Electronic Supplementary Material (ESI) for Organic & Biomolecular Chemistry.

Preparation of Isoquinazolines via Metal-Free [4 + 2] Cycloaddition of Ynamides with Nitriles

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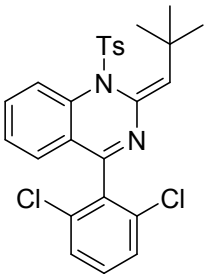
Contents

1. X-Ray crystallography

Figure S1: X-Ray crystallography and structural formula of compound **3k**. Displacement ellipsoids are drawn at the 30% probability level.



3k

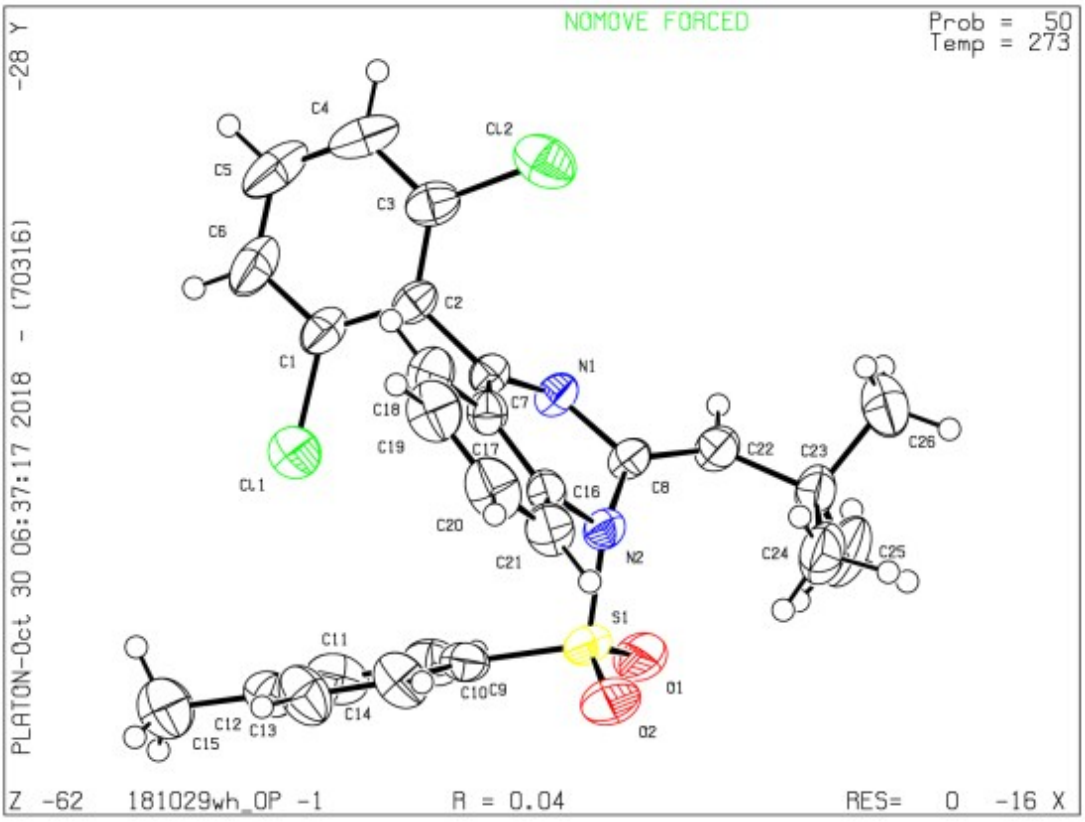
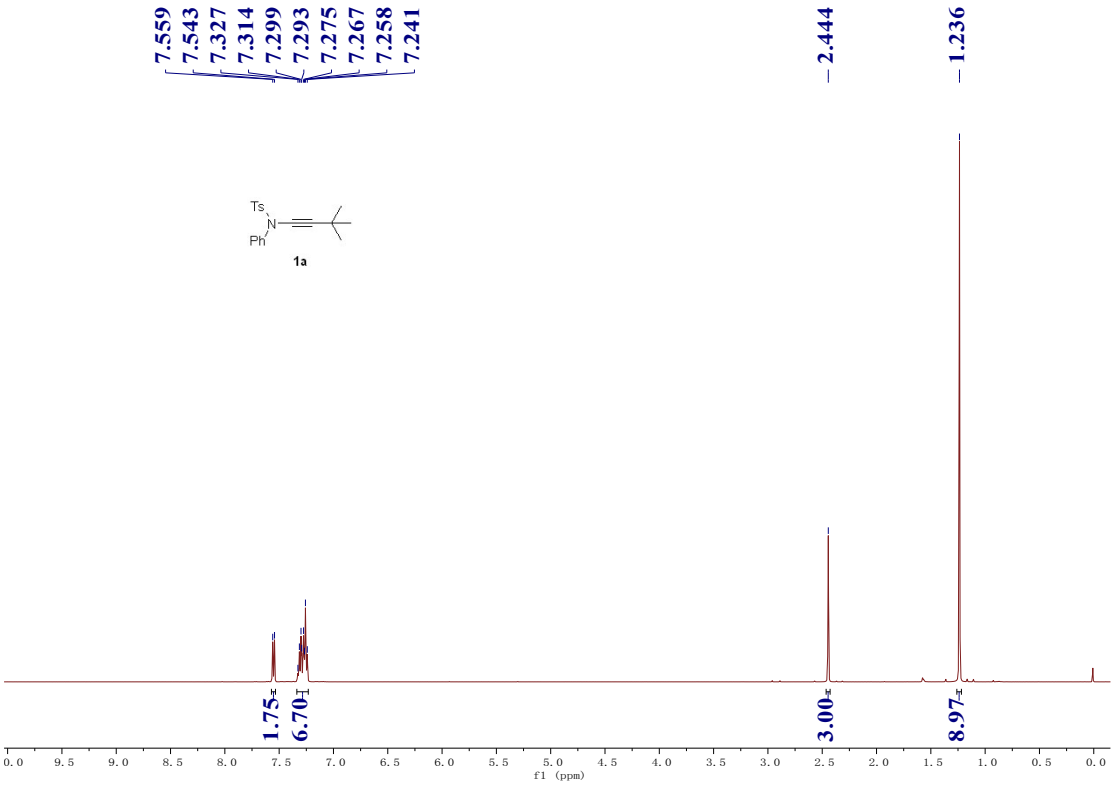


Table S1. Crystal data and structure refinement for C:81029WH_.

Identification code	181029wh_0m	
Empirical formula	C26 H24 Cl2 N2 O2 S	
Formula weight	499.43	
Temperature	273.15 K	
Wavelength	0.71073 Å	
Crystal system	Triclinic	
Space group	P-1	
Unit cell dimensions	a = 8.7442(10) Å	α= 95.3140(10)°.
	b = 11.0021(12) Å	β= 106.9550(10)°.
	c = 14.9590(16) Å	γ = 109.2400(10)°.
Volume	1271.0(2) $Å^3$	
Z	2	
Density (calculated)	1.305 Mg/m^3	
Absorption coefficient	0.363 mm^{-1}	
F(000)	520	
Crystal size	? x ? x ? mm^3	
Theta range for data collection	2.529 to 27.614°.	
Index ranges	-11<=h<=11, -14<=k<=13, -18<=l<=19	
Reflections collected	10247	
Independent reflections	5439 [R(int) = 0.0205]	
Completeness to theta = 25.242°	99.6 %	
Absorption correction	Semi-empirical from equivalents	
Max. and min. transmission	0.7456 and 0.6983	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	5439 / 0 / 302	
Goodness-of-fit on F^2	1.028	
Final R indices [I>2sigma(I)]	R1 = 0.0439, wR2 = 0.1046	
R indices (all data)	R1 = 0.0693, wR2 = 0.1168	
Extinction coefficient	n/a	
Largest diff. peak and hole	0.239 and -0.297 $e.Å^{-3}$	

