

Supporting Information

Transition Metal-Free Directly Regioselective Acylation of Quinazolines for the Synthesis of Acylquinazoline Derivatives

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,YiyuanPeng*

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Avenue, Nanchang 330022, China.*

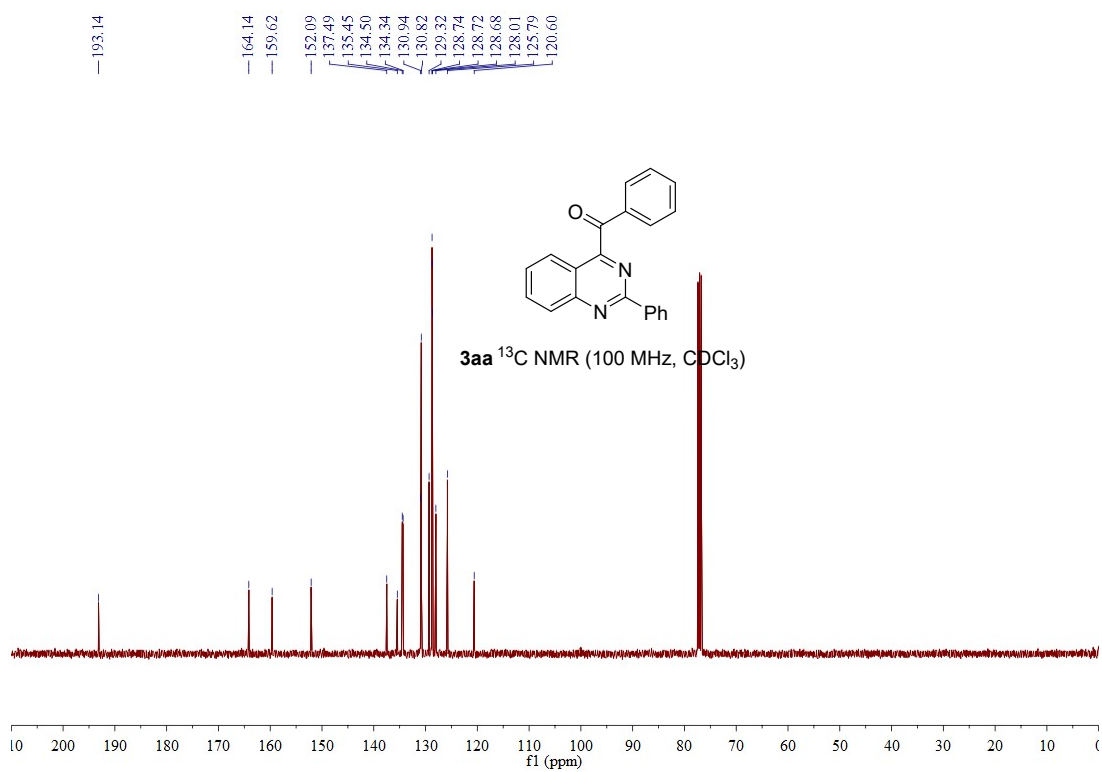
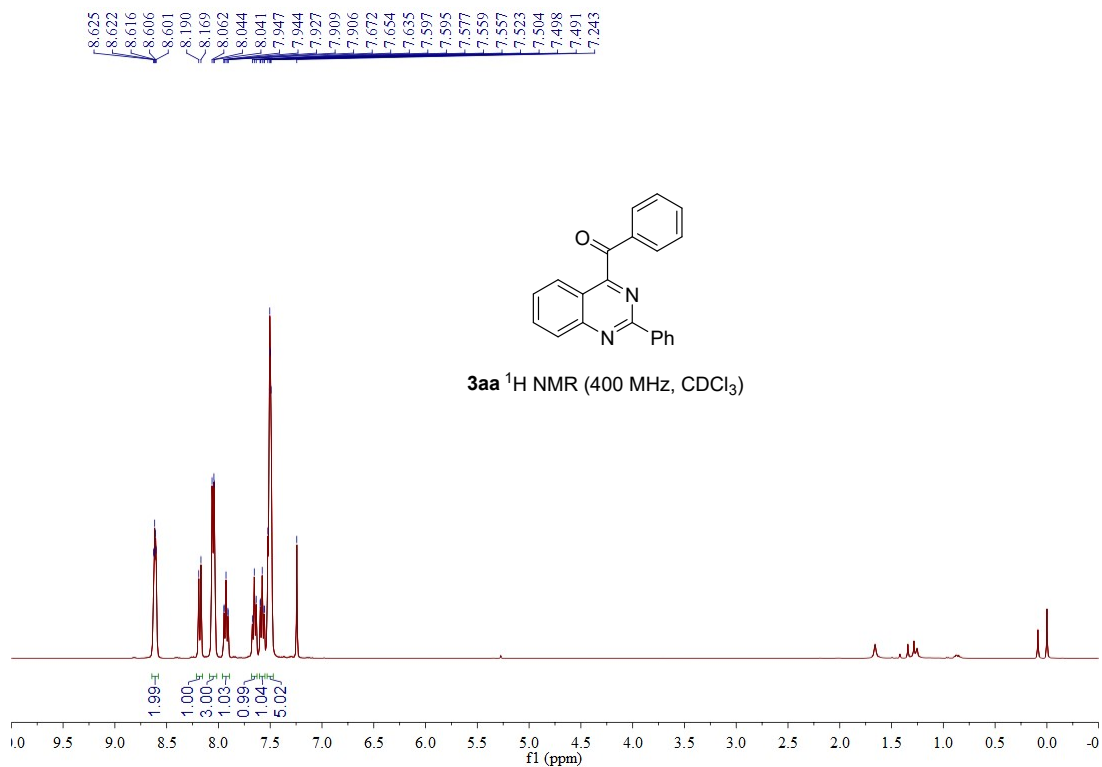
yypeng@jxnu.edu.cn

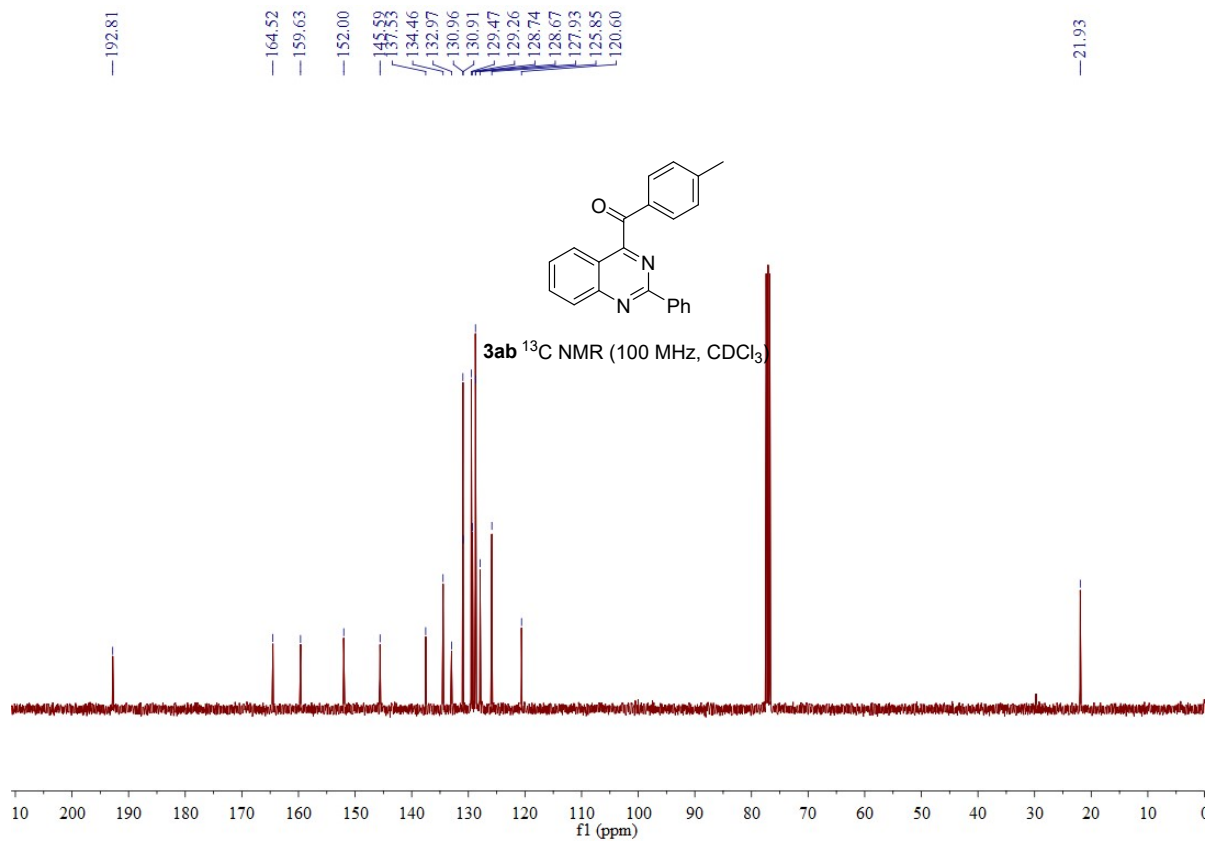
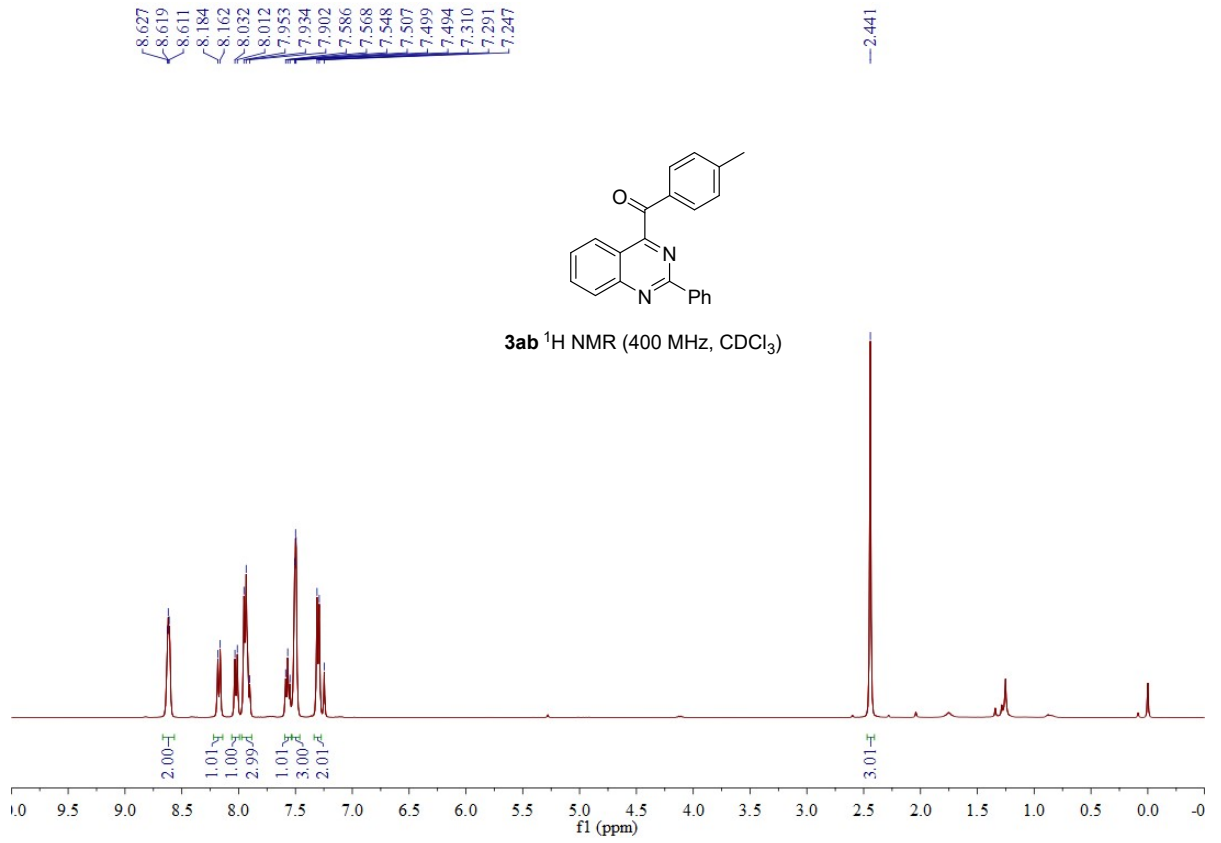
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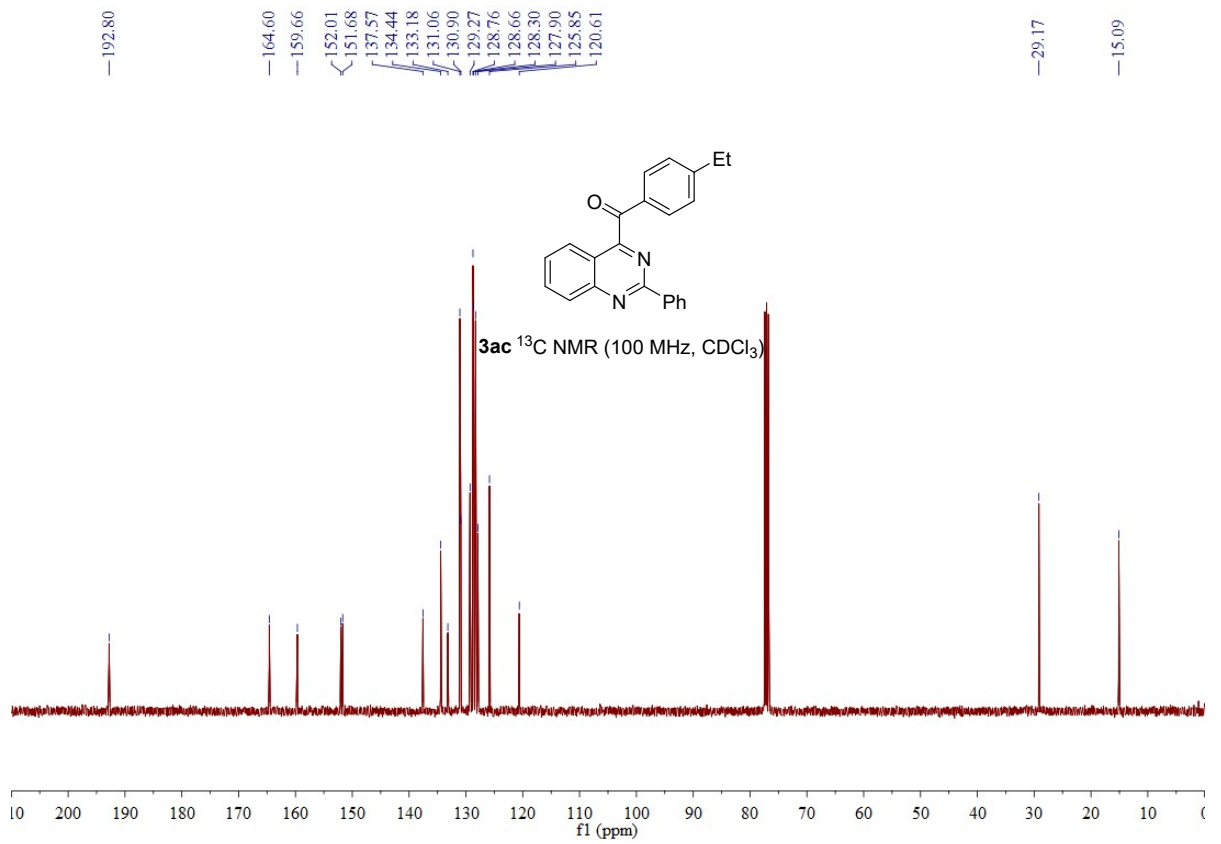
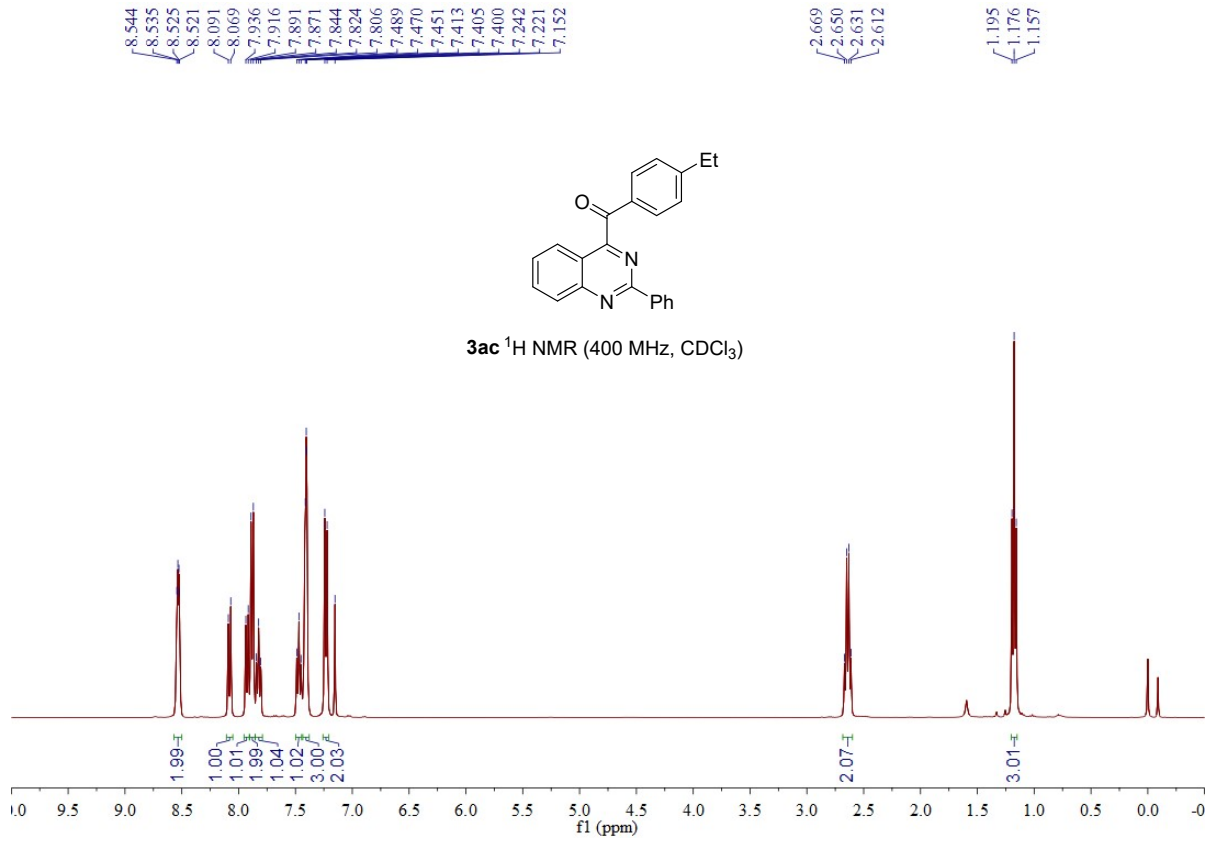
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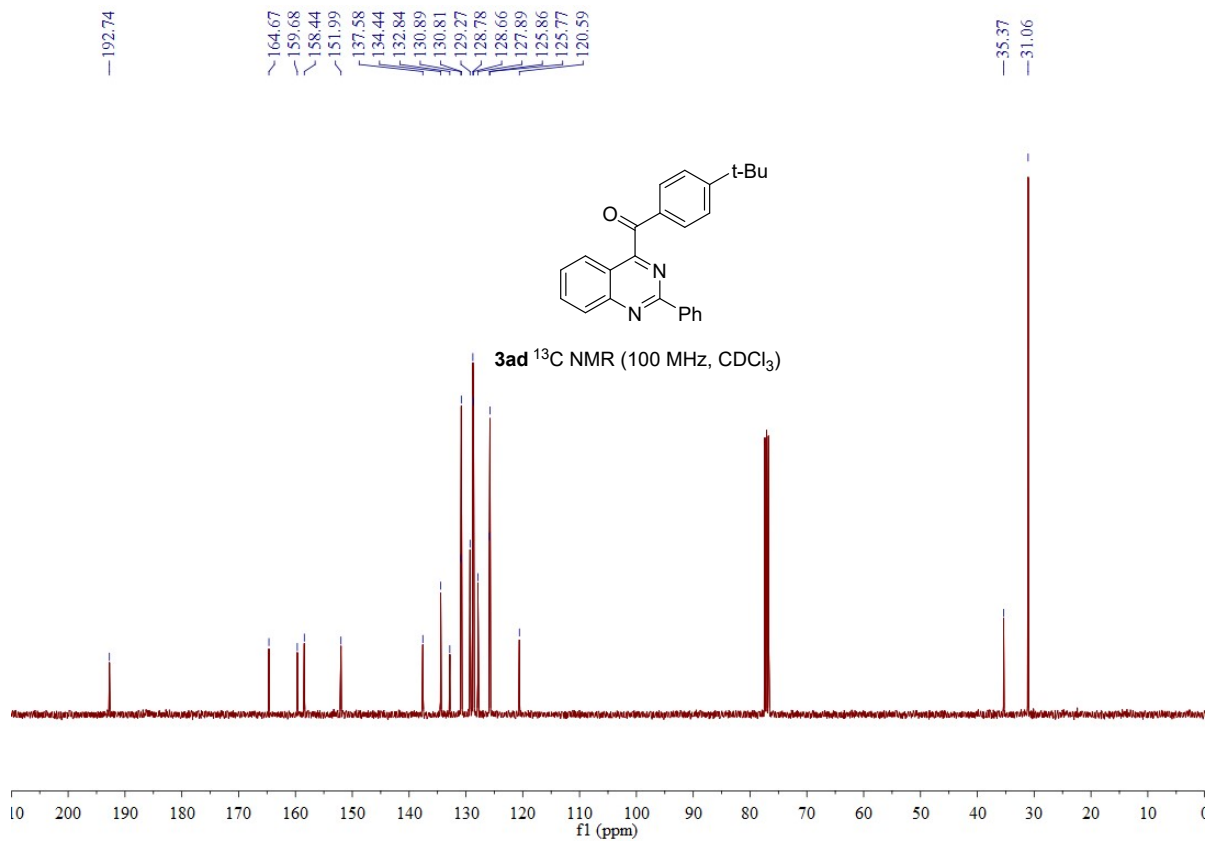
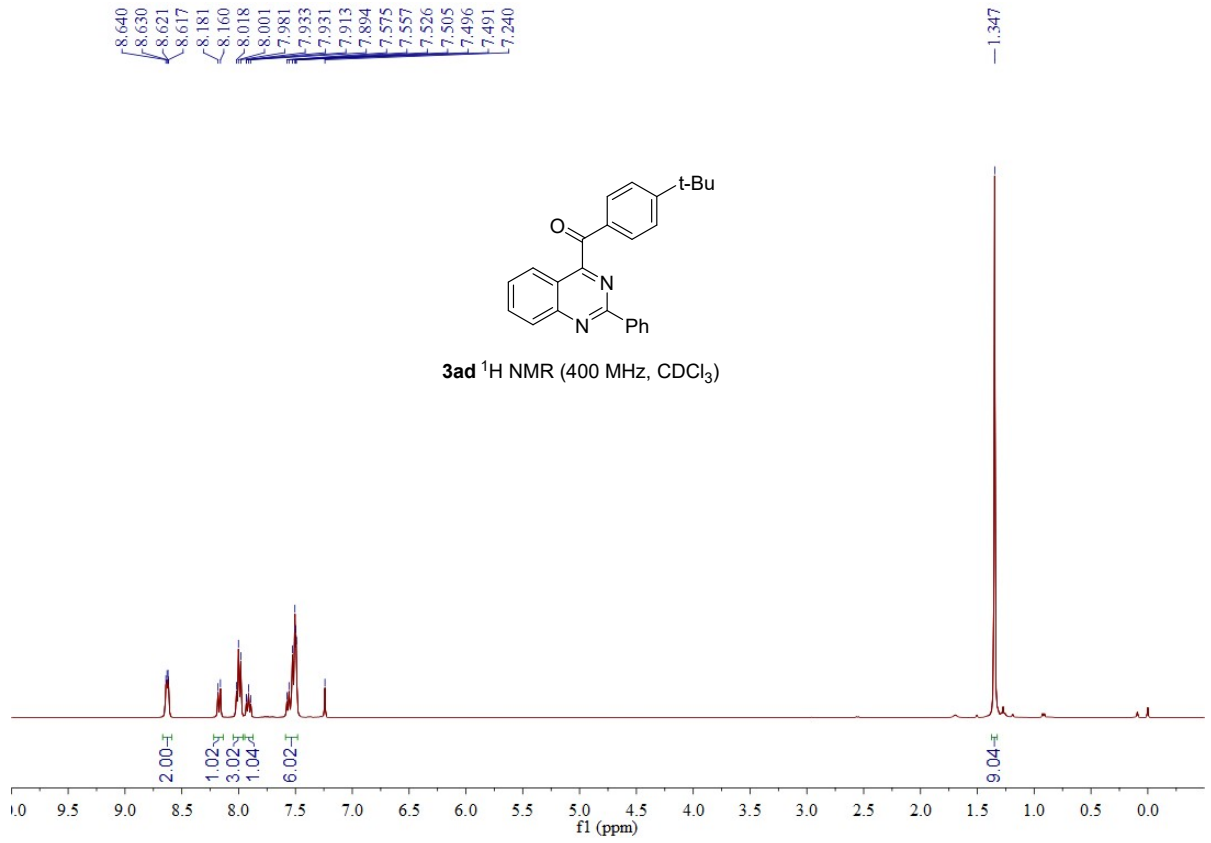
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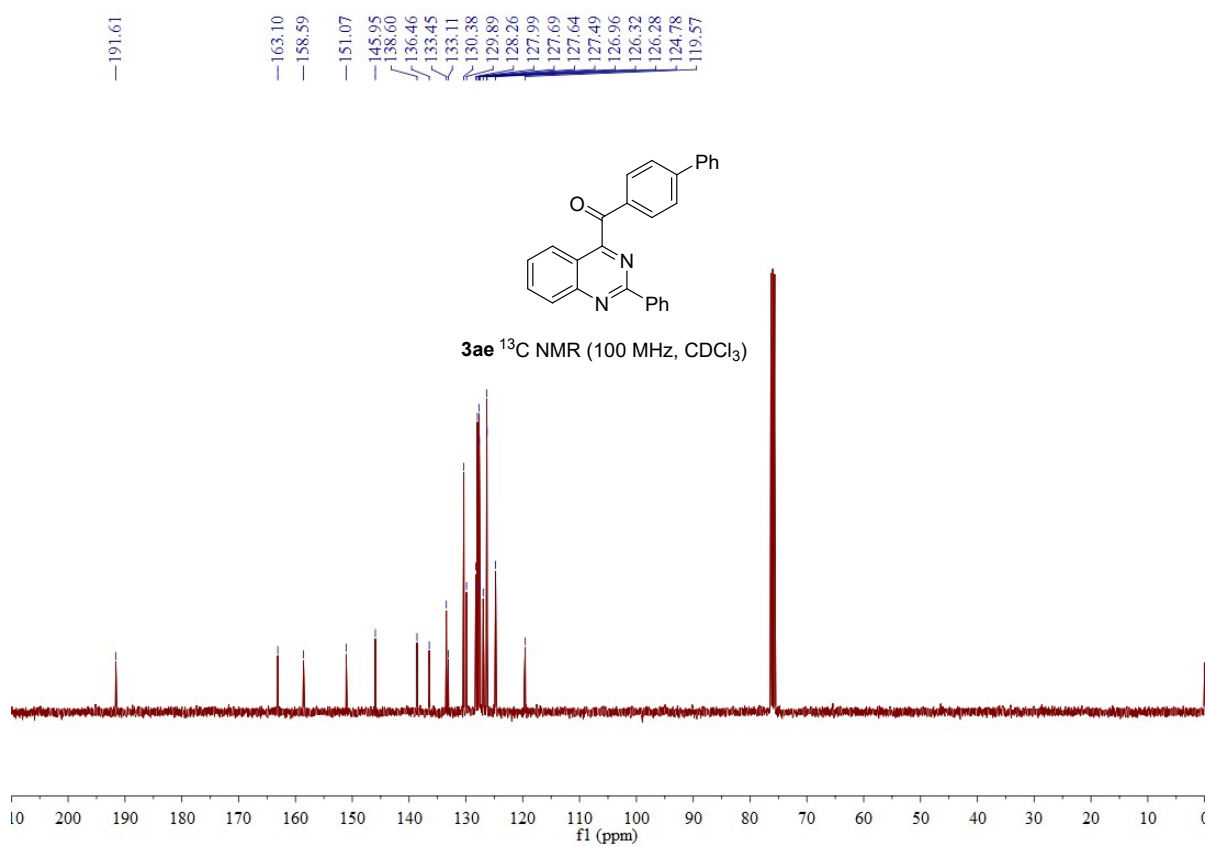
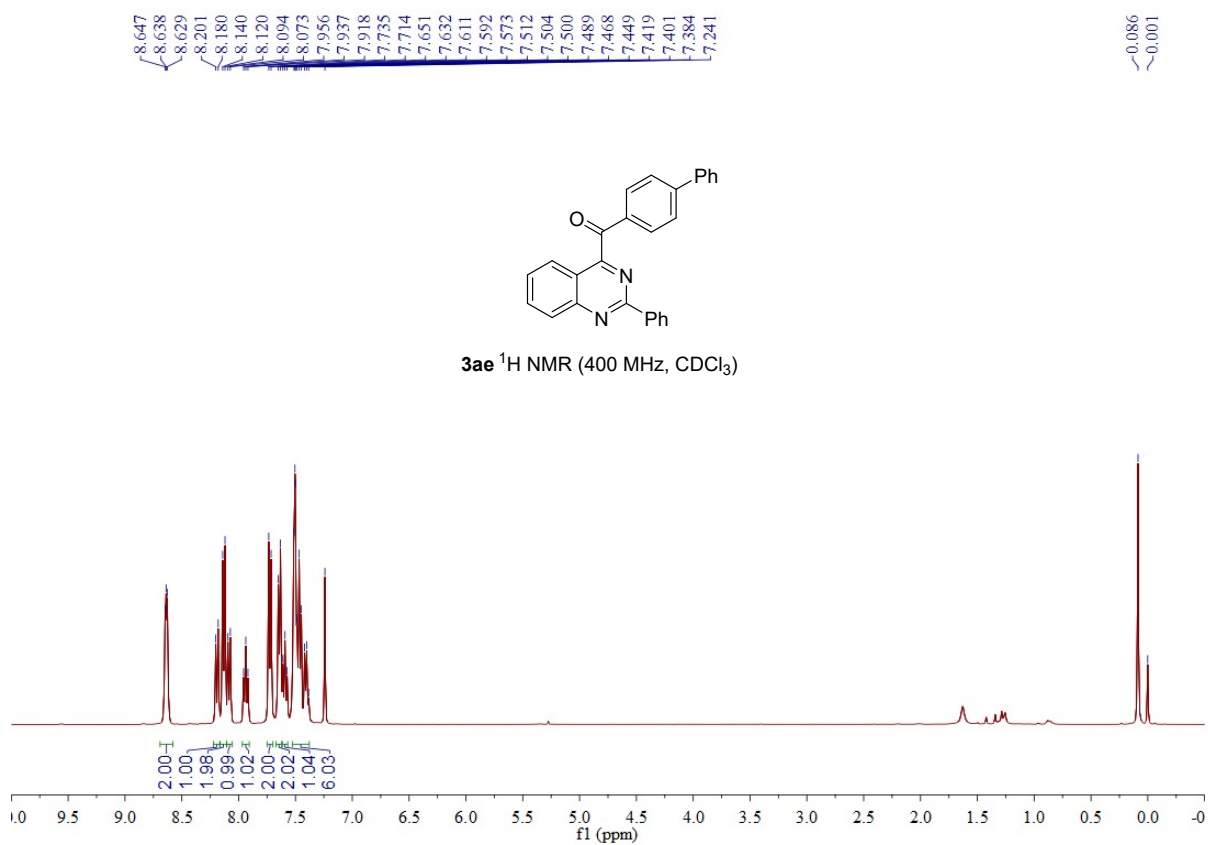
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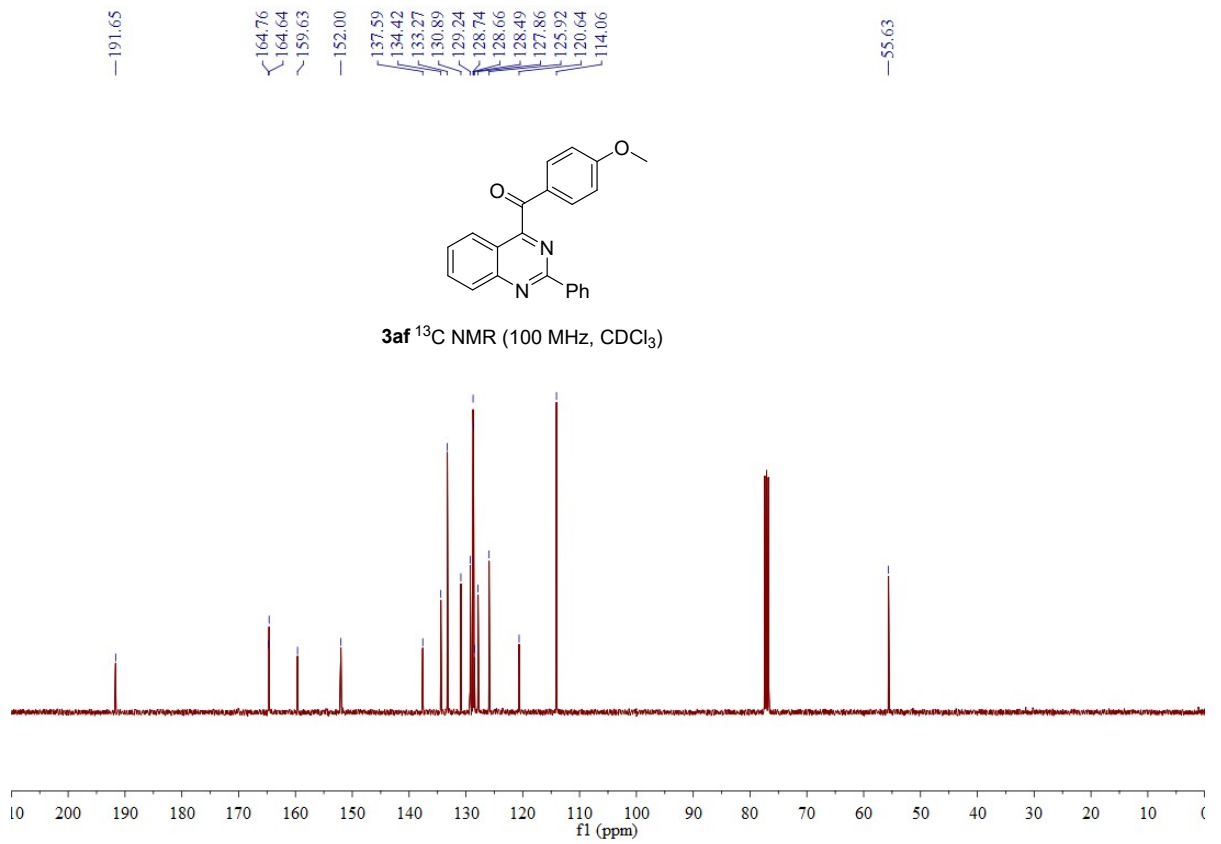
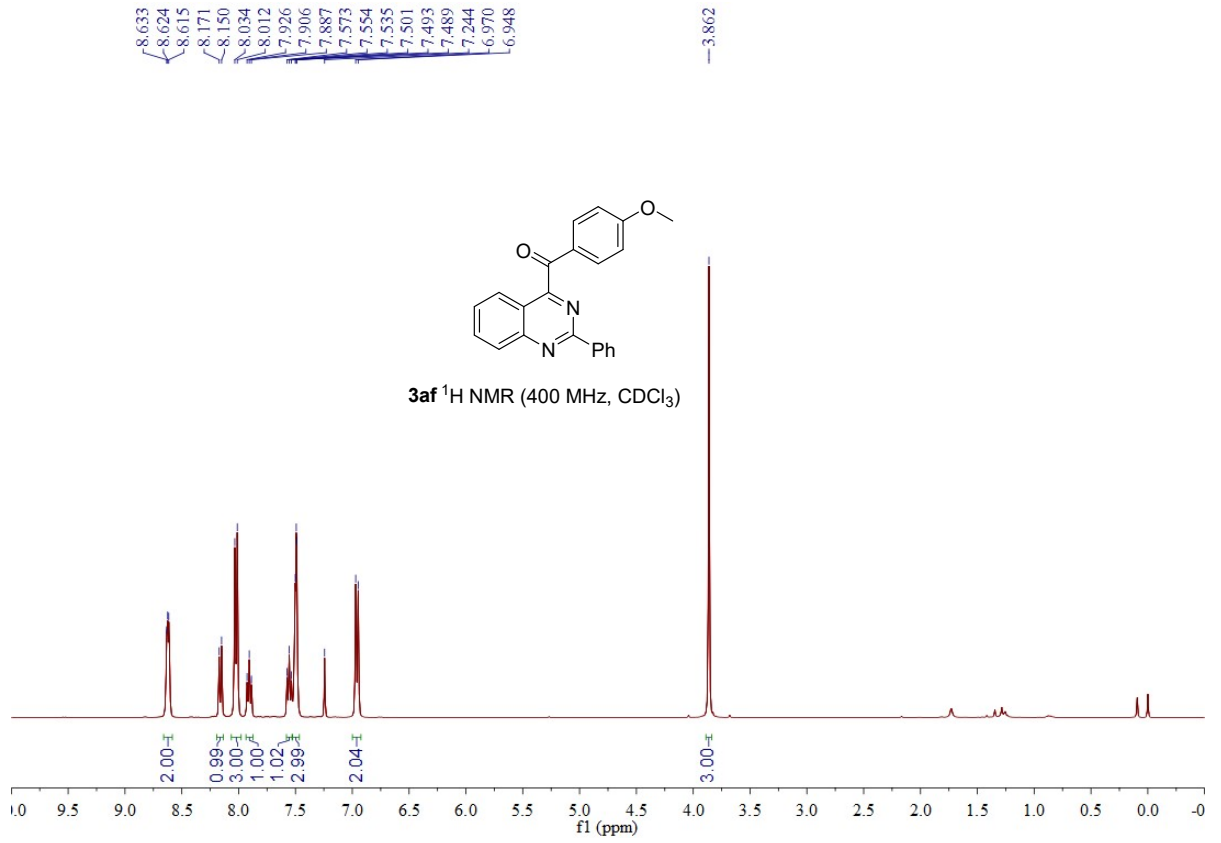


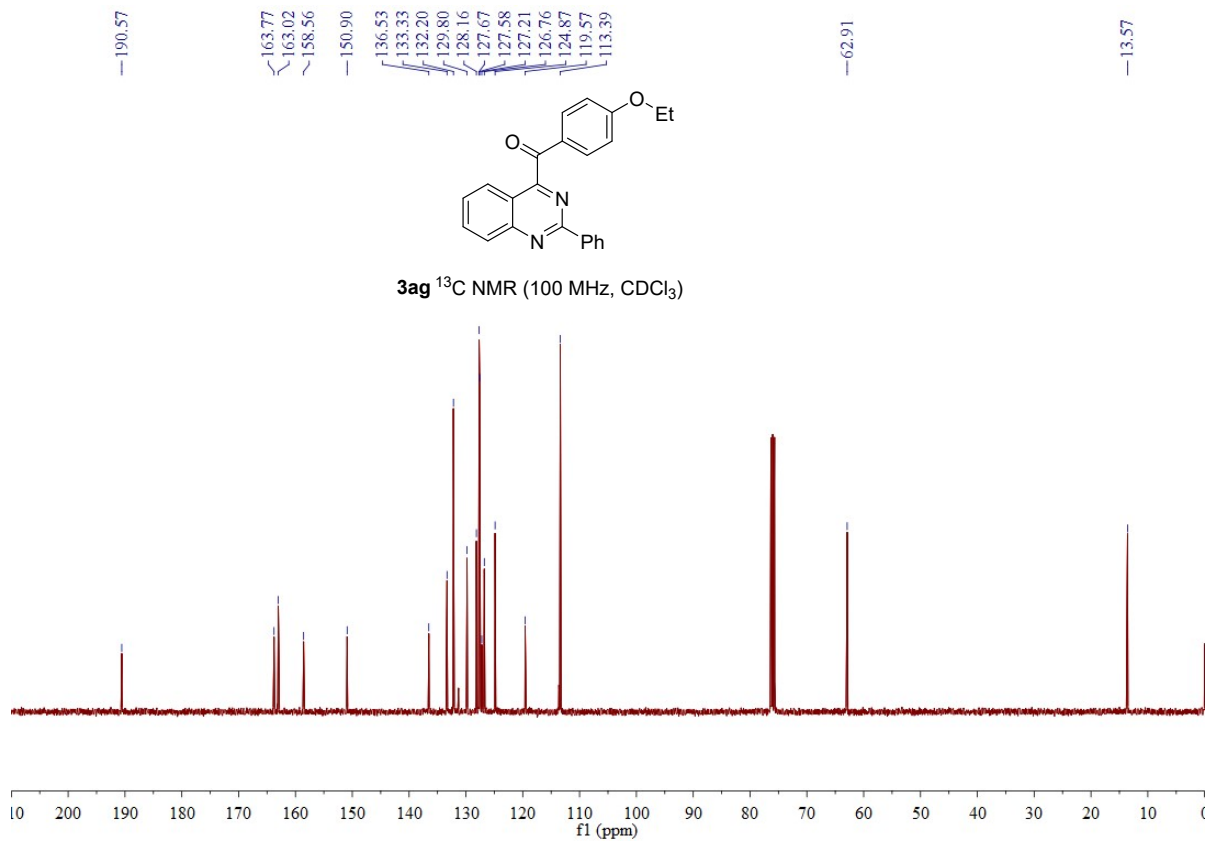
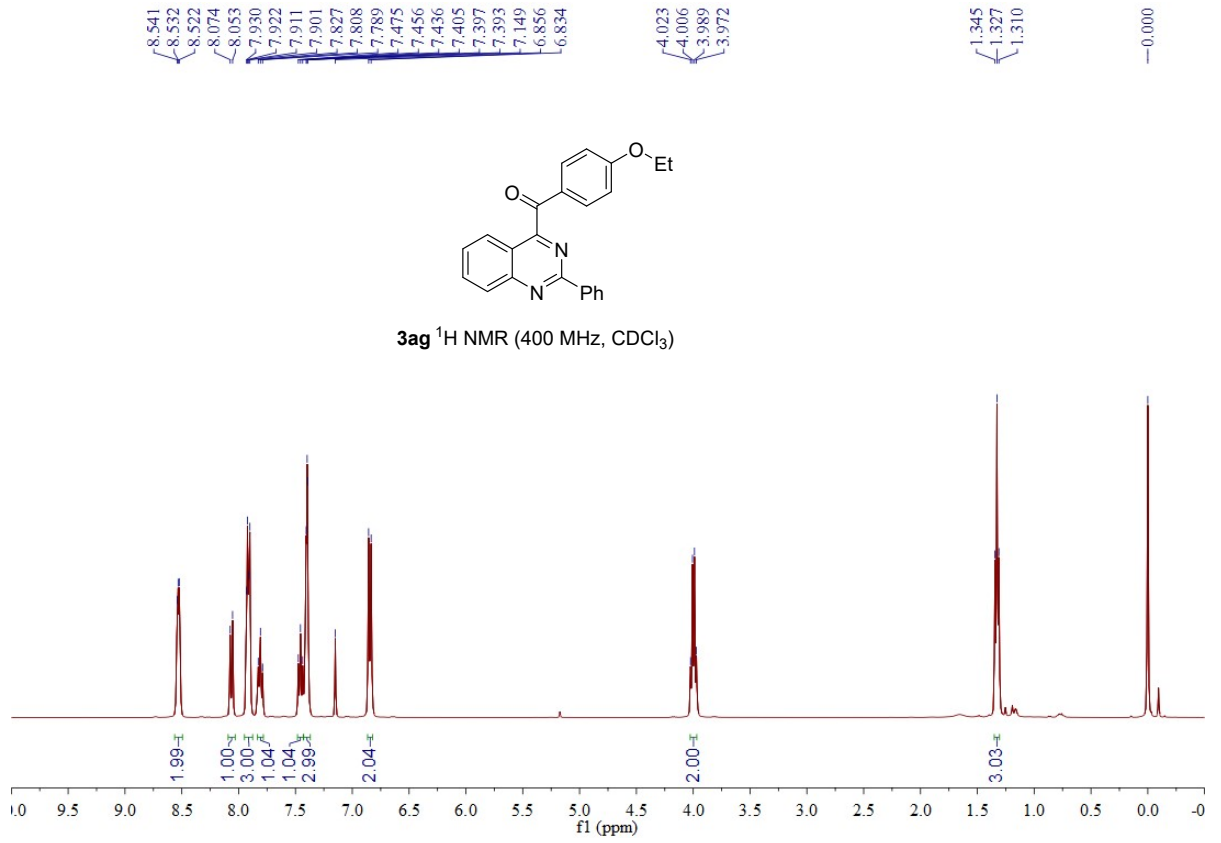


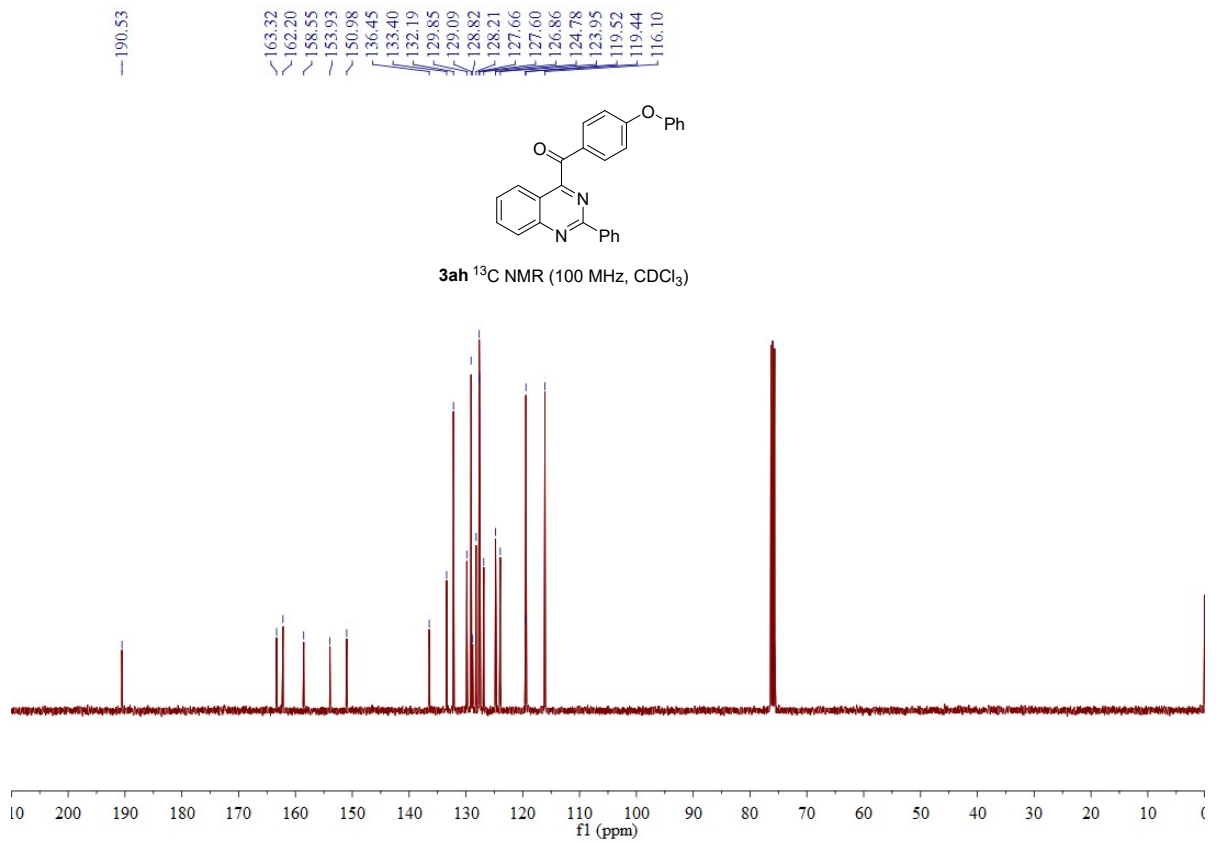
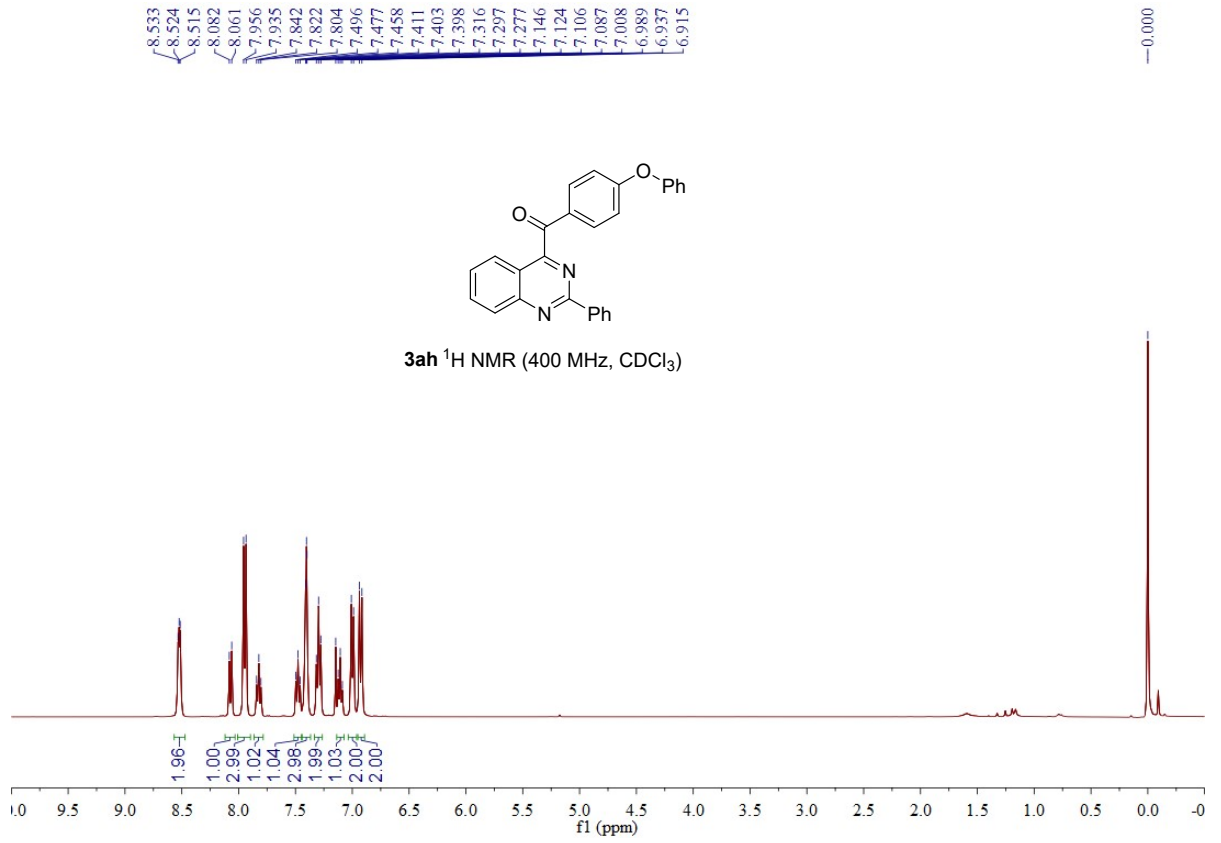


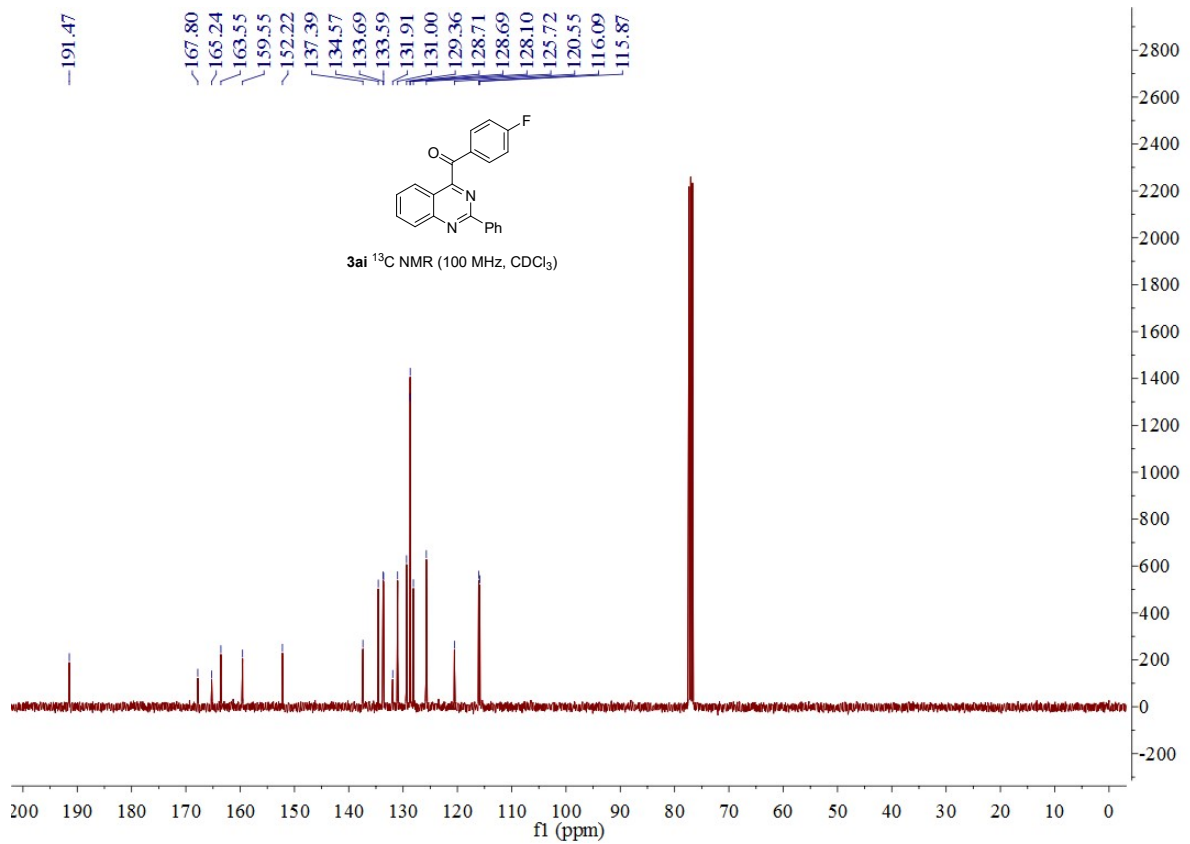
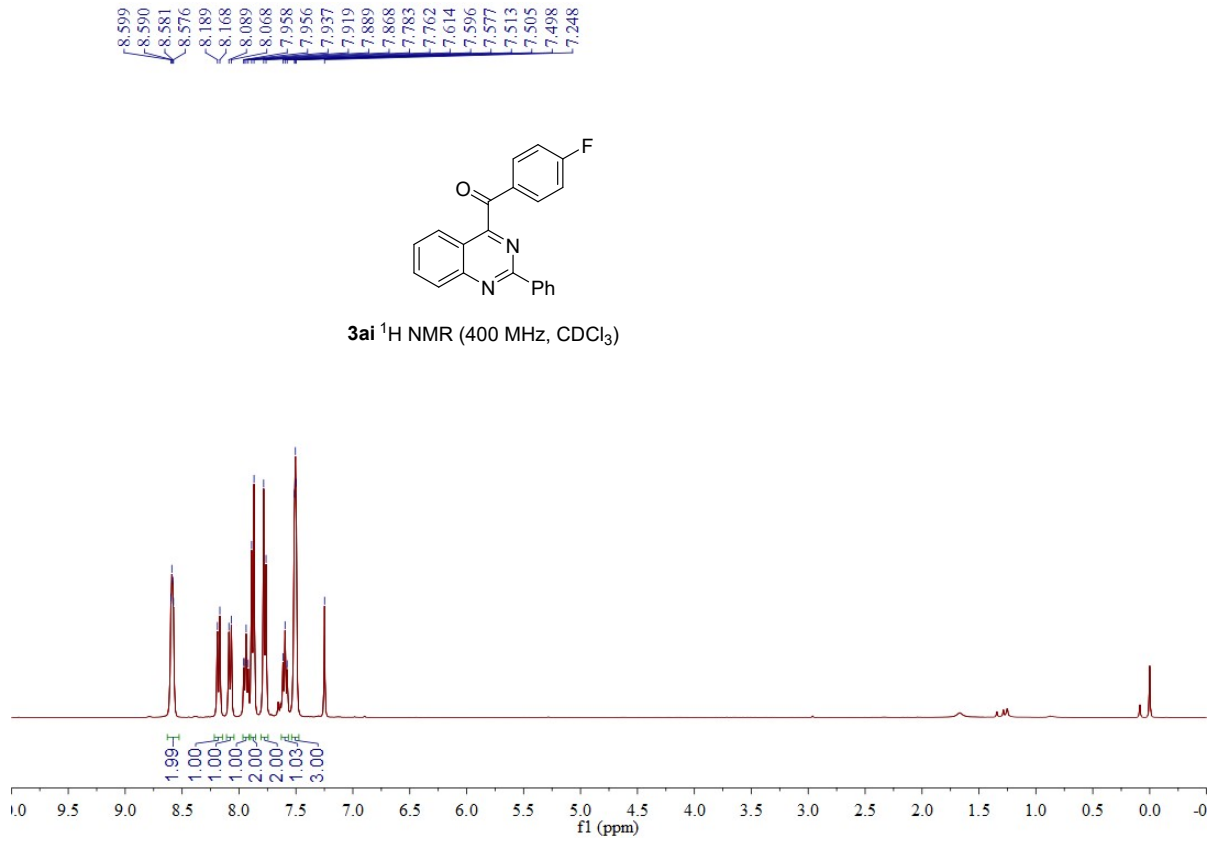


