

Supporting Information

A novel PIFA/KOH promoted approach to synthesize C2-arylacylated benzothiazoles as potential drug scaffolds

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College of Chemical Engineering, Zhejiang University of Technology, Hangzhou 310014, P. R. China

**E-mail: jqweng@zjut.edu.cn.*

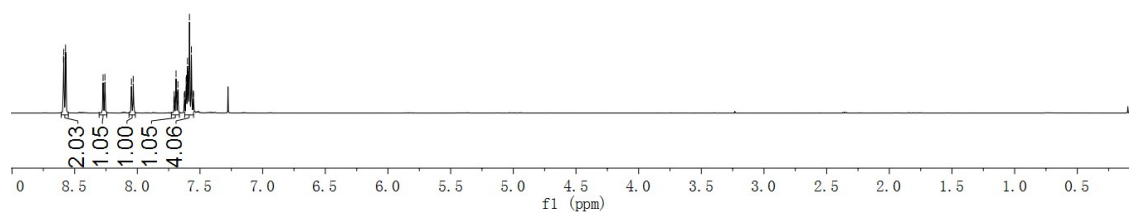
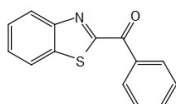
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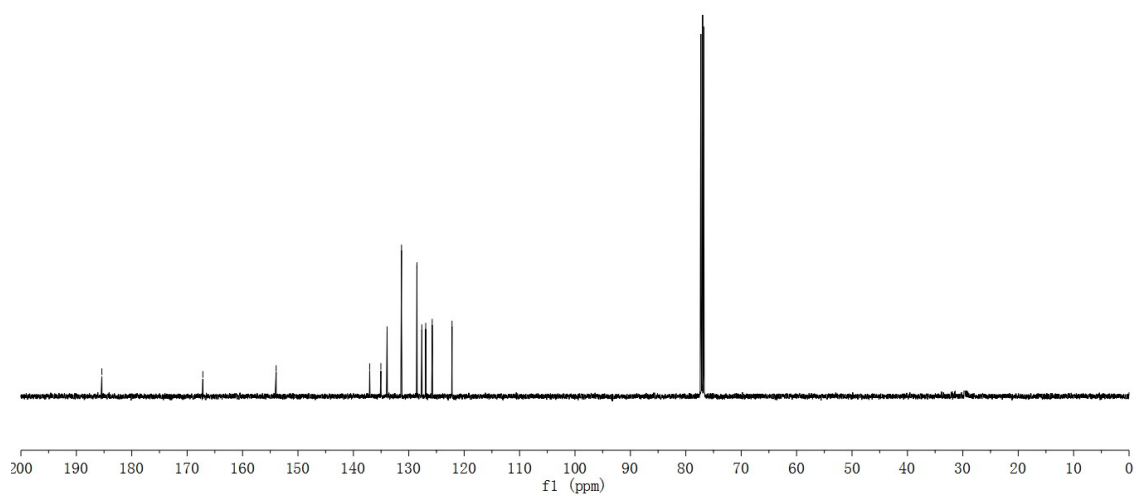
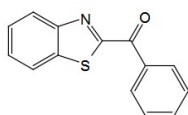
1. NMR Spectrum of compounds 3aa~3br

^1H and ^{13}C NMR Spectra of 3aa

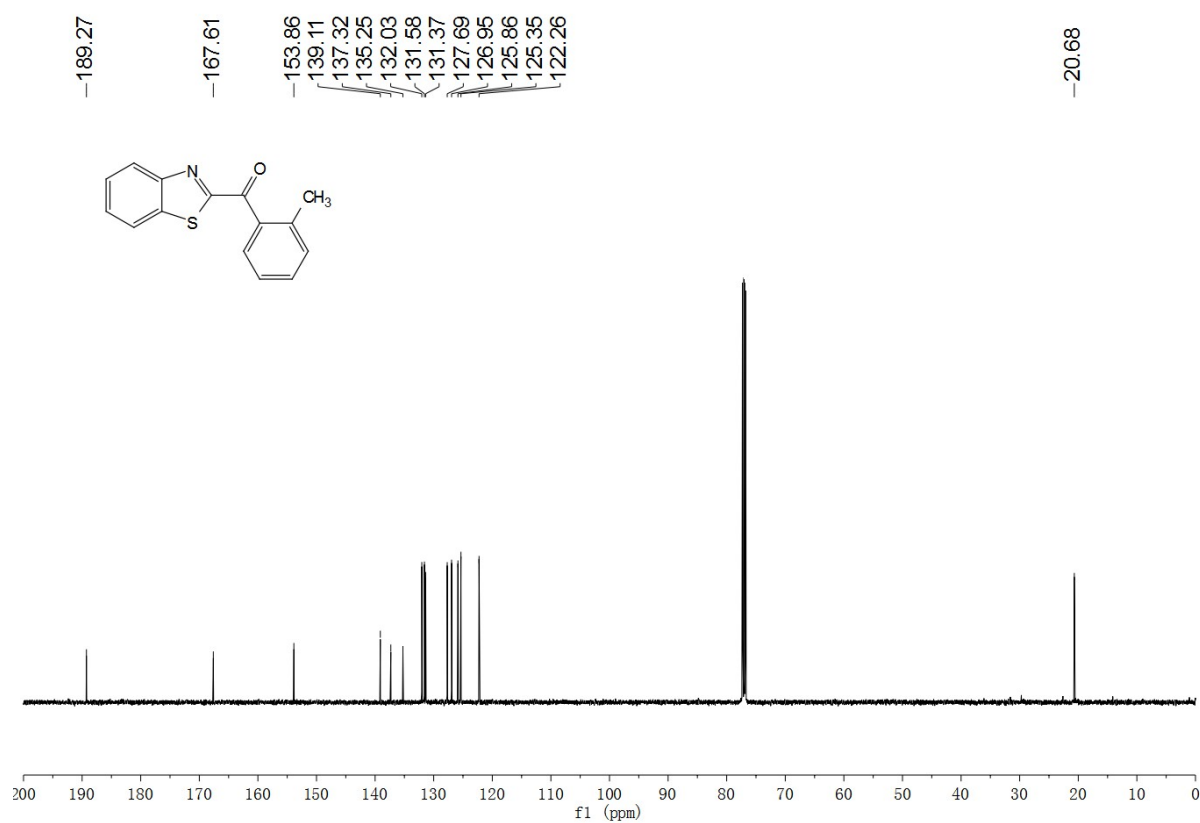
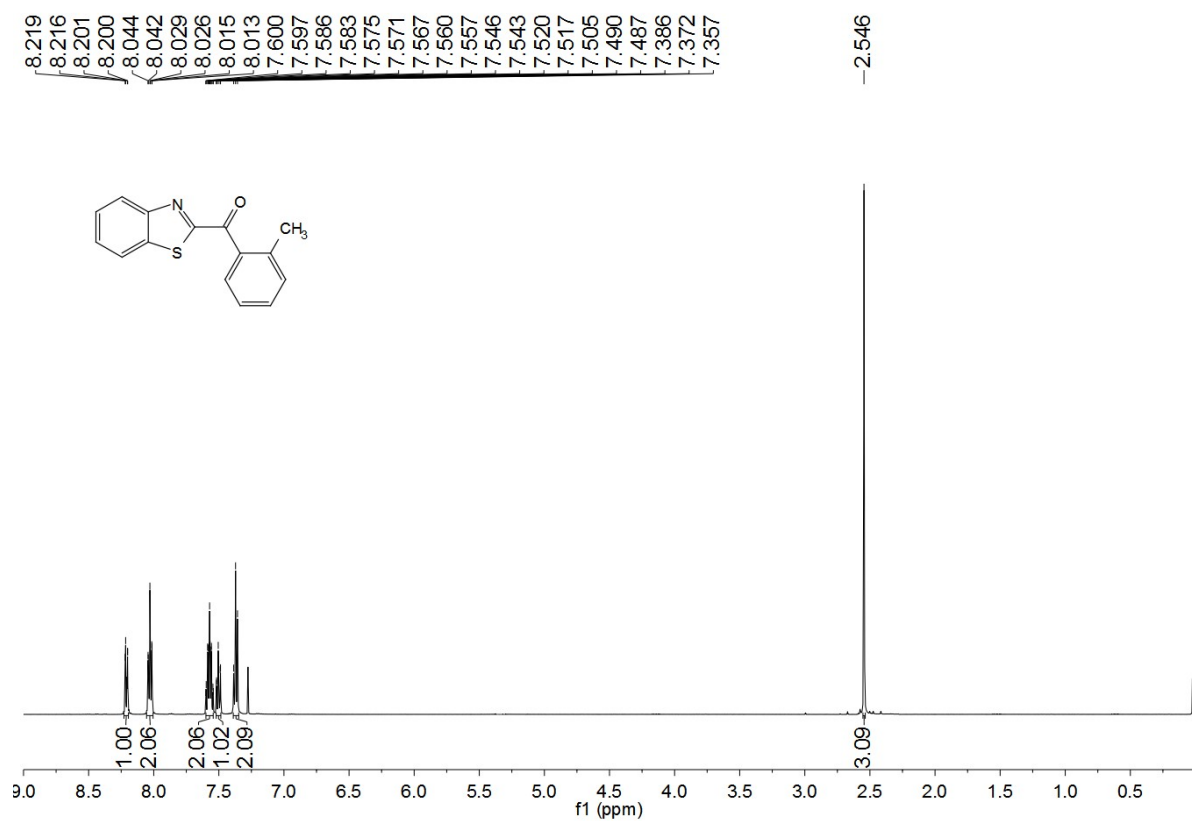
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8.573
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8.258
8.047
8.033
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7.691
7.687
7.679
7.676
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7.600
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7.592
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7.568
7.554
7.551



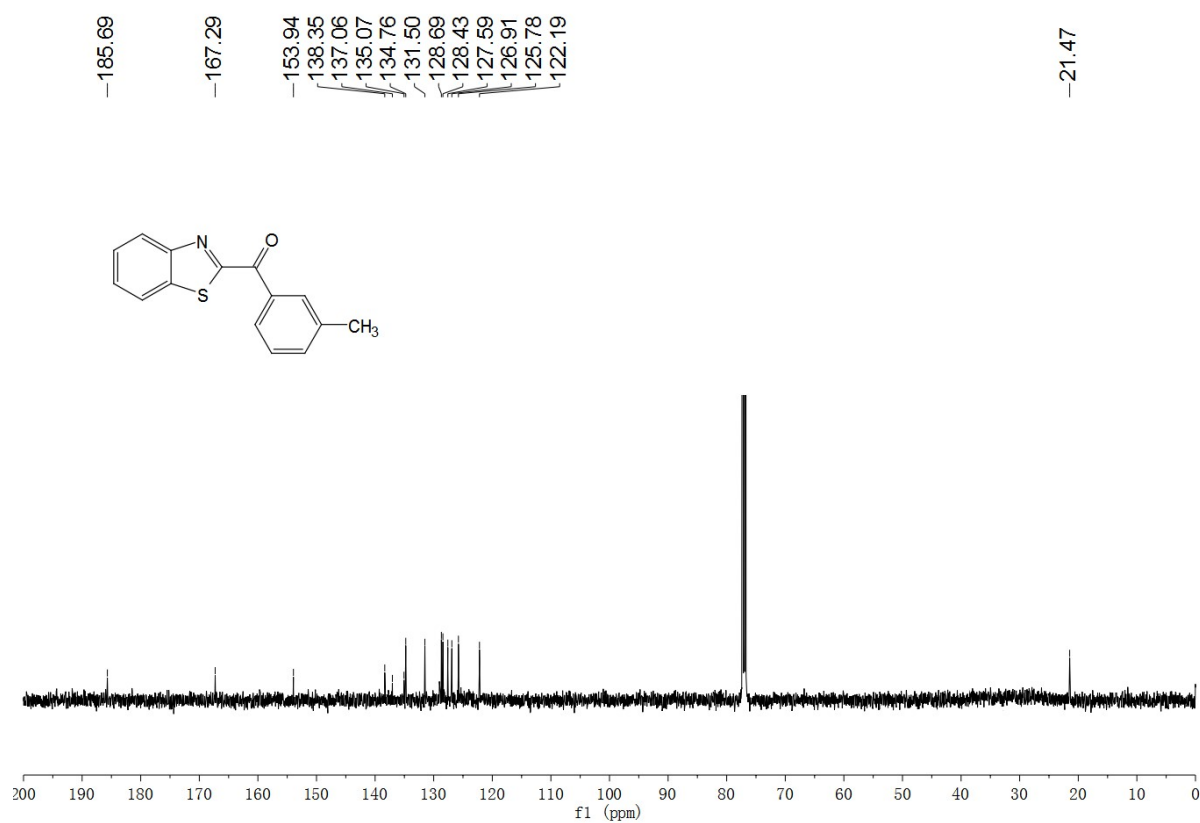
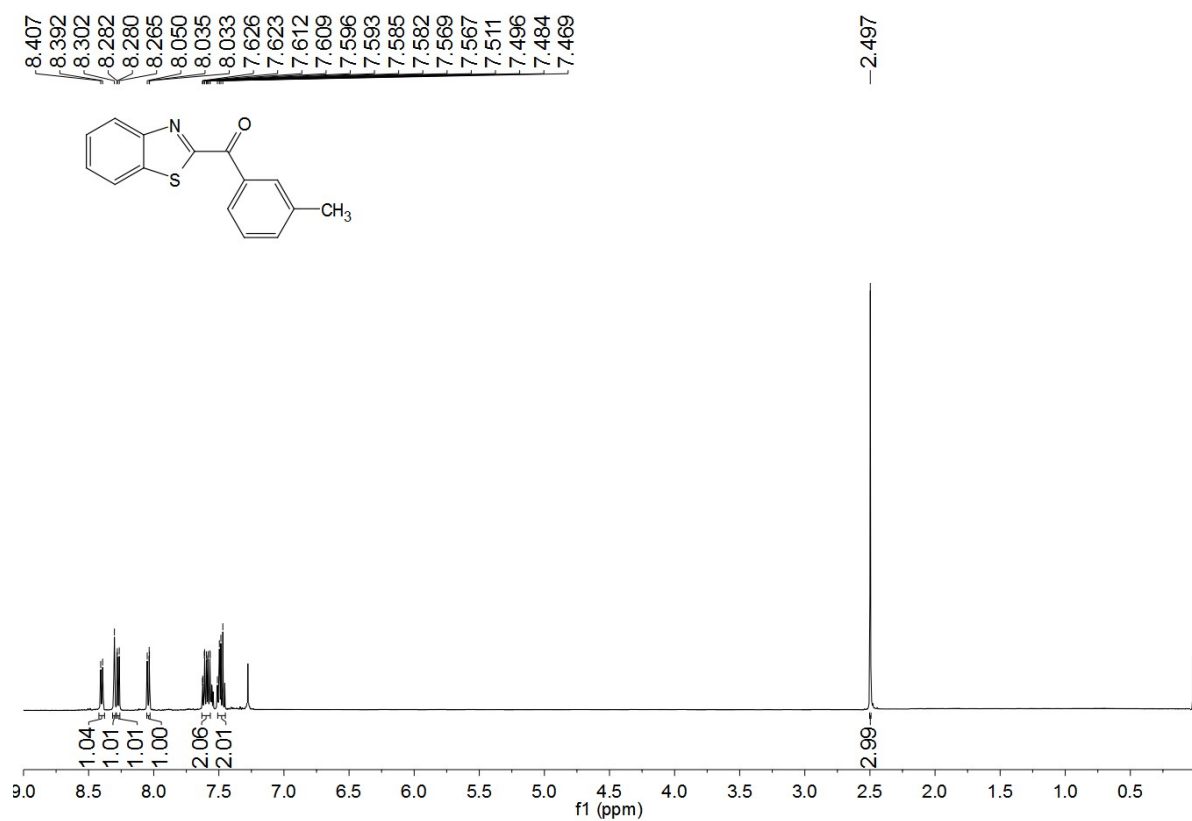
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167.17
153.94
137.06
135.03
133.91
131.31
128.53
127.64
126.95
125.77
122.19



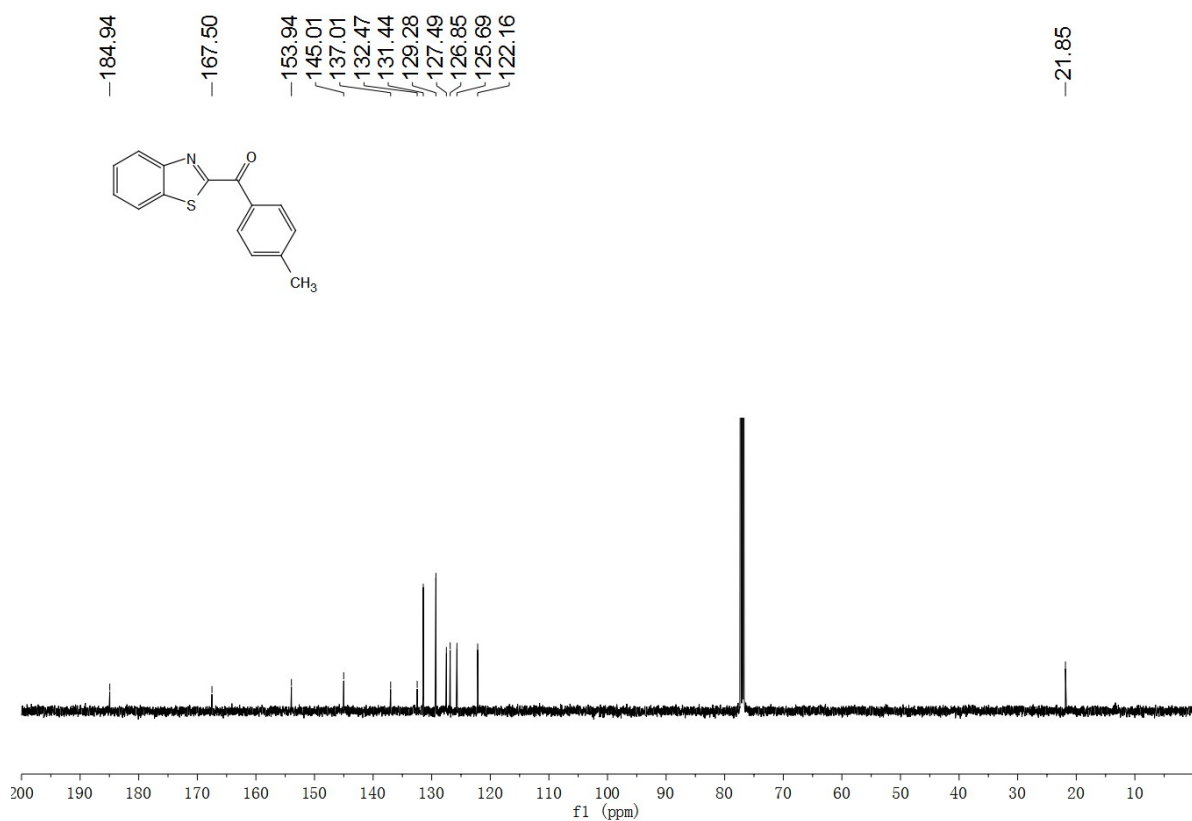
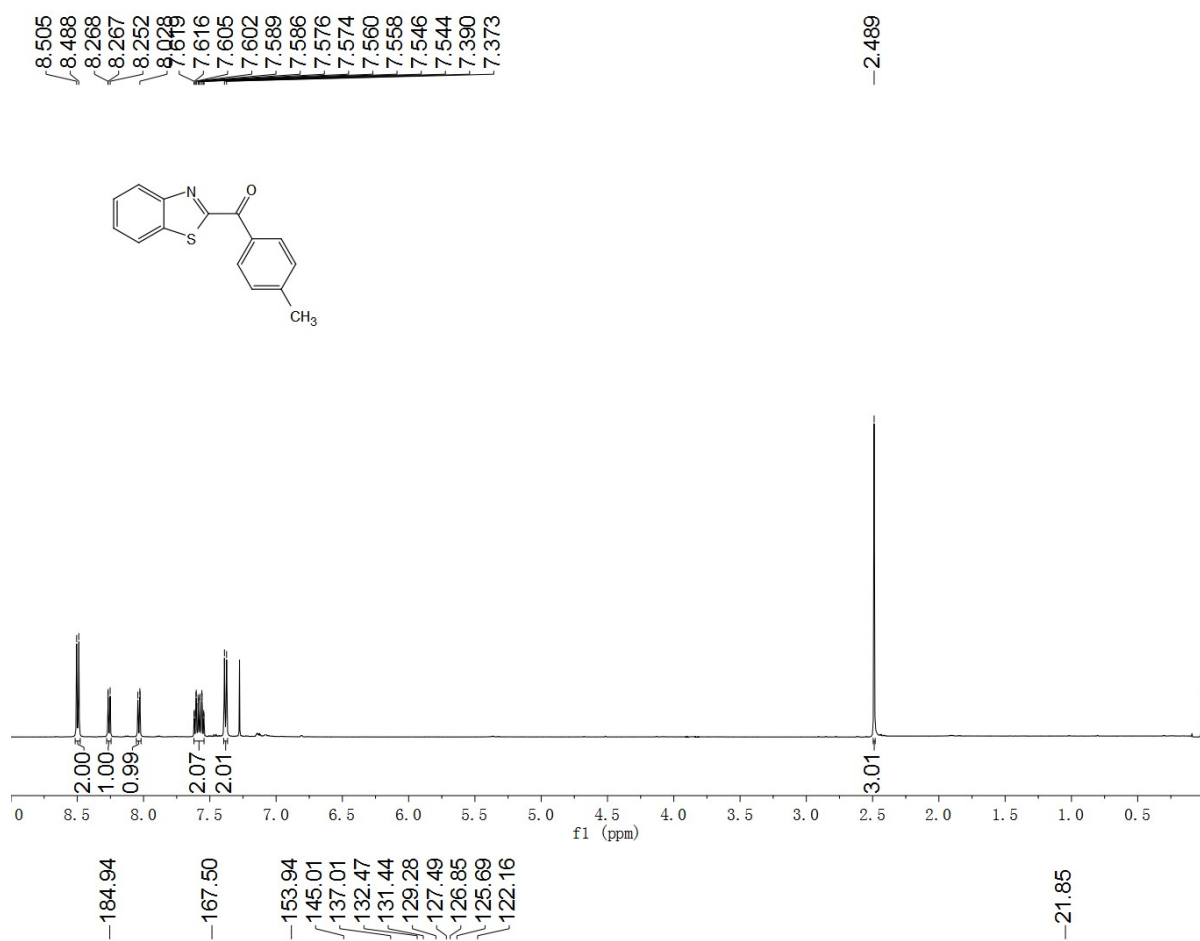
¹H and ¹³C NMR Spectra of 3ab