2 ^{1}H, ^{19}F and ^{13}C Spectra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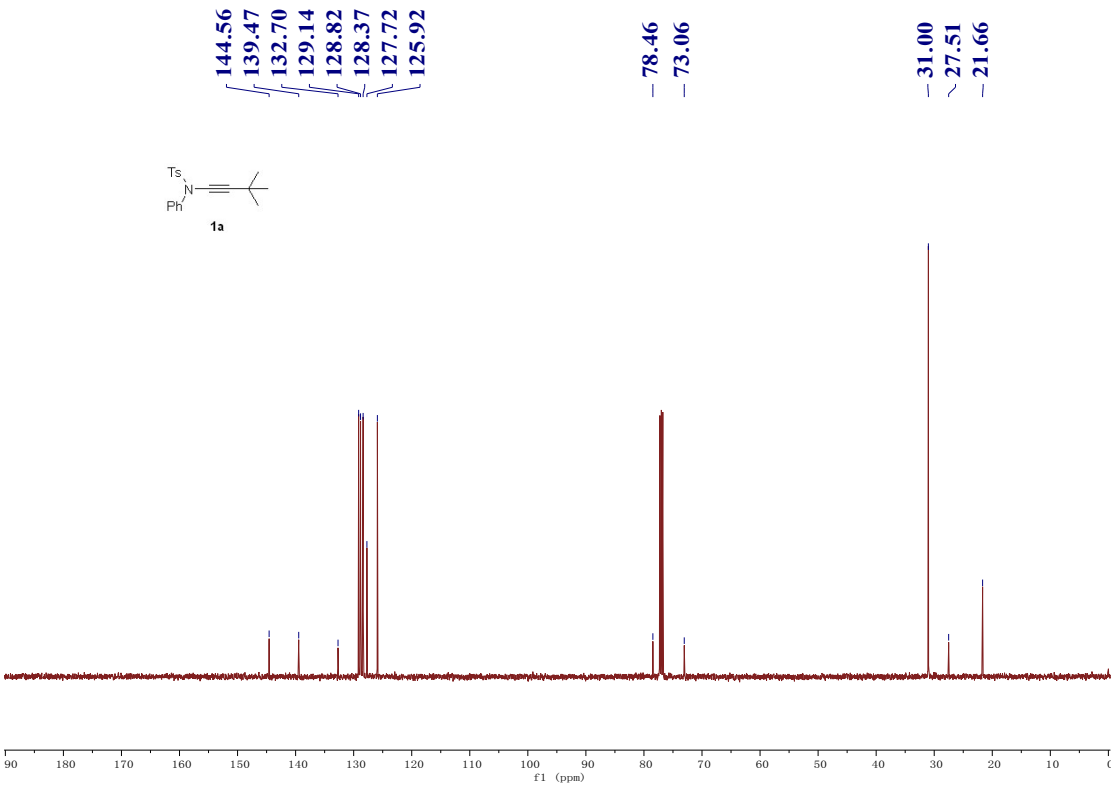
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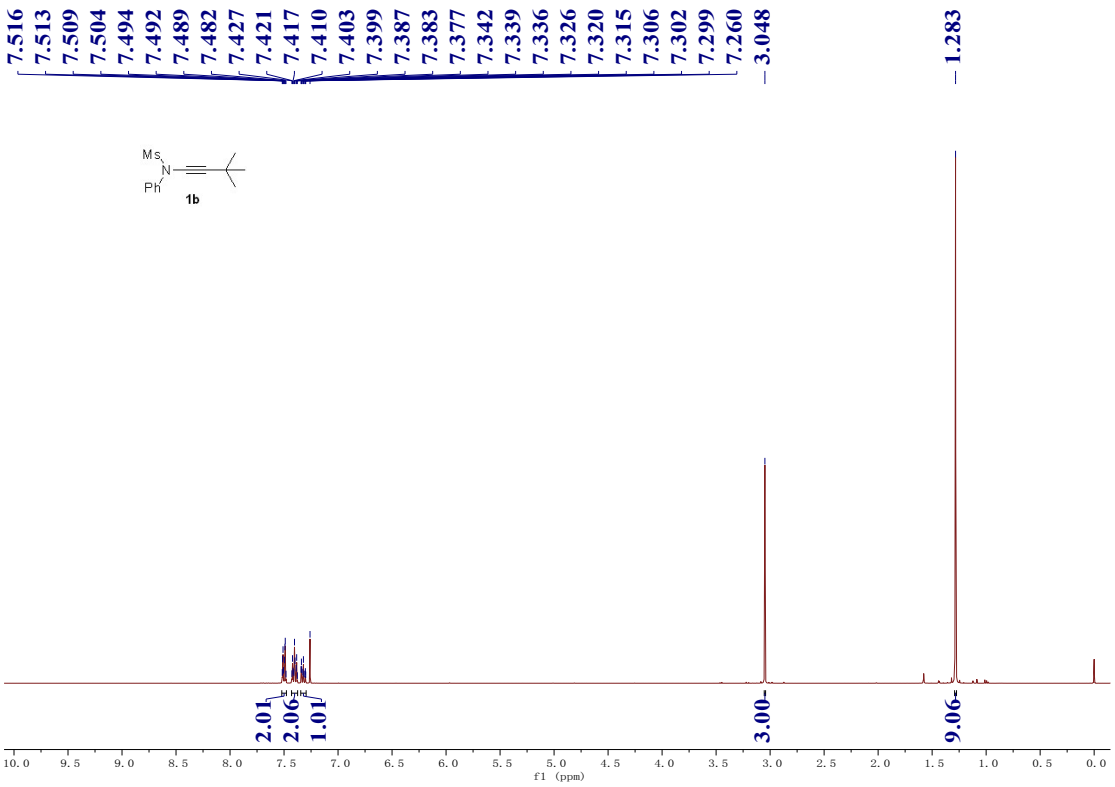
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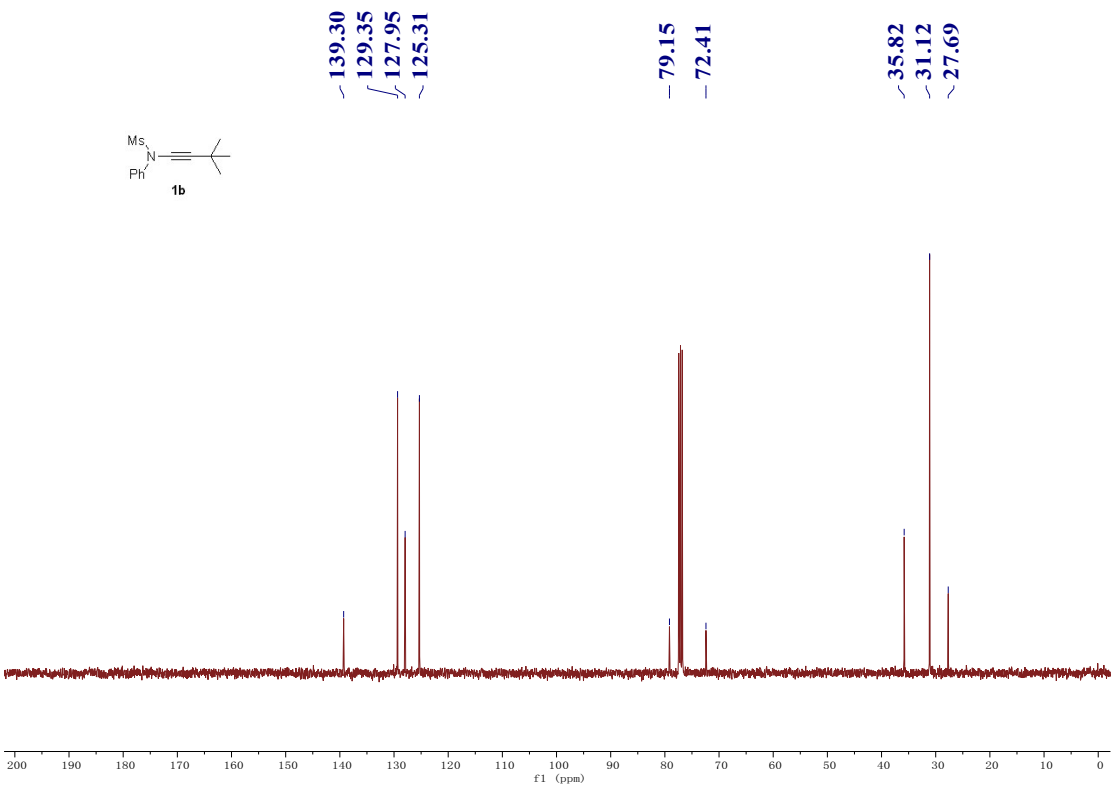
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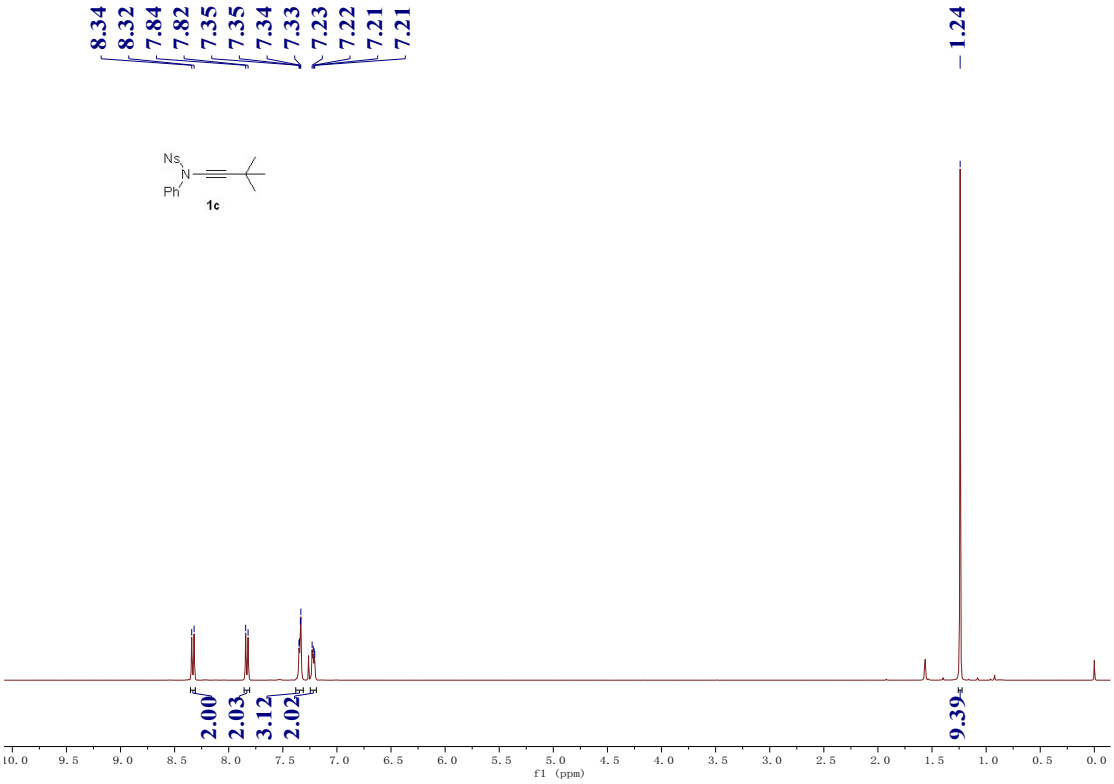
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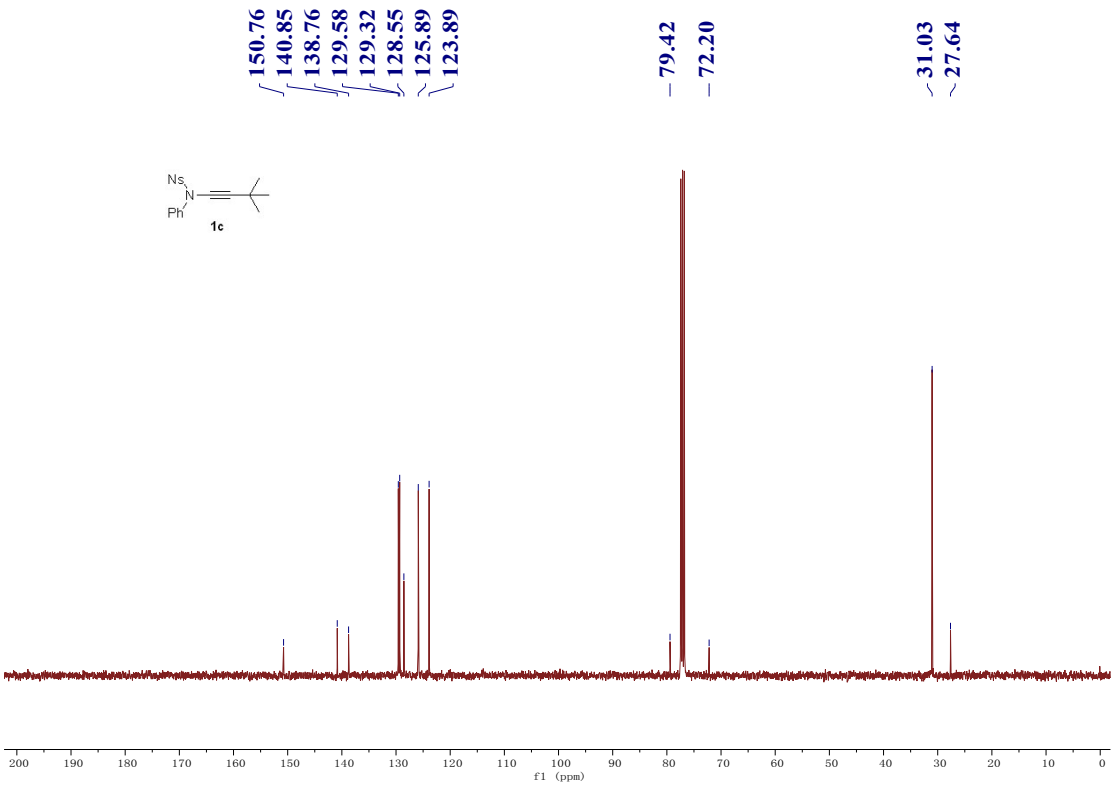
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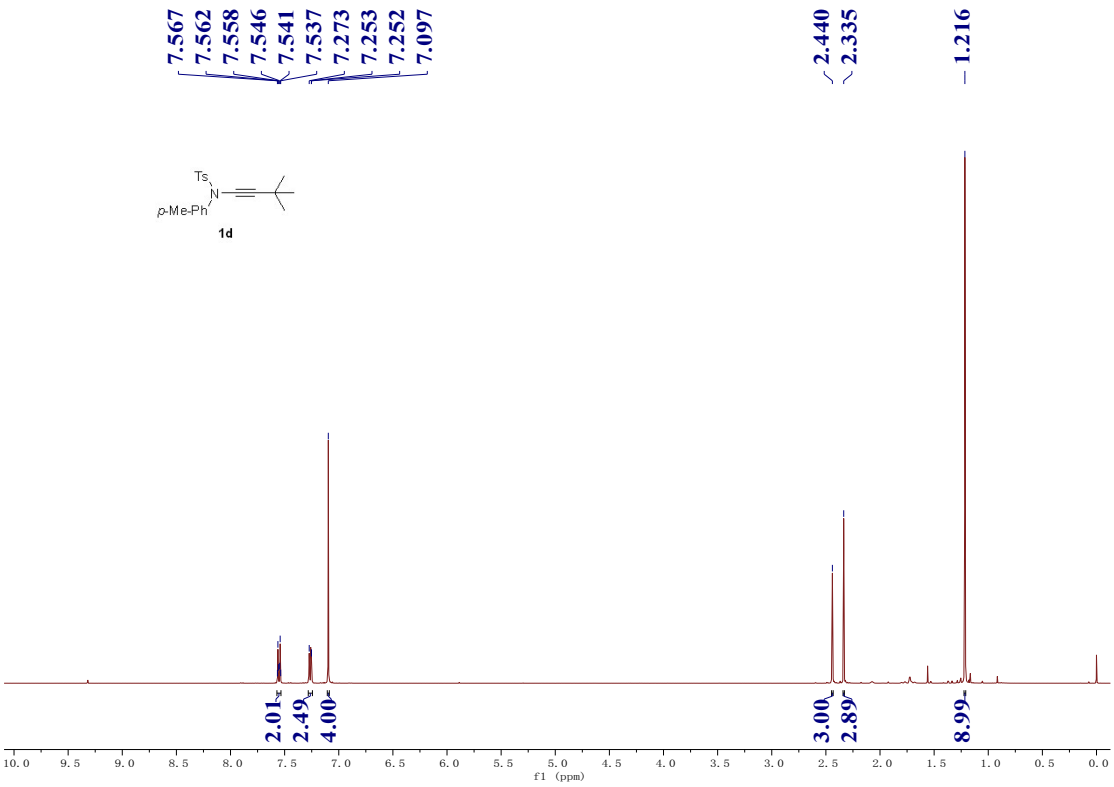
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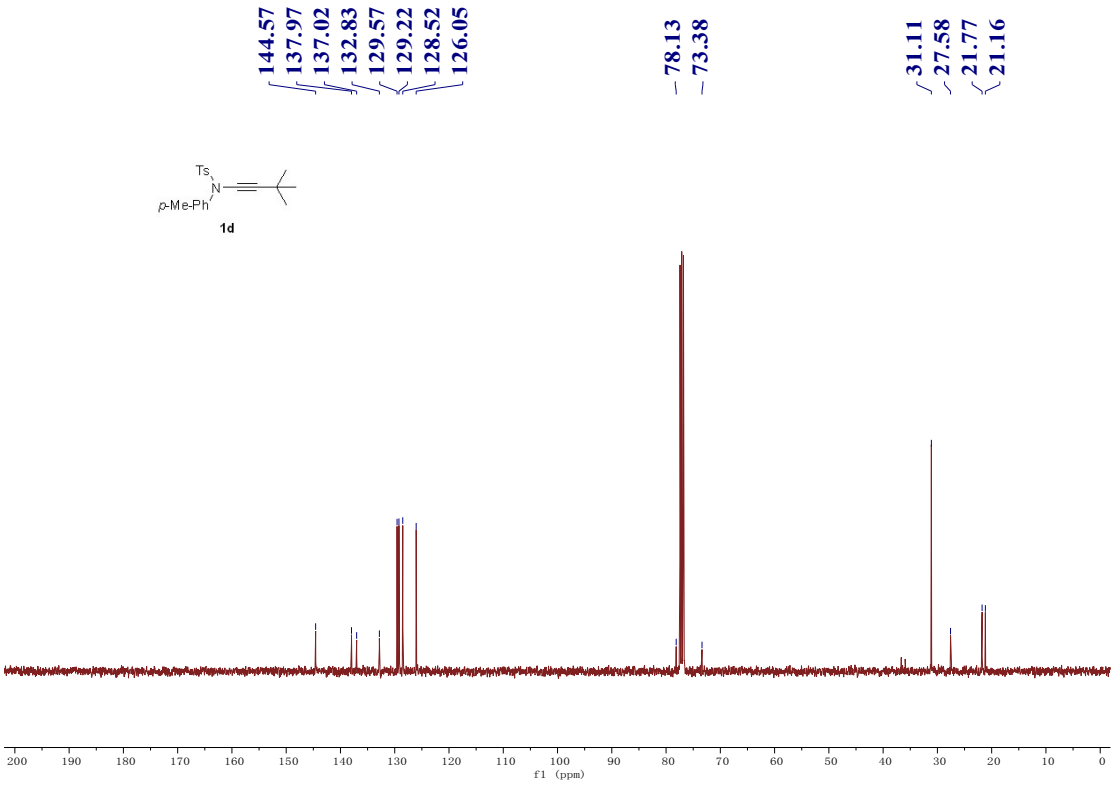
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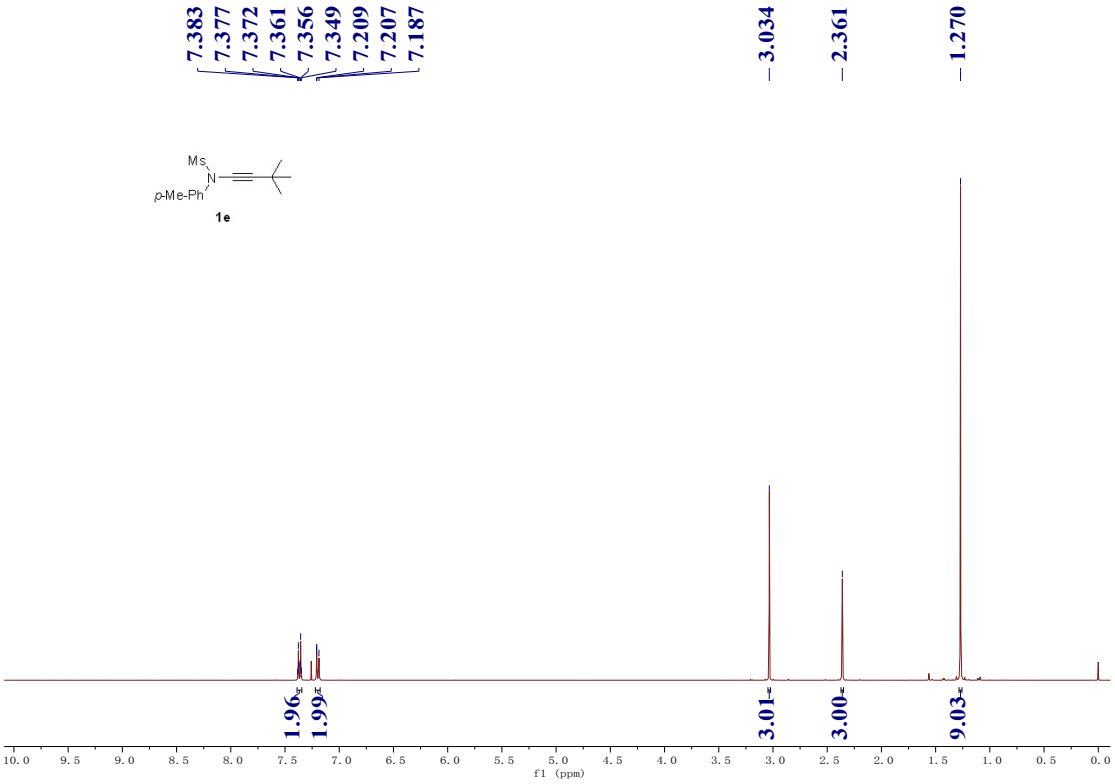
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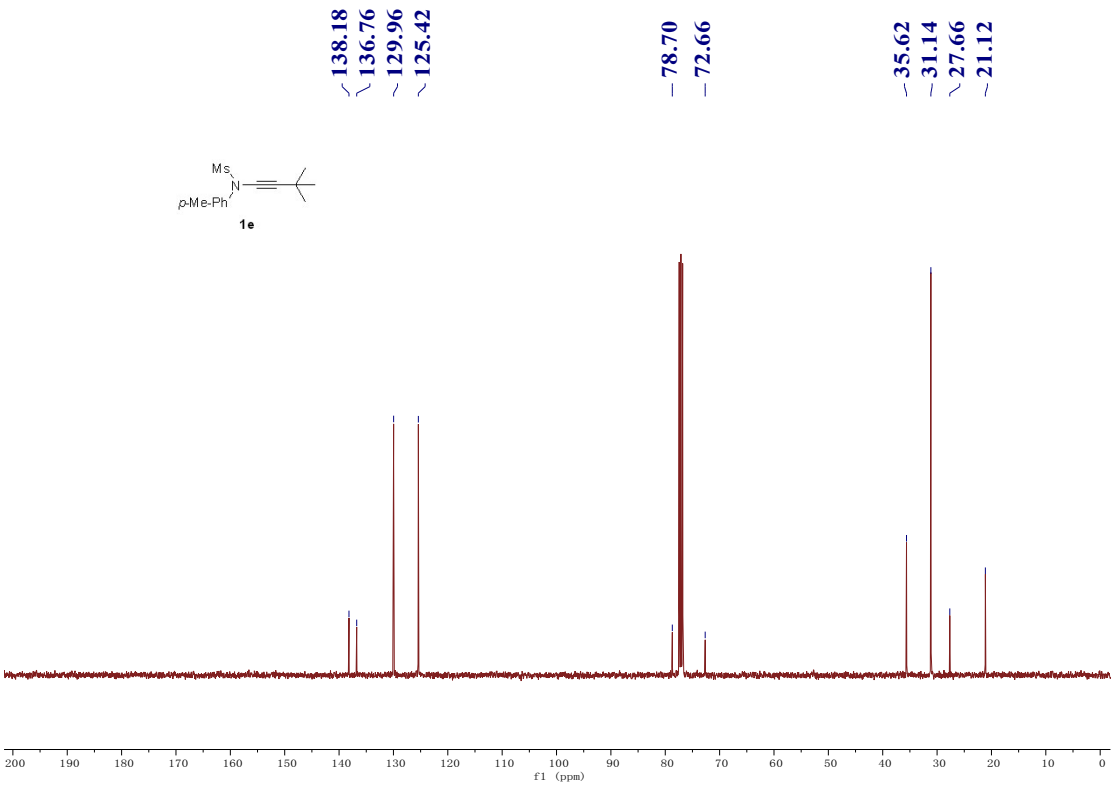
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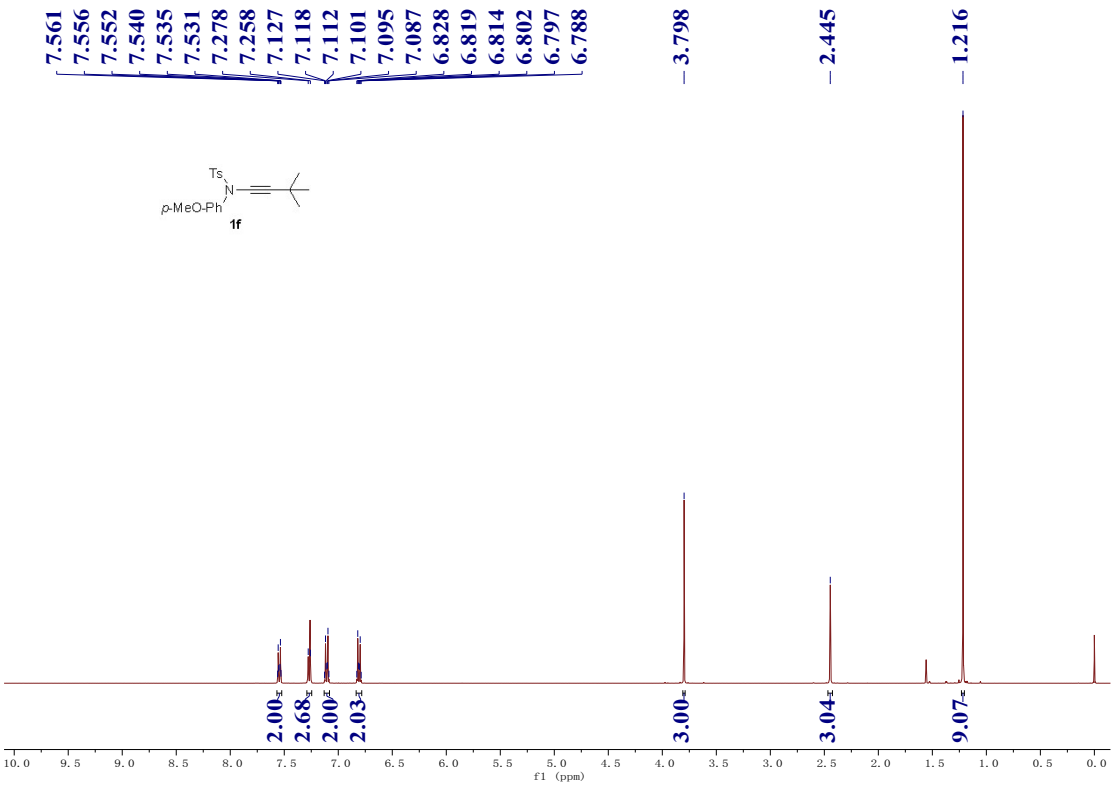
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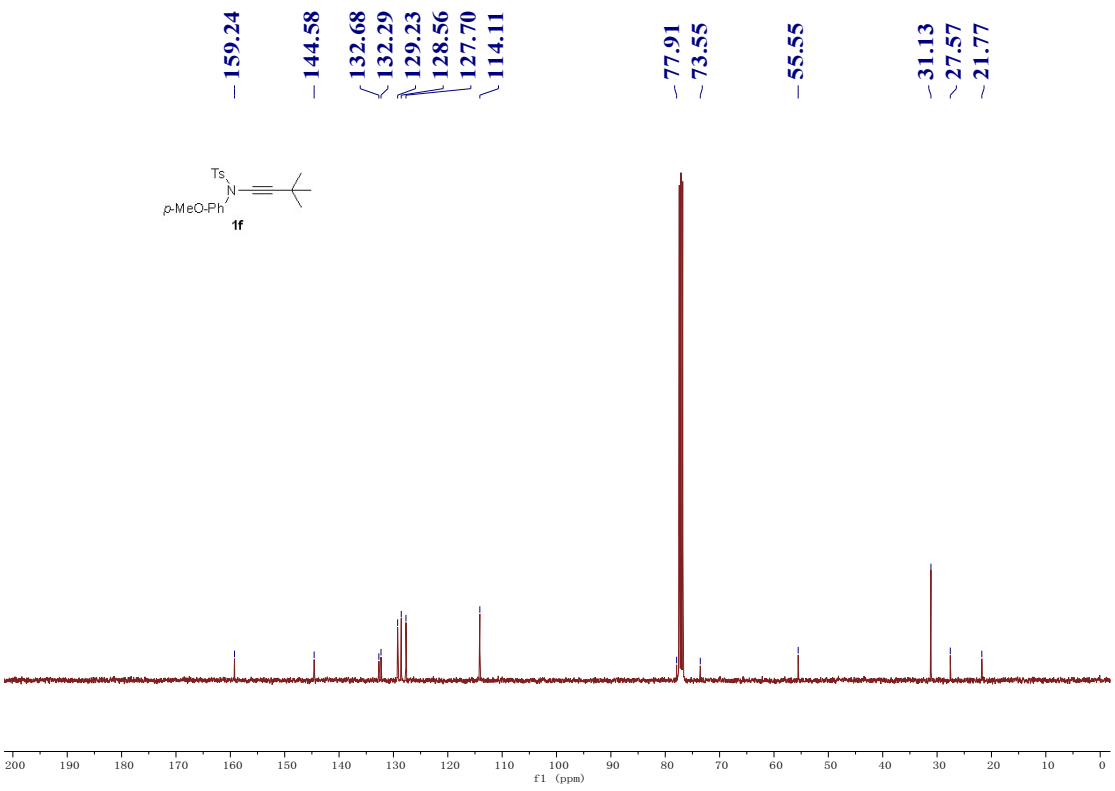
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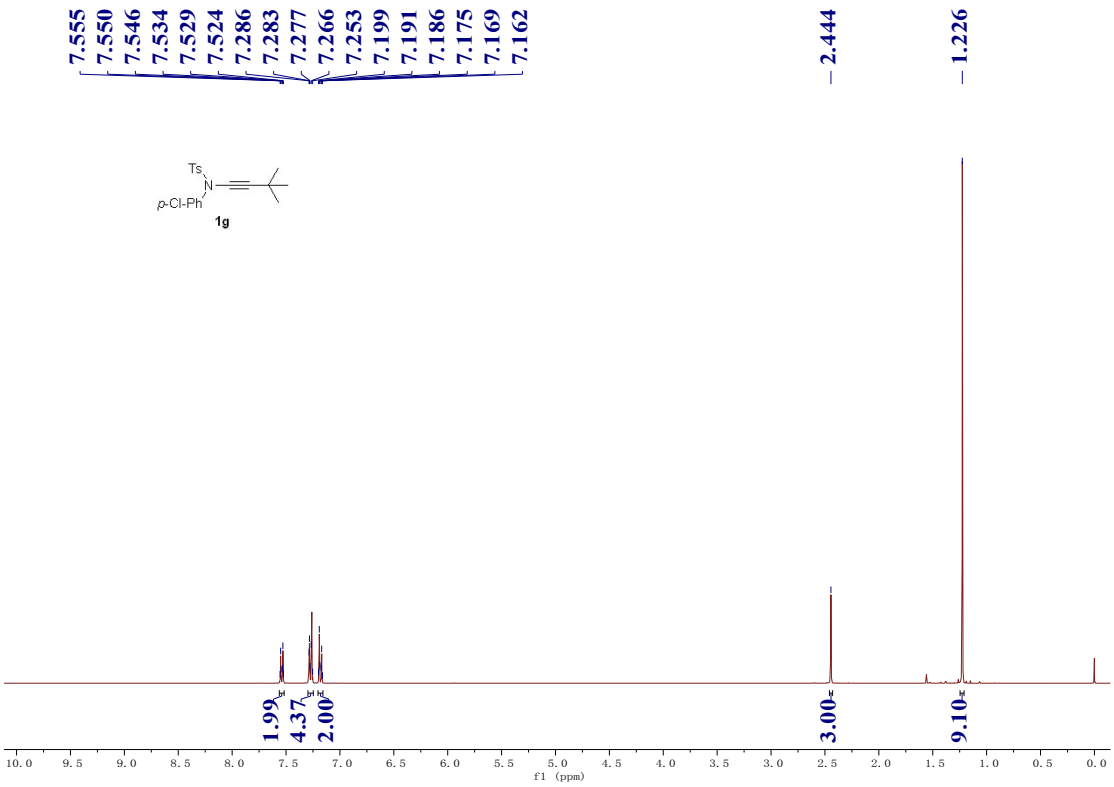
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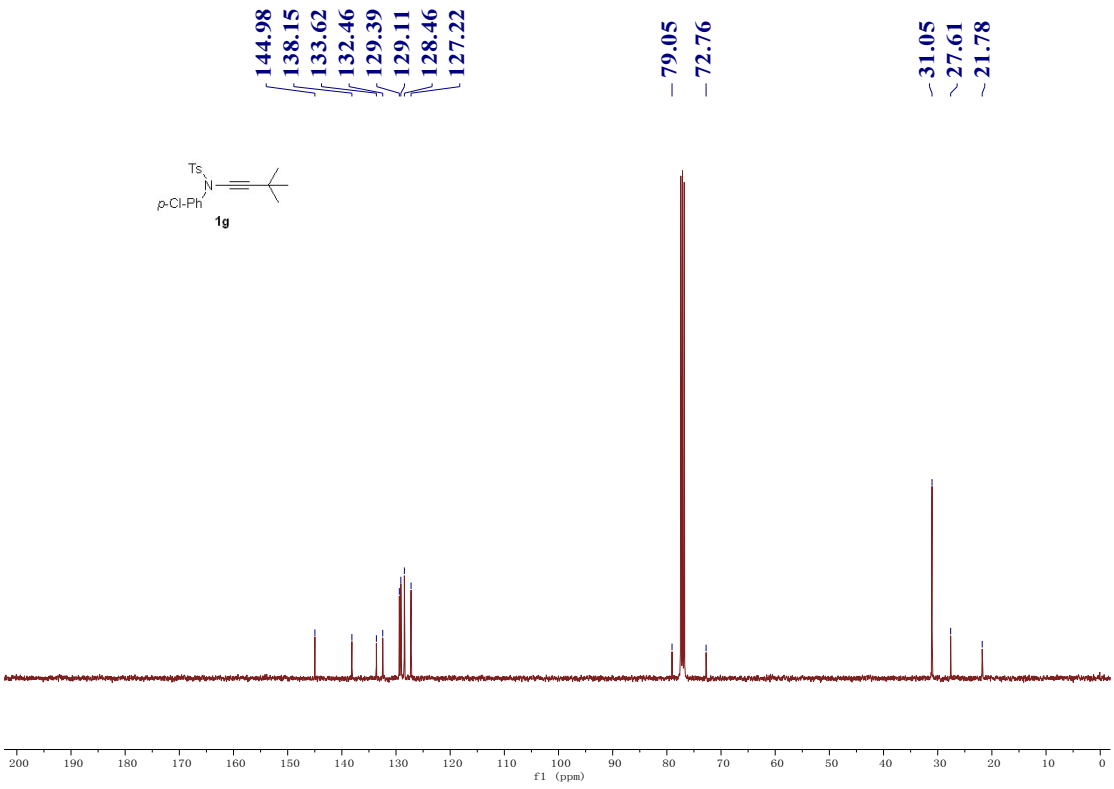
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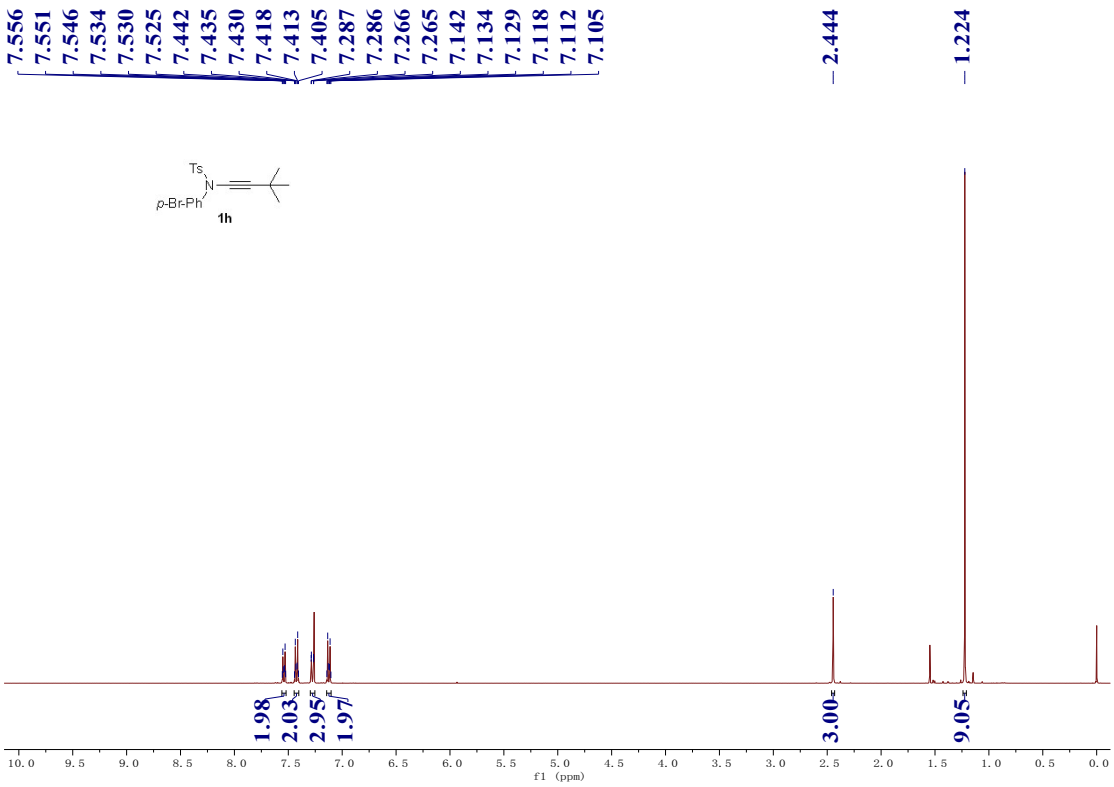
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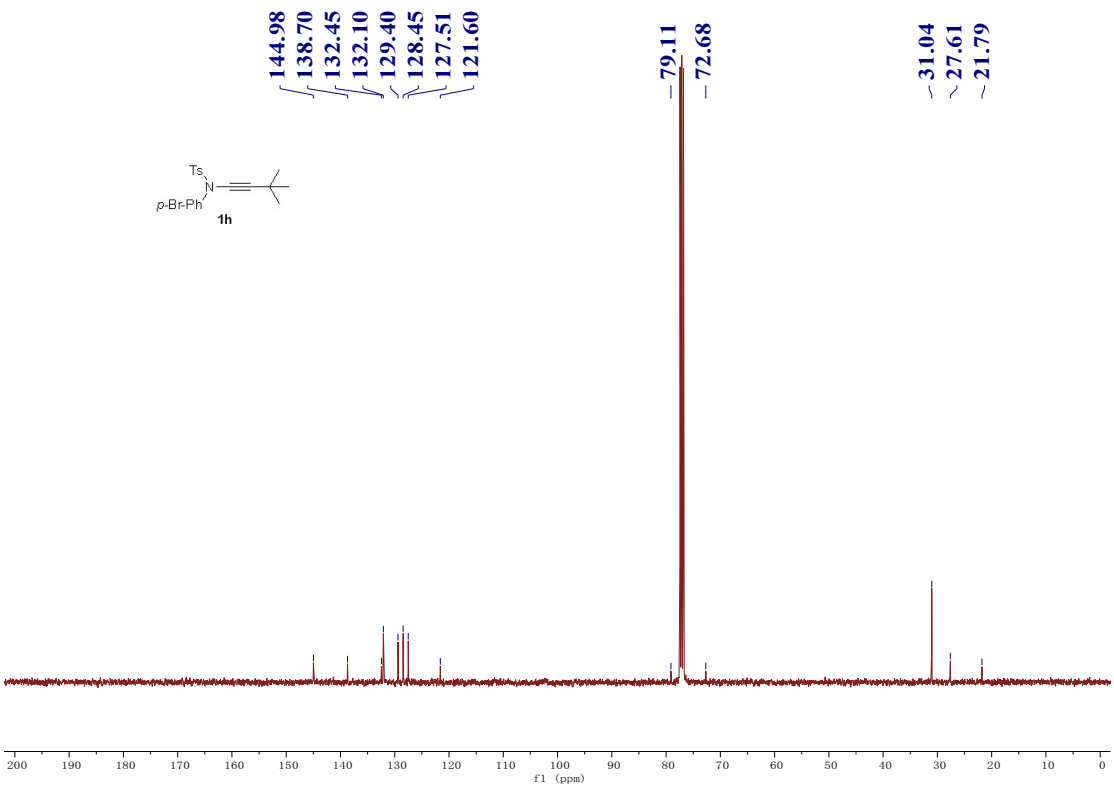
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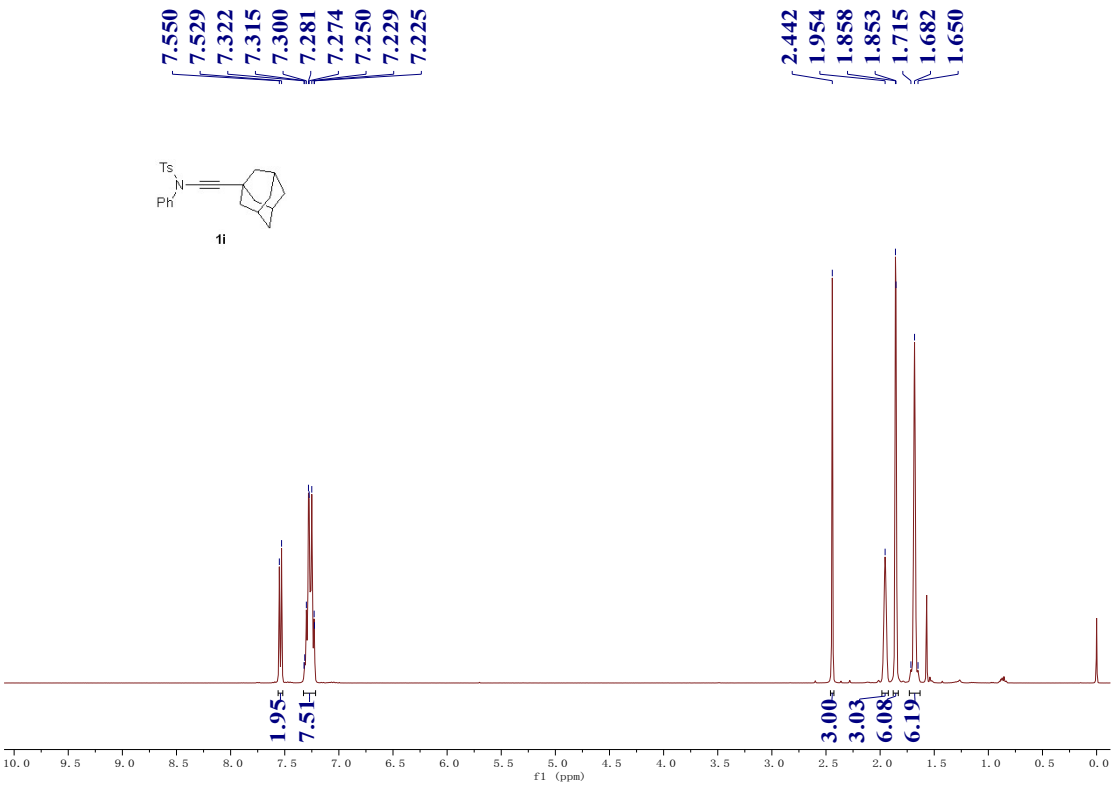
