

## *Supporting Information*

### **An efficient transition-metal-free route to quinazolin-4(3H)-ones via 2-aminobenzamides and thiols**

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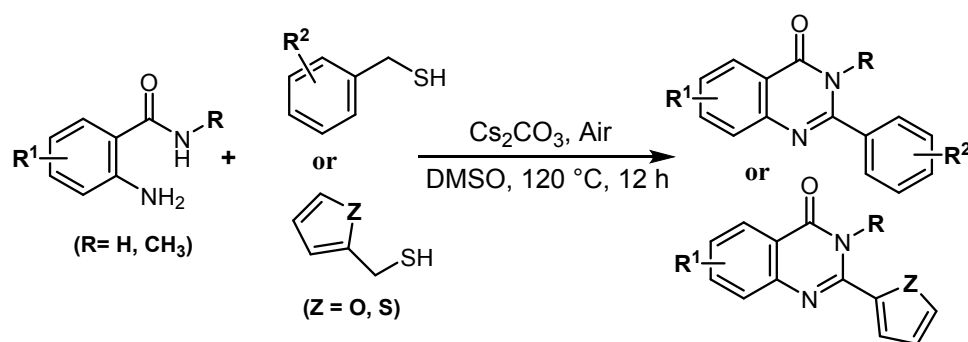
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## 1. General Information

$^1\text{H}$  NMR,  $^{13}\text{C}$  NMR were recorded in  $\text{DMSO-}d_6$  at room temperature on the Bruker DPX-400 spectrometer (400 MHz, 101 MHz). The chemical-shifts scale is based on internal TMS. For spectra, chemical shifts were reported in ppm ( $\delta$ ), multiplicity (s = singlet, d = doublet, t = triplet, q = quartet, m = multiplet) and coupling constant (Hz). Melting points were measured using a WC-1 microscopic apparatus and are uncorrected. High resolution mass spectra were ensured on a MALDI-FTMS. The structures of known compounds were further corroborated by comparing their  $^1\text{H}$  NMR,  $^{13}\text{C}$  NMR data with those of literature.

All reactions were monitored and post-processing by TLC with Qingdao GF<sub>254</sub> silica gel coated plates. Reagents were obtained from commercial suppliers such as Aladdin Scientific and used without further purification unless otherwise noted.

## 2. General Procedure for Quinazolin-4(3H)-ones Synthesis



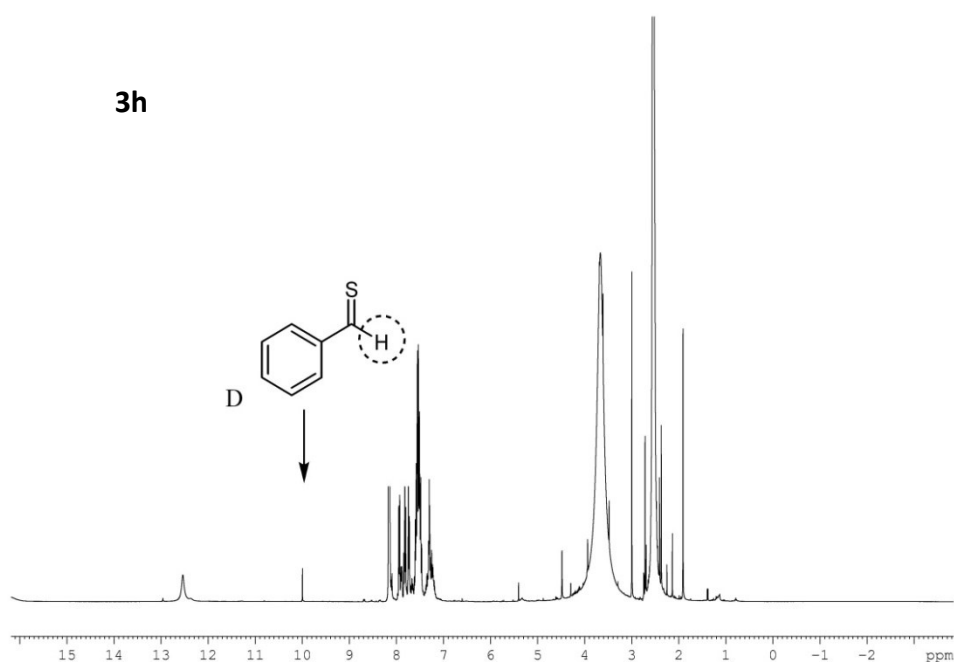
To a mixture of 2-anthranilamide (0.20 mmol), arylmethylmercaptan (0.40 mmol),  $\text{Cs}_2\text{CO}_3$  (130.3 mg, 2.0 equiv.) and DMSO (1 mL) were added in a 10 mL screw-cap Schlenk test tube. Then the mixture was stirred at 120 °C for 12 h under air atmosphere. The progress of the reaction was monitored by TLC. After the reaction was completed, the reaction mixture was cooled to room temperature then filtered with diatomite. The mixture was extracted with ethyl acetate (3.0 mL  $\times$  3) and the combined organic phases were dried over anhydrous  $\text{Na}_2\text{SO}_4$  and the solvent was evaporated under vacuum. The residue was purified by column chromatography to give the corresponding products (petroleum ether/ ethyl acetate = 2:1 to 6:1, 25%-98%).

### 3. Exploring the Mechanism by Mass Spectrometry Tracking

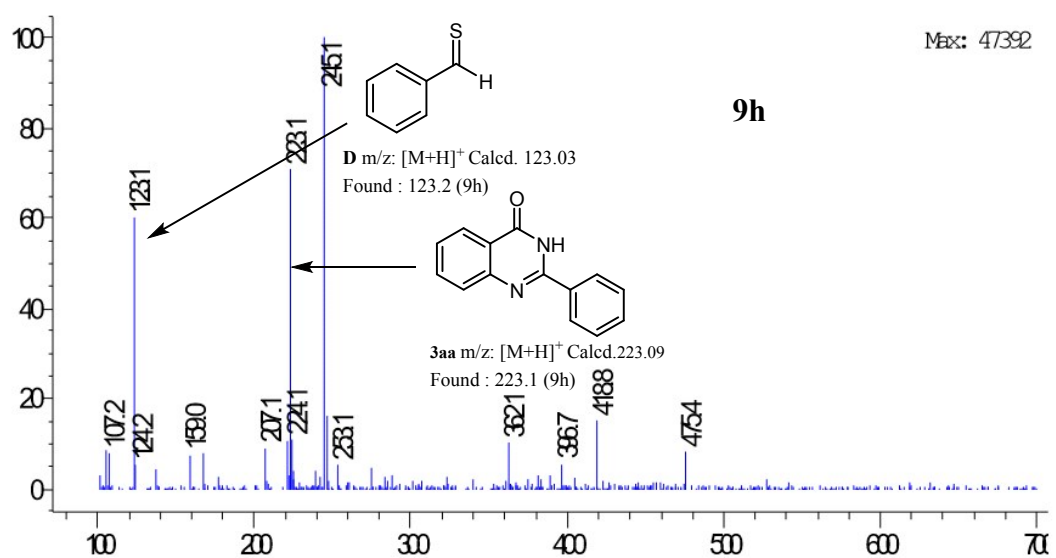
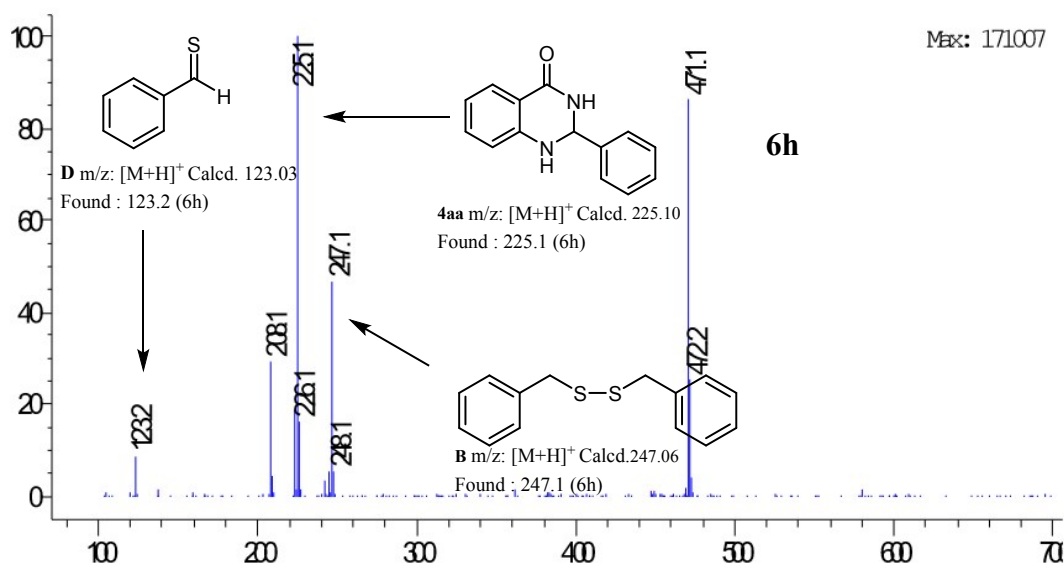
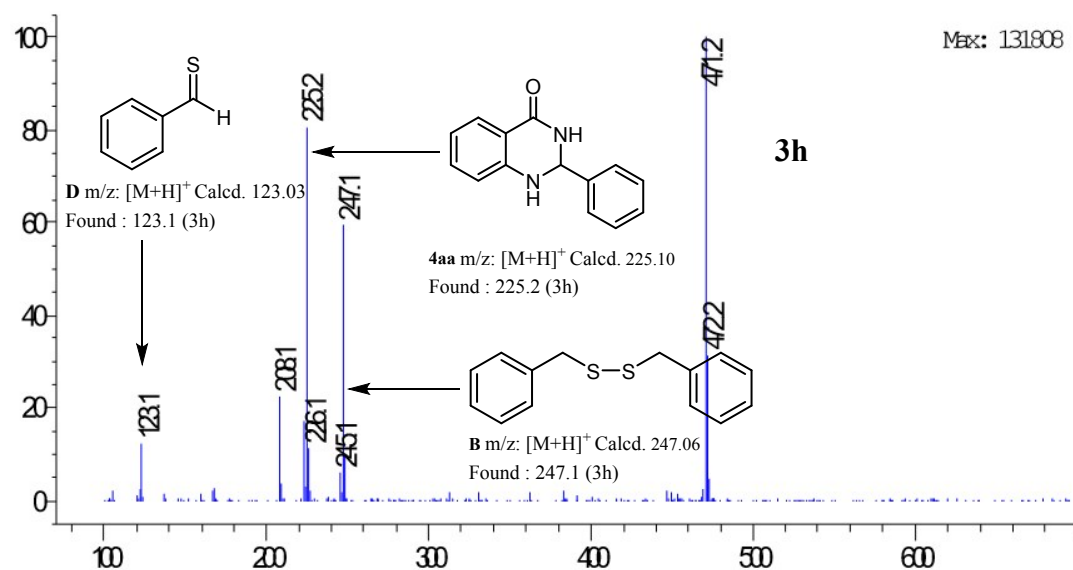
#### Experiments

