

## ***Supporting Information***

# **Facile synthesis of carbamoylated benzimidazo[2,1-*a*]isoquinolin-6(5*H*)-ones via radical cascade cyclization under metal- free conditions**

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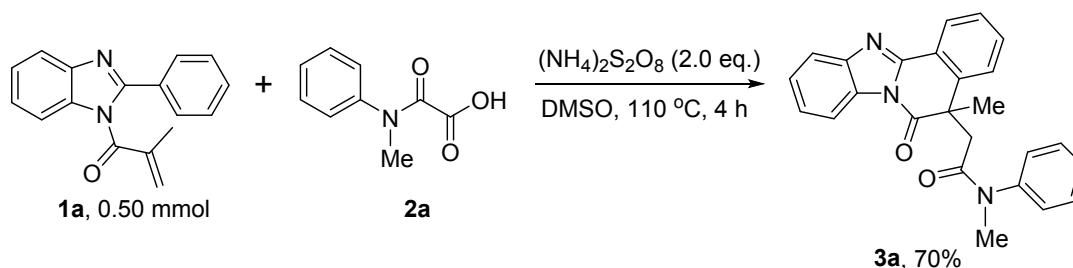
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## 1. General considerations

The  $^1\text{H}$  NMR and  $^{13}\text{C}$  NMR spectra were recorded on a 400 MHz Bruker FT-NMR spectrometer (400/100 MHz), and  $^{19}\text{F}$  NMR spectra were recorded on a 400 MHz Bruker FT-NMR spectrometer (377 MHz). All chemical shifts are given as  $\delta$  value (ppm) with reference to tetramethylsilane (TMS) as an internal standard. The peak patterns are indicated as follows: s, singlet; d, doublet; t, triplet; m, multiplet; q, quartet. The coupling constants,  $J$ , are reported in Hertz (Hz). High resolution mass spectroscopy data of the product were collected on an Agilent Technologies 6540 UHD Accurate-Mass Q-TOF LC/MS (ESI). All the solvents and commercially available reagents were purchased from commercial suppliers. Products were purified by flash chromatography on 200–300 mesh silica gels,  $\text{SiO}_2$ .

## 2. Representative procedure for the model reaction

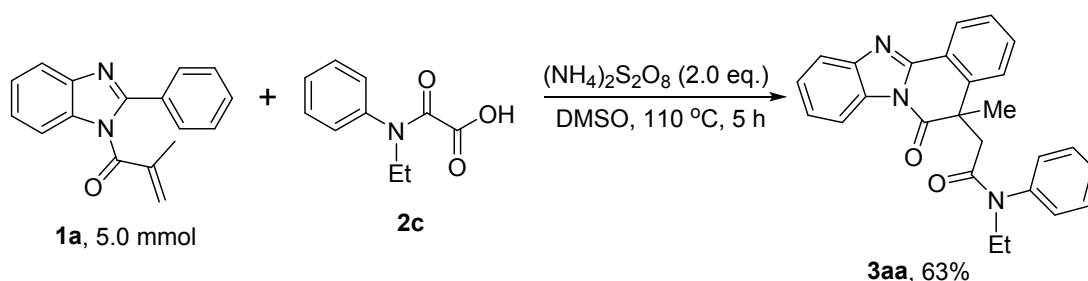
### 2.1 Representative procedure for the reaction in 0.50 mmol scale



A 5 mL oven-dried reaction vessel equipped with a magnetic stirrer bar was charged with *N*-methacryloyl-2-phenylbenzimidazole (**1a**, 0.50 mmol), *N*-methyl-*N*-phenyl oxamic acid (**2a**, 0.60 mmol),  $(\text{NH}_4)_2\text{S}_2\text{O}_8$  (2.0 eq.) and DMSO (2.0 mL). The reaction vessel was stirred at 110 °C

for 4 h. After completion of the reaction, The mixture was then diluted with EtOAc and H<sub>2</sub>O, the aqueous layer was extracted with EtOAc (7.0 mL×3), the combined organic layer was washed with brine, dried with Na<sub>2</sub>SO<sub>4</sub>, concentrated under reduced pressure to afford crude product, which was further purified by flash chromatography (silica gel, petroleum ether/ethyl acetate = 5/1) to give the desired product **3a** (70% yield).

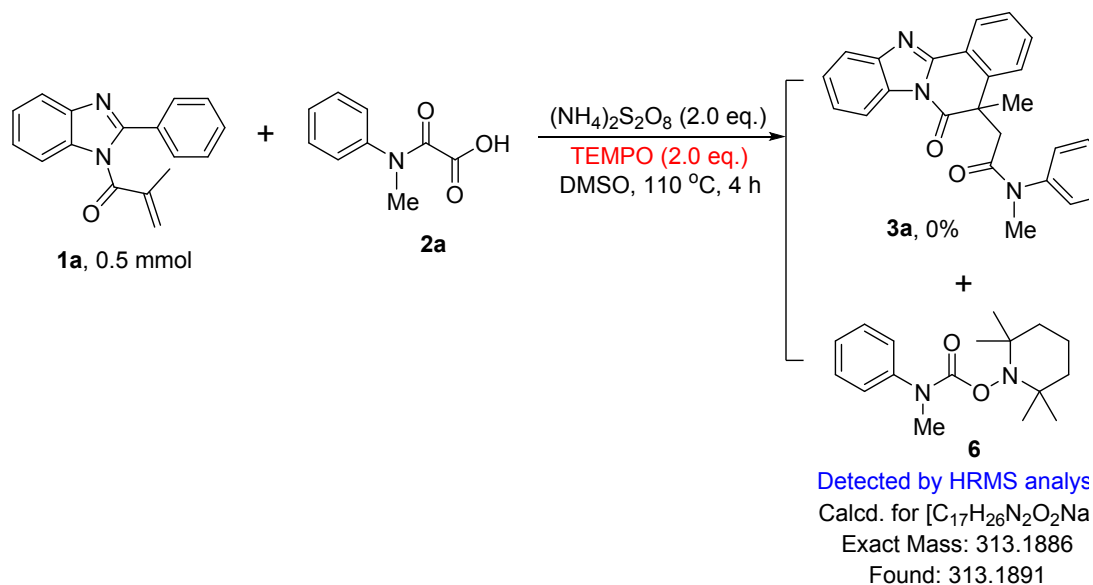
## 2.2 Representative procedure for the reaction in 5.0 mmol scale



A 50 mL oven-dried reaction vessel equipped with a magnetic stirrer bar was charged with *N*-methacryloyl-2-phenylbenzimidazole (**1a**, 1.31 g, 5.0 mmol), *N*-ethyl-*N*-phenyl oxamic acid (**2c**, 6.0 mmol), (NH<sub>4</sub>)<sub>2</sub>S<sub>2</sub>O<sub>8</sub> (2.0 eq.) and DMSO (15.0 mL). The reaction vessel was stirred at 110 °C for 4 h. After completion of the reaction, The mixture was then diluted with EtOAc and H<sub>2</sub>O, the aqueous layer was extracted with EtOAc (30 ml×3), the combined organic layer was washed with brine, dried with Na<sub>2</sub>SO<sub>4</sub>, concentrated under reduced pressure to afford crude product, which was further purified by flash chromatography (silica gel, EtOAc/petroleum ether = 1:10) to give the desired product **3aa** (1.30 g, 63% yield).

### 3. Preliminary mechanistic investigation

#### Free-radical inhibition and trapping experiment



A 5 mL oven-dried sealed tube equipped with a magnetic stirrer bar was charged with *N*-methacryloyl-2-phenylbenzimidazole (**1a**, 0.50 mmol), *N*-methyl-*N*-phenyl oxamic acid (**2a**, 0.60 mmol),  $(\text{NH}_4)_2\text{S}_2\text{O}_8$  (2.0 eq.), TEMPO (1.00 mmol, 2.0 eq.) and DMSO (2.0 mL). The reaction vessel was stirred at 110 °C for 4 h. After completion of the reaction, TLC detection showed that the reaction was completely inhibited and no desired product **3a** was found, indicating a radical pathway involved in the reaction. Meanwhile, the key intermediate **A** was captured by TEMPO as a free-radical trapping reagent and its corresponding adduct **6** was detected by high-resolution mass spectrum (HRMS) analysis (Figure S1).

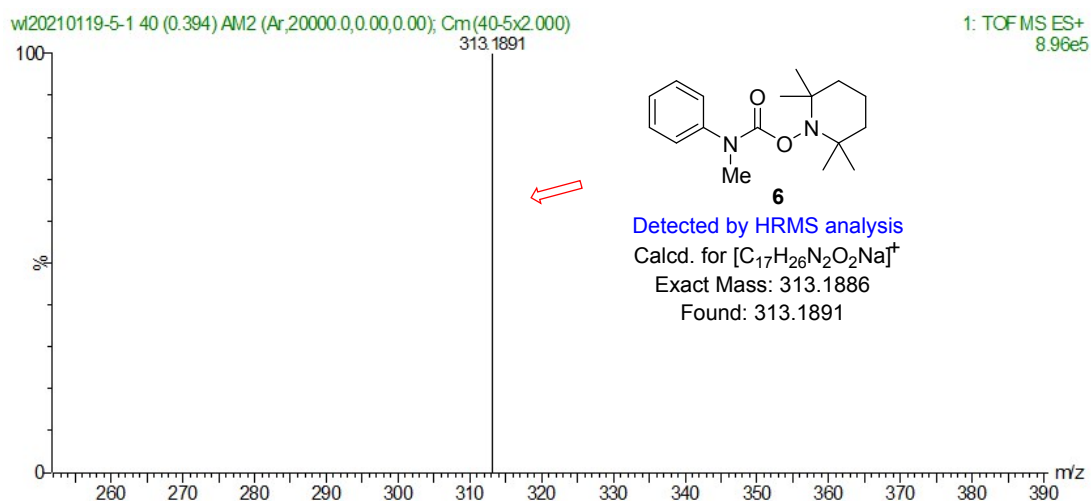
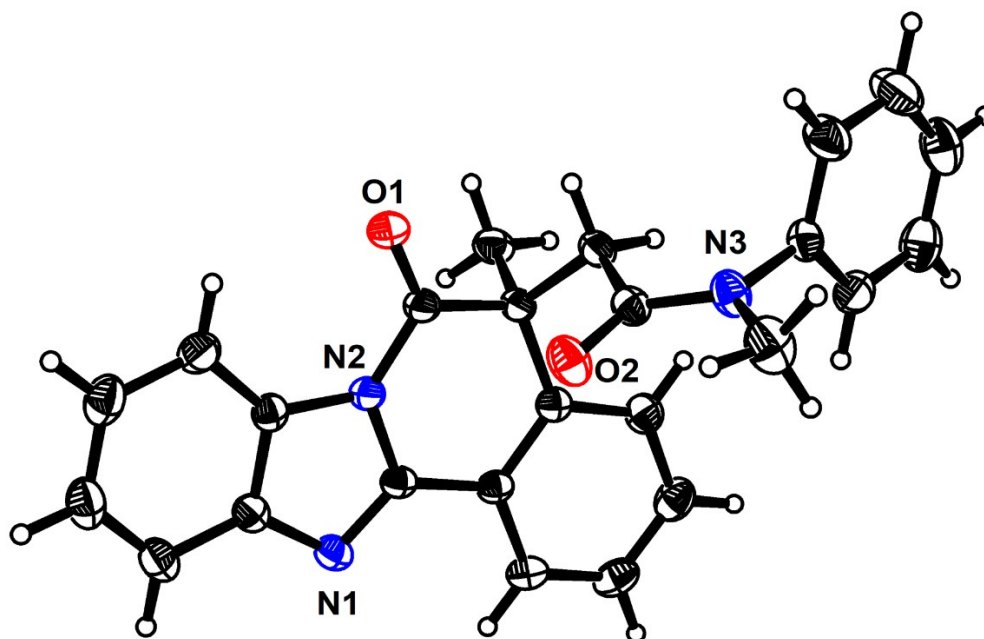


Figure S1. HRMS analysis of the adduct **6** from intermediate **A** and TEMPO

#### 4. X-Ray single crystal diffraction analysis of **3a** (CCDC: 2053319) and **5c** (CCDC: 2053320)

*N*-Methyl-2-(5-methyl-6-oxo-5,6-dihydrobenzo[4,5]imidazo[2,1-*a*]isoquinolin-5-yl)-*N*-phenylacetamide (**3a**, CCDC: 2053319)



## checkCIF/PLATON report

Structure factors have been supplied for datablock(s) 1

THIS REPORT IS FOR GUIDANCE ONLY. IF USED AS PART OF A REVIEW PROCEDURE FOR PUBLICATION, IT SHOULD NOT REPLACE THE EXPERTISE OF AN EXPERIENCED CRYSTALLOGRAPHIC REFEREE.

No syntax errors found. [CIF dictionary](#) [Interpreting this report](#)

### Datablock: 1

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Bond precision:	C-C = 0.0021 A	Wavelength=0.71073	
Cell:	a=14.7925 (18) alpha=90	b=10.7843 (13) beta=111.899 (2)	c=13.5803 (17) gamma=90
Temperature:	296 K		
	Calculated	Reported	
Volume	2010.1 (4)	2010.1 (4)	
Space group	P 21/c	P 21/c	
Hall group	-P 2ybc	-P 2ybc	
Moiety formula	C25 H21 N3 O2	?	
Sum formula	C25 H21 N3 O2	C25 H21 N3 O2	
Mr	395.45	395.45	
Dx, g cm <sup>-3</sup>	1.307	1.307	
Z	4	4	
Mu (mm <sup>-1</sup> )	0.084	0.084	
F000	832.0	832.0	
F000'	832.33		
h, k, lmax	17, 12, 16	17, 12, 16	
Nref	3537	3529	
Tmin, Tmax	0.978, 0.982		
Tmin'	0.978		

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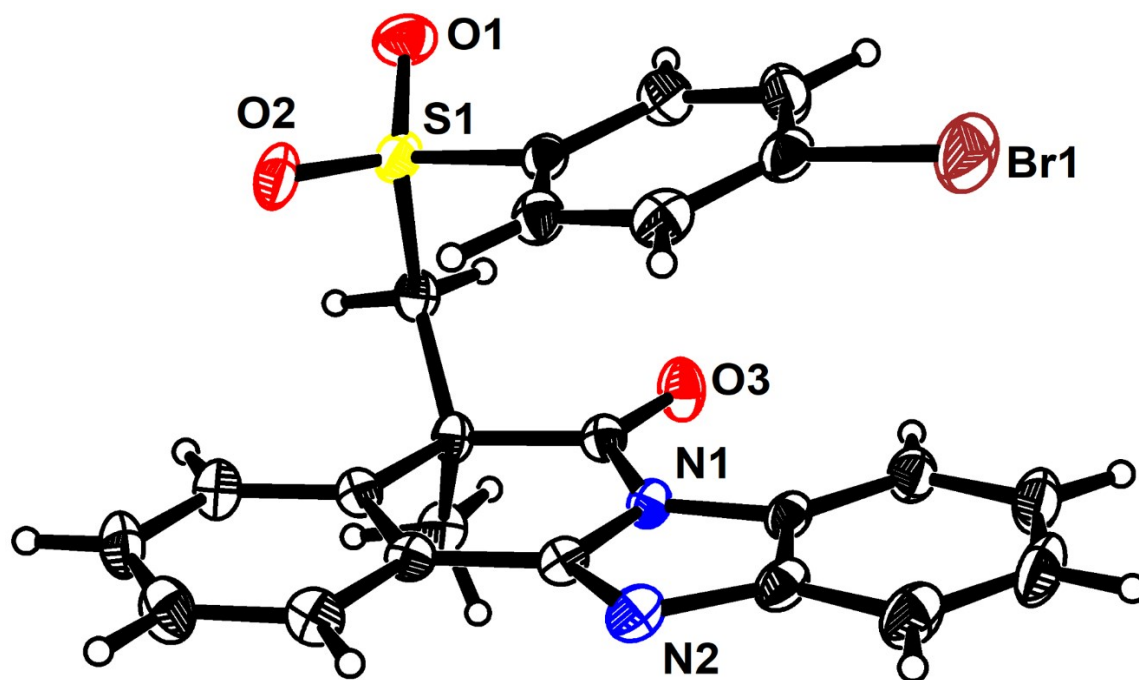
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Click on the hyperlinks for more details of the test.

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**5-(((4-Bromophenyl)sulfonyl)methyl)-5-methylbenzo[4,5]imidazo[2,1-*a*]isoquinolin-6(5*H*)-one (5c, CCDC: 2053320)**



## checkCIF/PLATON report

Structure factors have been supplied for datablock(s) 1

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No syntax errors found. [CIF dictionary](#) [Interpreting this report](#)

### Datablock: 1

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alpha=90 beta=94.098(2) gamma=90  
Temperature: 296 K

	Calculated	Reported
Volume	2001.2(3)	2001.2(3)
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Hall group	-P 2yn	-P 2yn
Moiety formula	C23 H17 Br N2 O3 S	?
Sum formula	C23 H17 Br N2 O3 S	C23 H17 Br N2 O3 S
Mr	481.35	481.35
Dx, g cm-3	1.598	1.598
Z	4	4
Mu (mm-1)	2.187	2.187
F000	976.0	976.0
F000'	975.72	
h, k, lmax	15, 8, 24	15, 8, 24
Nref	3518	3511
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Tmin'	0.561	

Correction method= Not given

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S = 0.987 Npar= 272

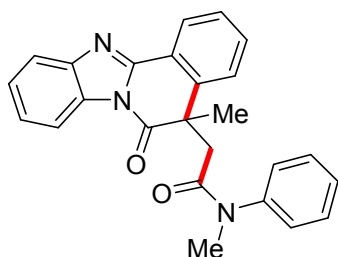
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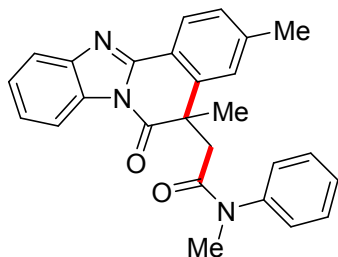
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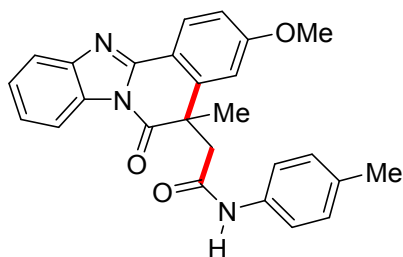
## 5. Characterization data for the products



***N*-Methyl-2-(5-methyl-6-oxo-5,6-dihydrobenzo[4,5]imidazo[2,1-*a*]isoquinolin-5-yl)-*N*-phenylacetamide (3a):** White solid; mp: 190.8–192.4 °C; <sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>) δ: 8.53 (dd, *J*<sub>1</sub> = 1.6 Hz, *J*<sub>2</sub> = 7.6 Hz, 1H), 8.41–8.39 (m, 1H), 7.84–7.82 (m, 1H), 7.53–7.37 (m, 7H), 7.20 (d, *J* = 7.2 Hz, 2H), 7.13 (d, *J* = 7.6 Hz, 1H), 3.49 (d, *J* = 17.2 Hz, 1H), 3.02–2.98 (m, 4H), 1.45 (s, 3H). <sup>13</sup>C NMR (100 MHz, CDCl<sub>3</sub>) δ: 173.5, 169.0, 150.0, 144.0, 143.5, 142.2, 131.8, 131.5, 130.2, 128.4, 127.5, 127.3, 126.5, 125.5, 125.3, 124.5, 123.1, 119.7, 115.7, 47.1, 45.0, 37.2, 29.9. HRMS (ESI) ([M+H]<sup>+</sup>) Calcd. For [C<sub>25</sub>H<sub>22</sub>N<sub>3</sub>O<sub>2</sub>]<sup>+</sup>: 396.1707, Found: 396.1705.