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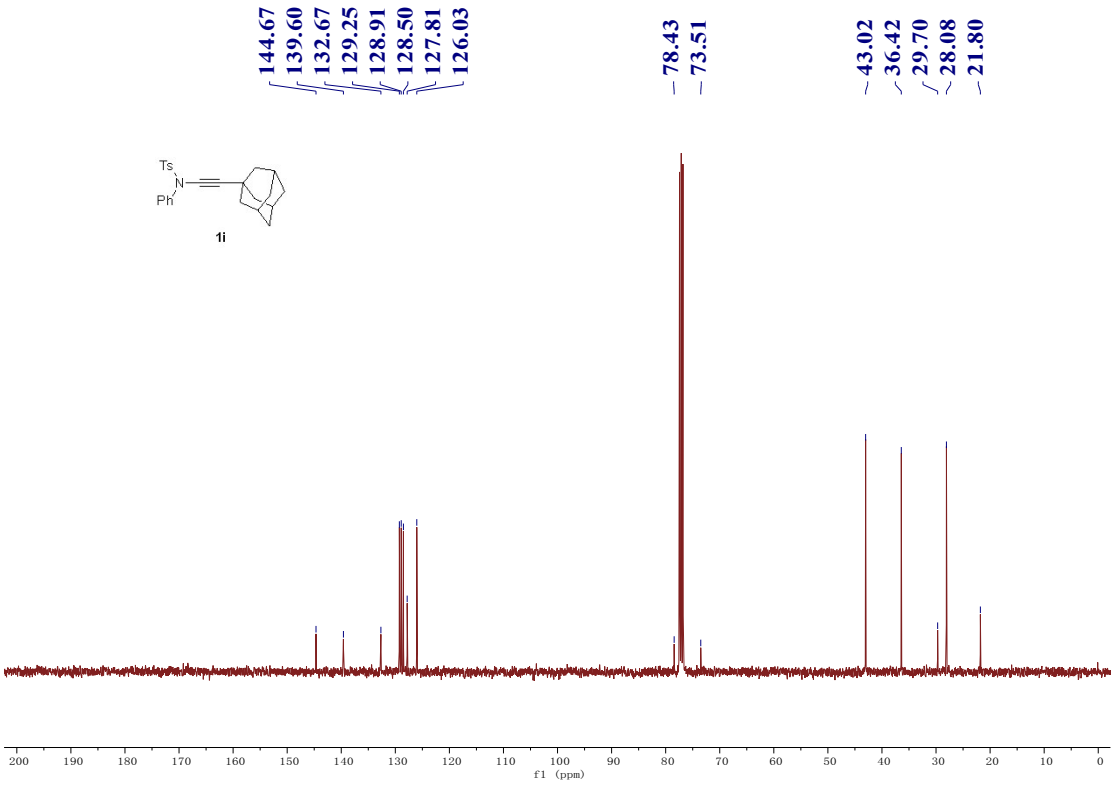
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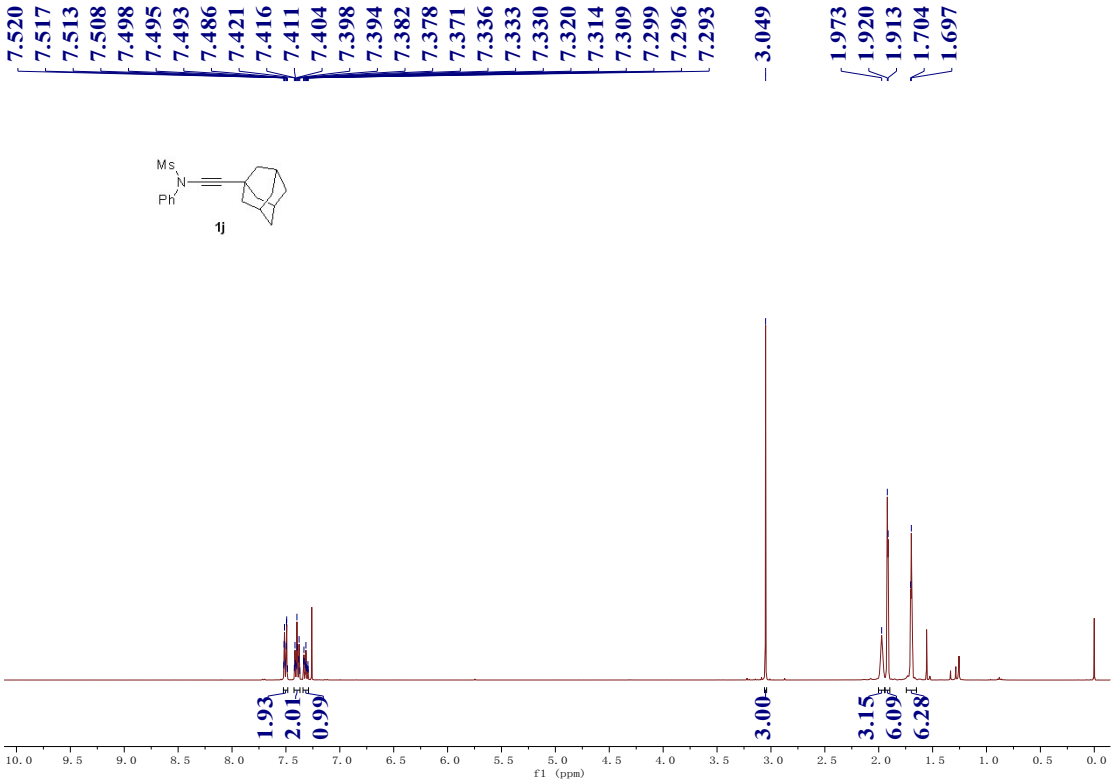
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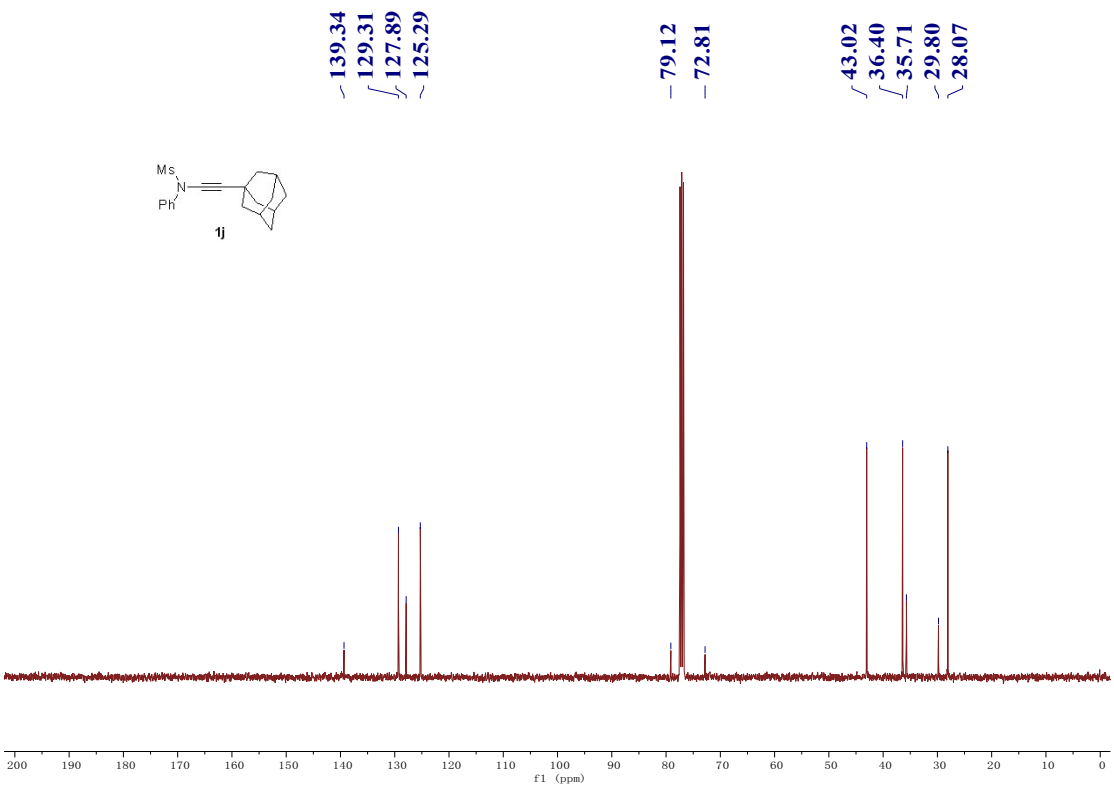
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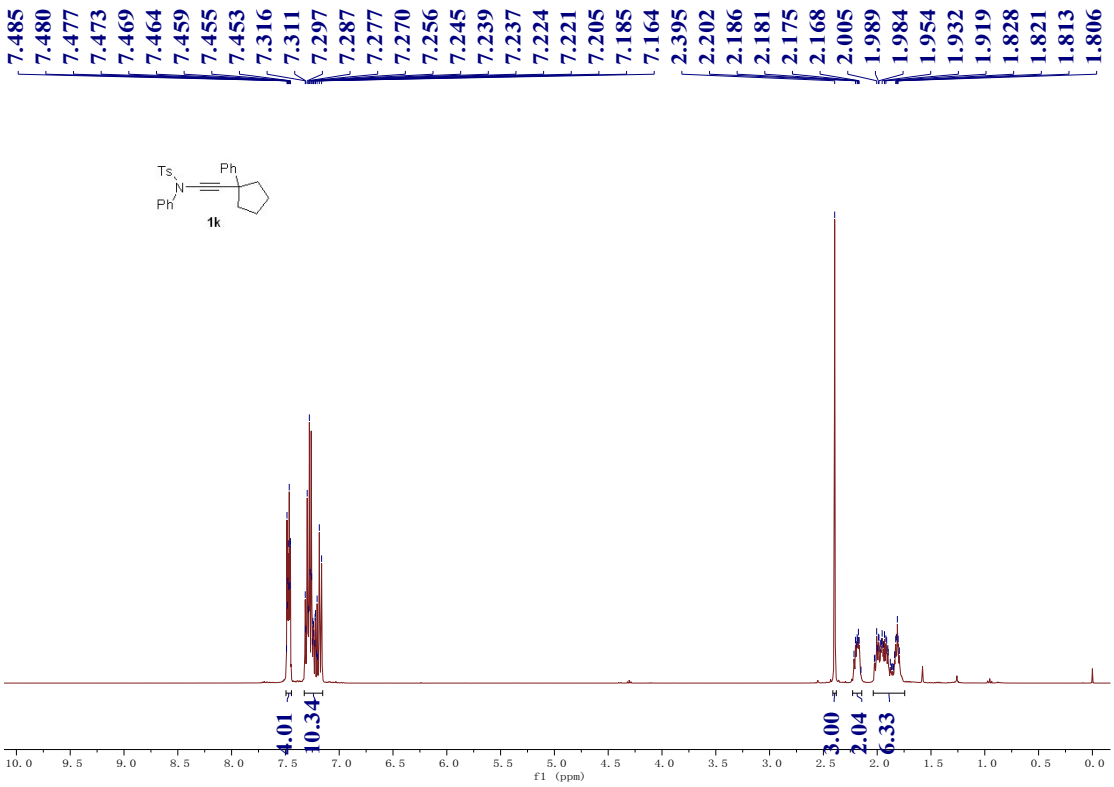
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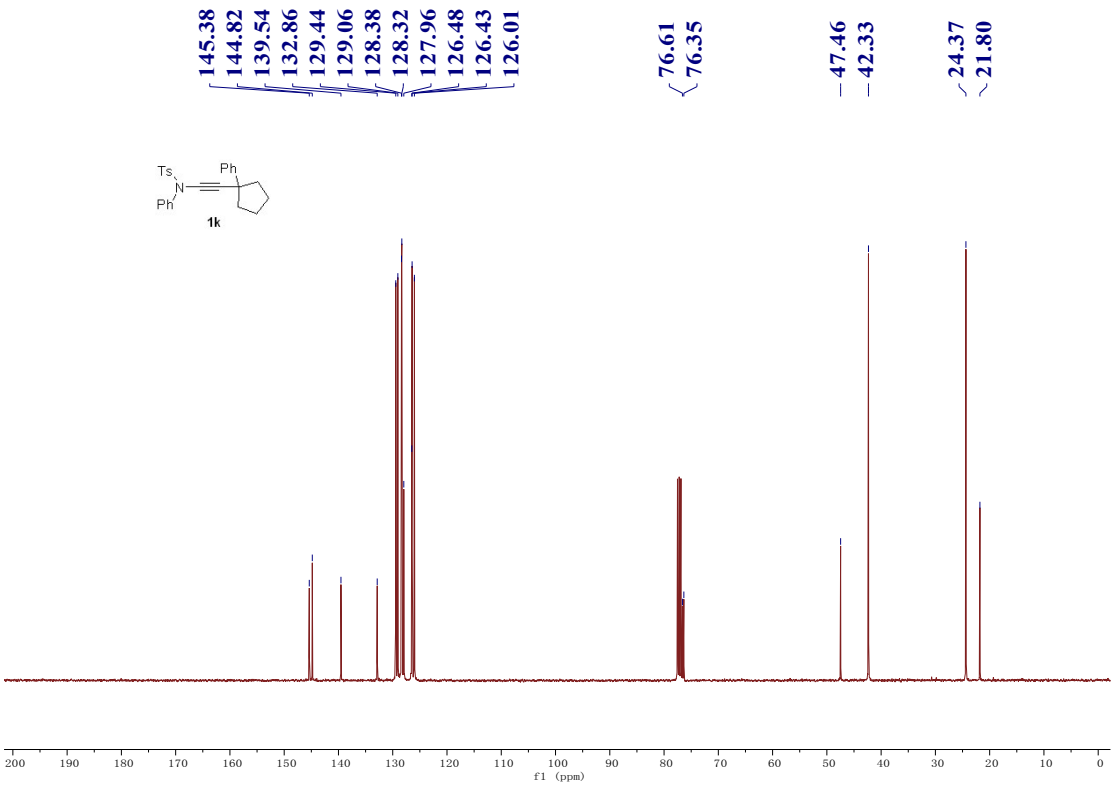
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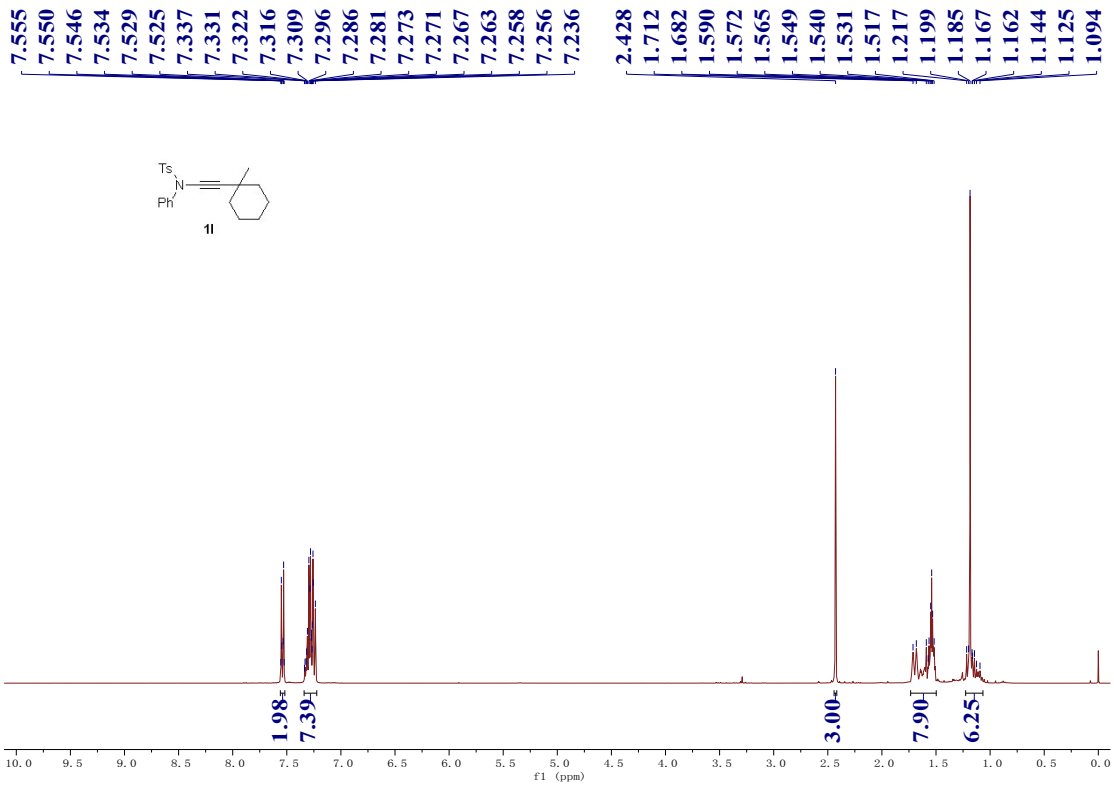
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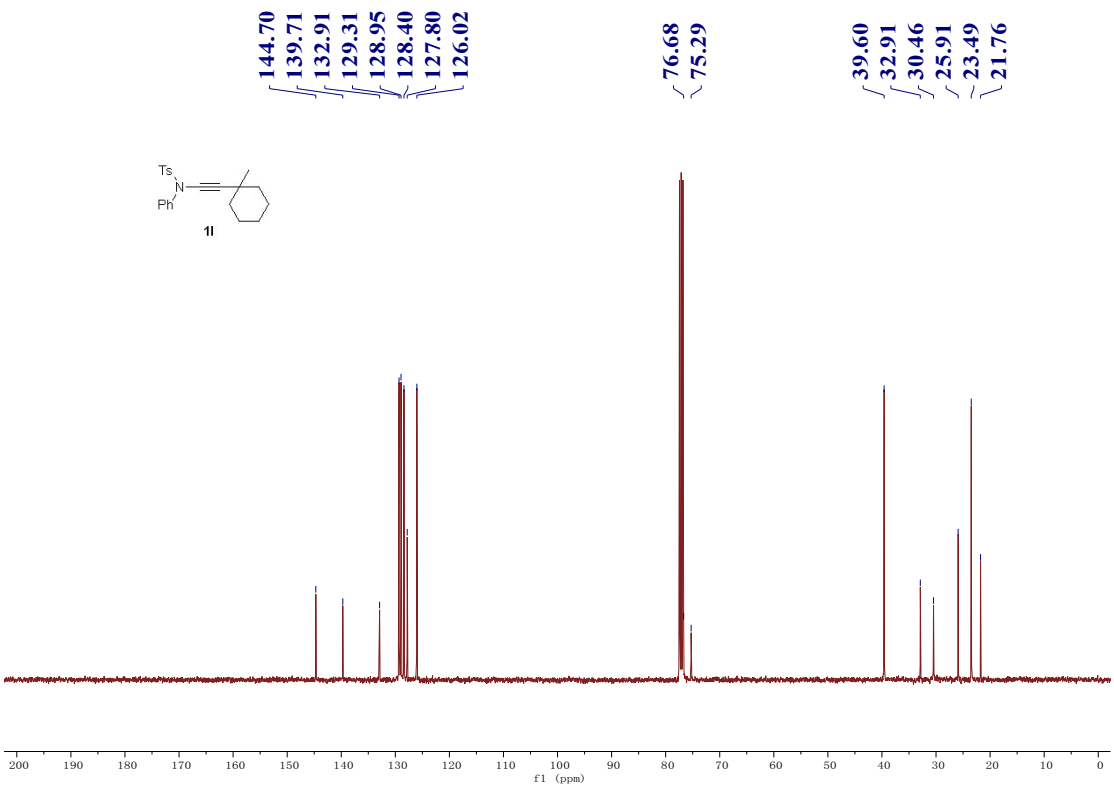
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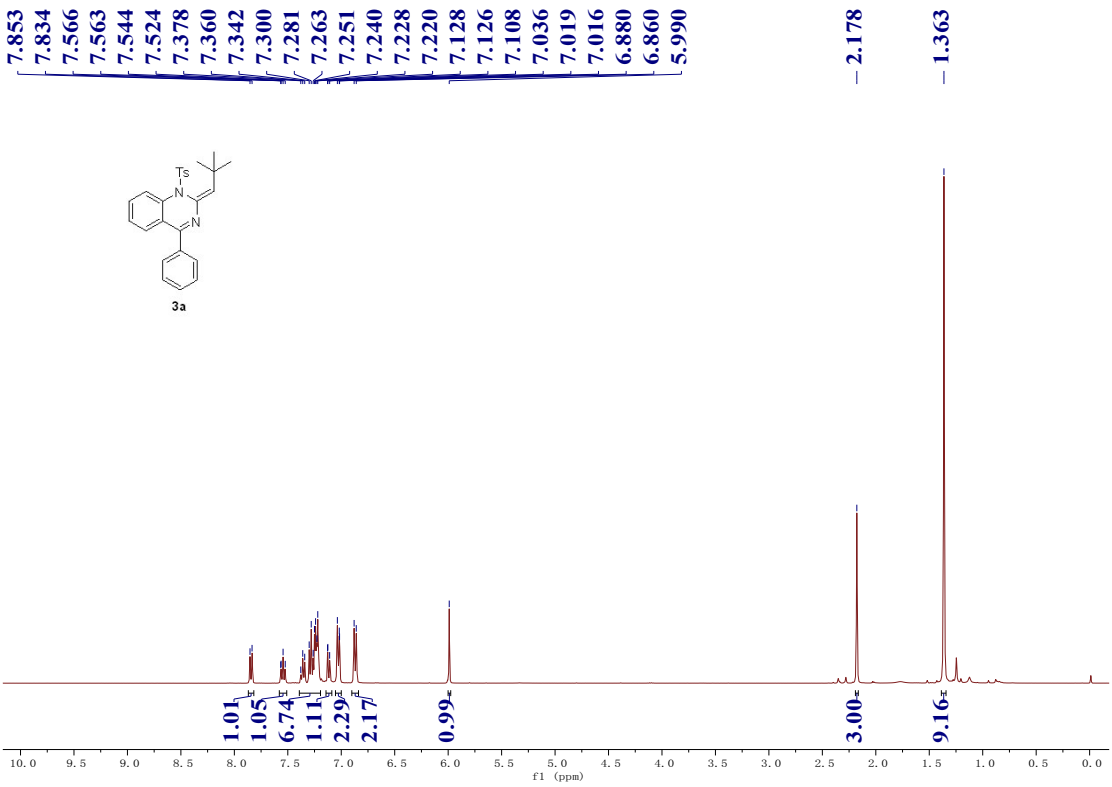
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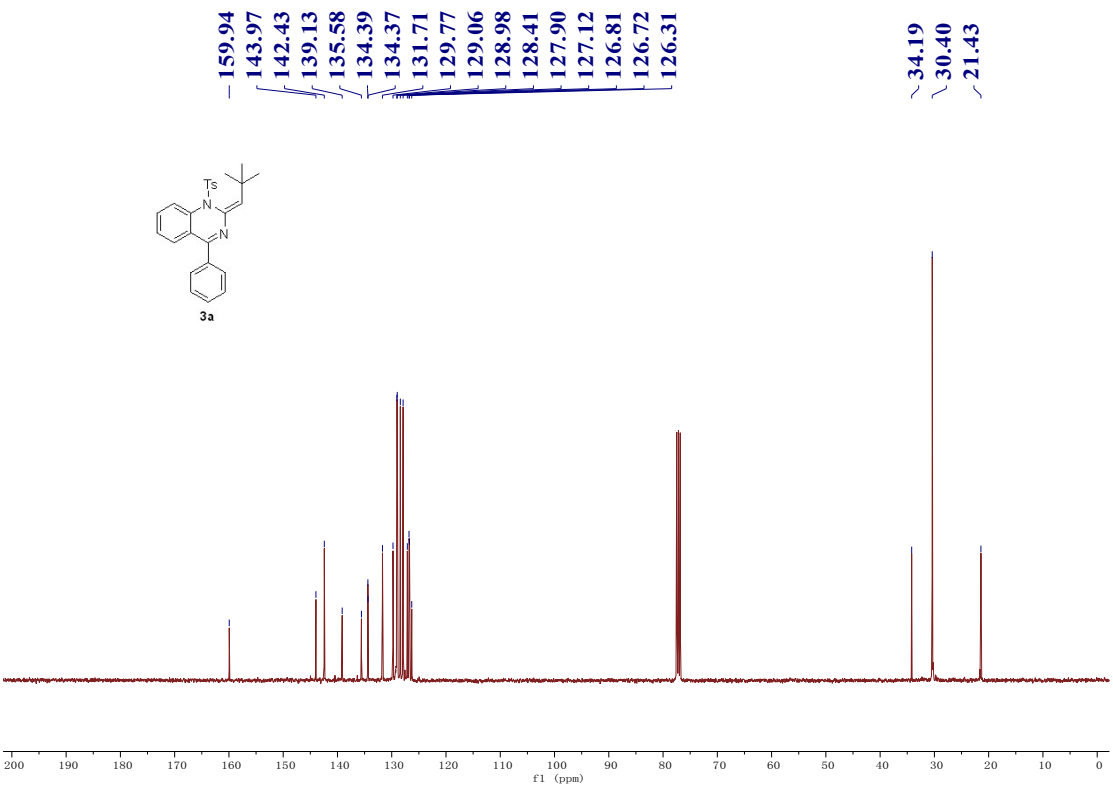
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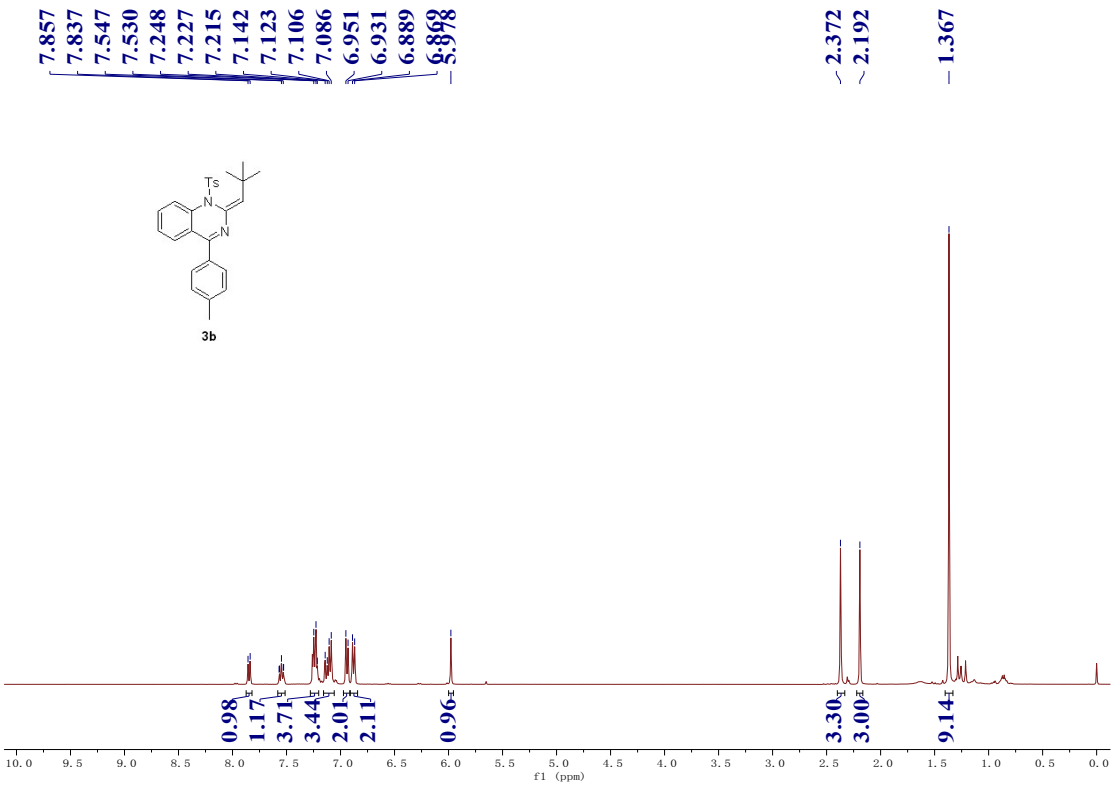
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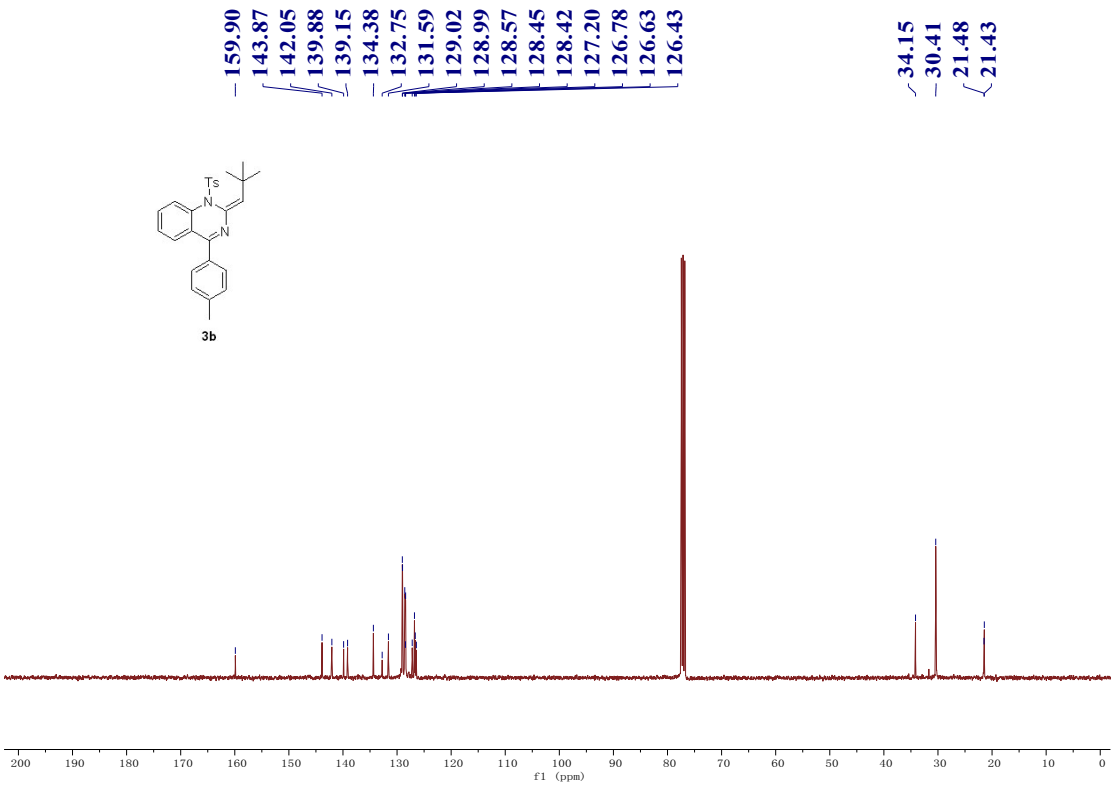
9.14
f1 (ppm)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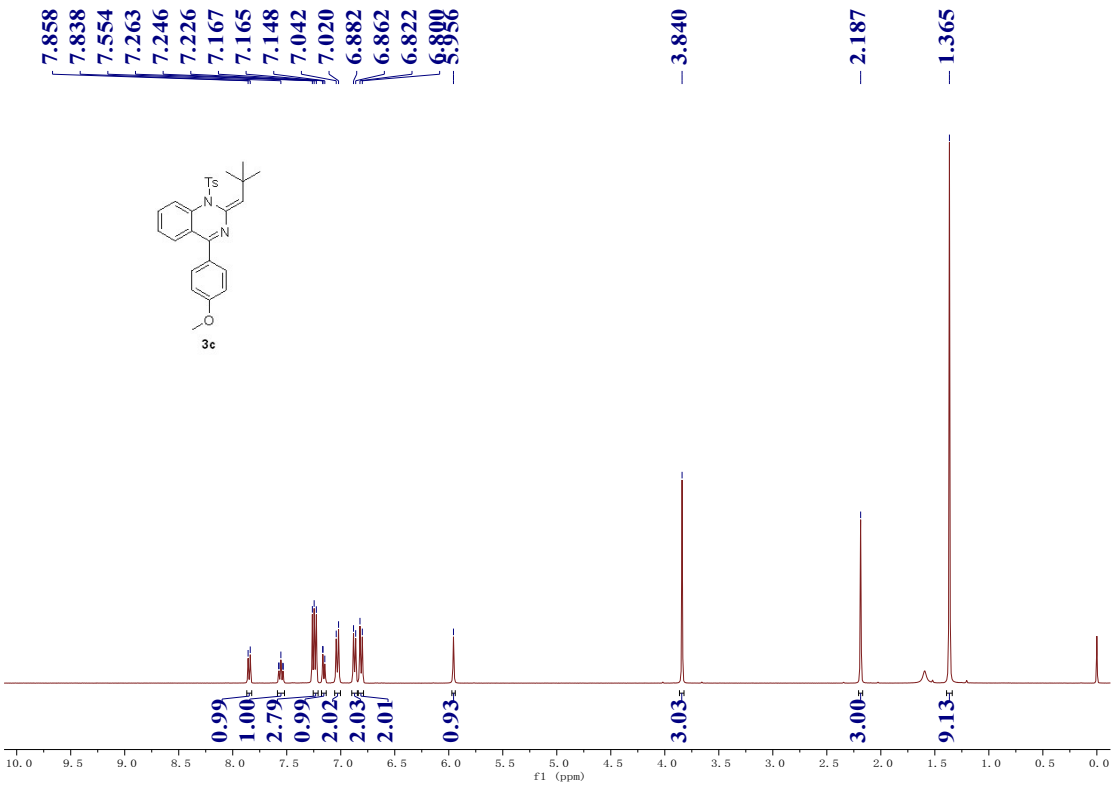
143.87
142.05
139.88
139.15
134.38
132.75
131.59
129.02
128.99
128.57
128.45
128.42
127.20
126.78
126.63
126.43
34.15
30.41
21.48
21.43
Ts
N
N
3b
f1 (ppm)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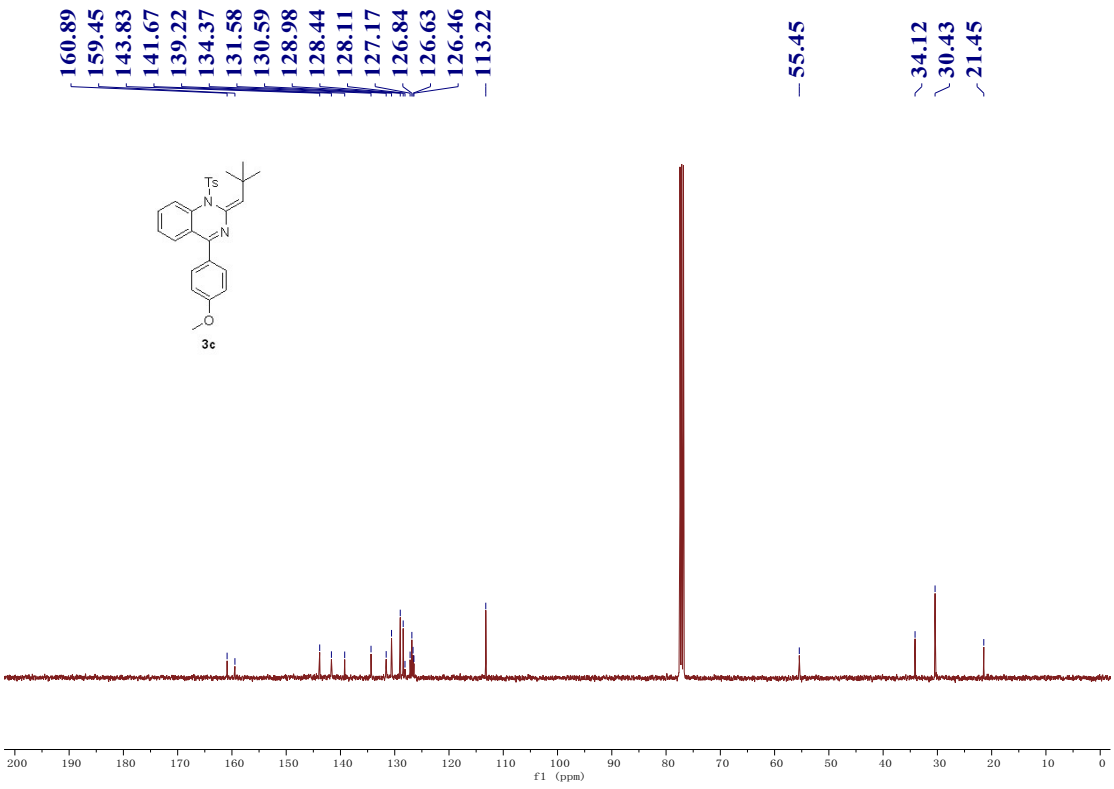
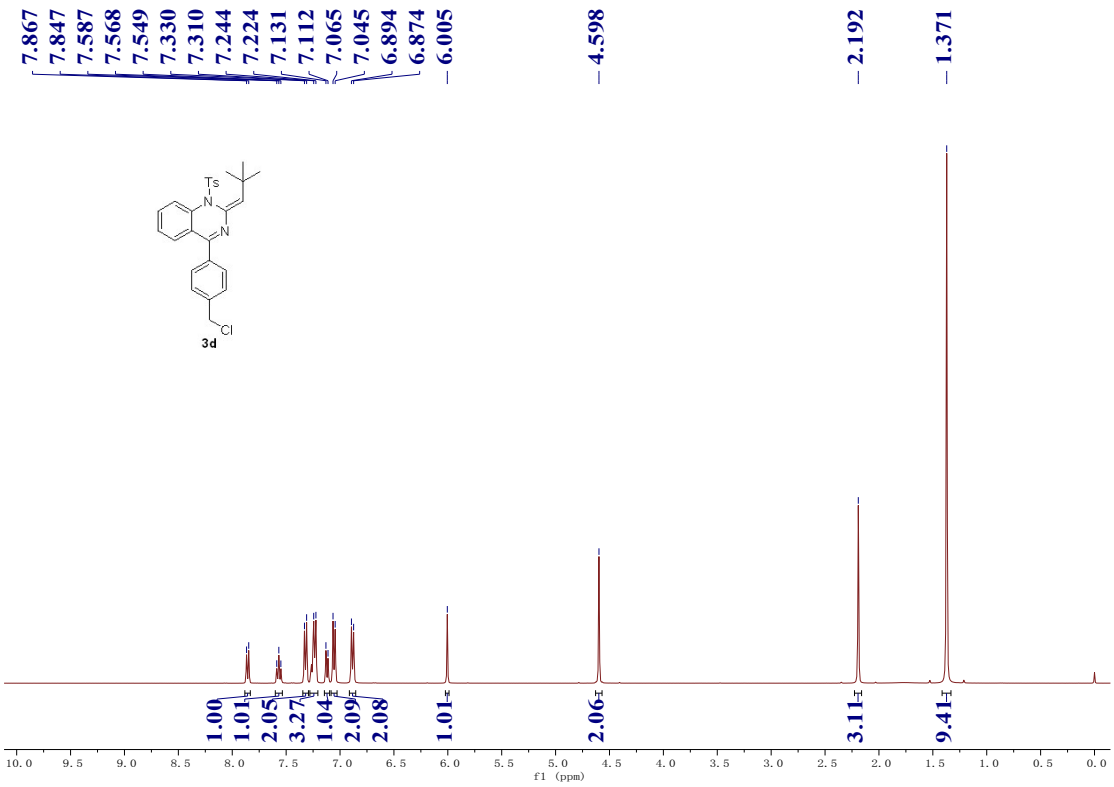
7.838
7.554
7.263
7.246
7.226
7.167
7.165
7.148
7.042
7.020
6.882
6.862
6.822
6.800
5.956
3.840
2.187
1.365
Ts
N
N
O
3c
0.99
1.00
2.79
0.99
2.02
2.03
2.01
0.93
3.03
3.00
9.13
f1 (ppm)


