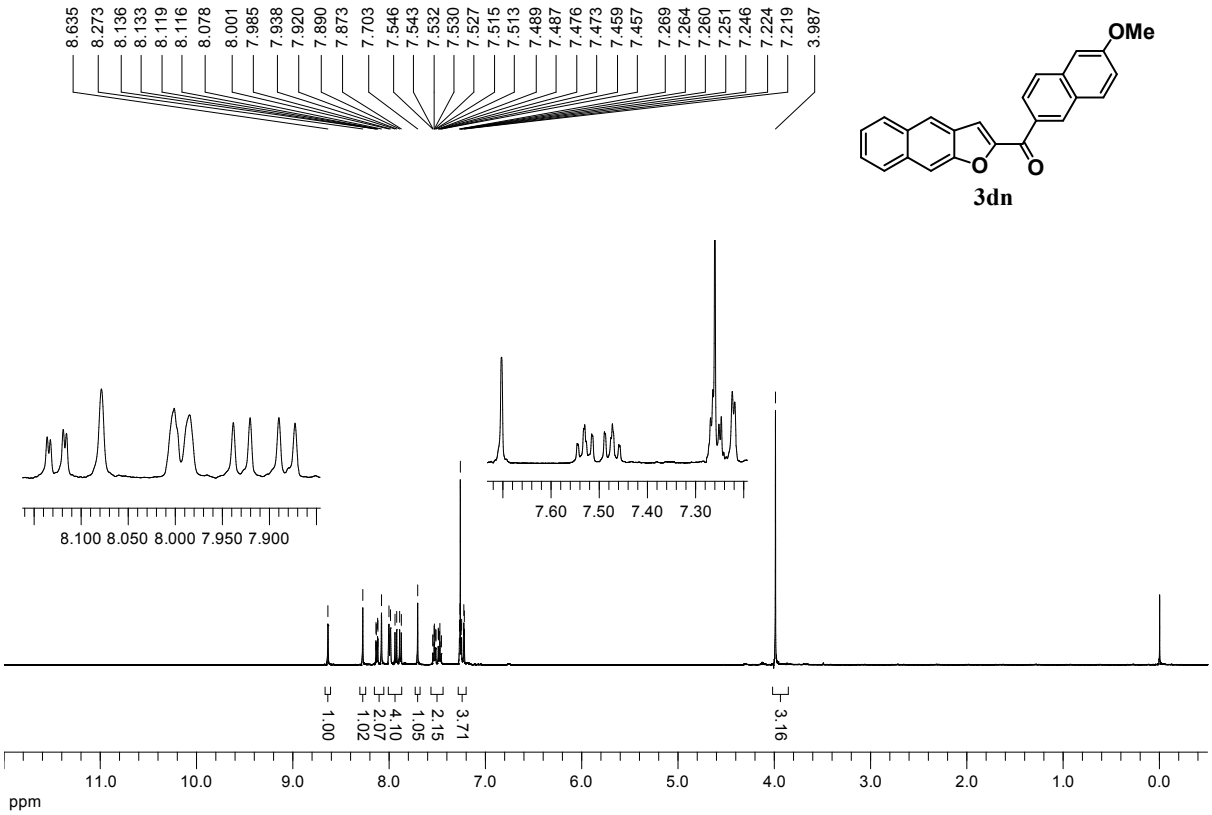
ppm (t1)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7.873
7.703
7.546
7.543
7.532
7.530
7.527
7.515
7.513
7.489
7.487
7.476
7.473
7.459
7.457
7.269
7.264
7.260
7.251
7.246
7.224
7.219
3.987
OMe
O
O
3dn
8.100 8.050 8.000 7.950 7.900
7.60 7.50 7.40 7.30
1.00
1.02
2.07
4.10
1.05
2.15
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3.16
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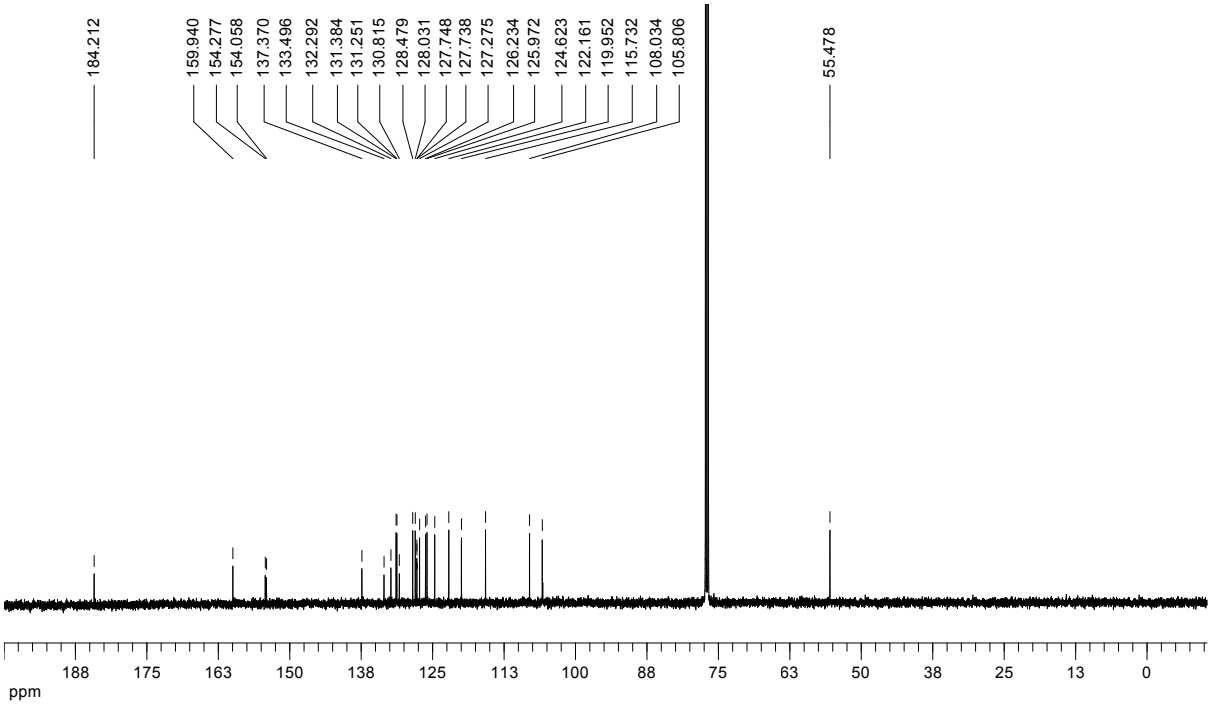
ppm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131.384
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128.479
128.031
127.748
127.738
127.275
126.234
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119.952
115.732
108.034
105.806
55.478
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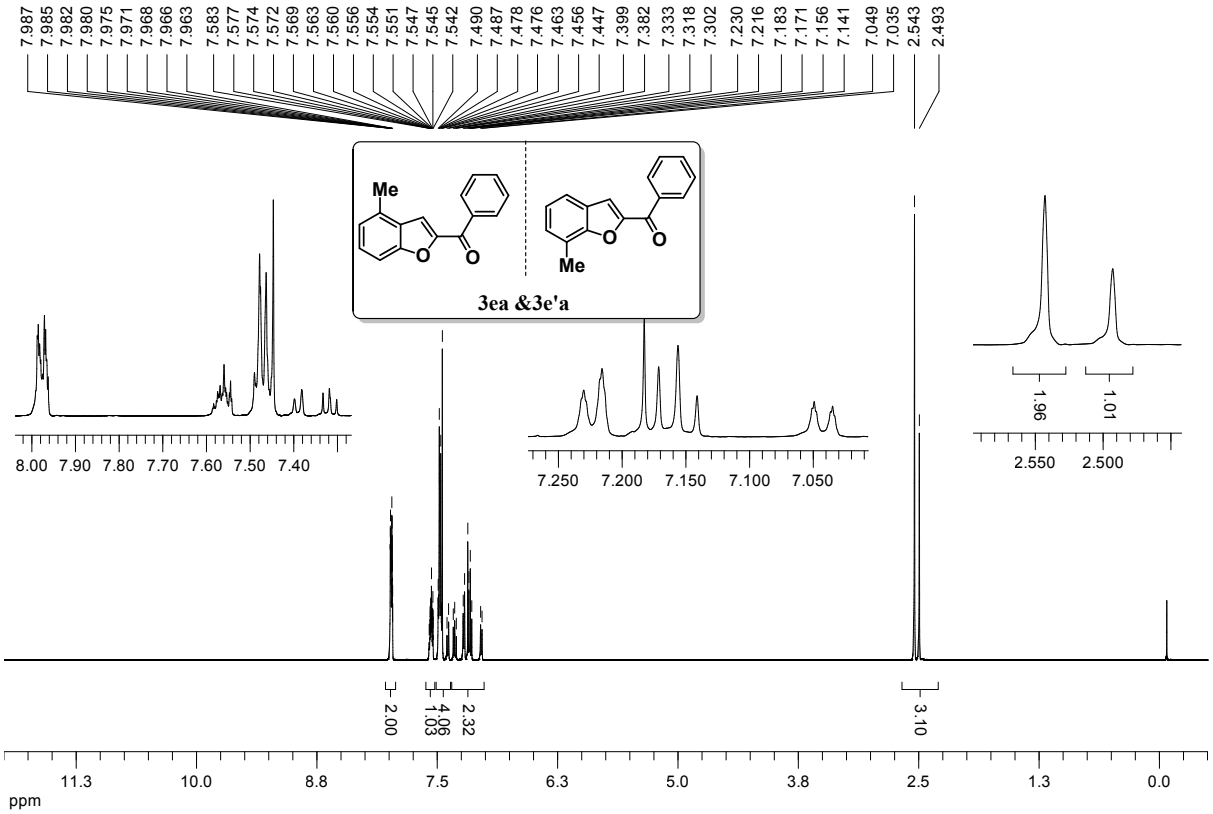
ppm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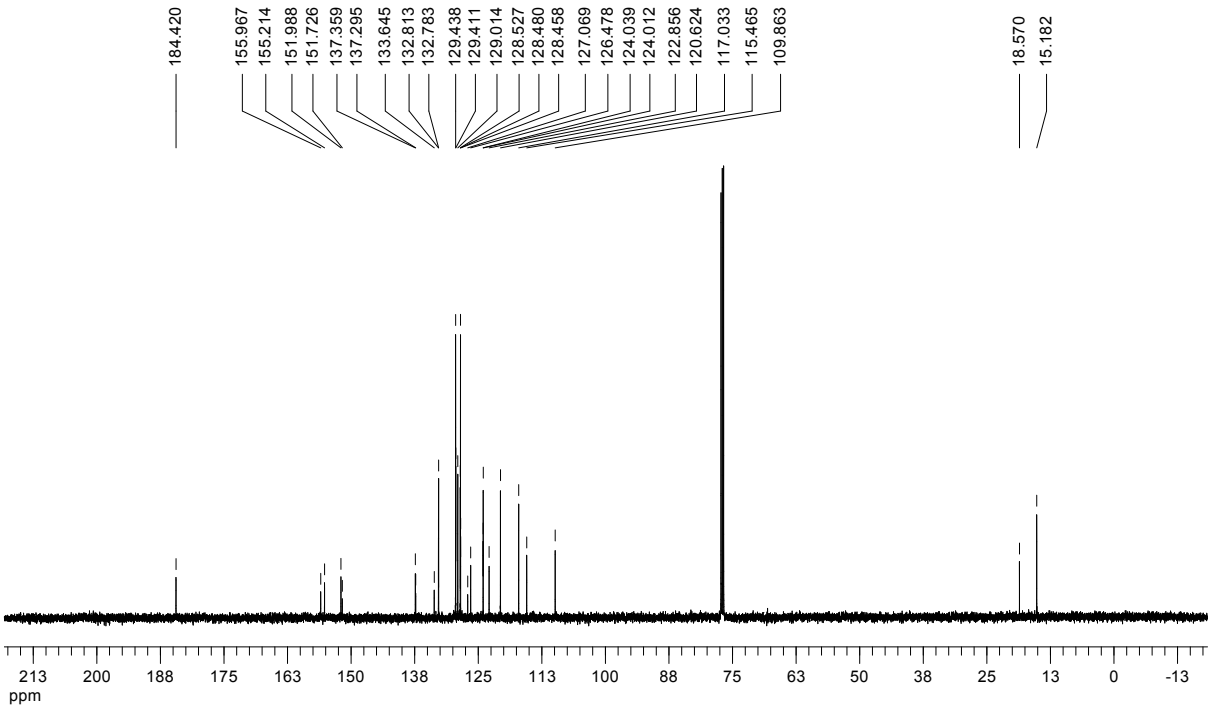
Me
O
O
Me
3ea &3e'a
8.00 7.90 7.80 7.70 7.60 7.50 7.40
7.250 7.200 7.150 7.100 7.050
1.96
1.01
2.550 2.500
2.00
1.03
4.06
2.32
3.10
11.3 10.0 8.8 7.5 6.3 5.0 3.8 2.5 1.3 0.0
ppm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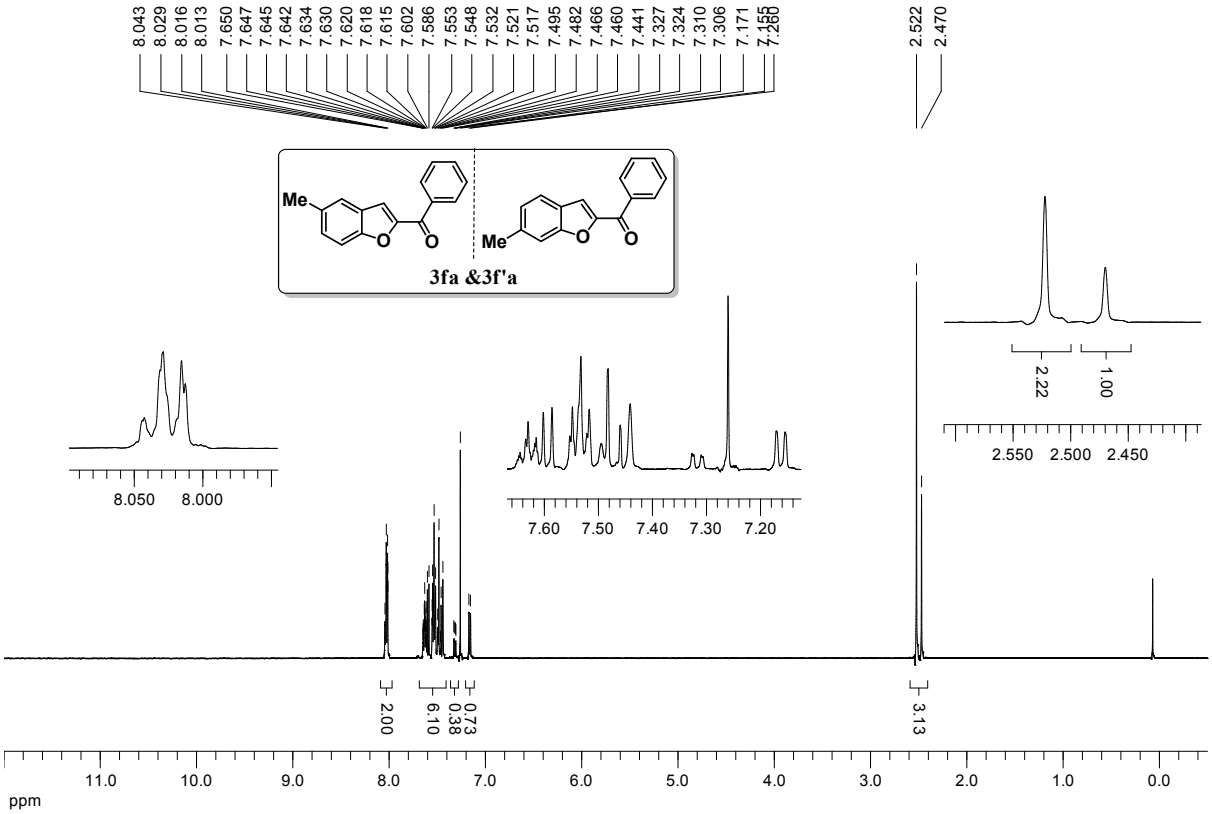
18.570 15.182
213 200 188 175 163 150 138 125 113 100 88 75 63 50 38 25 13 0 -13
ppm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7.482
7.466
7.460
7.441
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7.324
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7.306
7.171
7.155
7.260
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2.470
Me
O
O
Me
O
O
3fa &3f'a
8.050
8.000
7.60
7.50
7.40
7.30
7.20
2.550
2.500
2.450
2.22
1.00
2.00
6.10
0.38
0.73
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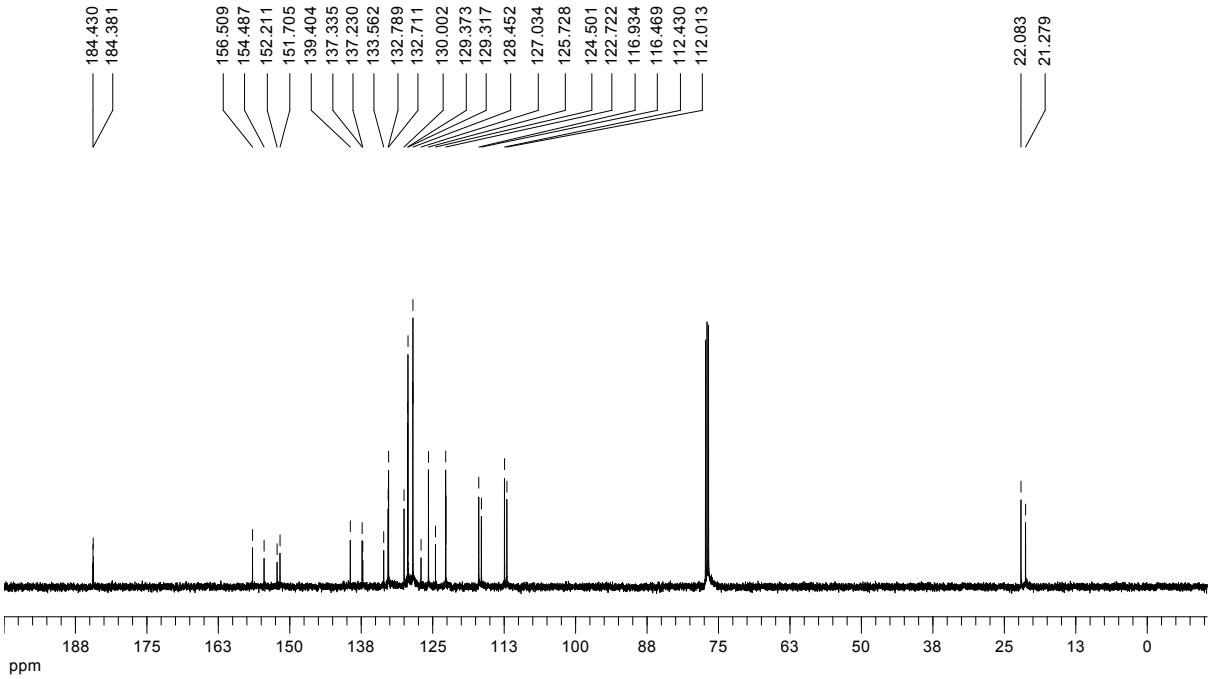
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129.373
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128.452
127.034
125.728
124.501
122.722
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116.469
112.430
112.013
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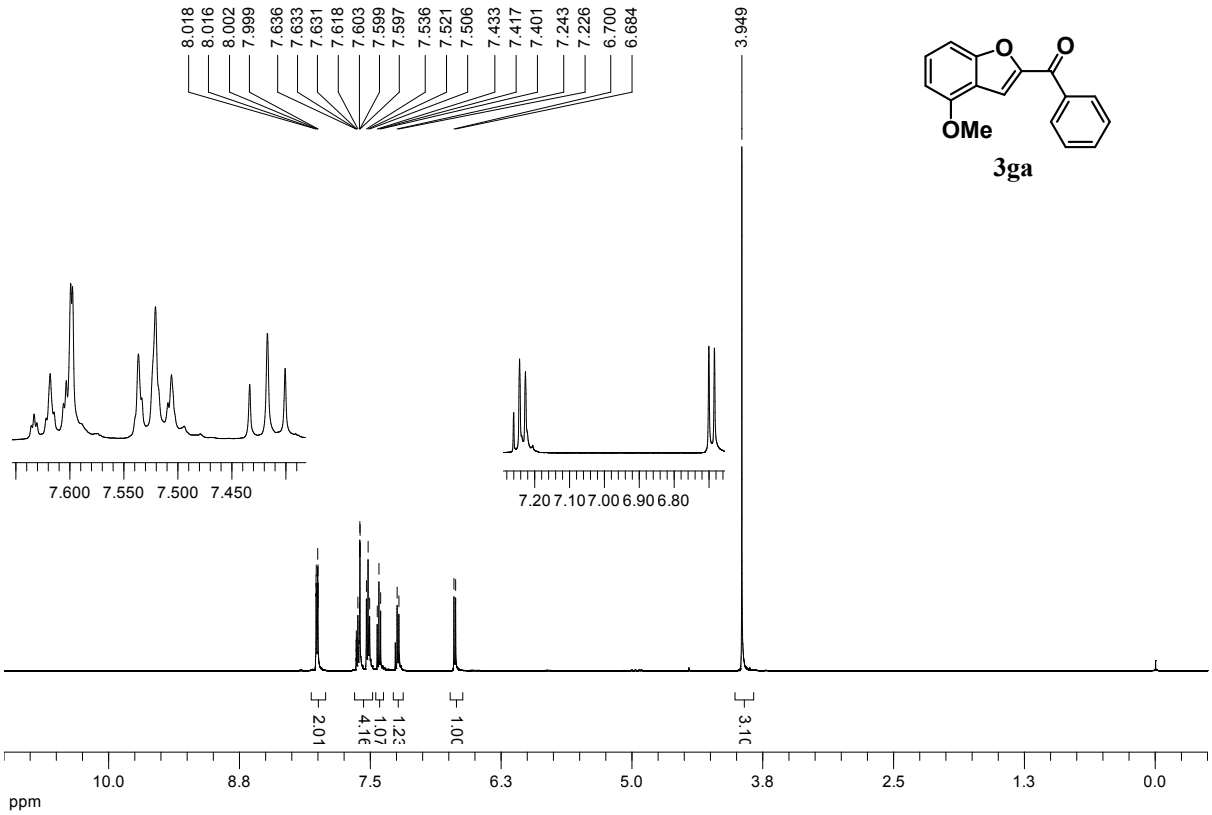
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7.618
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7.536
7.521
7.506
7.433
7.417
7.401
7.243
7.226
6.700
6.684
3.949
OMe
O
O
3ga
7.600 7.550 7.500 7.450
7.20 7.10 7.00 6.90 6.80
2.01
4.16
1.07
1.23
1.00
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10.0
8.8
7.5
6.3
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3.8
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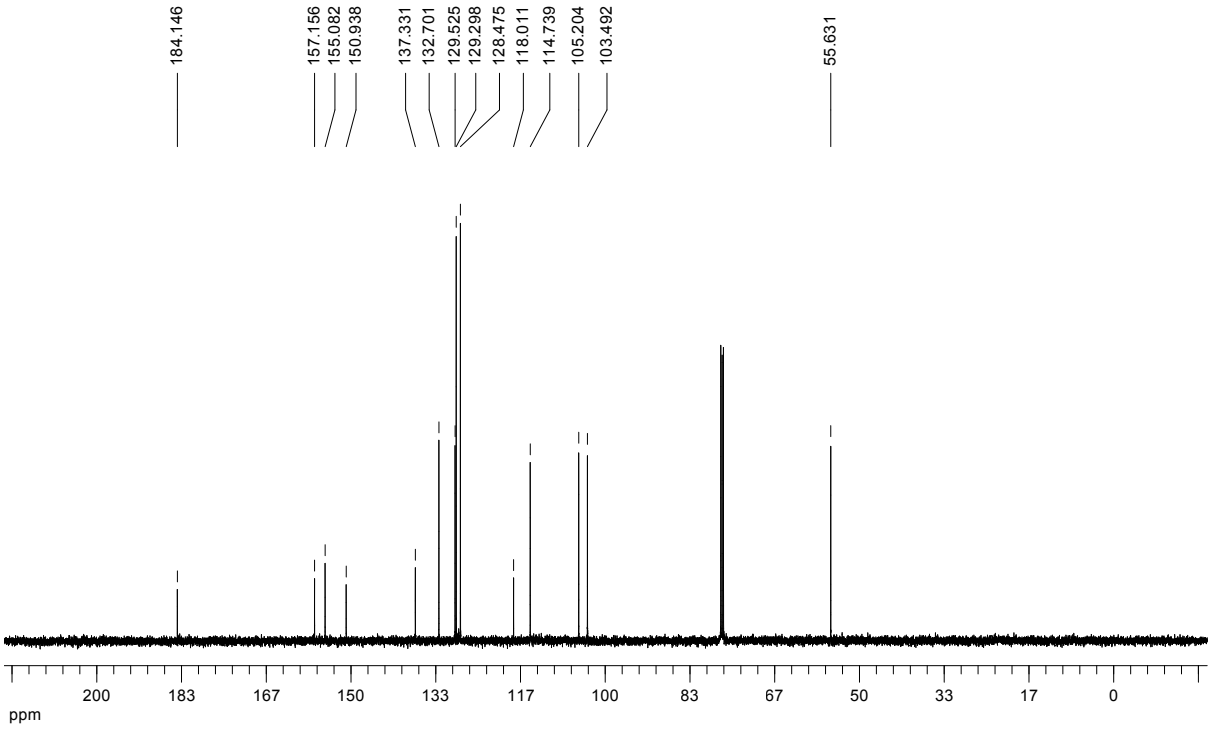
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55.631
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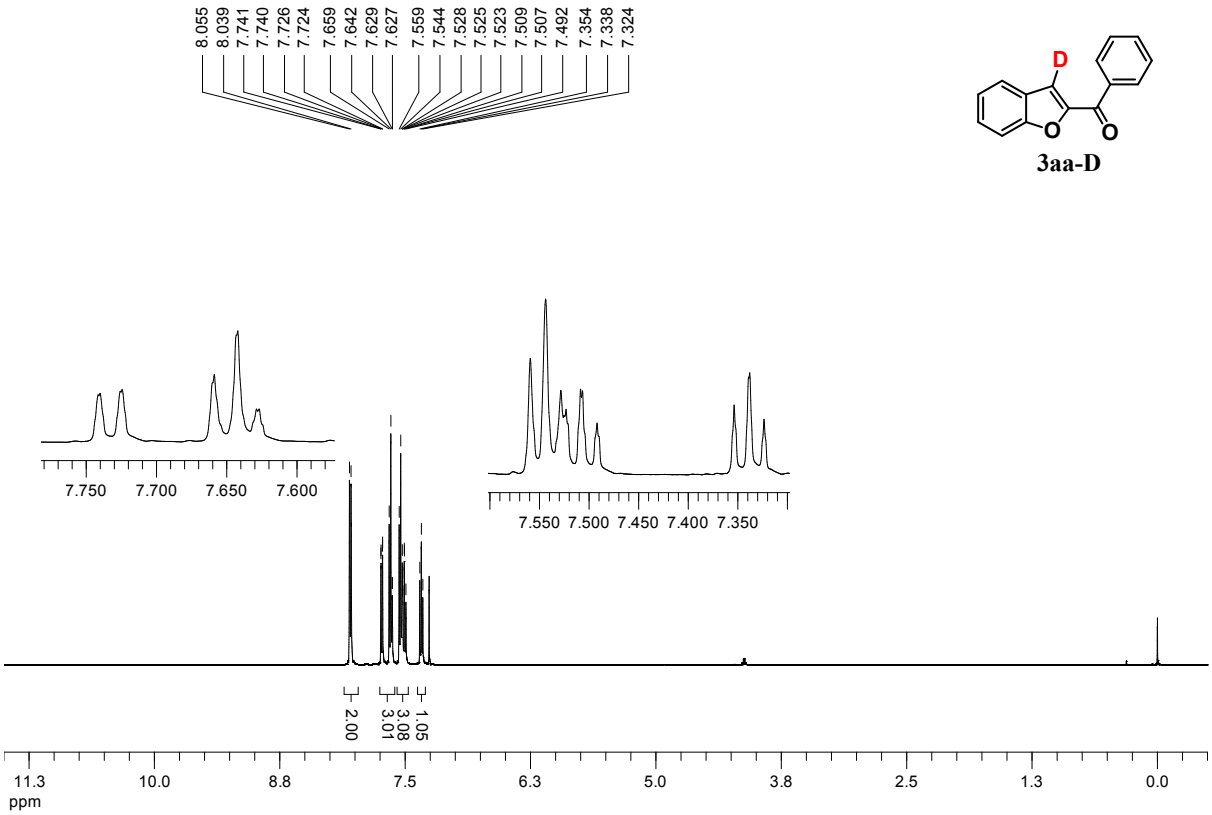
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7.642
7.629
7.627
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7.544
7.528
7.525
7.523
7.509
7.507
7.492
7.354
7.338
7.324
7.750 7.700 7.650 7.600
7.550 7.500 7.450 7.400 7.350
2.00
3.01
3.08
1.05
11.3 10.0 8.8 7.5 6.3 5.0 3.8 2.5 1.3 0.0
ppm

D
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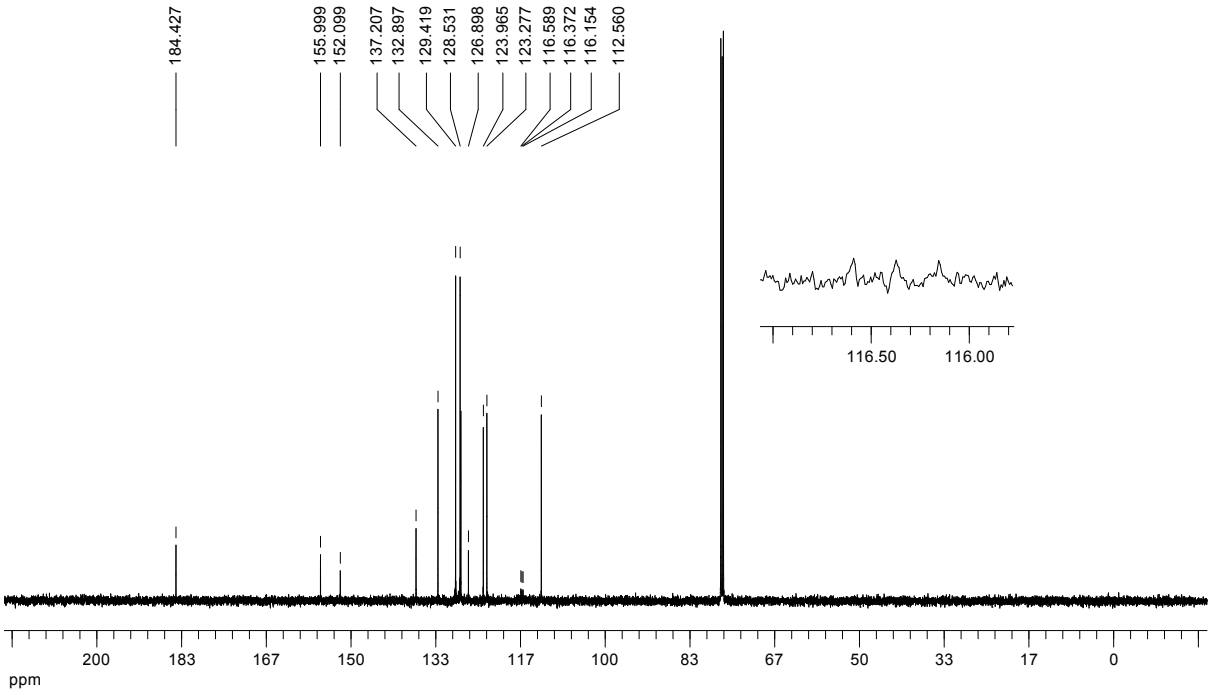
O