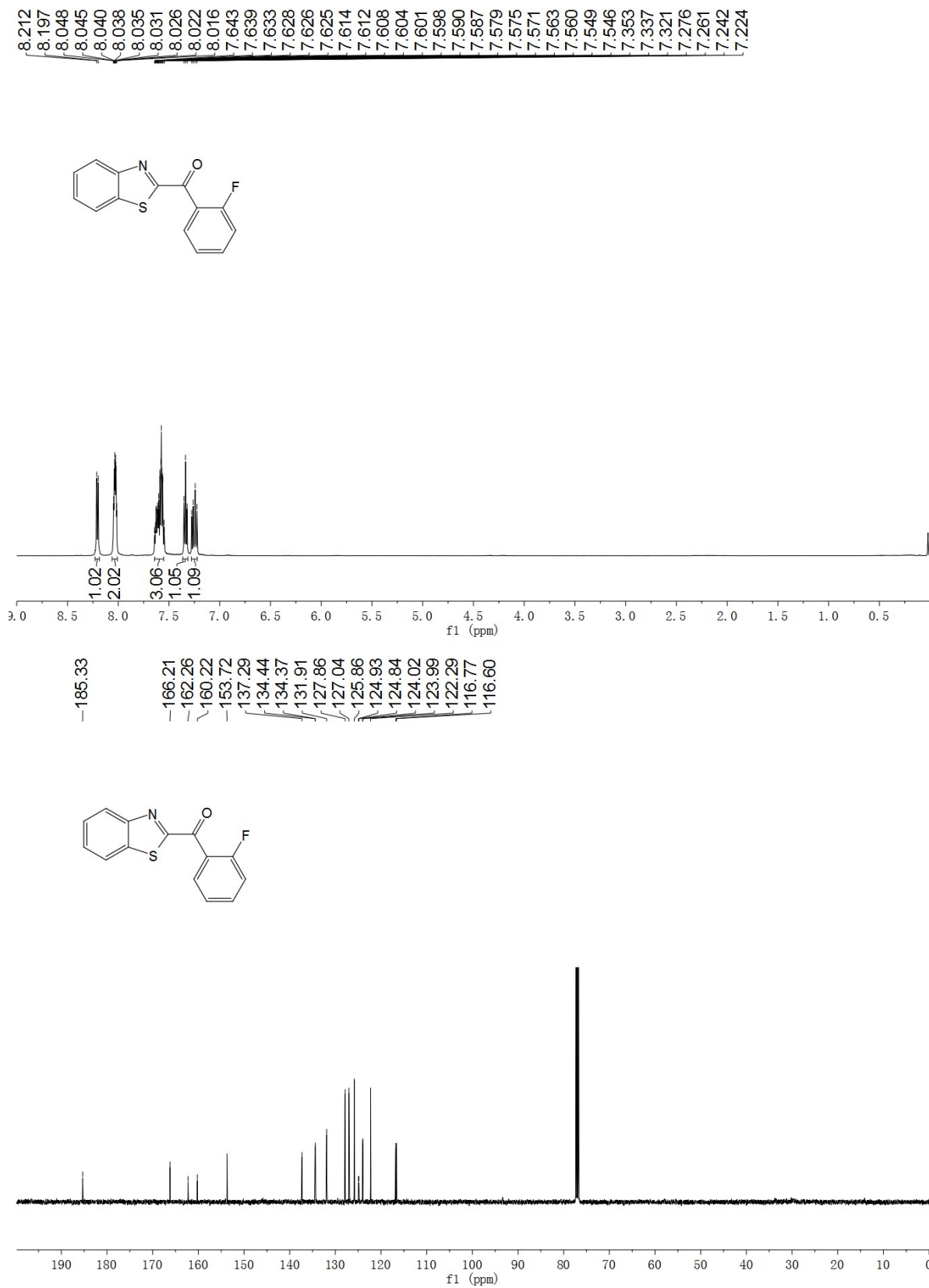
¹H and ¹³C NMR Spectra of 3ac



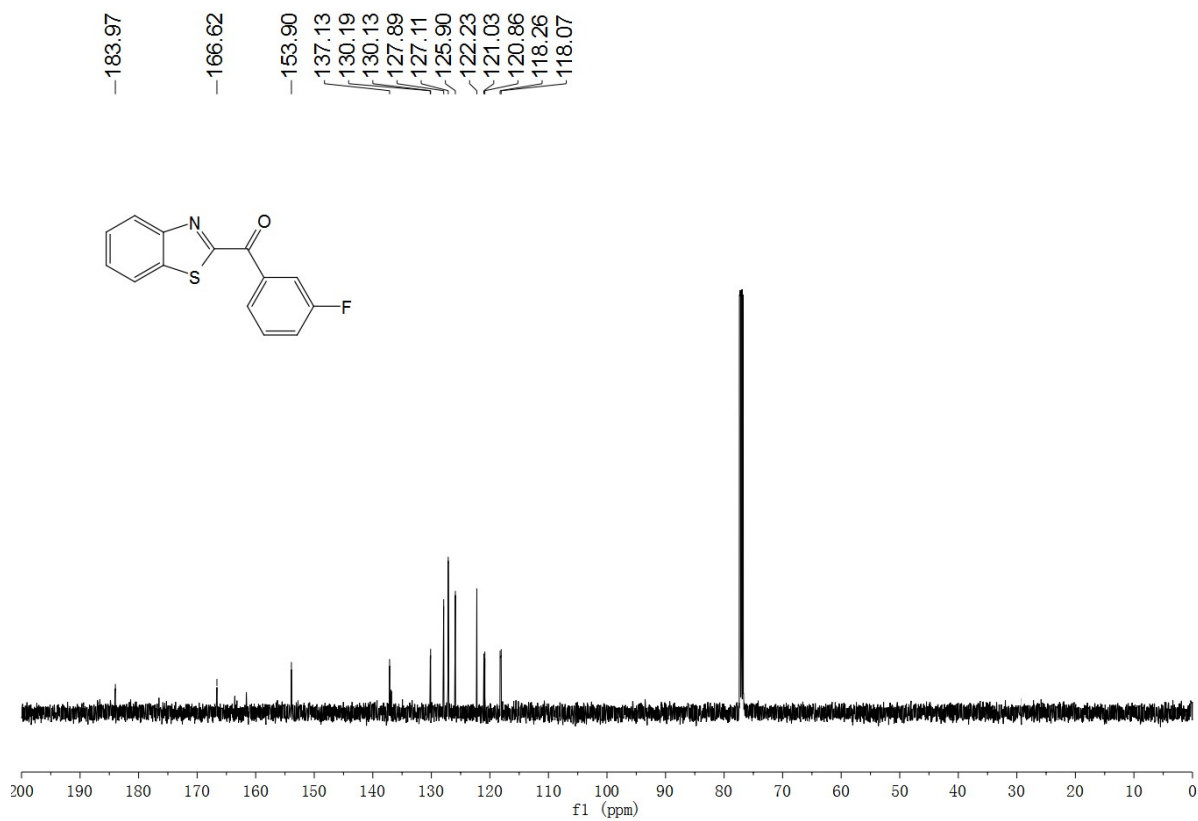
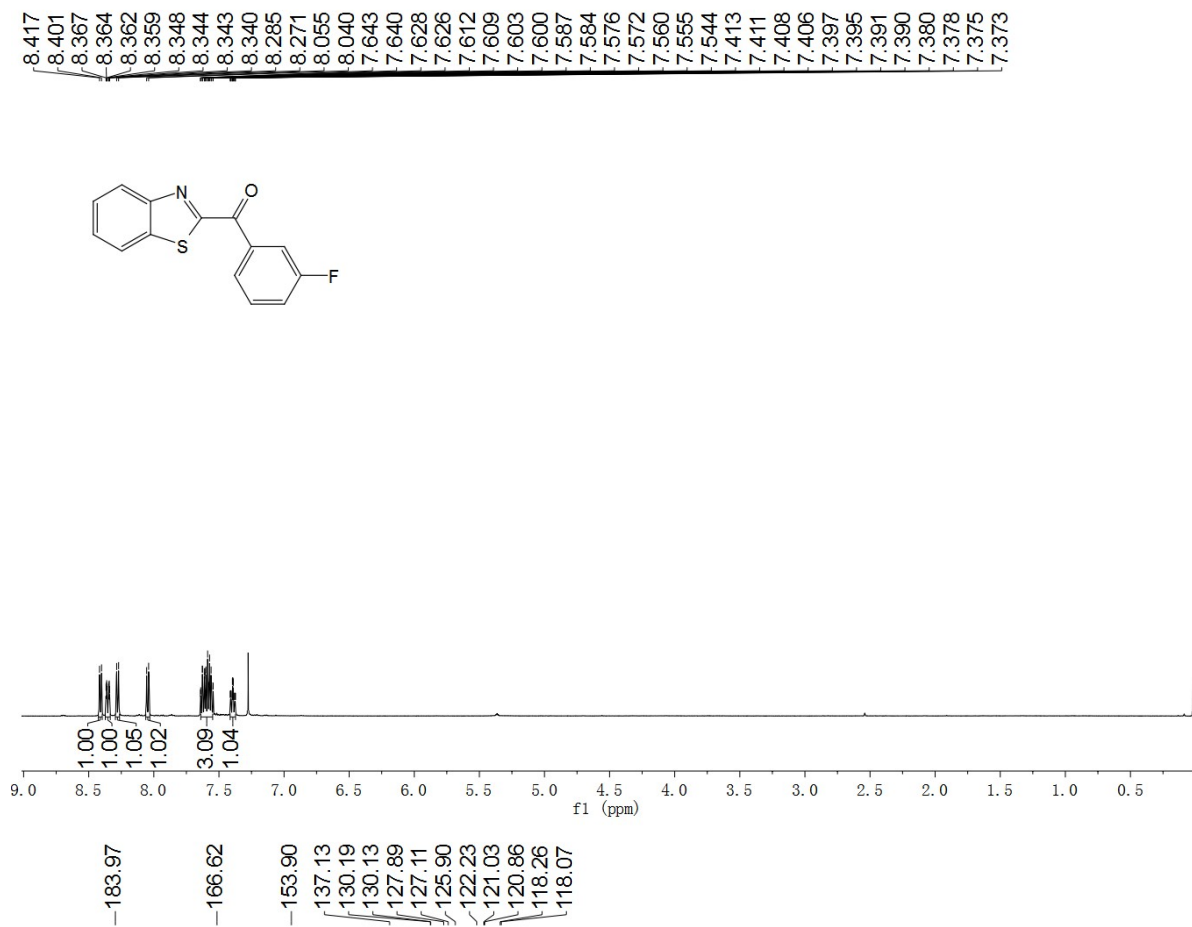
¹H and ¹³C NMR Spectra of 3ad



¹H and ¹³C NMR Spectra of 3ae

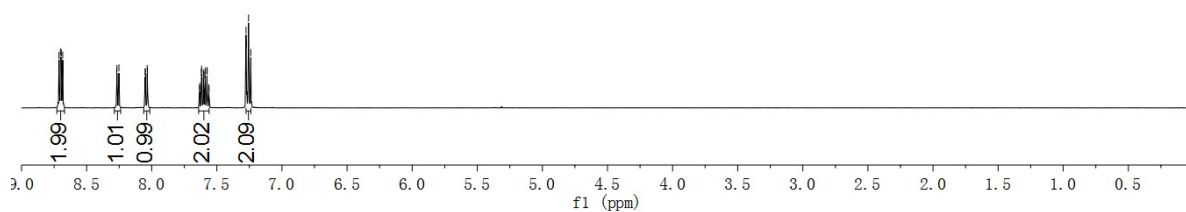
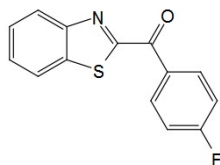


¹H and ¹³C NMR Spectra of 3af

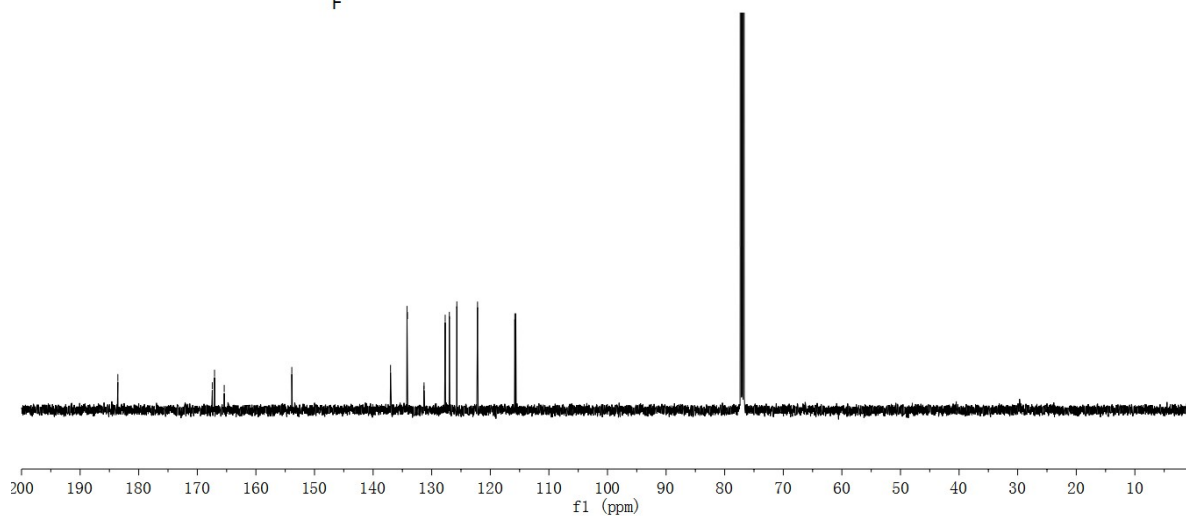
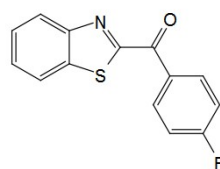


¹H and ¹³C NMR Spectra of 3ag

8.712
8.701
8.695
8.684
8.269
8.267
8.252
8.050
8.049
8.048
8.035
8.033
7.634
7.631
7.619
7.617
7.603
7.600
7.592
7.589
7.576
7.574
7.562
7.559
7.276
7.274
7.256
7.239

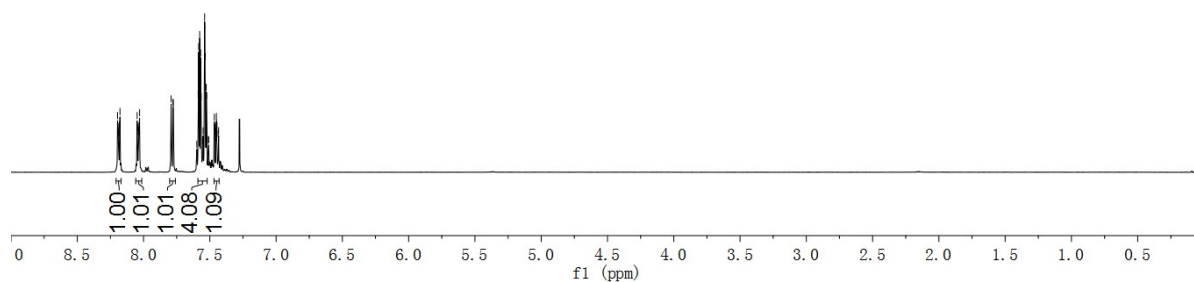
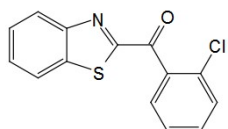


183.56
167.45
167.06
165.40
153.87
137.03
134.21
134.14
131.33
131.31
127.70
126.99
125.71
122.18
115.82
115.64

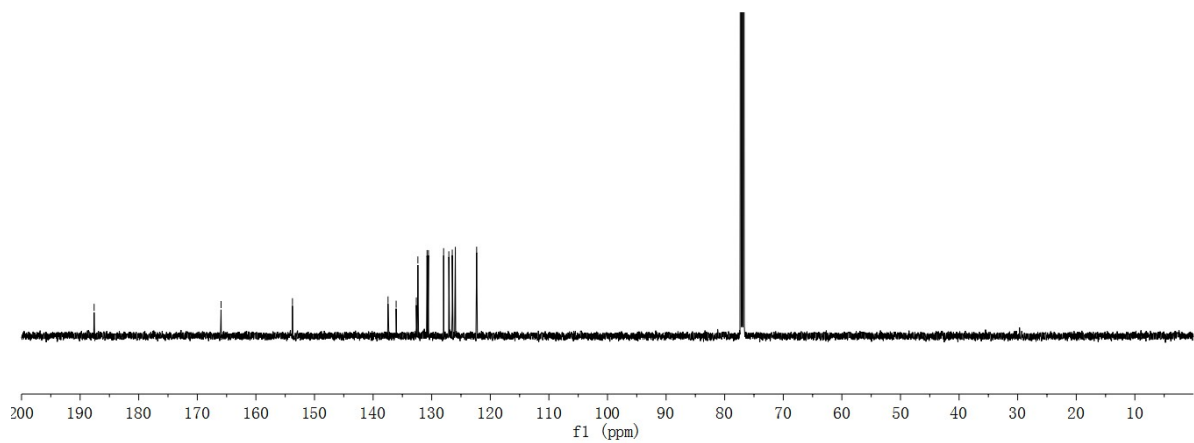
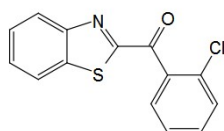


¹H and ¹³C NMR Spectra of 3ah

8.196
8.192
8.189
8.186
8.181
8.178
8.048
8.045
8.040
8.037
8.035
8.030
7.792
7.778
7.775
7.598
7.588
7.584
7.577
7.569
7.566
7.555
7.550
7.539
7.538
7.534
7.527
7.524
7.511
7.508
7.466
7.461
7.454
7.451
7.449
7.446
7.438
7.434

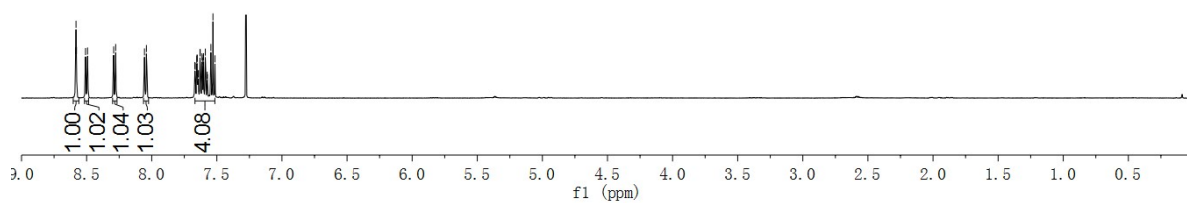
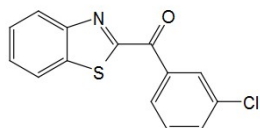


-187.61
-165.95
-153.76
-137.45
-136.07
-132.63
-132.36
-130.79
-130.55
-127.97
-127.07
-126.49
-125.97
-122.33

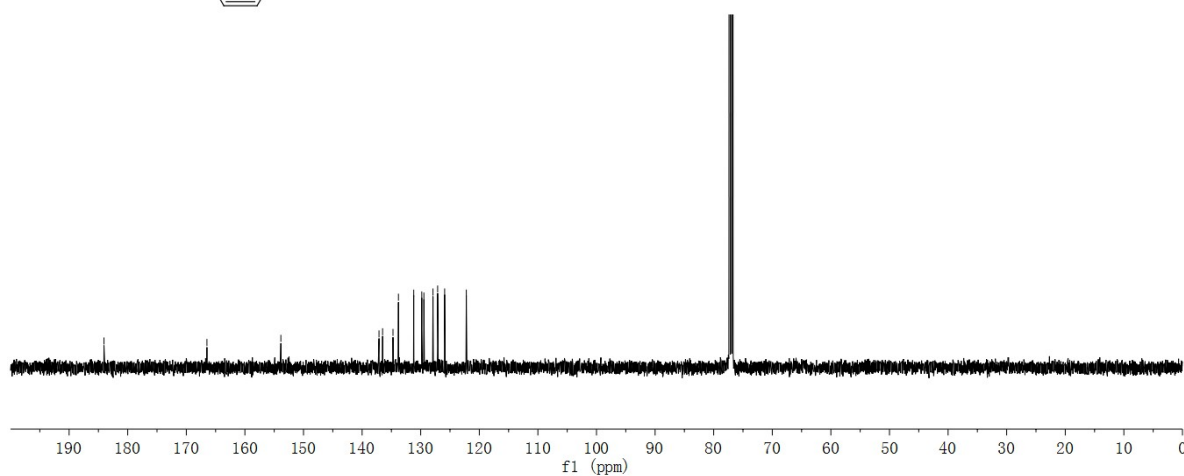
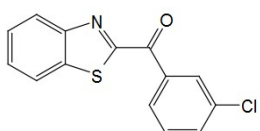