160.89
159.45
143.83
141.67
139.22
134.37
131.58
130.59
128.98
128.44
128.11
127.17
126.84
126.63
126.46
113.22
55.45
34.12
30.43
21.45
Ts
N
N
O
3c
f1 (ppm)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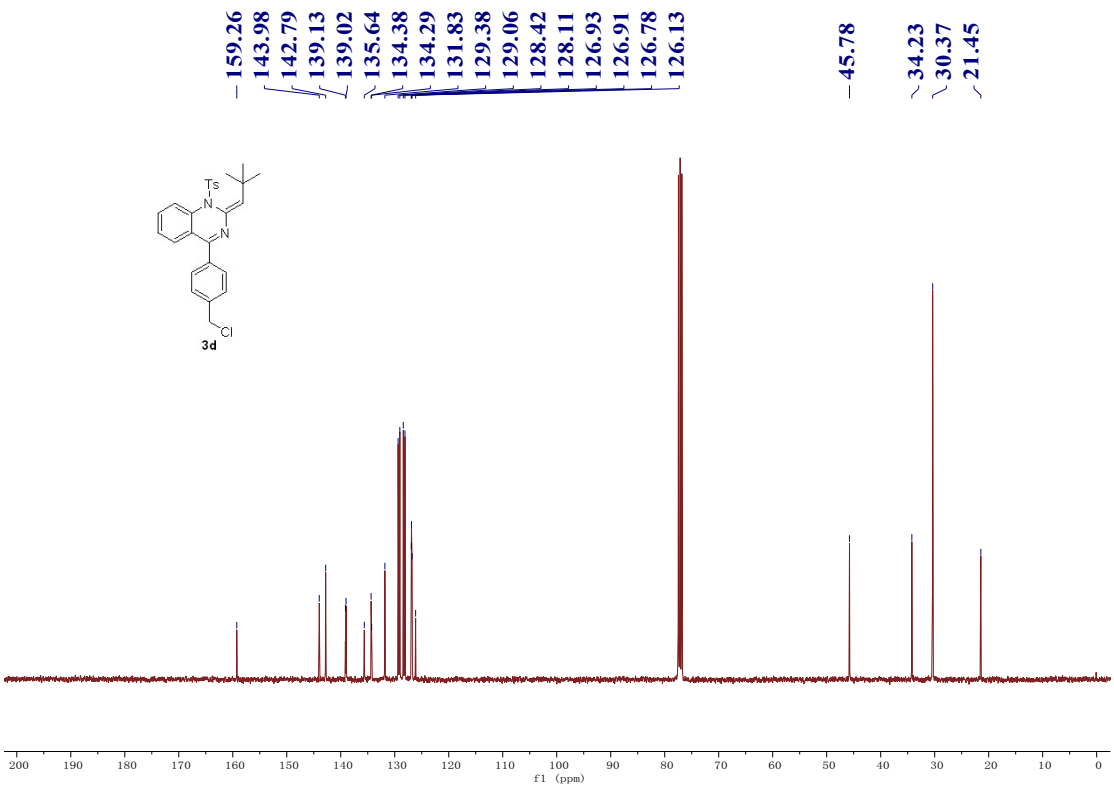
7.847
7.587
7.568
7.549
7.330
7.310
7.244
7.224
7.131
7.112
7.065
7.045
6.894
6.874
6.005
4.598
2.192
1.371
Ts
N
N
Cl
3d
1.00
1.01
2.05
3.27
1.04
2.09
2.08
1.01
2.06
3.11
9.41
f1 (ppm)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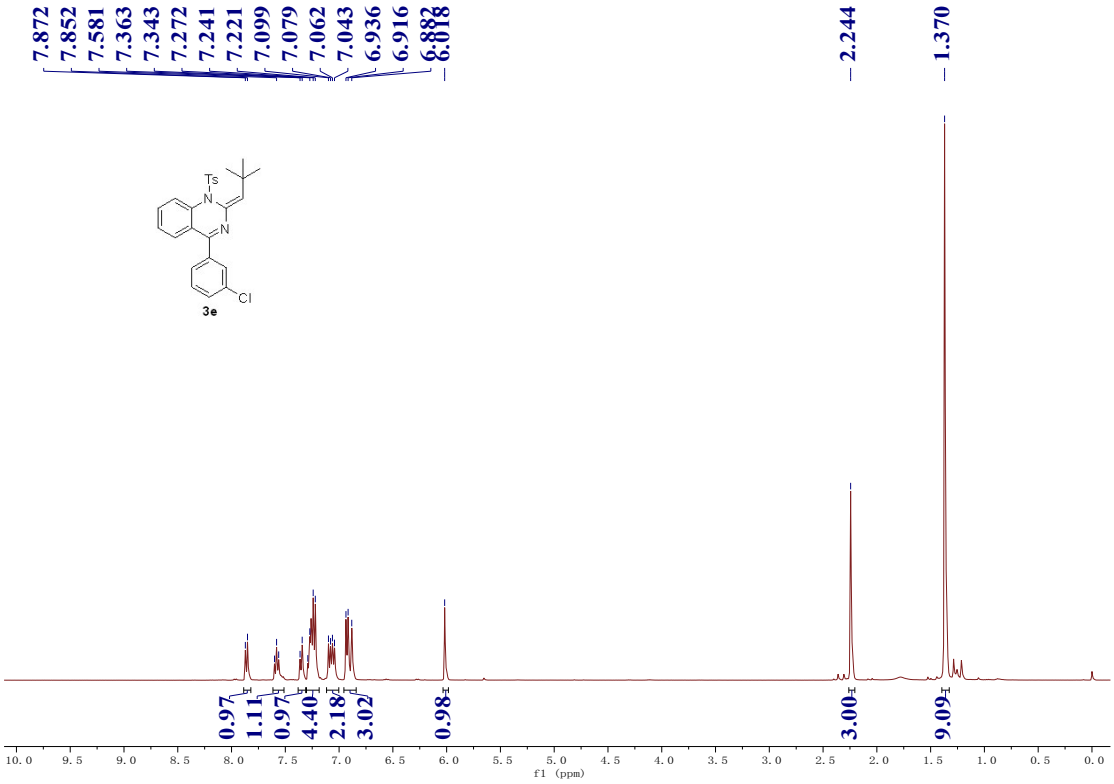
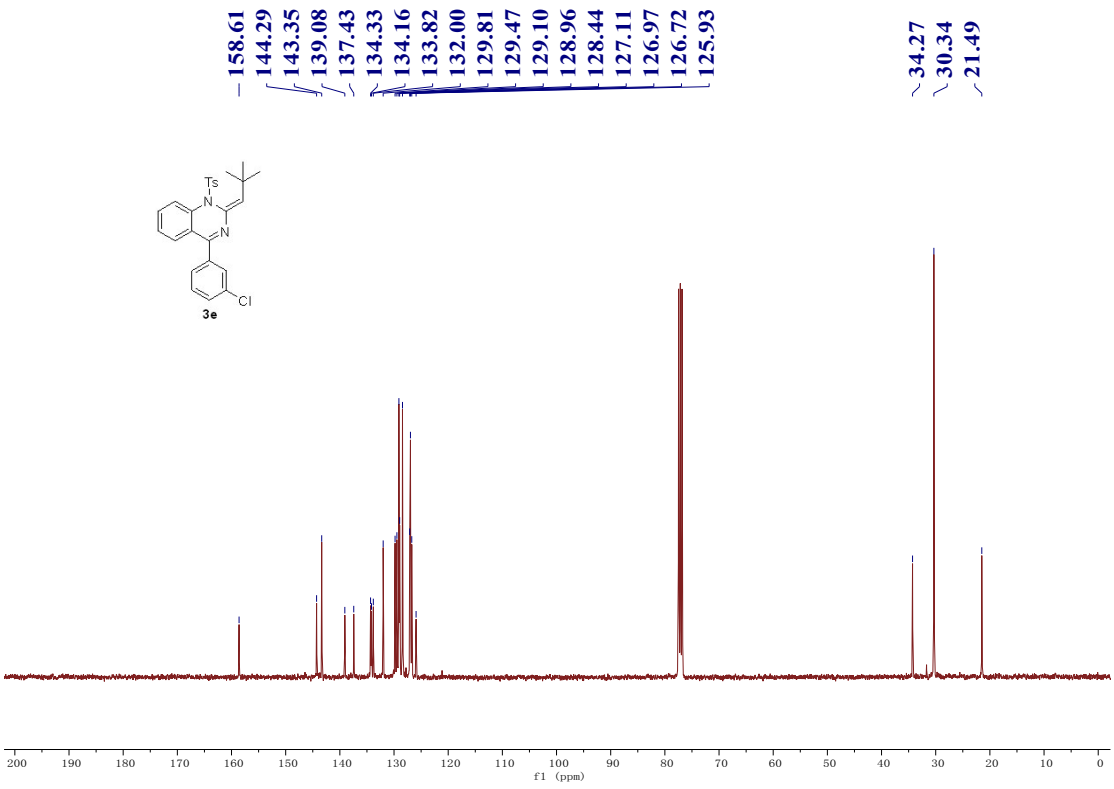
143.98
142.79
139.13
139.02
135.64
134.38
134.29
131.83
129.38
129.06
128.42
128.11
126.93
126.91
126.78
126.13
45.78
34.23
30.37
21.45
Ts
N
N
Cl
3d
f1 (ppm)