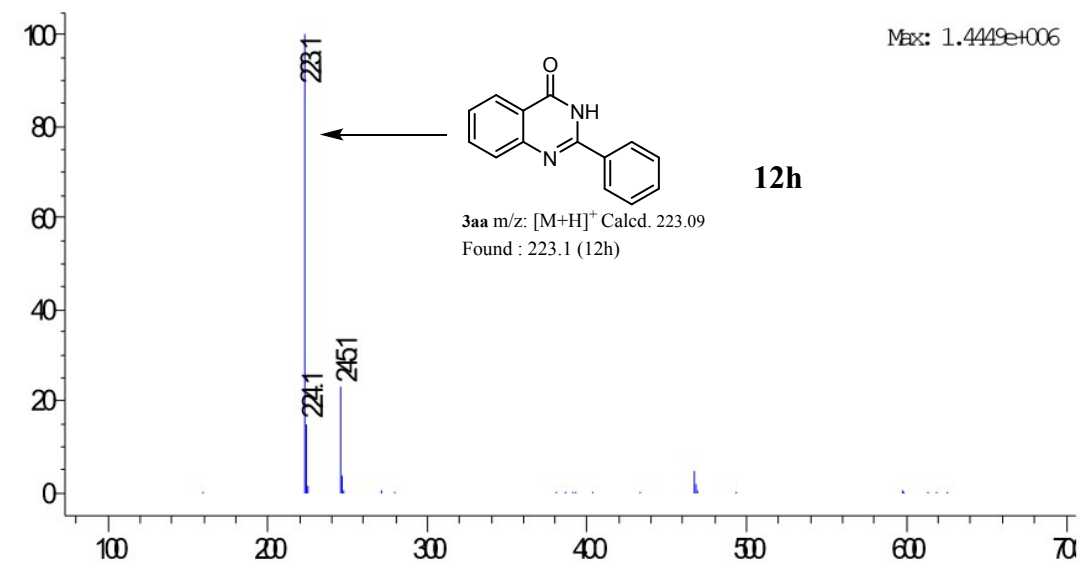
To a solution of the 2-aminobenzamide **1a** (0.20 mmol) in DMSO (1.0 mL) was added benzyl thiol **2a** (0.40 mmol), Cs<sub>2</sub>CO<sub>3</sub> (2.0 equiv.) under air atmosphere in five screw-cap Schlenk test tube. The reaction mixture was stirred at 120 °C for 3 h, 6 h, 9 h and 12 h in sequence. After the reaction was finished, the reaction mixture was cooled to room temperature. The mixture was extracted with ethyl acetate (3.0 mL × 3), the combined organic phases were dried over anhydrous Na<sub>2</sub>SO<sub>4</sub> and the solvent was evaporated under vacuum. Then, the mixture was detected by NMR and mass spectrometry separately and selected test results are as follows:

#### 3.1 Nuclear magnetic tracking results

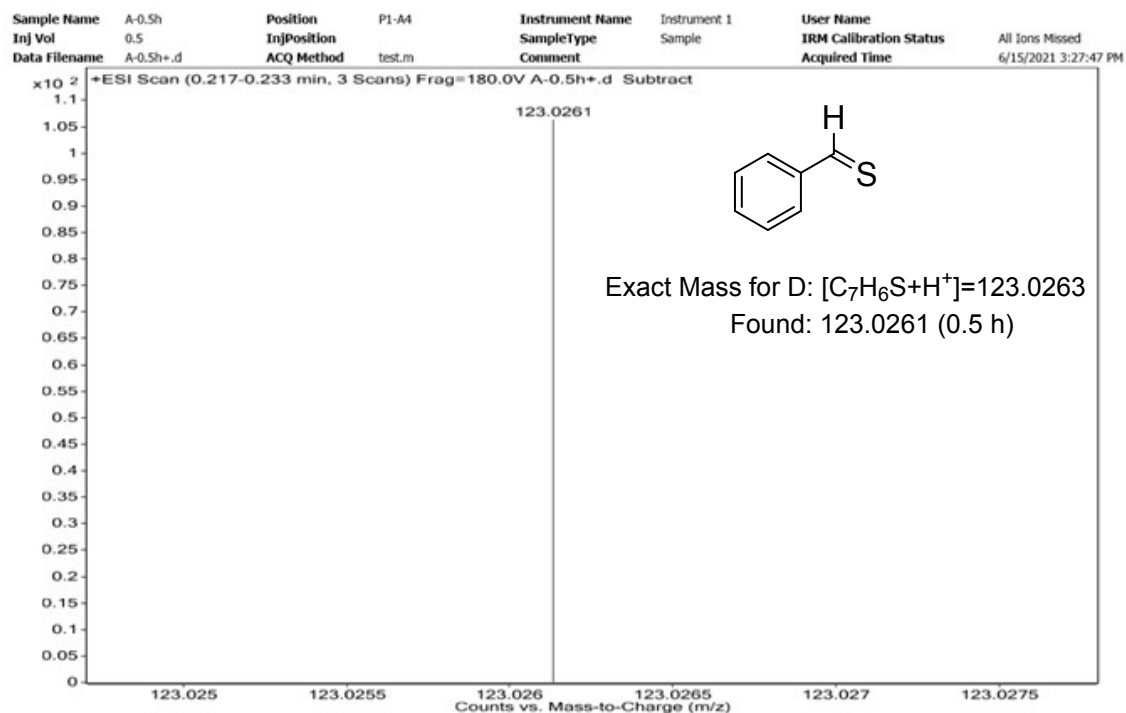
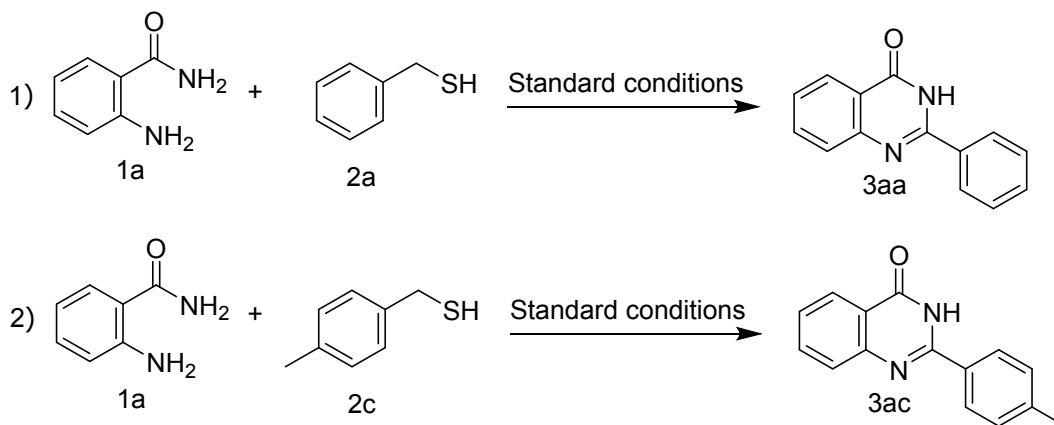