¹H and ¹³C NMR Spectra of 3ai

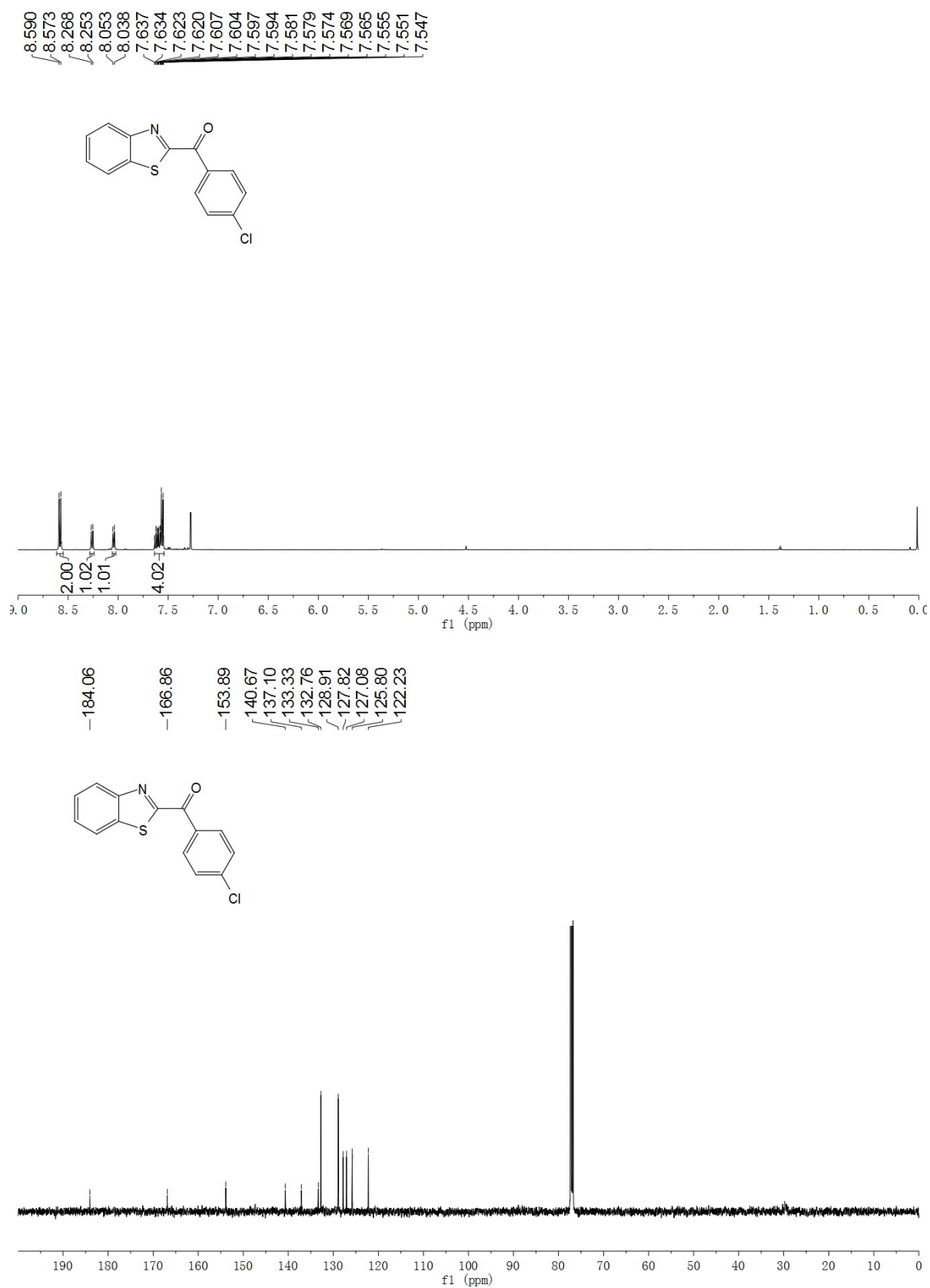
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8.581
8.578
8.509
8.493
8.292
8.277
8.056
8.041
7.668
7.666
7.654
7.652
7.651
7.644
7.642
7.630
7.628
7.614
7.611
7.605
7.602
7.588
7.574
7.572
7.546
7.530
7.514



184.05
166.48
153.86
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136.50
134.73
133.80
131.19
129.82
129.45
127.90
127.11
125.91
122.22

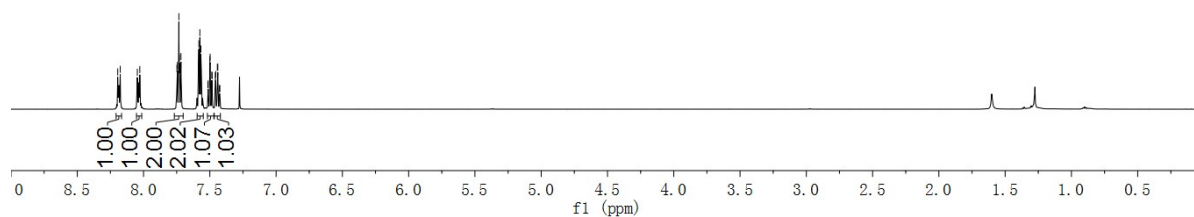
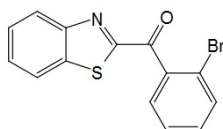


¹H and ¹³C NMR Spectra of 3aj

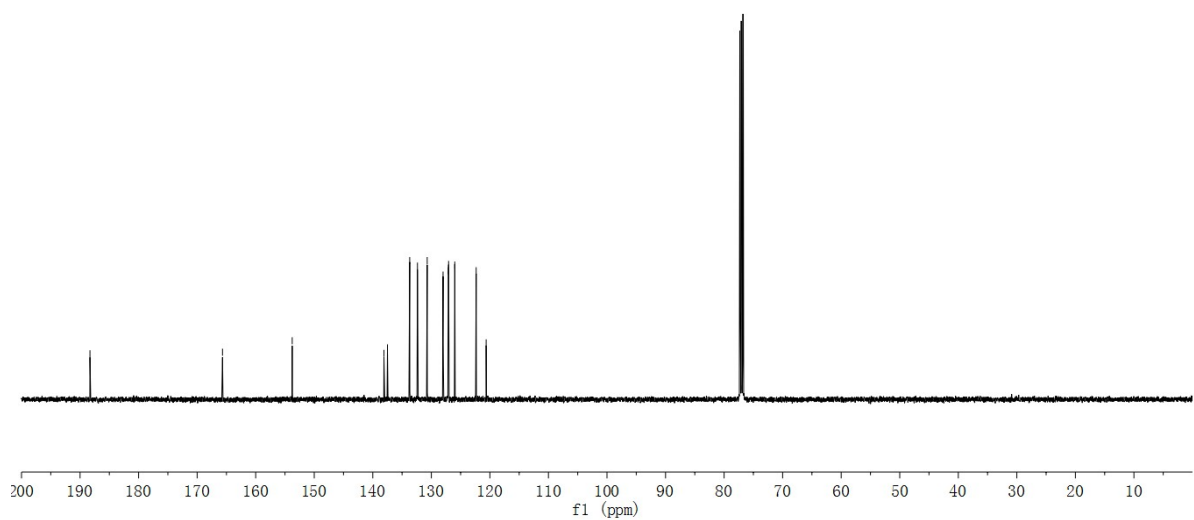
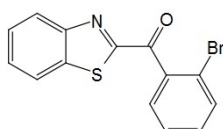


¹H and ¹³C NMR Spectra of 3ak

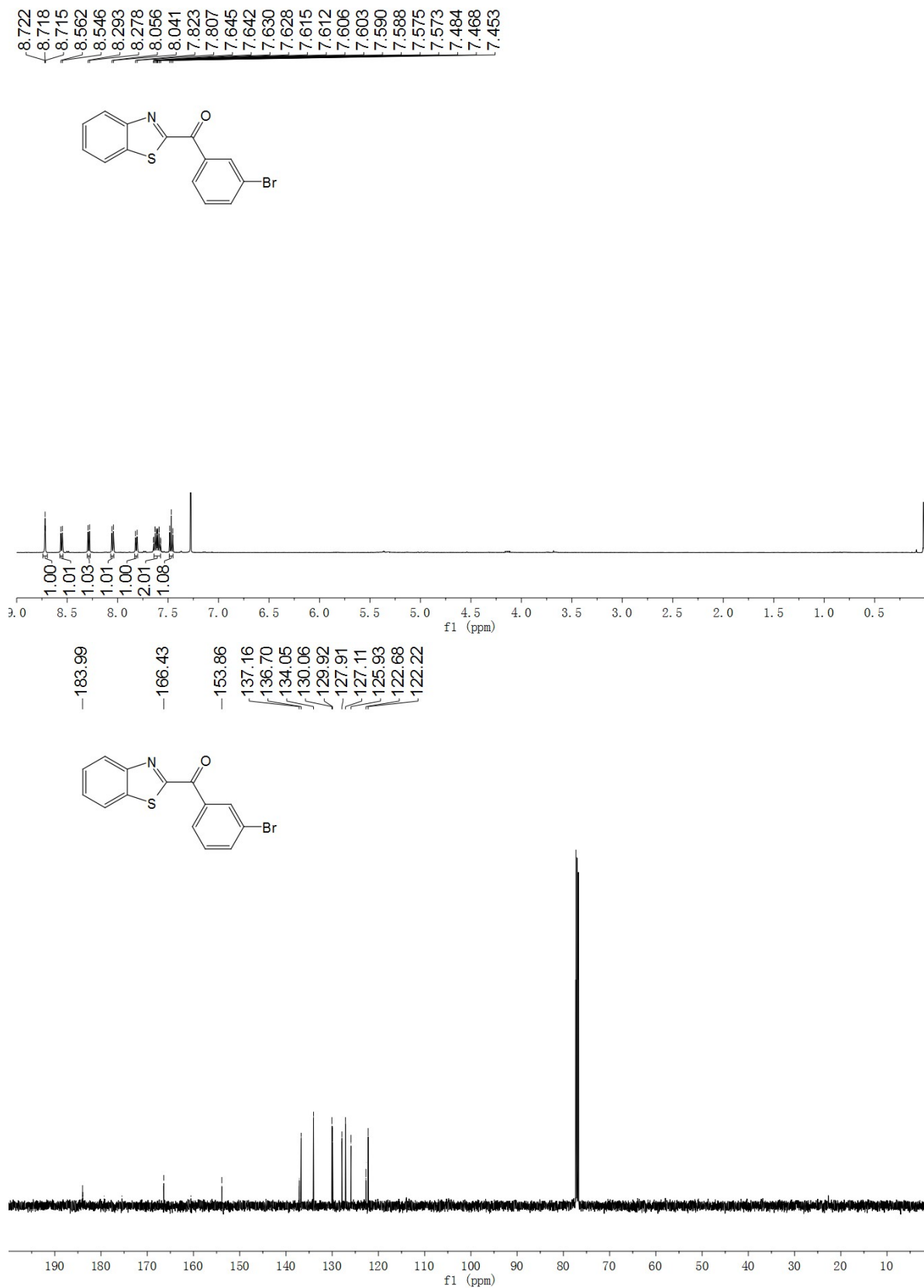
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8.047
8.028
7.748
7.745
7.733
7.730
7.718
7.583
7.575
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7.498
7.485
7.483
7.459
7.455
7.443
7.440
7.428
7.424



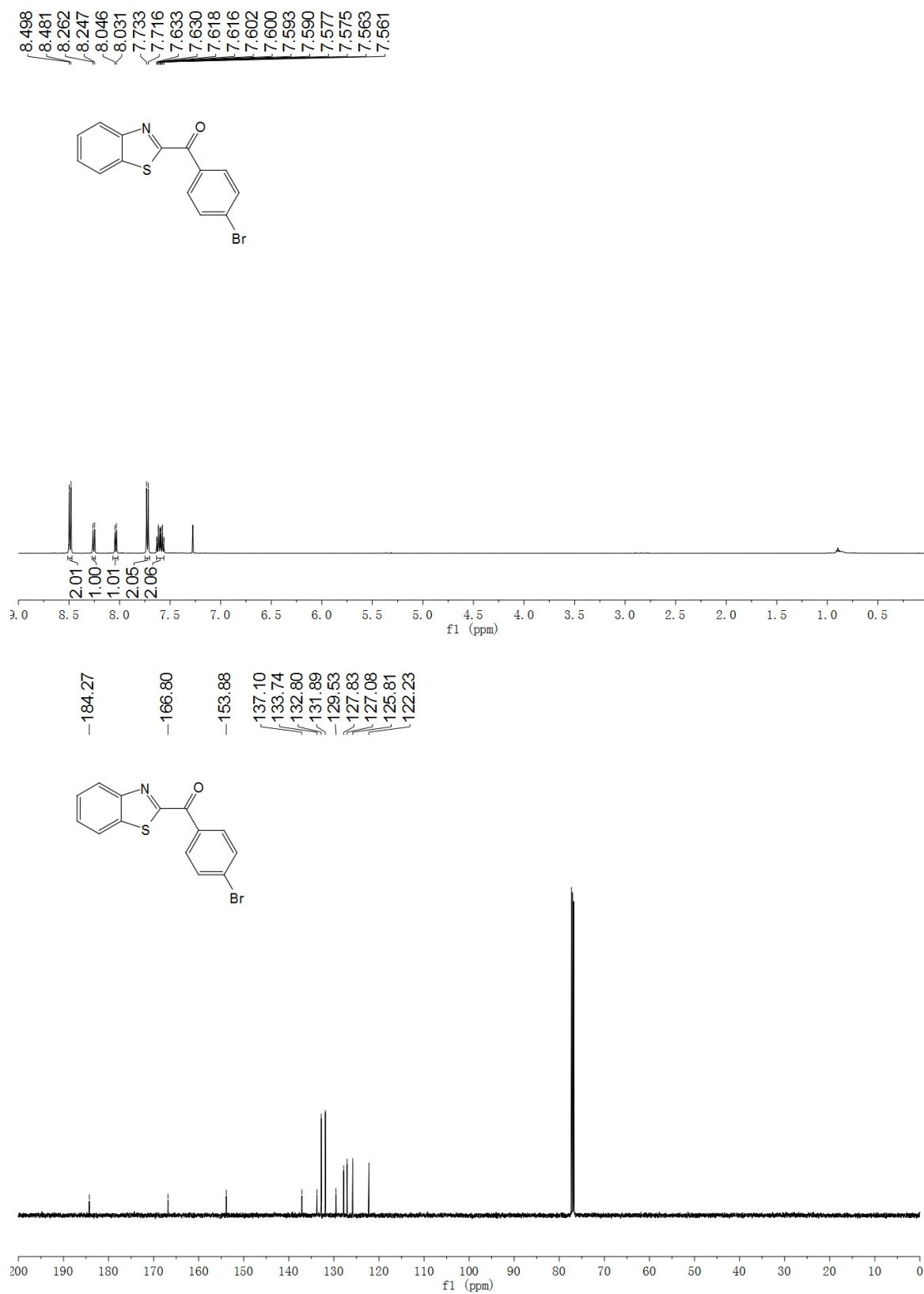
188.31
165.67
153.76
138.09
137.50
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127.09
127.05
125.99
122.34
120.64



¹H and ¹³C NMR Spectra of 3aI

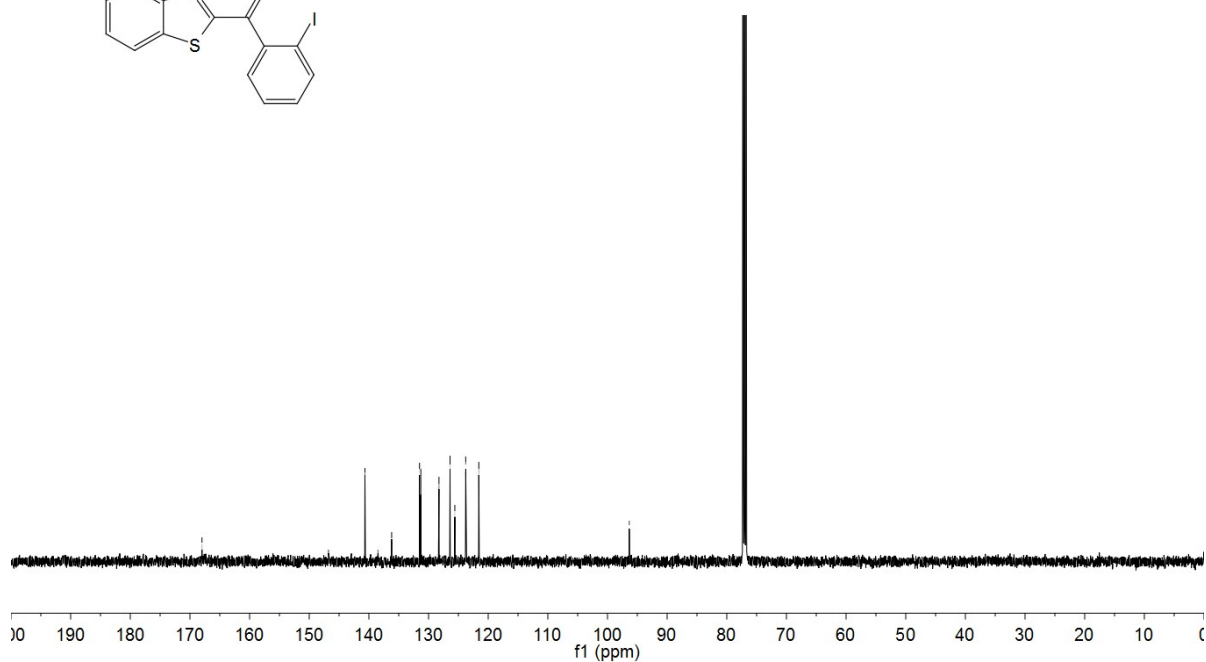
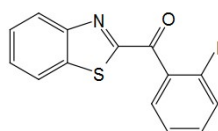
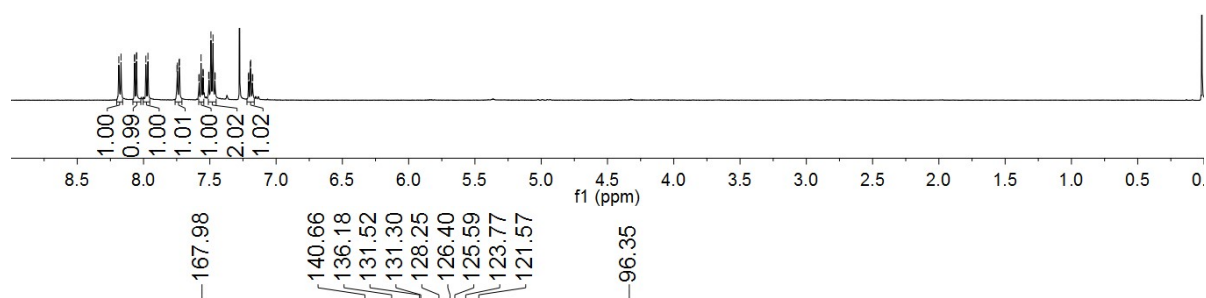
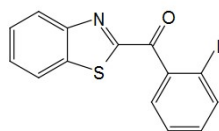


¹H and ¹³C NMR Spectra of 3am



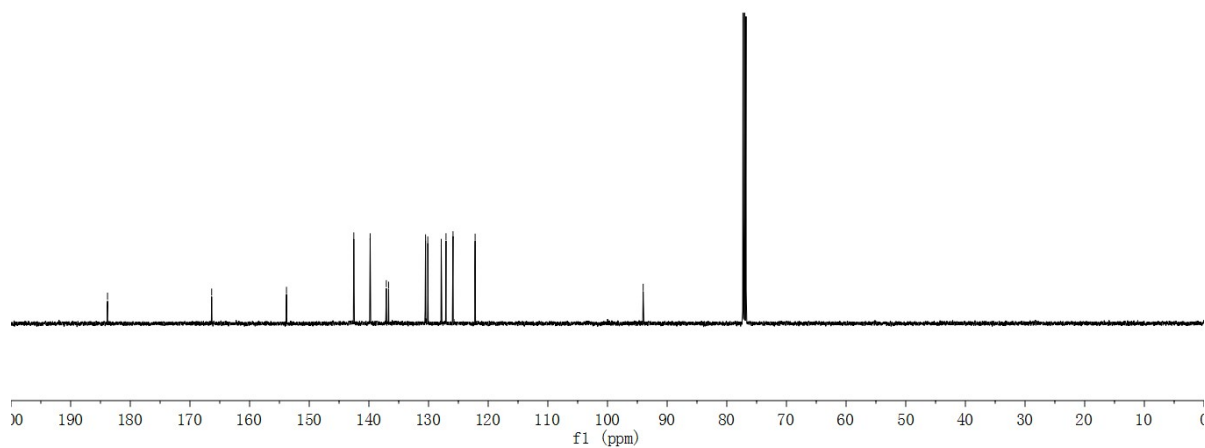
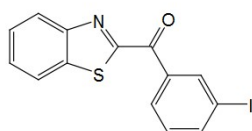
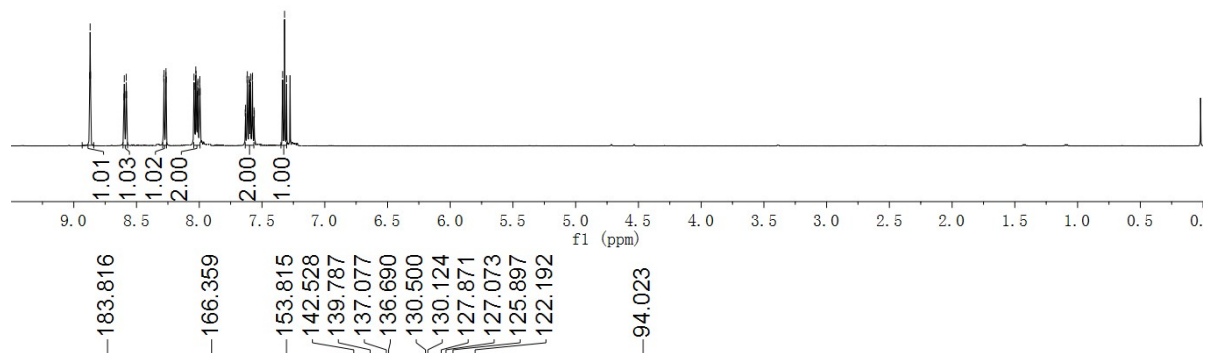
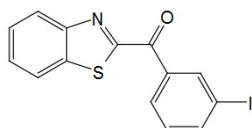
¹H and ¹³C NMR Spectra of 3an

8.186
8.170
8.069
8.067
8.053
8.051
7.982
7.967
7.748
7.744
7.732
7.729
7.583
7.580
7.566
7.552
7.549
7.509
7.506
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7.476
7.462
7.460
7.210
7.207
7.194
7.191
7.179
7.176



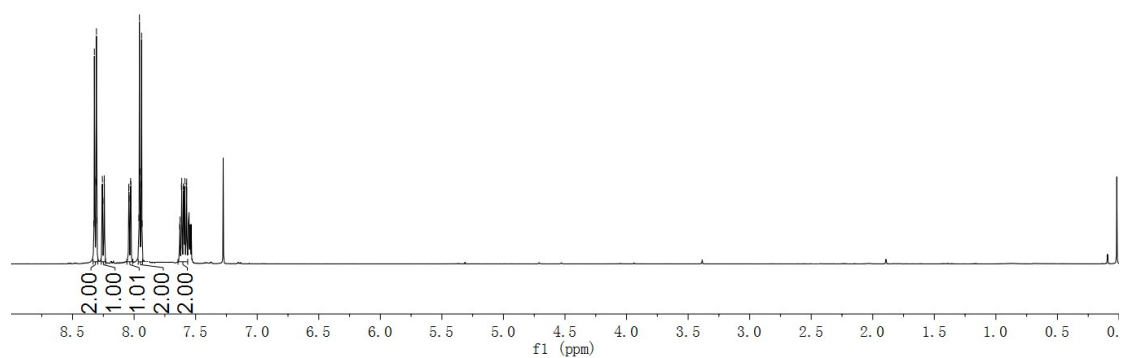
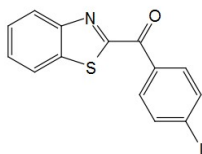
¹H and ¹³C NMR Spectra of 3ao

