Supporting Information for:

An effective organocatalytic preparation of both 1,3-diketones and nitriles from alkynones with oximes as hydroxide source

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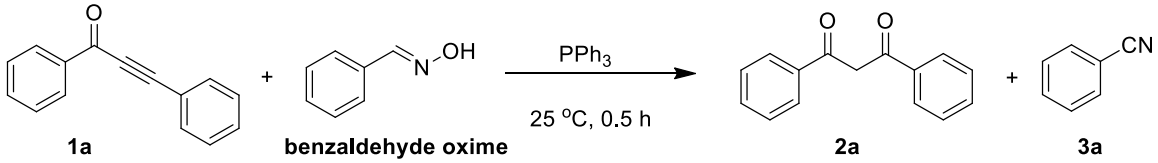
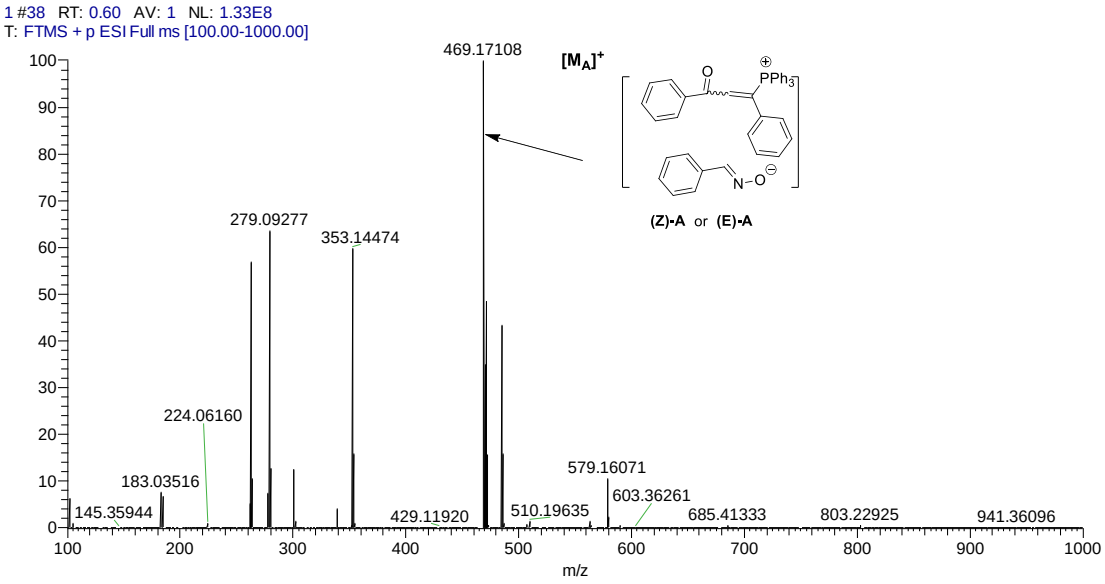
Contents:

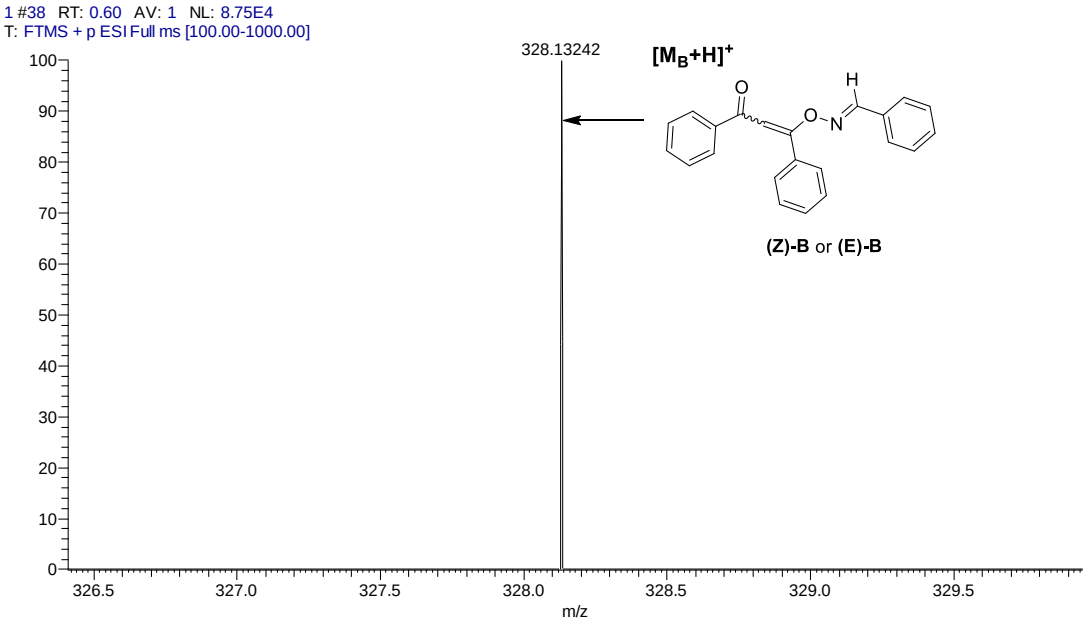
1. Mechanism Studies

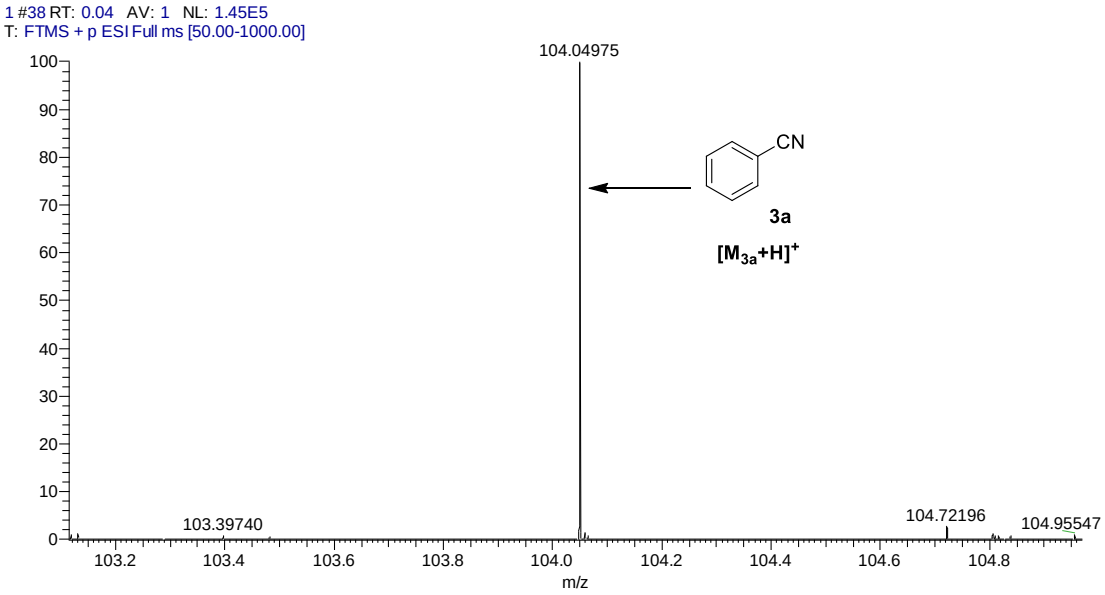
1.1 ESI-HRMS detection of the reaction mixture

Reaction intermediates and products were captured by monitoring the reaction mixture of 1,3-diphenylprop-2-yn-1-one **1a** with benzaldehyde oxime by ESI-HRMS at 0.5 h (Fig. S1).









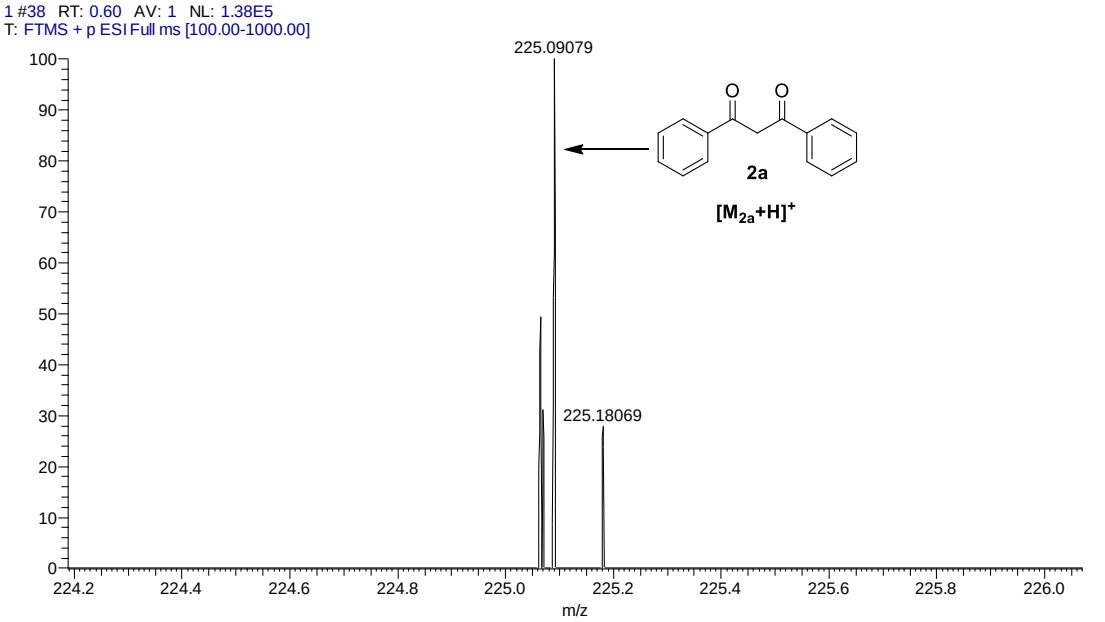


Fig. S1 ESI-HRMS detection of the reaction mixture using **1a** as substrate with 0.5 h under the standard conditions.

1.2 Monitoring the process of reaction by ^{1}H NMR.

We monitored the reaction of 1,3-diphenylprop-2-yn-1-one **1a** with 4-methyl-benzaldehyde oxime by ^{1}H NMR at 0 h, 1 h, 5.5 h and 7.5 h (Fig. S2). Form the

characteristic peak changes, the starting material **1a** and 4-methyl-benzaldehyde oxime were continuously consumed. In the meanwhile, the product **2a** and 4-methylbenzonitrile were constantly obtained.

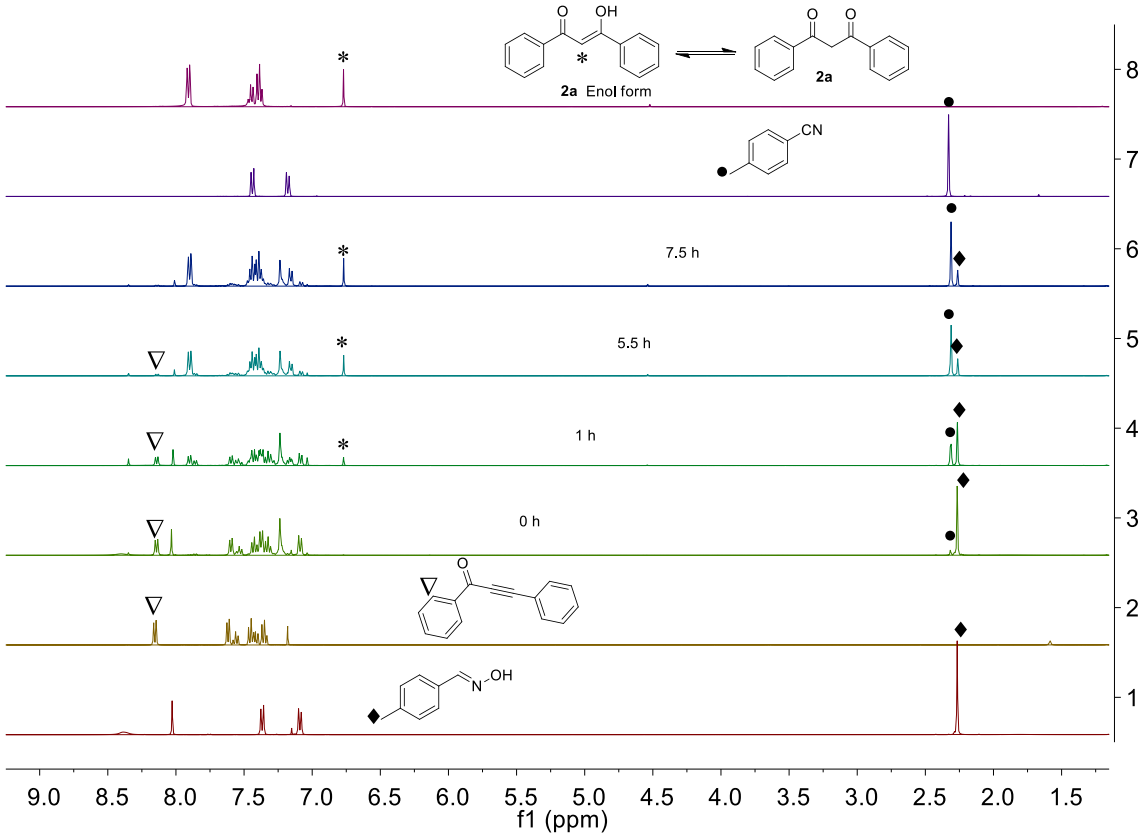
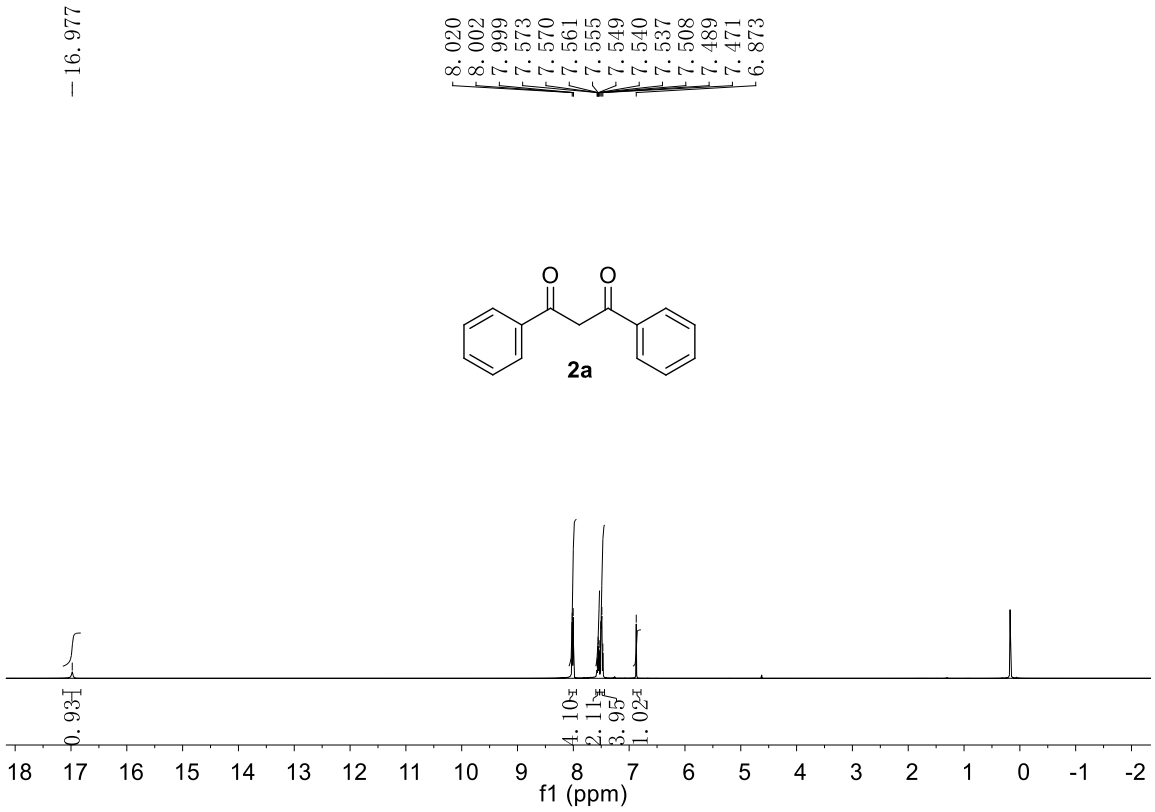
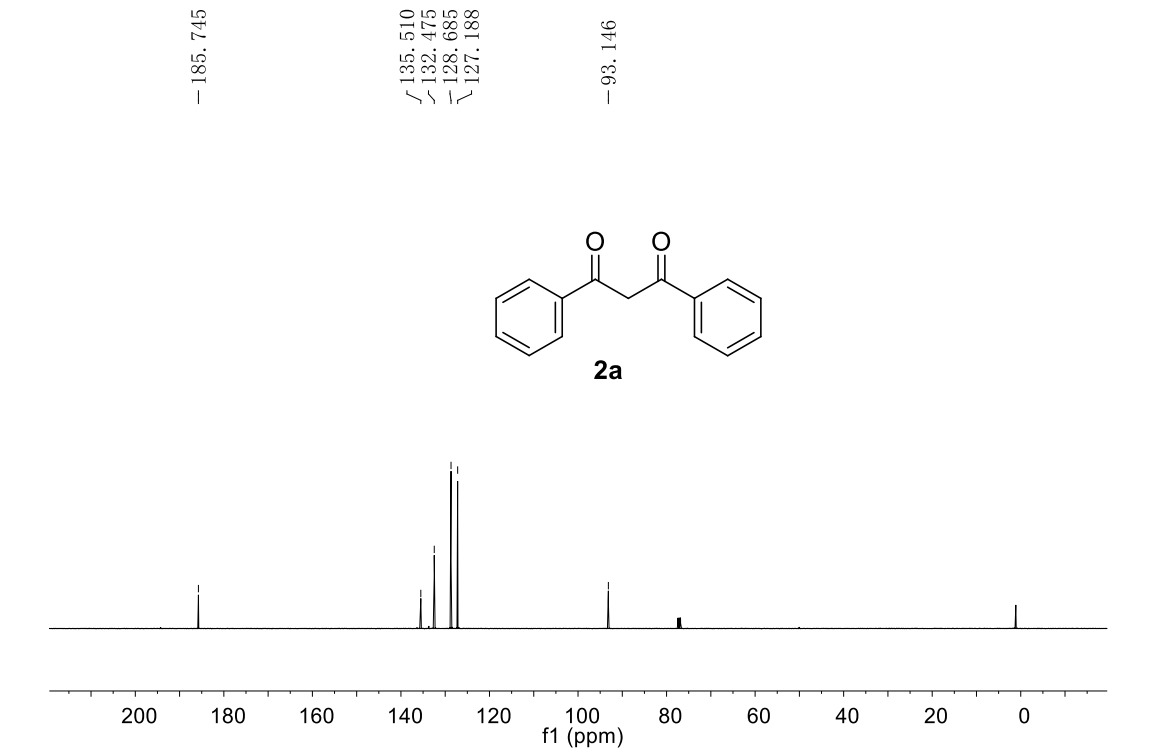
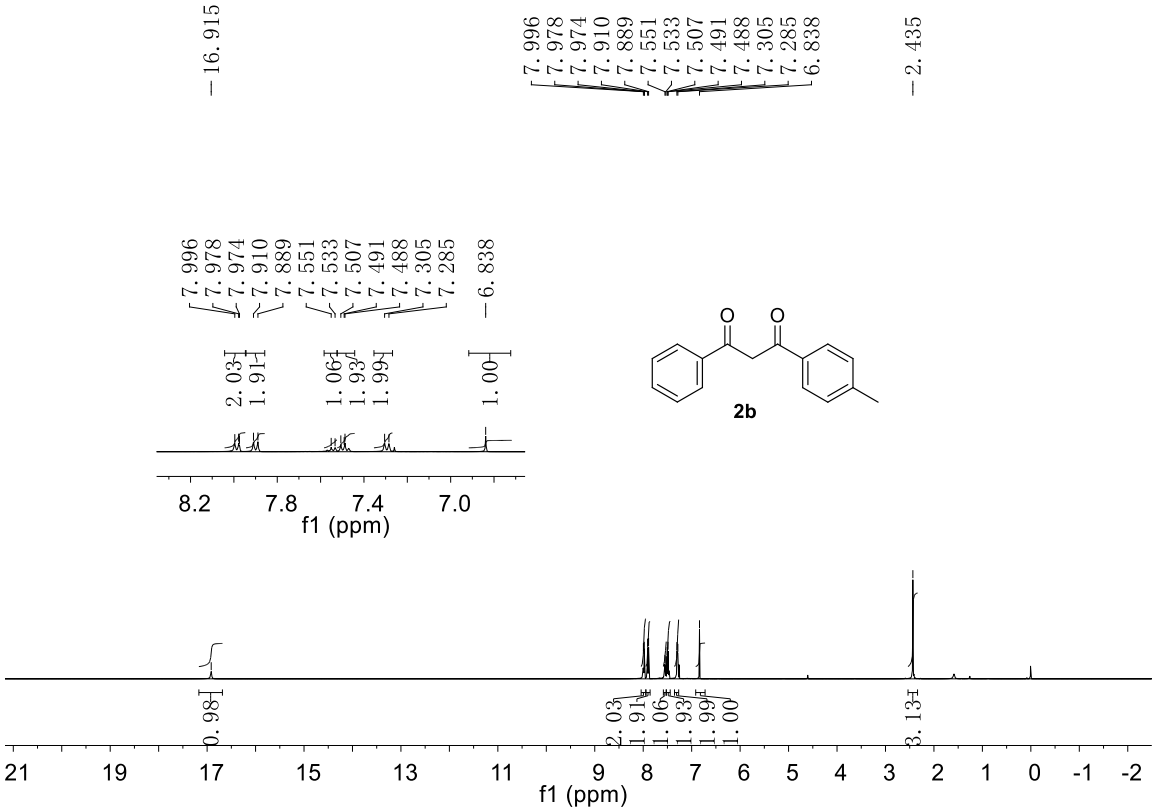


Fig. S2 Monitoring the reaction by ^{1}H NMR.

2. ^{1}H NMR and ^{13}C NMR Spectra of Products 2 and 3



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7.305
7.285
6.838
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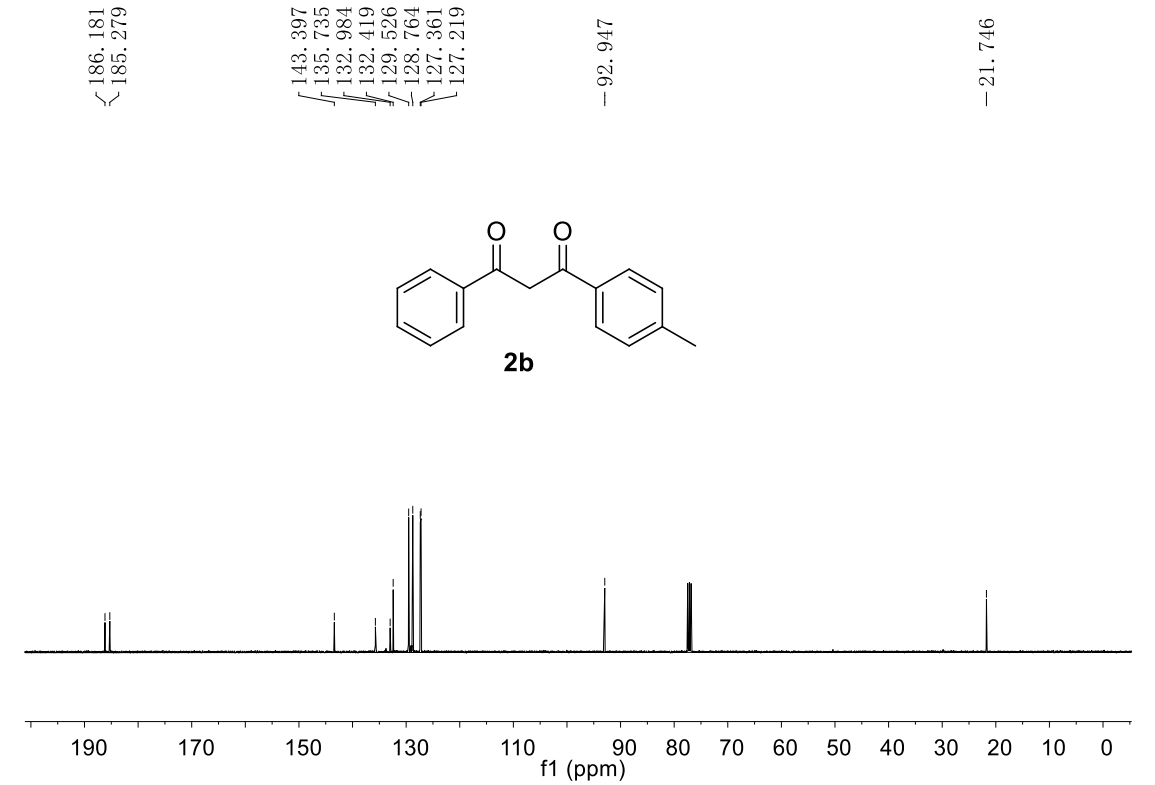
1.91
1.06
1.93
1.99
1.00
0.98
3.13
f1 (ppm)
2b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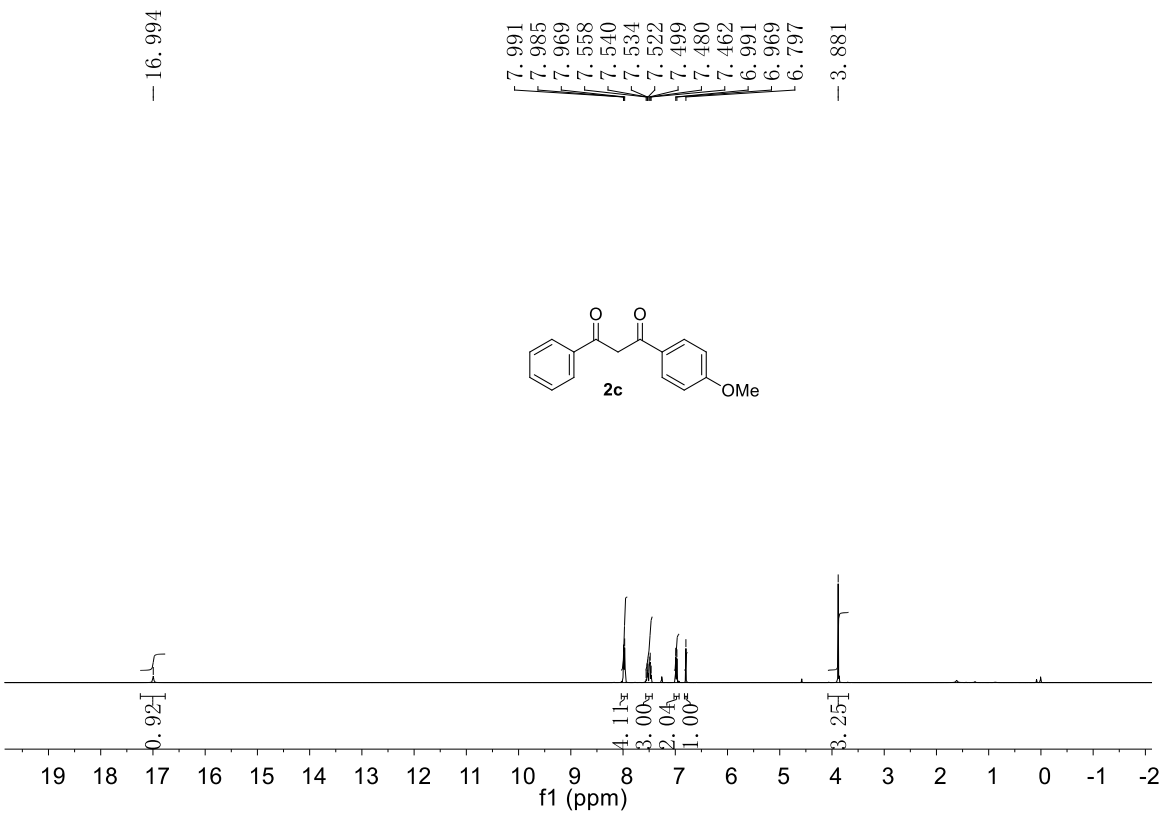
2b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7.558
7.540
7.534
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7.499
7.480
7.462
6.991
6.969
6.797
3.881
O
O
2c
OMe
0.92
4.11
3.00
2.04
1.00
3.25
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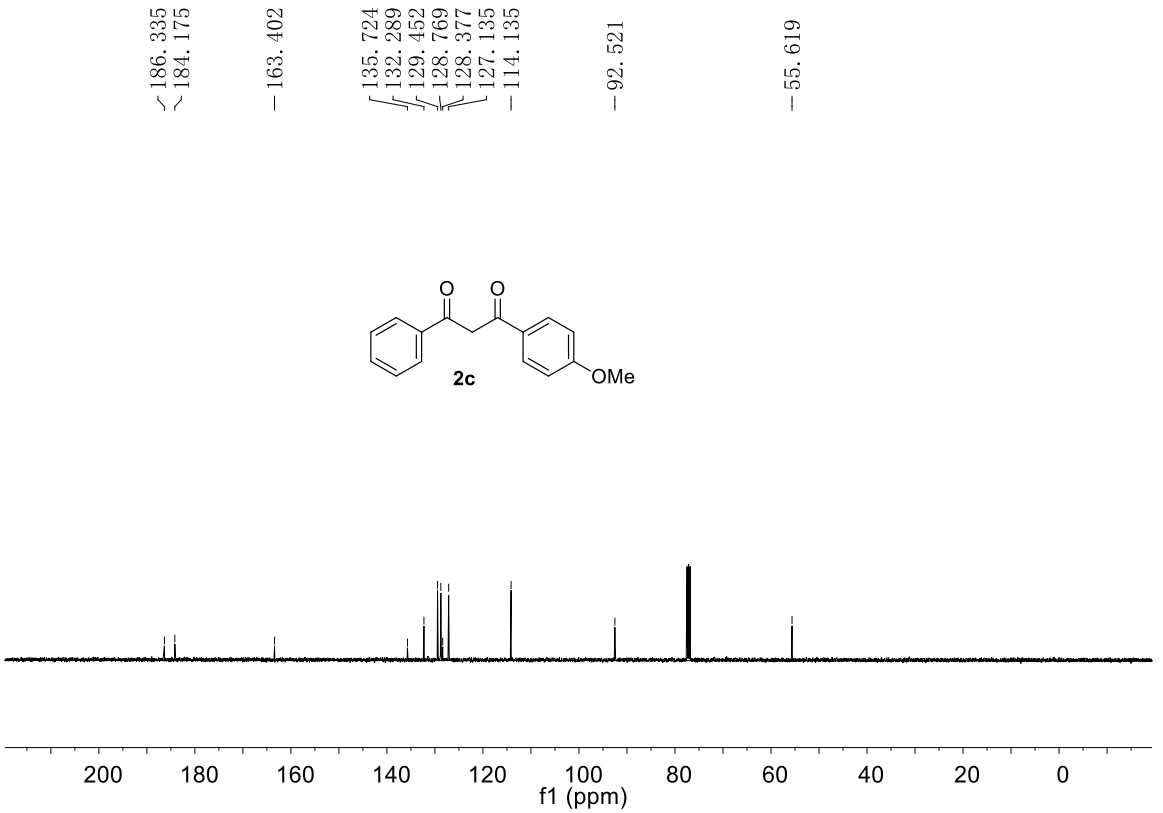
f1 (ppm)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O
2c
OMe
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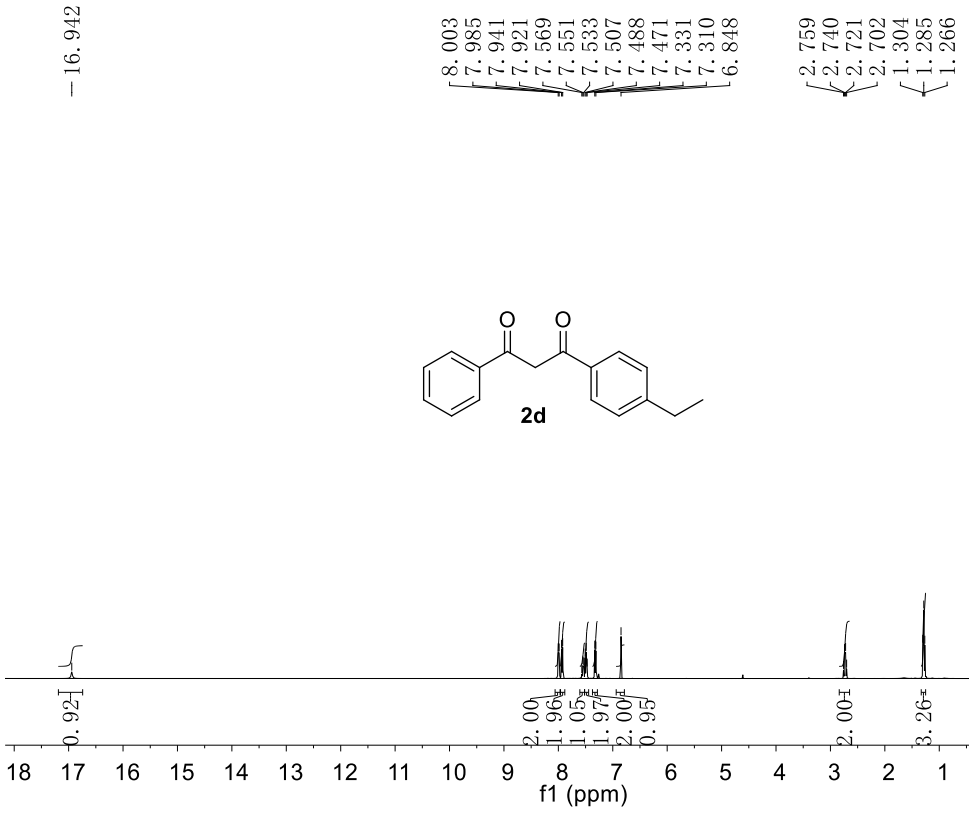
f1 (ppm)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7.507
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7.331
7.310
6.848
2.759
2.740
2.721
2.702
1.304
1.285
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0.95
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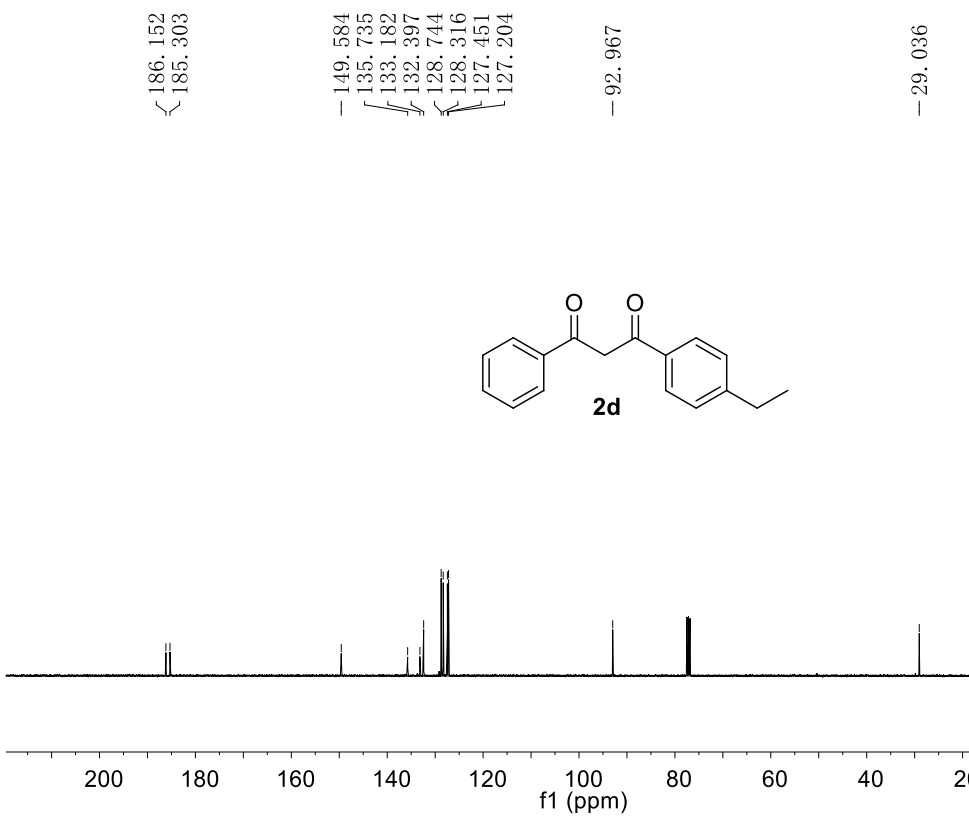
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2d
f1 (ppm)