7.872
7.852
7.581
7.363
7.343
7.272
7.241
7.221
7.099
7.079
7.062
7.043
6.936
6.916
6.882
6.018
2.244
1.370
Ts
N
N
Cl
3e
0.97
1.11
0.97
4.40
2.18
3.02
0.98
3.00
9.09
f1 (ppm)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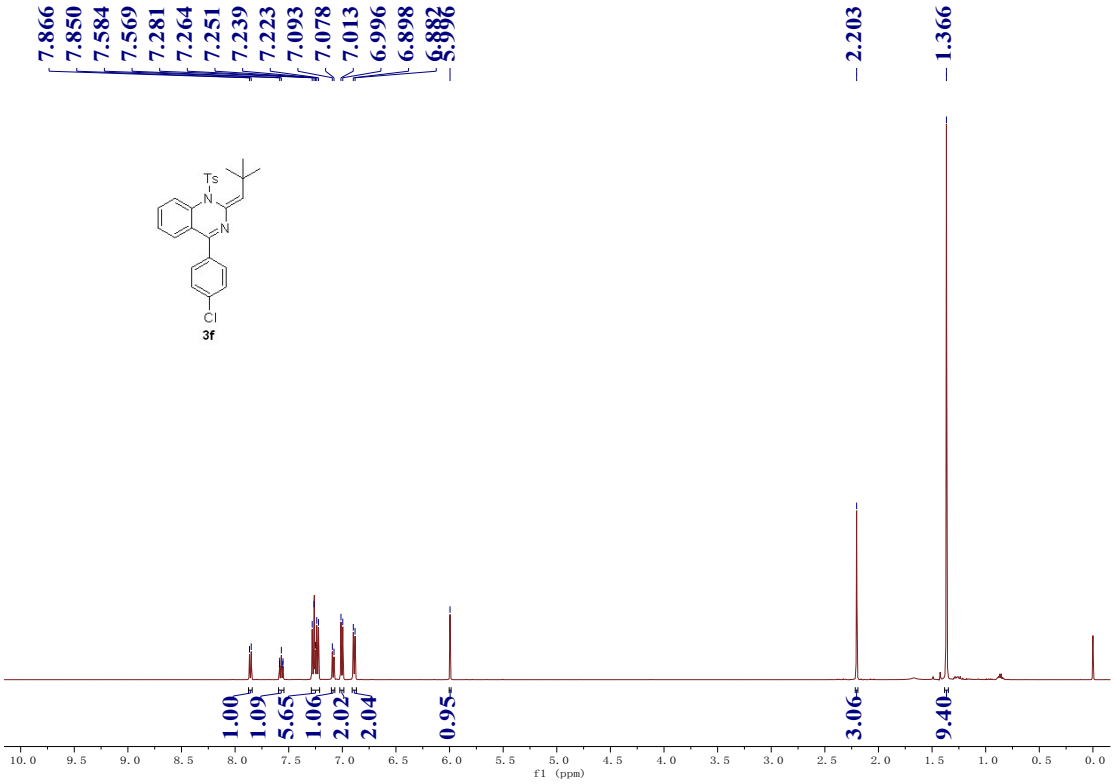
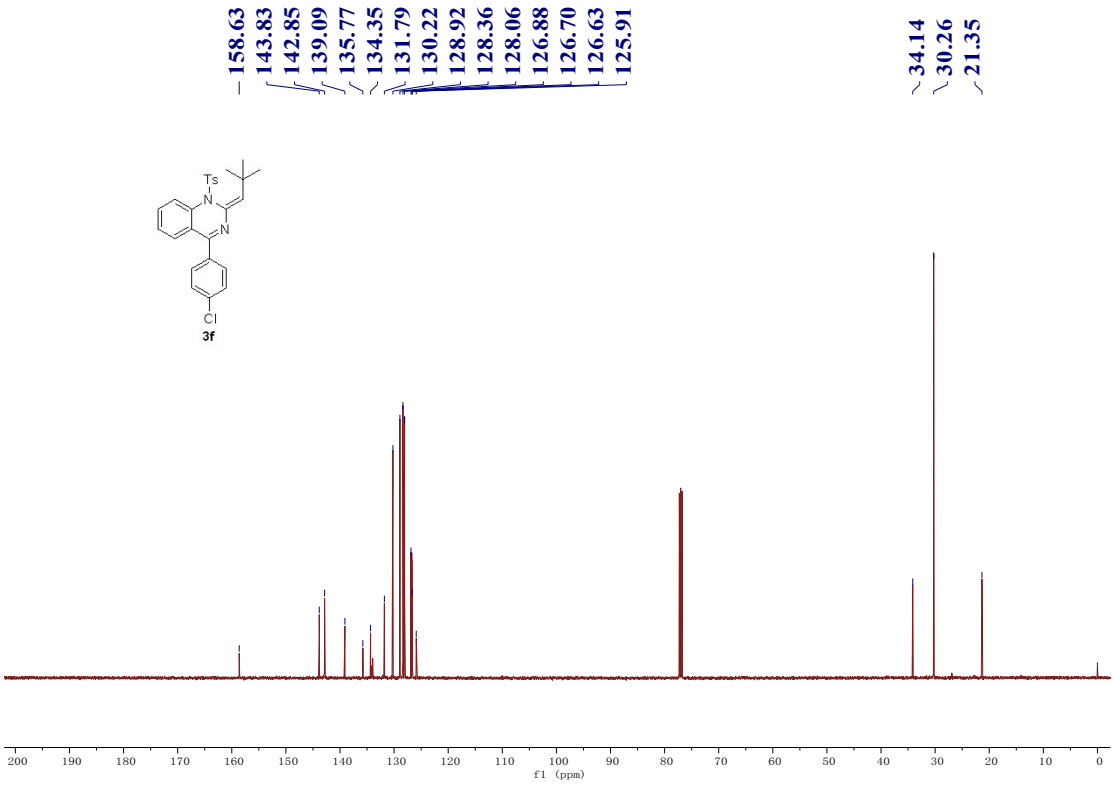
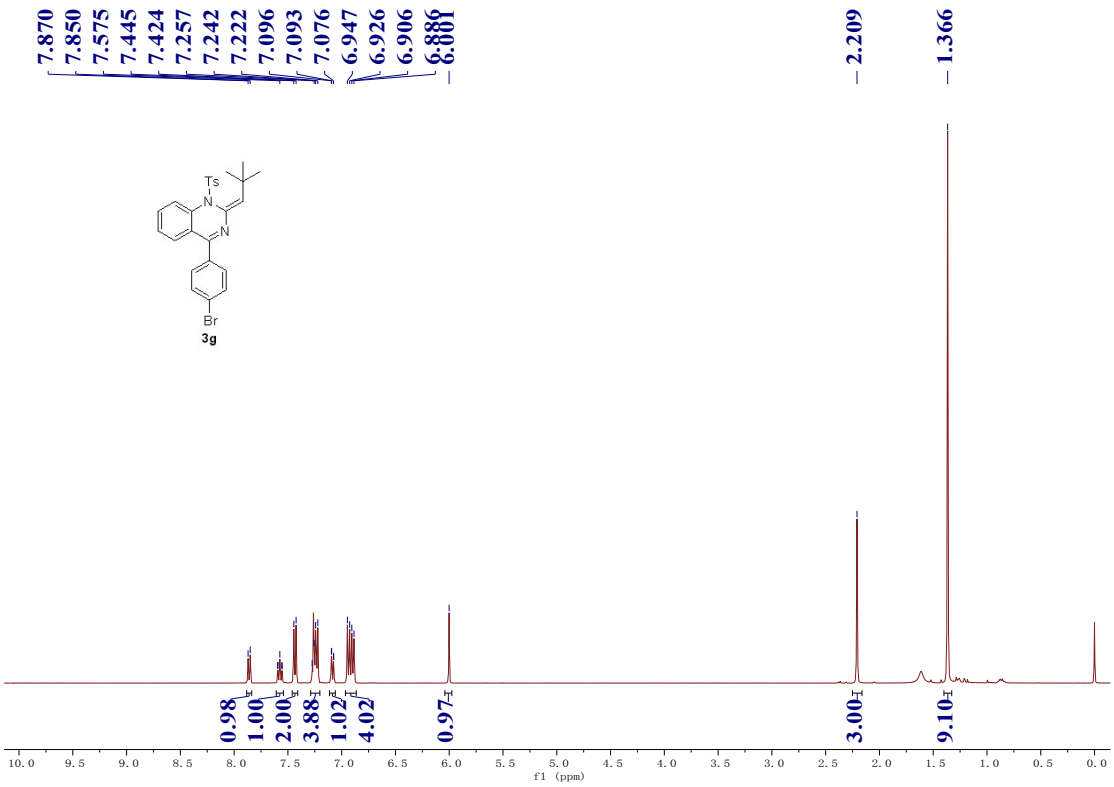
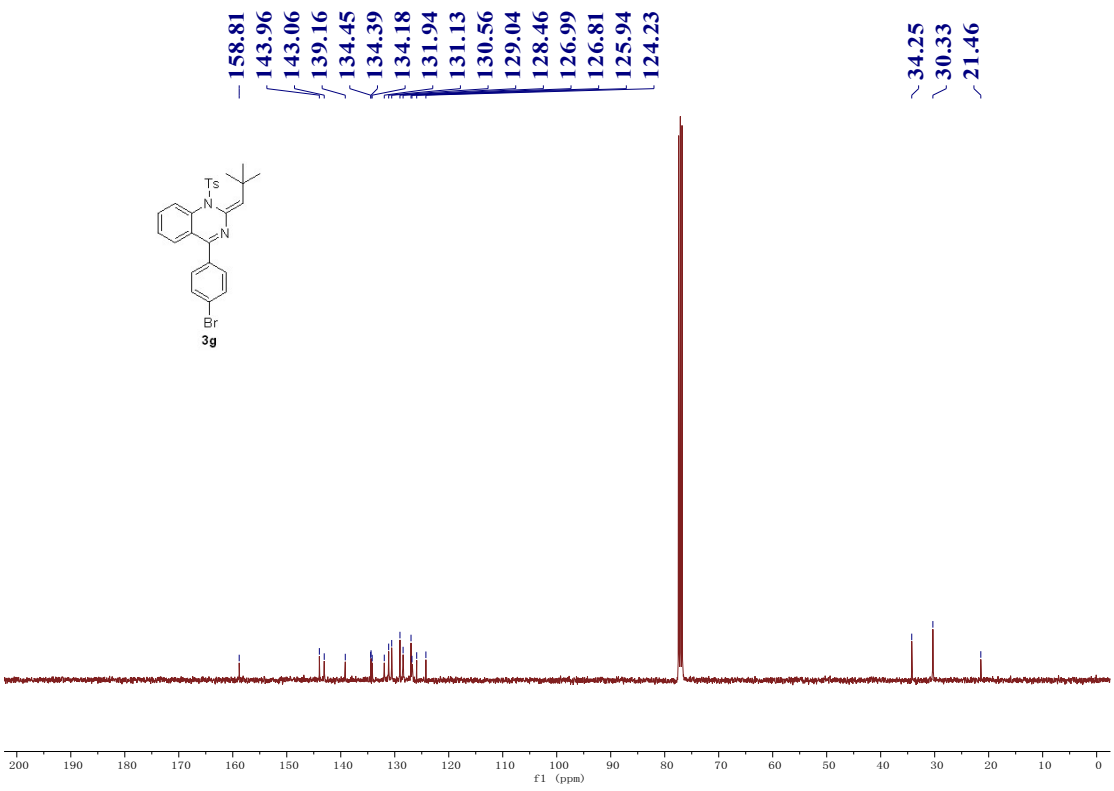
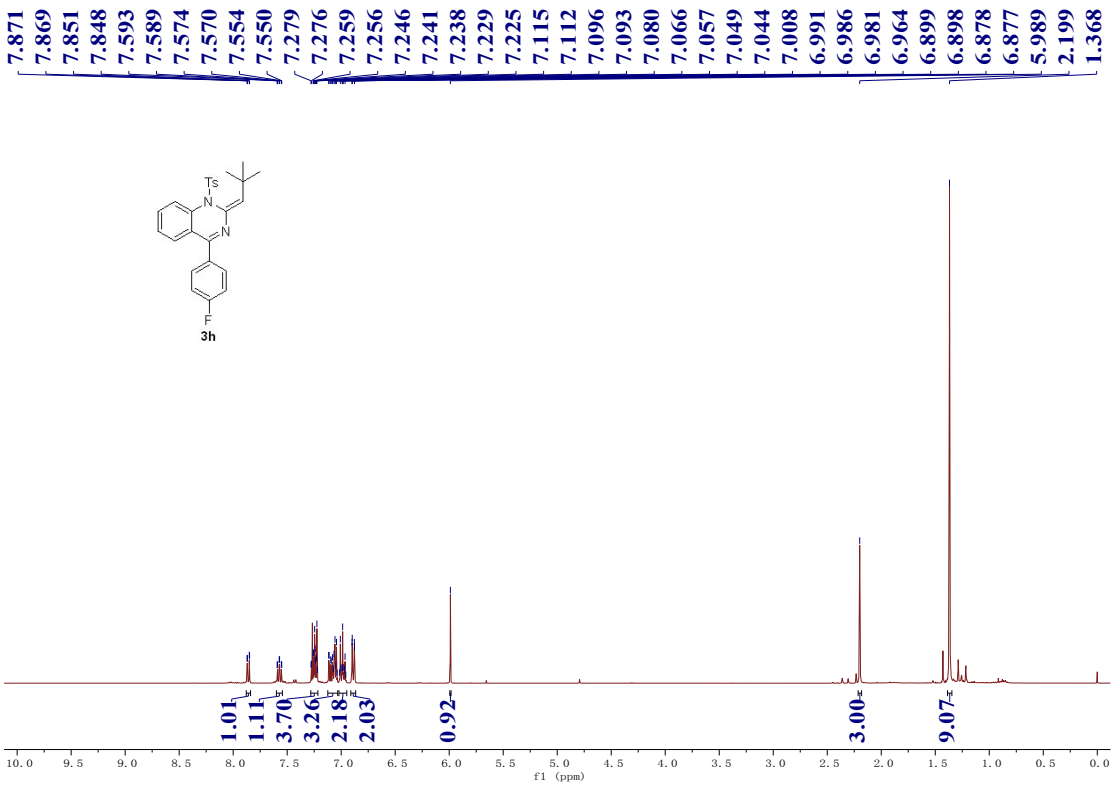
144.29
143.35
139.08
137.43
134.33
134.16
133.82
132.00
129.81
129.47
129.10
128.96
128.44
127.11
126.97
126.72
125.93
34.27
30.34
21.49
Ts
N
N
Cl
3e
f1 (ppm)


7.866
7.850
7.584
7.569
7.281
7.264
7.251
7.239
7.223
7.093
7.078
7.013
6.996
6.898
6.882
5.996
2.203
1.366
Ts
N
N
Cl
3f
1.00
1.09
5.65
1.06
2.02
2.04
0.95
3.06
9.40
f1 (ppm)


158.63
143.83
142.85
139.09
135.77
134.35
131.79
130.22
128.92
128.36
128.06
126.88
126.70
126.63
125.91
34.14
30.26
21.35
Ts
N
N
Cl
3f
f1 (ppm)


7.870
7.850
7.575
7.445
7.424
7.257
7.242
7.222
7.096
7.093
7.076
6.947
6.926
6.906
6.886
6.881
2.209
1.366
Ts
N
N
Br
3g
0.98
1.00
2.00
3.88
1.02
4.02
0.97
3.00
9.10
f1 (ppm)


158.81
143.96
143.06
139.16
134.45
134.39
134.18
131.94
131.13
130.56
129.04
128.46
126.99
126.81
125.94
124.23
34.25
30.33
21.46
Ts
N
N
Br
3g
f1 (ppm)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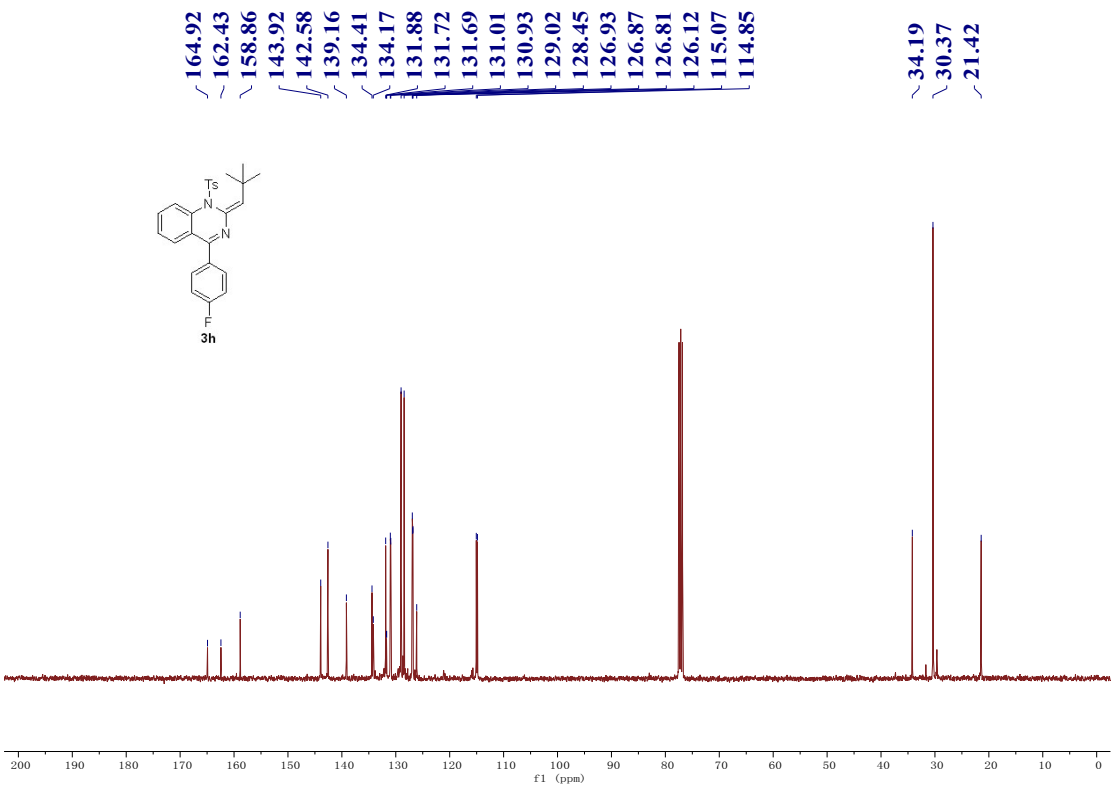
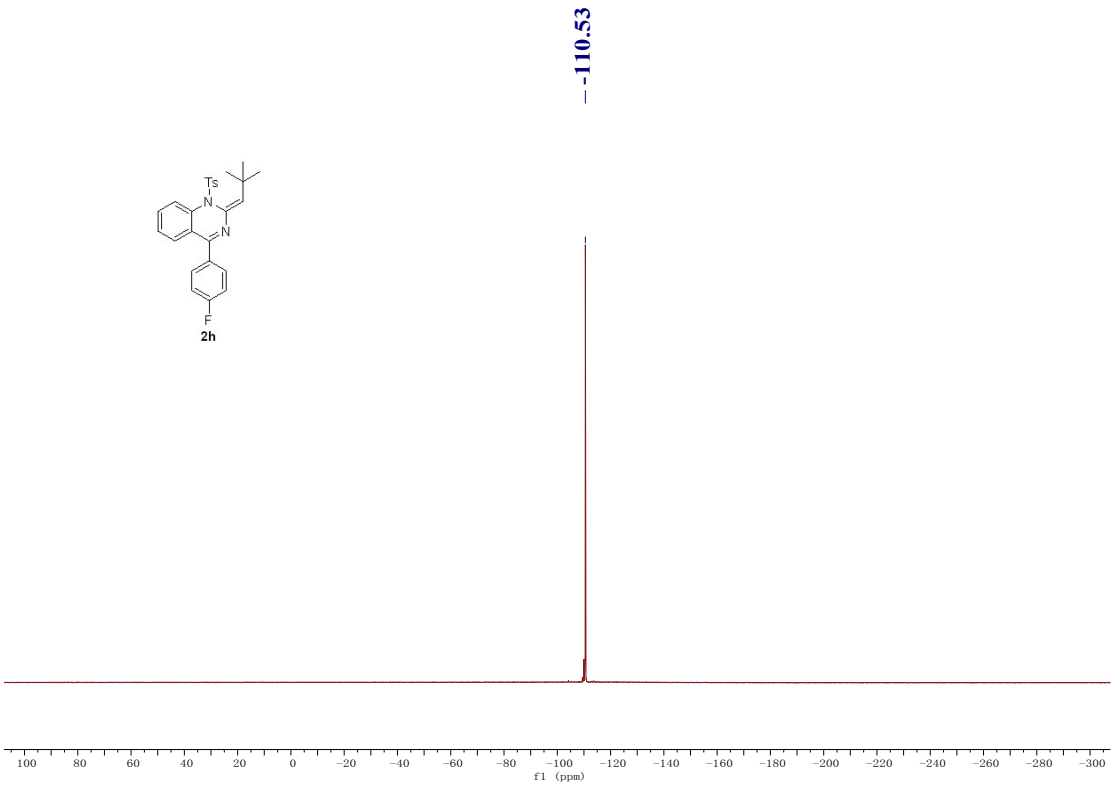
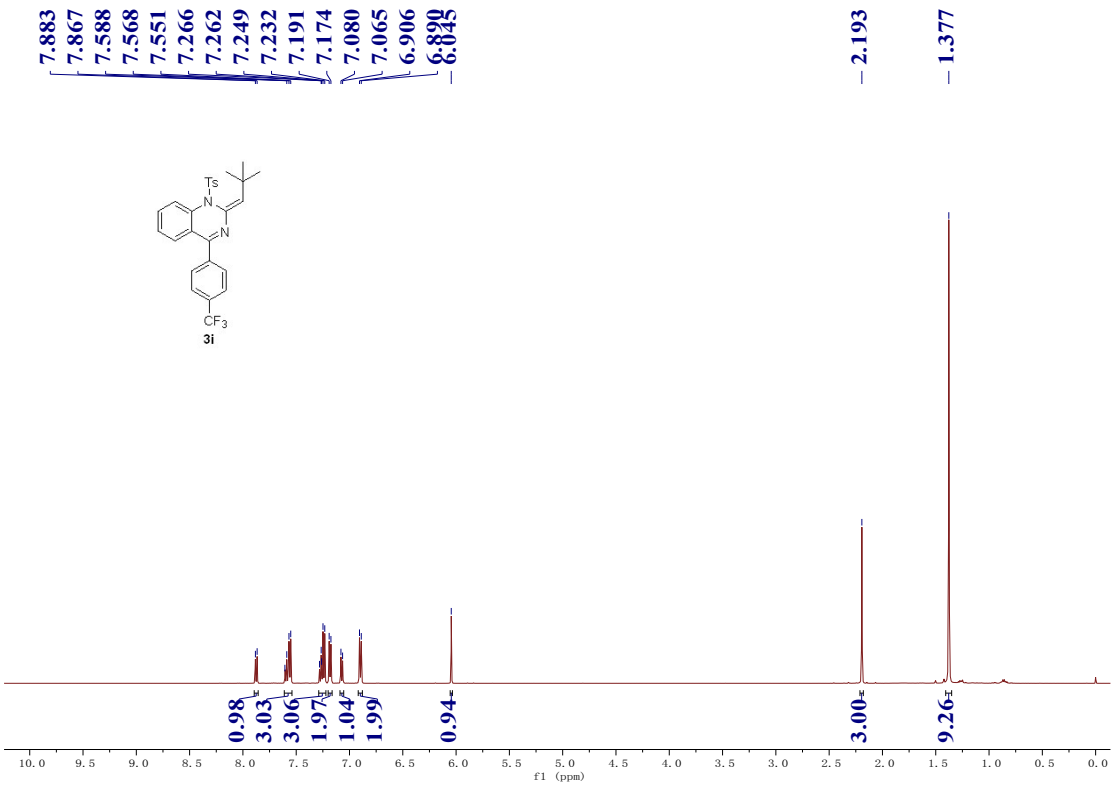
7.869
7.851
7.848
7.593
7.589
7.574
7.570
7.554
7.550
7.279
7.276
7.259
7.256
7.246
7.241
7.238
7.229
7.225
7.115
7.112
7.096
7.093
7.080
7.066
7.057
7.049
7.044
7.008
6.991
6.986
6.981
6.964
6.899
6.898
6.878
6.877
5.989
2.199
1.368
Ts
N
N
F
3h
1.01
1.11
3.70
3.26
2.18
2.03
0.92
3.00
9.07
f1 (ppm)