3aa-D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128.531
126.898
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116.154
112.560
116.50 116.00
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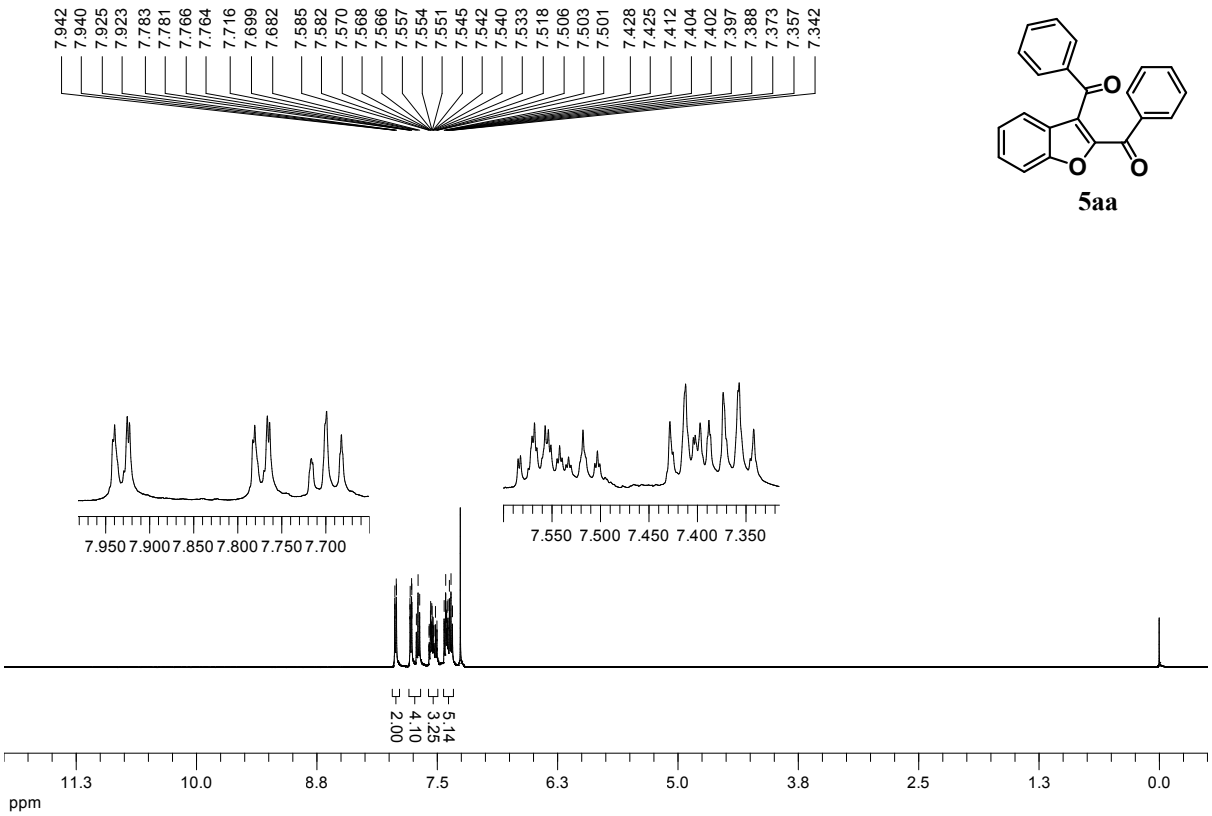
ppm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5aa
7.950 7.900 7.850 7.800 7.750 7.700
7.550 7.500 7.450 7.400 7.350
2.00 4.10 3.25 5.14
11.3 10.0 8.8 7.5 6.3 5.0 3.8 2.5 1.3 0.0
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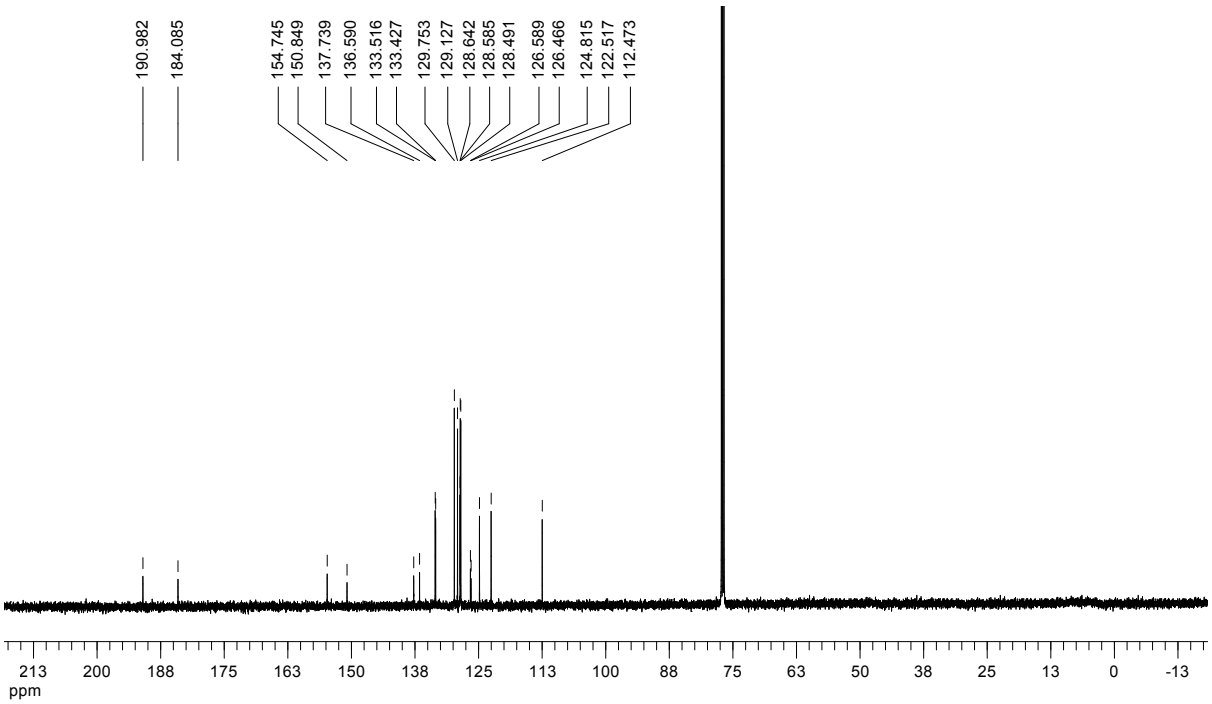
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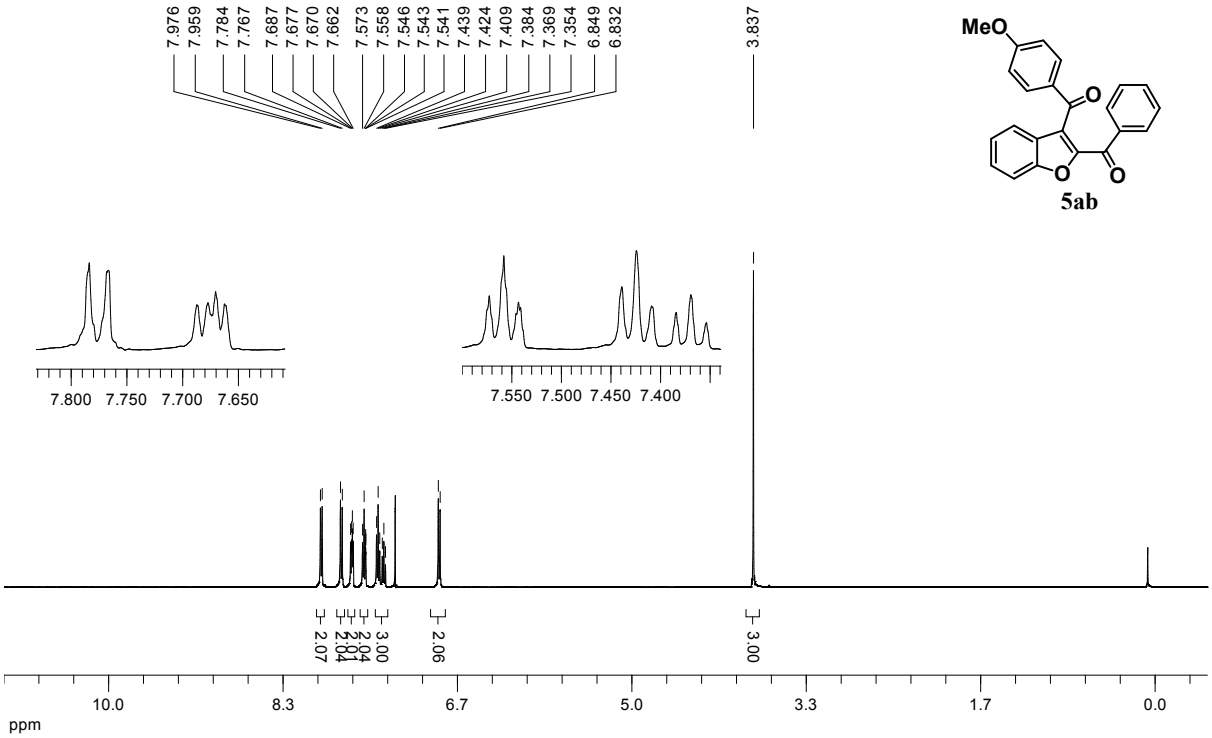
213 200 188 175 163 150 138 125 113 100 88 75 63 50 38 25 13 0 -13
ppm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7.543
7.541
7.439
7.424
7.409
7.384
7.369
7.354
6.849
6.832
3.837
MeO
O
O
O
5ab
7.800 7.750 7.700 7.650
7.550 7.500 7.450 7.400
2.07
2.04
2.04
2.02
3.00
2.06
3.00
10.0
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5.0
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1.7
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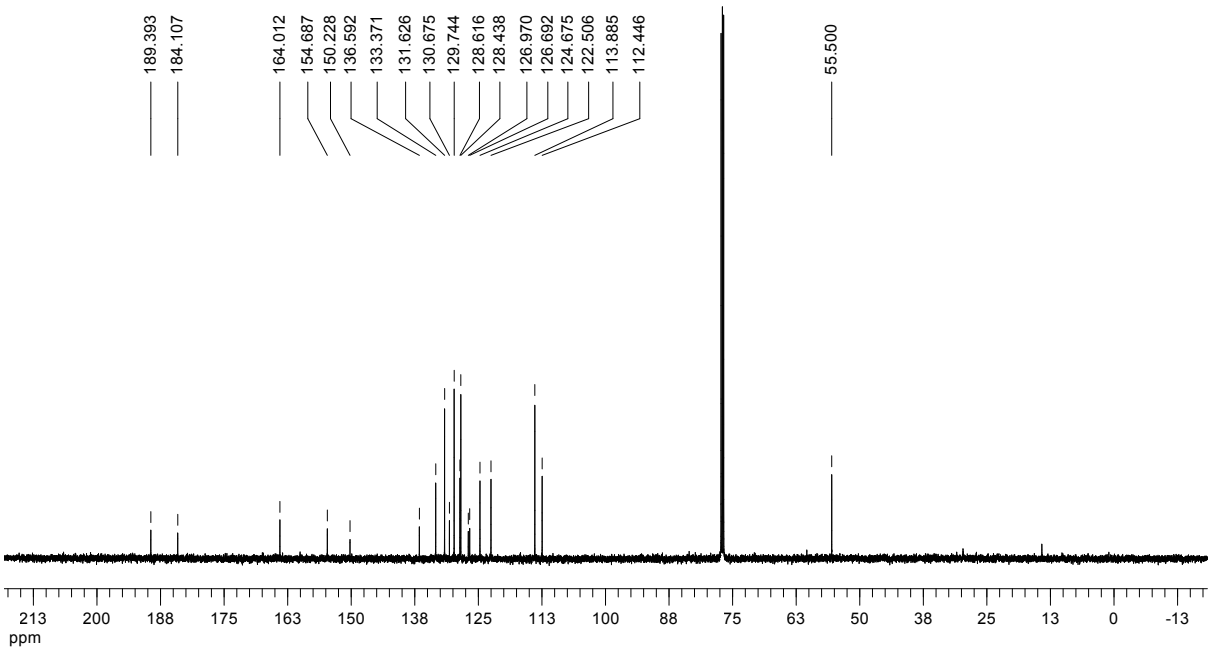
ppm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131.626
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129.744
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122.506
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112.446
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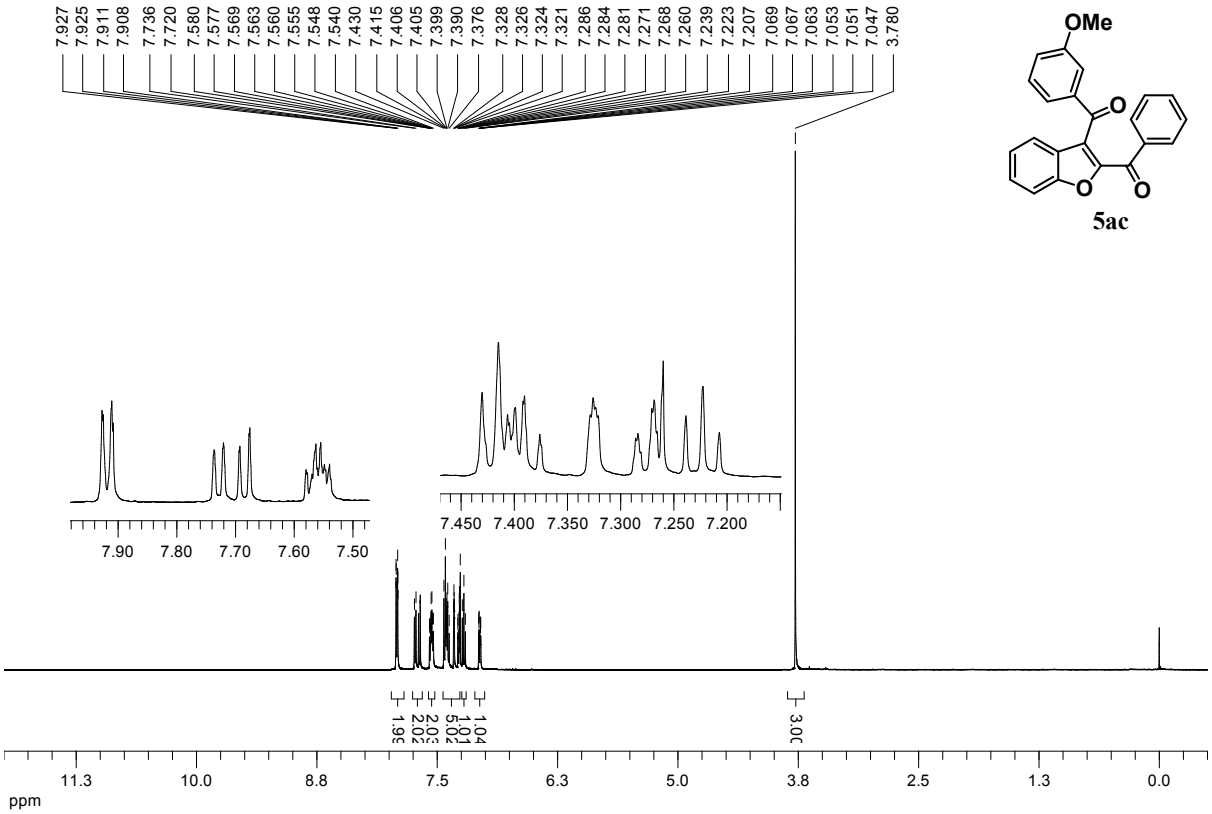
213 200 188 175 163 150 138 125 113 100 88 75 63 50 38 25 13 0 -13
ppm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7.577
7.569
7.563
7.560
7.555
7.548
7.540
7.430
7.415
7.406
7.405
7.399
7.390
7.376
7.328
7.326
7.324
7.321
7.286
7.284
7.281
7.271
7.268
7.260
7.239
7.223
7.207
7.069
7.067
7.063
7.053
7.051
7.047
3.780
OMe
O
O
O
5ac
7.90 7.80 7.70 7.60 7.50
7.450 7.400 7.350 7.300 7.250 7.200
1.96
2.02
2.03
5.02
1.01
1.04
3.00
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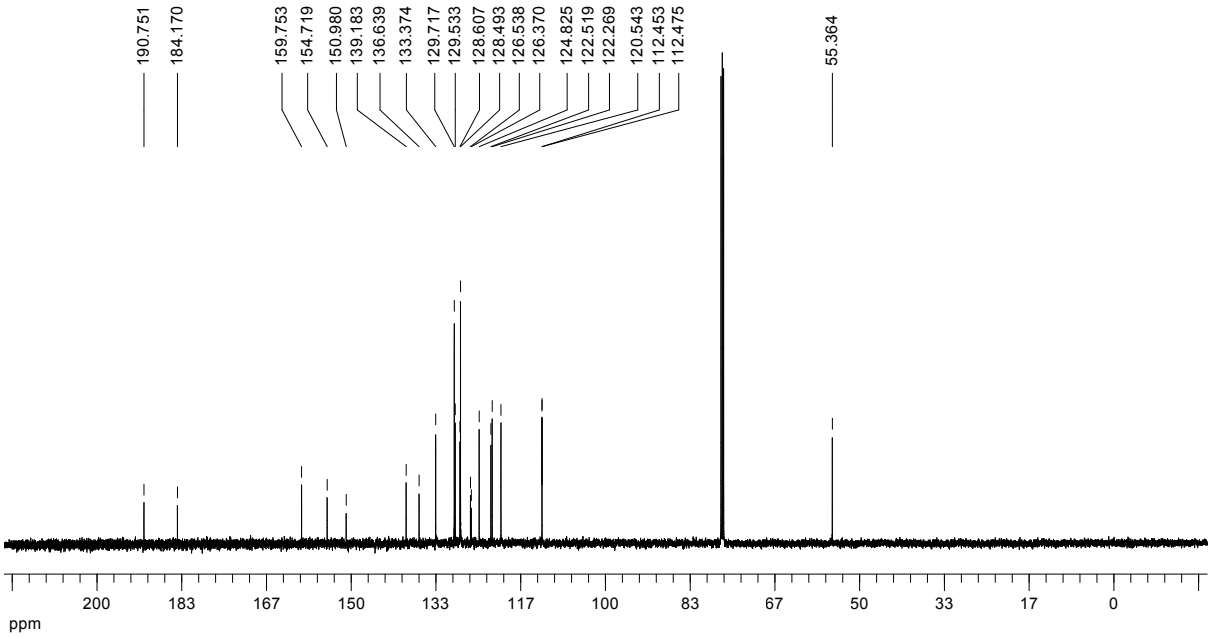
ppm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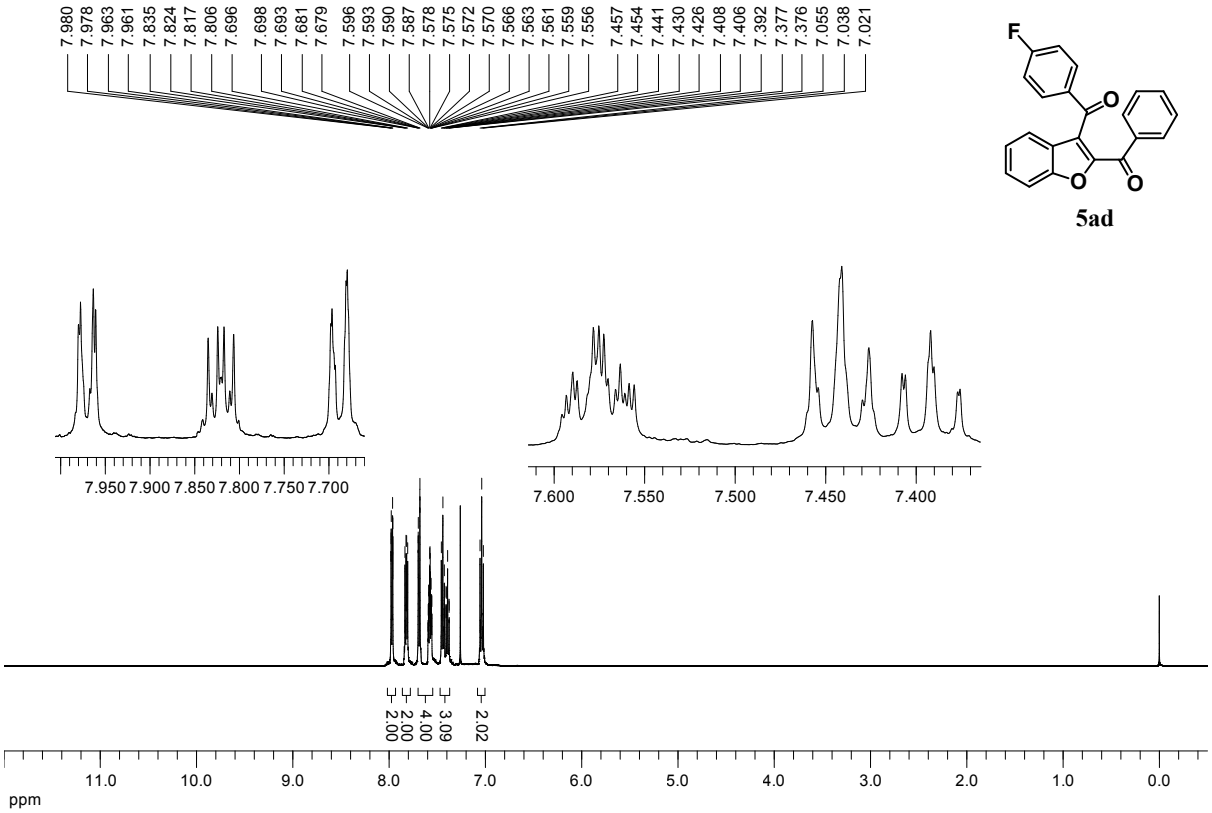
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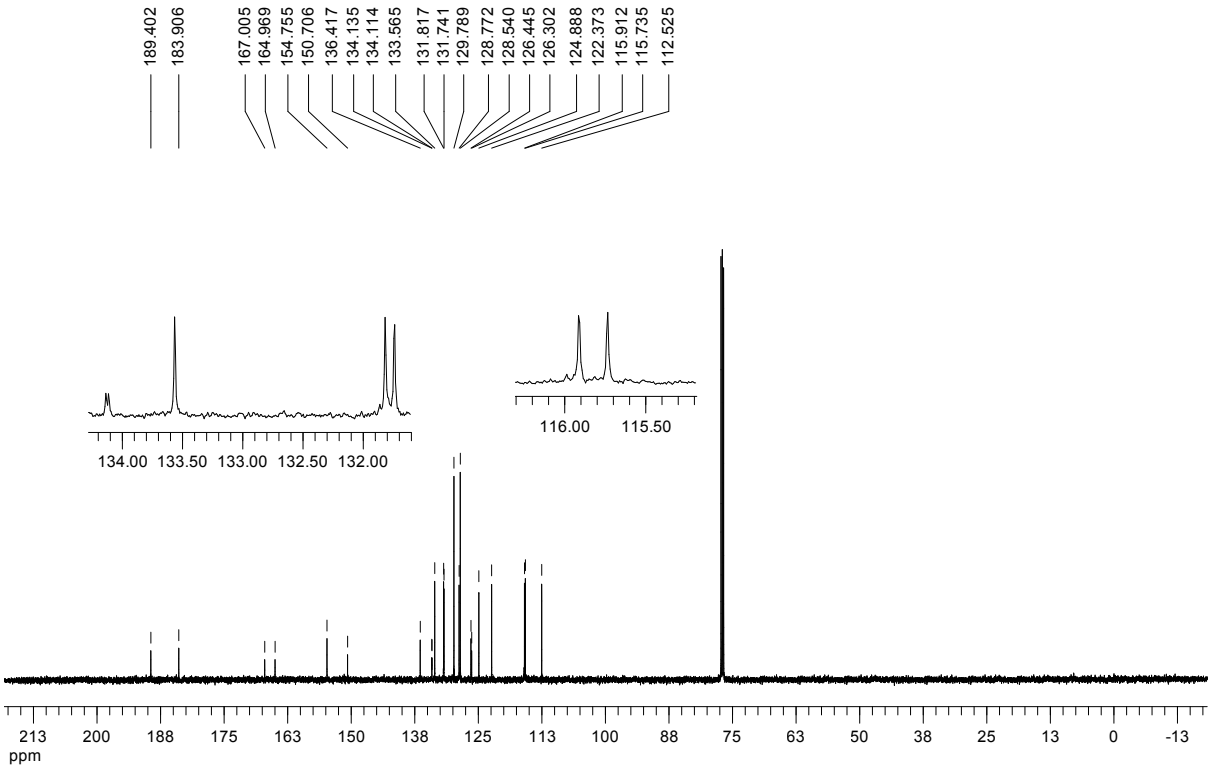
F
O
O
O
5ad
7.950 7.900 7.850 7.800 7.750 7.700
7.600 7.550 7.500 7.450 7.400
2.00 2.00 4.00 3.09 2.02
11.0 10.0 9.0 8.0 7.0 6.0 5.0 4.0 3.0 2.0 1.0 0.0
ppm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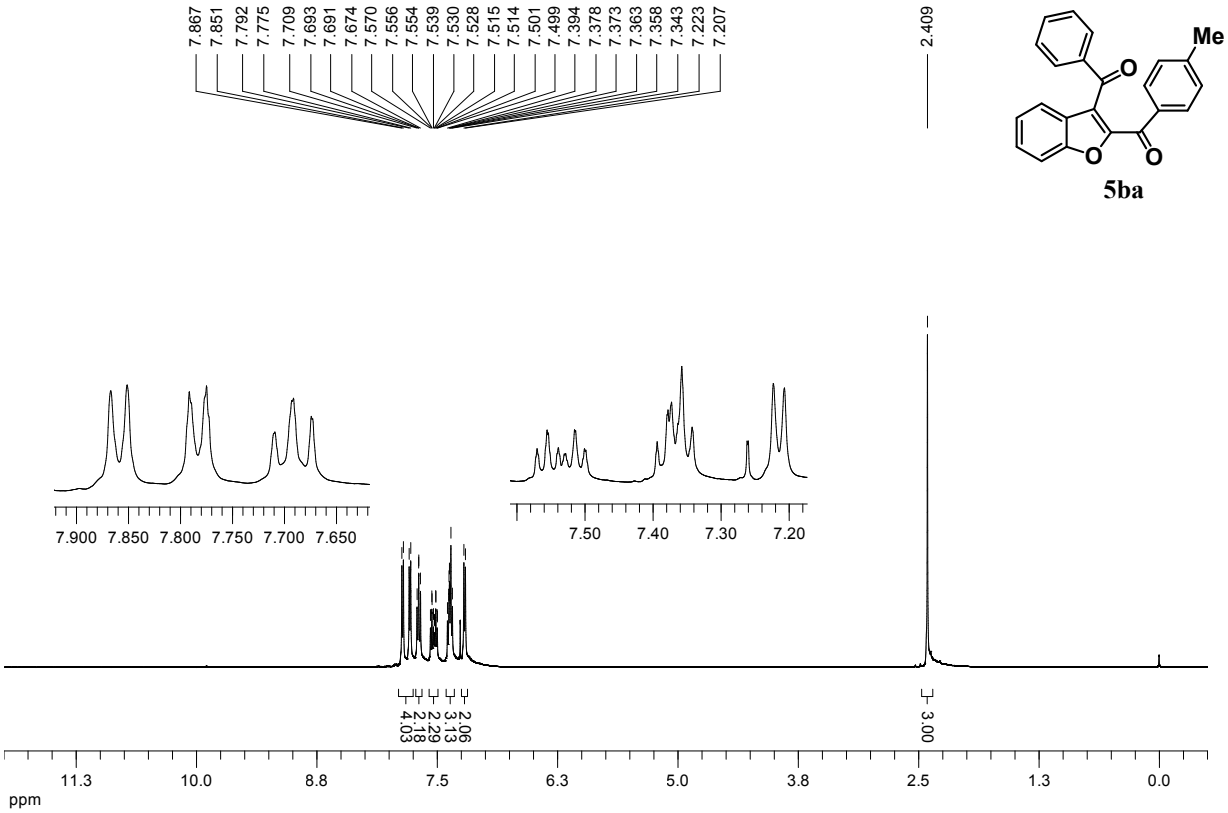
134.00 133.50 133.00 132.50 132.00
116.00 115.50
213 200 188 175 163 150 138 125 113 100 88 75 63 50 38 25 13 0 -13
ppm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7.530
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7.515
7.514
7.501
7.499
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7.378
7.373
7.363
7.358
7.343
7.223
7.207
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Me
O
O
O
5ba
7.900 7.850 7.800 7.750 7.700 7.650
7.50 7.40 7.30 7.20
4.03
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3.13
2.06
3.00
11.3 10.0 8.8 7.5 6.3 5.0 3.8 2.5 1.3 0.0
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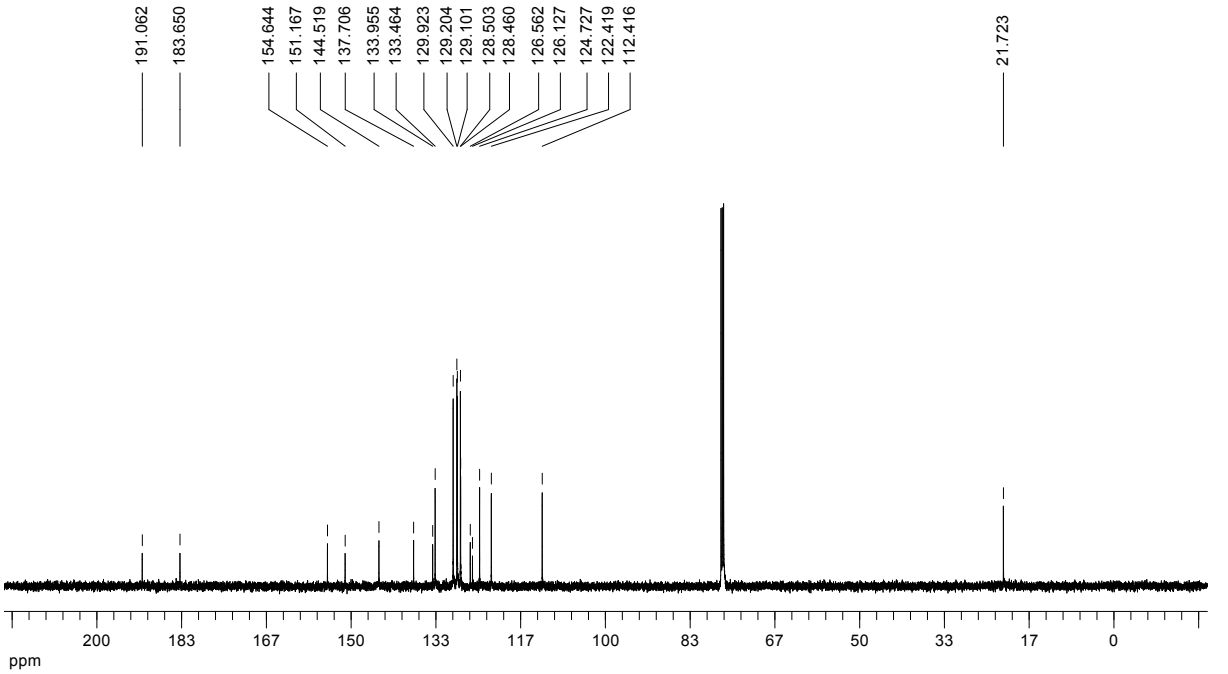
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126.562
126.127
124.727
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21.723
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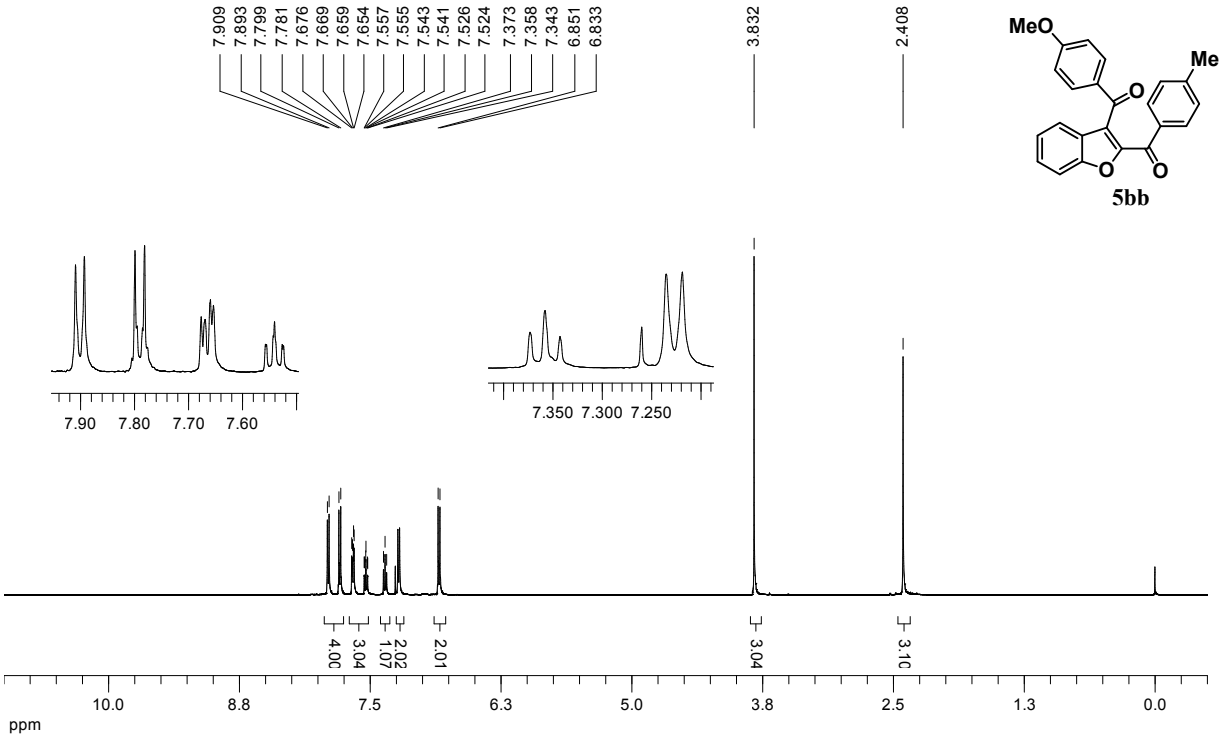