8.873
8.870
8.867
8.600
8.598
8.595
8.585
8.582
8.579
8.283
8.281
8.268
8.266
8.265
8.264
8.042
8.040
8.028
8.026
8.014
8.012
8.011
8.009
7.999
7.996
7.995
7.993
7.634
7.631
7.620
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7.304

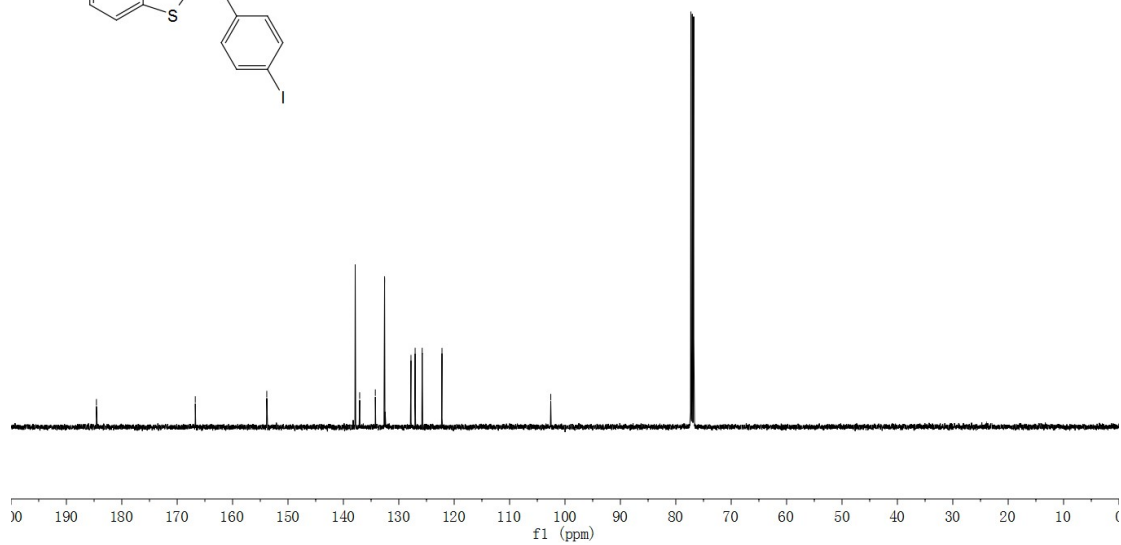
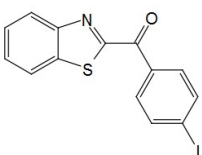


¹H and ¹³C NMR Spectra of 3ap

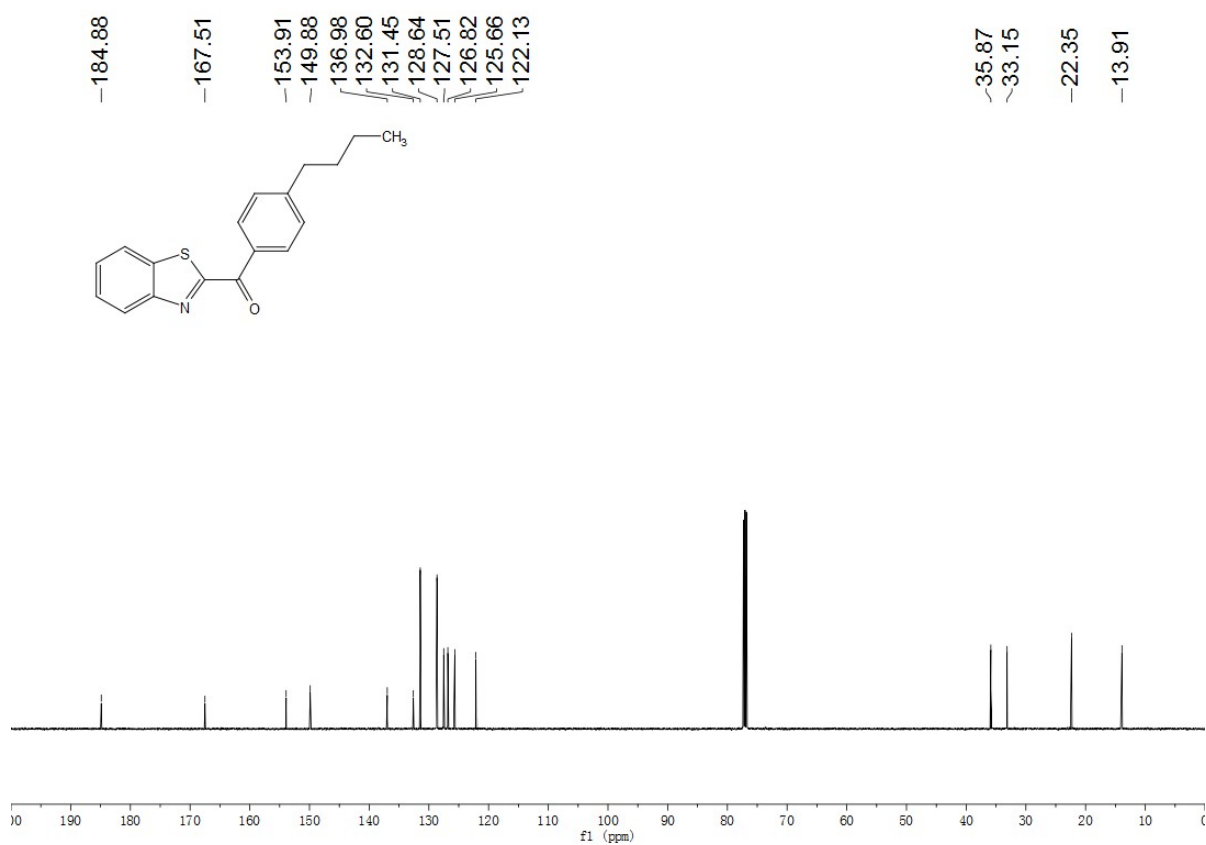
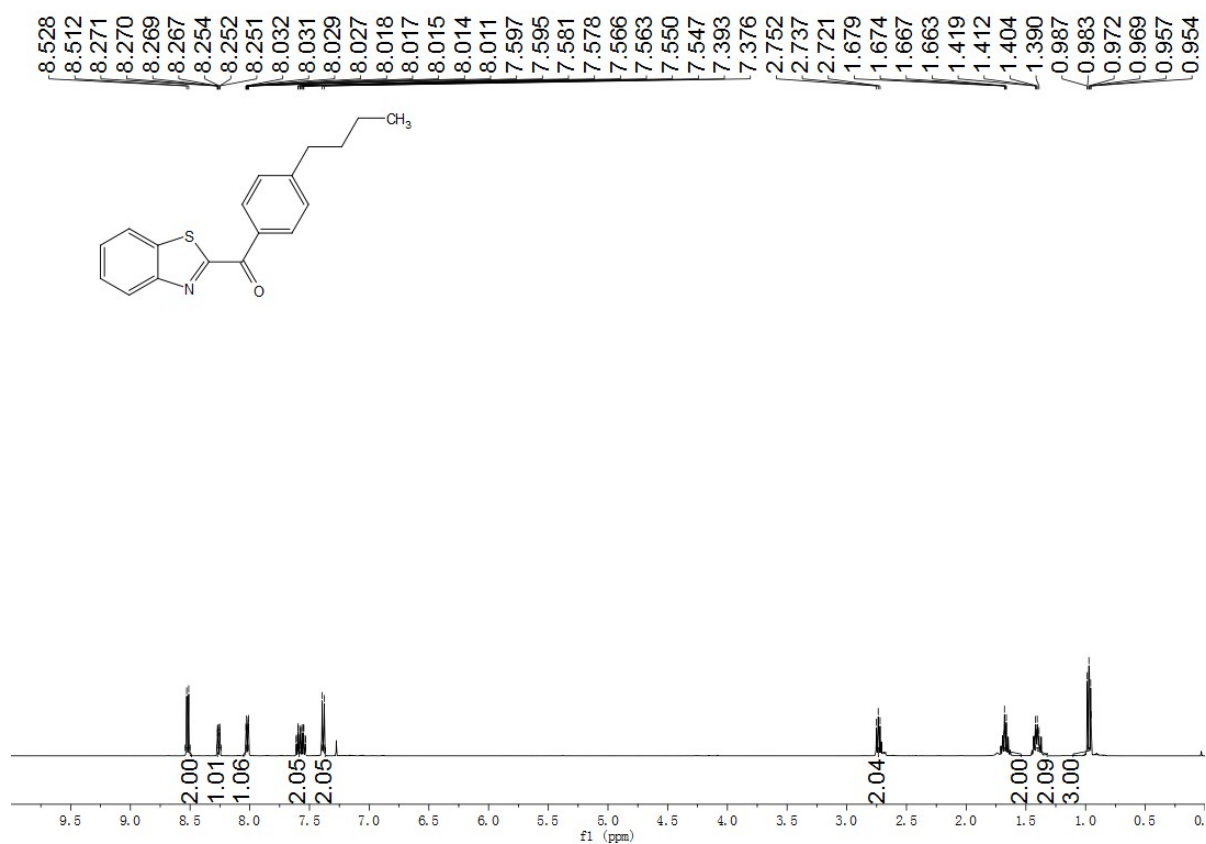
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8.042
8.041
8.028
8.026
7.961
7.957
7.953
7.943
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7.613
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7.597
7.591
7.588
7.575
7.572



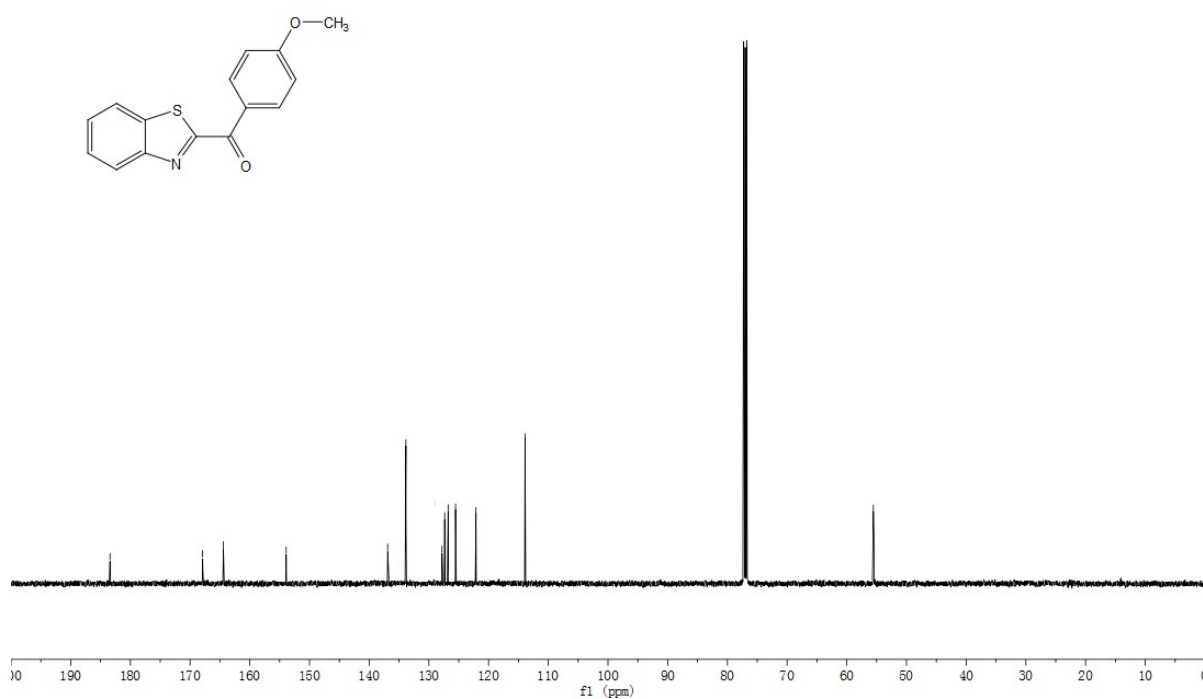
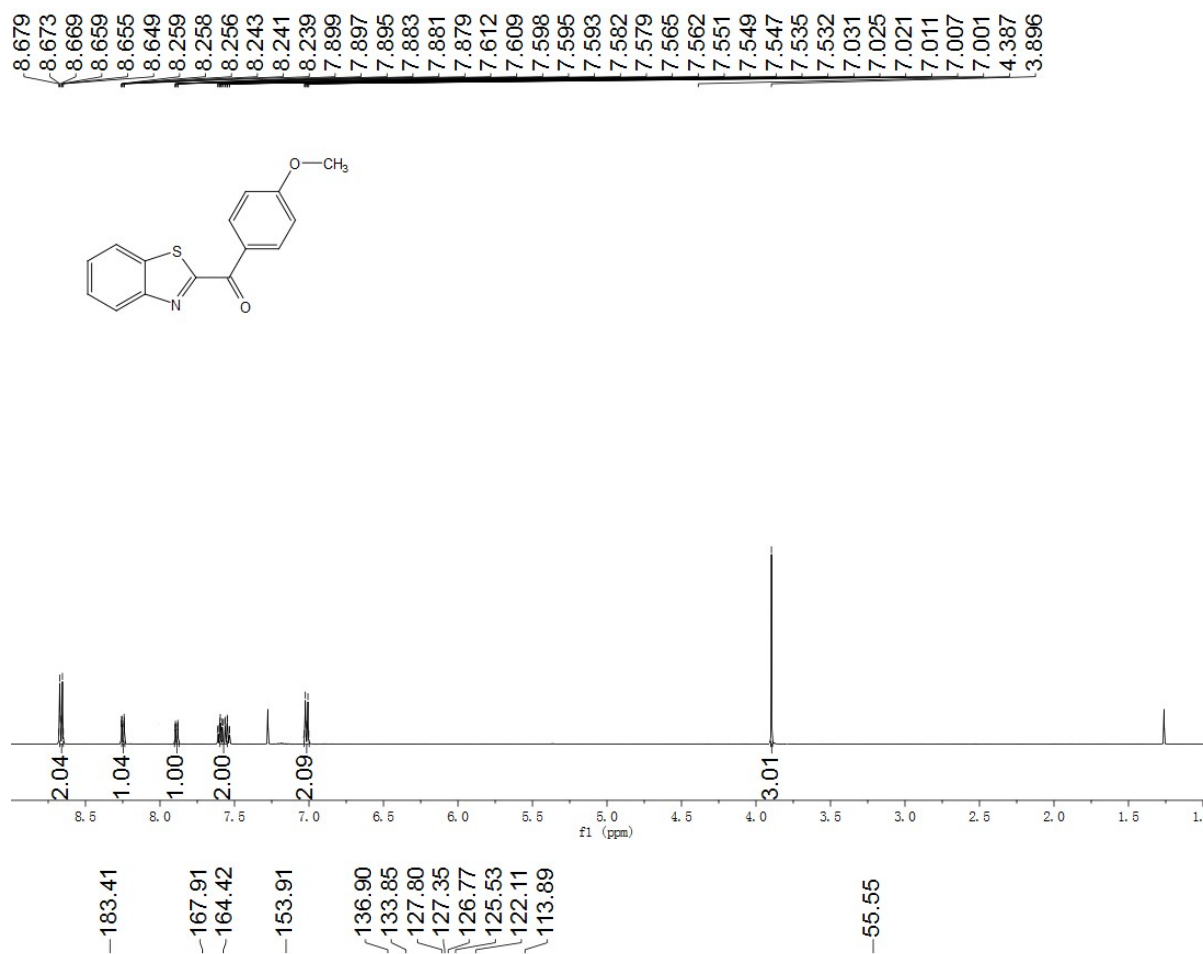
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-166.73
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-127.05
-125.78
-122.20
-102.57



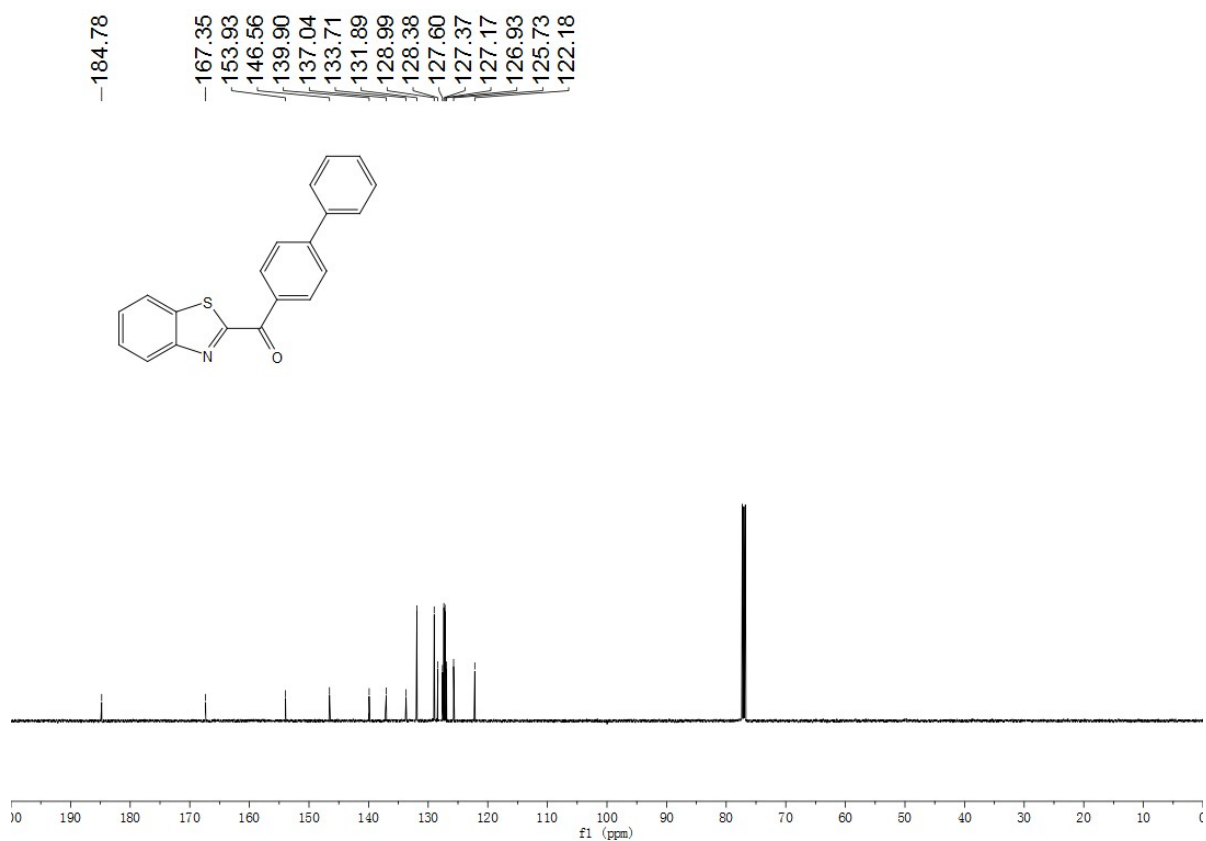
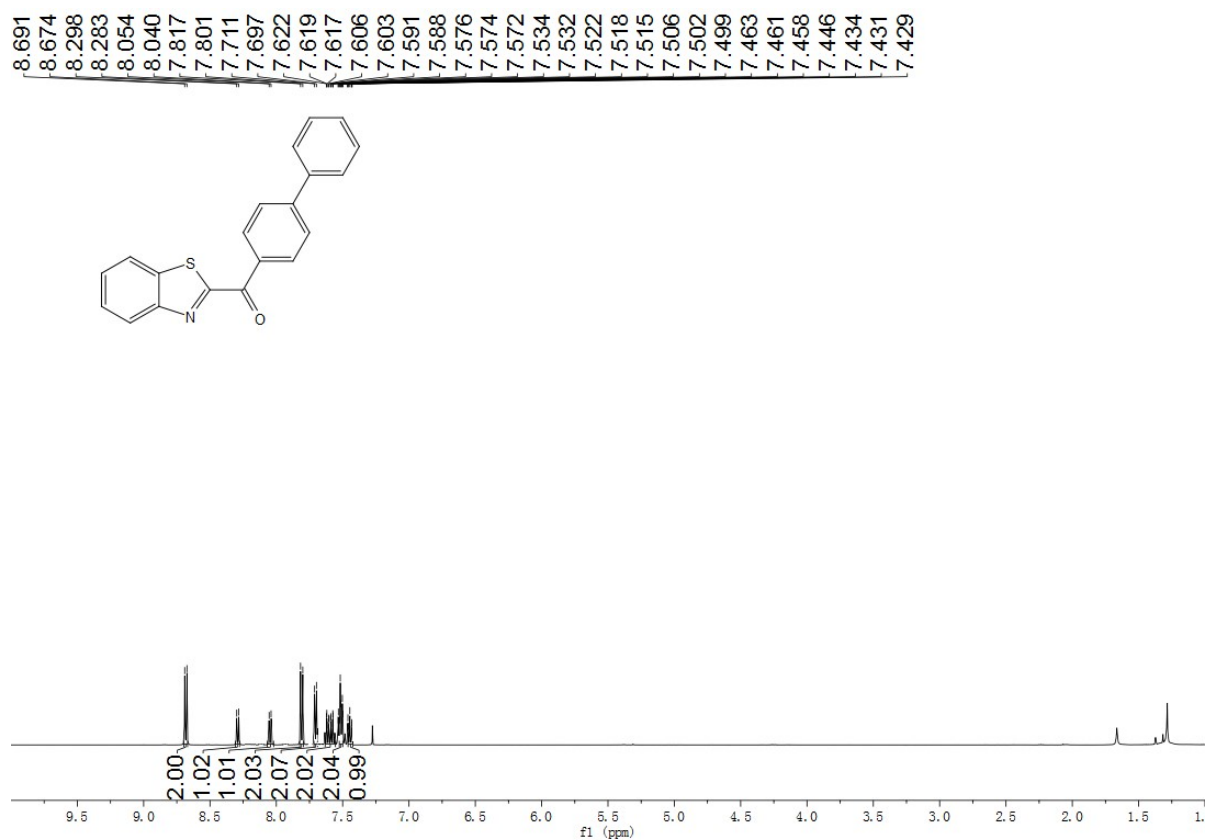
¹H and ¹³C NMR Spectra of 3aq