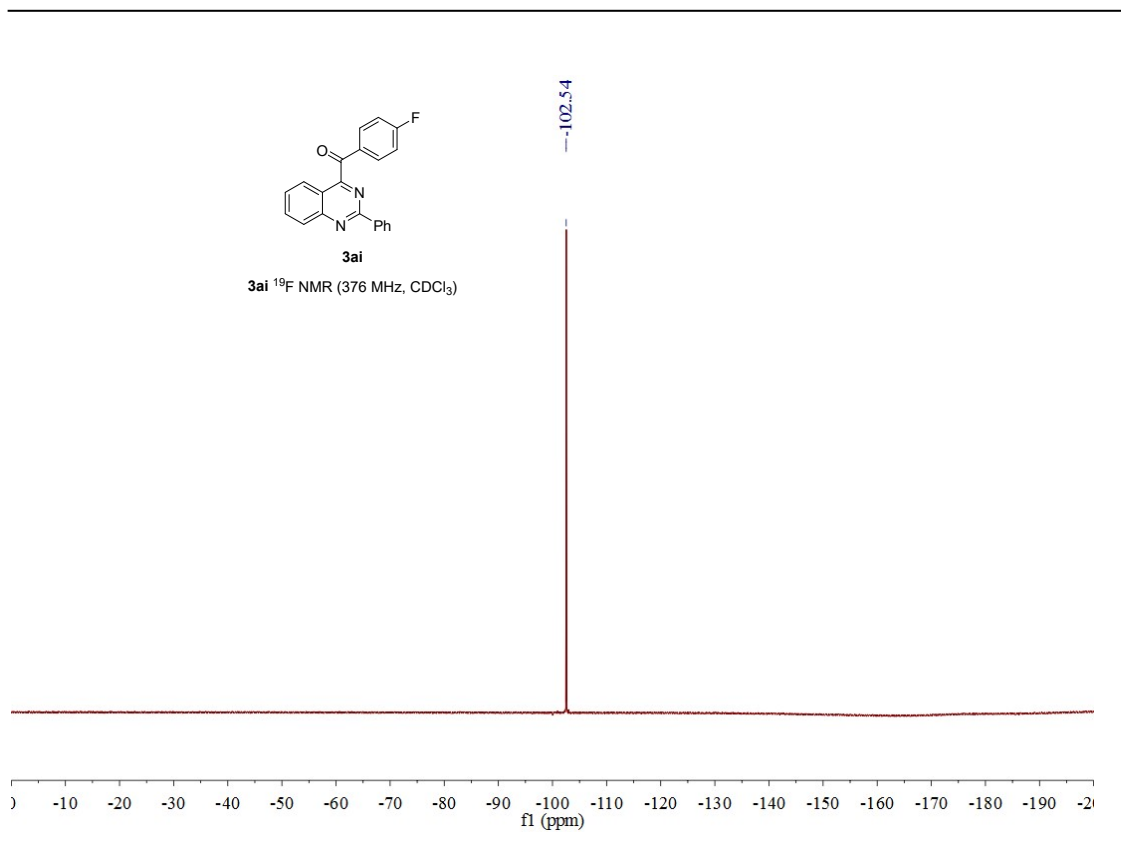


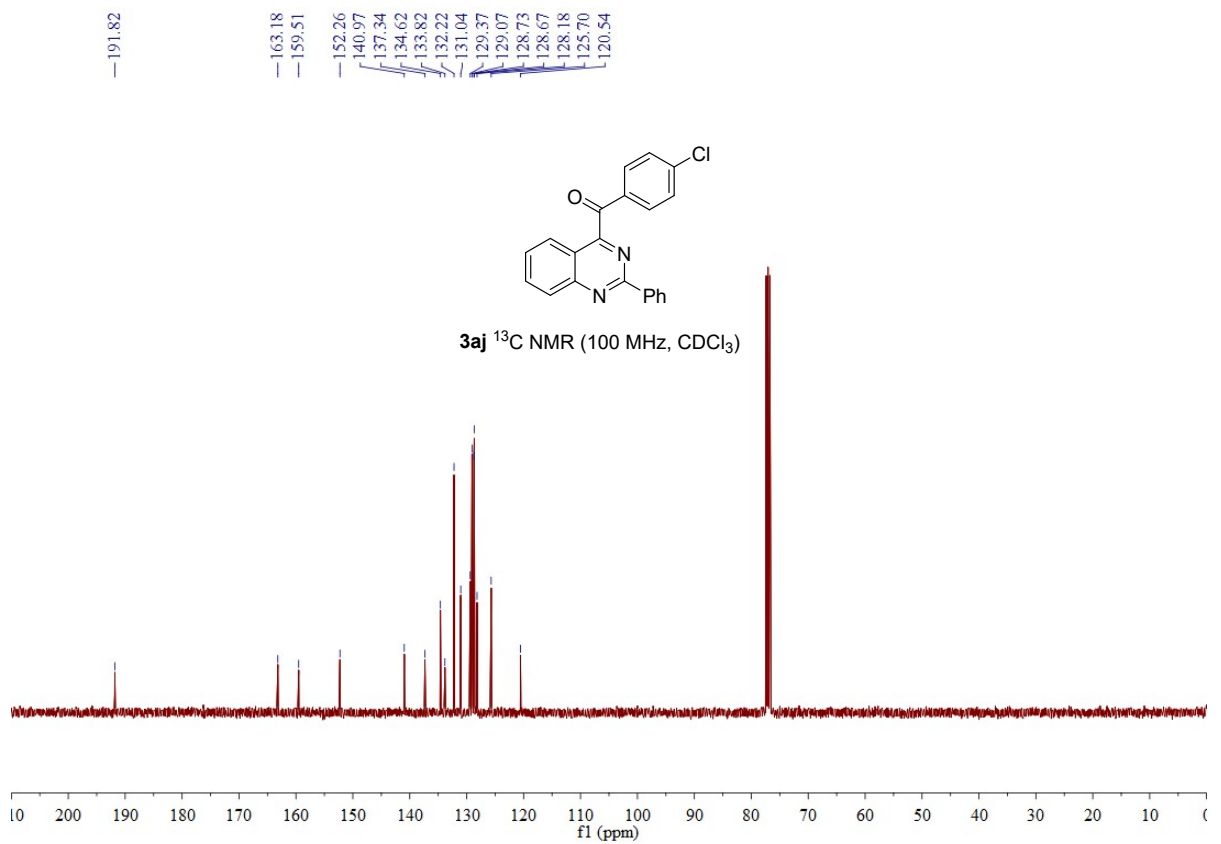
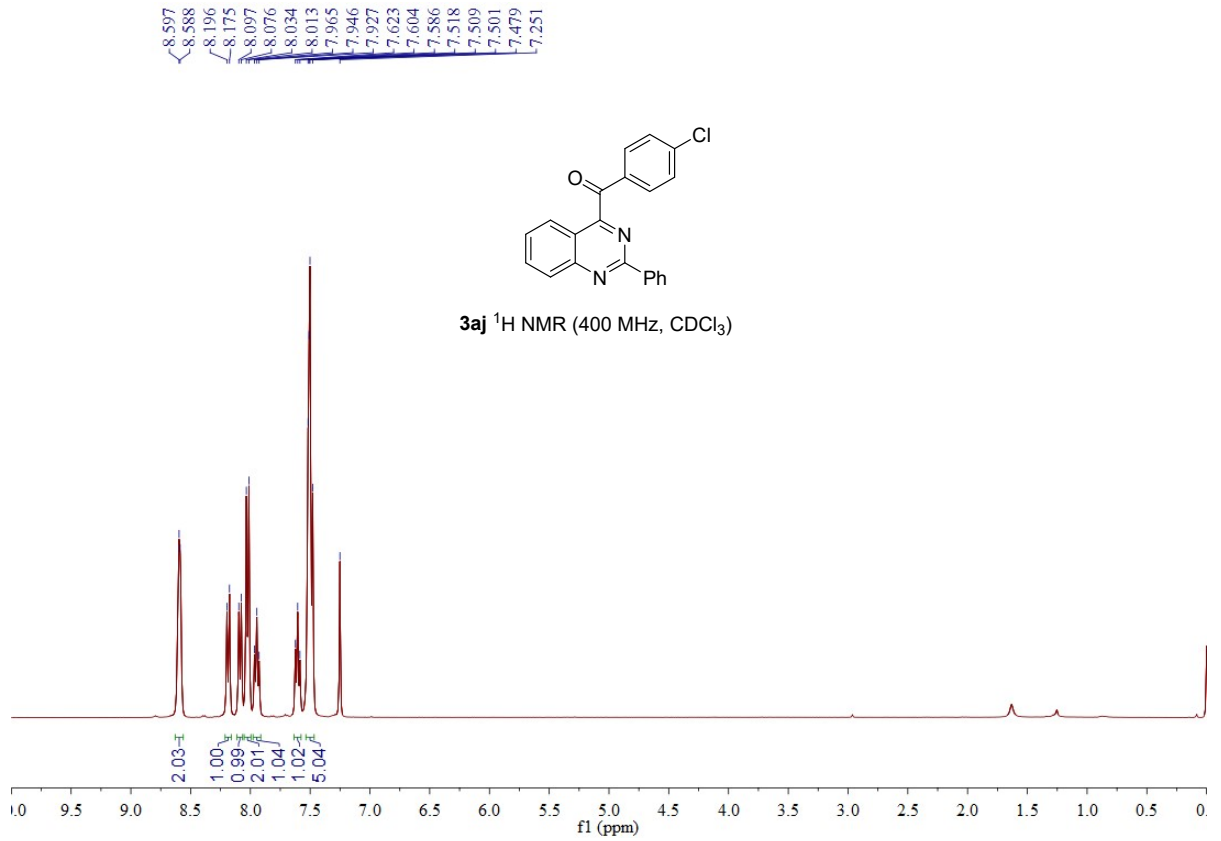




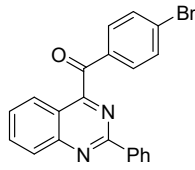




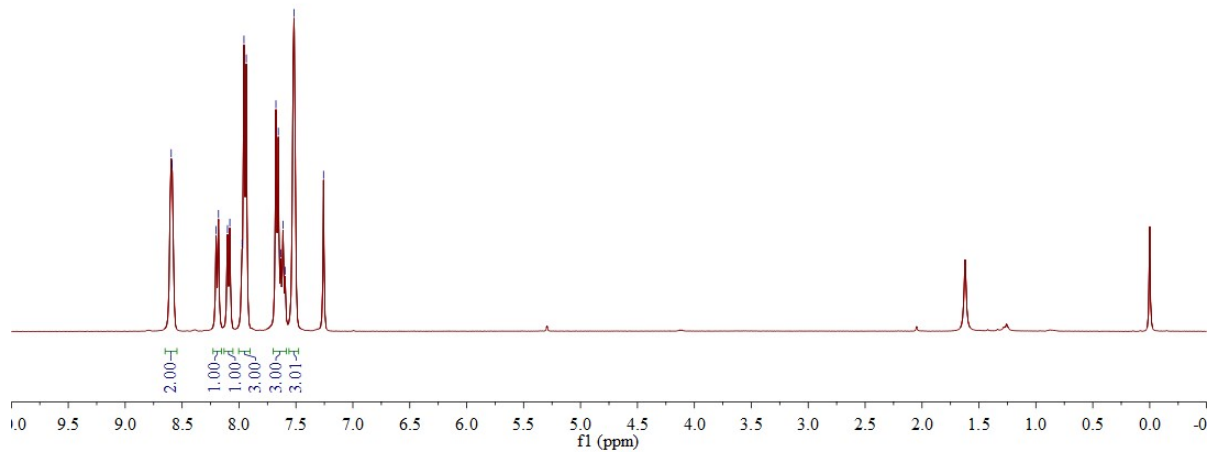




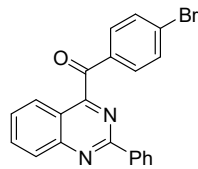
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7.257



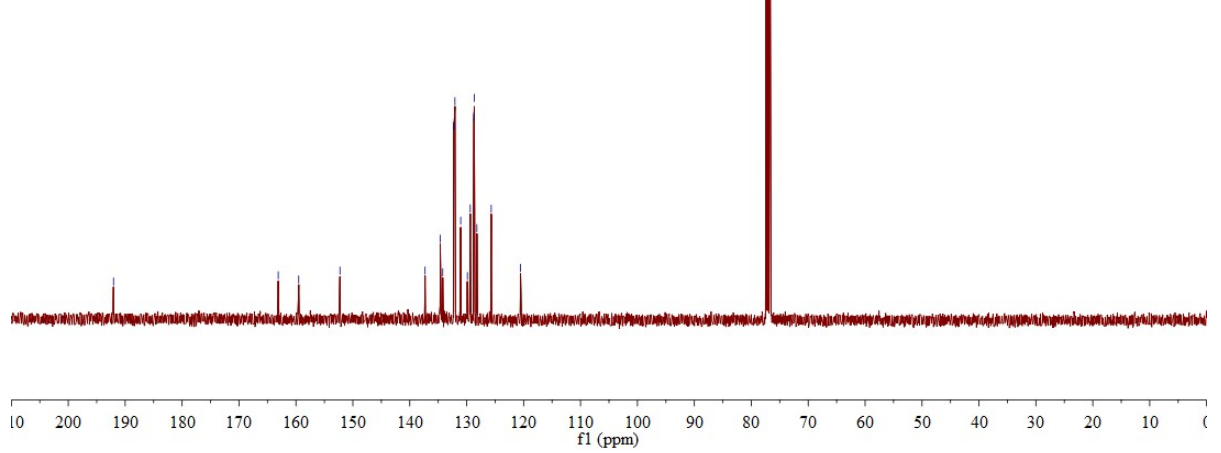
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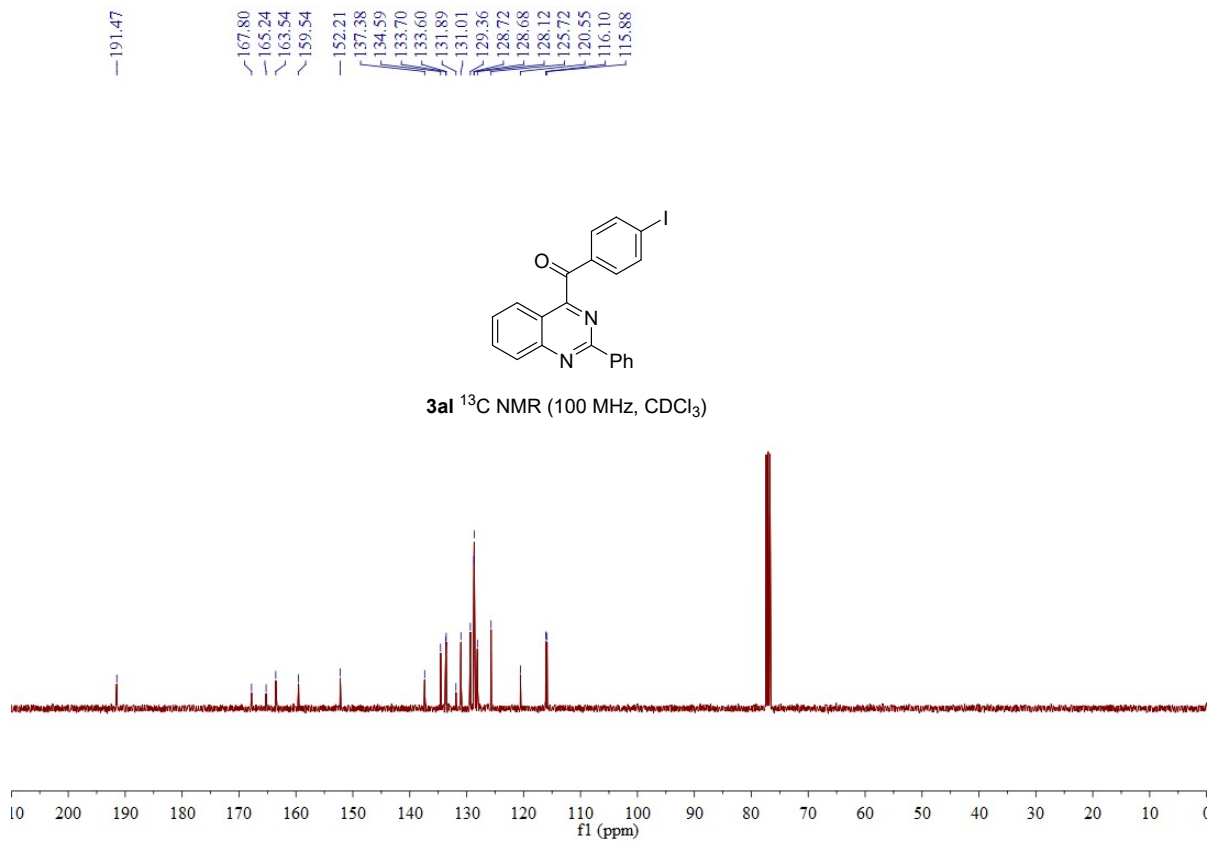
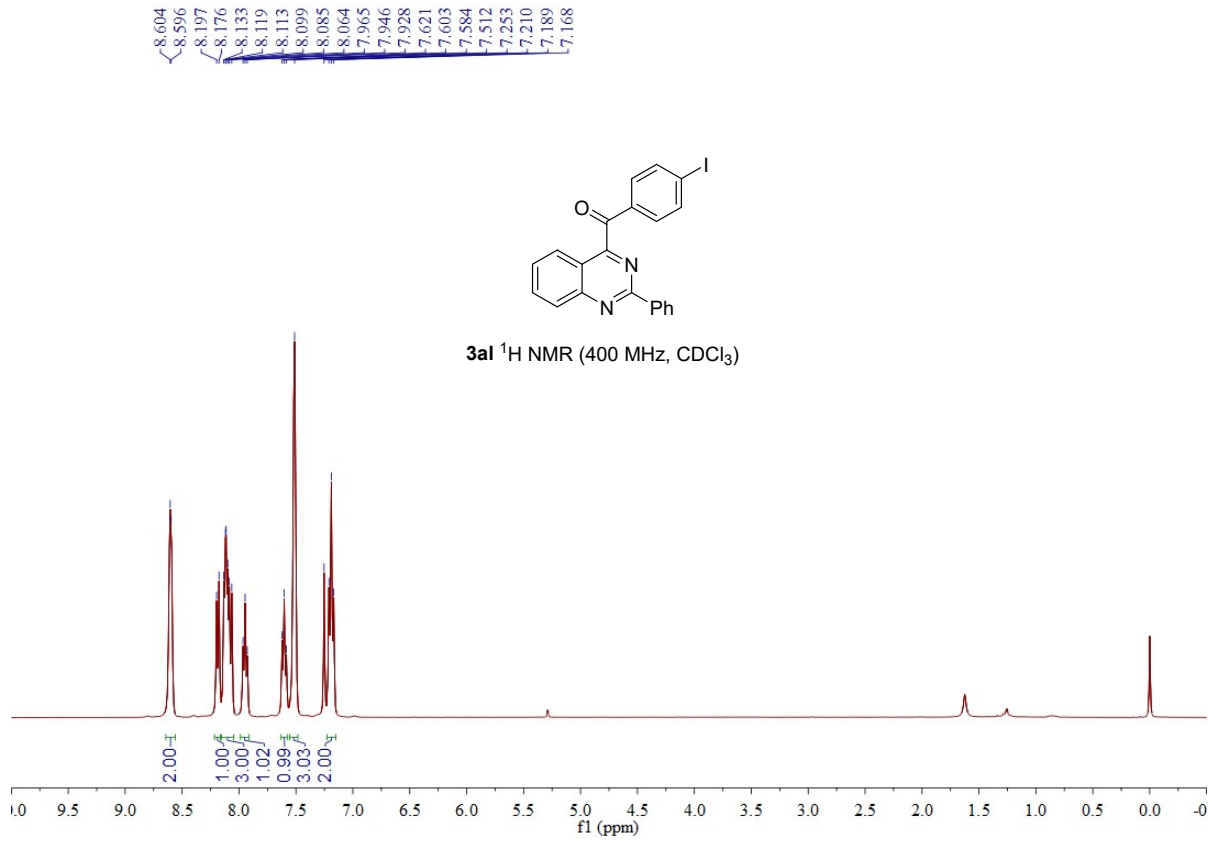


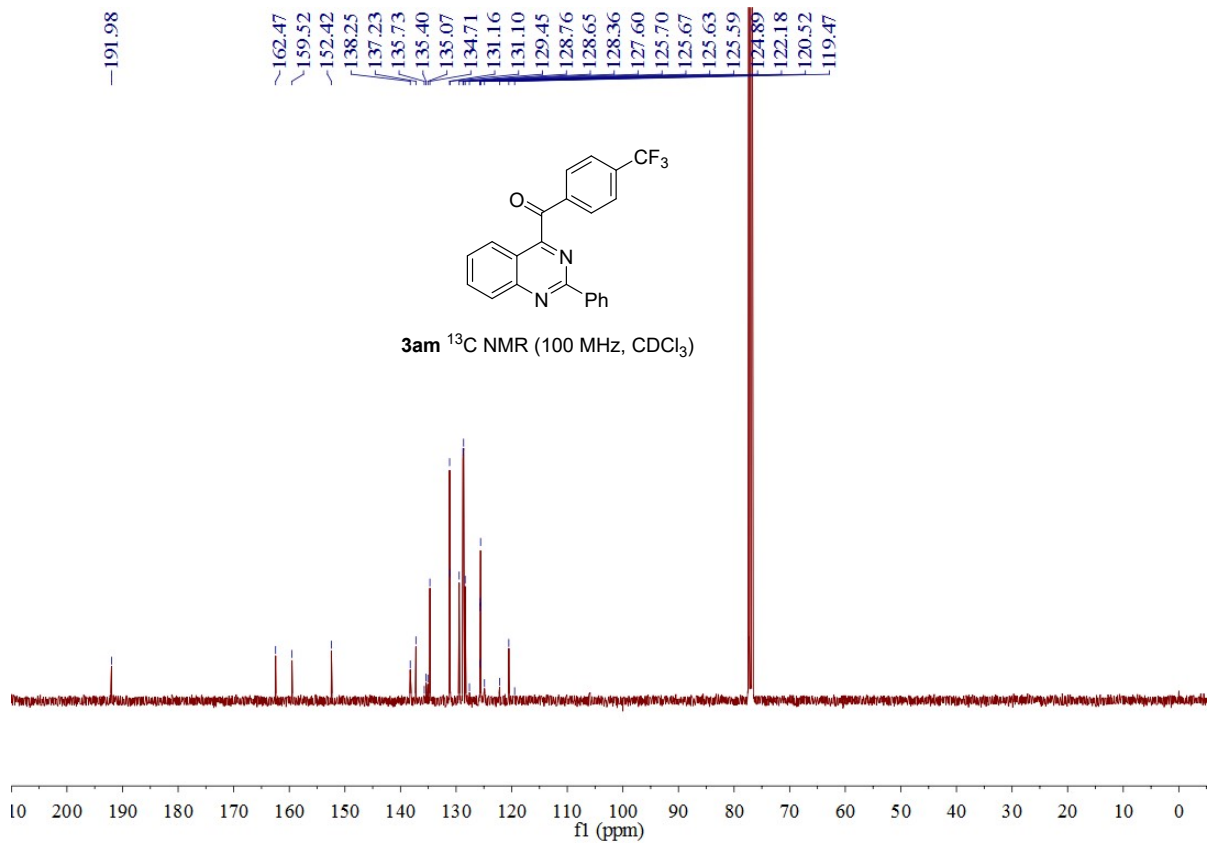
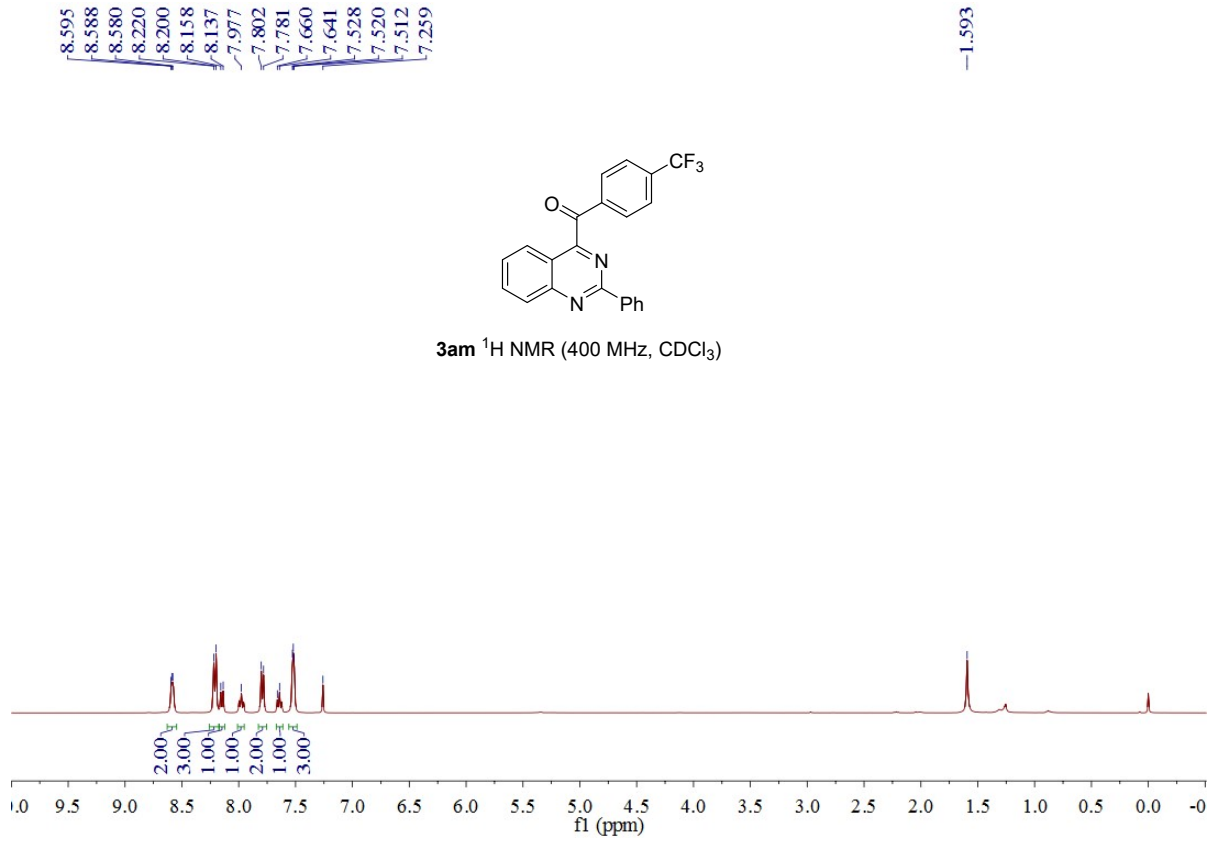
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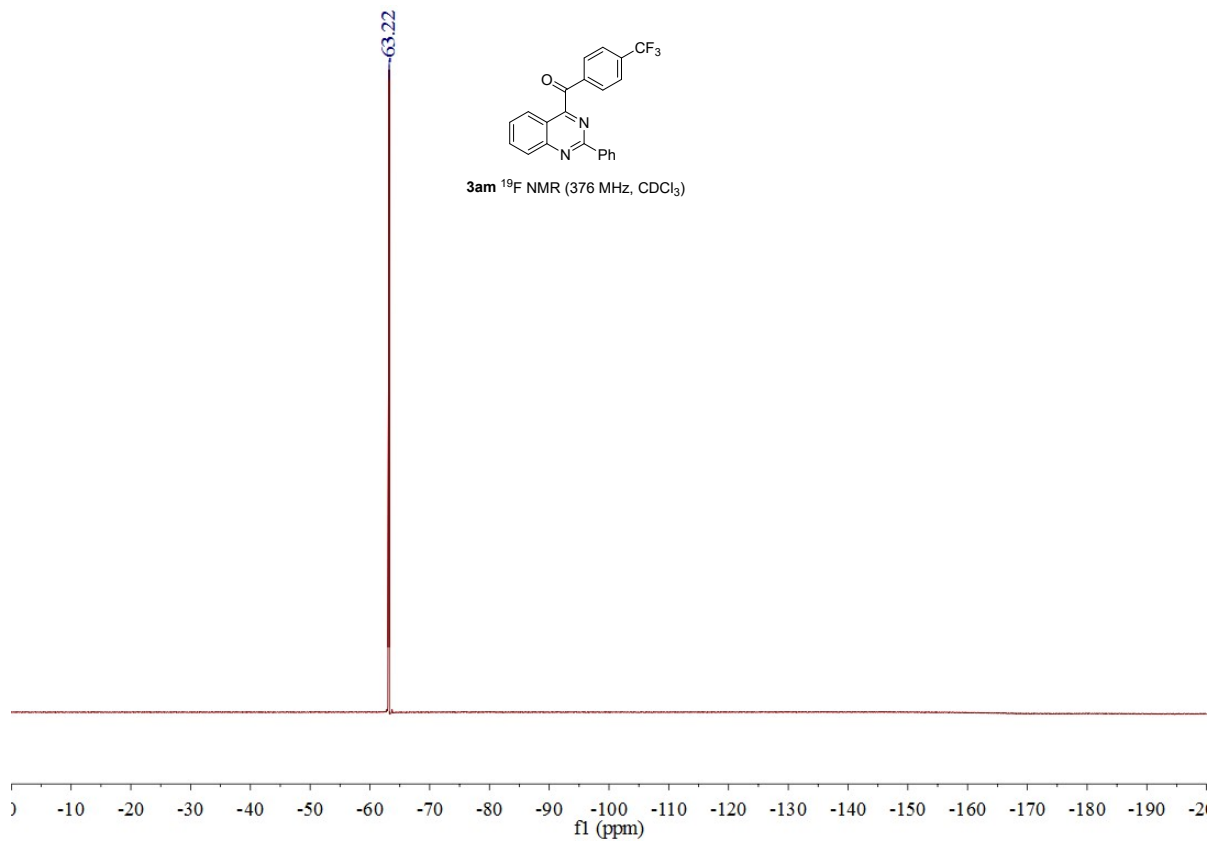


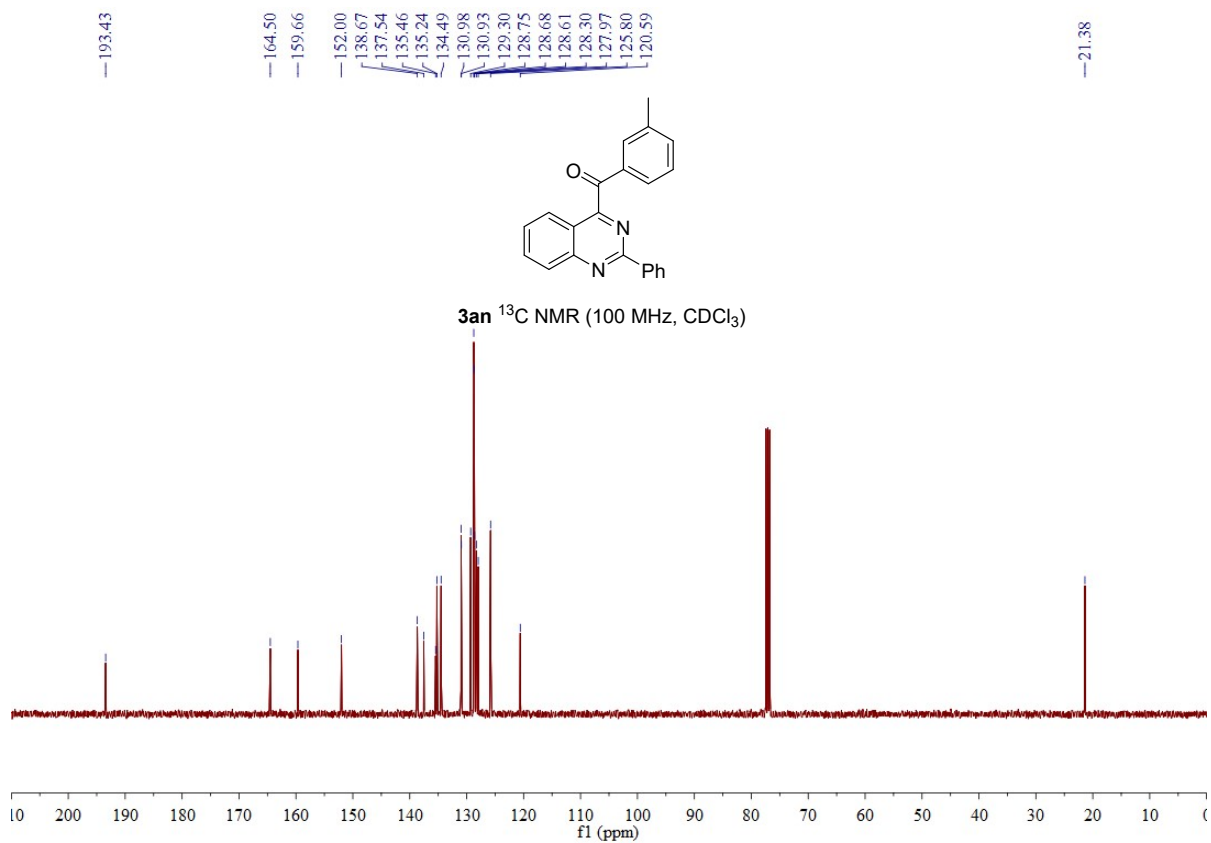
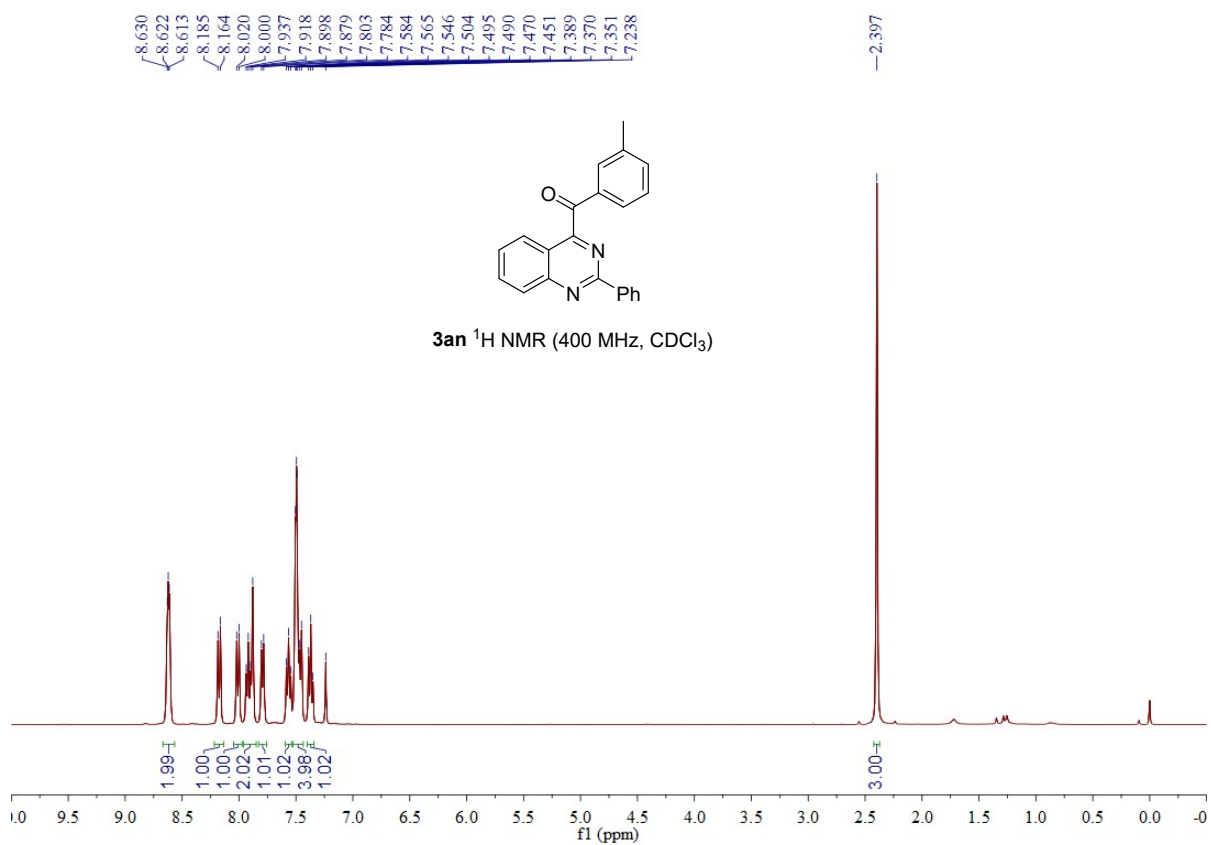
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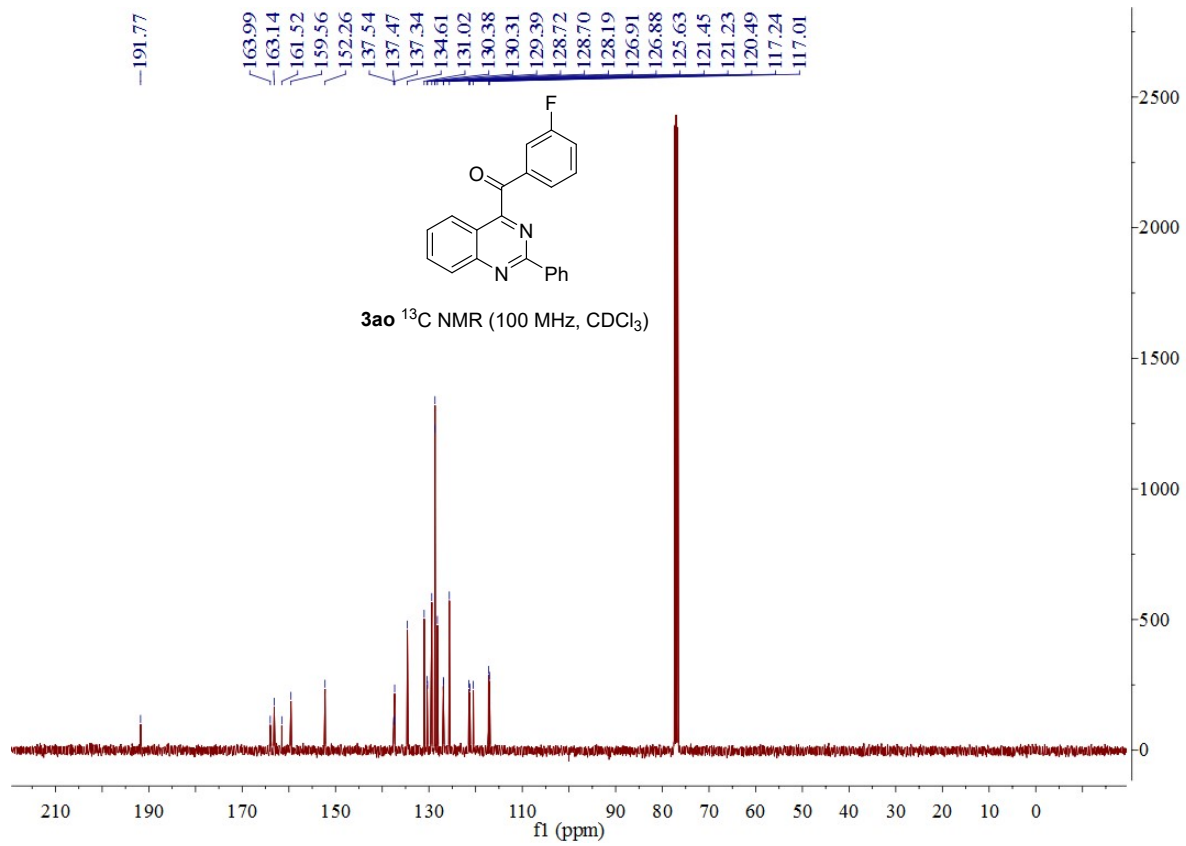
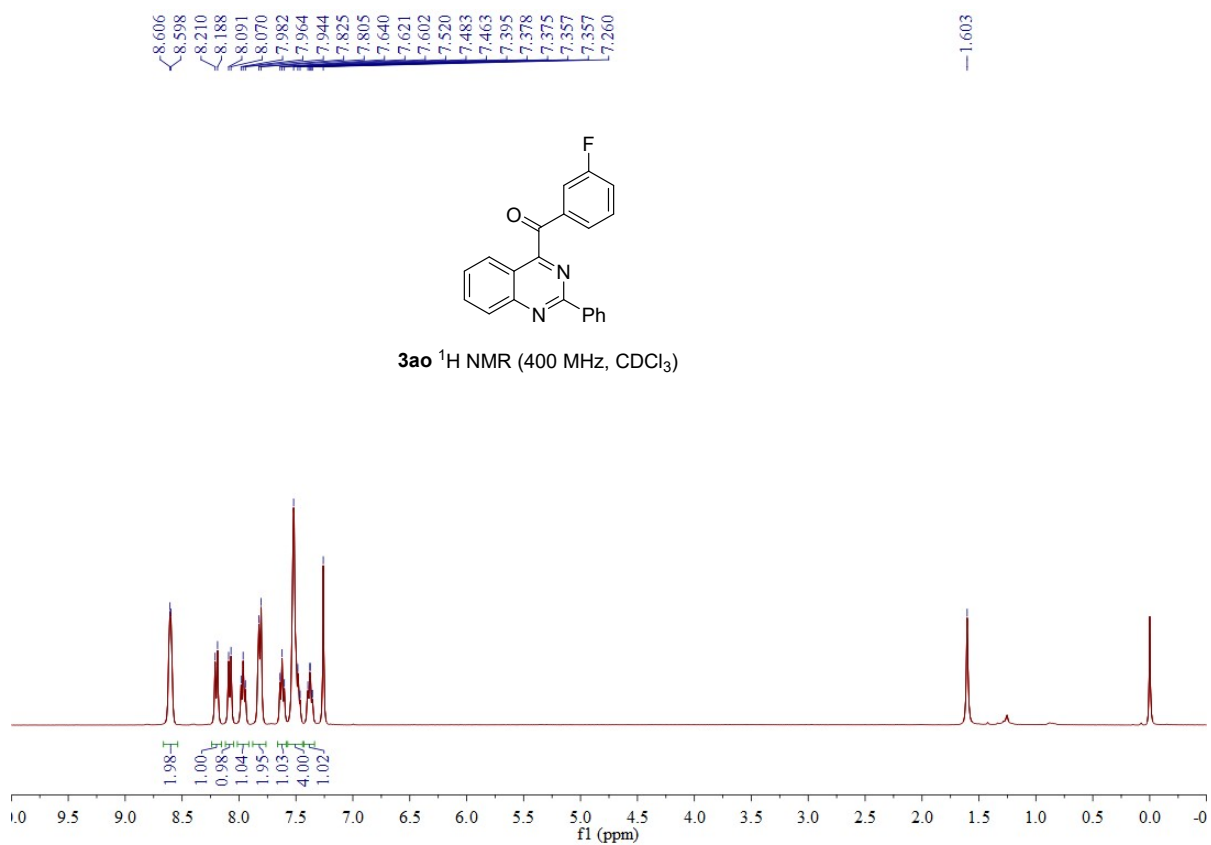


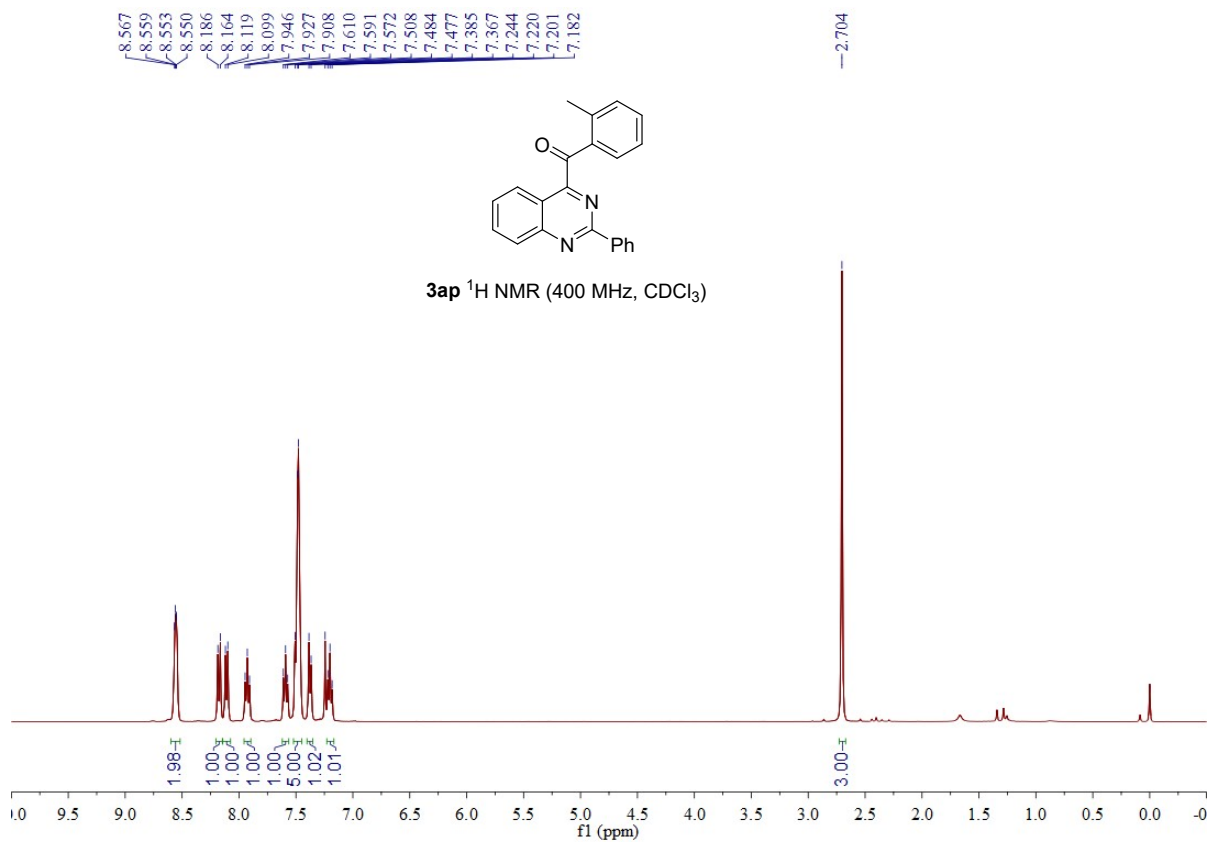
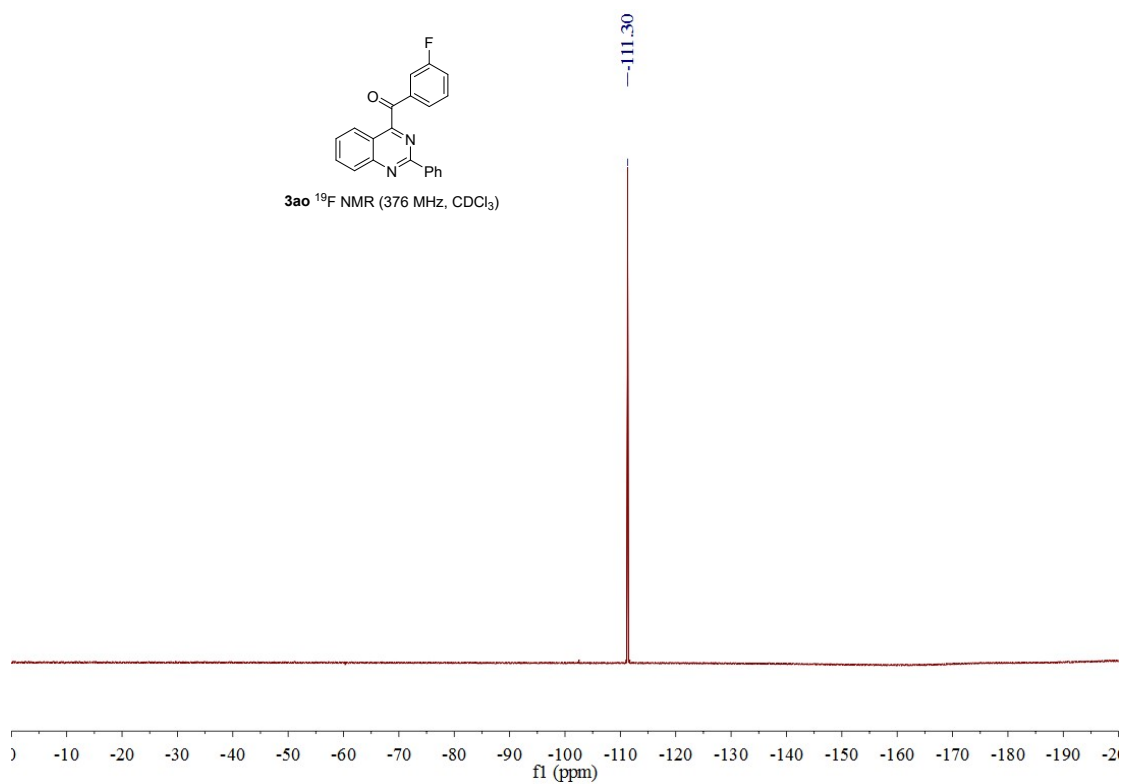