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7.985
7.805
7.791
7.777
7.576
7.558
7.553
7.540
7.512
7.493
7.476
7.402
7.383
7.378
7.370
7.368
6.850
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1.99
2.07
1.12
1.95
2.01
8.0
7.5
f1 (ppm)
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O
2e
1.01
1.99
2.07
1.12
1.95
2.01
1.00
2.99
18 17 16 15 14 13 12 11 10 9 8 7 6 5 4 3 2 1 0 -1
f1 (ppm)
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132.531
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O
2e
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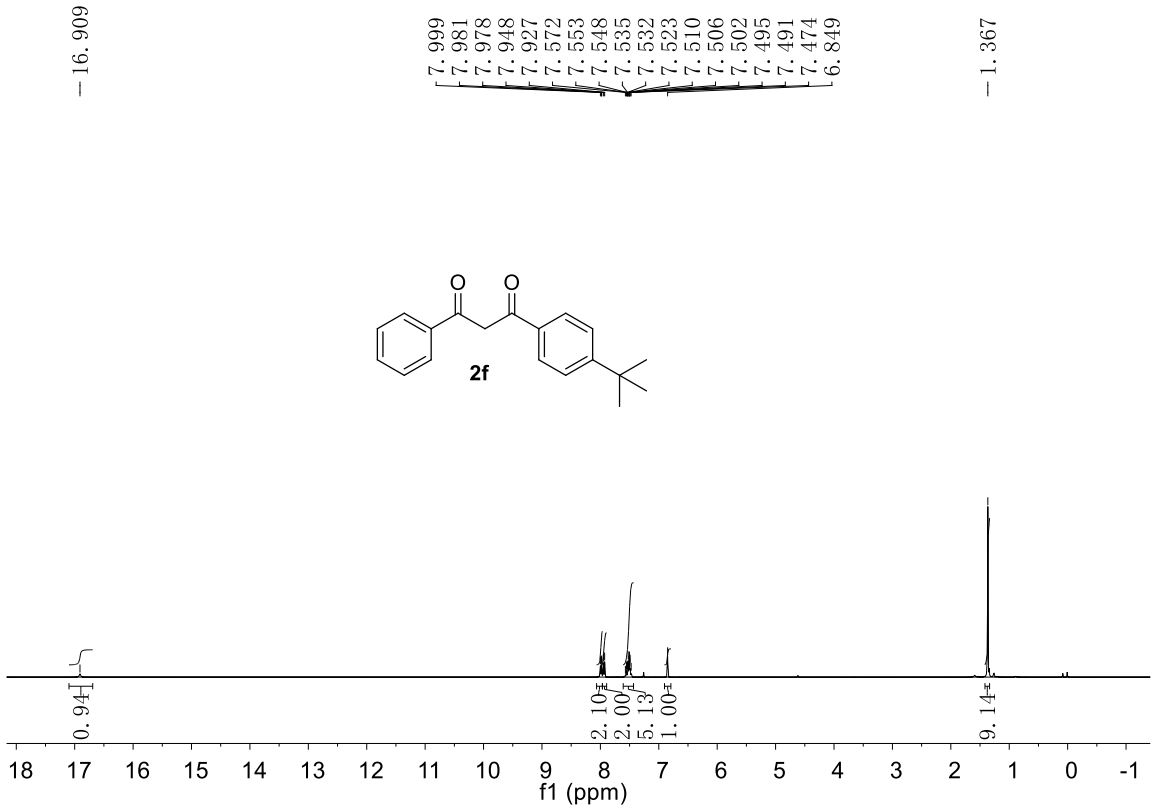
f1 (ppm)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7.535
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7.523
7.510
7.506
7.502
7.495
7.491
7.474
6.849
1.367
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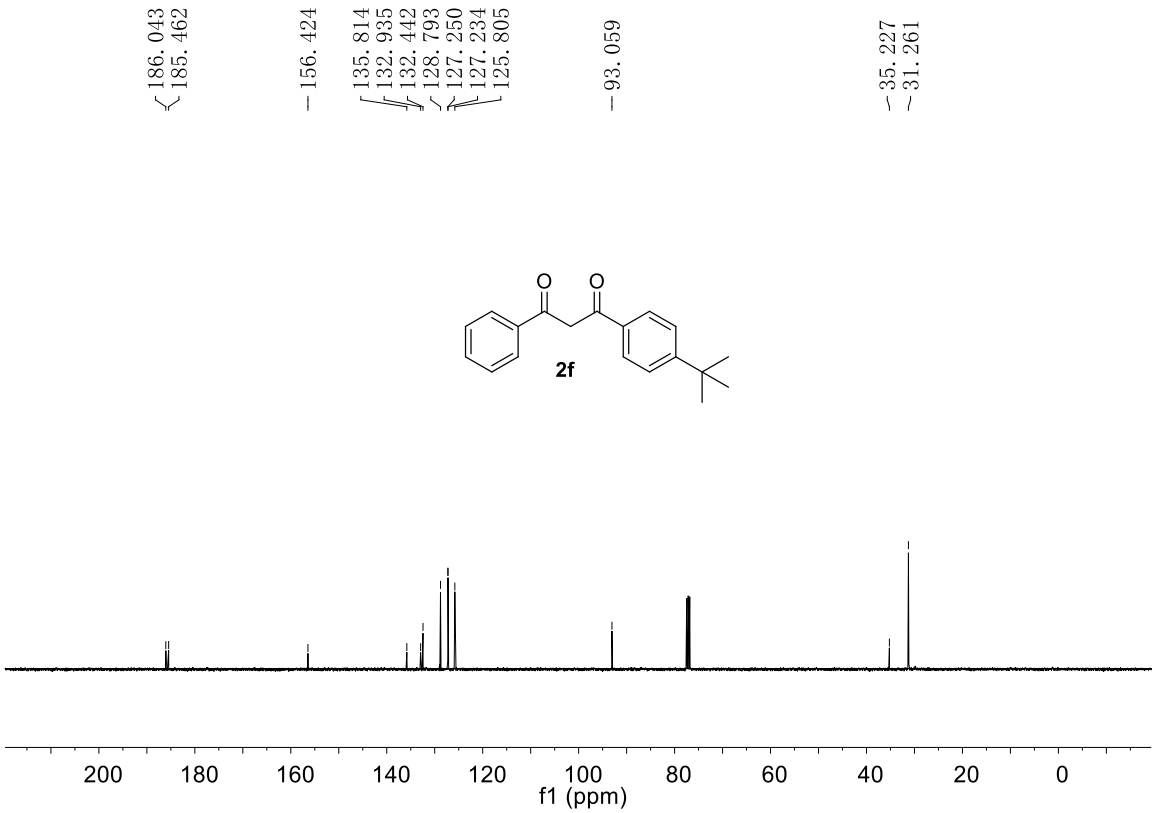
5.13
1.00
9.14
f1 (ppm)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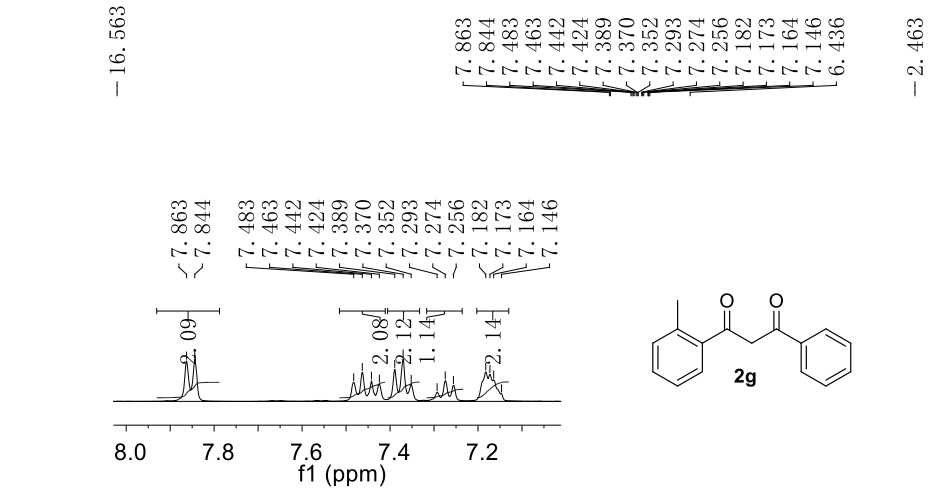
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7.442
7.424
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7.370
7.352
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7.256
7.182
7.173
7.164
7.146
6.436
2.463
2.09
2.08
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2.14
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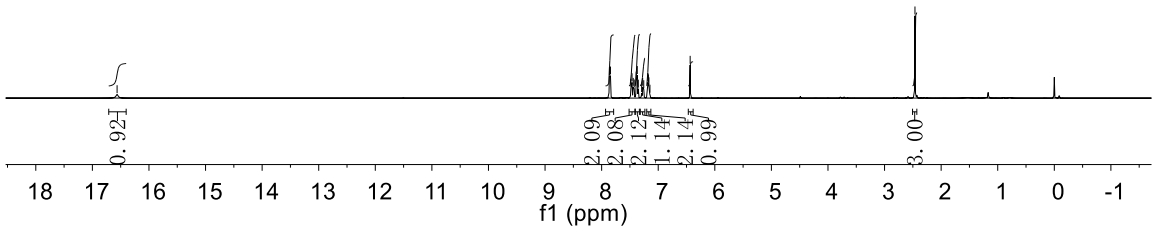
7.6
7.4
7.2
f1 (ppm)
O
O
2g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3.00
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17
16
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12
11
10
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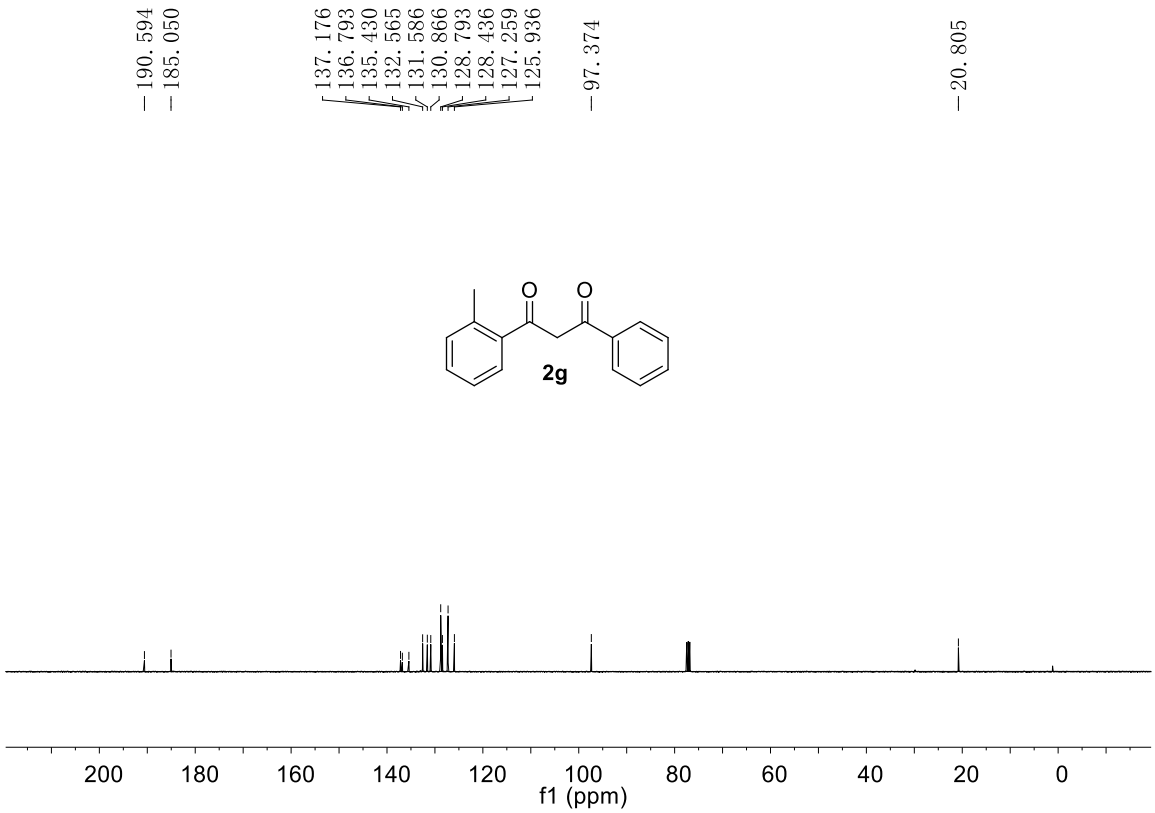
8
7
6
5
4
3
2
1
0
-1
f1 (ppm)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131.586
130.866
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O
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100
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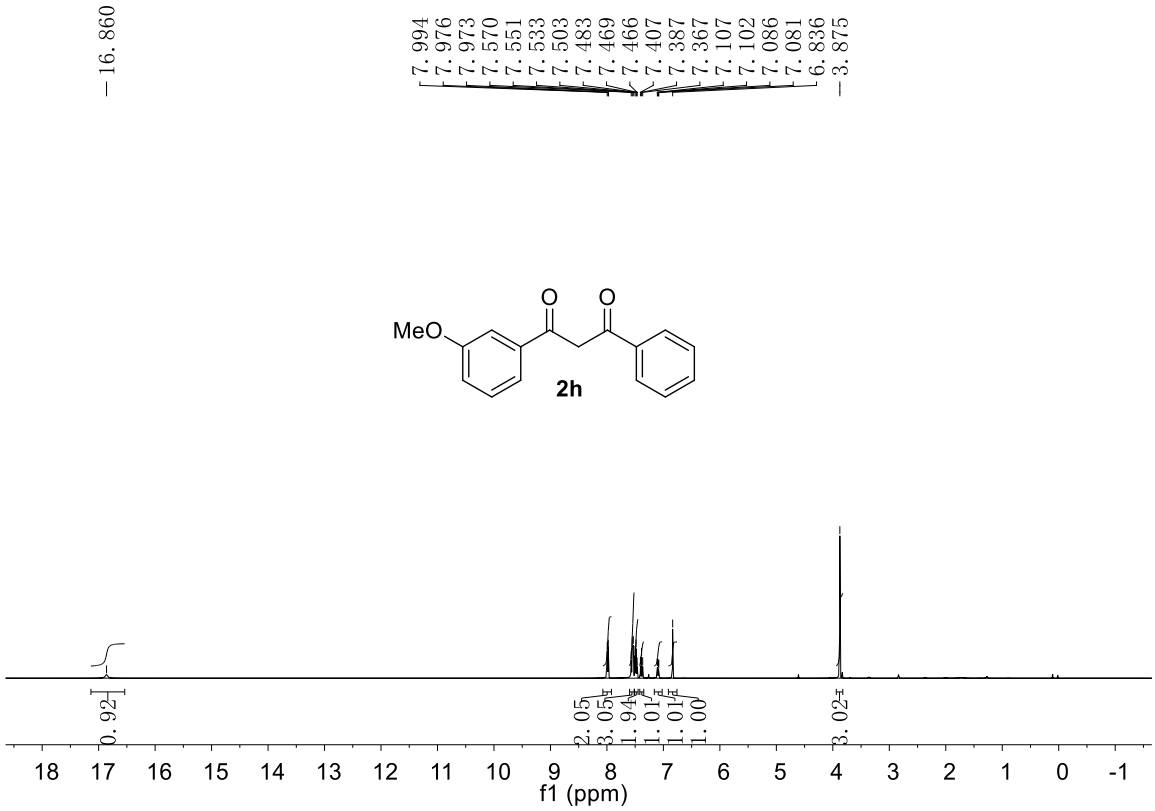
40
20
0
f1 (ppm)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7.387
7.367
7.107
7.102
7.086
7.081
6.836
3.875
MeO
O
O
2h
0.92
2.05
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1.01
1.00
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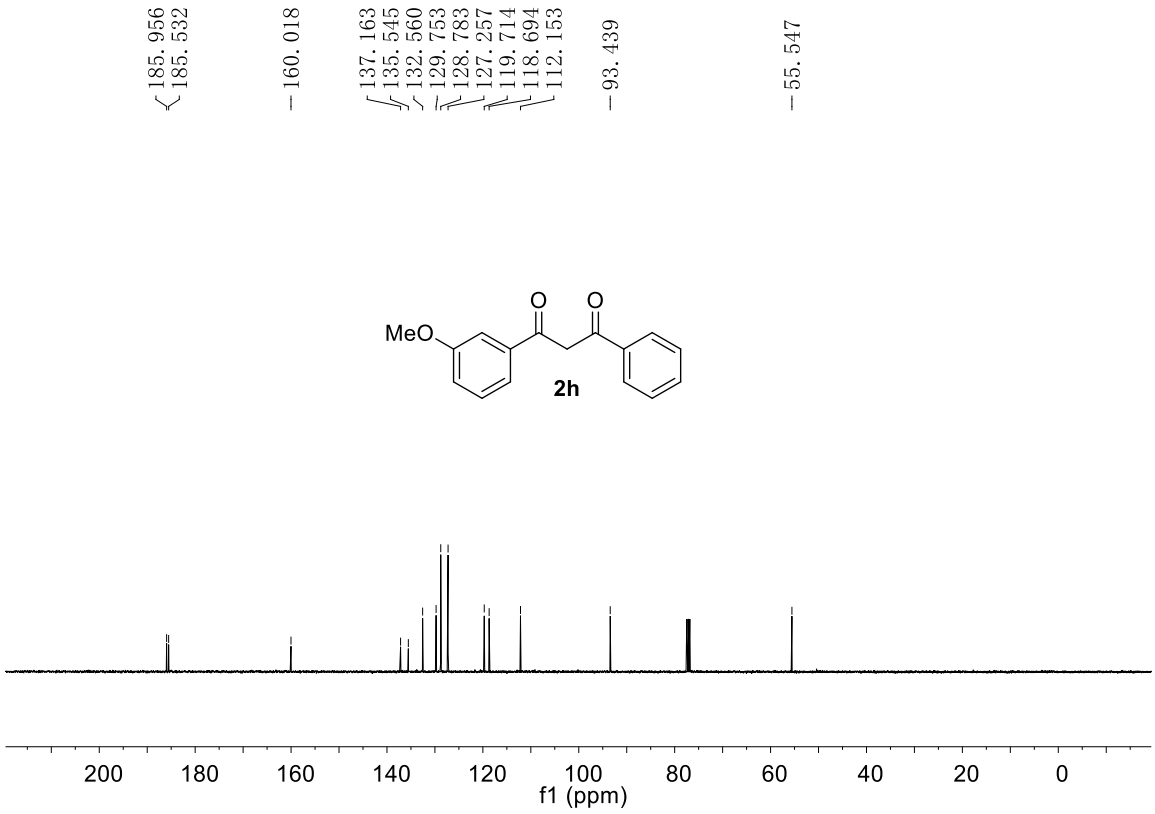
f1 (ppm)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MeO
O
O
2h
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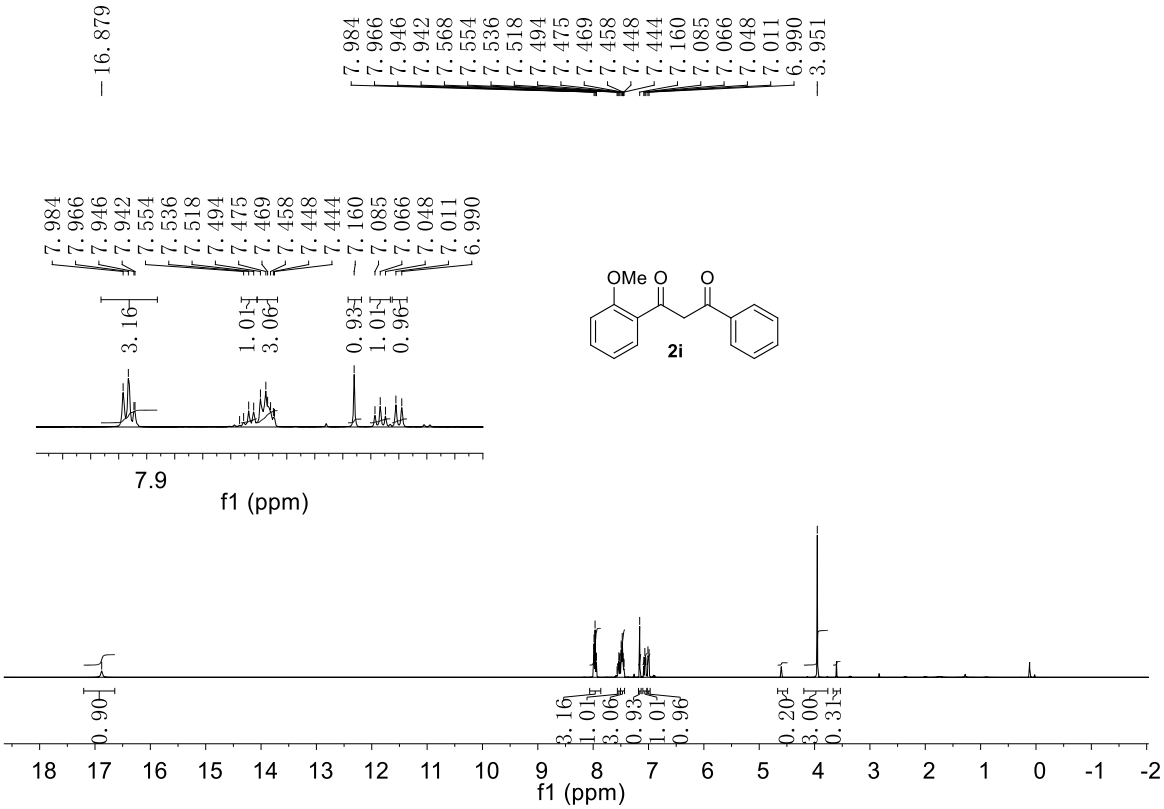
f1 (ppm)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7.458
7.448
7.444
7.160
7.085
7.066
7.048
7.011
6.990
3.951
3.16
1.01
3.06
0.93
1.01
0.96
0.90
0.20
3.00
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2i
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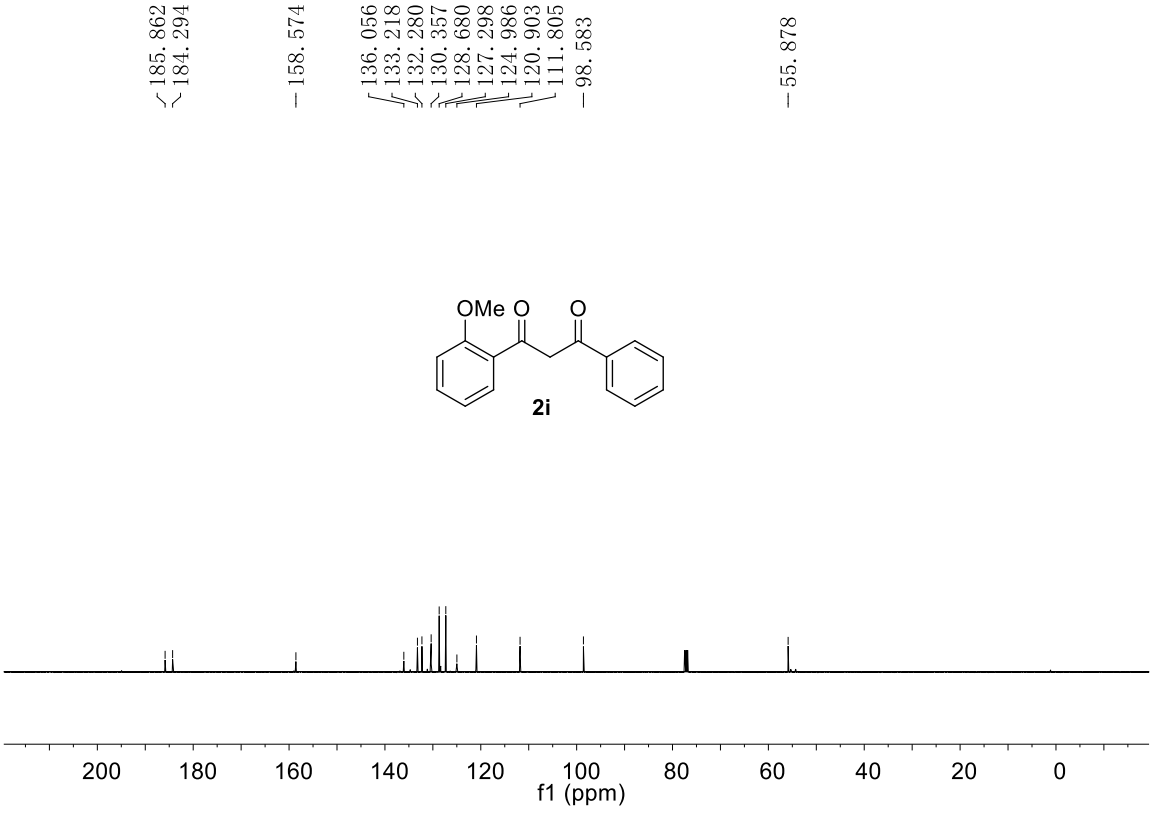
f1 (ppm)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2i
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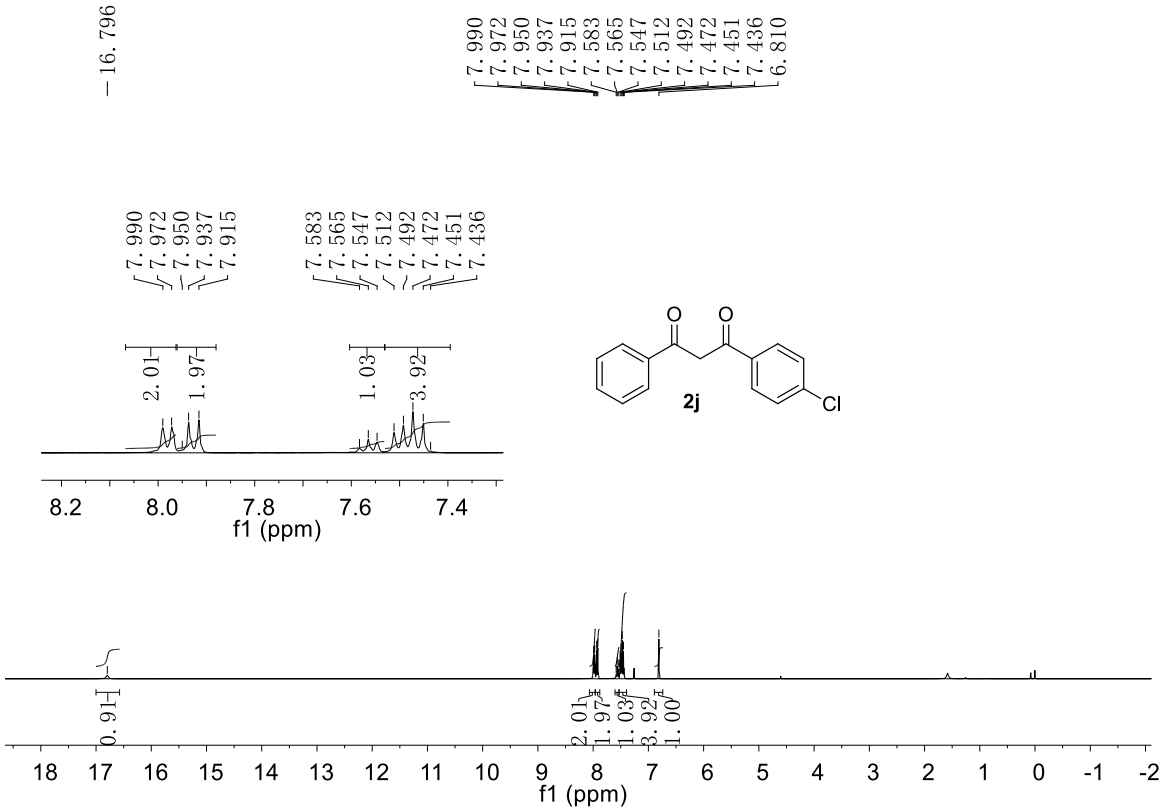
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1.97
1.03
3.92
8.2
8.0
7.8
7.6
7.4
f1 (ppm)
O
O
Cl
2j
0.91
2.01
1.97
1.03
3.92
1.00
18
17
16
15
14
13
12
11
10
9
8
7
6
5
4
3
2
1
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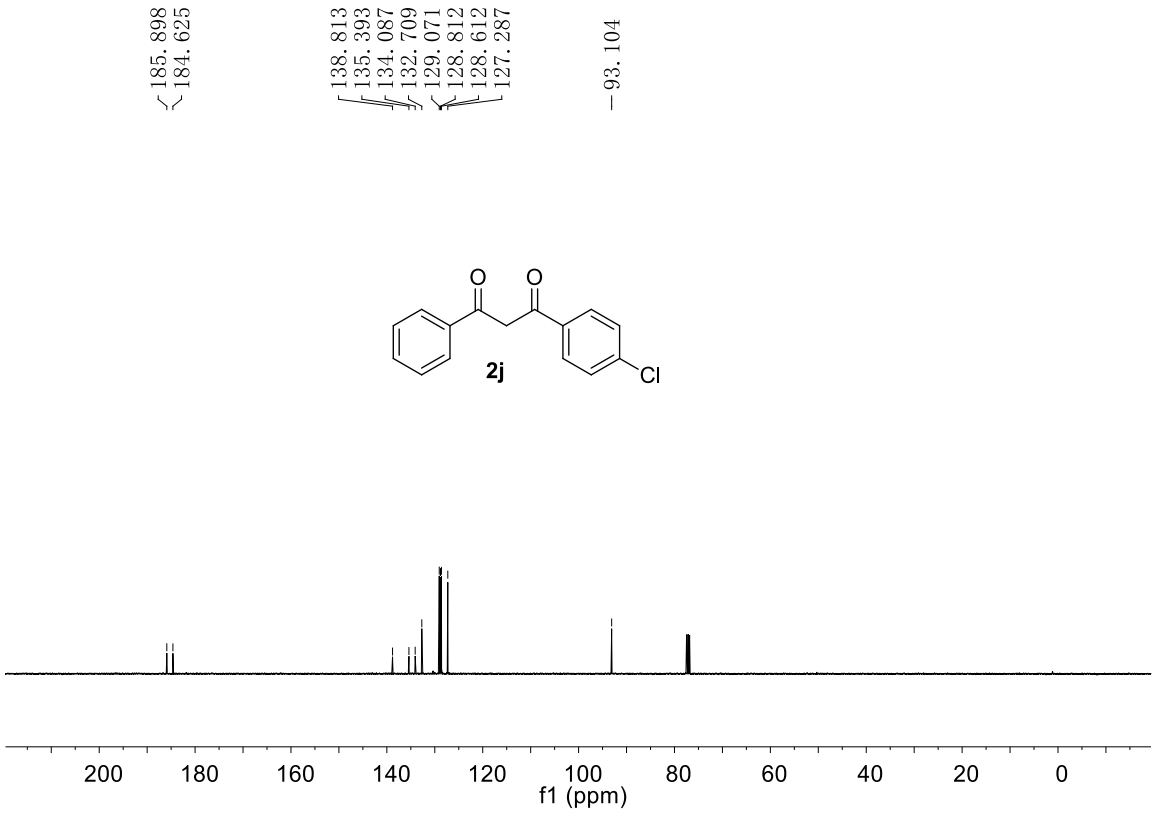
-1
-2
f1 (ppm)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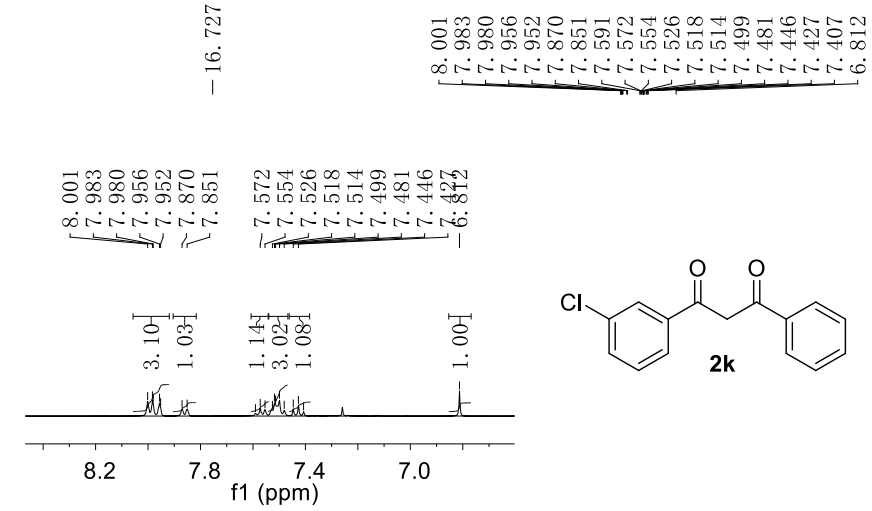
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7.427
7.407
6.812
3.10
1.03
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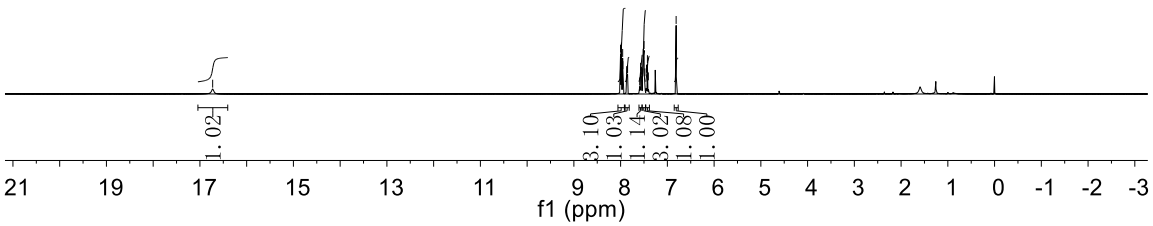
7.0
f1 (ppm)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19
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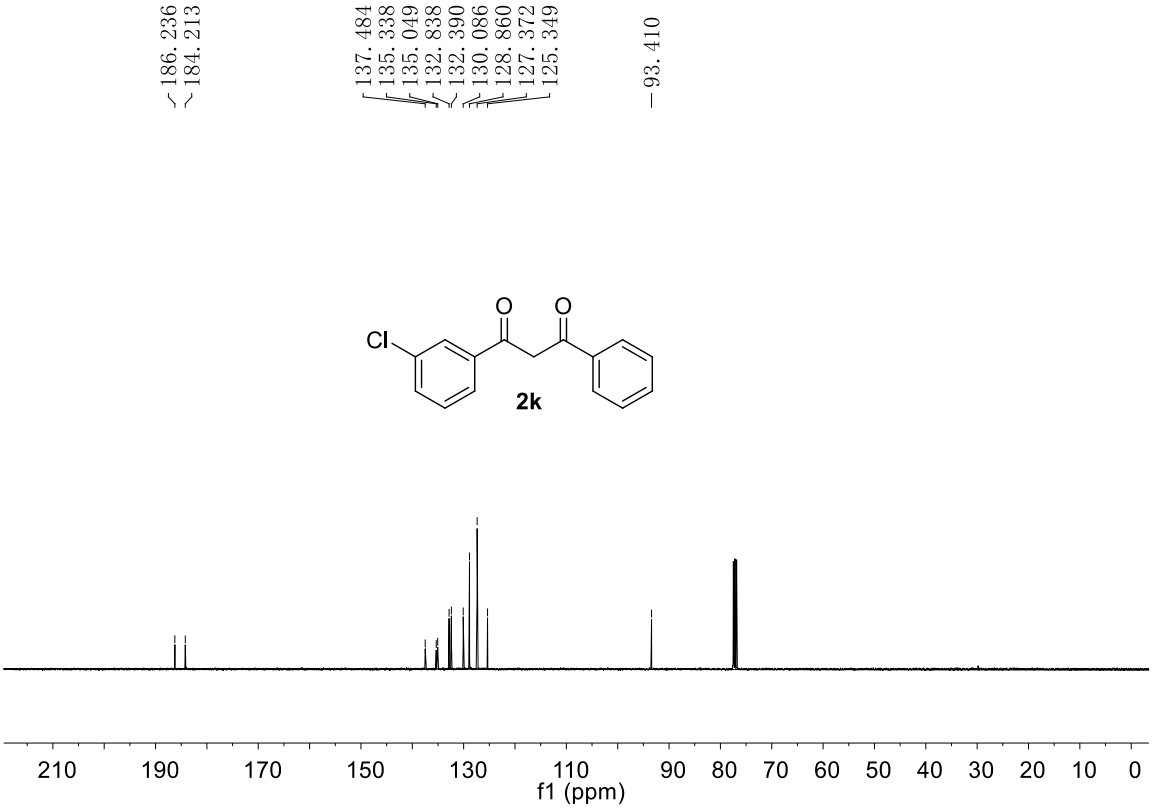
-3
f1 (ppm)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50
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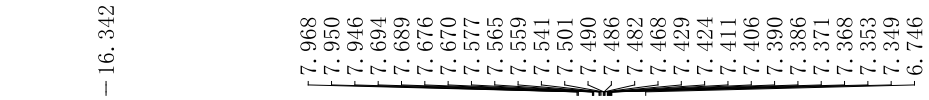
30
20
10
0
f1 (ppm)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7.501
7.490
7.486
7.482
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7.368
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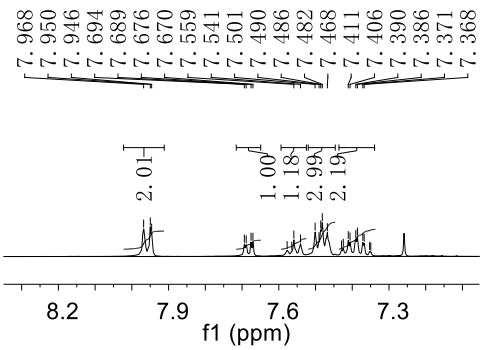
7.349
6.746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7.490
7.486
7.482
7.468
7.411
7.406
7.390
7.386
7.371
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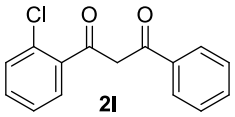
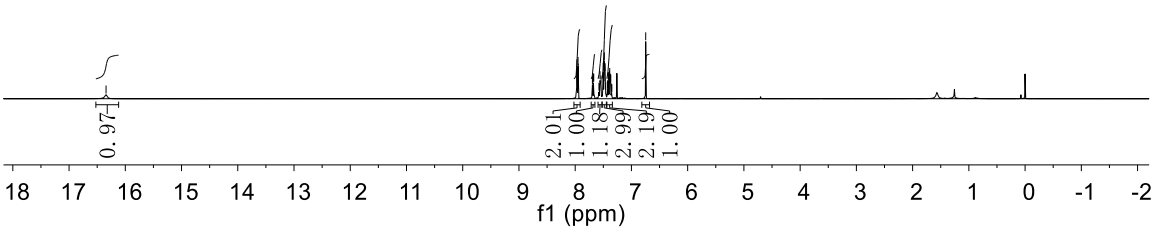
7.3
f1 (ppm)