164.92
162.43
158.86
143.92
142.58
139.16
134.41
134.17
131.88
131.72
131.69
131.01
130.93
129.02
128.45
126.93
126.87
126.81
126.12
115.07
114.85
34.19
30.37
21.42
Ts
N
N
F
3h
f1 (ppm)


-110.53
Ts
N
N
F
2h
100 80 60 40 20 0 -20 -40 -60 -80 -100 -120 -140 -160 -180 -200 -220 -240 -260 -280 -300
f1 (ppm)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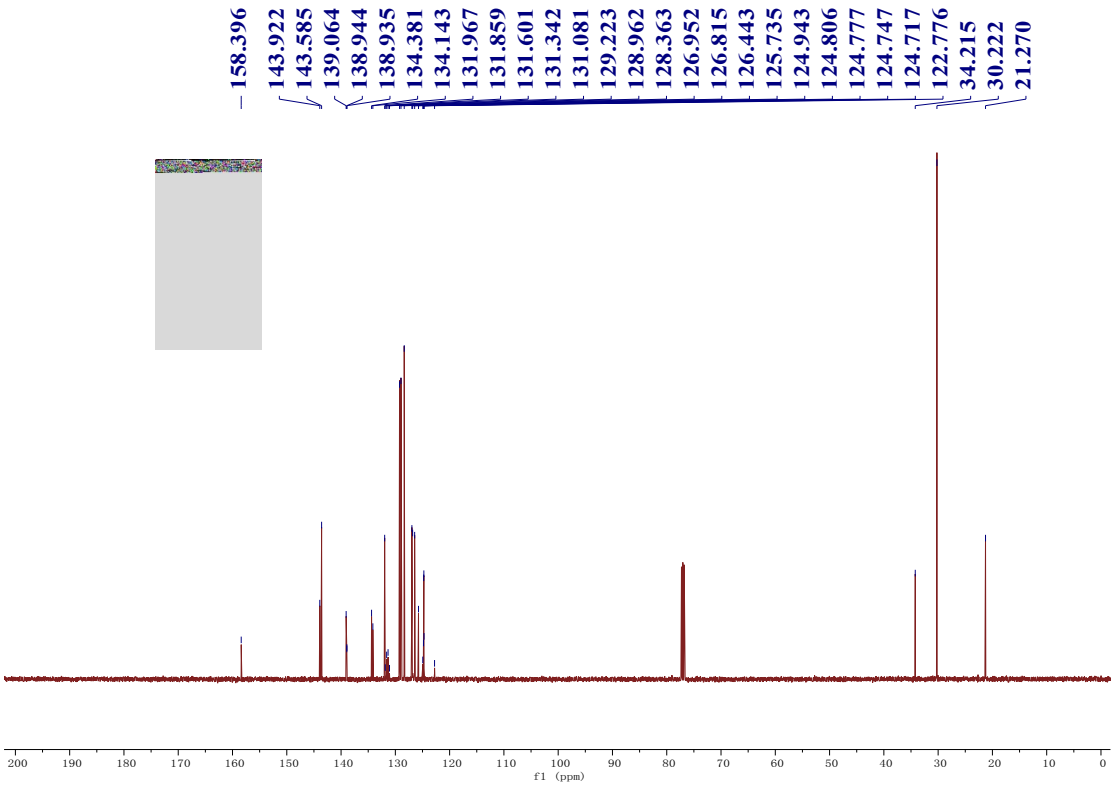
7.867
7.588
7.568
7.551
7.266
7.262
7.249
7.232
7.191
7.174
7.080
7.065
6.906
2.193
1.377
Ts
N
N
CF3
3i
0.98
3.03
3.06
1.97
1.04
1.99
0.94
3.00
9.26
10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)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143.585
139.064
138.944
138.935
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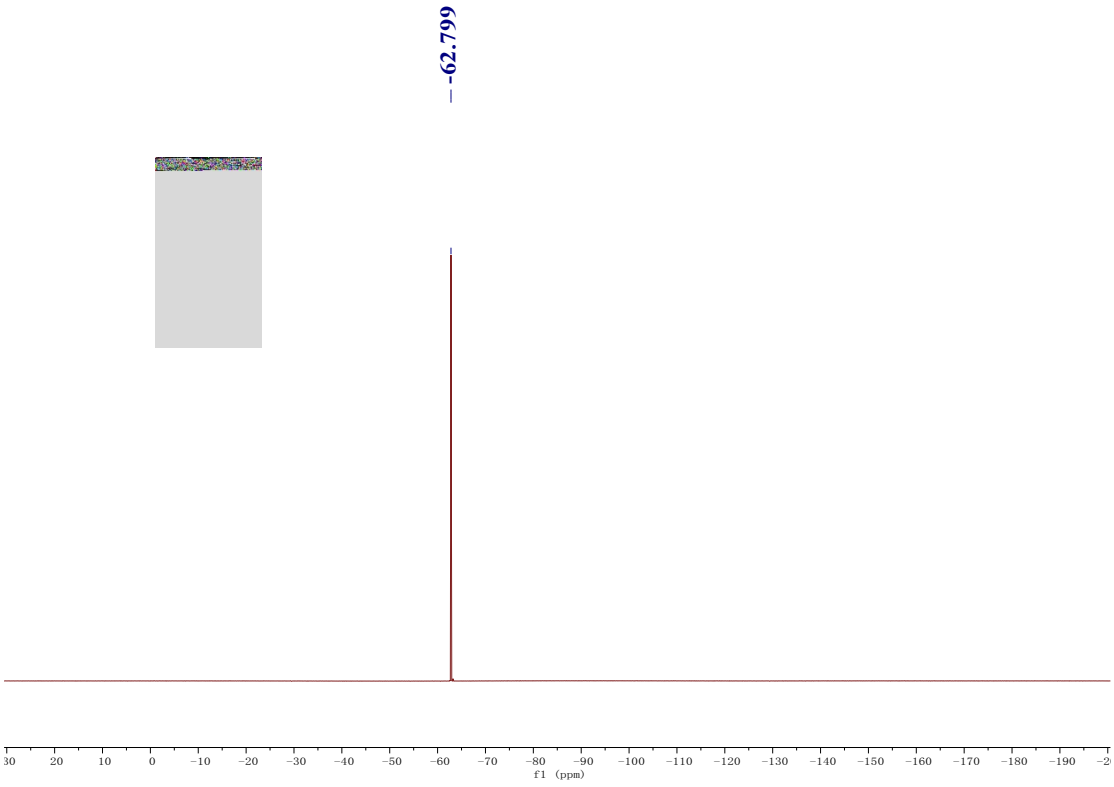
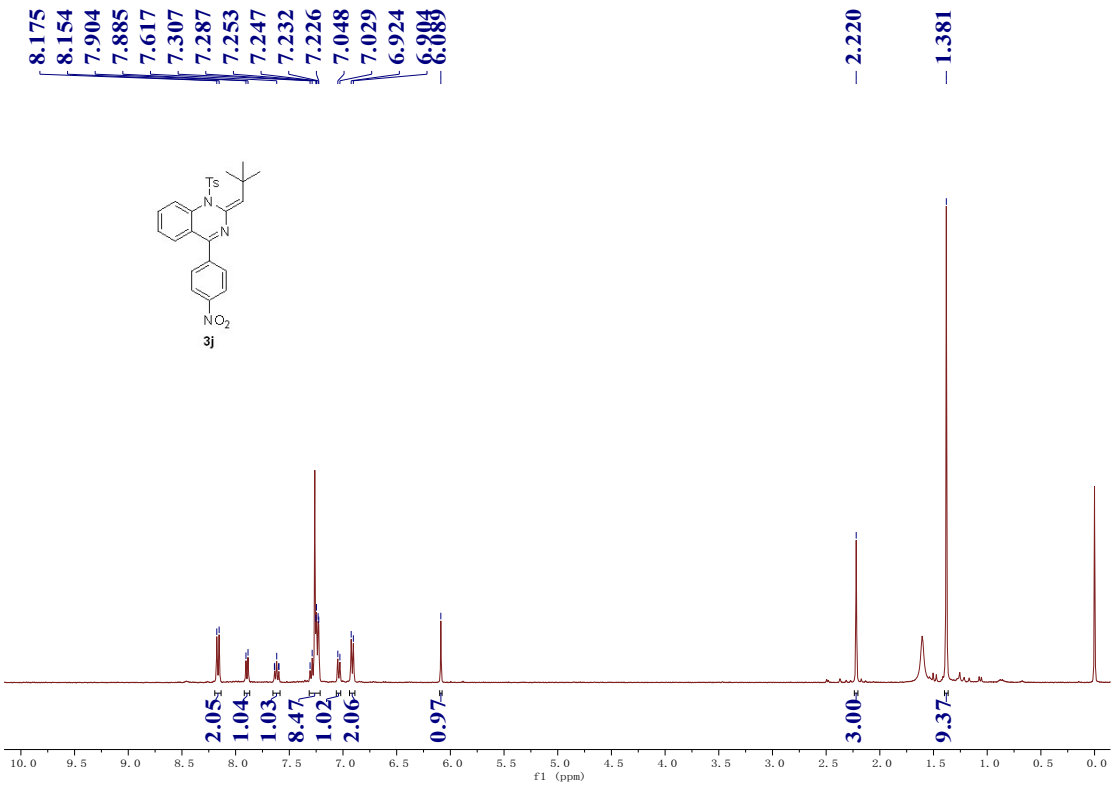
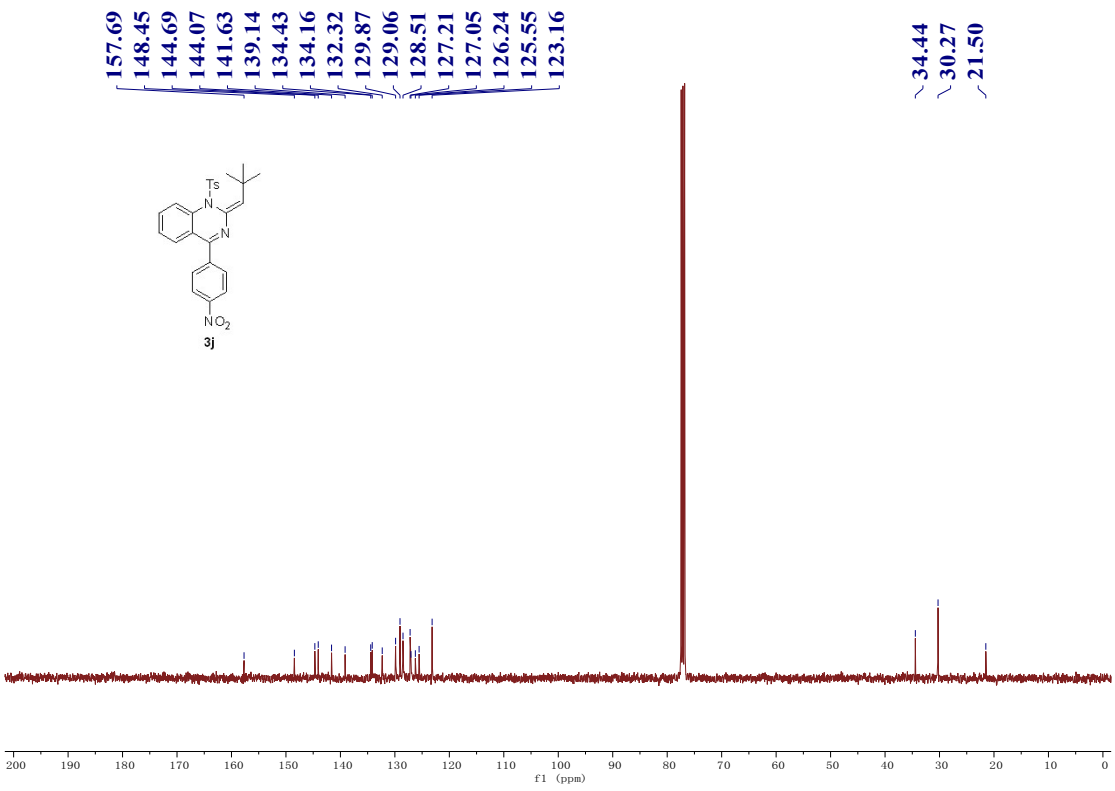
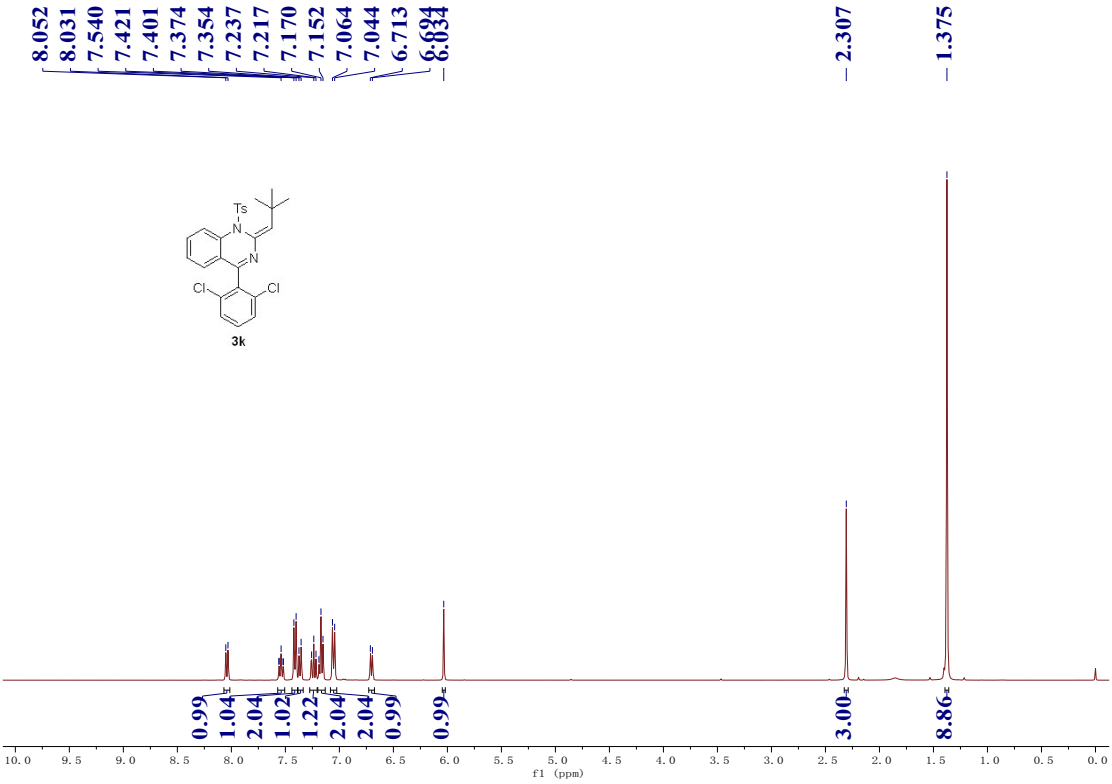
134.143
131.967
131.859
131.601
131.342
131.081
129.223
128.962
128.363
126.952
126.815
126.443
125.735
124.943
124.806
124.777
124.747
124.717
122.776
34.215
30.222
21.270
200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)


-62.799
30 20 10 0 -10 -20 -30 -40 -50 -60 -70 -80 -90 -100 -110 -120 -130 -140 -150 -160 -170 -180 -190
f1 (ppm)


8.175
8.154
7.904
7.885
7.617
7.307
7.287
7.253
7.247
7.232
7.226
7.048
7.029
6.924
2.220
1.381
Ts
N
N
NO2
3j
2.05
1.04
1.03
8.47
1.02
2.06
0.97
3.00
9.37
f1 (ppm)


157.69
148.45
144.69
144.07
141.63
139.14
134.43
134.16
132.32
129.87
129.06
128.51
127.21
127.05
126.24
125.55
123.16
34.44
30.27
21.50
Ts
N
N
NO2
3j
f1 (ppm)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7.540
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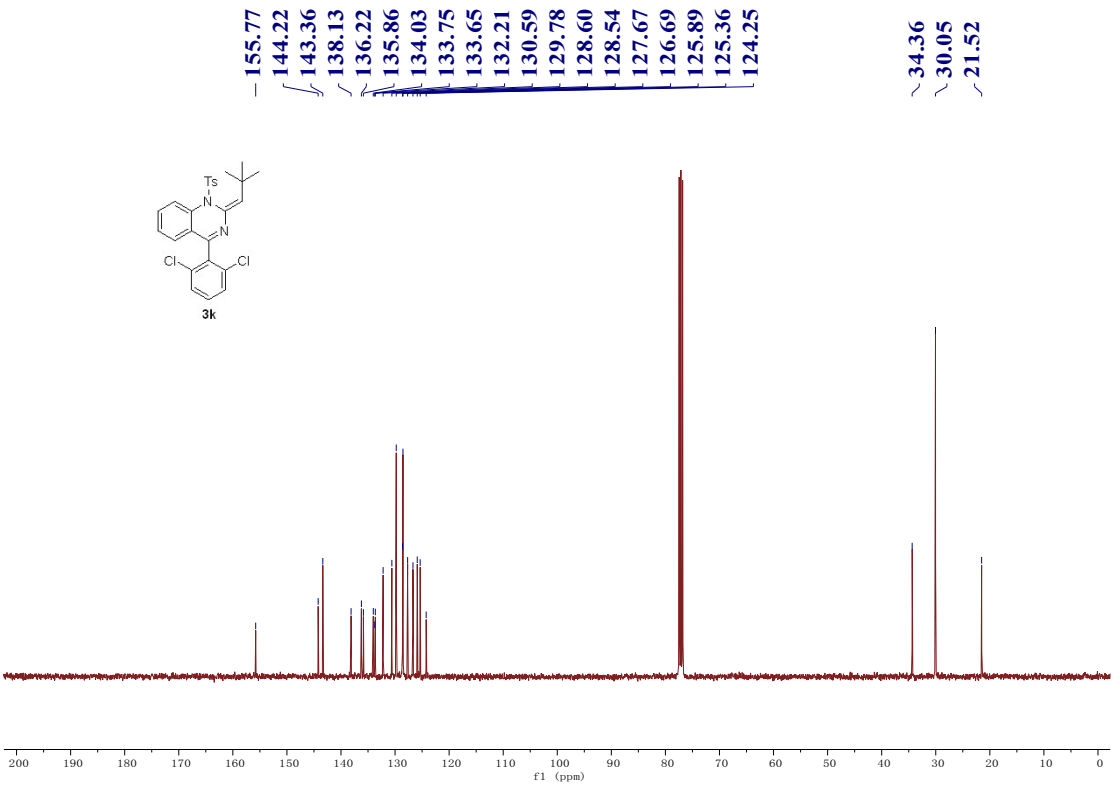
7.401
7.374
7.354
7.237
7.217
7.170
7.152
7.064
7.044
6.713
6.694
6.034
2.307
1.375
Ts
N
N
Cl
Cl
3k
0.99
1.04
2.04
1.02
1.22
2.04
2.04
0.99
0.99
3.00
8.86
f1 (ppm)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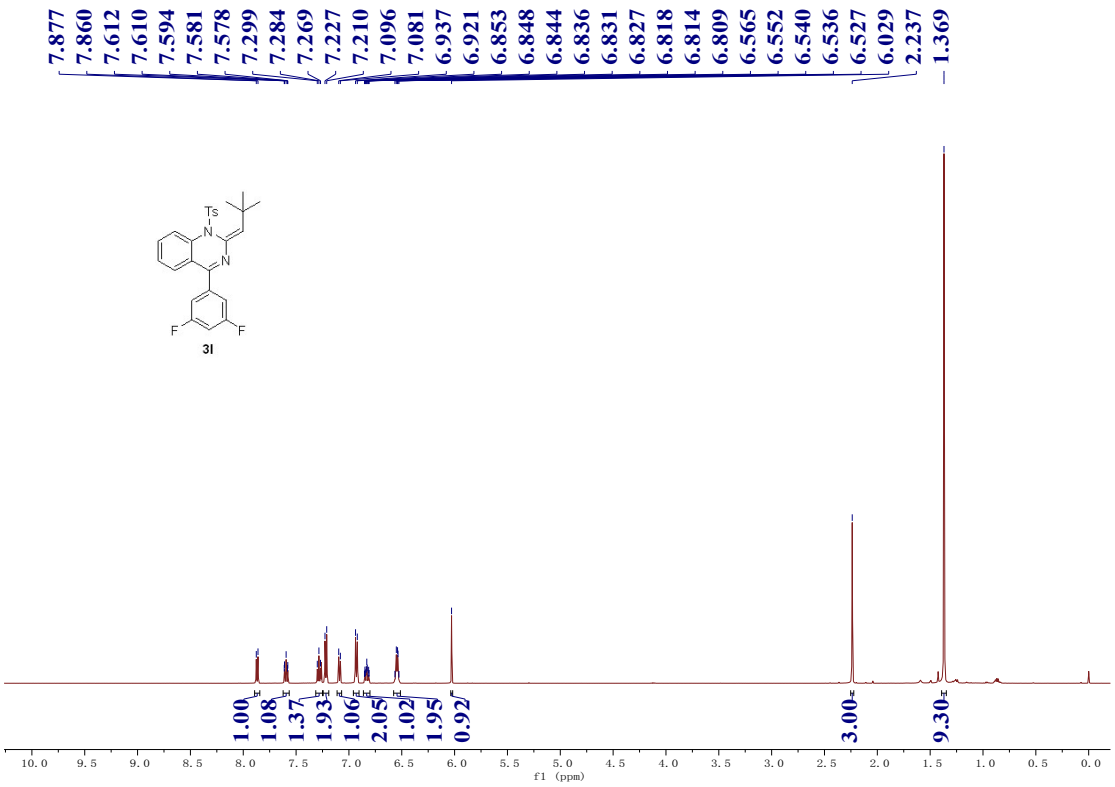
143.36
138.13
136.22
135.86
134.03
133.75
133.65
132.21
130.59
129.78
128.60
128.54
127.67
126.69
125.89
125.36
124.25
34.36
30.05
21.52
Ts
N
N
Cl
Cl
3k
f1 (ppm)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7.581
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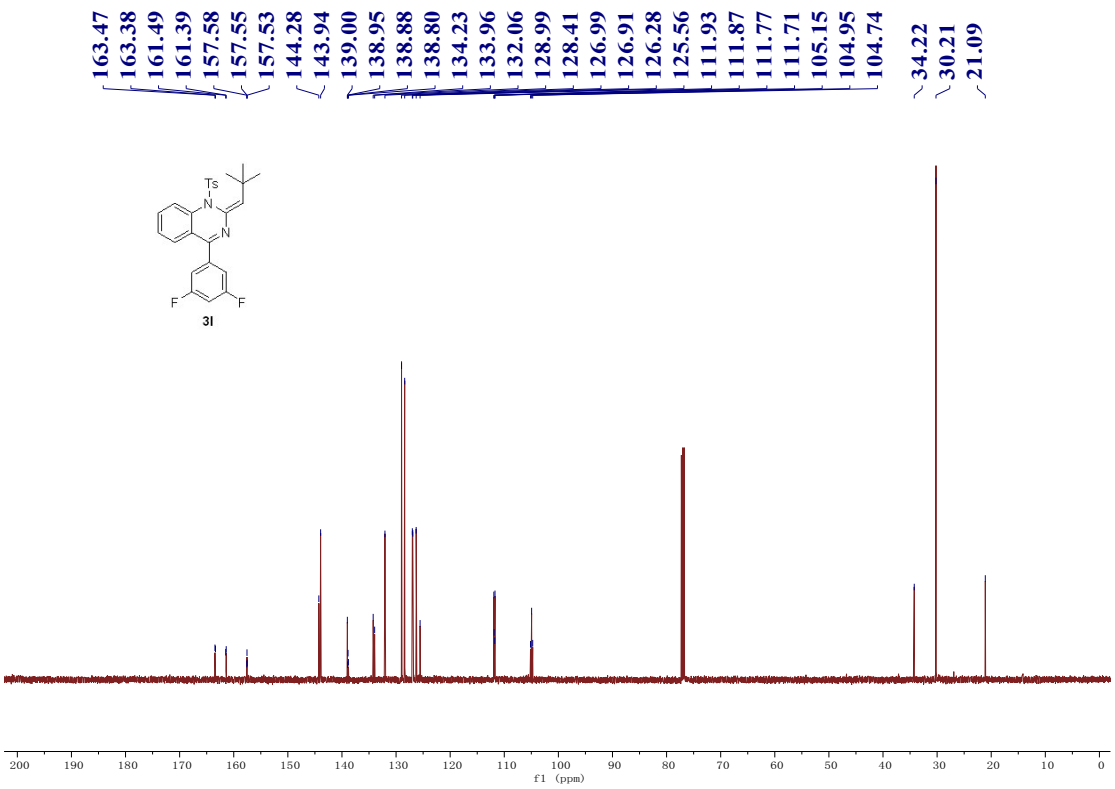
7.299
7.284
7.269
7.227
7.210
7.096
7.081
6.937
6.921
6.853
6.848
6.844
6.836
6.831
6.827
6.818
6.814
6.809
6.565
6.552
6.540
6.536
6.527
6.029
2.237
1.369
Ts
N
N
F
F
3l
1.00
1.08
1.37
1.93
1.06
2.05
1.02
1.95
0.92
3.00
9.30
f1 (ppm)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161.39
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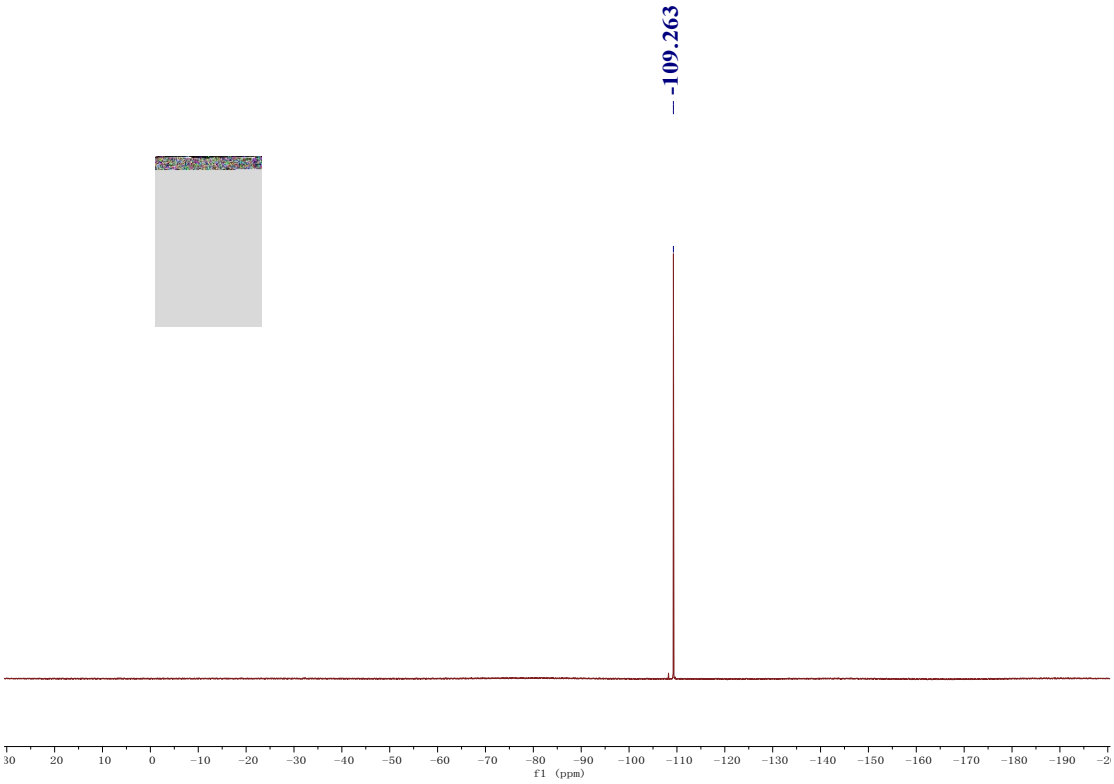
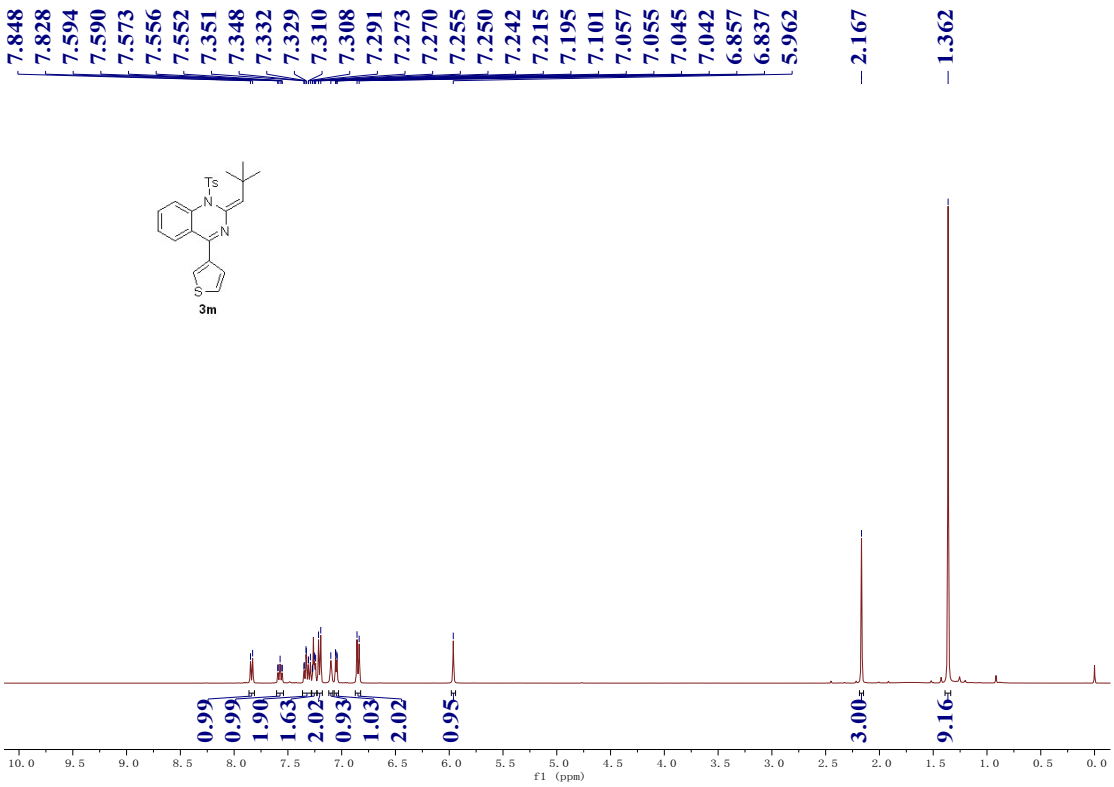
157.55
157.53
144.28
143.94
139.00
138.95
138.88
138.80
134.23
133.96
132.06
128.99
128.41
126.99
126.91
126.28
125.56
111.93
111.87
111.77
111.71
105.15
104.95
104.74
34.22
30.21
21.09
Ts
N
N
F
F
3l
f1 (ppm)