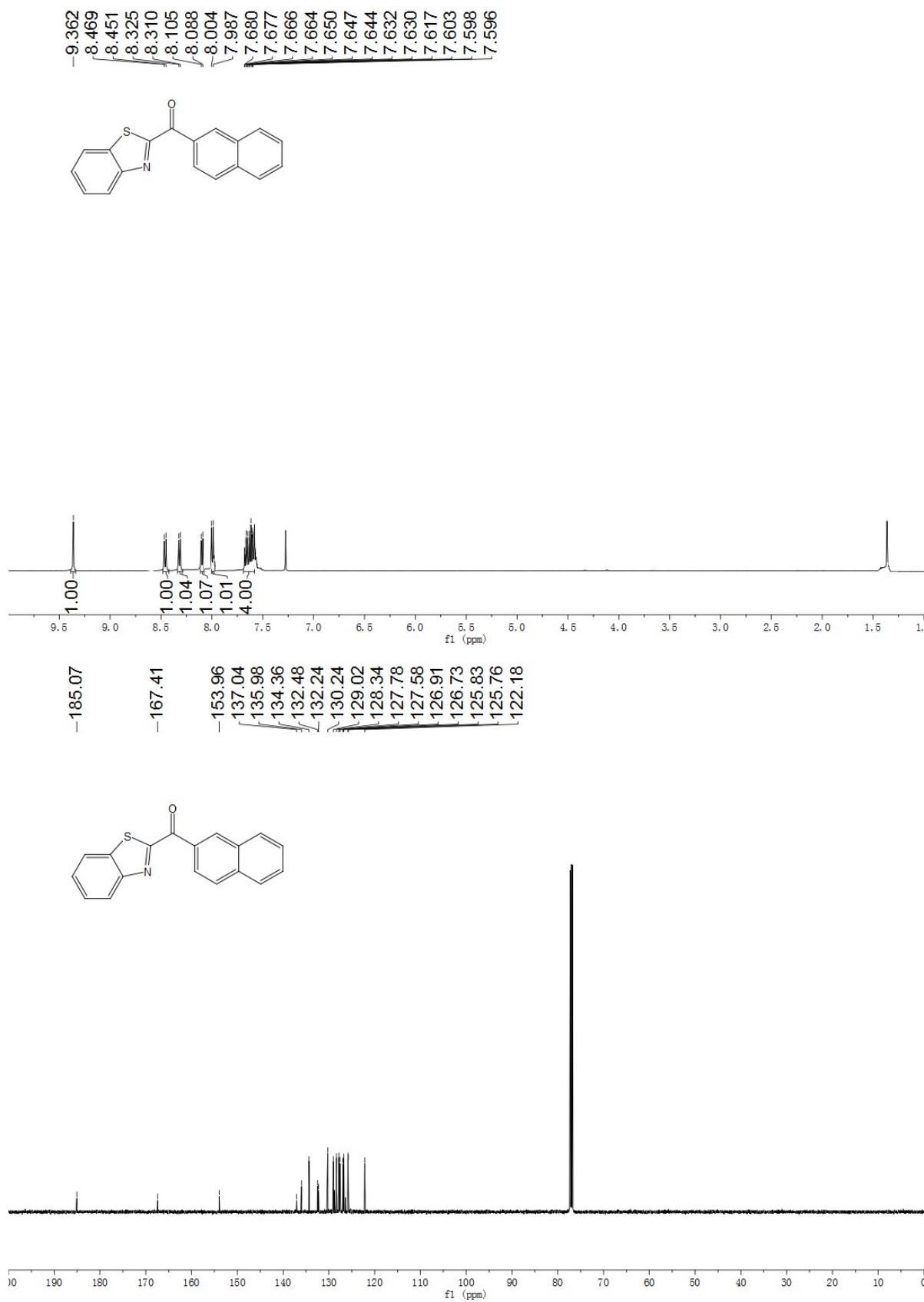
¹H and ¹³C NMR Spectra of 3ar



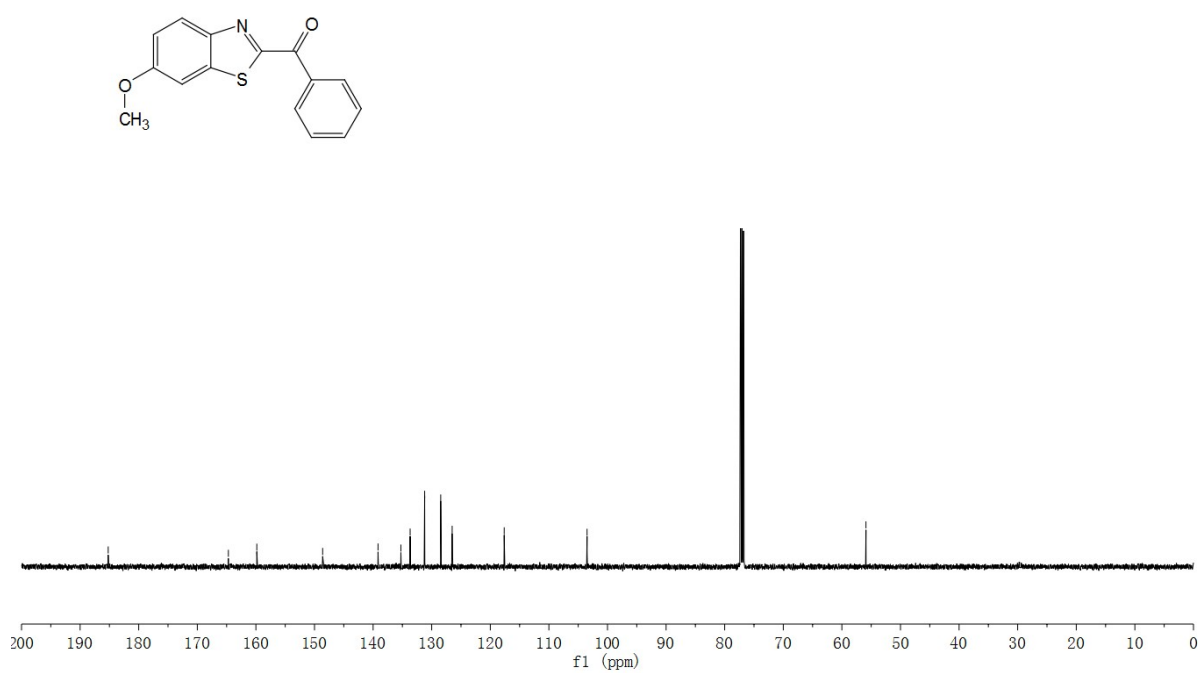
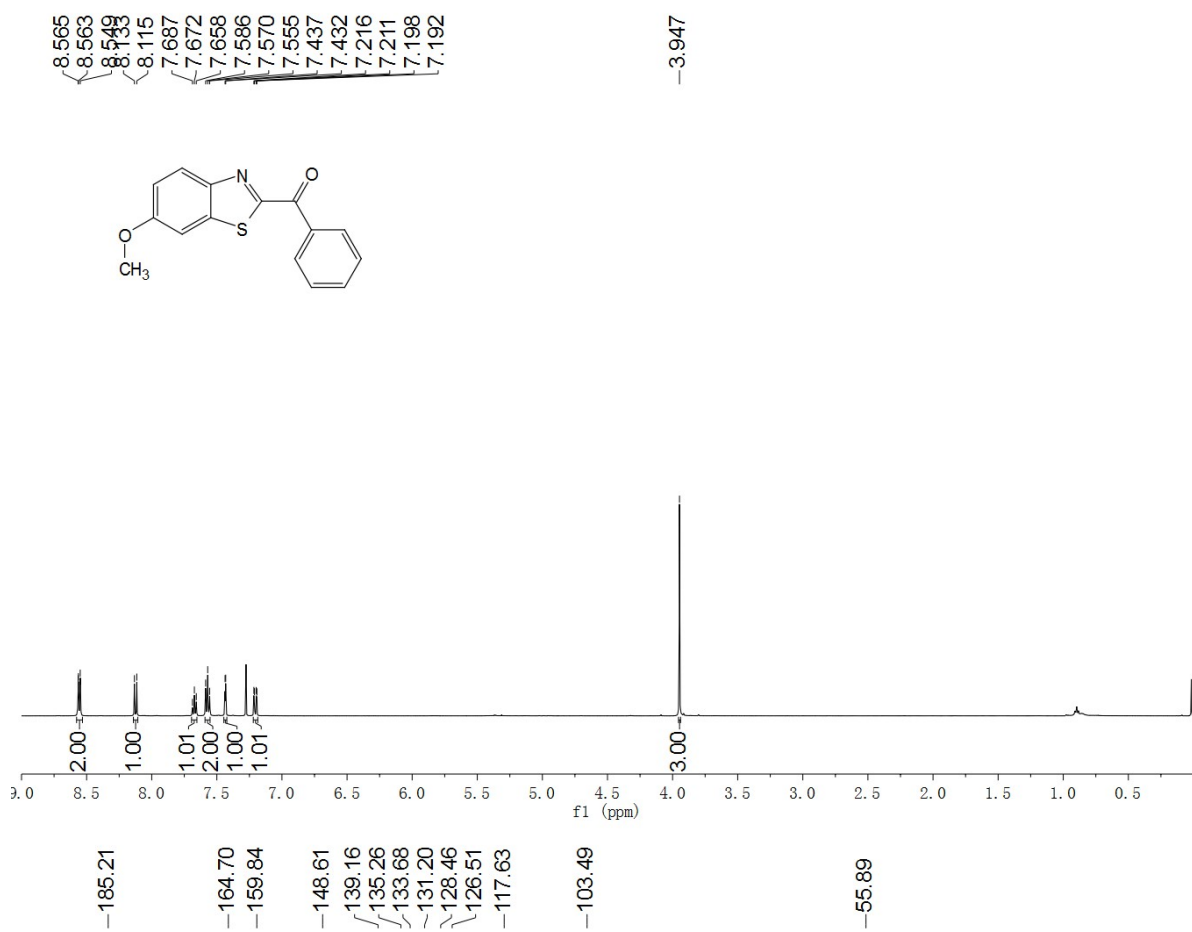
¹H and ¹³C NMR Spectra of 3as



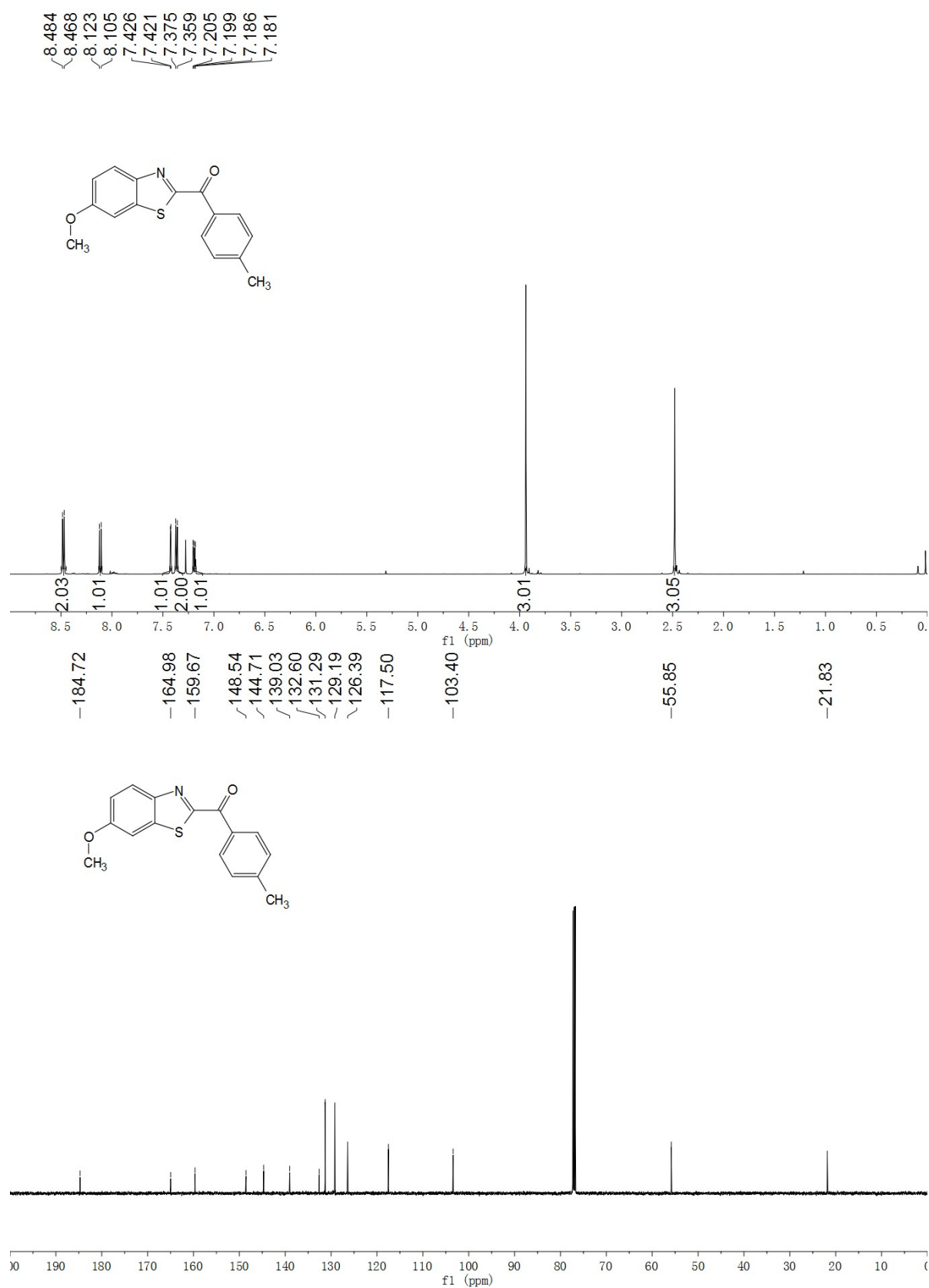
¹H and ¹³C NMR Spectra of 3at



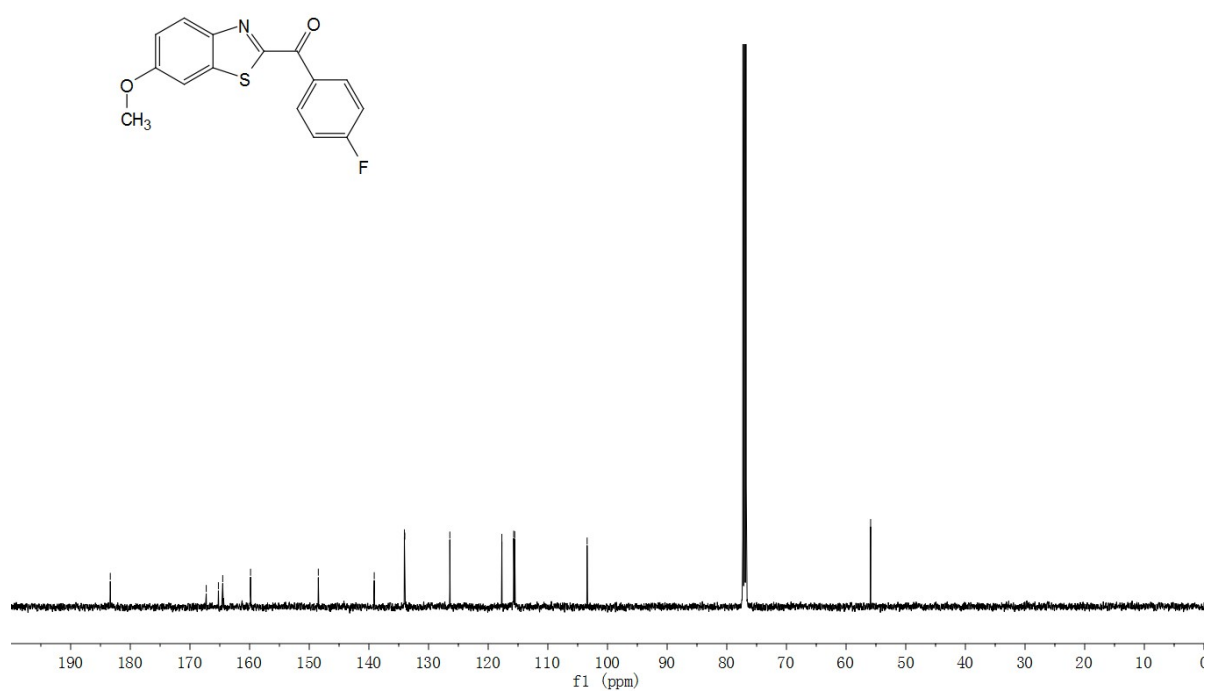
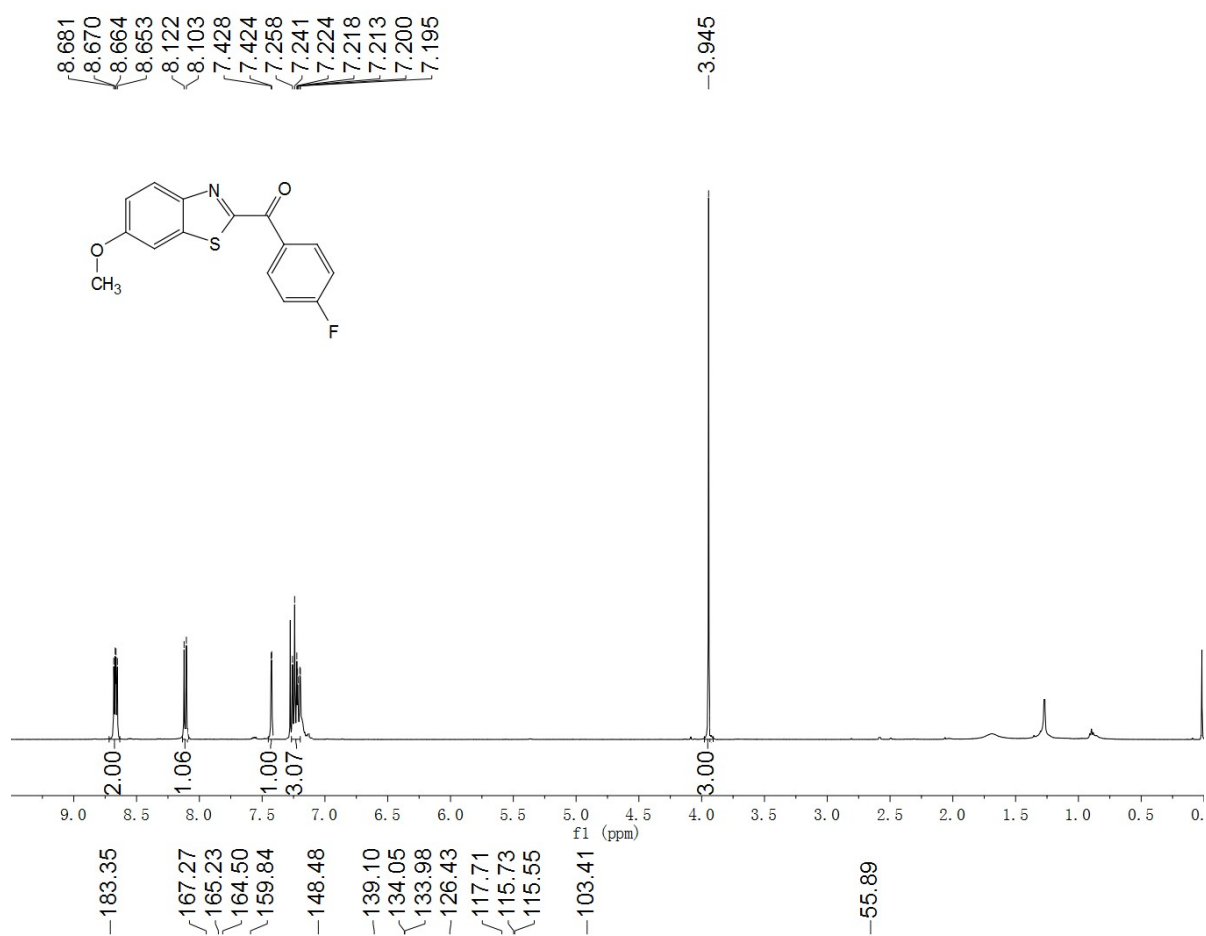
¹H and ¹³C NMR Spectra of 3ba



¹H and ¹³C NMR Spectra of 3bb



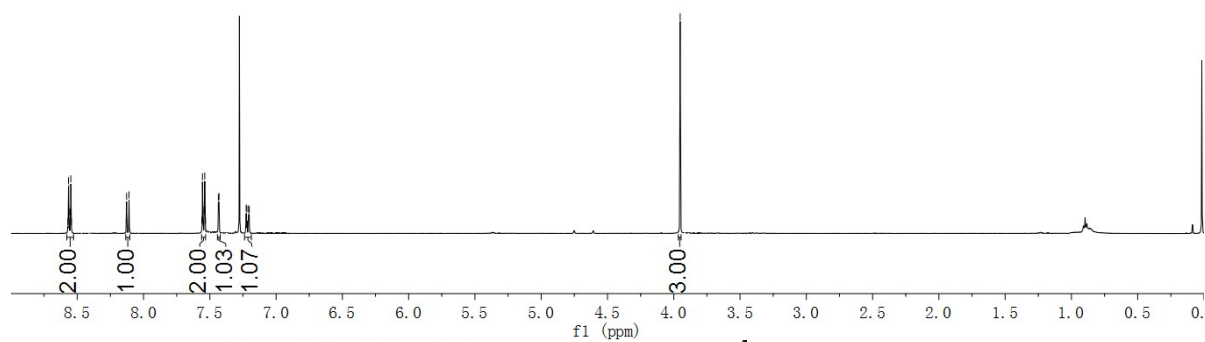
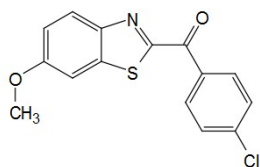
¹H and ¹³C NMR Spectra of 3bc



¹H and ¹³C NMR Spectra of 3bd

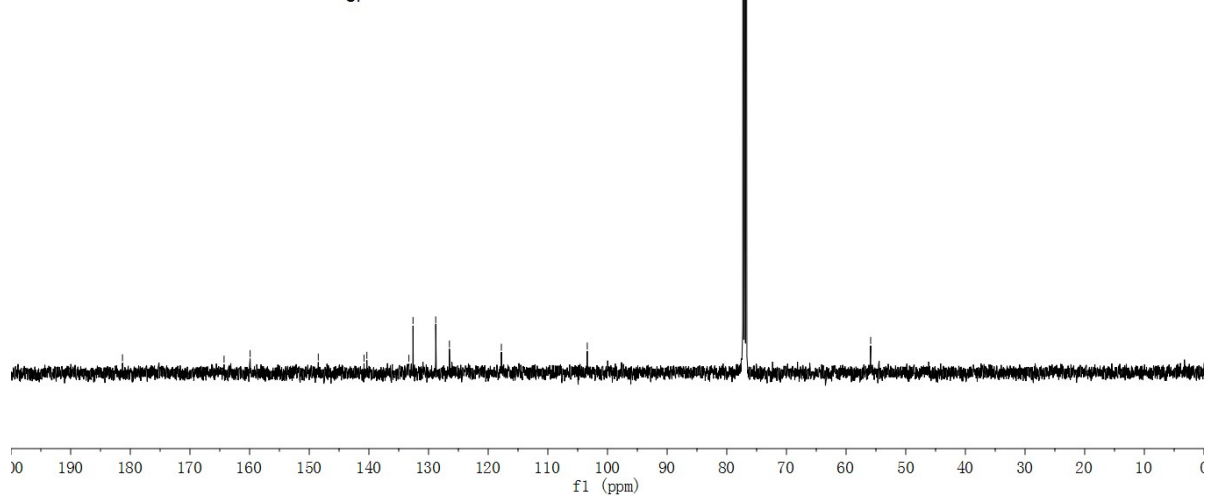
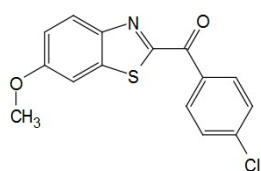
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8.566
8.563
8.553
8.549
8.544
8.128
8.110
7.560
7.556
7.552
7.542
7.538
7.534
7.436
7.431
7.226
7.221
7.208
7.203