Cl
O
O
2l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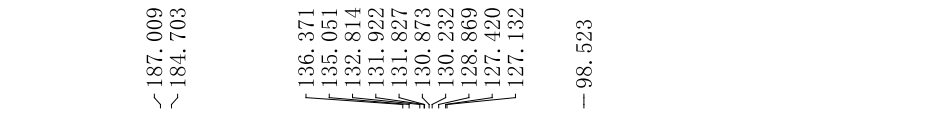
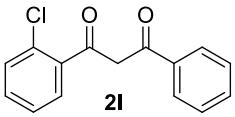
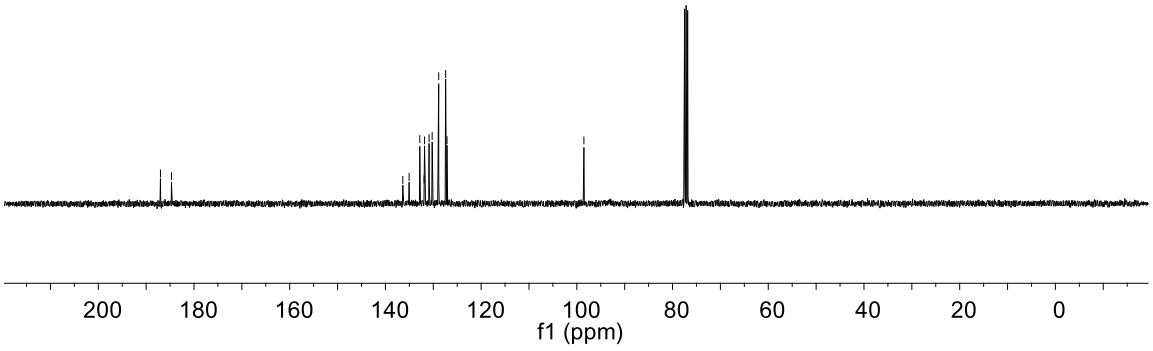
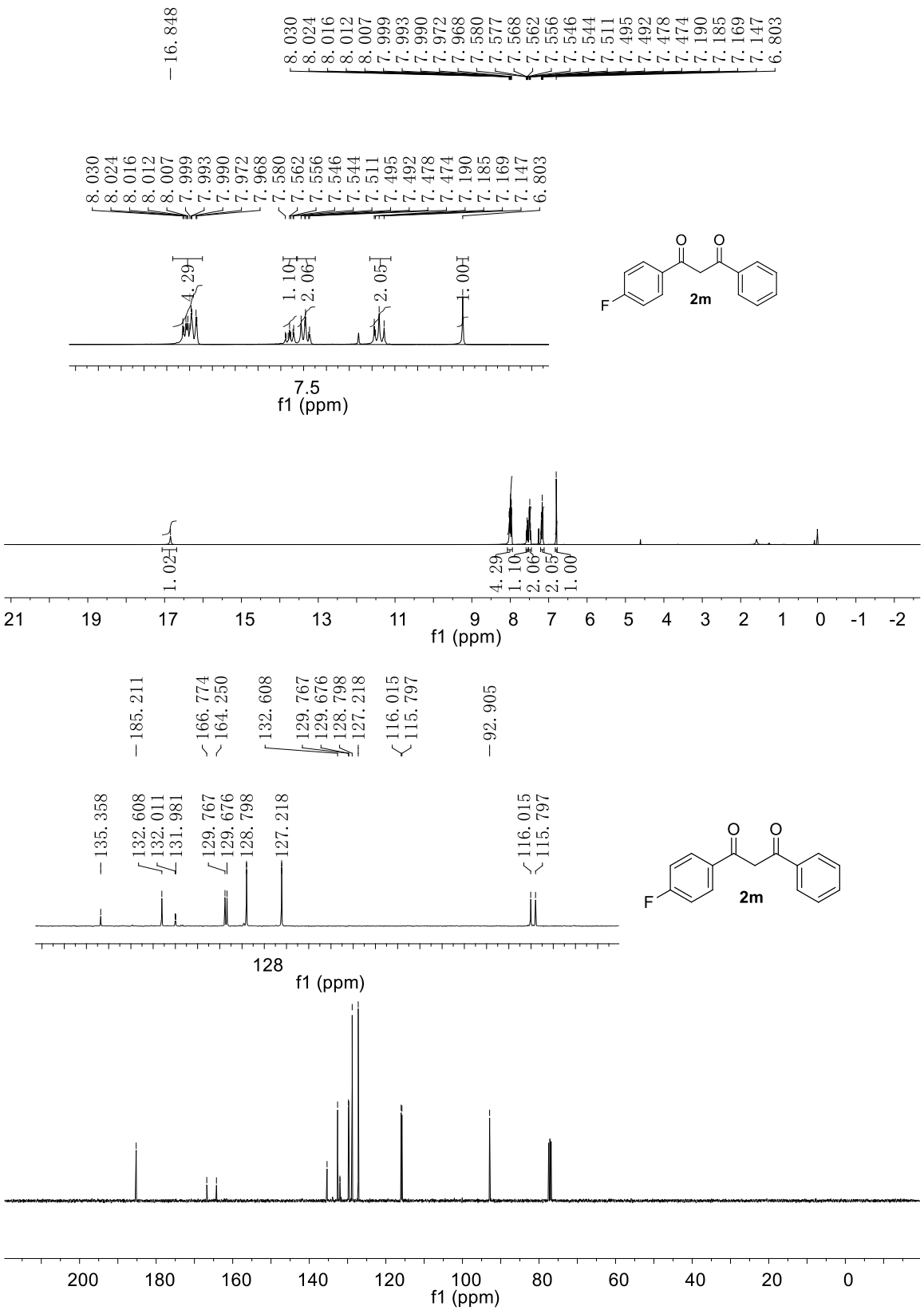
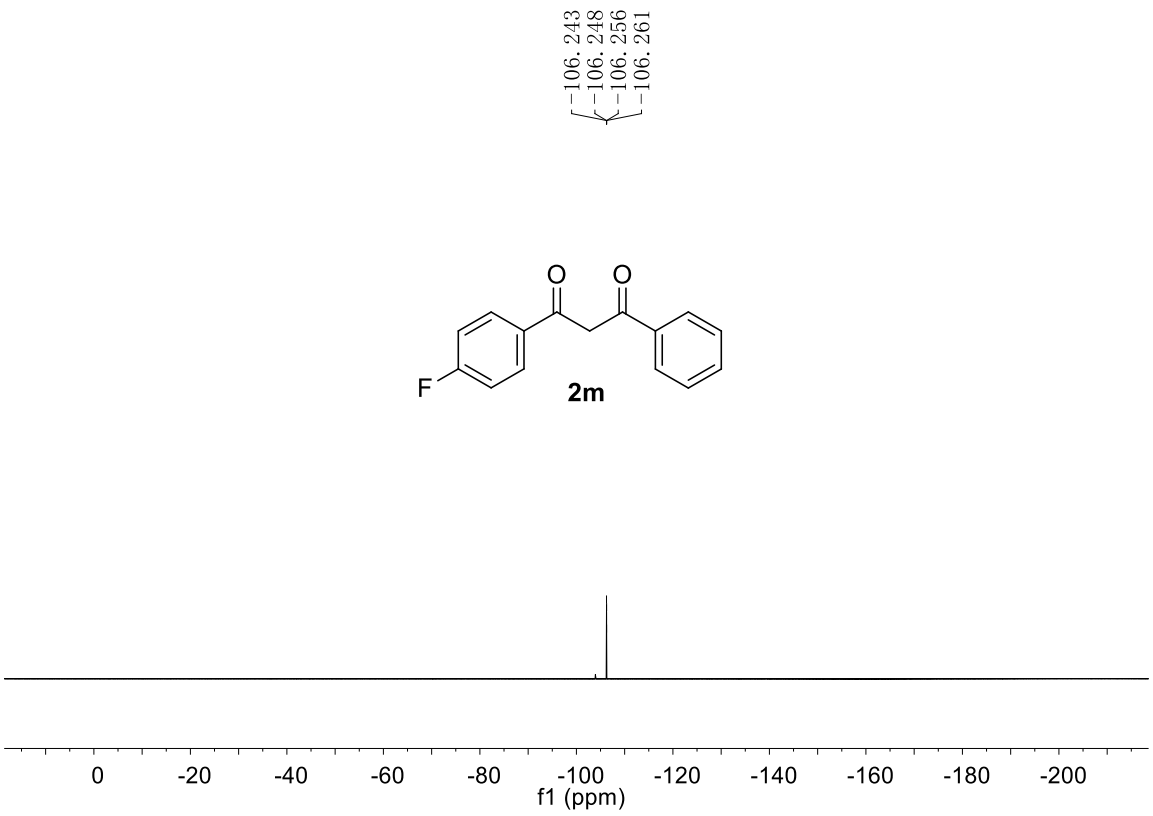
1.18
2.99
2.19
1.00
18
17
16
15
14
13
12
11
10
9
8
7
6
5
4
3
2
1
0
-1
-2
f1 (ppm)

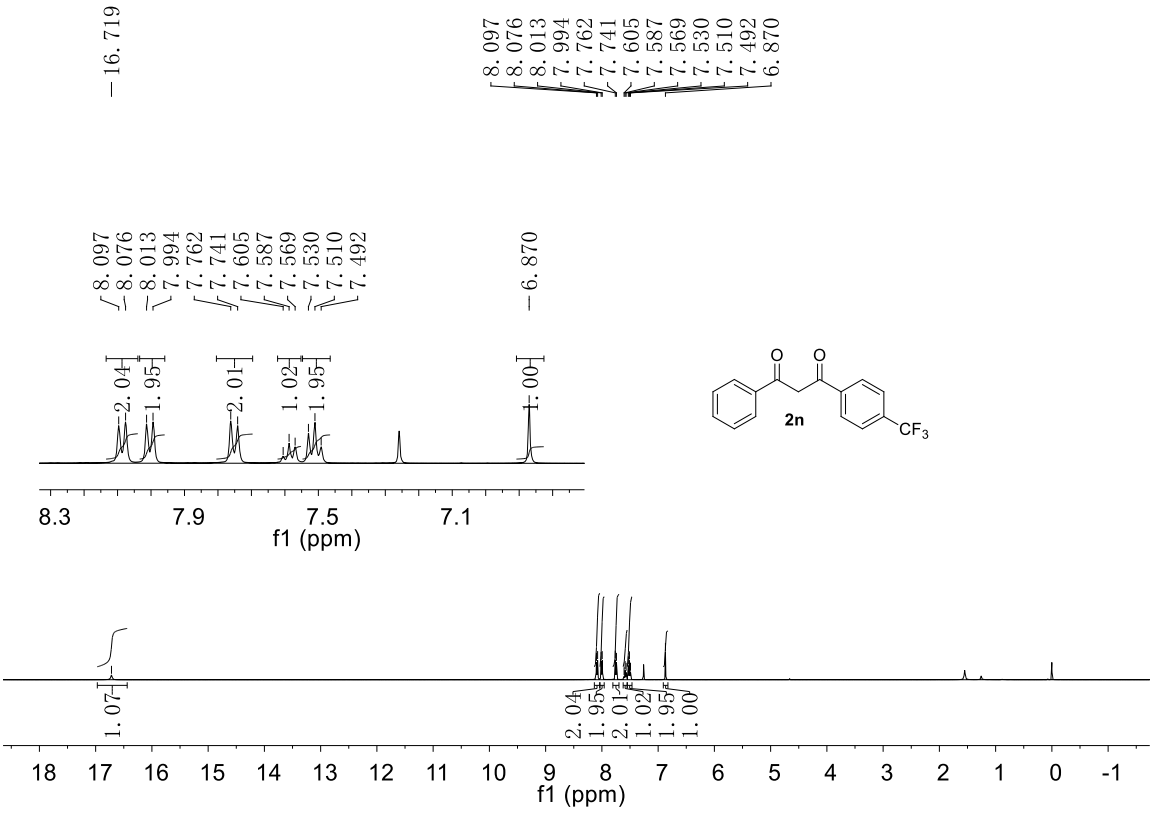

187.009
184.703
136.371
135.051
132.814
131.922
131.827
130.873
130.232
128.869
127.420
127.132
98.523

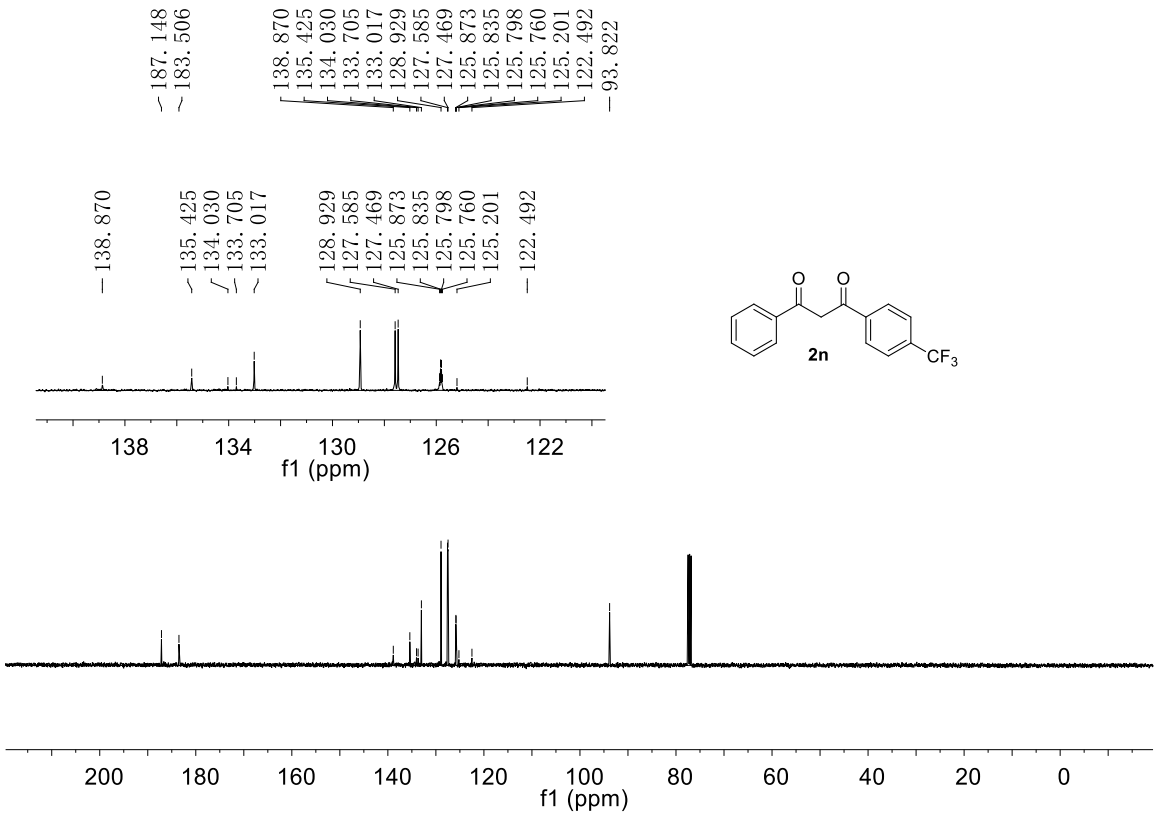

Cl
O
O
2l

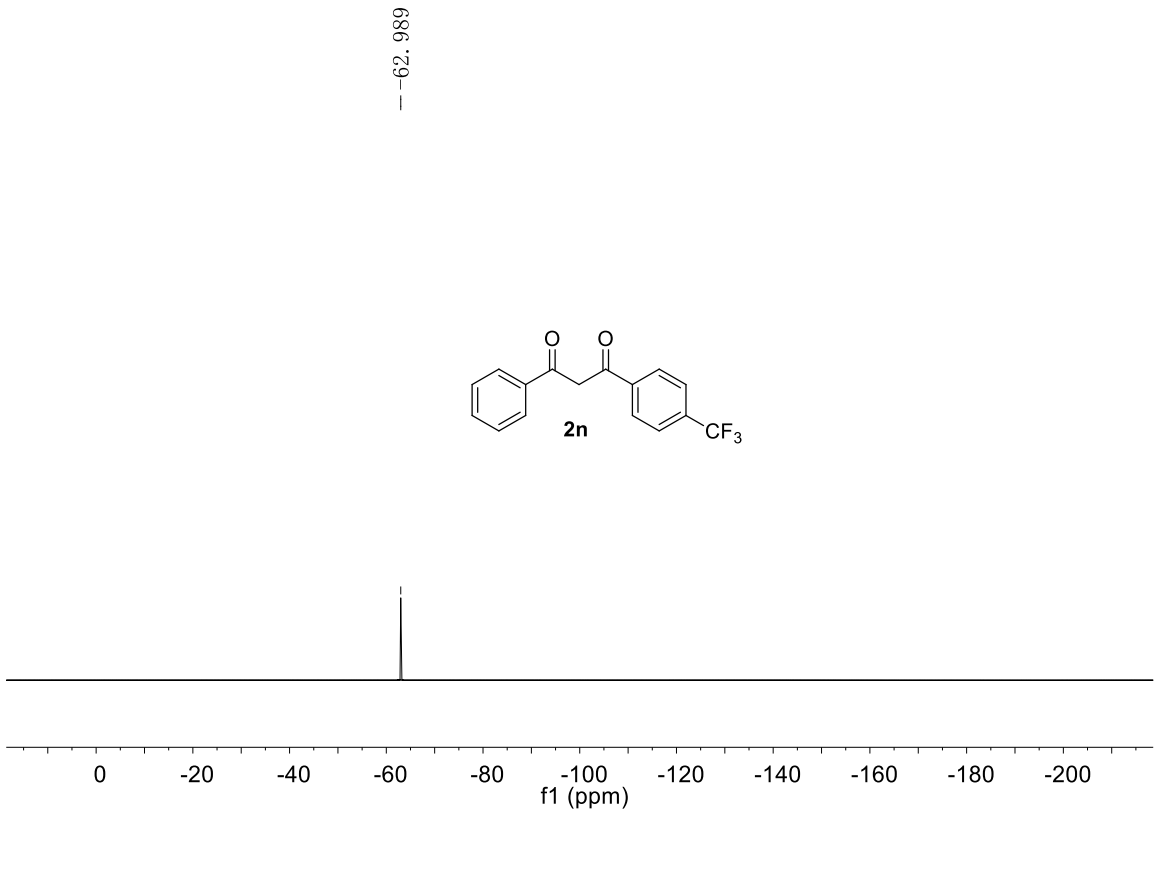

200
180
160
140
120
100
80
60
40
20
0
f1 (ppm)