ppm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7.526
7.524
7.373
7.358
7.343
6.851
6.833
3.832
2.408
MeO
Me
O
O
O
5bb
7.90 7.80 7.70 7.60
7.350 7.300 7.250
4.00
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1.07
2.02
2.01
3.04
3.10
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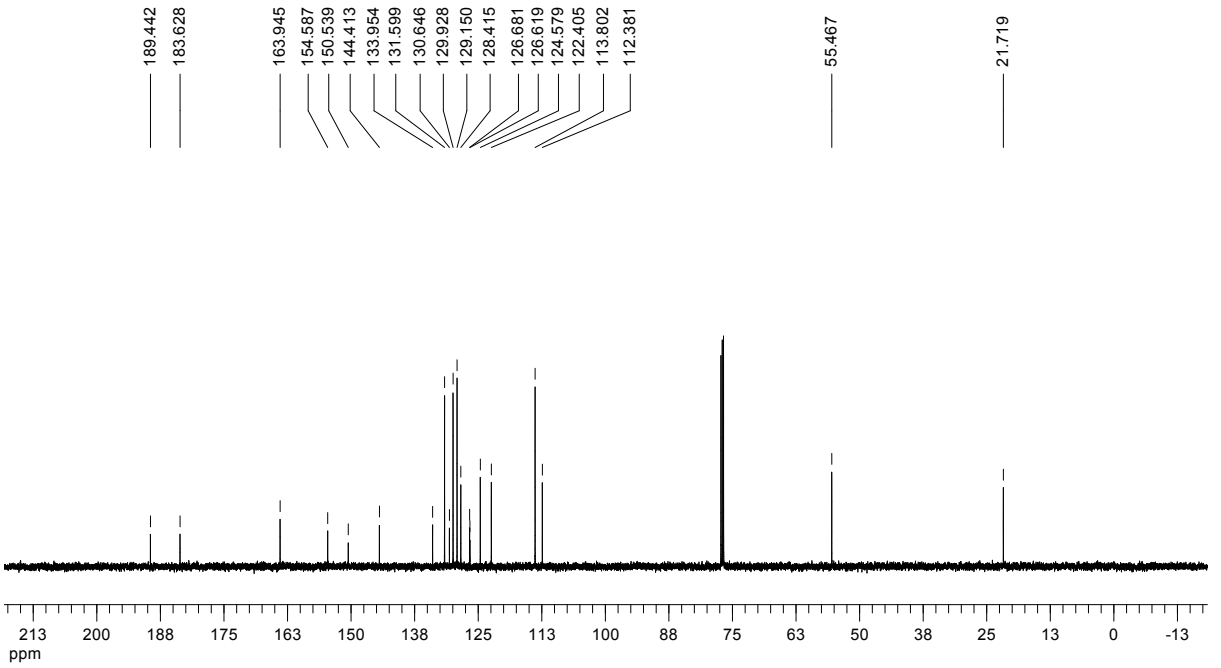
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55.467
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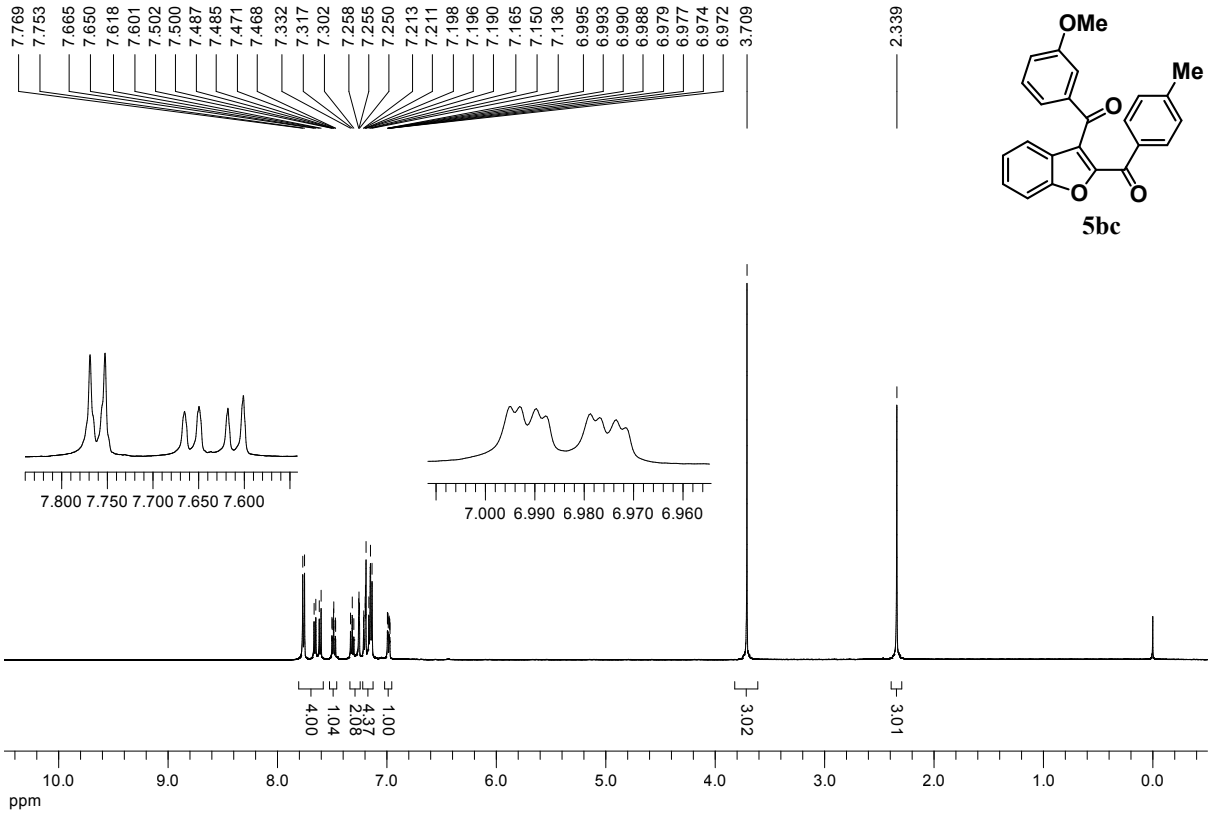
ppm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7.332
7.317
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7.258
7.255
7.250
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7.190
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7.150
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6.988
6.979
6.977
6.974
6.972
3.709
2.339
OMe
Me
O
O
O
5bc
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7.000 6.990 6.980 6.970 6.960
4.00
1.04
2.08
2.27
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3.02
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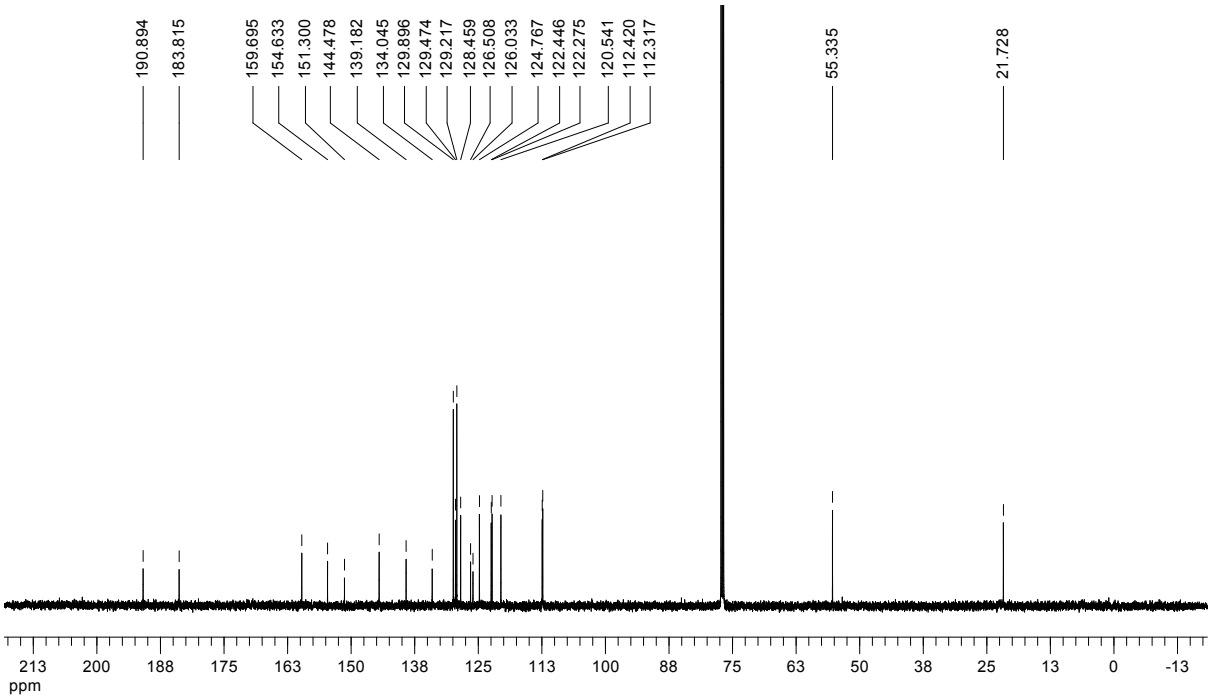
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126.033
124.767
122.446
122.275
120.541
112.420
112.317
55.335
21.728
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175
163
150
138
125
113
100
88
75
63
50
38
25
13
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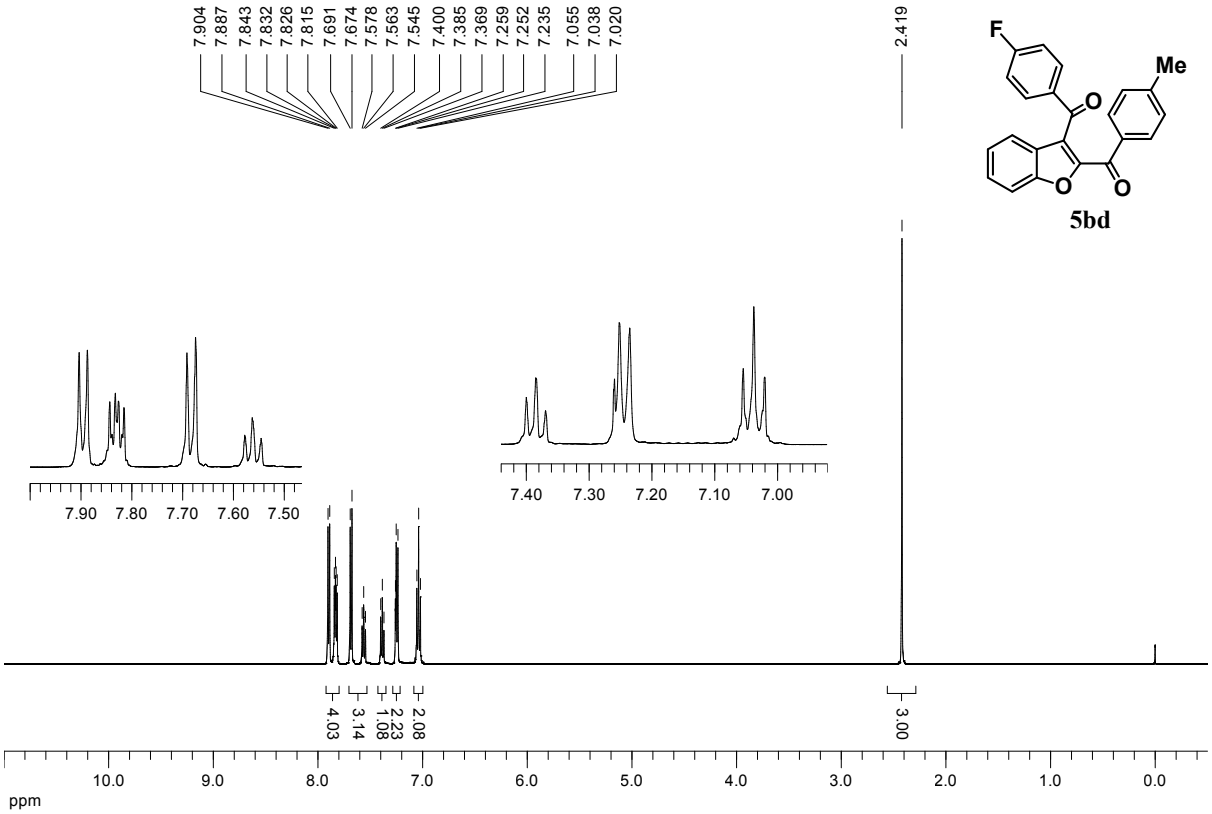
ppm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7.400
7.385
7.369
7.259
7.252
7.235
7.055
7.038
7.020
2.419
F
Me
O
O
O
5bd
7.90 7.80 7.70 7.60 7.50
7.40 7.30 7.20 7.10 7.00
4.03
3.14
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2.08
3.00
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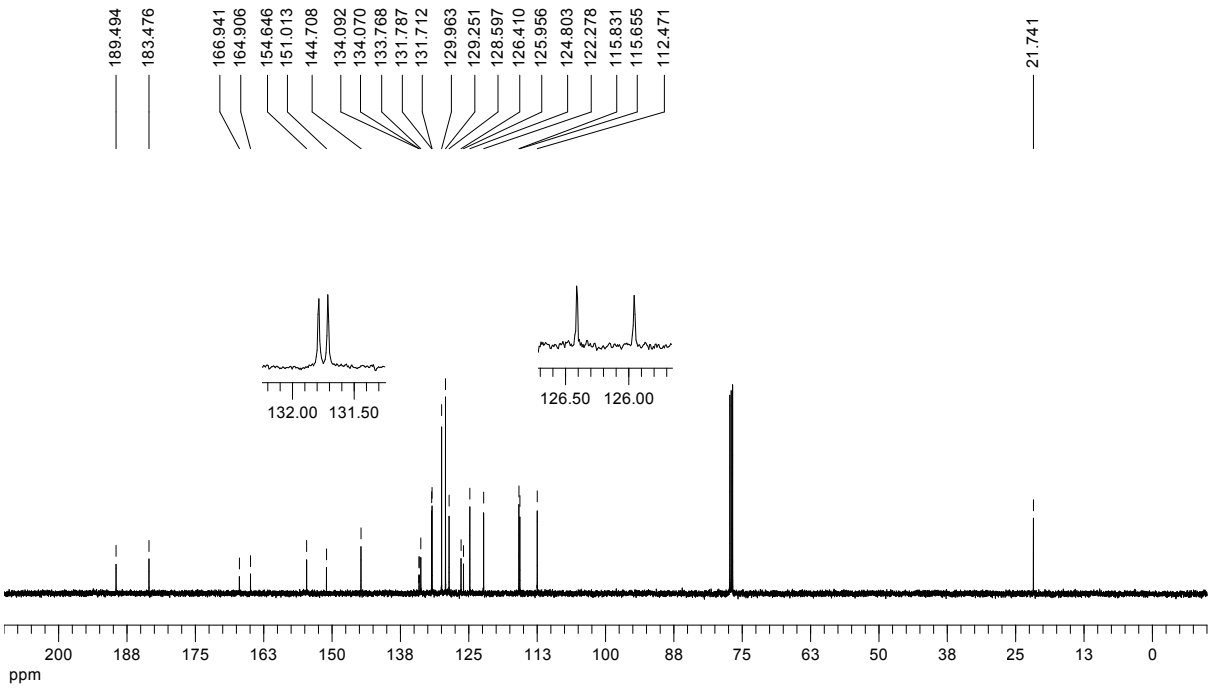
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129.963
129.251
128.597
126.410
125.956
124.803
122.278
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112.471
21.741
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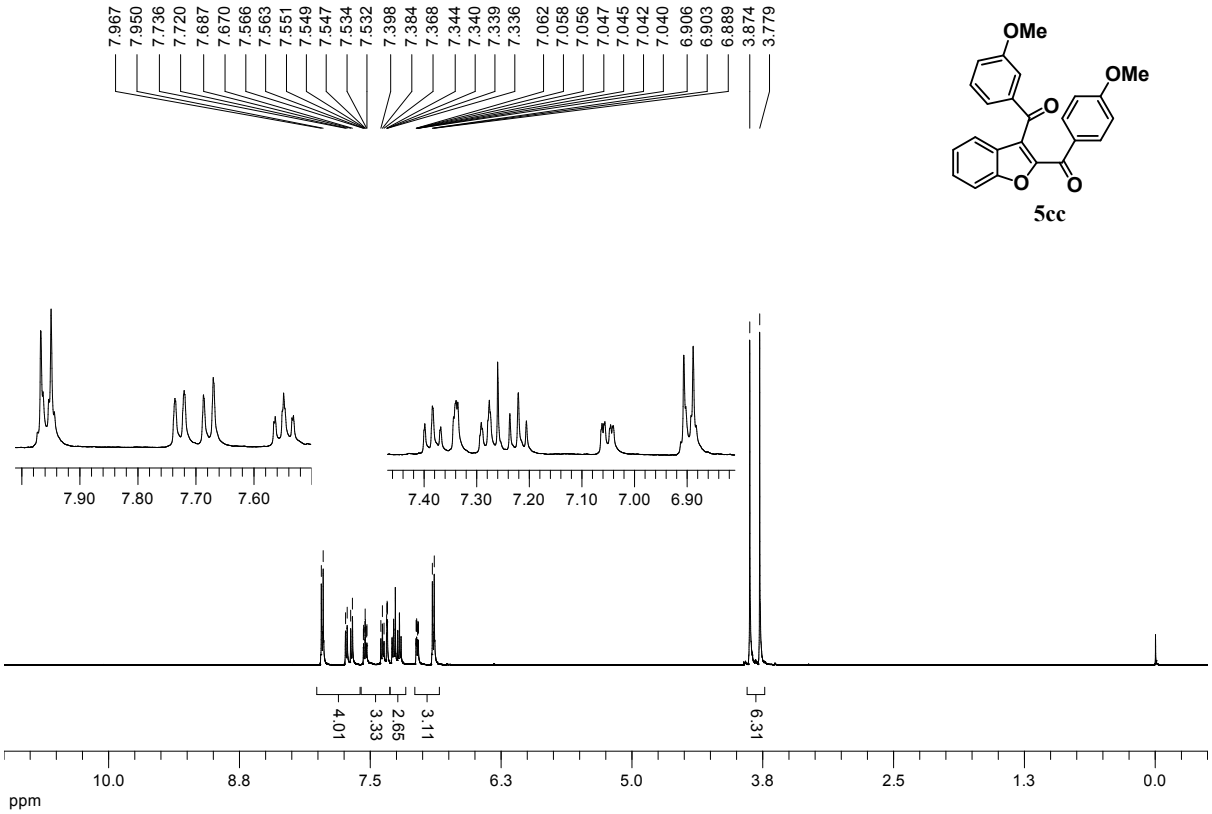
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7.532
7.398
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7.045
7.042
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6.906
6.903
6.889
3.874
3.779
OMe
OMe
O
O
O
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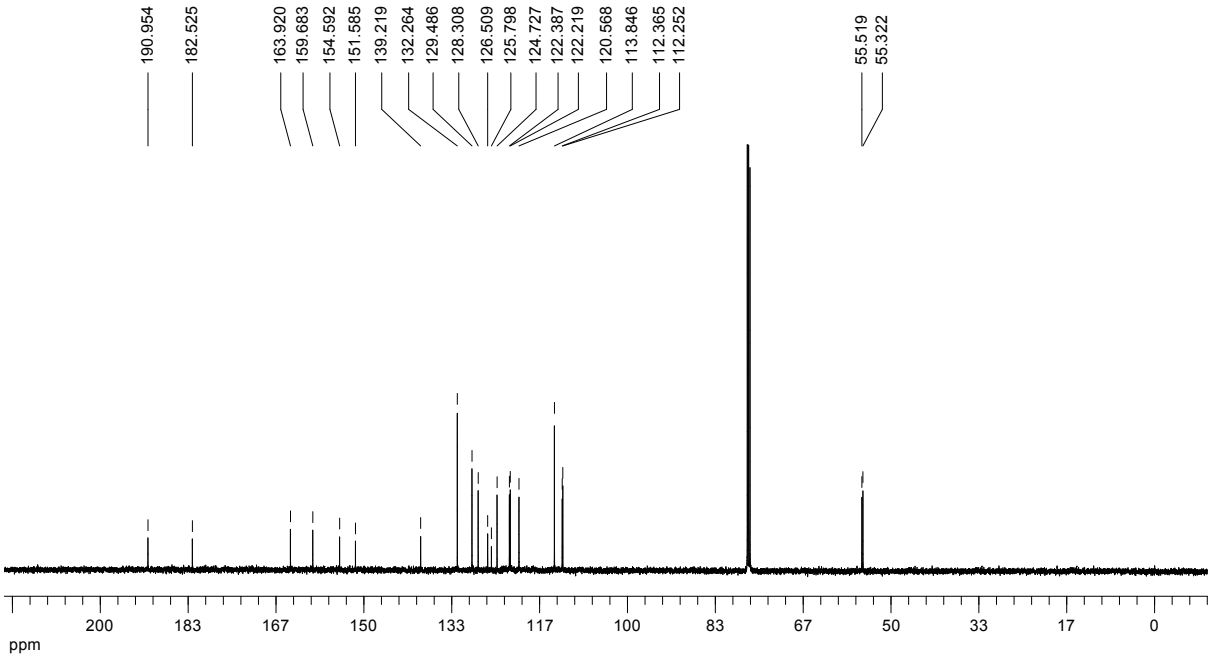
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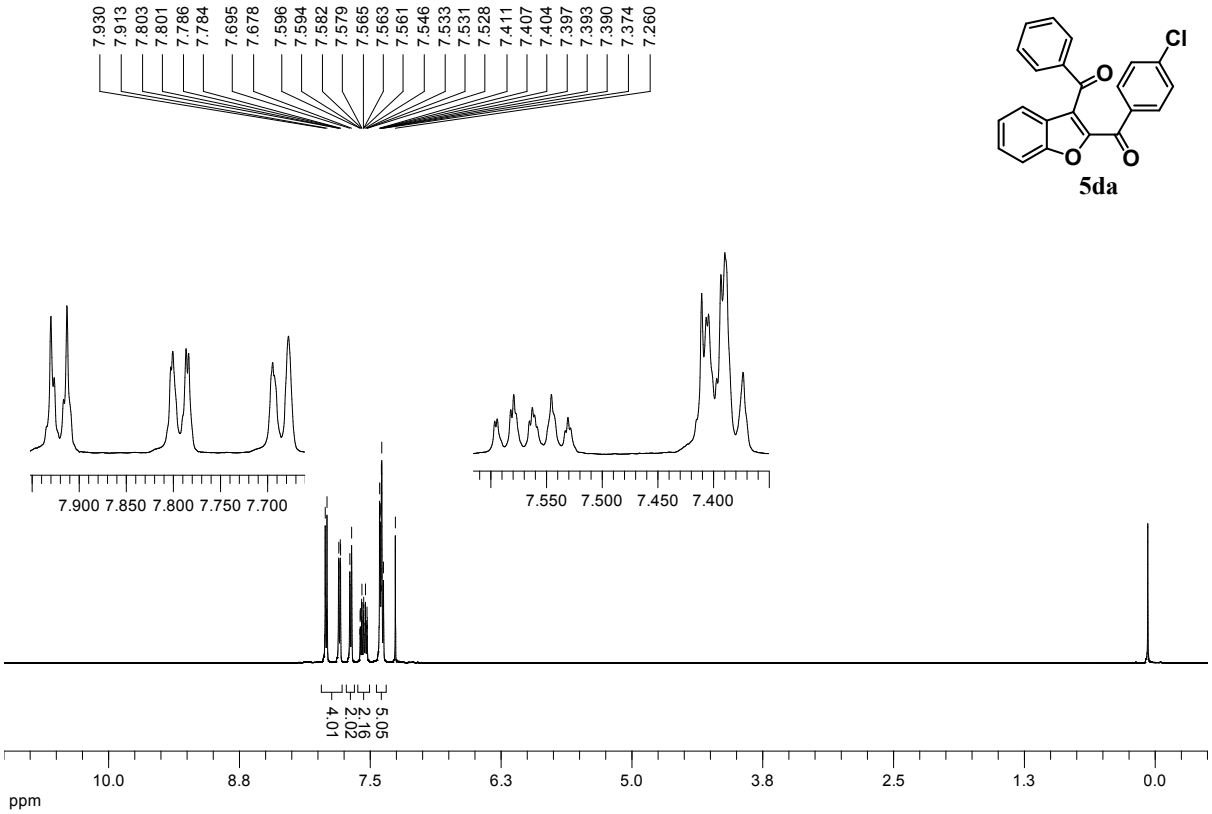
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7.531
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7.411
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7.397
7.393
7.390
7.374
7.260
Cl
O
O
O
5da
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7.550 7.500 7.450 7.400
4.01
2.02
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10.0
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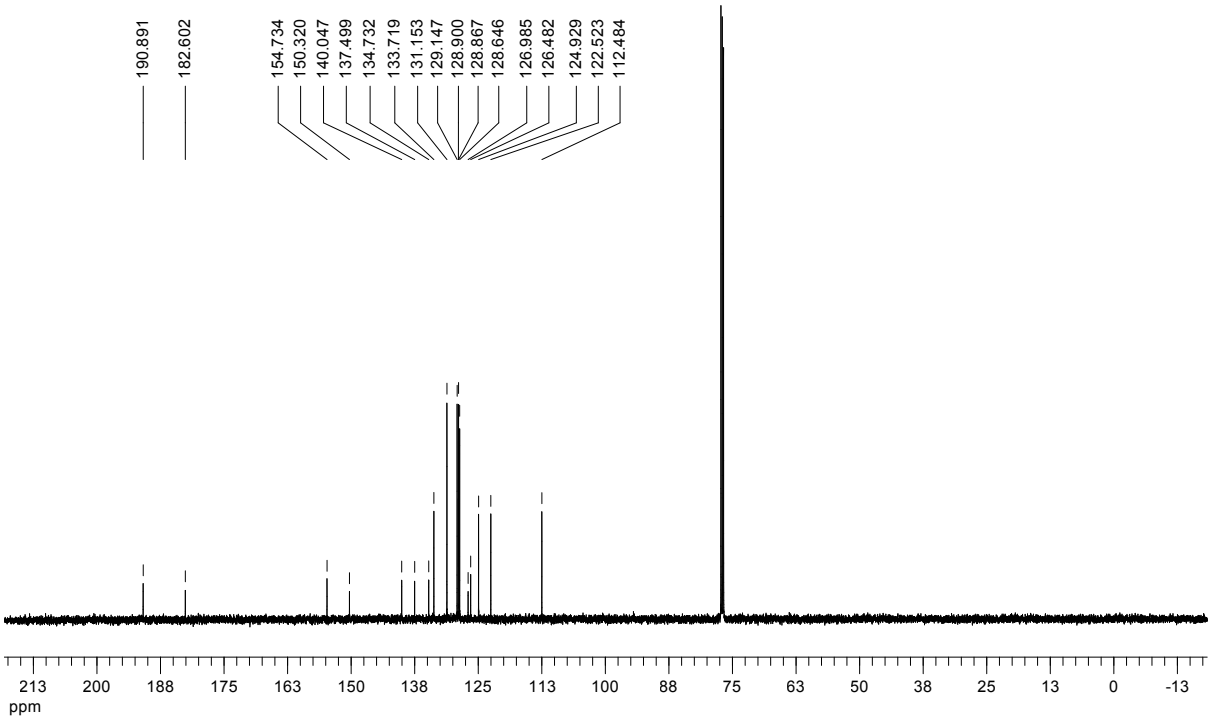
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126.482
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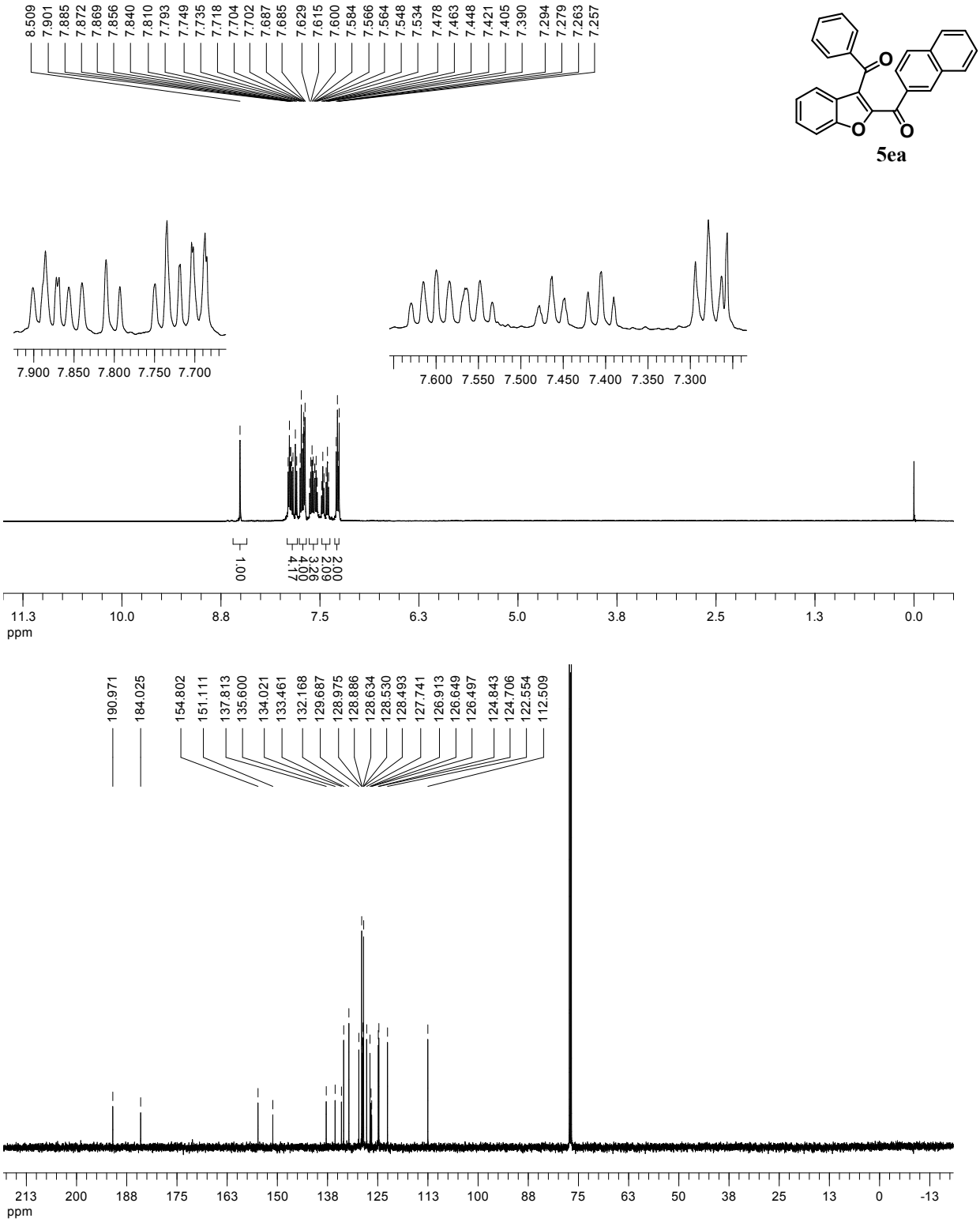
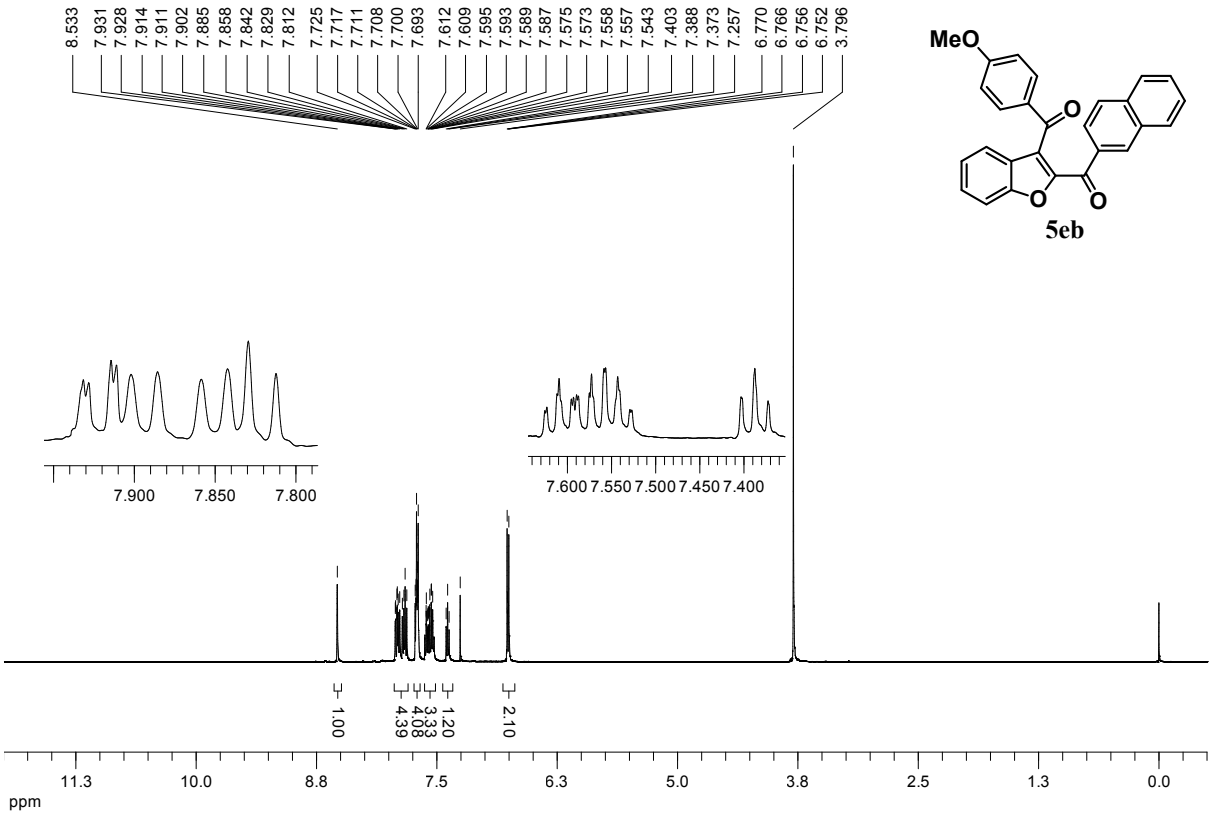
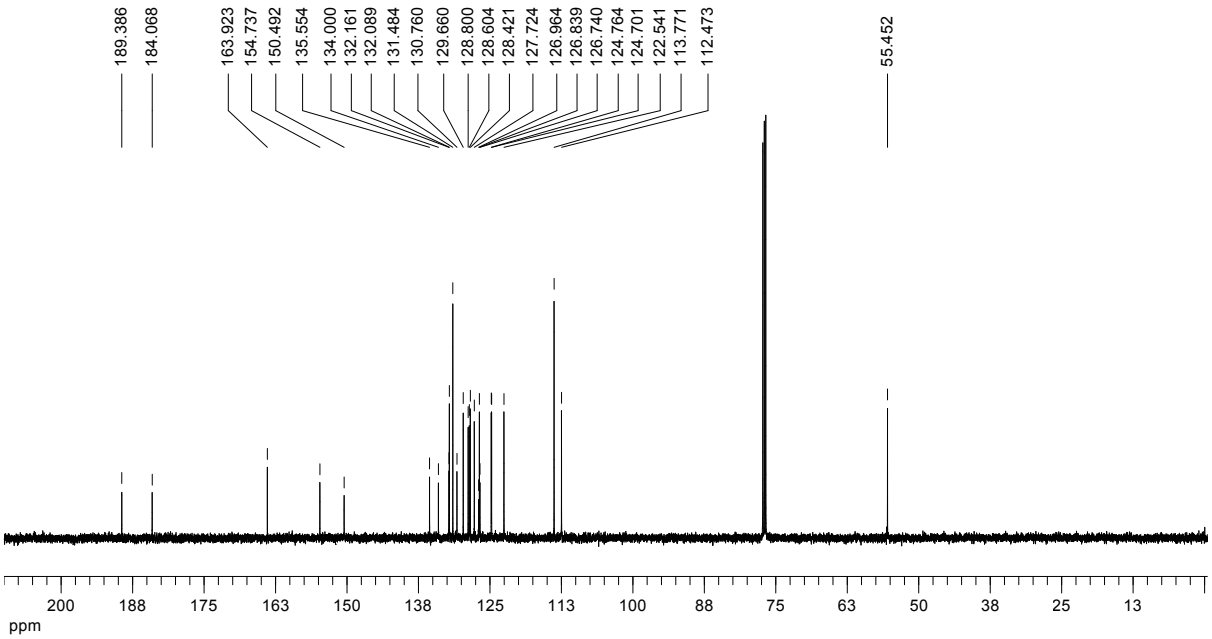
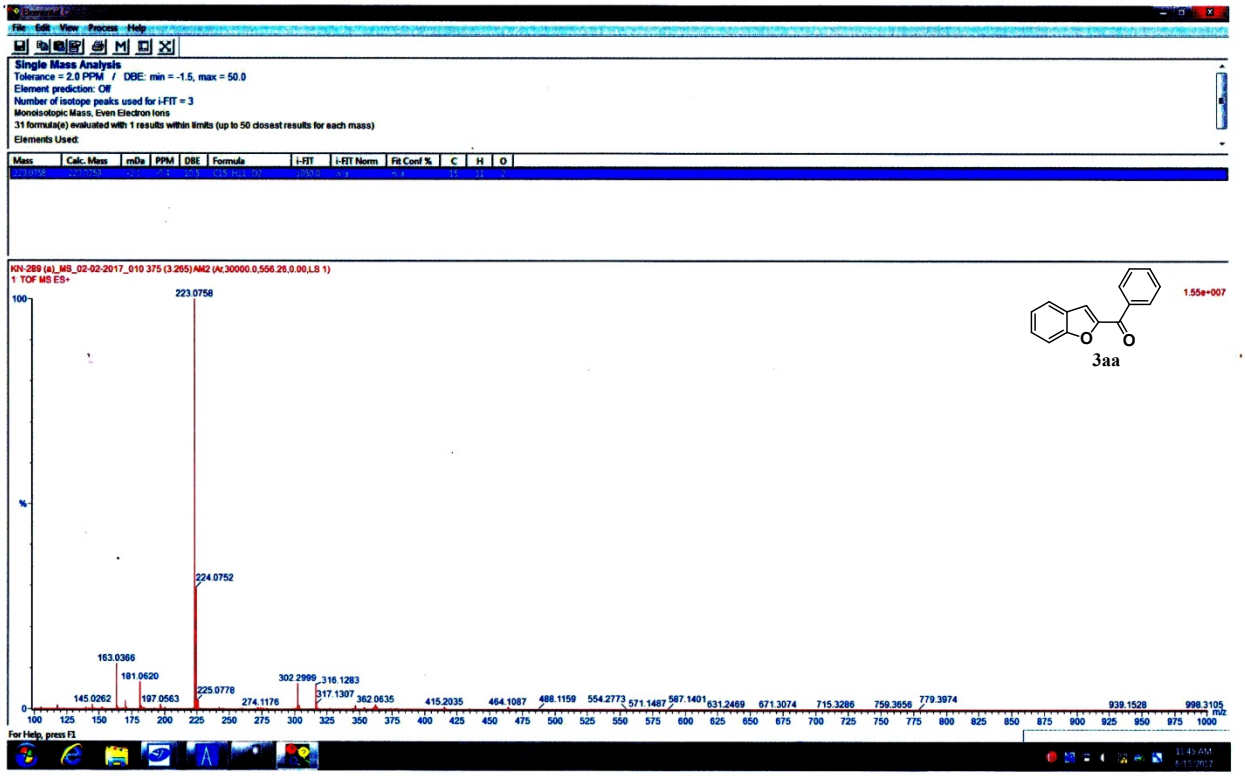
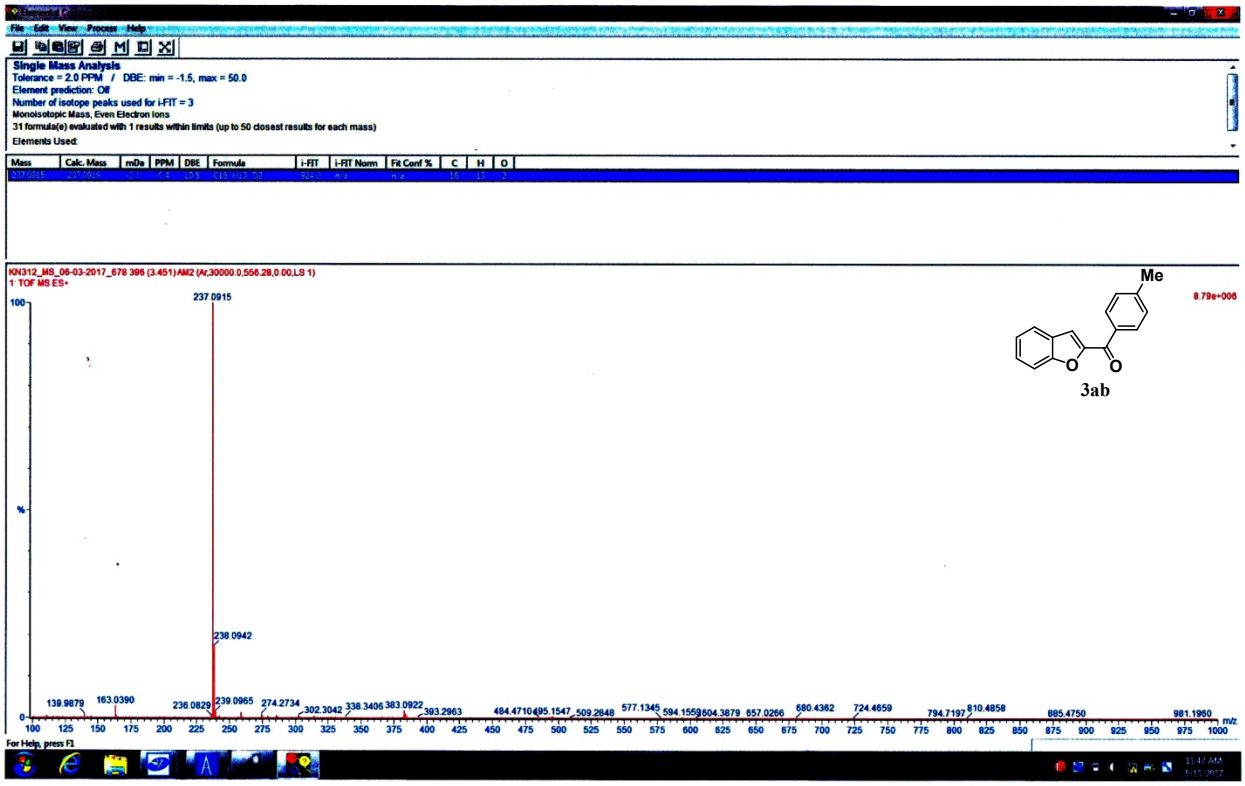
122.523
112.484
213
200
188
175
163
150
138
125
113
100
88
75
63
50
38
25
13
0
-13
ppm