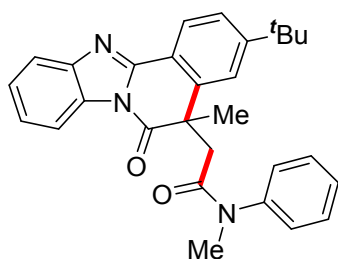


**2-(3,5-Dimethyl-6-oxo-5,6-dihydrobenzo[4,5]imidazo[2,1-*a*]isoquinolin-5-yl)-*N*-methyl-*N*-phenylacetamide (3b):** White solid; mp: 212.1–213.5 °C; <sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>) δ: 8.41–8.38 (m, 2H), 7.84–7.77 (m, 1H), 7.51 (t, *J* = 7.5 Hz, 2H), 7.44–7.35 (m, 3H), 7.28–7.26 (m, 1H), 7.19 (d, *J* = 7.2 Hz, 2H), 6.90 (s, 1H), 3.47 (d, *J* = 16.8 Hz, 1H), 3.01–2.97 (m, 4H), 2.44 (s, 3H), 1.43 (s, 3H). <sup>13</sup>C NMR (100 MHz, CDCl<sub>3</sub>) δ: 173.4, 168.9, 150.0, 144.0, 143.3, 141.9, 141.6, 131.6, 130.0, 128.4, 128.2, 127.1, 126.1, 125.2, 124.9, 124.8, 120.3, 119.3, 115.5, 46.8, 44.6, 37.0, 29.7, 21.8. HRMS (ESI) ([M+H]<sup>+</sup>) Calcd. For [C<sub>26</sub>H<sub>24</sub>N<sub>3</sub>O<sub>2</sub>]<sup>+</sup>: 410.1863, Found: 410.1859.

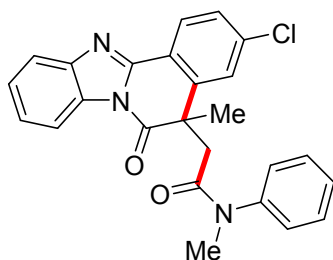


**2-(3-Methoxy-5-methyl-6-oxo-5,6-dihydrobenzo[4,5]imidazo[2,1-*a*]isoquinolin-5-yl)-*N*-(*p*-tolyl)acetamide (3c):** White solid; mp: 214.3–216.7 °C; <sup>1</sup>H NMR (400 MHz, DMSO-*d*<sub>6</sub>) δ: 10.02 (s, 1H), 8.33–8.28 (m, 2H), 7.82–7.80 (m, 1H), 7.47–7.39 (m, 2H), 7.23–7.21 (m, 3H), 7.10 (dd, *J*<sub>1</sub> = 2.4 Hz, *J*<sub>2</sub> = 8.8 Hz, 1H), 6.96 (d, *J* = 8.4 Hz, 1H), 3.89 (s, 3H), 3.66 (d, *J* = 16.8 Hz, 1H), 3.55 (d, *J* =

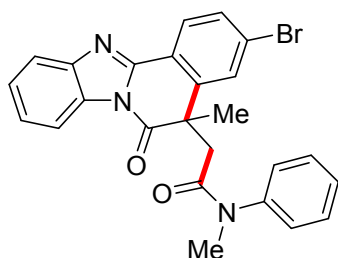
16.8 Hz, 1H), 2.15 (s, 3H), 1.63 (s, 3H).  $^{13}\text{C}$  NMR (100 MHz, DMSO- $d_6$ )  $\delta$ : 173.2, 167.8, 162.1, 150.0, 144.3, 143.9, 136.0, 132.2, 131.2, 129.0, 127.3, 125.4, 124.6, 119.1, 118.9, 115.2, 115.0, 113.5, 111.4, 55.6, 46.6, 46.5, 29.3, 20.3. HRMS (ESI) ( $[\text{M}+\text{H}]^+$ ) Calcd. For  $[\text{C}_{26}\text{H}_{24}\text{N}_3\text{O}_3]^+$ : 426.1812, Found: 426.1815.



**2-(3-(*tert*-Butyl)-5-methyl-6-oxo-5,6-dihydrobenzo[4,5]imidazo[2,1-*a*]isoquinolin-5-yl)-*N*-methyl-*N*-phenylacetamide (3d):** White solid; mp: 184.1–186.4 °C;  $^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ )  $\delta$ : 8.45–8.39 (m, 2H), 7.83–7.81 (m, 1H), 7.52–7.37 (m, 6H), 7.18 (d,  $J = 7.2$  Hz, 2H), 7.11–7.10 (m, 1H), 3.50 (d,  $J = 16.8$  Hz, 1H), 3.05–3.00 (m, 4H), 1.46 (s, 3H), 1.37 (s, 10H).  $^{13}\text{C}$  NMR (100 MHz,  $\text{CDCl}_3$ )  $\delta$ : 173.7, 168.9, 154.7, 150.0, 144.1, 143.4, 141.6, 131.7, 130.0, 128.2, 127.1, 126.1, 125.2, 124.9, 120.9, 120.4, 119.4, 115.6, 47.0, 45.1, 37.1, 35.1, 31.1, 29.9. HRMS (ESI) ( $[\text{M}+\text{H}]^+$ ) Calcd. For  $[\text{C}_{29}\text{H}_{30}\text{N}_3\text{O}_2]^+$ : 452.2333, Found: 452.2337.

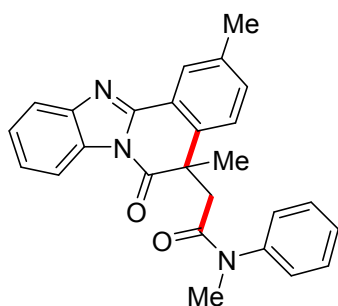


**2-(3-Chloro-5-methyl-6-oxo-5,6-dihydrobenzo[4,5]imidazo[2,1-a]isoquinolin-5-yl)-N-methyl-N-phenylacetamide (3e):** White solid; mp: 192.9–194.6 °C;  $^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ )  $\delta$ : 8.46 (d,  $J = 8.4$  Hz, 1H), 8.39–8.37 (m, 1H), 7.82–7.80 (m, 1H), 7.54 (t,  $J = 7.6$  Hz, 2H), 7.47–7.40 (m, 4H), 7.22 (d,  $J = 7.2$  Hz, 2H), 7.10–7.09 (m, 1H), 3.50 (d,  $J = 16.8$  Hz, 1H), 3.01 (s, 3H), 2.92 (d,  $J = 16.8$  Hz, 1H), 1.45 (s, 3H).  $^{13}\text{C}$  NMR (100 MHz,  $\text{CDCl}_3$ )  $\delta$ : 172.5, 168.7, 148.9, 143.9, 143.6, 143.1, 137.2, 131.5, 130.1, 128.3, 127.9, 127.6, 127.2, 125.5, 125.3, 124.8, 121.7, 119.6, 115.5, 47.0, 44.6, 37.1, 29.4. HRMS (ESI) ( $[\text{M}+\text{H}]^+$ ) Calcd. For  $[\text{C}_{25}\text{H}_{21}\text{ClN}_3\text{O}_2]^+$ : 430.1317, Found: 430.1320.



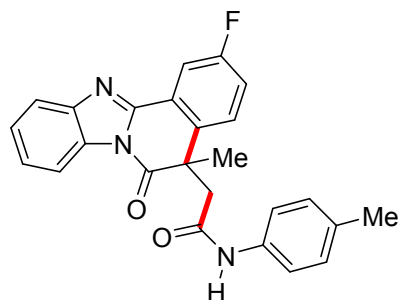
**2-(3-Bromo-5-methyl-6-oxo-5,6-dihydrobenzo[4,5]imidazo[2,1-a]isoquinolin-5-yl)-N-methyl-N-phenylacetamide (3f):** White solid;

mp: 214.6–216.2 °C; <sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>) δ: 8.39–8.37 (m, 2H), 7.82–7.80 (m, 1H), 7.61–7.52 (m, 3H), 7.47–7.39 (m, 3H), 7.27–7.21 (m, 3H), 3.50 (d, *J* = 16.8 Hz, 1H), 3.01 (s, 3H), 2.92 (d, *J* = 16.8 Hz, 1H), 1.45 (s, 3H). <sup>13</sup>C NMR (100 MHz, CDCl<sub>3</sub>) δ: 172.5, 168.7, 148.9, 143.9, 143.7, 143.2, 131.6, 130.8, 130.2, 128.4, 127.8, 127.7, 127.2, 125.7, 125.5, 125.4, 122.1, 119.6, 115.6, 47.0, 44.6, 37.1, 29.4. HRMS (ESI) ([M+H]<sup>+</sup>) Calcd. For [C<sub>25</sub>H<sub>20</sub>BrN<sub>3</sub>O<sub>2</sub>]<sup>+</sup>: 474.0812, Found: 474.0820.

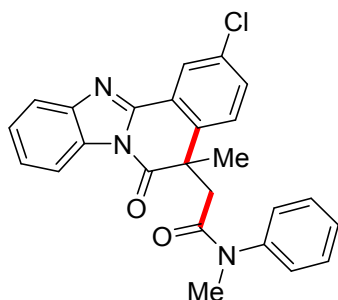


**2-(2,5-Dimethyl-6-oxo-5,6-dihydrobenzo[4,5]imidazo[2,1-a]isoquinolin-5-yl)-N-methyl-N-phenylacetamide (3g):** White solid; mp: 178.4–181.3 °C; <sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>) δ: 8.41–8.38 (m, 1H), 8.34 (s, 1H), 7.83–7.81 (m, 1H), 7.50 (t, *J* = 7.6 Hz, 2H), 7.44–7.37 (m, 3H), 7.32 (dd, *J*<sub>1</sub> = 2.0 Hz, *J*<sub>2</sub> = 8.0 Hz, 1H), 7.21–7.19 (m, 2H), 7.02 (d, *J* = 8.0 Hz, 1H), 3.47 (d, *J* = 16.8 Hz, 1H), 2.99–2.95 (m, 4H), 2.44 (s, 3H), 1.42 (s, 3H). <sup>13</sup>C NMR (100 MHz, CDCl<sub>3</sub>) δ: 173.5, 168.9, 150.0, 143.9, 143.3, 139.1, 137.2,

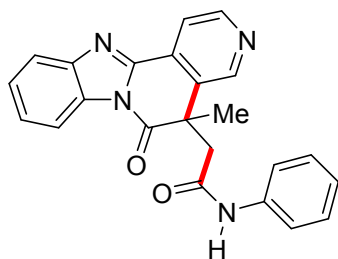
132.3, 131.6, 130.0, 128.2, 127.2, 126.4, 125.3, 125.0, 124.2, 122.7, 119.4, 115.6, 46.6, 44.8, 37.0, 29.7, 20.8. HRMS (ESI) ( $[M+H]^+$ ) Calcd. For  $[C_{26}H_{24}N_3O_2]^+$ : 410.1863, Found: 410.1867.



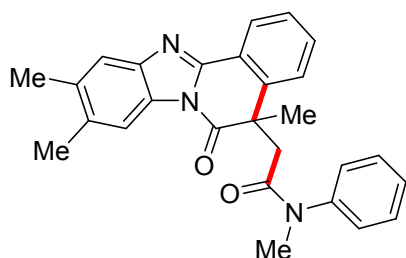
**2-(2-Fluoro-5-methyl-6-oxo-5,6-dihydrobenzo[4,5]imidazo[2,1-*a*]isoquinolin-5-yl)-*N*-(*p*-tolyl)acetamide (3h):** White solid; mp: 267.3–269.6 °C;  $^1H$  NMR (400 MHz,  $CDCl_3$ )  $\delta$ : 10.03 (s, 1H), 8.31–8.29 (m, 1H), 8.05 (dd,  $J_1 = 2.8$  Hz,  $J_2 = 8.8$  Hz, 1H), 7.88–7.86 (m, 1H), 7.81–7.77 (m, 1H), 7.49–7.47 (m, 3H), 7.19 (d,  $J = 8.0$  Hz, 2H), 6.95 (d,  $J = 8.0$  Hz, 2H), 3.65 (d,  $J = 16.8$  Hz, 1H), 3.54–3.48 (m, 2H), 2.13 (s, 3H), 1.66 (s, 3H).  $^{13}C$  NMR (100 MHz,  $CDCl_3$ )  $\delta$ : 173.0, 167.7, 160.9 ( $J = 242.8$  Hz), 148.9 ( $J = 3.6$  Hz), 143.5, 138.4 ( $J = 3.2$  Hz), 135.9, 132.3, 131.3, 129.0, 128.8 ( $J = 8.3$  Hz), 125.6 ( $J = 8.7$  Hz), 124.5, 124.5, 119.8, 119.0 ( $J = 21.8$  Hz), 118.9, 115.2, 111.9 ( $J = 23.6$  Hz), 47.0, 46.1, 28.8, 20.3.  $^{19}F$  NMR (377 MHz,  $CDCl_3$ )  $\delta$ : -114.29. HRMS (ESI) ( $[M+H]^+$ ) Calcd. For  $[C_{25}H_{21}FN_3O_2]^+$ : 414.1612, Found: 414.1620.



**2-(2-Chloro-5-methyl-6-oxo-5,6-dihydrobenzo[4,5]imidazo[2,1-a]isoquinolin-5-yl)-N-methyl-N-phenylacetamide (3i):** White solid; mp: 208.7–211.5 °C;  $^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ )  $\delta$ : 8.52 (d,  $J = 2.4$  Hz, 1H), 8.39–8.37 (m, 1H), 7.84–7.82 (m, 1H), 7.54–7.41 (m, 6H), 7.21 (d,  $J = 7.2$  Hz, 2H), 7.07 (d,  $J = 8.4$  Hz, 1H), 3.50 (d,  $J = 17.2$  Hz, 1H), 3.00–2.92 (m, 4H), 1.44 (s, 3H).  $^{13}\text{C}$  NMR (100 MHz,  $\text{CDCl}_3$ )  $\delta$ : 172.8, 168.8, 148.6, 143.9, 143.2, 140.4, 133.6, 131.7, 131.3, 130.2, 128.3, 127.2, 126.0, 125.9, 125.6, 125.5, 124.8, 119.8, 115.7, 46.8, 45.0, 37.1, 29.5. HRMS (ESI) ( $[\text{M}+\text{H}]^+$ ) Calcd. For  $[\text{C}_{25}\text{H}_{21}\text{ClN}_3\text{O}_2]^+$ : 430.1317, Found: 430.1322.



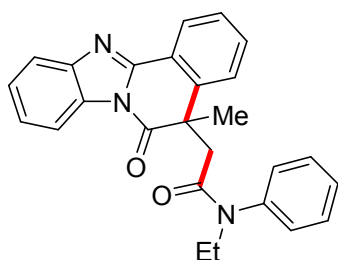
**2-(5-Methyl-6-oxo-5,6-dihydrobenzo[4,5]imidazo[2,1-*a*][2,6]naphthyridin-5-yl)-*N*-phenylacetamide (3j):** White solid; mp: 157.8–162.4 °C; <sup>1</sup>H NMR (400 MHz, DMSO-*d*<sub>6</sub>) δ: 10.17 (s, 1H), 9.08 (s, 1H), 8.71 (d, *J* = 5.2 Hz, 1H), 8.34–8.32 (m, 1H), 8.22 (d, *J* = 5.2 Hz, 1H), 7.95–7.93 (m, 1H), 7.55–7.53 (m, 2H), 7.28 (d, *J* = 8.0 Hz, 2H), 7.17–7.13 (m, 2H), 6.94 (t, *J* = 7.2 Hz, 1H), 3.69 (s, 2H), 1.75 (s, 3H). <sup>13</sup>C NMR (100 MHz, DMSO-*d*<sub>6</sub>) δ: 172.4, 167.9, 148.3, 147.9, 143.4, 138.2, 136.2, 131.3, 129.4, 128.6, 126.3, 125.9, 123.4, 120.2, 119.0, 117.7, 115.3, 46.7, 44.9, 28.1. HRMS (ESI) ([M+H]<sup>+</sup>) Calcd. For [C<sub>23</sub>H<sub>19</sub>N<sub>4</sub>O<sub>2</sub>]<sup>+</sup>: 383.1503, Found: 383.1512.



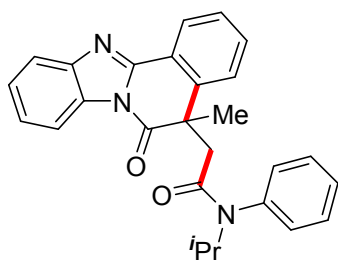
***N*-Methyl-*N*-phenyl-2-(5,9,10-trimethyl-6-oxo-5,6-dihydrobenzo[4,5]imidazo[2,1-*a*]isoquinolin-5-yl)acetamide (3k):** White solid; mp: 204.2–206.9 °C; <sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>) δ: 8.40 (dd, *J*<sub>1</sub> = 1.6, *J*<sub>2</sub> = 7.6 Hz, 1H), 8.10 (s, 1H), 7.50 (s, 1H), 7.44–7.32 (m, 5H), 7.12 (d, *J* = 6.8 Hz, 2H), 7.03 (d, *J* = 7.6 Hz, 1H), 3.39 (d, *J* = 16.8 Hz, 1H), 2.92–2.88 (m, 4H), 2.32 (d, *J* = 3.2 Hz, 6H), 1.35 (s, 3H). <sup>13</sup>C NMR (100 MHz, CDCl<sub>3</sub>) δ: 173.4, 168.9,



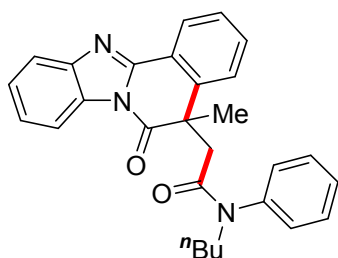
149.1, 143.4, 142.5, 141.8, 134.3, 134.2, 130.9, 130.1, 130.0, 128.2, 127.3, 127.2, 126.1, 124.3, 123.3, 119.8, 115.9, 46.8, 44.8, 37.1, 29.8, 20.4. HRMS (ESI) ( $[M+H]^+$ ) Calcd. For  $[C_{27}H_{26}N_3O_2]^+$ : 424.2020, Found: 424.2019.



***N*-Ethyl-2-(5-methyl-6-oxo-5,6-dihydrobenzo[4,5]imidazo[2,1-*a*]isoquinolin-5-yl)-*N*-phenylacetamide (3aa):** White solid; mp: 175.6–178.9 °C;  $^1H$  NMR (400 MHz,  $CDCl_3$ )  $\delta$ : 8.45 (dd,  $J_1 = 1.6$  Hz,  $J_2 = 7.6$  Hz, 1H), 8.33–8.31 (m, 1H), 7.76–7.74 (m, 1H), 7.46–7.30 (m, 7H), 7.11–7.04 (m, 3H), 3.49–3.26 (m, 3H), 2.84 (d,  $J = 16.4$  Hz, 1H), 1.37 (s, 3H), 0.78 (t,  $J = 7.2$  Hz, 3H).  $^{13}C$  NMR (100 MHz,  $CDCl_3$ )  $\delta$ : 173.4, 168.9, 149.1, 143.4, 142.5, 141.8, 134.3, 134.2, 130.9, 130.1, 130.0, 128.2, 127.3, 127.2, 126.1, 124.3, 123.3, 119.8, 115.9, 46.8, 44.8, 37.1, 29.8, 20.4. HRMS (ESI) ( $[M+H]^+$ ) Calcd. For  $[C_{26}H_{24}N_3O_2]^+$ : 410.1863, Found: 410.1866.