3.952



181.31
164.28
159.91
148.48
140.82
140.34
133.29
132.60
128.79
126.50
117.79
103.39

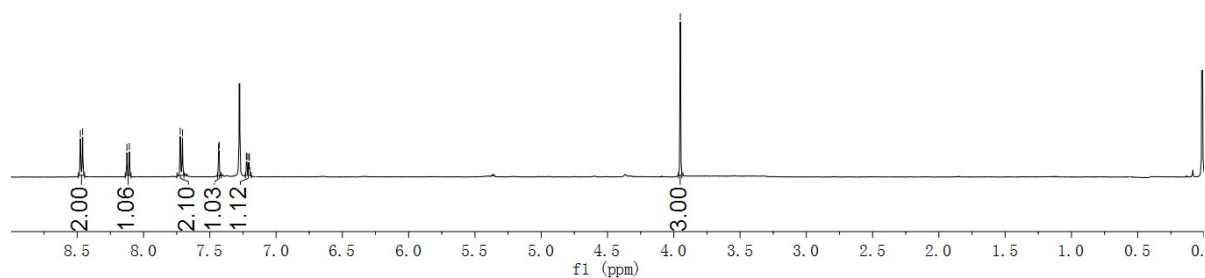
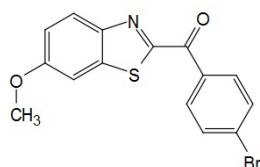
55.88



¹H and ¹³C NMR Spectra of 3be

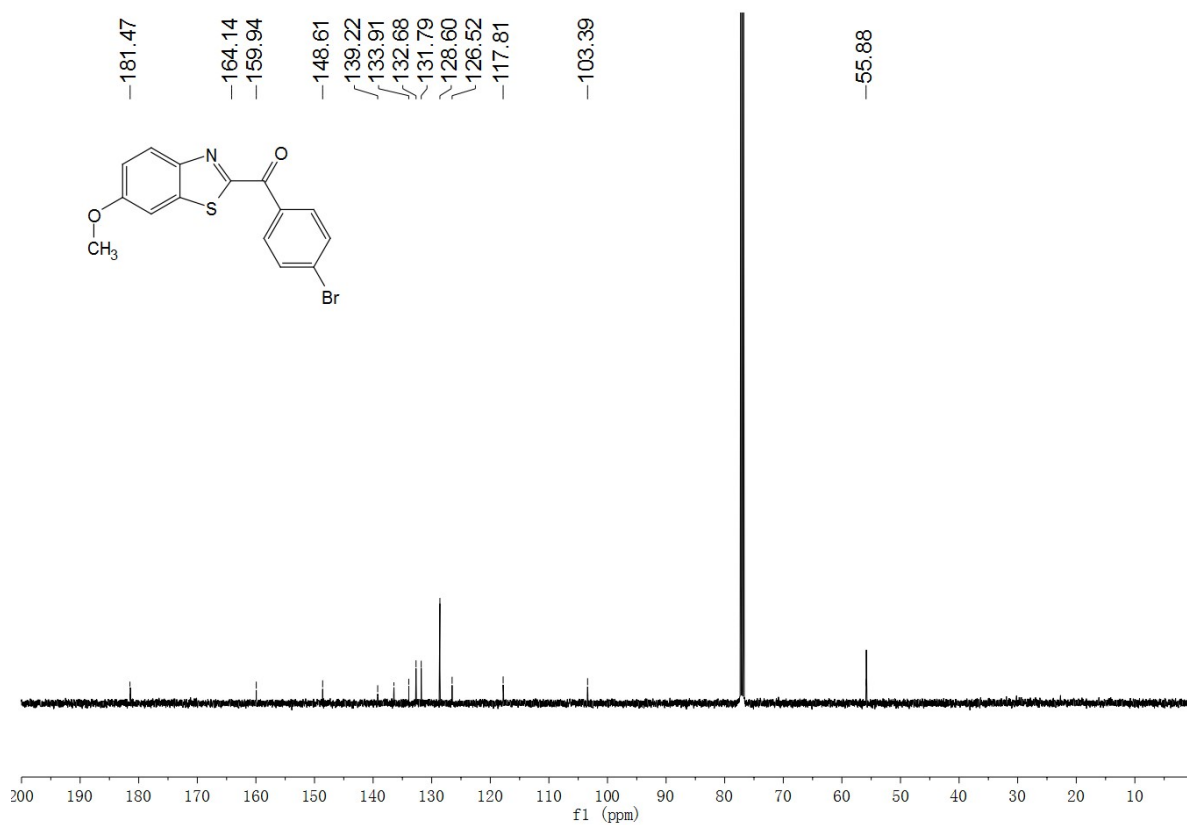
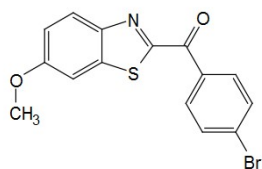
8.477
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7.723
7.706
7.434
7.429
7.225
7.220
7.206
7.201

3.951



181.47
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148.61
139.22
133.91
132.68
131.79
128.60
126.52
117.81
103.39

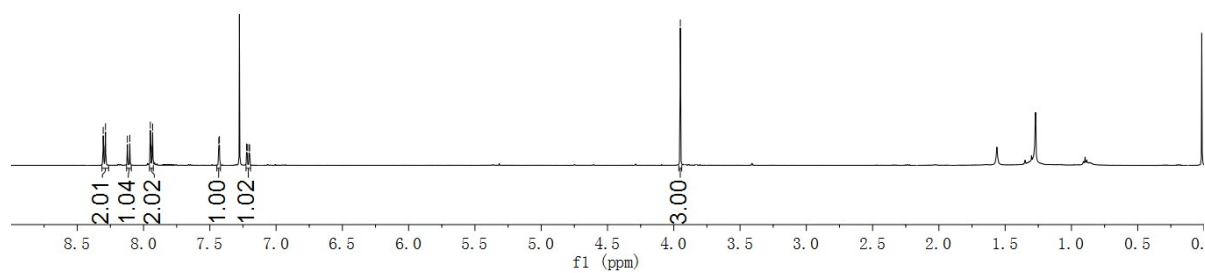
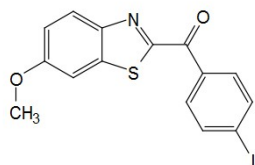
55.88



¹H and ¹³C NMR Spectra of 3bf

8.304
8.301
8.291
8.287
8.122
8.104
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7.945
7.935
7.931
7.432
7.428
7.223
7.218
7.205
7.200

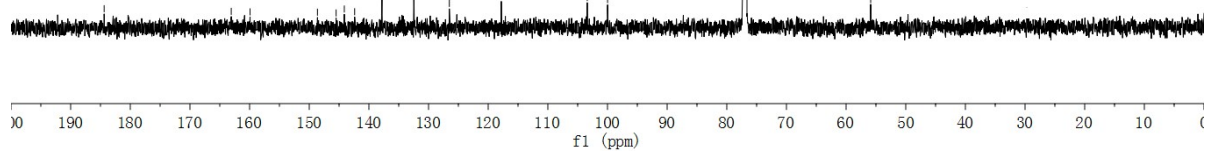
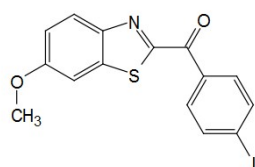
3.950



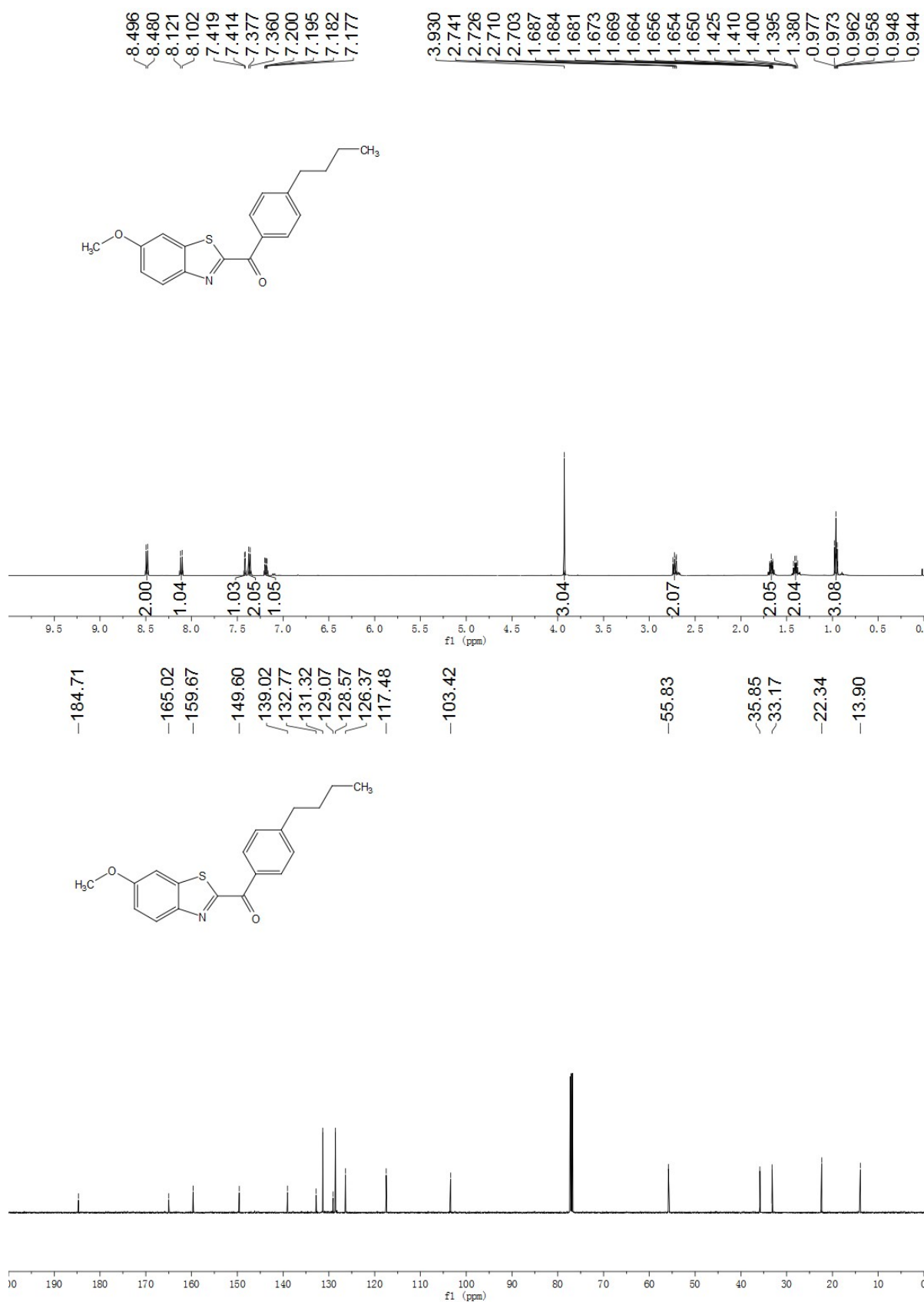
184.38
163.07
159.92
148.62
145.50
144.12
142.39
137.79
132.47
126.52
117.80

103.39
99.99

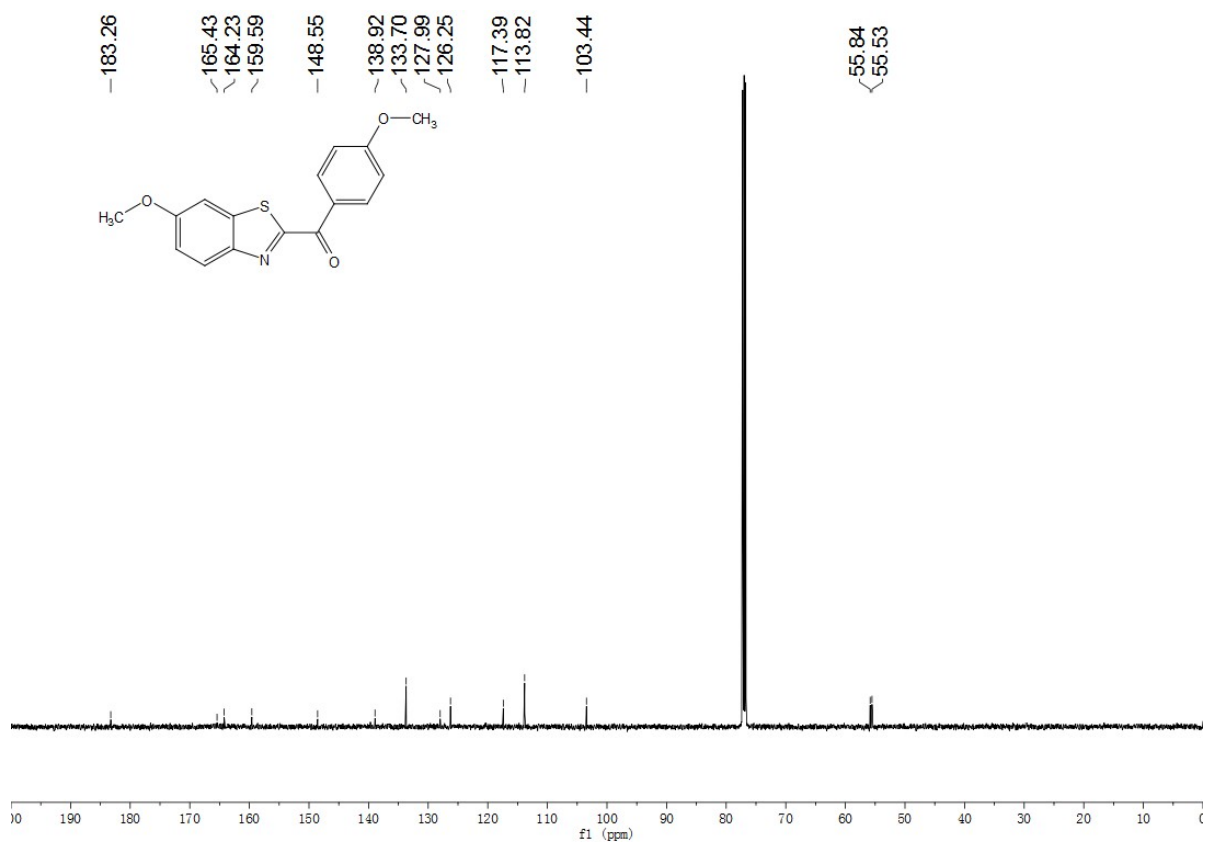
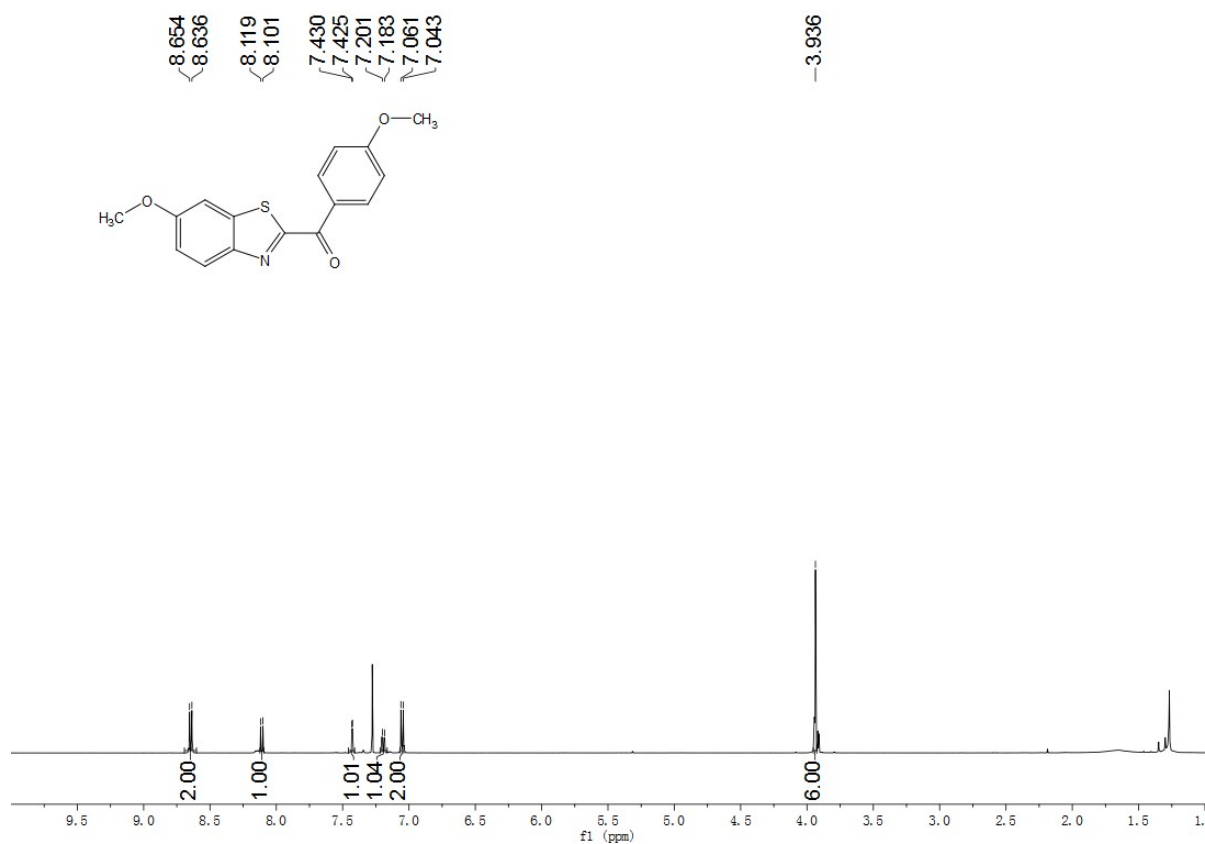
55.88



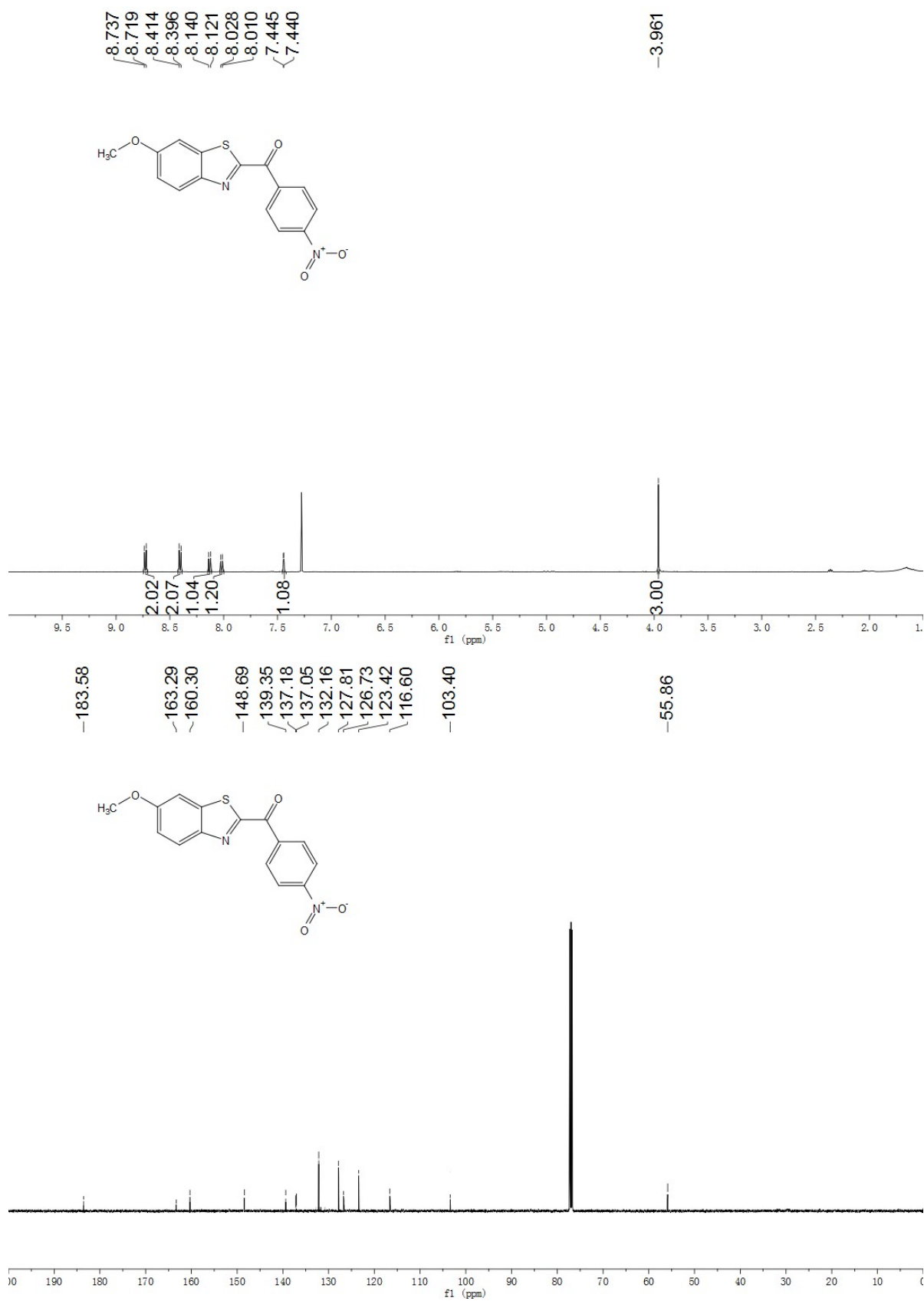
¹H and ¹³C NMR Spectra of 3bg



¹H and ¹³C NMR Spectra of 3bh

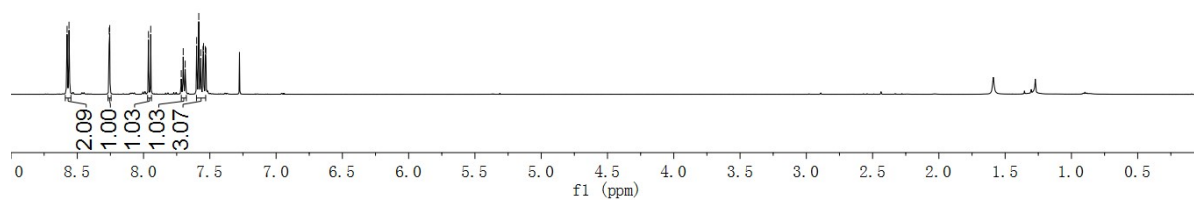
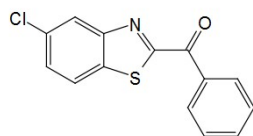