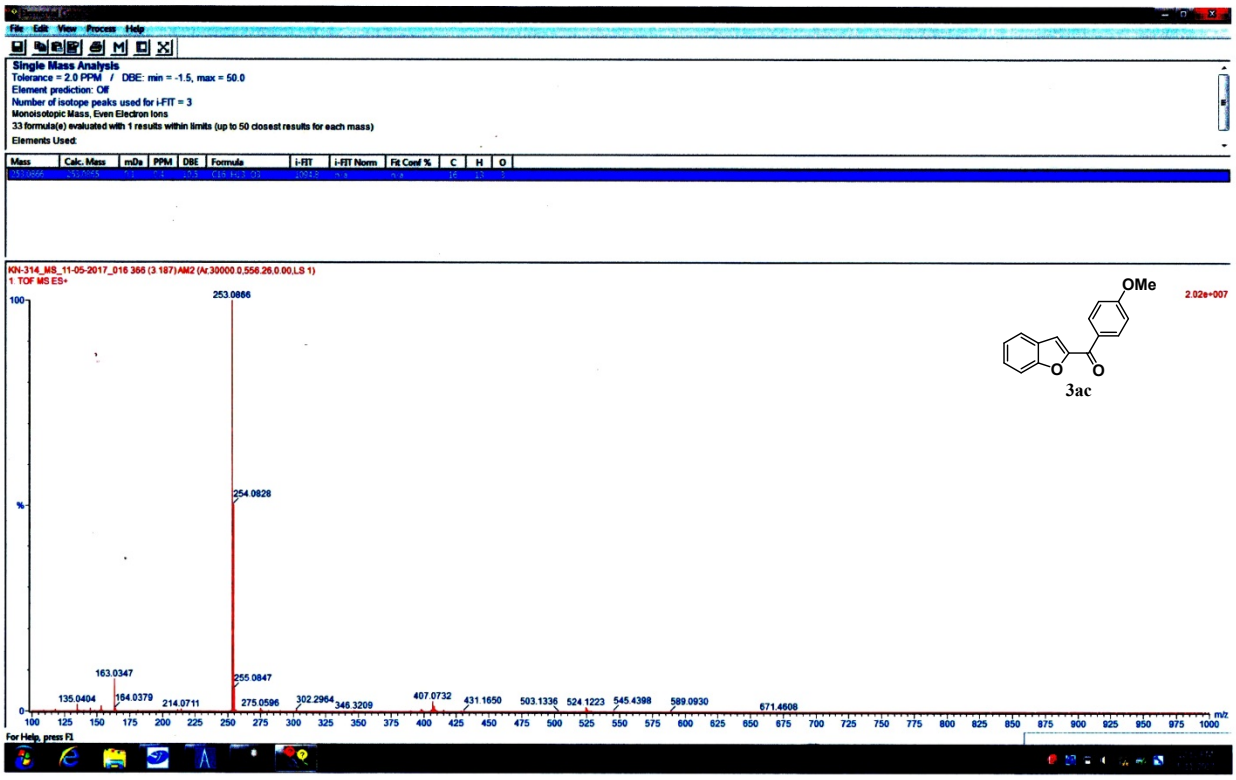

8.509 7.901 7.885 7.872 7.869 7.856 7.840 7.810 7.793 7.749 7.735 7.718 7.704 7.702 7.687 7.685 7.629 7.615 7.600 7.584 7.566 7.564 7.548 7.534 7.478 7.463 7.448 7.421 7.405 7.390 7.294 7.279 7.263 7.257
5ea
7.900 7.850 7.800 7.750 7.700
7.600 7.550 7.500 7.450 7.400 7.350 7.300
1.00 4.17 4.08 3.28 2.09 2.00
11.3 10.0 8.8 7.5 6.3 5.0 3.8 2.5 1.3 0.0
ppm
190.971 184.025 154.802 151.111 137.813 135.600 134.021 133.461 132.168 129.687 128.975 128.886 128.634 128.530 128.493 127.741 126.913 126.649 126.497 124.843 124.706 122.554 112.509
213 200 188 175 163 150 138 125 113 100 88 75 63 50 38 25 13 0 -13
ppm


8.533
7.931
7.928
7.914
7.911
7.902
7.885
7.858
7.842
7.829
7.812
7.725
7.717
7.711
7.708
7.700
7.693
7.612
7.609
7.595
7.593
7.589
7.587
7.575
7.573
7.558
7.557
7.543
7.403
7.388
7.373
7.257
6.770
6.766
6.756
6.752
3.796
MeO
O
O
O
5eb
7.900
7.850
7.800
7.600 7.550 7.500 7.450 7.400
1.00
4.39
4.08
3.33
1.20
2.10
11.3
10.0
8.8
7.5
6.3
5.0
3.8
2.5
1.3
0.0
ppm

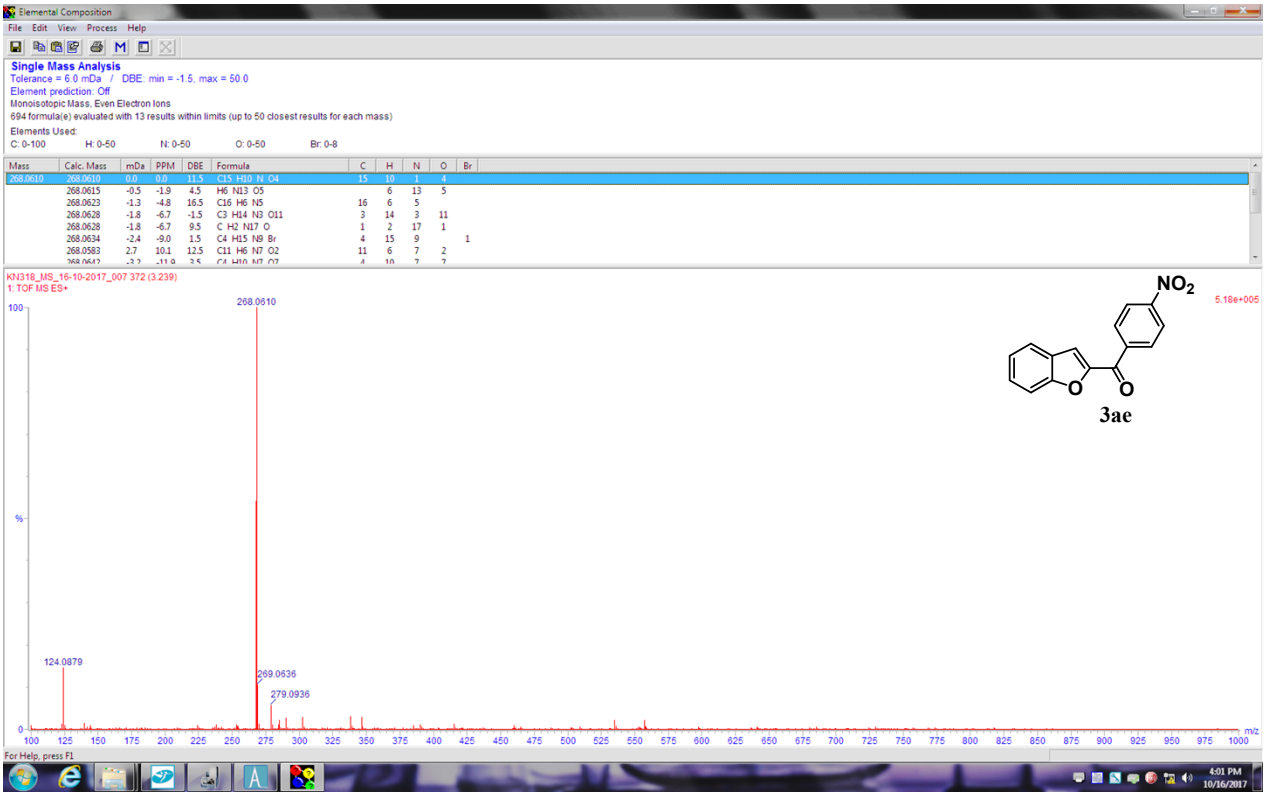

189.386
184.068
163.923
154.737
150.492
135.554
134.000
132.161
132.089
131.484
130.760
129.660
128.800
128.604
128.421
127.724
126.964
126.839
126.740
124.764
124.701
122.541
113.771
112.473
55.452
200
188
175
163
150
138
125
113
100
88
75
63
50
38
25
13
ppm


Single Mass Analysis
Tolerance = 2.0 PPM / DBE: min = -1.5, max = 50.0
Element prediction: Off
Number of isotope peaks used for i-FIT = 3
Monoisotopic Mass, Even Electron Ions
31 formula(e) evaluated with 1 results within limits (up to 50 closest results for each mass)
Elements Used:
Mass
Calc. Mass
mDa
PPM
DBE
Formula
i-FIT
i-FIT Norm
Fit Conf %
C
H
O
KN-289 (a)_MS_02-02-2017_010 375 (3.265)AM2 (Ar,30000.0,556.26,0.00,LS 1)
1: TOF MS ES+
223.0758
224.0752
163.0366
181.0620
145.0262
197.0563
225.0778
274.1176
302.2999
316.1283
317.1307
362.0635
415.2035
464.1087
488.1159
554.2773
571.1487
587.1401
631.2469
671.3074
715.3286
759.3656
779.3974
939.1528
998.3105
1.55e+007
3aa
For Help, press F1

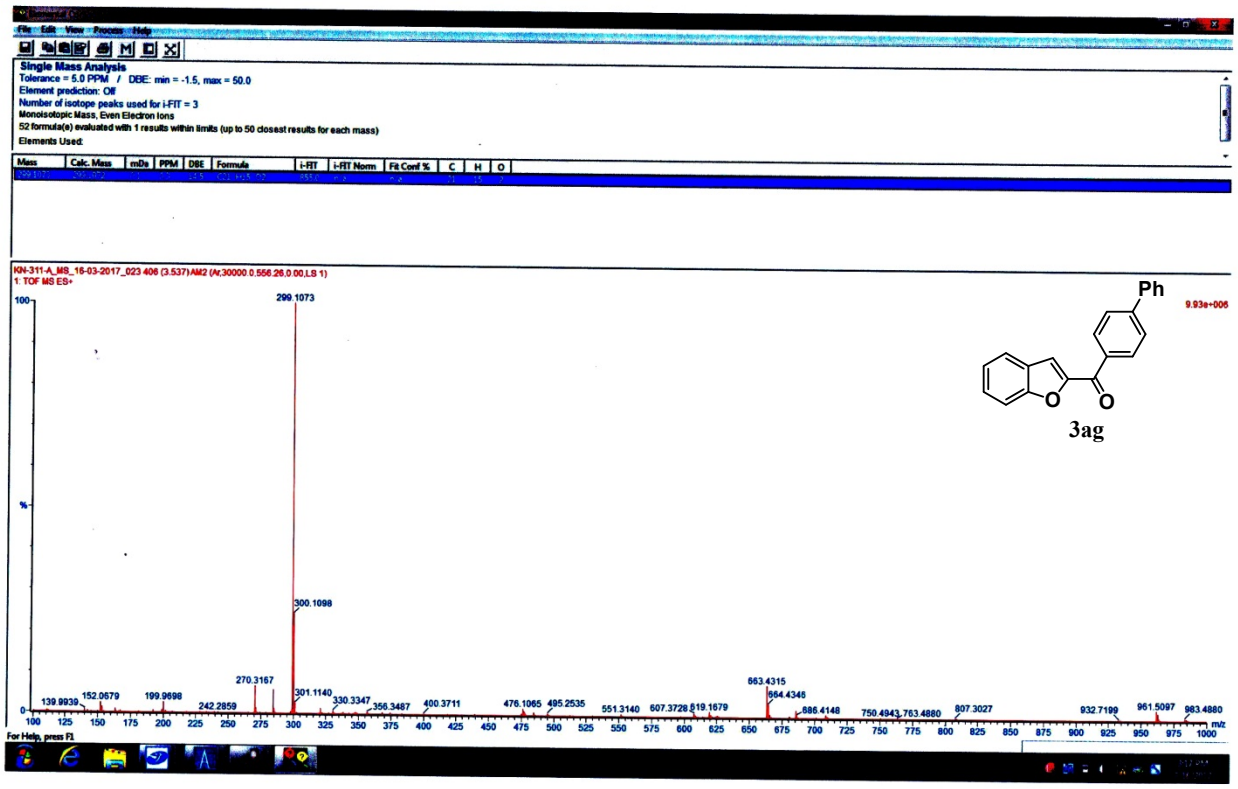

Single Mass Analysis
Tolerance = 2.0 PPM / DBE: min = -1.5, max = 50.0
Element prediction: Off
Number of isotope peaks used for i-FIT = 3
Monoisotopic Mass, Even Electron Ions
31 formula(e) evaluated with 1 results within limits (up to 50 closest results for each mass)
Elements Used:
Mass
Calc. Mass
mDa
PPM
DBE
Formula
i-FIT
i-FIT Norm
Fit Conf %
C
H
O
KN312_MS_06-03-2017_678 396 (3.451)AM2 (Ar,30000.0,556.28,0.00,LS 1)
1: TOF MS ES+
237.0915
238.0942
139.9879
163.0390
236.0829
239.0965
274.2734
302.3042
338.3406
383.0922
393.2963
484.4710
495.1547
509.2848
577.1345
594.1559
604.3879
657.0266
680.4362
724.4659
794.7197
810.4858
885.4750
981.1960
Me
8.79e+006
3ab
For Help, press F1


Single Mass Analysis
Tolerance = 2.0 PPM / DBE: min = -1.5, max = 50.0
Element prediction: Off
Number of isotope peaks used for i-FIT = 3
Monoisotopic Mass, Even Electron Ions
33 formula(e) evaluated with 1 results within limits (up to 50 closest results for each mass)
Elements Used:
Mass | Calc. Mass | mDa | PPM | DBE | Formula | i-FIT | i-FIT Norm | Fit Conf % | C | H | O
KN-314_MS_11-05-2017_016 365 (3.187) AM2 (Ar,30000.0,556.26,0.00,LS 1)
1: TOF MS ES+
253.0866
254.0828
255.0847
163.0347
135.0404
164.0379
214.0711
275.0596
302.2964
346.3209
407.0732
431.1650
503.1336
524.1223
545.4398
589.0930
671.4608
OMe
2.02e+007
3ac

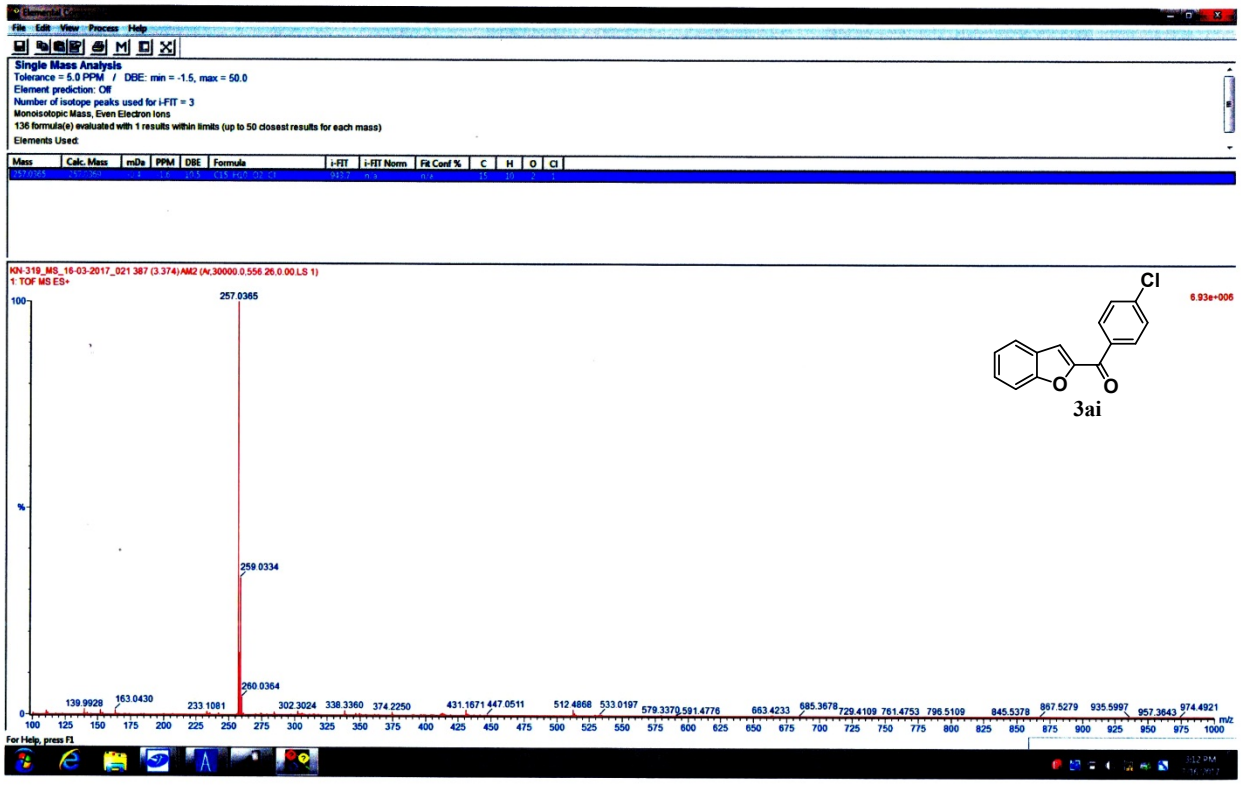

Single Mass Analysis
Tolerance = 2.0 PPM / DBE: min = -1.5, max = 50.0
Element prediction: Off
Number of isotope peaks used for i-FIT = 3
Monoisotopic Mass, Even Electron Ions
183 formula(e) evaluated with 1 results within limits (up to 50 closest results for each mass)
Elements Used:
Mass | Calc. Mass | mDa | PPM | DBE | Formula | i-FIT | i-FIT Norm | Fit Conf % | C | H | O | F
291.0635 | 291.0633 | 0.2 | 0.7 | 10.5 | C16 H10 O2 F3 | 777.2
KN-322_MS_04-04-2017_003 393 (3.425) AM2 (Ar,30000.0,556.28,0.00,LS 1)
1: TOF MS ES+
291.0635
292.0666
294.1105
330.3369
111.0210
139.9885
181.0654
235.1698
264.1381
295.1135
374.3628
384.1565
418.3884
478.1982
502.3366
579.1031
600.0928
611.2700
673.4572
689.2191
745.1177
908.2543
CF3
4.54e+006
3ad