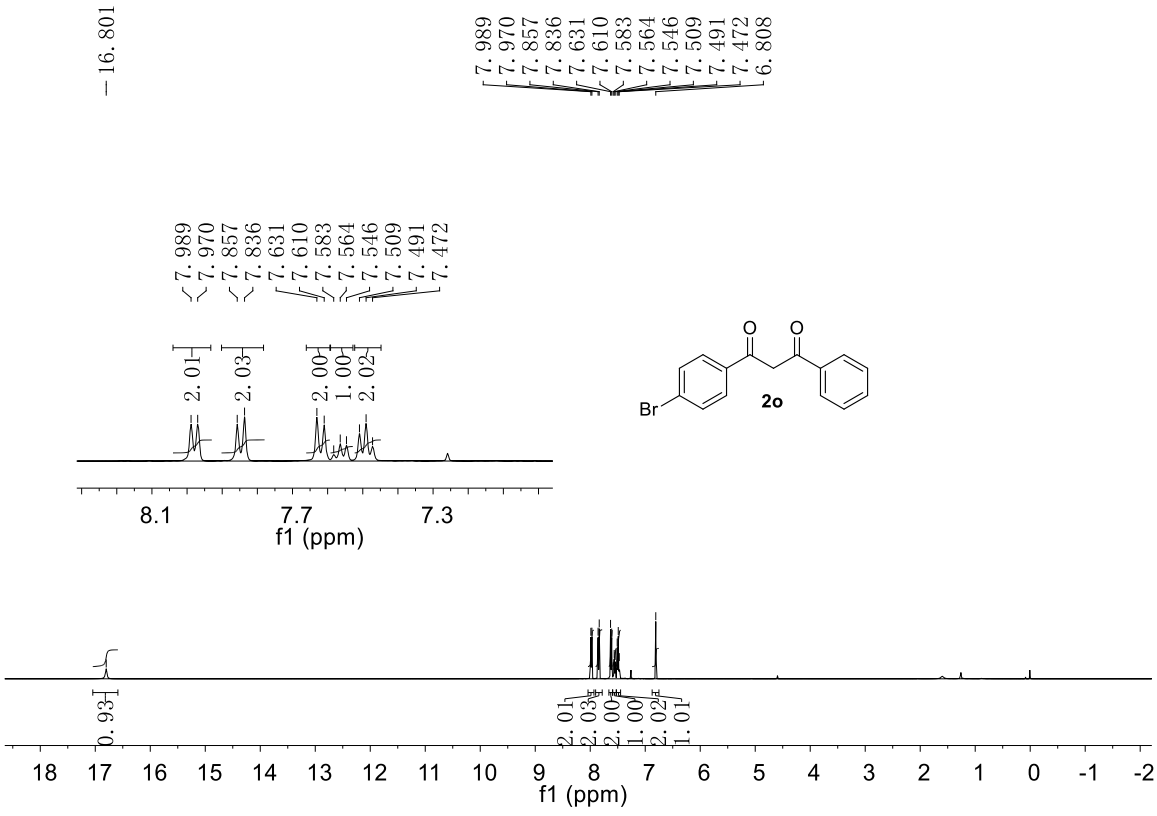

16.848
8.030
8.024
8.016
8.012
8.007
7.999
7.993
7.990
7.972
7.968
7.580
7.562
7.556
7.546
7.544
7.511
7.495
7.492
7.478
7.474
7.190
7.185
7.169
7.147
6.803
4.29
1.10
2.06
2.05
1.00
7.5
f1 (ppm)
O
O
F
2m
1.02
4.29
1.10
2.06
2.05
1.00
21
19
17
15
13
11
9
8
7
6
5
4
3
2
1
0
-1
-2
f1 (ppm)
185.211
166.774
164.250
132.608
129.767
129.676
128.798
127.218
116.015
115.797
92.905
135.358
132.608
132.011
131.981
129.767
129.676
128.798
127.218
116.015
115.797
O
O
F
2m
128
f1 (ppm)
200
180
160
140
120
100
80
60
40
20
0
f1 (ppm)

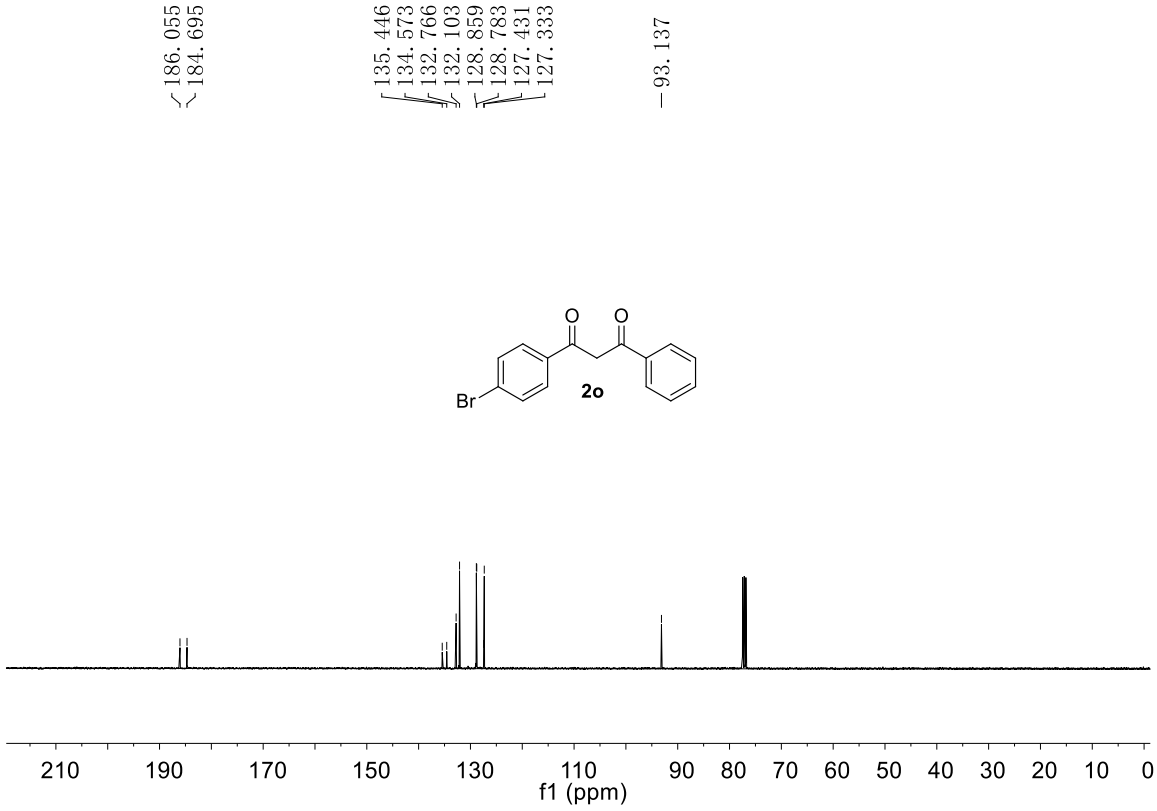

-106.243
-106.248
-106.256
-106.261
O
O
F
2m
0
-20
-40
-60
-80
-100
-120
-140
-160
-180
-200
f1 (ppm)

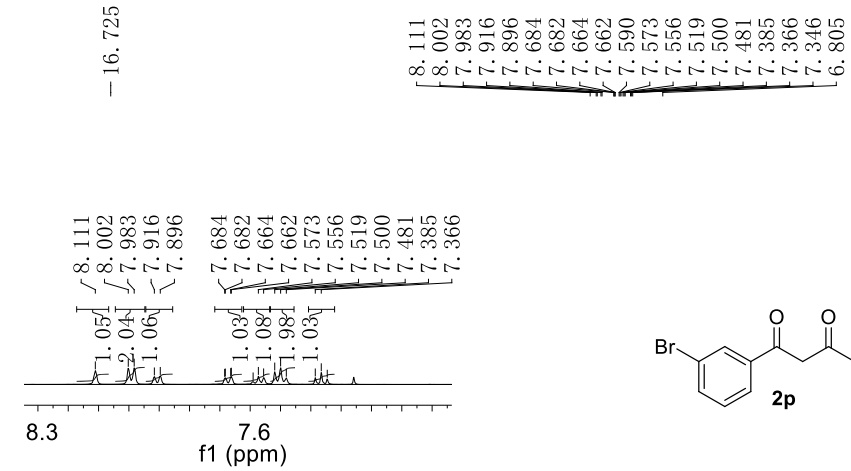

-16.719
8.097
8.076
8.013
7.994
7.762
7.741
7.605
7.587
7.569
7.530
7.510
7.492
6.870
2.04
1.95
2.01
1.02
1.95
1.00
O
O
2n
CF3
8.3
7.9
7.5
7.1
f1 (ppm)
1.07
2.04
1.95
2.01
1.02
1.95
1.00
18
17
16
15
14
13
12
11
10
9
8
7
6
5
4
3
2
1
0
-1
f1 (ppm)

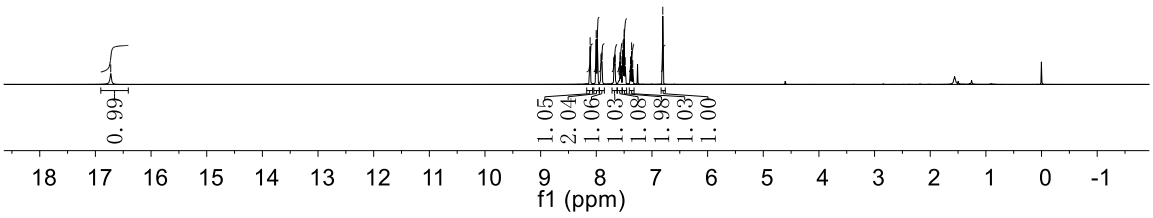

187.148
183.506
138.870
135.425
134.030
133.705
133.017
128.929
127.585
127.469
125.873
125.835
125.798
125.760
125.201
122.492
93.822
O
O
2n
CF3
f1 (ppm)

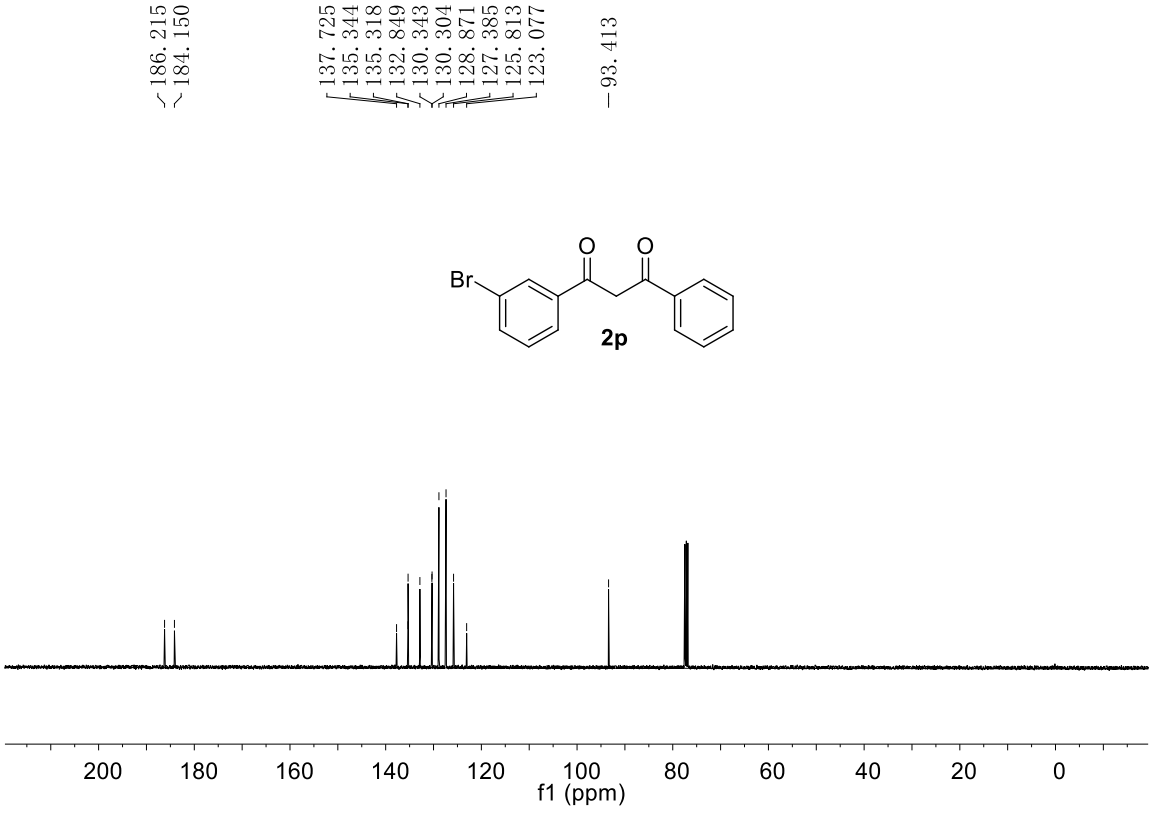

-62.989
O
O
2n
CF3
f1 (ppm)

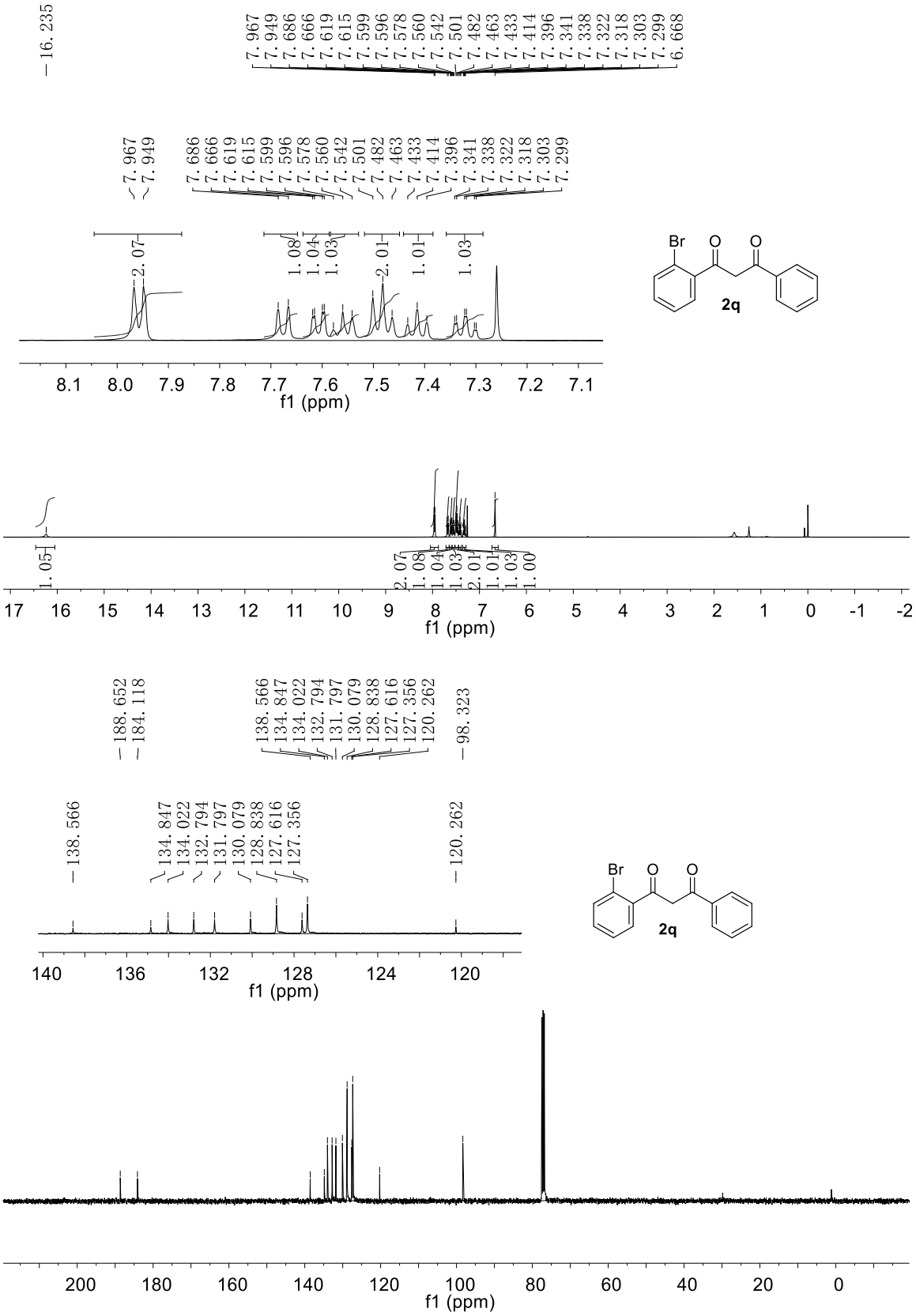

16.801
7.989
7.970
7.857
7.836
7.631
7.610
7.583
7.564
7.546
7.509
7.491
7.472
6.808
2.01
2.03
2.00
1.00
2.02
8.1
7.7
7.3
f1 (ppm)
O
O
Br
2o
0.93
2.01
2.03
2.00
1.00
2.02
1.01
18 17 16 15 14 13 12 11 10 9 8 7 6 5 4 3 2 1 0 -1 -2
f1 (ppm)

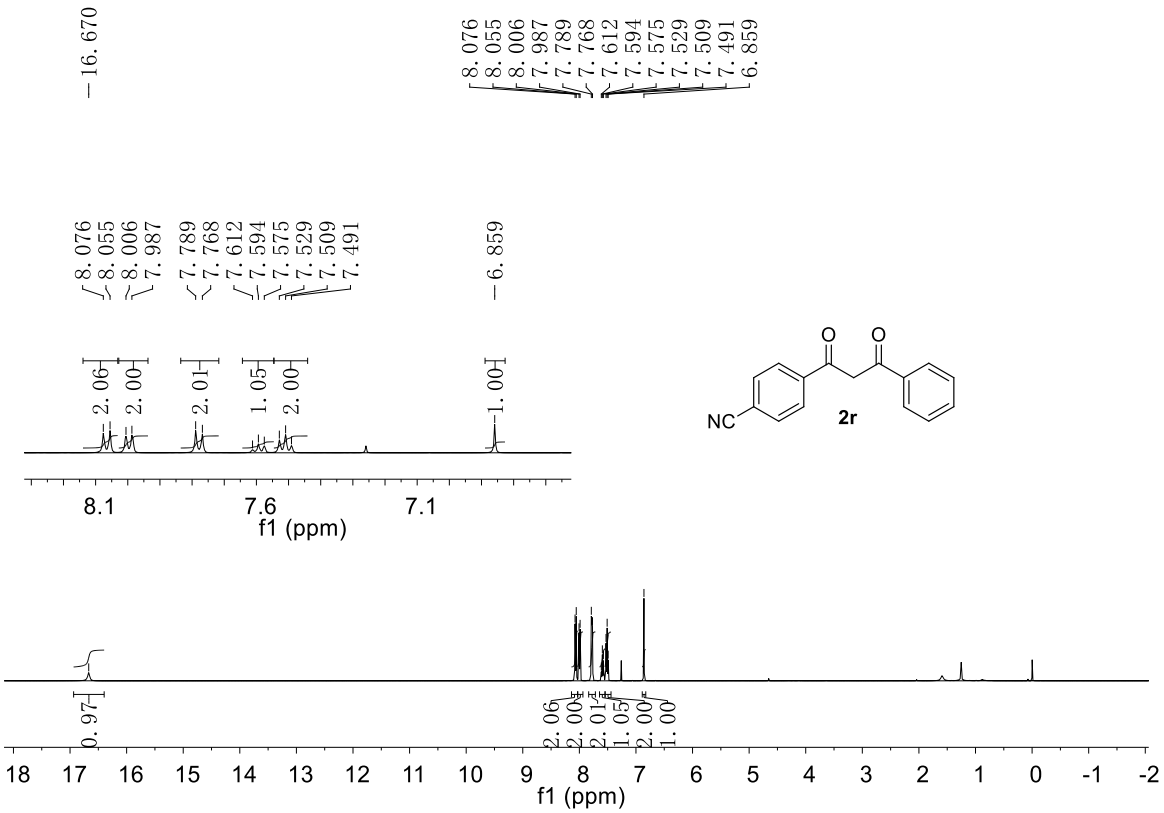

186.055
184.695
135.446
134.573
132.766
132.103
128.859
128.783
127.431
127.333
93.137
O
O
Br
2o
210 190 170 150 130 110 90 80 70 60 50 40 30 20 10 0
f1 (ppm)

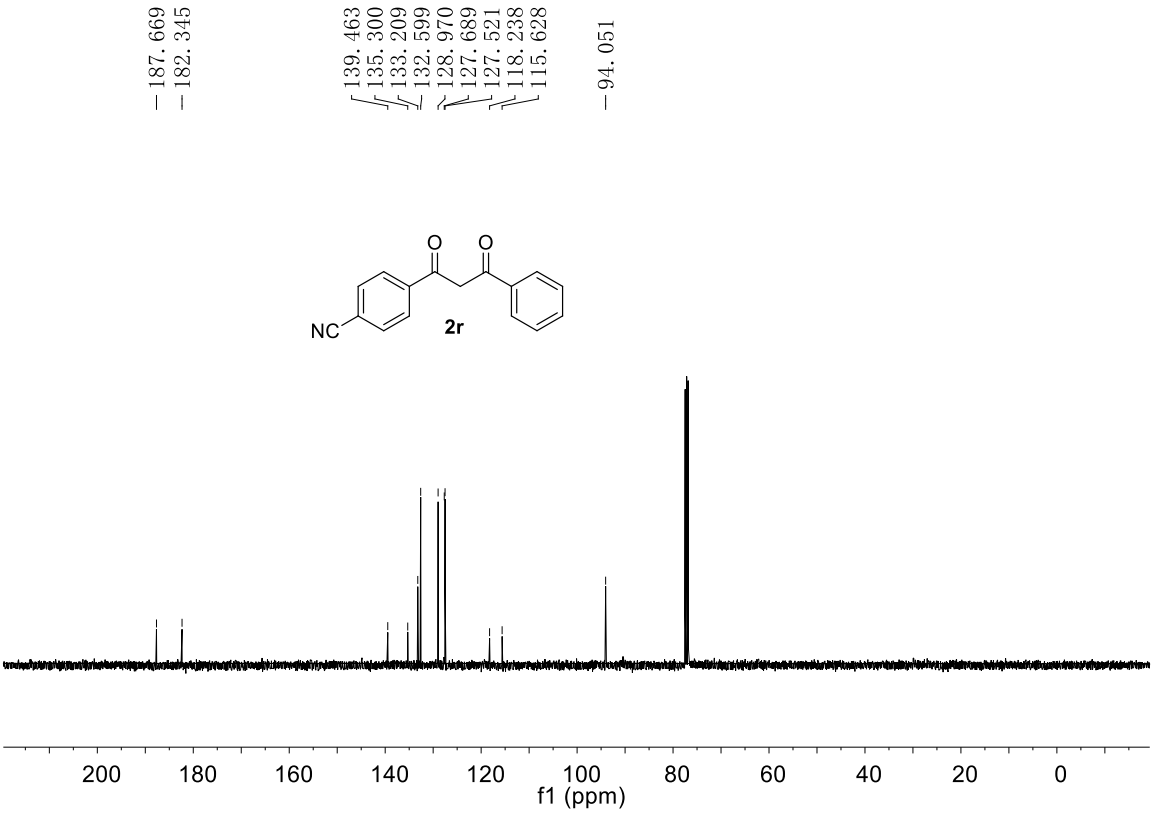

16.725
8.111
8.002
7.983
7.916
7.896
7.684
7.682
7.664
7.662
7.590
7.573
7.556
7.519
7.500
7.481
7.385
7.366
7.346
6.805
1.05
2.04
1.06
1.03
1.08
1.98
1.03
8.3
7.6
f1 (ppm)
Br
O
O
2p

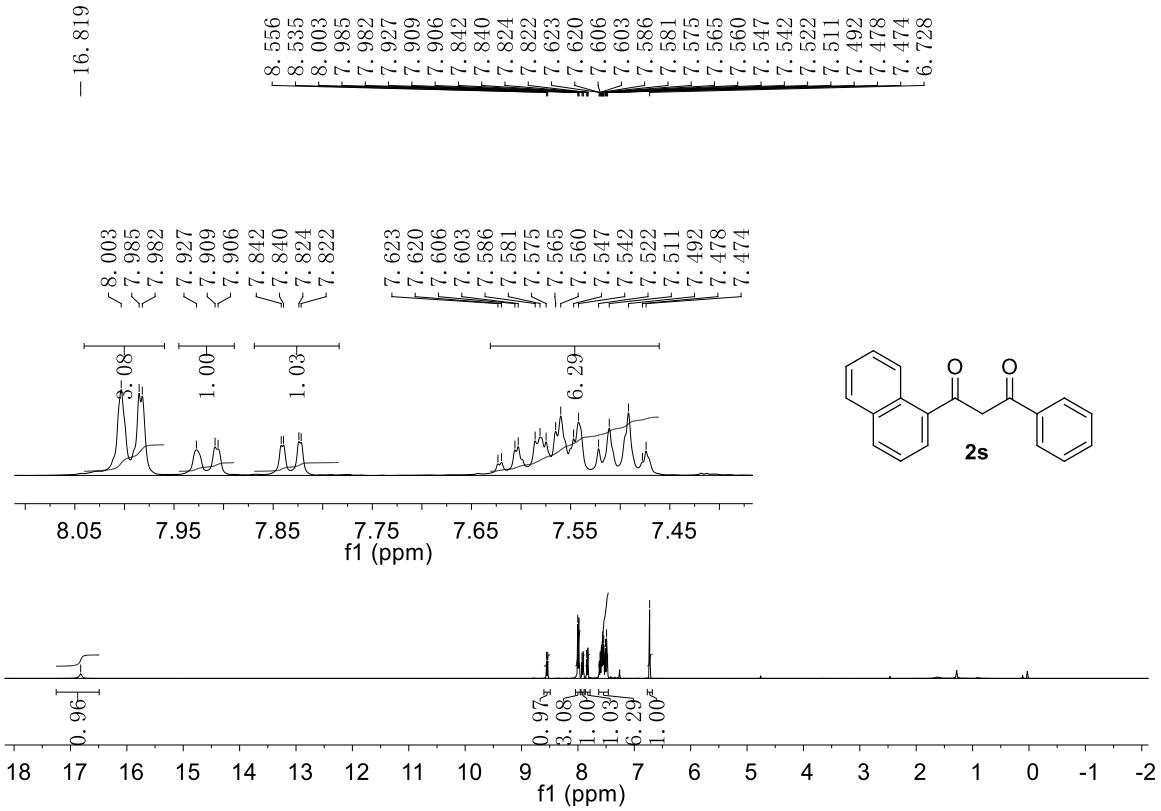

0.99
1.05
2.04
1.06
1.03
1.08
1.98
1.03
1.00
18 17 16 15 14 13 12 11 10 9 8 7 6 5 4 3 2 1 0 -1
f1 (ppm)

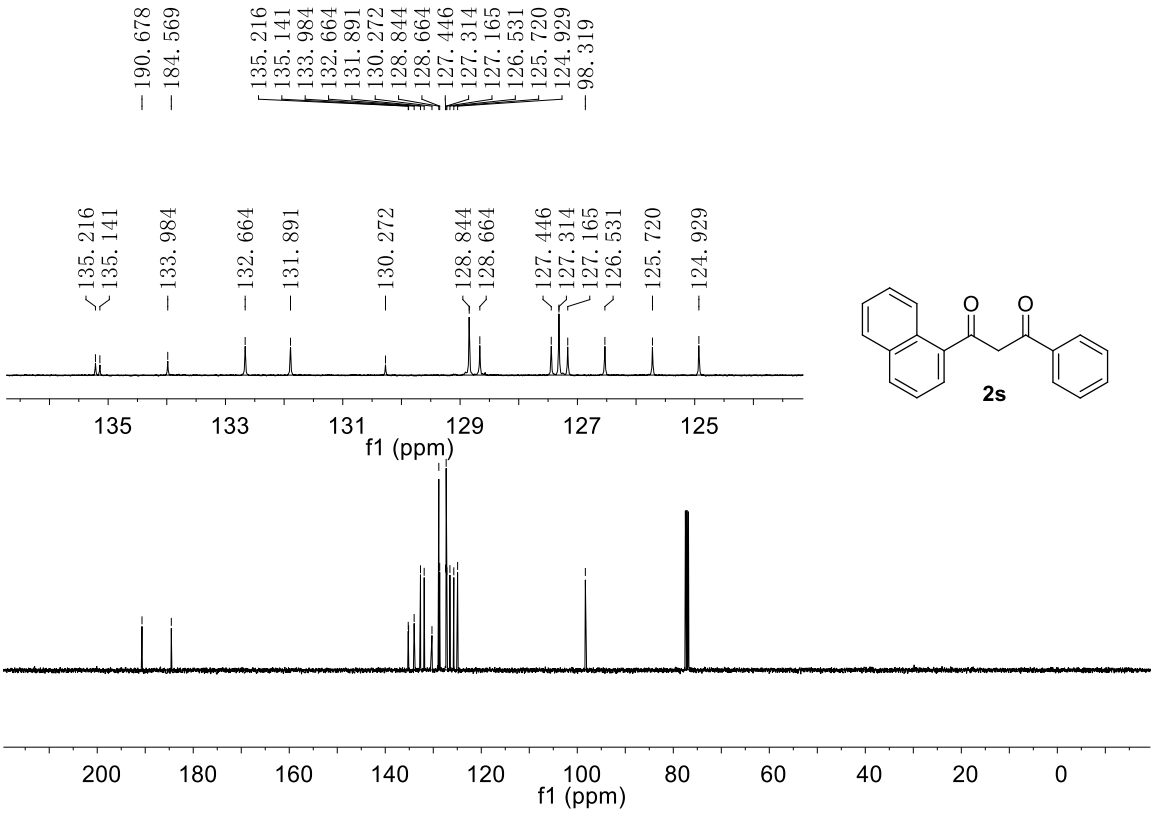

186.215
184.150
137.725
135.344
135.318
132.849
130.343
130.304
128.871
127.385
125.813
123.077
93.413
Br
O
O
2p
200 180 160 140 120 100 80 60 40 20 0
f1 (ppm)