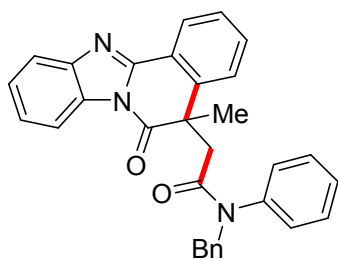


***N*-(*iso*-Propyl)-2-(5-methyl-6-oxo-5,6-dihydrobenzo[4,5]imidazo[2,1-*a*]isoquinolin-5-yl)-*N*-phenylacetamide (3ab):** White solid; mp: 209.5–211.6 °C; <sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>) δ: 8.53 (d, *J* = 8.0 Hz, 1H), 8.41–8.39 (m, 1H), 7.84–7.82 (m, 1H), 7.55–7.38 (m, 7H), 7.18–7.07 (m, 3H), 4.66–4.59 (m, 1H), 3.37 (d, *J* = 16.4 Hz, 1H), 2.80 (d, *J* = 16.8 Hz, 1H), 1.43 (s, 3H), 0.81 (dd, *J*<sub>1</sub> = 6.8 Hz, *J*<sub>2</sub> = 25.6 Hz, 6H). <sup>13</sup>C NMR (100 MHz, CDCl<sub>3</sub>) δ: 173.4, 168.3, 149.9, 144.0, 142.1, 138.1, 131.7, 131.1, 130.6, 129.5, 128.6, 127.4, 126.3, 125.3, 125.1, 124.4, 123.1, 119.6, 115.6, 47.1, 45.9, 45.8, 29.6, 20.9, 20.5. HRMS (ESI) ([M+H]<sup>+</sup>) Calcd. For [C<sub>27</sub>H<sub>26</sub>N<sub>3</sub>O<sub>2</sub>]<sup>+</sup>: 424.2020, Found: 424.2026.



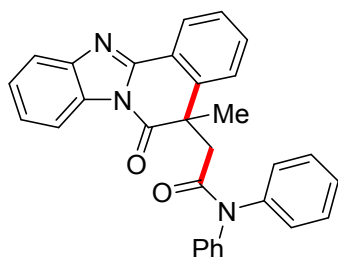
***N*-(*n*-Butyl)-2-(5-methyl-6-oxo-5,6-dihydrobenzo[4,5]imidazo[2,1-*a*]isoquinolin-5-yl)-*N*-phenylacetamide (3ac):** White solid; mp:

107.1–110.2 °C; <sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>) δ: 8.44–8.31 (m, 2H), 7.73 (d, *J* = 7.2 Hz, 1H), 7.41–7.32 (m, 7H), 7.08–7.03 (m, 3H), 3.39–3.26 (m, 3H), 2.82 (d, *J* = 16.8 Hz, 1H), 1.34 (s, 3H), 1.16–1.11 (m, 2H), 0.91 (s, 2H), 0.59 (s, 3H). <sup>13</sup>C NMR (100 Mhz, CDCl<sub>3</sub>) δ: 173.3, 168.4, 149.8, 143.9, 141.92, 141.89, 131.6, 131.1, 129.9, 128.2, 128.1, 127.3, 126.2, 125.3, 125.0, 124.3, 123.0, 119.5, 115.6, 48.7, 47.0, 45.0, 29.6, 29.4, 19.5, 13.5. HRMS (ESI) ([M+Na]<sup>+</sup>) Calcd. For [C<sub>28</sub>H<sub>27</sub>N<sub>3</sub>NaO<sub>2</sub>]<sup>+</sup>: 460.1995, Found: 460.1997.

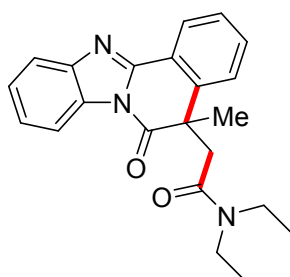


***N*-Benzyl-2-(5-methyl-6-oxo-5,6-dihydrobenzo[4,5]imidazo[2,1-*a*]isoquinolin-5-yl)-*N*-phenylacetamide (3ad):** White solid; mp: 183.6–185.0 °C; <sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>) δ: 8.60–8.57 (m, 1H), 8.44–8.42 (m, 1H), 7.85–7.83 (m, 1H), 7.54–7.52 (m, 2H), 7.44–7.38 (m, 5H), 7.15–7.06 (m, 4H), 6.95–6.93 (m, 2H), 6.71–6.68 (m, 2H), 4.89 (d, *J* = 14.4 Hz, 1H), 4.27 (d, *J* = 14.4 Hz, 1H), 3.55 (d, *J* = 16.4 Hz, 1H), 2.97 (d, *J* = 16.4 Hz, 1H), 1.49 (s, 3H). <sup>13</sup>C NMR (100 MHz, CDCl<sub>3</sub>) δ: 173.4, 169.1, 149.9, 144.0, 141.9, 141.8, 136.8, 131.7, 131.2, 129.8,

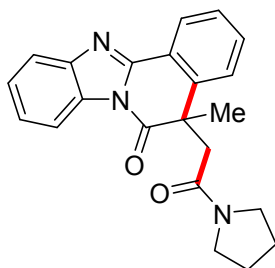
128.4, 128.2, 128.1, 128.0, 127.5, 127.1, 126.3, 125.4, 125.2, 124.6, 123.3, 119.6, 115.7, 52.6, 47.3, 45.2, 29.5. HRMS (ESI) ( $[M+H]^+$ ) Calcd. For  $[C_{31}H_{26}N_3O_2]^+$ : 472.2020, Found: 472.2024.



**2-(5-Methyl-6-oxo-5,6-dihydrobenzo[4,5]imidazo[2,1-*a*]isoquinolin-5-yl)-*N,N*-diphenylacetamide (3ae):** White solid; mp: 180.3–182.4 °C;  $^1H$  NMR (400 MHz,  $CDCl_3$ )  $\delta$ : 8.55 (dd,  $J_1 = 1.6$  Hz,  $J_2 = 8.0$  Hz, 1H), 8.39–8.36 (m, 1H), 7.81–7.79 (m, 1H), 7.58–7.21 (m, 11H), 7.10–7.00 (m, 3H), 6.80 (d,  $J = 8.0$  Hz, 2H), 3.71 (d,  $J = 16.8$  Hz, 1H), 3.15 (d,  $J = 16.8$  Hz, 1H), 1.50 (s, 3H).  $^{13}C$  NMR (100 MHz,  $CDCl_3$ )  $\delta$ : 173.1, 169.3, 149.8, 143.9, 141.8, 131.7, 131.2, 130.1, 128.7, 128.3, 127.5, 126.3, 126.1, 125.9, 125.3, 125.1, 124.3, 123.3, 119.5, 115.5, 47.4, 45.8, 29.6. HRMS (ESI) ( $[M+H]^+$ ) Calcd. For  $[C_{30}H_{24}N_3O_2]^+$ : 458.1863, Found: 458.1861.

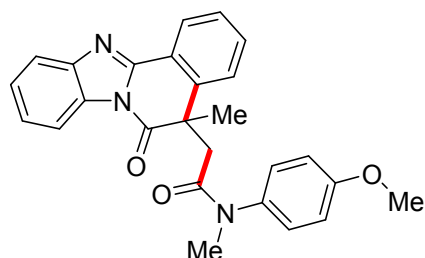


***N,N*-Diethyl-2-(5-methyl-6-oxo-5,6-dihydrobenzo[4,5]imidazo[2,1-*a*]isoquinolin-5-yl)acetamide (3af):** White solid; mp: 173.8–176.4 °C; <sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>) δ: 8.51 (dd, *J*<sub>1</sub> = 1.6 Hz, *J*<sub>2</sub> = 7.6 Hz, 1H), 8.38–8.35 (m, 1H), 7.83–7.80 (m, 1H), 7.51–7.36 (m, 4H), 7.31–7.27 (m, 1H), 3.68 (d, *J* = 16.8 Hz, 1H), 3.36–3.29 (m, 3H), 3.13–3.07 (m, 2H), 1.61 (s, 3H), 1.22 (t, *J* = 7.2 Hz, 3H), 0.83 (t, *J* = 7.2 Hz, 3H). <sup>13</sup>C NMR (100 MHz, CDCl<sub>3</sub>) δ: 173.4, 167.9, 150.0, 144.0, 142.5, 131.7, 131.2, 127.2, 126.3, 125.3, 125.0, 124.1, 123.0, 119.5, 115.6, 46.9, 43.8, 41.8, 39.9, 29.9, 14.3, 12.8. HRMS (ESI) ([M+H]<sup>+</sup>) Calcd. For [C<sub>22</sub>H<sub>24</sub>N<sub>3</sub>O<sub>2</sub>]<sup>+</sup>: 362.1863, Found: 362.1865.



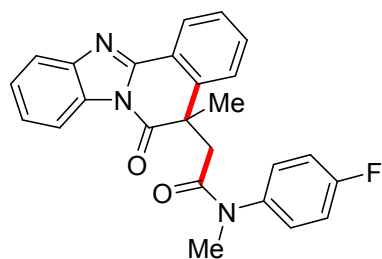
***N,N*-Diethyl-2-(5-methyl-6-oxo-5,6-dihydrobenzo[4,5]imidazo[2,1-*a*]isoquinolin-5-yl)acetamide (3ag):** White solid; mp: 149.5–152.0 °C; <sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>) δ: 8.51 (dd, *J*<sub>1</sub> = 1.6 Hz, *J*<sub>2</sub> = 7.6 Hz, 1H), 8.37–8.35 (m, 1H), 7.83–7.81 (m, 1H), 7.52–7.31 (m, 5H), 3.63 (d, *J* = 16.8 Hz, 1H), 3.49–3.37 (m, 2H), 3.27–3.19 (m, 2H), 3.14–3.07 (m, 1H), 1.90 (p, *J* = 6.8 Hz, 2H), 1.78–1.67 (m, 2H), 1.62 (s, 3H). <sup>13</sup>C NMR (100 MHz, CDCl<sub>3</sub>) δ: 173.5, 167.2, 150.0, 144.0, 142.3, 131.6, 131.3, 127.2, 126.3, 125.3, 125.0, 124.4, 123.0, 119.5, 115.6, 46.5, 46.4, 45.38, 45.35,

29.9, 25.9, 24.1. HRMS (ESI) ( $[M+H]^+$ ) Calcd. For  $[C_{22}H_{22}N_3O_2]^+$ :  
360.1707, Found: 360.1708.



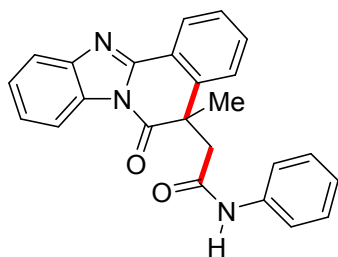
***N*-(4-Methoxyphenyl)-*N*-methyl-2-(5-methyl-6-oxo-5,6-dihydrobenzo[4,5]imidazo[2,1-*a*]isoquinolin-5-yl)acetamide (3ah):**

White solid; mp: 165.0–168.4 °C;  $^1H$  NMR (400 MHz,  $CDCl_3$ )  $\delta$  8.52 (dd,  $J_1 = 1.6$  Hz,  $J_2 = 7.6$  Hz, 1H), 8.41–8.39 (m, 1H), 7.84–7.82 (m, 1H), 7.53–7.39 (m, 4H), 7.16–7.11 (m, 3H), 7.01–6.99 (m, 2H), 3.86 (s, 3H), 3.47 (d,  $J = 16.8$  Hz, 1H), 3.01 (d,  $J = 16.8$  Hz, 1H), 2.95 (s, 3H), 1.45 (s, 3H).  $^{13}C$  NMR (100 MHz,  $CDCl_3$ )  $\delta$ : 173.6, 169.4, 159.3, 150.0, 144.1, 142.2, 136.2, 131.8, 131.4, 128.4, 127.5, 126.4, 125.5, 125.2, 124.5, 123.2, 119.7, 115.7, 115.3, 55.6, 47.1, 45.0, 37.3, 29.9. HRMS (ESI) ( $[M+H]^+$ ) Calcd. For  $[C_{26}H_{24}N_3O_3]^+$ : 426.1812, Found: 426.1811.



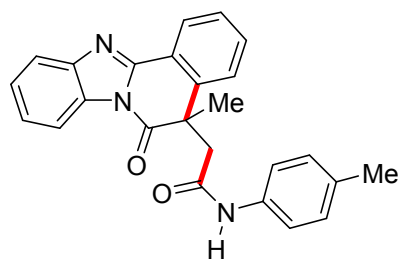
***N*-(4-Fluorophenyl)-*N*-methyl-2-(5-methyl-6-oxo-5,6-dihydrobenzo[4,5]imidazo[2,1-*a*]isoquinolin-5-yl)acetamide (3ai):**

White solid; mp: 195.5–196.3 °C; <sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>) δ: 8.52 (dd, *J*<sub>1</sub> = 1.6 Hz, *J*<sub>2</sub> = 8.0 Hz, 1H), 8.40–8.38 (m, 1H), 7.84–7.82 (m, 1H), 7.53–7.37 (m, 4H), 7.19 (d, *J* = 6.8 Hz, 4H), 7.13 (d, *J* = 7.6 Hz, 1H), 3.46 (d, *J* = 16.8 Hz, 1H), 2.99–2.95 (m, 4H), 1.47 (s, 3H). <sup>13</sup>C NMR (100 MHz, CDCl<sub>3</sub>) δ: 173.3, 168.9, 163.4 (*J* = 247.0 Hz), 149.8, 143.9, 141.9, 139.3 (*J* = 3.5 Hz), 131.6, 131.3, 129.0 (*J* = 8.5 Hz), 127.4, 126.3, 125.4, 125.1, 124.2, 123.0, 119.5, 117.0 (*J* = 22.6 Hz), 115.5, 46.9, 44.9, 37.1, 29.7. <sup>19</sup>F NMR (377 MHz, CDCl<sub>3</sub>) δ: –112.38. HRMS (ESI) ([*M*+*H*]<sup>+</sup>) Calcd. For [C<sub>25</sub>H<sub>21</sub>FN<sub>3</sub>O<sub>2</sub>]<sup>+</sup>: 414.1612, Found: 414.1614.



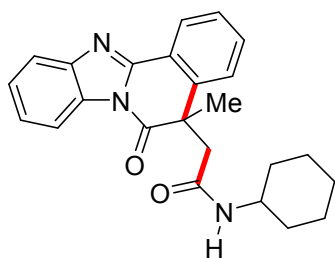
**2-(5-Methyl-6-oxo-5,6-dihydrobenzo[4,5]imidazo[2,1-*a*]isoquinolin-5-yl)-*N*-phenylacetamide (3aj):** White solid; mp: 165.5–165.9 °C; <sup>1</sup>H NMR (400 MHz, DMSO-*d*<sub>6</sub>) δ: 10.11 (s, 1H), 8.39 (d, *J* = 7.6 Hz, 1H), 8.33–8.30 (m, 1H), 7.88–7.86 (m, 1H), 7.73 (d, *J* = 7.6 Hz, 1H), 7.65–7.61 (m, 1H), 7.53–7.44 (m, 3H), 7.30 (d, *J* = 8.0 Hz, 2H), 7.17–7.13 (m, 2H), 6.94 (t, *J* = 7.2 Hz, 1H), 3.68 (d, *J* = 16.8 Hz, 1H), 3.55 (d, *J* = 16.8 Hz, 1H), 1.66 (s, 3H). <sup>13</sup>C NMR (100 MHz, DMSO-*d*<sub>6</sub>) δ:

173.2, 168.0, 149.9, 143.7, 142.1, 138.4, 131.8, 131.3, 128.6, 127.5, 125.9, 125.5, 125.20, 125.16, 123.3, 122.4, 119.6, 118.9, 115.1, 46.8, 46.2, 29.0. HRMS (ESI) ( $[M+H]^+$ ) Calcd. For  $[C_{24}H_{20}N_3O_2]^+$ : 382.1550, Found: 382.1549.



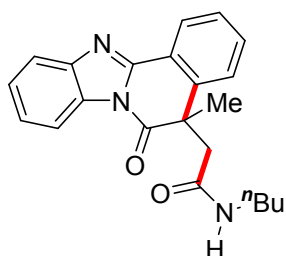
**2-(5-Methyl-6-oxo-5,6-dihydrobenzo[4,5]imidazo[2,1-a]isoquinolin-5-yl)-N-(p-tolyl)acetamide (3ak):** White solid; mp: 204.2–205.8 °C;  $^1H$  NMR (400 MHz,  $CDCl_3$ )  $\delta$ : 8.57 (s, 1H), 8.43–8.40 (m, 2H), 7.77–7.75 (m, 1H), 7.42–7.33 (m, 4H), 7.10 (d,  $J = 7.6$  Hz, 1H), 6.98 (d,  $J = 8.4$  Hz, 2H), 6.78 (d,  $J = 8.0$  Hz, 2H), 3.56 (d,  $J = 16.4$  Hz, 1H), 2.98 (d,  $J = 16.4$  Hz, 1H), 2.14 (s, 3H), 1.43 (s, 3H).  $^{13}C$  NMR (100 MHz,  $CDCl_3$ )  $\delta$ : 173.0, 167.6, 149.9, 143.6, 141.7, 134.8, 133.6, 131.7, 131.5, 129.1, 127.6, 126.0, 125.6, 125.4, 124.9, 122.5, 119.7, 119.4, 115.7, 46.5, 46.0, 29.8, 20.7. HRMS (ESI) ( $[M+H]^+$ ) Calcd. For  $[C_{25}H_{22}N_3O_2]^+$ : 396.1707, Found: 396.1704.





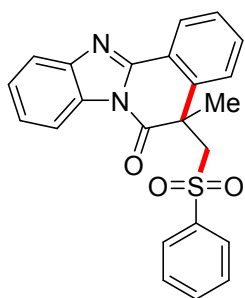
***N*-Cyclohexyl-2-(5-methyl-6-oxo-5,6-dihydrobenzo[4,5]imidazo[2,1-*a*]isoquinolin-5-yl)acetamide (3a):**

White solid; mp: 226.7–228.3 °C; <sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>) δ: 8.49 (dd, *J*<sub>1</sub> = 1.6 Hz, *J*<sub>2</sub> = 7.2 Hz, 1H), 8.42–8.40 (m, 1H), 7.83–7.81 (m, 1H), 7.51–7.39 (m, 4H), 7.34 (d, *J* = 7.6 Hz, 1H), 5.84 (d, *J* = 8.4 Hz, 1H), 3.57 (d, *J* = 15.6 Hz, 1H), 3.42–3.33 (m, 1H), 2.92 (d, *J* = 15.6 Hz, 1H), 1.69–1.40 (m, 8H), 1.26–0.76 (m, 6H). <sup>13</sup>C NMR (100 MHz, CDCl<sub>3</sub>) δ: 173.0, 167.8, 149.8, 143.9, 141.5, 131.6, 131.3, 127.5, 126.1, 125.5, 125.2, 125.0, 122.8, 119.5, 115.7, 48.0, 46.8, 46.6, 32.75, 32.69, 29.5, 25.2, 24.62, 24.55. HRMS (ESI) ([M+H]<sup>+</sup>) Calcd. For [C<sub>24</sub>H<sub>26</sub>N<sub>3</sub>O<sub>2</sub>]: 388.2020, Found: 388.2027.