### 3.2 Mass spectrometry tracking results

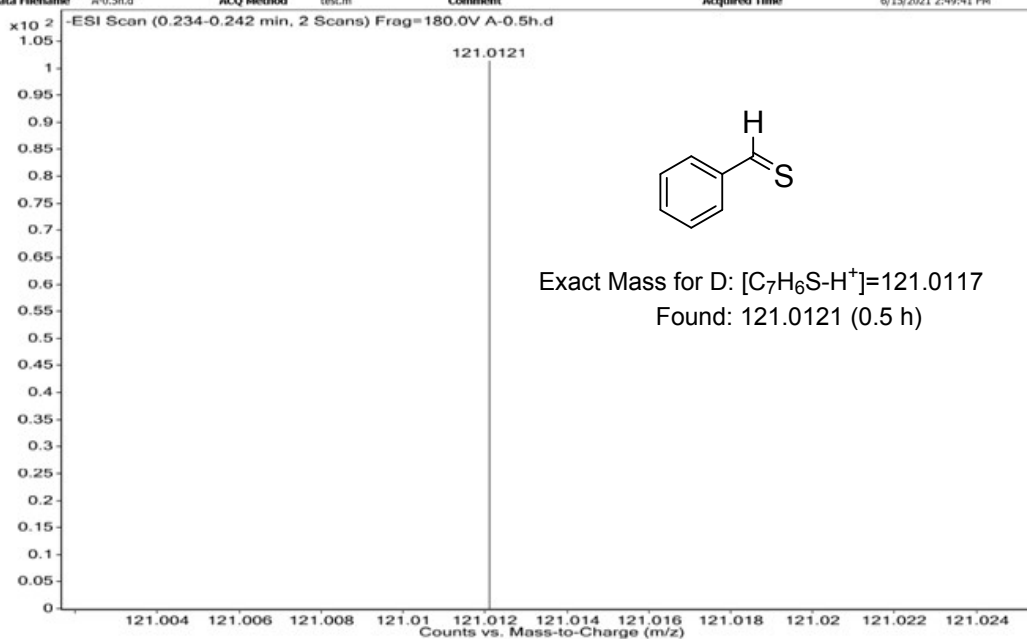




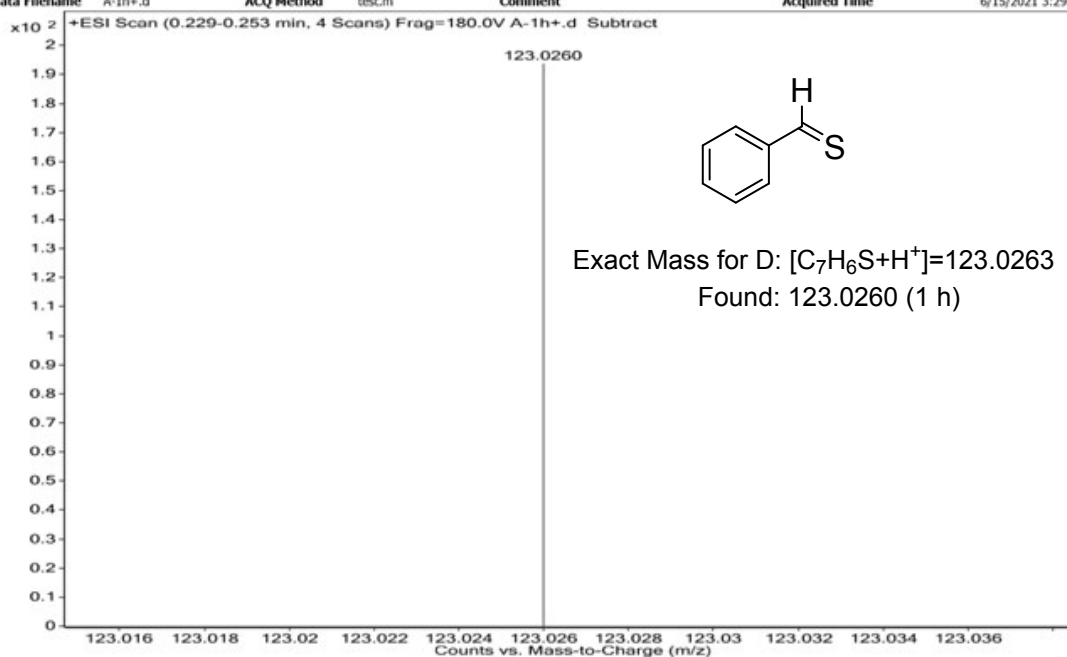
High resolution mass spectrometry in +ESI mode and -ESI mode



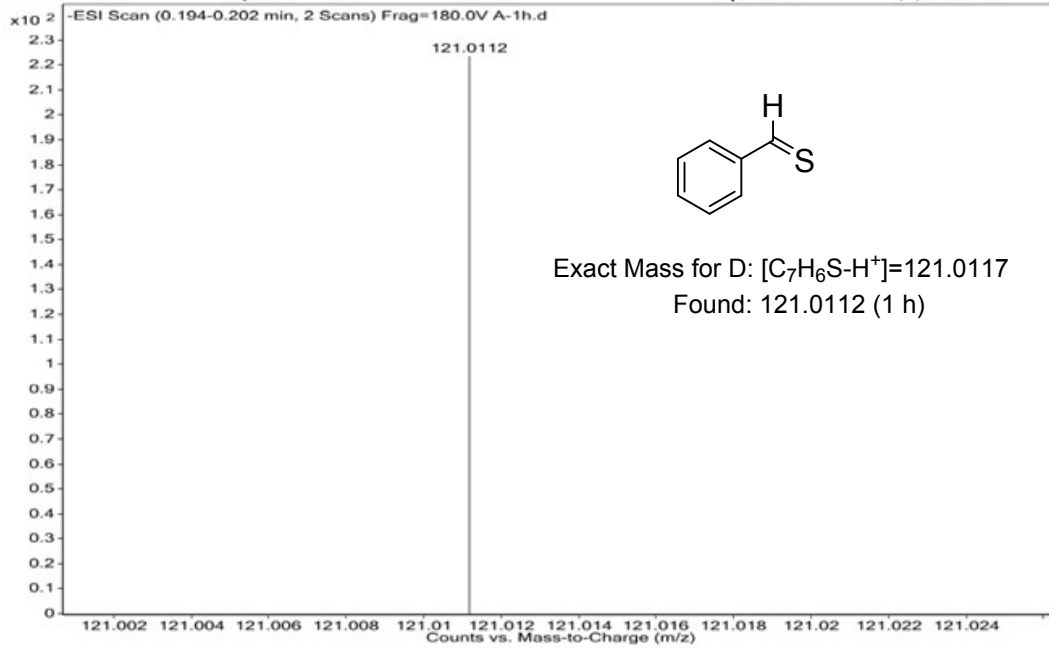
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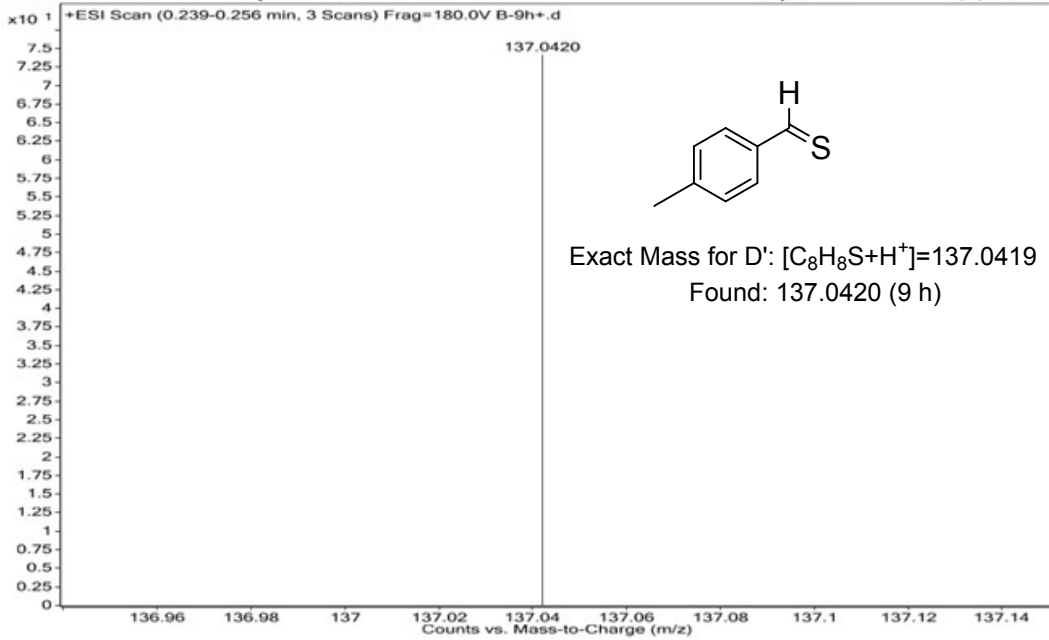
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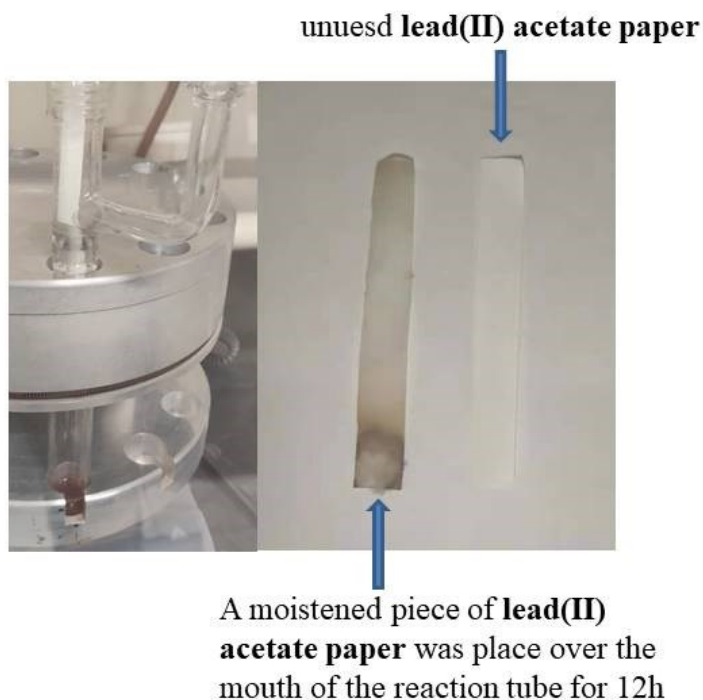
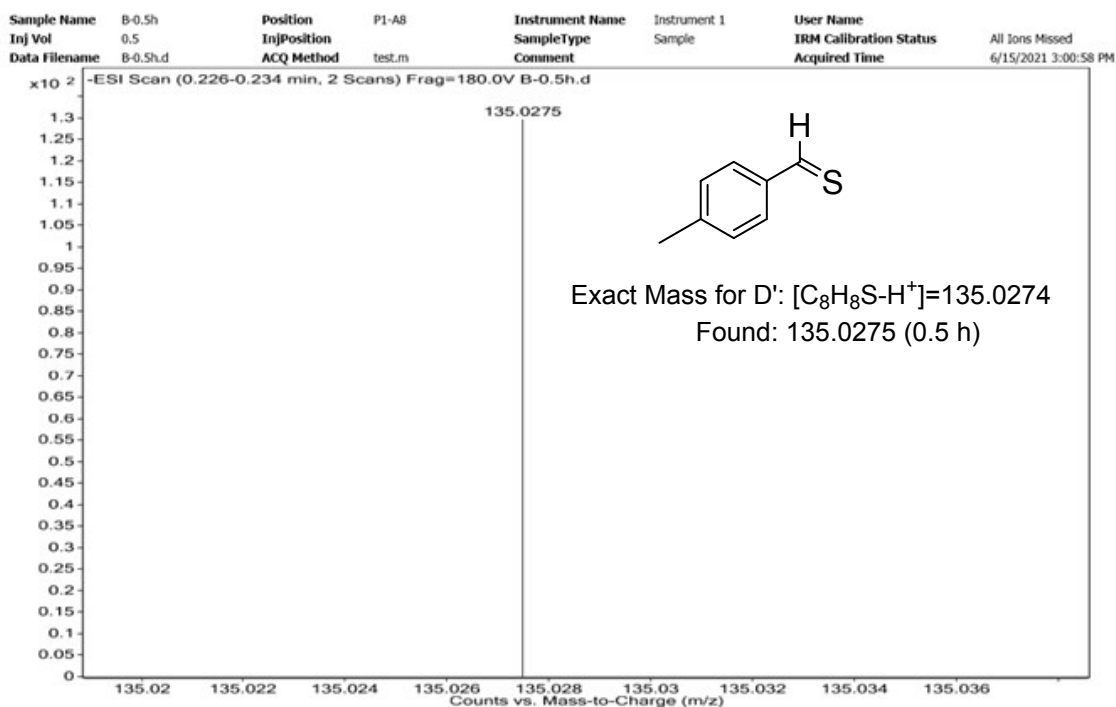


Sample Name	A-1h	Position	P1-A5	Instrument Name	Instrument 1	User Name	
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Sample Name	B-9h	Position	P1-B2	Instrument Name	Instrument 1	User Name	
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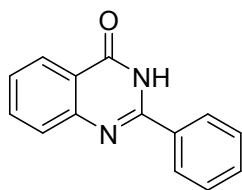


**Figure 1**

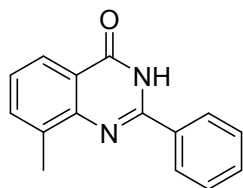
In order to examine the existence of H<sub>2</sub>S, lead (II) acetate paper was used to the model reaction. As shown in Figure 1, the determination of H<sub>2</sub>S was found by the coloring of lead acetate paper to black when a moistened piece of lead acetate paper was placed over the mouth of the flask for 12 h.