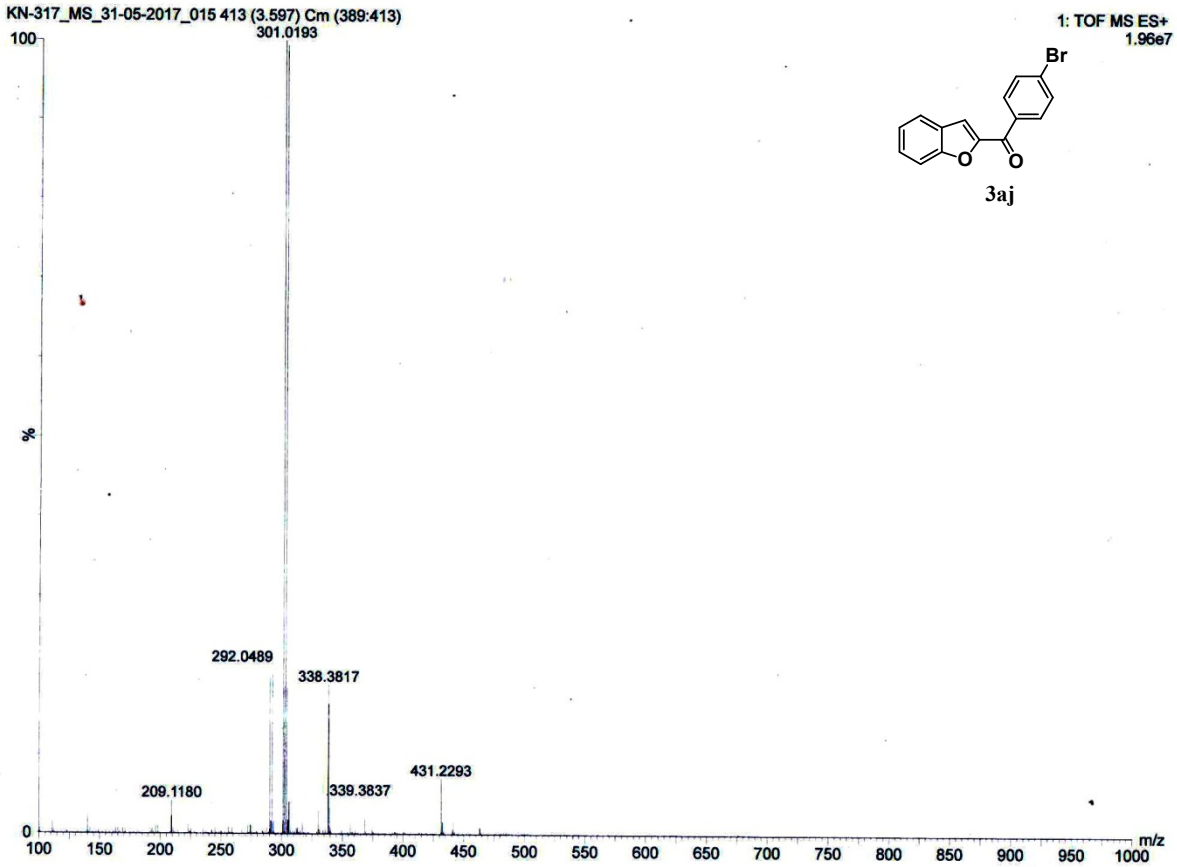

Elemental Composition
Single Mass Analysis
Tolerance = 6.0 mDa / DBE: min = -1.5, max = 50.0
Element prediction: Off
Monoisotopic Mass, Even Electron Ions
694 formula(e) evaluated with 13 results within limits (up to 50 closest results for each mass)
Elements Used:
C: 0-100 H: 0-50 N: 0-50 O: 0-50 Br: 0-8
Mass Calc. Mass mDa PPM DBE Formula C H N O Br
268.0610 268.0610 0.0 0.0 11.5 C15 H10 N O4 15 10 1 4
268.0615 -0.5 -1.9 4.5 H6 N13 O5 6 13 5
268.0623 -1.3 -4.8 16.5 C16 H6 N5 16 6 5
268.0628 -1.8 -6.7 -1.5 C3 H14 N3 O11 3 14 3 11
268.0628 -1.8 -6.7 9.5 C H2 N17 O 1 2 17 1
268.0634 -2.4 -9.0 1.5 C4 H15 N9 Br 4 15 9 1
268.0583 2.7 10.1 12.5 C11 H6 N7 O2 11 6 7 2
KN318_MS_16-10-2017_007 372 (3.239)
1: TOF MS ES+
5.18e+005
268.0610
124.0879
269.0636
279.0936
NO2
O
O
3ae
For Help, press F1

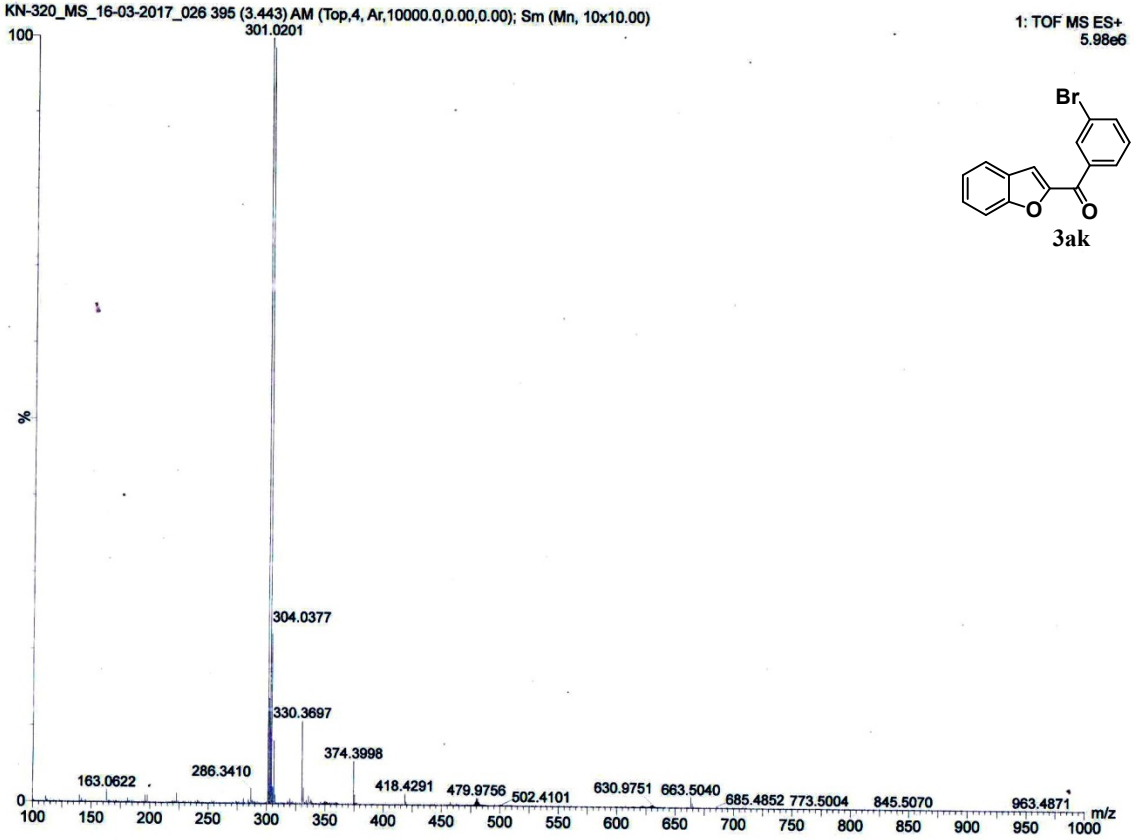

Single Mass Analysis
Tolerance = 2.0 PPM / DBE: min = -1.5, max = 50.0
Element prediction: Off
Number of isotope peaks used for i-FIT = 3
Monoisotopic Mass, Even Electron Ions
285 formula(e) evaluated with 1 results within limits (up to 50 closest results for each mass)
Elements Used:
Mass Calc. Mass mDa PPM DBE Formula i-FIT i-FIT Norm Fit Conf % C H N O
248.0711 248.0712 -0.1 -0.4 12.5 C16 H10 N O2 756.1 n/a n/a 16 10 1 2
KN-324_MS_04-04-2017_006 354 (3.085) AM2 (Ar,30000.0,556.27,0.00,LS 1)
1 TOF MS ES+
3.31e+006
248.0711
249.0746
251.1177
415.2115
431.1783
CN
O
O
3af
For Help, press F1

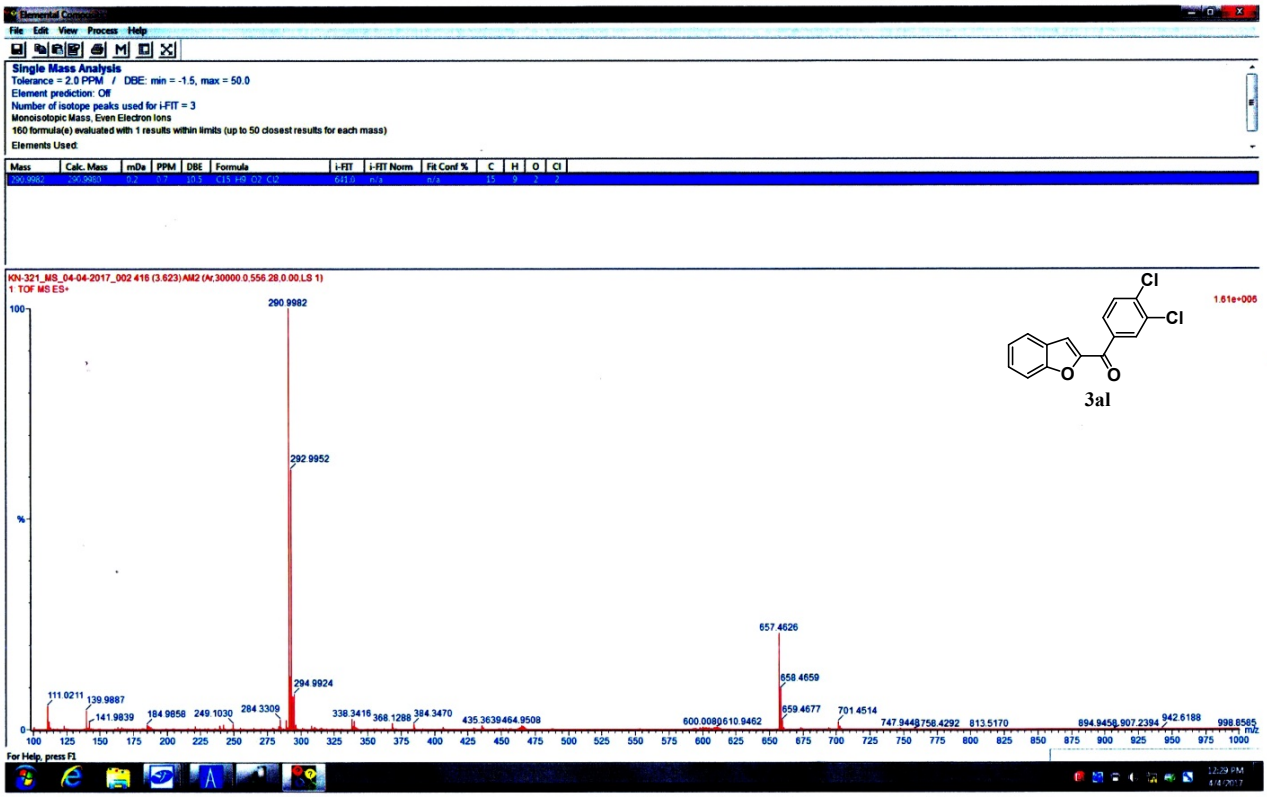

Single Mass Analysis
Tolerance = 5.0 PPM / DBE: min = -1.5, max = 50.0
Element prediction: Off
Number of isotope peaks used for i-FIT = 3
Monoisotopic Mass, Even Electron Ions
52 formula(e) evaluated with 1 results within limits (up to 50 closest results for each mass)
Elements Used:
Mass | Calc. Mass | mDa | PPM | DBE | Formula | i-FIT | i-FIT Norm | Fit Conf % | C | H | O
KN-311-A_MS_16-03-2017_023 406 (3.537) AM2 (Ar,30000 0.556 26.0 00 LS 1)
1: TOF MS ES+
299.1073
300.1098
270.3167
301.1140
330.3347
356.3487
400.3711
476.1065
495.2535
551.3140
607.3728
619.1679
663.4315
664.4346
886.4148
750.4943
763.4880
807.3027
932.7199
961.5097
983.4880
139.9939
152.0679
199.9698
242.2859
For Help, press F1
Ph
O
O
3ag


Single Mass Analysis
Tolerance = 5.0 PPM / DBE: min = -1.5, max = 50.0
Element prediction: Off
Number of isotope peaks used for i-FIT = 3
Monoisotopic Mass, Even Electron Ions
154 formula(e) evaluated with 2 results within limits (up to 50 closest results for each mass)
Elements Used:
Mass | Calc. Mass | mDa | PPM | DBE | Formula | i-FIT | i-FIT Norm | Fit Conf % | C | H | O | F
241.0676 | -0.9 | -3.7 | 6.5 | C12 H11 O3 F2 | 1303.3 | 1.199 | 30.15 | 12 | 11 | 3 | 2
KN-315_MS_16-03-2017_025 372 (3.239) AM2 (Ar,30000 0.556 25.0 00 LS 1); Cm (368:383)
1: TOF MS ES+
241.0667
242.0655
243.0678
136.0583
163.0401
181.0647
240.0542
302.2968
346.3194
390.3418
415.1934
447.0423
500.0731
512.4770
561.4204
637.0744
663.4122
685.3871
817.4978
845.5280
867.5062
For Help, press F1
F
O
O
3ah


Single Mass Analysis
Tolerance = 5.0 PPM / DBE: min = -1.5, max = 50.0
Element prediction: Off
Number of isotope peaks used for i-FIT = 3
Monoisotopic Mass, Even Electron Ions
136 formula(e) evaluated with 1 results within limits (up to 50 closest results for each mass)
Elements Used:
Mass
Calc. Mass
mDa
PPM
DBE
Formula
i-FIT
i-FIT Norm
Fit Conf %
C
H
O
Cl
KN-319_MS_16-03-2017_021 387 (3.374)AM2 (Ar,30000.0,556 26.0 00 LS 1)
1: TOF MS ES+
6.93e+006
257.0365
259.0334
260.0364
139.9928
163.0430
233.1081
302.3024
338.3360
374.2250
431.1671
447.0511
512.4868
533.0197
579.3370
591.4776
663.4233
685.3678
729.4109
761.4753
796.5109
845.5378
867.5279
935.5997
957.3643
974.4921
m/z
For Help, press F1
Cl
O
O
3ai

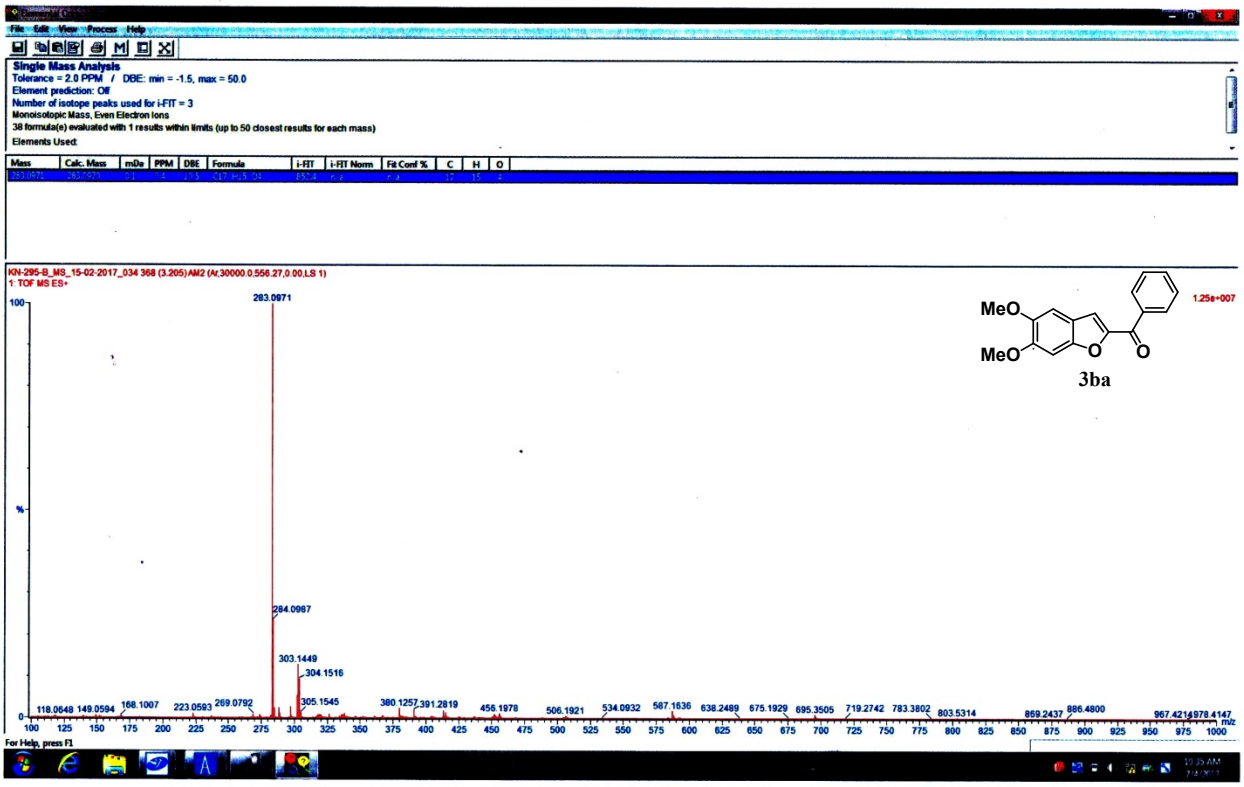

KN-317_MS_31-05-2017_015 413 (3.597) Cm (389:413)
1: TOF MS ES+
1.96e7
301.0193
292.0489
338.3817
431.2293
209.1180
339.3837
%
m/z
Br
O
O
3aj

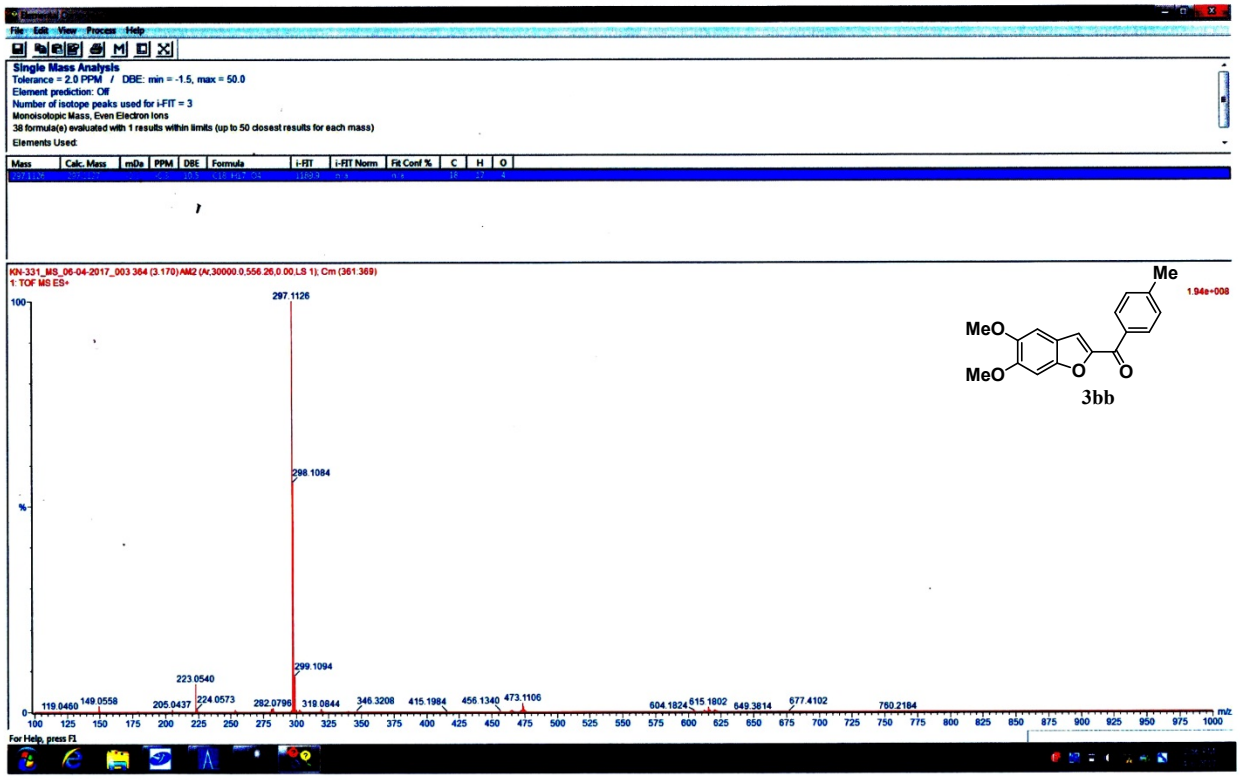

KN-320_MS_16-03-2017_026 395 (3.443) AM (Top,4, Ar,10000.0,0.00,0.00); Sm (Mn, 10x10.00)
1: TOF MS ES+
5.98e6
301.0201
304.0377
330.3697
374.3998
286.3410
163.0622
418.4291
479.9756
502.4101
630.9751
663.5040
685.4852
773.5004
845.5070
963.4871
m/z
Br
O
O
3ak

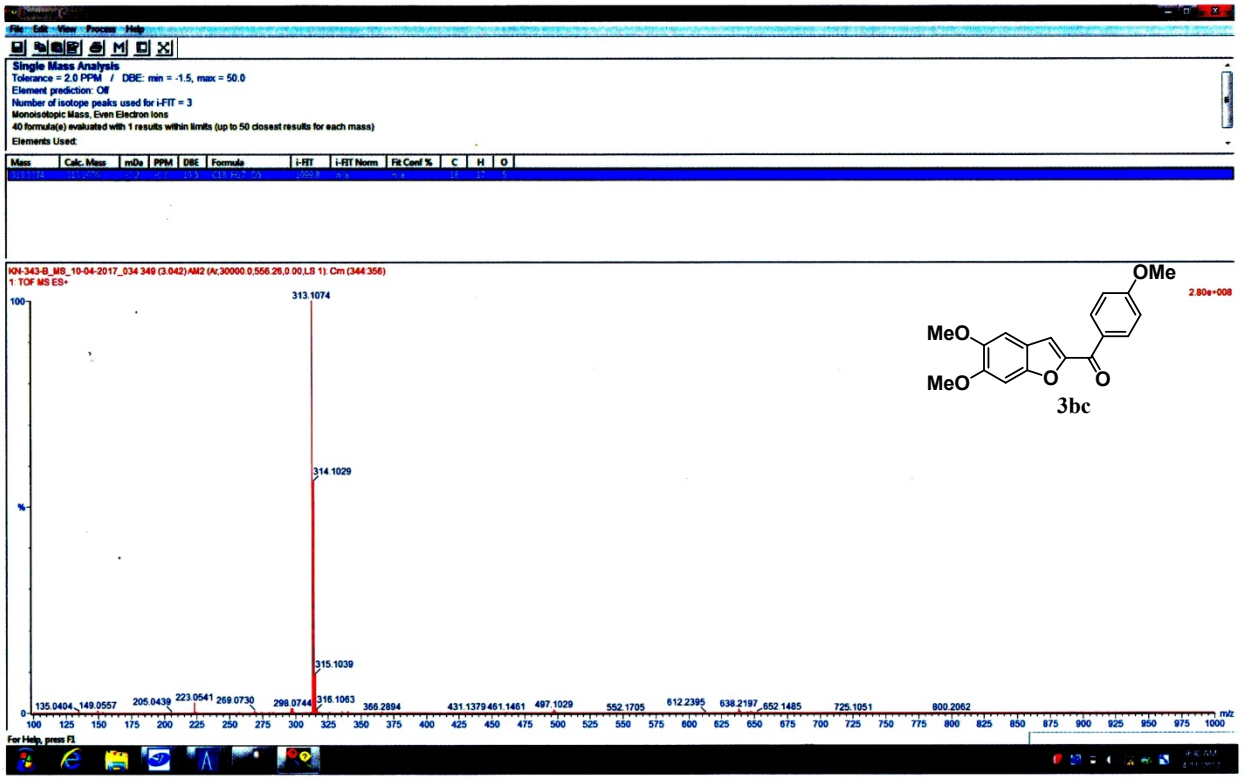

Single Mass Analysis
Tolerance = 2.0 PPM / DBE: min = -1.5, max = 50.0
Element prediction: Off
Number of isotope peaks used for i-FIT = 3
Monoisotopic Mass, Even Electron Ions
160 formula(e) evaluated with 1 results within limits (up to 50 closest results for each mass)
Elements Used:
KN-321_MS_04-04-2017_002 416 (3.623) AM2 (Ar,30000.0,556.28,0.00,LS 1)
1: TOF MS ES+
1.61e+006
290.9982
292.9952
294.9924
657.4626
658.4659
659.4677
701.4514
111.0211
139.9887
141.9839
184.9858
249.1030
284.3309
338.3416
368.1288
384.3470
435.3639
464.9508
600.0080
610.9462
747.9448
758.4292
813.5170
894.9458
907.2394
942.6188
998.8565
m/z
Cl
Cl
O
O
3al

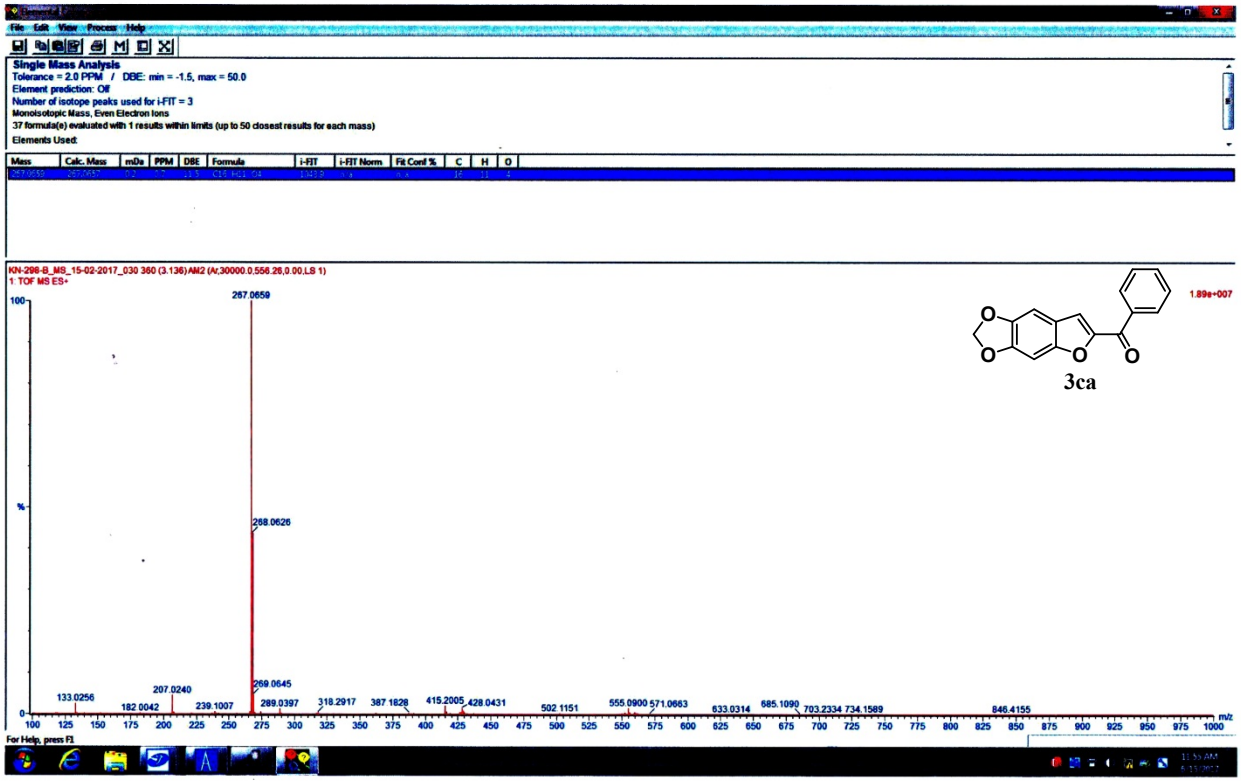

File Edit View Process Help
Single Mass Analysis
Tolerance = 5.0 PPM / DBE: min = -1.5, max = 50.0
Element prediction: Off
Number of isotope peaks used for i-FIT = 3
Monoisotopic Mass, Even Electron Ions
44 formula(e) evaluated with 1 results within limits (up to 50 closest results for each mass)
Elements Used:
Mass Calc. Mass mDa PPM DBE Formula i-FIT i-FIT Norm Fit Conf % C H O
KN-313_MS_16-03-2017_027 398 (3.468) AM2 (Ar,30000,0.556,25.0,00,LS 1)
1: TOF MS ES+
273.0914
274.0916
163.0421
145.0322
168.0835
272.0801
275.0943
330.3297
356.3435
374.3527
400.3649
437.0789
439.5789
484.4589
556.6372
567.1329
583.1024
628.0706
663.4225
700.6555
839.1915
935.4789
1.42e+007
O
O
3am
For Help, press F1