***N*-Butyl-2-(5-methyl-6-oxo-5,6-dihydrobenzo[4,5]imidazo[2,1-*a*]isoquinolin-5-yl)acetamide (3am):** White solid; mp: 154.1–155.9 °C;

$^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ )  $\delta$ : 8.48 (dd,  $J_1 = 1.6$  Hz,  $J_2 = 7.2$  Hz, 1H), 8.41–8.38 (m, 1H), 7.82–7.80 (m, 1H), 7.49–7.40 (m, 4H), 7.34 (dd,  $J_1 = 1.6$  Hz,  $J_2 = 7.6$  Hz, 1H), 5.92–5.89 (m, 1H), 3.58 (d,  $J = 15.6$  Hz, 1H), 2.97–2.86 (m, 3H), 1.59 (s, 3H), 1.18–1.11 (m, 2H), 1.07–1.00 (m, 2H), 0.71 (t,  $J = 7.2$  Hz, 3H).  $^{13}\text{C}$  NMR (100 MHz,  $\text{CDCl}_3$ )  $\delta$ : 173.1, 168.7, 149.8, 143.9, 141.4, 131.6, 131.4, 127.5, 126.1, 125.5, 125.3, 125.0, 122.9, 119.5, 115.7, 46.8, 46.4, 39.0, 31.2, 29.6, 19.6, 13.5. HRMS (ESI) ( $[\text{M}+\text{H}]^+$ ) Calcd. For  $[\text{C}_{22}\text{H}_{24}\text{N}_3\text{O}_2]^+$ : 362.1863, Found: 362.1872.

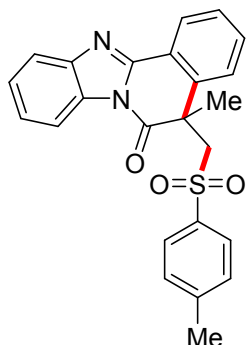


**5-Methyl-5-((phenylsulfonyl)methyl)benzo[4,5]imidazo[2,1-**

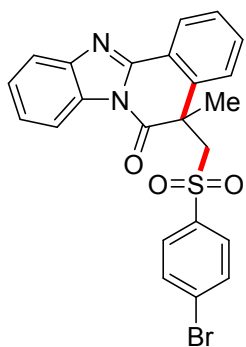
***a*]isoquinolin-6(5*H*)-one (5a):** White solid; mp: 186.8–189.9 °C;

$^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ )  $\delta$ : 8.50 (dd,  $J_1 = 1.6$  Hz,  $J_2 = 8.0$  Hz, 1H), 8.35–8.33 (m, 1H), 7.85–7.83 (m, 1H), 7.48–7.37 (m, 6H), 7.27–7.22 (m, 3H), 7.15 (d,  $J = 8.0$  Hz, 1H), 4.55 (d,  $J = 14.8$  Hz, 1H), 4.04 (d,  $J = 14.8$  Hz, 1H), 1.67 (s, 3H).  $^{13}\text{C}$  NMR (100 MHz,  $\text{CDCl}_3$ )  $\delta$ : 170.6, 149.2, 143.8, 139.6, 137.0, 133.3, 131.4, 131.2, 128.9, 128.4, 127.5, 126.6, 126.1, 126.0, 125.6, 122.8, 119.8, 115.7,

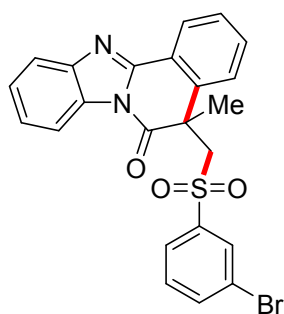
64.4, 46.8, 31.0. HRMS (ESI) ( $[M+Na]^+$ ) Calcd. For  $[C_{23}H_{18}N_2NaO_3S]^+$ : 425.0930, Found: 425.0937.



**5-Methyl-5-(tosylmethyl)benzo[4,5]imidazo[2,1-*a*]isoquinolin-6(5*H*)-one (5b):** White solid; mp: 188.7–189.8 °C;  $^1H$  NMR (400 MHz,  $CDCl_3$ )  $\delta$ : 8.51–8.48 (m, 1H), 8.26–8.23 (m, 1H), 7.83–7.81 (m, 1H), 7.49–7.35 (m, 4H), 7.30–7.26 (m, 4H), 6.99–6.97 (m, 2H), 4.54 (d,  $J = 14.8$  Hz, 1H), 3.99 (d,  $J = 14.8$  Hz, 1H), 2.14 (s, 3H), 1.67 (s, 3H).  $^{13}C$  NMR (100 MHz,  $CDCl_3$ )  $\delta$ : 170.4, 149.2, 144.8, 143.9, 137.1, 136.1, 131.4, 131.3, 129.5, 128.4, 127.9, 127.0, 126.1, 126.0, 125.6, 122.8, 119.8, 115.7, 64.4, 46.9, 31.5, 21.3. HRMS (ESI) ( $[M+Na]^+$ ) Calcd. For  $[C_{24}H_{20}N_2NaO_3S]^+$ : 439.1087, Found: 439.1089.



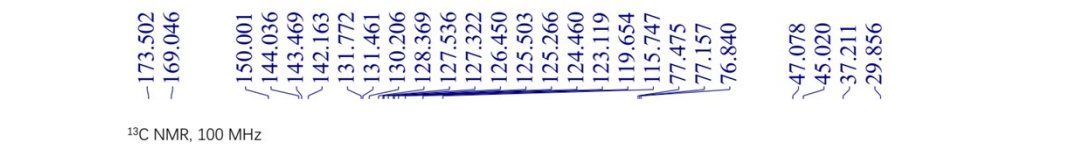
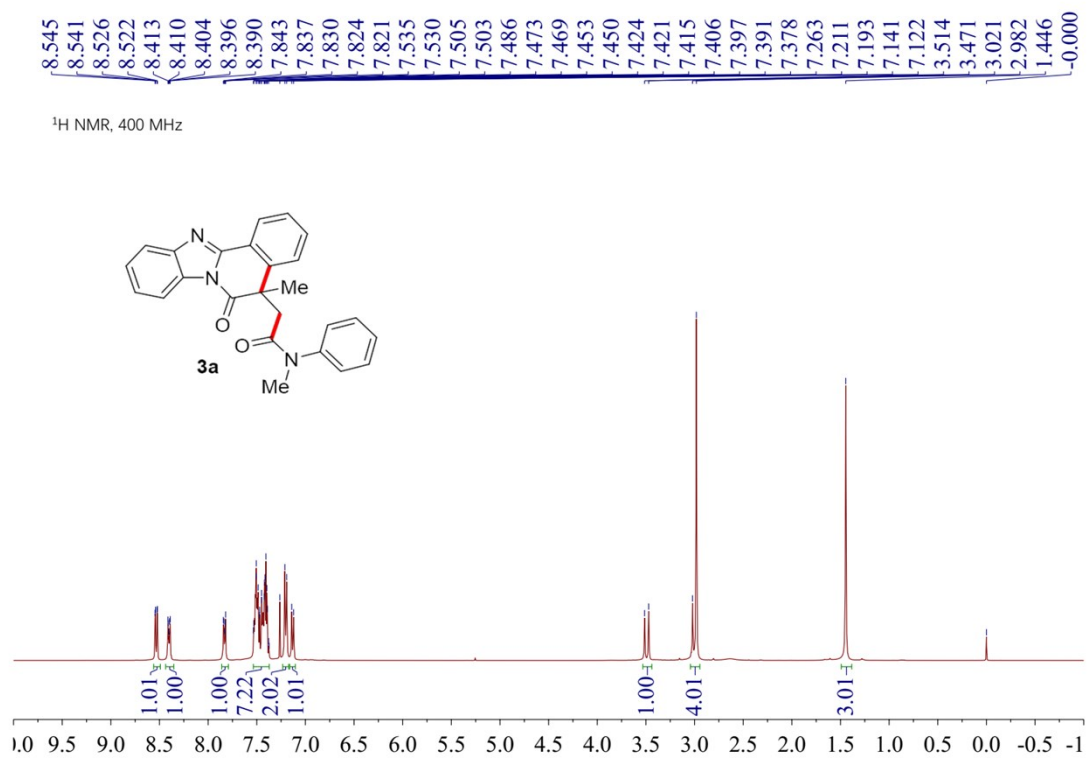
**5-(((4-Bromophenyl)sulfonyl)methyl)-5-methylbenzo[4,5]imidazo[2,1-*a*]isoquinolin-6(5*H*)-one (5c):** White solid; mp: 216.8–218.8 °C; <sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>) δ: 8.51–8.49 (m, 1H), 8.31–8.29 (m, 1H), 7.85–7.83 (m, 1H), 7.49–7.43 (m, 3H), 7.39–7.35 (m, 2H), 7.32–7.23 (m, 3H), 7.16 (d, *J* = 7.6 Hz, 1H), 4.52 (d, *J* = 14.8 Hz, 1H), 4.00 (d, *J* = 14.8 Hz, 1H), 1.67 (s, 3H). <sup>13</sup>C NMR (100 MHz, CDCl<sub>3</sub>) δ: 170.4, 149.0, 143.8, 138.5, 136.9, 132.2, 131.34, 131.28, 129.1, 128.9, 128.4, 126.6, 126.2, 126.1, 125.9, 122.9, 119.9, 115.7, 64.5, 46.8, 31.1. HRMS (ESI) ([*M*+*H*]<sup>+</sup>) Calcd. For [C<sub>23</sub>H<sub>18</sub>BrN<sub>2</sub>O<sub>3</sub>S]<sup>+</sup>: 481.0216, Found: 481.0221.

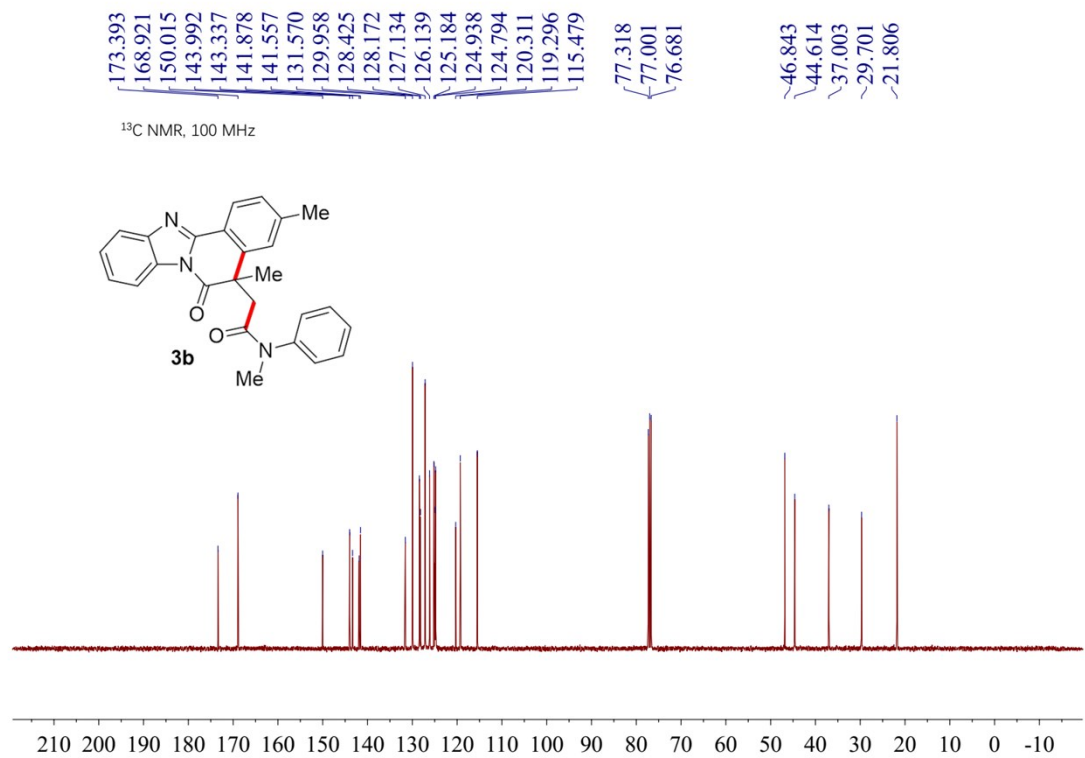
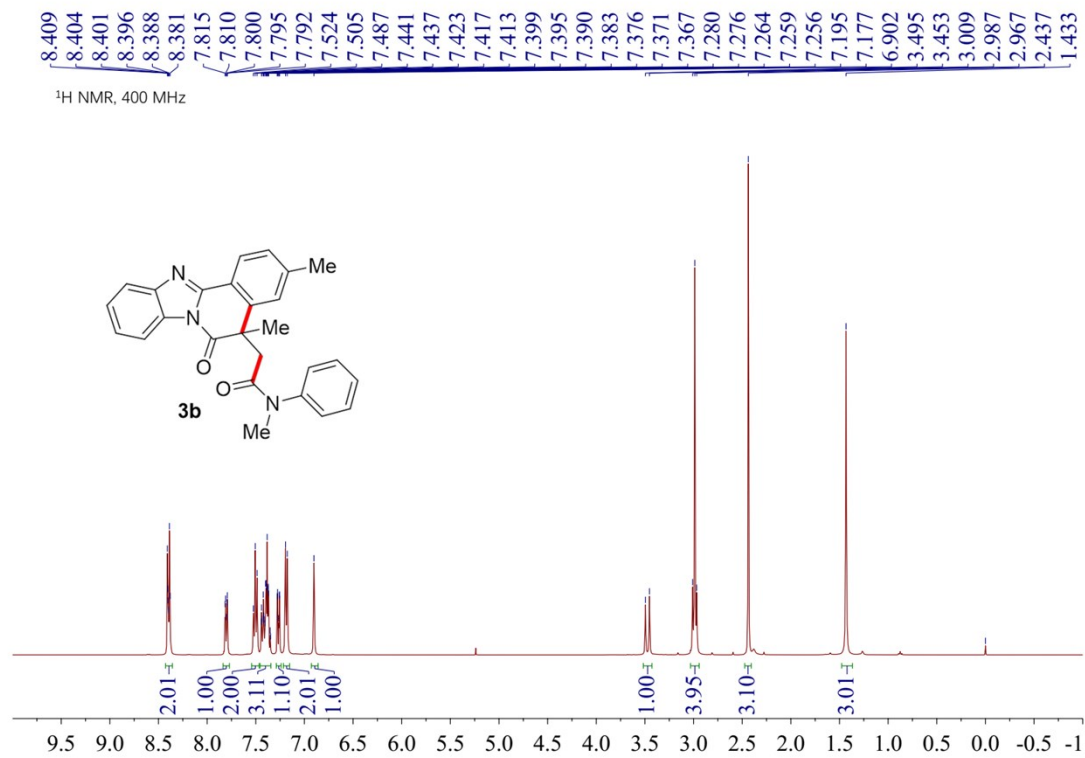


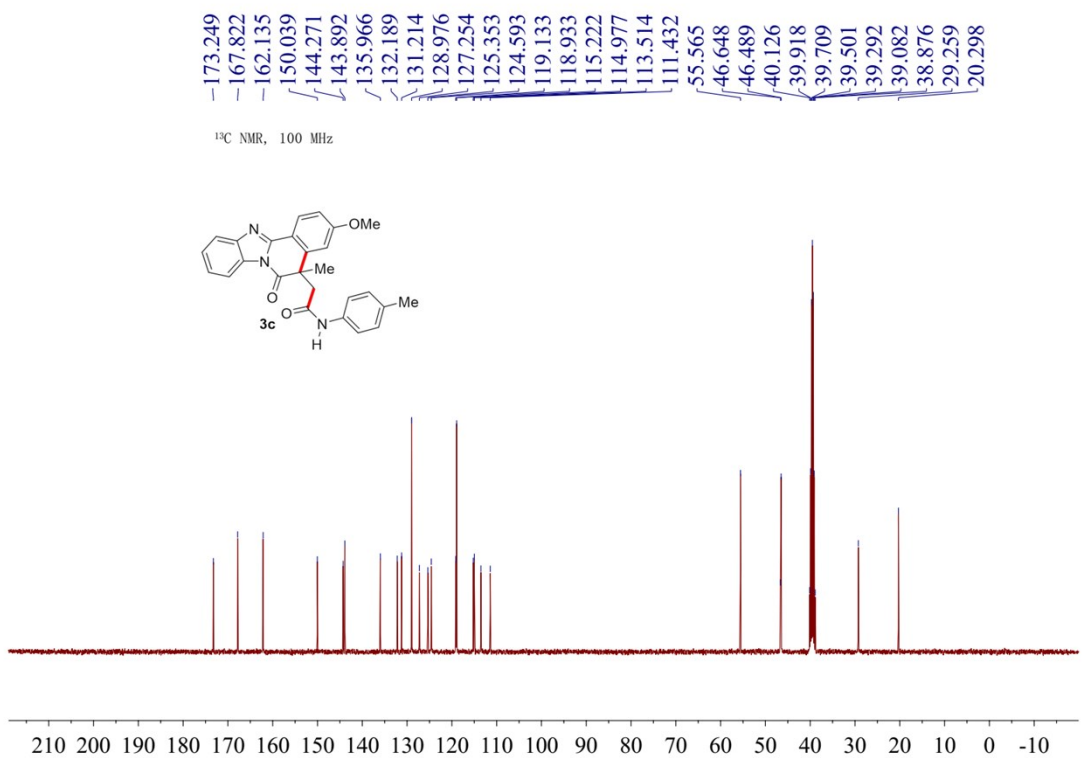
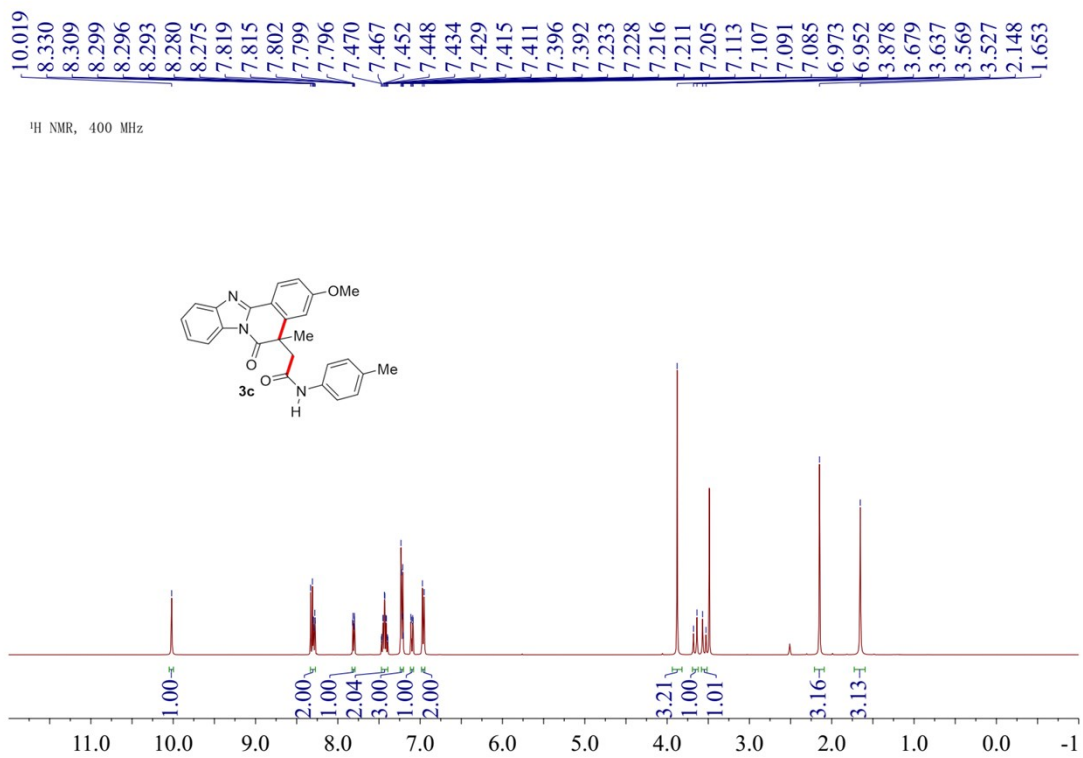
**5-(((3-Bromophenyl)sulfonyl)methyl)-5-methylbenzo[4,5]imidazo[2,1-*a*]isoquinolin-6(5*H*)-one (5d):** White solid; mp: 170.6–172.9 °C; <sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>) δ: 8.52 (dd, *J*<sub>1</sub> = 1.2 Hz, *J*<sub>2</sub> = 8.0 Hz, 1H), 8.36–8.34 (m, 1H), 7.85–7.83 (m, 1H), 7.51–7.36 (m, 6H), 7.22–7.18 (m, 1H), 7.15–7.08 (m, 2H), 4.54 (d, *J* = 14.8 Hz, 1H), 4.03 (d, *J* = 14.8 Hz, 1H), 1.66 (s, 3H). <sup>13</sup>C NMR (100 MHz, CDCl<sub>3</sub>) δ: 170.4, 149.0, 143.8, 141.4, 136.6, 136.4, 131.4, 131.0, 130.44, 130.42, 128.7, 126.4, 126.1, 126.01, 125.96, 125.7, 122.91, 122.88, 119.8, 115.7,