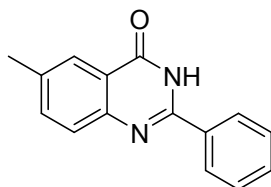
#### 4. Characterization Data of Products



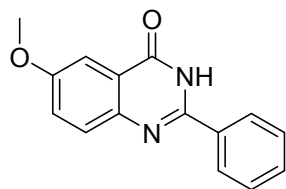
**2-Phenylquinazolin-4(3H)-one (3aa)<sup>1</sup>:** White solid; 98% yield (43.5 mg); mp 236-237 °C; TLC (PE: EA=3:1), R<sub>f</sub> = 0.40. <sup>1</sup>H NMR (400 MHz, DMSO-*d*<sub>6</sub>) δ 12.56 (s, 1H), 8.20-8.15 (m, 3H), 7.86-7.82 (m, 1H), 7.75 (d, *J* = 7.64 Hz, 1H), 7.62-7.50 (m, 4H). <sup>13</sup>C NMR (101 MHz, DMSO-*d*<sub>6</sub>) δ 162.7, 152.8, 149.2, 135.1, 133.2, 131.9, 129.1, 128.2, 128.0, 127.1, 126.3, 121.5.



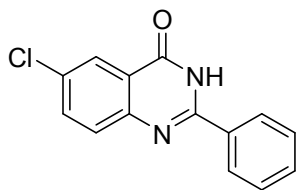
**8-Methyl-2-phenylquinazolin-4(3H)-one (3ba)<sup>2</sup>:** White solid; 82% yield (38.7 mg); mp 237-239 °C; TLC (PE: EA=3:1), R<sub>f</sub> = 0.42. <sup>1</sup>H NMR (400 MHz, DMSO-*d*<sub>6</sub>) δ 12.53 (s, 1H), 8.24-8.22 (dd, *J* = 7.68, 1.36 Hz 2H), 7.99 (d, *J* = 7.52 Hz, 1H), 7.68 (d, *J* = 6.8 Hz, 1H), 7.61-7.51 (m, 3H), 7.39 (t, *J* = 7.6 Hz, 1H), 2.62 (s, 3H). <sup>13</sup>C NMR (101 MHz, DMSO-*d*<sub>6</sub>) δ 163.0, 151.5, 147.6, 136.1, 135.4, 133.4, 131.8, 129.1, 128.2, 126.5, 124.0, 121.3, 17.6.



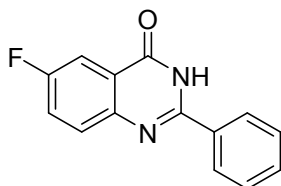
**6-Methyl-2-phenylquinazolin-4(3H)-one (3ca)<sup>3</sup>:** White solid; 86% yield (40.6 mg); mp 238-240 °C; TLC (PE: EA=3:1), R<sub>f</sub> = 0.42. <sup>1</sup>H NMR (400 MHz, DMSO-*d*<sub>6</sub>) δ 12.47 (s, 1H), 8.22-8.14 (m, 2H), 7.97 (s, 1H), 7.69-7.65 (m, 2H), 7.62-7.52 (m, 3H), 2.48 (s, 3H). <sup>13</sup>C NMR (101 MHz, DMSO-*d*<sub>6</sub>) δ 162.4, 151.7, 146.6, 136.3, 135.9, 132.8, 131.3, 128.6, 127.6, 127.2, 125.2, 120.6, 20.8.



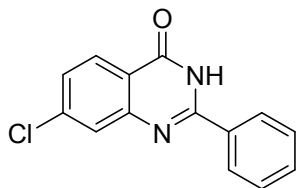
**6-Methoxy-2-phenylquinazolin-4(3H)-one (3da)<sup>3</sup>:** White solid; 74% yield (37.3 mg); mp 249-251 °C; TLC (PE: EA=2:1), R<sub>f</sub> = 0.40. <sup>1</sup>H NMR (400 MHz, DMSO-*d*<sub>6</sub>) δ 12.52 (s, 1H), 8.34-7.99 (m, 2H), 7.71 (d, *J* = 8.9 Hz, 1H), 7.65-7.49 (m, 4H), 7.45 (dd, *J* = 8.9, 3.0 Hz, 1H), 3.90 (s, 3H). <sup>13</sup>C NMR (101 MHz, DMSO-*d*<sub>6</sub>) δ 162.5, 158.2, 150.6, 143.7, 133.3, 131.5, 129.7, 129.1, 128.0, 124.6, 122.2, 106.3, 56.1.



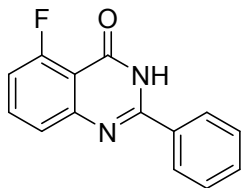
**6-Chloro-2-phenylquinazolin-4(3H)-one (3ea)<sup>1</sup>:** White solid; 72% yield (36.9 mg); mp 212-213 °C; TLC (PE: EA=2:1), R<sub>f</sub> = 0.44. <sup>1</sup>H NMR (400 MHz, DMSO-*d*<sub>6</sub>) δ 12.72 (s, 1H), 8.22-8.15 (m, 2H), 8.09 (d, *J* = 2.5 Hz, 1H), 7.87 (dd, *J* = 8.7, 2.5 Hz, 1H), 7.77 (d, *J* = 8.7 Hz, 1H), 7.64-7.53 (m, 3H). <sup>13</sup>C NMR (101 MHz, DMSO-*d*<sub>6</sub>) δ 161.8, 153.4, 147.9, 135.2, 132.9, 132.1, 131.2, 130.2, 129.1, 128.3, 125.3, 122.7.



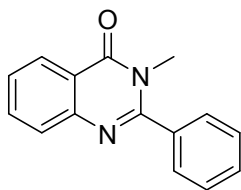
**6-Fluoro-2-phenylquinazolin-4(3H)-one (3fa)<sup>4</sup>:** White solid; 73% yield (35.0 mg); mp 282-284 °C; TLC (PE: EA=3:1 to 5:1) R<sub>f</sub> = 0.44. <sup>1</sup>H NMR (400 MHz, DMSO-*d*<sub>6</sub>) δ 12.68 (s, 1H), 8.17 (d, *J* = 7.56 Hz, 2H), 7.87-7.79 (m, 2H), 7.73 (td, *J* = 8.7, 3.0 Hz, 1H), 7.64-7.52 (m, 3H). <sup>13</sup>C NMR (101 MHz, DMSO-*d*<sub>6</sub>) δ 161.9(d, *J* = 51.0 Hz), 159.2, 152.4, 146.1, 133.0, 131.9, 130.8, 129.1, 128.2, 123.6(d, *J* = 51.0 Hz), 122.7(d, *J* = 8.3 Hz), 111.0(d, *J* = 23.35 Hz). <sup>19</sup>F NMR (376 MHz, DMSO-*d*<sub>6</sub>) δ -113.50.



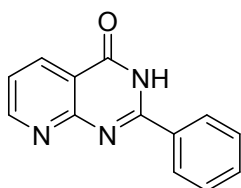
**7-Chloro-2-phenylquinazolin-4(3H)-one (3ga)<sup>3</sup>:** White solid; 43% yield (22.0 mg); mp 291-292 °C; TLC (PE: EA=2:1 to 4:1) R<sub>f</sub> = 0.40. <sup>1</sup>H NMR (400 MHz, DMSO-*d*<sub>6</sub>) δ 12.67 (s, 1H), 8.22-8.10 (m, 3H), 7.78 (d, *J* = 2.0 Hz, 1H), 7.64-7.51 (m, 4H). <sup>13</sup>C NMR (101 MHz, DMSO-*d*<sub>6</sub>) δ 162.2, 154.3, 150.3, 139.6, 132.8, 132.2, 129.1, 128.4, 128.4, 127.3, 127.0, 120.2.



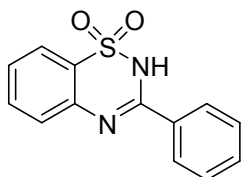
**5-Fluoro-2-phenylquinazolin-4(3H)-one (3ha)<sup>3</sup>:** White solid; 49% yield (23.5 mg); mp > 300 °C; TLC (PE: EA=3:1) R<sub>f</sub> = 0.42. <sup>1</sup>H NMR (400 MHz, DMSO-*d*<sub>6</sub>) δ 12.57 (s, 1H), 8.23-8.09 (m, 2H), 7.80 (td, *J* = 8.2, 5.6 Hz, 1H), 7.65-7.47 (m, 4H), 7.28-7.23 (m, 1H). <sup>13</sup>C NMR (101 MHz, DMSO-*d*<sub>6</sub>) δ 162.3, 159.9(d, *J* = 34.9 Hz), 153.8, 151.3, 135.6(d, *J* = 10.8 Hz), 132.7, 132.2, 129.1, 128.3, 124.0, 113.4(d, *J* = 20.57 Hz), 110.9(d, *J* = 6.1 Hz). <sup>19</sup>F NMR (376 MHz, DMSO-*d*<sub>6</sub>) δ -111.5.



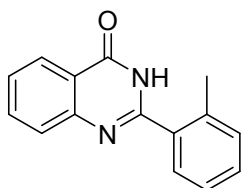
**3-Methyl-2-phenylquinazolin-4(3H)-one (3ia)**<sup>5</sup>: White solid; 90% yield (42.5 mg); mp 101-103 °C; TLC (PE: EA=2:1) R<sub>f</sub> = 0.40. <sup>1</sup>H NMR (400 MHz, DMSO-*d*<sub>6</sub>): δ 8.15 (dd, *J* = 8.0, 1.5 Hz, 1H), 7.83-7.79 (m, 1H), 7.66-7.62 (m, 3H), 7.56-7.52 (m, 4H), 3.34 (s, 3H). <sup>13</sup>C NMR (101 MHz, DMSO-*d*<sub>6</sub>) δ 162.1, 156.6, 147.5, 135.9, 134.8, 130.3, 128.9, 128.7, 127.6, 127.3, 126.6, 120.6, 34.4.