¹H and ¹³C NMR Spectra of 3bi

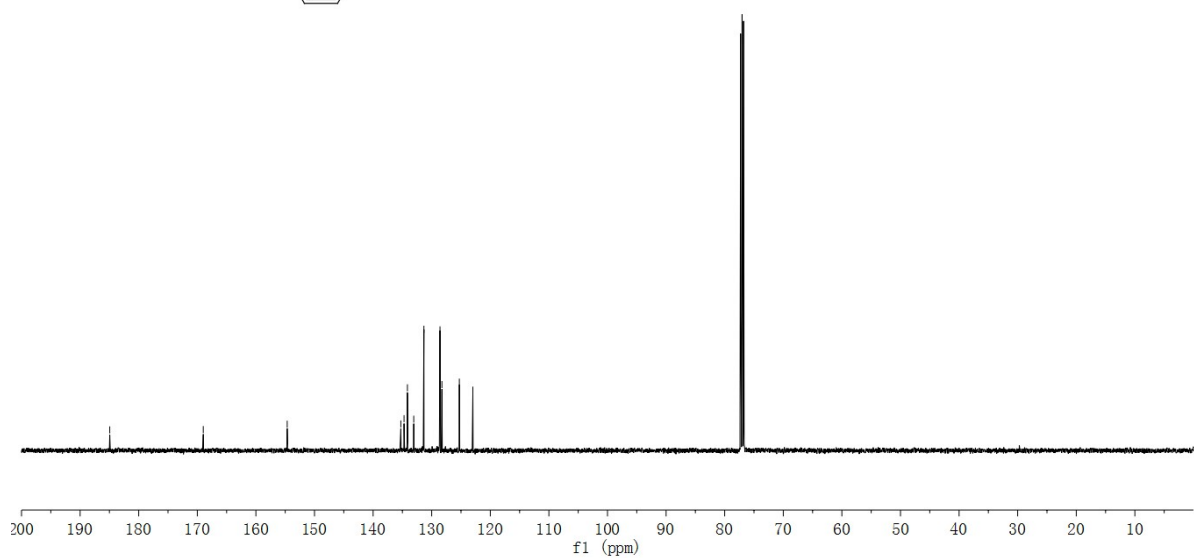
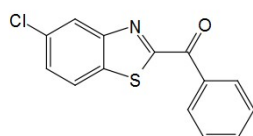


¹H and ¹³C NMR Spectra of 3bj

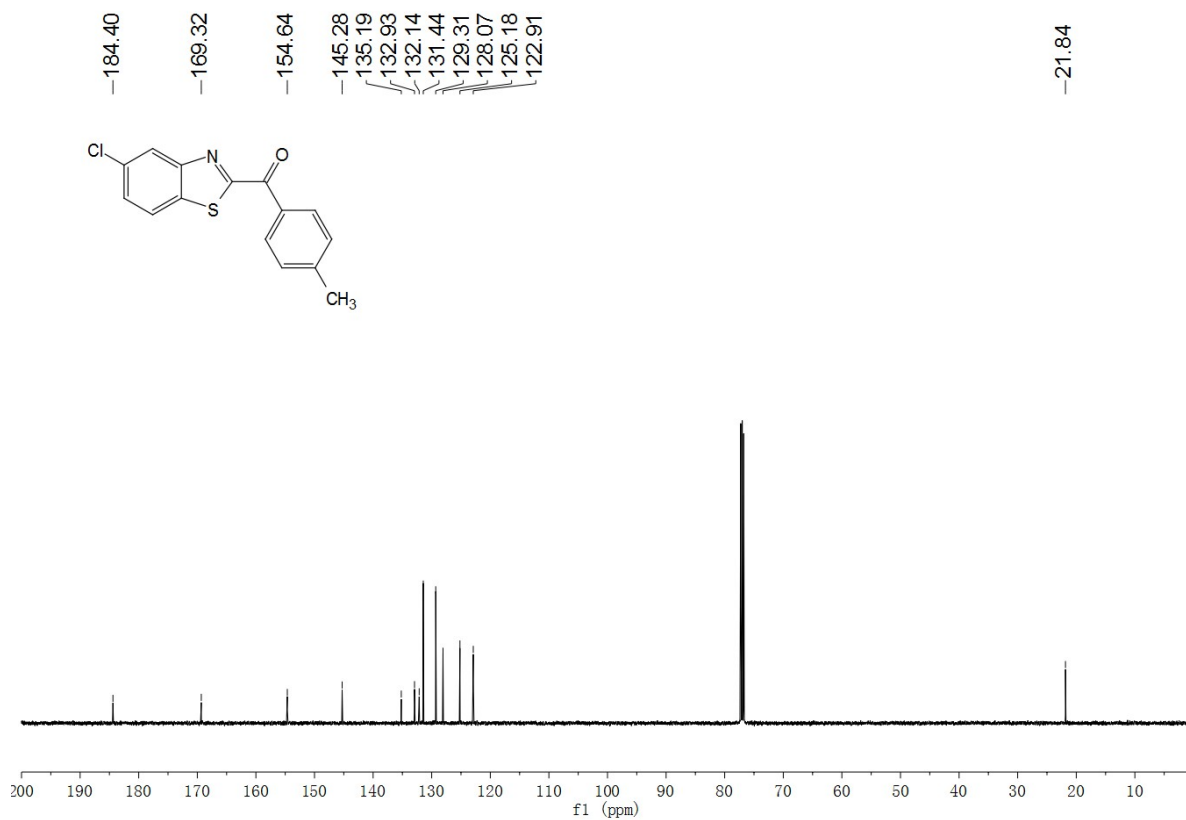
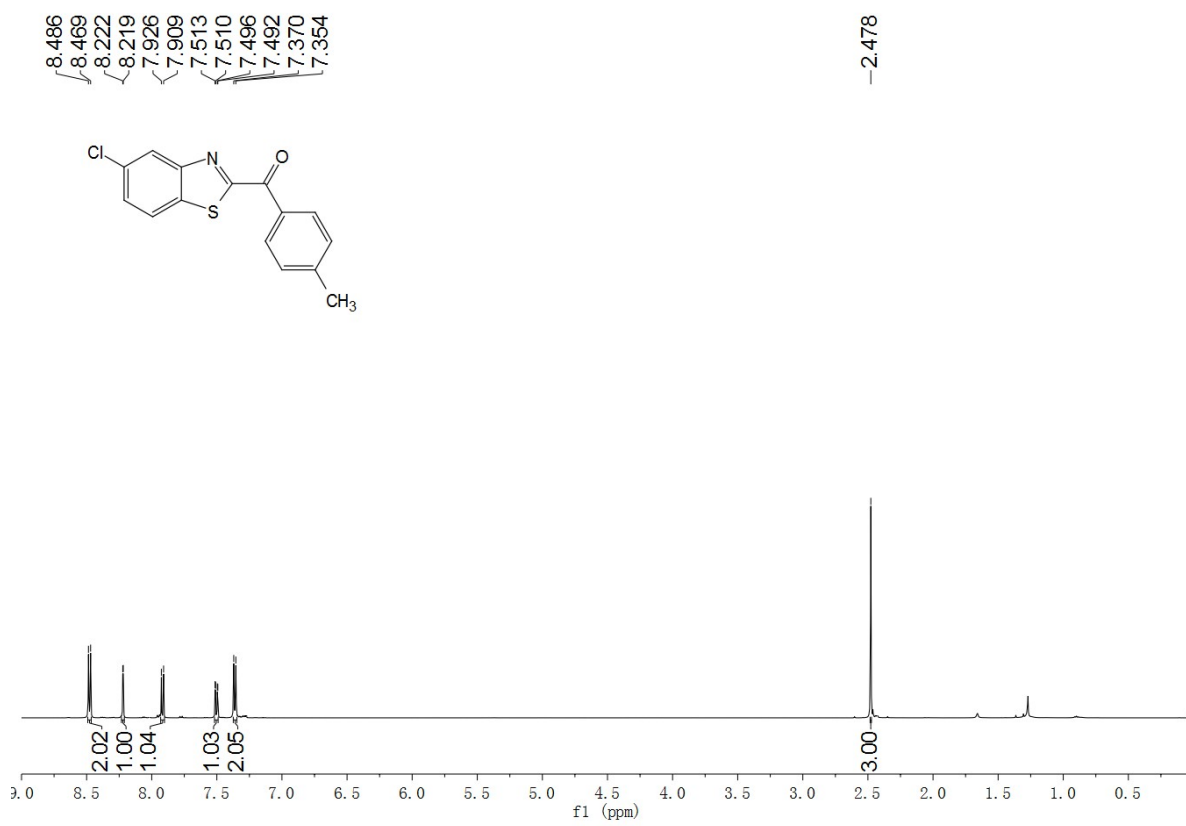
8.577
8.562
8.560
8.259
8.255
7.963
7.946
7.716
7.701
7.686
7.599
7.583
7.568
7.551
7.547
7.534
7.530



184.94
168.98
154.66
135.26
134.72
134.14
133.06
131.33
128.59
128.26
125.28
122.98

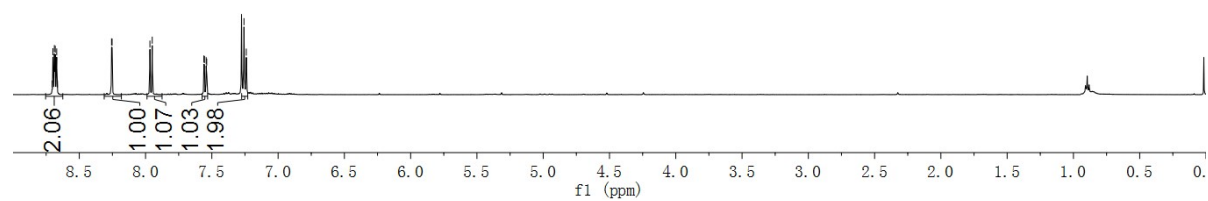
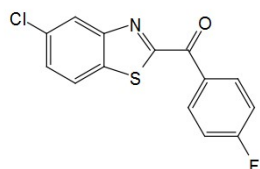


¹H and ¹³C NMR Spectra of 3bk

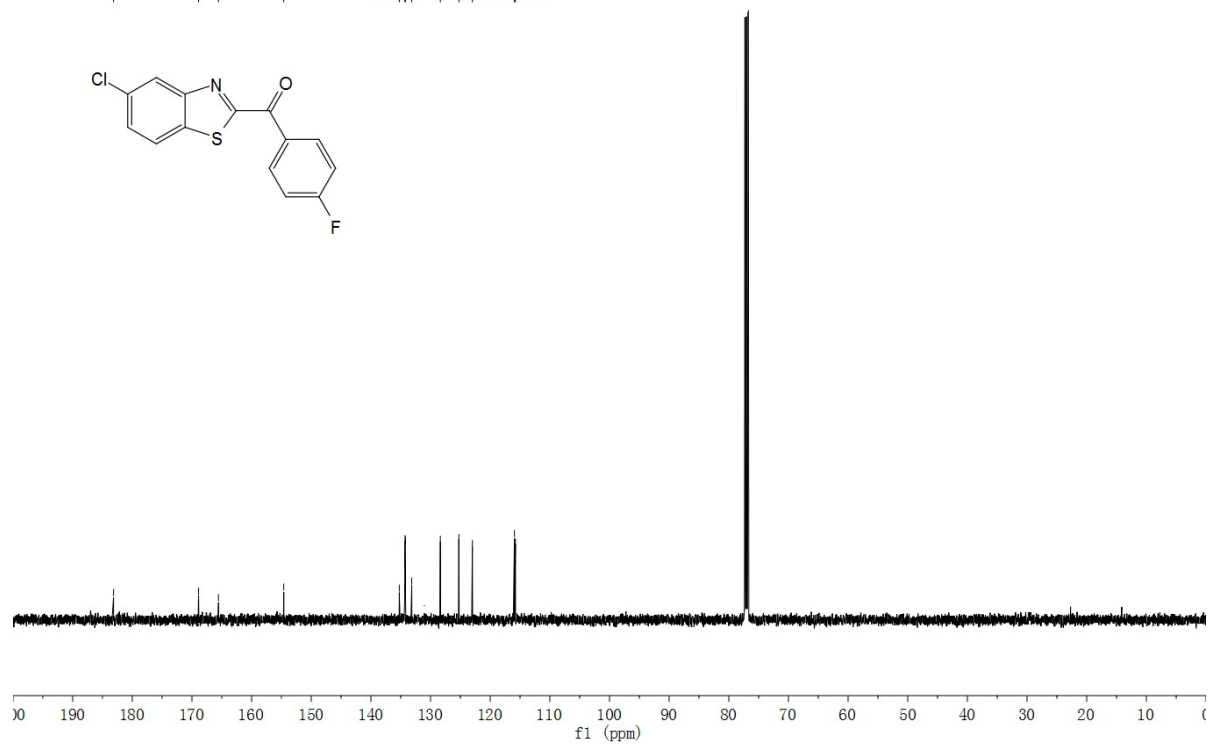
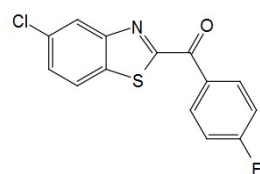


¹H and ¹³C NMR Spectra of 3bl

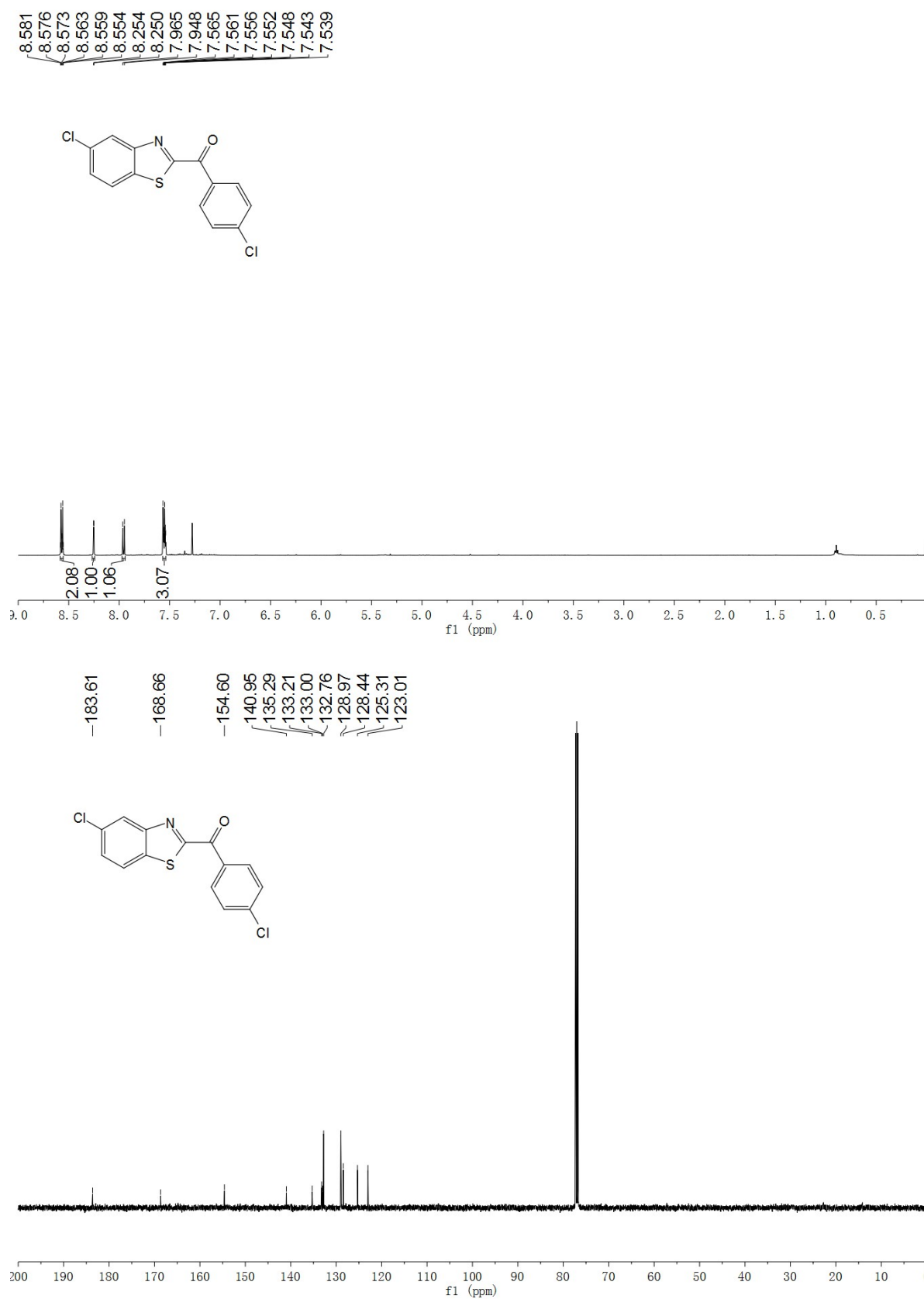
8.70
8.69
8.69
8.68
8.67
8.66
8.26
8.25
7.97
7.95
7.56
7.56
7.54
7.54
7.26
7.24



183.15
168.89
165.55
154.60
135.24
134.28
134.21
133.15
128.35
125.25
122.99
115.94
115.76

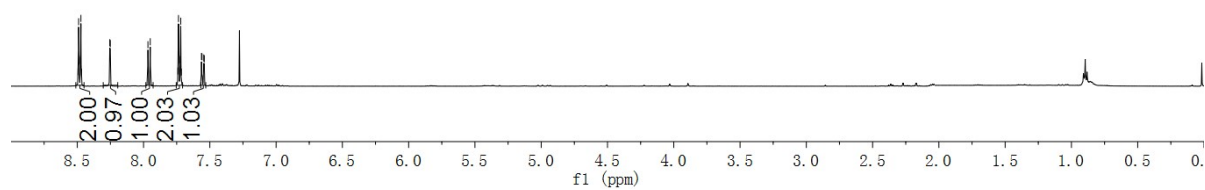
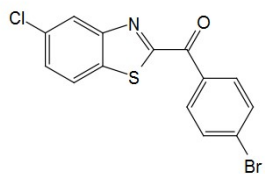


¹H and ¹³C NMR Spectra of 3bm

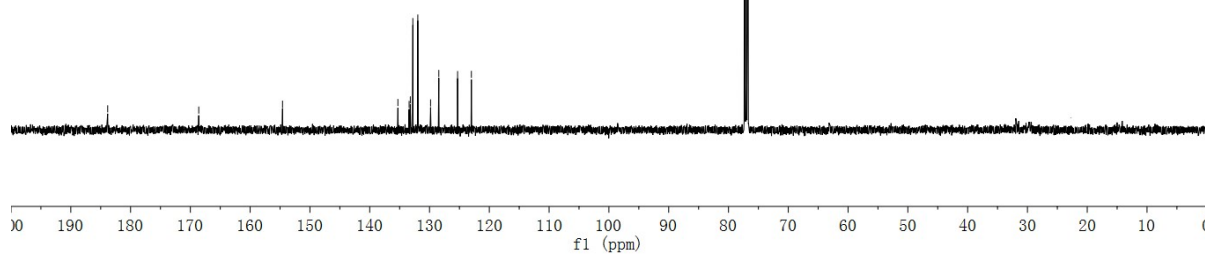
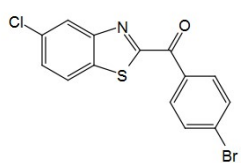


¹H and ¹³C NMR Spectra of 3bn

8.494
8.490
8.486
8.476
8.472
8.468
8.255
8.251
7.967
7.949
7.741
7.736
7.733
7.723
7.719
7.715
7.563
7.559
7.546
7.542

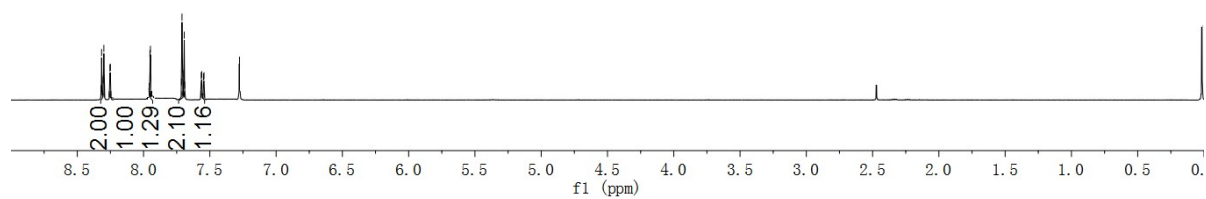
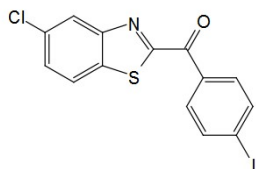


183.83
168.60
154.59
135.29
133.41
133.22
132.79
131.96
129.83
128.45
125.31
123.00