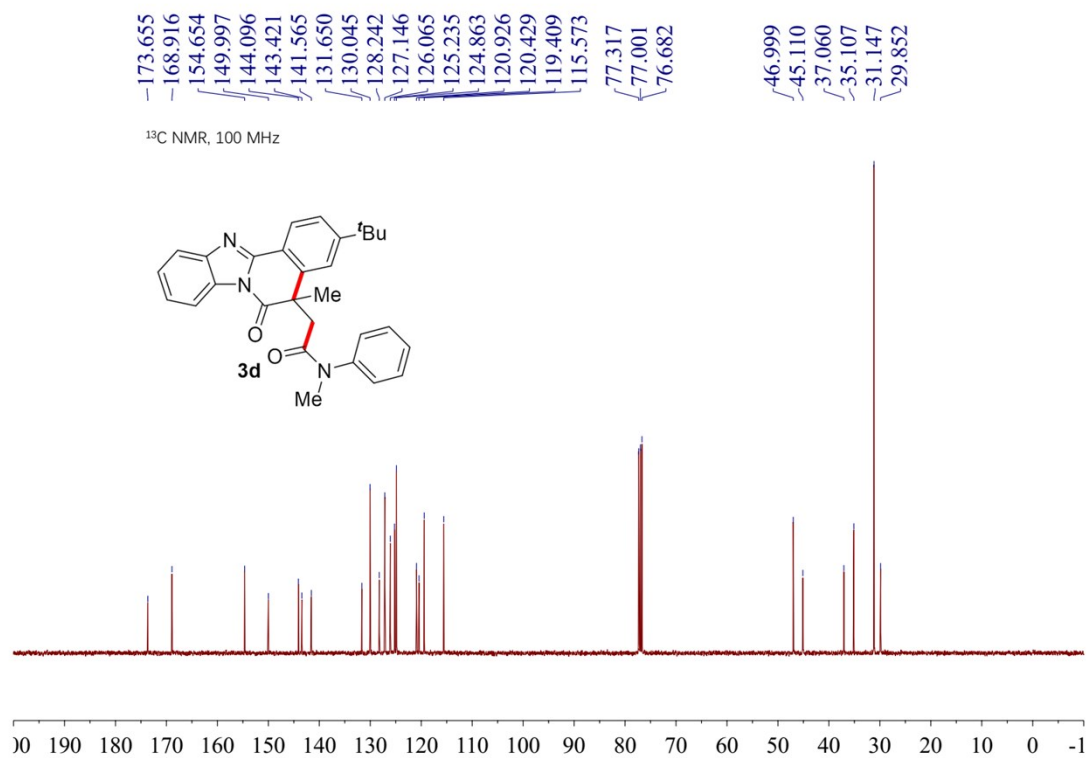
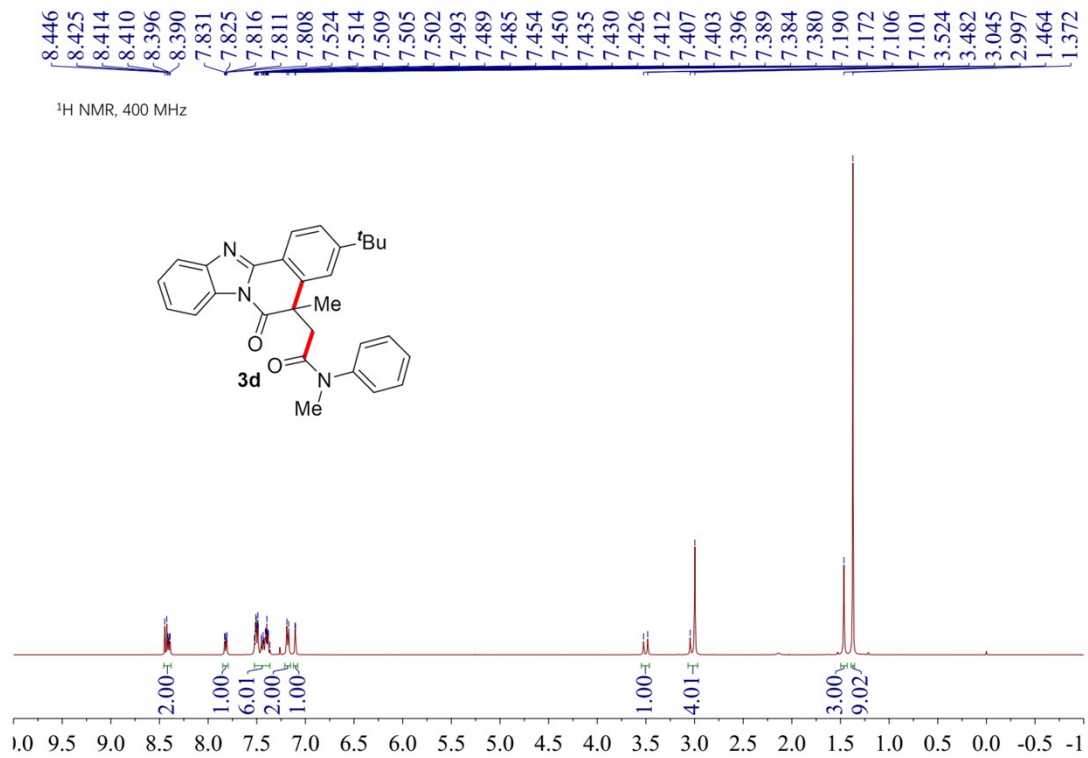
64.6, 46.8, 30.8. HRMS (ESI) ( $[M+Na]^+$ ) Calcd. For  $[C_{23}H_{17}BrN_2NaO_3S]^+$ : 503.0035, Found: 503.0039.

## 6. $^1H$ and $^{13}C$ NMR spectra of the products

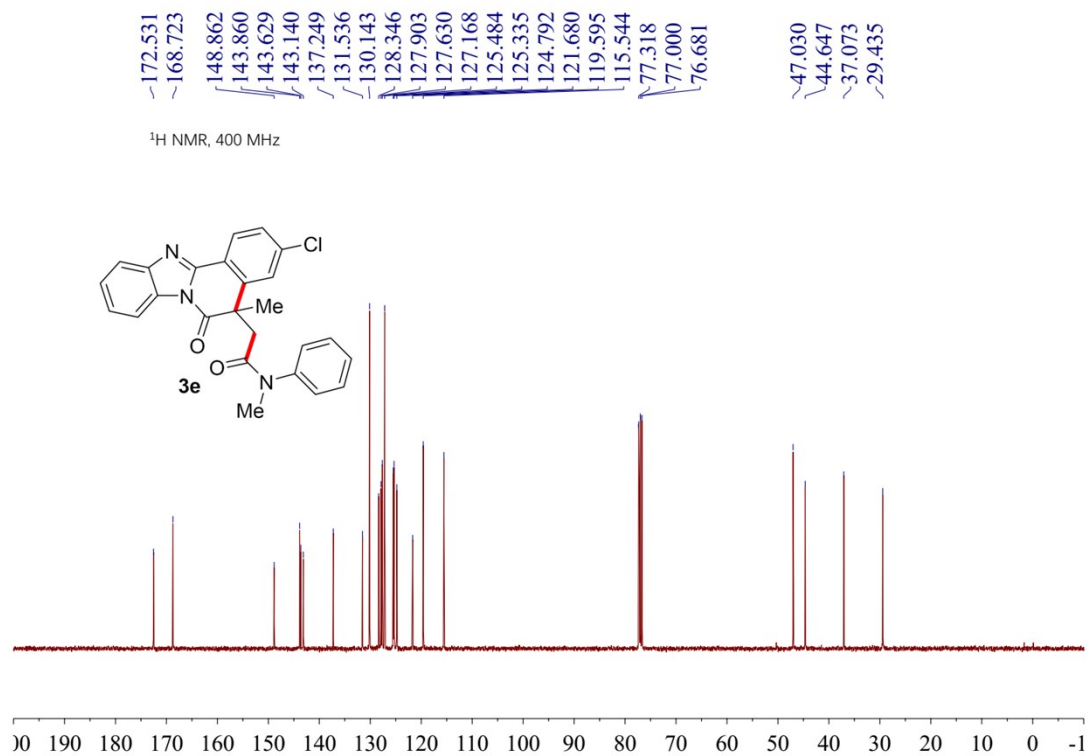
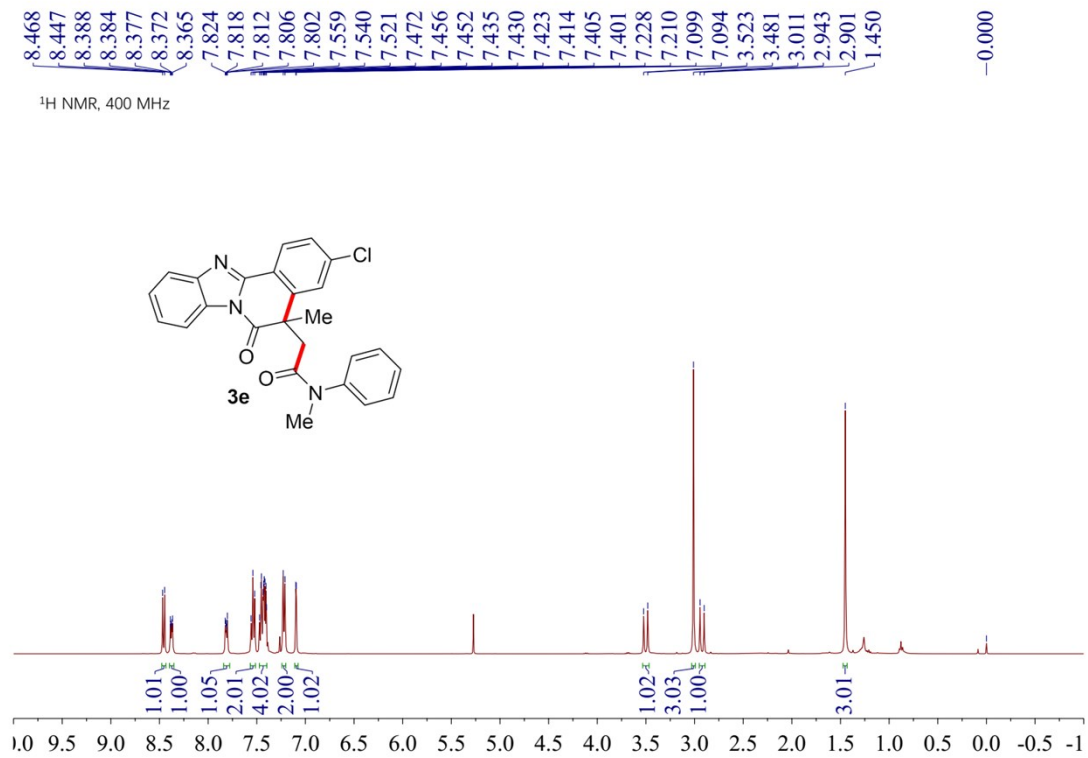


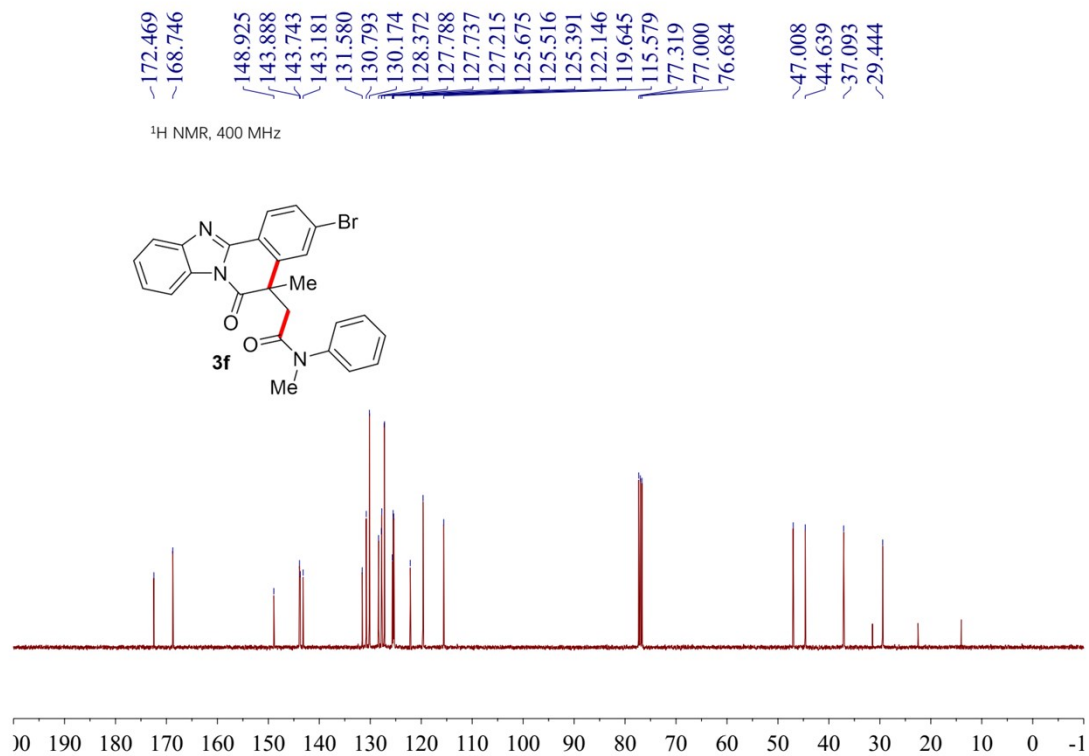
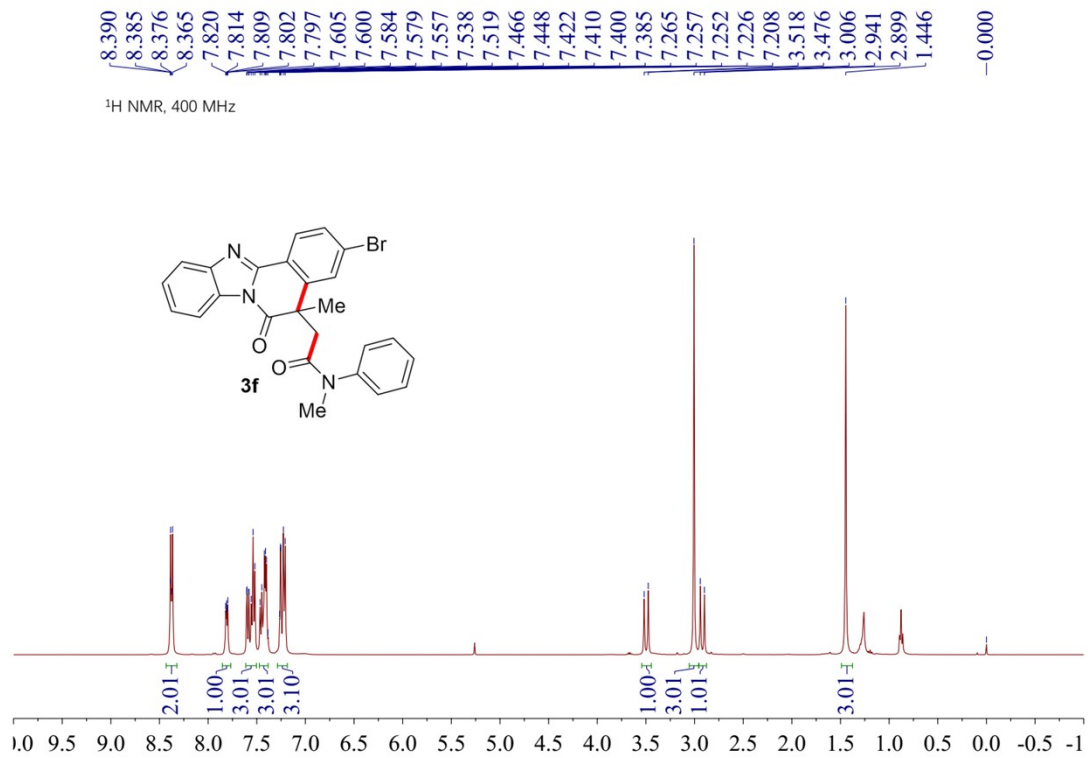