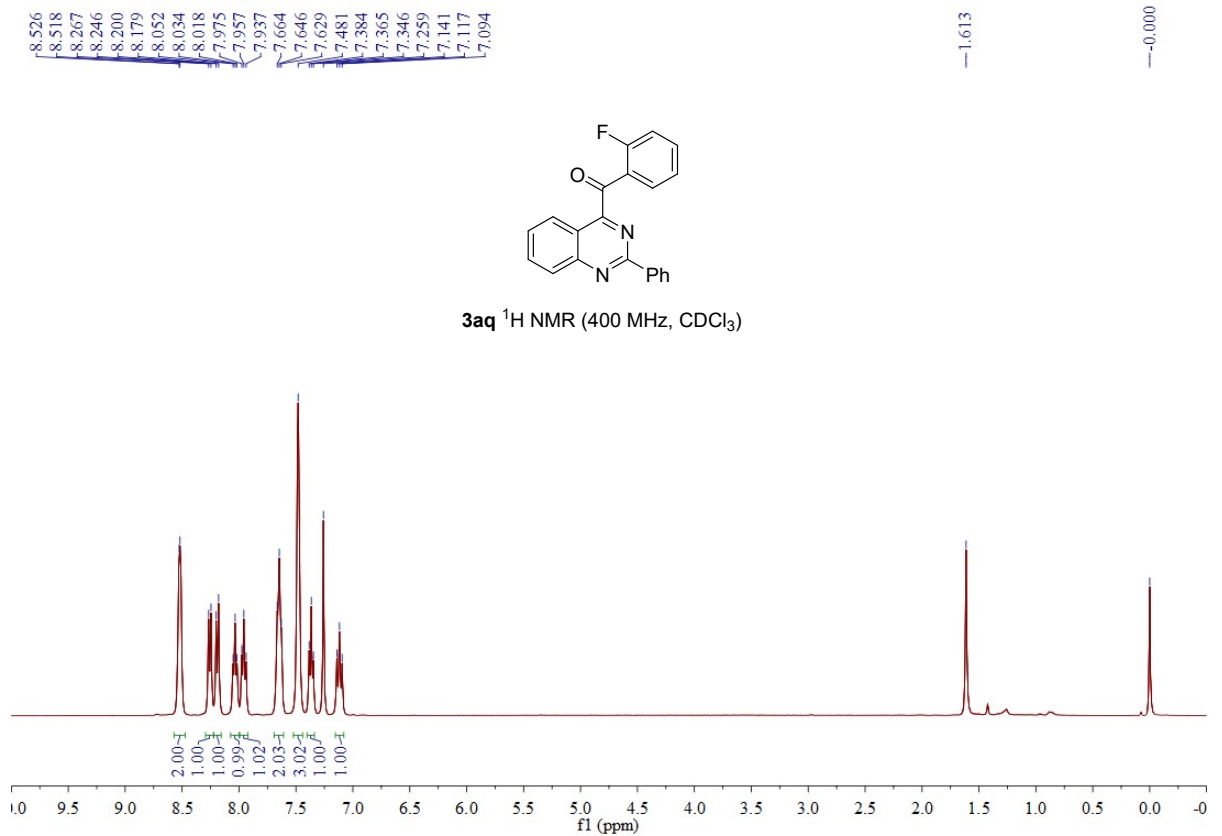
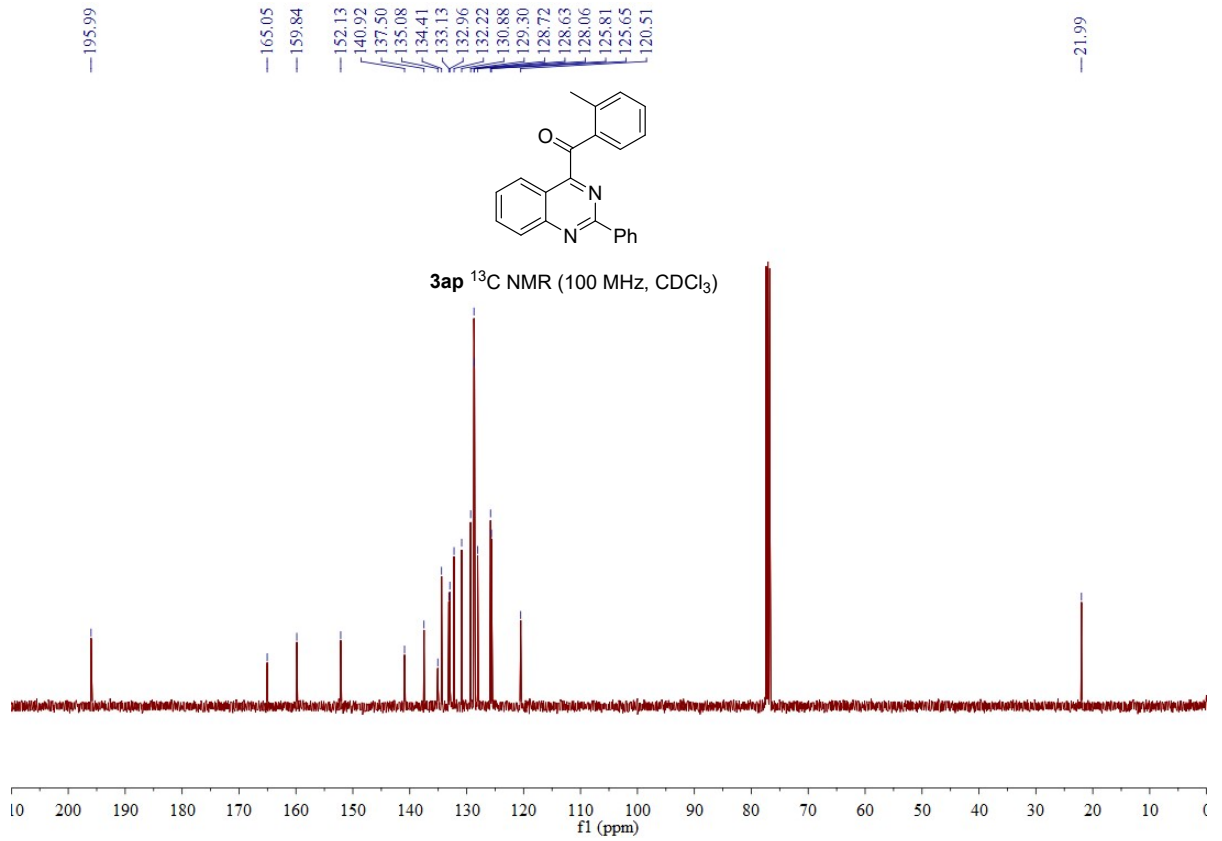


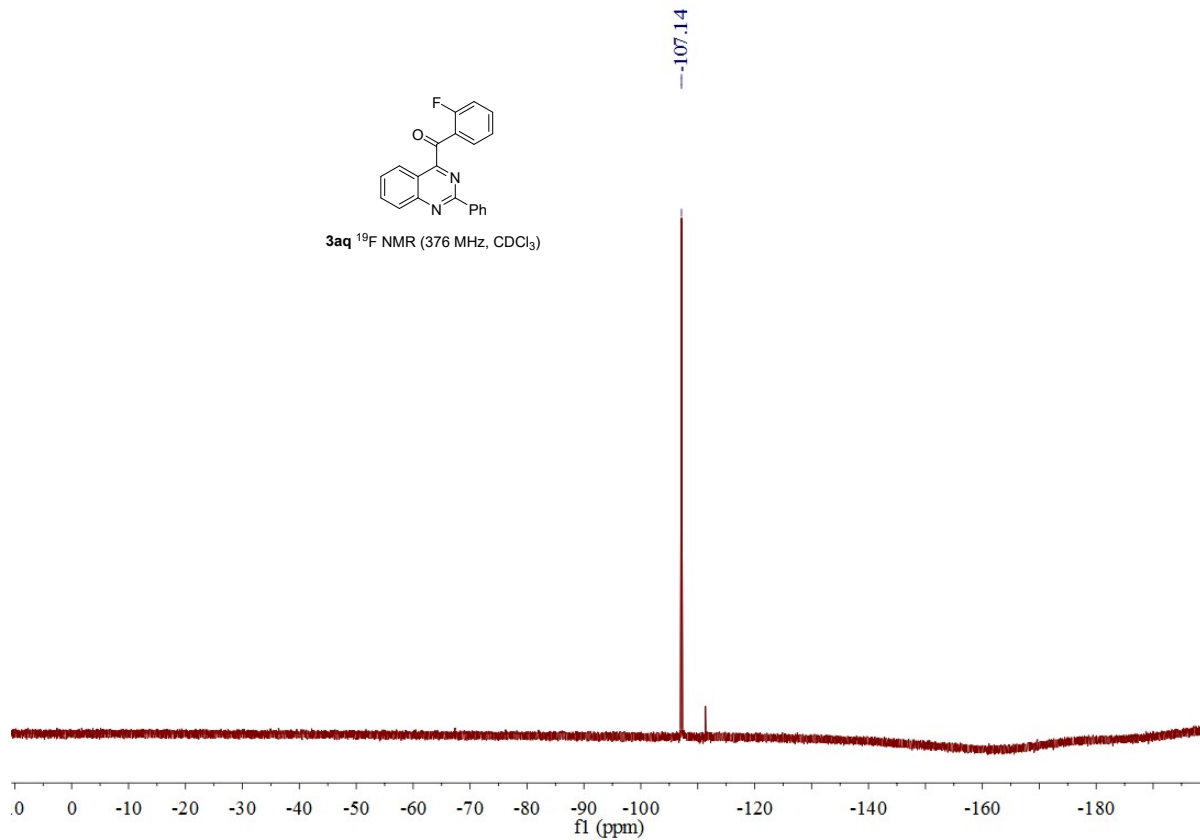
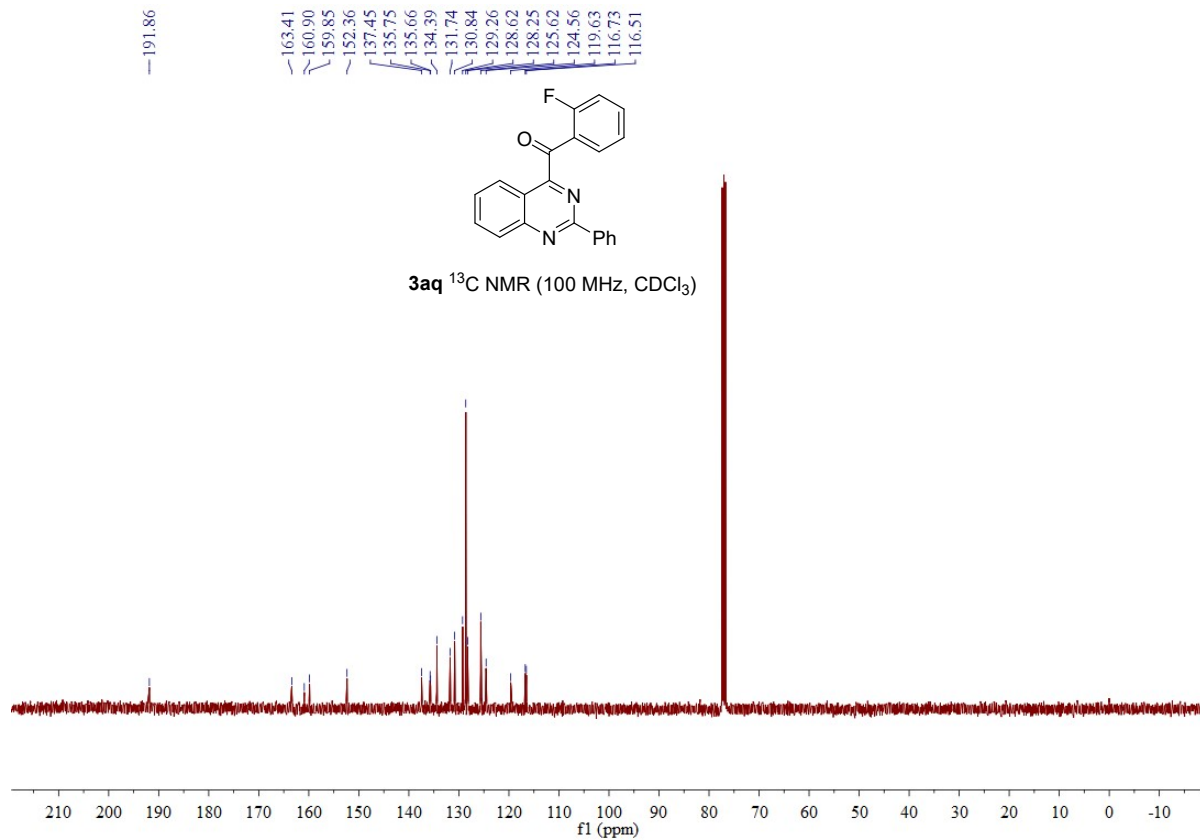


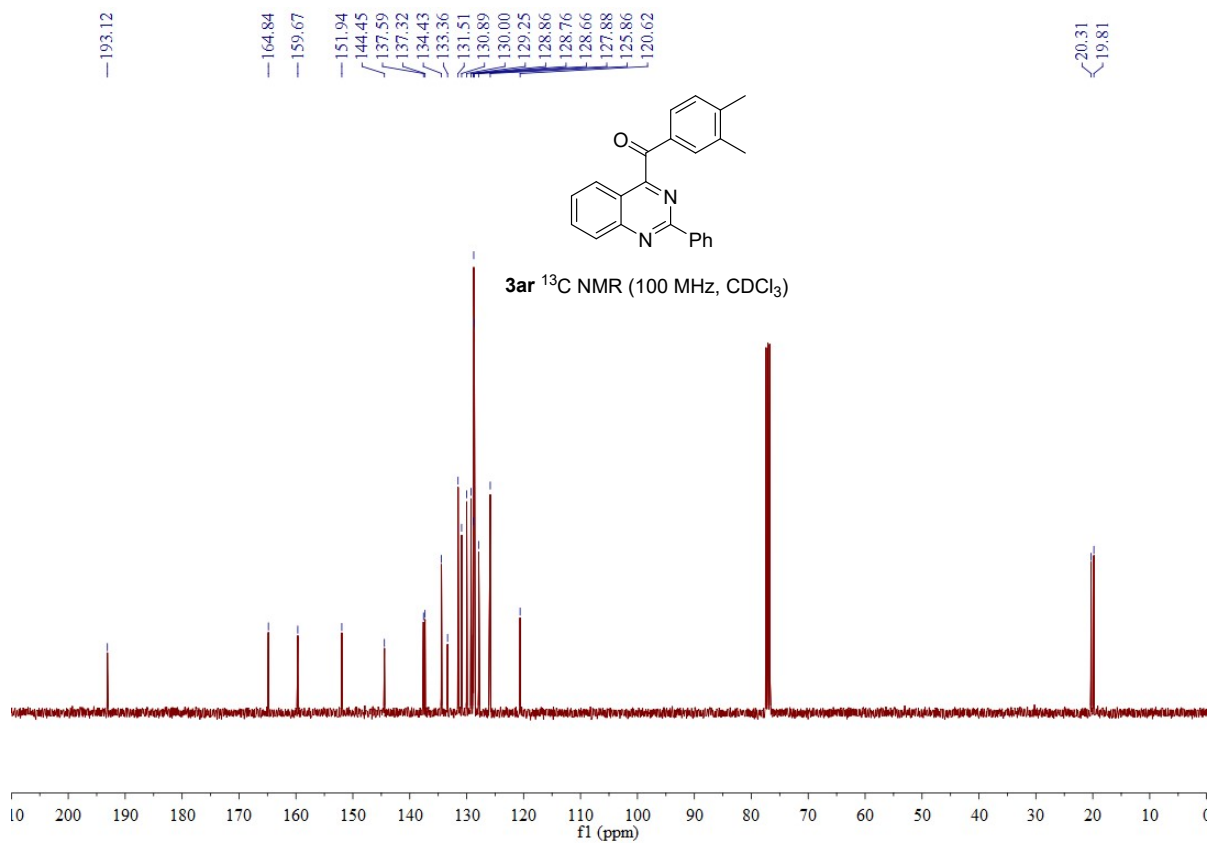
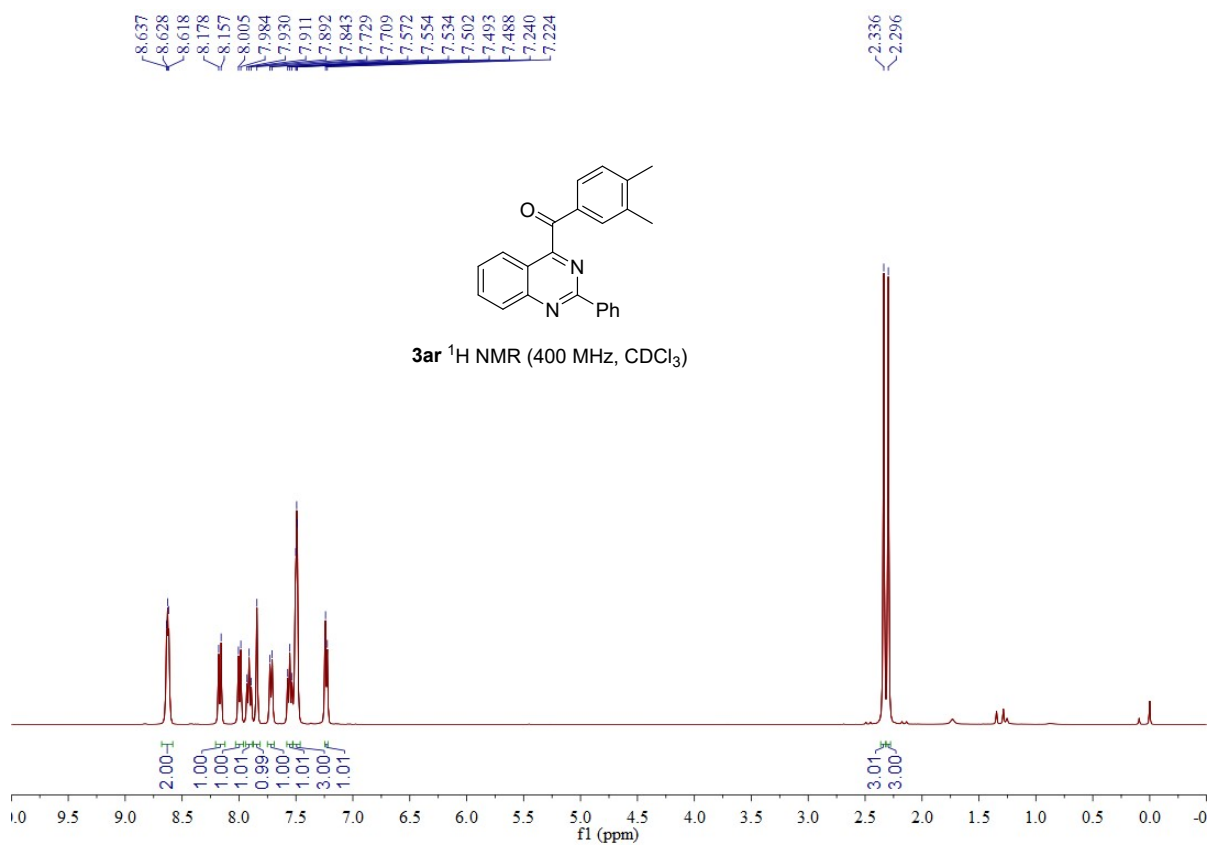




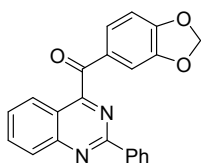




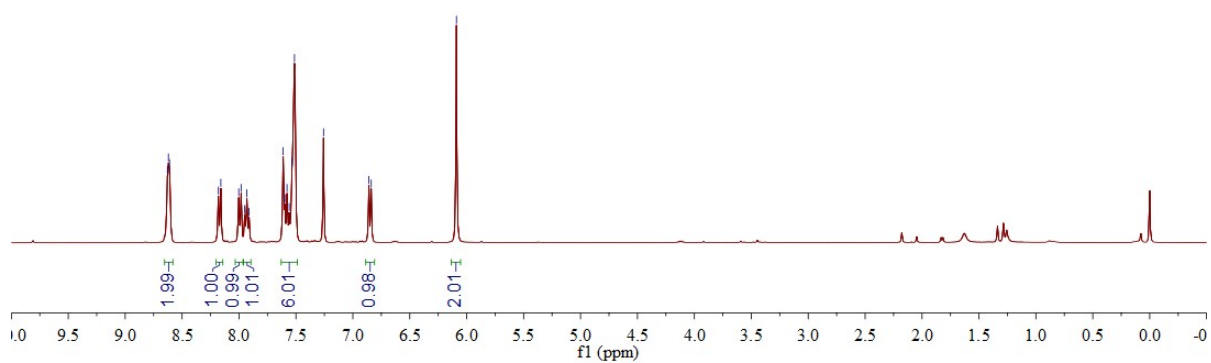




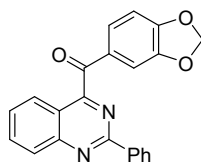
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-6.090



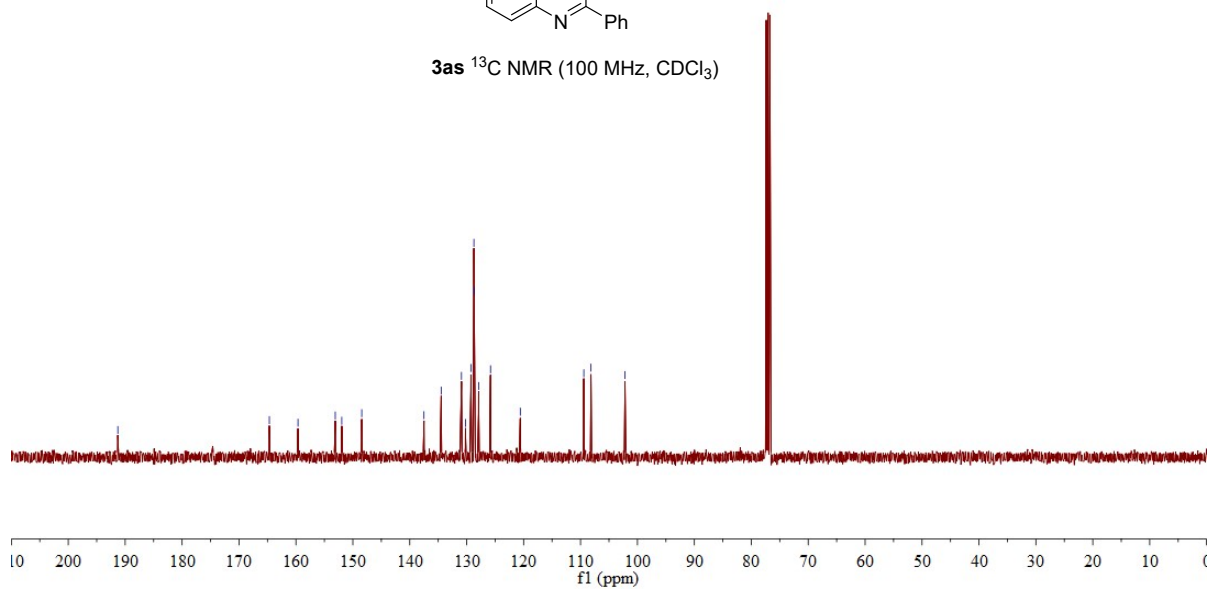
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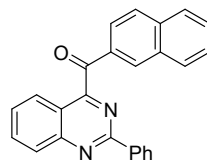
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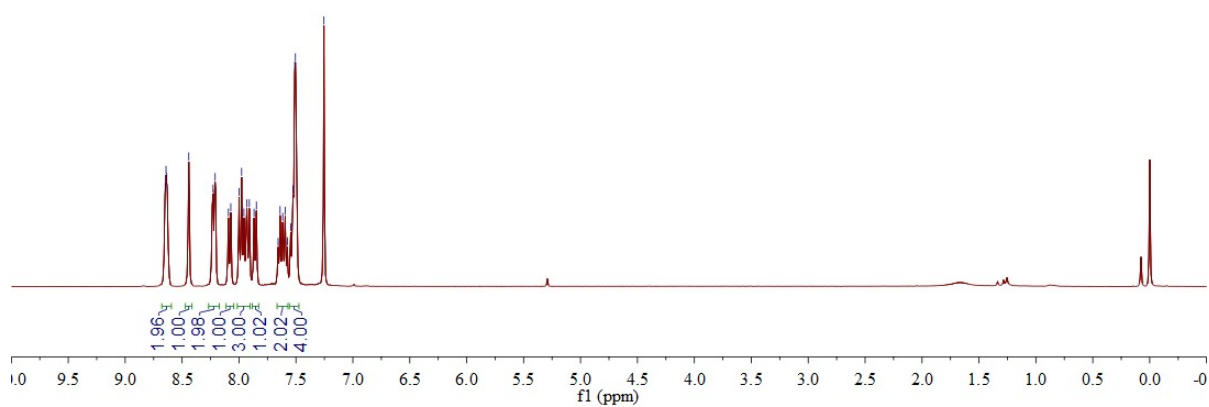
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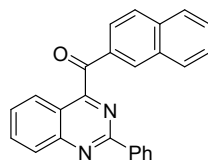
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7.504
7.254



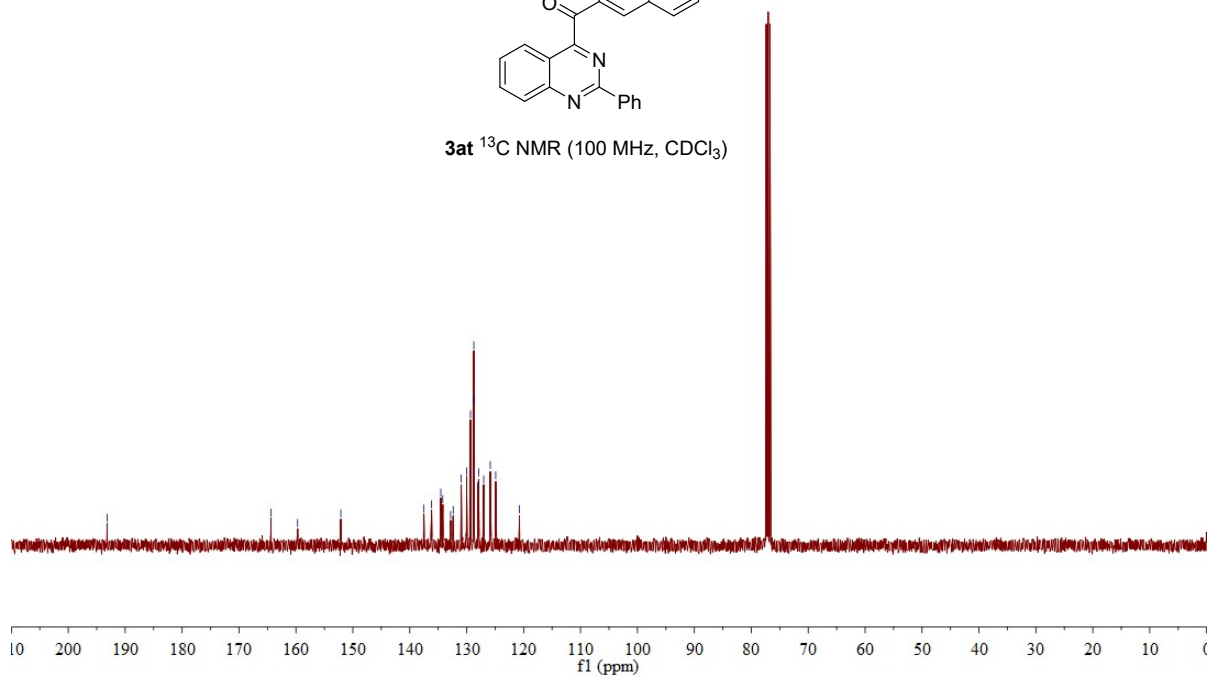
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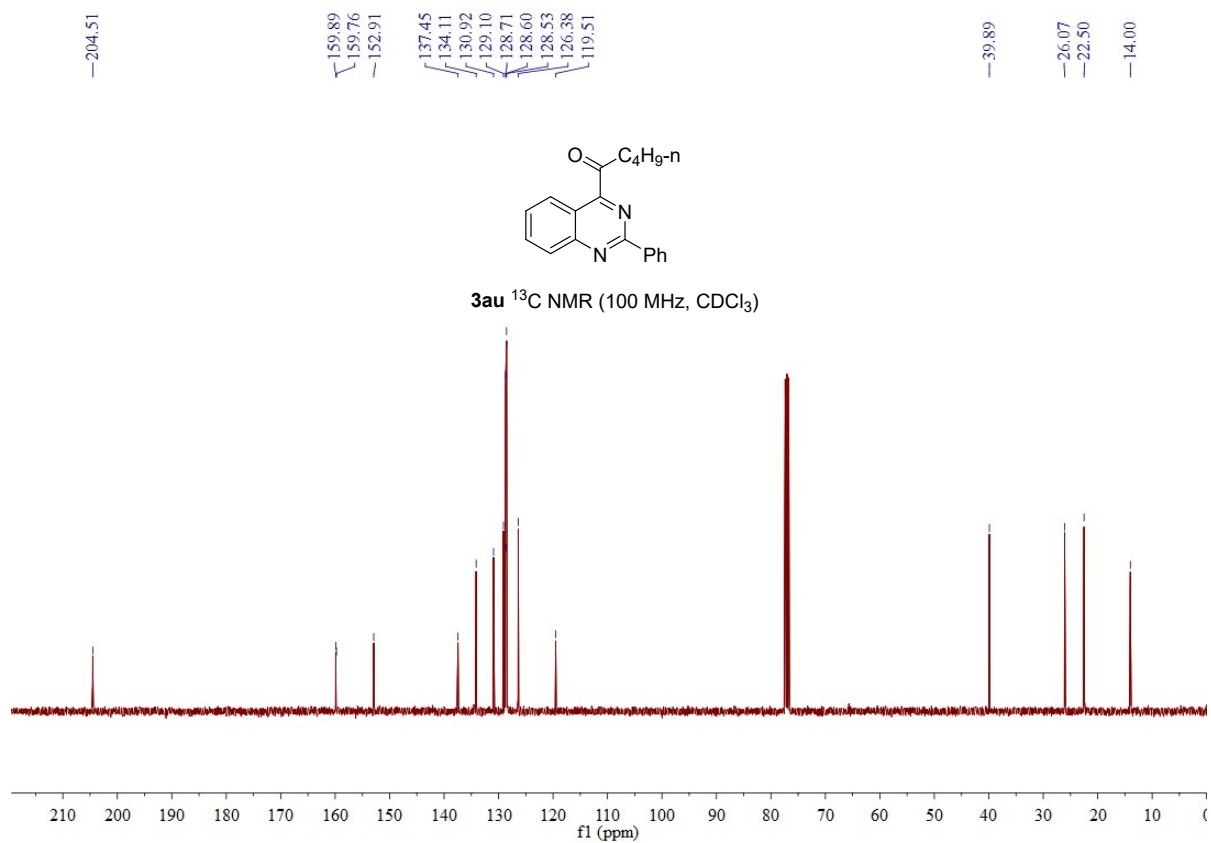
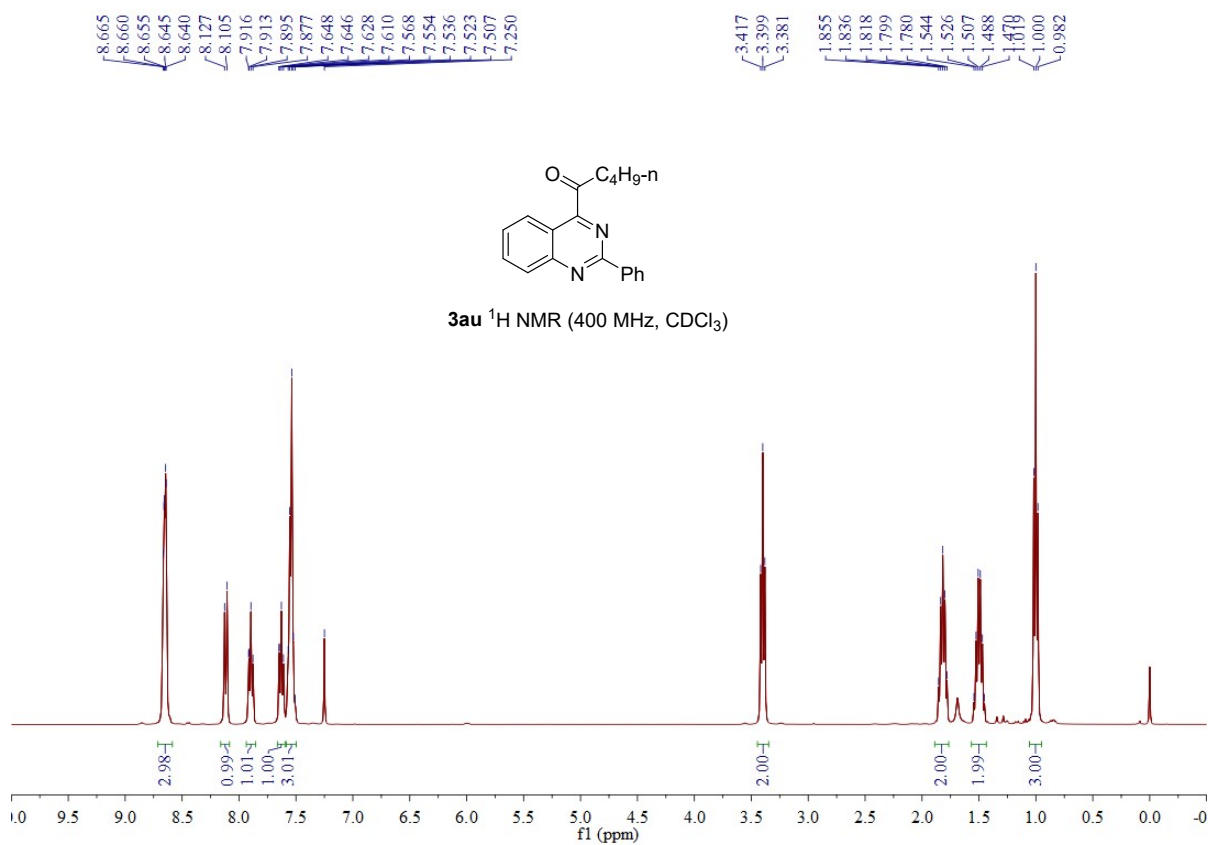


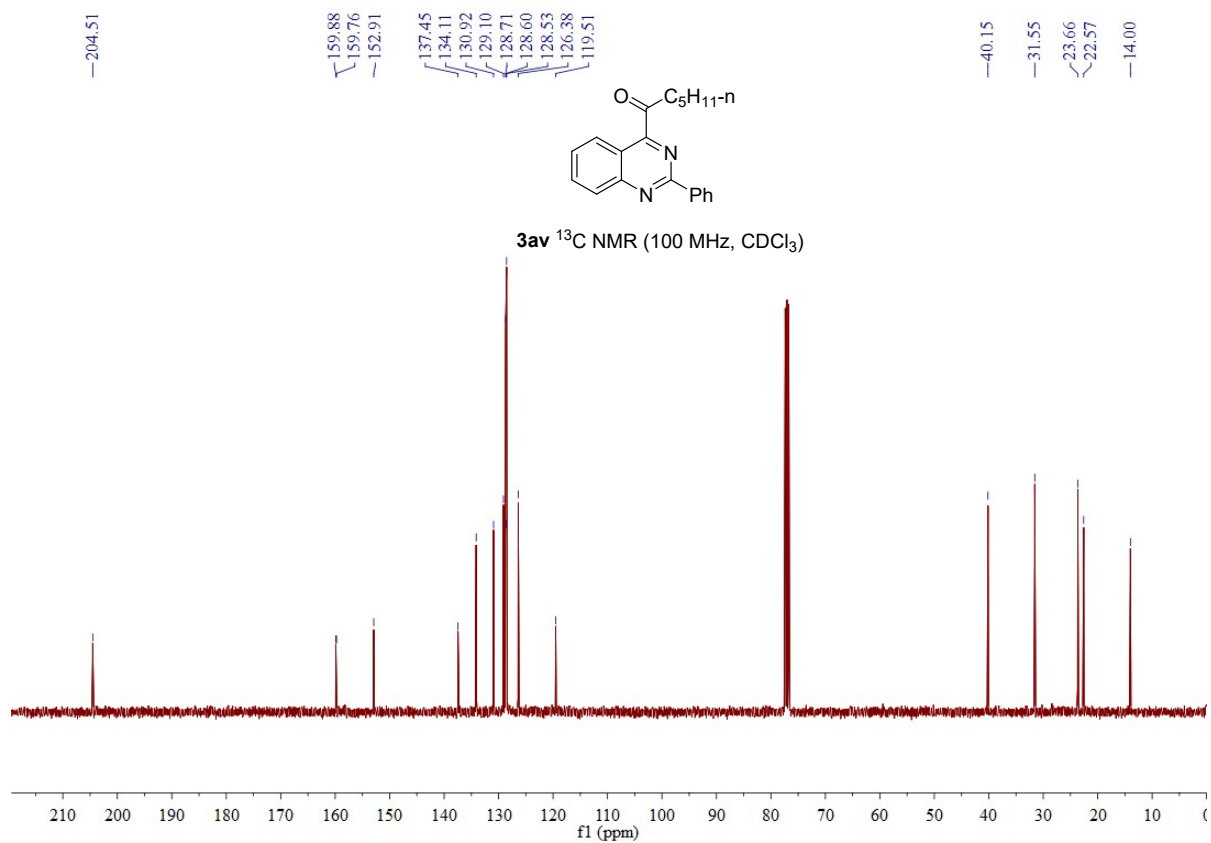
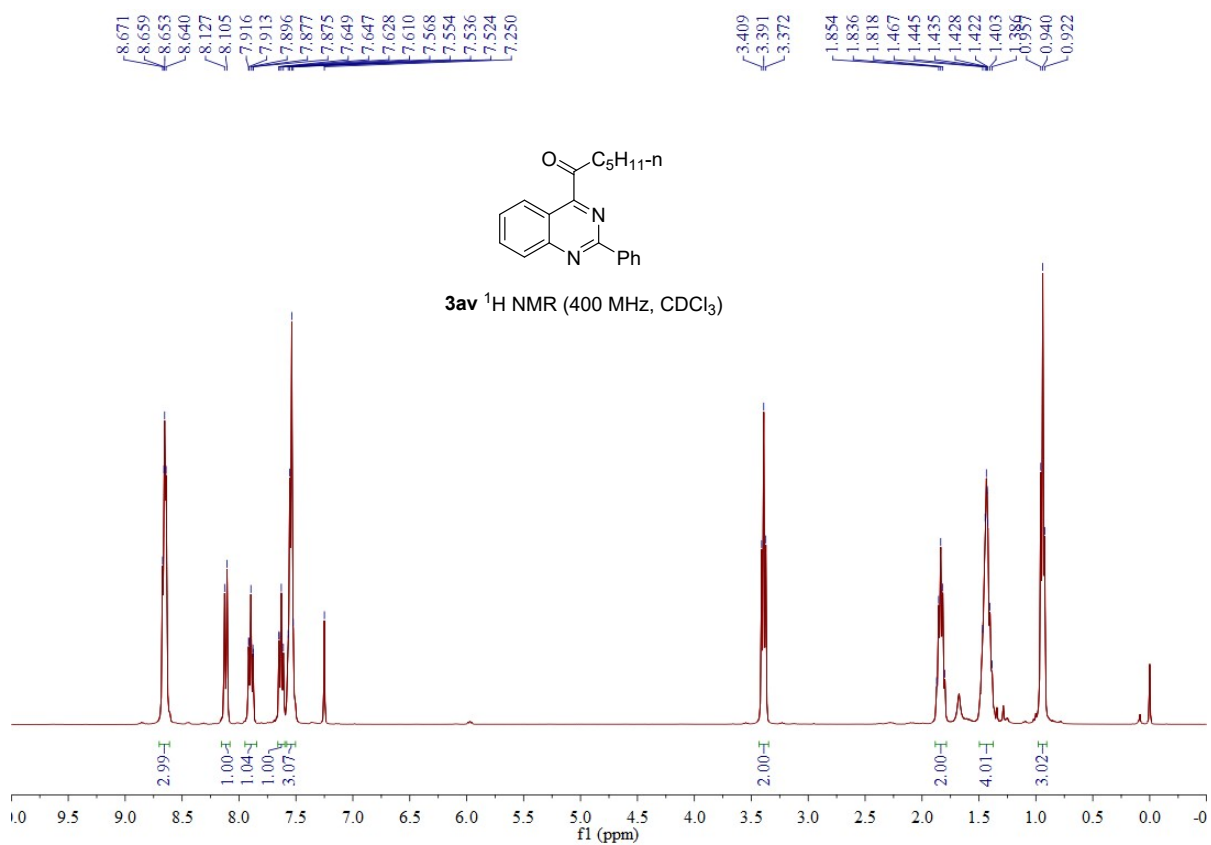
193.17
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152.11
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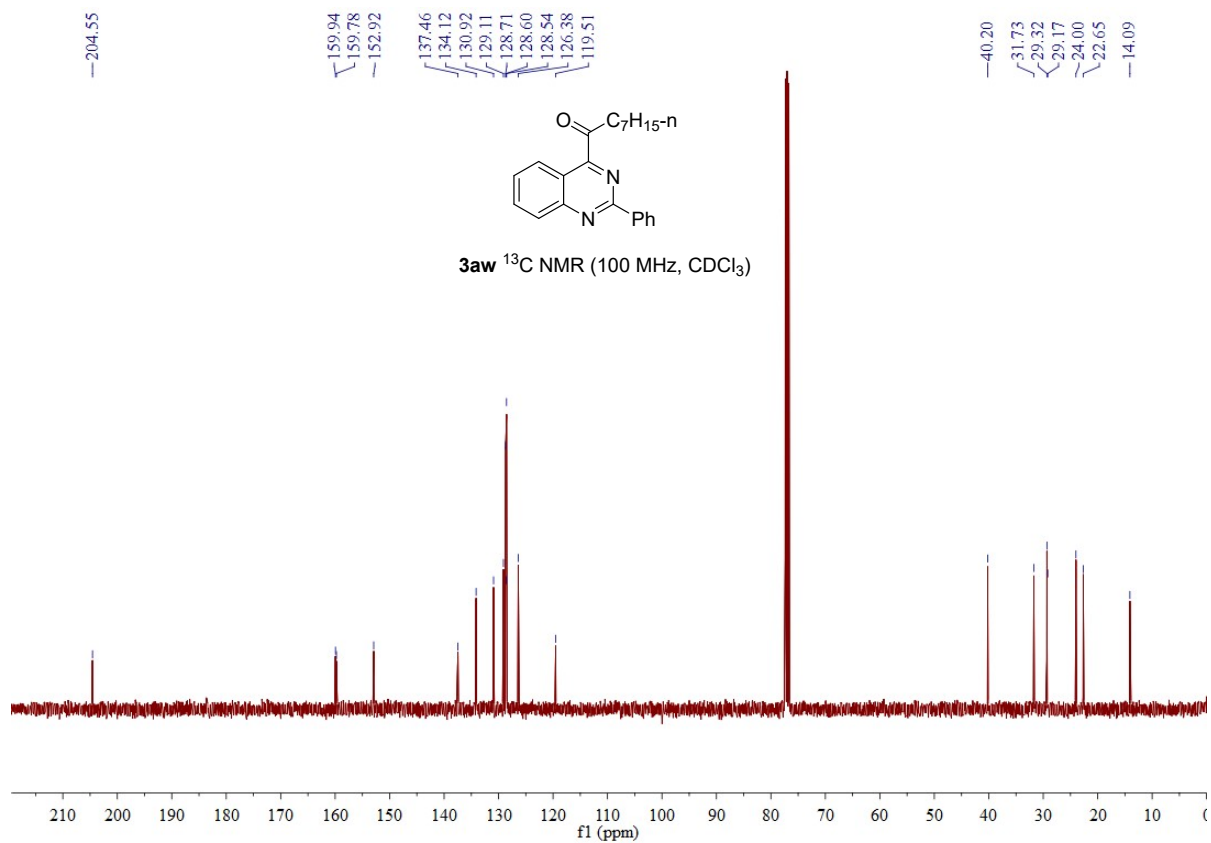
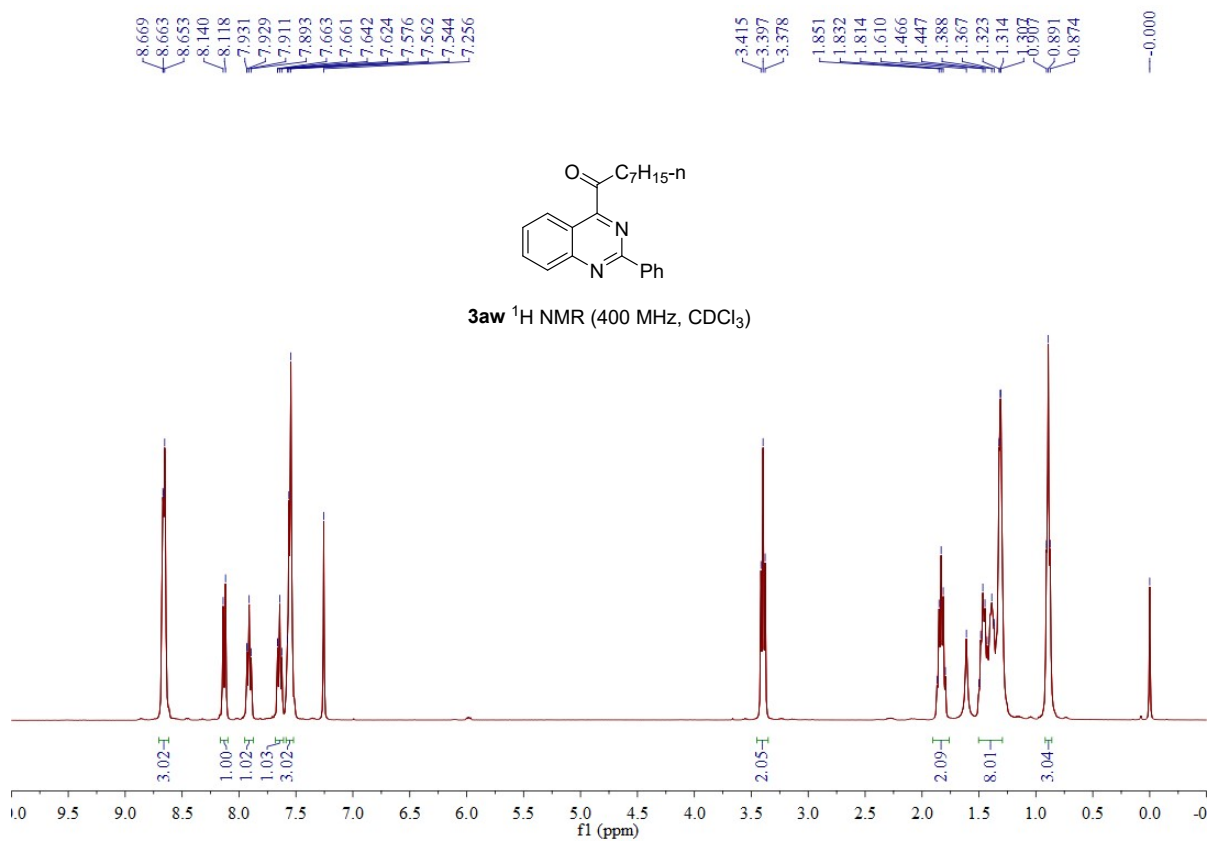


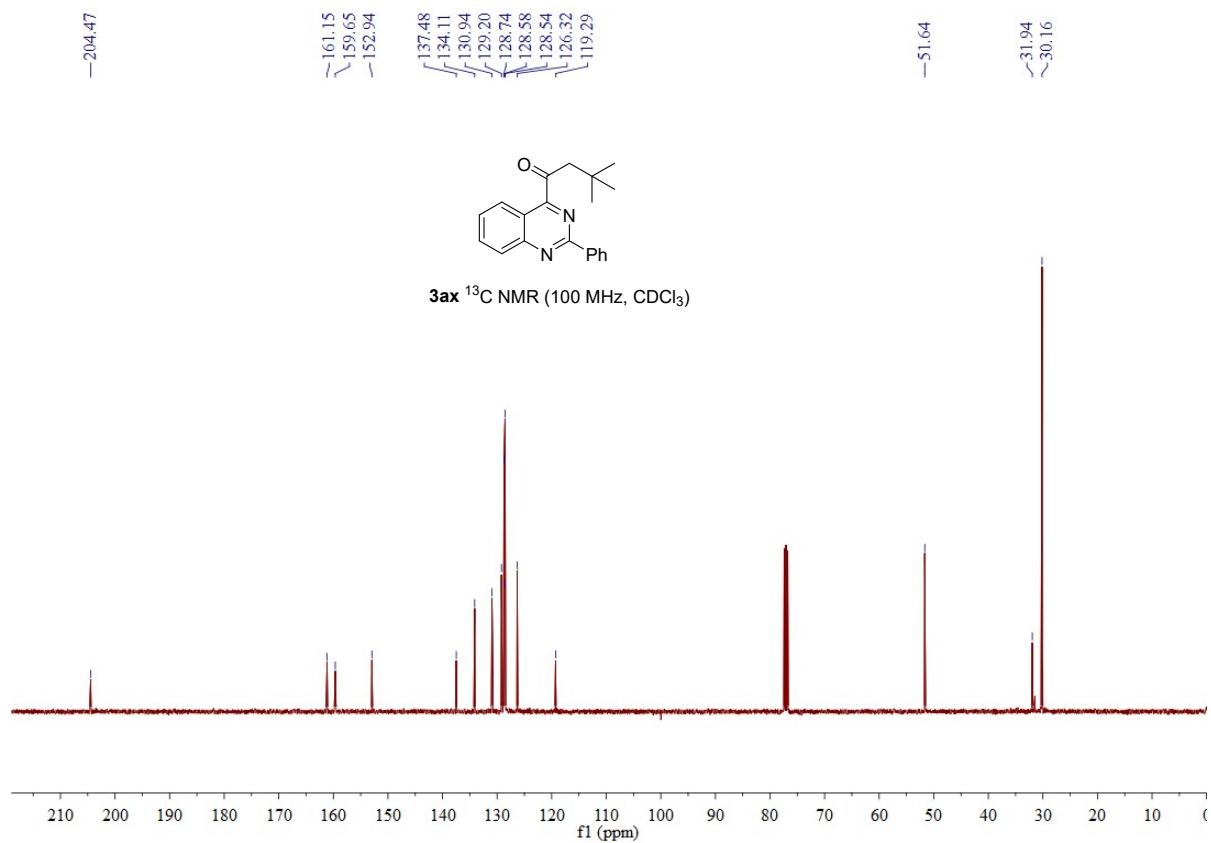
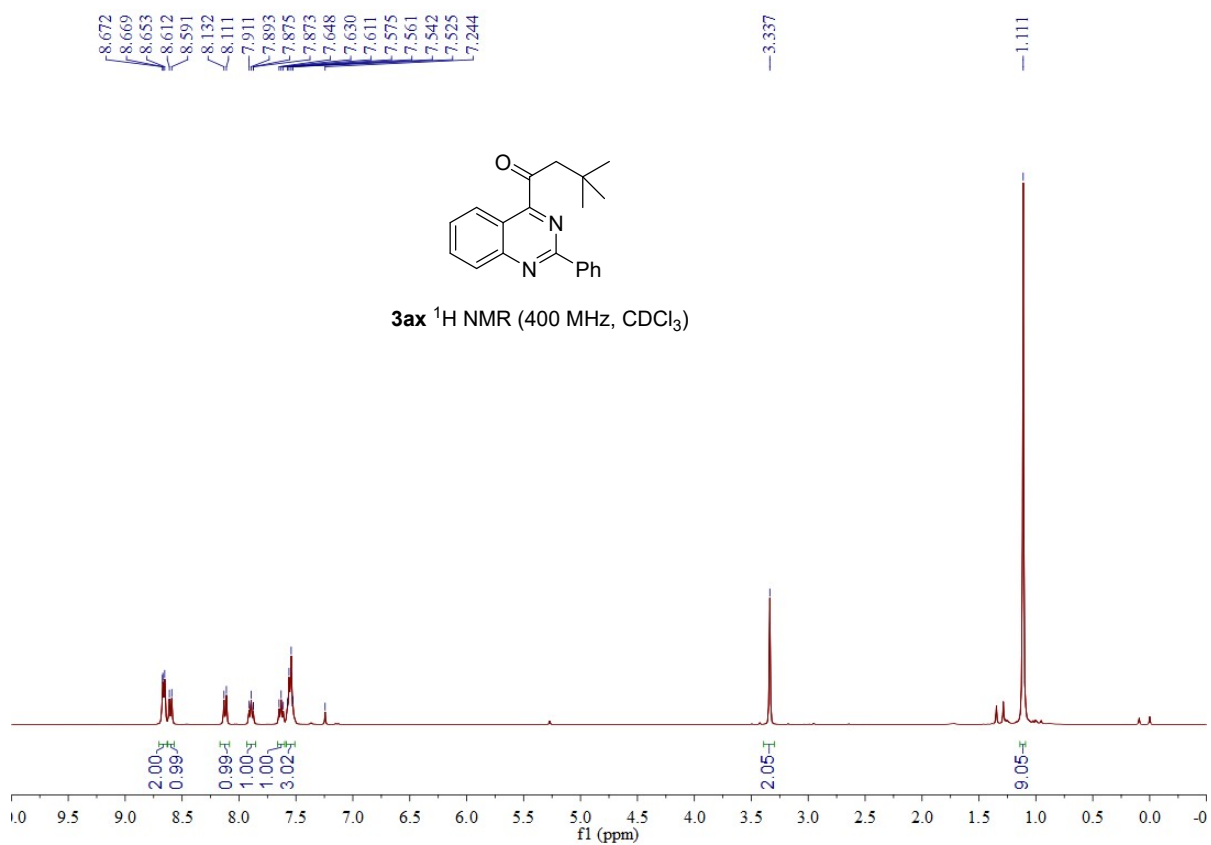
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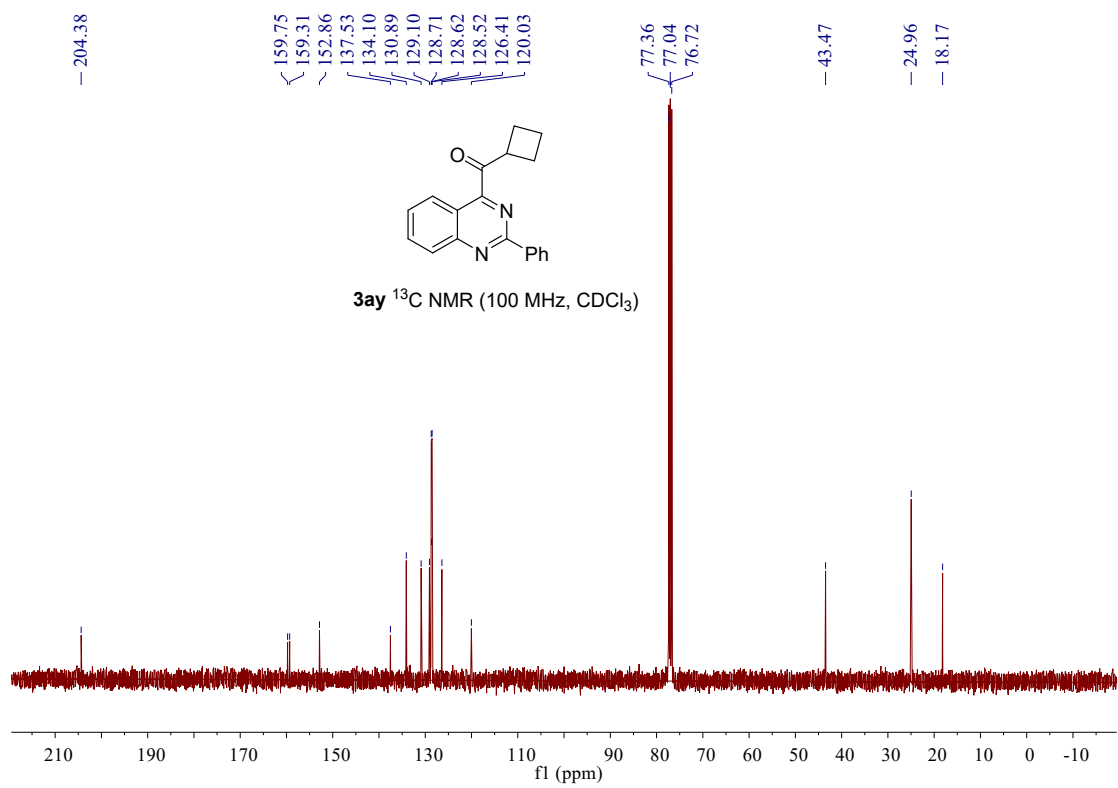
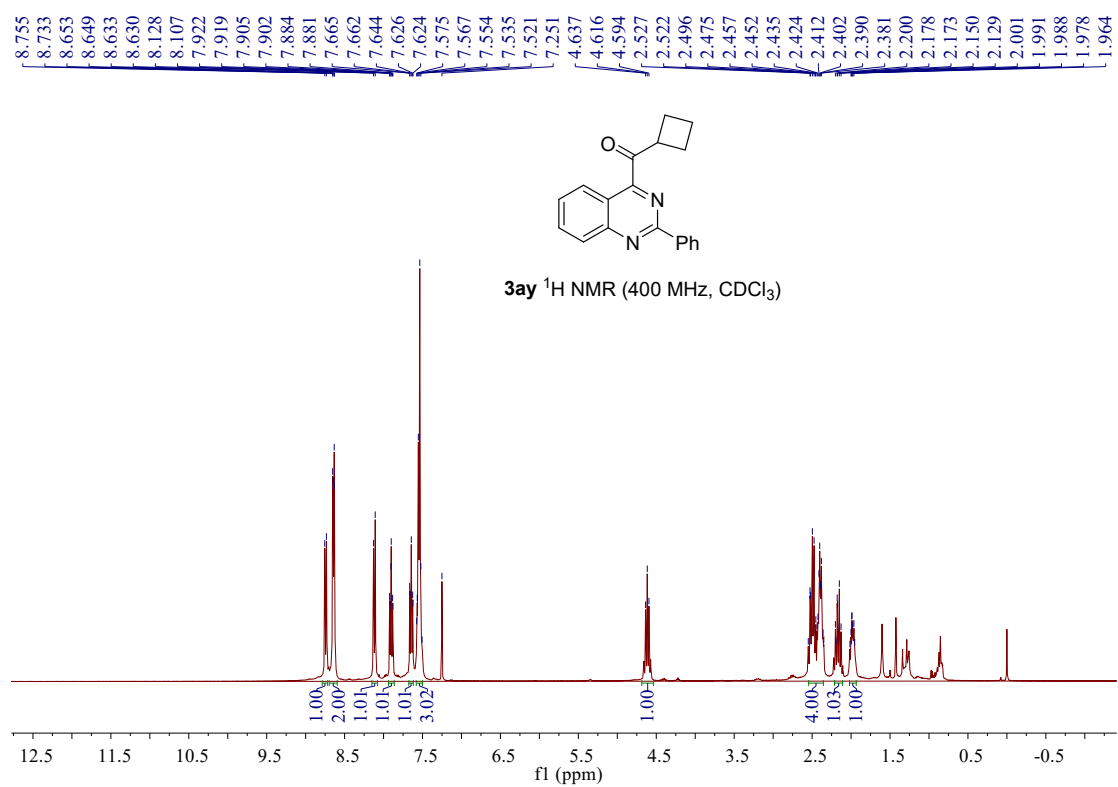