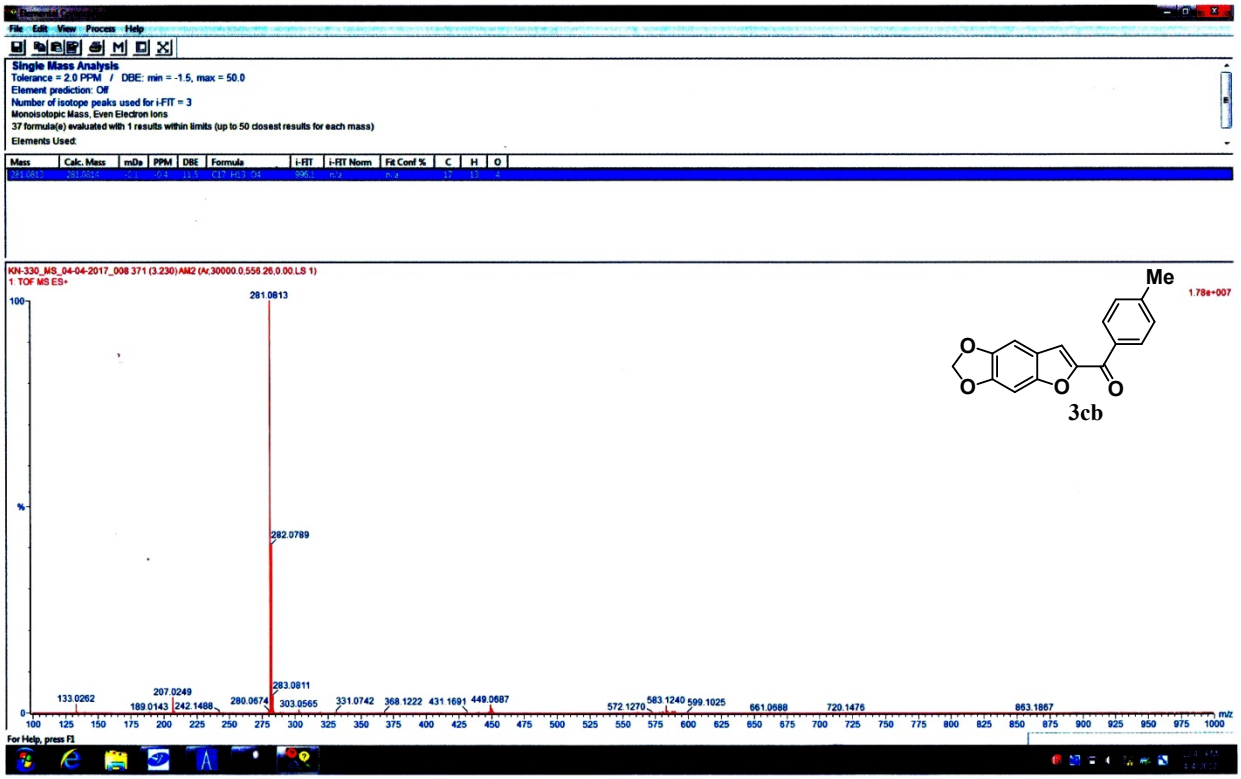

File Edit View Process Help
Single Mass Analysis
Tolerance = 2.0 PPM / DBE: min = -1.5, max = 50.0
Element prediction: Off
Number of isotope peaks used for i-FIT = 3
Monoisotopic Mass, Even Electron Ions
41 formula(e) evaluated with 1 results within limits (up to 50 closest results for each mass)
Elements Used:
Mass Calc. Mass mDa PPM DBE Formula i-FIT i-FIT Norm Fit Conf % C H O
KN-323_MS_04-04-2017_004 389 (3.391) AM2 (Ar,30000,0.556,27.0,00,LS 1)
1: TOF MS ES+
303.1022
304.1041
305.1068
139.9877
163.0387
203.9707
249.1011
302.0927
330.3352
368.1276
431.1767
482.1075
503.6050
588.1180
627.1748
643.1489
715.3586
775.7111
929.2612
965.5564
1.22e+007
OMe
O
O
3an
For Help, press F1

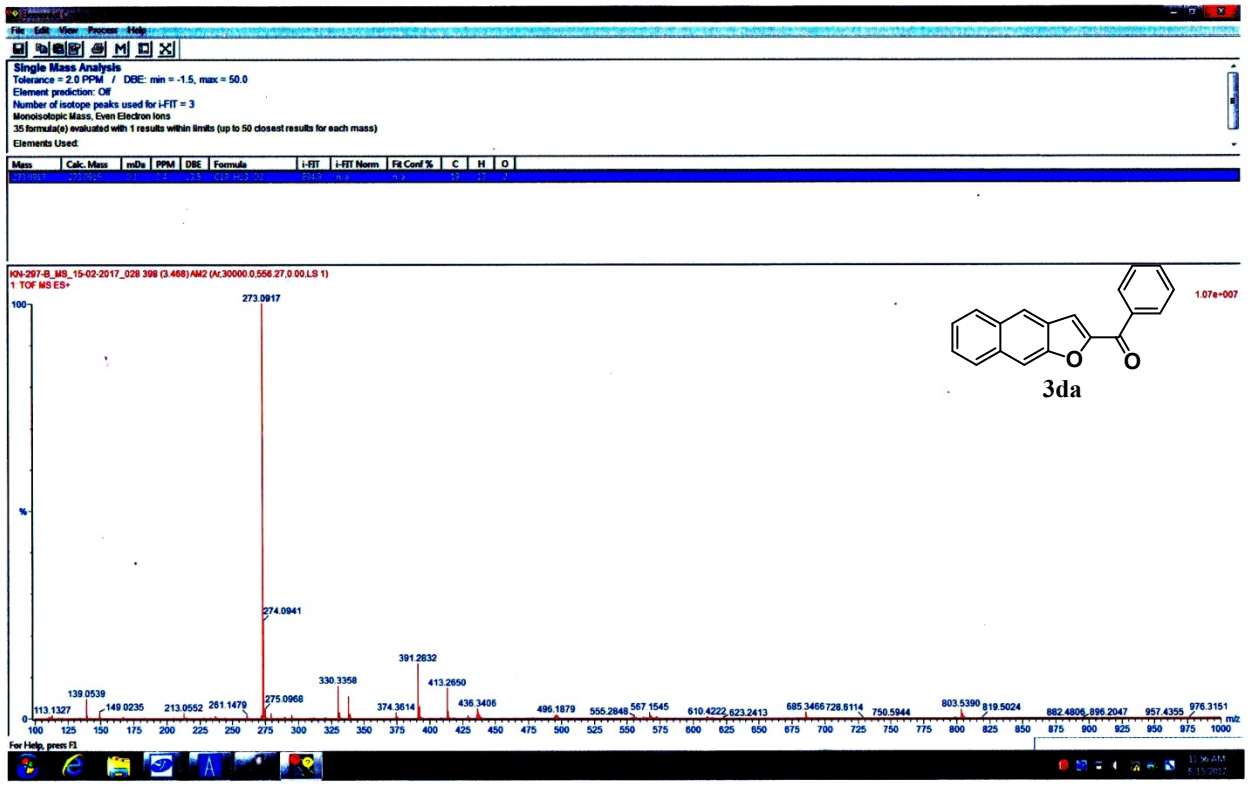

File Edit View Process Help
Single Mass Analysis
Tolerance = 2.0 PPM / DBE: min = -1.5, max = 50.0
Element prediction: Off
Number of isotope peaks used for i-FIT = 3
Monoisotopic Mass, Even Electron Ions
38 formula(e) evaluated with 1 results within limits (up to 50 closest results for each mass)
Elements Used:
Mass Calc. Mass mDa PPM DBE Formula i-FIT i-FIT Norm Fit Conf % C H O
KN-295-B_MS_15-02-2017_034 368 (3.205) AM2 (Ar,30000.0,556.27,0.00,LS 1)
1: TOF MS ES+
283.0971
284.0987
303.1449
304.1516
305.1545
1.25e+007
MeO
MeO
O
O
3ba
For Help, press F1


File Edit View Process Help
Single Mass Analysis
Tolerance = 2.0 PPM / DBE: min = -1.5, max = 50.0
Element prediction: Off
Number of isotope peaks used for i-FIT = 3
Monoisotopic Mass, Even Electron Ions
38 formula(e) evaluated with 1 results within limits (up to 50 closest results for each mass)
Elements Used:
Mass Calc. Mass mDa PPM DBE Formula i-FIT i-FIT Norm Fit Conf % C H O
KN-331_MS_06-04-2017_003 364 (3.170) AM2 (Ar,30000.0,556.26,0.00,LS 1); Cm (361:369)
1: TOF MS ES+
297.1126
298.1084
299.1094
223.0540
1.94e+008
Me
MeO
MeO
O
O
3bb
For Help, press F1

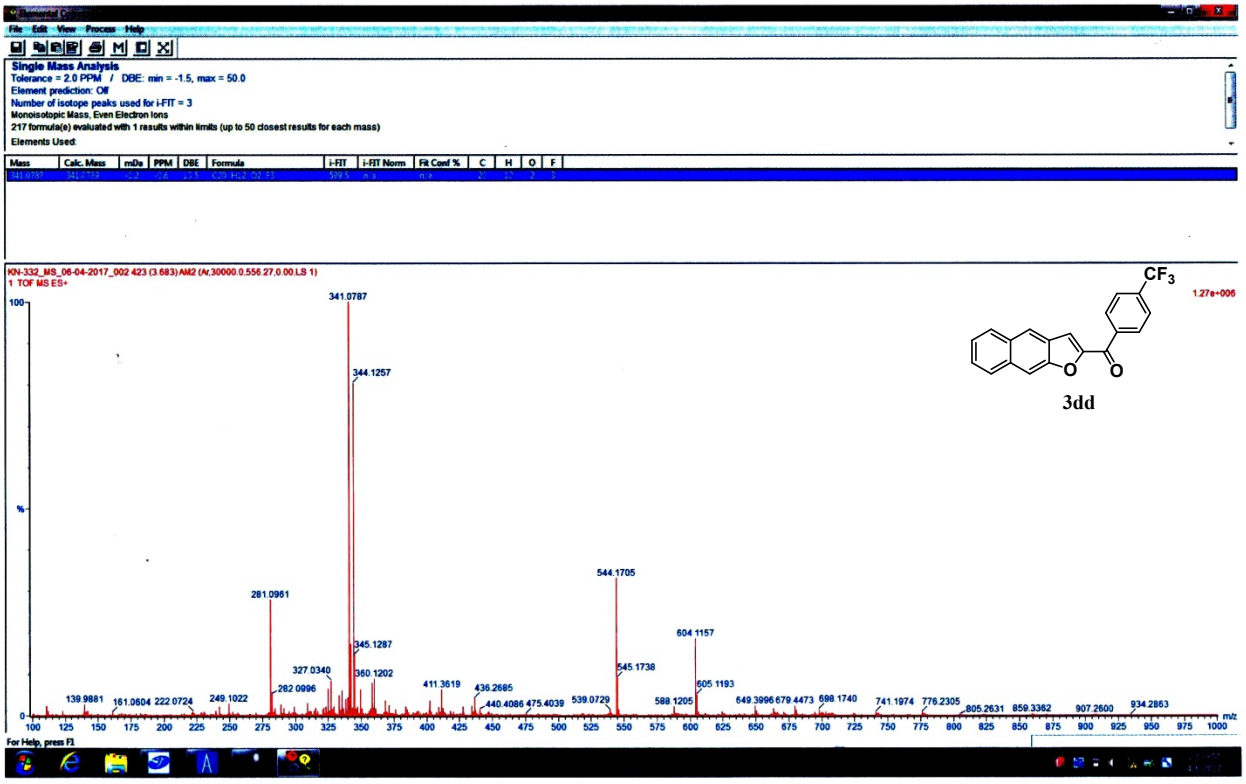

Single Mass Analysis
Tolerance = 2.0 PPM / DBE: min = -1.5, max = 50.0
Element prediction: Off
Number of isotope peaks used for i-FIT = 3
Monoisotopic Mass, Even Electron Ions
40 formula(e) evaluated with 1 results within limits (up to 50 closest results for each mass)
Elements Used:
Mass Calc. Mass mDa PPM DBE Formula i-FIT i-FIT Norm Fit Conf % C H O
KN-343-B_MS_10-04-2017_034 349 (3.042) AM2 (Ar,30000.0,556.26,0.00,LS 1): Cm (344:356)
1: TOF MS ES+
313.1074
314.1029
315.1039
2.80e+008
OMe
MeO
MeO
O
O
3bc
For Help, press F1

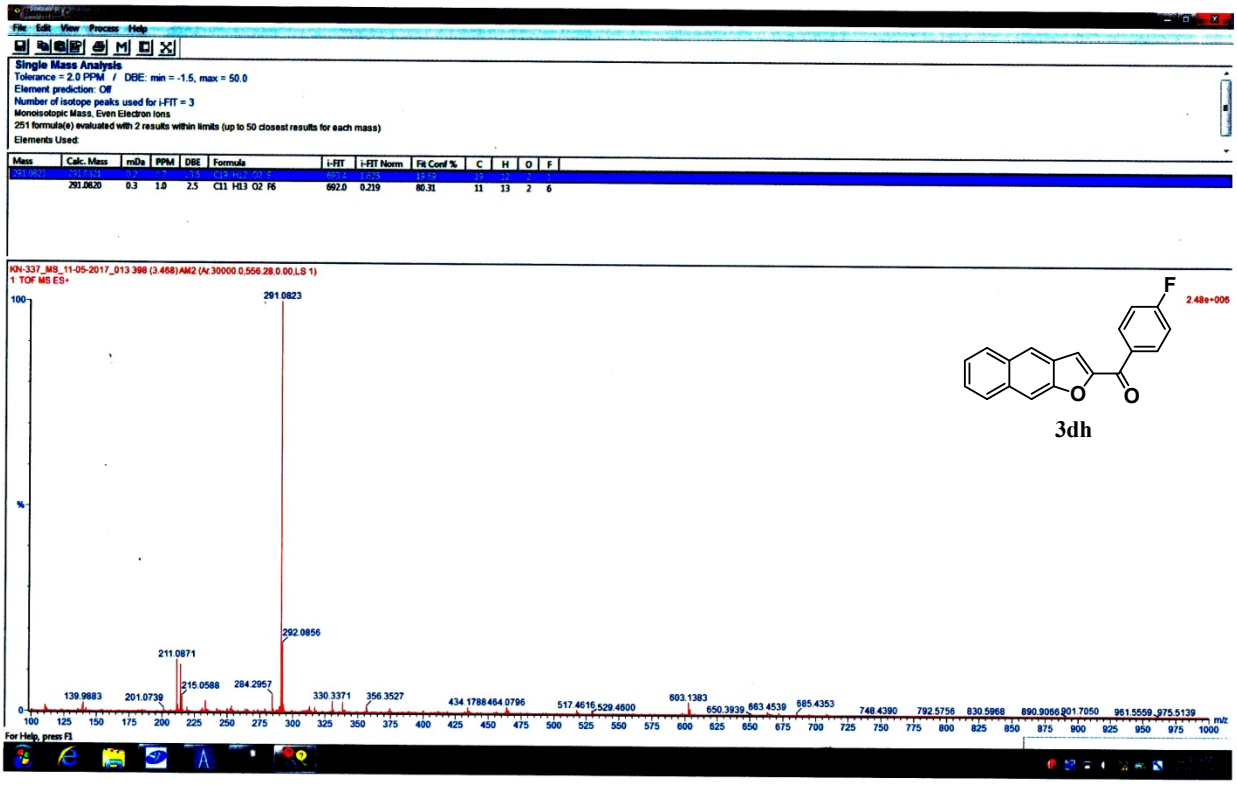

Single Mass Analysis
Tolerance = 2.0 PPM / DBE: min = -1.5, max = 50.0
Element prediction: Off
Number of isotope peaks used for i-FIT = 3
Monoisotopic Mass, Even Electron Ions
37 formula(e) evaluated with 1 results within limits (up to 50 closest results for each mass)
Elements Used:
Mass Calc. Mass mDa PPM DBE Formula i-FIT i-FIT Norm Fit Conf % C H O
KN-298-B_MS_15-02-2017_030 360 (3.136) AM2 (Ar,30000.0,556.26,0.00,LS 1)
1: TOF MS ES+
267.0659
268.0626
269.0645
1.89e+007
O
O
O
O
3ca
For Help, press F1

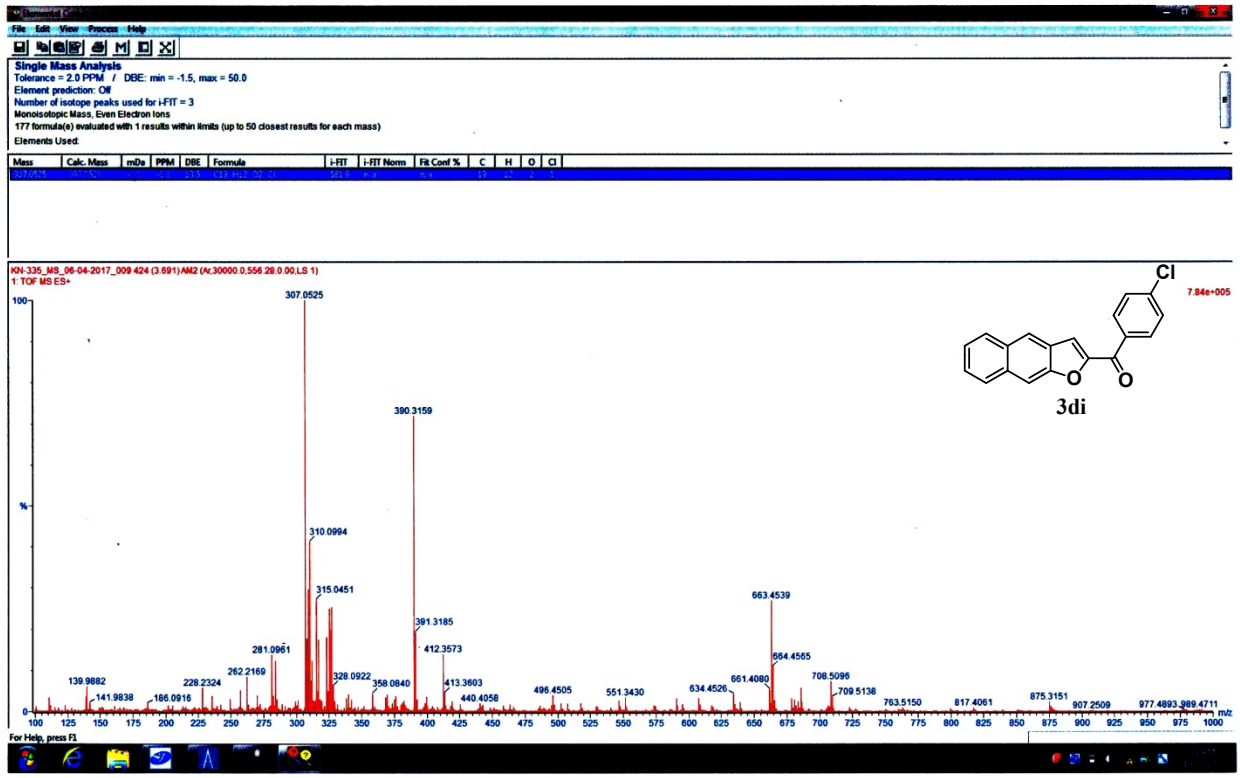

File Edit View Process Help
Single Mass Analysis
Tolerance = 2.0 PPM / DBE: min = -1.5, max = 50.0
Element prediction: Off
Number of isotope peaks used for i-FIT = 3
Monoisotopic Mass, Even Electron Ions
37 formula(e) evaluated with 1 results within limits (up to 50 closest results for each mass)
Elements Used:
Mass Calc. Mass mDa PPM DBE Formula i-FIT i-FIT Norm Fit Conf % C H O
KN-330_MS_04-04-2017_008 371 (3.230) AM2 (Ar,30000,0.556,26,0.00,LS 1)
1: TOF MS ES+
281.0813
282.0789
283.0811
133.0262
207.0249
189.0143
242.1488
280.0674
303.0565
331.0742
368.1222
431.1691
449.0687
572.1270
583.1240
599.1025
661.0588
720.1476
863.1867
1.78e+007
Me
3cb
For Help, press F1

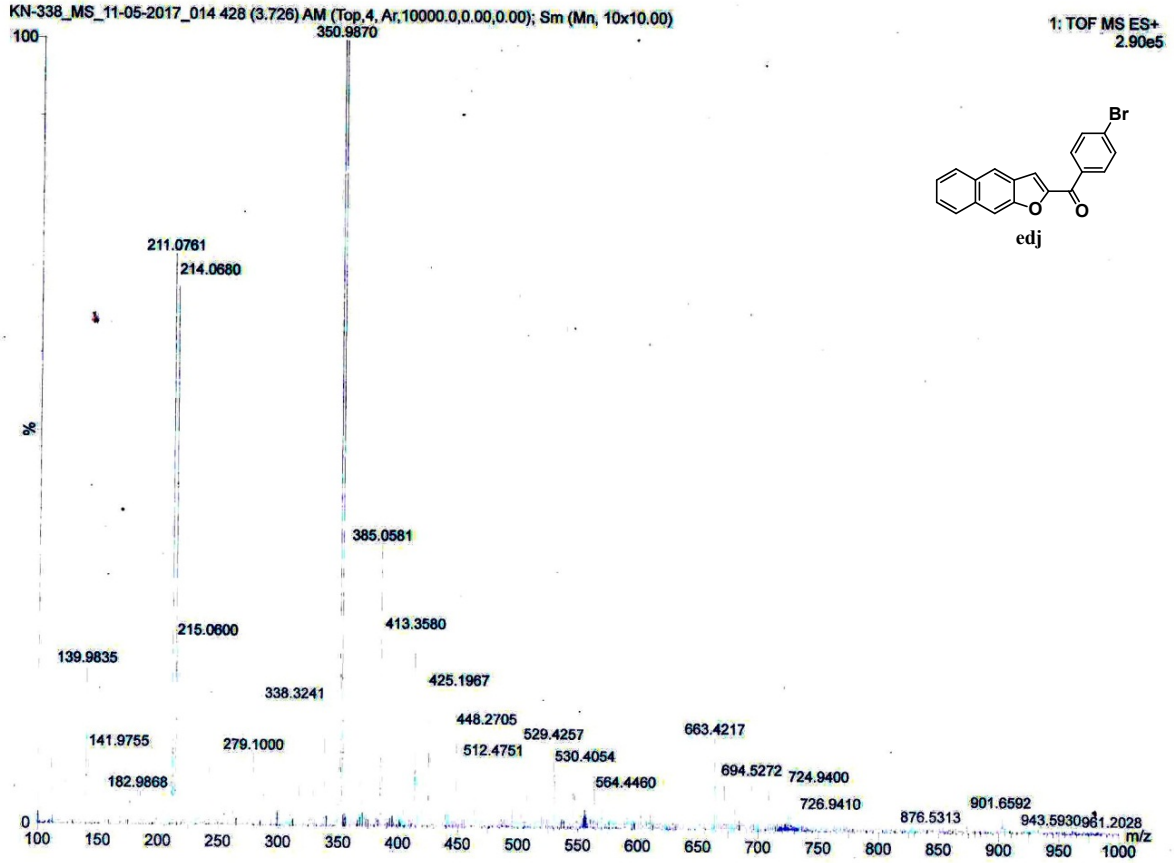

File Edit View Process Help
Single Mass Analysis
Tolerance = 2.0 PPM / DBE: min = -1.5, max = 50.0
Element prediction: Off
Number of isotope peaks used for i-FIT = 3
Monoisotopic Mass, Even Electron Ions
35 formula(e) evaluated with 1 results within limits (up to 50 closest results for each mass)
Elements Used:
Mass Calc. Mass mDa PPM DBE Formula i-FIT i-FIT Norm Fit Conf % C H O
KN-297-B_MS_15-02-2017_028 398 (3.468) AM2 (Ar,30000,0.556,27,0.00,LS 1)
1: TOF MS ES+
273.0917
274.0941
391.2832
413.2650
330.3358
139.0539
149.0235
113.1327
213.0552
261.1479
275.0968
374.3614
436.3406
496.1879
555.2848
567.1545
610.4222
623.2413
685.3466
728.6114
750.5944
803.5390
819.5024
882.4806
896.2047
957.4355
976.3151
1.07e+007
3da
For Help, press F1

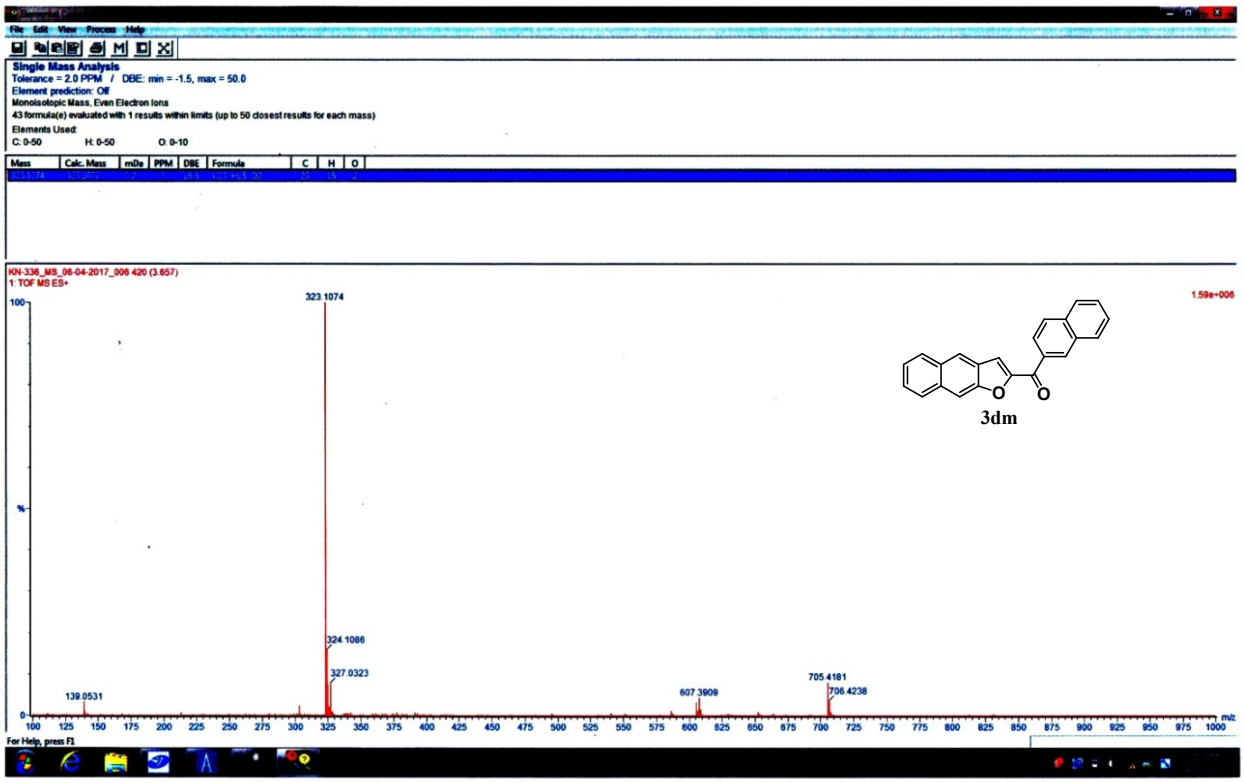

File Edit View Process Help
Single Mass Analysis
Tolerance = 2.0 PPM / DBE: min = -1.5, max = 50.0
Element prediction: Off
Number of isotope peaks used for i-FIT = 3
Monoisotopic Mass, Even Electron Ions
41 formula(e) evaluated with 1 results within limits (up to 50 closest results for each mass)
Elements Used:
Mass Calc. Mass mDa PPM DBE Formula i-FIT i-FIT Norm Fit Conf % C H O
KN-325_MS_06-04-2017_005 406 (3.537) AM2 (Ar,30000.0,556.27,0.00,LS 1)
1: TOF MS ES+
1.49e+007
303.1022
304.1022
OMe
O
O
3dc
For Help, press F1

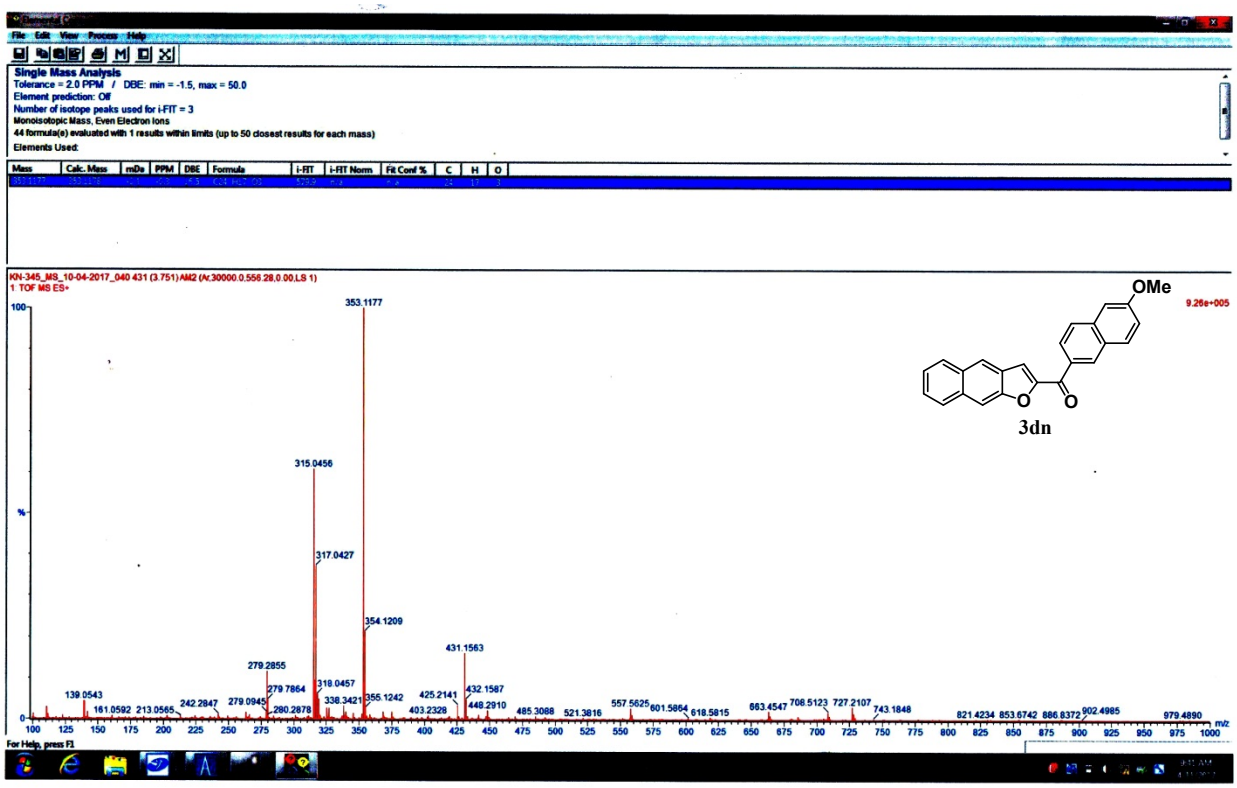

File Edit View Process Help
Single Mass Analysis
Tolerance = 2.0 PPM / DBE: min = -1.5, max = 50.0
Element prediction: Off
Number of isotope peaks used for i-FIT = 3
Monoisotopic Mass, Even Electron Ions
217 formula(e) evaluated with 1 results within limits (up to 50 closest results for each mass)
Elements Used:
Mass Calc. Mass mDa PPM DBE Formula i-FIT i-FIT Norm Fit Conf % C H O F
KN-332_MS_06-04-2017_002 423 (3.683) AM2 (Ar,30000.0,556.27,0.00,LS 1)
1: TOF MS ES+
1.27e+006
341.0787
344.1257
281.0961
345.1287
327.0340
360.1202
282.0996
544.1705
545.1738
604.1157
605.1193
CF3
O
O
3dd
For Help, press F1