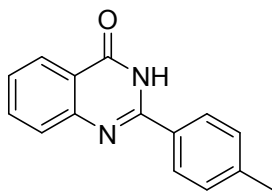
**2-Phenyl-Pyrido[2,3-*d*]pyrimidin-4(3H)-one (3ja)**<sup>5</sup>: Light yellow solid; 44% yield (19.6 mg); mp 284-285 °C; TLC (PE: EA=3:1) R<sub>f</sub> = 0.40. <sup>1</sup>H NMR (400 MHz, DMSO-*d*<sub>6</sub>) δ 12.83 (s, 1H), 8.98 (dd, *J* = 4.6, 2.1 Hz, 1H), 8.54 (dd, *J* = 7.8, 2.0 Hz, 1H), 8.23 (d, *J* = 6.9 Hz, 2H), 7.68-7.50 (m, 4H). <sup>13</sup>C NMR (101 MHz, DMSO-*d*<sub>6</sub>) δ 163.1, 158.6, 156.1, 155.5, 135.5, 132.5, 131.9, 128.7, 128.1, 122.2, 116.1.



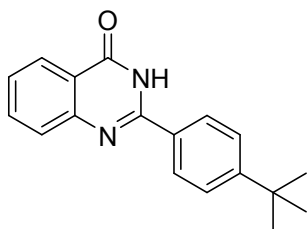
**3-Phenyl-2H-1,2,4-benzothiadiazine-1,1-dioxide (3ka)**<sup>5</sup>: White solid; 32% yield (16.5 mg); mp > 300 °C; TLC (PE: EA=3:1) R<sub>f</sub> = 0.40. <sup>1</sup>H NMR (400 MHz, DMSO-*d*<sub>6</sub>) δ 12.63 (s, 1H), 8.17-8.15 (m, 2H), 7.90-7.85 (m, 2H), 7.75-7.67 (m, 2H), 7.61 (t, *J* = 7.84 Hz, 2H), 7.53-7.49 (m, 1H). <sup>13</sup>C NMR (101 MHz, DMSO-*d*<sub>6</sub>) δ 155.3, 136.2, 133.5, 133.3, 132.2, 129.3, 128.9, 127.1, 123.7, 121.9, 119.2.



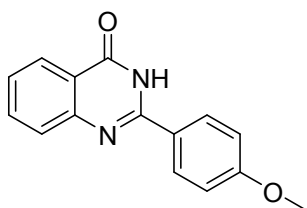
**2-(2-Methylphenyl)-4(3H)-quinazolinone (3ab)**<sup>1</sup>: White solid; 70% yield (33.0 mg); mp 217-218 °C; TLC (PE: EA=3:1) R<sub>f</sub> = 0.40. <sup>1</sup>H NMR (400 MHz, DMSO-*d*<sub>6</sub>) δ 12.45 (s, 1H), 8.17 (d, *J* = 7.0 Hz, 1H), 7.86-7.82 (m, 1H), 7.69 (d, *J* = 8.1 Hz, 1H), 7.60-7.47 (m, 2H), 7.46-7.42 (m, 1H), 7.37-7.32 (m, 2H), 2.39 (s, 3H). <sup>13</sup>C NMR (101 MHz, DMSO-*d*<sub>6</sub>) δ 161.8, 154.4, 148.7, 136.1, 134.5, 134.2, 130.5, 129.9, 129.1, 127.3, 126.6, 125.8, 125.7, 120.9, 19.5.



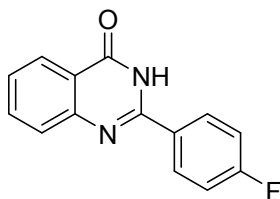
**2-(4-Methylphenyl)-4(3H)-quinazolinone (3ac)<sup>1</sup>:** White solid; 75% yield (35.4 mg); mp 242-243 °C; TLC (PE: EA=3:1) R<sub>f</sub> = 0.40. <sup>1</sup>H NMR (400 MHz, DMSO-*d*<sub>6</sub>) δ 12.46 (s, 1H), 8.16 (dd, *J* = 8.0, 1.6 Hz, 1H), 8.13-8.06 (m, 2H), 7.85-7.81 (m, 1H), 7.73 (d, *J* = 7.9 Hz, 1H), 7.53-7.49 (m, 1H), 7.34 (d, *J* = 8.1 Hz, 2H), 2.38 (s, 3H). <sup>13</sup>C NMR (101 MHz, DMSO-*d*<sub>6</sub>) δ 162.2, 152.2, 148.8, 141.4, 134.5, 129.9, 129.2, 127.6, 127.4, 126.3, 125.8, 120.9, 20.9.



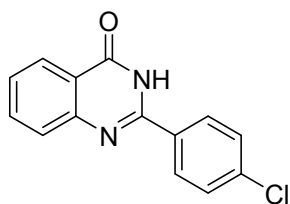
**2-[4-(1,1-Dimethylethyl)phenyl]-4(3H)-quinazolinone (3ad)<sup>6</sup>:** White solid; 78% yield (43.4 mg); mp 207-209 °C; TLC (PE: EA=2:1) R<sub>f</sub> = 0.40. <sup>1</sup>H NMR (400 MHz, DMSO-*d*<sub>6</sub>) δ 12.51 (s, 1H), 8.18-8.14 (m, 3H), 7.86-7.82 (m, 1H), 7.74 (d, *J* = 8.3 Hz, 1H), 7.58-7.50 (m, 3H), 1.33 (s, 9H). <sup>13</sup>C NMR (101 MHz, DMSO-*d*<sub>6</sub>) δ 162.8, 154.8, 152.6, 149.3, 135.1, 130.4, 128.0, 127.9, 126.9, 126.3, 125.9, 121.4, 35.1, 31.4.



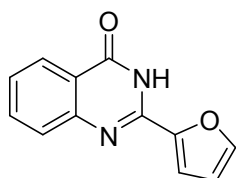
**2-(4-Methoxyphenyl)-4(3H)-quinazolinone (3ae)<sup>1</sup>:** White solid; 75% yield (37.8 mg); mp 200-201 °C; TLC (PE: EA=2:1) R<sub>f</sub> = 0.44. <sup>1</sup>H NMR (400 MHz, DMSO-*d*<sub>6</sub>) δ 12.41 (s, 1H), 8.22-8.18 (m, 2H), 8.14 (dd, *J* = 7.9, 1.5 Hz, 1H), 7.84-7.80 (m, 1H), 7.71 (d, *J* = 7.7 Hz, 1H), 7.51-7.47 (m, 1H), 7.09 (d, *J* = 8.9 Hz, 2H), 3.85 (s, 3H). <sup>13</sup>C NMR (101 MHz, DMSO-*d*<sub>6</sub>) δ 162.4, 161.8, 151.9, 148.8, 134.5, 129.4, 127.1, 126.1, 125.8, 124.8, 120.6, 114.0, 55.4.



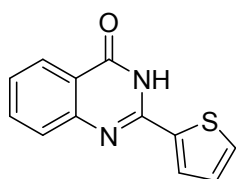
**2-(4-Fluorophenyl)quinazolin-4(3H)-one (3af)<sup>1</sup>:** White solid; 31% yield (14.9 mg); mp 284-286 °C; TLC (PE: EA=3:1 to 6:1) R<sub>f</sub> = 0.40. <sup>1</sup>H NMR (400 MHz, DMSO-*d*<sub>6</sub>) δ 12.58 (s, 1H), 8.31-8.23 (m, 2H), 8.17 (dd, *J* = 7.9, 1.6 Hz, 1H), 7.88-7.84 (m, 1H), 7.75 (d, *J* = 8.3 Hz, 1H), 7.56-7.52 (m, 1H), 7.43-7.39 (m, 2H). <sup>13</sup>C NMR (101 MHz, DMSO-*d*<sub>6</sub>) δ 165.8, 162.7, 151.9, 149.1, 135.1, 130.9 (d, *J* = 9.1 Hz), 129.7, 128.0, 127.1, 126.3, 121.4, 116.1 (d, *J* = 21.2 Hz). <sup>19</sup>F NMR (376 MHz, DMSO-*d*<sub>6</sub>) δ -109.1.



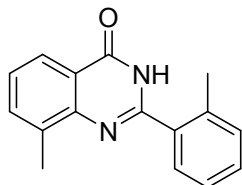
**2-(4-Chlorophenyl)-4(3H)-quinazolinone (3ag)<sup>1</sup>:** White solid; 29% yield (14.8 mg); mp 171-172 °C; TLC (PE: EA=3:1 to 6:1) R<sub>f</sub> = 0.40. <sup>1</sup>H NMR (400 MHz, DMSO-*d*<sub>6</sub>) δ 12.62 (s, 1H), 8.24-8.20 (m, 2H), 8.17 (dd, *J* = 7.9, 1.6 Hz, 1H), 7.88-7.84 (m, 1H), 7.76 (d, *J* = 7.7 Hz, 1H), 7.66-7.63 (m, 2H), 7.57-7.53 (m, 1H). <sup>13</sup>C NMR (101 MHz, DMSO-*d*<sub>6</sub>) δ 162.2, 151.4, 148.5, 136.3, 134.6, 131.6, 129.6, 128.6, 127.4, 126.8, 125.9, 121.0.



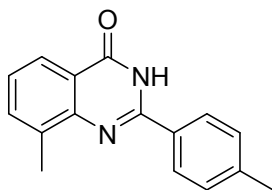
**2-(Furan-2-yl)-4(3H)-quinazolinone (3ah)<sup>7</sup>:** Light yellow solid; 40% yield (16.9 mg); mp 219-221 °C; TLC (PE: EA=3:1) R<sub>f</sub> = 0.40. <sup>1</sup>H NMR (400 MHz, DMSO-*d*<sub>6</sub>) δ 12.56 (s, 1H), 8.17 (dd, *J* = 7.9, 1.6 Hz, 1H), 8.05 (d, *J* = 1.7 Hz, 1H), 7.88-7.84 (m, 1H), 7.74 (d, *J* = 7.7 Hz, 1H), 7.68 (d, *J* = 3.6 Hz, 1H), 7.56-7.52 (m, 1H), 6.80 (dd, *J* = 3.6, 1.8 Hz, 1H). <sup>13</sup>C NMR (101 MHz, DMSO-*d*<sub>6</sub>) δ 161.5, 148.6, 146.6, 146.1, 144.0, 134.6, 127.2, 126.5, 125.9, 121.1, 114.5, 112.5.