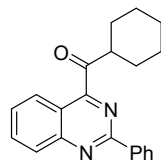




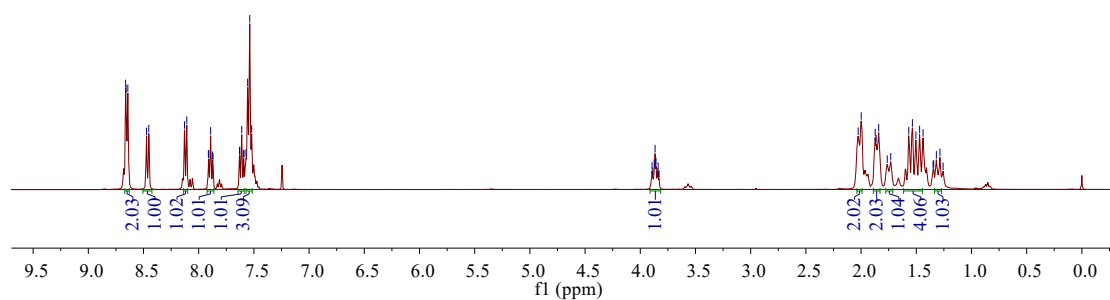




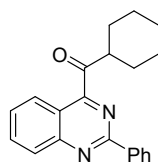
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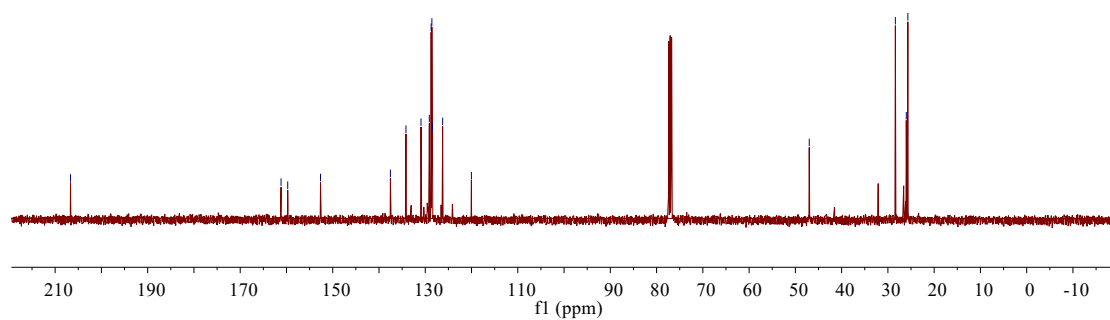
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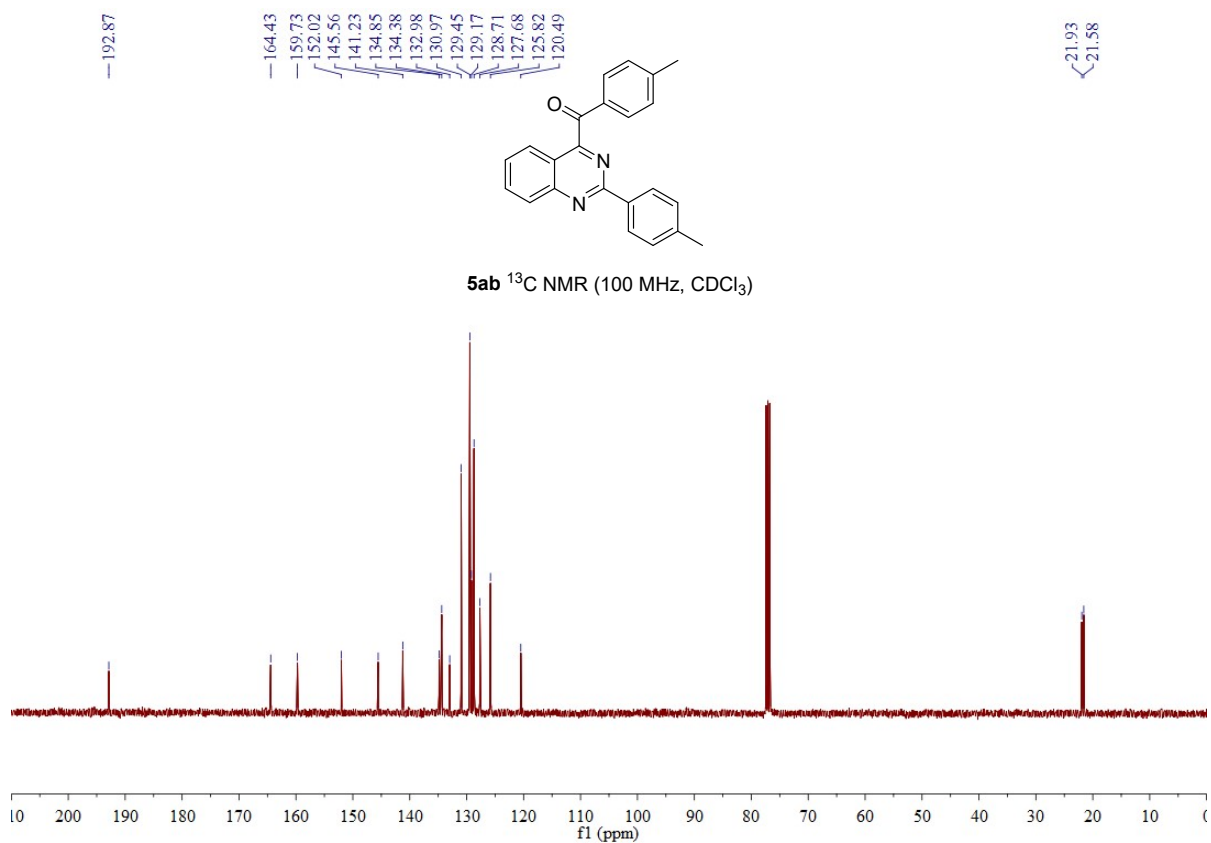
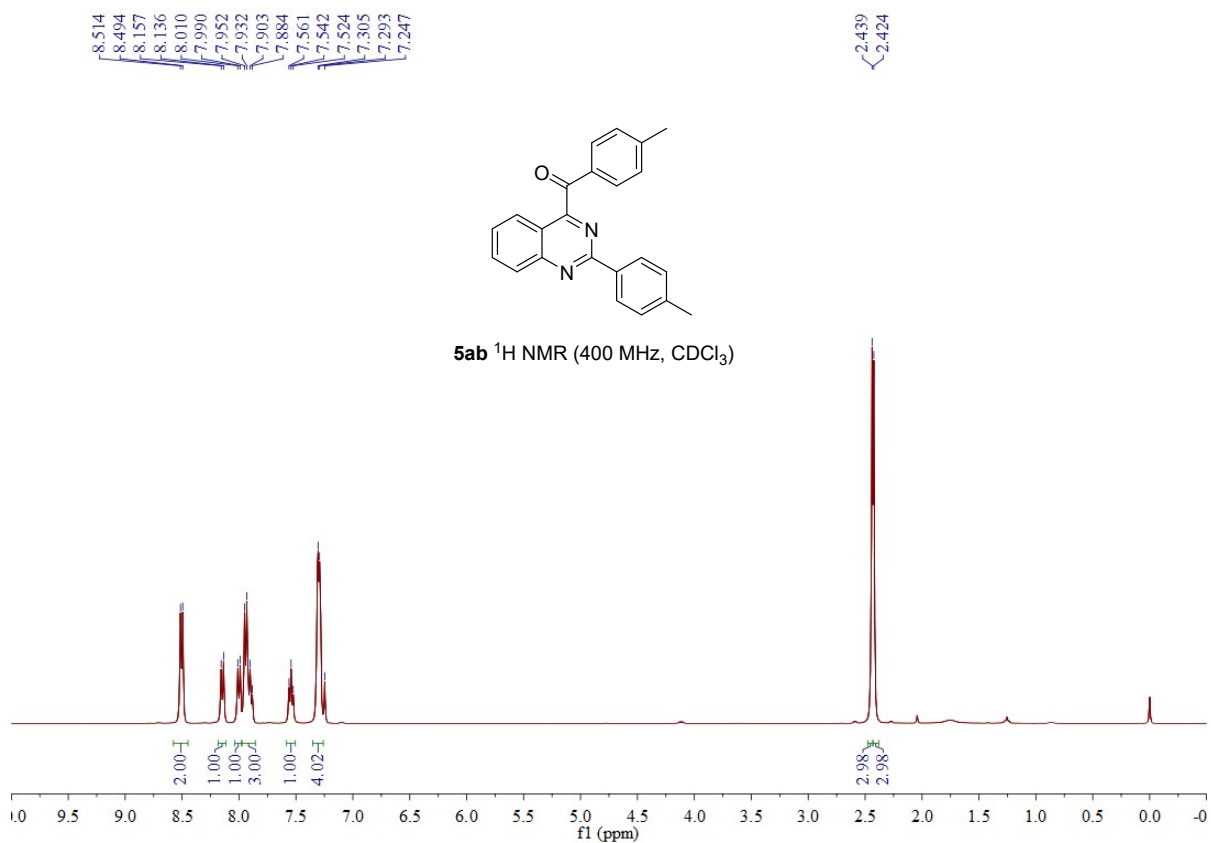
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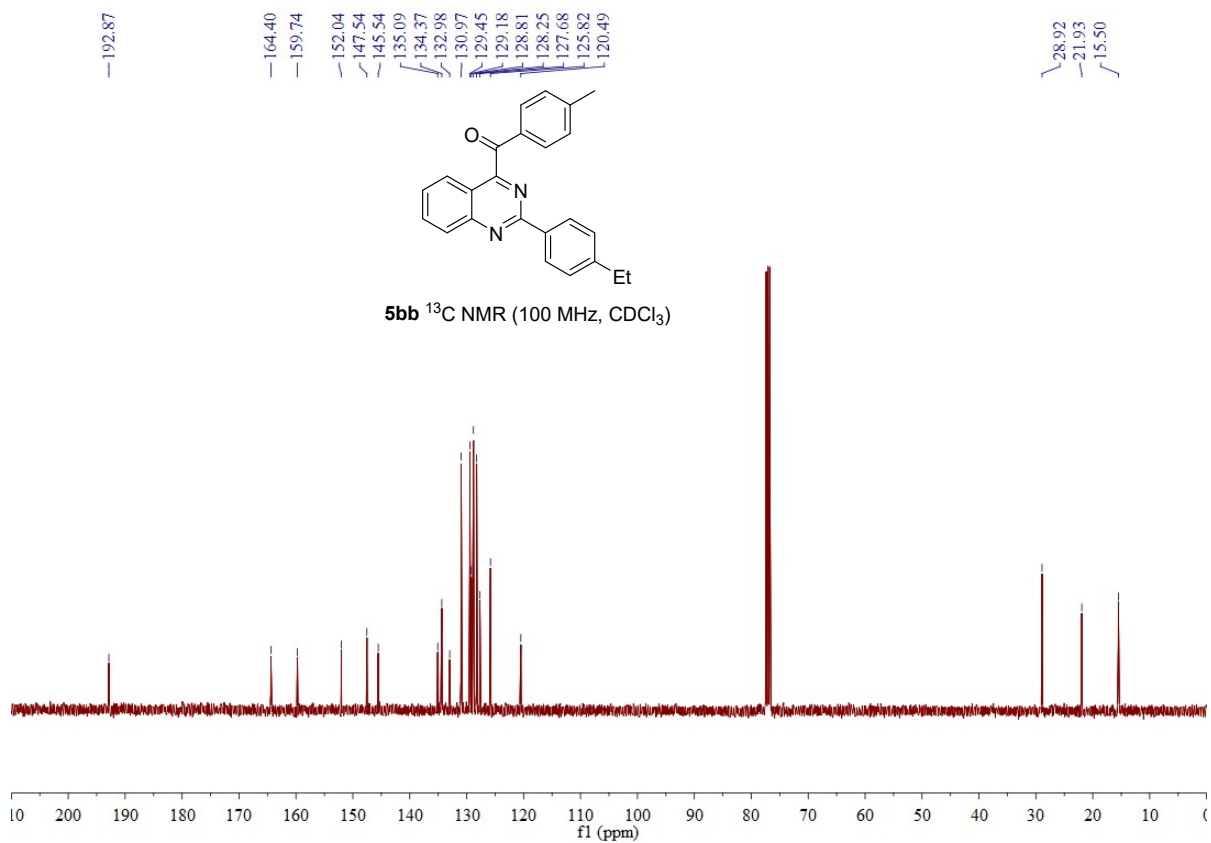
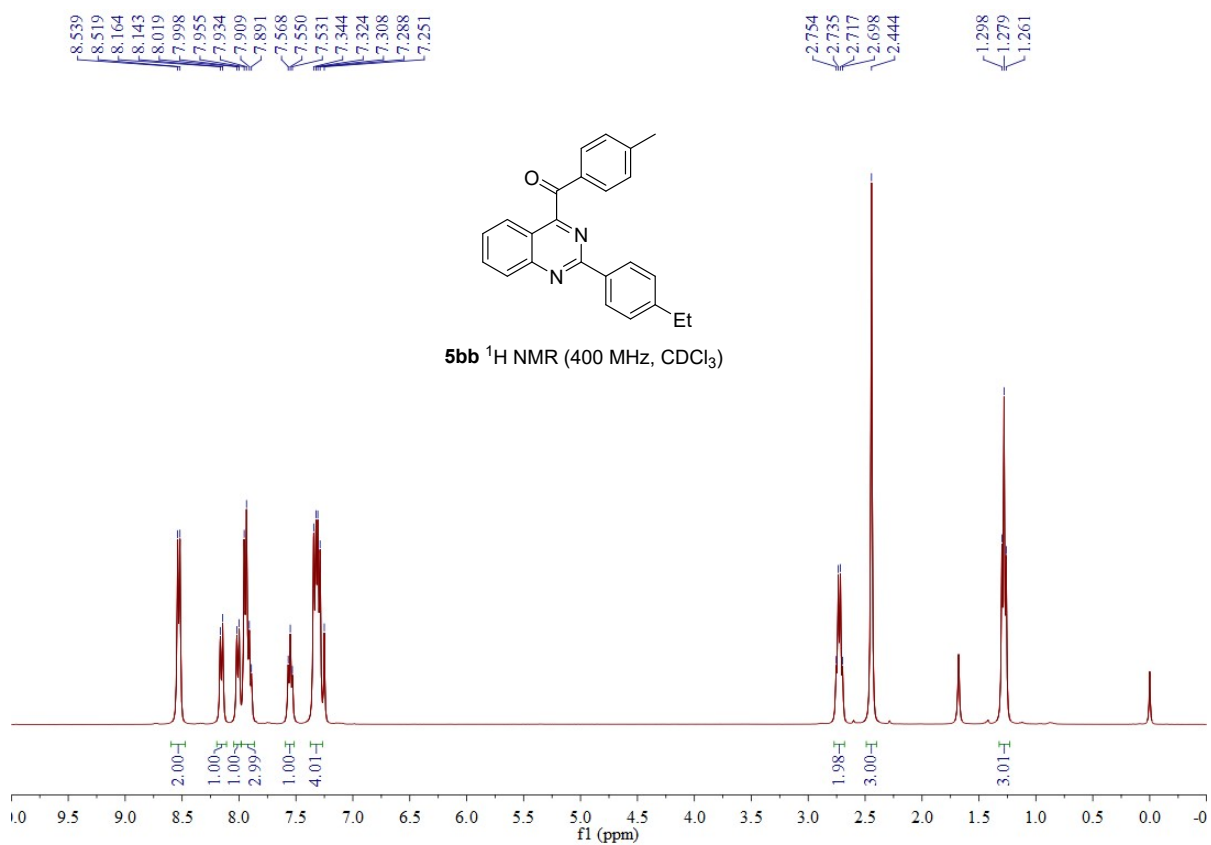


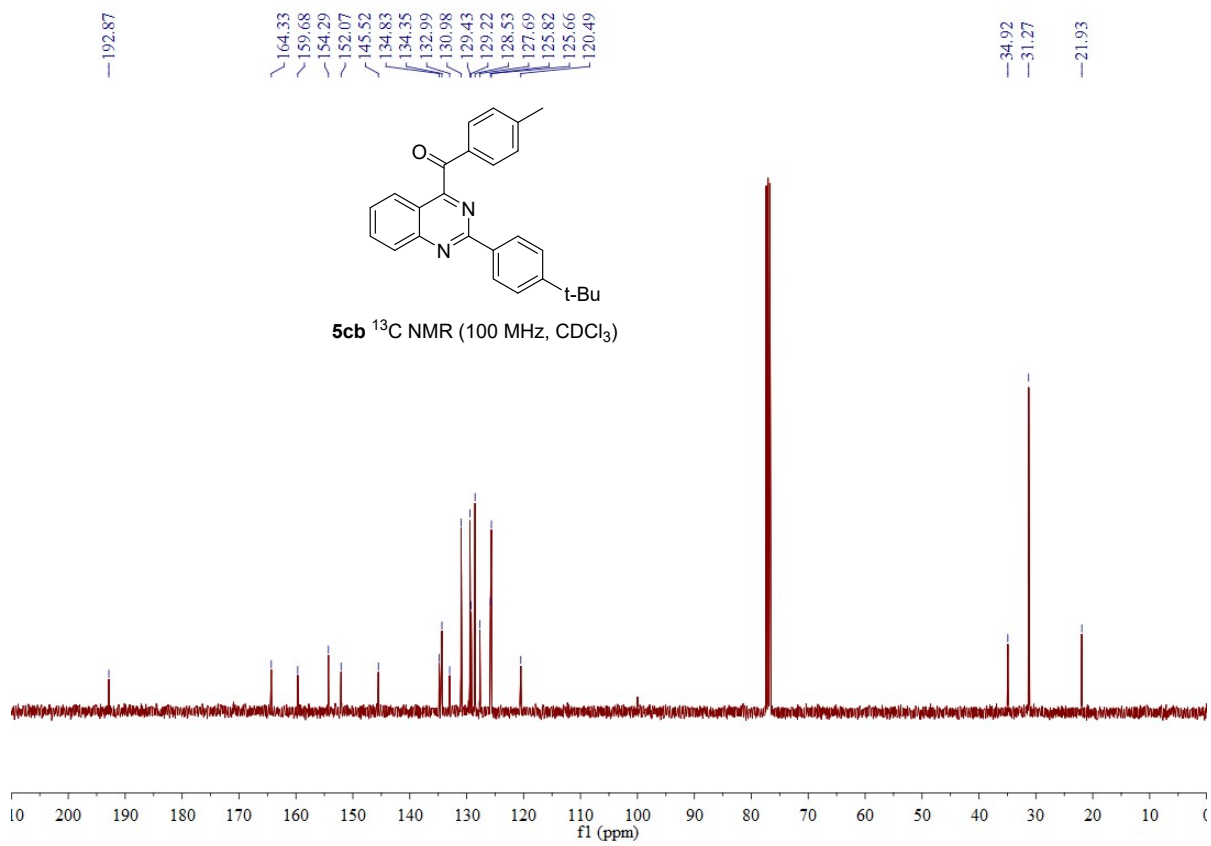
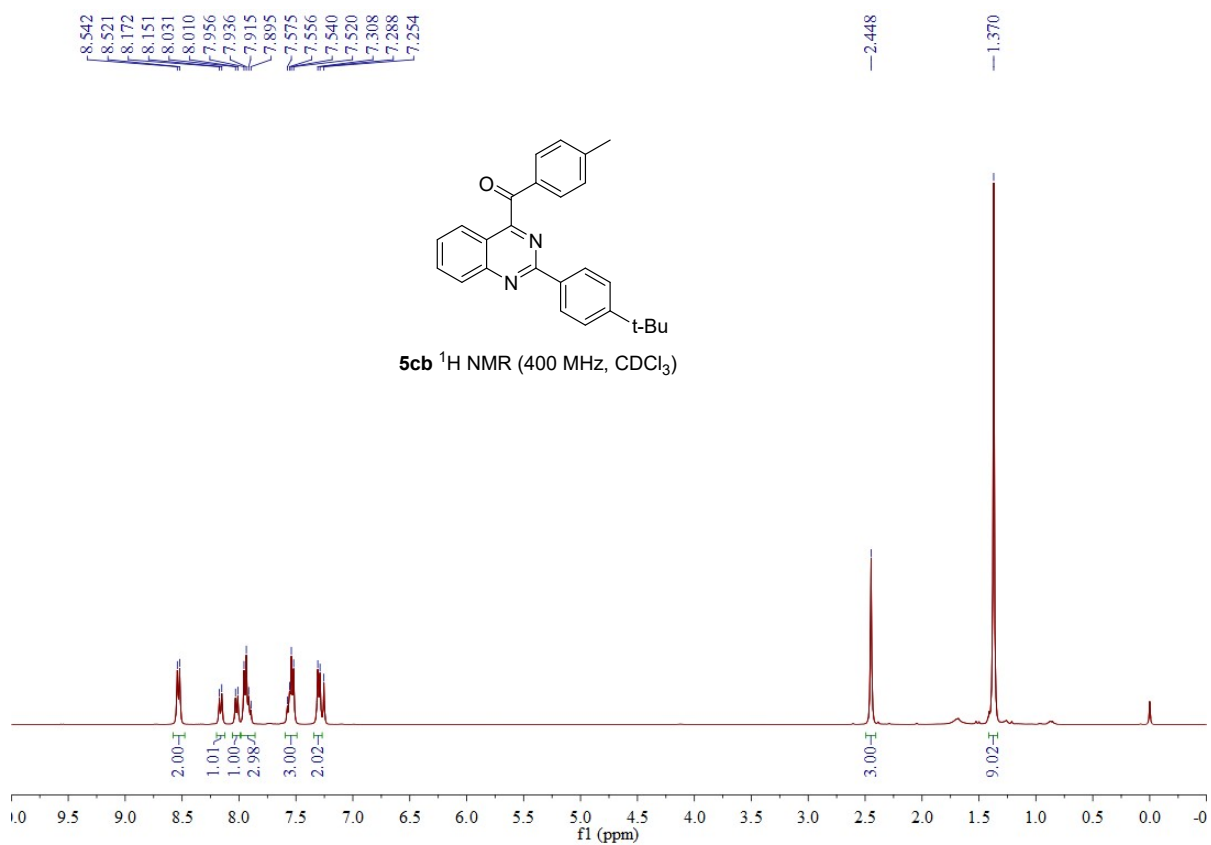
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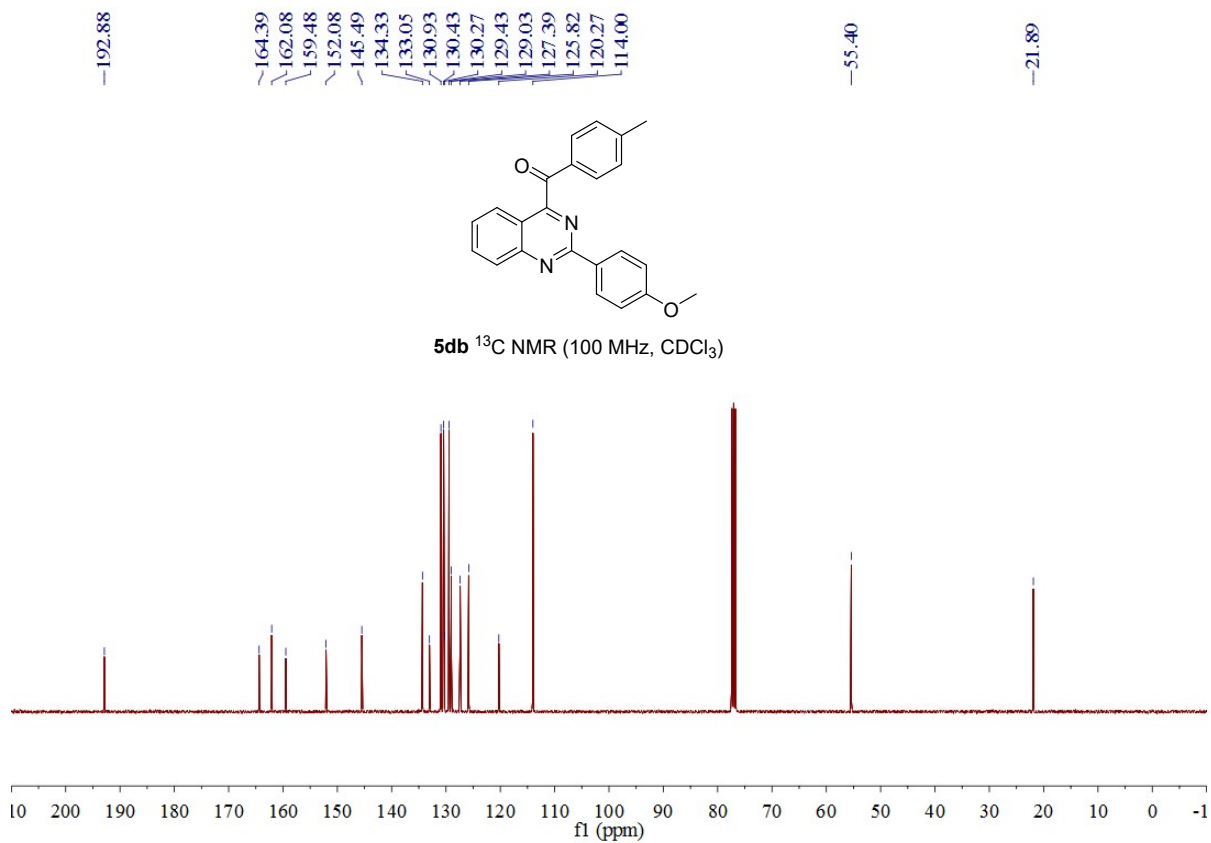
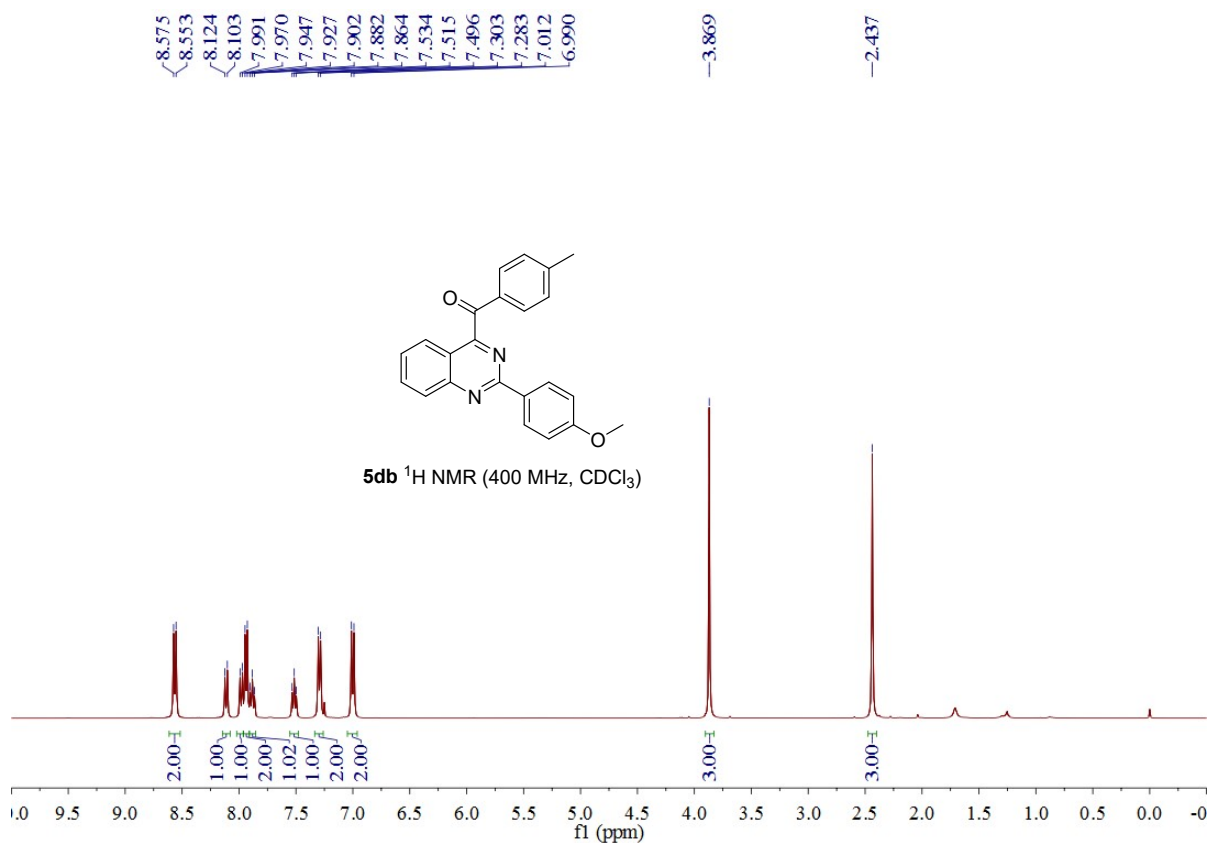


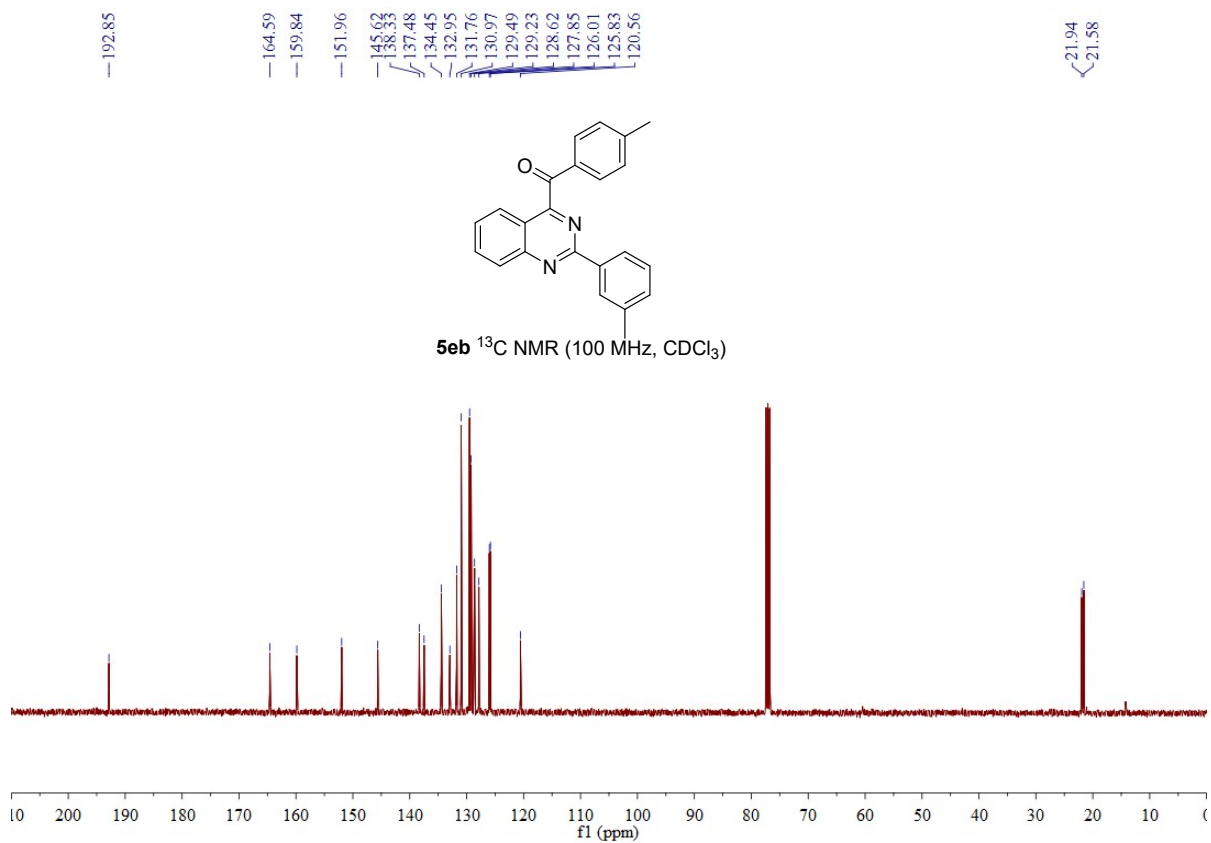
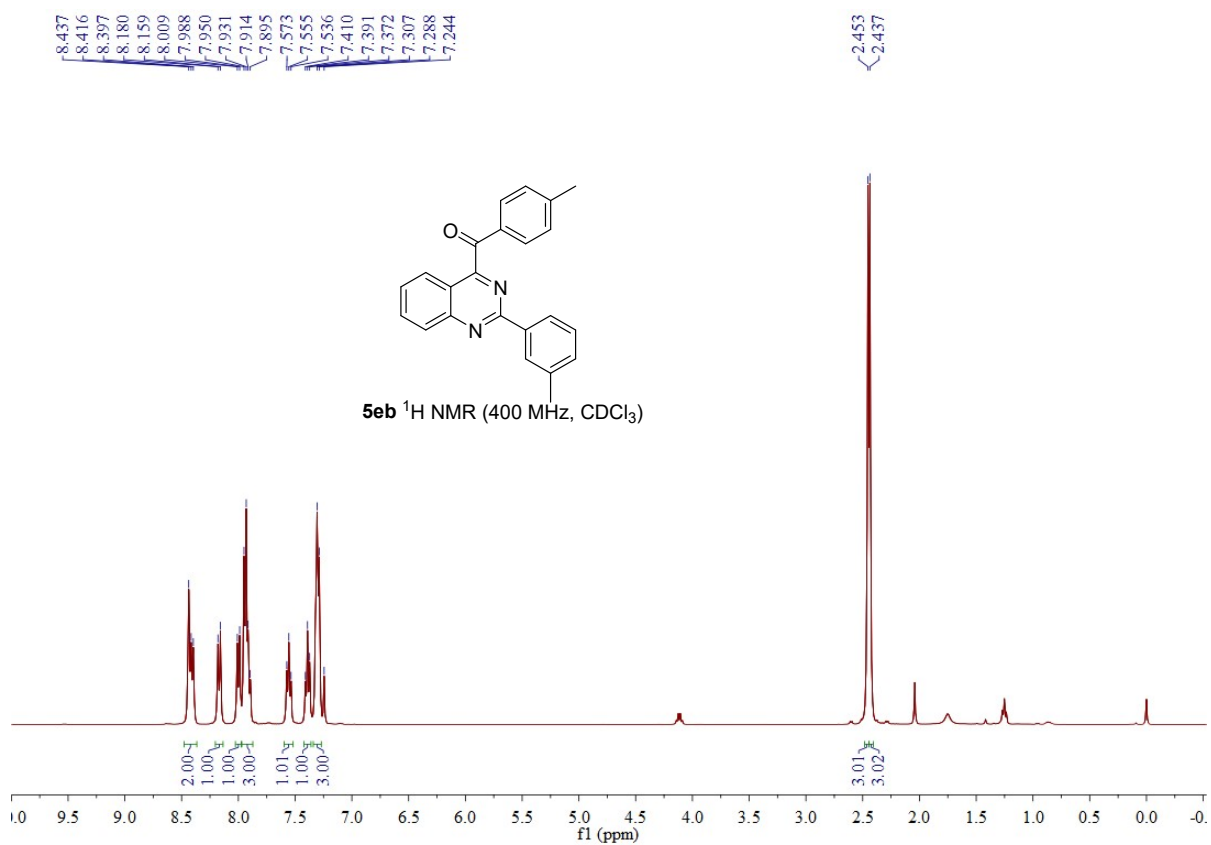
Copy of Products 5 NMR

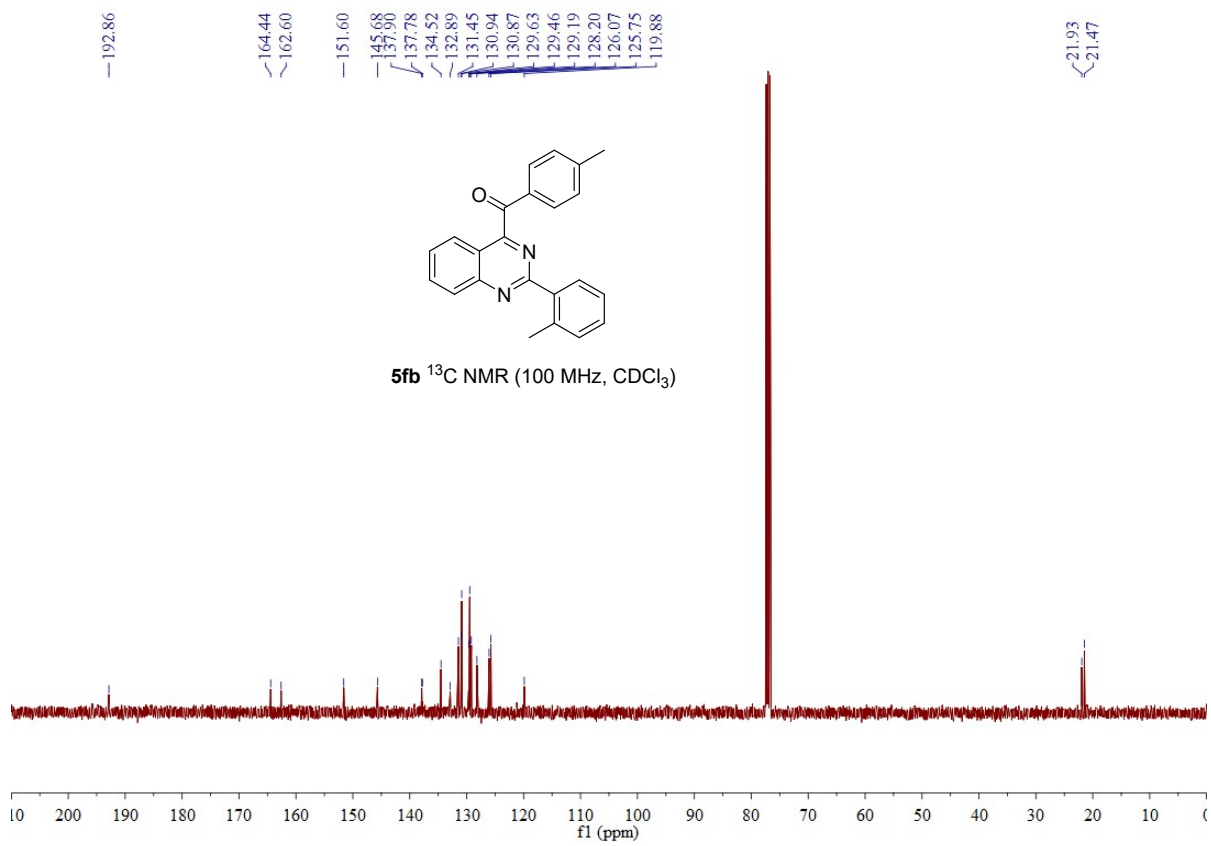
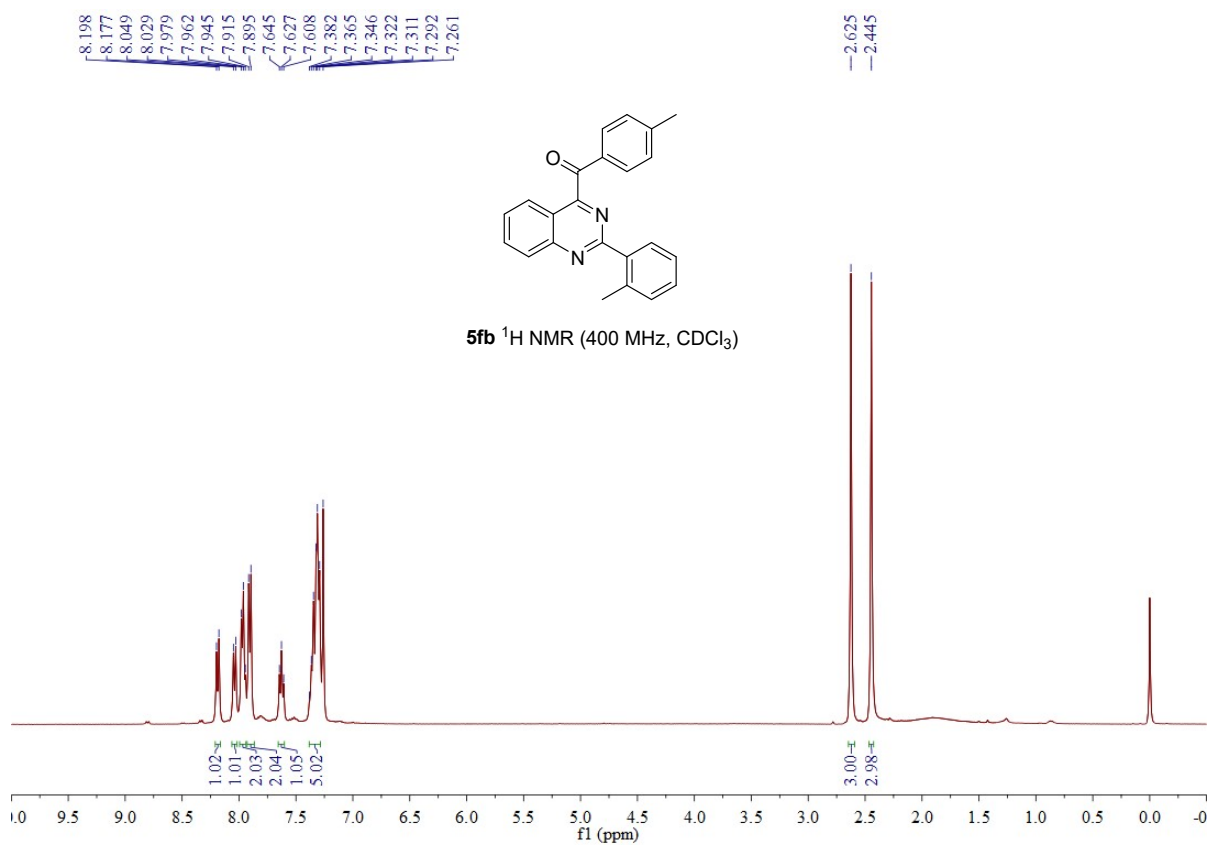


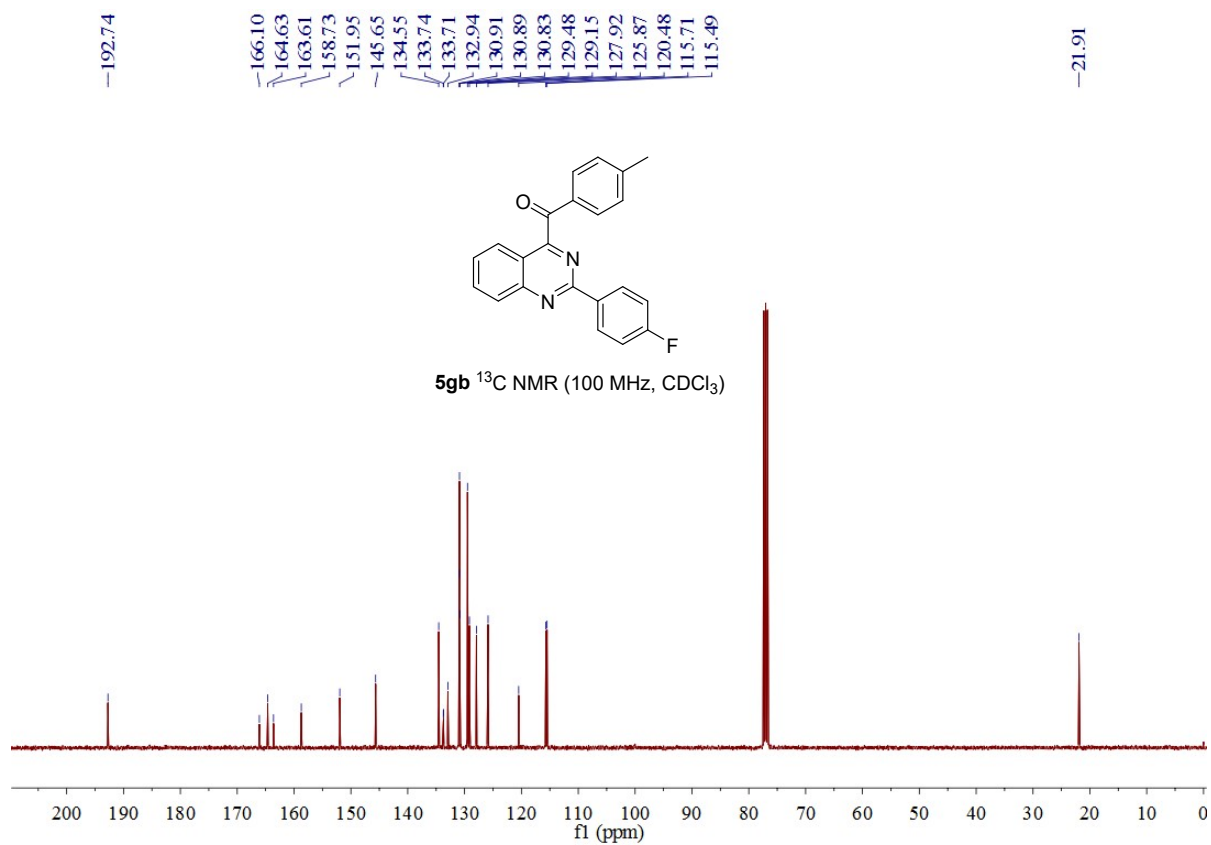
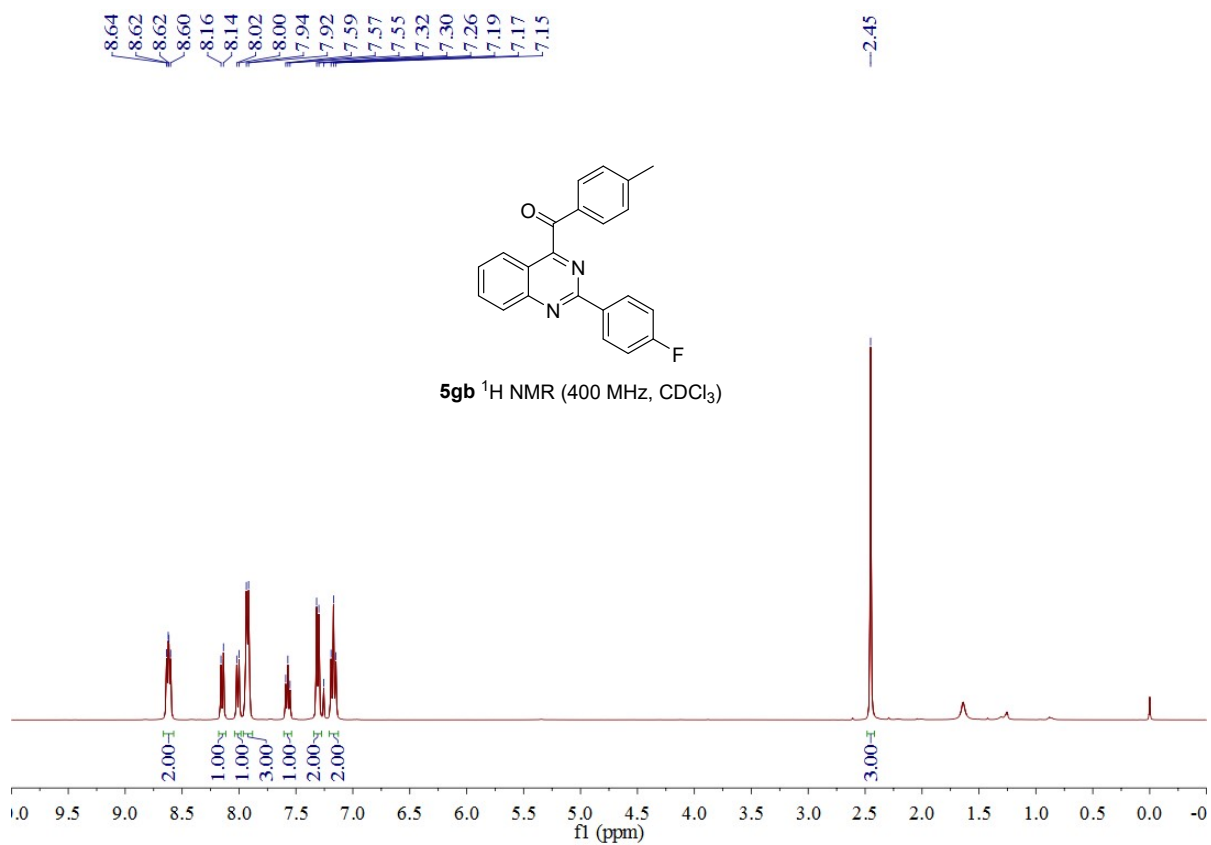


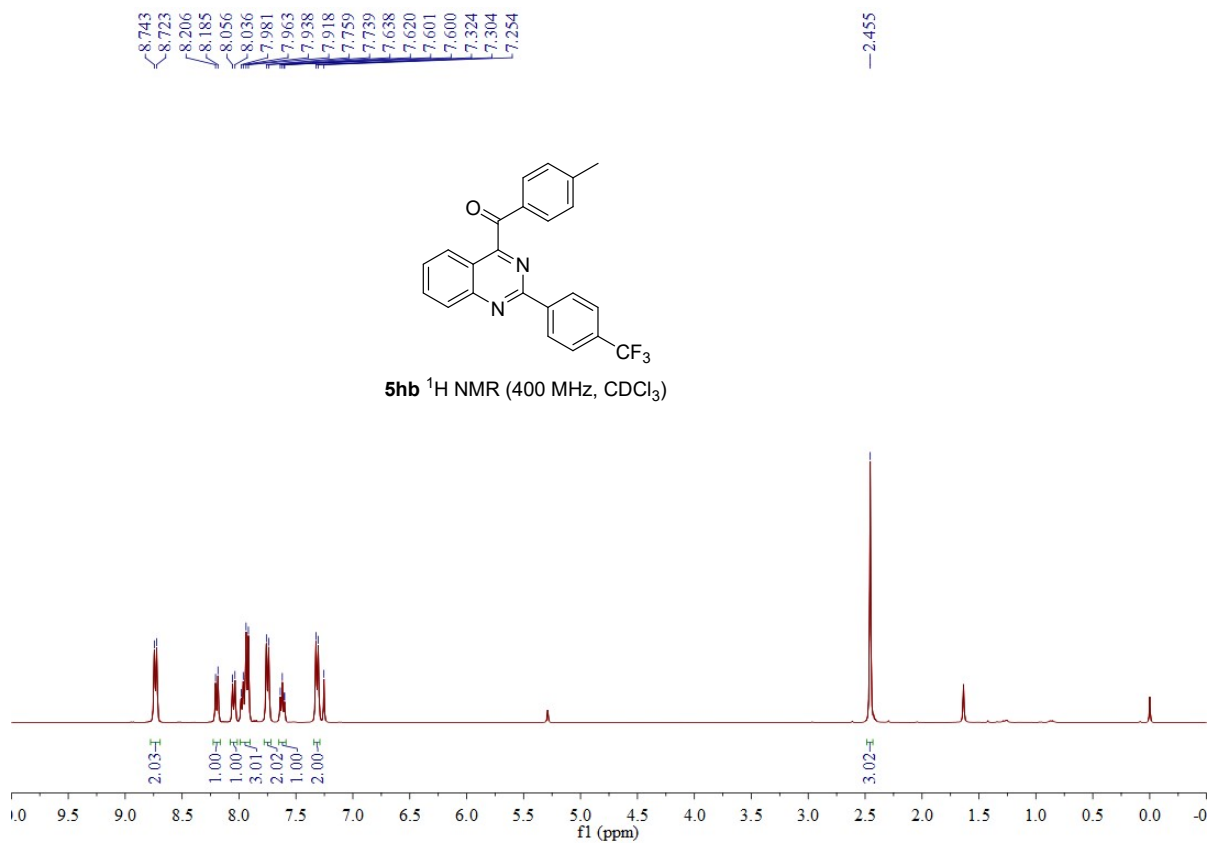
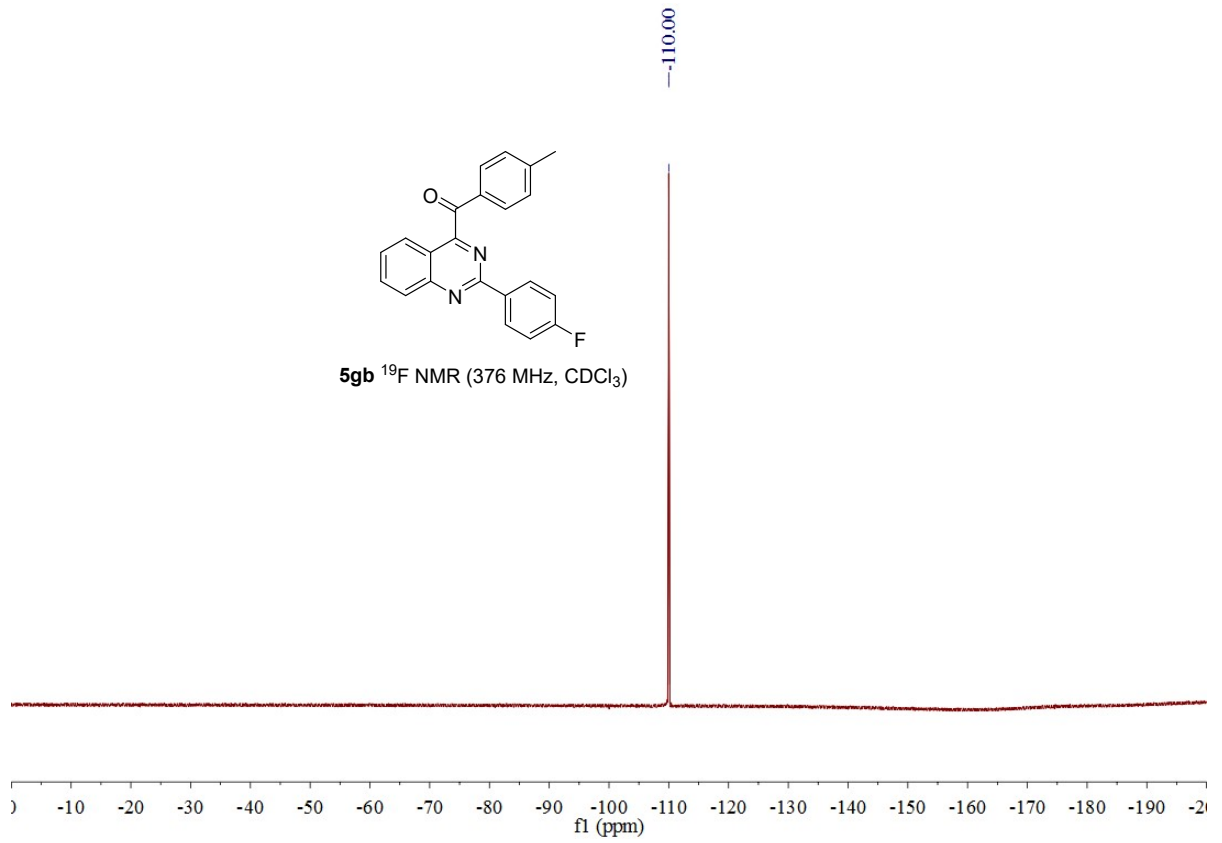