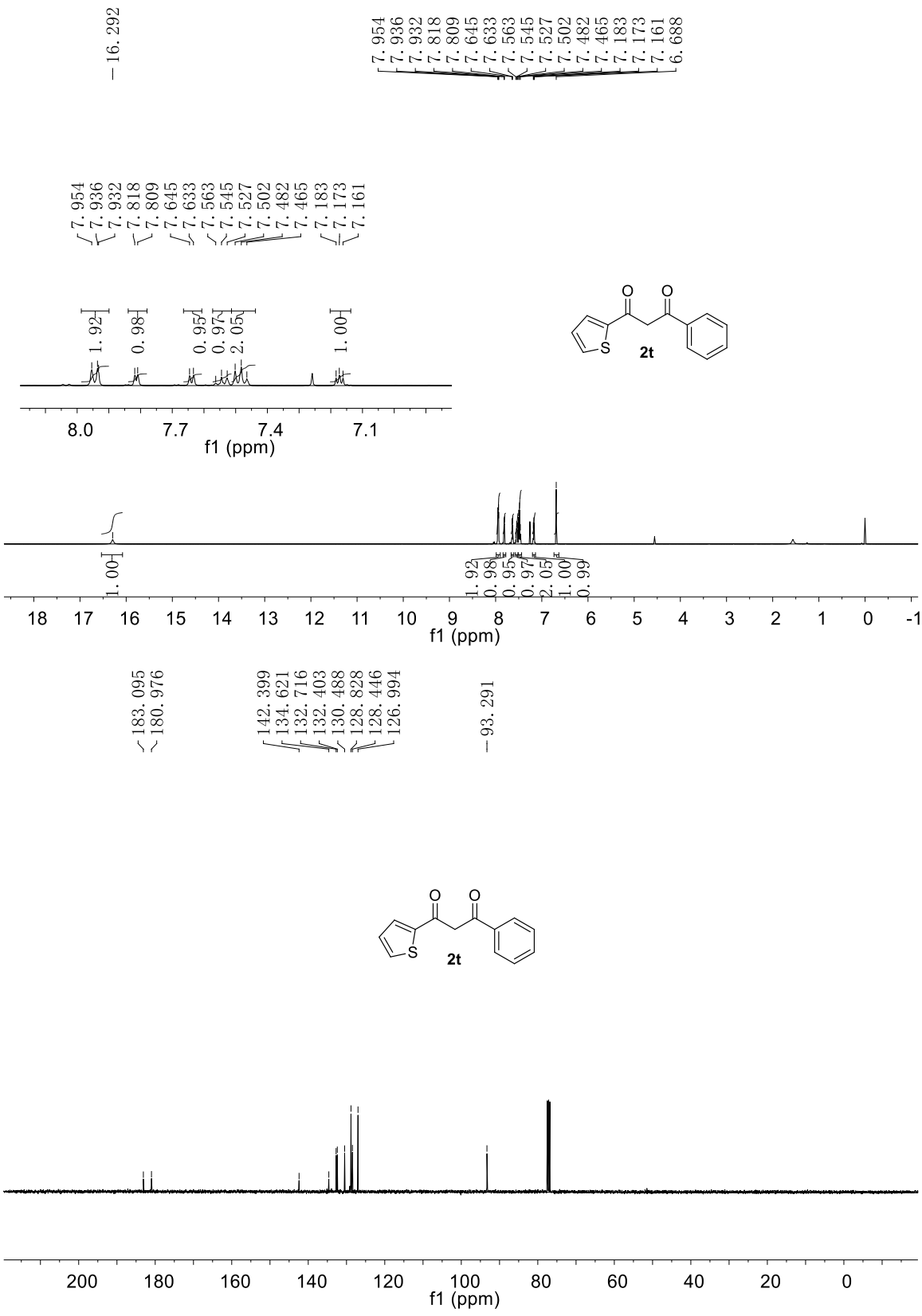

16.235
7.967
7.949
7.686
7.666
7.619
7.615
7.599
7.596
7.578
7.560
7.542
7.501
7.482
7.463
7.433
7.414
7.396
7.341
7.338
7.322
7.318
7.303
7.299
6.668
2.07
1.08
1.04
1.03
2.01
1.01
1.03
Br
O
O
2q
f1 (ppm)
1.05
2.07
1.08
1.04
1.03
2.01
1.01
1.03
1.00
f1 (ppm)
188.652
184.118
138.566
134.847
134.022
132.794
131.797
130.079
128.838
127.616
127.356
120.262
98.323
f1 (ppm)
f1 (ppm)


16.670
8.076
8.055
8.006
7.987
7.789
7.768
7.612
7.594
7.575
7.529
7.509
7.491
6.859
2.06
2.00
2.01
1.05
2.00
1.00
0.97
NC
2r
f1 (ppm)

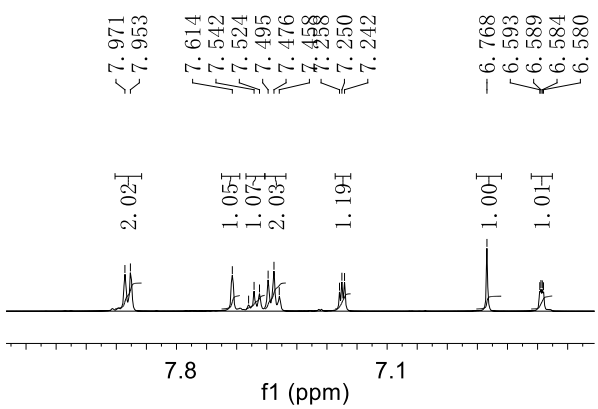

187.669
182.345
139.463
135.300
133.209
132.599
128.970
127.689
127.521
118.238
115.628
94.051
NC
2r
f1 (ppm)

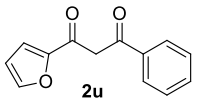

16.819
8.556
8.535
8.003
7.985
7.982
7.927
7.909
7.906
7.842
7.840
7.824
7.822
7.623
7.620
7.606
7.603
7.586
7.581
7.575
7.565
7.560
7.547
7.542
7.522
7.511
7.492
7.478
7.474
6.728
3.08
1.00
1.03
6.29
0.96
0.97
f1 (ppm)
2s

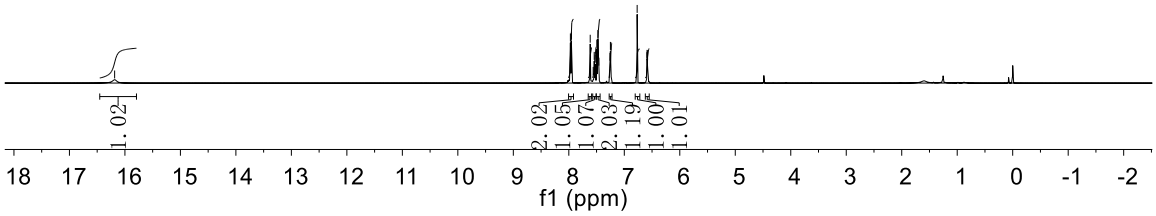

190.678
184.569
135.216
135.141
133.984
132.664
131.891
130.272
128.844
128.664
127.446
127.314
127.165
126.531
125.720
124.929
98.319
f1 (ppm)
2s

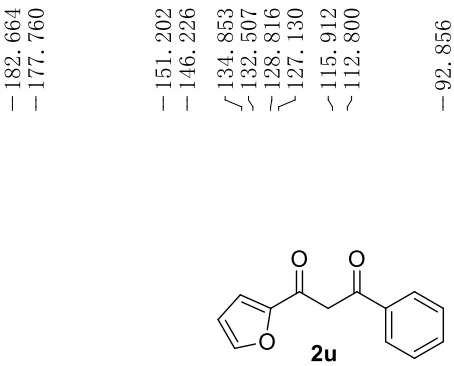

16.292
7.954
7.936
7.932
7.818
7.809
7.645
7.633
7.563
7.545
7.527
7.502
7.482
7.465
7.183
7.173
7.161
6.688
1.92
0.98
0.95
0.97
2.05
1.00
f1 (ppm)
O
O
S
2t
1.00
1.92
0.98
0.95
0.97
2.05
1.00
0.99
f1 (ppm)
183.095
180.976
142.399
134.621
132.716
132.403
130.488
128.828
128.446
126.994
93.291
f1 (ppm)


16.185
7.971
7.953
7.614
7.560
7.542
7.524
7.495
7.476
7.458
7.258
7.250
7.242
6.768
6.593
6.589
6.584
6.580

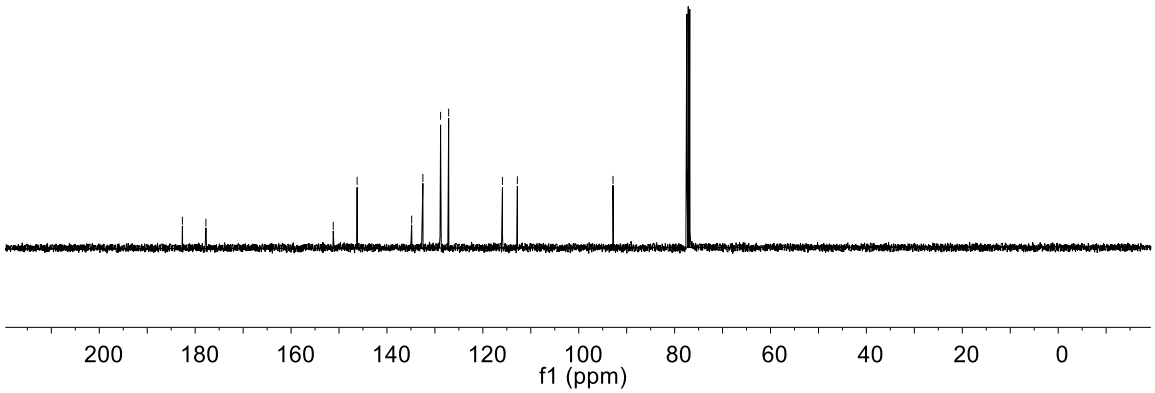

7.971
7.953
7.614
7.542
7.524
7.495
7.476
7.458
7.258
7.250
7.242
6.768
6.593
6.589
6.584
6.580
2.02
1.05
1.07
2.03
1.19
1.00
1.01
7.8
7.1
f1 (ppm)

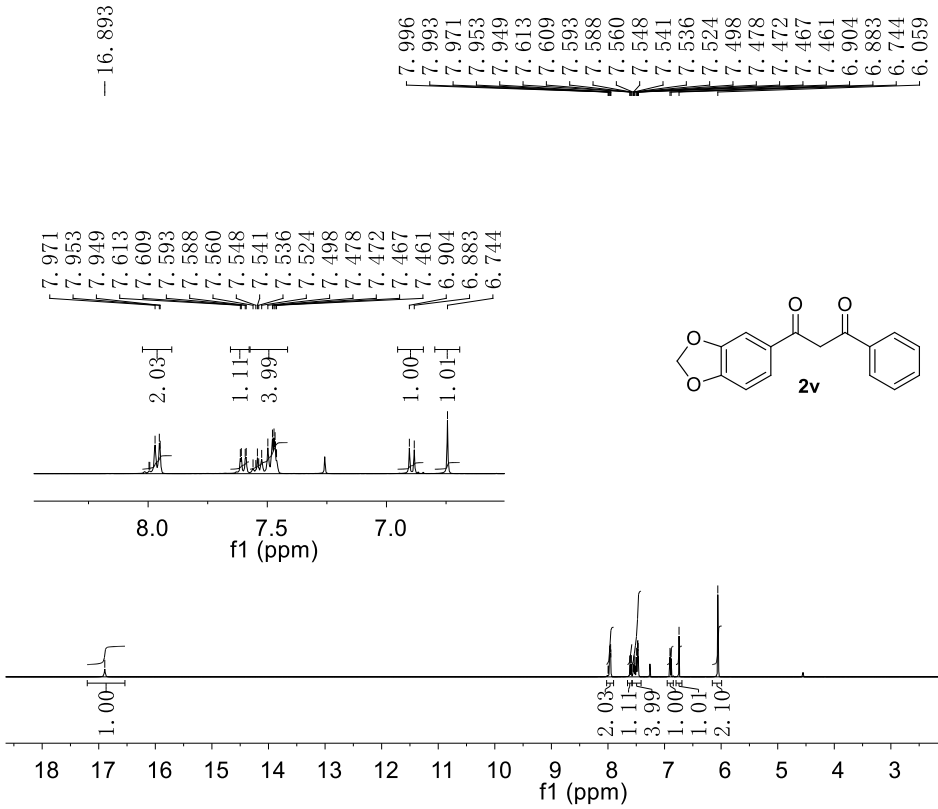

O
O
O
2u


1.02
2.02
1.05
1.07
2.03
1.19
1.00
1.01
18
17
16
15
14
13
12
11
10
9
8
7
6
5
4
3
2
1
0
-1
-2
f1 (ppm)


182.664
177.760
151.202
146.226
134.853
132.507
128.816
127.130
115.912
112.800
92.856

O
O
O
2u


200
180
160
140
120
100
80
60
40
20
0
f1 (ppm)


16.893
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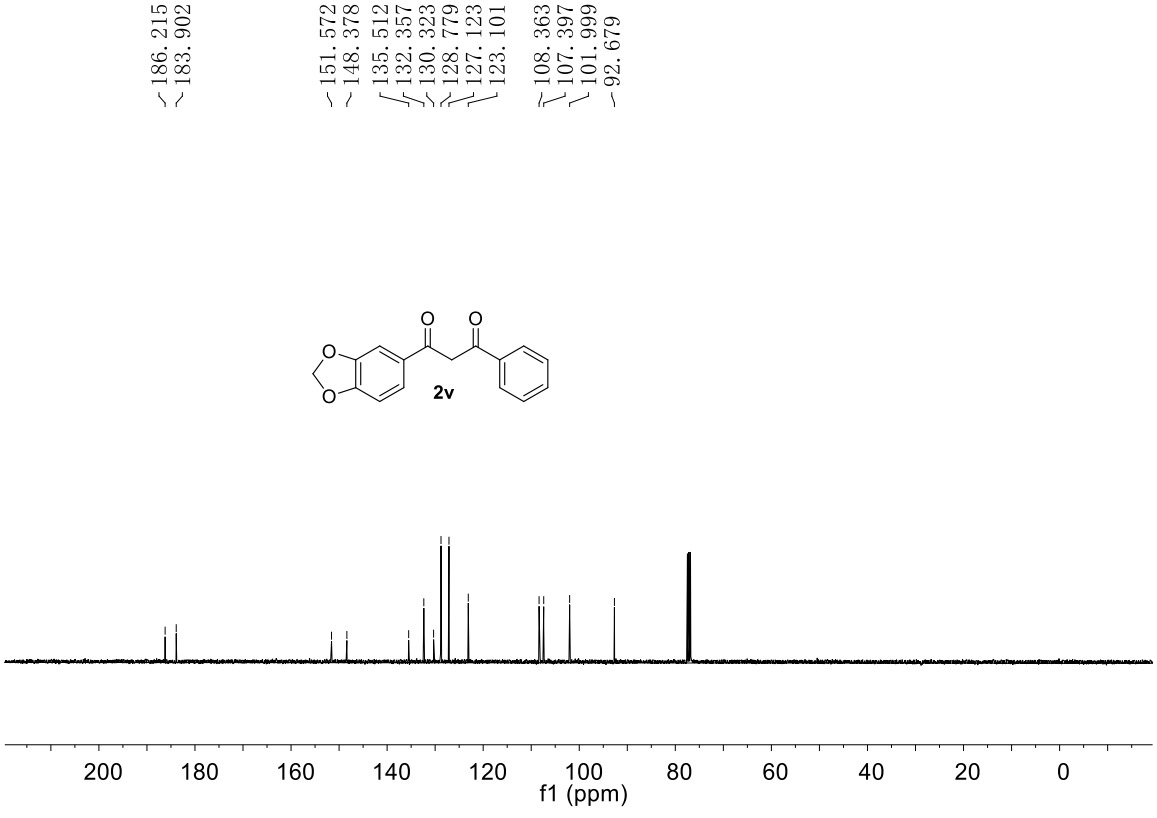
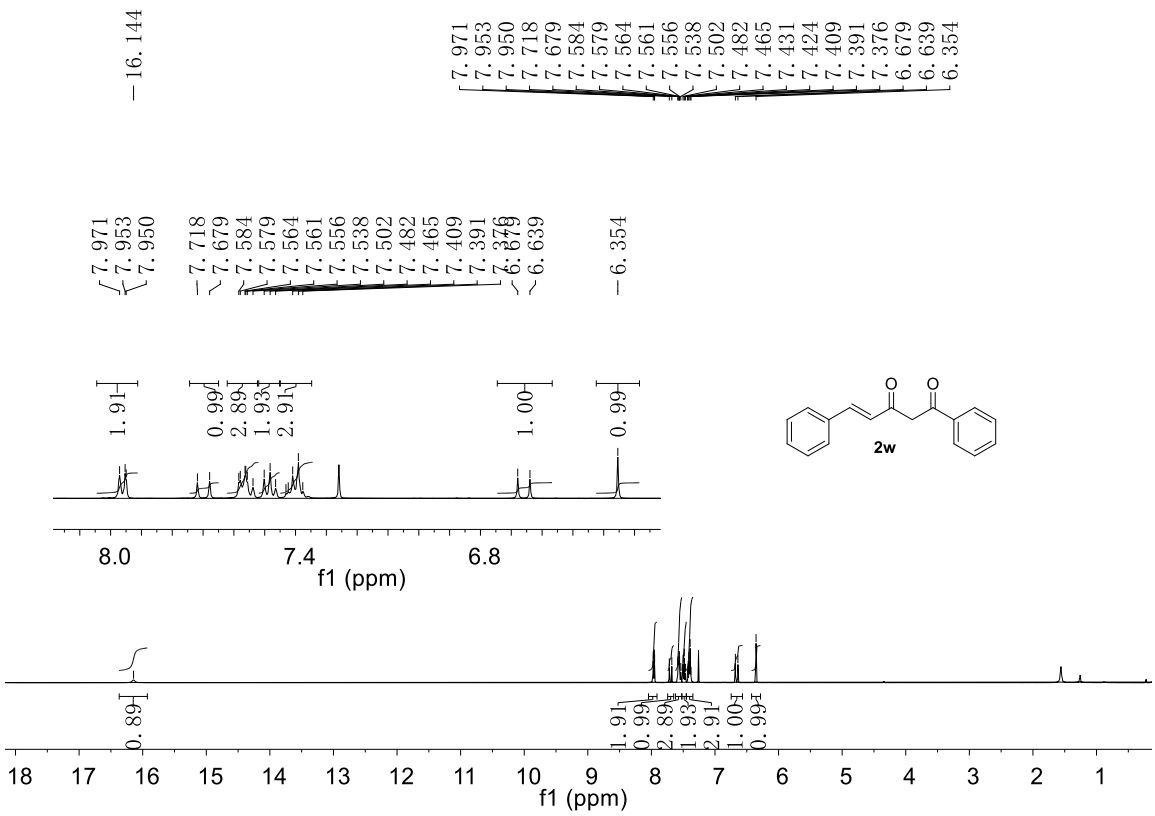
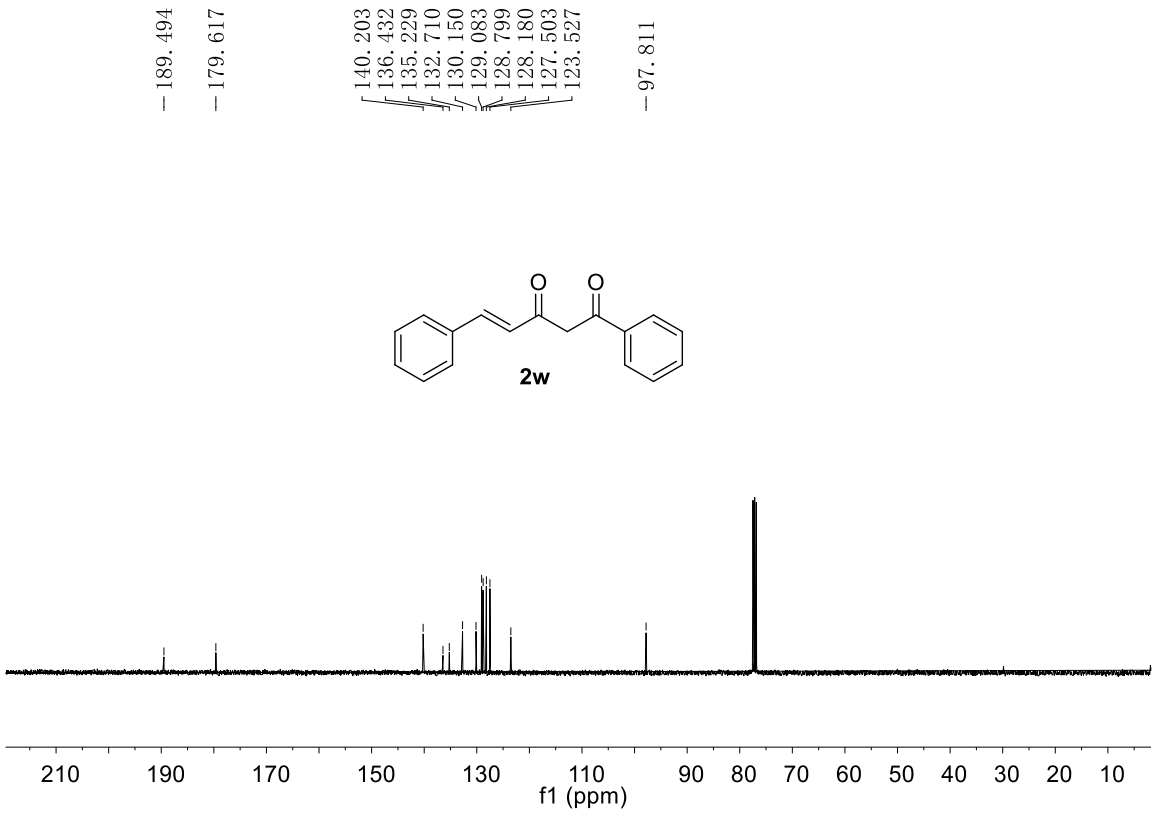
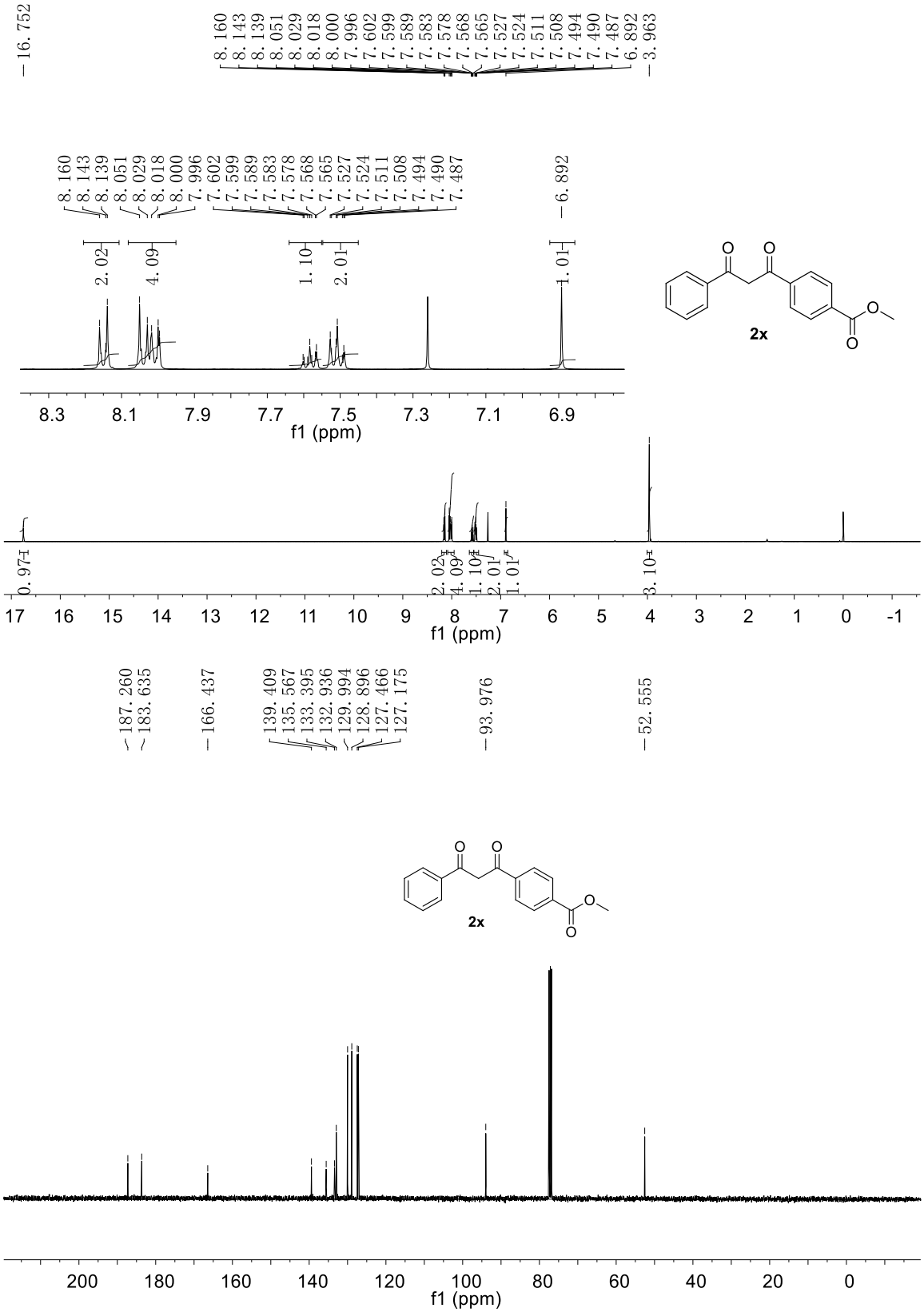
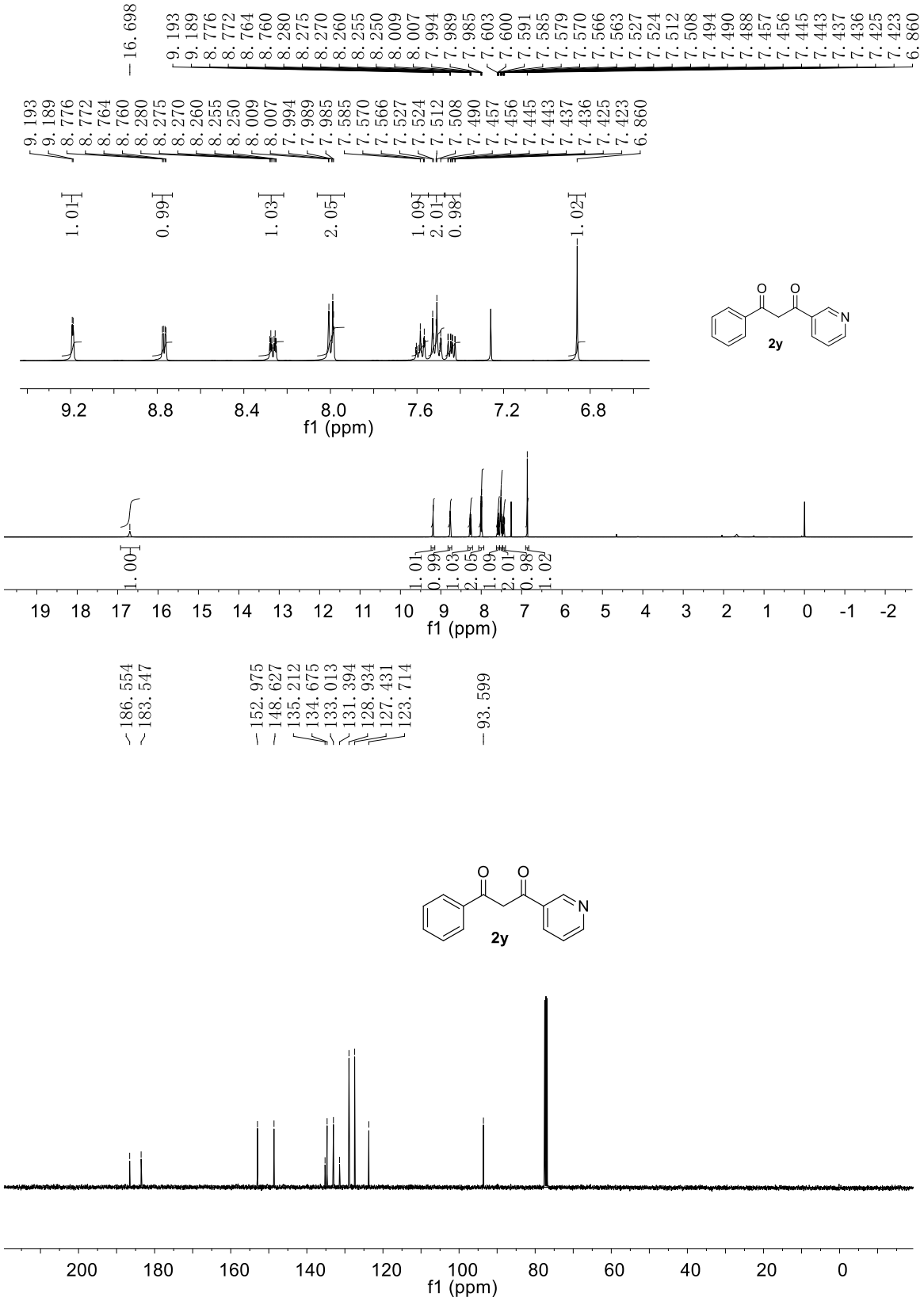
7.993
7.971
7.953
7.949
7.613
7.609
7.593
7.588
7.560
7.548
7.541
7.536
7.524
7.498
7.478
7.472
7.467
7.461
6.904
6.883
6.744
6.059
2v
2.03
1.11
3.99
1.00
1.01
8.0
7.5
7.0
f1 (ppm)
1.00
2.03
1.11
3.99
1.00
1.01
2.10
18 17 16 15 14 13 12 11 10 9 8 7 6 5 4 3 2 1 0 -1
f1 (ppm)