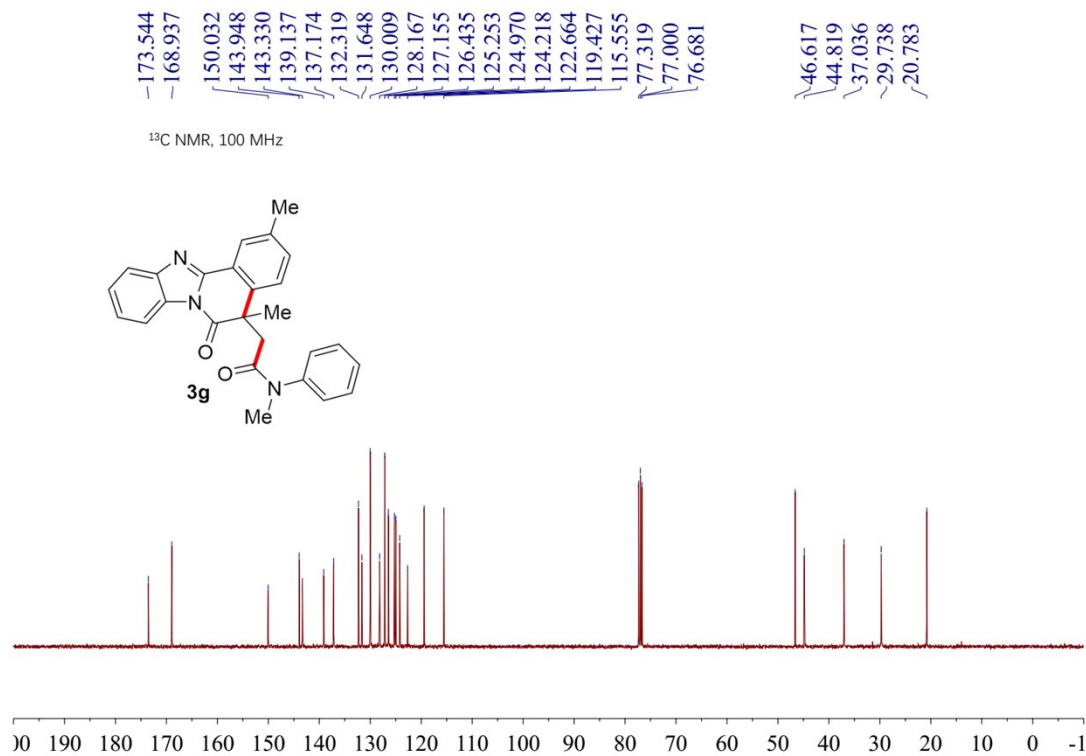
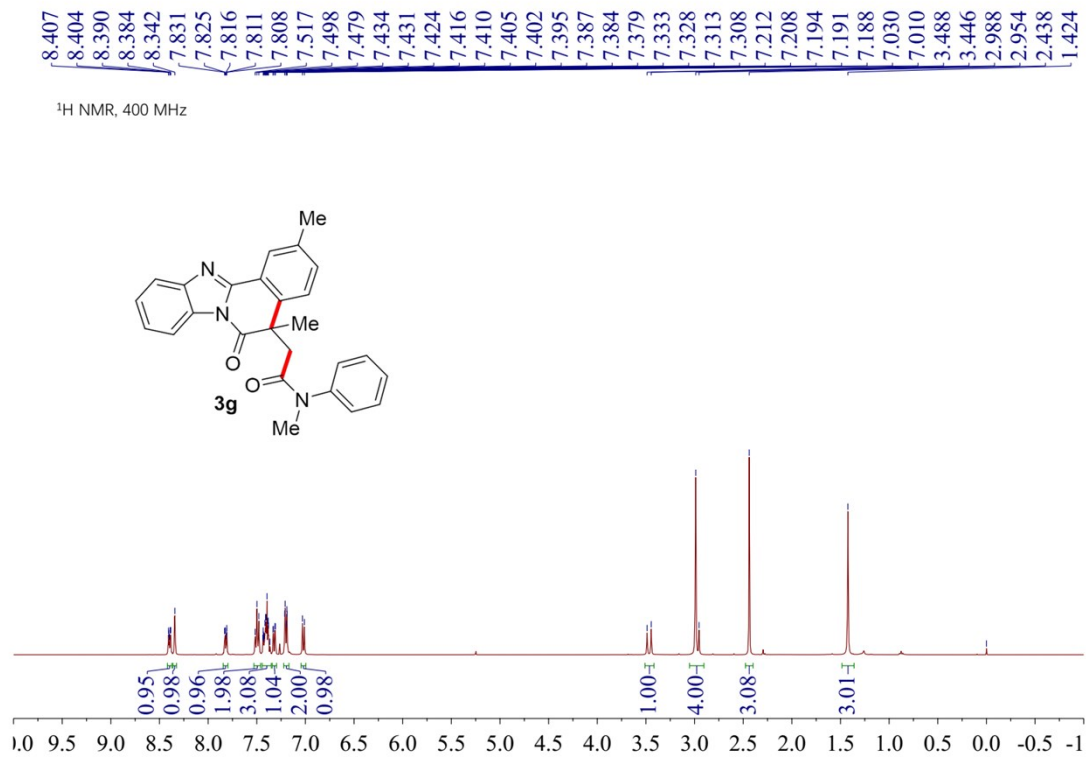


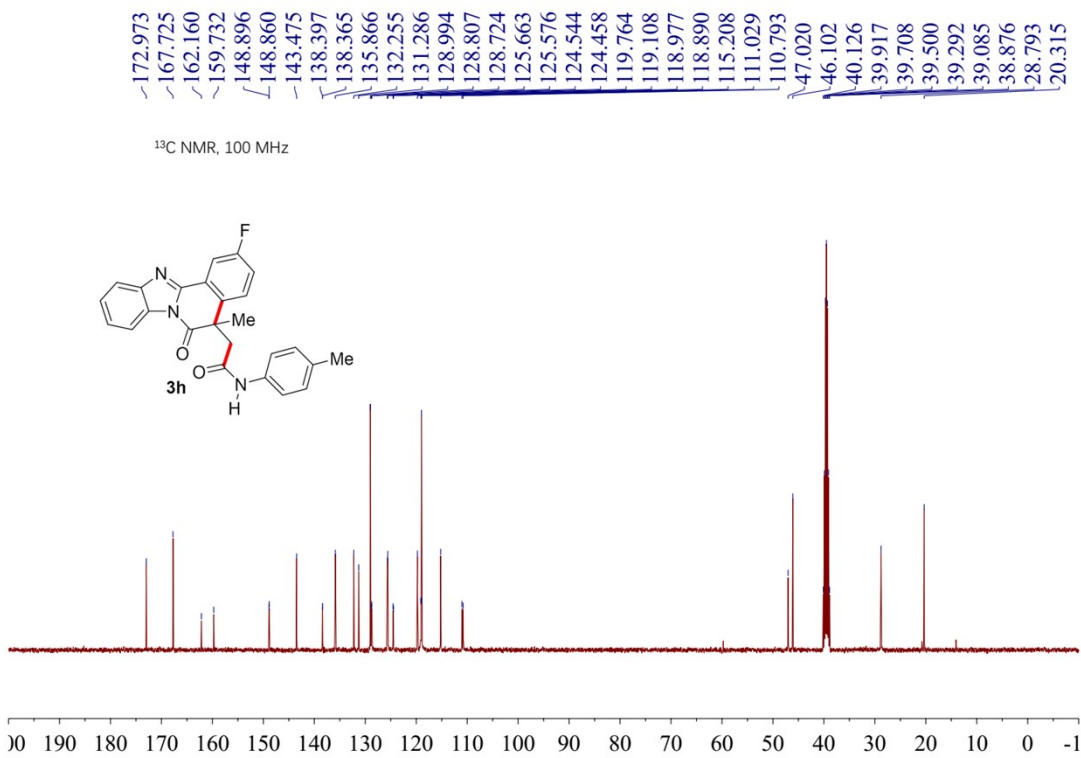
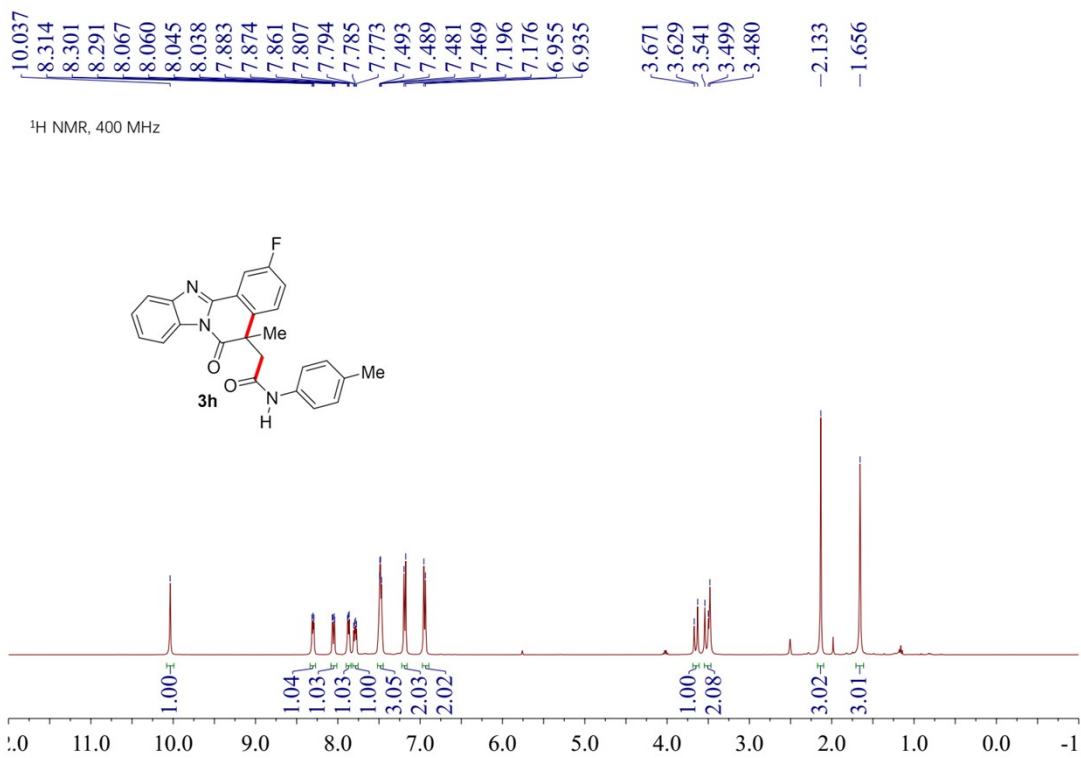




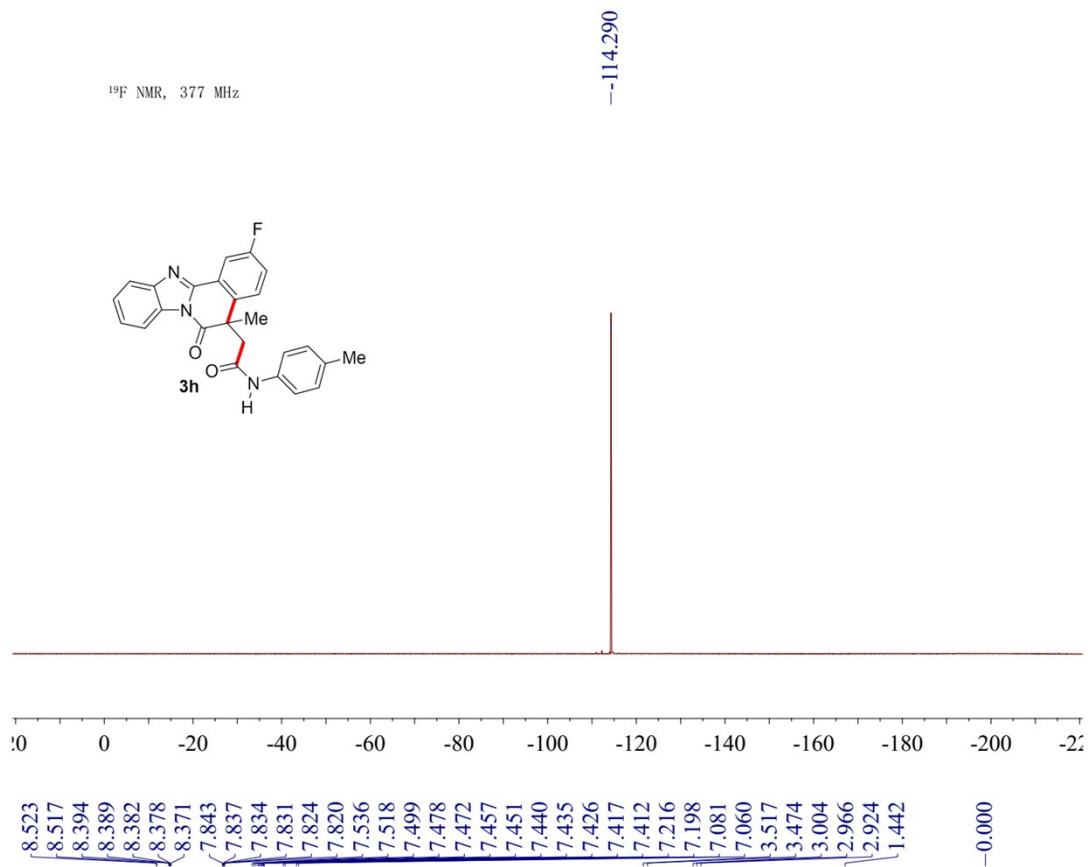
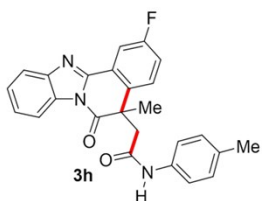




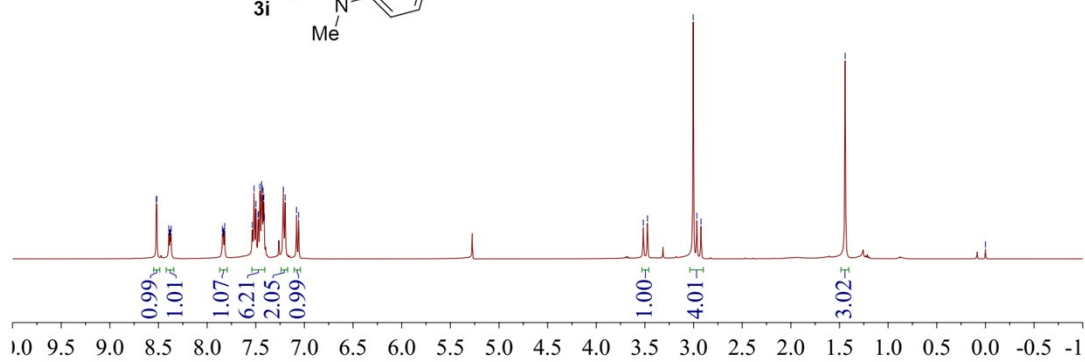
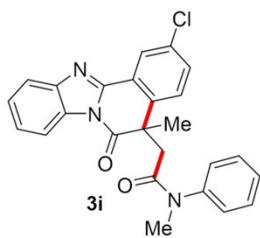


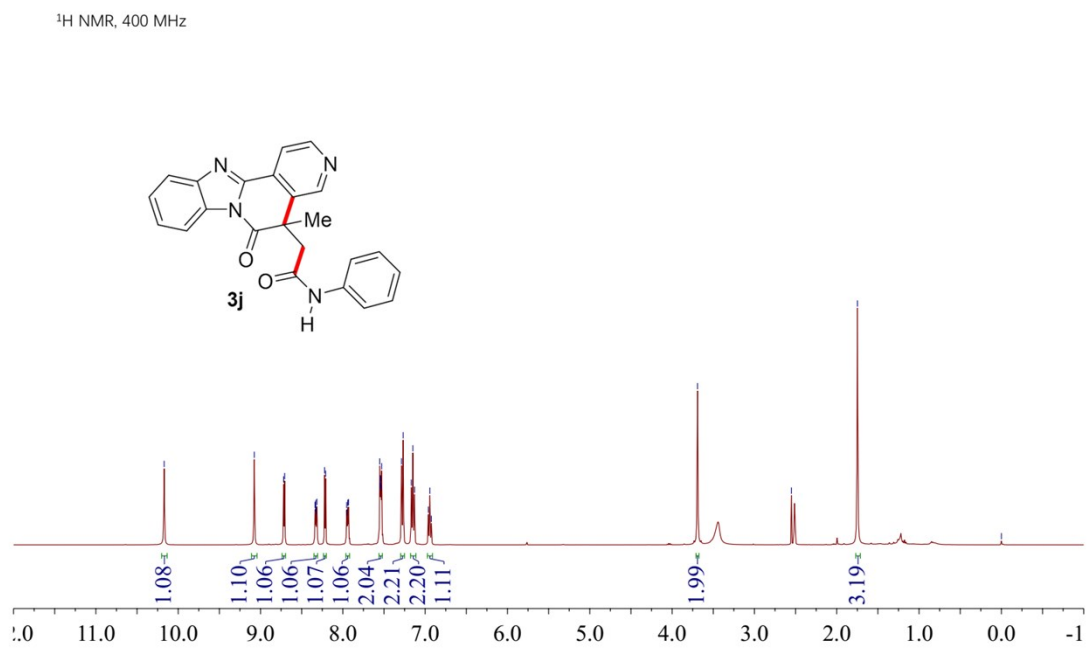
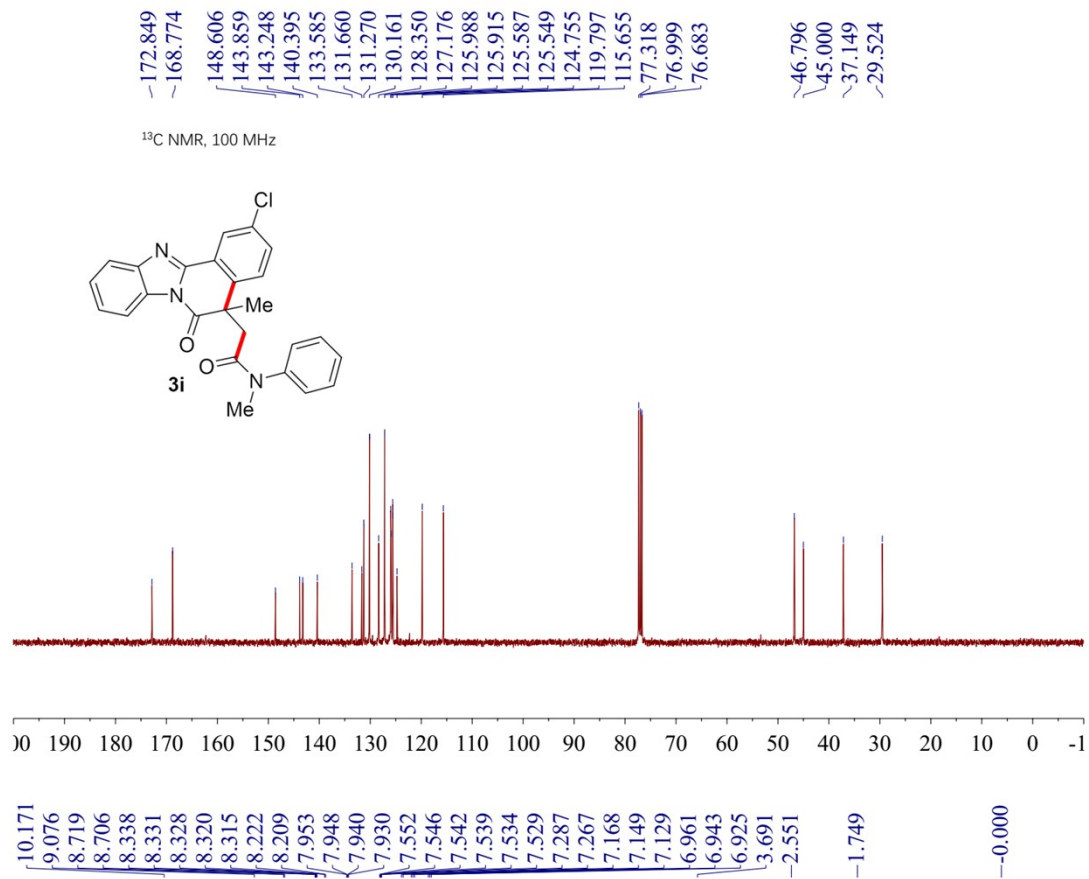