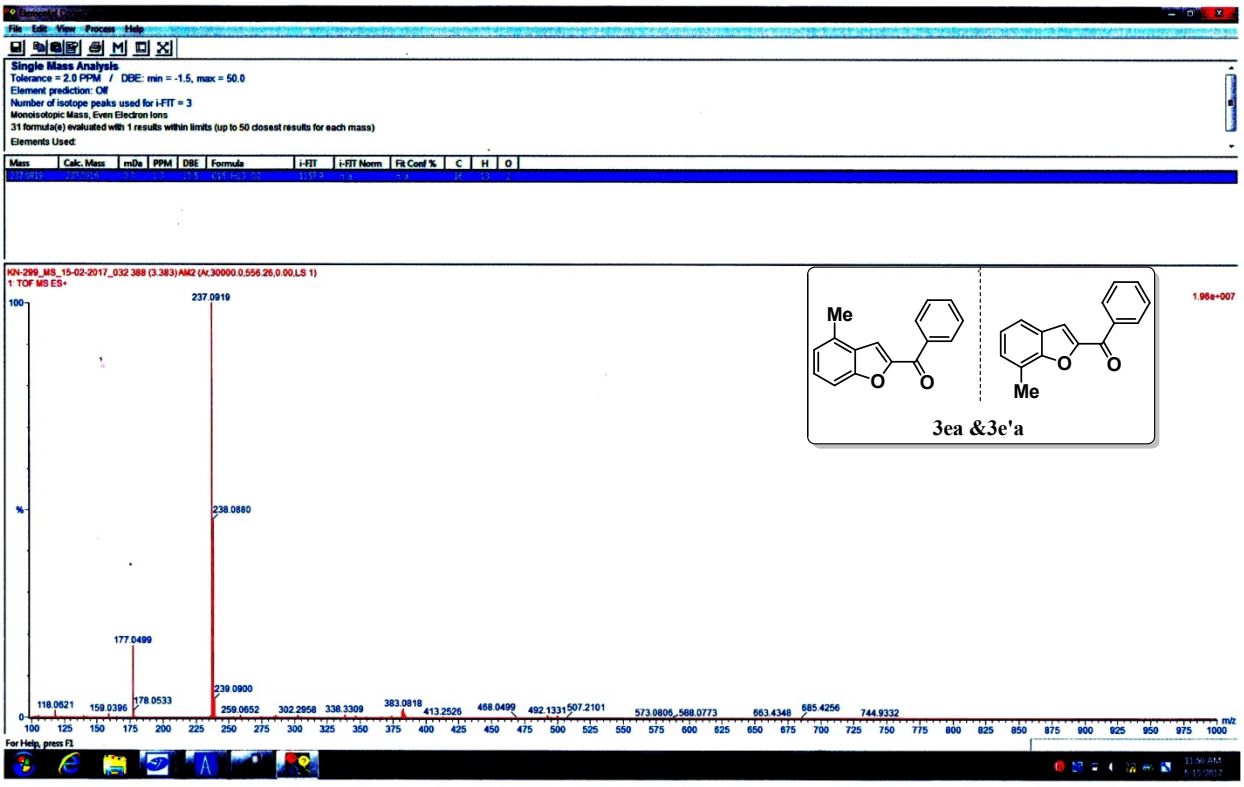

Single Mass Analysis
Tolerance = 2.0 PPM / DBE: min = -1.5, max = 50.0
Element prediction: Off
Number of isotope peaks used for i-FIT = 3
Monoisotopic Mass, Even Electron Ions
251 formula(e) evaluated with 2 results within limits (up to 50 closest results for each mass)
Elements Used:
Mass Calc. Mass mDa PPM DBE Formula i-FIT i-FIT Norm Fit Conf % C H O F
291.0820 0.3 1.0 2.5 C11 H13 O2 F6 692.0 0.219 80.31 11 13 2 6
291.0823
292.0856
211.0871
139.9883
201.0739
215.0588
284.2957
330.3371
356.3527
434.1788 464.0796
517.4616 529.4600
603.1383
650.3939 663.4539
685.4353
748.4390
792.5756
830.5968
890.9066 901.7050
961.5559 975.5139
F
O
O
3dh

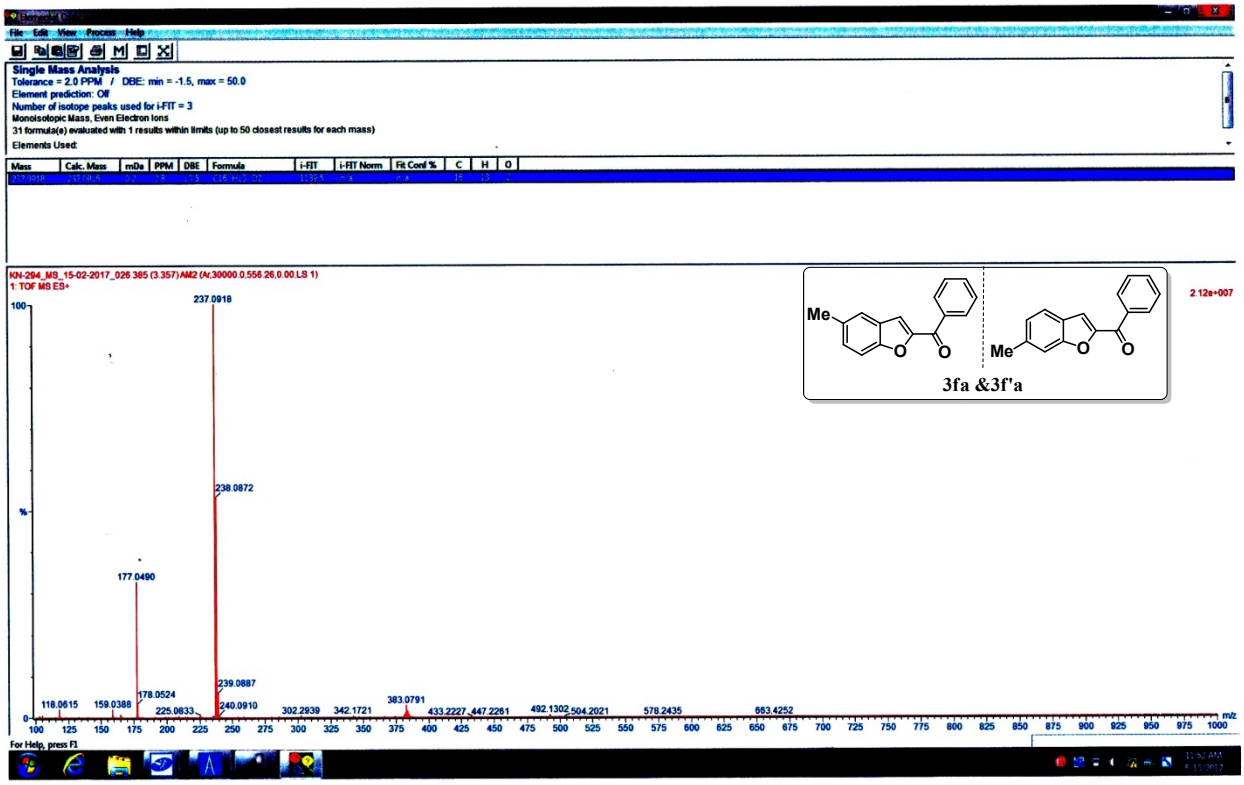

Single Mass Analysis
Tolerance = 2.0 PPM / DBE: min = -1.5, max = 50.0
Element prediction: Off
Number of isotope peaks used for i-FIT = 3
Monoisotopic Mass, Even Electron Ions
177 formula(e) evaluated with 1 results within limits (up to 50 closest results for each mass)
Elements Used:
Mass Calc. Mass mDa PPM DBE Formula i-FIT i-FIT Norm Fit Conf % C H O Cl
307.0525
390.3159
310.0994
315.0451
391.3185
412.3573
281.0961
262.2169
139.9882
141.9838
186.0916
228.2324
328.0922
358.0840
413.3603
440.4058
496.4505
551.3430
634.4526
661.4080
663.4539
664.4565
708.5096
709.5138
763.5150
817.4061
875.3151
907.2509
977.4893 989.4711
Cl
O
O
3di

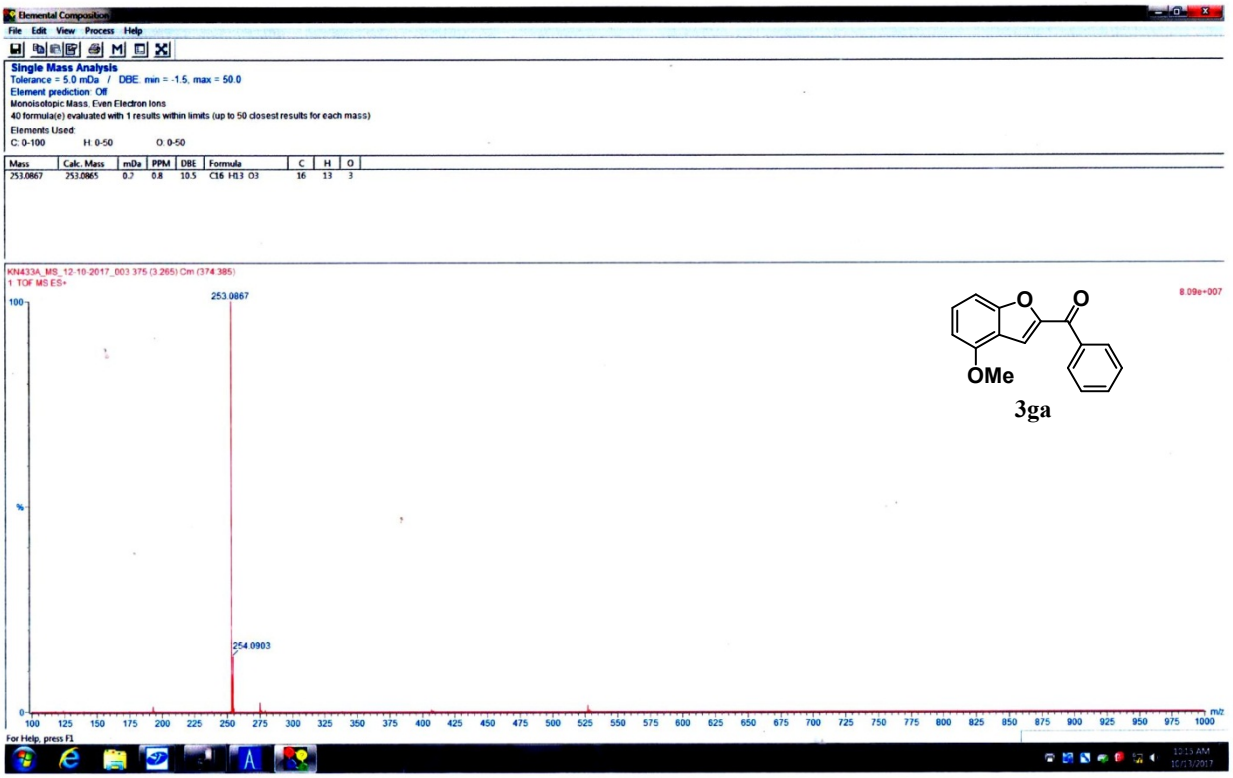

KN-338_MS_11-05-2017_014 428 (3.726) AM (Top,4, Ar,10000.0,0.00,0.00); Sm (Mn, 10x10.00)
1: TOF MS ES+
2.90e5
350.9870
211.0761
214.0680
385.0581
215.0600
413.3580
139.9835
425.1967
338.3241
448.2705
529.4257
663.4217
141.9755
279.1000
512.4751
530.4054
694.5272
724.9400
182.9868
564.4460
726.9410
901.6592
876.5313
943.5930
961.2028
m/z
Br
O
O
edj

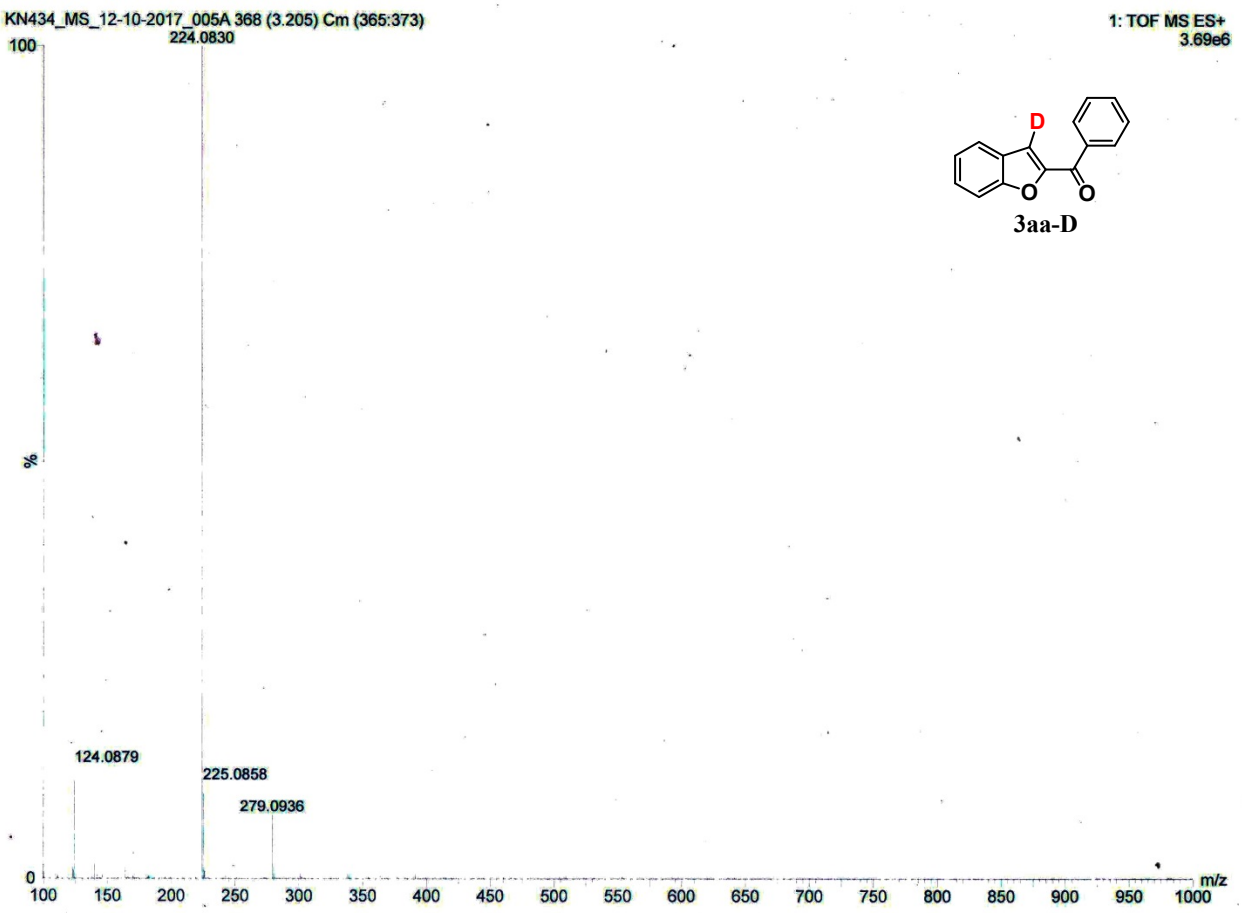

Single Mass Analysis
Tolerance = 2.0 PPM / DBE: min = -1.5, max = 50.0
Element prediction: Off
Monoisotopic Mass, Even Electron Ions
43 formula(e) evaluated with 1 results within limits (up to 50 closest results for each mass)
Elements Used:
C: 0-50 H: 0-50 O: 0-10
Mass
Calc. Mass
mDa
PPM
DBE
Formula
C
H
O
KN-336_MS_06-04-2017_006 420 (3.657)
1: TOF MS ES+
1.59e+006
323.1074
324.1086
327.0323
139.0531
607.3909
705.4181
706.4238
3dm
For Help, press F1


Single Mass Analysis
Tolerance = 2.0 PPM / DBE: min = -1.5, max = 50.0
Element prediction: Off
Number of isotope peaks used for i-FIT = 3
Monoisotopic Mass, Even Electron Ions
44 formula(e) evaluated with 1 results within limits (up to 50 closest results for each mass)
Elements Used:
KN-345_MS_10-04-2017_040 431 (3.751) AM2 (Ar,30000.0,556.28,0.00,LS 1)
1: TOF MS ES+
353.1177
315.0456
317.0427
354.1209
431.1563
OMe
3dn


Single Mass Analysis
Tolerance = 2.0 PPM / DBE: min = -1.5, max = 50.0
Element prediction: Off
Number of isotope peaks used for i-FIT = 3
Monoisotopic Mass, Even Electron Ions
31 formula(e) evaluated with 1 results within limits (up to 50 closest results for each mass)
Elements Used:
KN-299_MS_15-02-2017_032 388 (3.383) AM2 (Ar,30000.0,556.26,0.00,LS 1)
1: TOF MS ES+
237.0919
238.0880
177.0499
239.0900
Me
Me
3ea &3e'a

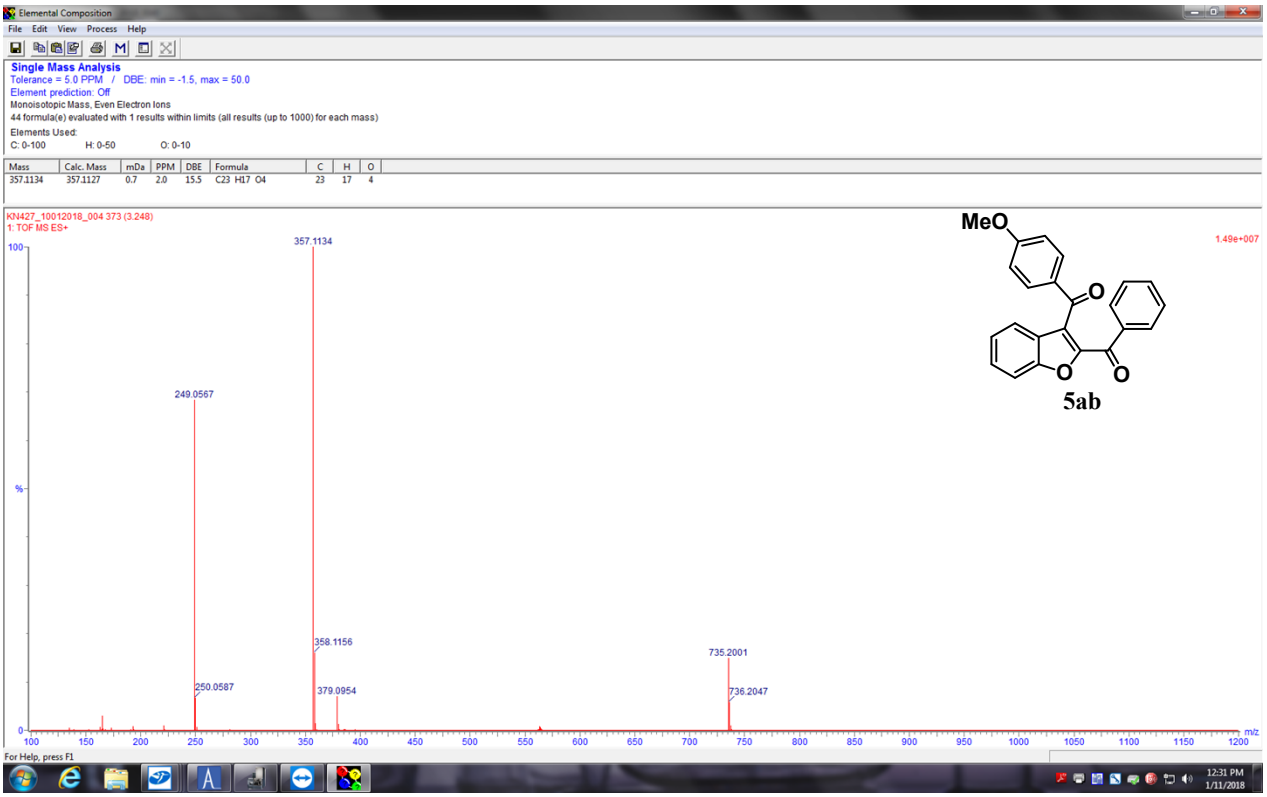

Single Mass Analysis
Tolerance = 2.0 PPM / DBE: min = -1.5, max = 50.0
Element prediction: Off
Number of isotope peaks used for i-FIT = 3
Monoisotopic Mass, Even Electron Ions
31 formula(e) evaluated with 1 results within limits (up to 50 closest results for each mass)
Elements Used:
Mass | Calc. Mass | mDa | PPM | DBE | Formula | i-FIT | i-FIT Norm | Fit Conf % | C | H | O
KN-294_MS_15-02-2017_026 385 (3.357) AM2 (Ar,30000,0.556,26.0,00,LS 1)
1: TOF MS ES+
237.0918
238.0872
177.0490
239.0887
118.0615
159.0388
178.0524
225.0833
240.0910
302.2939
342.1721
383.0791
433.2227
447.2261
492.1302
504.2021
578.2435
663.4252
2.12e+007
Me
Me
3fa &3f'a
For Help, press F1

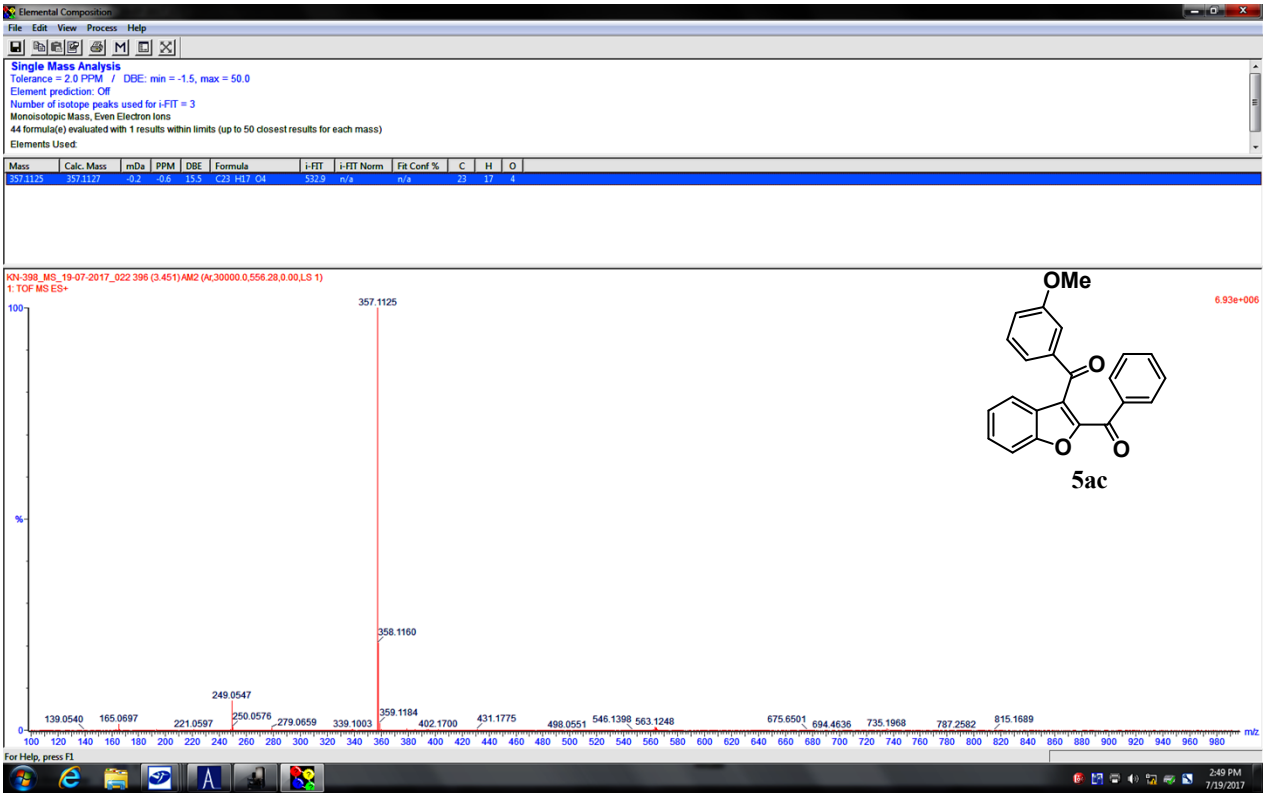

Elemental Composition
Single Mass Analysis
Tolerance = 5.0 mDa / DBE: min = -1.5, max = 50.0
Element prediction: Off
Monoisotopic Mass, Even Electron Ions
40 formula(e) evaluated with 1 results within limits (up to 50 closest results for each mass)
Elements Used:
C: 0-100 H: 0-50 O: 0-50
Mass | Calc. Mass | mDa | PPM | DBE | Formula | C | H | O
253.0867 | 253.0865 | 0.2 | 0.8 | 10.5 | C16 H13 O3 | 16 | 13 | 3
KN433A_MS_12-10-2017_003 375 (3.265) Cm (374:385)
1: TOF MS ES+
253.0867
254.0903
8.09e+007
OMe
3ga
For Help, press F1

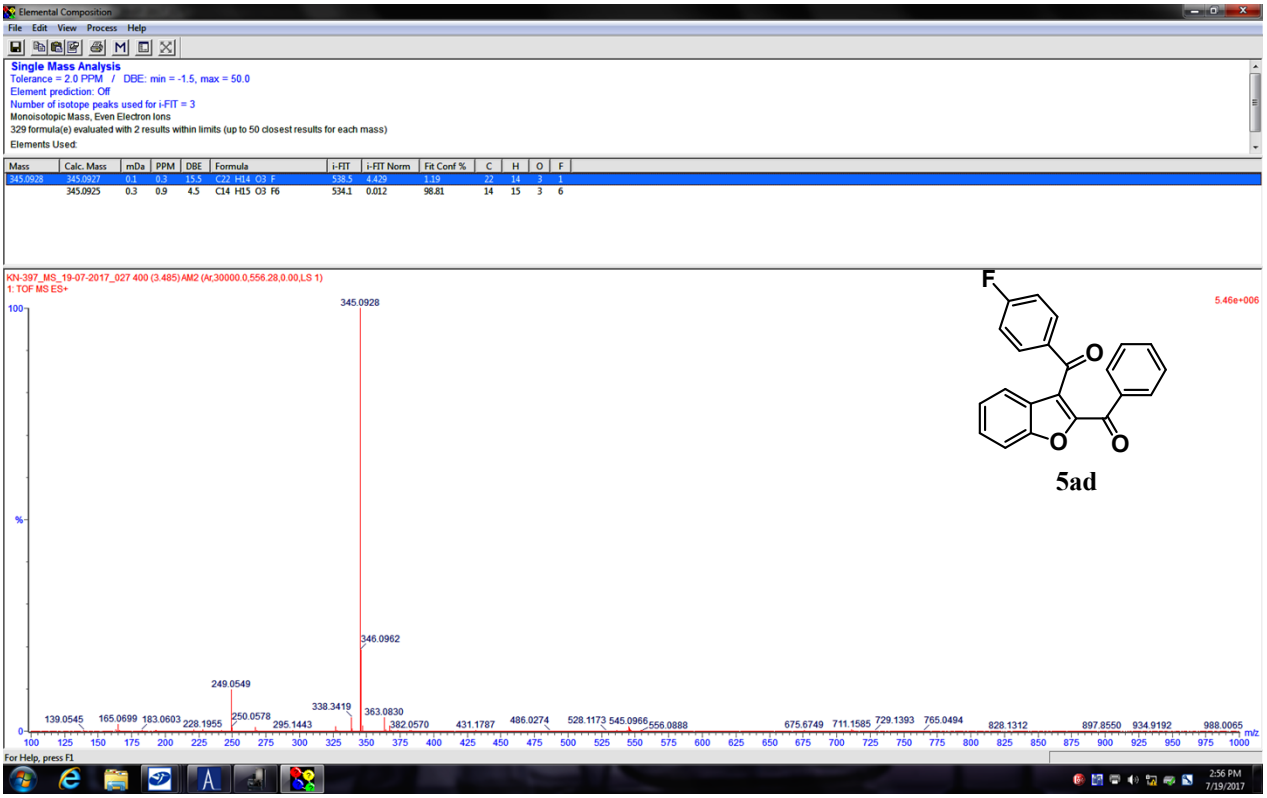

KN434_MS_12-10-2017_005A 368 (3.205) Cm (365:373)
1: TOF MS ES+
3.69e6
100
%
0
224.0830
124.0879
225.0858
279.0936
m/z
100 150 200 250 300 350 400 450 500 550 600 650 700 750 800 850 900 950 1000
D
O
O