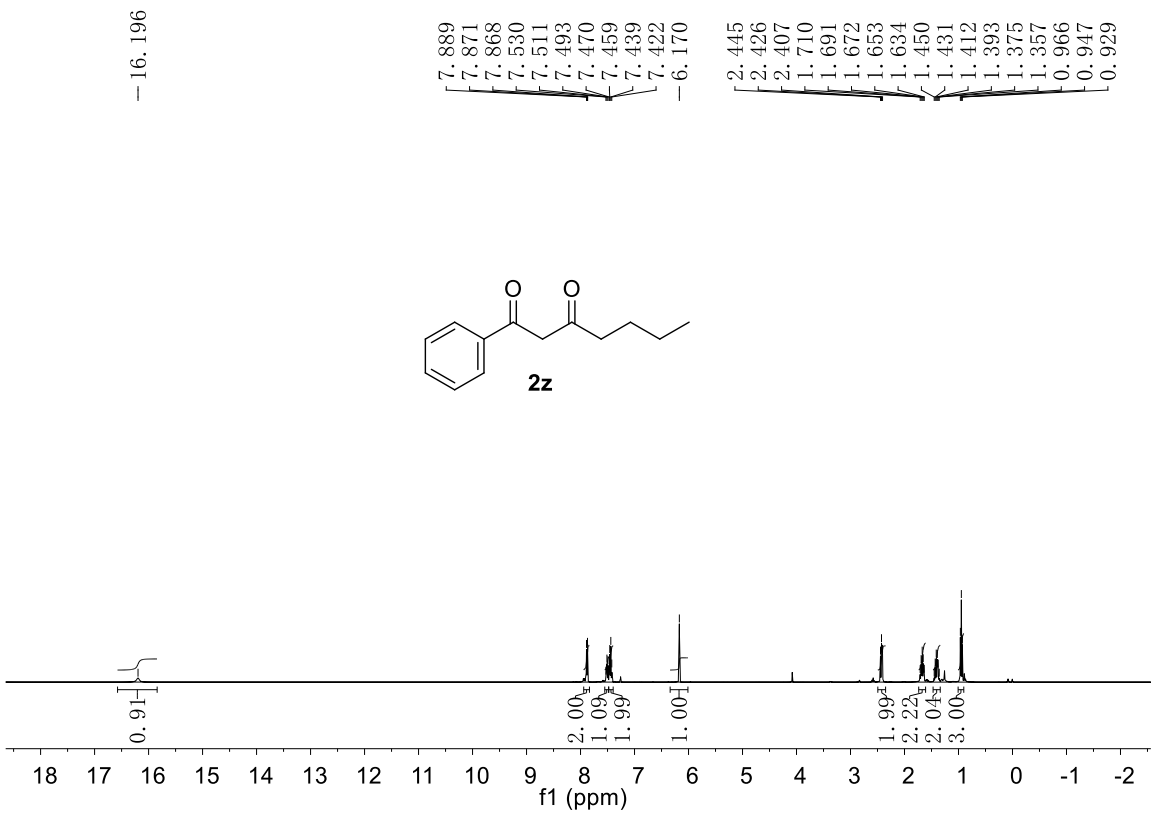

186.215
183.902
151.572
148.378
135.512
132.357
130.323
128.779
127.123
123.101
108.363
107.397
101.999
92.679
2v
200 180 160 140 120 100 80 60 40 20 0
f1 (ppm)

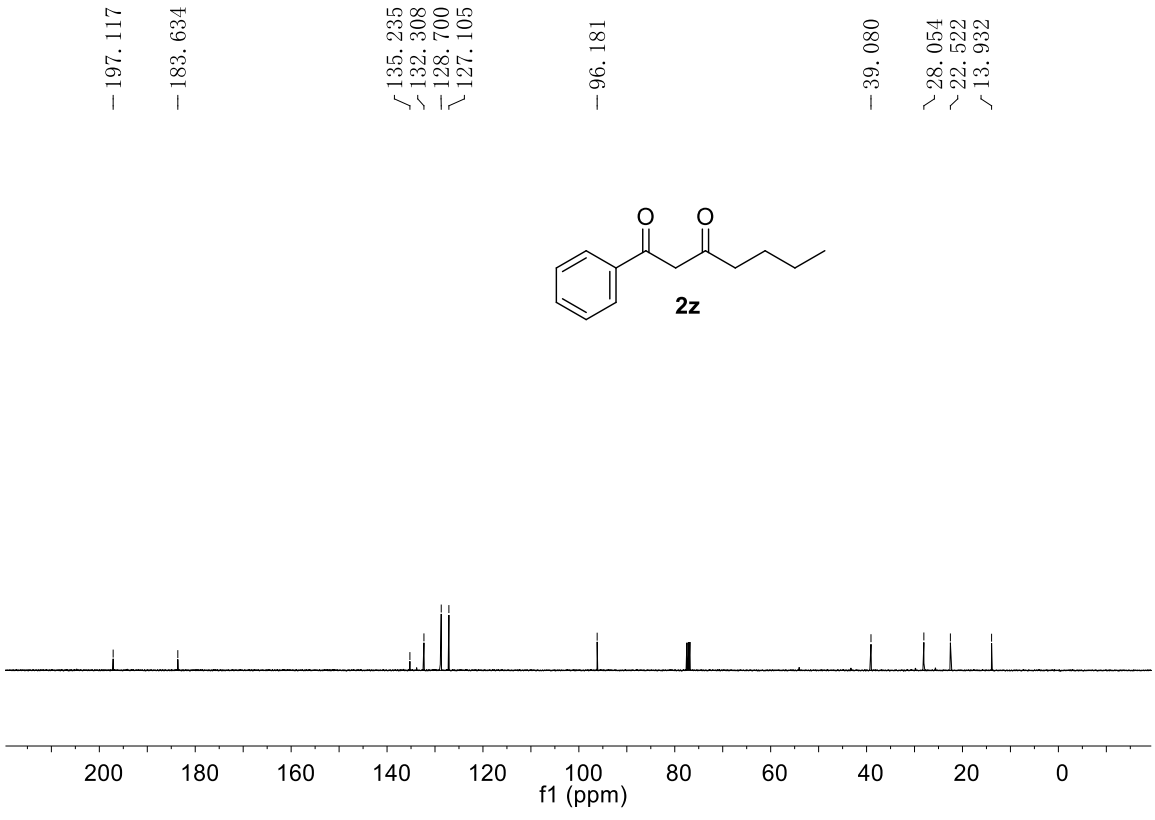

16.144
7.971
7.953
7.950
7.718
7.679
7.584
7.579
7.564
7.561
7.556
7.538
7.502
7.482
7.465
7.431
7.424
7.409
7.391
7.376
6.679
6.639
6.354
1.91
0.99
2.89
1.93
2.91
1.00
0.99
2w
8.0
7.4
6.8
f1 (ppm)
0.89
1.91
0.99
2.89
1.93
2.91
1.00
0.99
18 17 16 15 14 13 12 11 10 9 8 7 6 5 4 3 2 1
f1 (ppm)

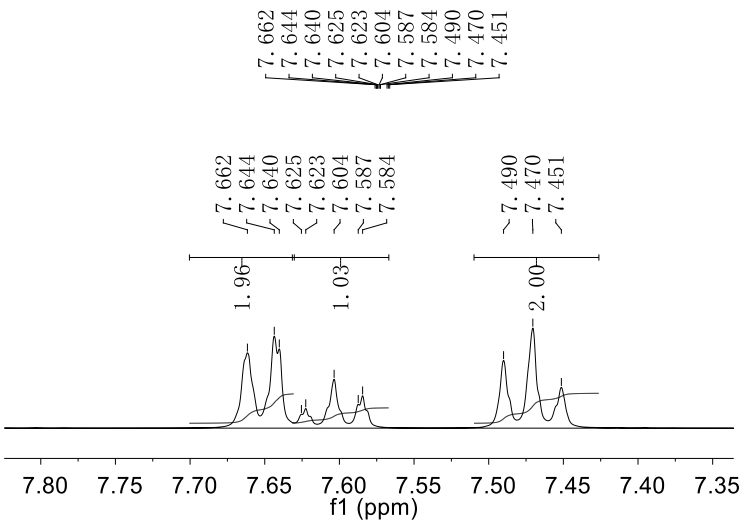

189.494
179.617
140.203
136.432
135.229
132.710
130.150
129.083
128.799
128.180
127.503
123.527
97.811
2w
210 190 170 150 130 110 90 80 70 60 50 40 30 20 10
f1 (ppm)


16.752
8.160
8.143
8.139
8.051
8.029
8.018
8.000
7.996
7.602
7.599
7.589
7.583
7.578
7.568
7.565
7.527
7.524
7.511
7.508
7.494
7.490
7.487
6.892
3.963
2.02
4.09
1.10
2.01
1.01
2x
f1 (ppm)
0.97
3.10
187.260
183.635
166.437
139.409
135.567
133.395
132.936
129.994
128.896
127.466
127.175
93.976
52.555


16.698
9.193
9.189
8.776
8.772
8.764
8.760
8.280
8.275
8.270
8.260
8.255
8.250
8.009
8.007
7.994
7.989
7.985
7.603
7.600
7.591
7.585
7.579
7.570
7.566
7.563
7.527
7.524
7.512
7.508
7.494
7.490
7.488
7.457
7.456
7.445
7.443
7.437
7.436
7.425
7.423
6.860
1.01
0.99
1.03
2.05
1.09
2.01
0.98
1.02
O
O
N
2y
f1 (ppm)
1.00
1.01
0.99
1.03
2.05
1.09
2.01
0.98
1.02
f1 (ppm)
186.554
183.547
152.975
148.627
135.212
134.675
133.013
131.394
128.934
127.431
123.714
93.599
O
O
N
2y
f1 (ppm)

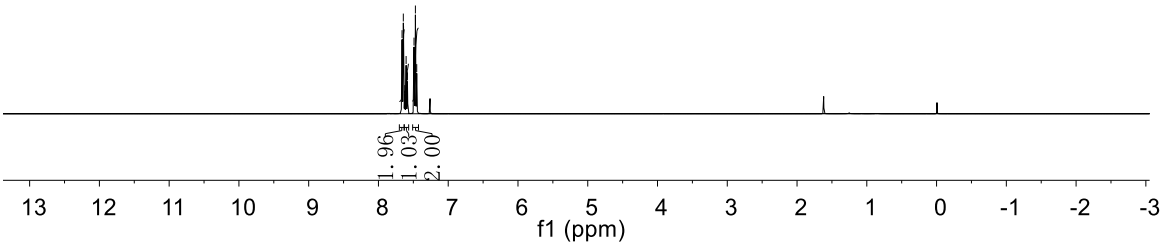

16.196
7.889
7.871
7.868
7.530
7.511
7.493
7.470
7.459
7.439
7.422
6.170
2.445
2.426
2.407
1.710
1.691
1.672
1.653
1.634
1.450
1.431
1.412
1.393
1.375
1.357
0.966
0.947
0.929
O
O
2z
0.91
2.00
1.09
1.99
1.00
1.99
2.22
2.04
3.00
18 17 16 15 14 13 12 11 10 9 8 7 6 5 4 3 2 1 0 -1 -2
f1 (ppm)


197.117
183.634
135.235
132.308
128.700
127.105
96.181
39.080
28.054
22.522
13.932
O
O
2z
200 180 160 140 120 100 80 60 40 20 0
f1 (ppm)


7.662
7.644
7.640
7.625
7.623
7.604
7.587
7.584
7.490
7.470
7.451
1.96
1.03
2.00
7.80 7.75 7.70 7.65 7.60 7.55 7.50 7.45 7.40 7.35
f1 (ppm)


CN

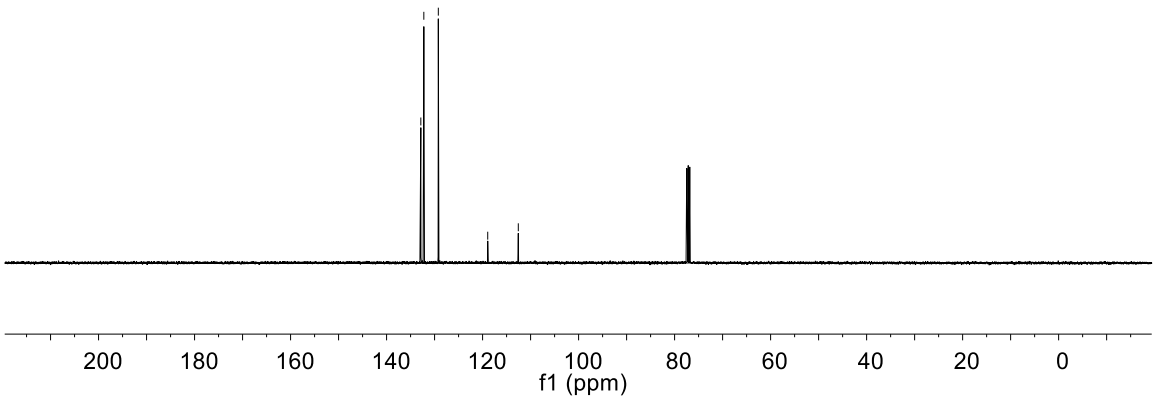
3a

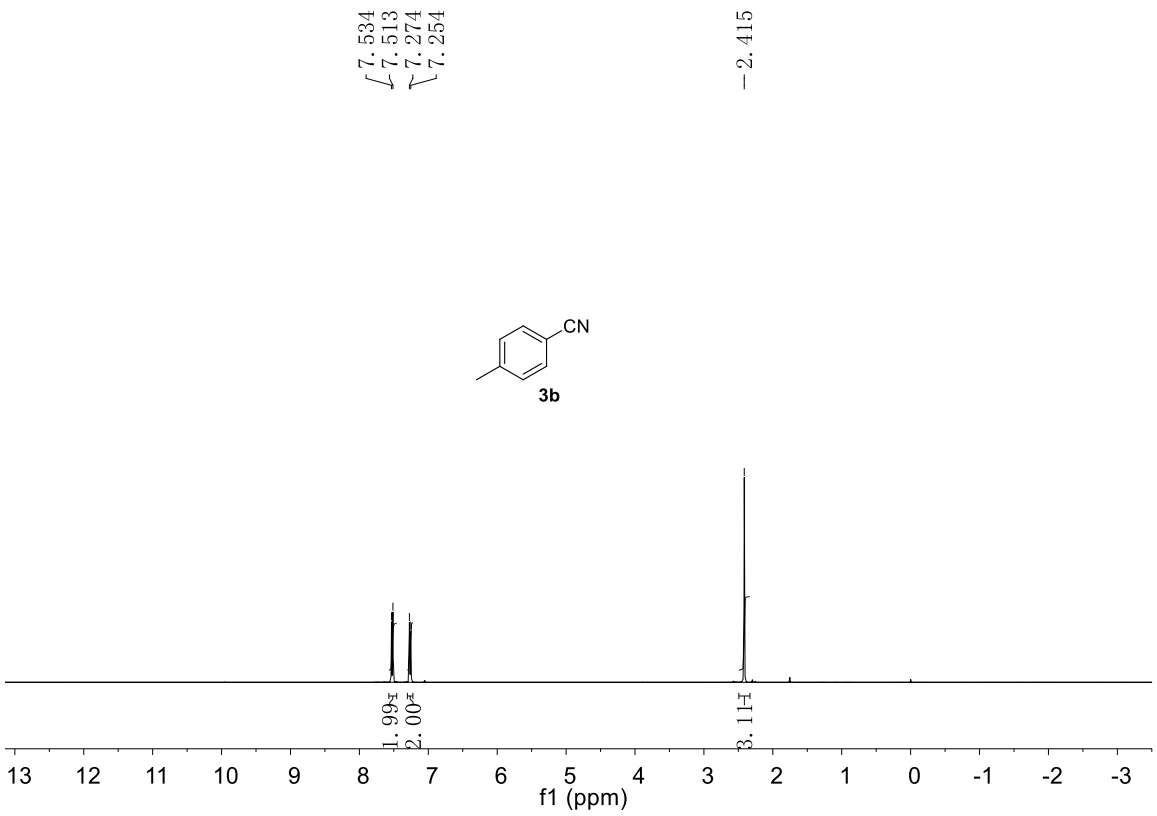

1.96
1.03
2.00
13 12 11 10 9 8 7 6 5 4 3 2 1 0 -1 -2 -3
f1 (ppm)

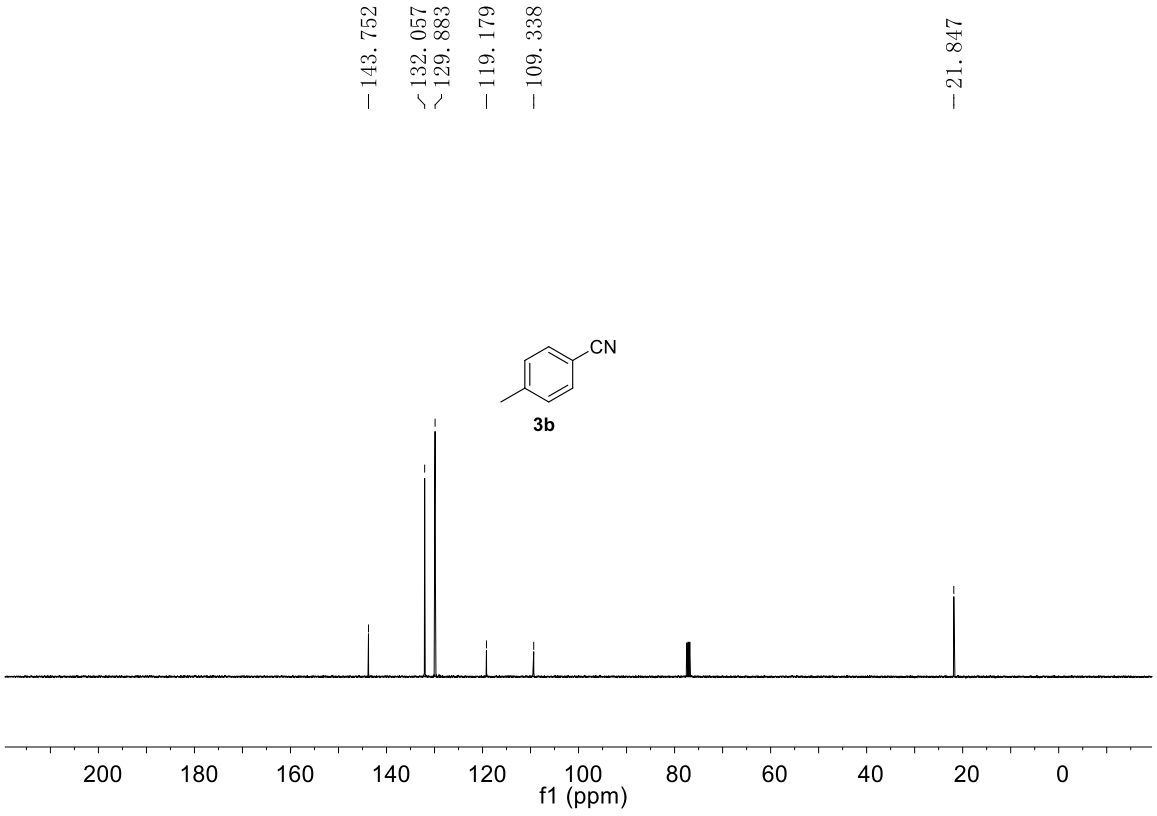

132.868
132.243
129.222
118.929
112.562

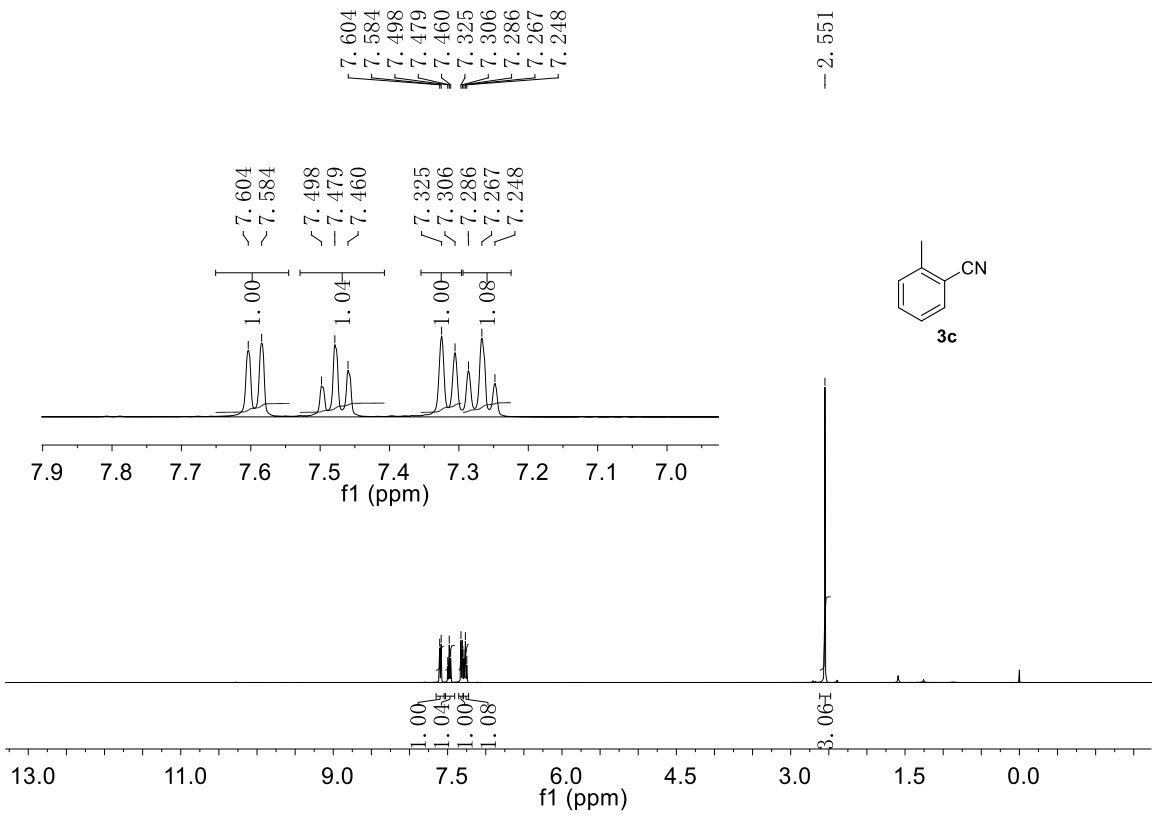

CN

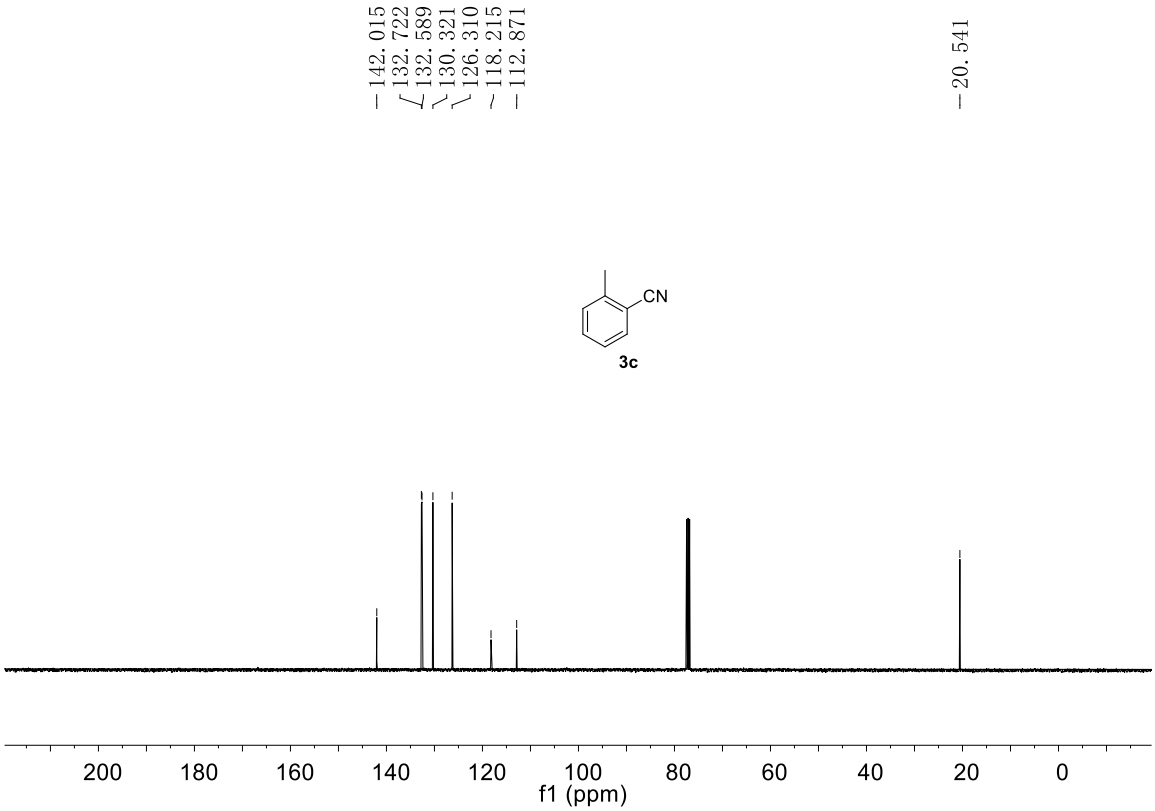
3a

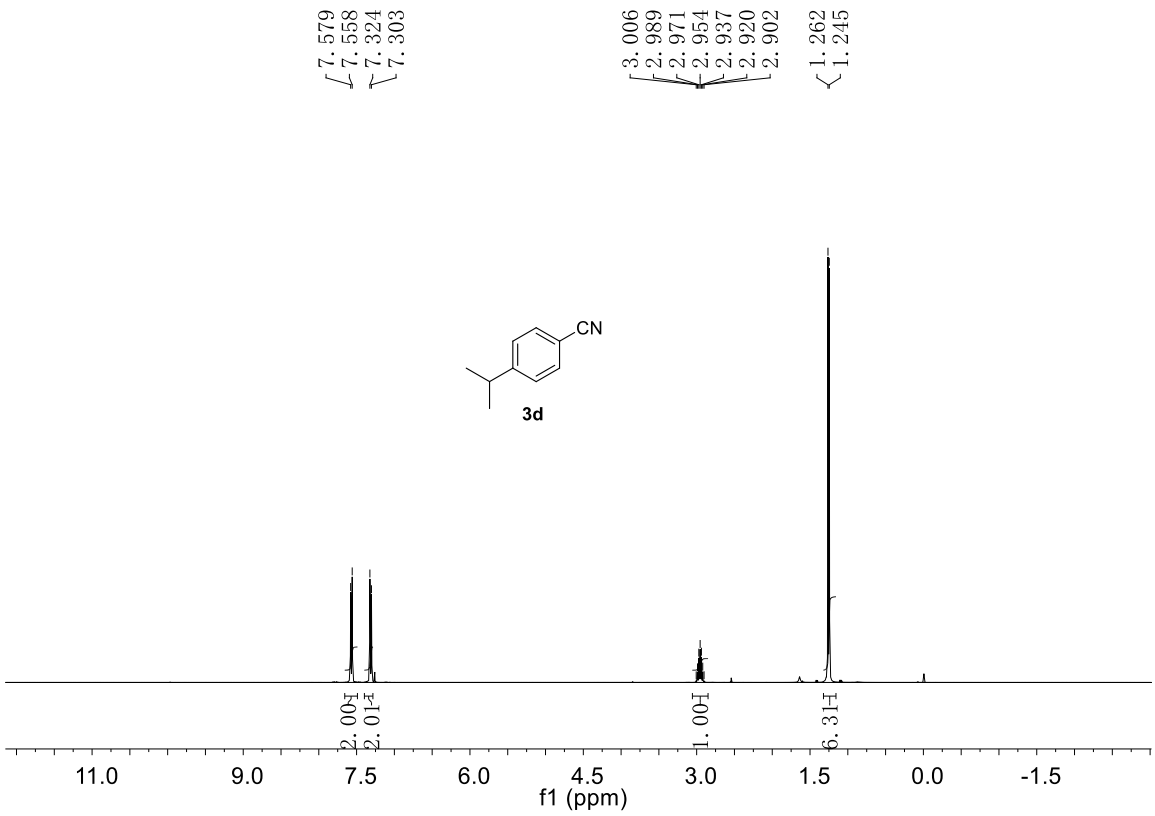

200 180 160 140 120 100 80 60 40 20 0
f1 (ppm)

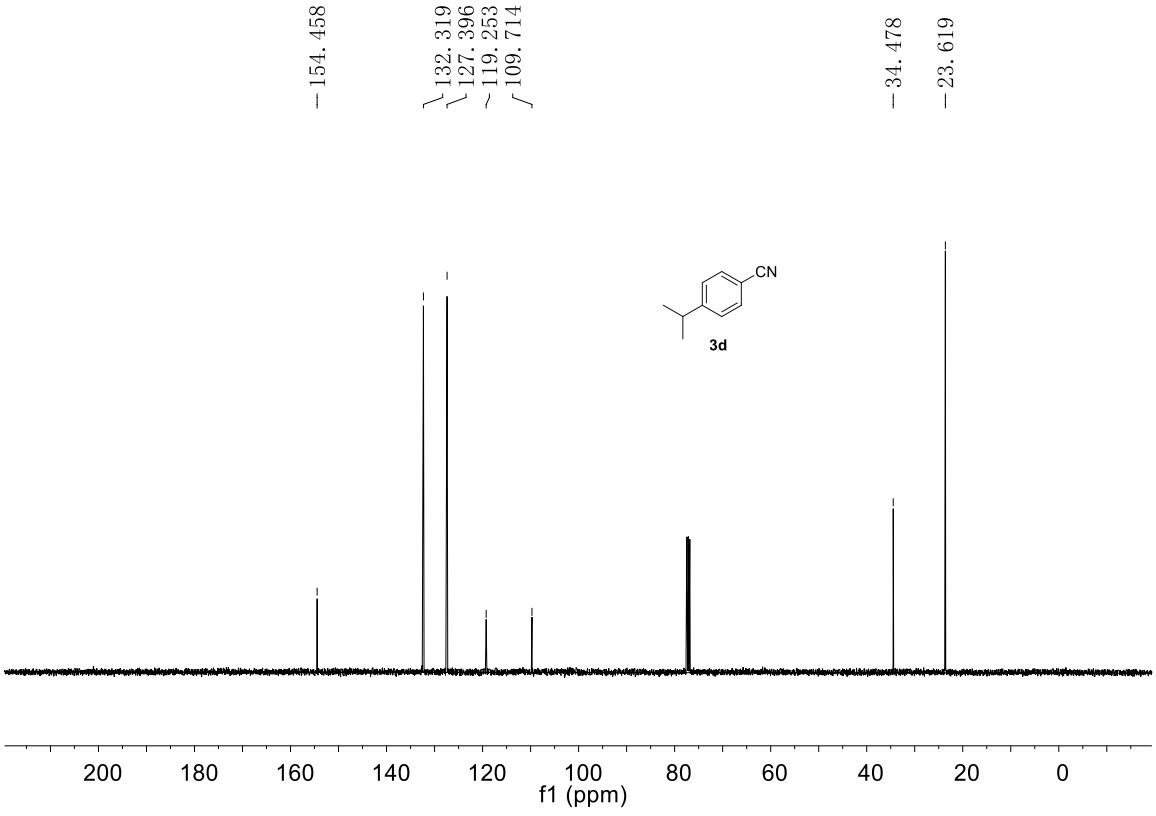

7.534
7.513
7.274
7.254
2.415
CN
3b
1.99
2.00
3.11
13 12 11 10 9 8 7 6 5 4 3 2 1 0 -1 -2 -3
f1 (ppm)