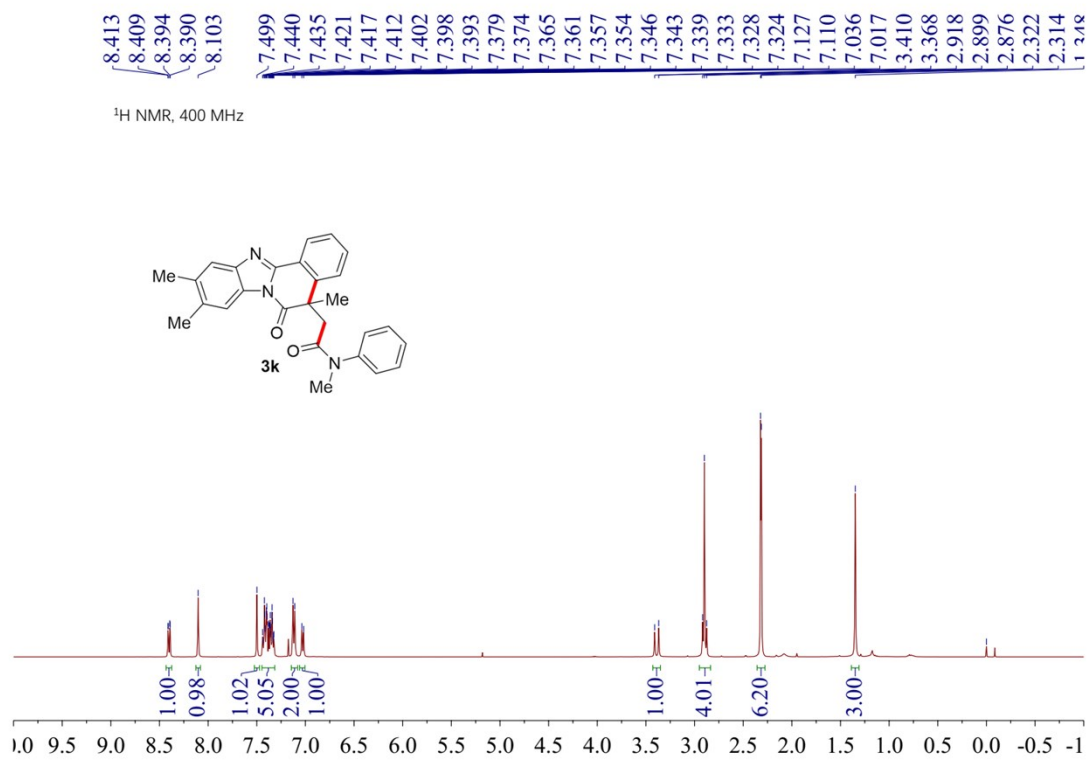
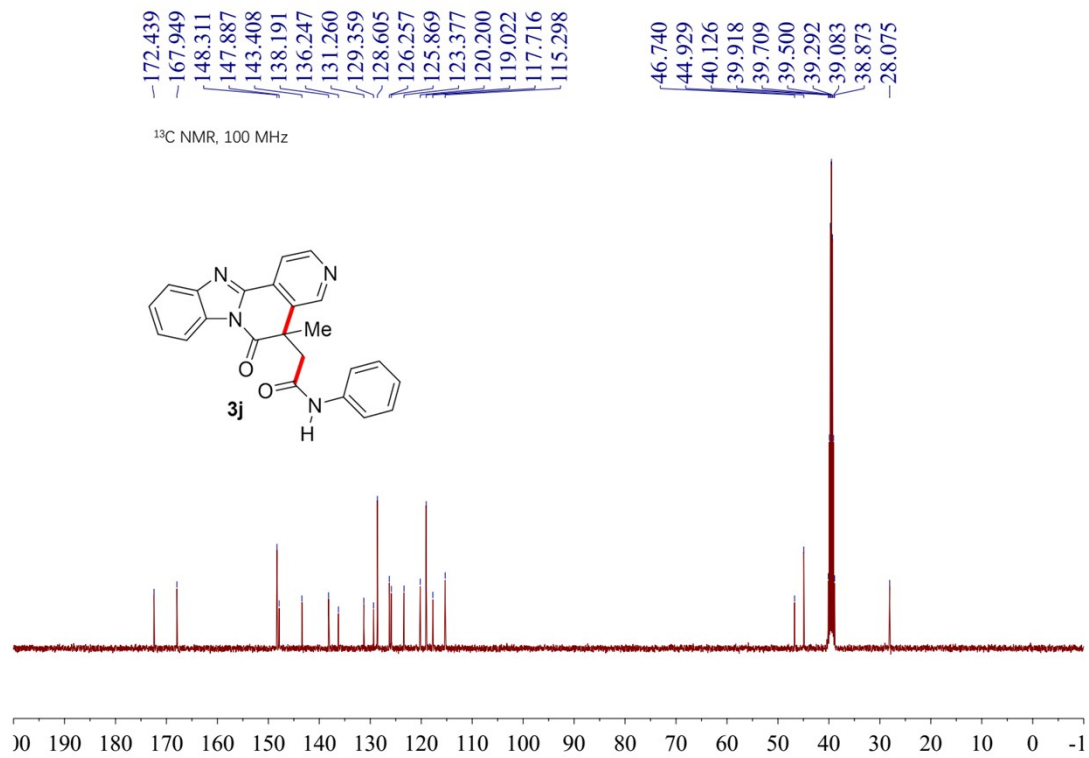
<sup>19</sup>F NMR, 377 MHz

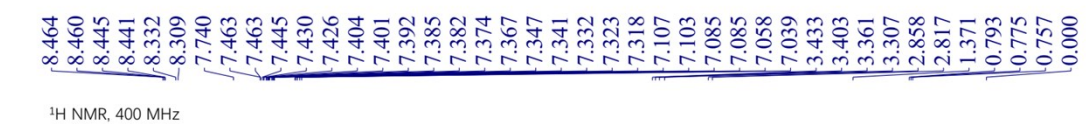
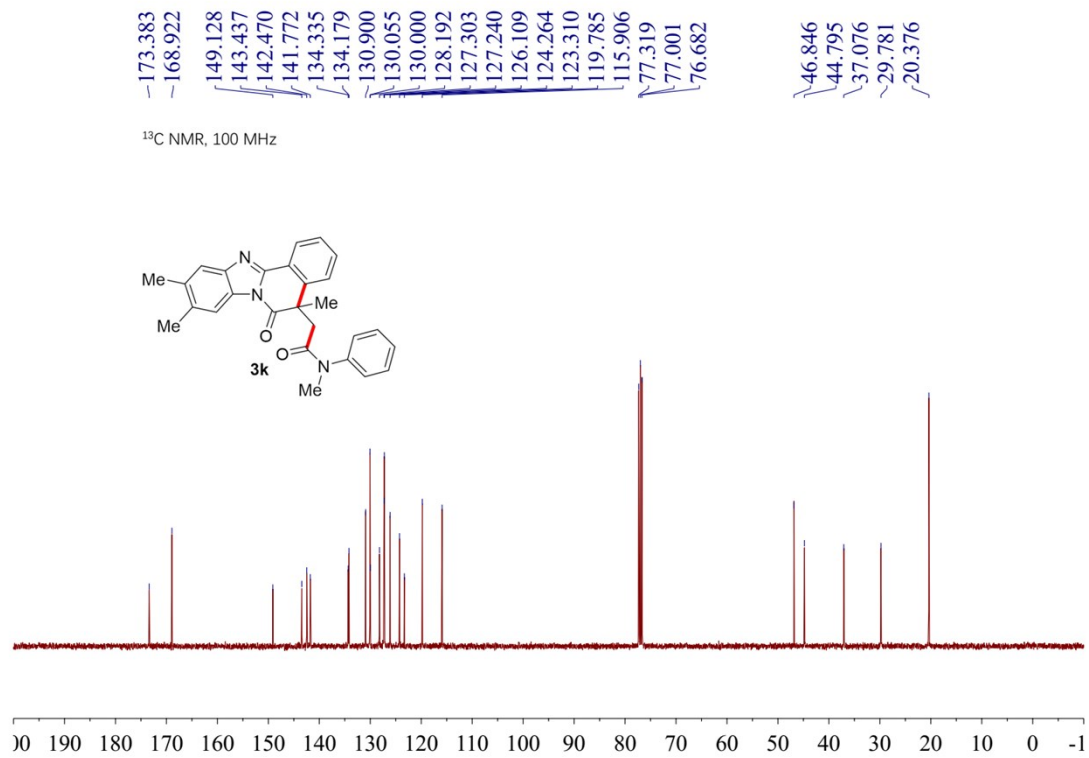


<sup>1</sup>H NMR, 400 MHz

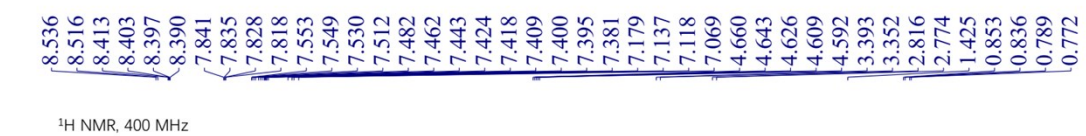
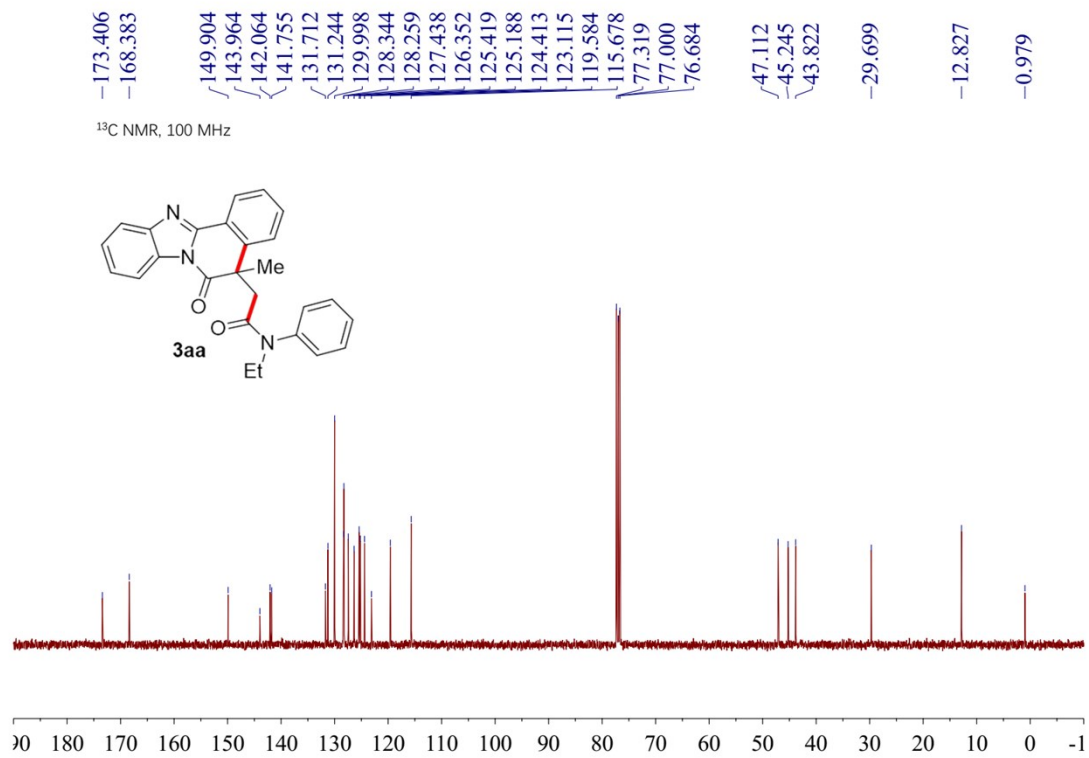


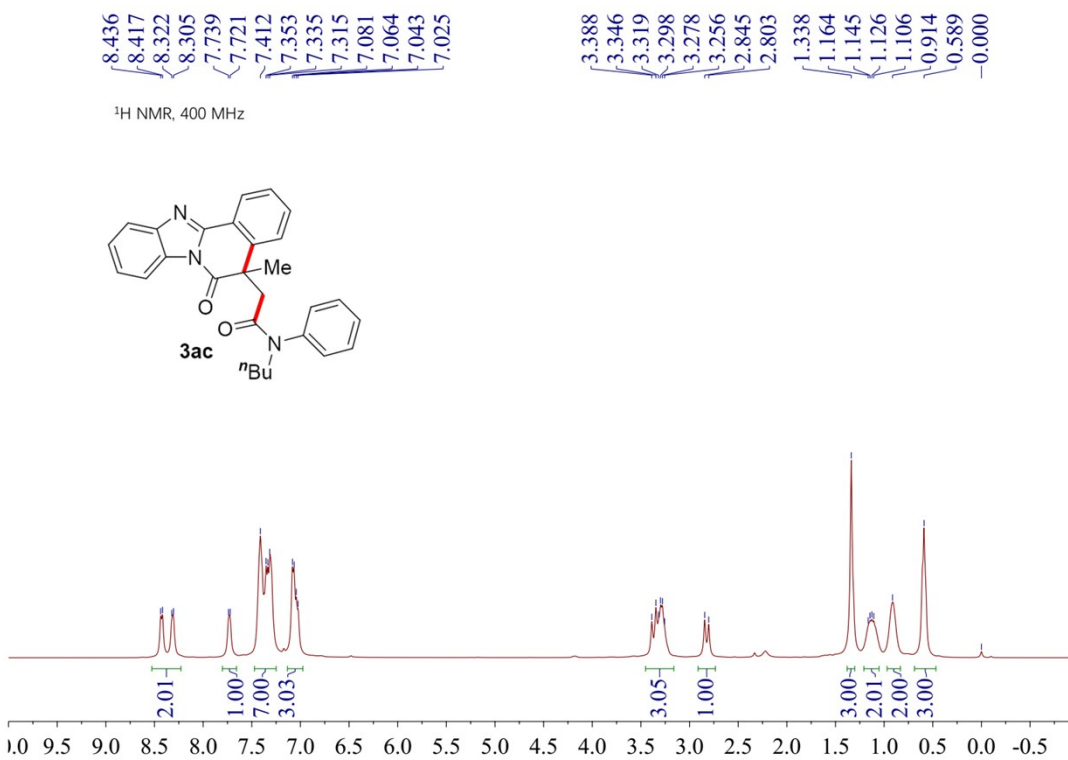
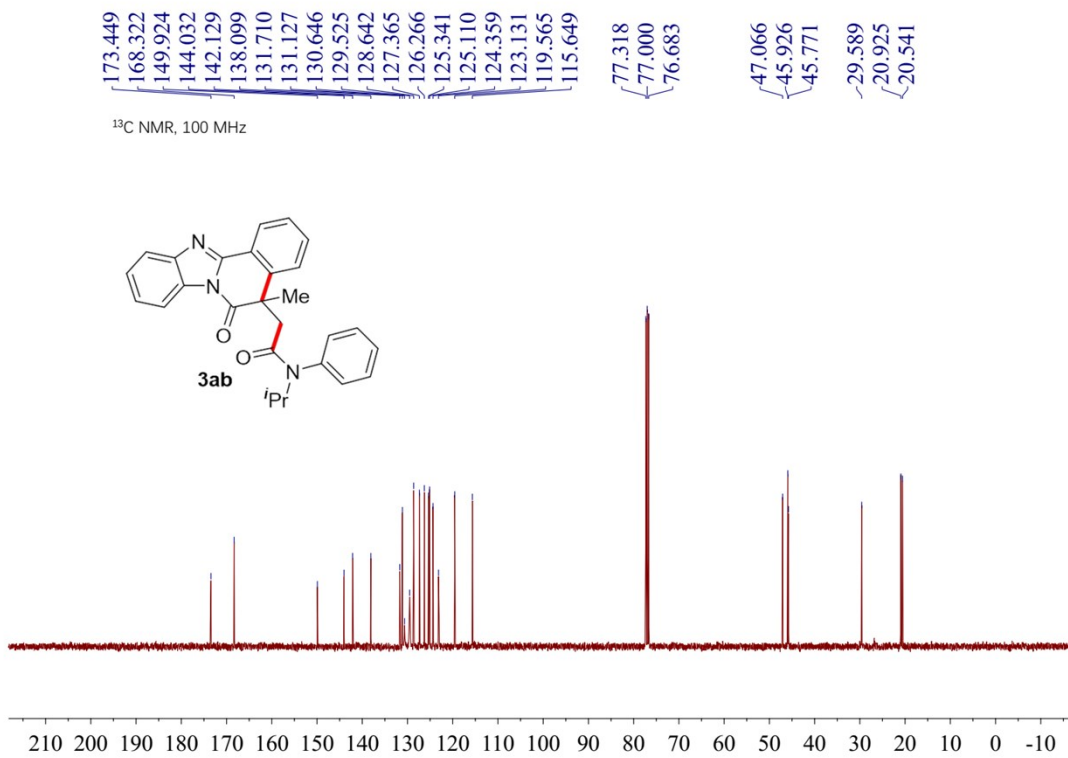












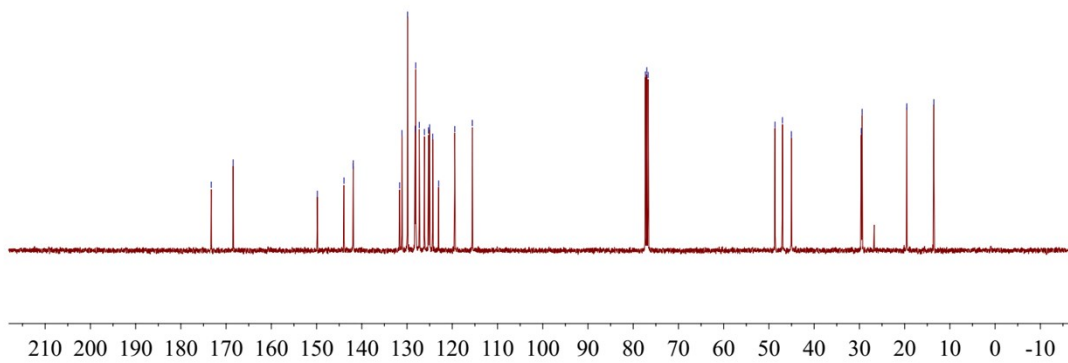
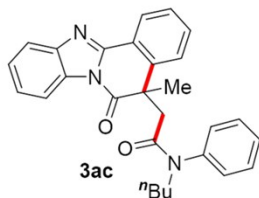
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128.077  
127.294  
126.151  
125.251  
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123.012  
119.459  
115.570