-109.263
f1 (ppm)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7.828
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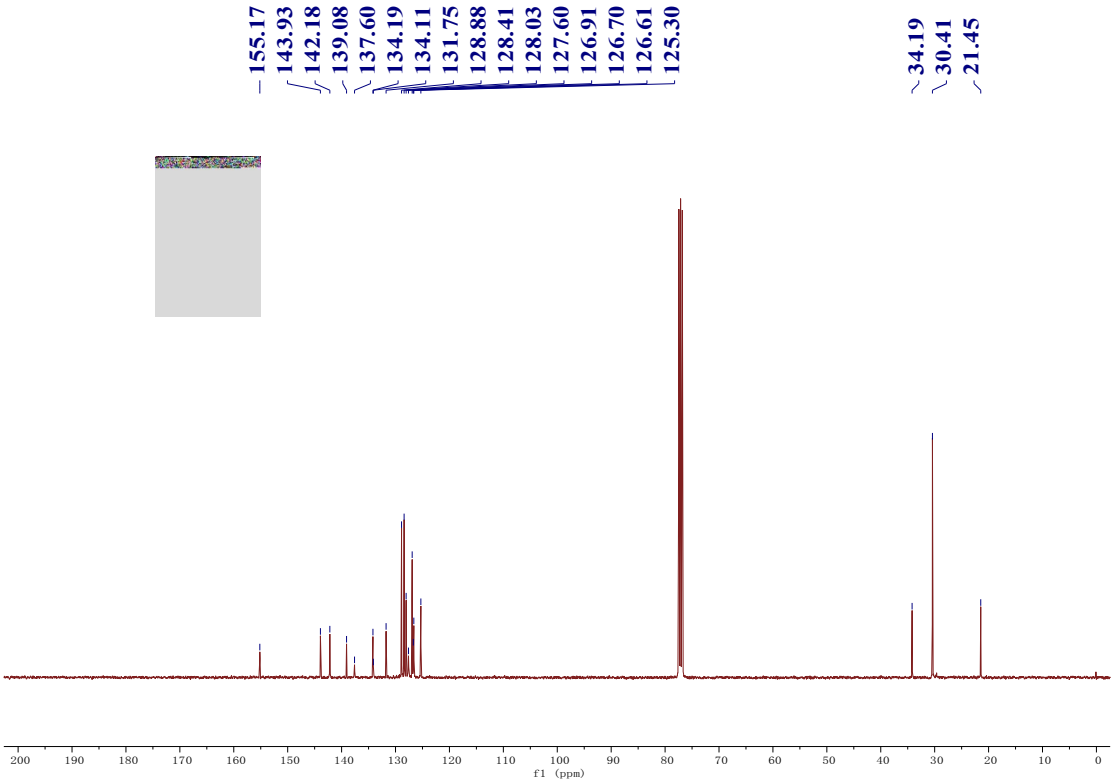
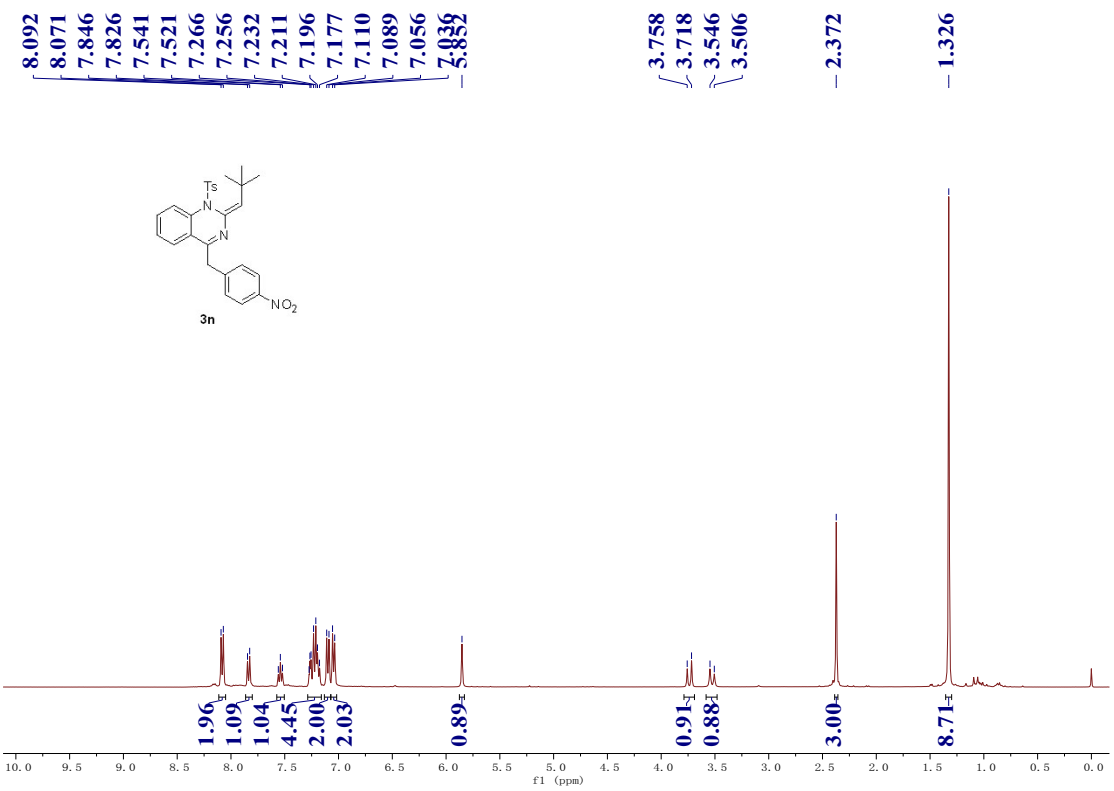
7.590
7.573
7.556
7.552
7.351
7.348
7.332
7.329
7.310
7.308
7.291
7.273
7.270
7.255
7.250
7.242
7.215
7.195
7.101
7.057
7.055
7.045
7.042
6.857
6.837
5.962
2.167
1.362
Ts
N
N
S
3m
0.99
0.99
1.90
1.63
2.02
0.93
1.03
2.02
0.95
3.00
9.16
f1 (ppm)


155.17
143.93
142.18
139.08
137.60
134.19
134.11
131.75
128.88
128.41
128.03
127.60
126.91
126.70
126.61
125.30
34.19
30.41
21.45
f1 (ppm)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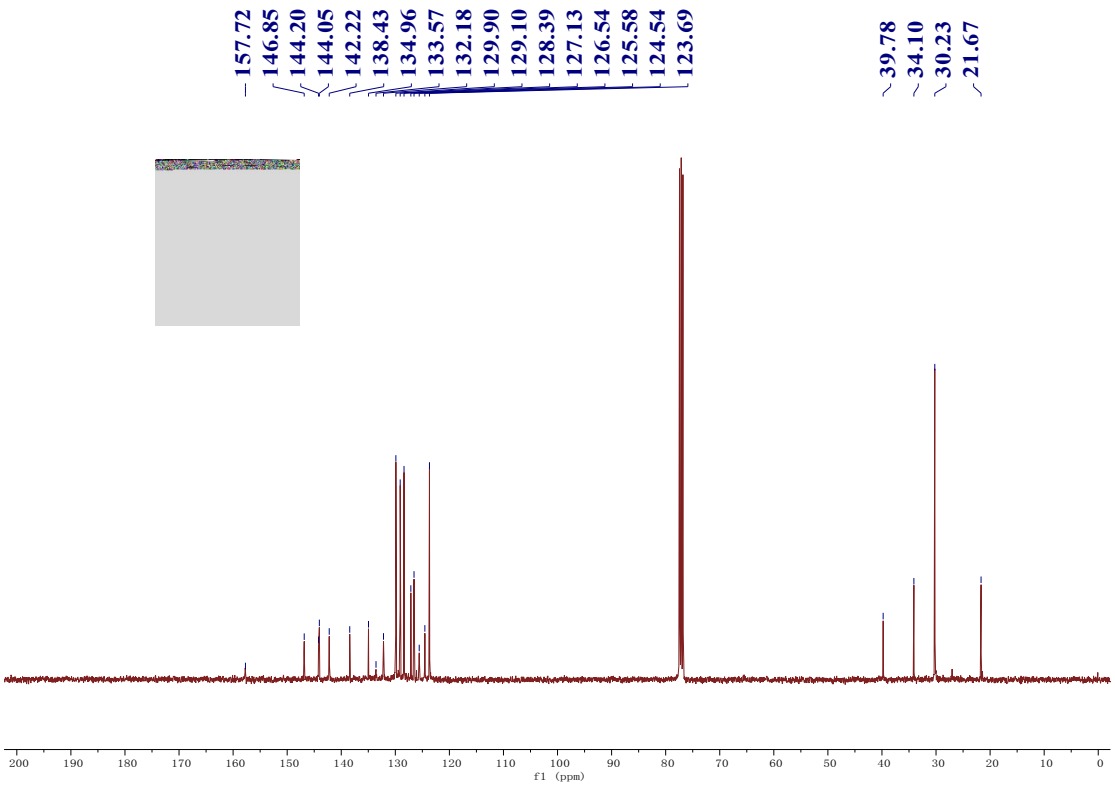
7.846
7.826
7.541
7.521
7.266
7.256
7.232
7.211
7.196
7.177
7.110
7.089
7.056
3.758
3.718
3.546
3.506
2.372
1.326
Ts
N
N
NO2
3n
1.96
1.09
1.04
4.45
2.00
2.03
0.89
0.91
0.88
3.00
8.71
f1 (ppm)


157.72
146.85
144.20
144.05
142.22
138.43
134.96
133.57
132.18
129.90
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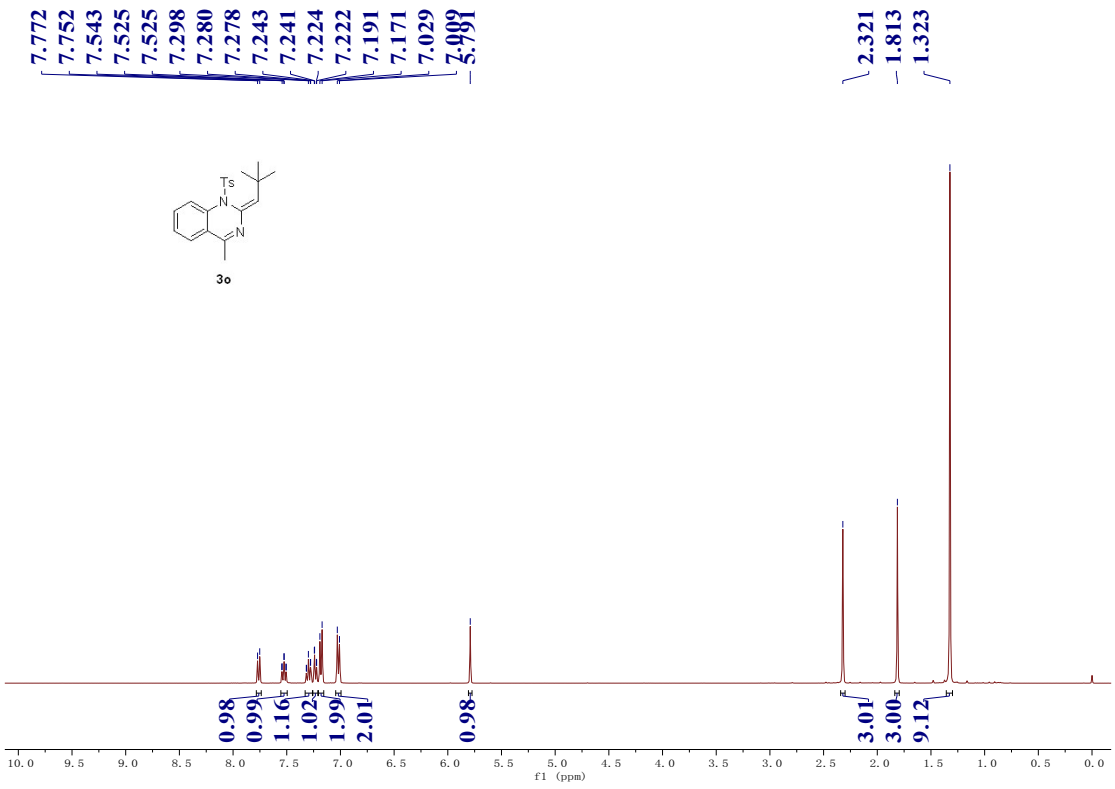
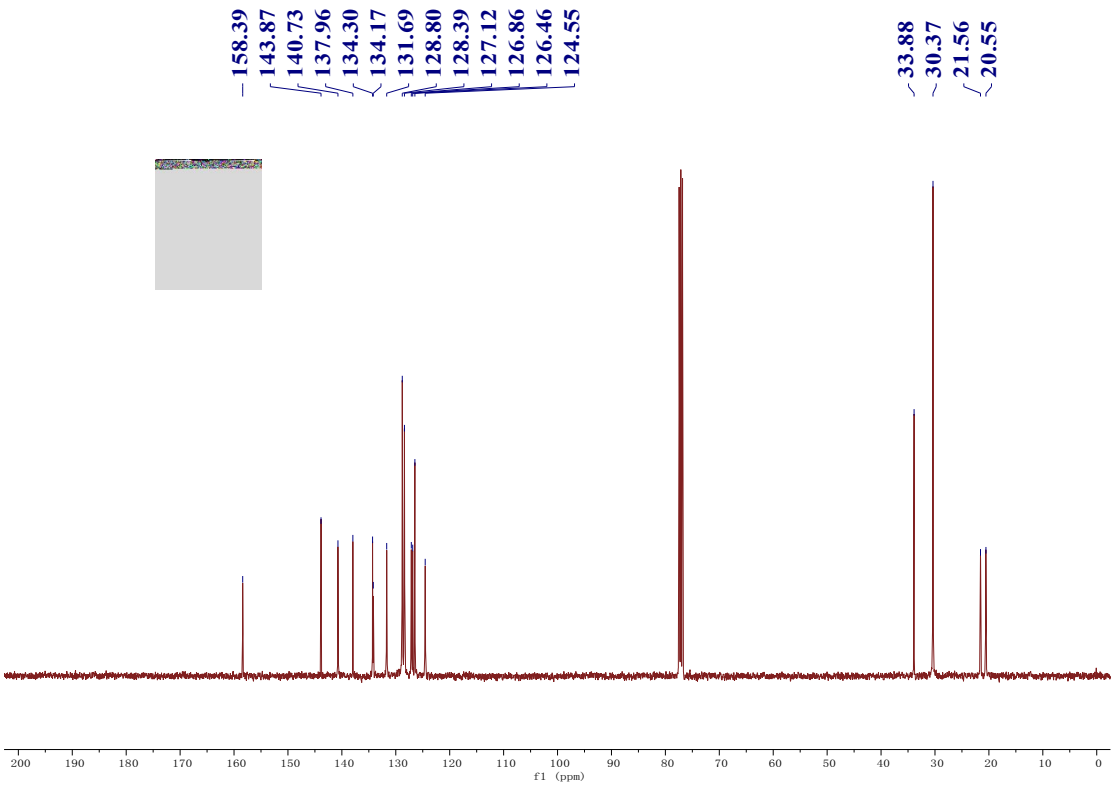
128.39
127.13
126.54
125.58
124.54
123.69
39.78
34.10
30.23
21.67
f1 (ppm)


7.772
7.752
7.543
7.525
7.525
7.298
7.280
7.278
7.243
7.241
7.224
7.222
7.191
7.171
7.029
2.321
1.813
1.323
Ts
N
N
3o
0.98
0.99
1.16
1.02
1.99
2.01
0.98
3.01
3.00
9.12
f1 (ppm)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140.73
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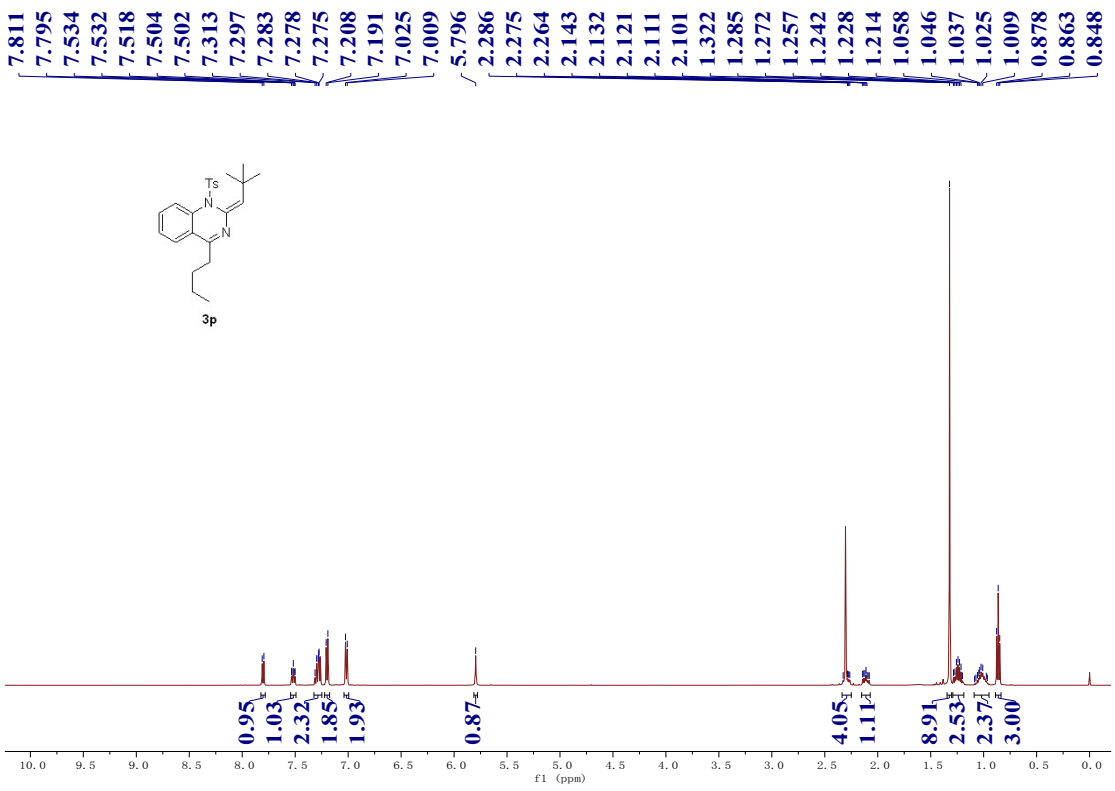
134.30
134.17
131.69
128.80
128.39
127.12
126.86
126.46
124.55
33.88
30.37
21.56
20.55
f1 (ppm)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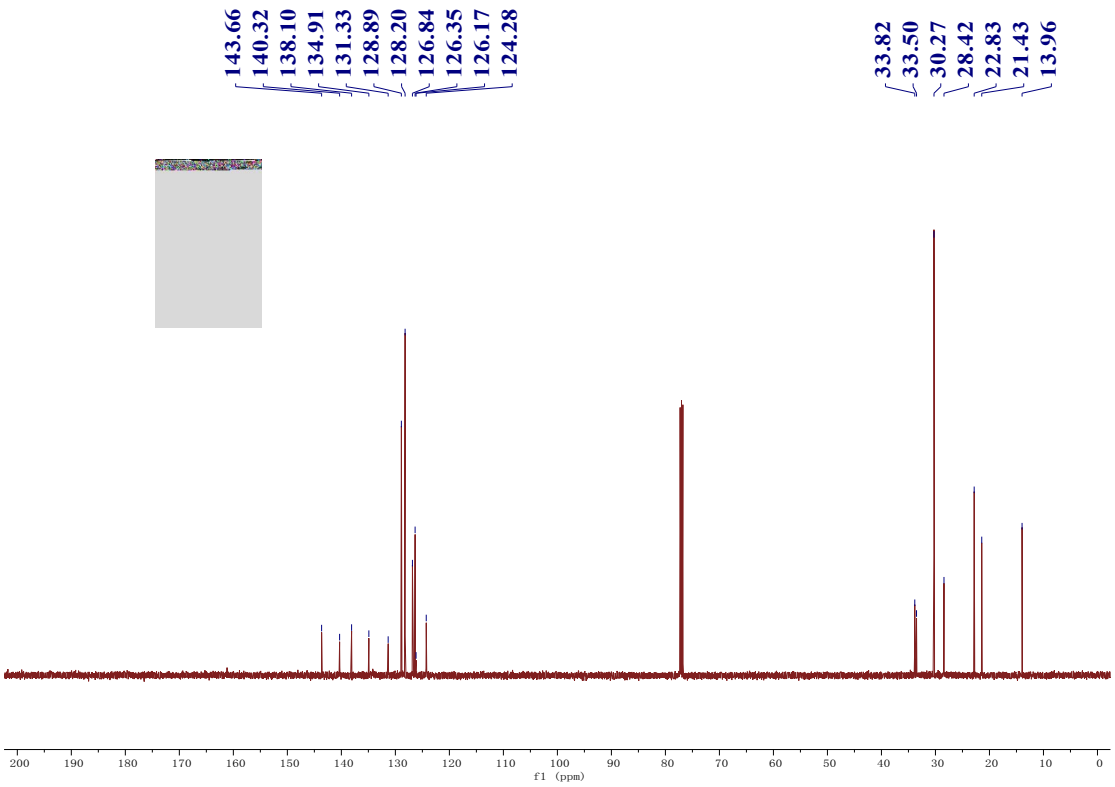
7.532
7.518
7.504
7.502
7.313
7.297
7.283
7.278
7.275
7.208
7.191
7.025
7.009
5.796
2.286
2.275
2.264
2.143
2.132
2.121
2.111
2.101
1.322
1.285
1.272
1.257
1.242
1.228
1.214
1.058
1.046
1.037
1.025
1.009
0.878
0.863
0.848
Ts
N
N
3p
0.95
1.03
2.32
1.85
1.93
0.87
4.05
1.11
8.91
2.53
2.37
3.00
f1 (ppm)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138.10
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128.89
128.20
126.84
126.35
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124.28
33.82
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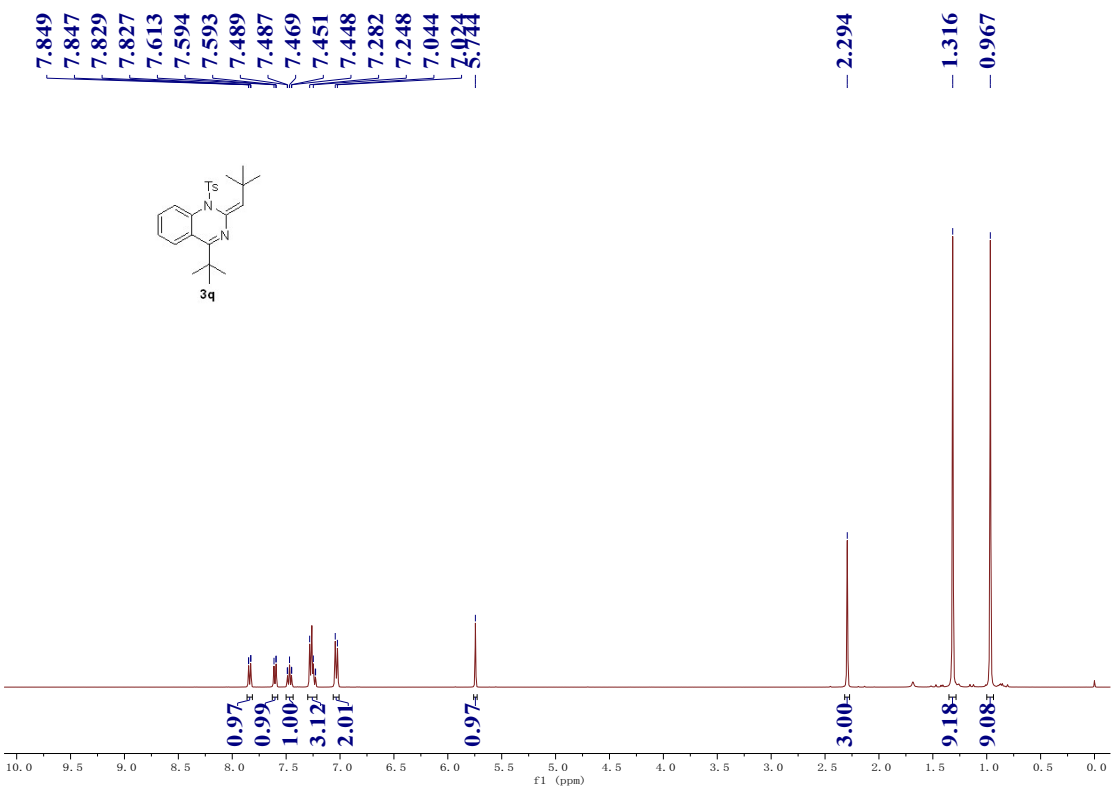
28.42
22.83
21.43
13.96
f1 (ppm)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7.594
7.593
7.489
7.487
7.469
7.451
7.448
7.282
7.248
7.044
2.294
1.316
0.967
Ts
N
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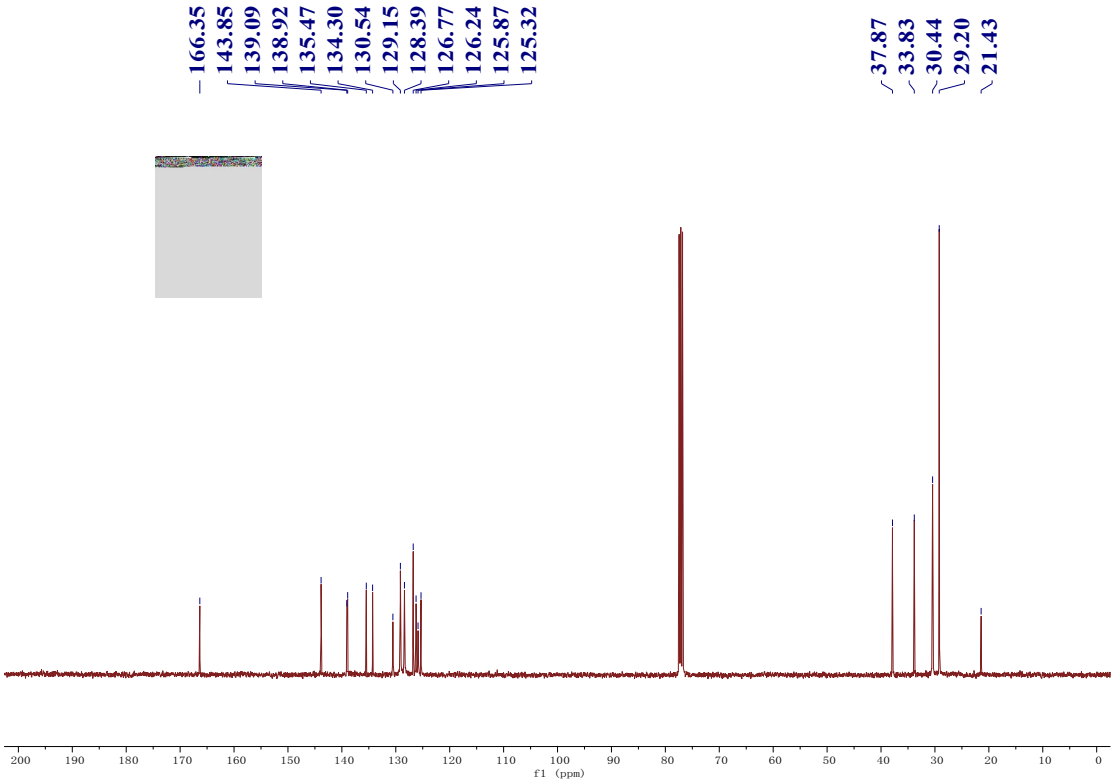
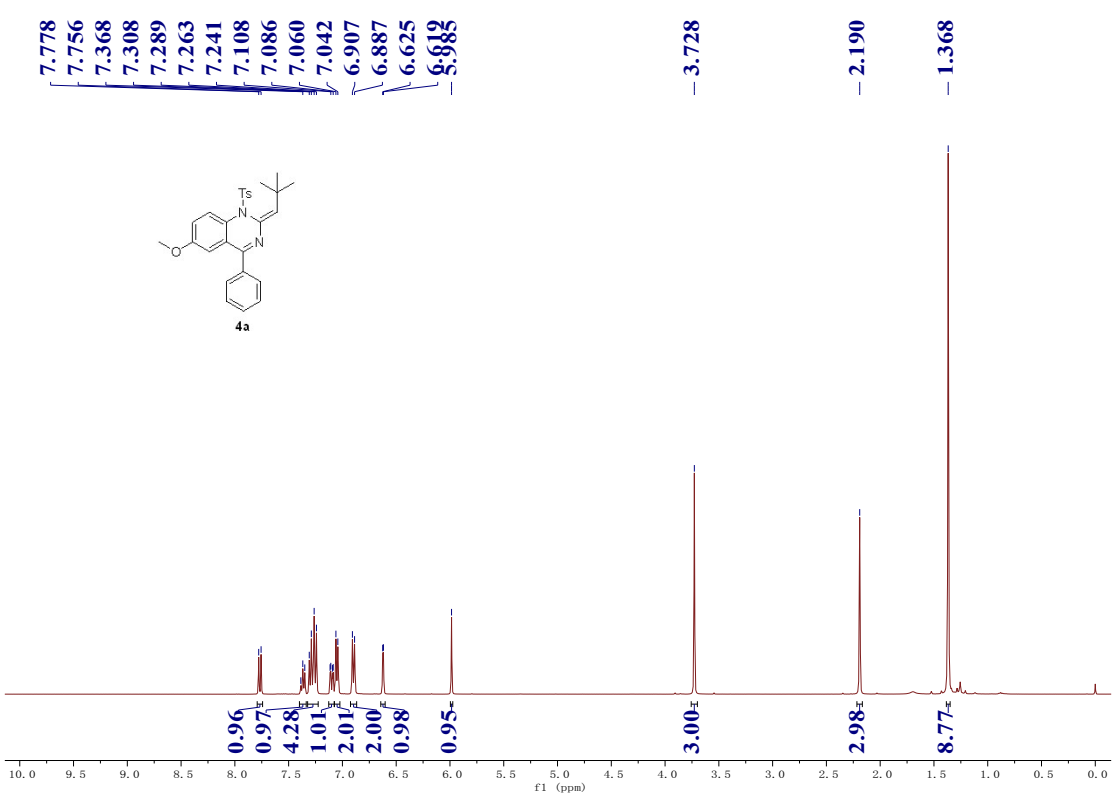
0.99
1.00
3.12
2.01
0.97
3.00
9.18
9.08
f1 (ppm)