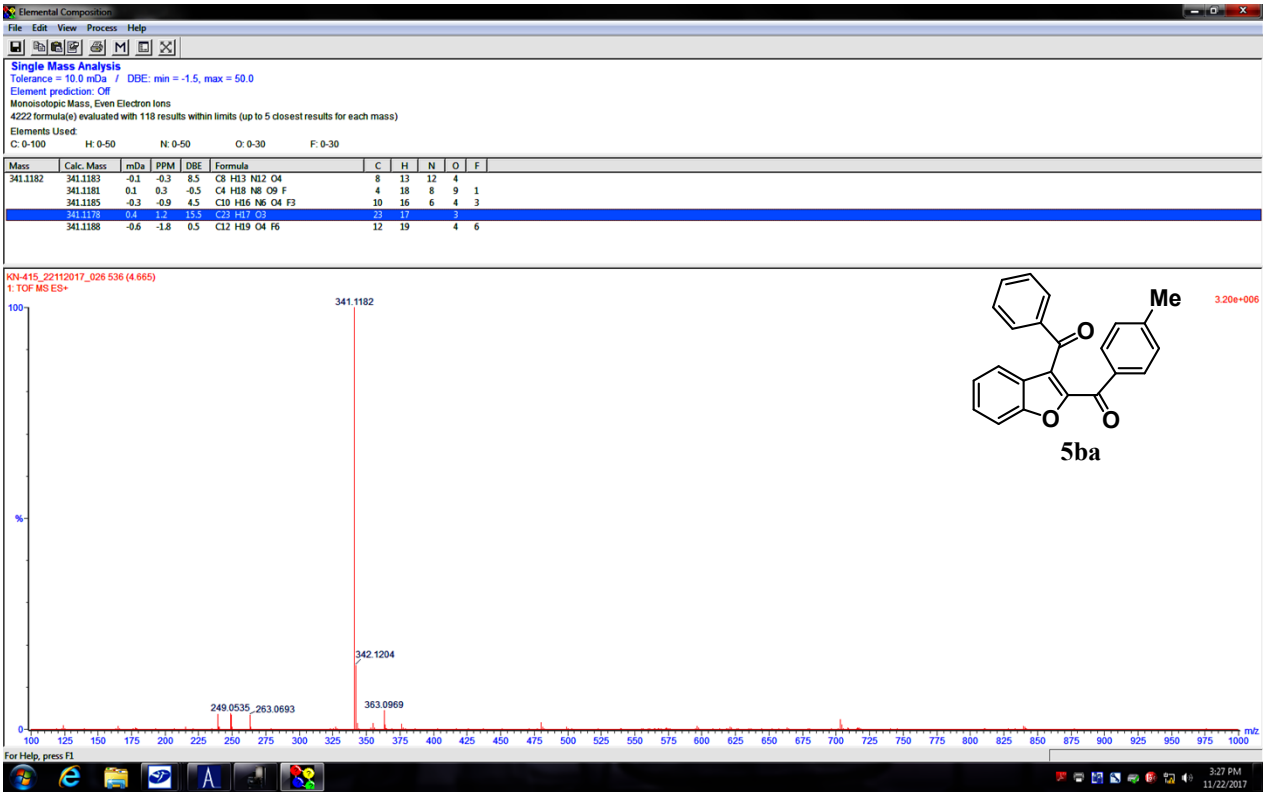
3aa-D

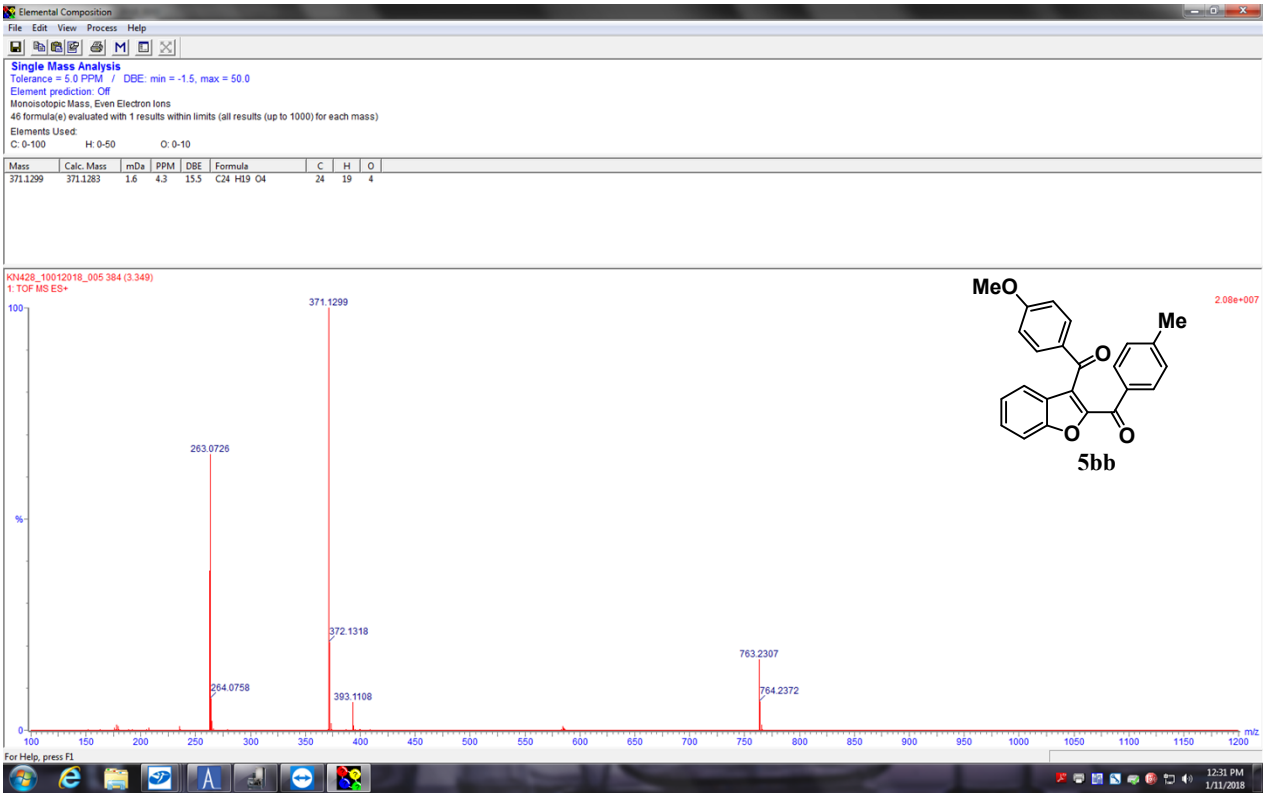

Elemental Composition
File Edit View Process Help
Single Mass Analysis
Tolerance = 2.0 PPM / DBE: min = -1.5, max = 50.0
Element prediction: Off
Number of isotope peaks used for i-FIT = 3
Monoisotopic Mass, Even Electron Ions
43 formula(e) evaluated with 1 results within limits (up to 50 closest results for each mass)
Elements Used:
Mass | Calc. Mass | mDa | PPM | DBE | Formula | i-FIT | i-FIT Norm | Fit Conf % | C | H | O
327.1022 | 327.1021 | 0.1 | 0.3 | 15.5 | C22 H15 O3 | 608.6 | n/a | n/a | 22 | 15 | 3
KN-379_MS_19-07-2017_021 394 (3.434) AM2 (Ar,30000.0,556.28,0.00,LS 1)
1: TOF MS ES+
8.78e+006
327.1022
328.1053
249.0549
139.0544
165.0699
221.0595
250.0581
309.0906
329.1075
364.0660
431.1780
501.1346
518.1094
605.0815
653.1936
675.1777
691.1345
755.1091
801.1322
855.0541
912.1169
930.6547
955.5978
m/z
For Help, press F1
5aa

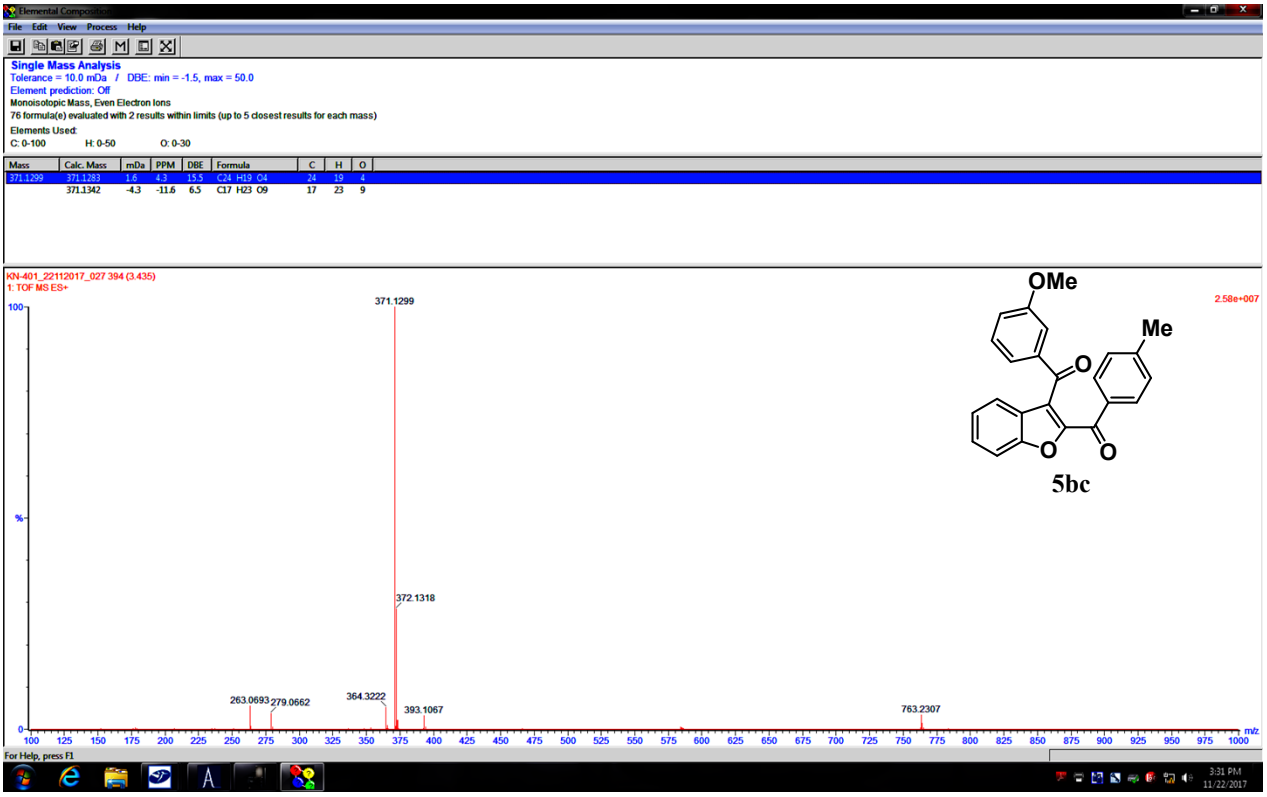

Elemental Composition
File Edit View Process Help
Single Mass Analysis
Tolerance = 5.0 PPM / DBE: min = -1.5, max = 50.0
Element prediction: Off
Monoisotopic Mass, Even Electron Ions
44 formula(e) evaluated with 1 results within limits (all results (up to 1000) for each mass)
Elements Used:
C: 0-100 H: 0-50 O: 0-10
Mass | Calc. Mass | mDa | PPM | DBE | Formula | C | H | O
357.1134 | 357.1127 | 0.7 | 2.0 | 15.5 | C23 H17 O4 | 23 | 17 | 4
KN427_10012018_004 373 (3.248)
1: TOF MS ES+
1.49e+007
357.1134
249.0567
358.1156
250.0587
379.0954
735.2001
736.2047
m/z
For Help, press F1
MeO
5ab

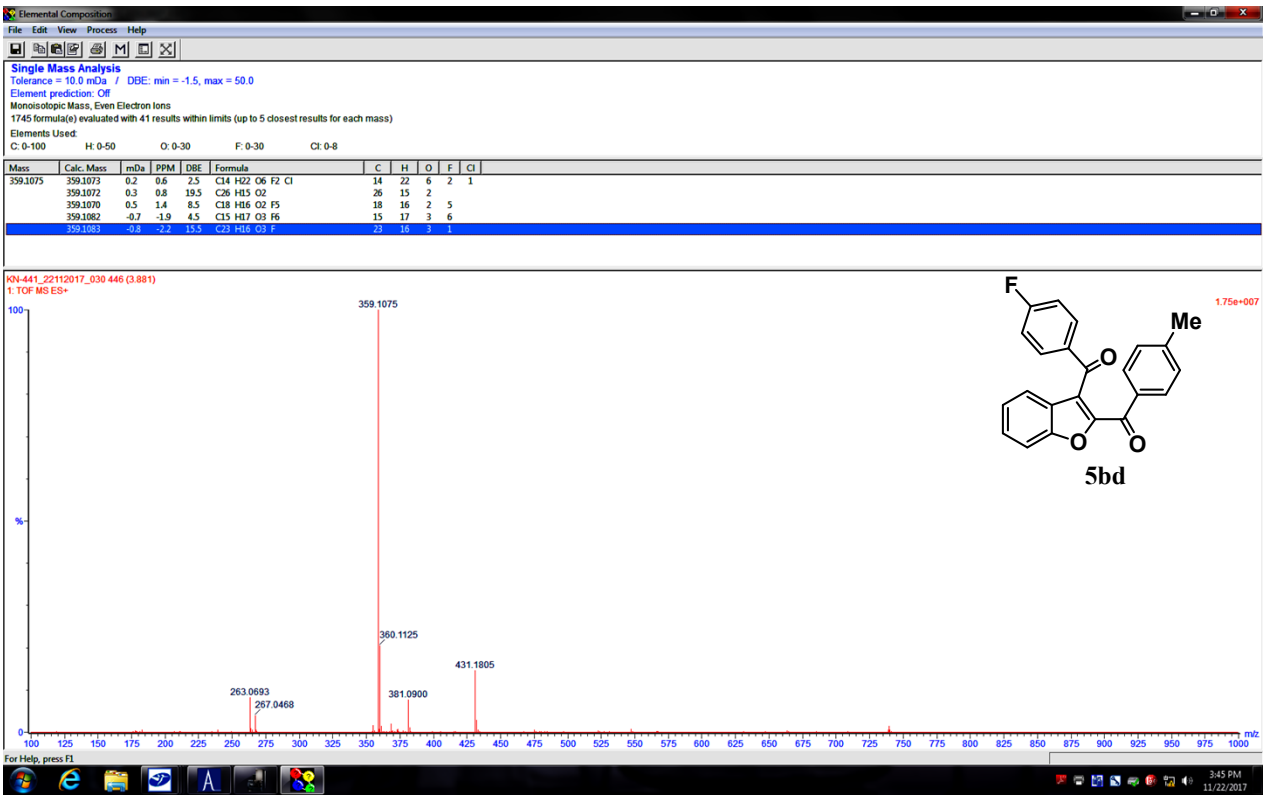

Elemental Composition
File Edit View Process Help
Single Mass Analysis
Tolerance = 2.0 PPM / DBE: min = -1.5, max = 50.0
Element prediction: Off
Number of isotope peaks used for i-FIT = 3
Monoisotopic Mass, Even Electron Ions
44 formula(e) evaluated with 1 results within limits (up to 50 closest results for each mass)
Elements Used:
Mass Calc. Mass mDa PPM DBE Formula i-FIT i-FIT Norm Fit Conf % C H O
357.1125 357.1127 -0.2 -0.6 15.5 C23 H17 O4 532.9 n/a n/a 23 17 4
KN-398_MS_19-07-2017_022 396 (3.451) AM2 (Ar,30000.0,556.28,0.00,LS 1)
1: TOF MS ES+
6.93e+006
357.1125
358.1160
359.1184
249.0547
139.0540
165.0697
221.0597
250.0576
279.0659
339.1003
402.1700
431.1775
498.0551
546.1398
563.1248
675.6501
694.4636
735.1968
787.2582
815.1689
OMe
O
O
O
5ac
For Help, press F1

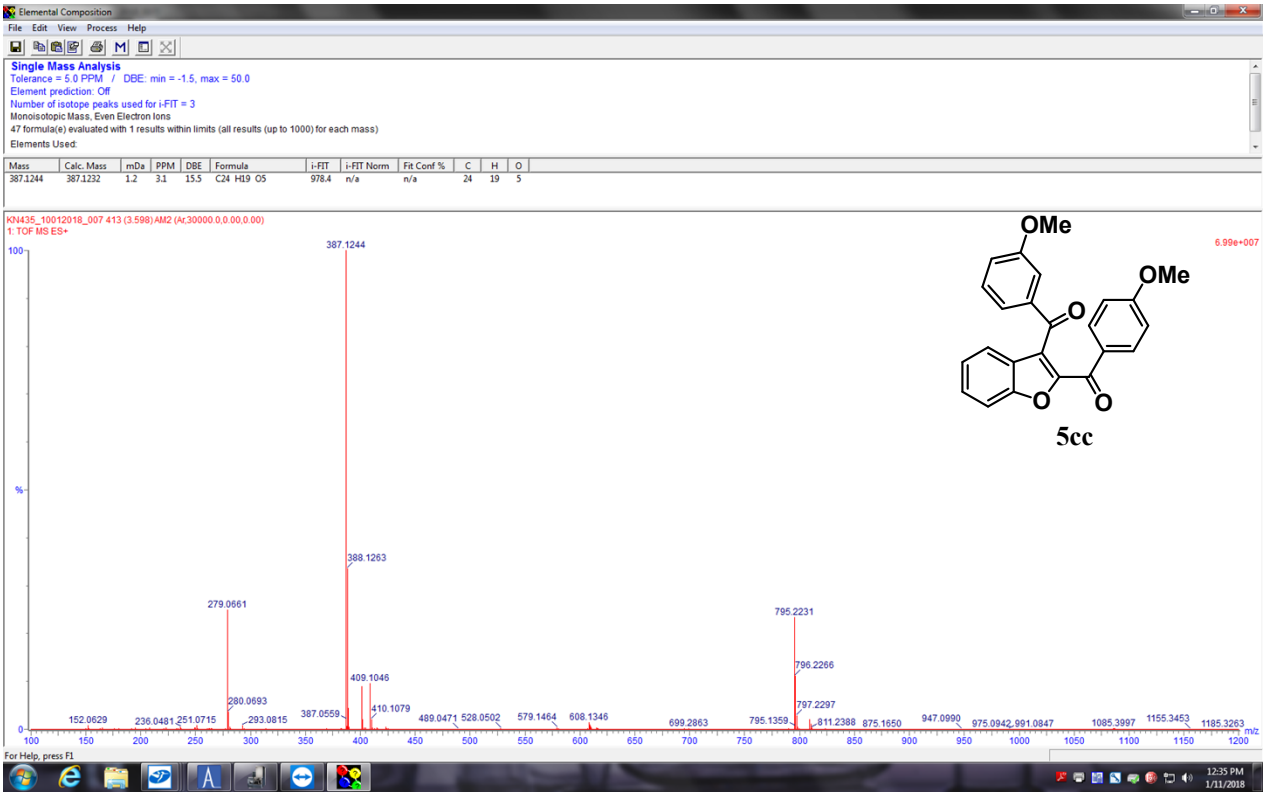

Elemental Composition
File Edit View Process Help
Single Mass Analysis
Tolerance = 2.0 PPM / DBE: min = -1.5, max = 50.0
Element prediction: Off
Number of isotope peaks used for i-FIT = 3
Monoisotopic Mass, Even Electron Ions
329 formula(e) evaluated with 2 results within limits (up to 50 closest results for each mass)
Elements Used:
Mass Calc. Mass mDa PPM DBE Formula i-FIT i-FIT Norm Fit Conf % C H O F
345.0928 345.0927 0.1 0.3 15.5 C22 H14 O3 F 538.5 4.429 1.19 22 14 3 1
345.0925 0.3 0.9 4.5 C14 H15 O3 F6 534.1 0.012 98.81 14 15 3 6
KN-397_MS_19-07-2017_027 400 (3.485) AM2 (Ar,30000.0,556.28,0.00,LS 1)
1: TOF MS ES+
5.46e+006
345.0928
346.0962
249.0549
139.0545
165.0699
183.0603
228.1955
250.0578
295.1443
338.3419
363.0830
382.0570
431.1787
486.0274
528.1173
545.0966
556.0888
675.6749
711.1585
729.1393
765.0494
828.1312
897.8550
934.9192
988.0065
F
O
O
O
5ad
For Help, press F1


Elemental Composition
File Edit View Process Help
Single Mass Analysis
Tolerance = 10.0 mDa / DBE: min = -1.5, max = 50.0
Element prediction: Off
Monoisotopic Mass, Even Electron Ions
4222 formula(e) evaluated with 118 results within limits (up to 5 closest results for each mass)
Elements Used:
C: 0-100 H: 0-50 N: 0-50 O: 0-30 F: 0-30
Mass Calc. Mass mDa PPM DBE Formula C H N O F
341.1182 341.1183 -0.1 -0.3 8.5 C8 H13 N12 O4 8 13 12 4
341.1181 0.1 0.3 -0.5 C4 H18 N8 O9 F 4 18 8 9 1
341.1185 -0.3 -0.9 4.5 C10 H16 N6 O4 F3 10 16 6 4 3
341.1178 0.4 1.2 15.5 C23 H17 O3 23 17 3
341.1188 -0.6 -1.8 0.5 C12 H19 O4 F6 12 19 4 6
KN-415_22112017_026 536 (4.665)
1: TOF MS ES+
341.1182
342.1204
363.0969
249.0535
263.0693
Me
O
O
O
5ba
3.20e+006
For Help, press F1

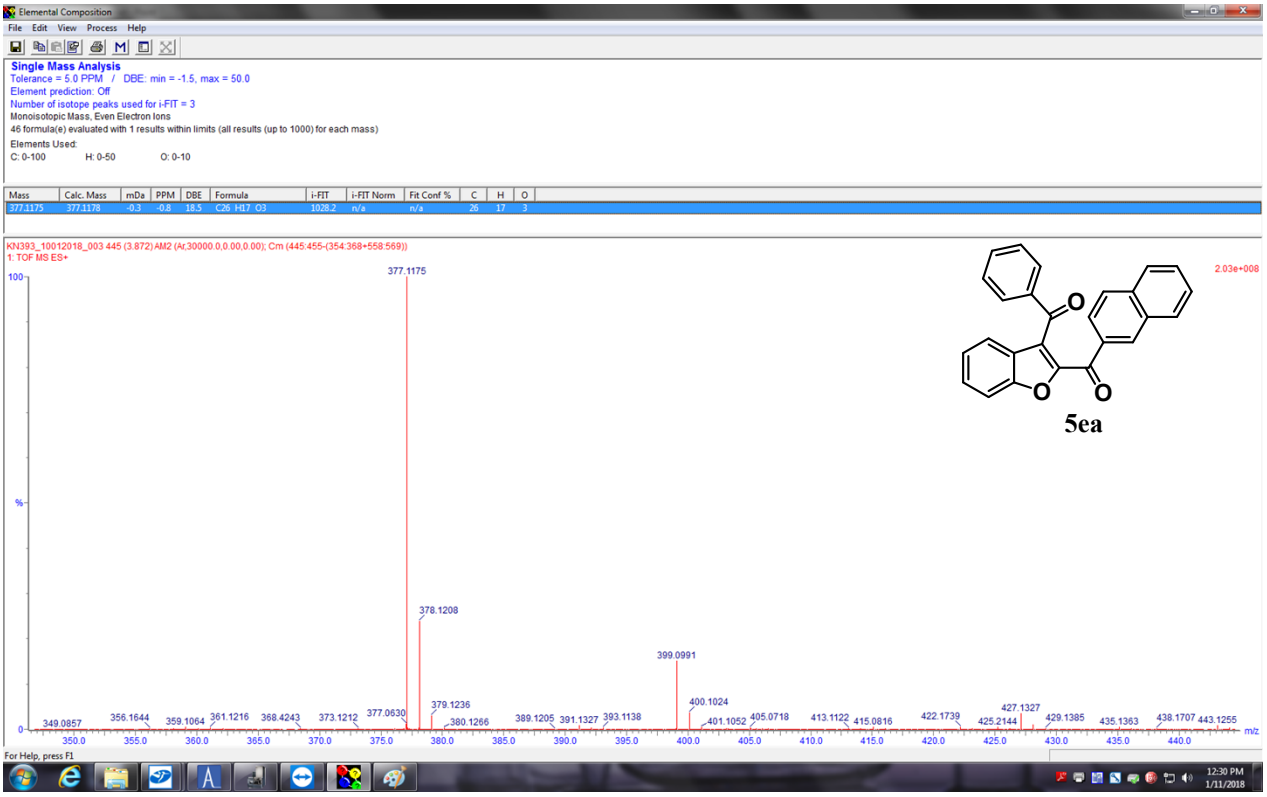

Elemental Composition
File Edit View Process Help
Single Mass Analysis
Tolerance = 5.0 PPM / DBE: min = -1.5, max = 50.0
Element prediction: Off
Monoisotopic Mass, Even Electron Ions
46 formula(e) evaluated with 1 results within limits (all results (up to 1000) for each mass)
Elements Used:
C: 0-100 H: 0-50 O: 0-10
Mass Calc. Mass mDa PPM DBE Formula C H O
371.1299 371.1283 1.6 4.3 15.5 C24 H19 O4 24 19 4
KN428_10012018_005 384 (3.349)
1: TOF MS ES+
371.1299
263.0726
372.1318
264.0758
393.1108
763.2307
764.2372
MeO
Me
O
O
O
5bb
2.08e+007
For Help, press F1

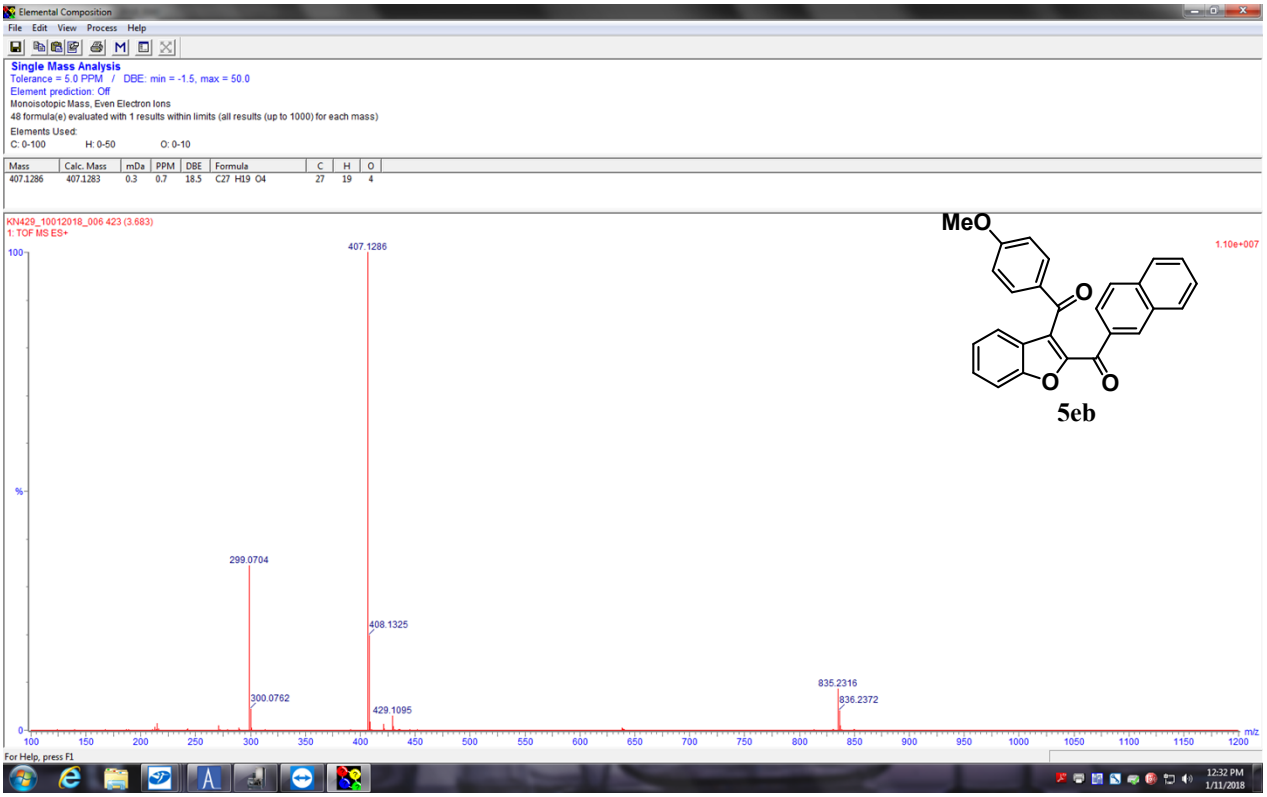

Elemental Composition
File Edit View Process Help
Single Mass Analysis
Tolerance = 10.0 mDa / DBE: min = -1.5, max = 50.0
Element prediction: Off
Monoisotopic Mass, Even Electron Ions
76 formula(e) evaluated with 2 results within limits (up to 5 closest results for each mass)
Elements Used:
C: 0-100 H: 0-50 O: 0-30
Mass Calc. Mass mDa PPM DBE Formula C H O
371.1299 371.1283 1.6 4.3 15.5 C24 H19 O4 24 19 4
371.1342 -4.3 -11.6 6.5 C17 H23 O9 17 23 9
KN-401_22112017_027 394 (3.435)
1: TOF MS ES+
2.58e+007
371.1299
372.1318
263.0693
279.0662
364.3222
393.1067
763.2307
OMe
Me
O
O
O
5bc
For Help, press F1


Elemental Composition
File Edit View Process Help
Single Mass Analysis
Tolerance = 10.0 mDa / DBE: min = -1.5, max = 50.0
Element prediction: Off
Monoisotopic Mass, Even Electron Ions
1745 formula(e) evaluated with 41 results within limits (up to 5 closest results for each mass)
Elements Used:
C: 0-100 H: 0-50 O: 0-30 F: 0-30 Cl: 0-8
Mass Calc. Mass mDa PPM DBE Formula C H O F Cl
359.1075 359.1073 0.2 0.6 2.5 C14 H22 O6 F2 Cl 14 22 6 2 1
359.1072 0.3 0.8 19.5 C26 H15 O2 26 15 2
359.1070 0.5 1.4 8.5 C18 H16 O2 F5 18 16 2 5
359.1082 -0.7 -1.9 4.5 C15 H17 O3 F6 15 17 3 6
359.1083 -0.8 -2.2 15.5 C23 H16 O3 F 23 16 3 1
KN-441_22112017_030 446 (3.881)
1: TOF MS ES+
1.75e+007
359.1075
360.1125
431.1805
263.0693
267.0468
381.0900
F
Me
O
O
O
5bd
For Help, press F1


Elemental Composition
File Edit View Process Help
Single Mass Analysis
Tolerance = 5.0 PPM / DBE: min = -1.5, max = 50.0
Element prediction: Off
Number of isotope peaks used for i-FIT = 3
Monoisotopic Mass, Even Electron Ions
47 formula(e) evaluated with 1 results within limits (all results (up to 1000) for each mass)
Elements Used:
Mass Calc. Mass mDa PPM DBE Formula i-FIT i-FIT Norm Fit Conf % C H O
387.1244 387.1232 1.2 3.1 15.5 C24 H19 O5 978.4 n/a n/a 24 19 5
KN435_10012018_007 413 (3.598) AM2 (Ar,30000.0,0.00,0.00)
1: TOF MS ES+
6.99e+007
387.1244
388.1263
279.0661
795.2231
796.2266
409.1046
280.0693
410.1079
797.2297
152.0629
236.0481
251.0715
293.0815
387.0559
489.0471
528.0502
579.1464
608.1346
699.2863
795.1359
811.2388
875.1650
947.0990
975.0942
991.0847
1085.3997
1155.3453
1185.3263
OMe
OMe
O
O
O
5cc
For Help, press F1


Elemental Composition
File Edit View Process Help
Single Mass Analysis
Tolerance = 10.0 mDa / DBE: min = -1.5, max = 50.0
Element prediction: Off
Monoisotopic Mass, Even Electron Ions
301 formula(e) evaluated with 10 results within limits (up to 5 closest results for each mass)
Elements Used:
C: 0-100 H: 0-50 O: 0-30 Cl: 0-8
Mass Calc. Mass mDa PPM DBE Formula C H O Cl
361.0645 361.0653 -0.8 -2.2 24.5 C28 H9 O 28 9 1
361.0631 1.4 3.9 15.5 C22 H14 O3 Cl 22 14 3 1
361.0660 -1.5 -4.2 1.5 C15 H25 O Cl4 15 25 1 4
361.0618 2.7 7.5 2.5 C10 H17 O14 10 17 14
361.0610 3.5 9.7 6.5 C16 H19 O5 Cl2 16 19 5 2
KN-424_22112017_031 432 (3.760)
1: TOF MS ES+
1.04e+007
361.0645
363.0618
383.0458
283.0144
338.3424
743.0995
Cl
O
O
O
5da
For Help, press F1


Elemental Composition
File Edit View Process Help
Single Mass Analysis
Tolerance = 5.0 PPM / DBE: min = -1.5, max = 50.0
Element prediction: Off
Number of isotope peaks used for i-FIT = 3
Monoisotopic Mass, Even Electron Ions
46 formula(e) evaluated with 1 results within limits (all results (up to 1000) for each mass)
Elements Used:
C: 0-100 H: 0-50 O: 0-10
Mass | Calc. Mass | mDa | PPM | DBE | Formula | i-FIT | i-FIT Norm | Fit Conf % | C | H | O
377.1175 | 377.1178 | -0.3 | -0.8 | 18.5 | C26 H17 O3 | 1028.2 | n/a | n/a | 26 | 17 | 3
KN393_10012018_003 445 (3.872) AM2 (Ar,30000.0,0.00,0.00); Cm (445:455-(354:368+558:569))
1: TOF MS ES+
2.03e+008
377.1175
378.1208
399.0991
400.1024
5ea
For Help, press F1


Elemental Composition
File Edit View Process Help
Single Mass Analysis
Tolerance = 5.0 PPM / DBE: min = -1.5, max = 50.0
Element prediction: Off
Monoisotopic Mass, Even Electron Ions
48 formula(e) evaluated with 1 results within limits (all results (up to 1000) for each mass)
Elements Used:
C: 0-100 H: 0-50 O: 0-10
Mass | Calc. Mass | mDa | PPM | DBE | Formula | C | H | O
407.1286 | 407.1283 | 0.3 | 0.7 | 18.5 | C27 H19 O4 | 27 | 19 | 4
KN429_10012018_006 423 (3.683)
1: TOF MS ES+
1.10e+007
MeO
407.1286
299.0704
300.0762
408.1325
429.1095
835.2316
836.2372
5eb
For Help, press F1