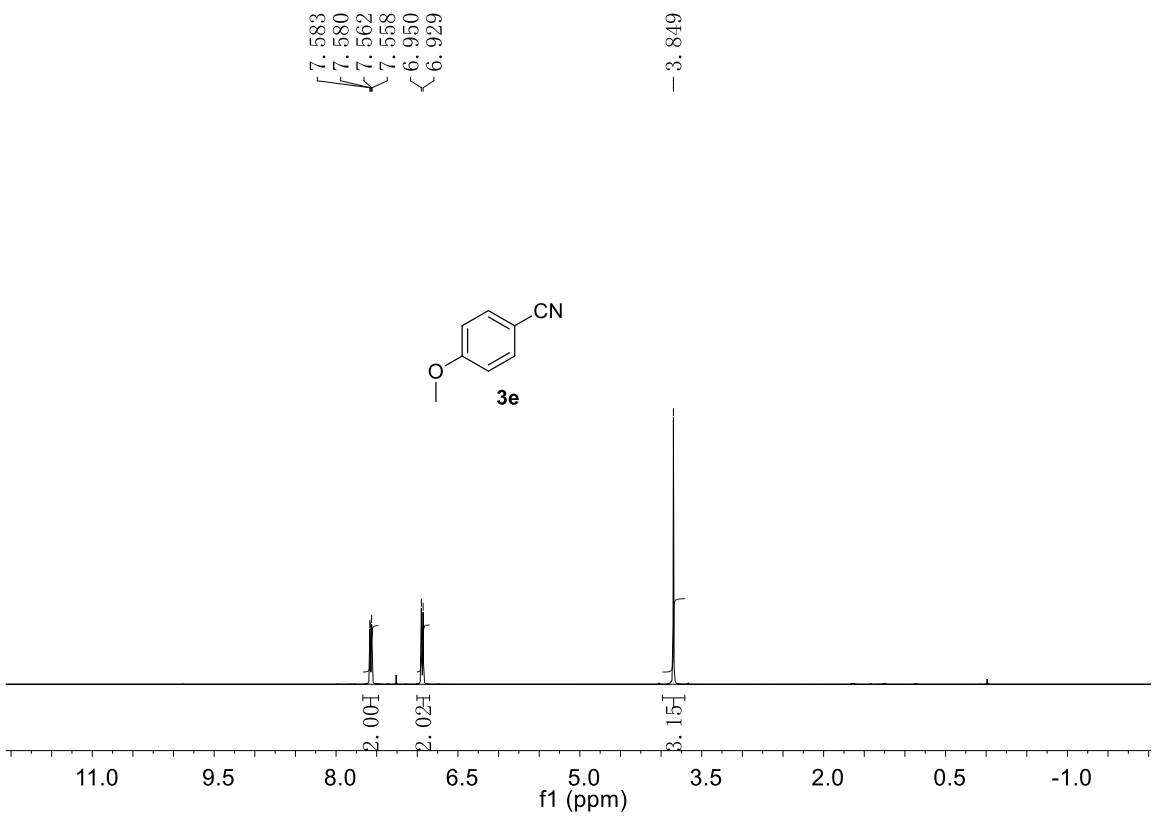

143.752
132.057
129.883
119.179
109.338
21.847
CN
3b
200 180 160 140 120 100 80 60 40 20 0
f1 (ppm)

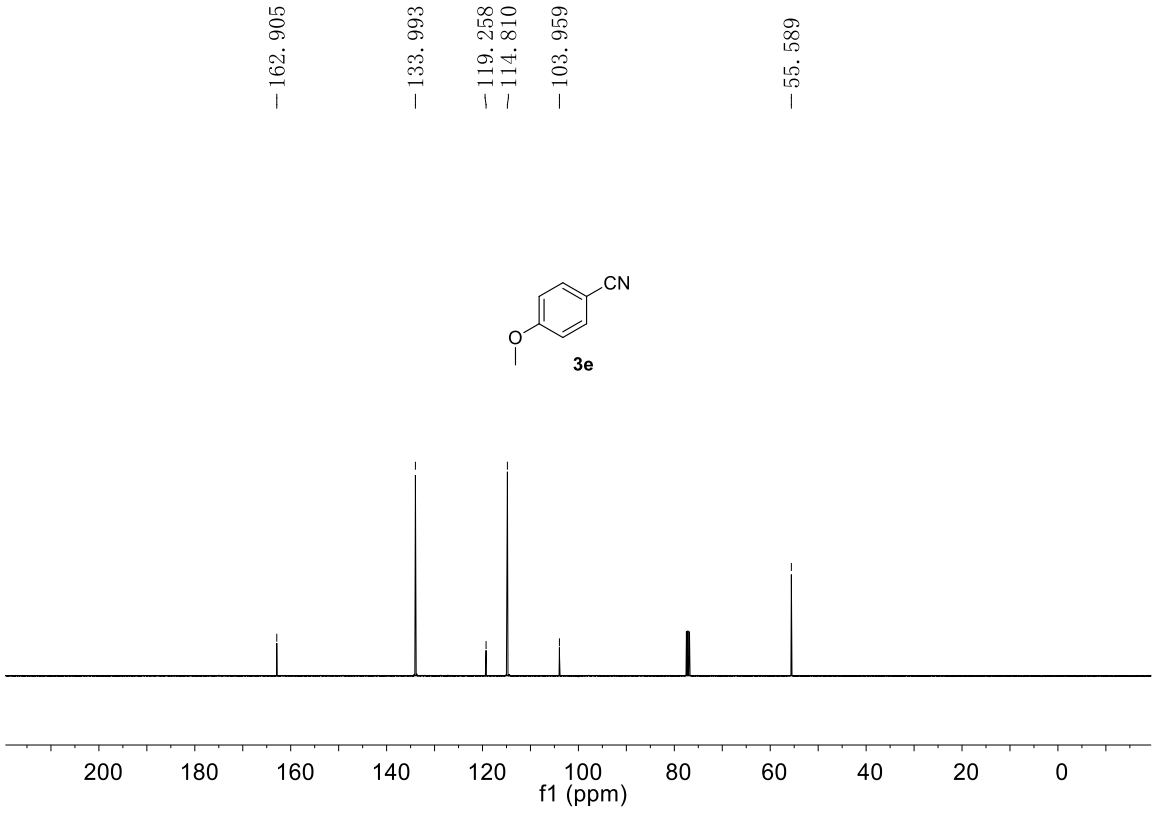

7.604
7.584
7.498
7.479
7.460
7.325
7.306
7.286
7.267
7.248
2.551
1.00
1.04
1.00
1.08
3.06
CN
3c
f1 (ppm)

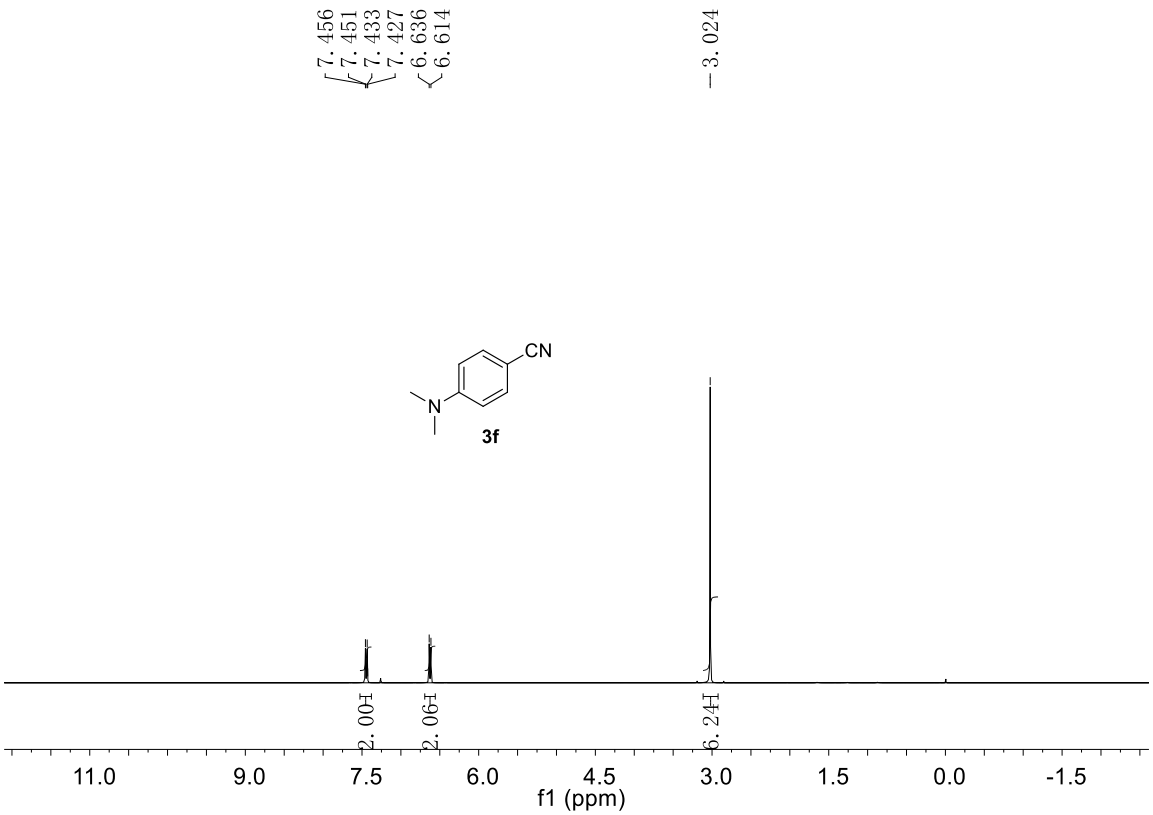

142.015
132.722
132.589
130.321
126.310
118.215
112.871
20.541
CN
3c
f1 (ppm)

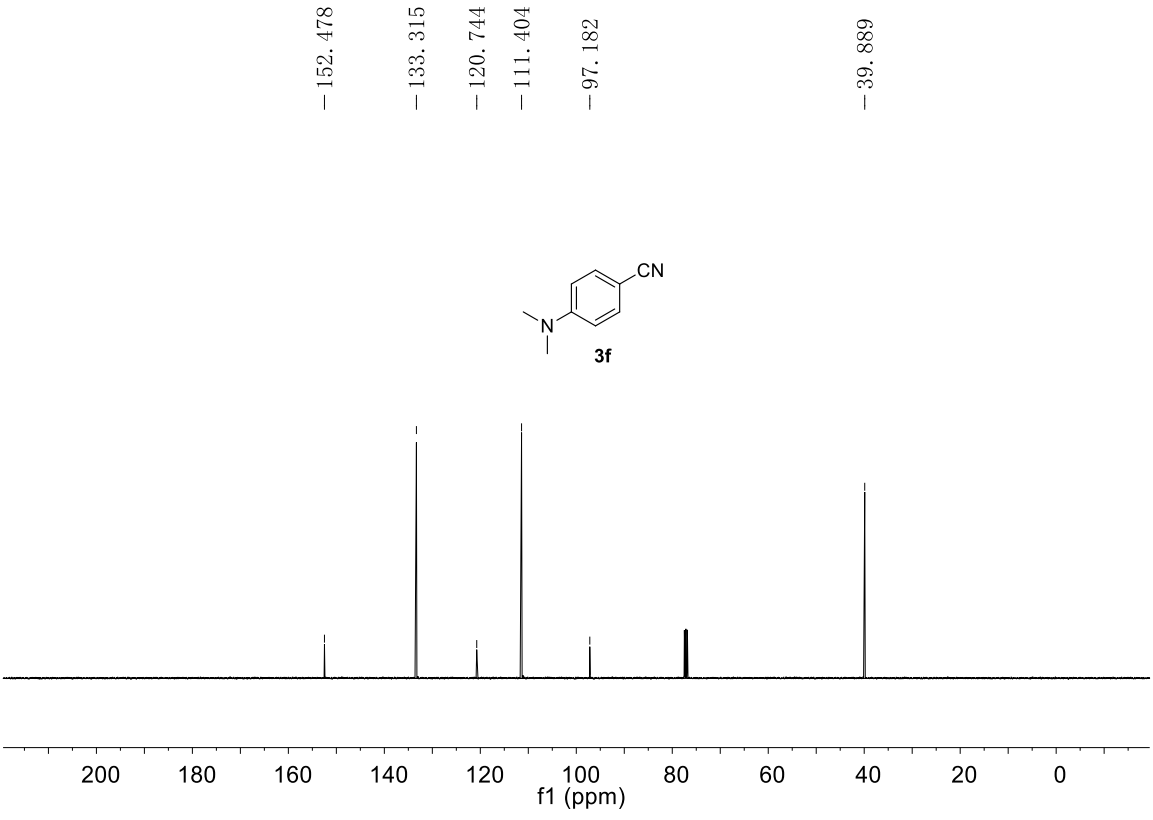

7.579
7.558
7.324
7.303
3.006
2.989
2.971
2.954
2.937
2.920
2.902
1.262
1.245
CN
3d
2.00
2.01
1.00
6.31
11.0
9.0
7.5
6.0
4.5
3.0
1.5
0.0
-1.5
f1 (ppm)

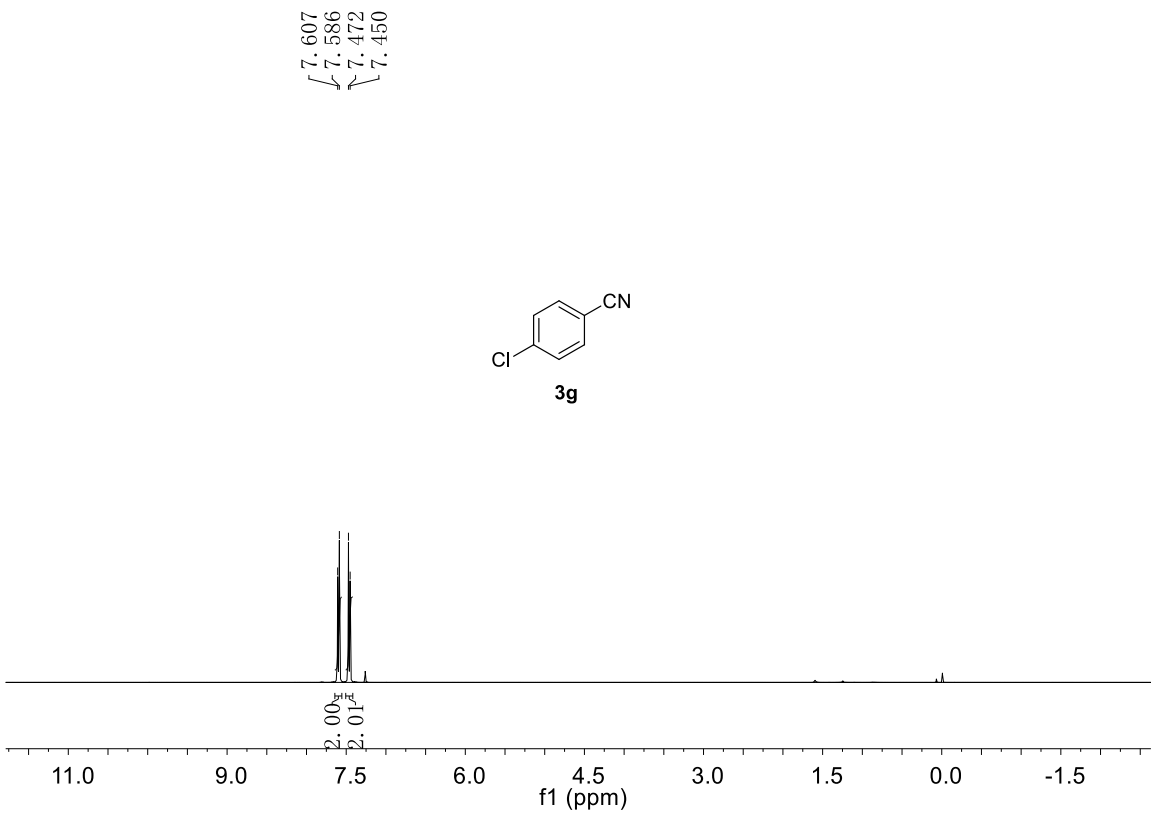

154.458
132.319
127.396
119.253
109.714
34.478
23.619
CN
3d
200
180
160
140
120
100
80
60
40
20
0
f1 (ppm)

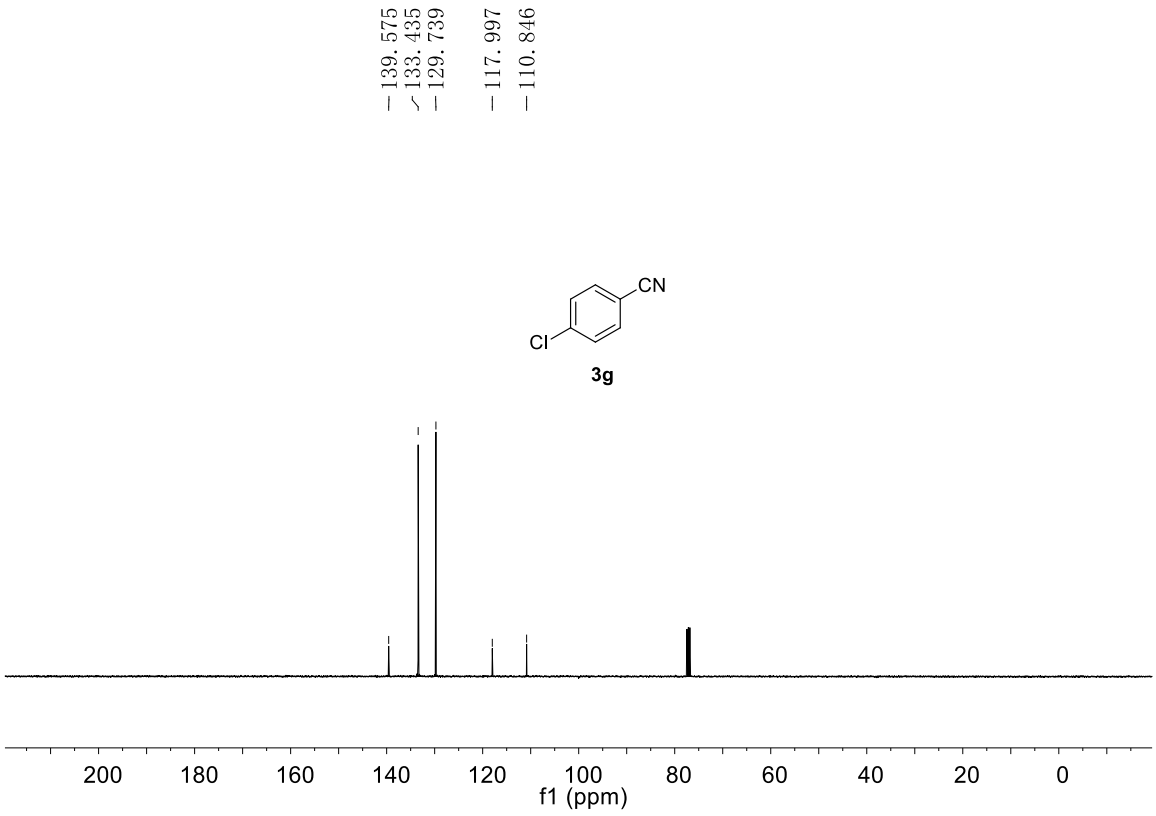

7.583
7.580
7.562
7.558
6.950
6.929
3.849
CN
O
3e
2.00
2.02
3.15
11.0
9.5
8.0
6.5
5.0
3.5
2.0
0.5
-1.0
f1 (ppm)


162.905
133.993
119.258
114.810
103.959
55.589
CN
O
3e
200
180
160
140
120
100
80
60
40
20
0
f1 (ppm)

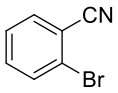

7.456
7.451
7.433
7.427
6.636
6.614
3.024
CN
N
3f
2.00H
2.06H
6.24H
11.0
9.0
7.5
6.0
4.5
3.0
1.5
0.0
-1.5
f1 (ppm)


152.478
133.315
120.744
111.404
97.182
39.889
CN
N
3f
200
180
160
140
120
100
80
60
40
20
0
f1 (ppm)

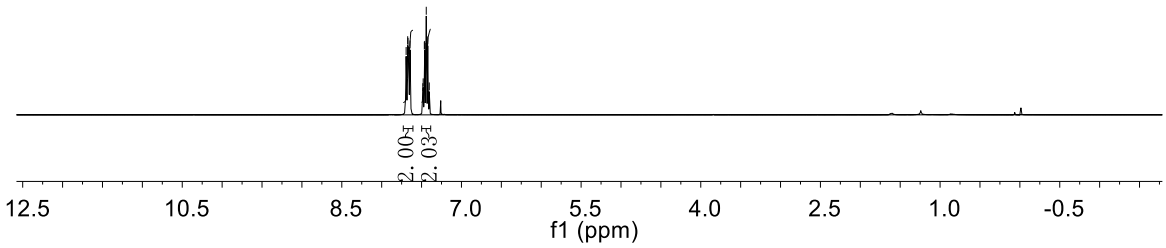

7.607
7.586
7.472
7.450
CN
Cl
3g
2.00
2.01
11.0
9.0
7.5
6.0
4.5
3.0
1.5
0.0
-1.5
f1 (ppm)

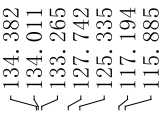

139.575
133.435
129.739
117.997
110.846
CN
Cl
3g
200
180
160
140
120
100
80
60
40
20
0
f1 (ppm)


7.693
7.690
7.674
7.670
7.663
7.645
7.640
7.484
7.480
7.465
7.461
7.446
7.441
7.422
7.404


CN
Br

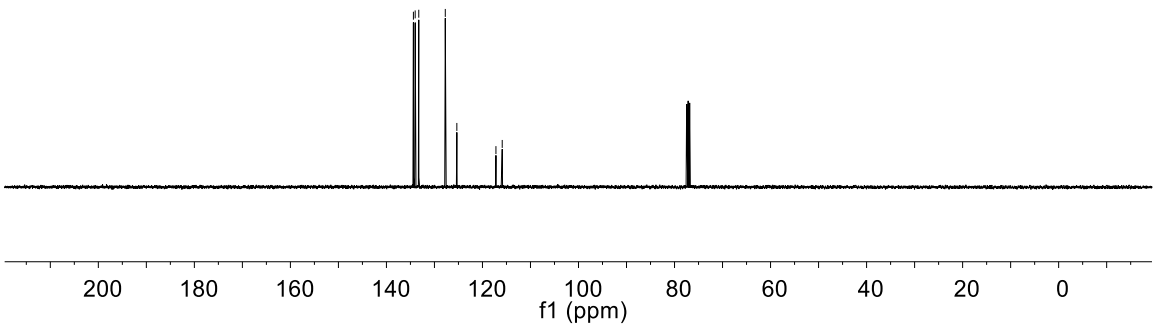
3h

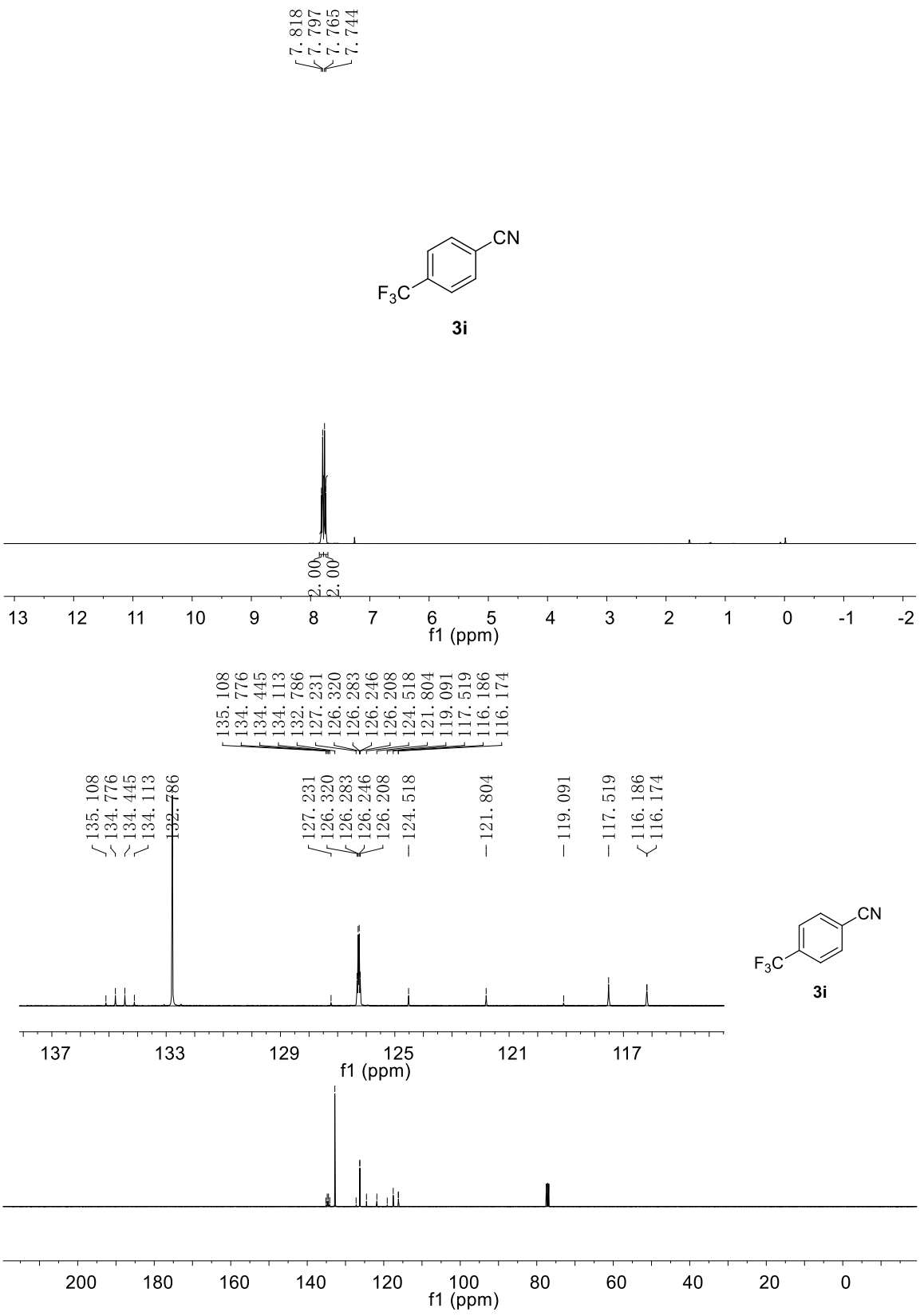

2.00
2.03
12.5
10.5
8.5
7.0
5.5
4.0
2.5
1.0
-0.5
f1 (ppm)