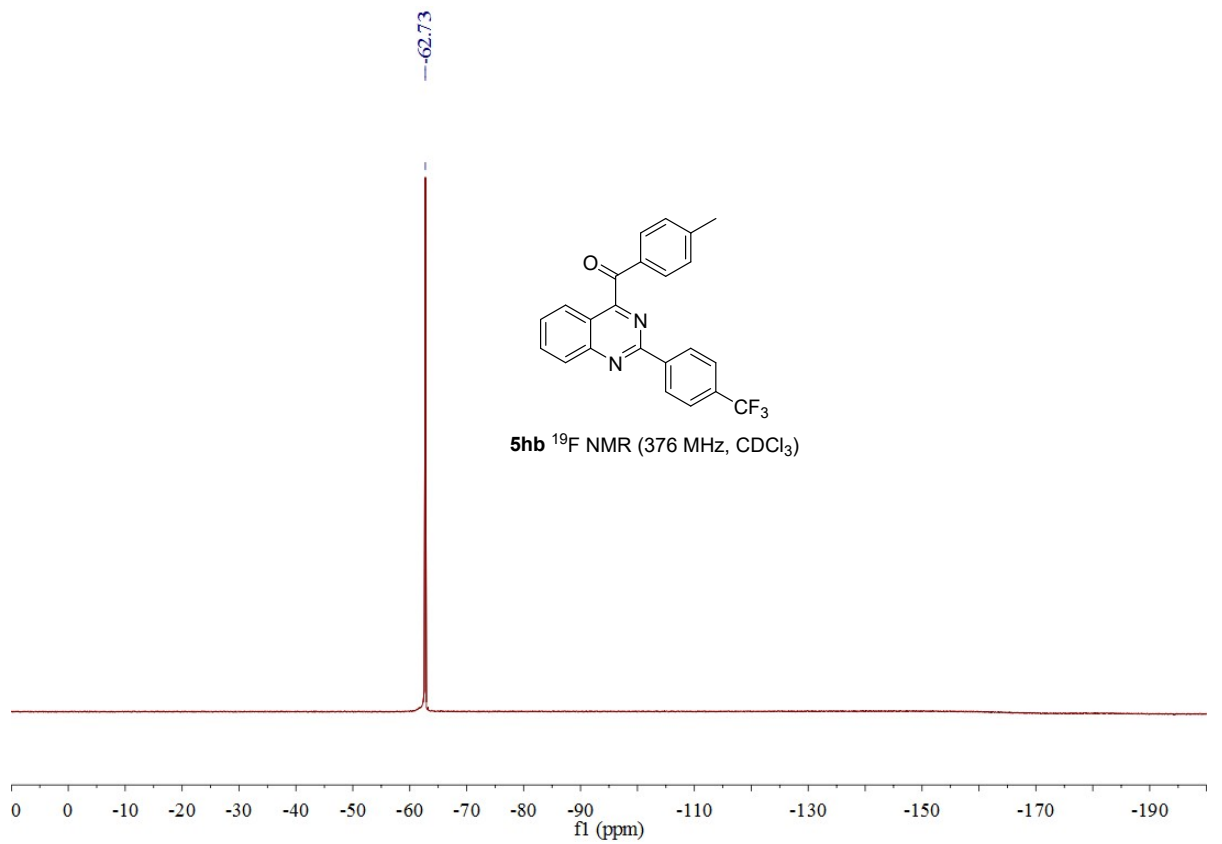
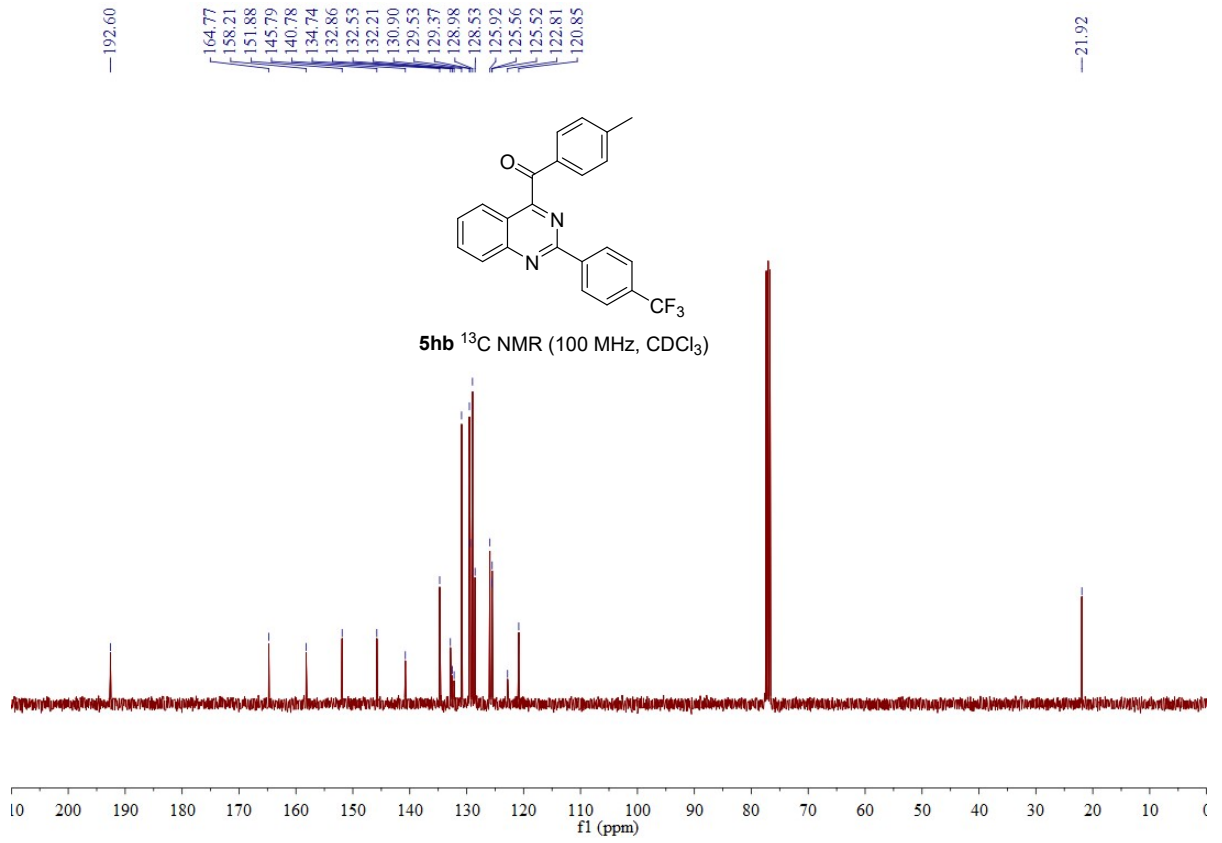


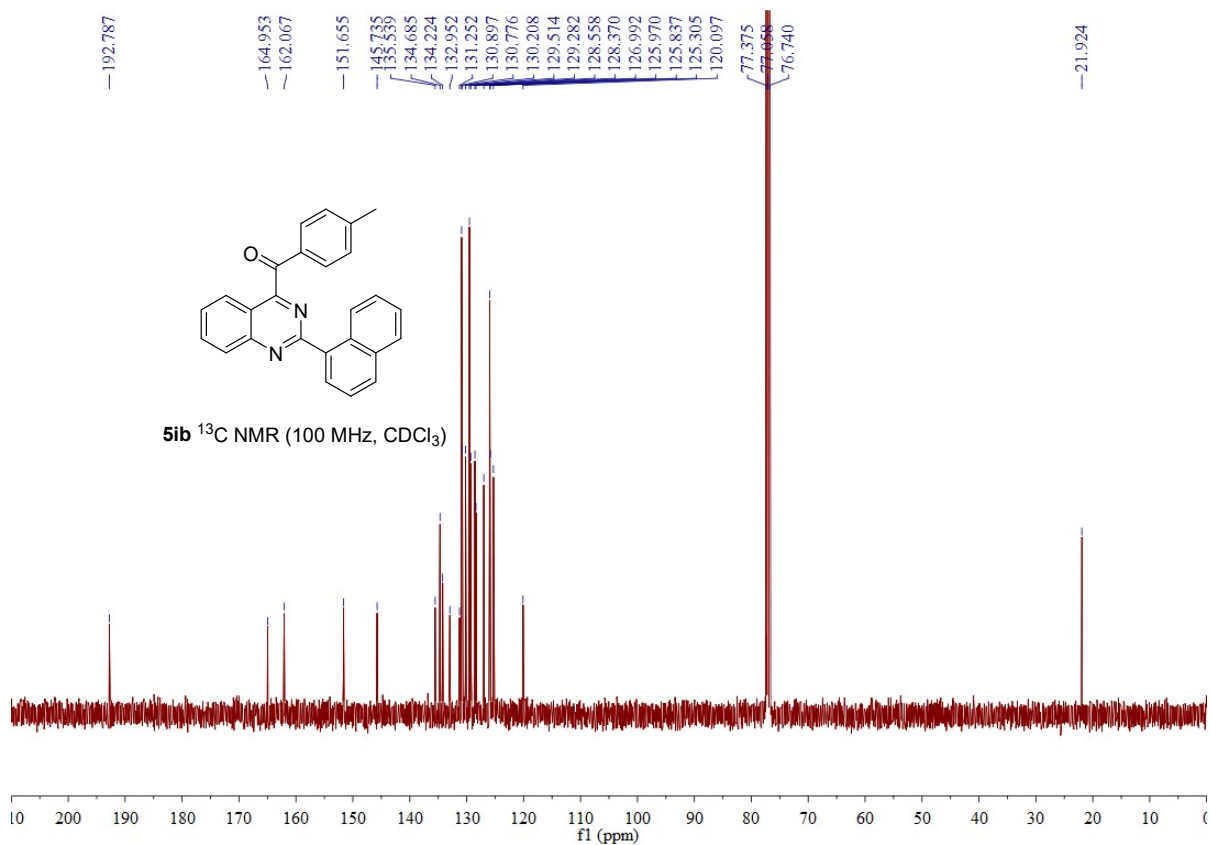
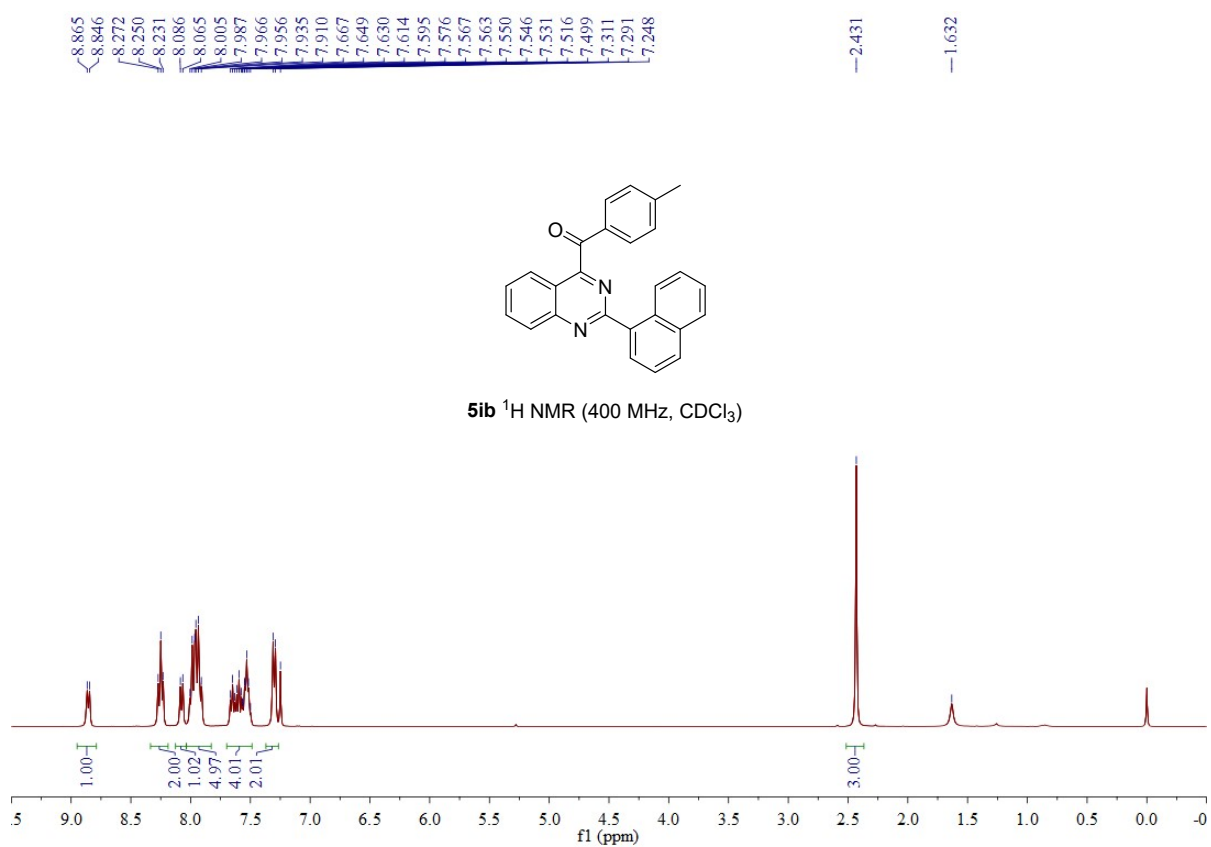


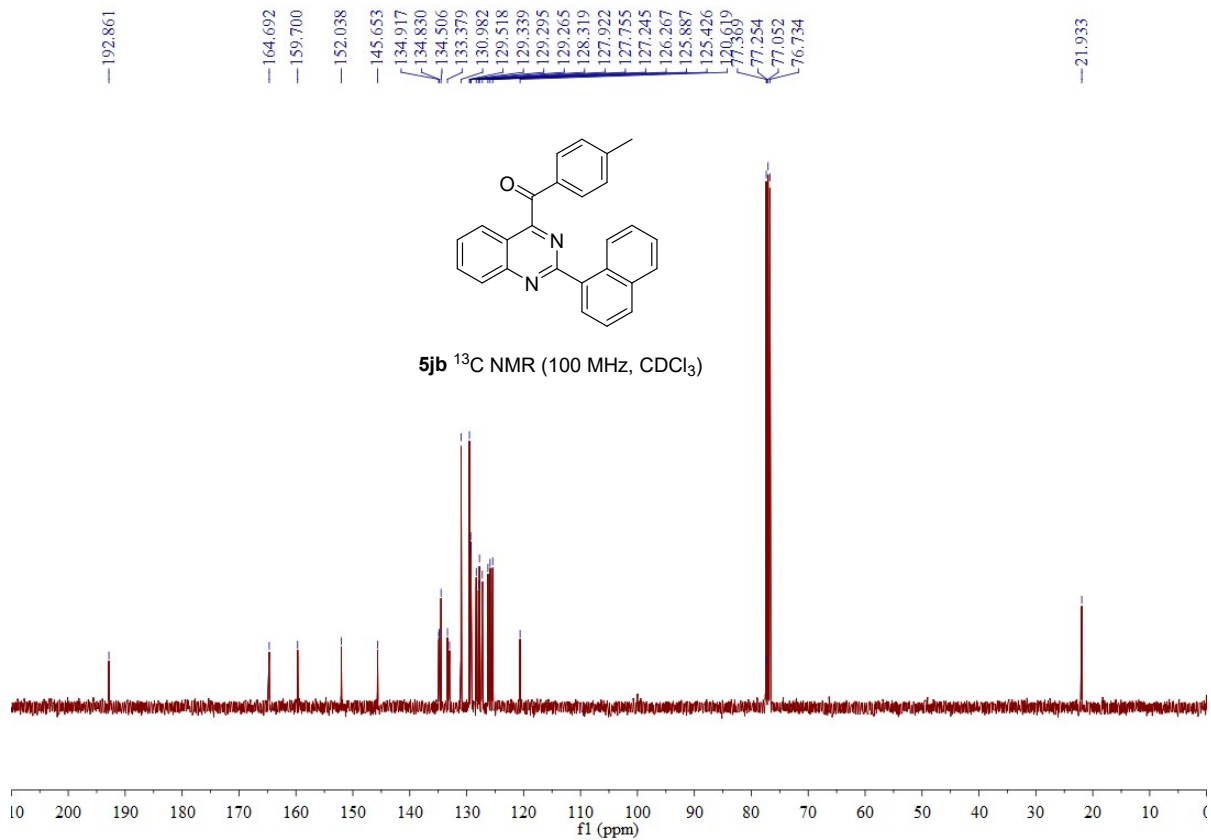
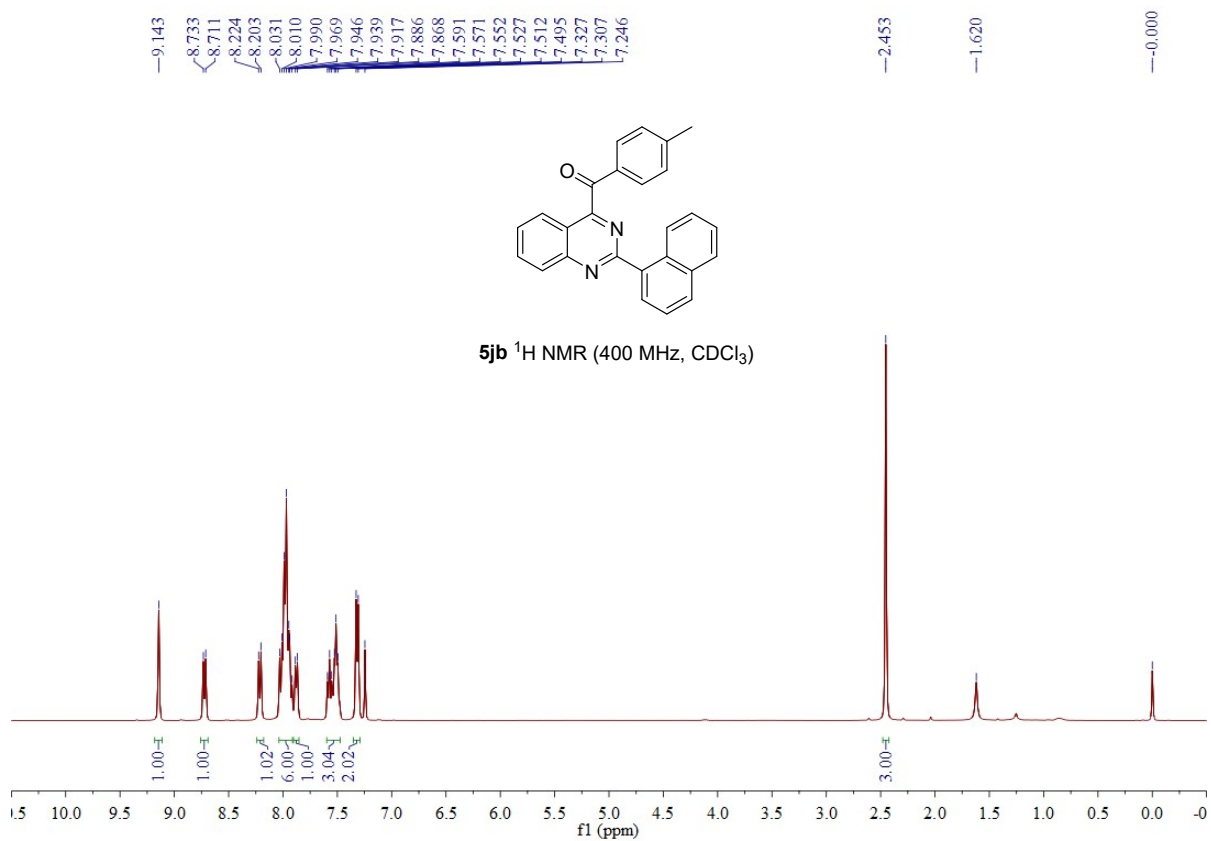




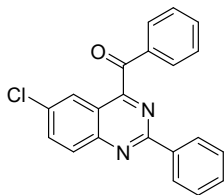




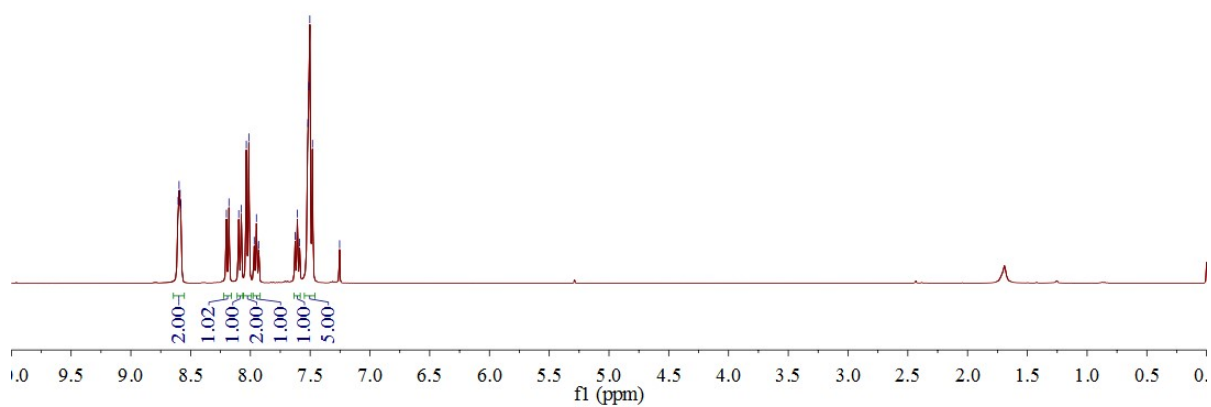




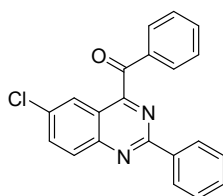
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8.077
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7.607
7.588
7.520
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7.481
7.254



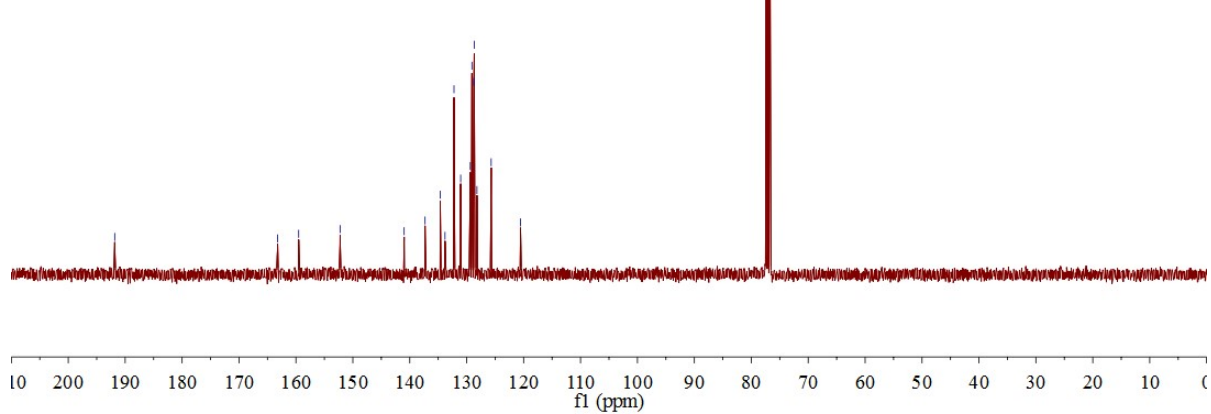
5la ¹H NMR (400 MHz, CDCl₃)



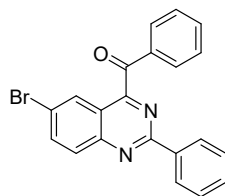
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152.24
140.98
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128.74
128.68
128.20
125.70
120.54



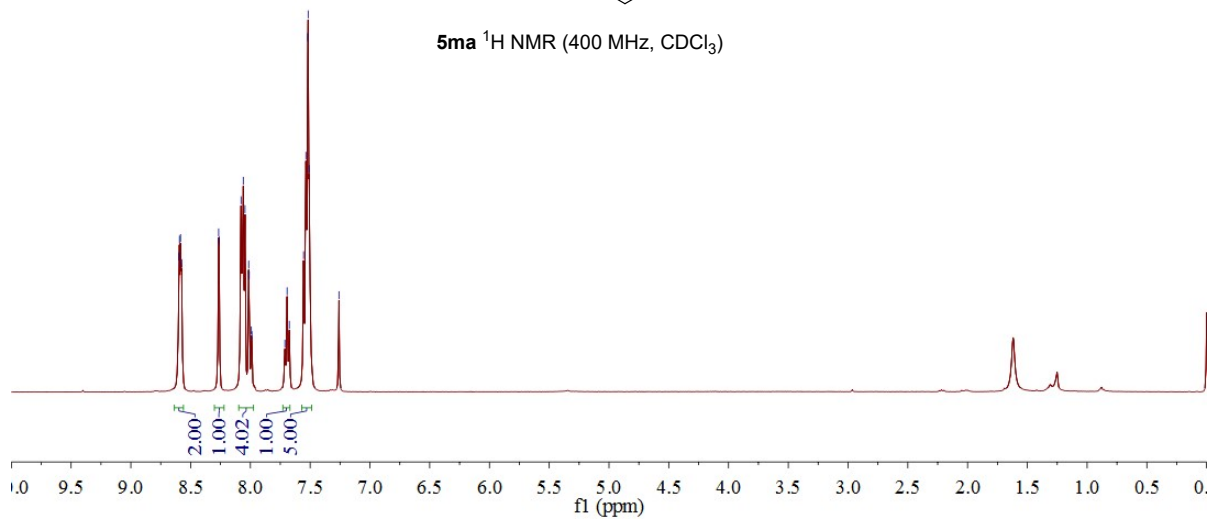
5la ¹³C NMR (100 MHz, CDCl₃)



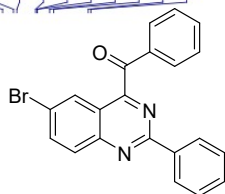
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8.060
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8.014
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7.693
7.674
7.555
7.536
7.521
7.517
7.509
7.259



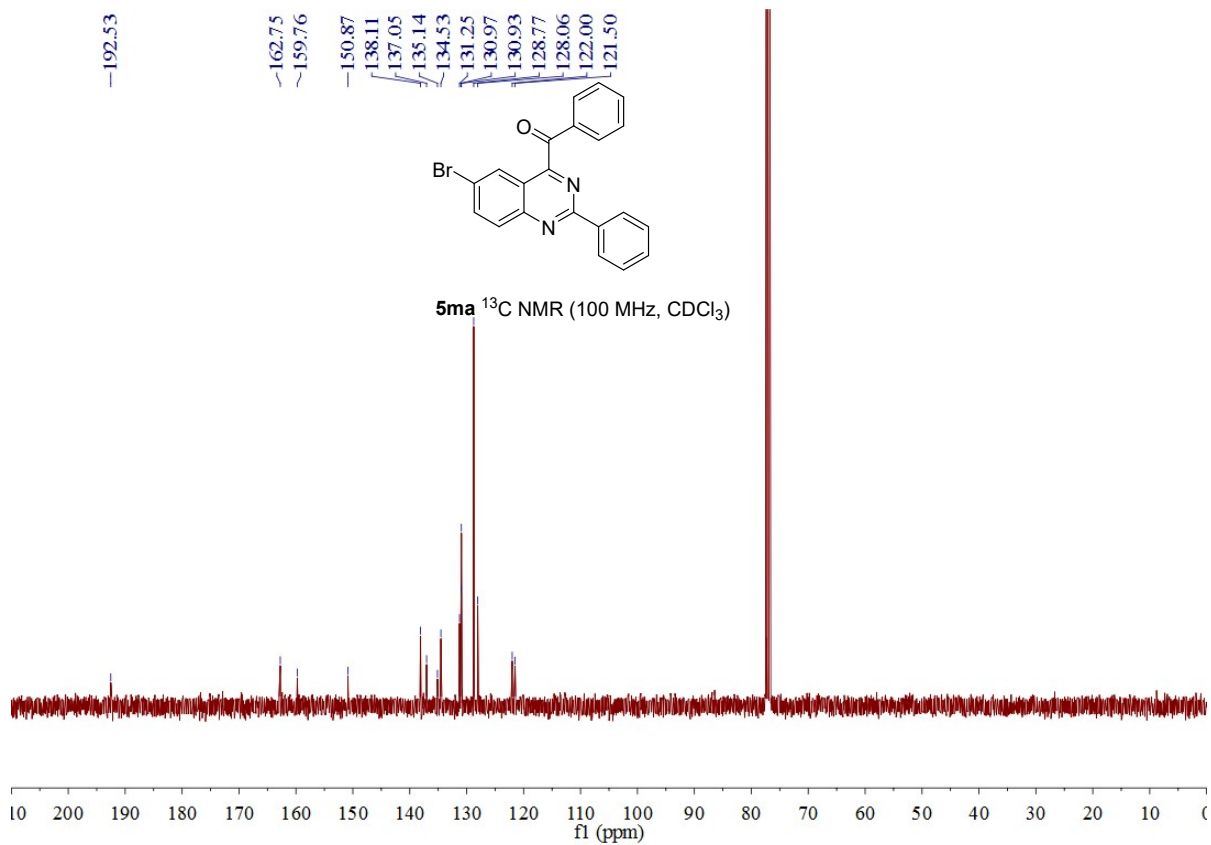
5ma ^1H NMR (400 MHz, CDCl_3)



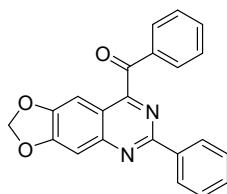
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162.75
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130.93
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128.06
122.00
121.50



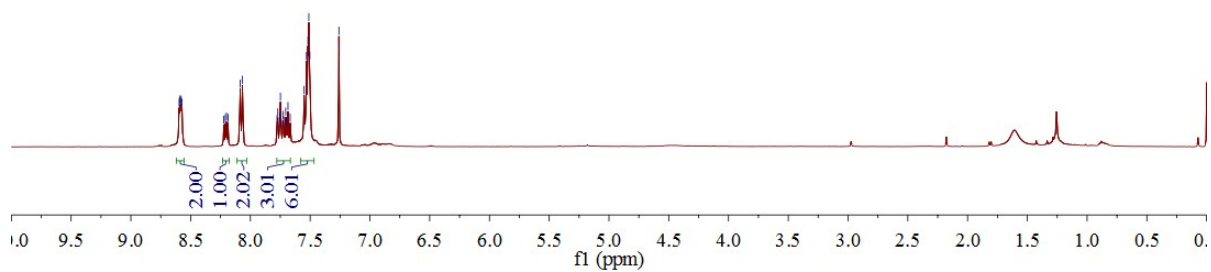
5ma ^{13}C NMR (100 MHz, CDCl_3)



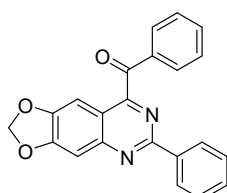
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8.210
8.200
8.187
8.085
8.067
7.777
7.771
7.756
7.749
7.742
7.728
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7.686
7.667
7.551
7.531
7.519
7.511
7.503
7.260



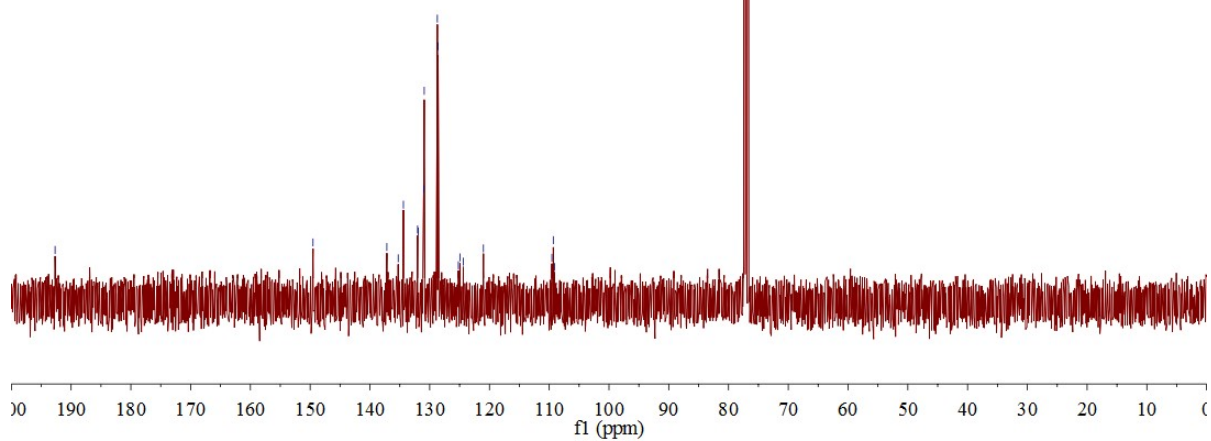
5na ¹H NMR (400 MHz, CDCl₃)



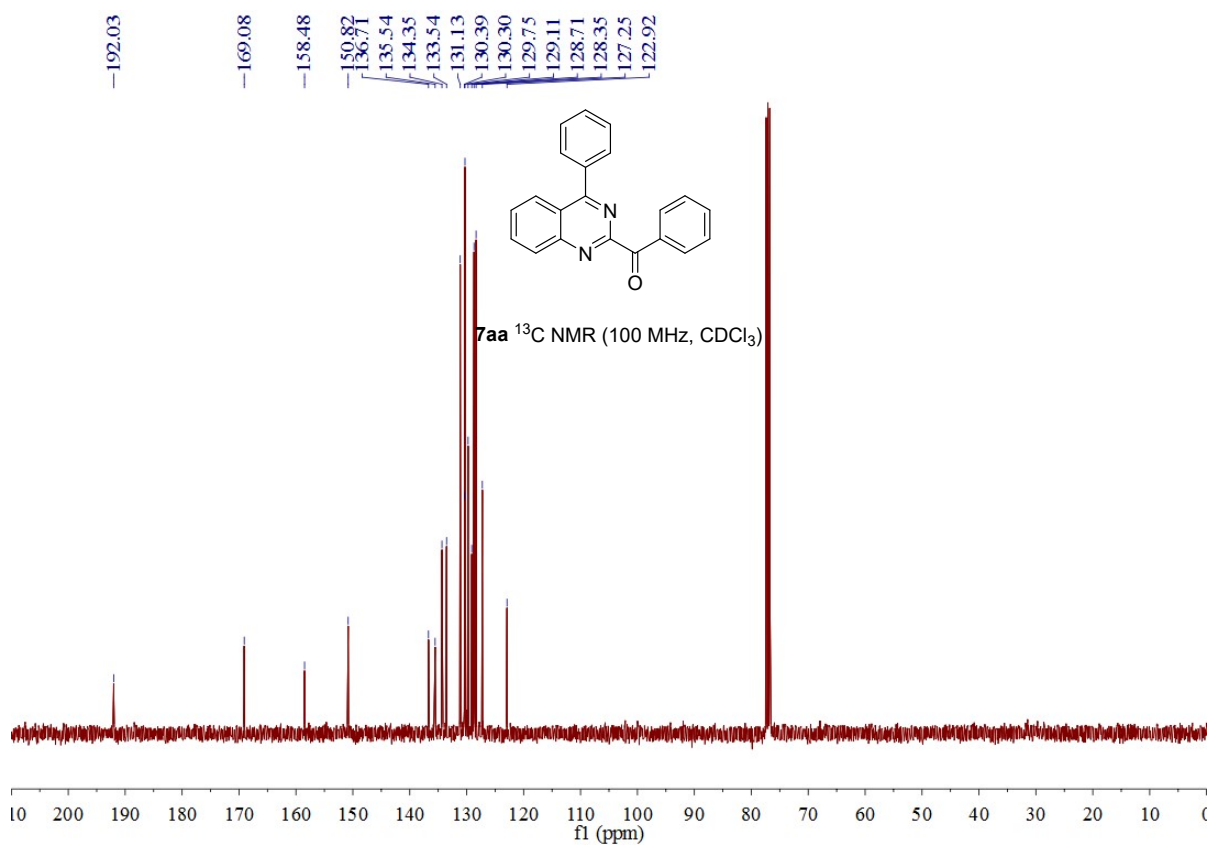
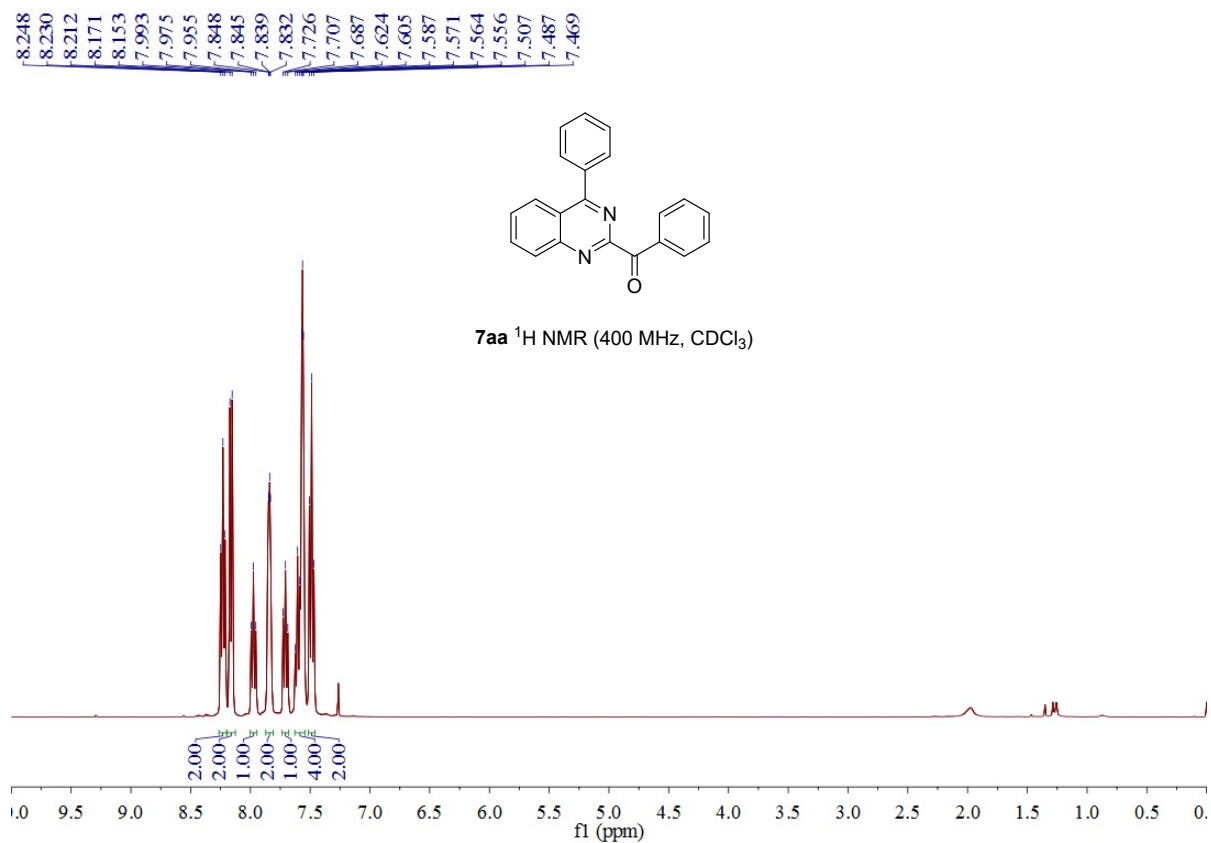
192.68
149.52
137.17
134.40
132.02
131.93
131.02
130.91
128.72
109.32
109.12

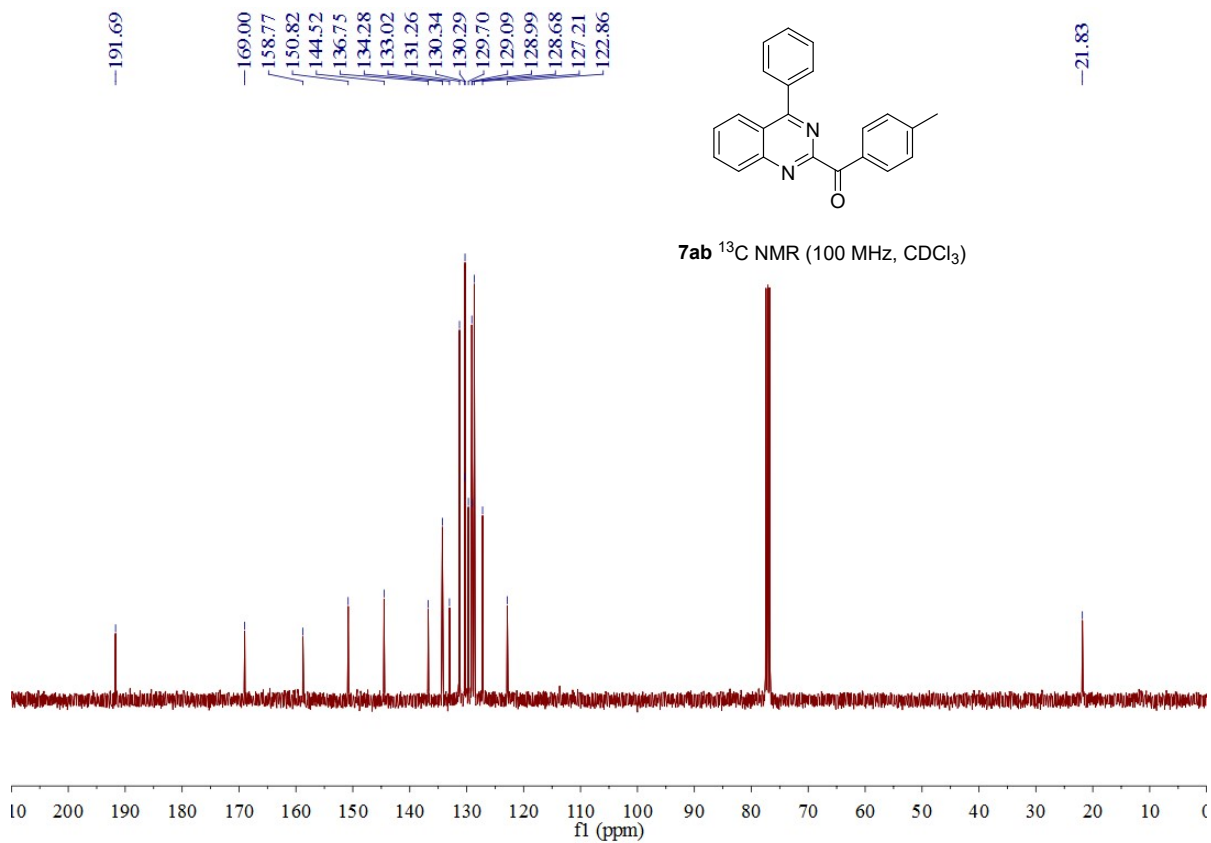
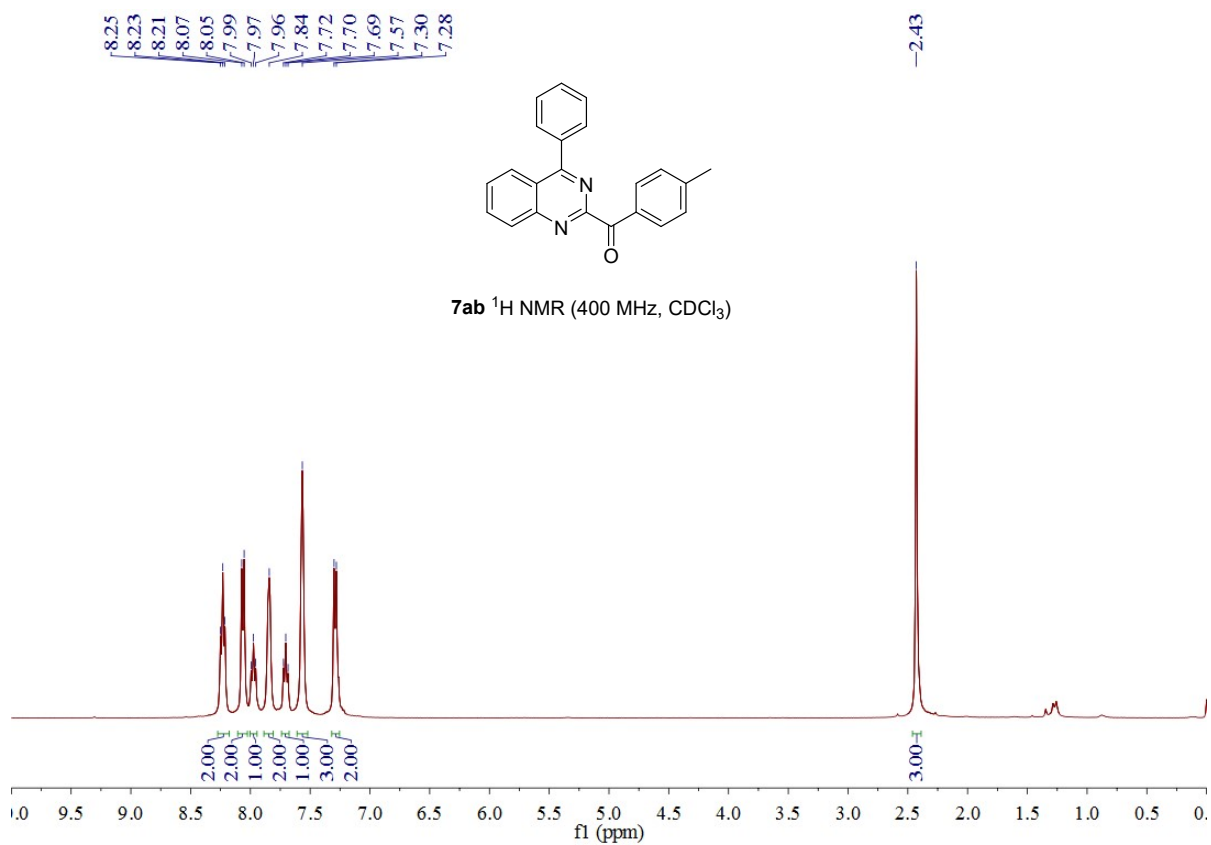


5na ¹³C NMR (100 MHz, CDCl₃)



Copy of Products 7 NMR

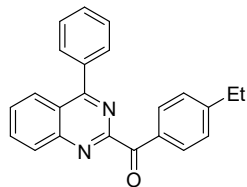




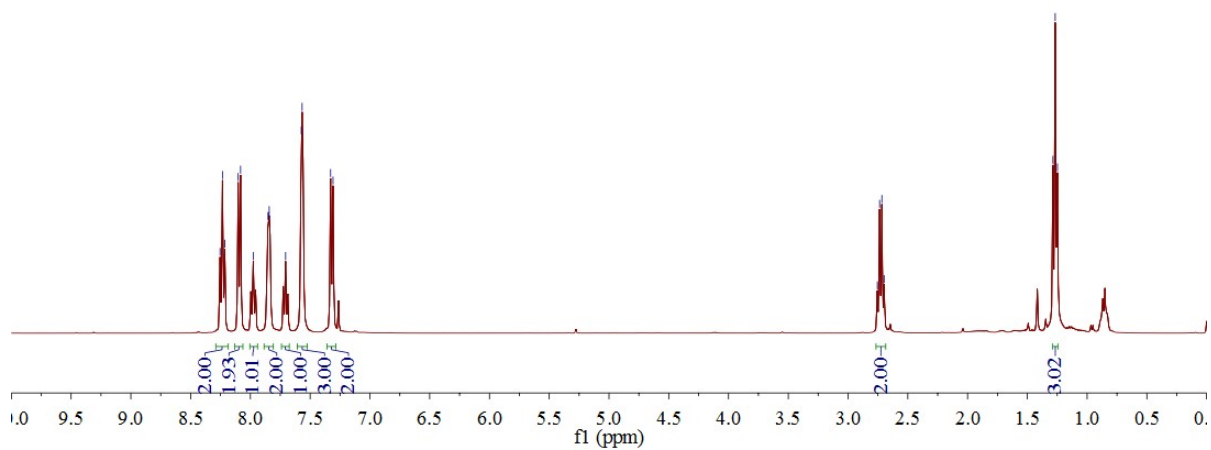
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8.23
8.22
8.10
8.08
7.98
7.85
7.85
7.84
7.71
7.57
7.57
7.33
7.31

2.75
2.74
2.72
2.70

1.29
1.27
1.25



7ac ^1H NMR (400 MHz, CDCl_3)



-191.69

-169.02

-158.78

-150.82

-150.67

-136.75

-134.29

-133.19

-131.38

-130.34

-130.29

-129.70

-128.99

-128.68

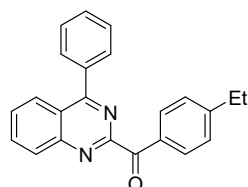
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-127.22