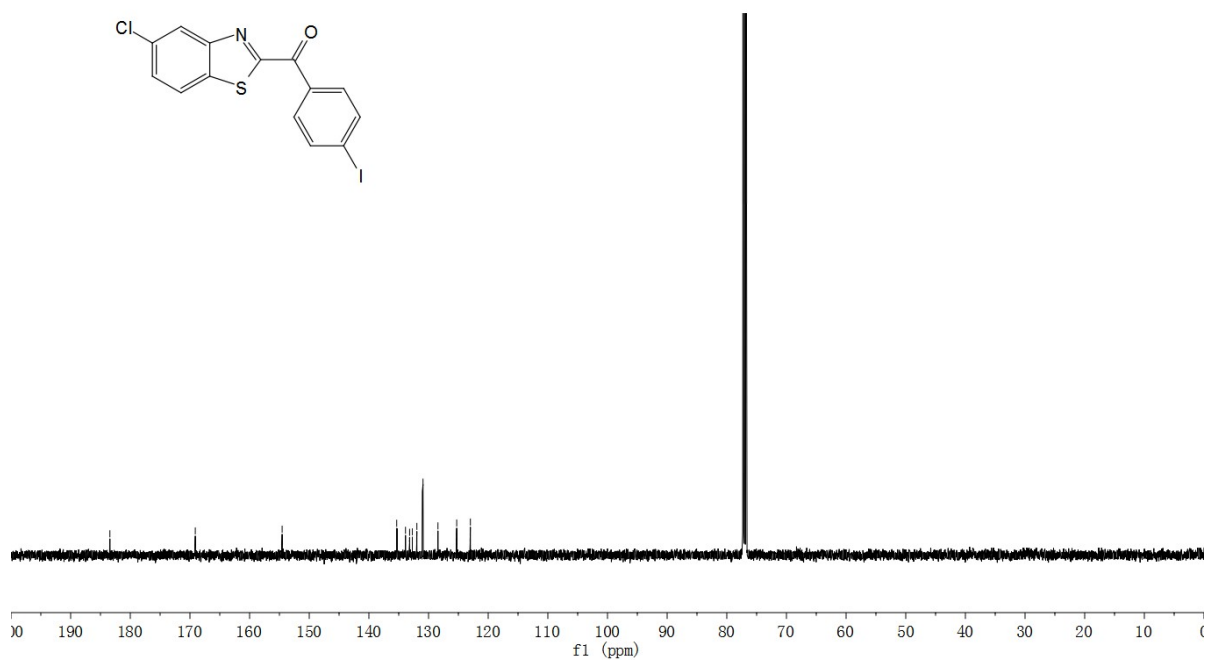
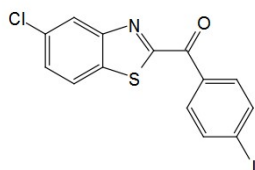


¹H and ¹³C NMR Spectra of 3bo

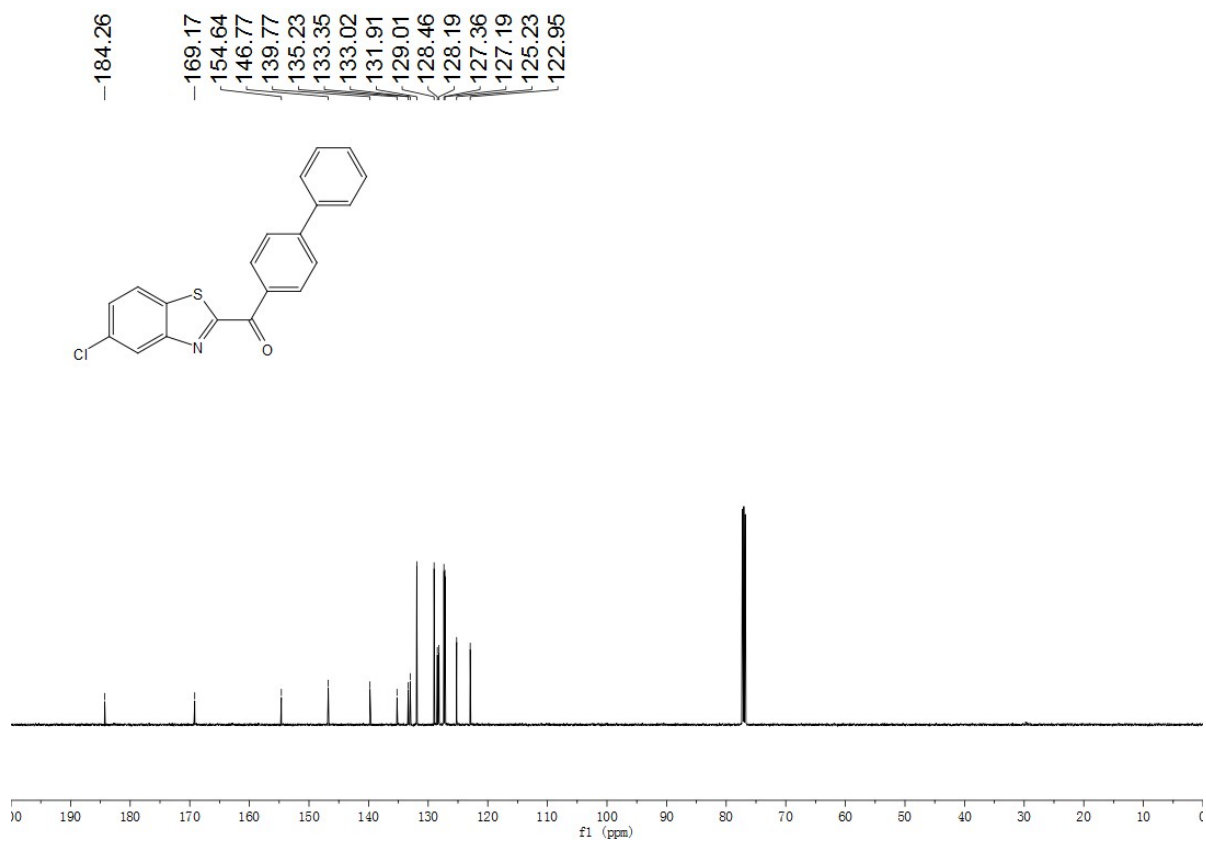
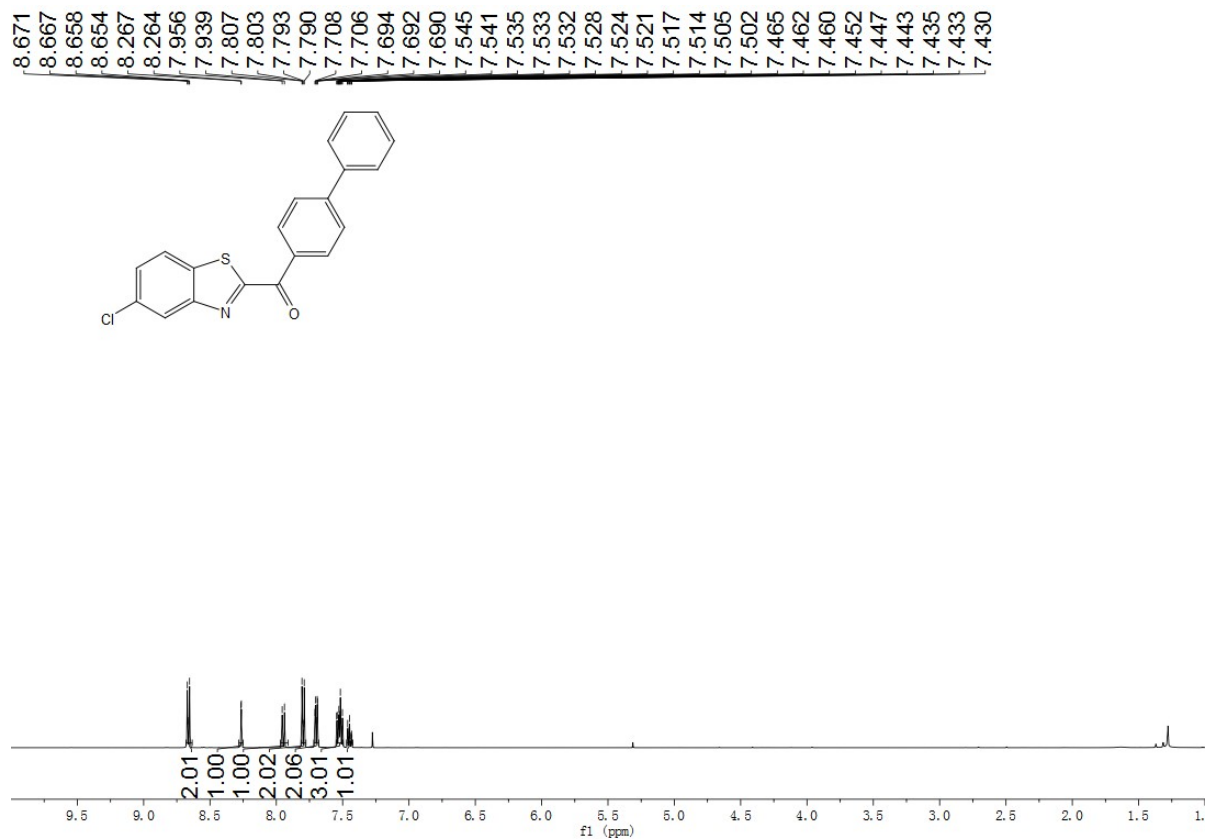
8.321
8.316
8.313
8.303
8.299
8.295
8.254
8.250
7.952
7.948
7.714
7.710
7.706
7.697
7.693
7.689
7.565
7.561
7.548
7.544



183.45
169.19
154.55
135.26
133.91
133.17
132.71
131.90
130.93
128.42
125.28
122.99

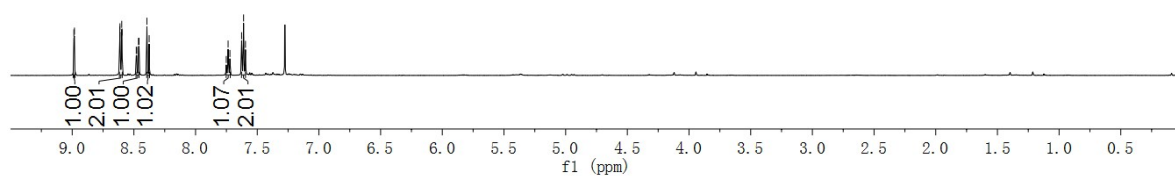
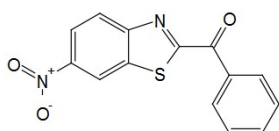


¹H and ¹³C NMR Spectra of 3bp

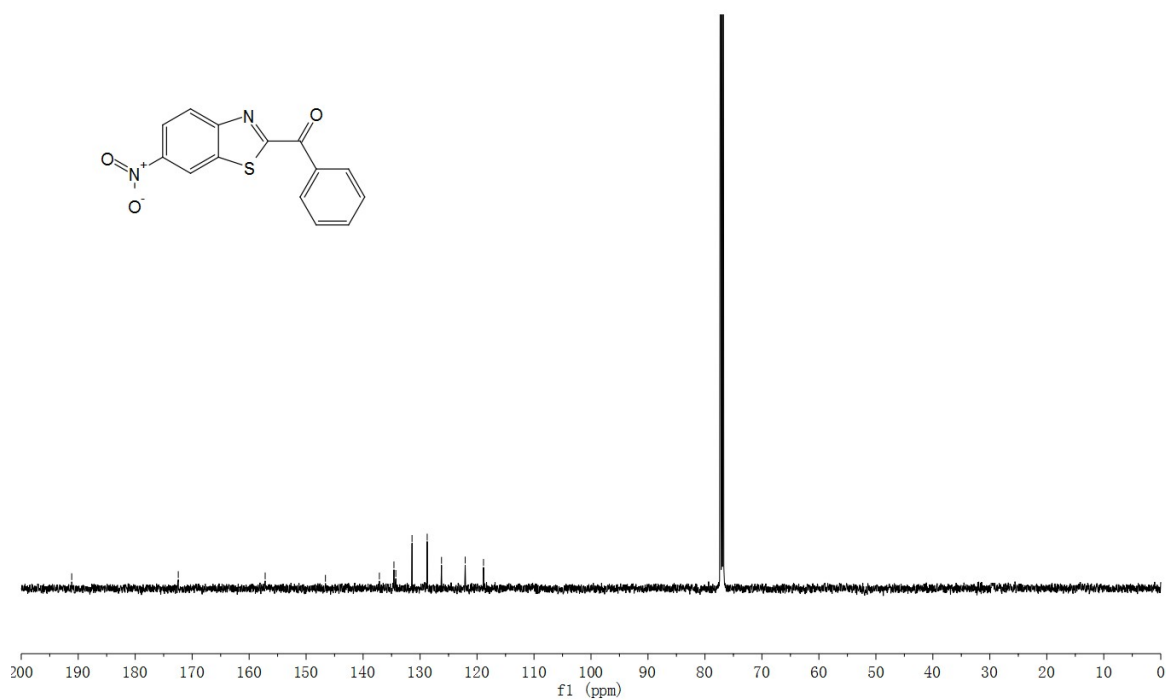
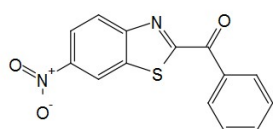


¹H and ¹³C NMR Spectra of 3bq

8.986
8.982
8.614
8.613
8.598
8.596
8.481
8.476
8.463
8.458
8.394
8.376
7.751
7.736
7.721
7.627
7.611
7.595

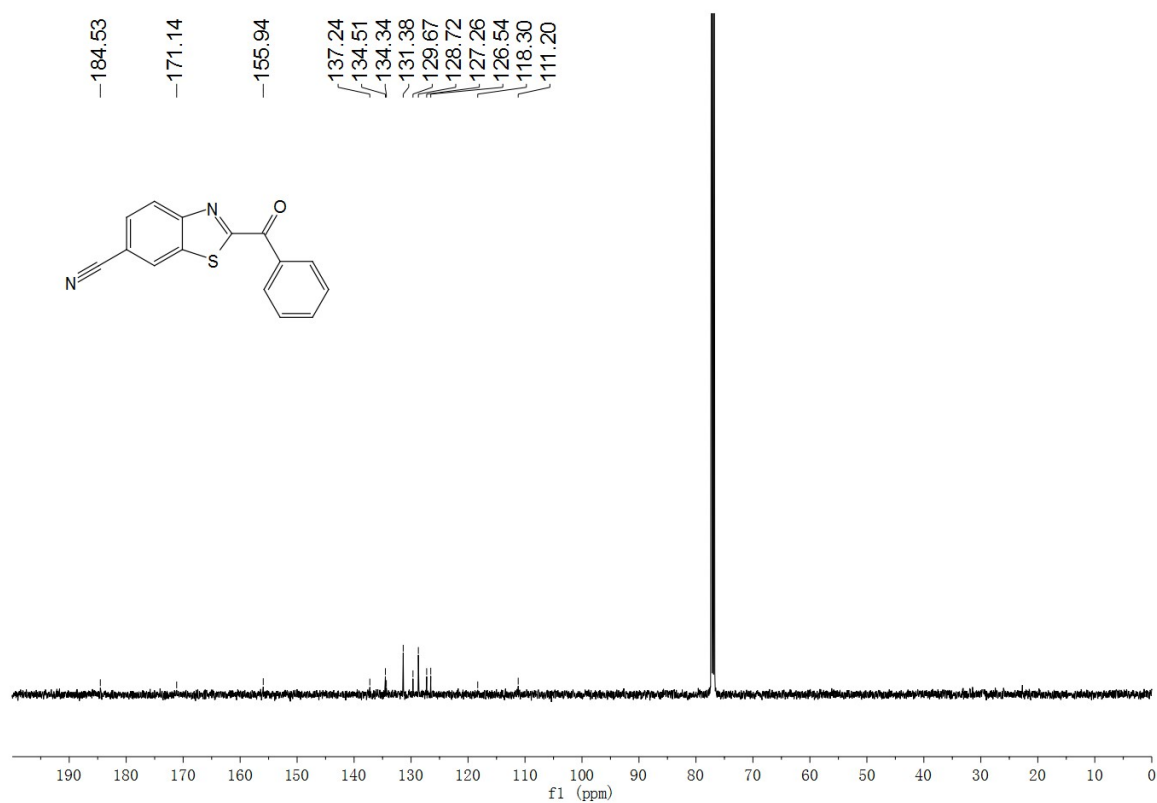
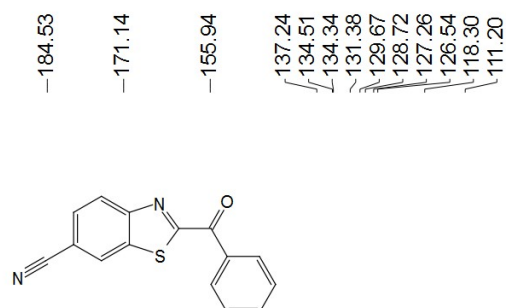
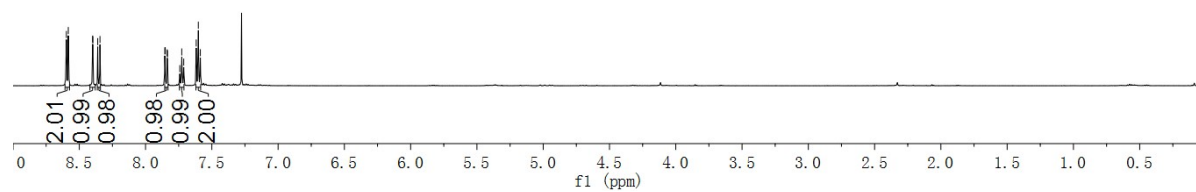
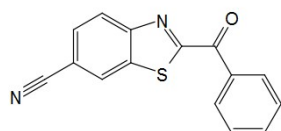


-191.14
-172.44
-157.19
-146.61
-137.14
-134.59
-134.26
-131.41
-128.75
-126.24
-122.08
-118.86



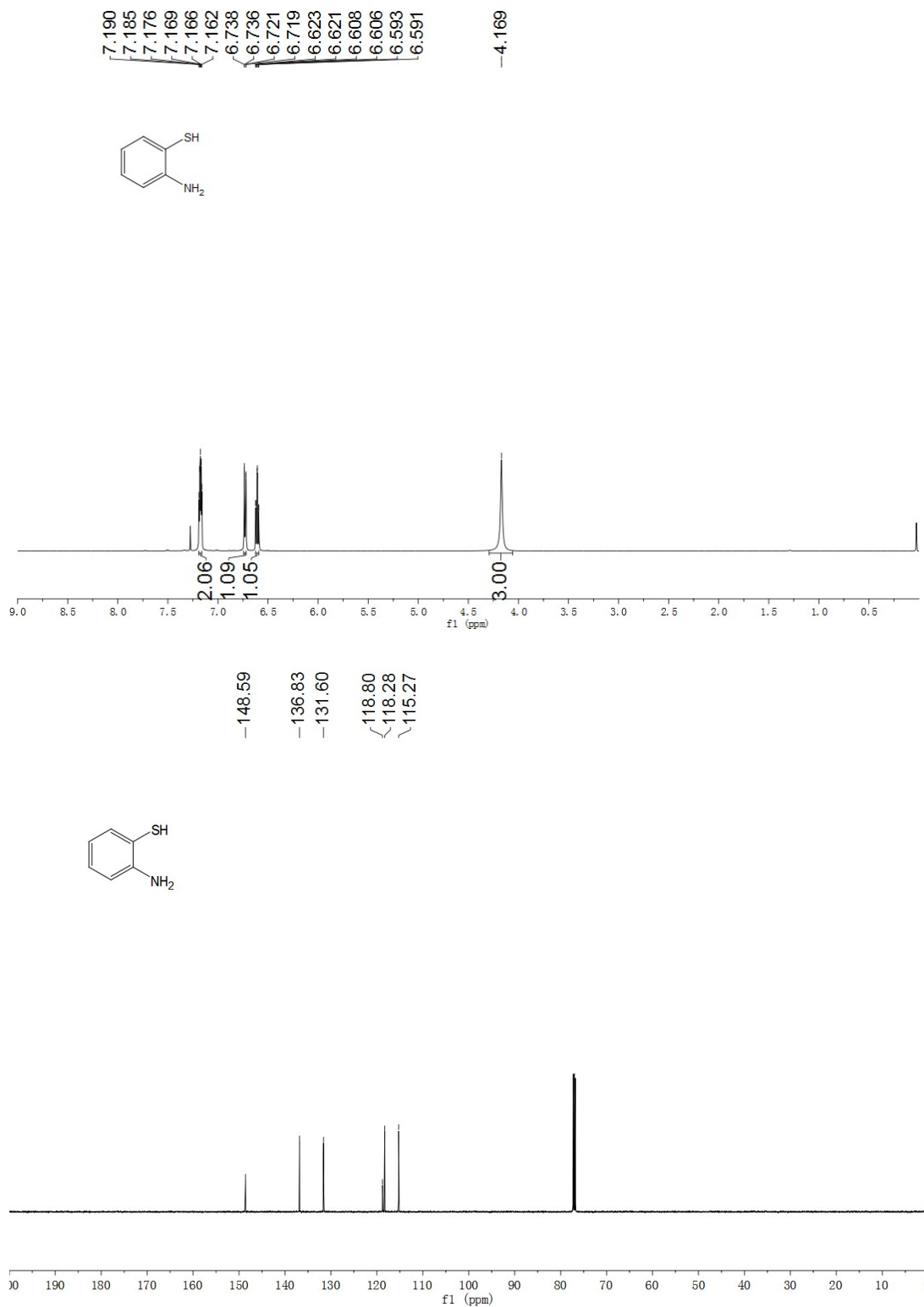
¹H and ¹³C NMR Spectra of 3br

8.597
8.583
8.399
8.397
8.361
8.344
7.855
7.852
7.838
7.834
7.742
7.727
7.712
7.618
7.602
7.587

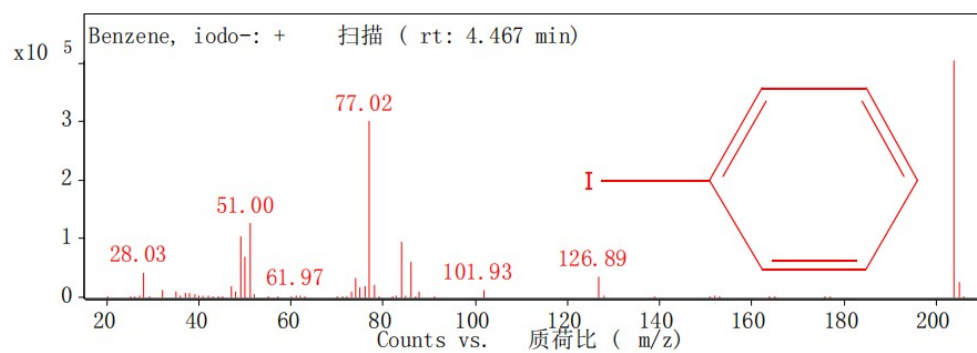


2. NMR Spectrum of 1b

2-Aminobenzenethiol (*1b*): Yellow solid; yield 83% (31 mg); m.p.: 70-71 °C; ^1H NMR (500 MHz, cdCl_3) δ 7.19 – 7.16 (m, 2H), 6.73 (dd, $J = 8.0, 1.0\text{ Hz}$, 1H), 6.61 (td, $J = 7.5, 1.5\text{ Hz}$, 1H), 4.17 (s, 3H); ^{13}C NMR (125 MHz, CDCl_3) δ 148.59, 136.83, 131.60, 118.80, 118.28, 115.27.



3. GC-MS Spectrum of PhI



质谱图结构

Benzenes, iodo-