77.319  
77.001  
76.684

48.657  
47.019  
45.032

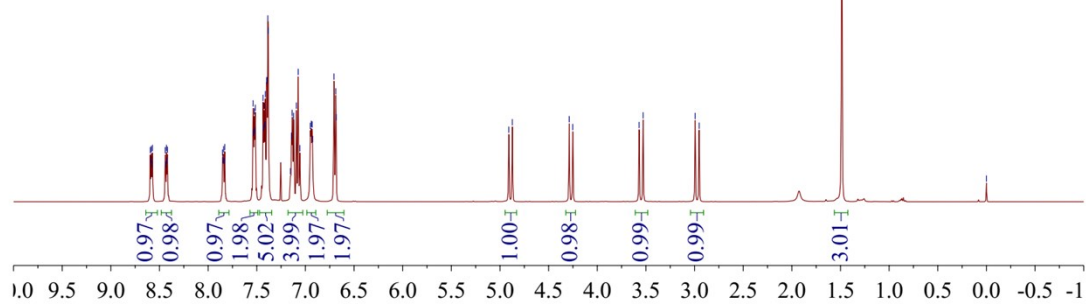
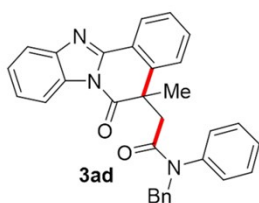
29.586  
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19.521  
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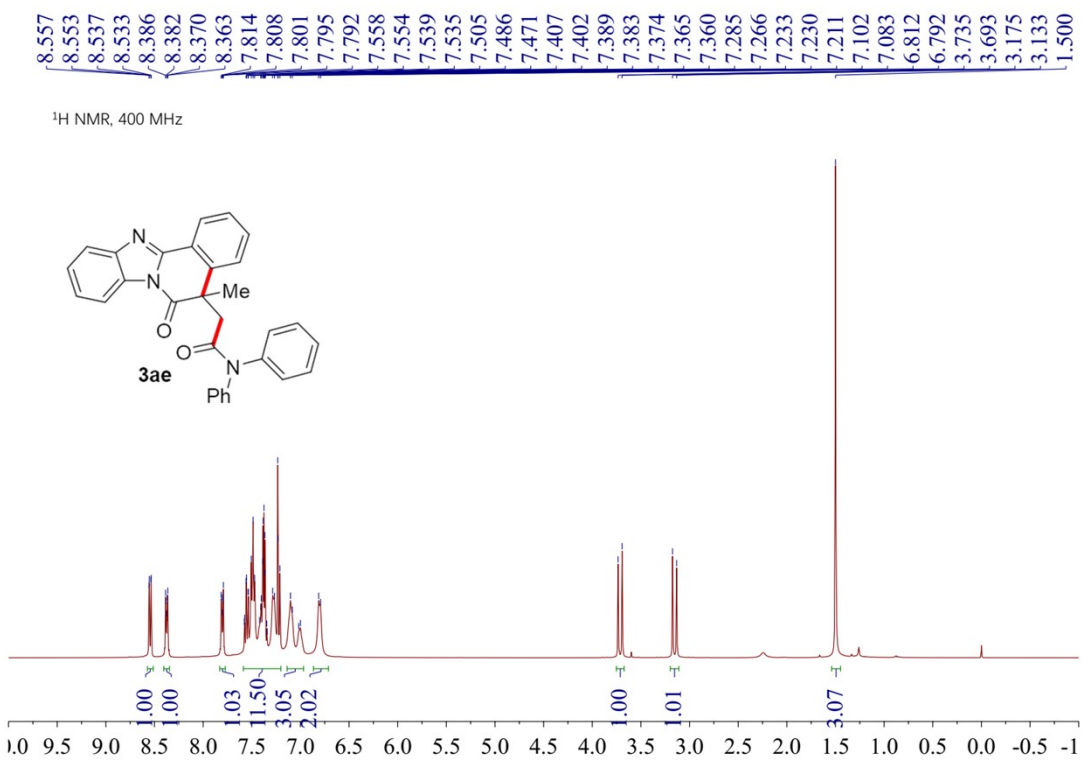
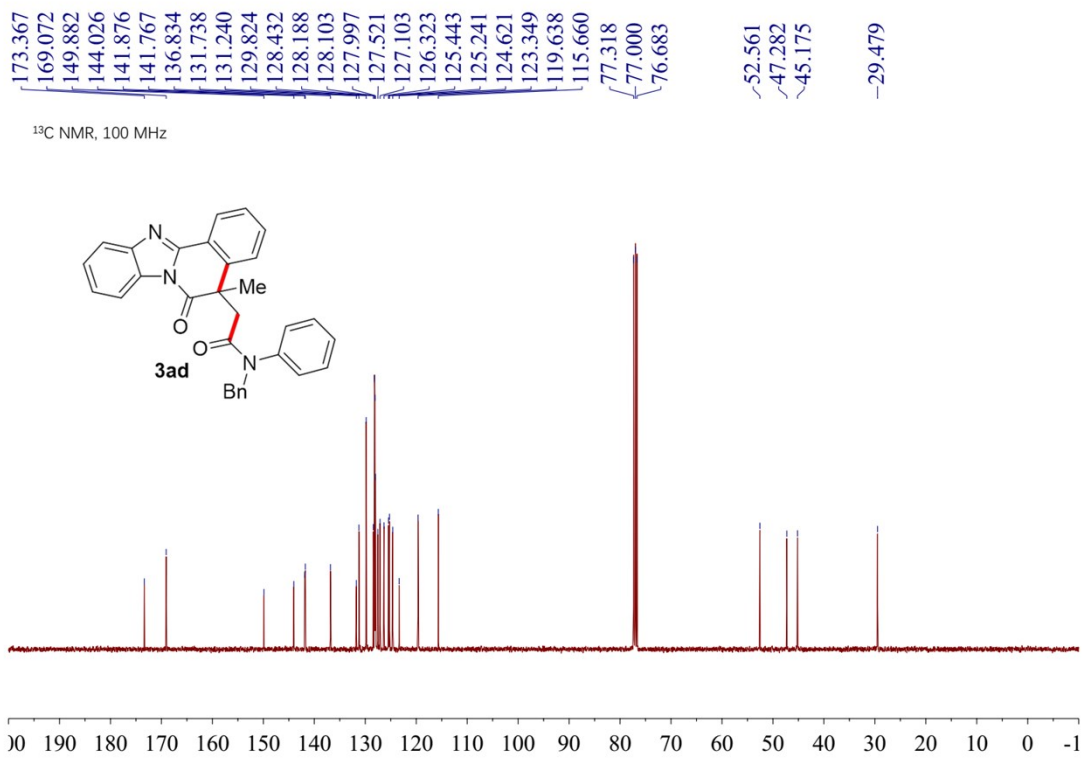
<sup>13</sup>C NMR, 100 MHz

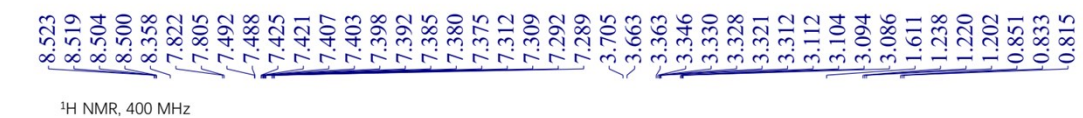
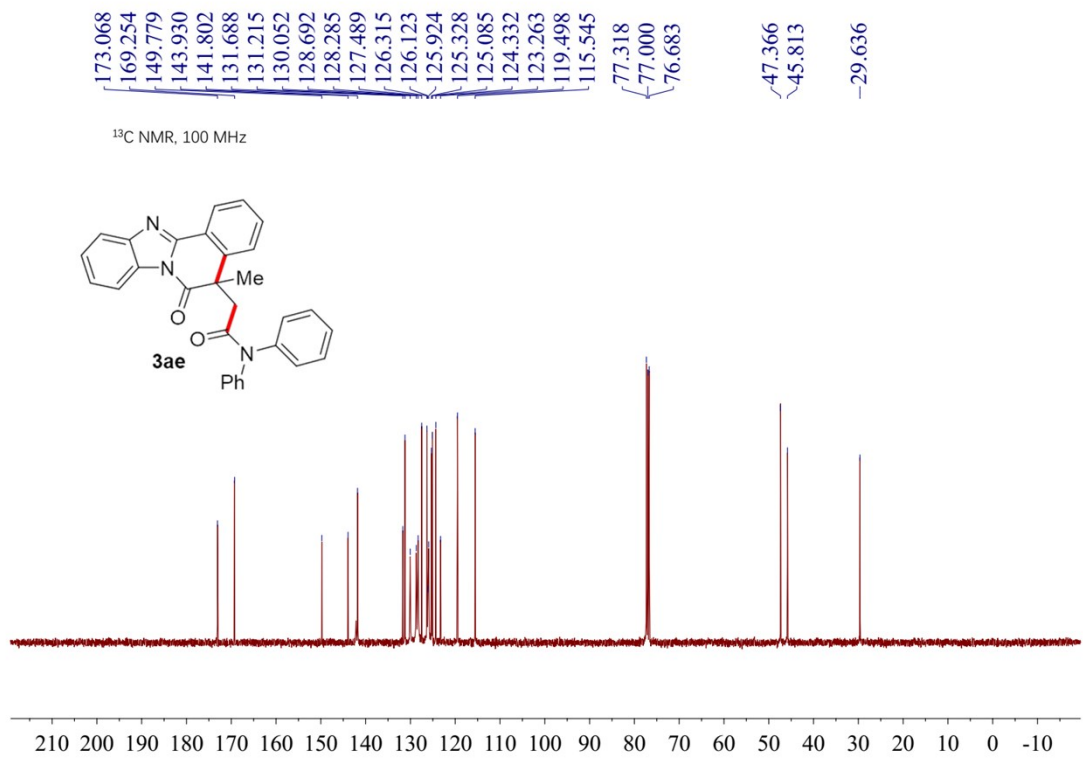


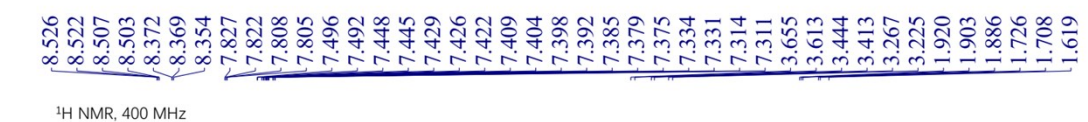
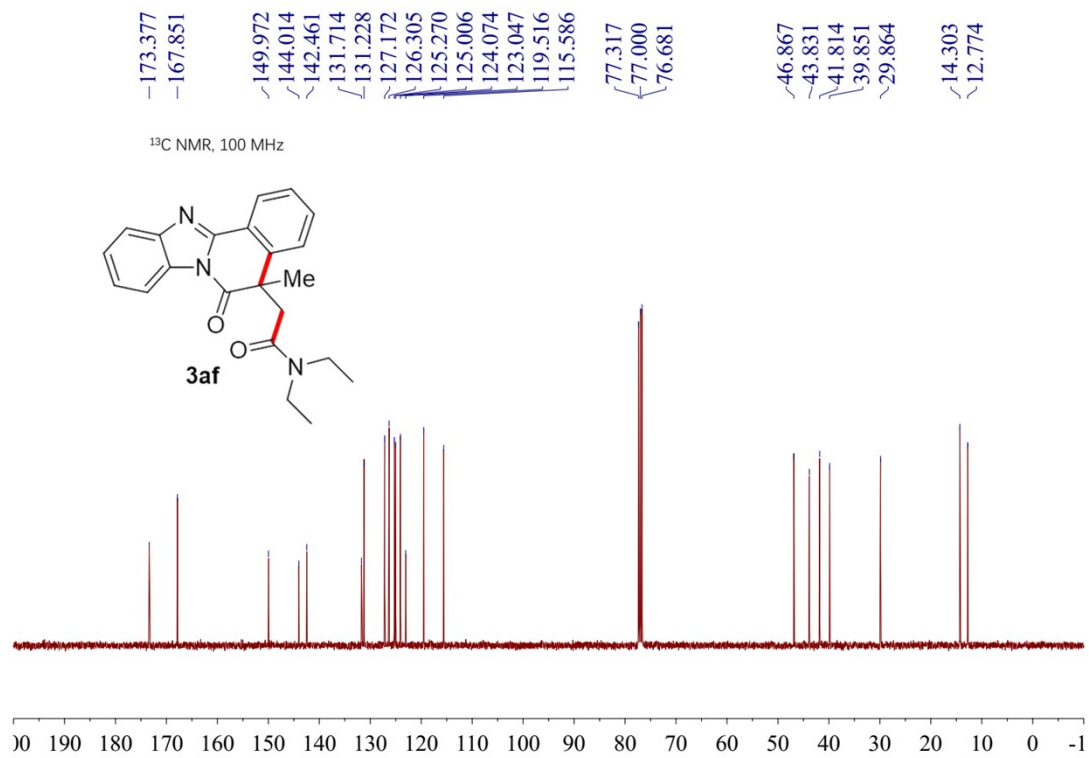
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7.424  
7.417  
7.412  
7.399  
7.394  
7.386  
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7.143  
7.137  
7.122  
7.093  
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7.057  
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6.940  
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1.487

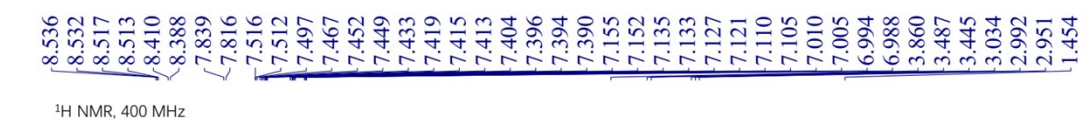
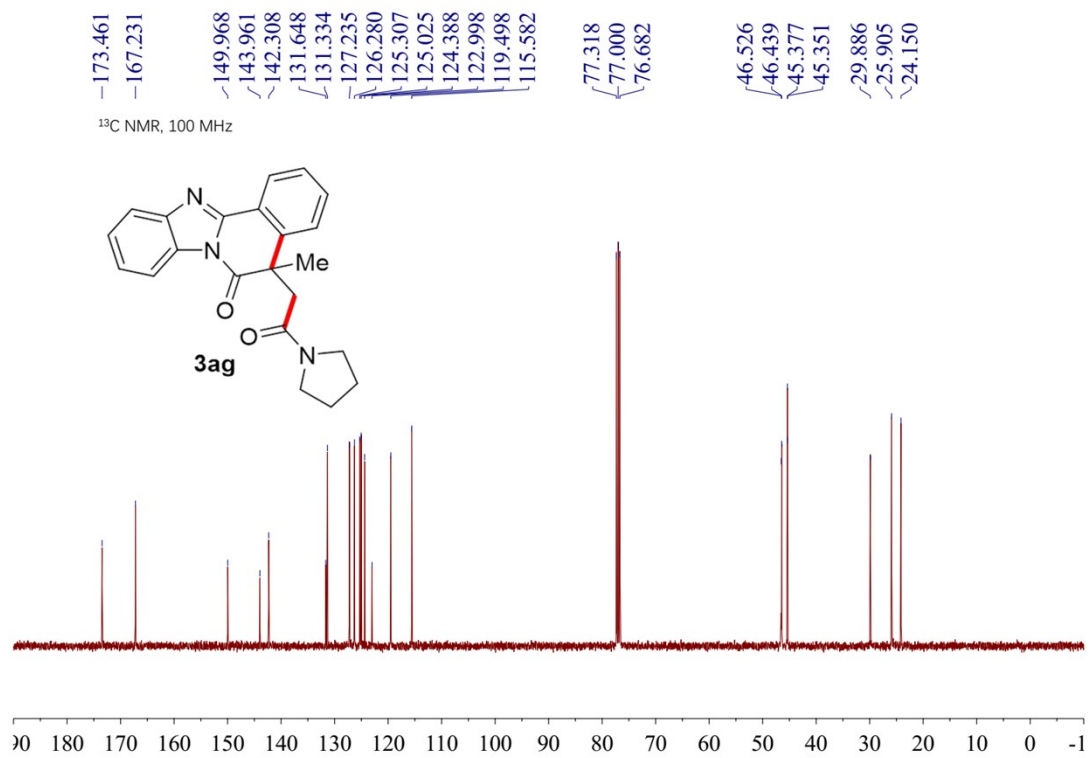
<sup>1</sup>H NMR, 400 MHz

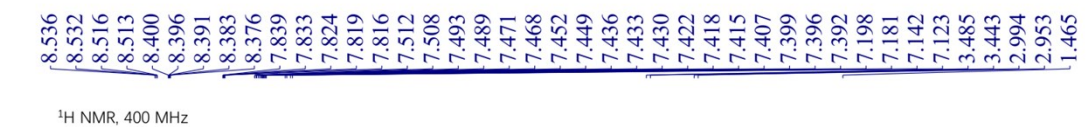
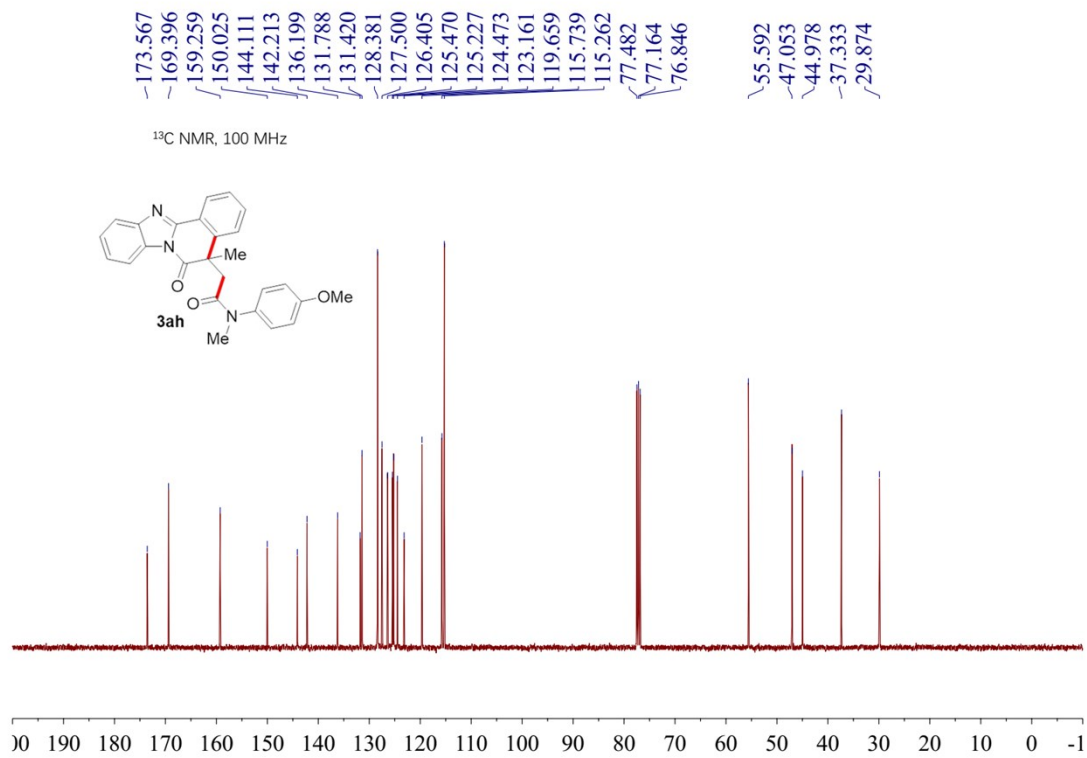








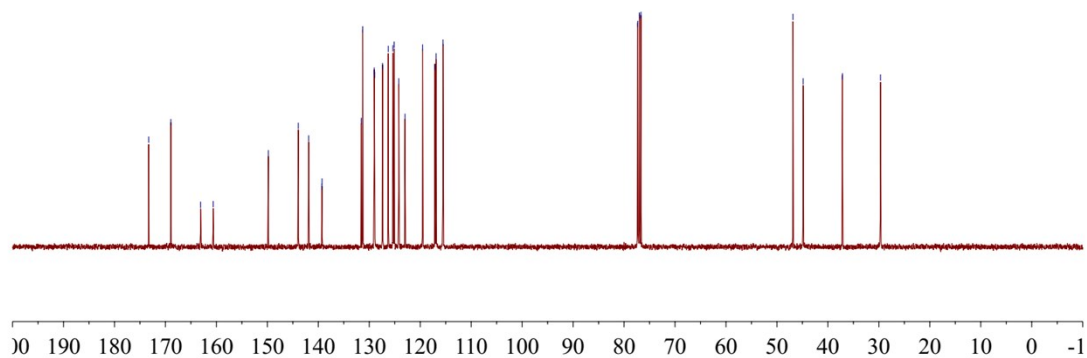
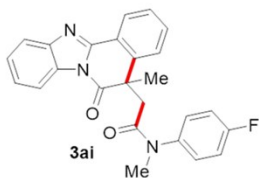






173.287  
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 77.000  
 76.682  
 46.856  
 44.855  
 37.148  
 29.677

<sup>13</sup>C NMR, 100 MHz



<sup>19</sup>F NMR, 377 MHz