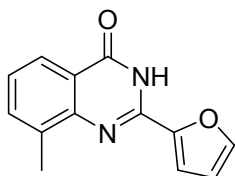
**2-(Thiophen-2-yl)quinazolin-4(3H)-one (3ai)<sup>1</sup>:** White solid; 60% yield (27.3 mg); mp 235-238 °C; TLC (PE: EA=3:1) R<sub>f</sub> = 0.40. <sup>1</sup>H NMR (400 MHz, DMSO-*d*<sub>6</sub>) δ 12.66 (s, 1H), 8.23 (dd, *J* = 3.8, 1.2 Hz, 1H), 8.13 (dd, *J* = 7.9, 1.6 Hz, 1H), 7.87 (d, *J* = 5.0 Hz, 1H), 7.83-7.78 (m, 1H), 7.65 (m, *J* = 8.1 Hz, 1H), 7.51-7.47 (m, 1H), 7.24 (dd, *J* = 5.1, 3.8 Hz, 1H). <sup>13</sup>C NMR (101 MHz, DMSO-*d*<sub>6</sub>) δ 162.4, 149.0, 148.4, 137.8, 135.2, 132.7, 129.9, 129.0, 127.3, 126.8, 126.5, 121.3.



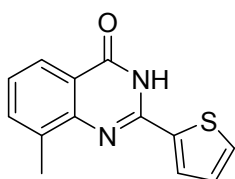
**8-Methyl-2-(2-methylphenyl)-4(3H)-quinazolinone (3bb):** White solid; 70% yield (35 mg); mp 249-251 °C; TLC (PE: EA=2:1) R<sub>f</sub> = 0.42. <sup>1</sup>H NMR (400 MHz, DMSO-*d*<sub>6</sub>) δ 12.43 (s, 1H), 8.01 (dd, *J* = 8.0, 1.6 Hz, 1H), 7.69 (dt, *J* = 7.1, 1.4 Hz, 1H), 7.54 (dd, *J* = 7.5, 1.5 Hz, 1H), 7.47-7.39 (m, 2H), 7.39-7.31 (m, 2H), 2.54 (s, 3H), 2.45 (s, 3H). <sup>13</sup>C NMR (101 MHz, DMSO-*d*<sub>6</sub>) δ 162.6, 153.5, 147.61, 136.9, 135.9, 135.3, 134.7, 131.2, 130.4, 129.8, 126.6, 126.2, 123.9, 121.3, 20.4, 17.7. Calcd. For C<sub>16</sub>H<sub>14</sub>N<sub>2</sub>O [M+H]<sup>+</sup> : 251.1184, found: 251.1183.



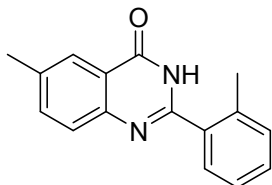
**8-Methyl-2-(4-methylphenyl)-4(3H)-quinazolinone (3bc)<sup>2</sup>:** White solid; 73% yield (36.5 mg); mp 269-271 °C; TLC (PE: EA=2:1) R<sub>f</sub> = 0.42. <sup>1</sup>H NMR (400 MHz, DMSO-*d*<sub>6</sub>) δ 12.46 (s, 1H), 8.13 (d, *J* = 8.3 Hz, 2H), 8.0-7.97 (m, 1H), 7.68 (d, *J* = 6.8 Hz, 1H), 7.40-7.35 (m, 3H), 2.61 (s, 3H), 2.39 (s, 3H). <sup>13</sup>C NMR (101 MHz, DMSO-*d*<sub>6</sub>) δ 163.1, 151.4, 147.7, 141.9, 136.0, 135.4, 130.6, 129.7, 128.1, 126.4, 123.9, 121.2, 21.5, 17.6.



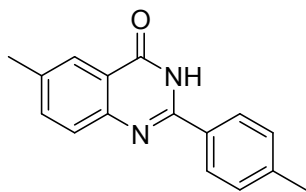
**8-Methyl-2-(2-furanyl)-quinazolinone-4(3H)-one (3bh):** Light yellow solid; 30% yield (13.6 mg); mp 292-293 °C; TLC (PE: EA=3:1) R<sub>f</sub> = 0.40. <sup>1</sup>H NMR (400 MHz, DMSO-*d*<sub>6</sub>) δ 12.50 (s, 1H), 8.02 (d, *J* = 1.7 Hz, 1H), 7.97 (dd, *J* = 8.0, 1.6 Hz, 1H), 7.68 (d, *J* = 7.2 Hz, 1H), 7.63 (d, *J* = 3.6 Hz, 1H), 7.38 (t, *J* = 7.6 Hz, 1H), 6.76 (dd, *J* = 3.6, 1.8 Hz, 1H), 2.58 (s, 3H). <sup>13</sup>C NMR (101 MHz, DMSO-*d*<sub>6</sub>) δ 162.4, 147.6, 147.0, 146.8, 143.5, 135.9, 135.5, 126.4, 124.1, 121.6, 114.8, 112.9, 17.7. Calcd. For C<sub>13</sub>H<sub>10</sub>N<sub>2</sub>O<sub>2</sub> [M+H]<sup>+</sup> : 227.0821, found: 227.0818.



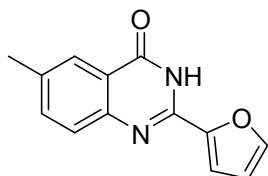
**8-Methyl-2-(2-thienyl)-quinazolinone-4(3H)-one (3bi):** White solid; 31% yield (15.0 mg); mp 237-243 °C; TLC (PE: EA=3:1) R<sub>f</sub> = 0.40. <sup>1</sup>H NMR (400 MHz, DMSO-*d*<sub>6</sub>) δ 12.66 (s, 1H), 8.21 (d, *J* = 3.7 Hz, 1H), 7.96 (d, *J* = 7.8 Hz, 1H), 7.86 (d, *J* = 5.0 Hz, 1H), 7.67 (d, *J* = 7.3 Hz, 1H), 7.37 (t, *J* = 7.6 Hz, 1H), 7.23 (dd, *J* = 5.1, 3.8 Hz, 1H), 2.57 (s, 3H). <sup>13</sup>C NMR (101 MHz, DMSO-*d*<sub>6</sub>) δ 162.6, 147.5, 147.2, 138.3, 135.5, 135.5, 132.6, 129.5, 129.0, 126.3, 124.1, 121.2, 17.3. Calcd. For C<sub>13</sub>H<sub>10</sub>N<sub>2</sub>OS [M+H]<sup>+</sup> : 243.0592, found: 243.0589.



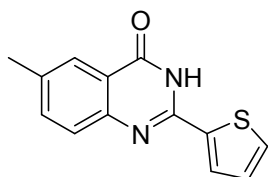
**6-Methyl-2-(2-methylphenyl)-4(3H)-quinazolinone (3cb)<sup>8</sup>:** White solid; 72% yield (36 mg); mp 215-217 °C; TLC (PE: EA=2:1) R<sub>f</sub> = 0.42. <sup>1</sup>H NMR (400 MHz, DMSO-*d*<sub>6</sub>) δ 12.37 (s, 1H), 8.01-7.92 (m, 1H), 7.66 (dd, *J* = 8.3, 2.1 Hz, 1H), 7.60 (d, *J* = 8.3 Hz, 1H), 7.50 (d, *J* = 7.6 Hz, 1H), 7.45-7.41 (m, 1H), 7.36-7.31 (m, 2H), 2.47 (s, 3H), 2.38 (s, 3H). <sup>13</sup>C NMR (101 MHz, DMSO-*d*<sub>6</sub>) δ 161.7, 153.5, 146.7, 136.3, 136.1, 135.7, 134.2, 130.5, 129.8, 129.0, 127.2, 125.7, 125.1, 120.6, 20.8, 19.5.



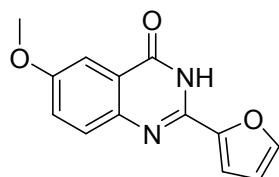
**6-Methyl-2-(4-methylphenyl)-4(3H)-quinazolinone (3cc)**<sup>7</sup>: White solid; 75% yield (37.5 mg); mp 271-272 °C; TLC (PE: EA=2:1) R<sub>f</sub> = 0.42. <sup>1</sup>H NMR (400 MHz, DMSO-*d*<sub>6</sub>) δ 12.39 (s, 1H), 8.12-8.04 (m, 2H), 7.95 (d, *J* = 1.8 Hz, 1H), 7.70-7.60 (m, 2H), 7.36 (d, *J* = 8.0 Hz, 2H), 2.46 (s, 3H), 2.40 (s, 3H). <sup>13</sup>C NMR (101 MHz, DMSO-*d*<sub>6</sub>) δ 162.2, 151.4, 141.3, 136.1, 135.8, 129.9, 129.3, 129.2, 127.5, 127.2, 125.2, 120.6, 20.9, 20.8.



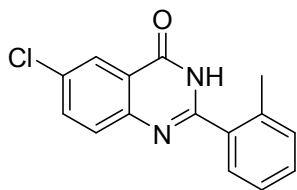
**6-Methyl-2-(2-furanyl)-quinazolinone-4(3H)-one (3ch)**<sup>9</sup>: Light yellow solid; 36% yield (16.3 mg); mp 256-257 °C; TLC (PE: EA=3:1) R<sub>f</sub> = 0.40. <sup>1</sup>H NMR (400 MHz, DMSO-*d*<sub>6</sub>) δ 12.42 (s, 1H), 7.99 (d, *J* = 1.7 Hz, 1H), 7.94-7.89 (m, 1H), 7.67-7.56 (m, 3H), 6.74 (dd, *J* = 3.6, 1.8 Hz, 1H), 2.44 (s, 3H). <sup>13</sup>C NMR (101 MHz, DMSO-*d*<sub>6</sub>) δ 161.5, 146.6, 146.3, 146.1, 143.3, 136.2, 135.9, 127.1, 125.3, 120.8, 114.1, 112.4, 20.8.