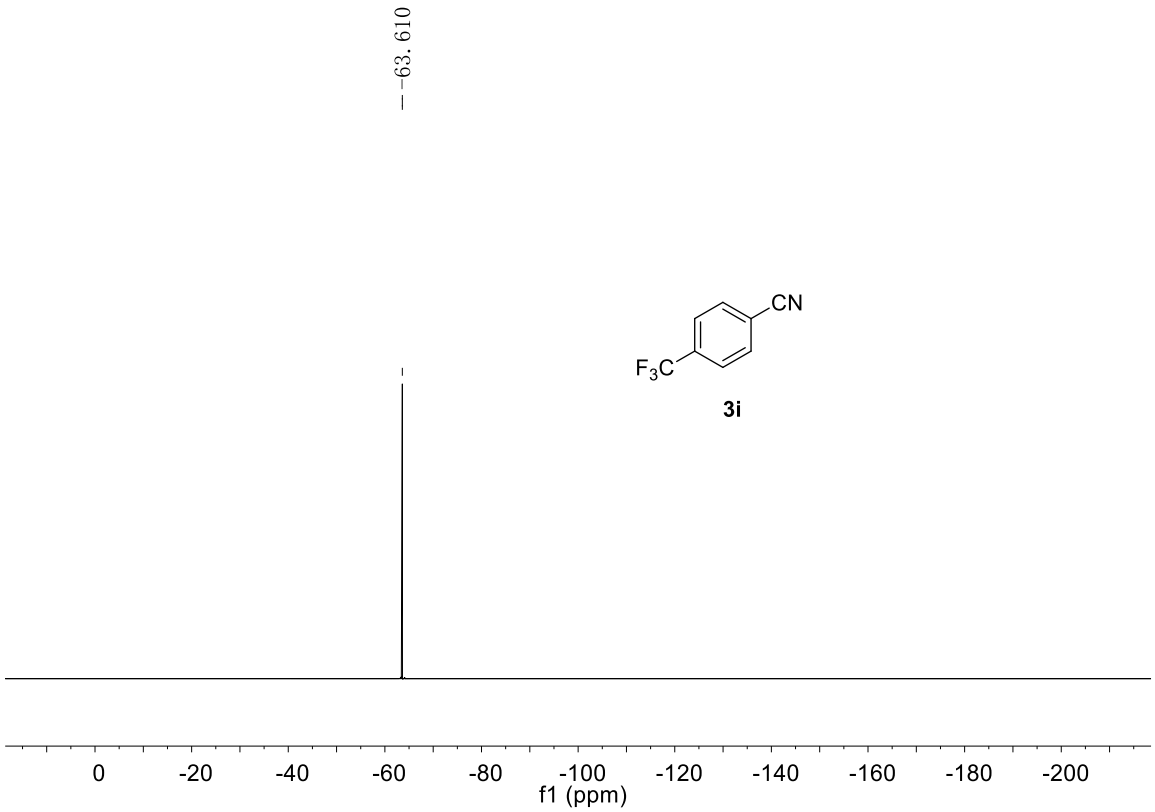

134.382
134.011
133.265
127.742
125.335
117.194
115.885

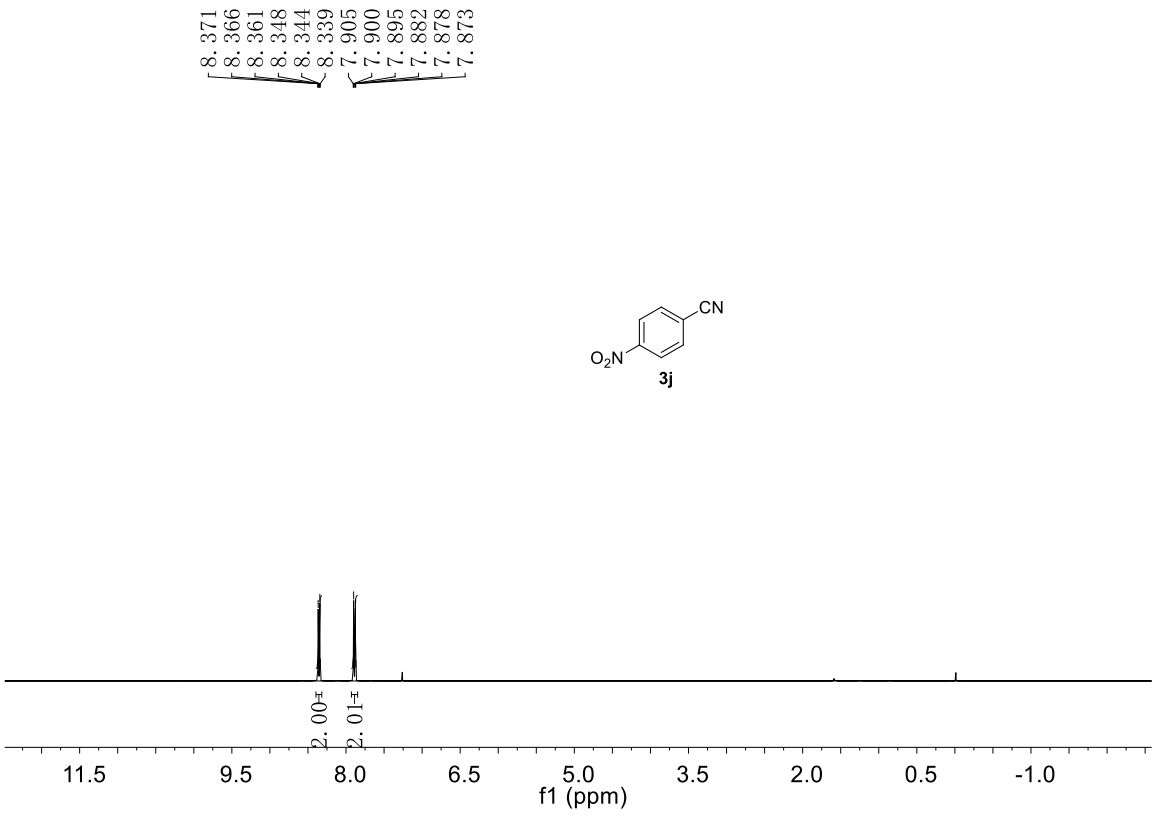

CN
Br

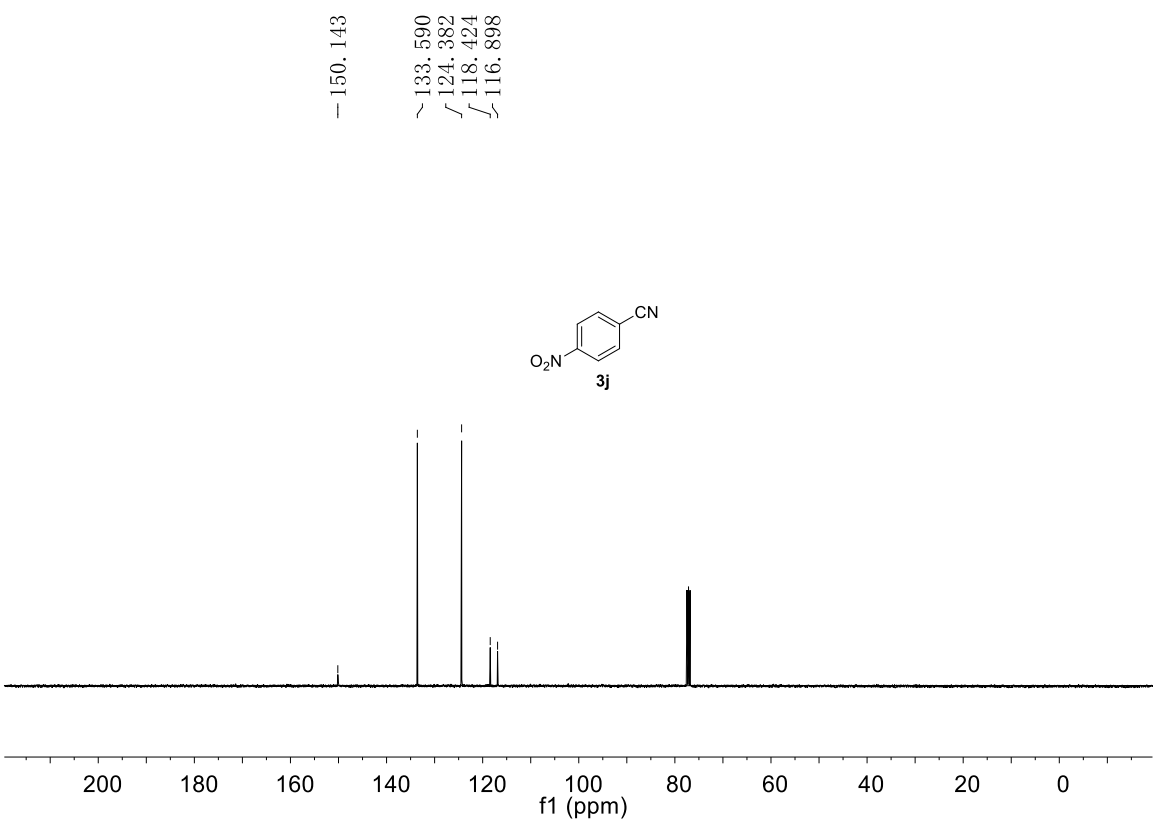
3h

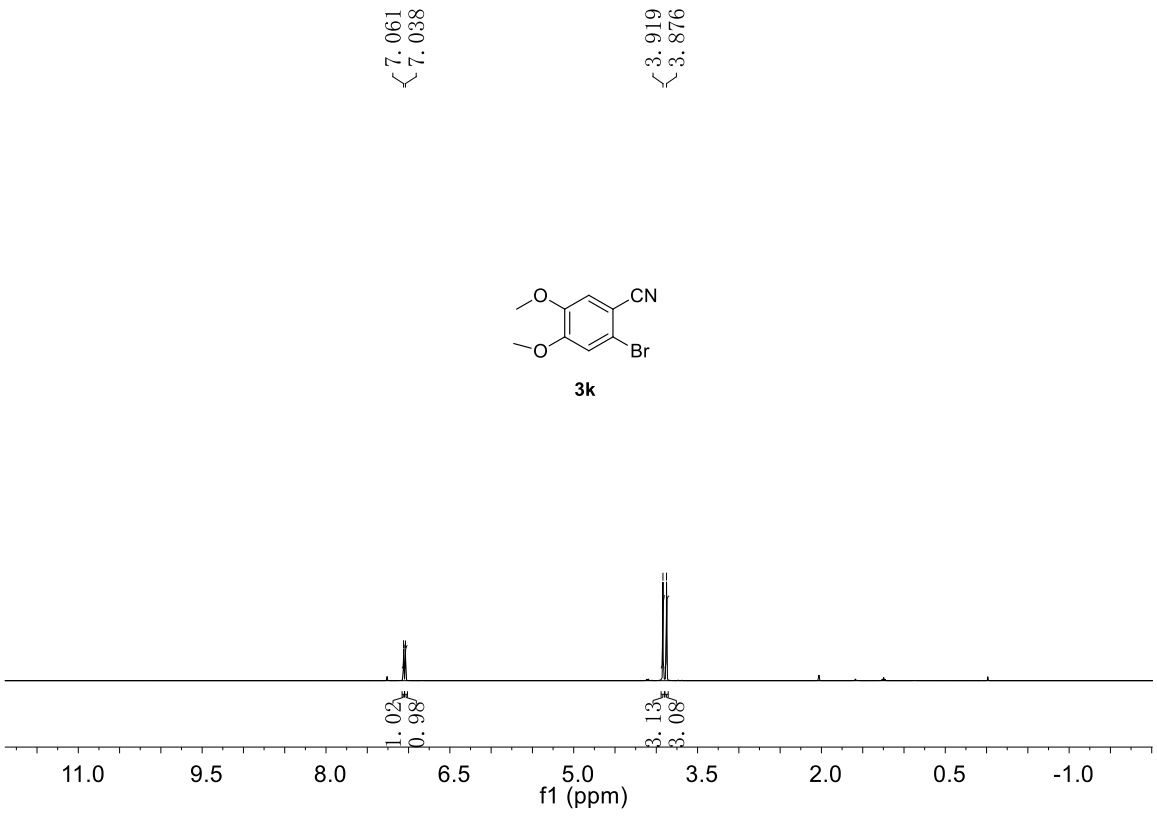

200
180
160
140
120
100
80
60
40
20
0
f1 (ppm)

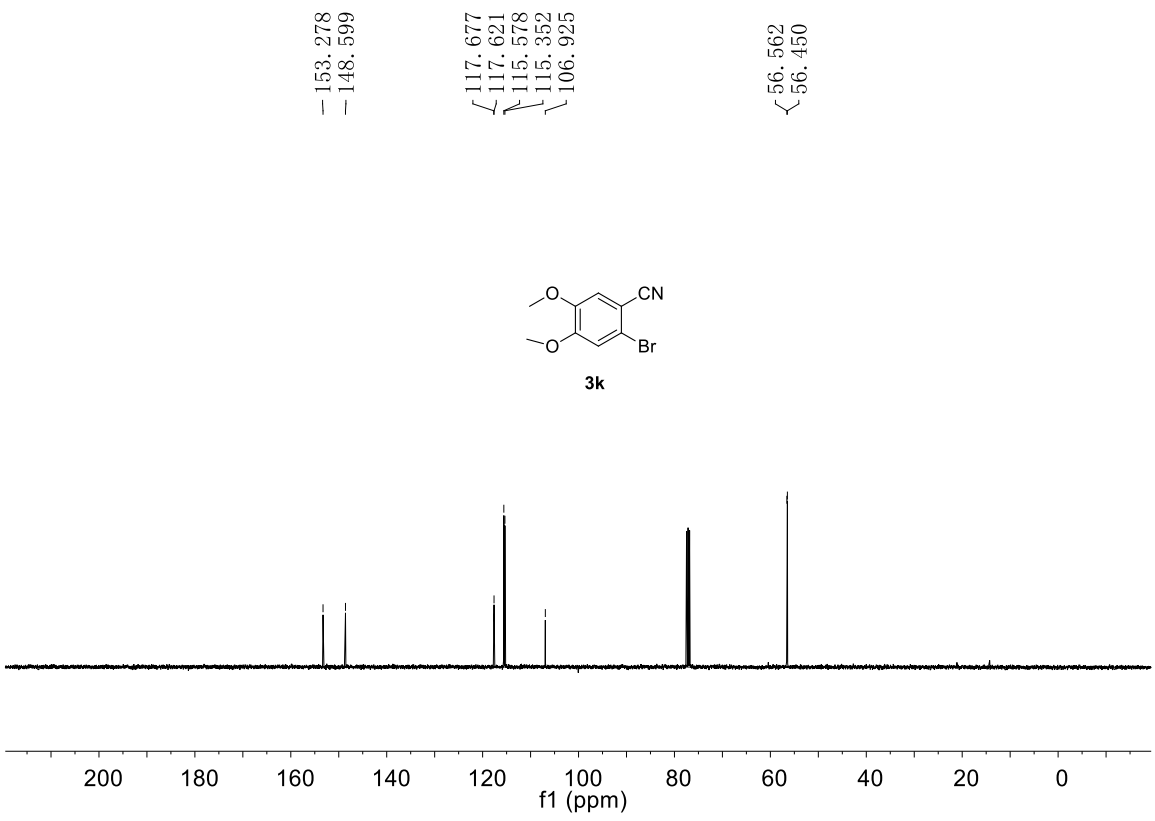

7.818
7.797
7.765
7.744
CN
F3C
3i
2.00
2.00
13 12 11 10 9 8 7 6 5 4 3 2 1 0 -1 -2
f1 (ppm)
135.108
134.776
134.445
134.113
132.786
127.231
126.320
126.283
126.246
126.208
124.518
121.804
119.091
117.519
116.186
116.174
CN
F3C
3i
137 133 129 125 121 117
f1 (ppm)
200 180 160 140 120 100 80 60 40 20 0
f1 (ppm)

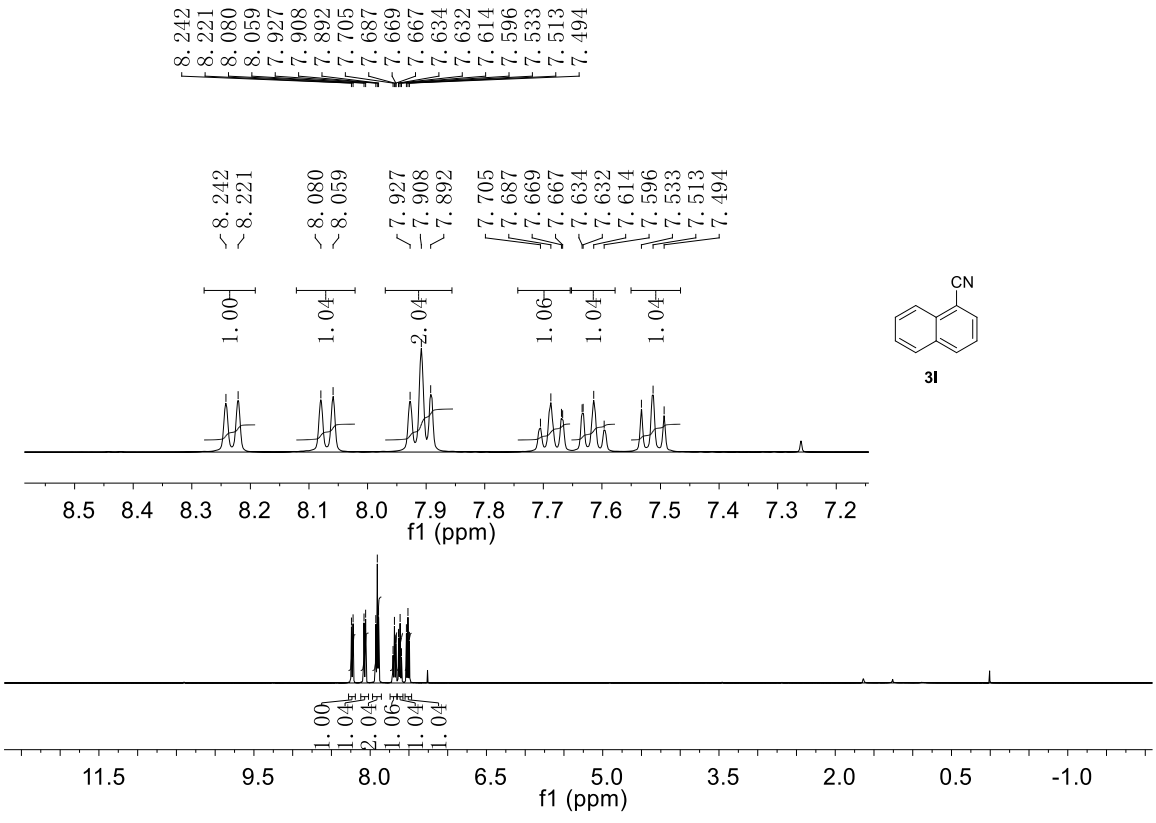

-63.610
CN
F3C
3i
0
-20
-40
-60
-80
-100
-120
-140
-160
-180
-200
f1 (ppm)

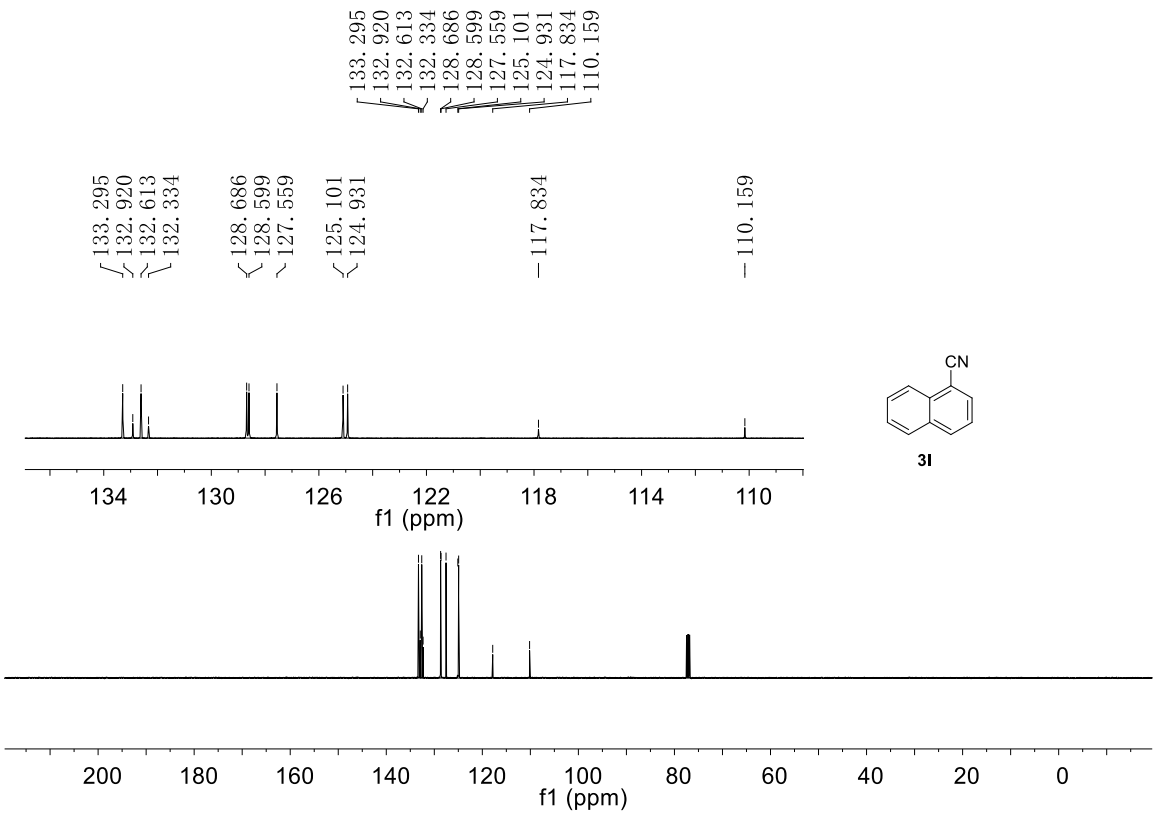

8.371
8.366
8.361
8.348
8.344
8.339
7.905
7.900
7.895
7.882
7.878
7.873
CN
O2N
3j
2.00
2.01
11.5
9.5
8.0
6.5
5.0
3.5
2.0
0.5
-1.0
f1 (ppm)

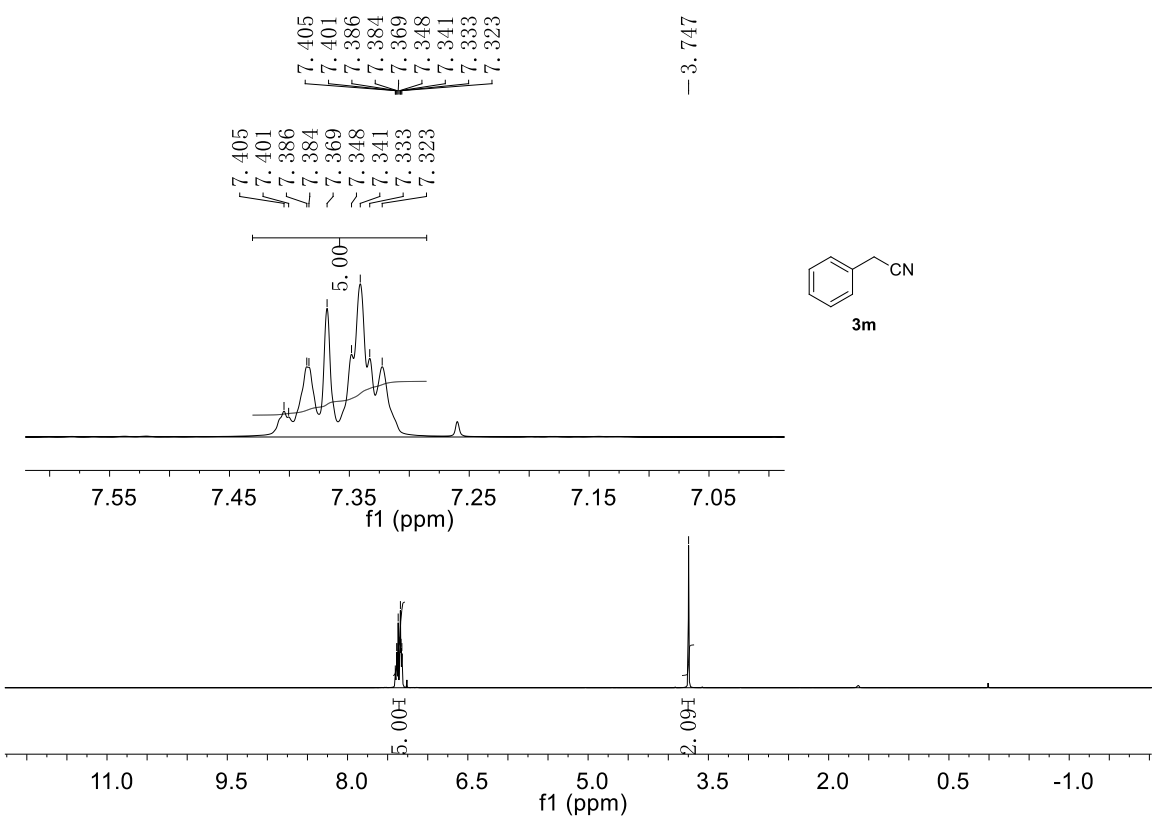

150.143
133.590
124.382
118.424
116.898
CN
O2N
3j
200
180
160
140
120
100
80
60
40
20
0
f1 (ppm)

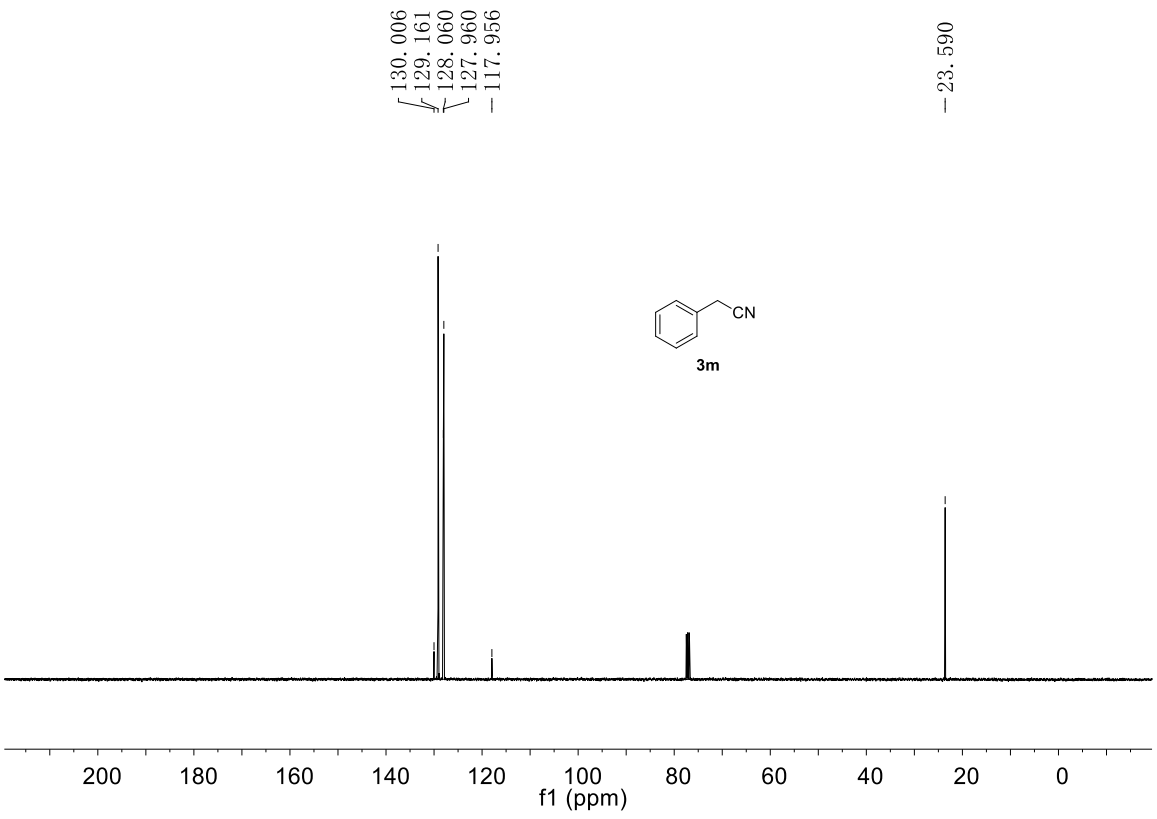

7.061
7.038
3.919
3.876
O
O
CN
Br
3k
1.02
0.98
3.13
3.08
11.0
9.5
8.0
6.5
5.0
3.5
2.0
0.5
-1.0
f1 (ppm)

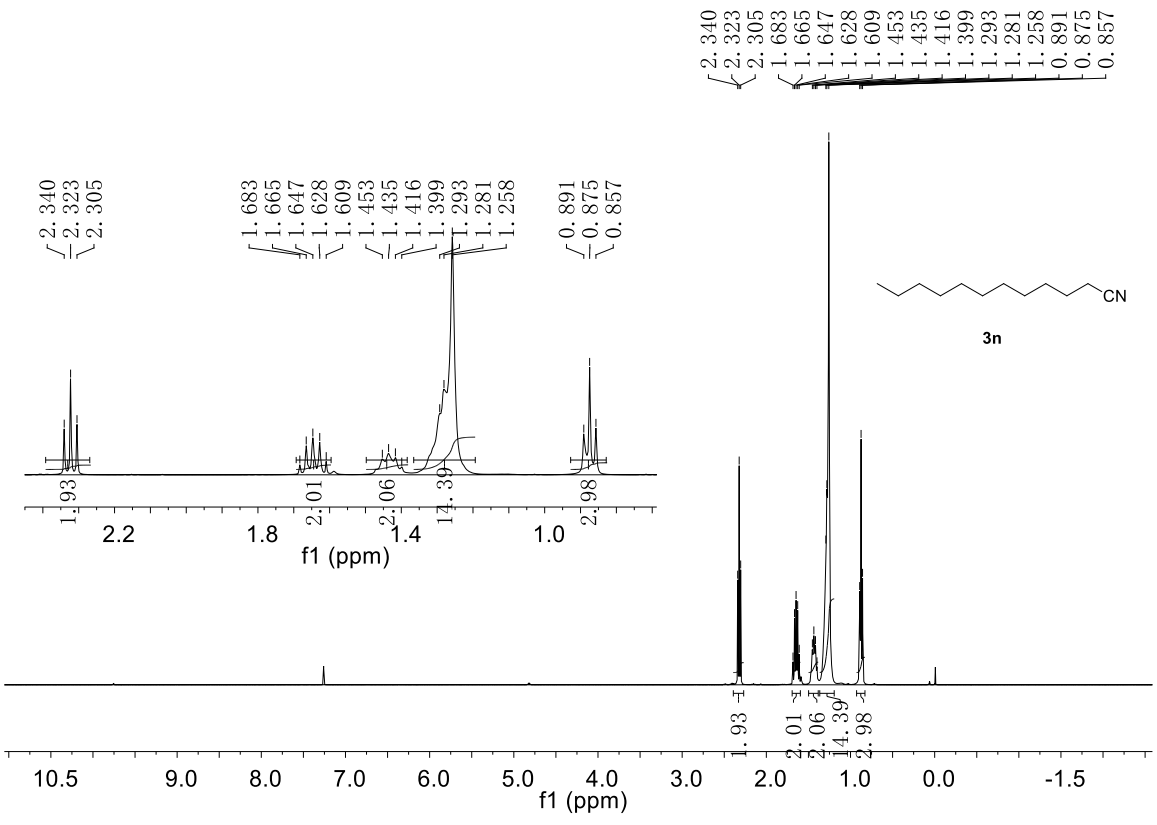

153.278
148.599
117.677
117.621
115.578
115.352
106.925
56.562
56.450
O
O
CN
Br
3k
200
180
160
140
120
100
80
60
40
20
0
f1 (ppm)

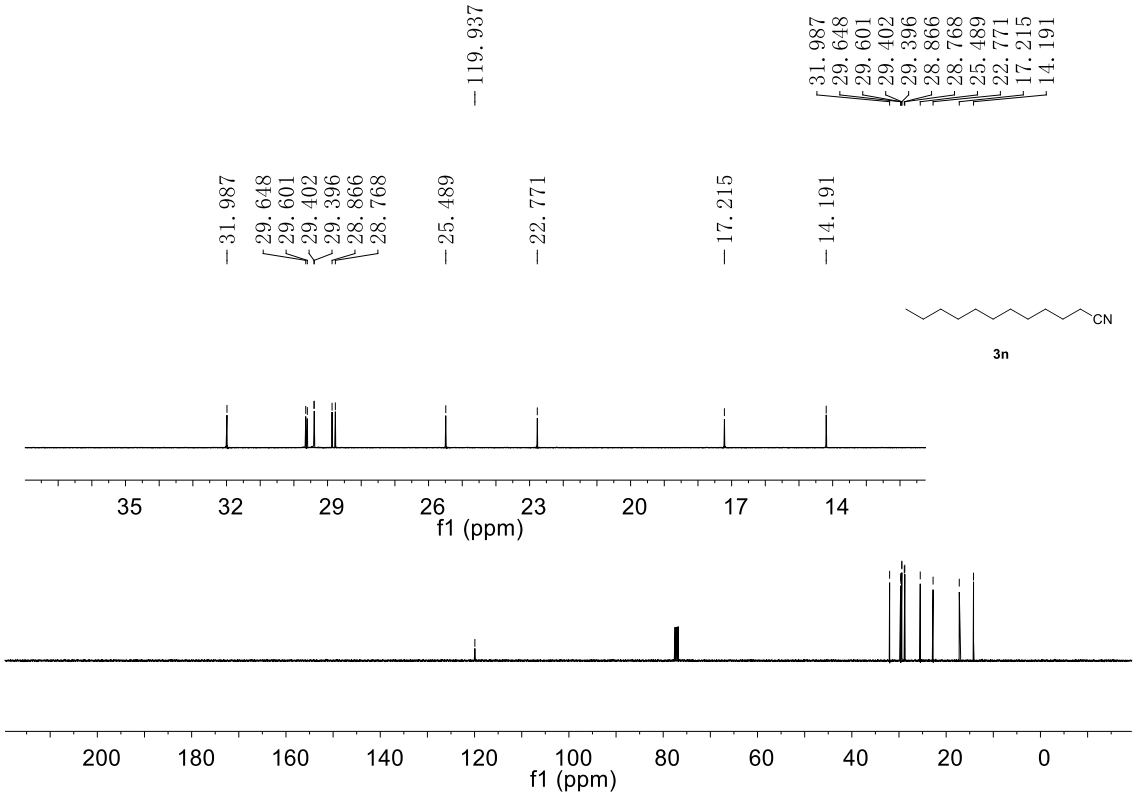

8.242
8.221
8.080
8.059
7.927
7.908
7.892
7.705
7.687
7.669
7.667
7.634
7.632
7.614
7.596
7.533
7.513
7.494
1.00
1.04
2.04
1.06
1.04
1.04
CN
3l
8.5
8.4
8.3
8.2
8.1
8.0
7.9
7.8
7.7
7.6
7.5
7.4
7.3
7.2
f1 (ppm)
11.5
9.5
8.0
6.5
5.0
3.5
2.0
0.5
-1.0
f1 (ppm)


133.295
132.920
132.613
132.334
128.686
128.599
127.559
125.101
124.931
117.834
110.159
CN
3l
f1 (ppm)


7.405
7.401
7.386
7.384
7.369
7.348
7.341
7.333
7.323
3.747
5.00
2.09
CN
3m
f1 (ppm)


130.006
129.161
128.060
127.960
117.956
23.590
CN
3m
200
180
160
140
120
100
80
60
40
20
0
f1 (ppm)


2.340
2.323
2.305
1.683
1.665
1.647
1.628
1.609
1.453
1.435
1.416
1.399
1.293
1.281
1.258
0.891
0.875
0.857
CN
3n
1.93
2.01
2.06
14.39
2.98
10.5
9.0
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0.0
-1.5
f1 (ppm)


119.937
31.987
29.648
29.601
29.402
29.396
28.866
28.768
25.489
22.771
17.215
14.191
CN
3n
f1 (ppm)
f1 (ppm)