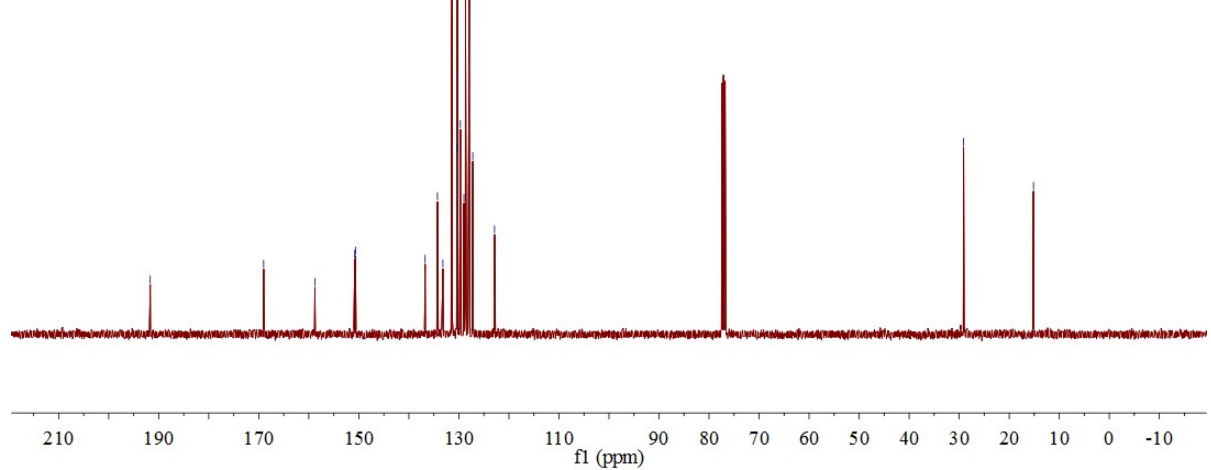
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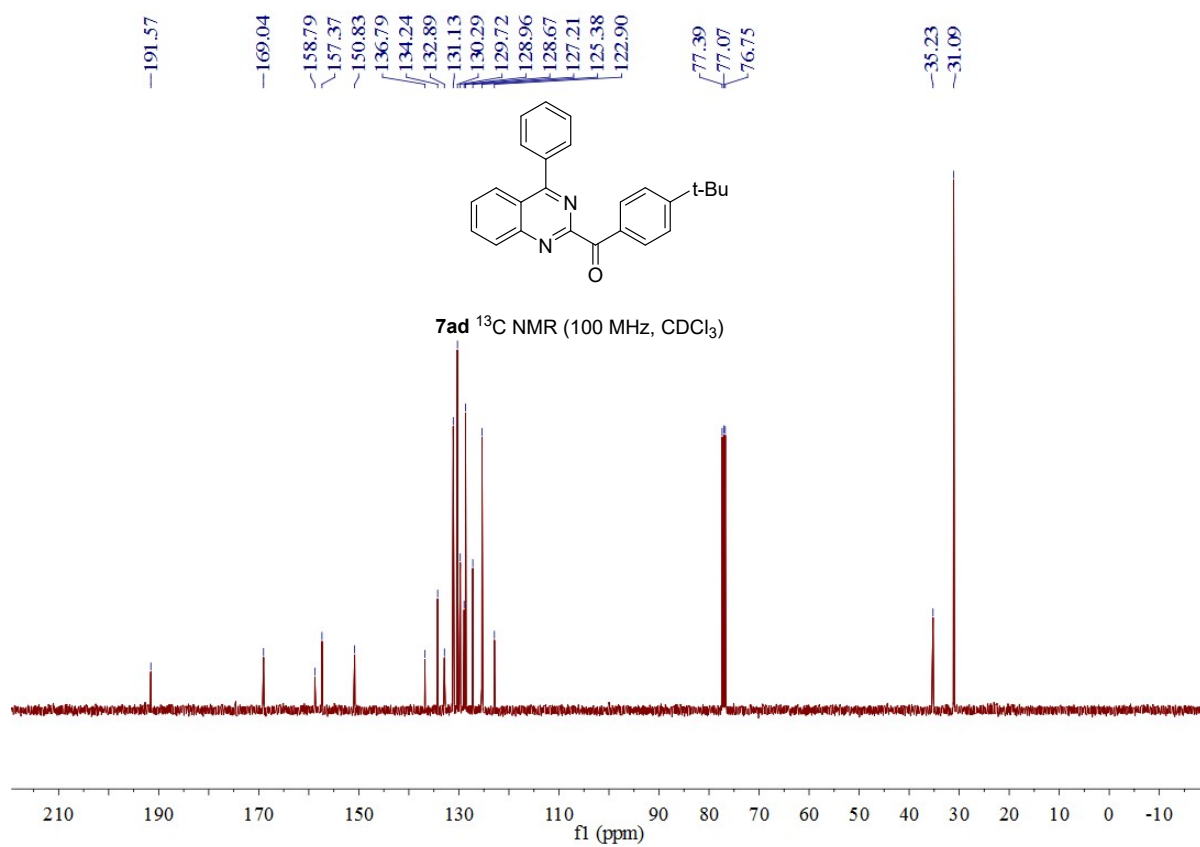
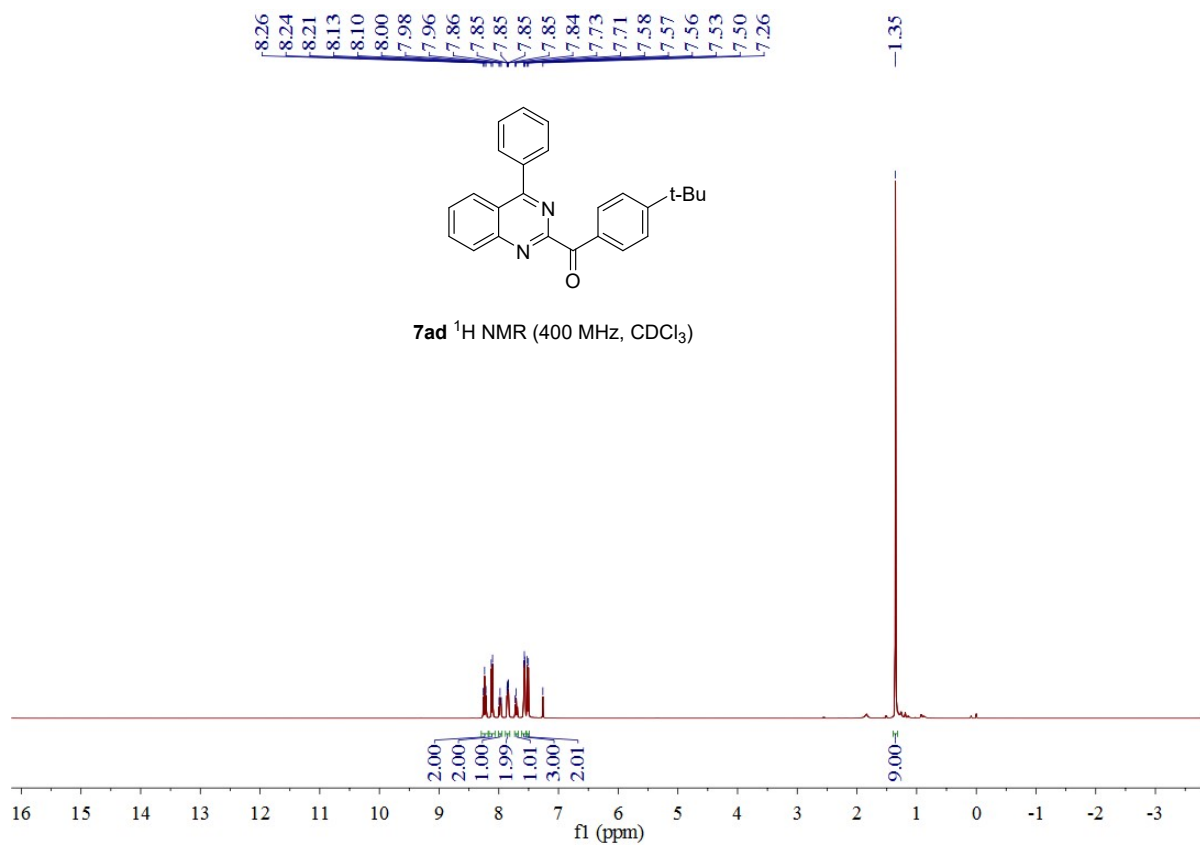
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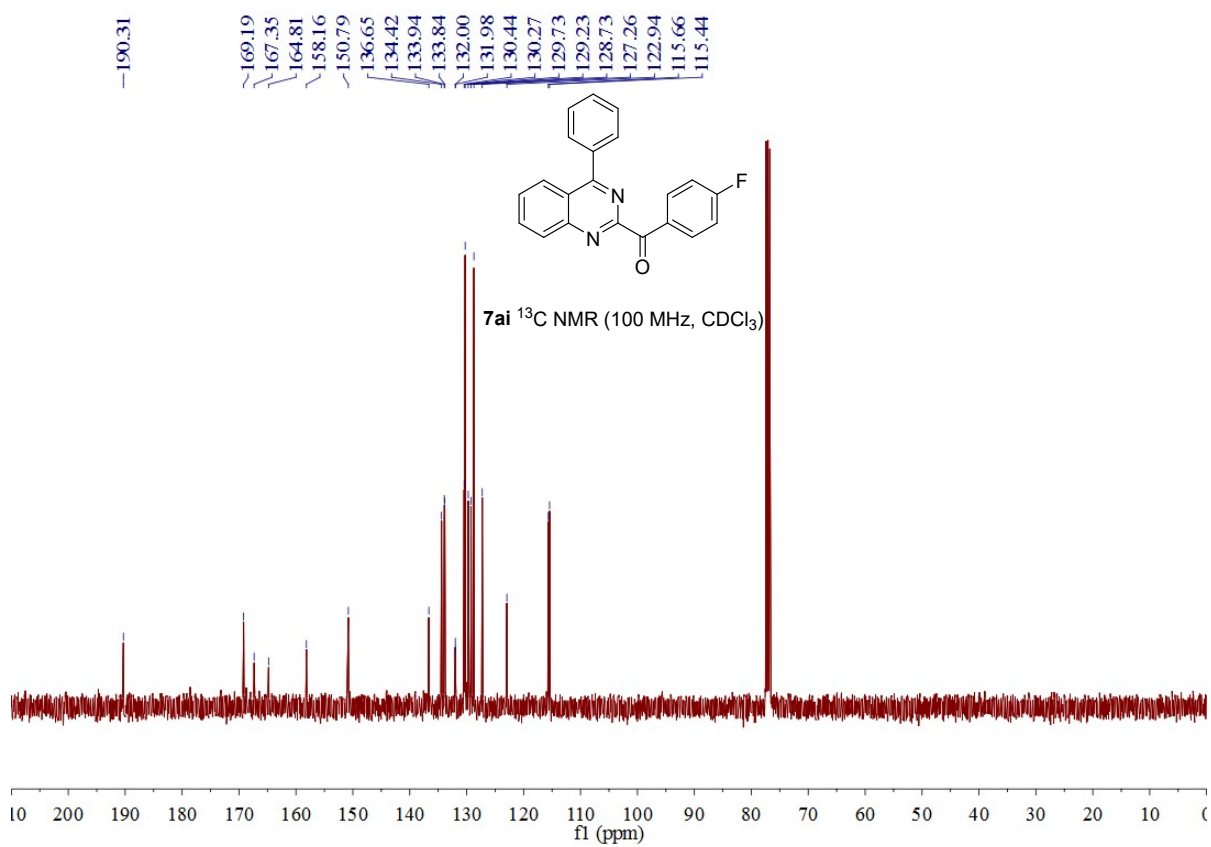
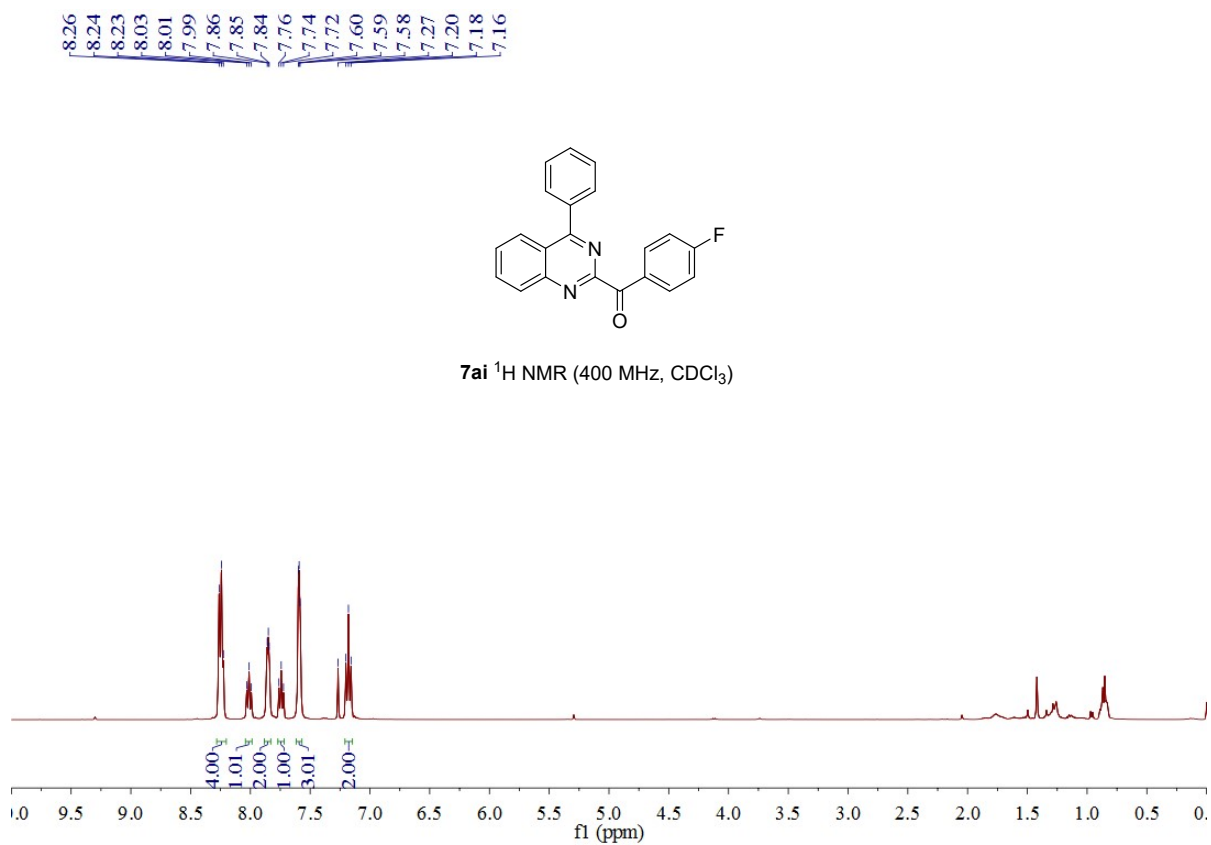
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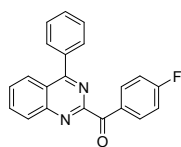


7ac ^{13}C NMR (100 MHz, CDCl_3)

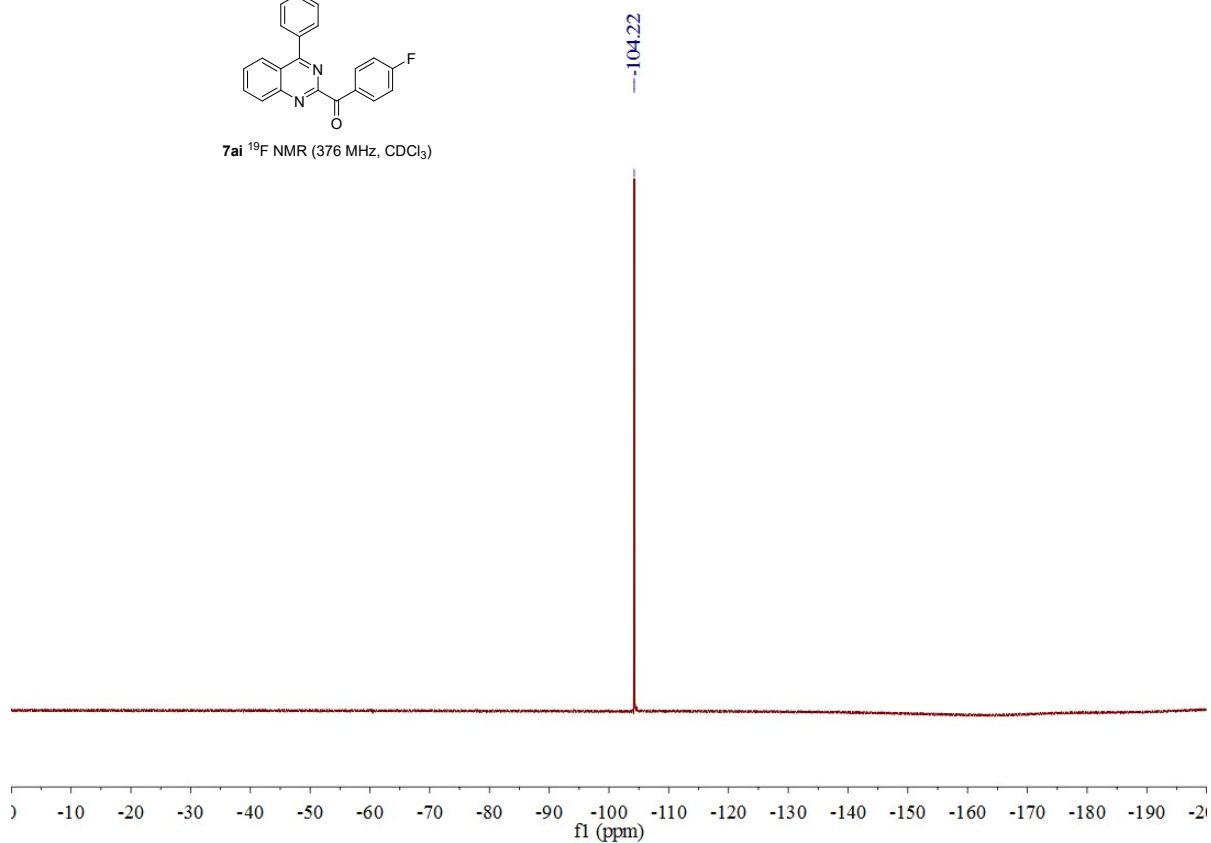




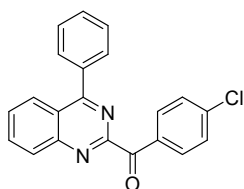




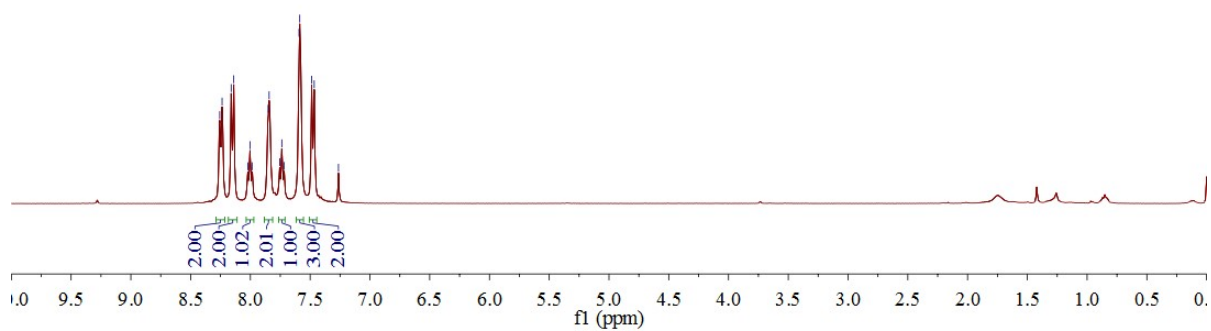
7ai ¹⁹F NMR (376 MHz, CDCl₃)

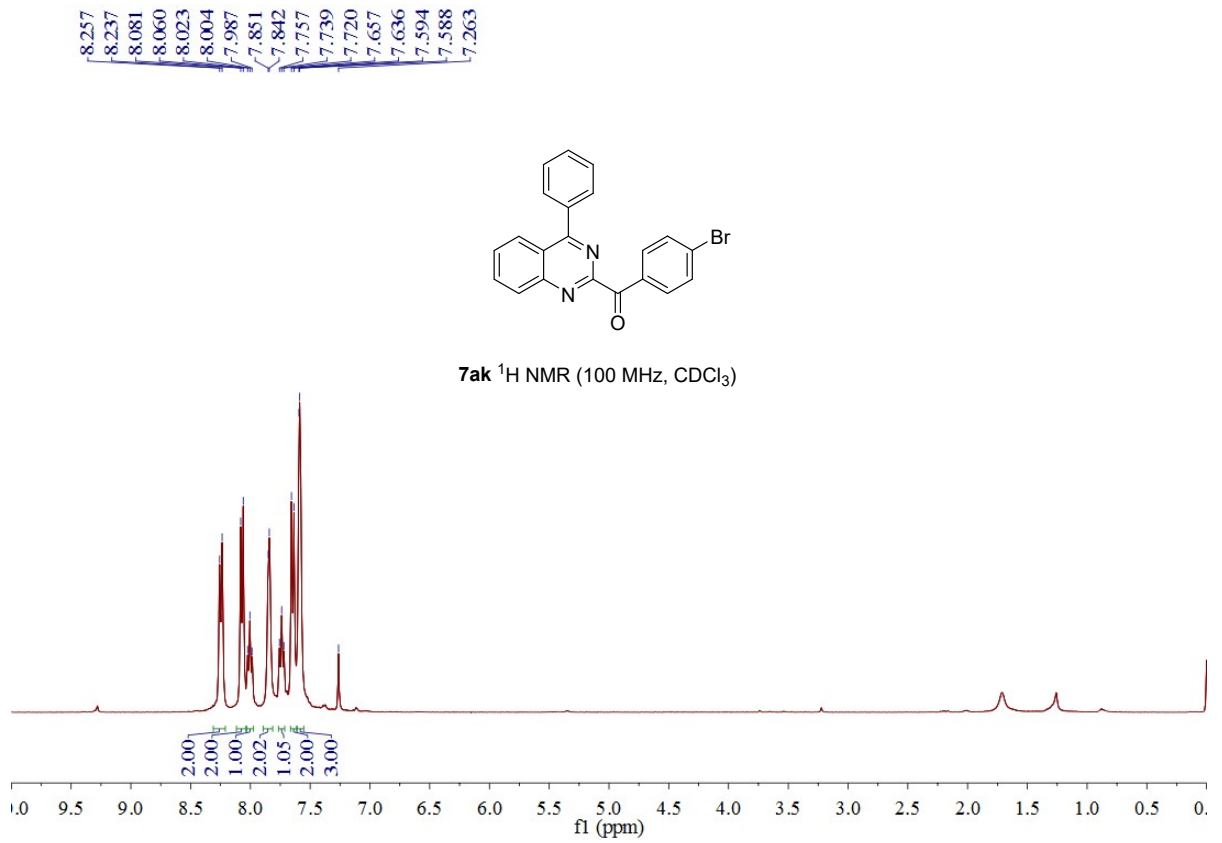
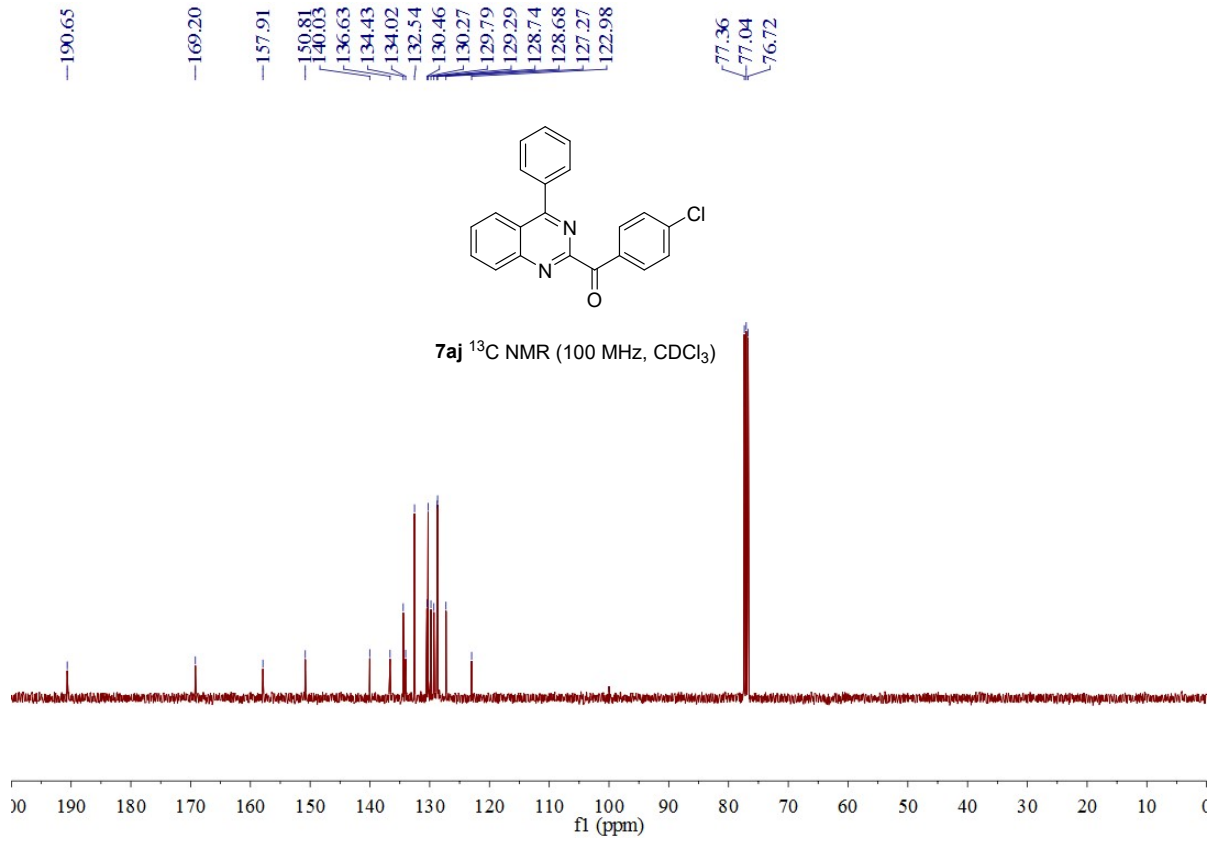


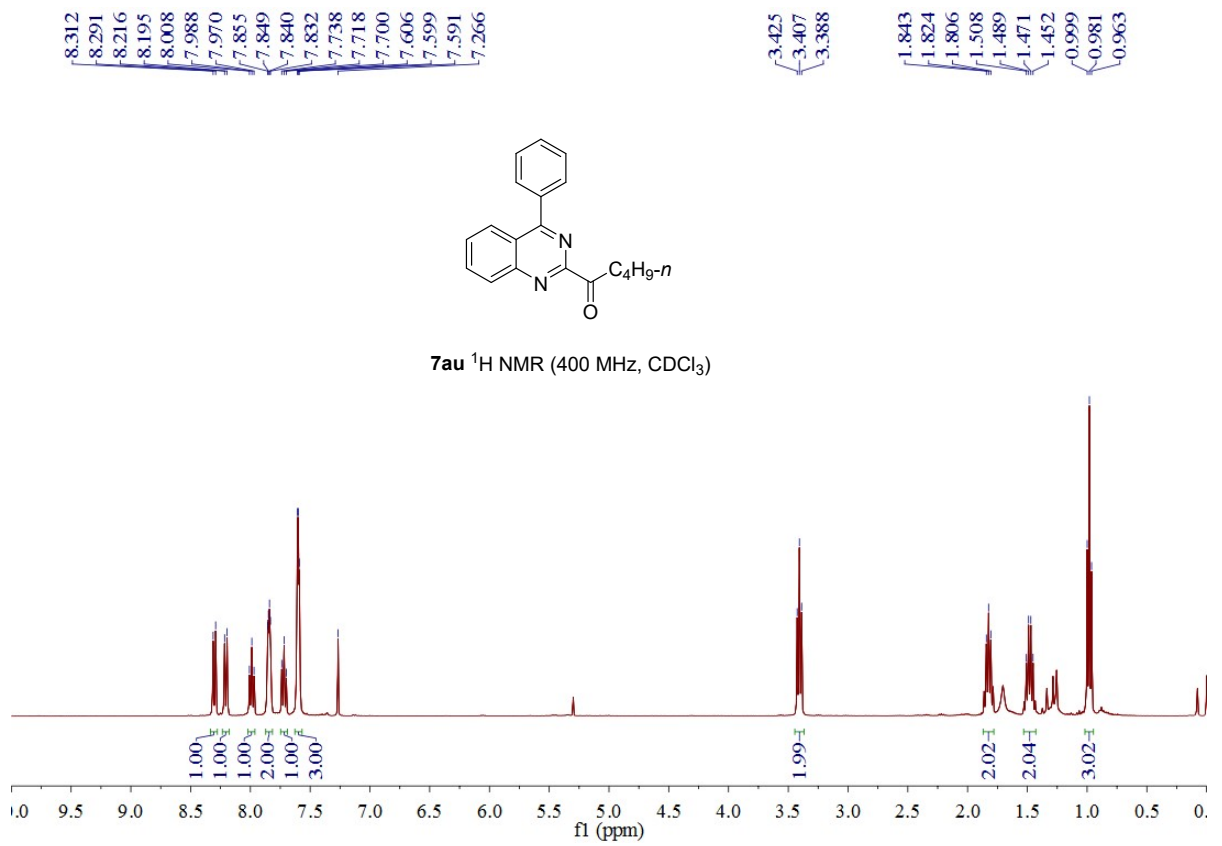
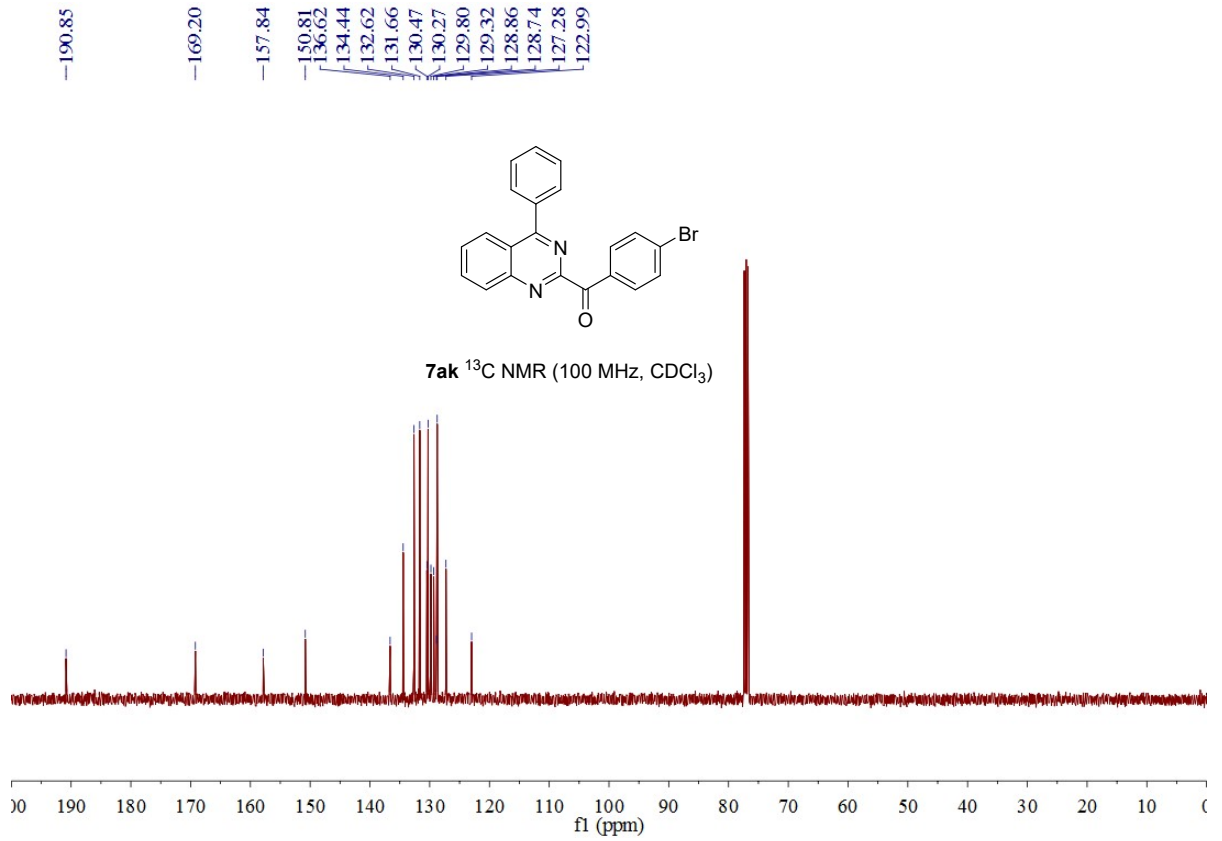
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8.139
8.022
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7.719
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7.587
7.487
7.466
7.263

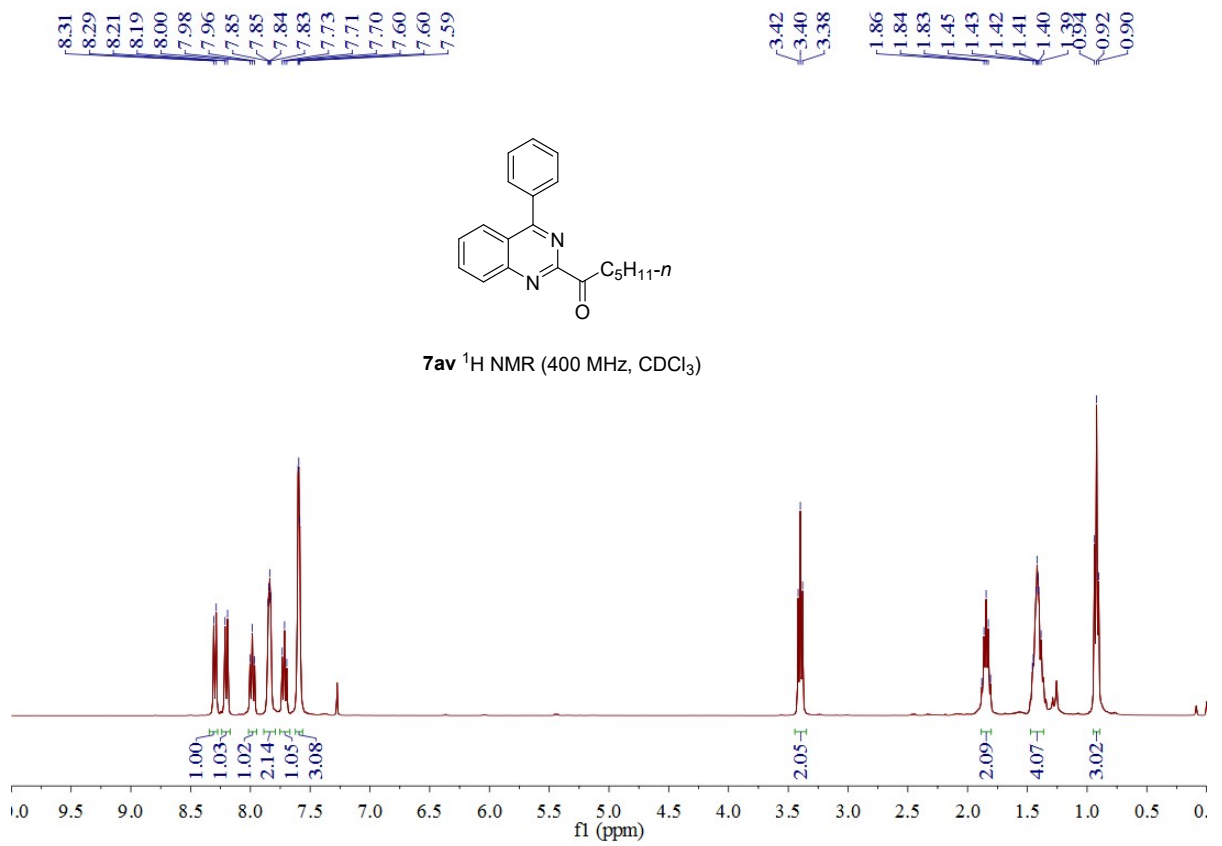
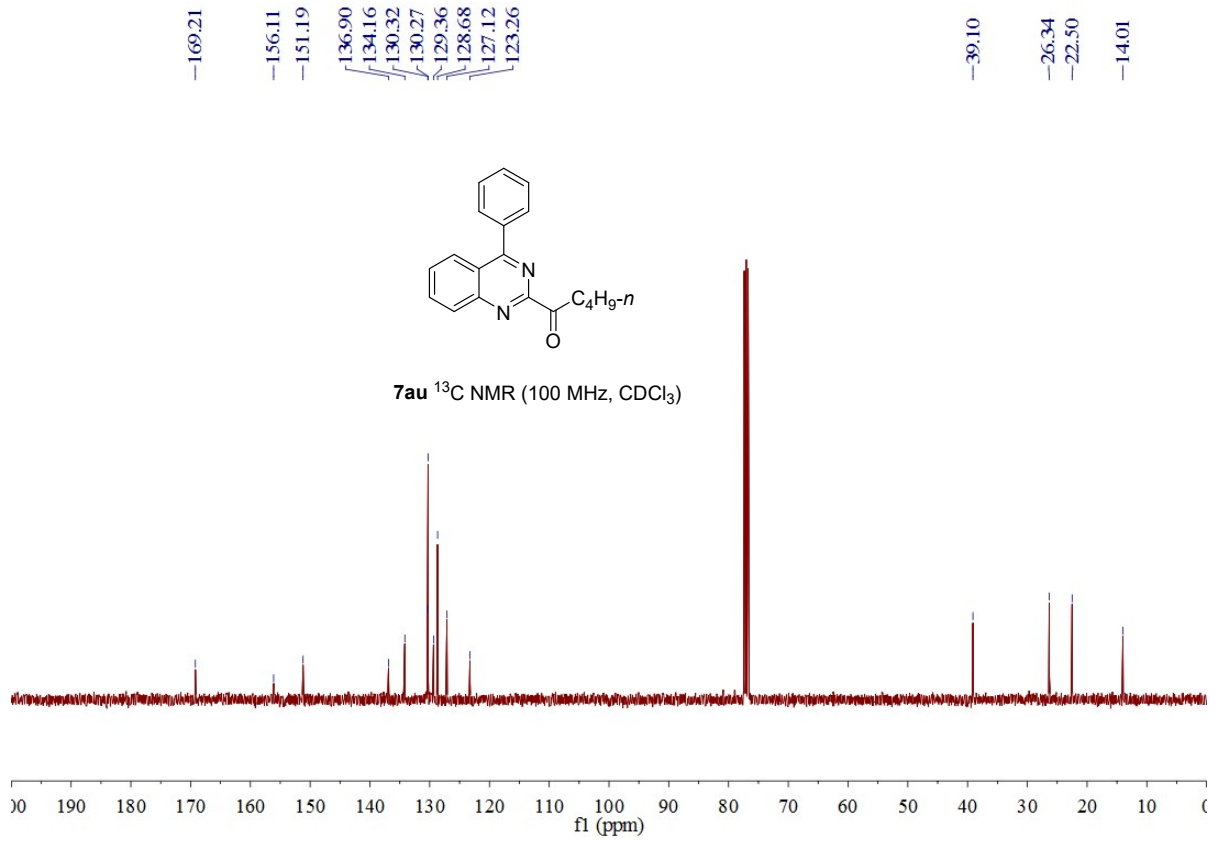


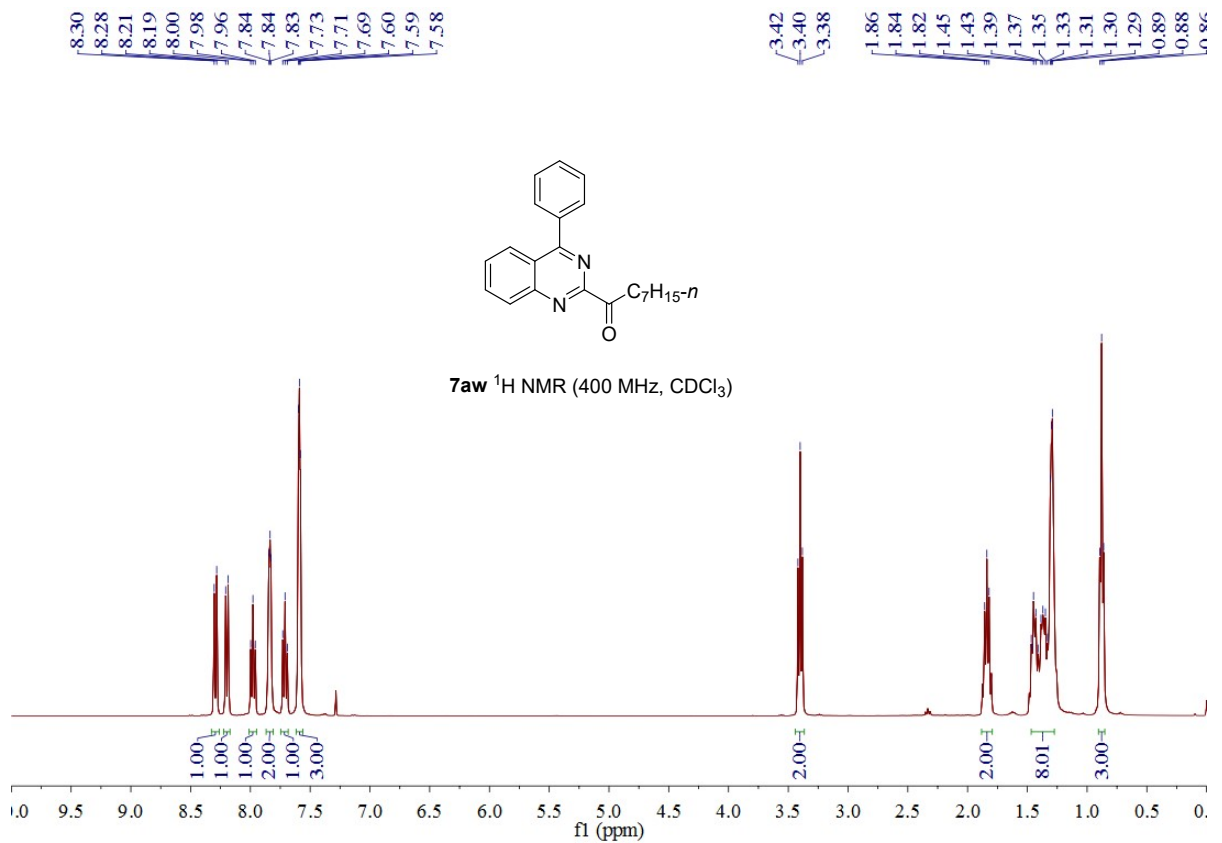
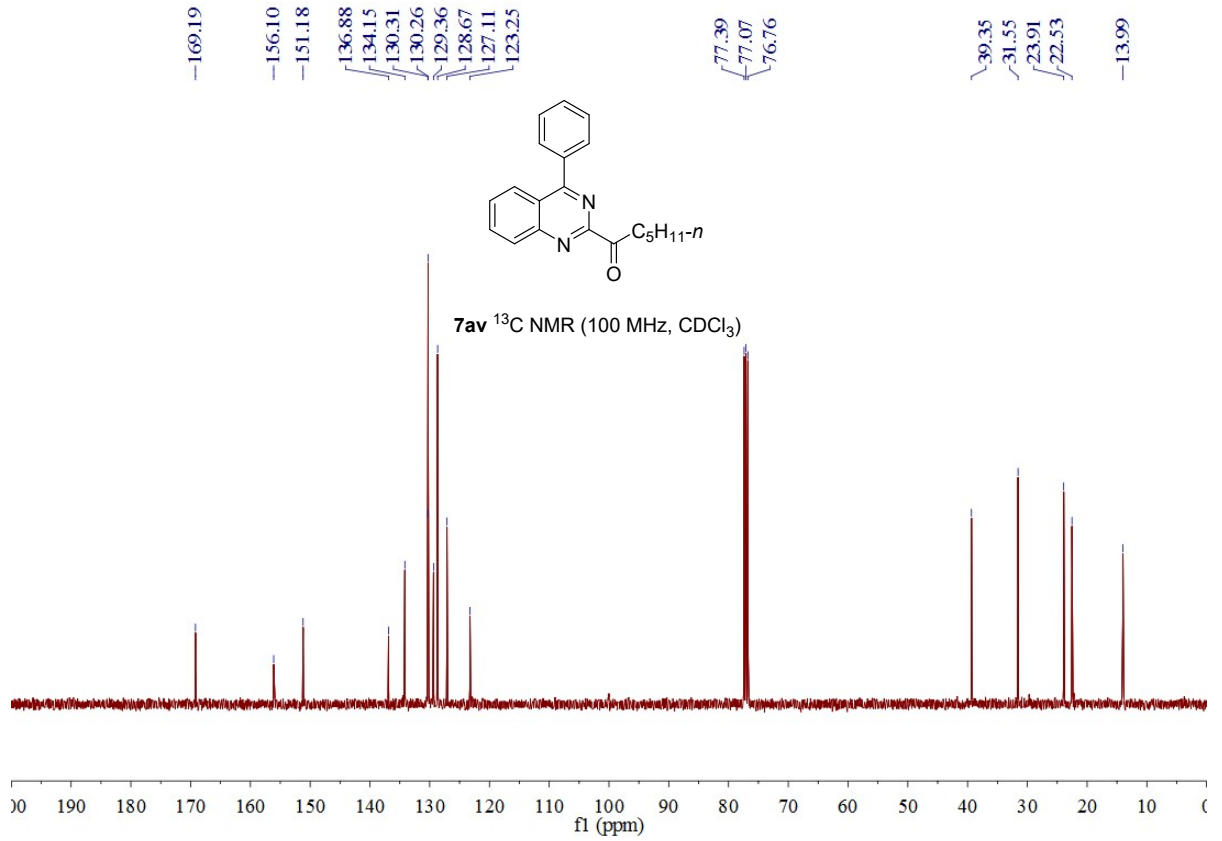
7aj ¹H NMR (400 MHz, CDCl₃)

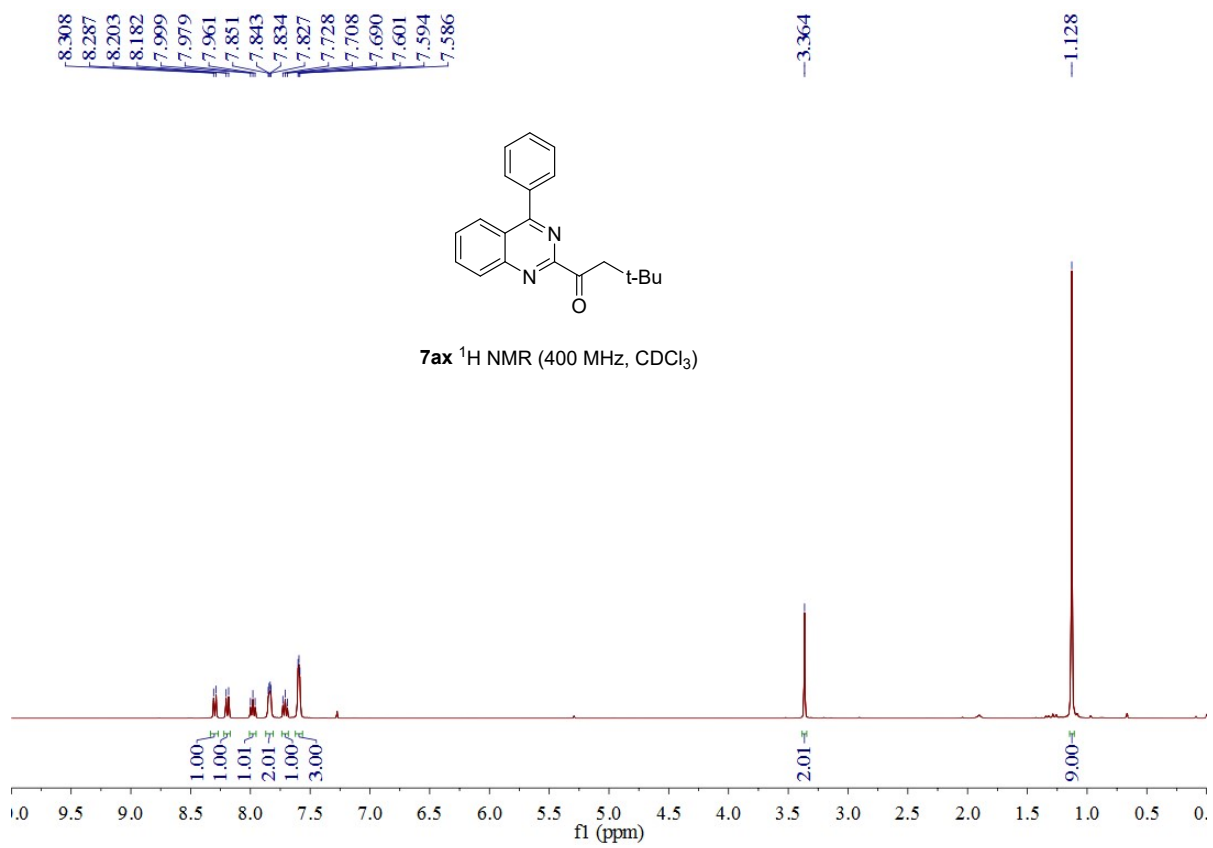
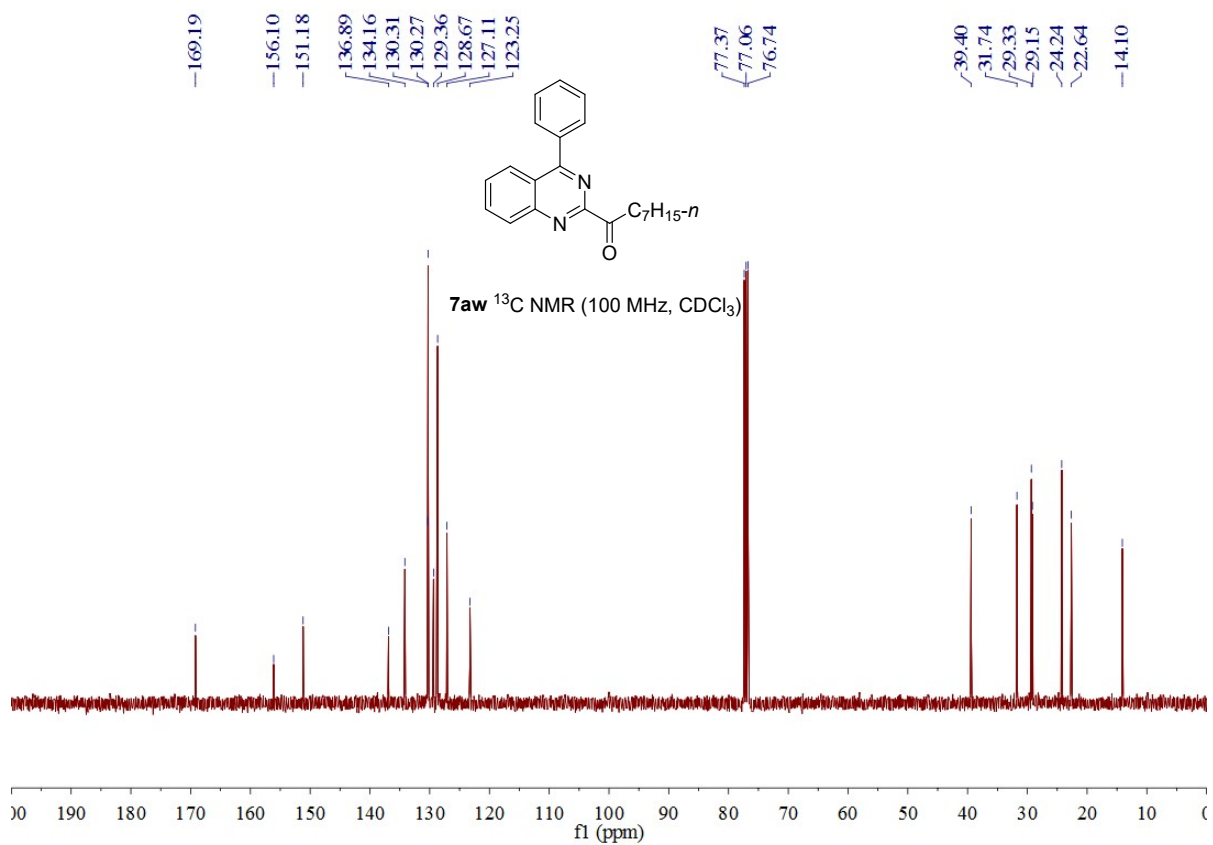


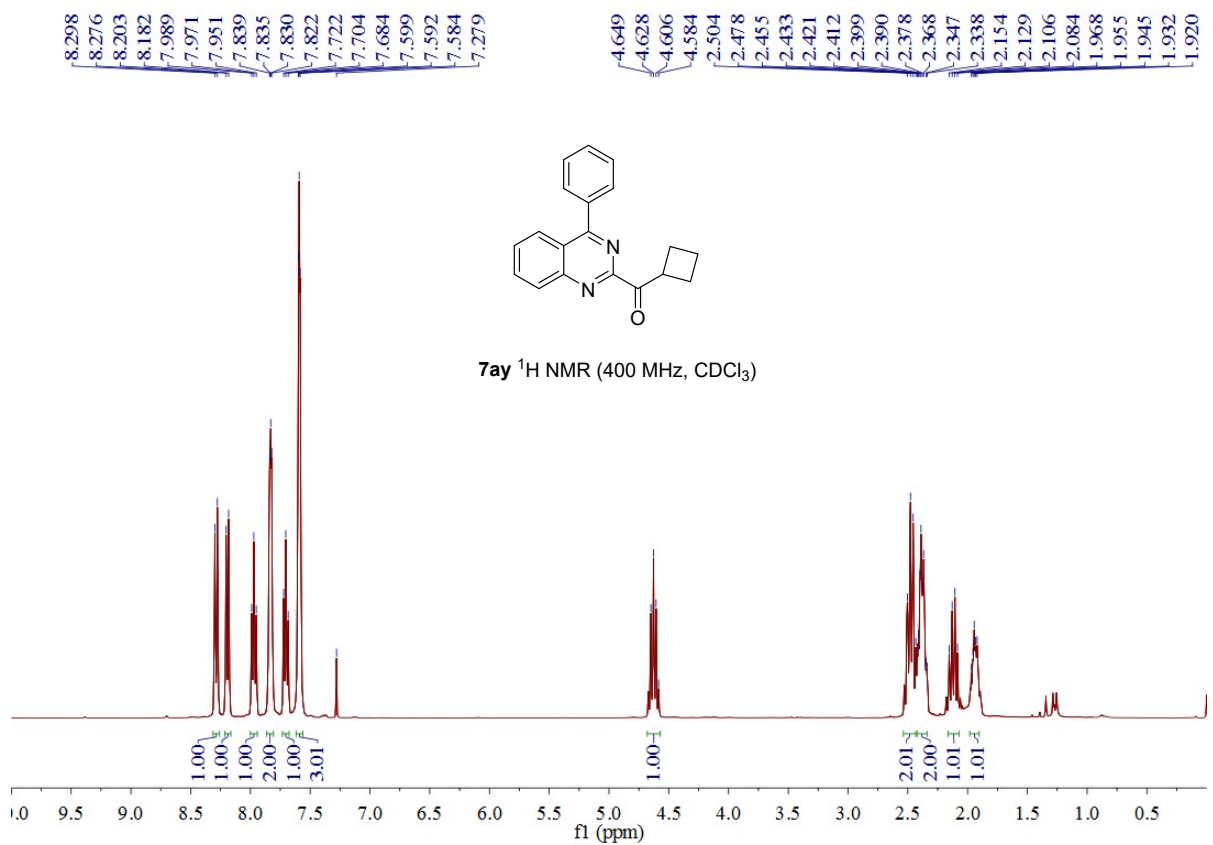
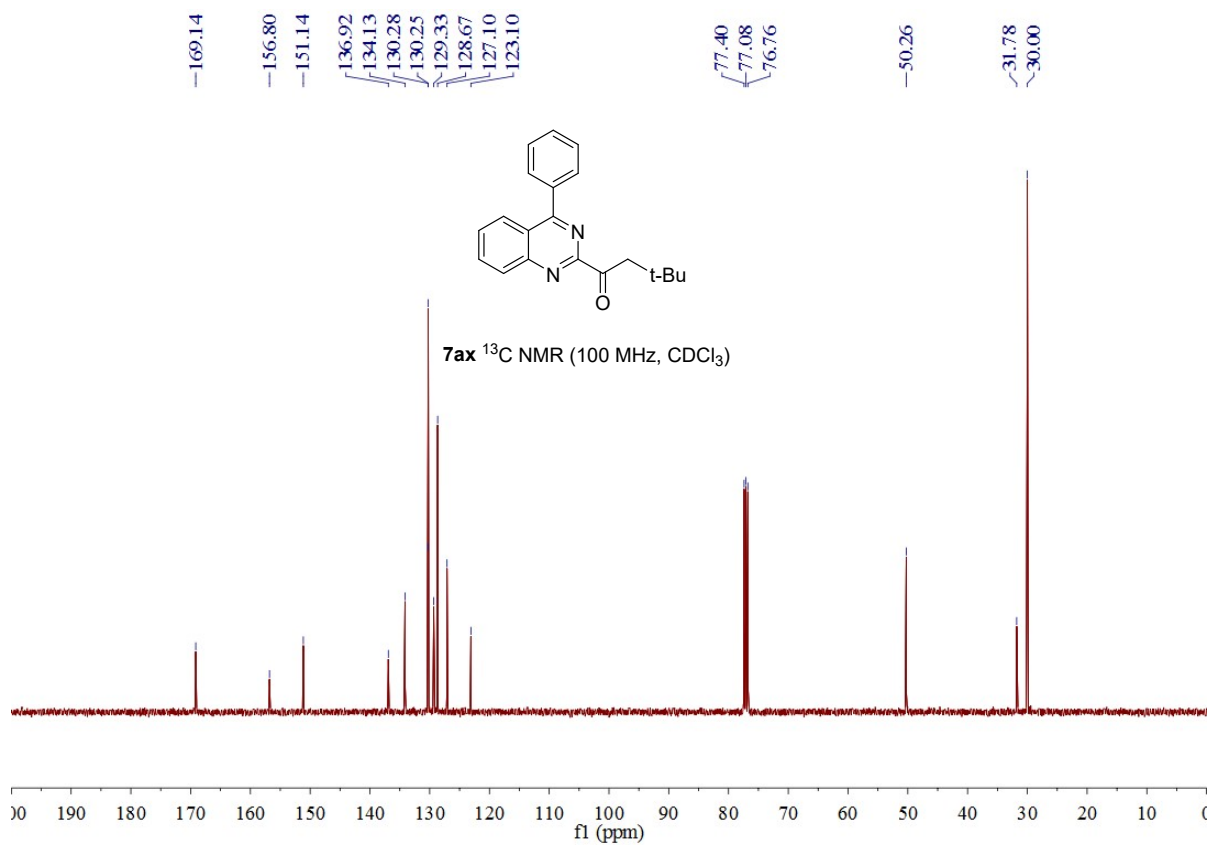


