

## *Supporting Information for*

### **(4+2) Cyclization of Aza-*o*-quinone Methides with Azlactones: Construction of Biologically Important Dihydroquinolinone Framework**

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Yu-Chen Zhang<sup>a,\*</sup> and Feng Shi<sup>a,\*</sup>

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*China*

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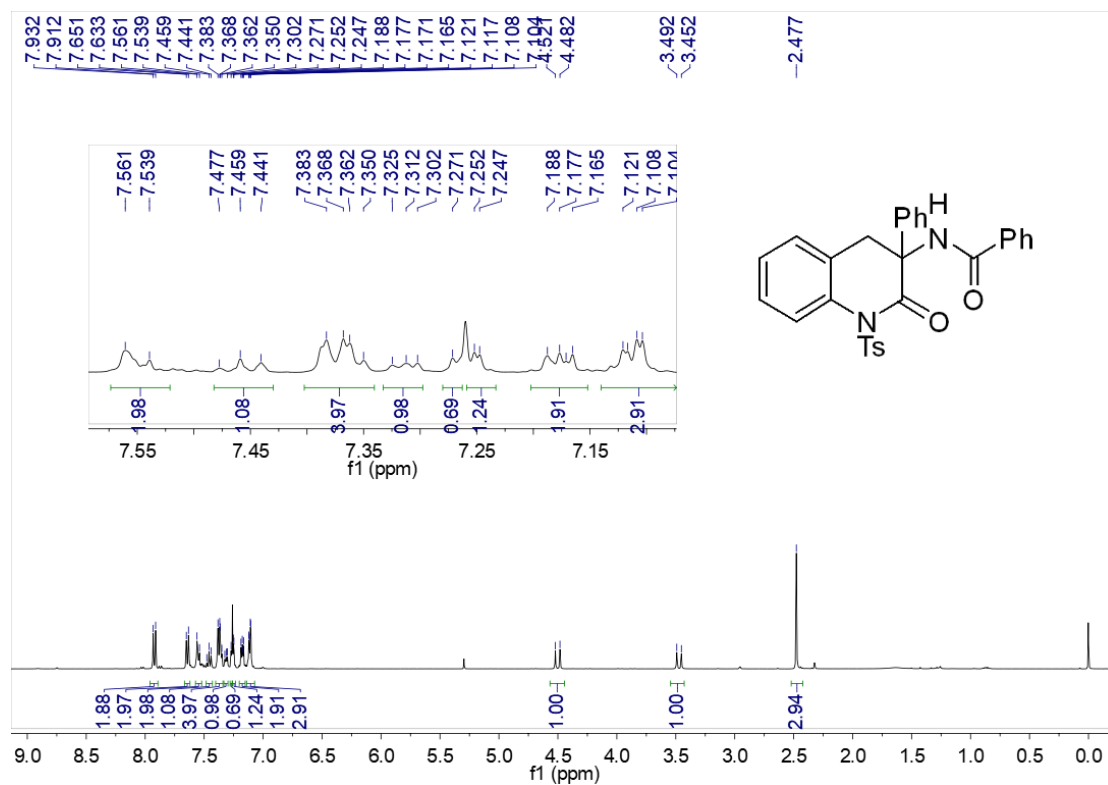
#### **Contents:**

**1. NMR spectra of products 3-5 and compound I (S2-S33)**

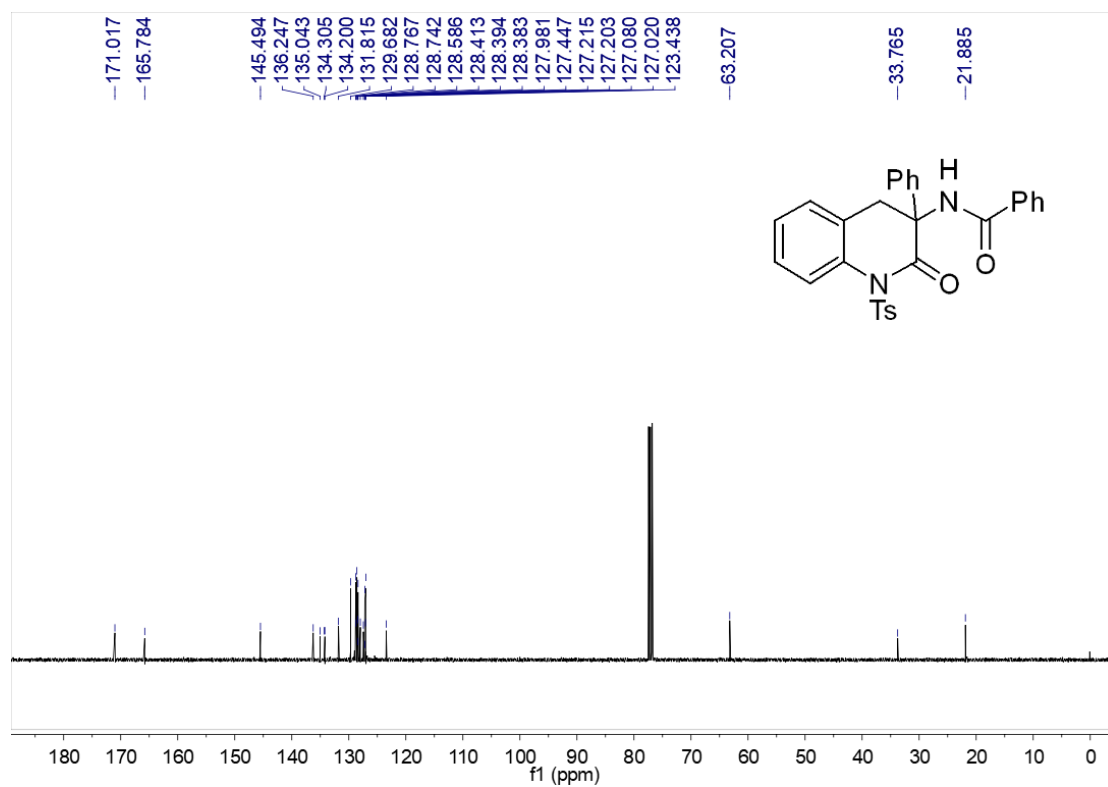
**2. X-ray single crystal data for product 3aa (S34-S35)**

## 1. NMR spectra of products 3-5 and compound I

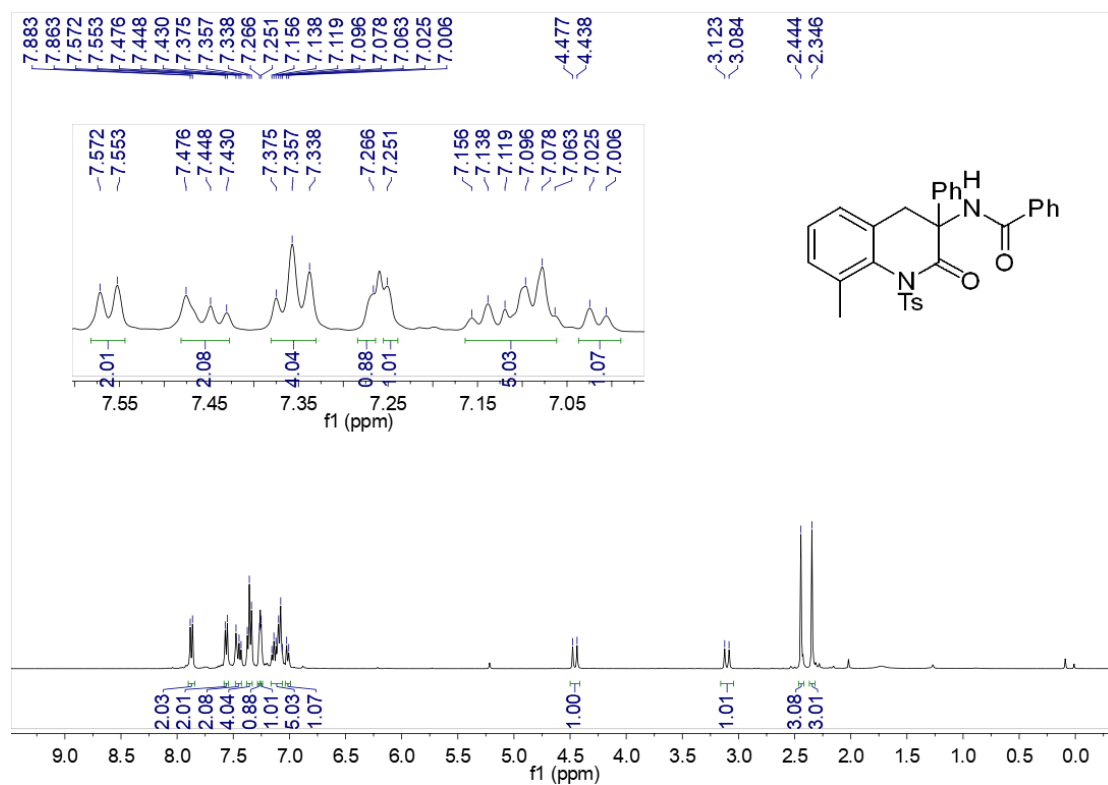
$^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ ) of compound **3aa**:



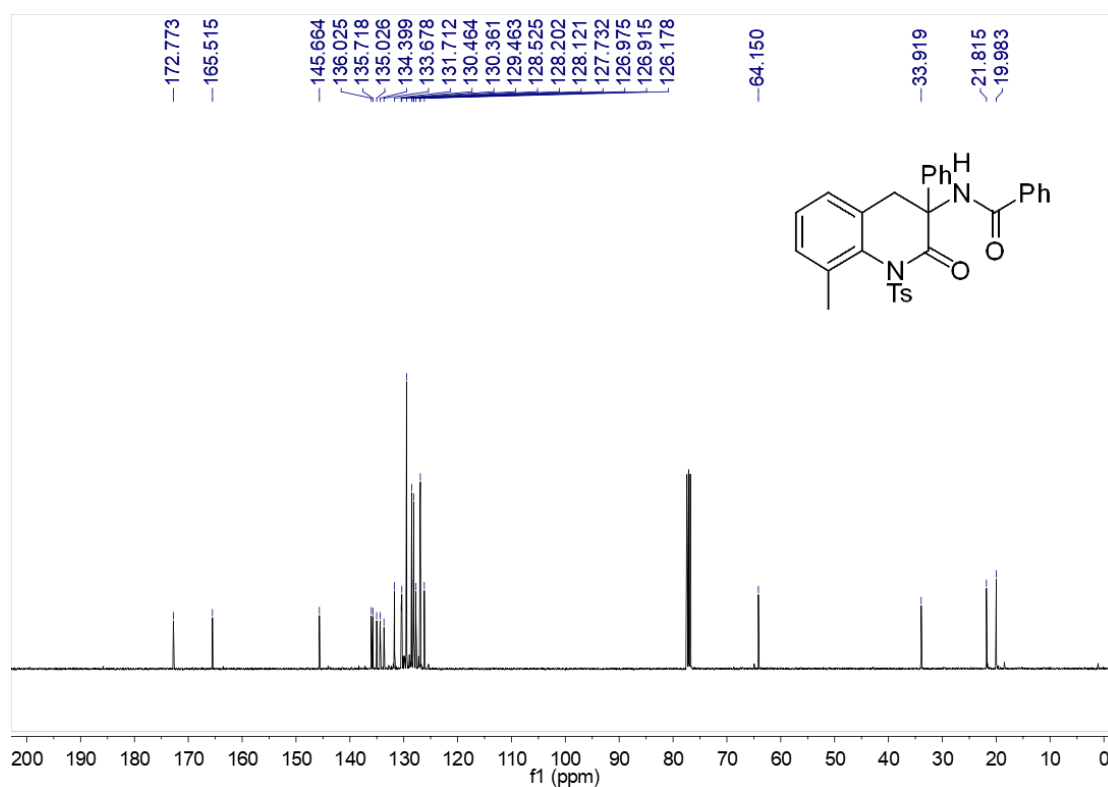
$^{13}\text{C}$  NMR (100 MHz,  $\text{CDCl}_3$ ) of compound **3aa**:



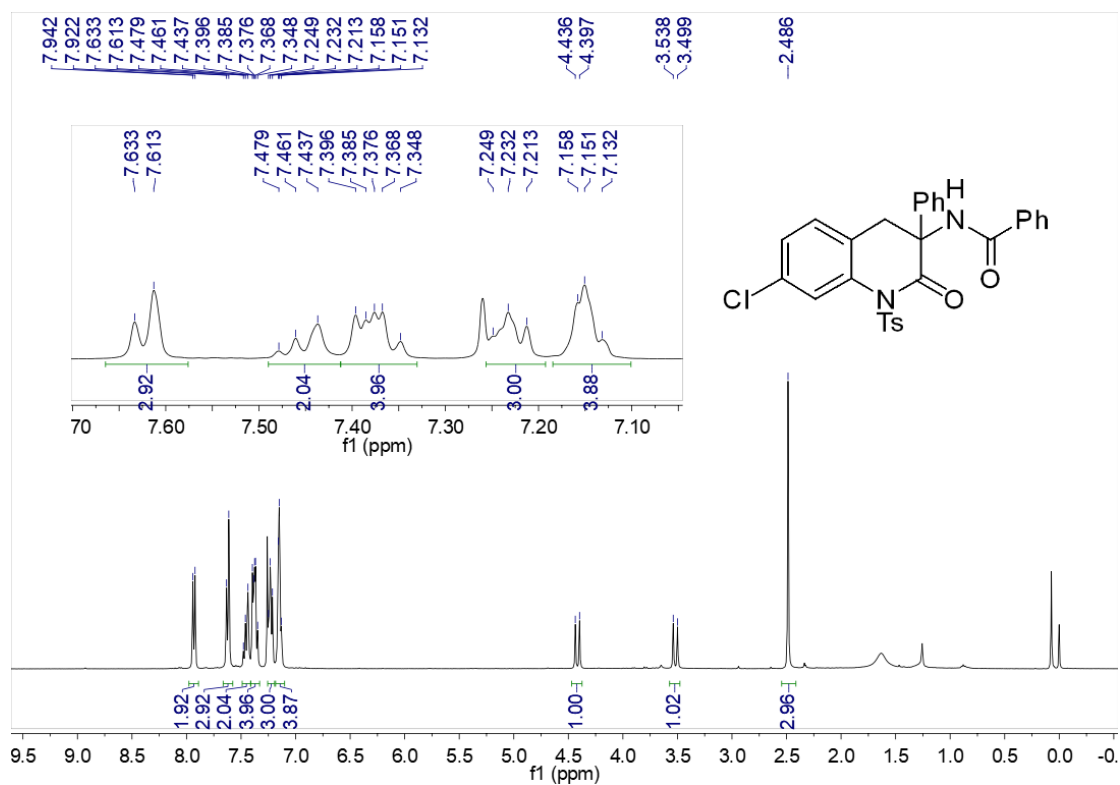
$^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ ) of compound **3ba**:



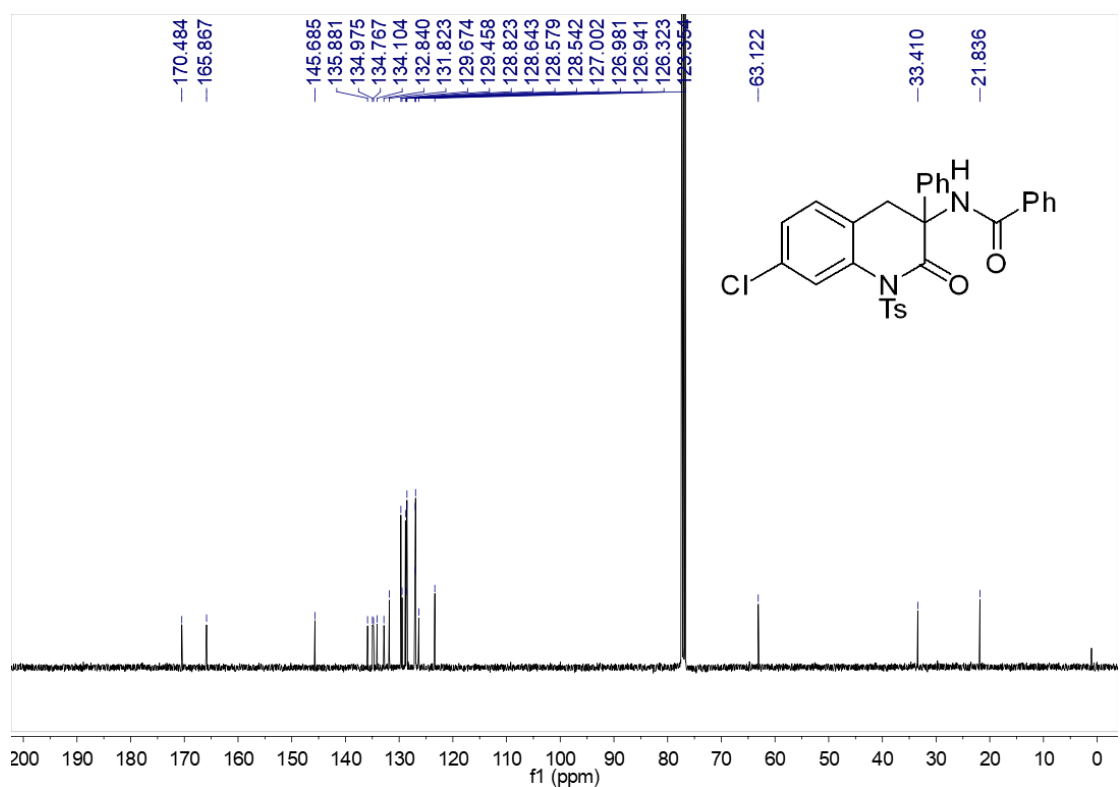
$^{13}\text{C}$  NMR (100 MHz,  $\text{CDCl}_3$ ) of compound **3ba**:



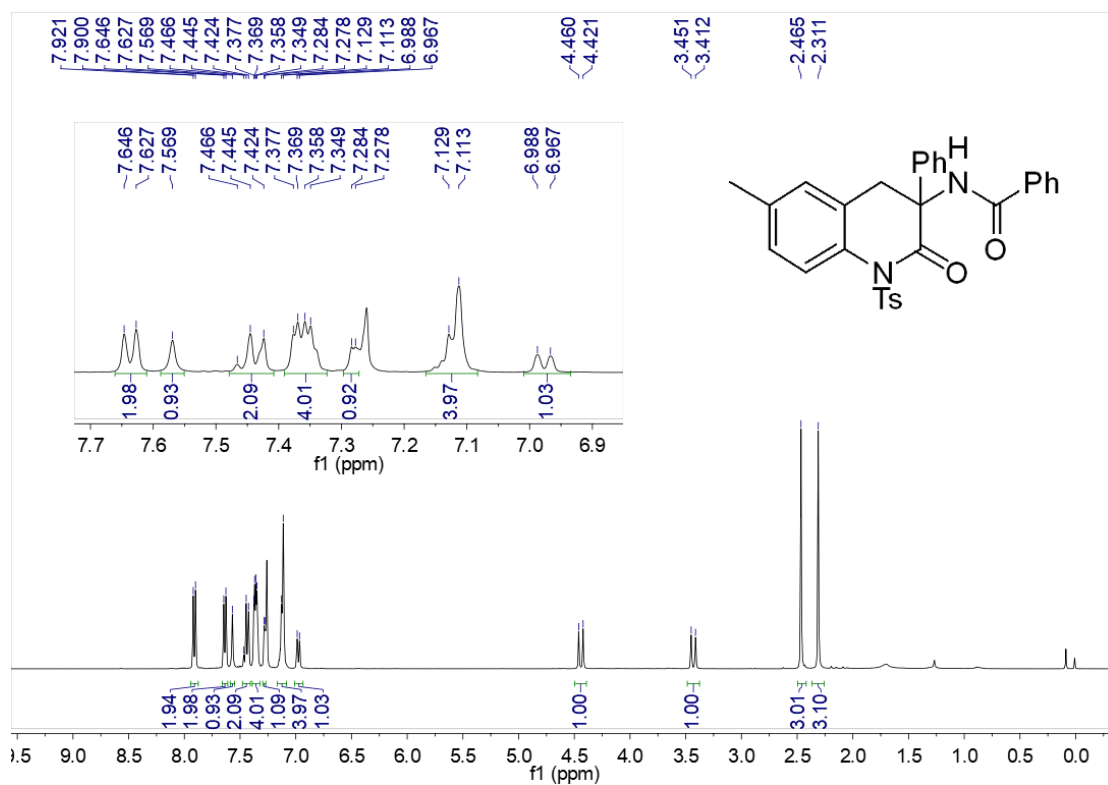
$^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ ) of compound **3ca**:



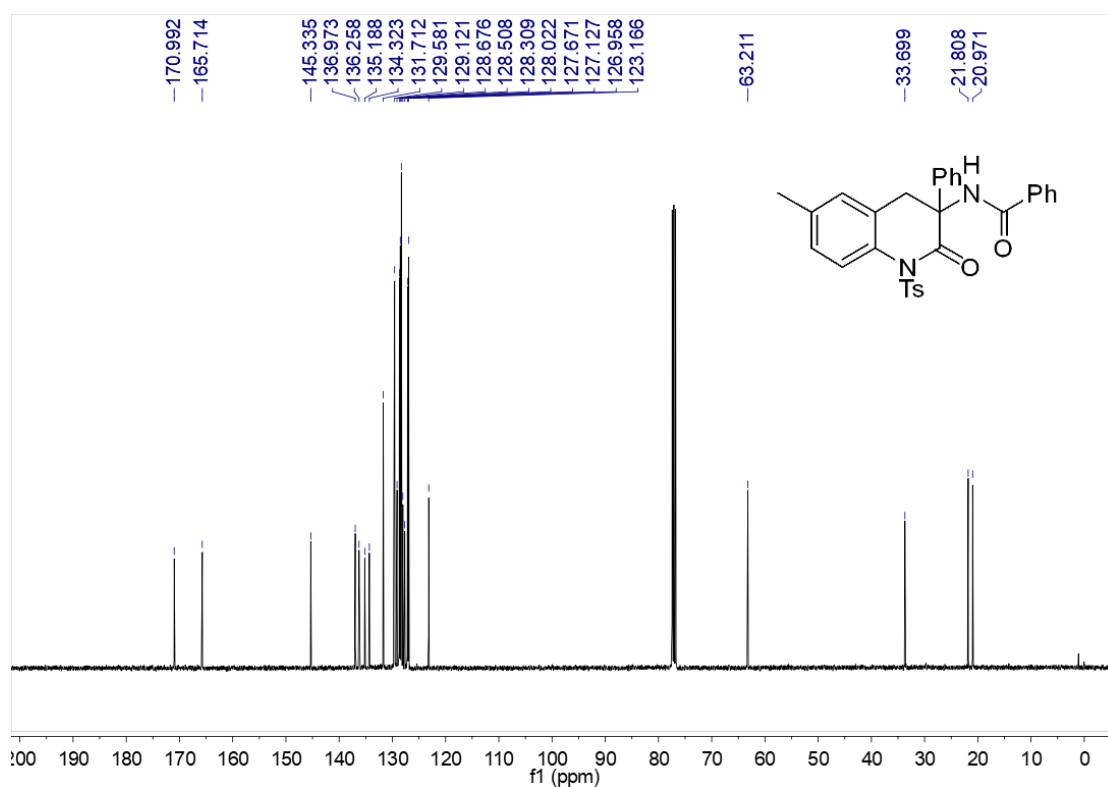
$^{13}\text{C}$  NMR (100 MHz,  $\text{CDCl}_3$ ) of compound **3ca**:



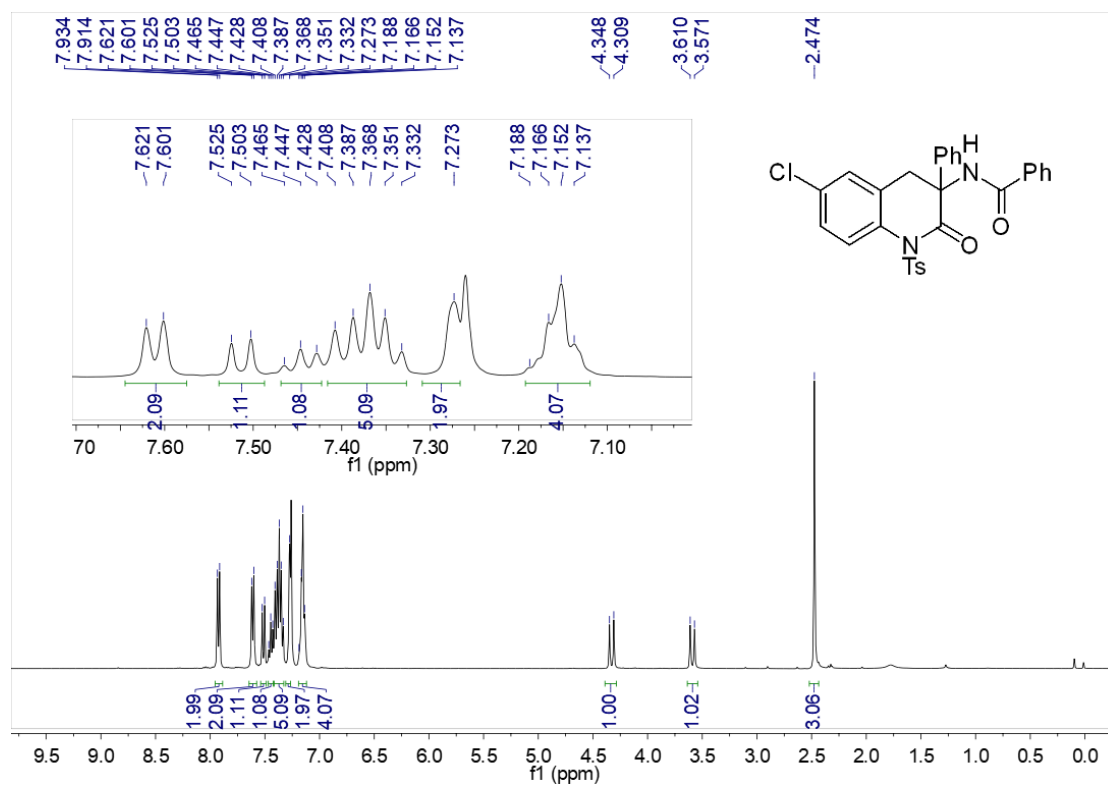
$^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ ) of compound **3da**:



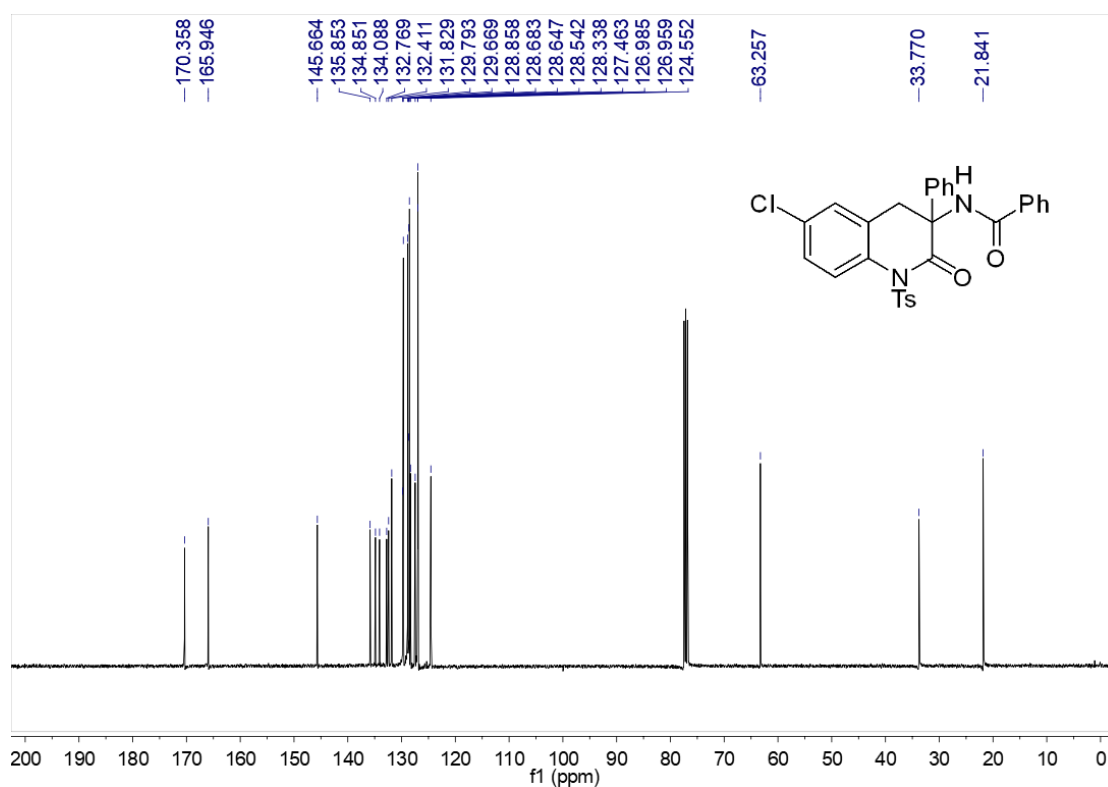
$^{13}\text{C}$  NMR (100 MHz,  $\text{CDCl}_3$ ) of compound **3da**:



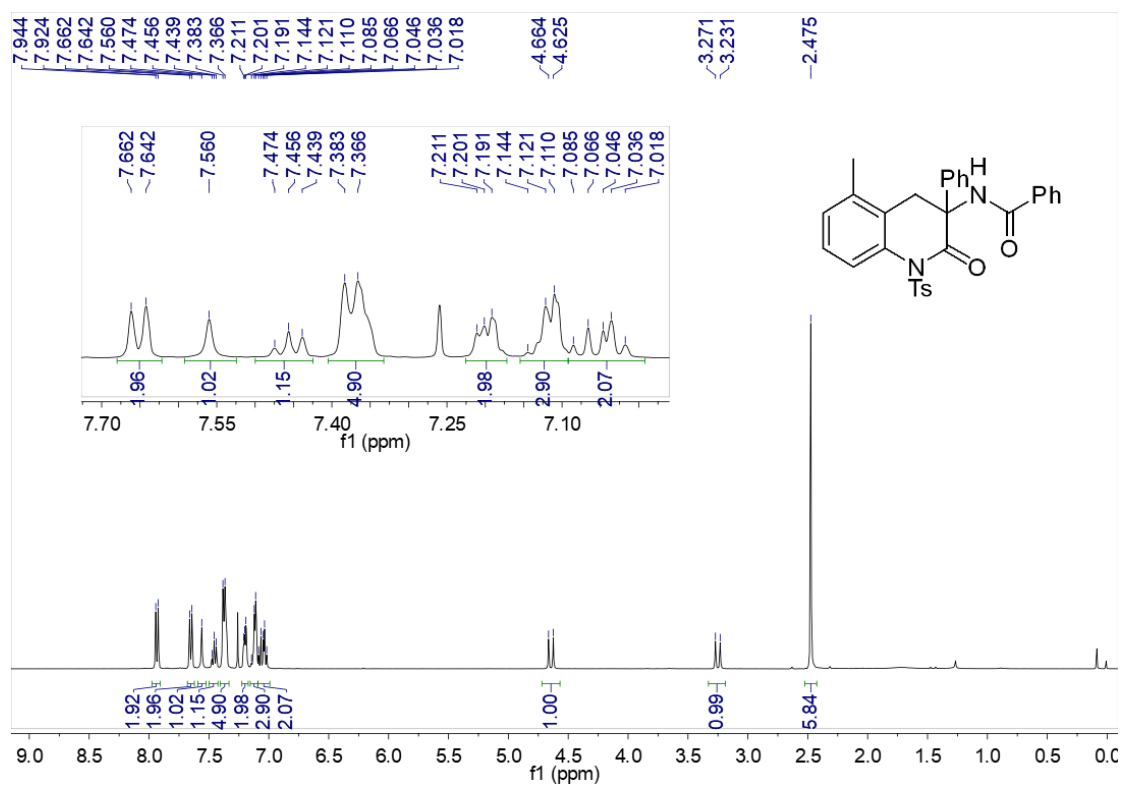
$^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ ) of compound **3ea**:



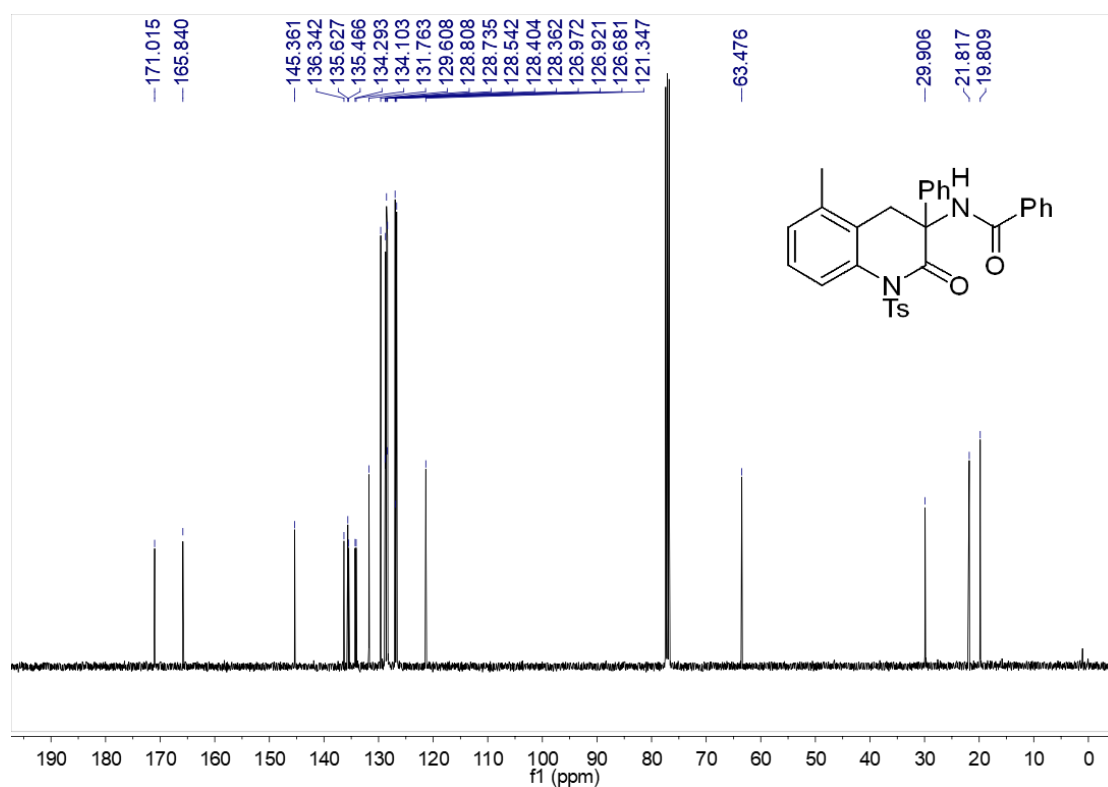
$^{13}\text{C}$  NMR (100 MHz,  $\text{CDCl}_3$ ) of compound **3ea**:



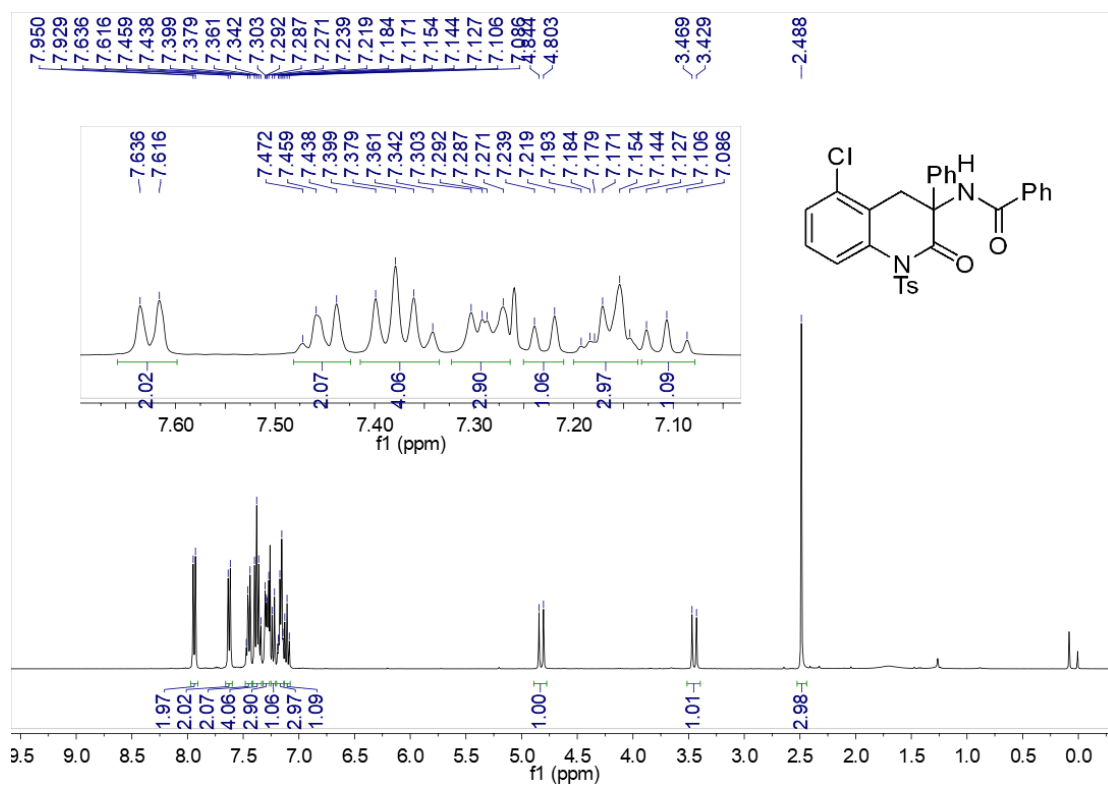
$^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ ) of compound **3fa**:



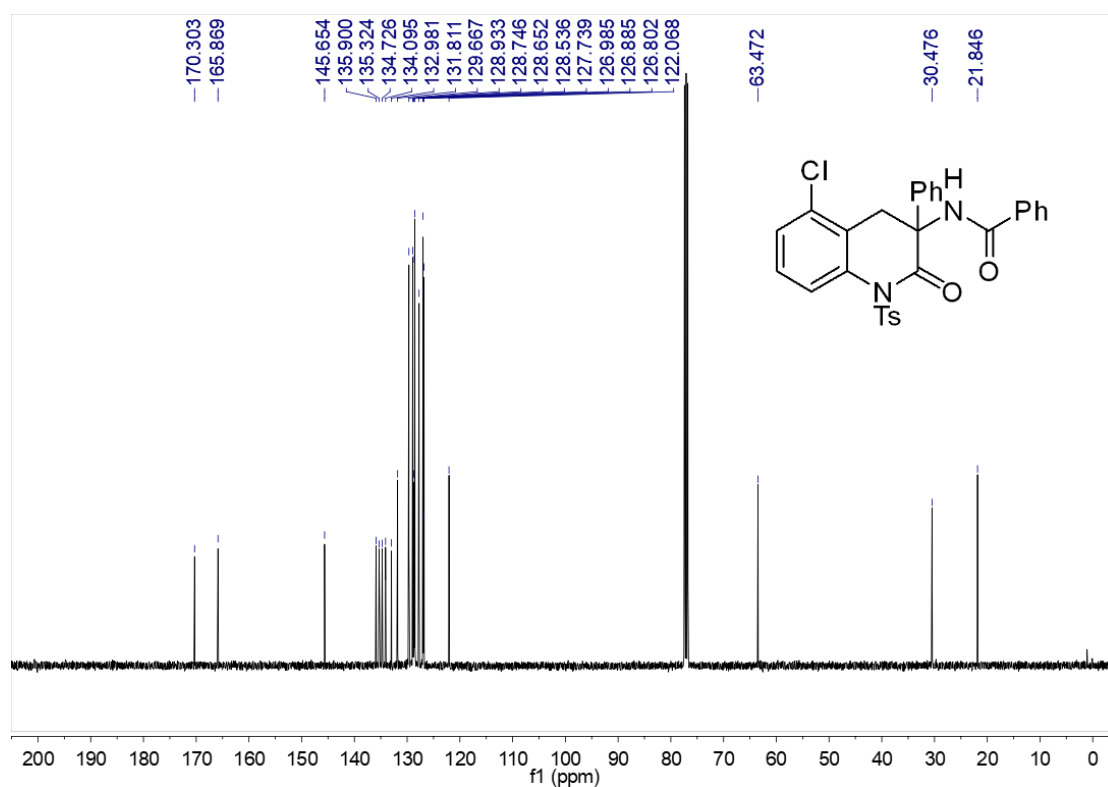
$^{13}\text{C}$  NMR (100 MHz,  $\text{CDCl}_3$ ) of compound **3fa**:



$^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ ) of compound **3ga**:

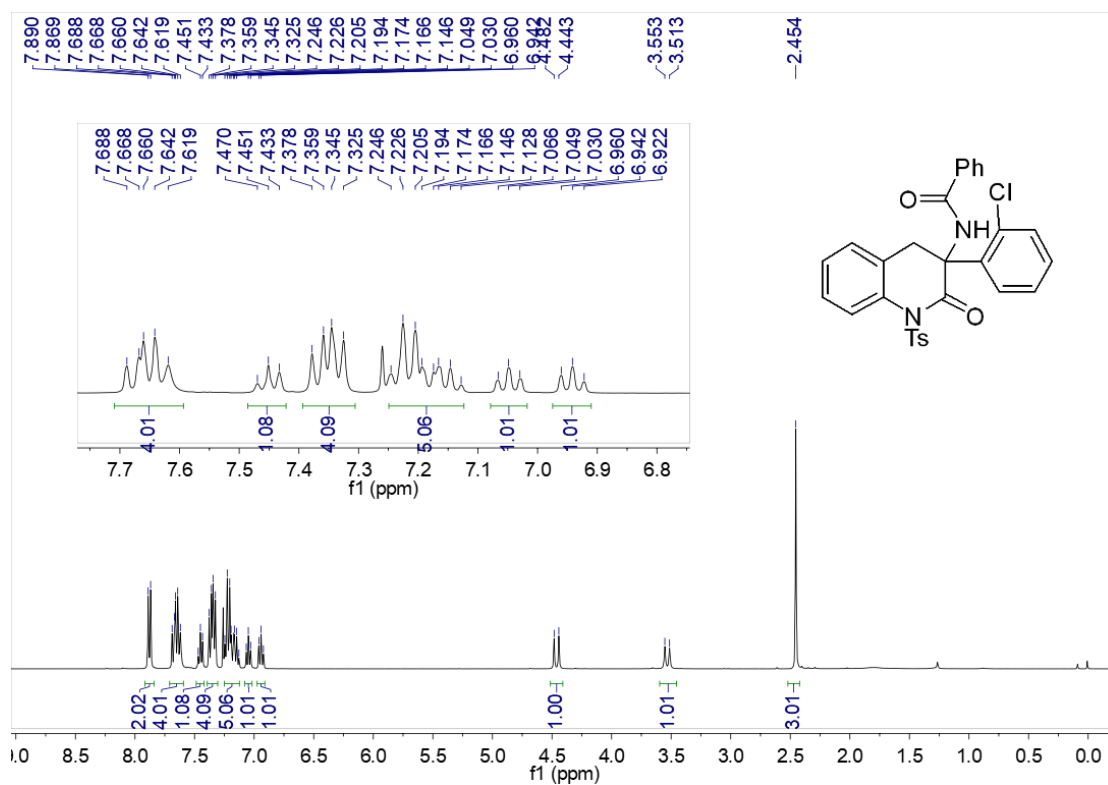


$^{13}\text{C}$  NMR (100 MHz,  $\text{CDCl}_3$ ) of compound **3ga**:

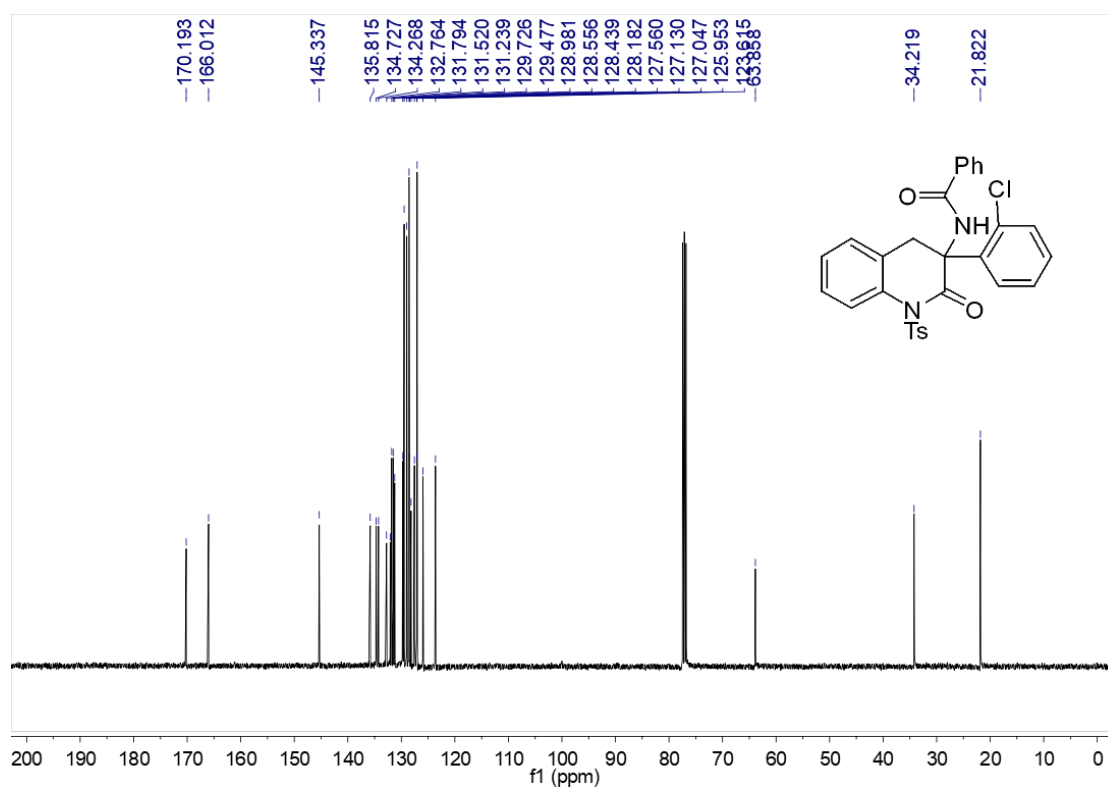




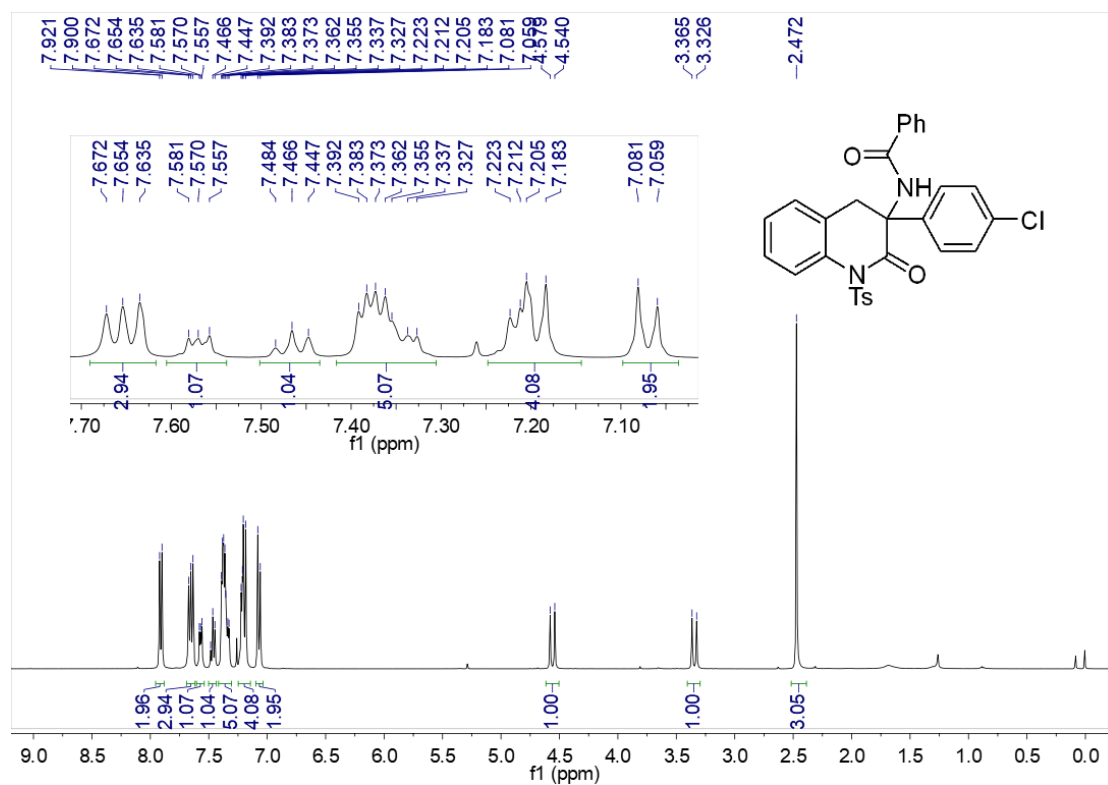
$^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ ) of compound **3ab**:



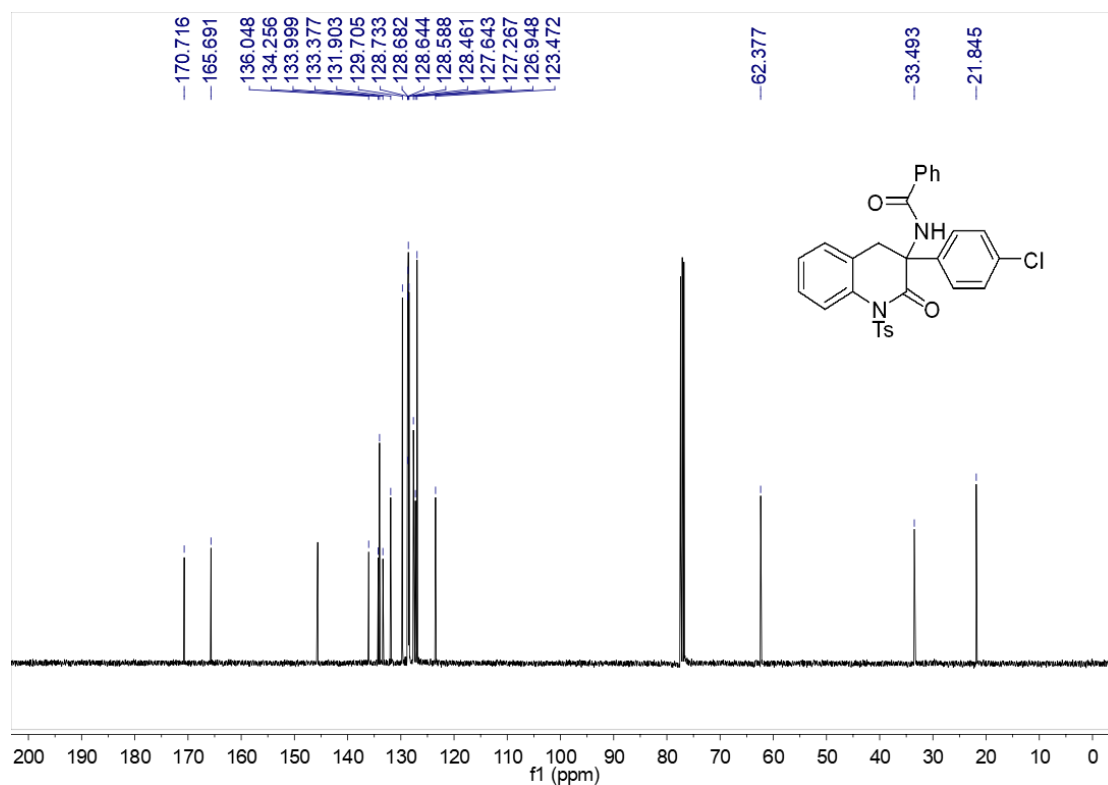
$^{13}\text{C}$  NMR (100 MHz,  $\text{CDCl}_3$ ) of compound **3ab**:



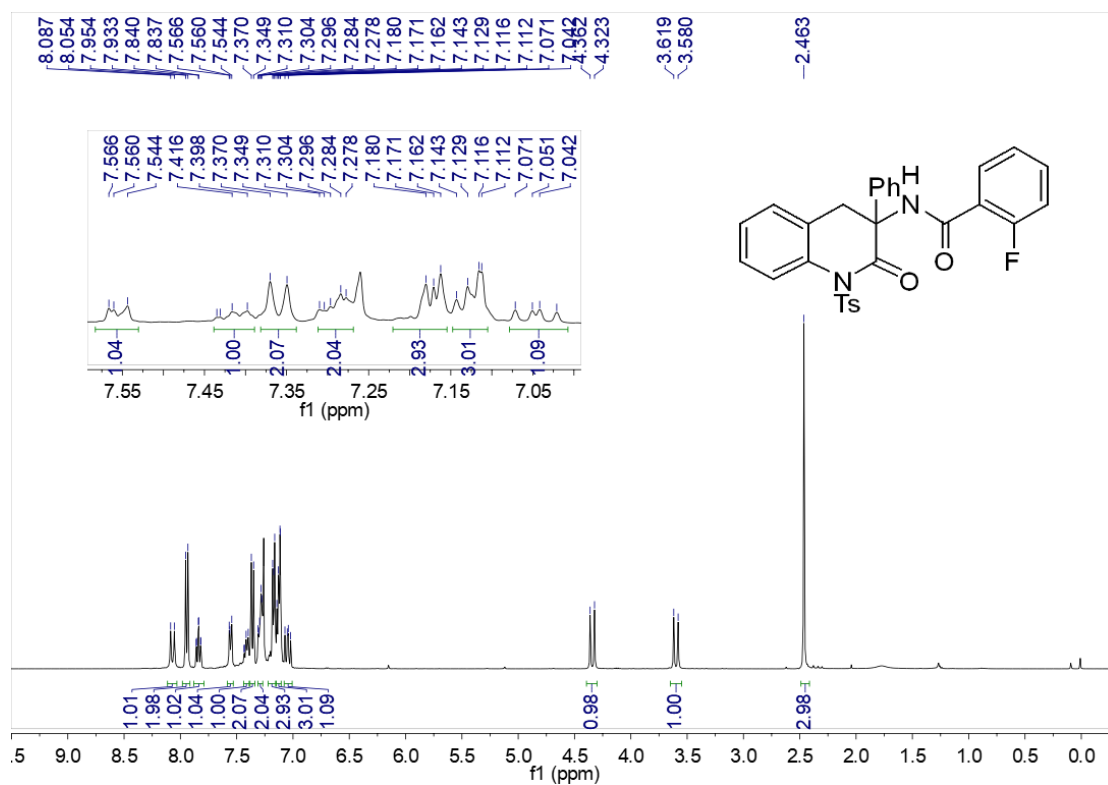
$^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ ) of compound **3ac**:



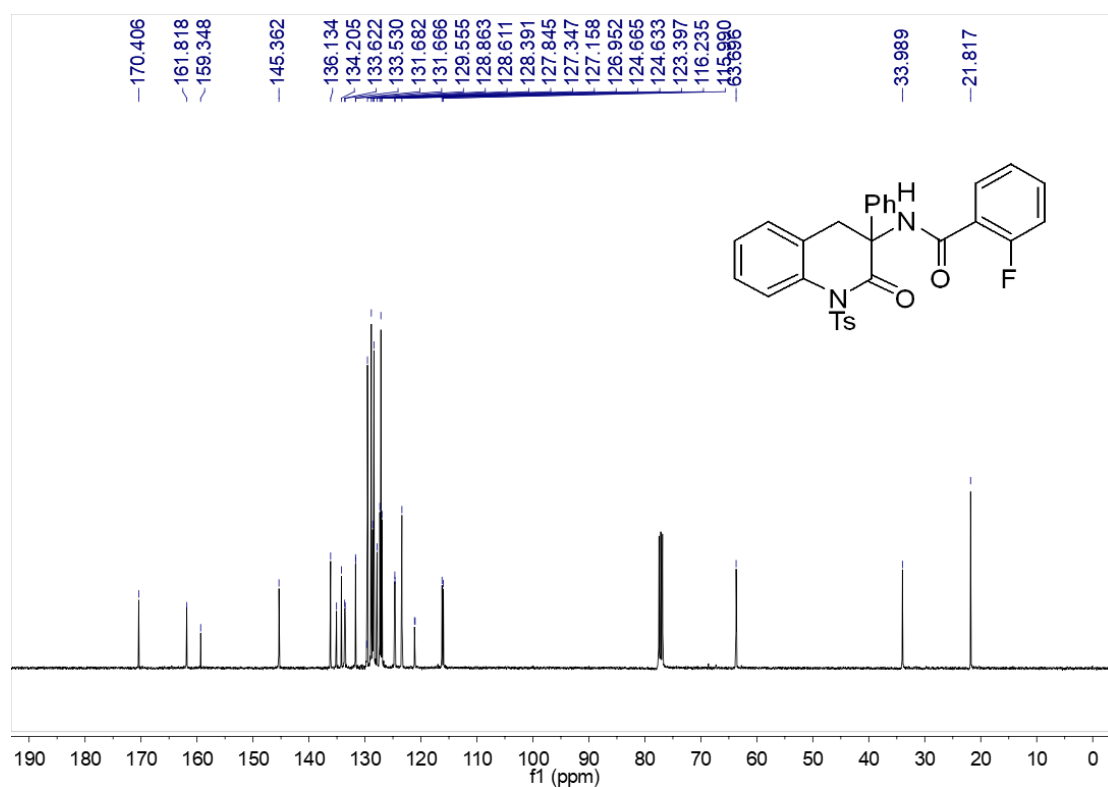
$^{13}\text{C}$  NMR (100 MHz,  $\text{CDCl}_3$ ) of compound **3ac**:



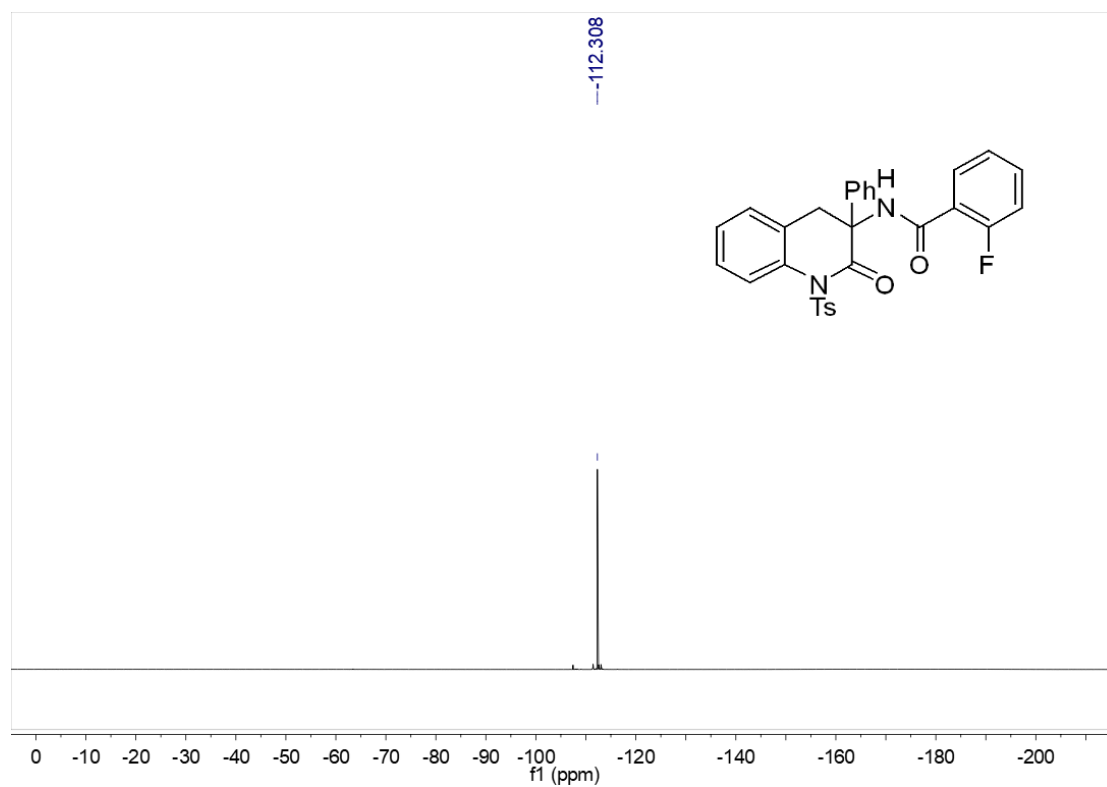
$^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ ) of compound **3ad**:



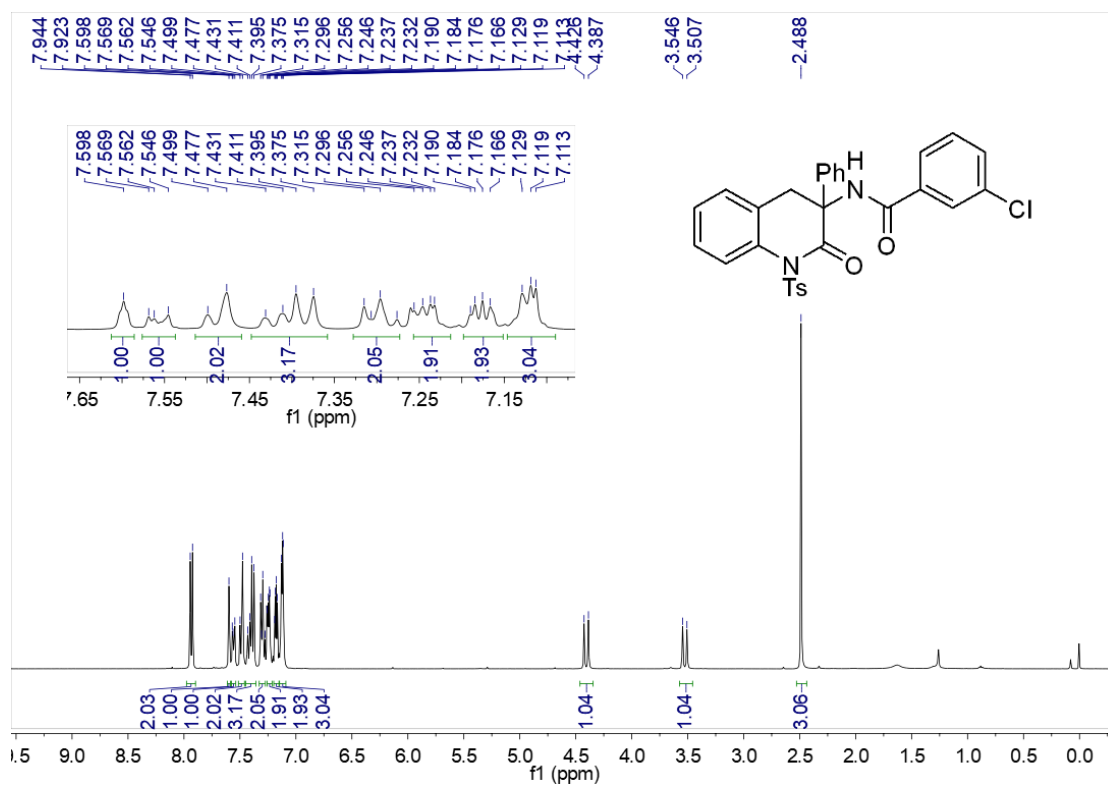
$^{13}\text{C}$  NMR (100 MHz,  $\text{CDCl}_3$ ) of compound **3ad**:



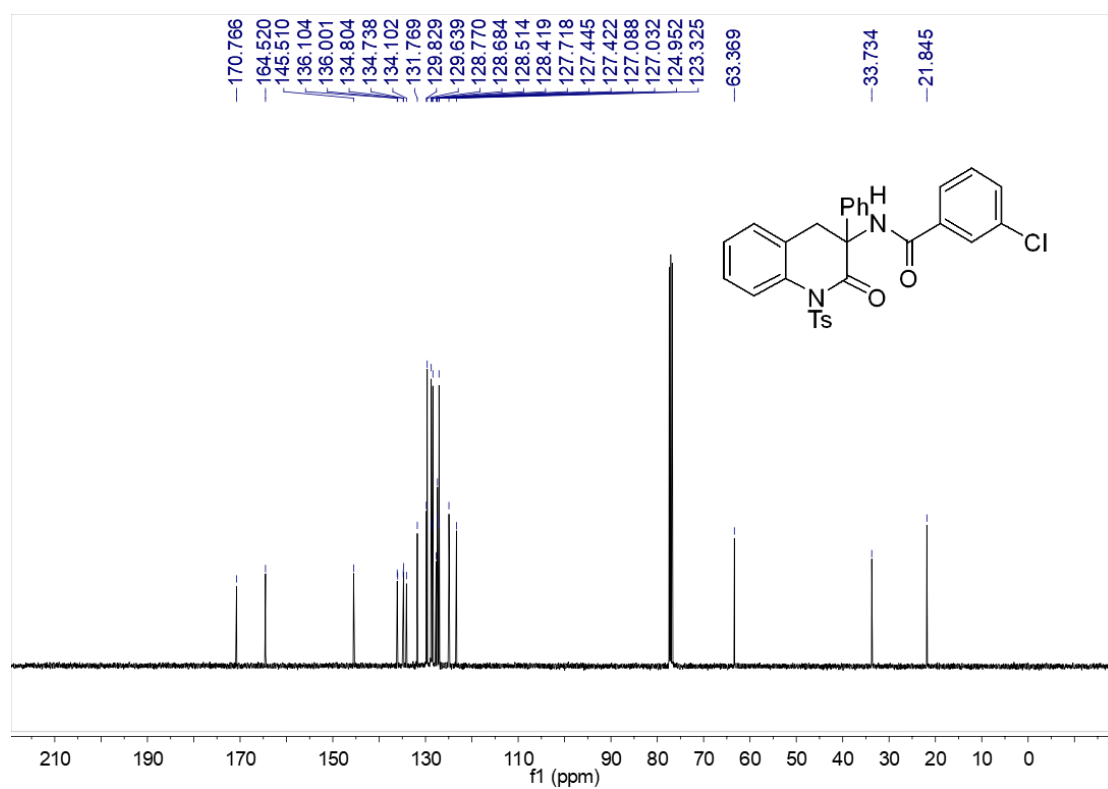
$^{19}\text{F}$  NMR (376 MHz,  $\text{CDCl}_3$ ) of compound **3ad**:



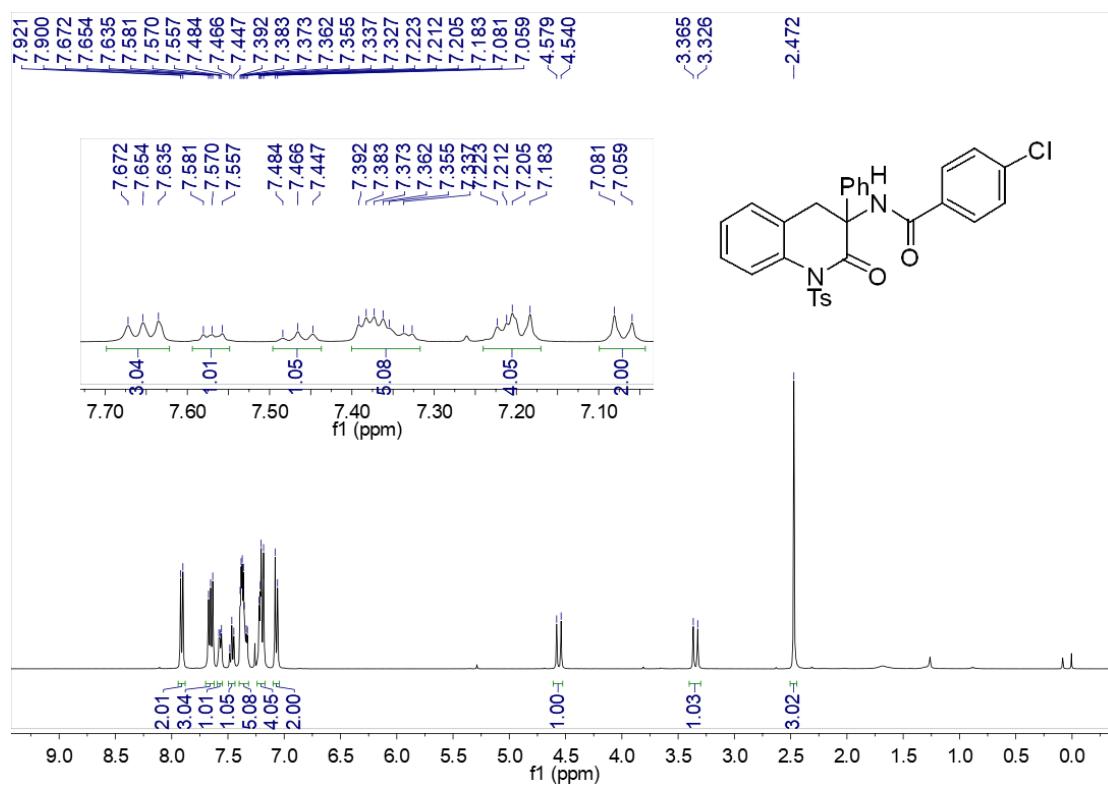
$^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ ) of compound **3ae**:



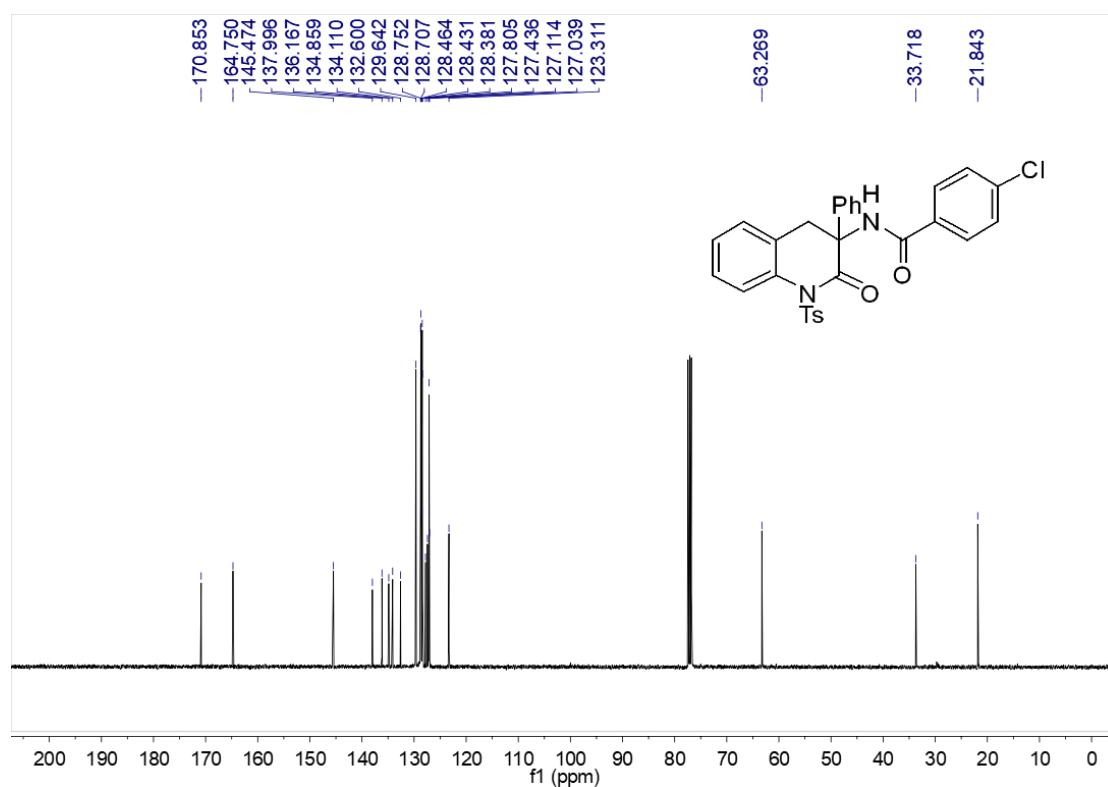
$^{13}\text{C}$  NMR (100 MHz,  $\text{CDCl}_3$ ) of compound **3ae**:



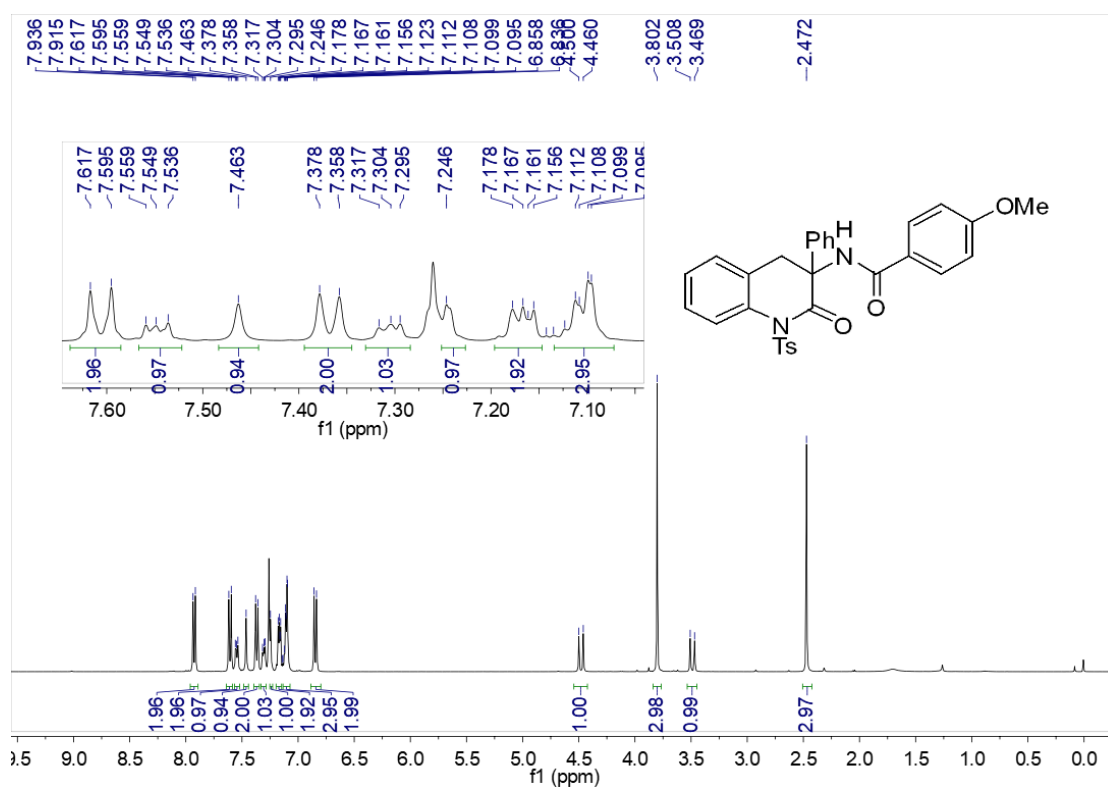
$^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ ) of compound **3af**:



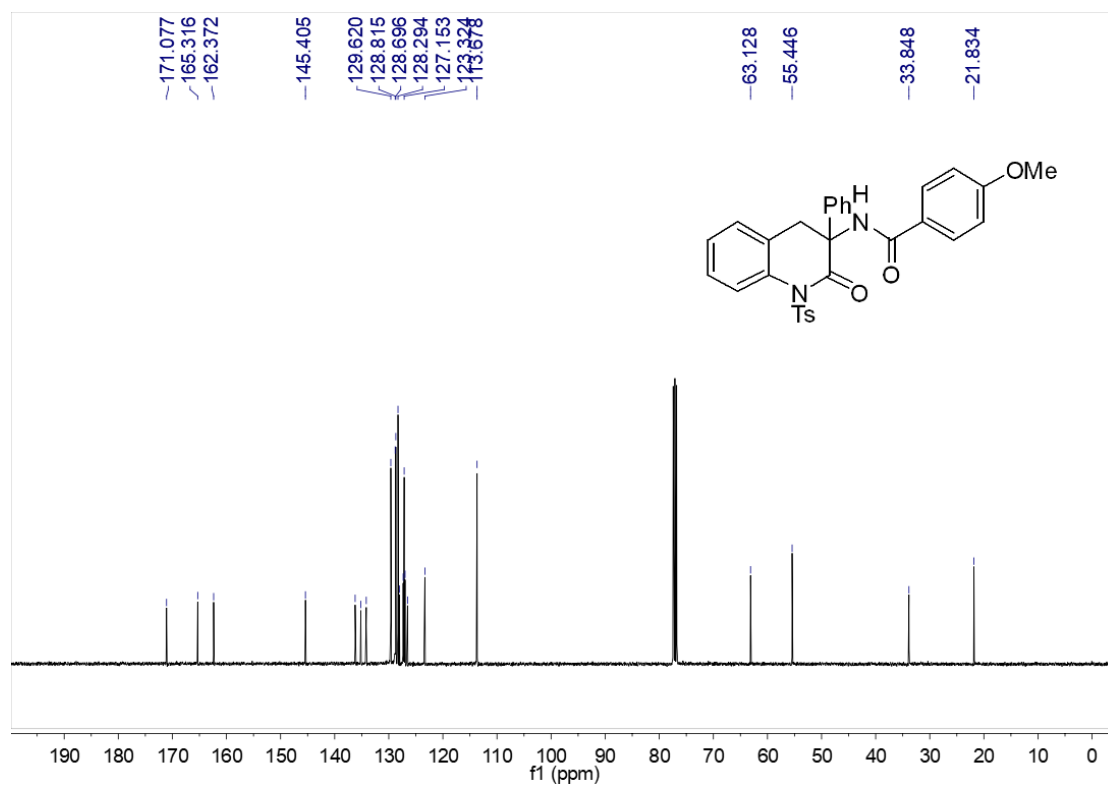
$^{13}\text{C}$  NMR (100 MHz,  $\text{CDCl}_3$ ) of compound **3af**:



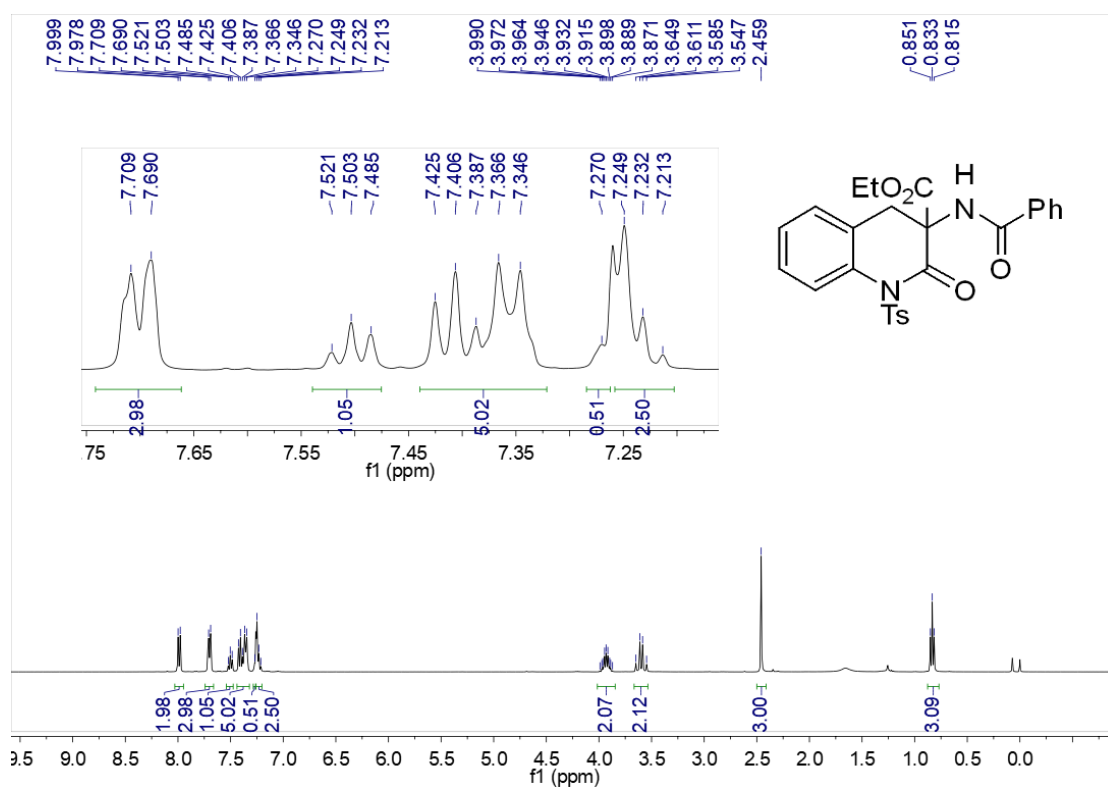
$^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ ) of compound **3ag**:



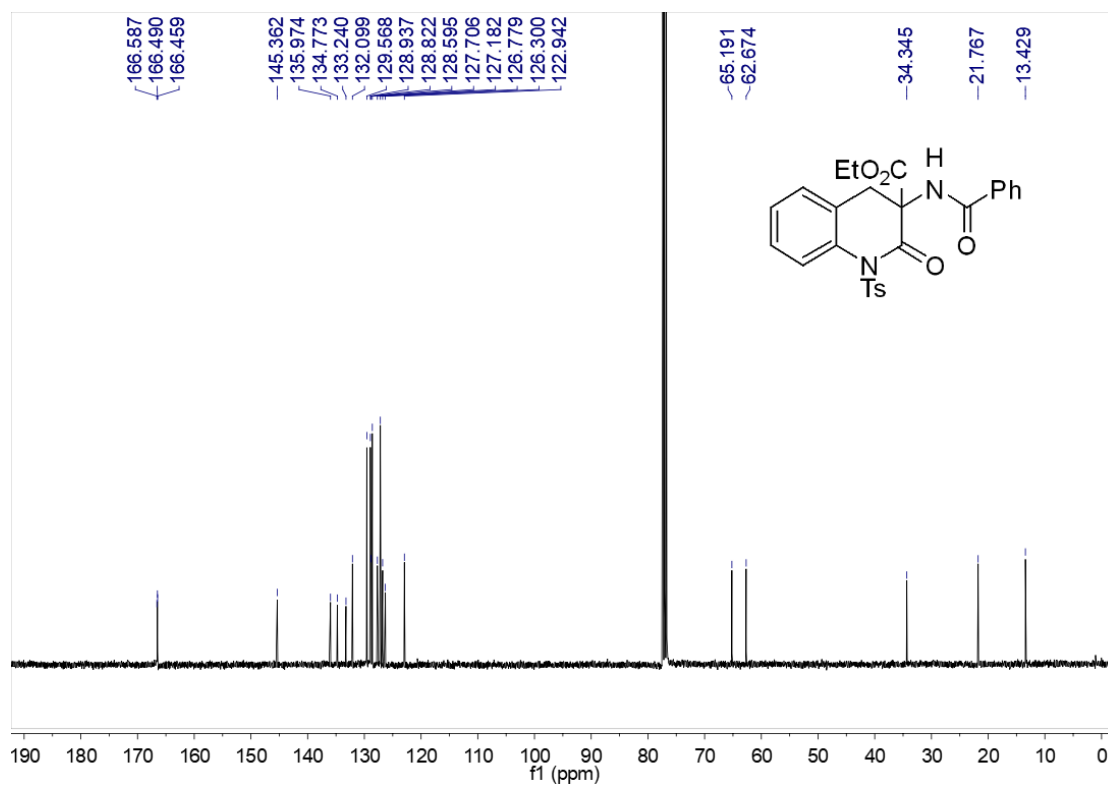
$^{13}\text{C}$  NMR (100 MHz,  $\text{CDCl}_3$ ) of compound **3ag**:



$^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ ) of compound **3ah**:

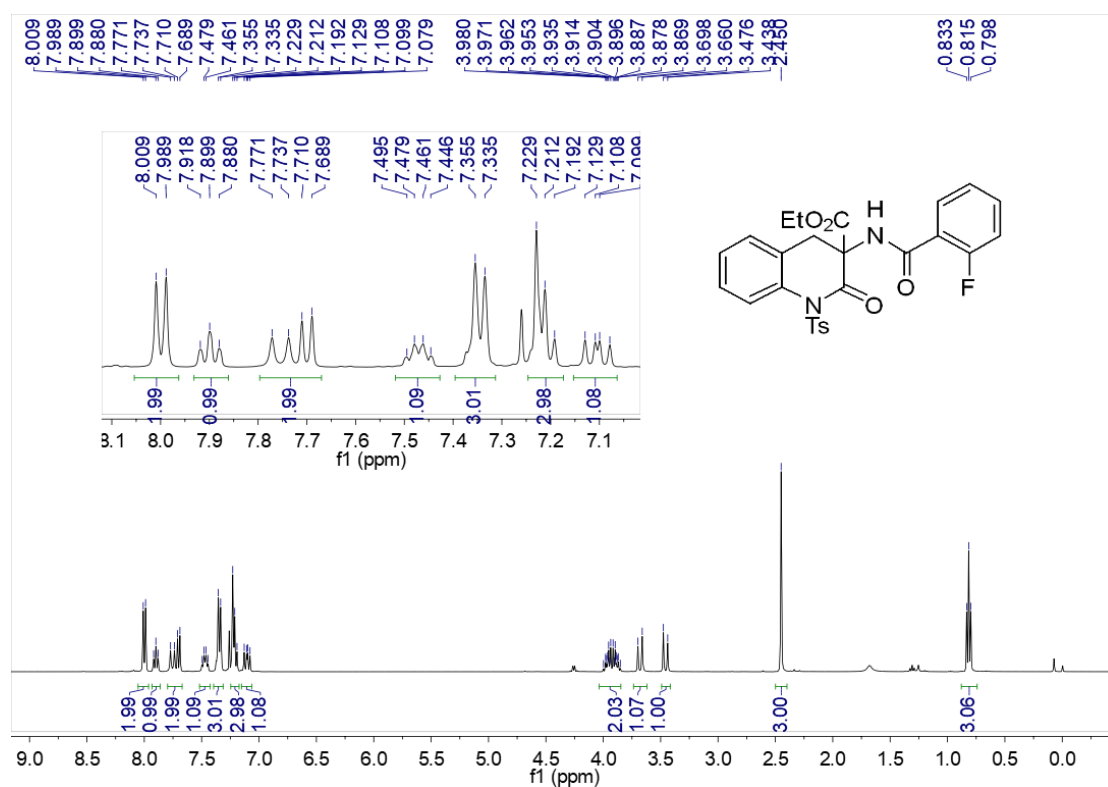


$^{13}\text{C}$  NMR (100 MHz,  $\text{CDCl}_3$ ) of compound **3ah**:

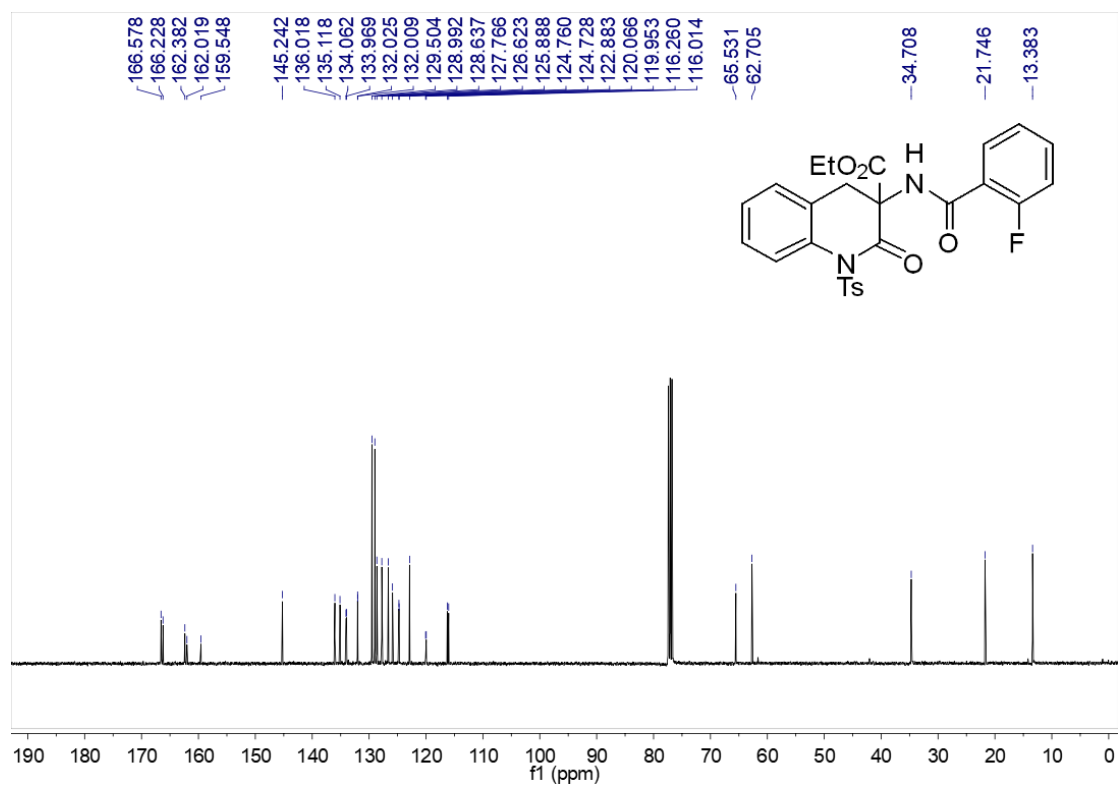




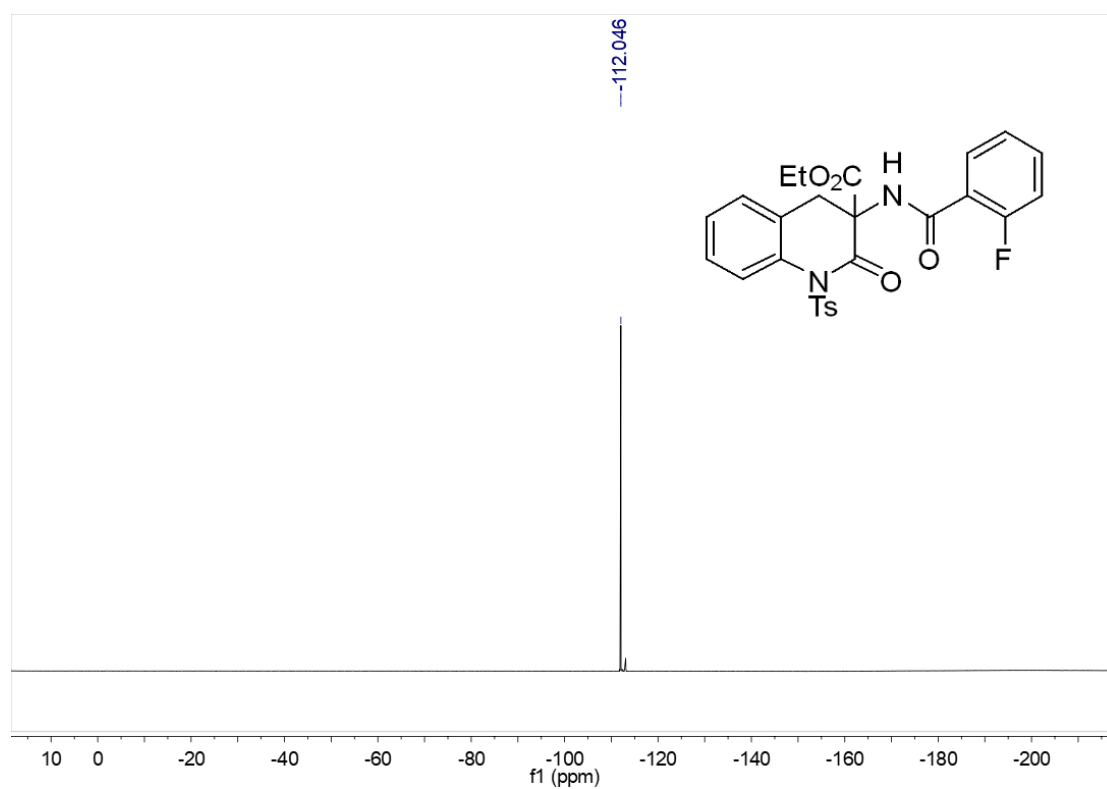
$^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ ) of compound **3ai**:



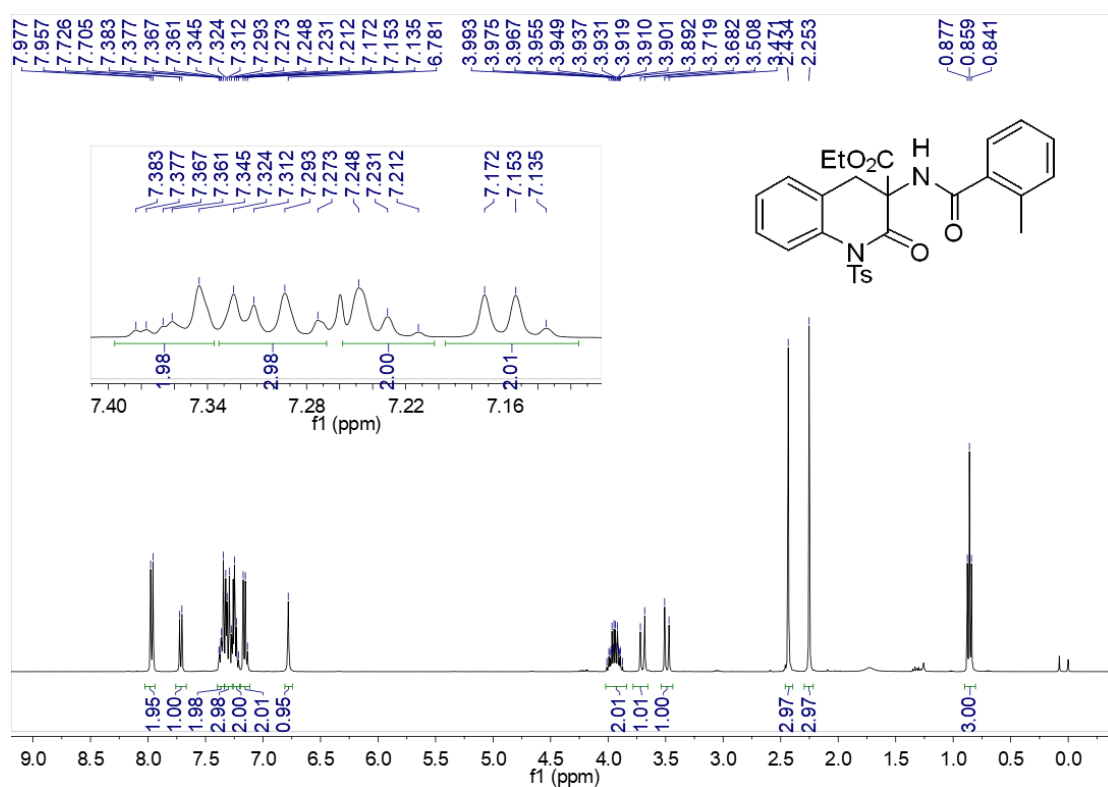
$^{13}\text{C}$  NMR (100 MHz,  $\text{CDCl}_3$ ) of compound **3ai**:



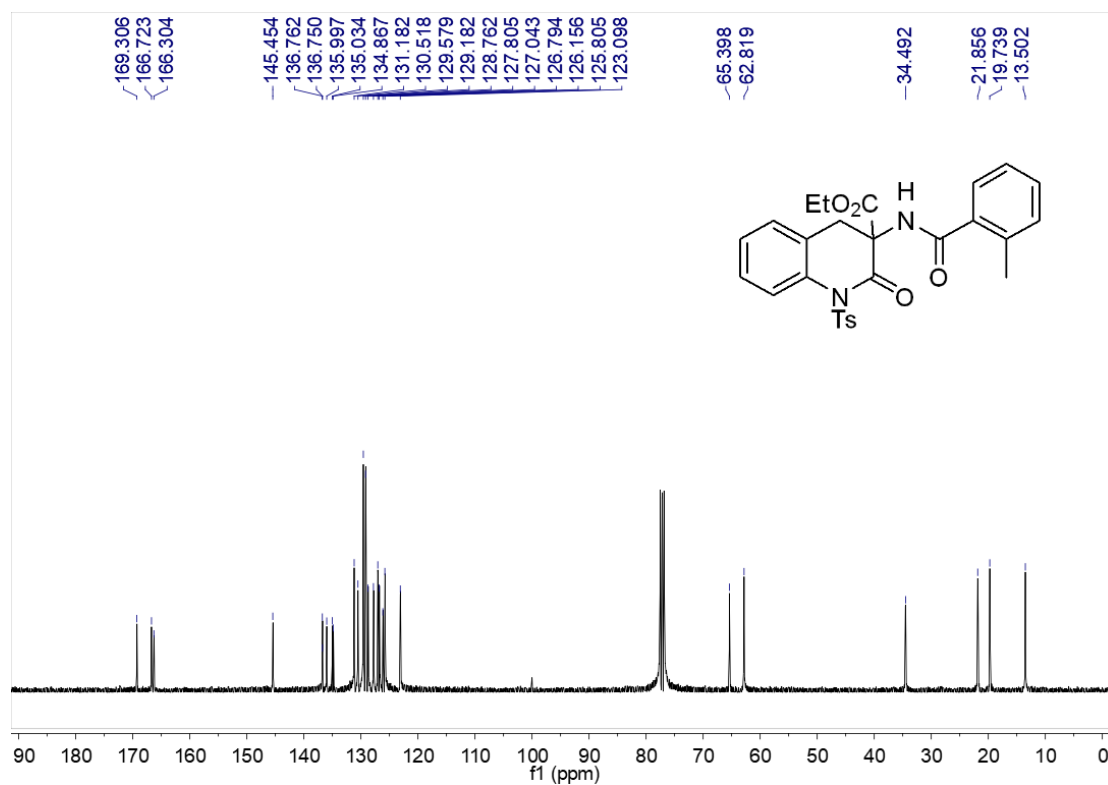
$^{19}\text{F}$  NMR (376 MHz,  $\text{CDCl}_3$ ) of compound **3ai**:



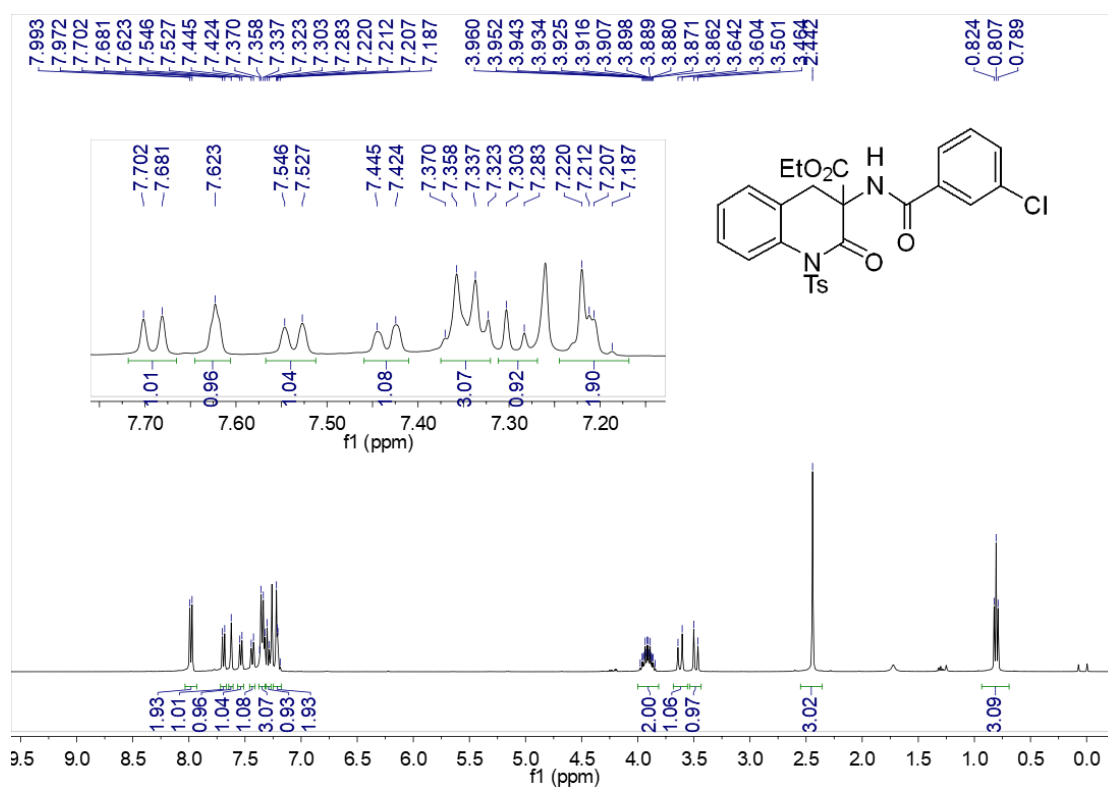
$^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ ) of compound **3aj**:



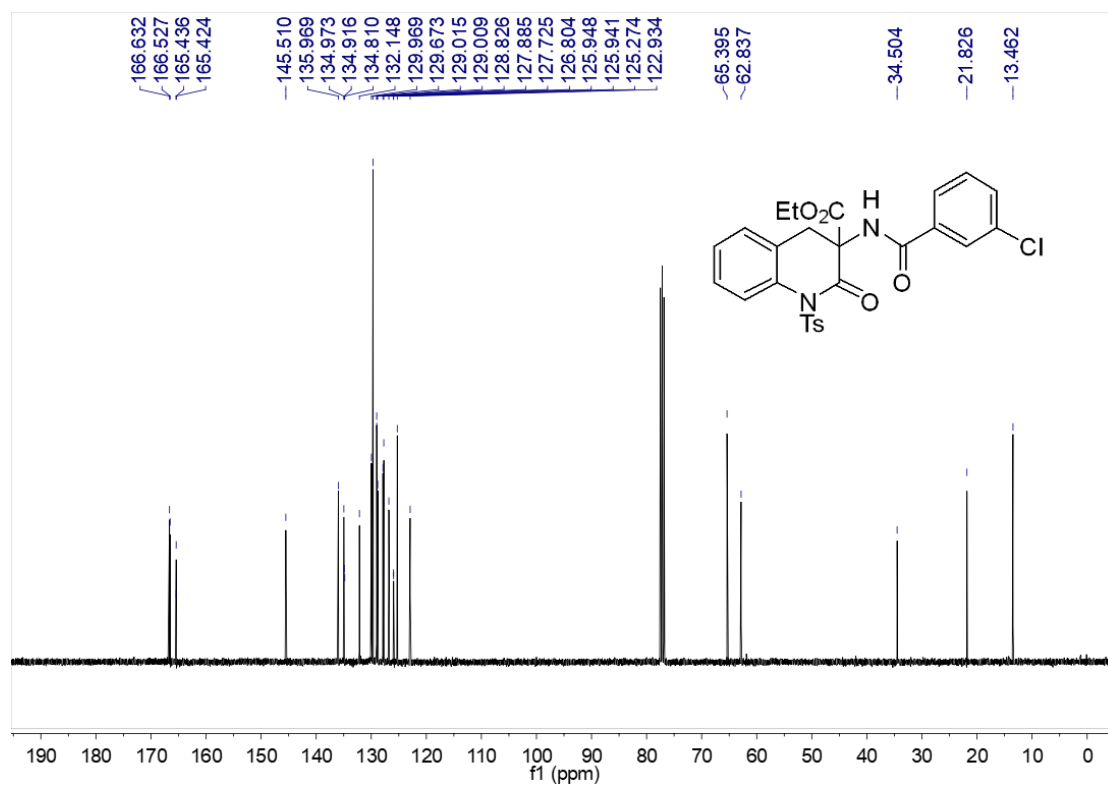
$^{13}\text{C}$  NMR (100 MHz,  $\text{CDCl}_3$ ) of compound **3aj**:



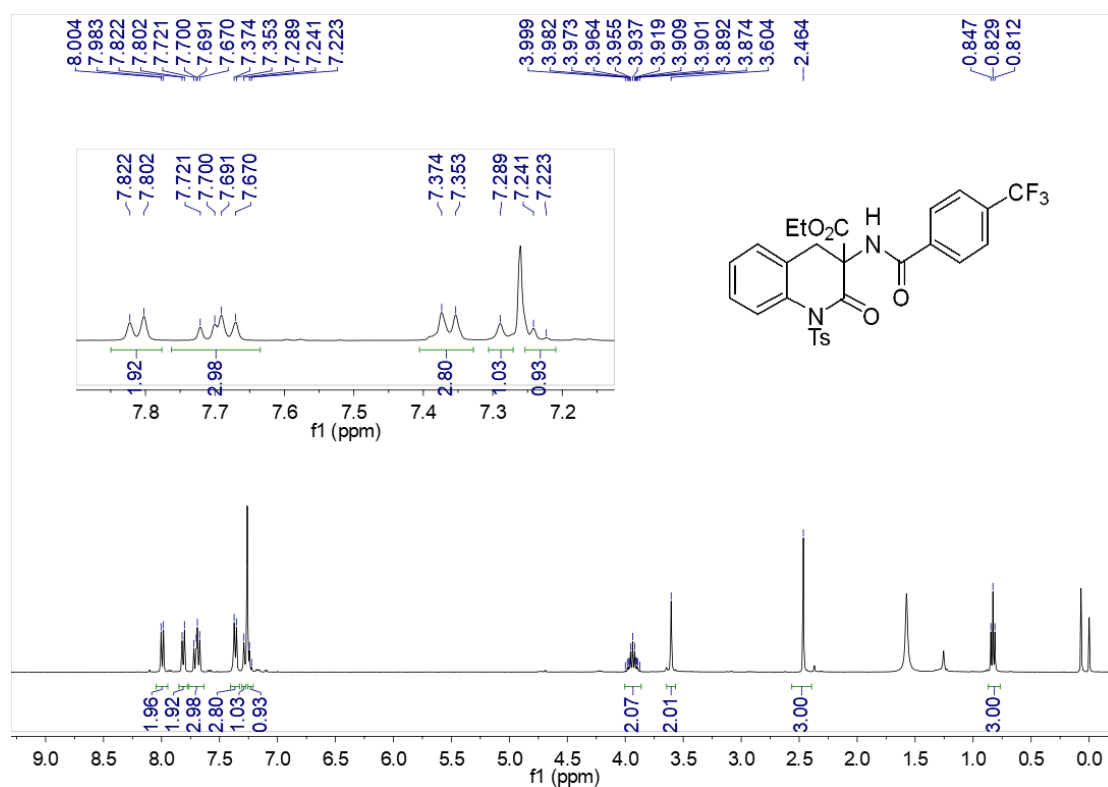
$^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ ) of compound **3ak**:



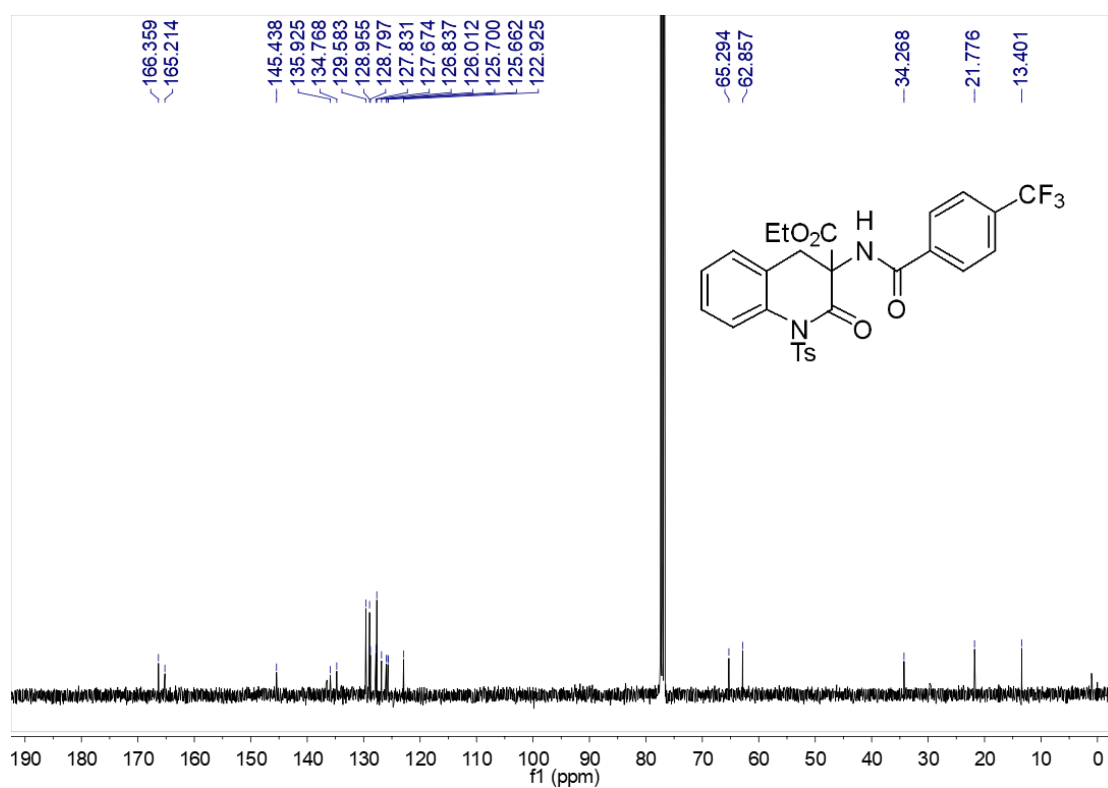
$^{13}\text{C}$  NMR (100 MHz,  $\text{CDCl}_3$ ) of compound **3ak**:



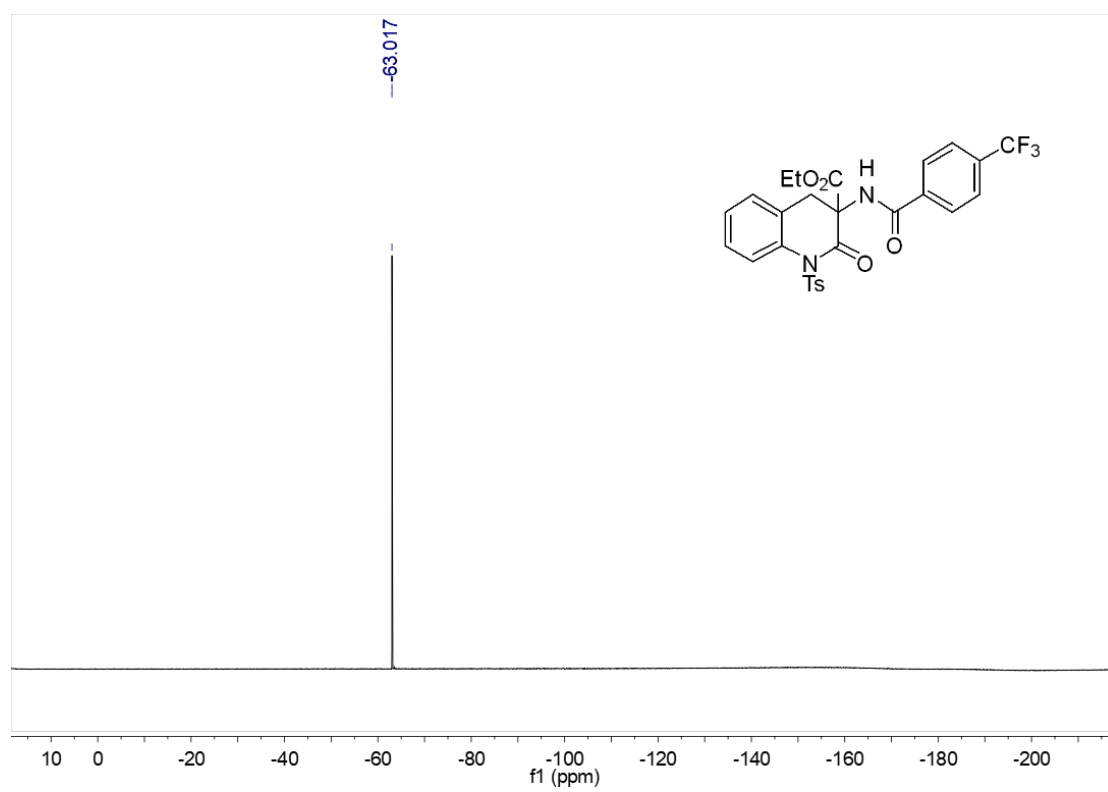
$^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ ) of compound **3al**:



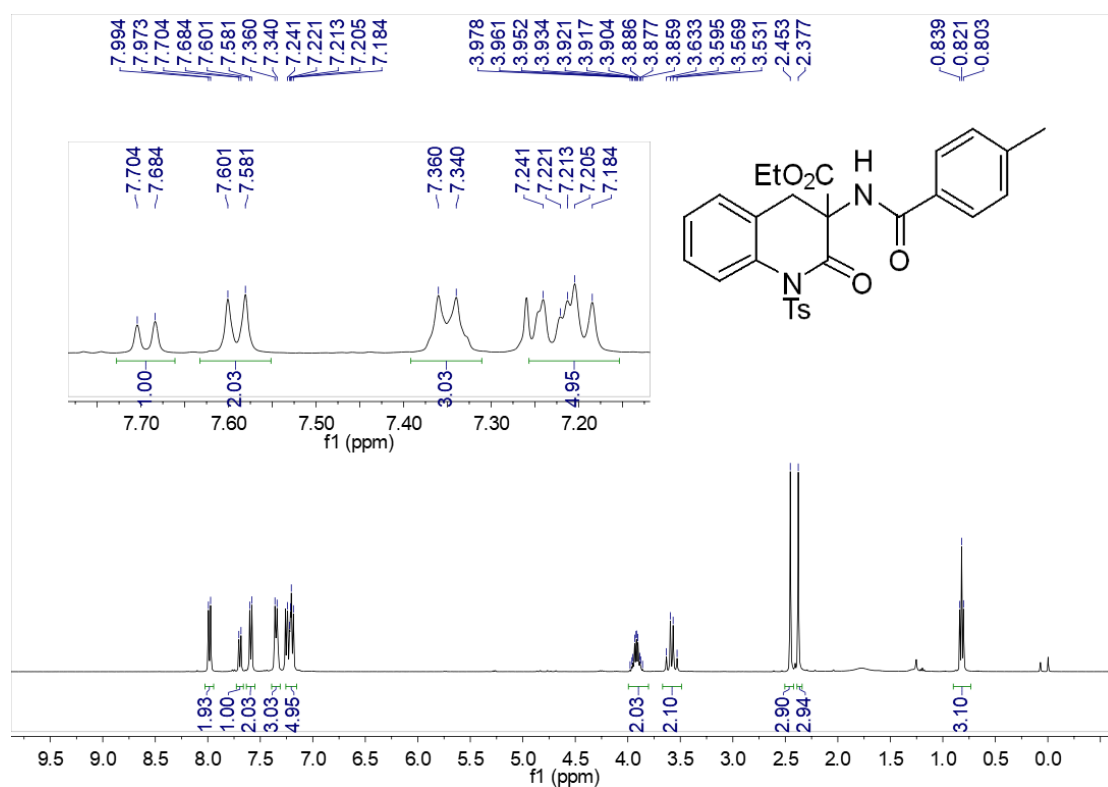
$^{13}\text{C}$  NMR (100 MHz,  $\text{CDCl}_3$ ) of compound **3al**:



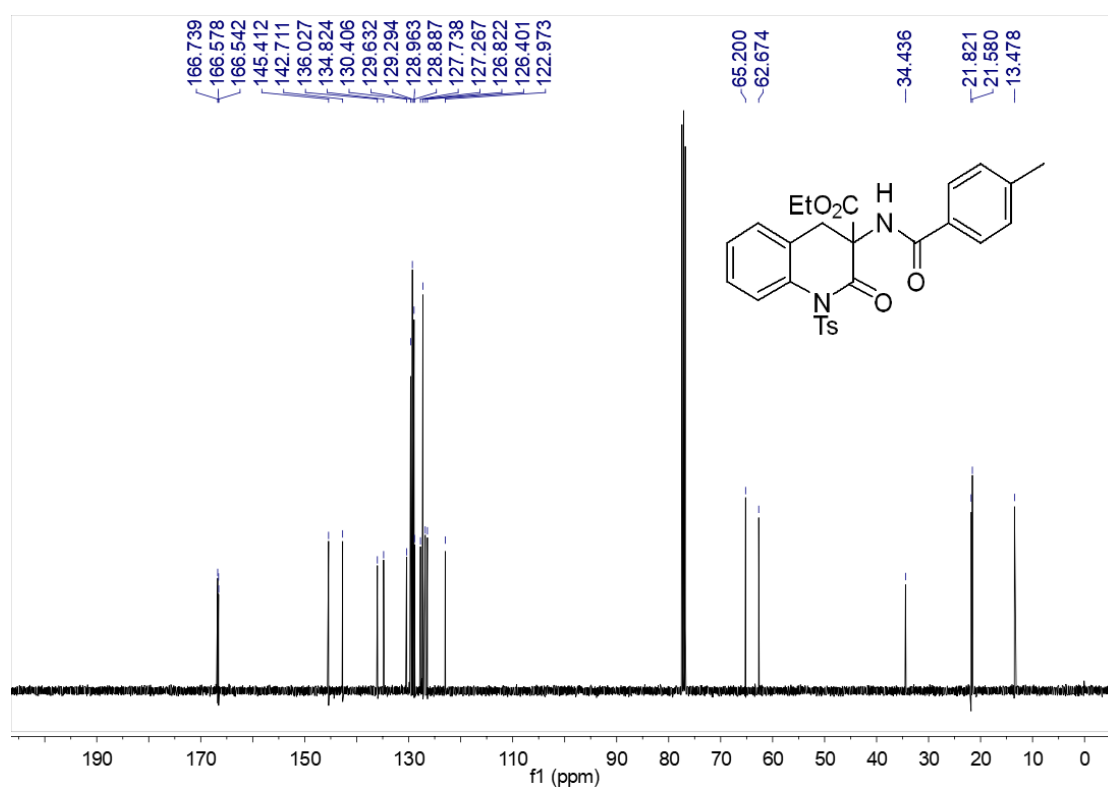
$^{19}\text{F}$  NMR (376 MHz,  $\text{CDCl}_3$ ) of compound **3al**:



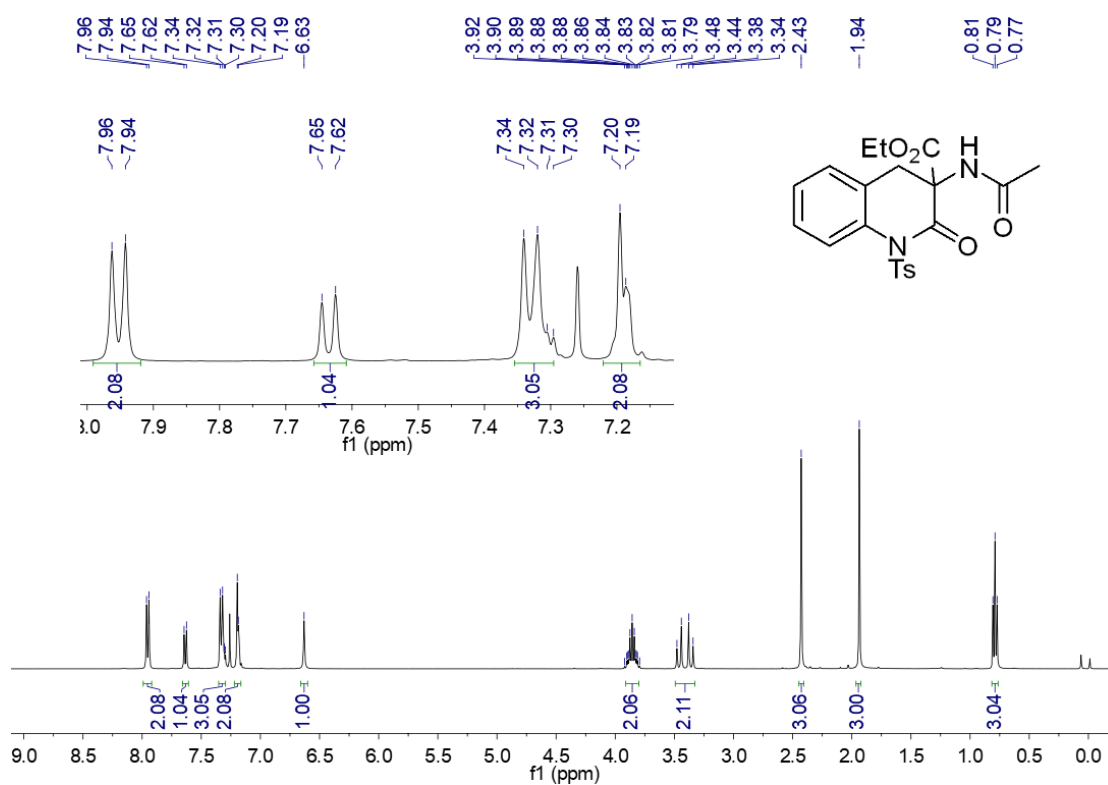
$^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ ) of compound **3am**:



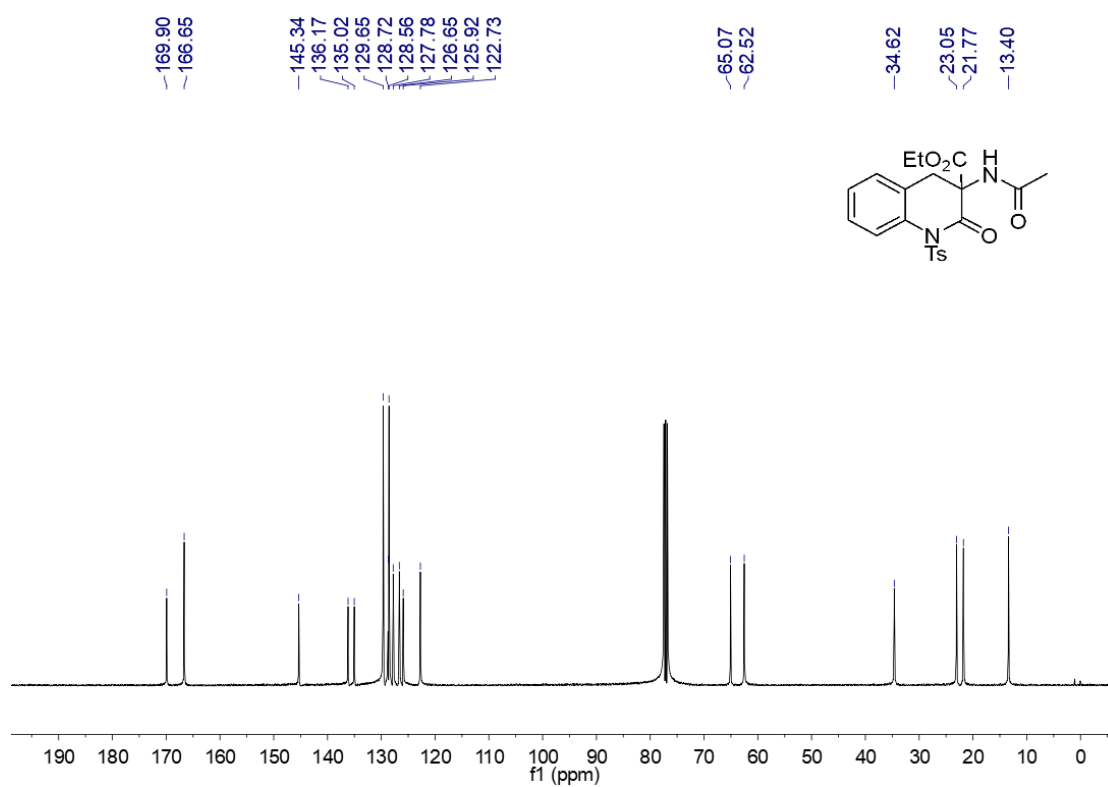
$^{13}\text{C}$  NMR (100 MHz,  $\text{CDCl}_3$ ) of compound **3am**:



$^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ ) of compound **3an**:

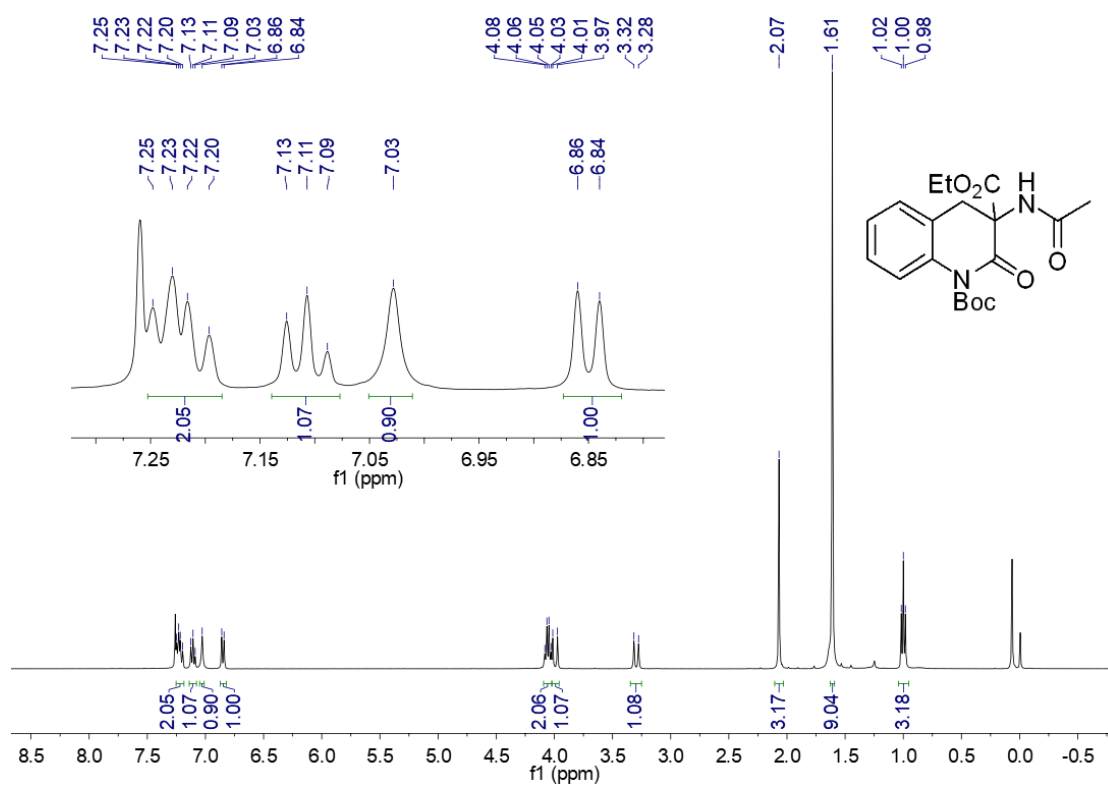


$^{13}\text{C}$  NMR (100 MHz,  $\text{CDCl}_3$ ) of compound **3an**:

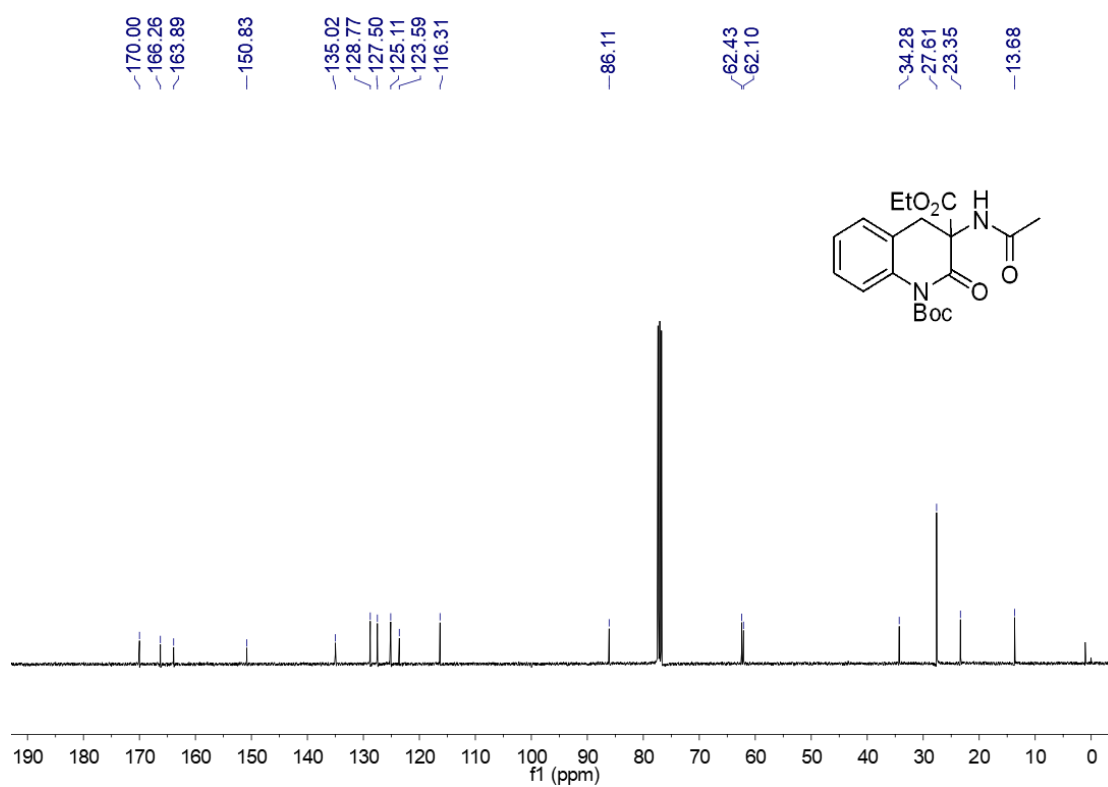




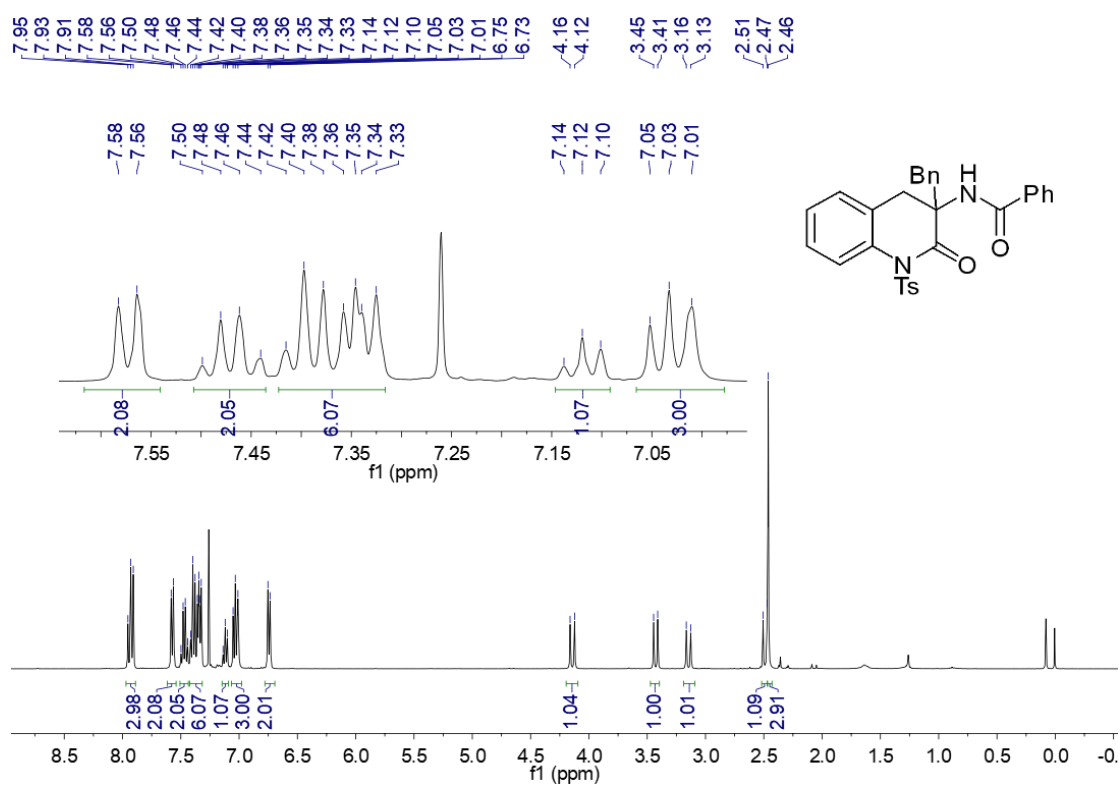
$^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ ) of compound **3hn**:



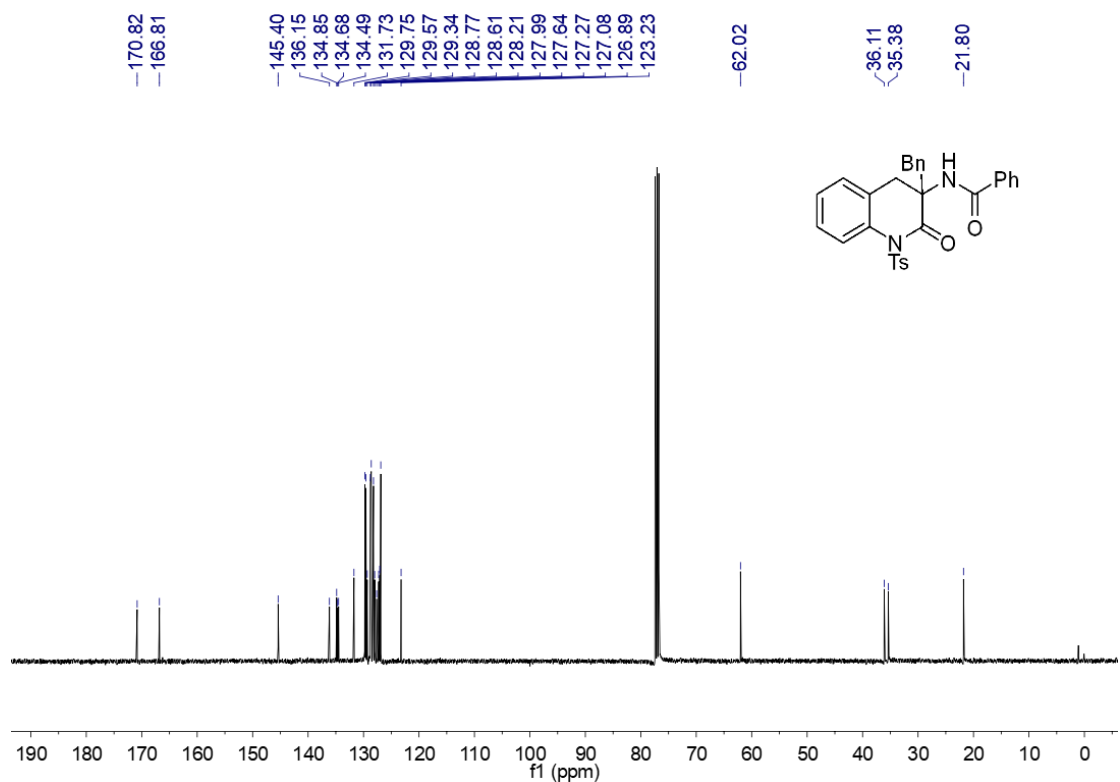
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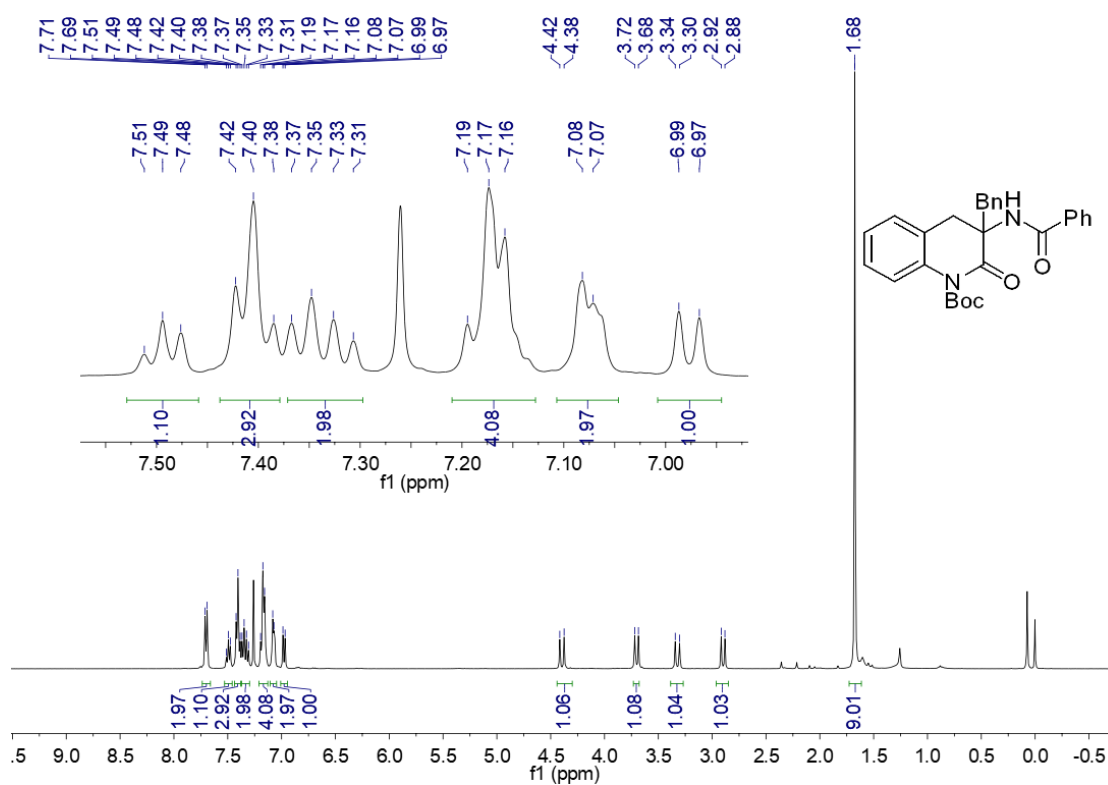
$^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ ) of compound **3ao**:



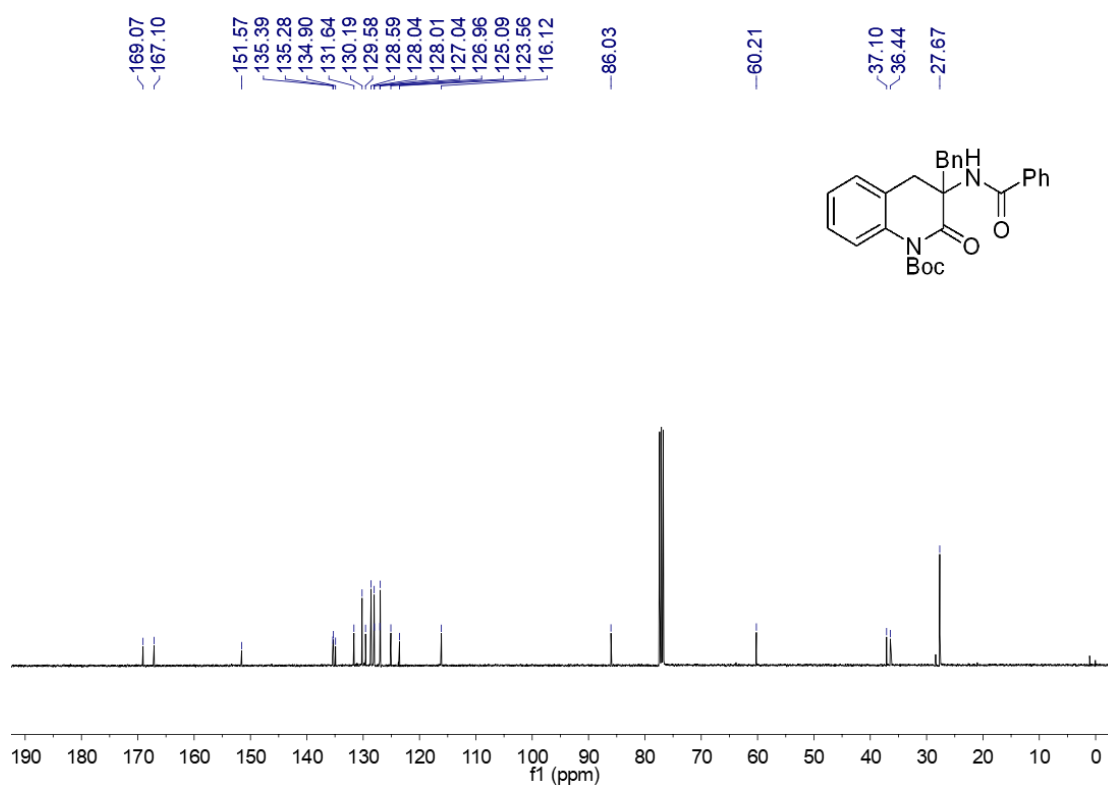
$^{13}\text{C}$  NMR (100 MHz,  $\text{CDCl}_3$ ) of compound **3ao**:



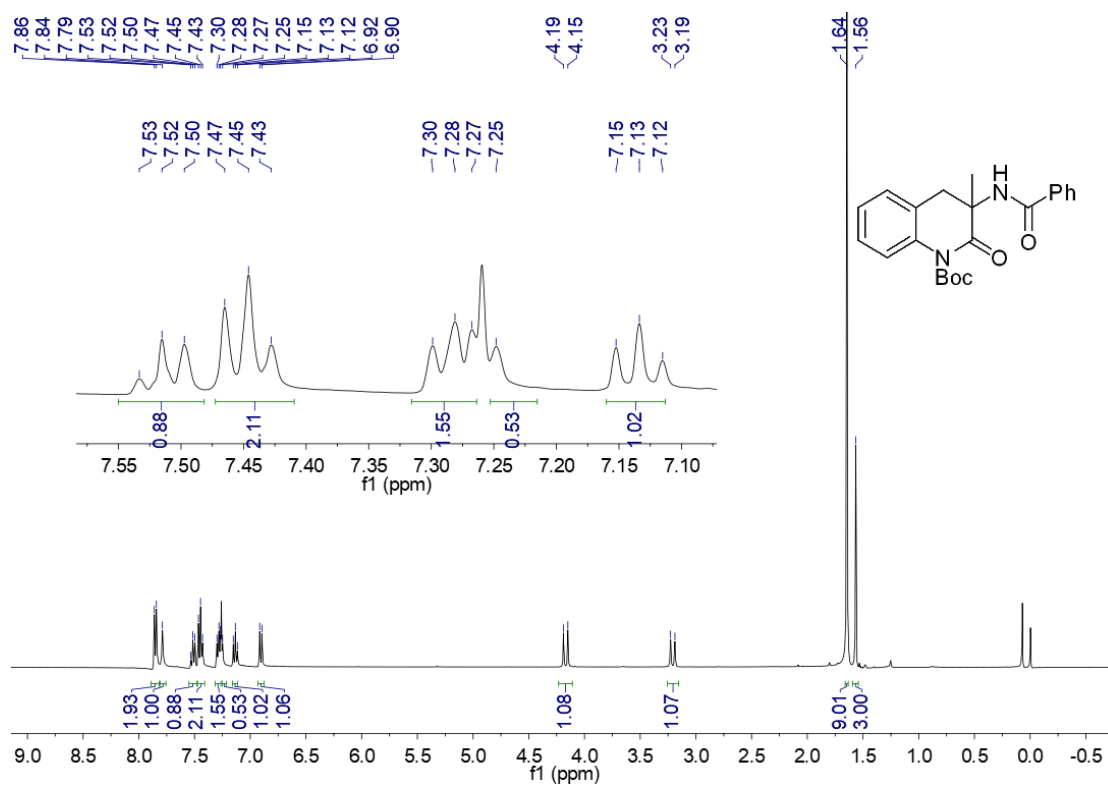
$^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ ) of compound **3ho**:



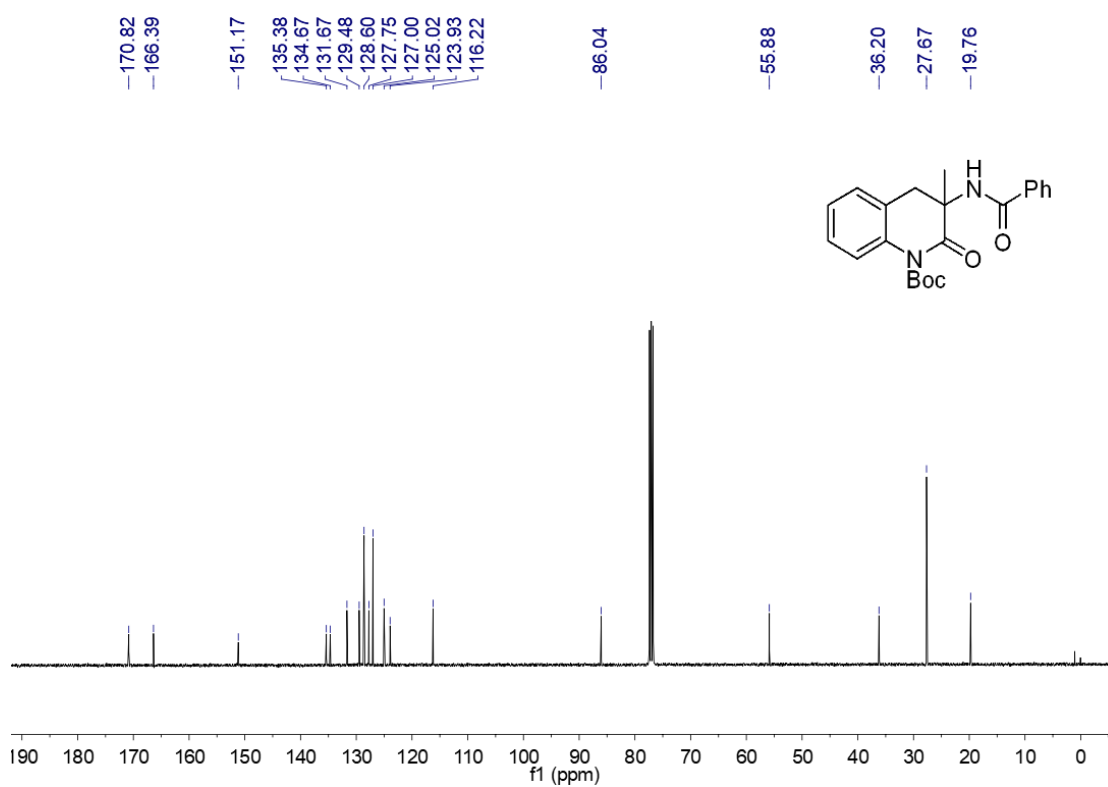
$^{13}\text{C}$  NMR (100 MHz,  $\text{CDCl}_3$ ) of compound **3ho**:



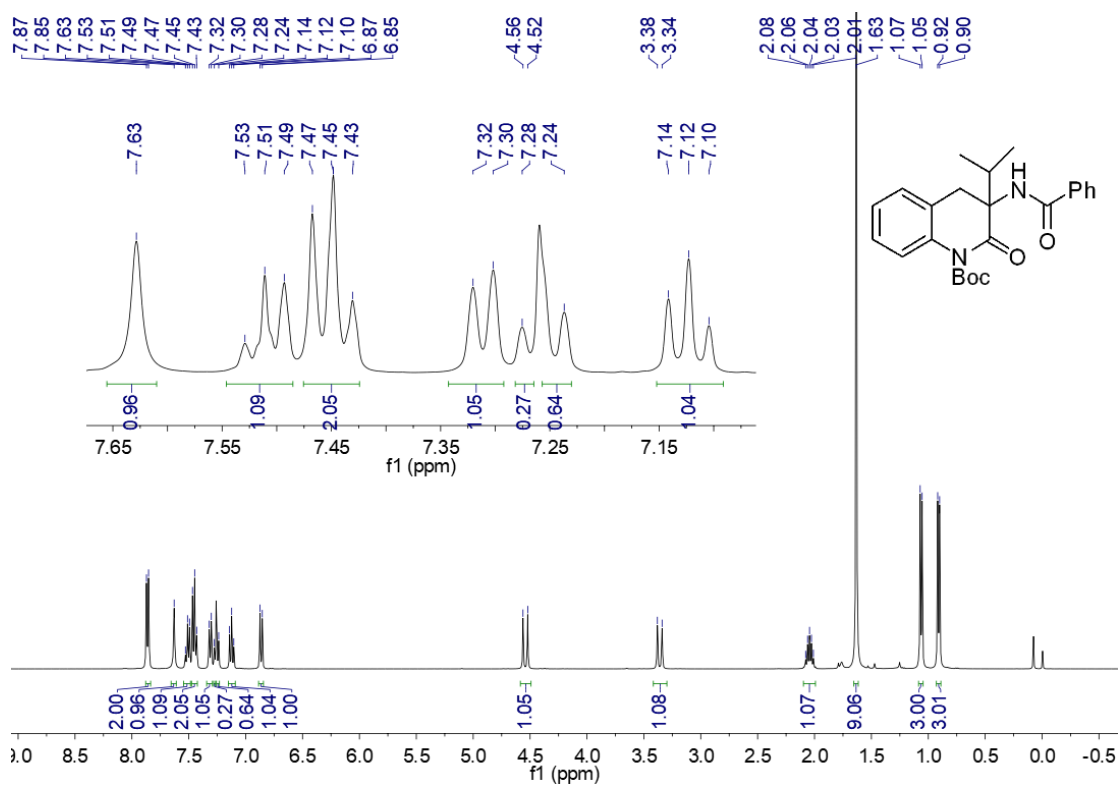
$^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ ) of compound **3hp**:



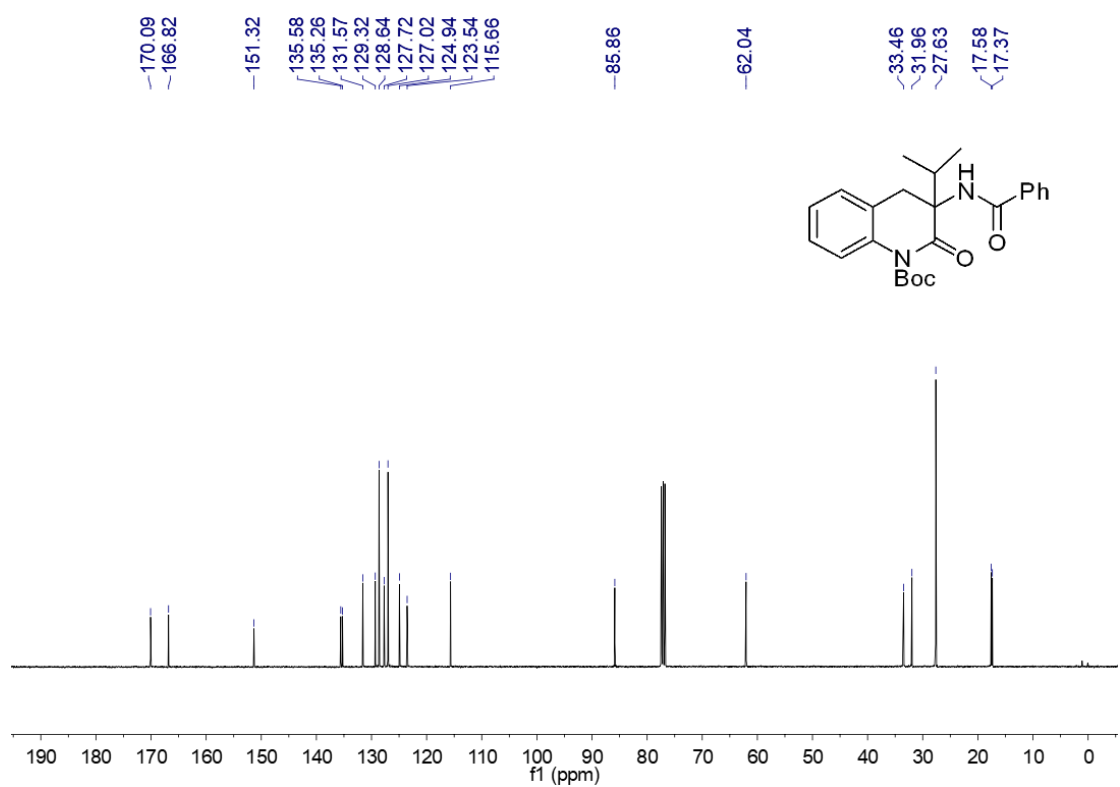
$^{13}\text{C}$  NMR (100 MHz,  $\text{CDCl}_3$ ) of compound **3hp**:



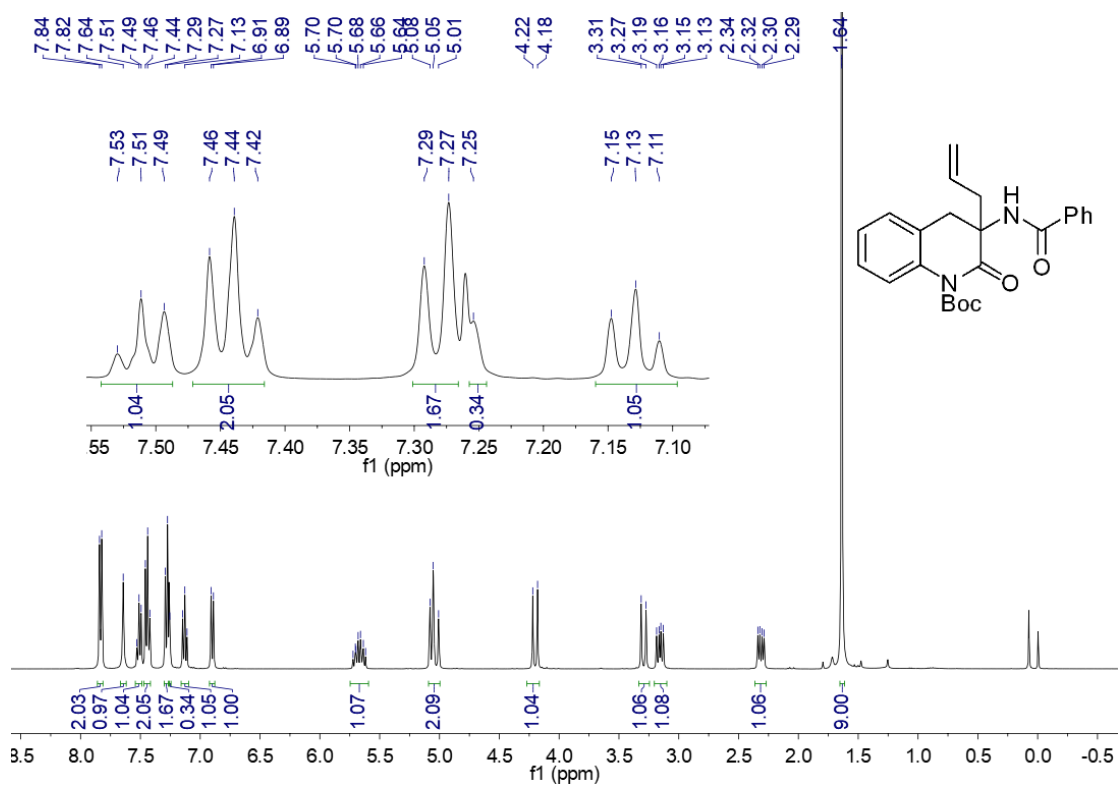
$^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ ) of compound **3hq**:



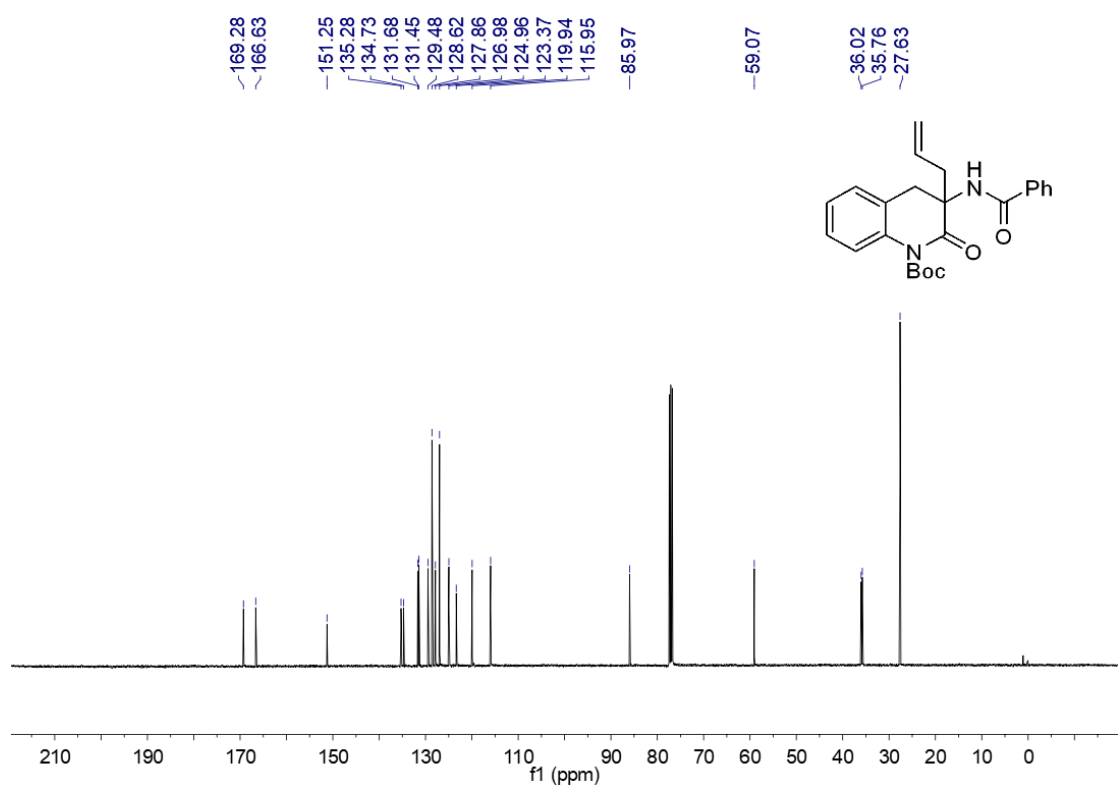
$^{13}\text{C}$  NMR (100 MHz,  $\text{CDCl}_3$ ) of compound **3hq**:



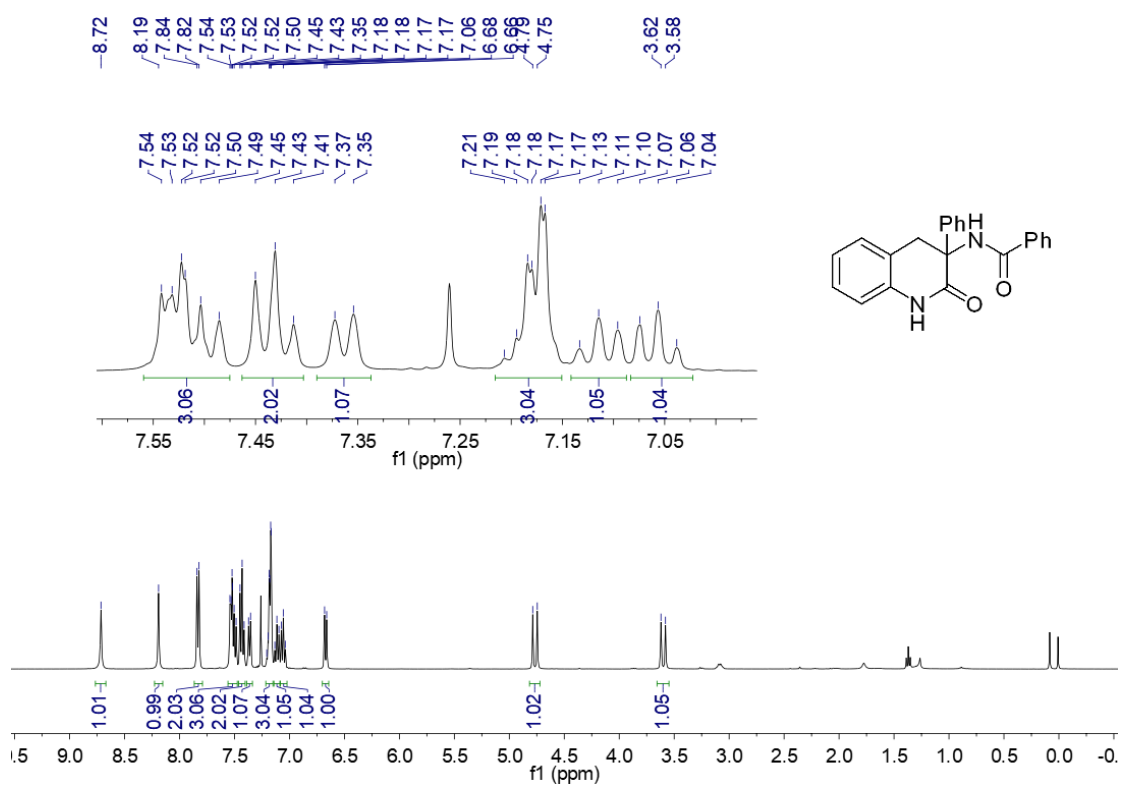
$^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ ) of compound **3hr**:



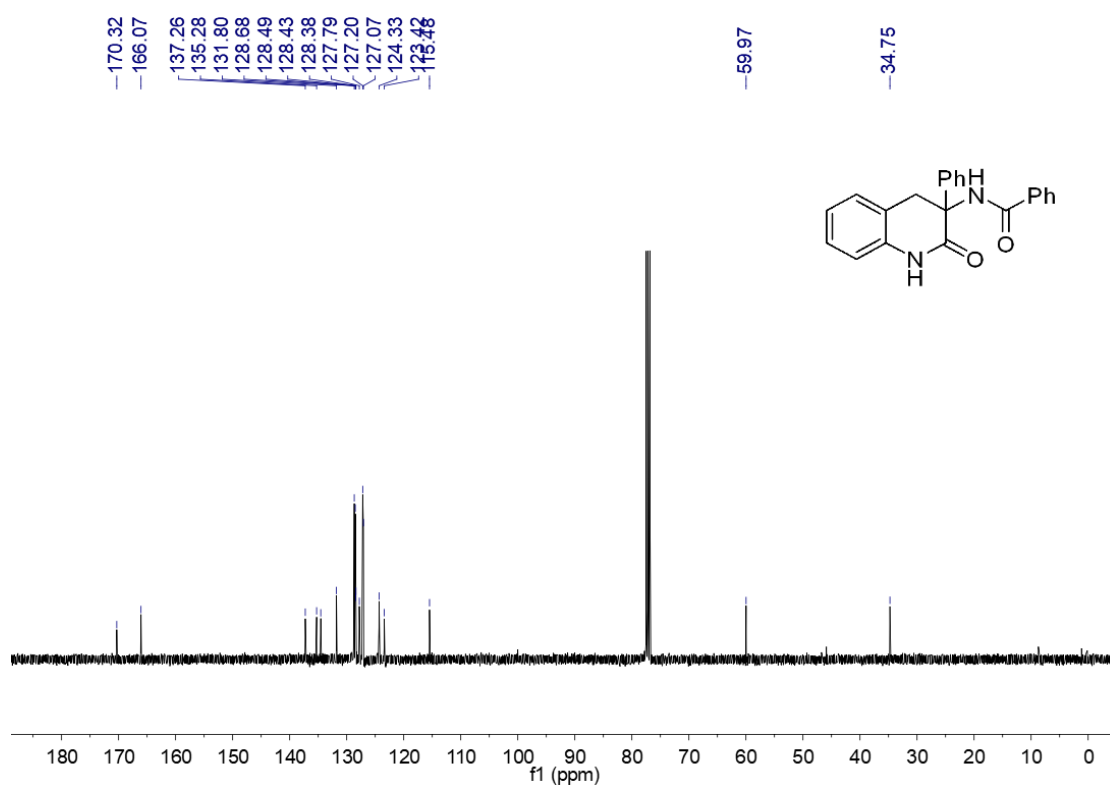
$^{13}\text{C}$  NMR (100 MHz,  $\text{CDCl}_3$ ) of compound **3hr**:



$^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ ) of compound **4**:



$^{13}\text{C}$  NMR (100 MHz,  $\text{CDCl}_3$ ) of compound **4**:



Chemical structure: CC(=O)NC(=O)c1c[nH]c2ccccc12C(=O)OCC

<sup>1</sup>H NMR spectrum (CDCl<sub>3</sub>) showing peaks and integrations:

- 10.54 ppm (s, 1H, integration 0.80)
- 7.16, 7.14, 7.12 ppm (m, 5H, integration 1.98)
- 6.93, 6.91, 6.89, 6.87, 6.85 ppm (m, 5H, integration 2.02)
- 4.00, 3.99, 3.98, 3.97, 3.96, 3.95, 3.94, 3.93, 3.92, 3.44, 3.40, 3.38, 3.34, 1.86 ppm (m, 4H, integration 2.00)
- 3.04 ppm (s, 3H, integration 2.33)
- 2.33 ppm (s, 3H, integration 3.04)
- 1.86 ppm (s, 3H, integration 3.00)

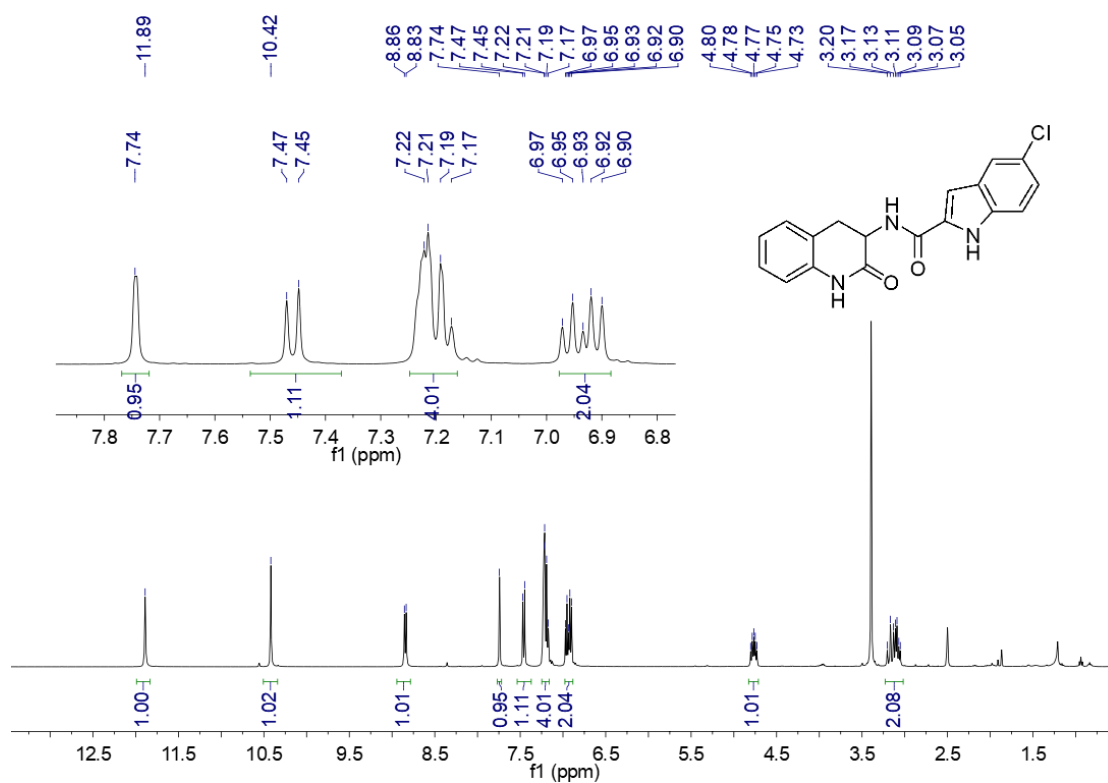
Chemical structure of 1-(2-ethoxycarbonyl-2-oxo-1-phenyl-1H-imidazol-5-yl)ethan-1-one is shown above the spectrum.

Peak list (ppm):

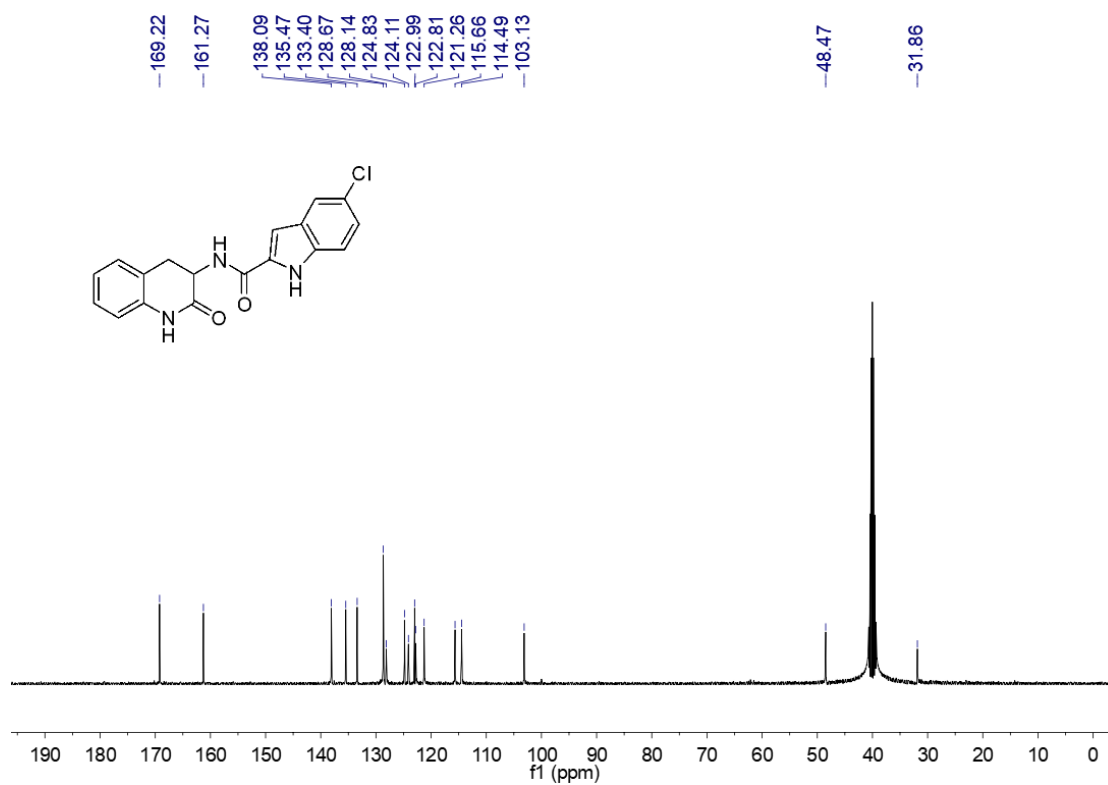
Peak List (ppm)
170.07
168.31
165.48
137.50
128.43
127.85
122.85
121.84
115.29
62.01
61.42
34.83
22.93
14.11



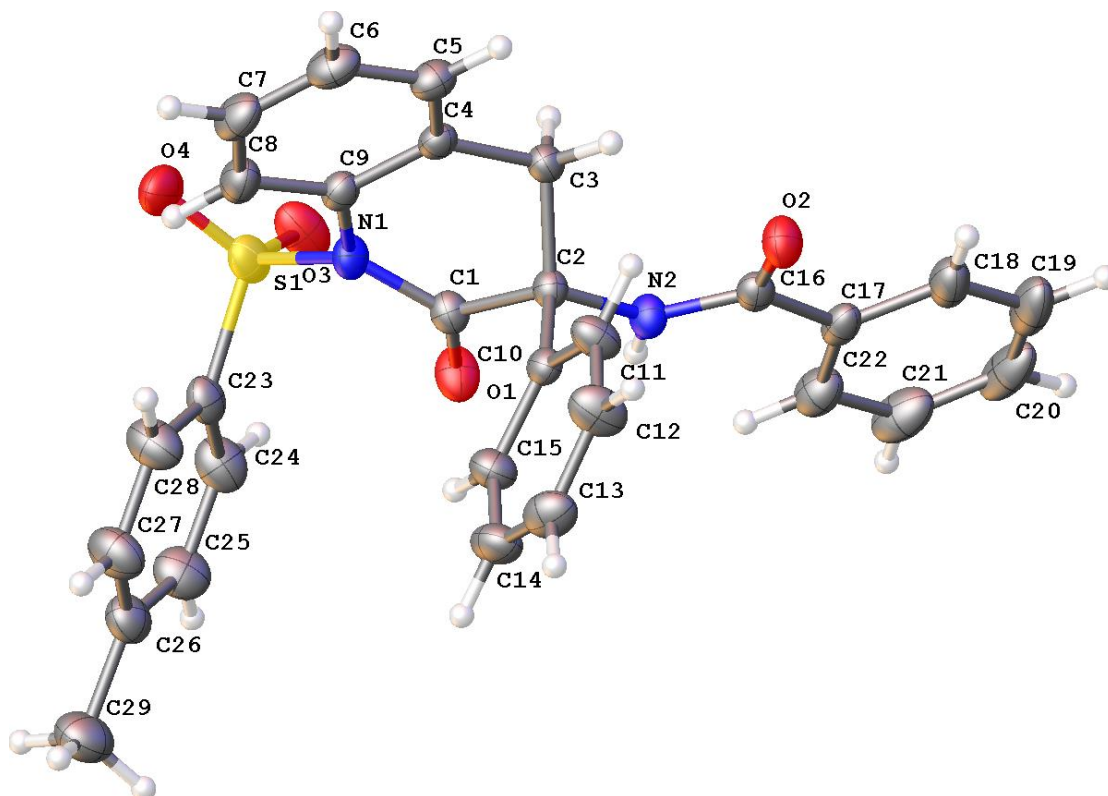
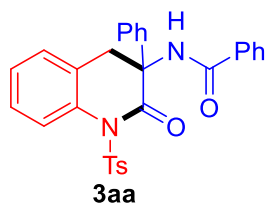
$^1\text{H}$  NMR (400 MHz,  $\text{DMSO}-d_6$ ) of compound **I**:



$^{13}\text{C}$  NMR (100 MHz,  $\text{DMSO}-d_6$ ) of compound **I**:



## 2. X-ray single crystal data for product 3aa



The thermal ellipsoid was drawn at the 30% probability level.

Identification code	sf20190405a_0m	
Empirical formula	C <sub>29</sub> H <sub>24</sub> N <sub>2</sub> O <sub>4</sub> S	
Formula weight	496.56	
Temperature	181.65 K	
Wavelength	0.71073 Å	
Crystal system	Triclinic	
Space group	P-1	
Unit cell dimensions	a = 8.3267(18) Å	α = 97.684(3) °
	b = 8.7156(19) Å	β = 91.300(2) °
	c = 16.902(4) Å	γ = 94.942(2) °
Volume	1210.3(5) Å <sup>3</sup>	
Z	2	
Density (calculated)	1.363 Mg/m <sup>3</sup>	

Absorption coefficient	0.173 mm <sup>-1</sup>
F(000)	520
Theta range for data collection	2.704 to 26.368 °
Index ranges	-10<=h<=10, -10<=k<=8, -16<=l<=21
Reflections collected	6813
Independent reflections	4826 [R(int) = 0.0142]
Completeness to theta = 25.242 °	98.3 %
Absorption correction	Semi-empirical from equivalents
Max. and min. transmission	0.7455 and 0.6519
Refinement method	Full-matrix least-squares on F <sup>2</sup>
Data / restraints / parameters	4826 / 0 / 326
Goodness-of-fit on F <sup>2</sup>	1.029
Final R indices [I>2sigma(I)]	R1 = 0.0480, wR2 = 0.1196
R indices (all data)	R1 = 0.0630, wR2 = 0.1288
Extinction coefficient	n/a
Largest diff. peak and hole	0.347 and -0.319 e.Å <sup>-3</sup>