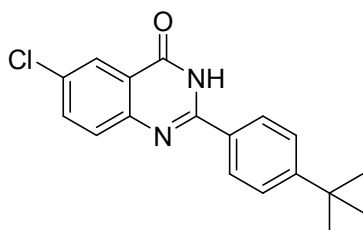
**6-Methyl-2-(2-thienyl)-quinazolinone-4(3H)-one (3ci)**<sup>10</sup>: White solid; 32% yield (15.5 mg); mp 266-267 °C; TLC (PE: EA=3:1) R<sub>f</sub> = 0.40. <sup>1</sup>H NMR (400 MHz, DMSO-*d*<sub>6</sub>): δ 12.58 (s, 1H), 8.20 (dd, *J* = 3.9, 1.2 Hz, 1H), 7.93 (d, *J* = 1.6 Hz, 1H), 7.85 (dd, *J* = 5.0, 1.1 Hz, 1H), 7.63 (dd, *J* = 8.3, 2.1 Hz, 1H), 7.56 (d, *J* = 8.3 Hz, 1H), 7.23 (dd, *J* = 5.0, 3.8 Hz, 1H), 2.44 (s, 3H). <sup>13</sup>C NMR (101 MHz, DMSO-*d*<sub>6</sub>) δ 161.7, 147.0, 146.6, 137.4, 136.1, 135.9, 131.8, 129.1, 128.4, 126.8, 125.4, 120.6, 20.8.



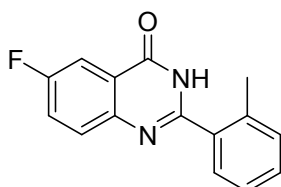
**6-Methoxy-2-(2-furanyl)-quinazolinone-4(3H)-one (3dh)**: Light yellow solid; 25% yield (12.1 mg); mp > 300 °C; TLC (PE: EA=2:1), R<sub>f</sub> = 0.40. <sup>1</sup>H NMR (400 MHz, DMSO-*d*<sub>6</sub>) δ 12.48 (s, 1H), 7.97 (s, 1H), 7.65 (d, *J* = 8.9 Hz, 1H), 7.58 (d, *J* = 3.5 Hz, 1H), 7.53 (d, *J* = 2.9 Hz, 1H), 7.43 (dd, *J* = 8.9, 3.0 Hz, 1H), 6.74 (dd, *J* = 3.3, 1.6 Hz, 1H), 3.88 (s, 3H). <sup>13</sup>C NMR (101 MHz, DMSO-*d*<sub>6</sub>+MeOD) δ 161.7, 158.2, 146.6, 146.4, 143.4, 142.4, 129.3, 124.4, 122.3, 113.9, 112.7, 106.5, 55.9. HR-MS (ESI<sup>+</sup>): Calcd. For C<sub>13</sub>H<sub>10</sub>N<sub>2</sub>O<sub>3</sub> [M+H]<sup>+</sup> : 243.0770, found: 243.0766.



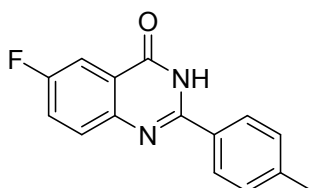
**6-Chloro-2-(2-methylphenyl)-4(3H)-quinazolinone (3eb)<sup>11</sup>:** White solid; 64% yield (34.6 mg); mp 255-259 °C; TLC (PE: EA=2:1), R<sub>f</sub> = 0.42. <sup>1</sup>H NMR (400 MHz, DMSO-*d*<sub>6</sub>) δ 12.63 (s, 1H), 8.11 (d, *J* = 2.5 Hz, 1H), 7.87 (dd, *J* = 8.7, 2.6 Hz, 1H), 7.73 (d, *J* = 8.7 Hz, 1H), 7.52 (d, *J* = 7.6 Hz, 1H), 7.47-7.43 (m, 1H), 7.37-7.32 (m, 2H), 2.39 (s, 3H). <sup>13</sup>C NMR (101 MHz, DMSO-*d*<sub>6</sub>) δ 160.9, 154.9, 147.4, 136.1, 134.5, 133.9, 130.8, 130.5, 130.0, 129.1, 125.7, 124.8, 122.2, 19.5.



**6-Chloro-2-[4-(1,1-dimethylethyl)phenyl]-4(3H)-quinazolinone (3ed):** White solid; 62% yield (38.7 mg); mp > 300 °C; TLC (PE: EA=2:1 to 3:1), R<sub>f</sub> = 0.42. <sup>1</sup>H NMR (400 MHz, DMSO-*d*<sub>6</sub>) δ 12.66 (s, 1H), 8.16-8.10 (m, 2H), 8.08 (d, *J* = 2.5 Hz, 1H), 7.85 (dd, *J* = 8.7, 2.5 Hz, 1H), 7.75 (d, *J* = 8.7 Hz, 1H), 7.60-7.53 (m, 2H), 1.33 (s, 10H). <sup>13</sup>C NMR (101 MHz, DMSO-*d*<sub>6</sub>) δ 161.9, 155.0, 153.2, 148.0, 135.1, 131.0, 130.1, 128.1, 126.8, 125.9, 125.3, 122.6, 35.2, 31.4. HR-MS (ESI<sup>+</sup>): Calcd. For C<sub>18</sub>H<sub>17</sub>ClN<sub>2</sub>O [M+H]<sup>+</sup> : 313.1108, found: 313.1107.



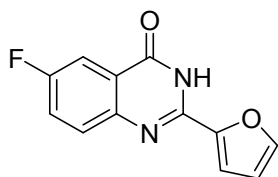
**6-Fluoro-2-(2-methylphenyl)-4(3H)-quinazolinone (3fb):** White solid; 67% yield (34.0 mg); mp 233-237 °C; TLC (PE: EA=3:1 to 5:1) R<sub>f</sub> = 0.40. <sup>1</sup>H NMR (400 MHz, DMSO-*d*<sub>6</sub>) δ 12.60 (s, 1H), 7.83 (dd, *J* = 8.6, 2.9 Hz, 1H), 7.79-7.67 (m, 2H), 7.50 (d, *J* = 7.6 Hz, 1H), 7.45-7.41 (m, 1H), 7.35-7.31 (m, 2H), 2.38 (s, 3H). <sup>13</sup>C NMR (101 MHz, DMSO-*d*<sub>6</sub>) δ 161.7 (d, *J* = 8.7 Hz), 159.3, 154.4, 146.0, 136.6, 134.5, 131.0, 130.7 (d, *J* = 13.0 Hz), 130.4, 129.6, 126.2, 123.4 (d, *J* = 44.4 Hz), 122.6 (d, *J* = 8.1 Hz), 110.9 (d, *J* = 23.2 Hz), 20.0. <sup>19</sup>F NMR (376 MHz, DMSO-*d*<sub>6</sub>) δ -113.5. HR-MS (ESI<sup>+</sup>): Calcd. For C<sub>15</sub>H<sub>11</sub>FN<sub>2</sub>O [M+H]<sup>+</sup>: 255.0934, found: 255.0930.



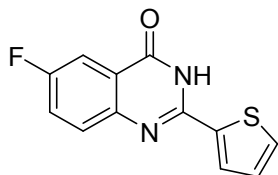
**6-Fluoro-2-(4-methylphenyl)-4(3H)-quinazolinone (3fc)<sup>4</sup>:** White solid; 70% yield (35.6 mg); mp 301-303 °C; TLC (PE: EA=3:1 to 5:1) R<sub>f</sub> = 0.40. <sup>1</sup>H NMR (400 MHz, DMSO-*d*<sub>6</sub>) δ



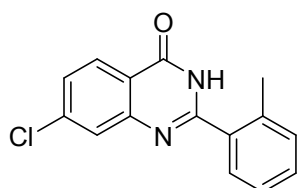
12.56 (s, 1H), 8.06 (d,  $J = 8.0$  Hz, 2H), 7.80-7.75 (m, 2H), 7.70-7.65 (m, 1H), 7.32 (d,  $J = 8.0$  Hz, 2H), 2.37 (s, 3H).  $^{13}\text{C}$  NMR (101 MHz,  $\text{DMSO-}d_6$ )  $\delta$  162.4, 161.5, 159.1, 152.4, 146.1, 141.9, 130.4 (d,  $J = 34.3$  Hz), 129.7, 128.1, 123.5 (d,  $J = 25.3$  Hz), 122.5 (d,  $J = 9.1$  Hz), 111.9 (d,  $J = 23.2$  Hz), 21.5.  $^{19}\text{F}$  NMR (376 MHz,  $\text{DMSO-}d_6$ )  $\delta$  -113.8.



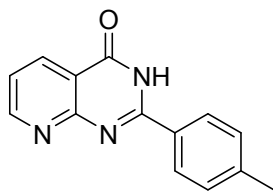
**6-Fluoro-2-(2-furanyl)-4(3H)-quinazolinone (3fh):** Light yellow solid; 30% yield (13.8 mg); mp > 300 °C; TLC (PE: EA=3:1 to 6:1)  $R_f = 0.40$ .  $^1\text{H}$  NMR (400 MHz,  $\text{DMSO-}d_6$ )  $\delta$  12.65 (s, 1H), 8.01 (dd,  $J = 1.8, 0.7$  Hz, 1H), 7.84-7.75 (m, 2H), 7.71 (td,  $J = 8.7, 3.0$  Hz, 1H), 7.63 (dd,  $J = 3.6, 0.8$  Hz, 1H), 6.76 (dd,  $J = 3.5, 1.7$  Hz, 1H).  $^{13}\text{C}$  NMR (101 MHz,  $\text{DMSO-}d_6$ )  $\delta$  161.5 (d,  $J = 3.0$  Hz), 159.2, 147.1, 146.4, 146.0, 144.0, 130.5 (d,  $J = 8.1$  Hz), 123.6 (d,  $J = 24.2$  Hz), 122.8 (d,  $J = 9.1$  Hz), 115.0, 113.0, 111.2 (d,  $J = 24.2$  Hz).  $^{19}\text{F}$  NMR (376 MHz,  $\text{DMSO-}d_6$ )  $\delta$  -113.6. Calcd. For  $\text{C}_{12}\text{H}_7\text{FN}_2\text{O}_2$   $[\text{M}+\text{H}]^+$  : 231.0570, found: 231.0566.