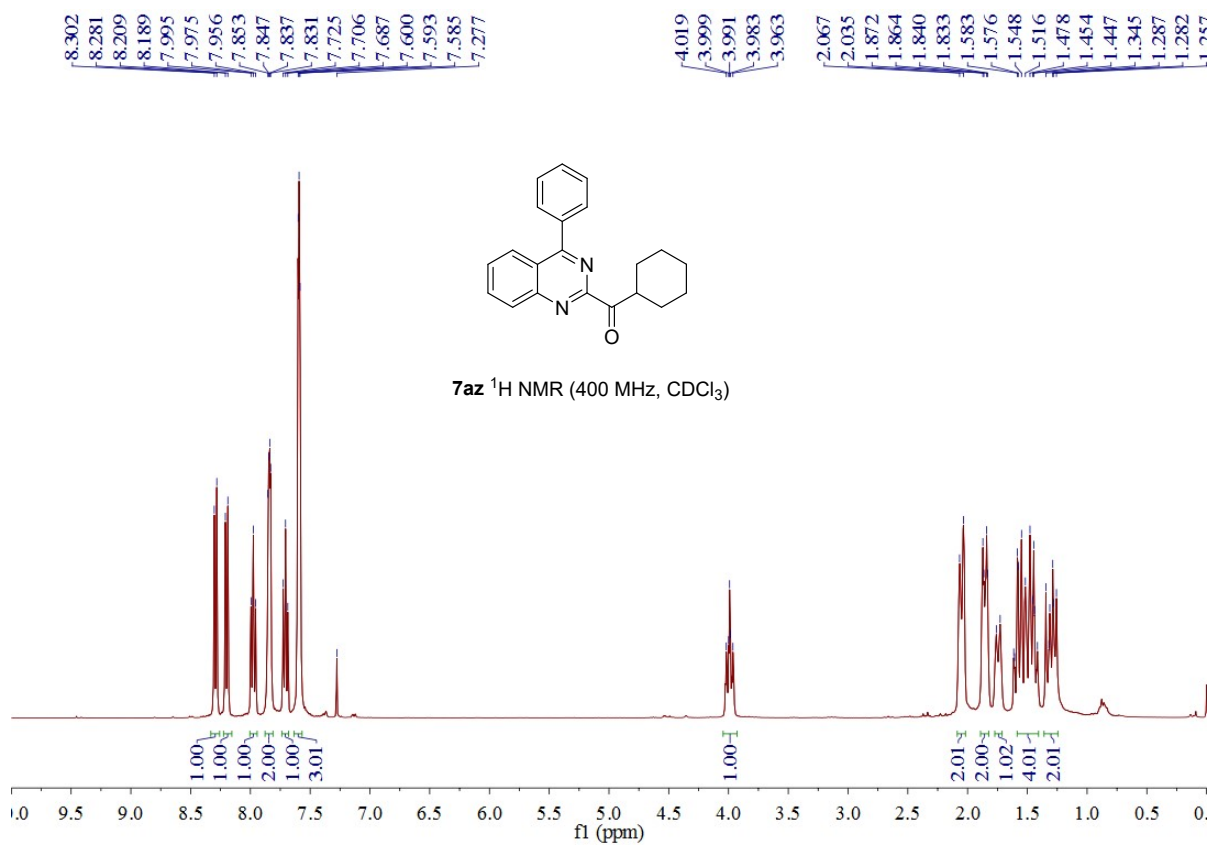


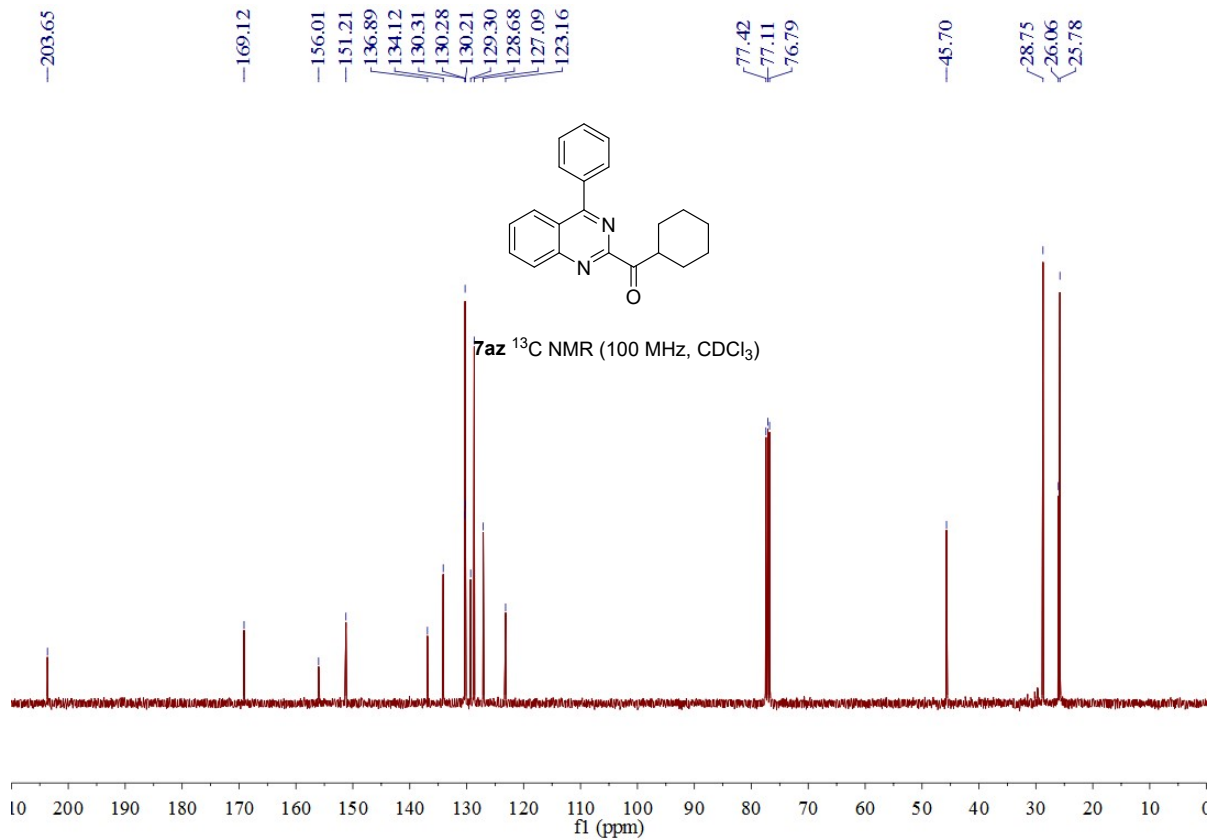




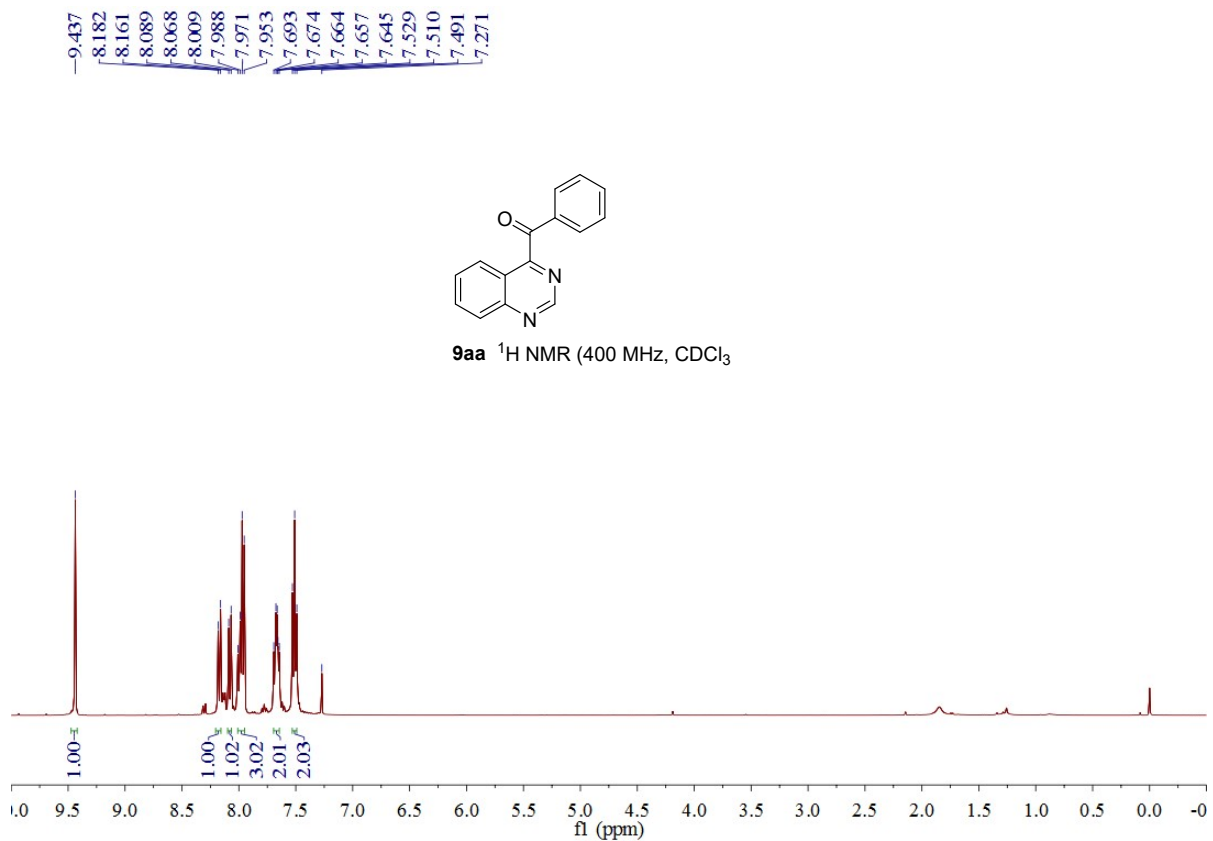


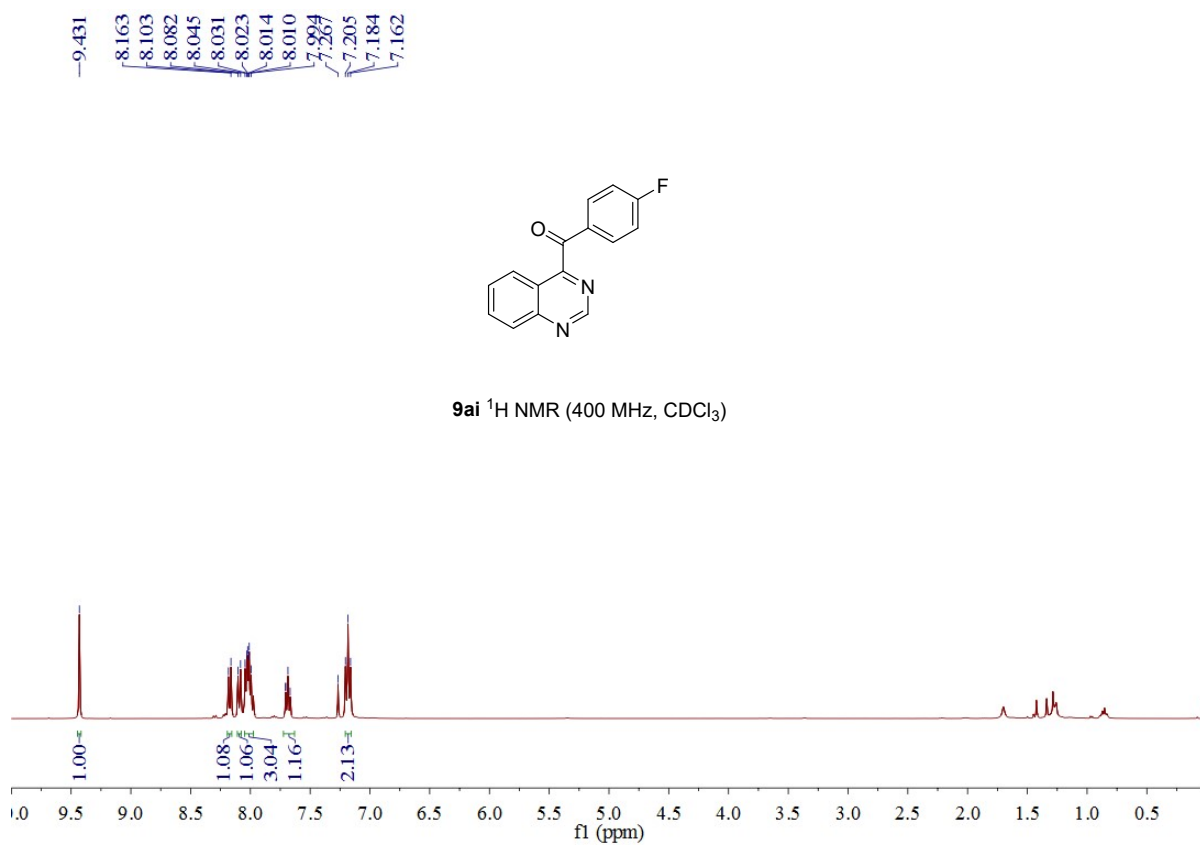
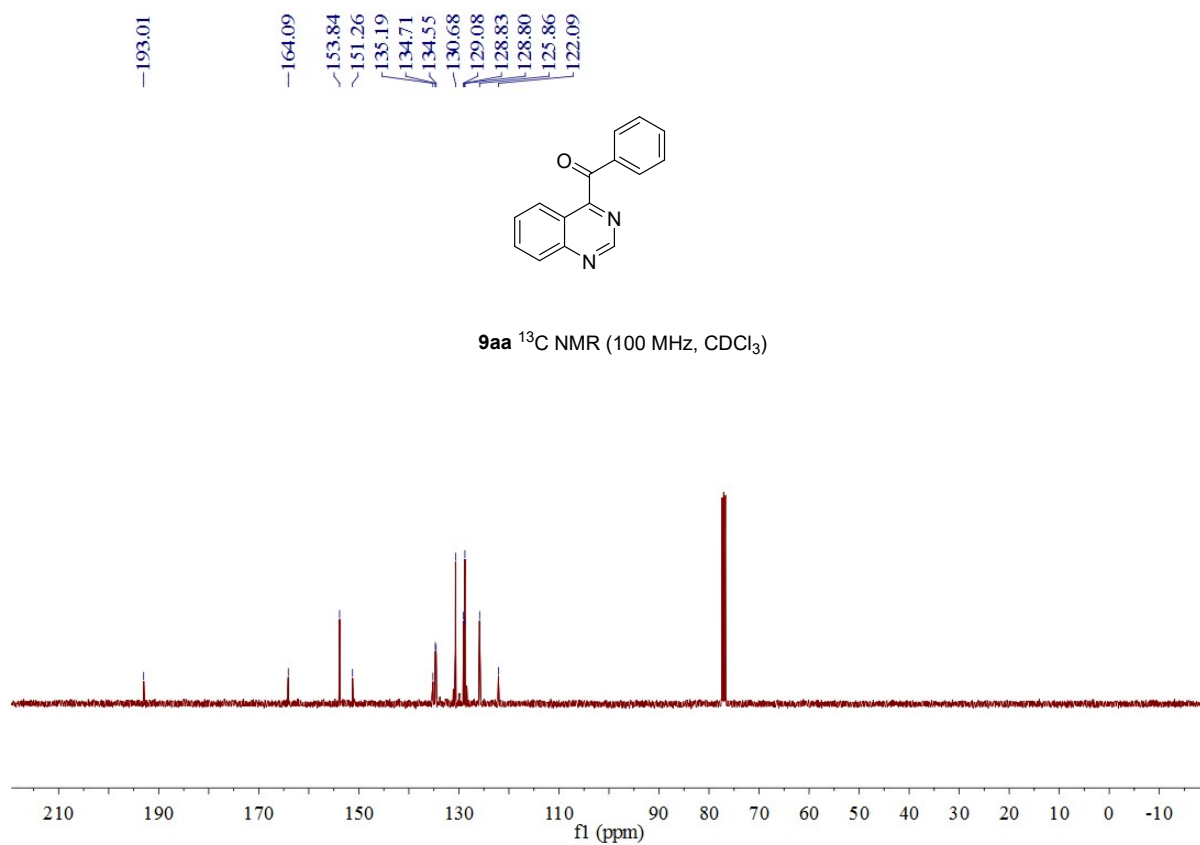


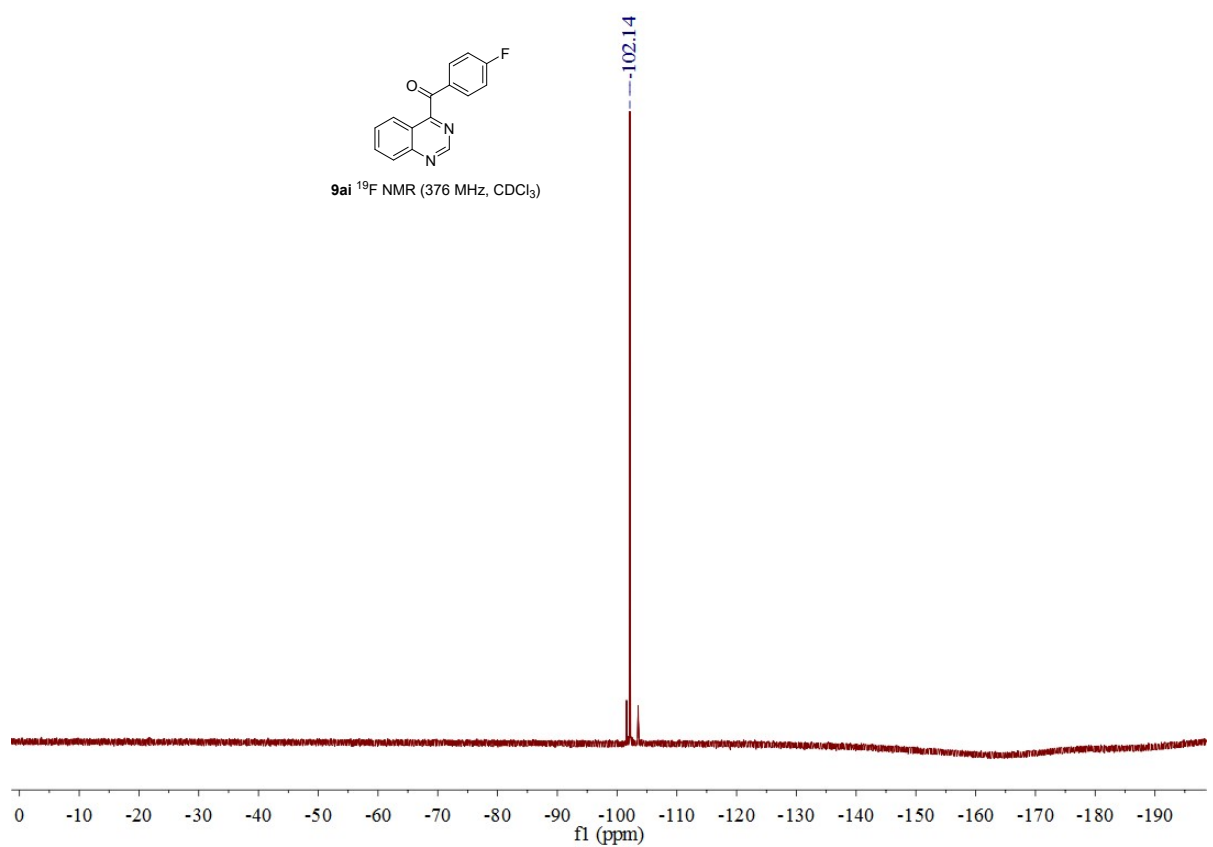
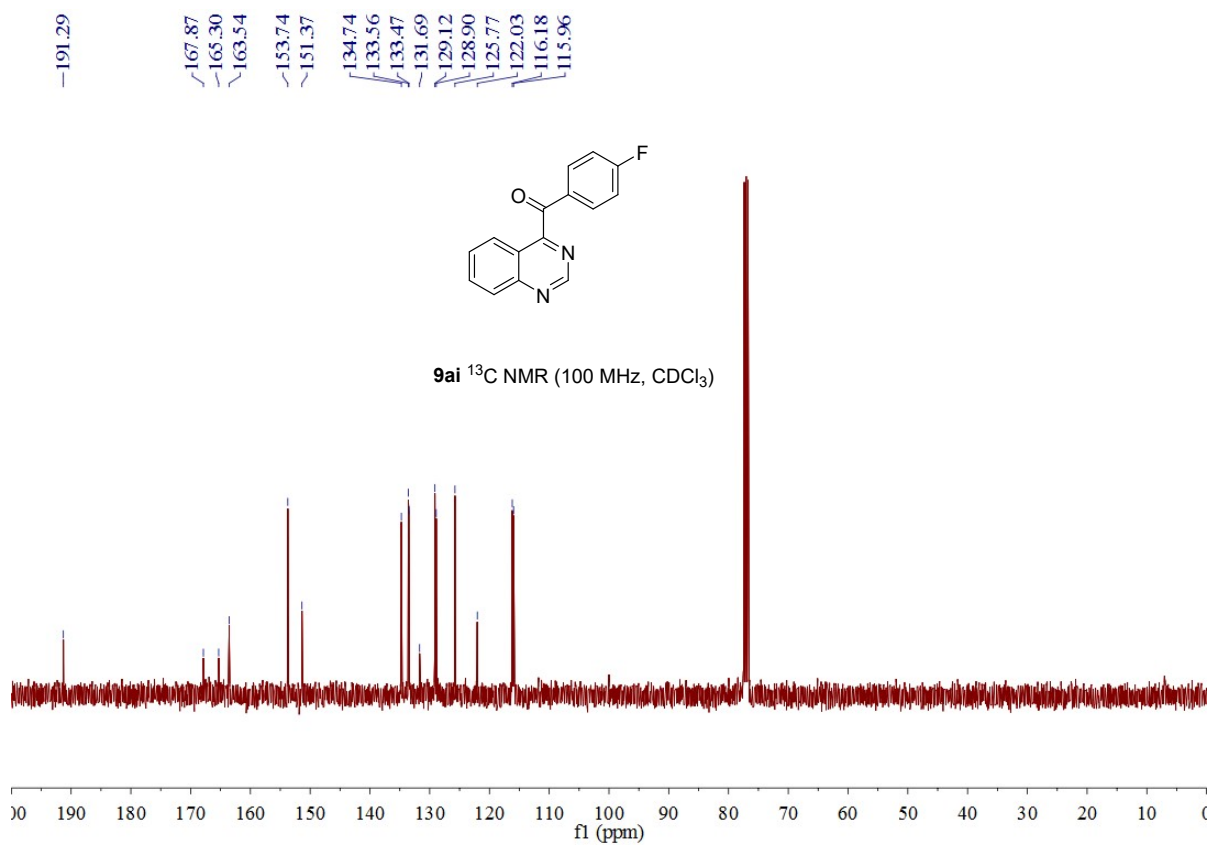




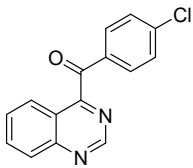
Copy of Products 9 NMR



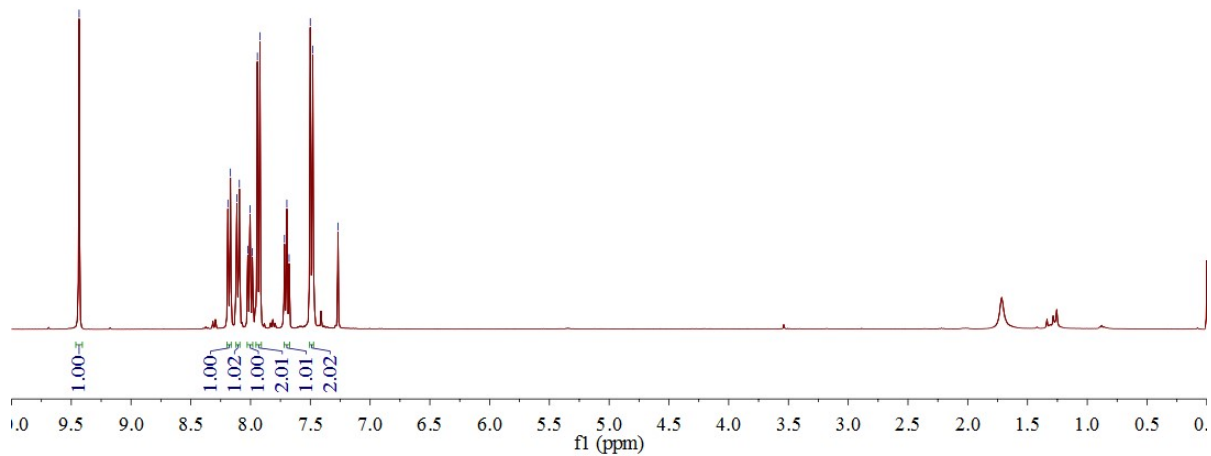




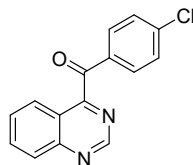
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8.189
8.168
8.114
8.094
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7.985
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7.479
7.268



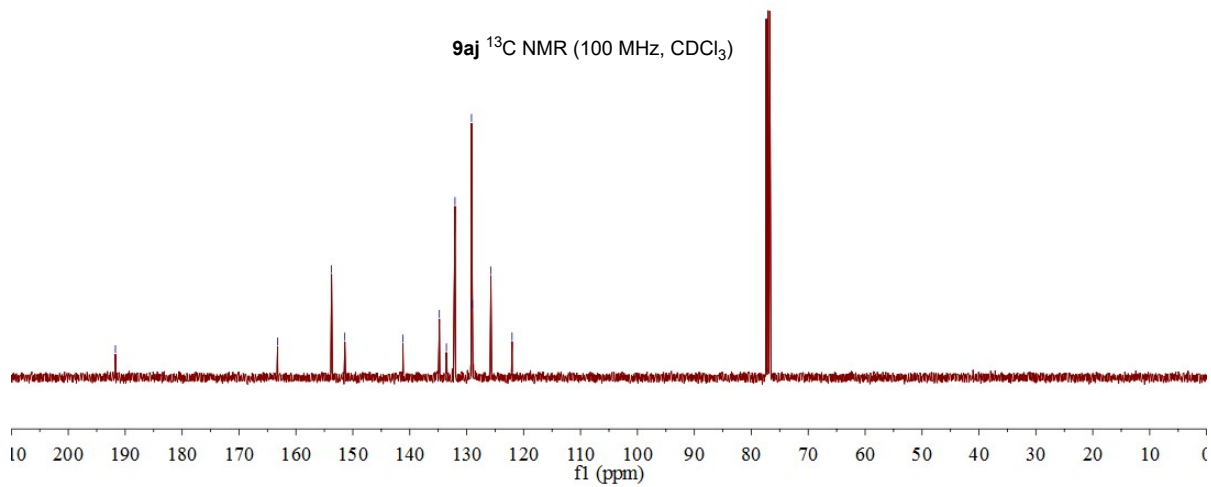
9aj ¹H NMR (400 MHz, CDCl₃)



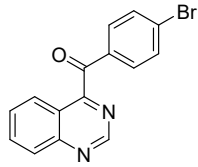
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153.74
151.41
141.20
134.80
133.57
132.06
129.15
128.99
125.75
122.03



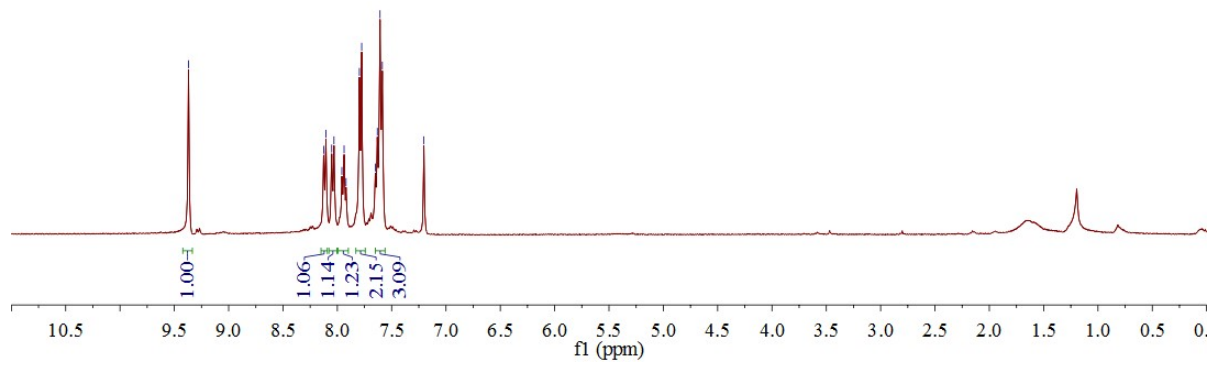
9aj ¹³C NMR (100 MHz, CDCl₃)



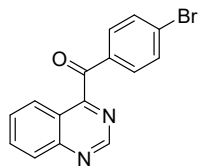
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7.586
7.203



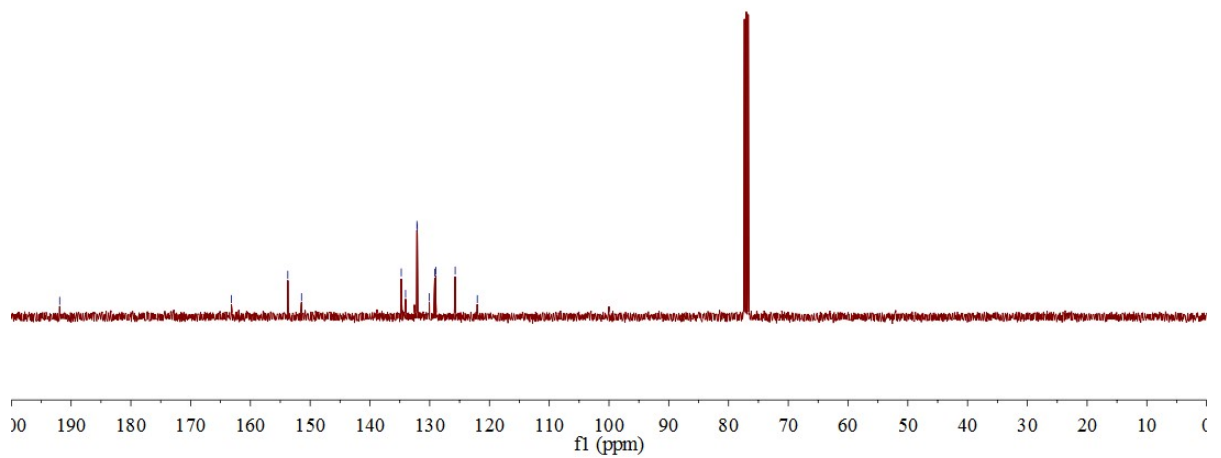
9ak ^1H NMR (400 MHz, CDCl_3)



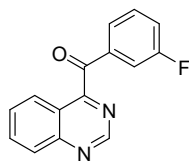
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151.45
134.76
134.03
132.13
132.07
130.05
129.16
128.97
125.73
122.03



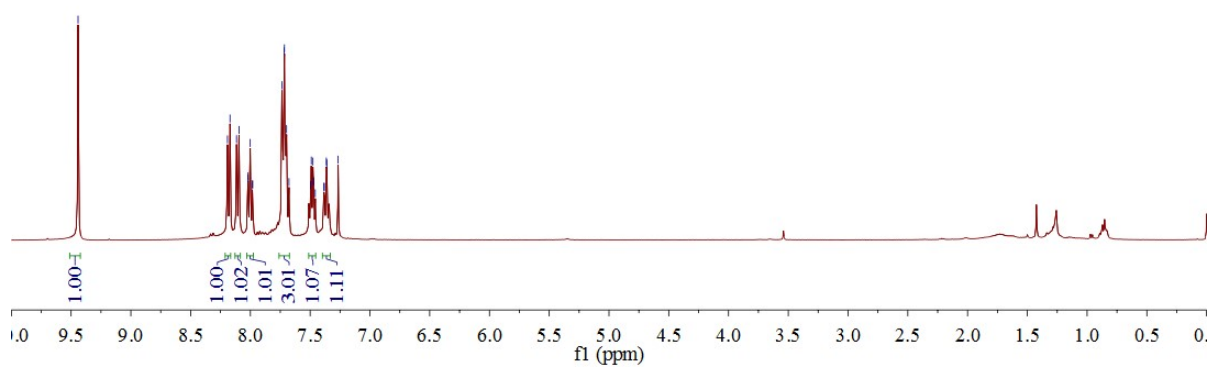
9ak ^{13}C NMR (100 MHz, CDCl_3)



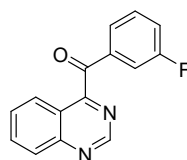
9.442
8.192
8.170
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8.095
8.022
8.019
8.001
7.983
7.981
7.737
7.717
7.715
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7.266



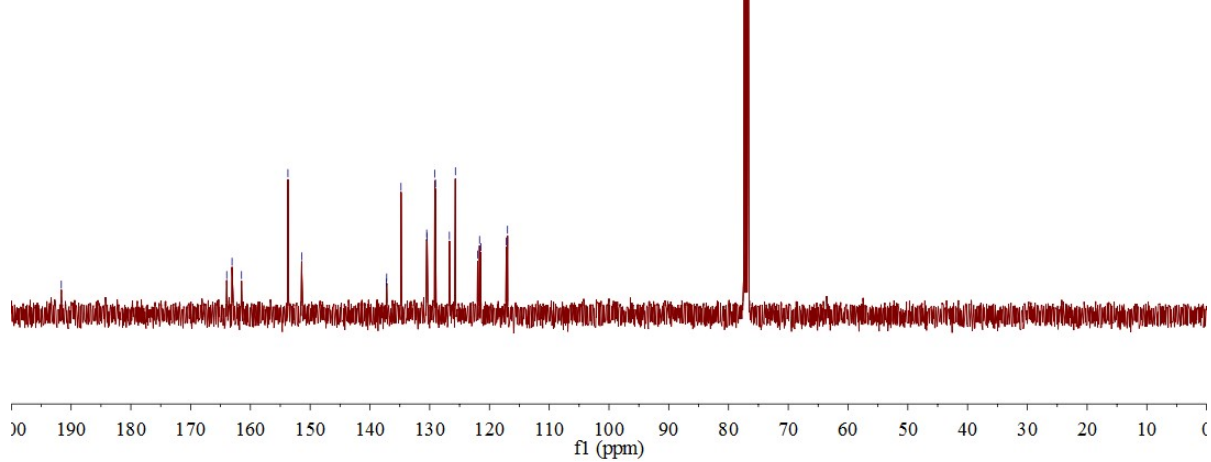
9ao ^1H NMR (400 MHz, CDCl_3)

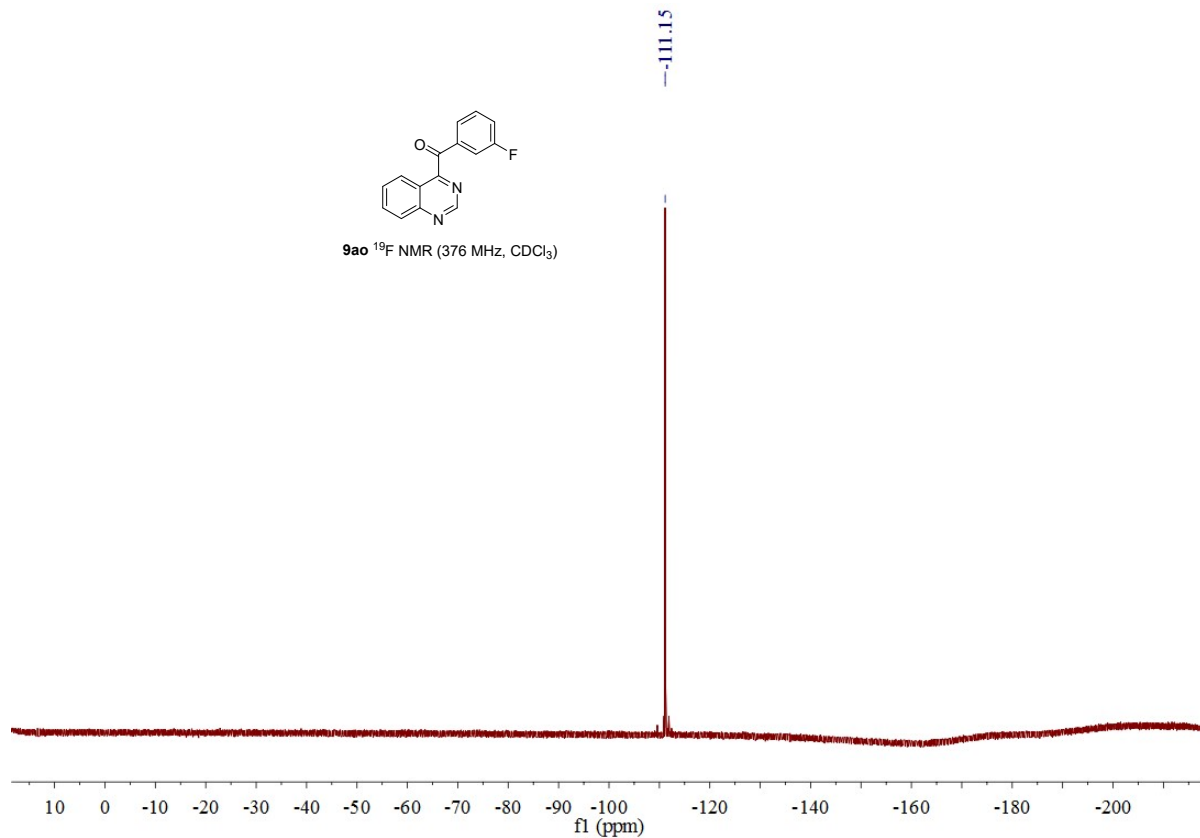


191.640
163.958
163.072
161.485
153.720
151.428
137.255
137.190
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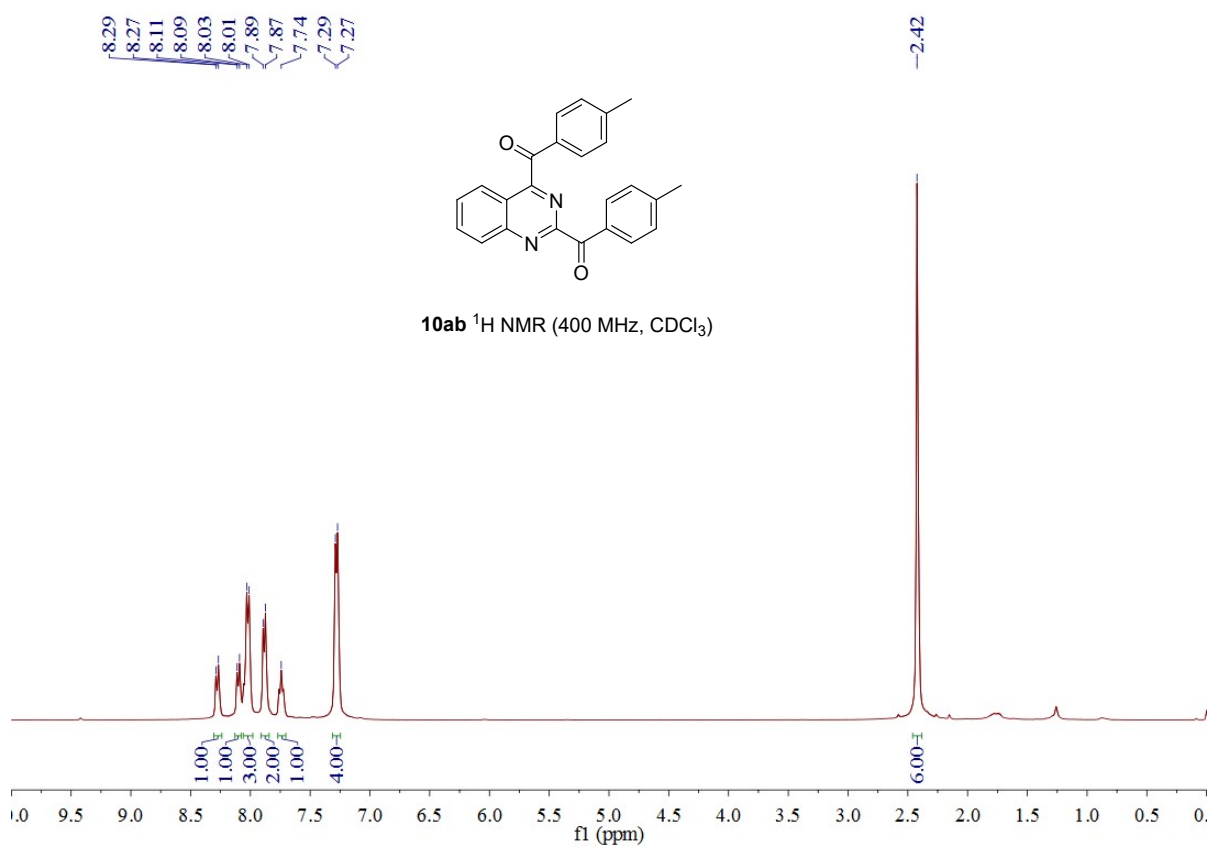


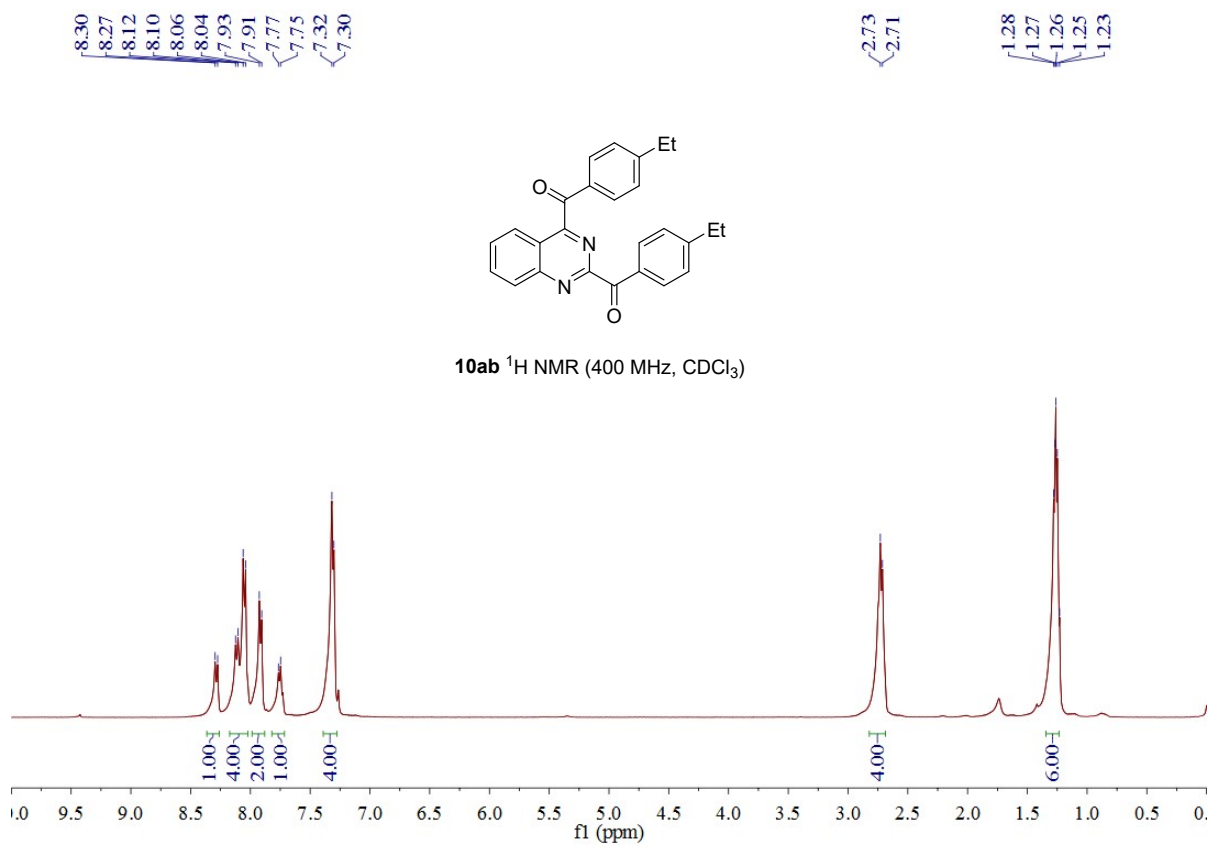
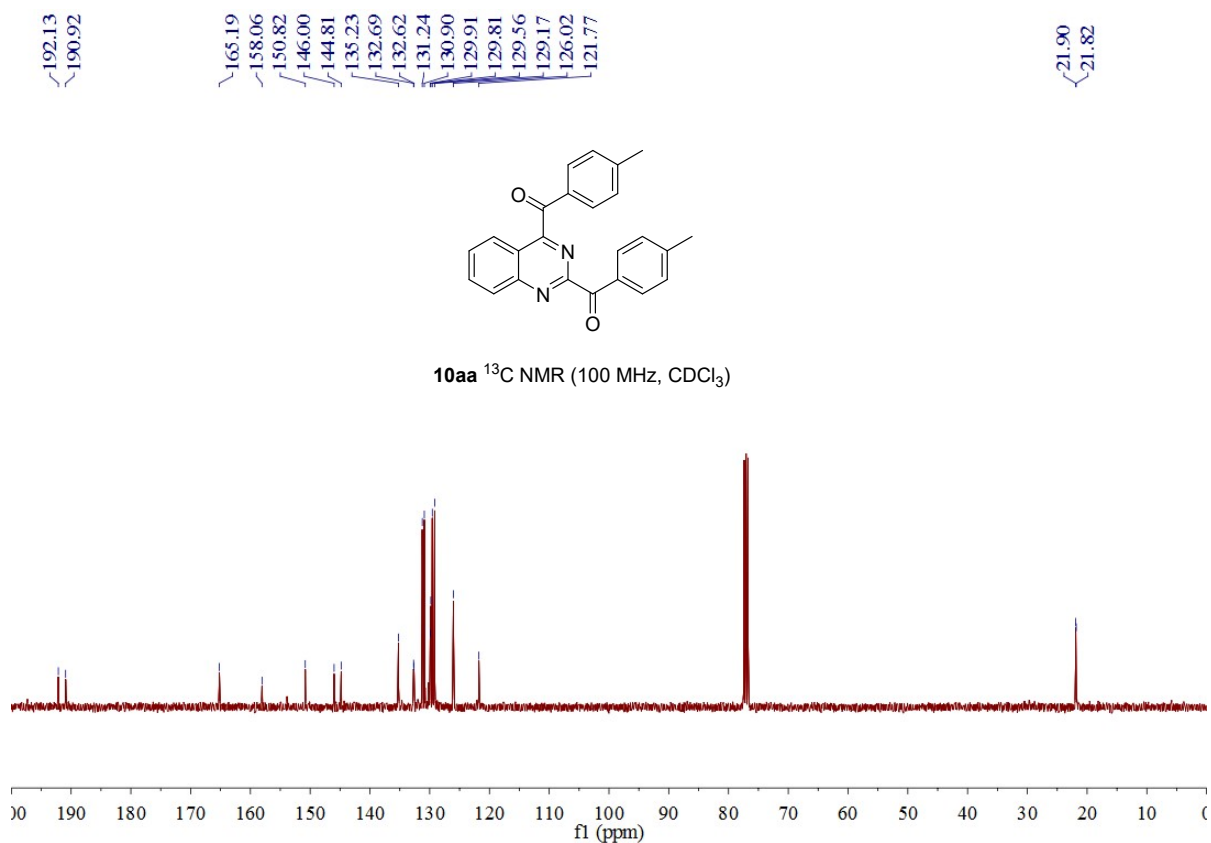
9ao ^{13}C NMR (100 MHz, CDCl_3)

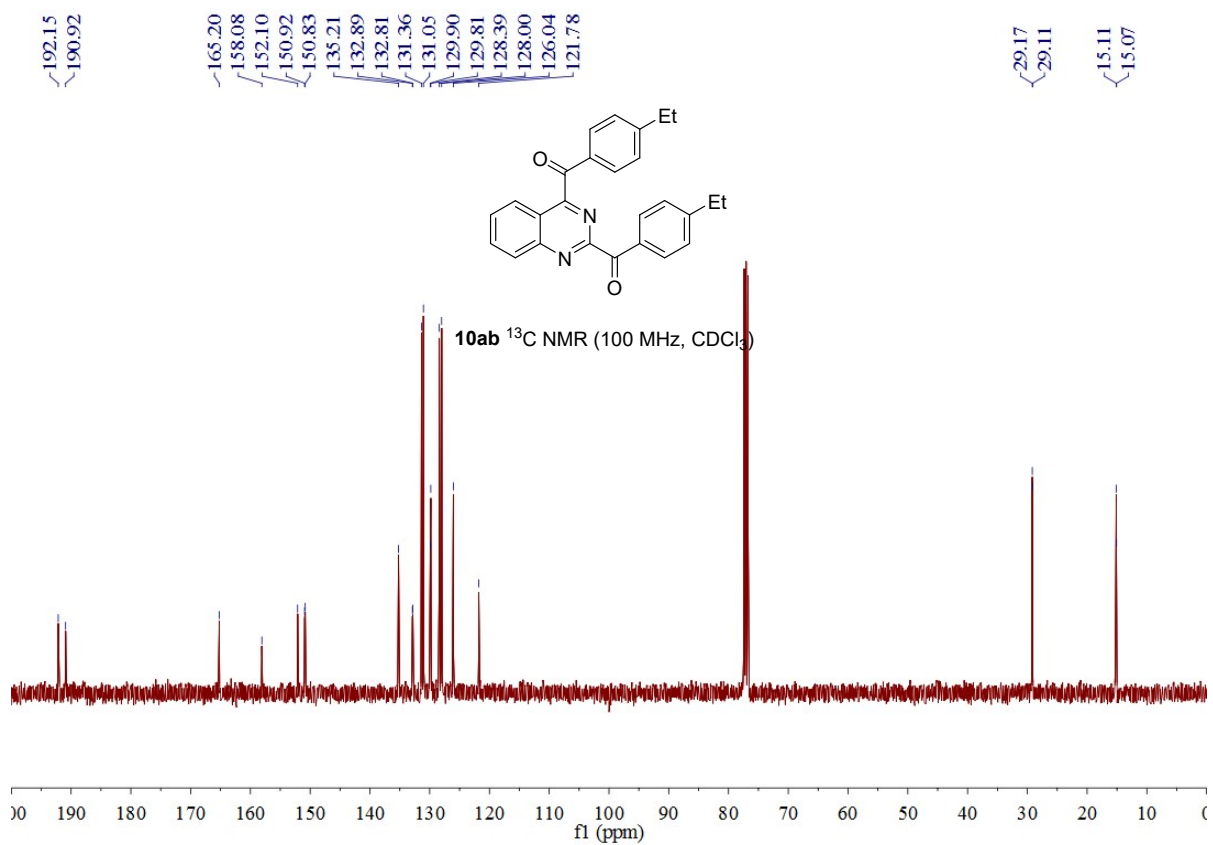


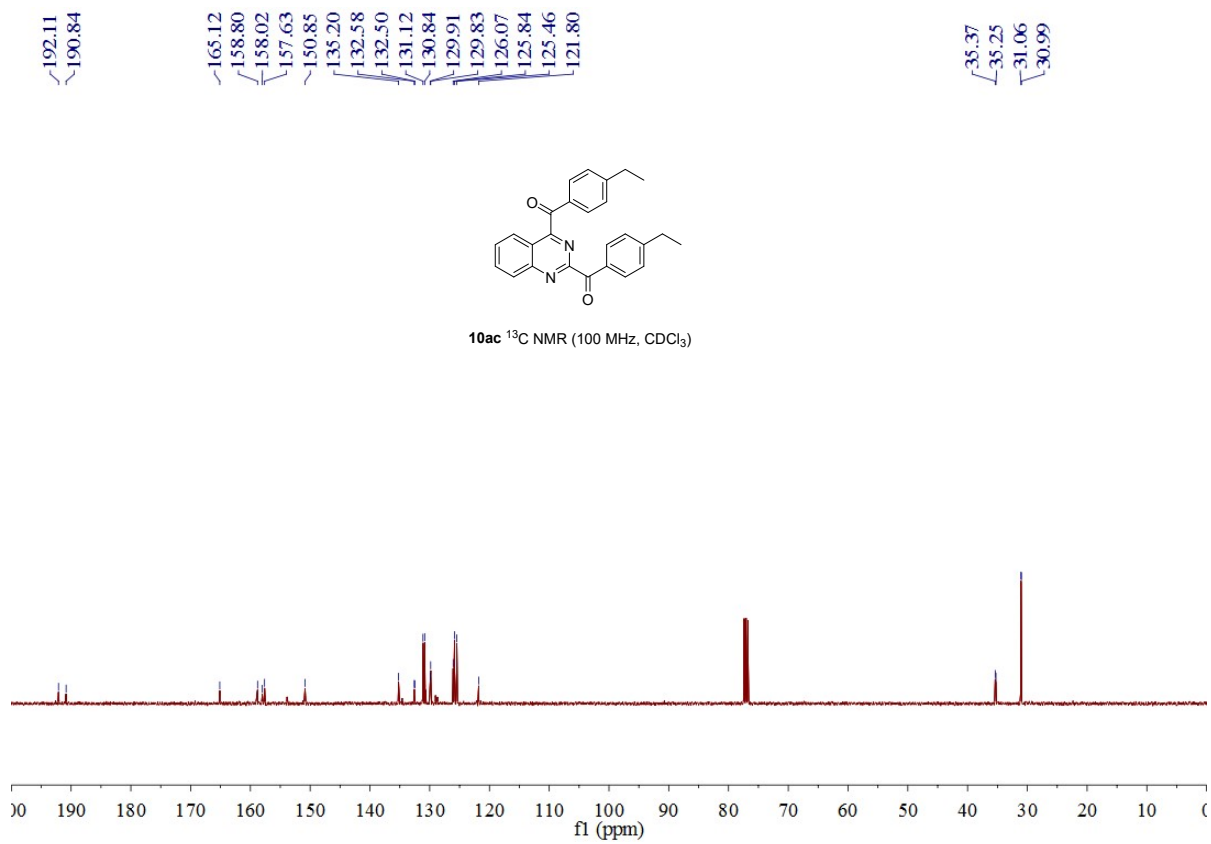
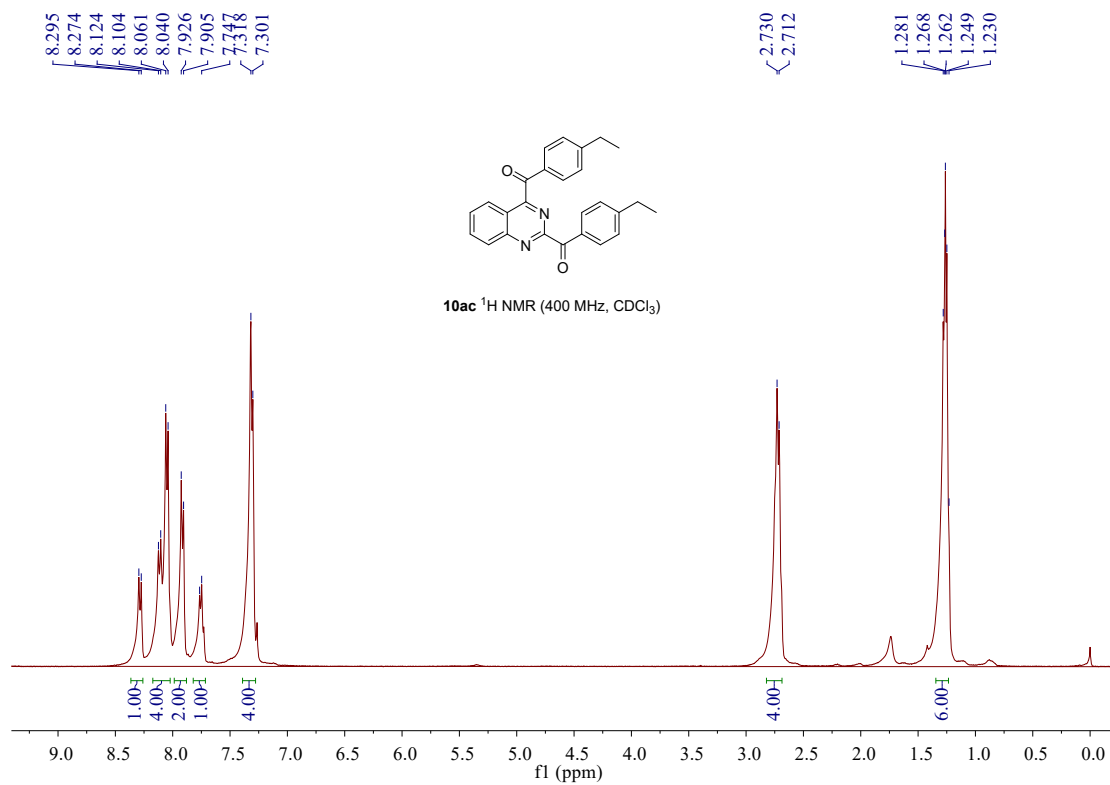