166.35
143.85
139.09
138.92
135.47
134.30
130.54
129.15
128.39
126.77
126.24
125.87
125.32
37.87
33.83
30.44
29.20
21.43
f1 (ppm)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7.289
7.263
7.241
7.108
7.086
7.060
7.042
6.907
6.887
6.625
6.619
3.885
3.728
2.190
1.368
Ts
N
N
O
4a
0.96
0.97
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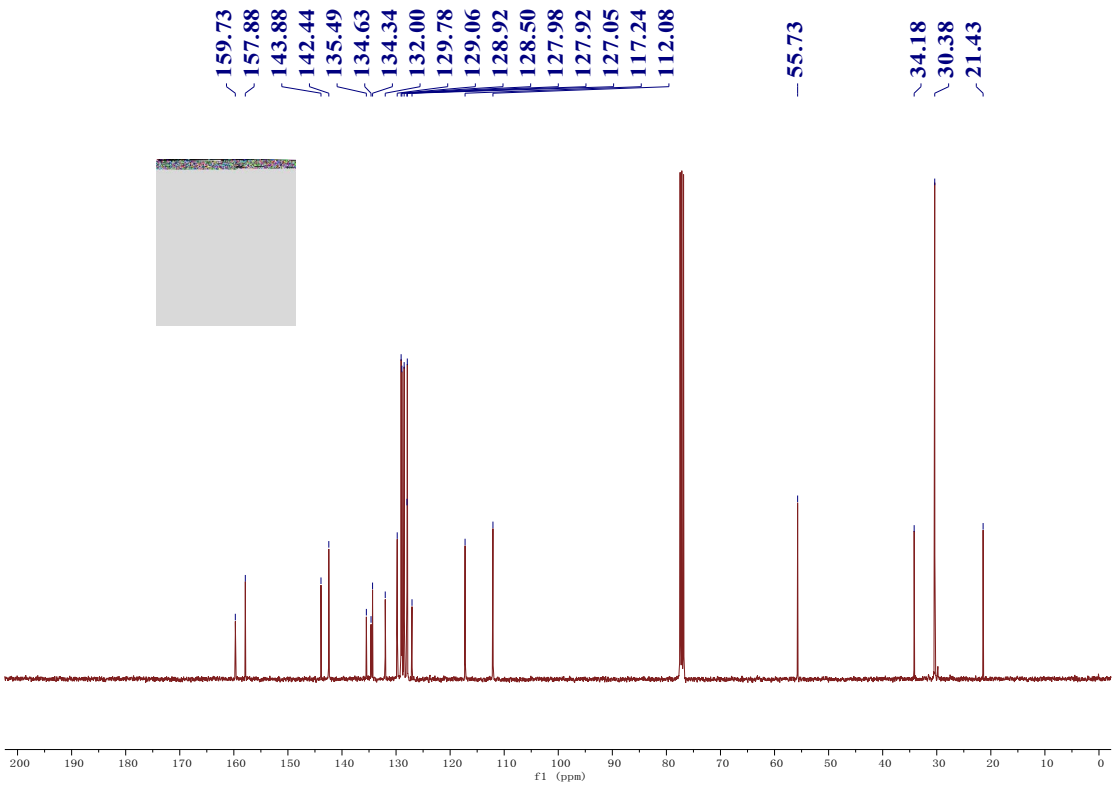
2.01
2.00
0.98
0.95
3.00
2.98
8.77
f1 (ppm)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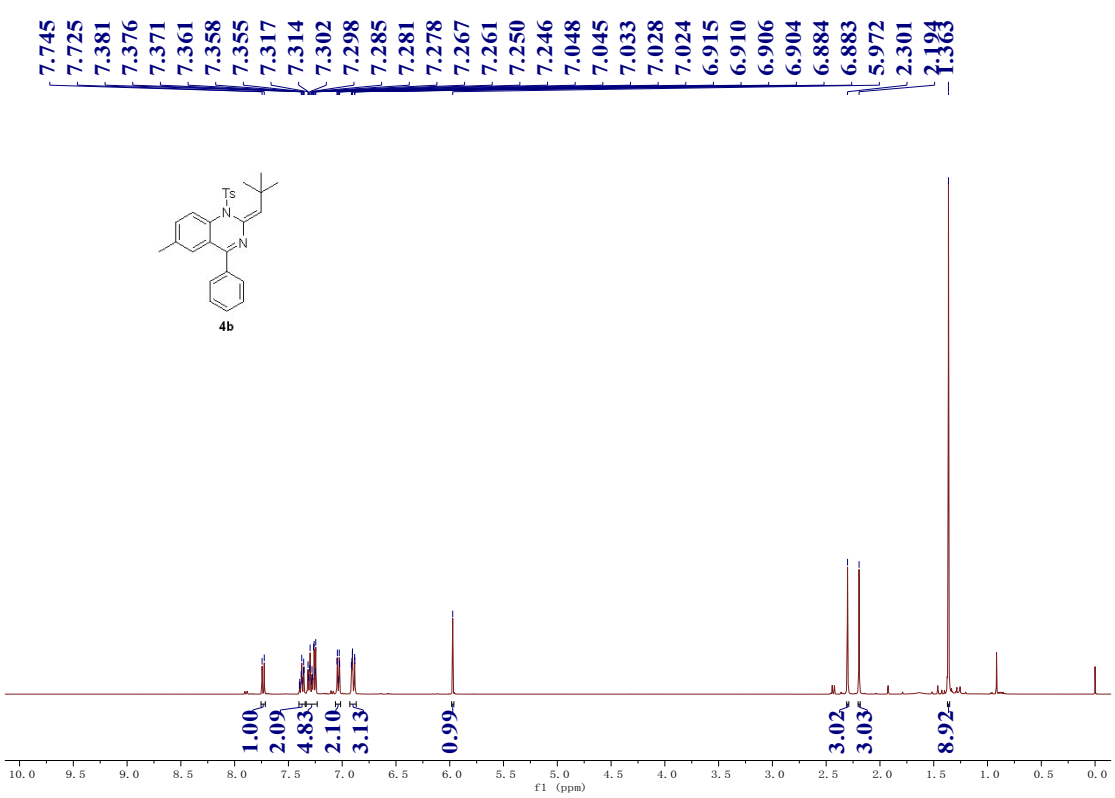
134.63
134.34
132.00
129.78
129.06
128.92
128.50
127.98
127.92
127.05
117.24
112.08
55.73
34.18
30.38
21.43
200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)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7.355
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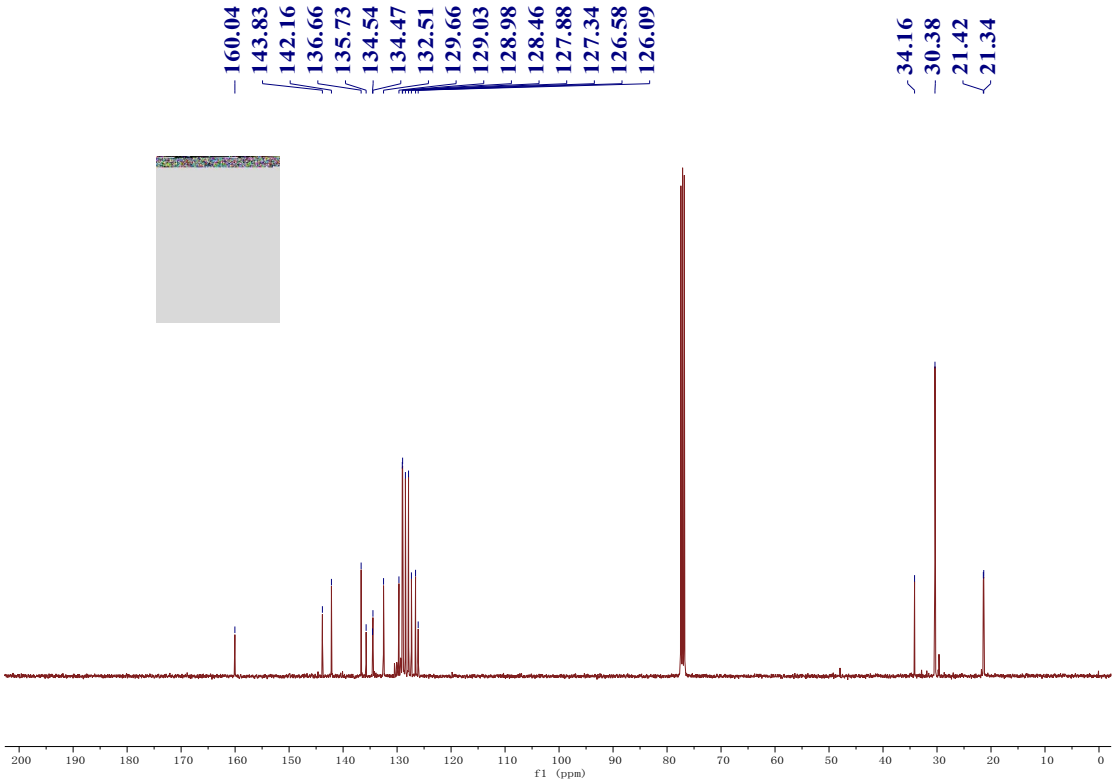
7.314
7.302
7.298
7.285
7.281
7.278
7.267
7.261
7.250
7.246
7.048
7.045
7.033
7.028
7.024
6.915
6.910
6.906
6.904
6.884
6.883
5.972
2.301
2.194
1.363
Ts
N
N
4b
1.00
2.09
4.83
2.10
3.13
0.99
3.02
3.03
8.92
10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)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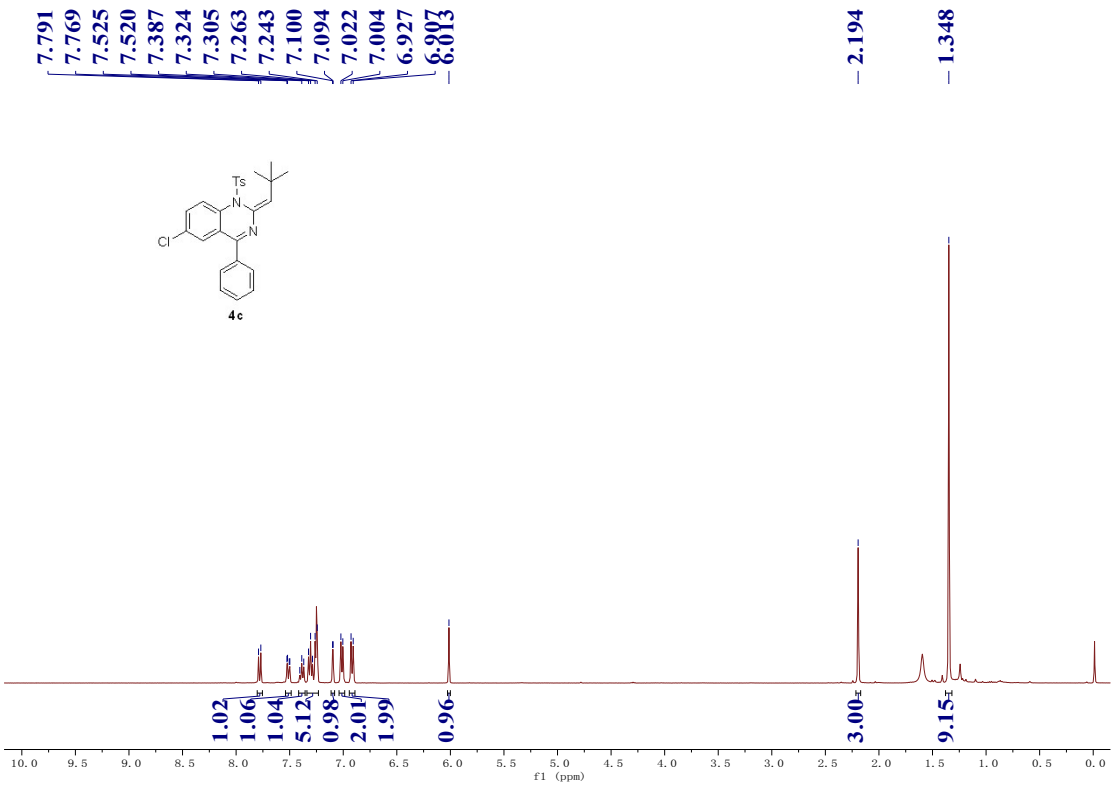
136.66
135.73
134.54
134.47
132.51
129.66
129.03
128.98
128.46
127.88
127.34
126.58
126.09
34.16
30.38
21.42
21.34
f1 (ppm)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7.305
7.263
7.243
7.100
7.094
7.022
7.004
6.927
6.907
6.013
2.194
1.348
Ts
N
N
Cl
4c
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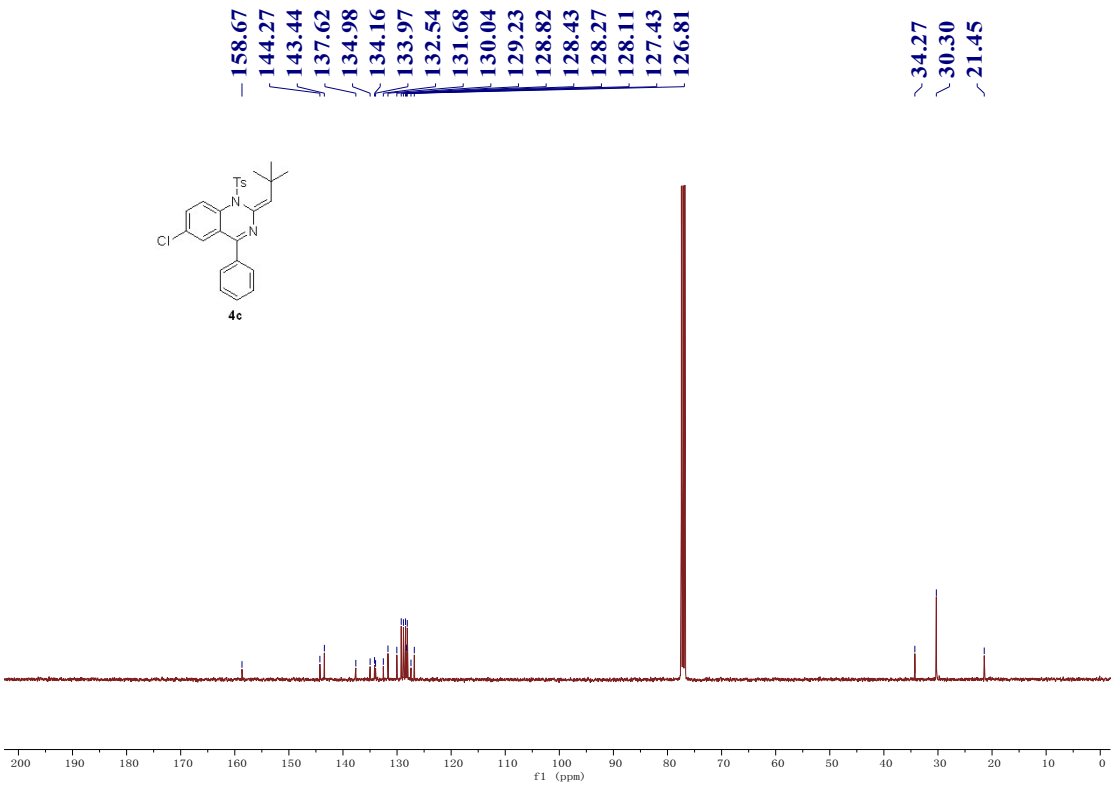
1.06
1.04
5.12
0.98
2.01
1.99
0.96
3.00
9.15
f1 (ppm)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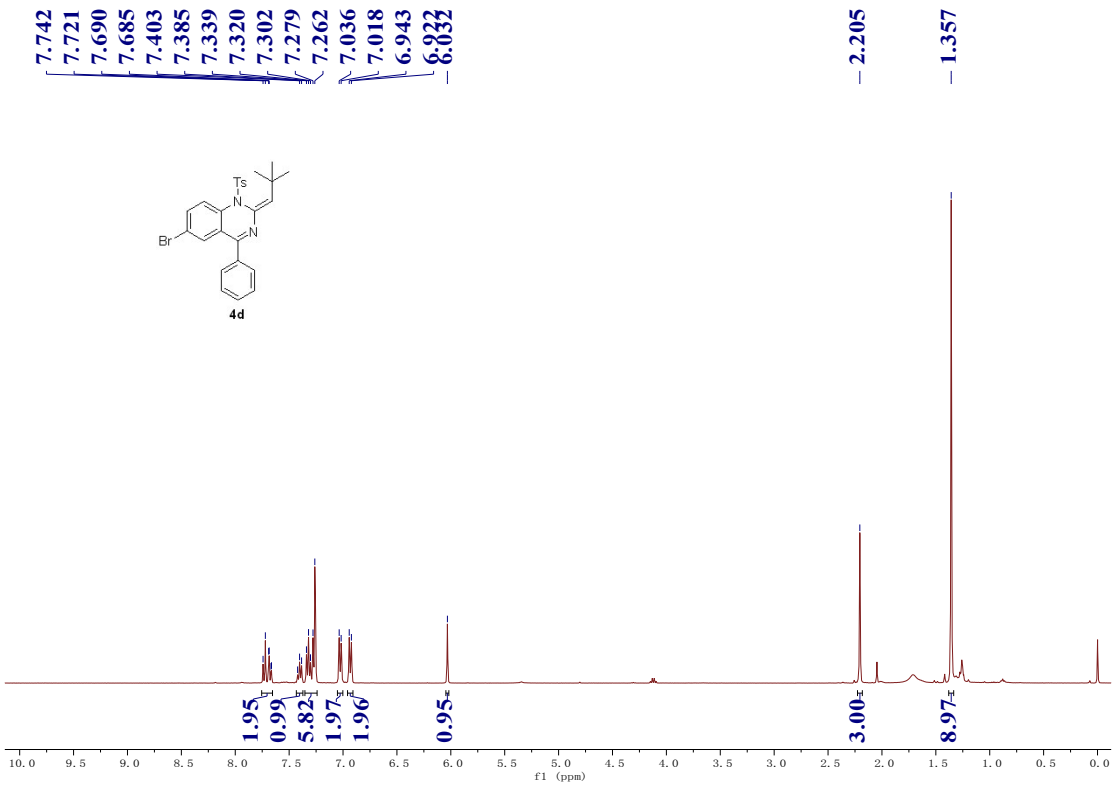
134.98
134.16
133.97
132.54
131.68
130.04
129.23
128.82
128.43
128.27
128.11
127.43
126.81
34.27
30.30
21.45
Ts
N
N
Cl
4c
200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)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7.403
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7.320
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7.279
7.262
7.036
7.018
6.943
6.932
6.032
2.205
1.357
Ts
N
N
Br
4d
1.95
0.99
5.82
1.97
1.96
0.95
3.00
8.97
10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
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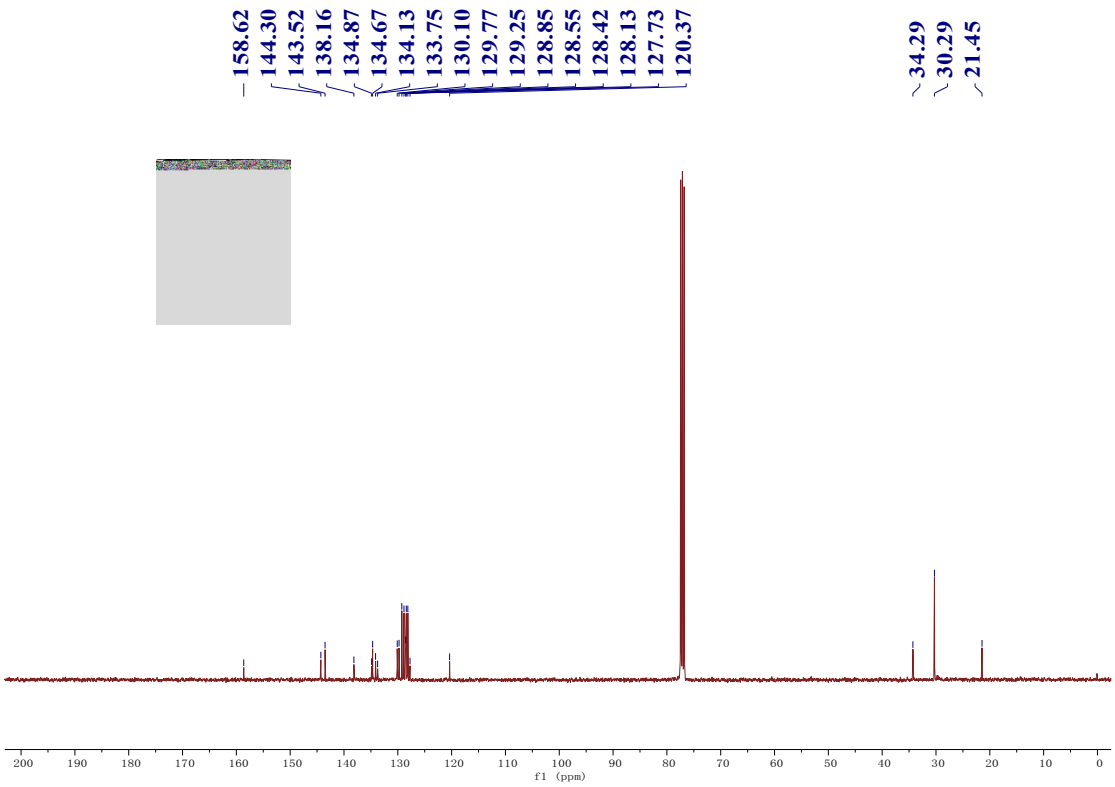
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134.67
134.13
133.75
130.10
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129.25
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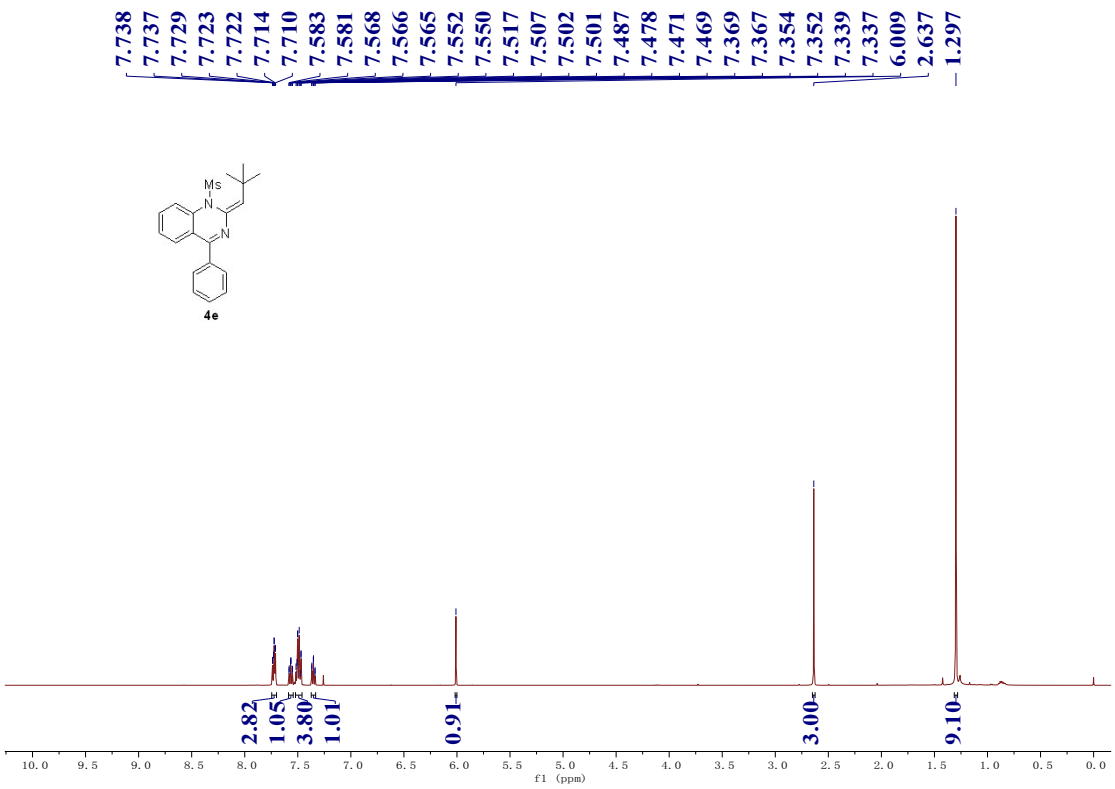
120.37
34.29
30.29
21.45
f1 (ppm)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7.729
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7.583
7.581
7.568
7.566
7.565
7.552
7.550
7.517
7.507
7.502
7.501
7.487
7.478
7.471
7.469
7.369
7.367
7.354
7.352
7.339
7.337
6.009
2.637
1.297
Ms
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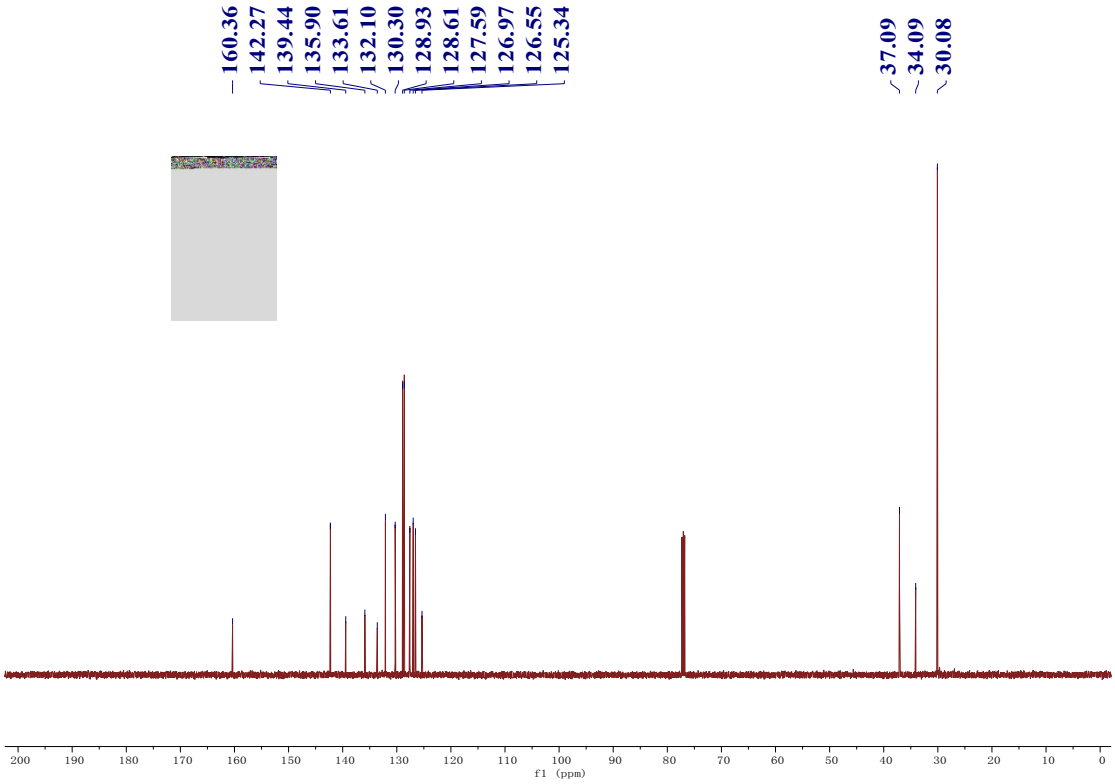
N
4e
2.82
1.05
3.80
1.01
0.91
3.00
9.10
f1 (ppm)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133.61
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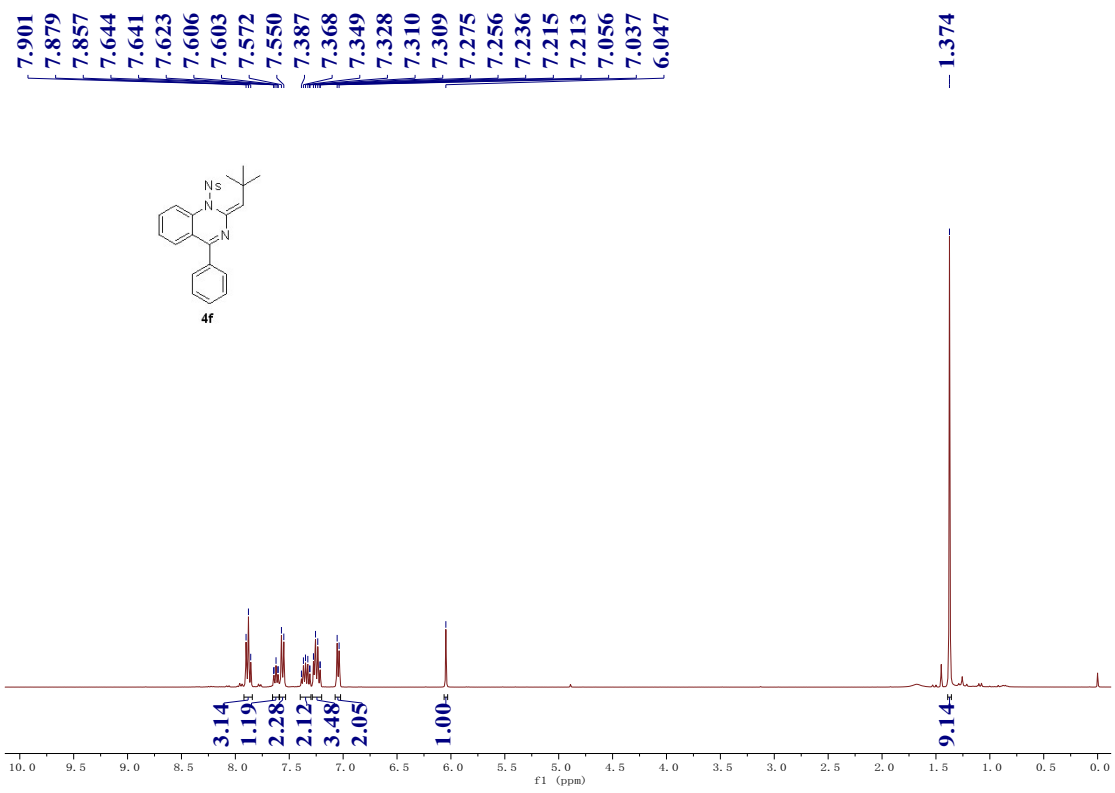
127.59
126.97
126.55
125.34
37.09
34.09
30.08
f1 (ppm)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7.349
7.328
7.310
7.309
7.275
7.256
7.236
7.215
7.213
7.056
7.037
6.047
1.374
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4f
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2.28
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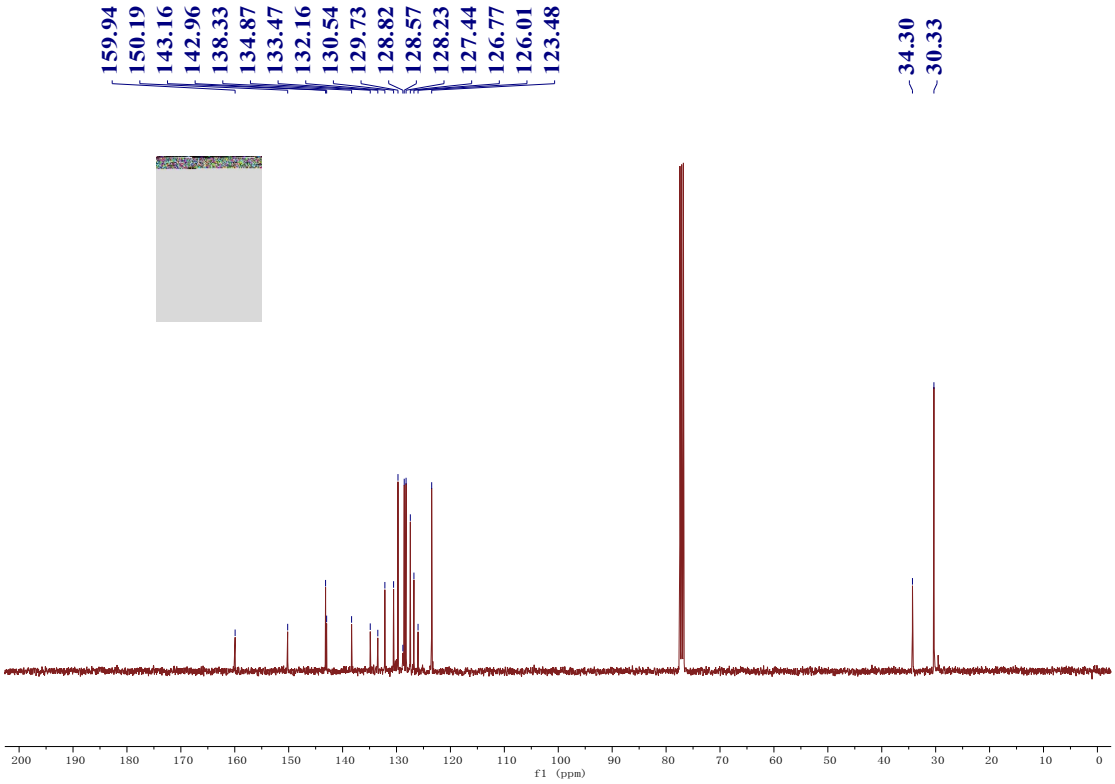
2.05
1.00
9.14
f1 (ppm)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142.96
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132.16
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129.73
128.82
128.57
128.23
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126.01
123.48
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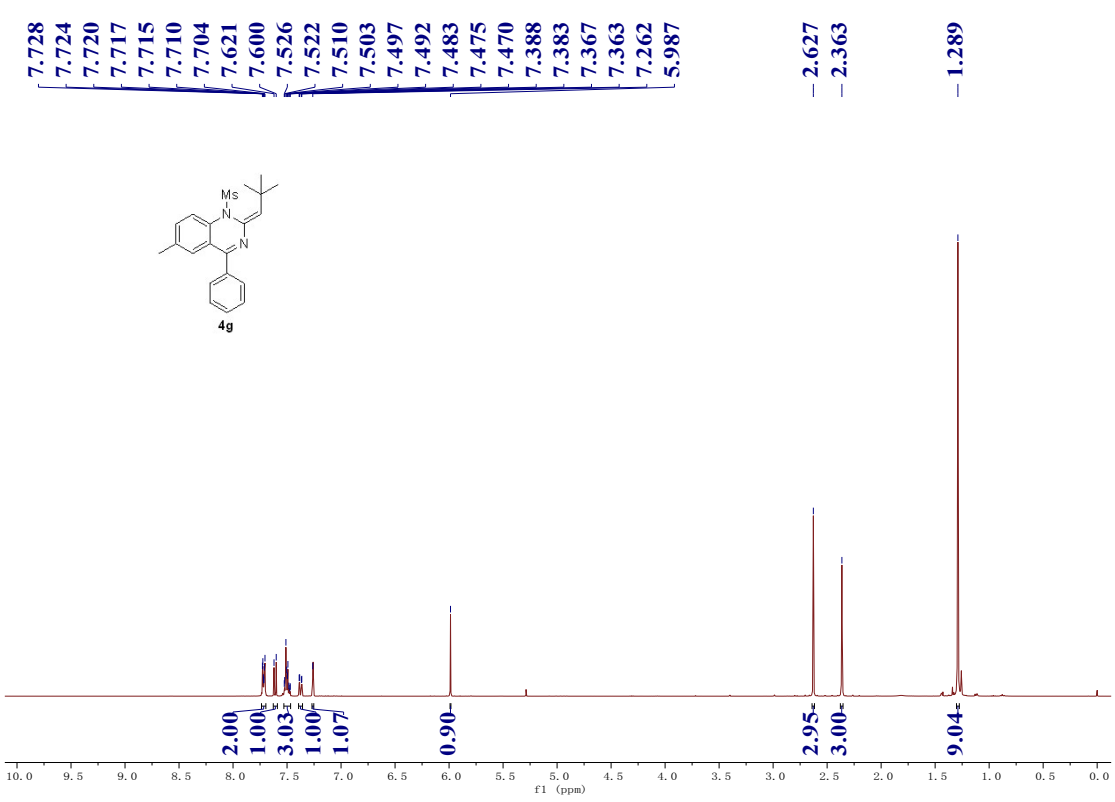
30.33
200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)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7.510
7.503
7.497
7.492
7.483
7.475
7.470
7.388
7.383
7.367
7.363
7.262
5.987
2.627
2.363
1.289
Ms
N
N
4g
2.00
1.00
3.03
1.00
1.07
0.90
2.95
3.00
9.04
10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
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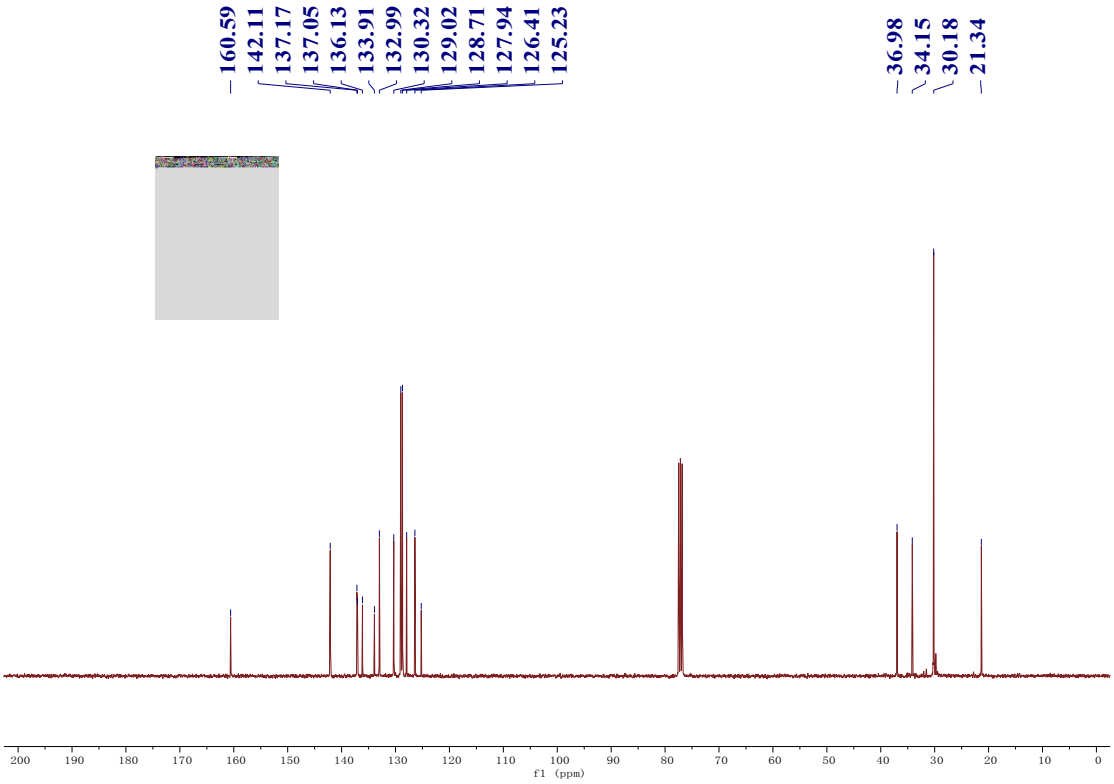
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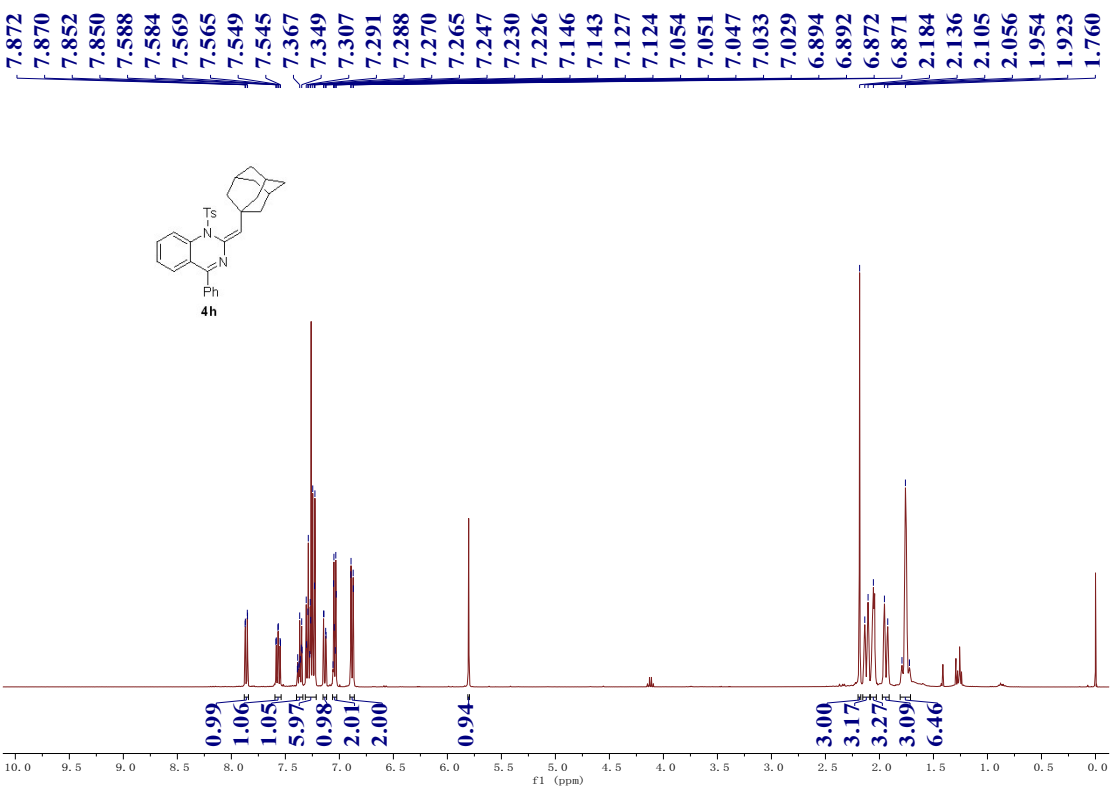
21.34
f1 (ppm)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7.247
7.230
7.226
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7.143
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7.029
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6.892
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6.871
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2.136
2.105
2.056
1.954
1.923
1.760
Ts
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N
Ph
4h
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1.06
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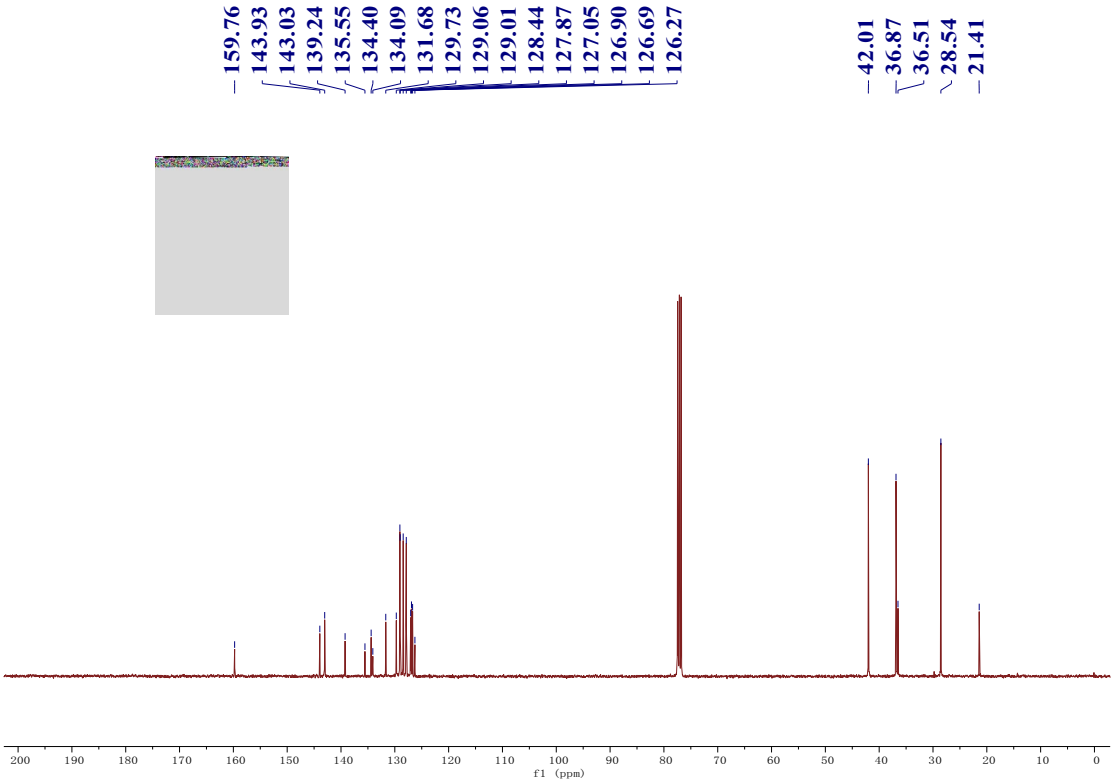
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126.27
42.01
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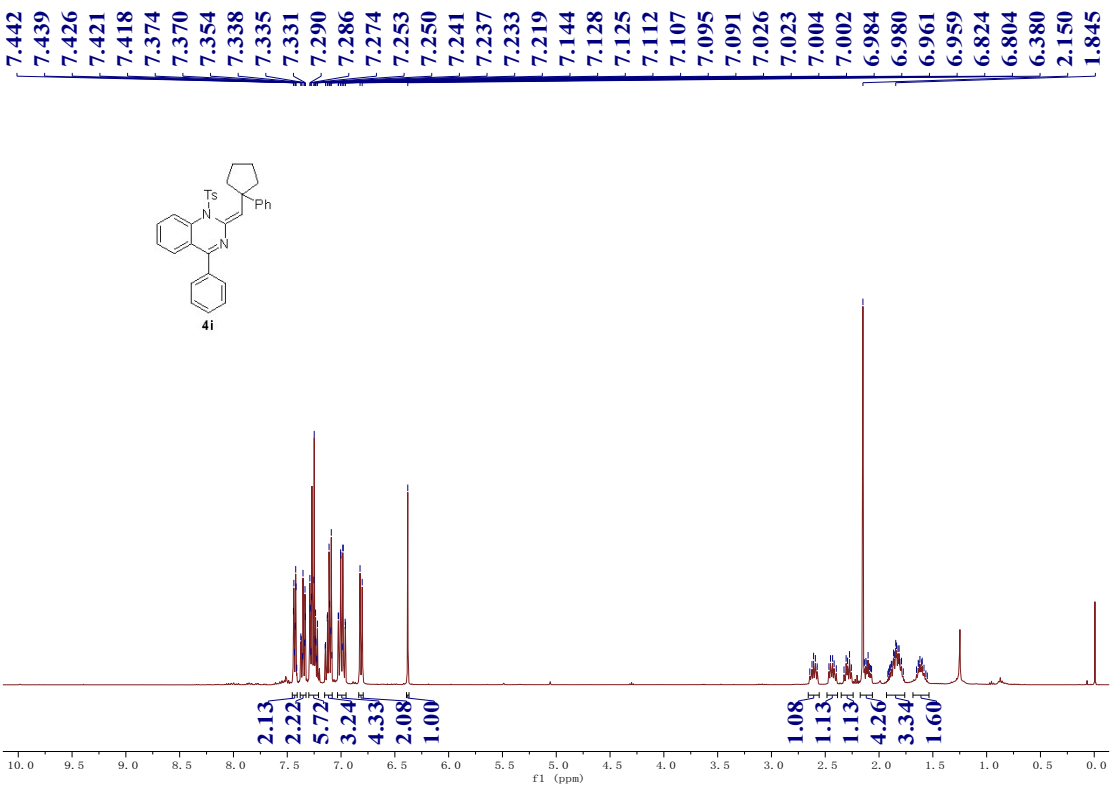
21.41
f1 (ppm)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7.125
7.112
7.107
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2.150
1.845
Ts
N
Ph
N
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2.13
2.22
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2.08
1.00
1.08
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1.13
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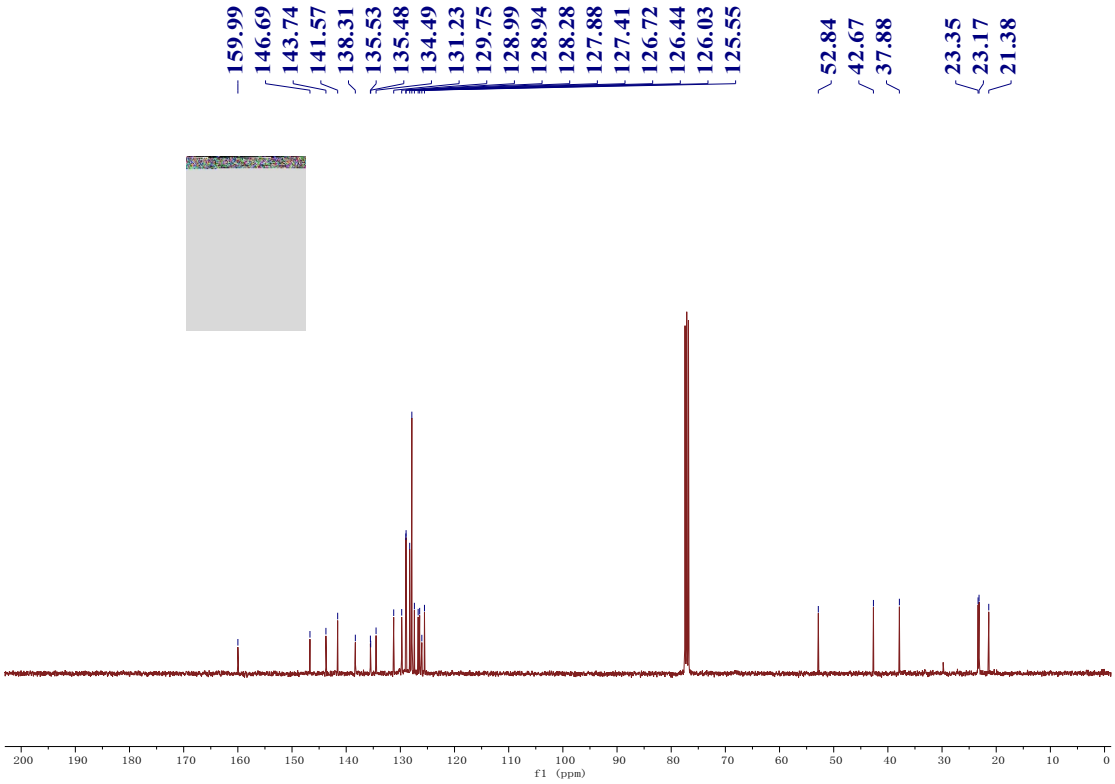
f1 (ppm)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128.28
127.88
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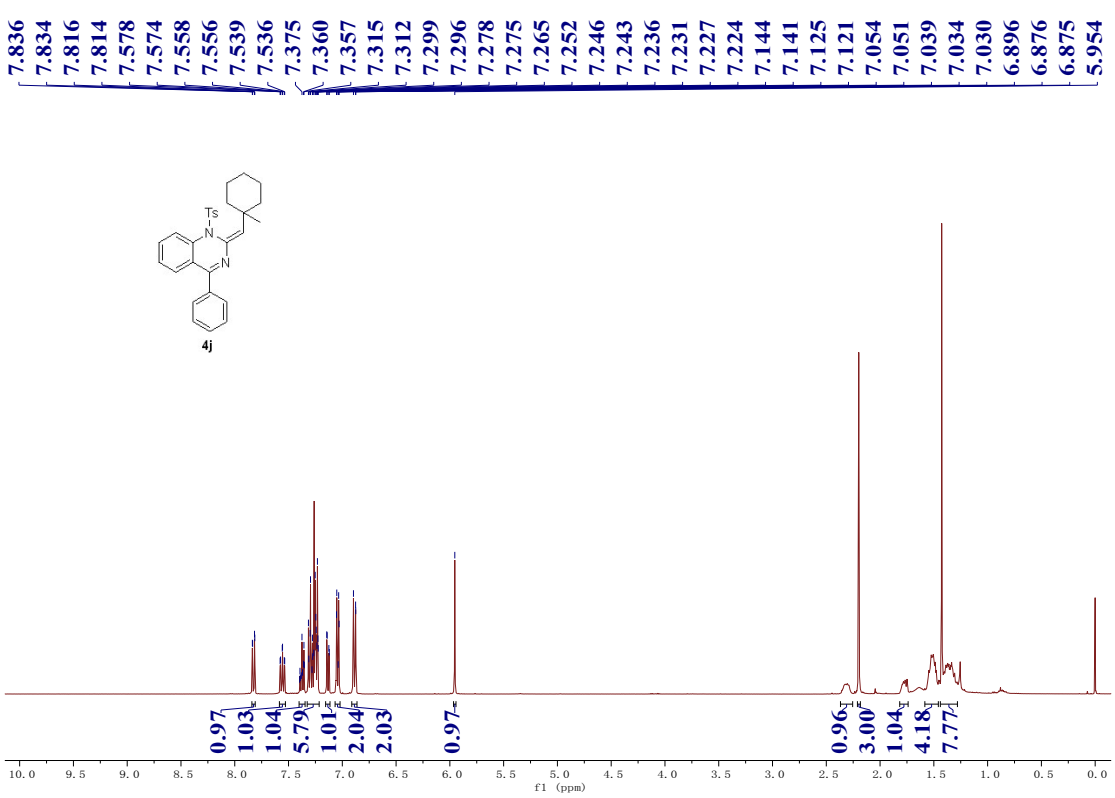
126.03
125.55
52.84
42.67
37.88
23.35
23.17
21.38
f1 (ppm)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7.296
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7.275
7.265
7.252
7.246
7.243
7.236
7.231
7.227
7.224
7.144
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7.125
7.121
7.054
7.051
7.039
7.034
7.030
6.896
6.876
6.875
5.954
Ts
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N
4j
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1.04
4.18
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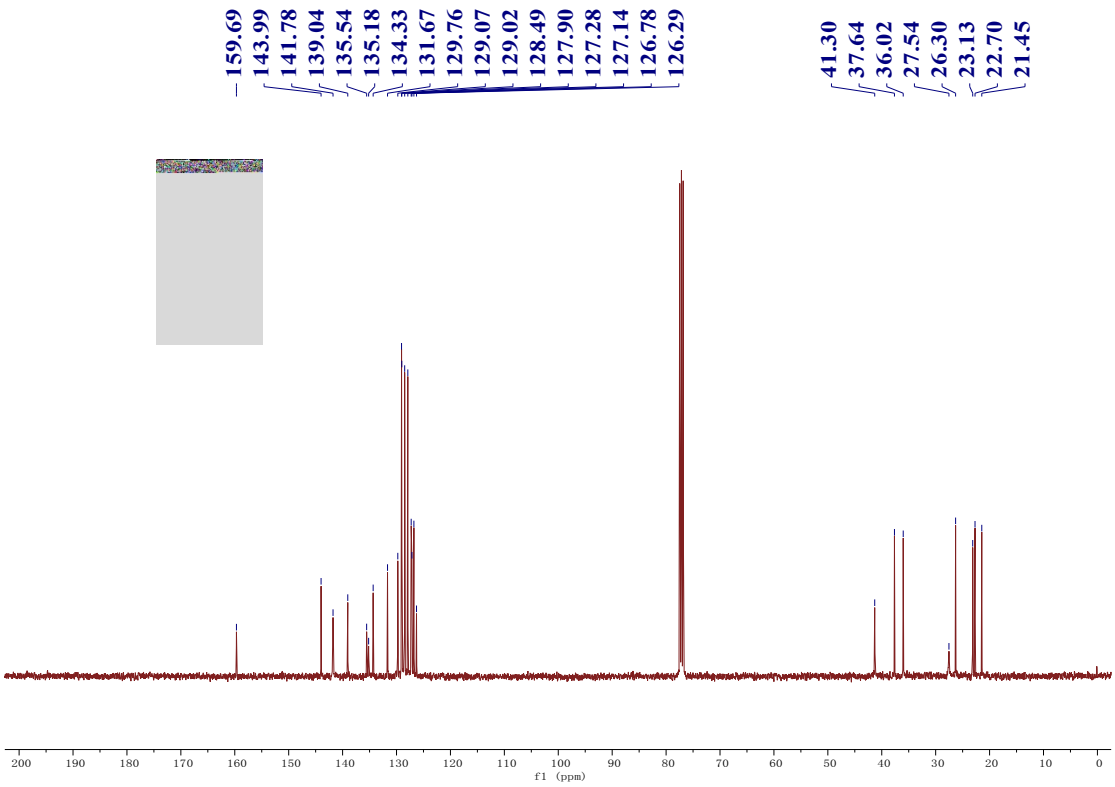
f1 (ppm)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127.90
127.28
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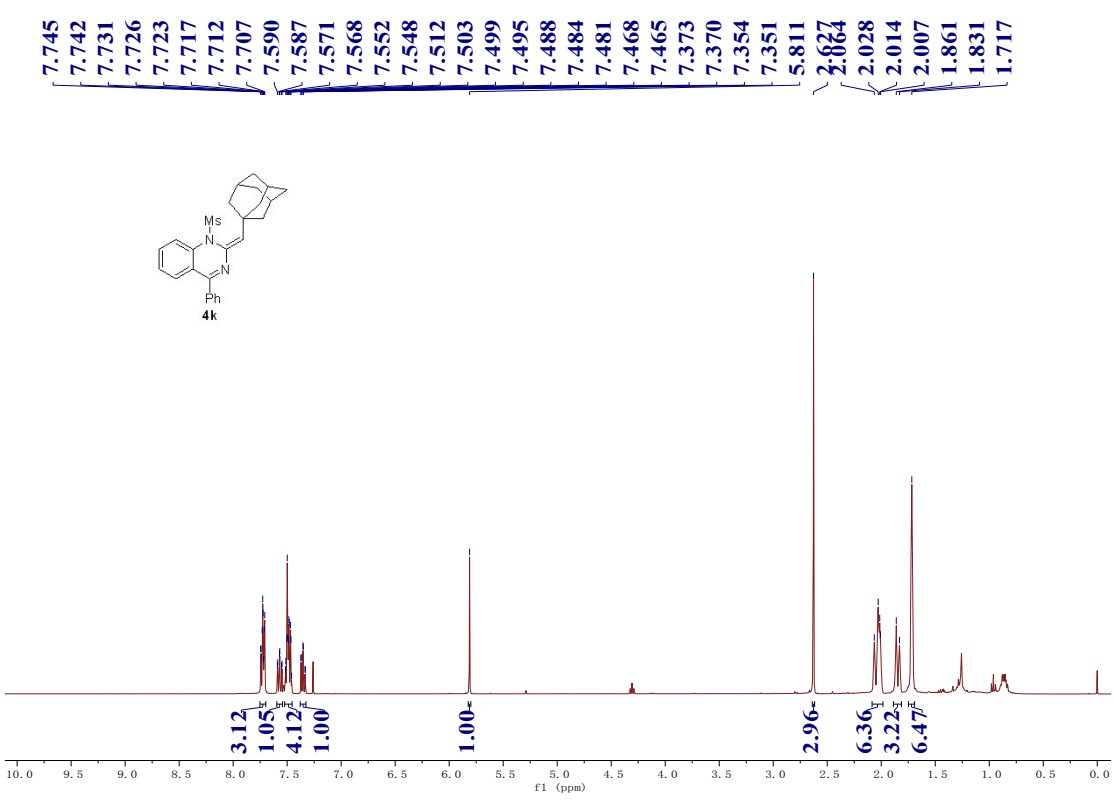
26.30
23.13
22.70
21.45
f1 (ppm)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7.552
7.548
7.512
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7.488
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7.468
7.465
7.373
7.370
7.354
7.351
5.811
2.627
2.064
2.028
2.014
2.007
1.861
1.831
1.717
Ms
N
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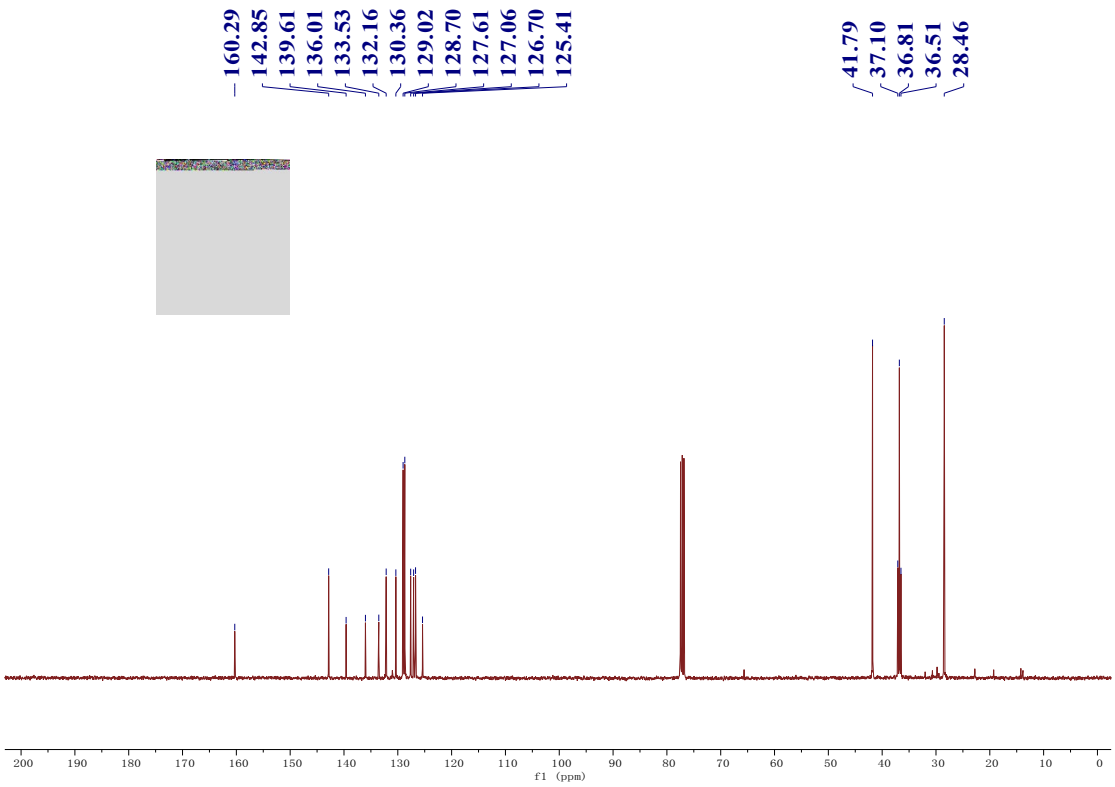
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127.06
126.70
125.41
41.79
37.10
36.81
36.51
28.46
200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)