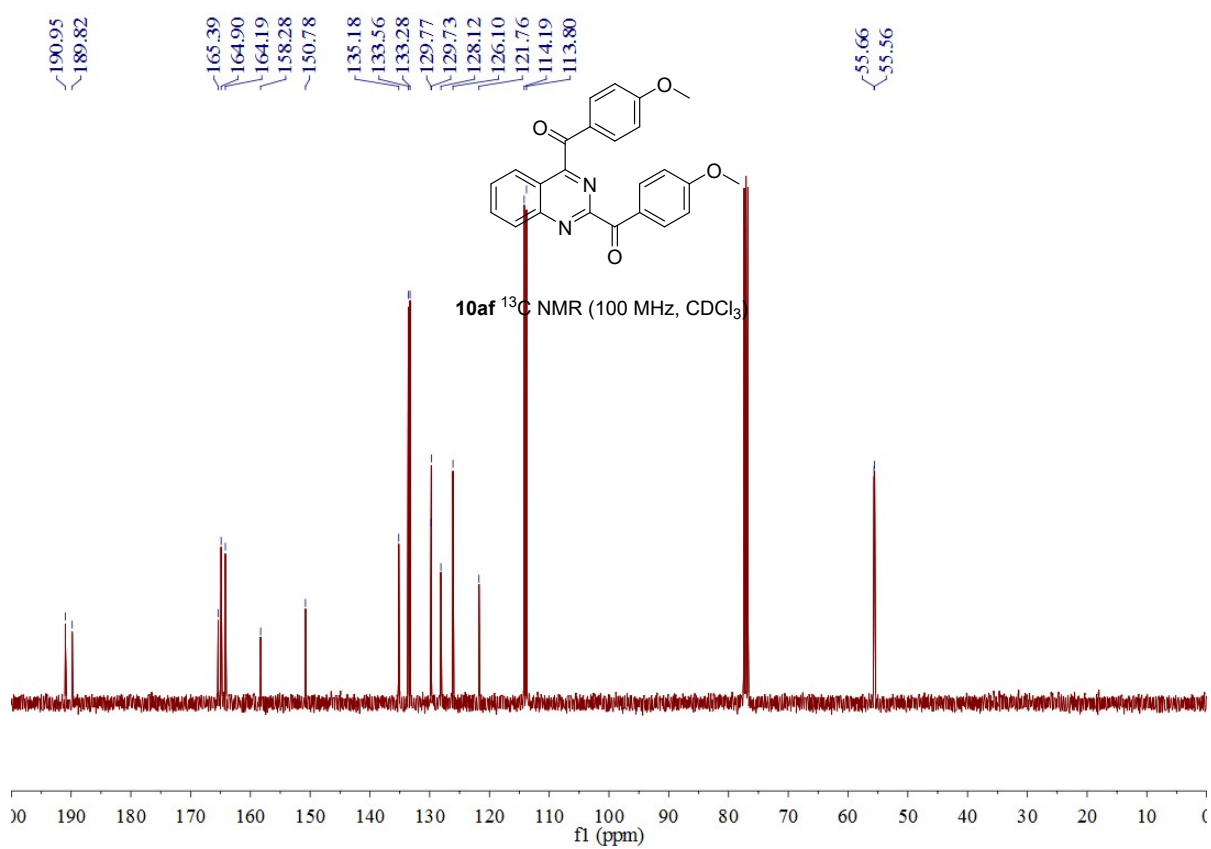
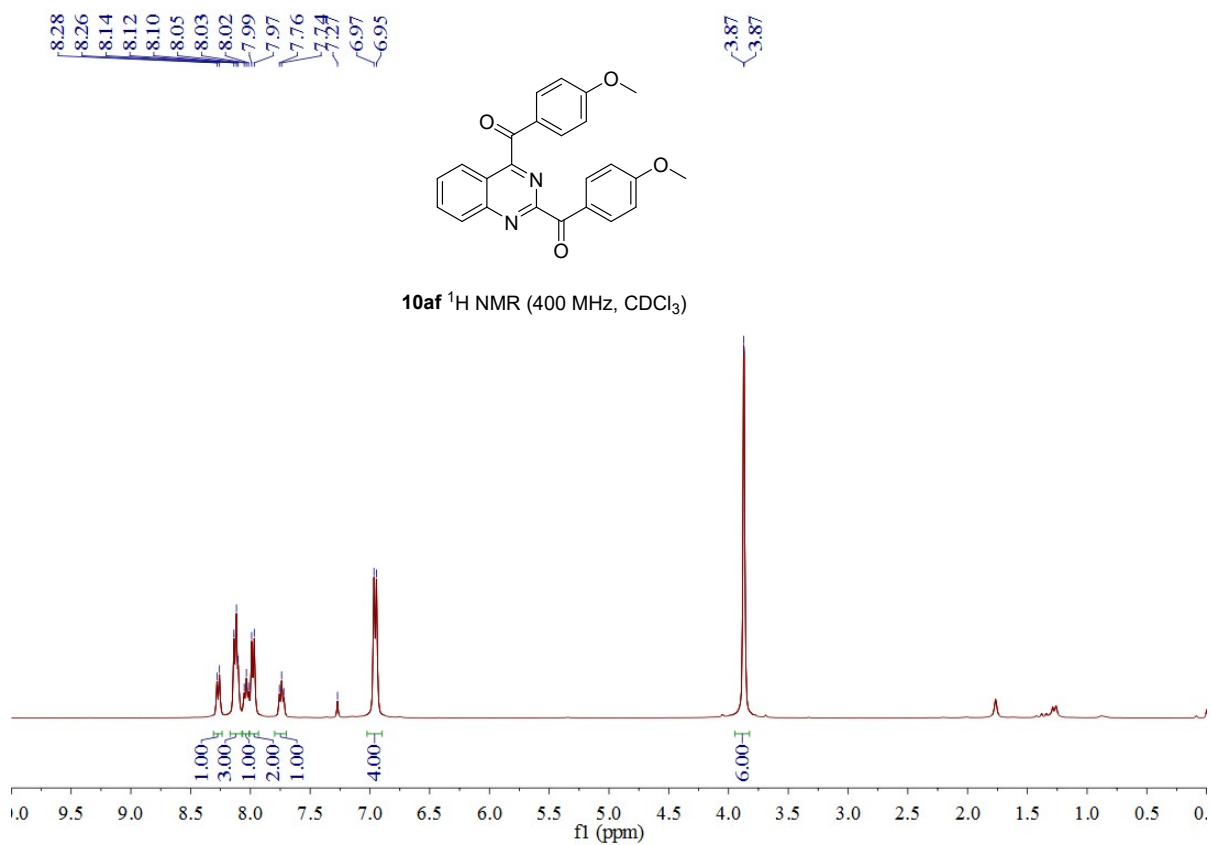
Copy of Products 10 NMR

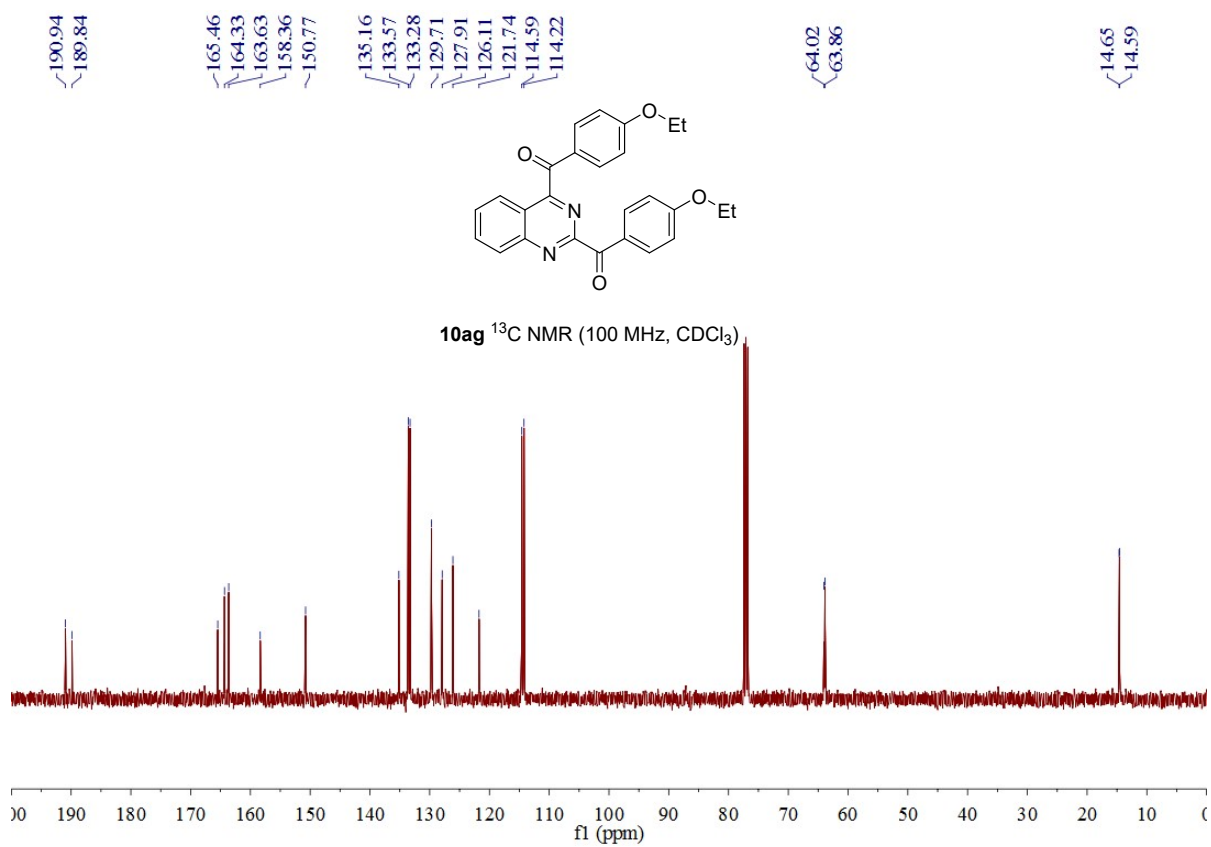
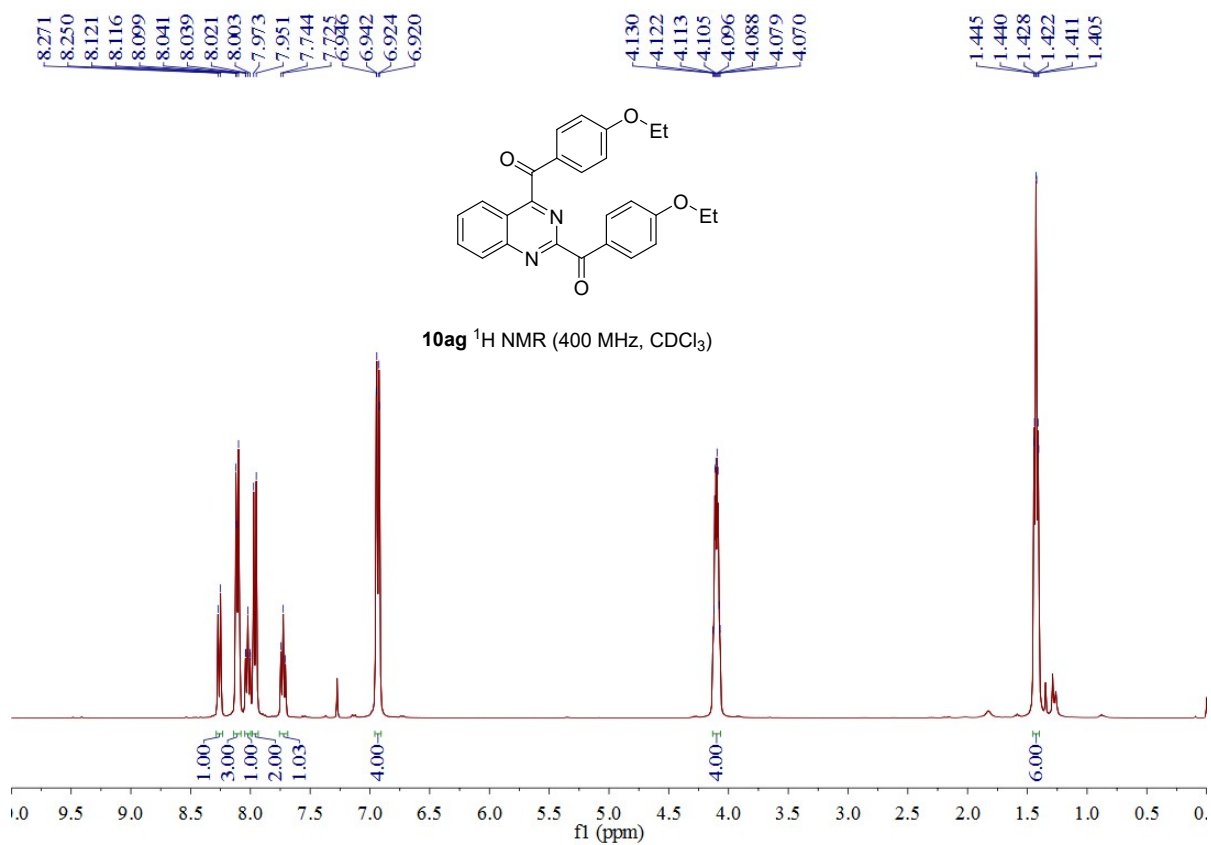




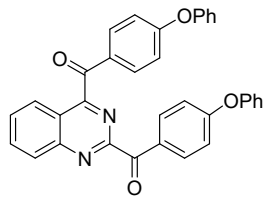




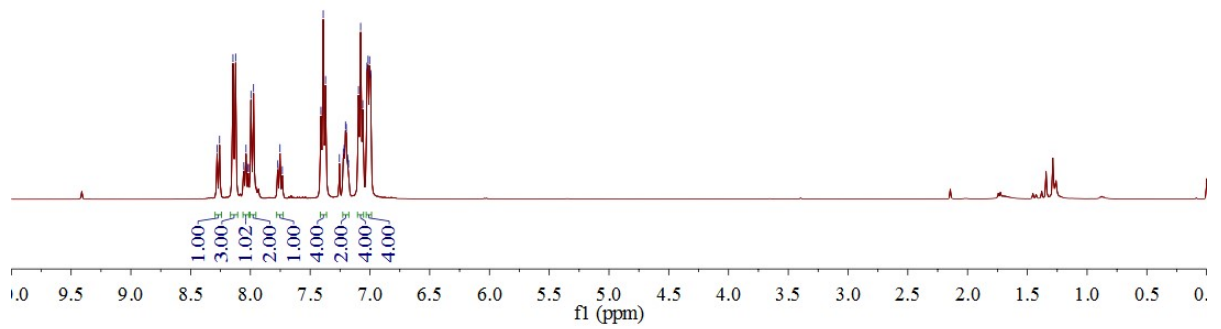




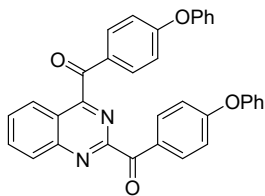
8.279
8.258
8.146
8.124
8.055
8.037
8.018
8.016
7.995
7.973
7.771
7.752
7.733
7.410
7.391
7.371
7.255
7.223
7.216
7.204
7.198
7.186
7.179
7.096
7.078
7.060
7.025
7.015
7.003
6.993



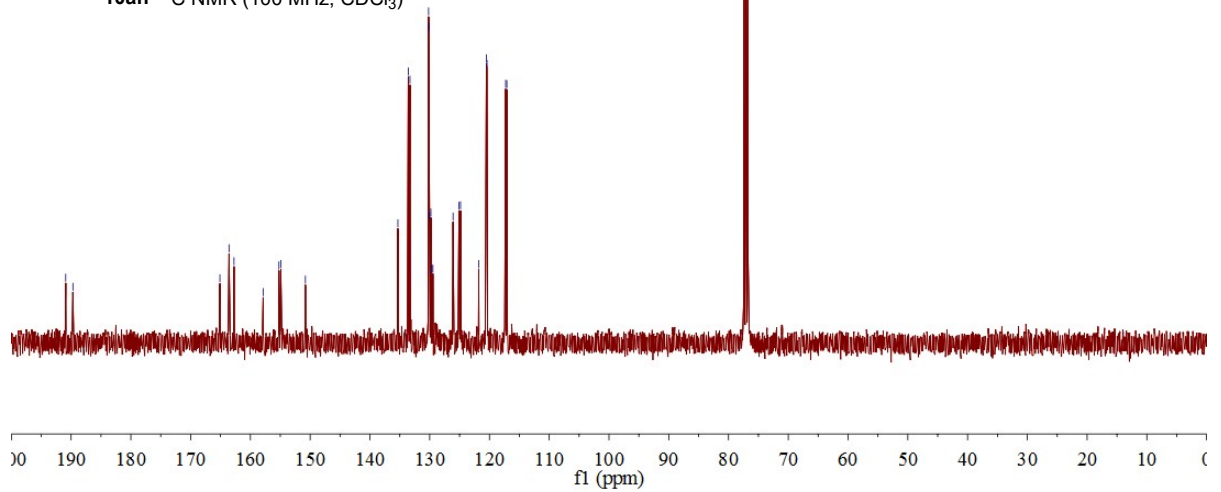
10ah ¹H NMR (400 MHz, CDCl₃)



190.90
189.70
165.10
163.58
162.74
157.87
155.22
154.90
150.80
135.32
133.58
133.30
130.19
130.11
130.02
129.80
129.64
129.46
126.09
125.10
124.84
121.79
120.51
120.41
117.28
117.09



10ah ¹³C NMR (100 MHz, CDCl₃)

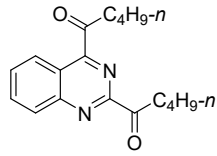


10 au

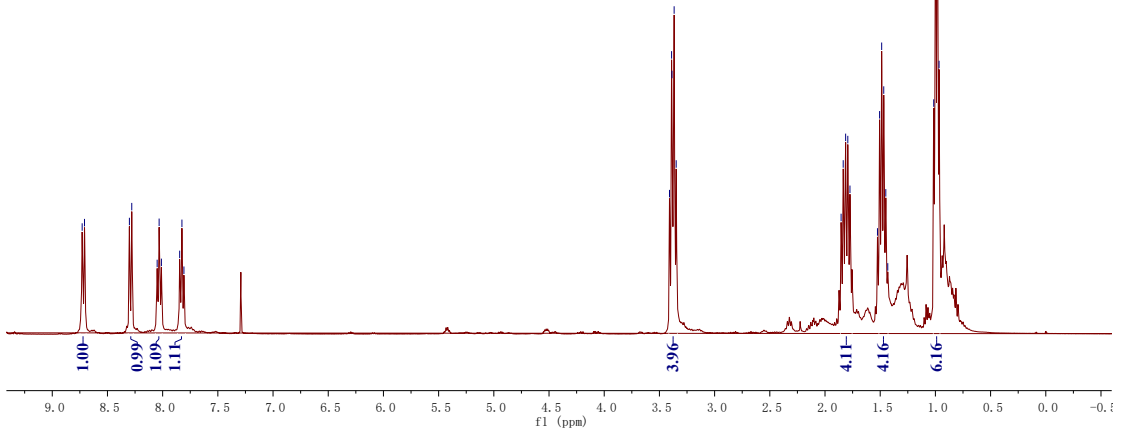
8.729
8.708
8.301
8.280
8.050
8.032
8.011
7.846
7.825
7.807

3.409
3.390
3.386
3.367
3.348

1.854
1.835
1.813
1.793
1.774
1.506
1.487
1.468
1.449
0.998
0.985
0.967



10au ¹H NMR (400 MHz, CDCl₃)



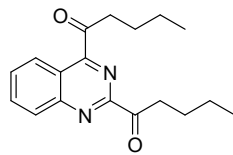
10 au

203.82
200.11

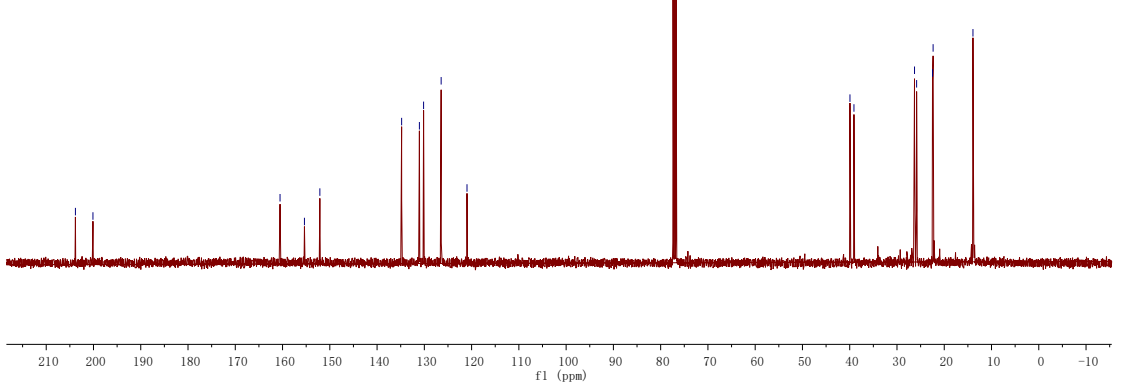
160.53
155.37
152.10

134.80
131.04
130.16
126.44
120.97

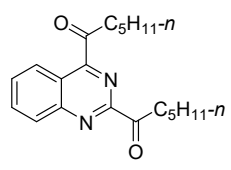
39.95
39.10
26.29
25.85
22.48
22.36
13.93



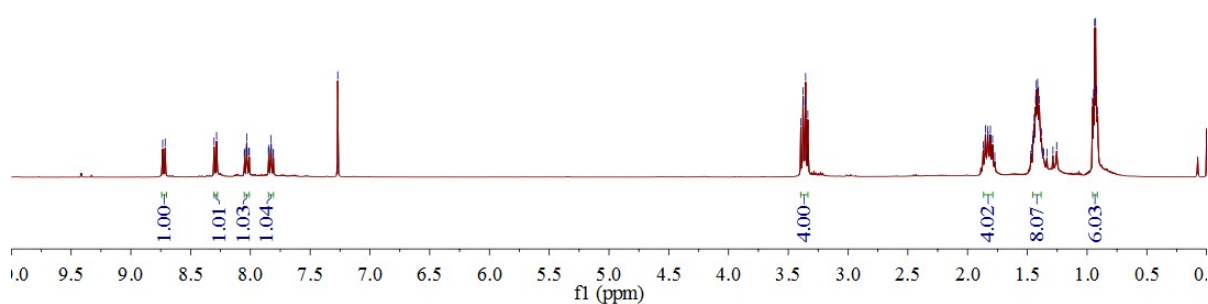
10au ¹³C NMR (100 MHz, CDCl₃)



8.73
8.71
8.30
8.28
8.05
8.03
8.03
8.01
8.01
7.85
7.83
7.83
7.82
7.27
3.40
3.38
3.37
3.36
3.36
3.34
1.87
1.85
1.83
1.83
1.81
1.81
1.79
1.46
1.45
1.45
1.44
1.43
1.43
1.42
1.41
1.41
1.40
1.38
1.37
1.36
1.34
1.29
1.25
-0.95
-0.94
-0.93
-0.92
-0.91



10av ¹H NMR (400 MHz, CDCl₃)

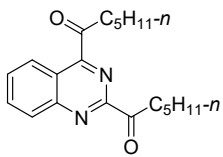


-203.88
-200.17

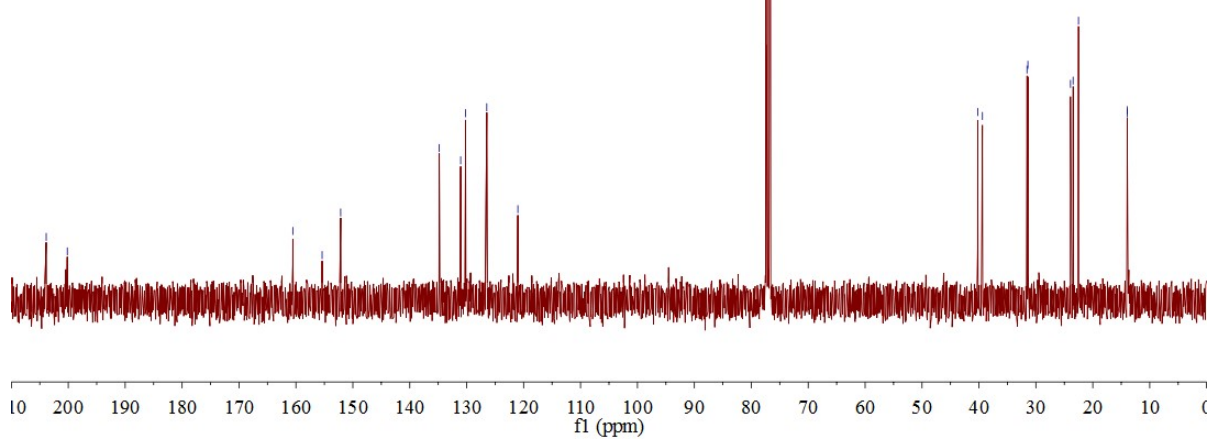
-160.55
-155.40
-152.14

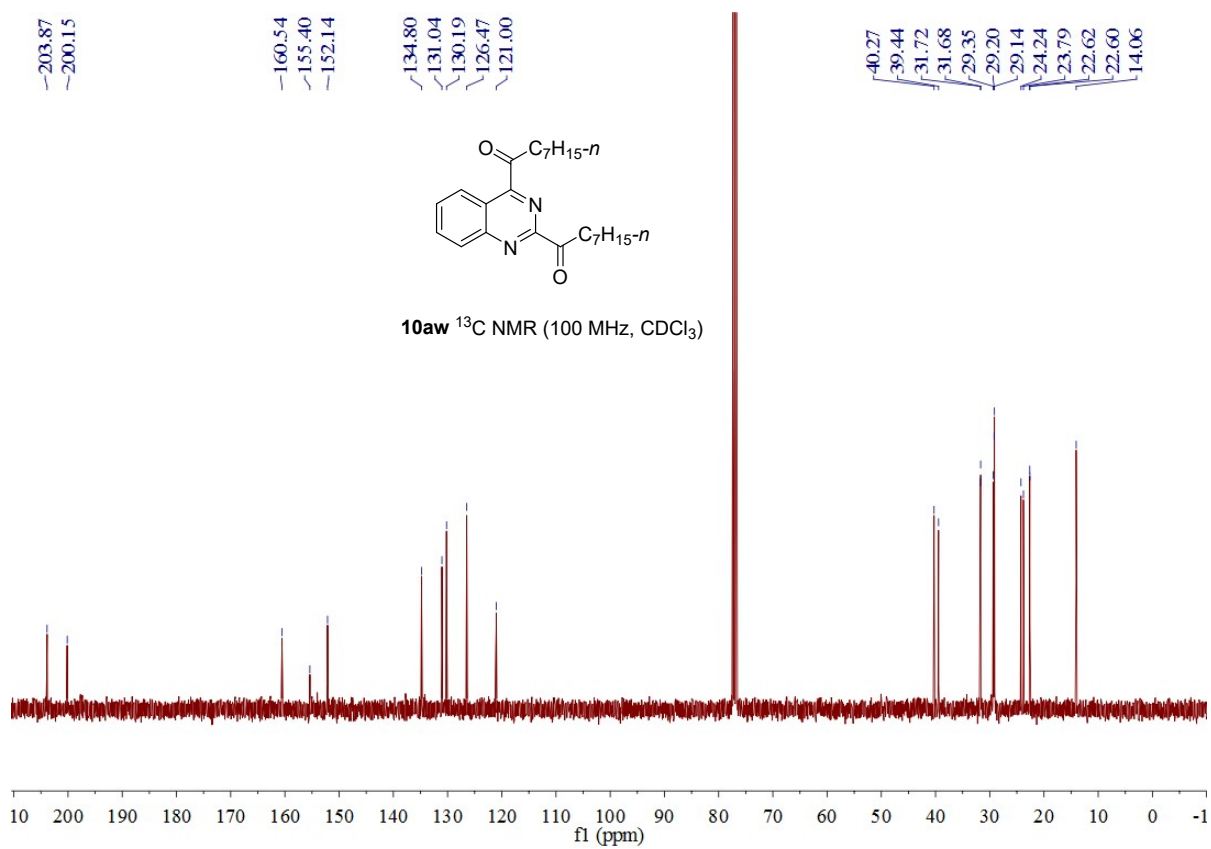
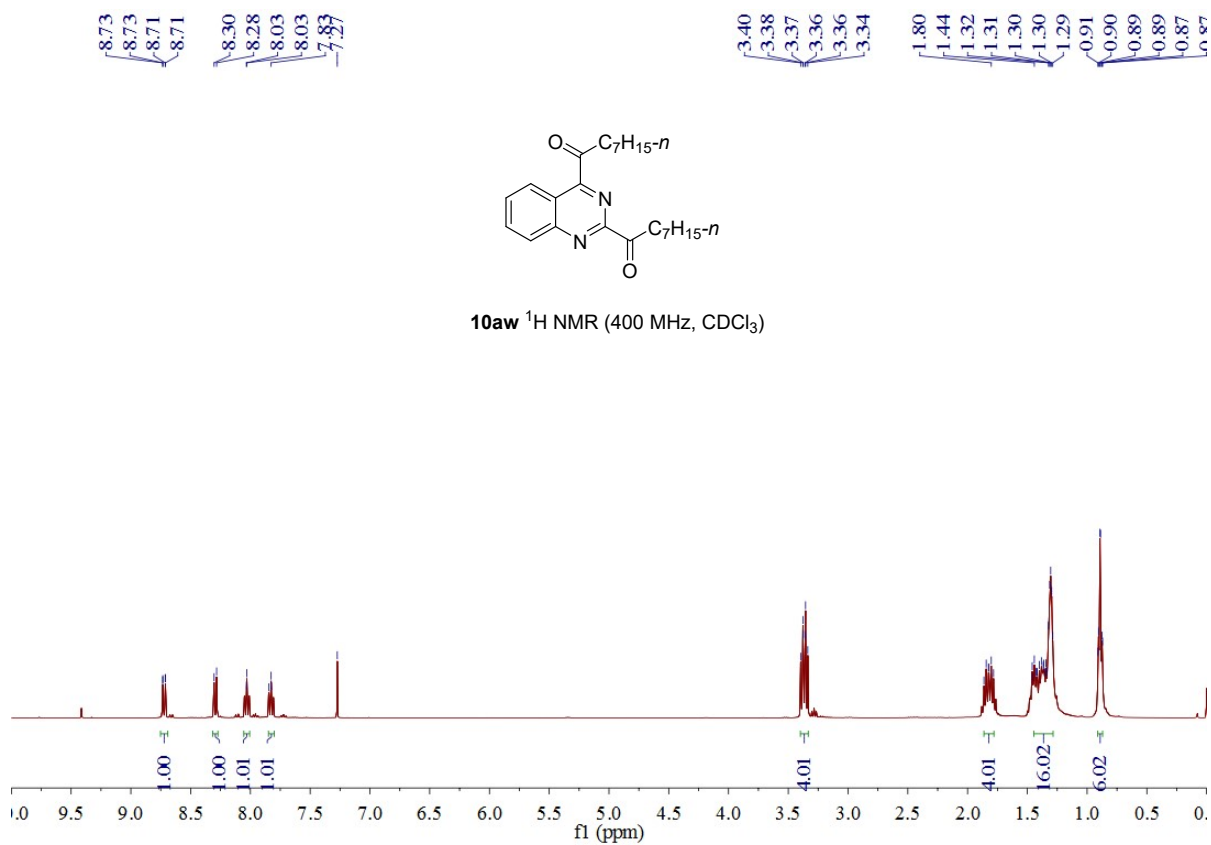
134.82
131.05
130.19
126.47
121.00

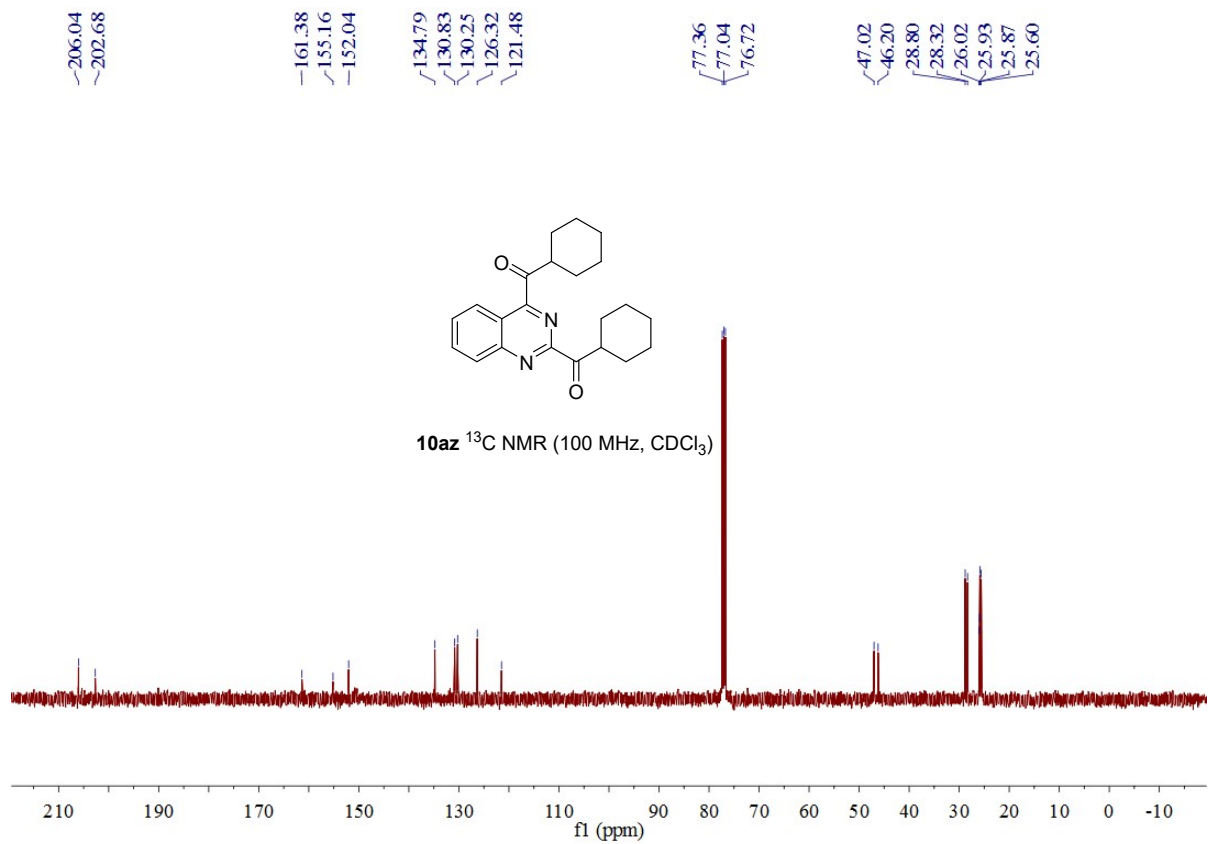
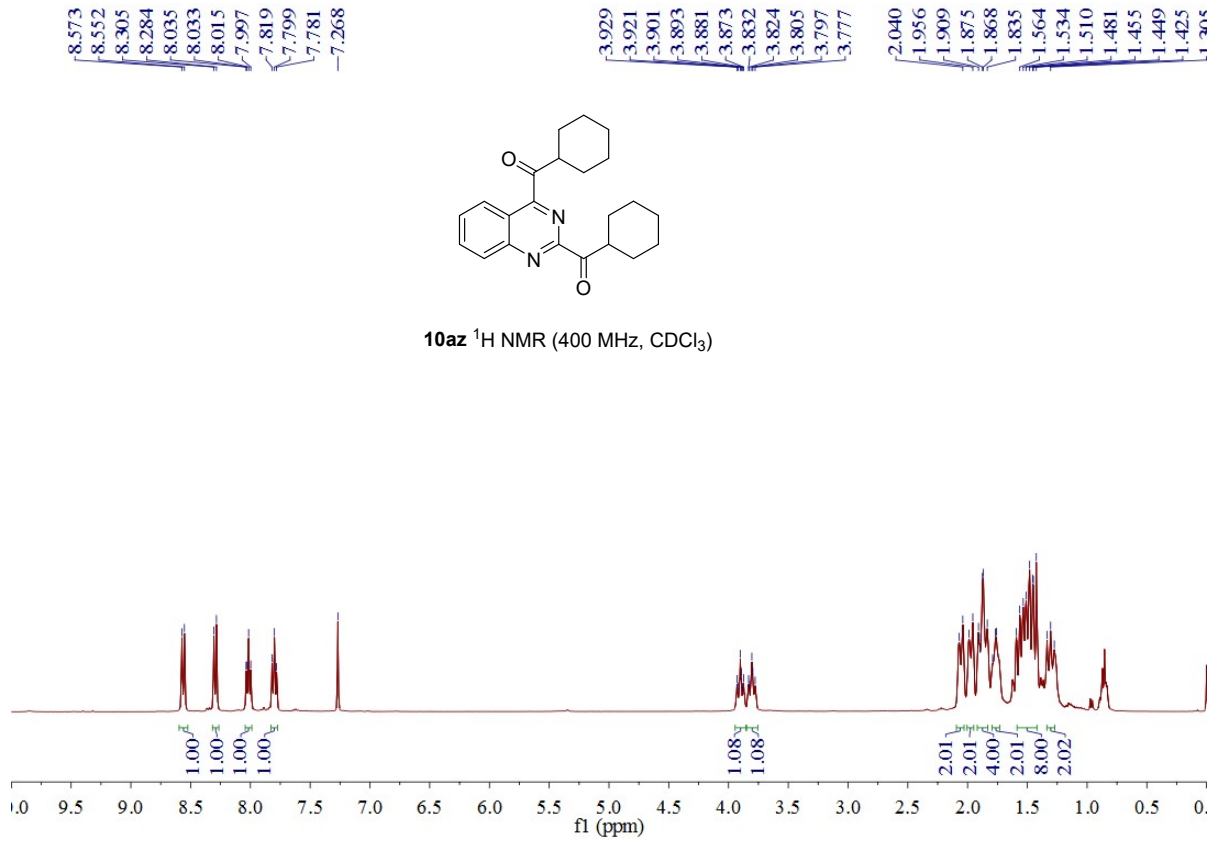
40.22
39.39
31.56
31.40
23.91
23.46
22.51
13.96
13.92



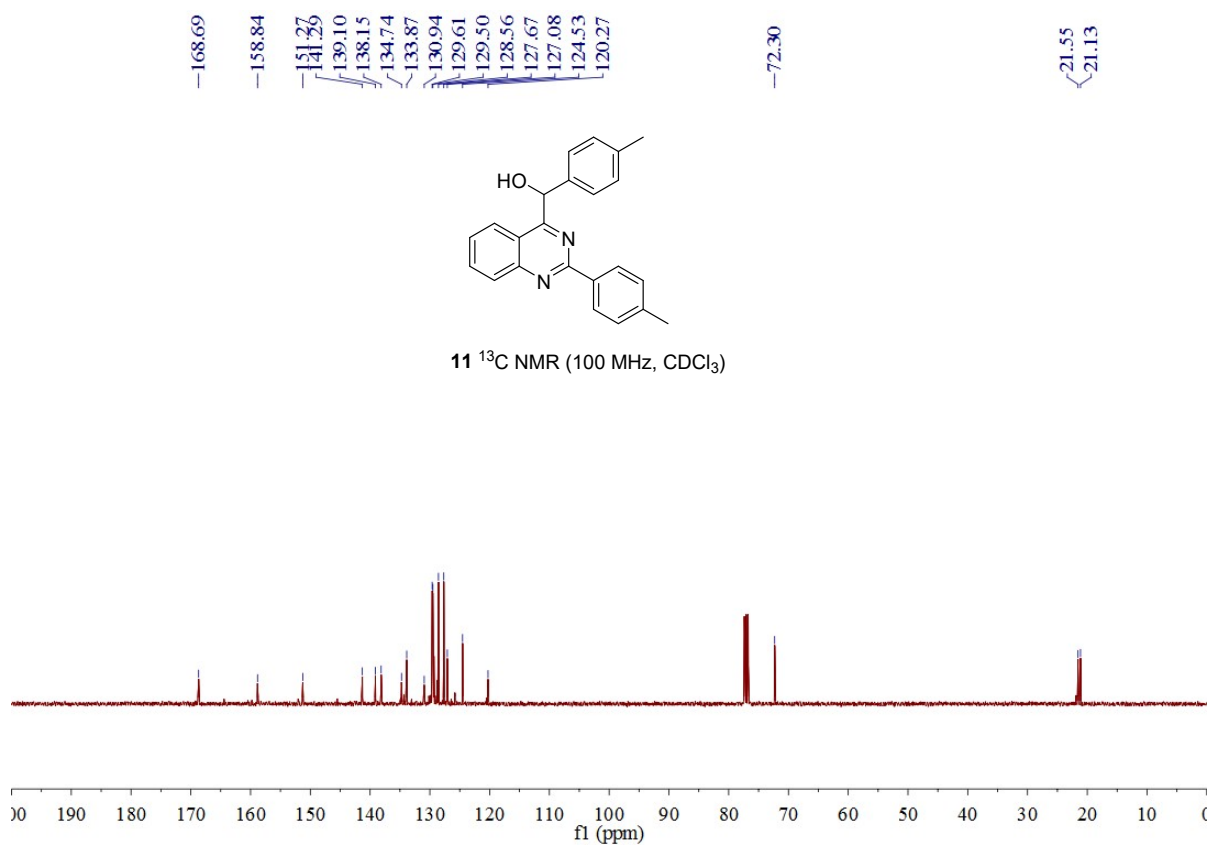
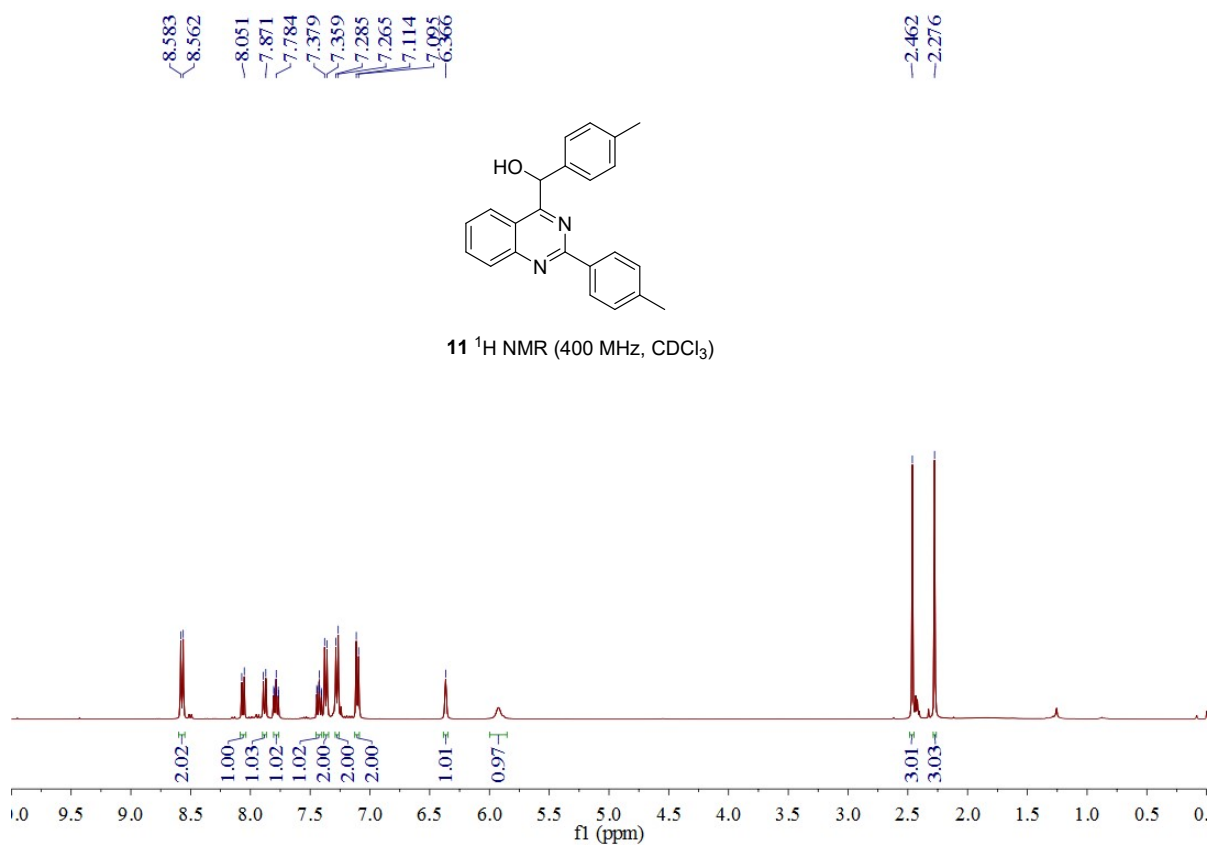
10av ¹³C NMR (100 MHz, CDCl₃)



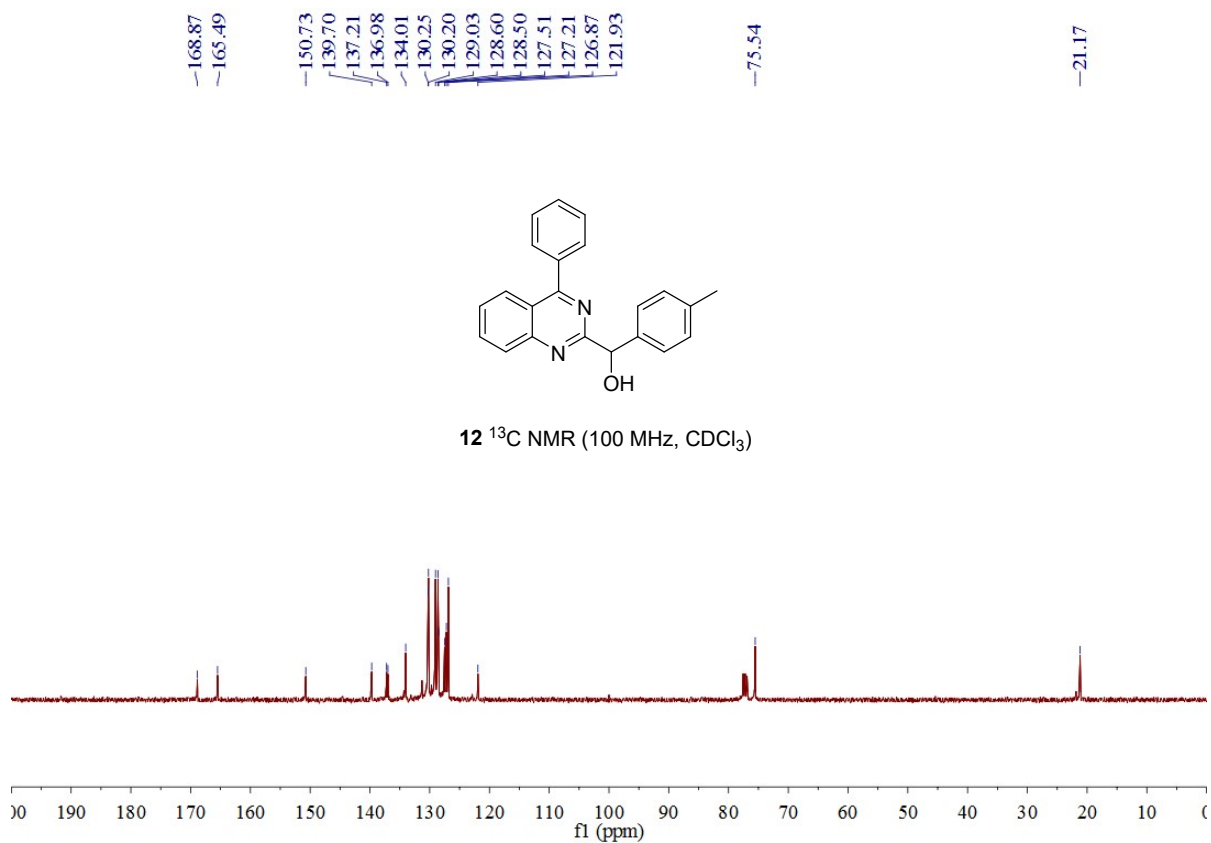
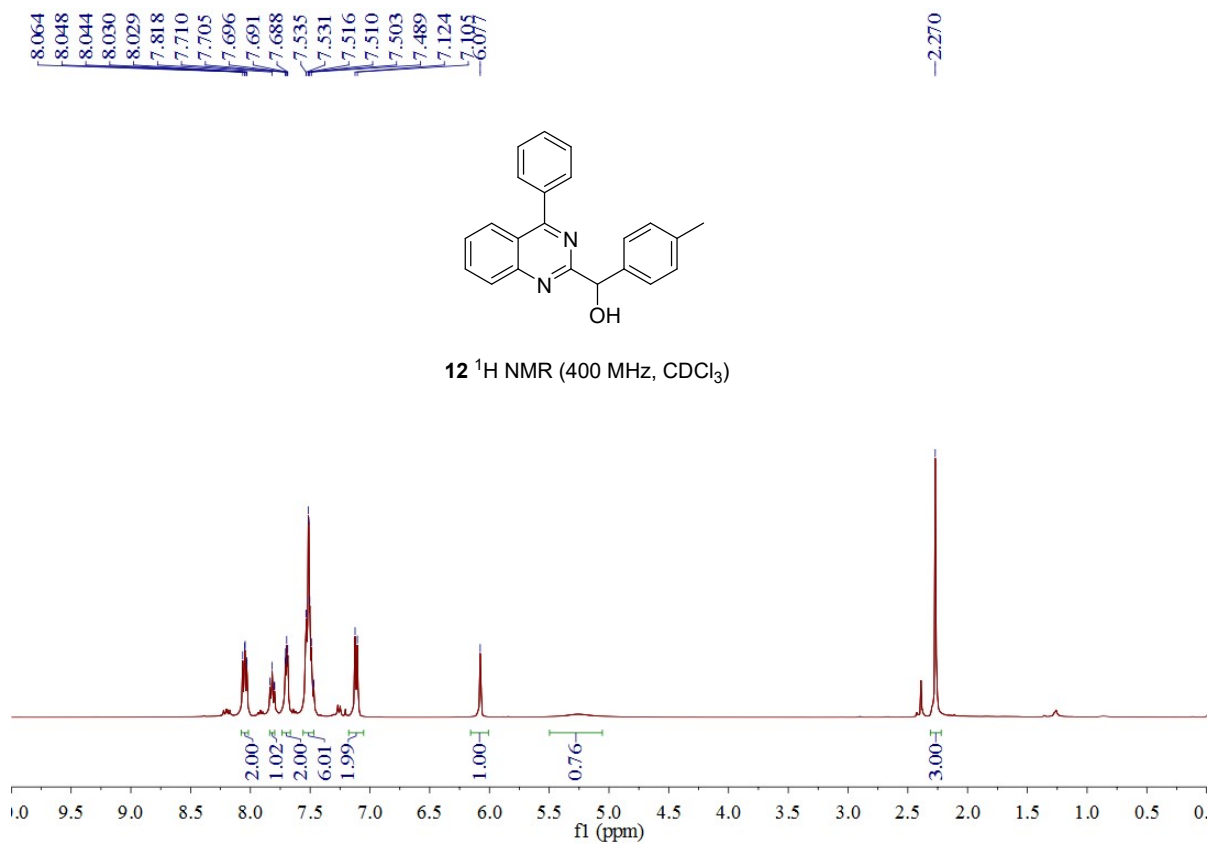




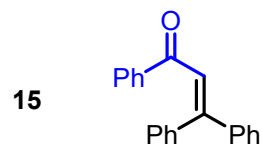
Copy of Products 11 NMR



Copy of Products 12 NMR



II The HPLC-MS Figure of adducts **15** and **16**

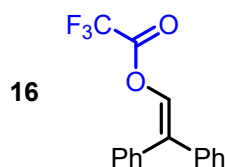
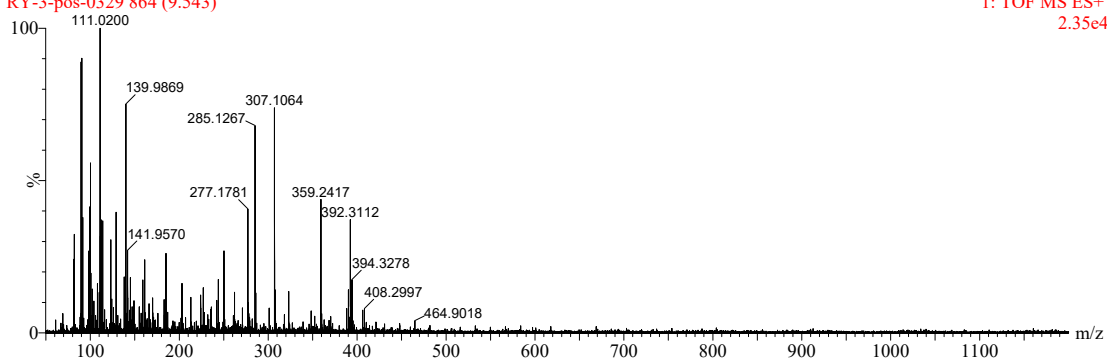


HRMS (ESI): m/z $[M+H]^+$ calcd for $C_{21}H_{17}O$: 285.1279, Found: 285.1267

R_Y-3-pos-0329

R_Y-3-pos-0329 864 (9.543)

1: TOF MS ES+
2.35e4



HRMS (ESI): m/z $[M+H]^+$ calcd for $C_{16}H_{12}O$: 293.0789, Found: 293.0790

R_Y-3-pos-0329

R_Y-3-pos-0329 688 (7.600)

1: TOF MS ES+
1.06e4