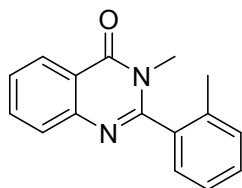
**6-Fluoro-2-(2-thienyl)-4(3H)-quinazolinone (3fi):** White solid; 40% yield (19.7 mg); mp 255-258 °C; TLC (PE: EA=3:1 to 6:1)  $R_f = 0.40$ .  $^1\text{H}$  NMR (400 MHz,  $\text{DMSO-}d_6$ )  $\delta$  12.79 (s, 1H), 8.23 (dd,  $J = 3.8, 1.2$  Hz, 1H), 7.88 (dd,  $J = 5.0, 1.1$  Hz, 1H), 7.82-7.80 (m, 1H), 7.76-7.67 (m, 2H), 7.25-7.23 (m, 1H).  $^{13}\text{C}$  NMR (101 MHz,  $\text{DMSO-}d_6$ )  $\delta$  161.7, 161.5, 159.1, 147.8, 145.9, 137.6, 132.7, 130.2 (d,  $J = 7.9$  Hz), 129.9, 129.0, 123.6 (d,  $J = 24.2$  Hz), 122.5 (d,  $J = 8.3$  Hz).  $^{19}\text{F}$  NMR (376 MHz,  $\text{DMSO-}d_6$ )  $\delta$  -113.8. Calcd. For  $\text{C}_{12}\text{H}_7\text{FN}_2\text{OS}$   $[\text{M}+\text{H}]^+$  : 247.0341, found: 247.0337.



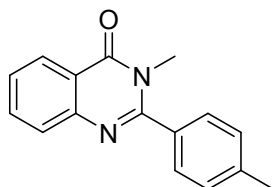
**7-Chloro-2-(2-methylphenyl)-4(3H)-quinazolinone (3gb):** White solid; 35% yield (18.9 mg); mp 227-236 °C; TLC (PE: EA=2:1 to 4:1)  $R_f = 0.42$ .  $^1\text{H}$  NMR (400 MHz,  $\text{DMSO-}d_6$ )  $\delta$  12.60 (s, 1H), 8.16 (d,  $J = 8.5$  Hz, 1H), 7.76 (d,  $J = 2.1$  Hz, 1H), 7.58 (dd,  $J = 8.5, 2.1$  Hz, 1H), 7.52 (d,  $J = 7.6$ , 1H), 7.47-7.43 (m, 1H), 7.37-7.32 (m, 2H), 2.39 (s, 3H).  $^{13}\text{C}$  NMR (101 MHz,  $\text{DMSO-}d_6$ )  $\delta$  161.7, 156.3, 150.3, 139.5, 136.7, 134.3, 131.1, 130.6, 129.6, 128.4, 127.4, 127.0, 126.2, 120.3, 20.0. HR-MS (ESI $^+$ ): Calcd. For  $\text{C}_{15}\text{H}_{11}\text{ClN}_2\text{O}$   $[\text{M}+\text{H}]^+$  : 271.0638, found: 271.0637.



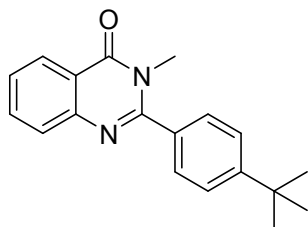
**2-(4-Methylphenyl)- Pyrido[2,3-d]pyrimidin-4(3H)-one (3jc)<sup>12</sup>:** Light yellow solid; 42% yield (19.9 mg); mp 228-229 °C; TLC (PE: EA=3:1) R<sub>f</sub> = 0.40. <sup>1</sup>H NMR (400 MHz, DMSO-*d*<sub>6</sub>) δ 12.75 (s, 1H), 8.96 (dd, *J* = 4.7, 2.1 Hz, 1H), 8.52 (dd, *J* = 7.8, 2.0 Hz, 1H), 8.18-8.10 (m, 2H), 7.52 (dd, *J* = 7.9, 4.5 Hz, 1H), 7.38 (d, *J* = 8.0 Hz, 2H), 2.40 (s, 3H). <sup>13</sup>C NMR (101 MHz, DMSO-*d*<sub>6</sub>) δ 163.0, 158.6, 156.0, 155.3, 142.1, 135.4, 129.6, 129.2, 128.0, 122.0, 116.0, 21.0.



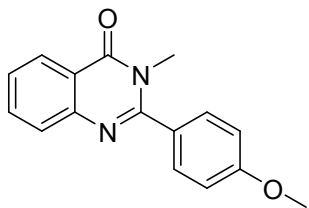
**3-Methyl-2-(2-methylphenyl)-4(3H)-quinazolinone (3ib)<sup>5</sup>:** White solid; 79% yield (39.5 mg); mp 138-139 °C; TLC (PE: EA=2:1) R<sub>f</sub> = 0.40. <sup>1</sup>H NMR (400 MHz, DMSO-*d*<sub>6</sub>) δ 8.22 (dd, *J* = 8.1, 1.5 Hz, 1H), 7.88-7.83 (m, 1H), 7.68 (d, *J* = 8.2 Hz, 1H), 7.48-7.44 (m, 1H), 7.49-7.42 (m, 2H), 7.41-7.35 (m, 2H), 3.22 (s, 3H), 2.19 (s, 3H). <sup>13</sup>C NMR (101 MHz, DMSO-*d*<sub>6</sub>) δ 161.4, 155.7, 147.1, 135.0, 134.9, 134.3, 130.3, 129.5, 127.7, 127.1, 126.9, 126.1, 126.0, 120.3, 32.4, 18.6.



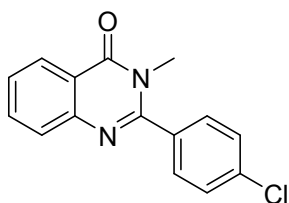
**3-Methyl-2-(4-methylphenyl)- 4(3H)-quinazolinone (3ic)<sup>7</sup>:** White solid; 83% yield (41.5 mg); mp 137-138 °C; TLC (PE: EA=2:1) R<sub>f</sub> = 0.40. <sup>1</sup>H NMR (400 MHz, DMSO-*d*<sub>6</sub>) δ 8.18 (dd, *J* = 8.0, 1.5 Hz, 1H), 7.84-7.80 (m, 1H), 7.66 (d, *J* = 7.8 Hz, 1H), 7.58-7.52 (m, 3H), 7.35 (d, *J* = 8.0 Hz, 2H), 3.38 (s, 3H), 2.40 (s, 3H). <sup>13</sup>C NMR (101 MHz, DMSO-*d*<sub>6</sub>) δ 161.7, 156.2, 147.1, 139.5, 134.3, 132.6, 128.9, 128.3, 127.1, 126.7, 126.0, 120.0, 33.9, 20.9.



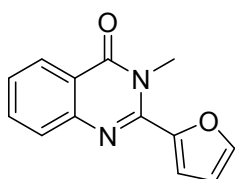
**2-[4-(1,1-Dimethylethyl)phenyl]-3-methyl-4(3H)-quinazolinone (3id)<sup>13</sup>:** White solid; 45% yield (26.3 mg); mp 192-194 °C; TLC (PE: EA=2:1 to 4:1) R<sub>f</sub> = 0.40. <sup>1</sup>H NMR (400 MHz, DMSO-*d*<sub>6</sub>) δ 8.18 (dd, *J* = 8.1, 1.5 Hz, 1H), 7.85-7.81 (m, 1H), 7.66-7.60 (m, 3H), 7.57-7.53 (m, 3H), 1.34 (s, 9H). <sup>13</sup>C NMR (101 MHz, DMSO-*d*<sub>6</sub>) δ 162.2, 156.7, 152.9, 147.6, 134.8, 133.1, 128.6, 127.6, 127.3, 126.5, 125.6, 120.5, 35.1, 34.5, 31.5.



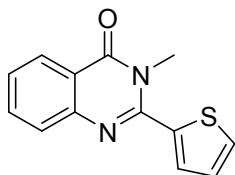
**2-(4-Methoxyphenyl)-3-methyl-4(3H)-quinazolinone (3ie)<sup>7</sup>:** White solid; 80% yield (42.6 mg); mp 140-142 °C; TLC (PE: EA=2:1 to 3:1) R<sub>f</sub> = 0.40. <sup>1</sup>H NMR (400 MHz, DMSO-*d*<sub>6</sub>) δ 8.17 (dd, *J* = 8.0, 1.5 Hz, 1H), 7.84-7.80 (m, 1H), 7.67-7.64 (m, 3H), 7.55-7.51 (m, 1H), 7.09 (d, *J* = 8.7 Hz, 2H), 3.85 (s, 3H), 3.41 (s, 3H). <sup>13</sup>C NMR (101 MHz, DMSO-*d*<sub>6</sub>) δ 161.8, 160.3, 156.0, 147.1, 134.2, 130.1, 127.6, 127.1, 126.6, 126.0, 119.9, 113.7, 55.3, 34.1.



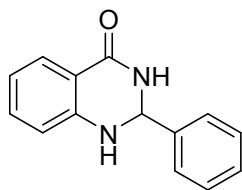
**2-(4-Chlorophenyl)-3-methyl-4(3H)-quinazolinone (3ig)<sup>7</sup>:** White solid; 35% yield (18.9 mg); mp 110-112 °C; TLC (PE: EA=3:1 to 5:1) R<sub>f</sub> = 0.40. <sup>1</sup>H NMR (400 MHz, DMSO-*d*<sub>6</sub>) δ 8.20 (dd, *J* = 8.0, 1.5 Hz, 1H), 7.87-7.83 (m, 1H), 7.75-7.73 (m, 2H), 7.69 (d, *J* = 8.0 Hz, 1H), 7.63 (d, *J* = 8.5 Hz, 2H), 7.60-7.56 (m, 1H), 3.37 (s, 3H). <sup>13</sup>C NMR (101 MHz, DMSO-*d*<sub>6</sub>) δ 161.5, 155.2, 146.9, 134.6, 134.4, 134.2, 130.3, 128.5, 127.2, 127.0, 126.1, 120.2, 33.8.



**2-(2-Furanyl)-3-methyl-4(3H)-quinazolinone (3ih)<sup>13</sup>:** yellow solid; 42% yield (19.0 mg); mp 106-108 °C; TLC (PE: EA=3:1 to 4:1) R<sub>f</sub> = 0.40. <sup>1</sup>H NMR (400 MHz, DMSO-*d*<sub>6</sub>) δ 8.16 (dd, *J* = 8.0, 1.6 Hz, 1H), 8.03 (d, *J* = 1.8 Hz, 1H), 7.86-7.81 (m, 1H), 7.69 (d, *J* = 7.8 Hz, 1H), 7.54 (t, *J* = 7.1 Hz, 1H), 7.33 (d, *J* = 3.5 Hz, 1H), 6.78 (dd, *J* = 3.5, 1.8 Hz, 1H), 3.68 (s, 3H). <sup>13</sup>C NMR (101 MHz, DMSO-*d*<sub>6</sub>) δ 162.0, 147.4, 147.2, 146.7, 146.2, 135.0, 127.6, 127.5, 126.7, 120.3, 116.6, 112.5, 33.2.

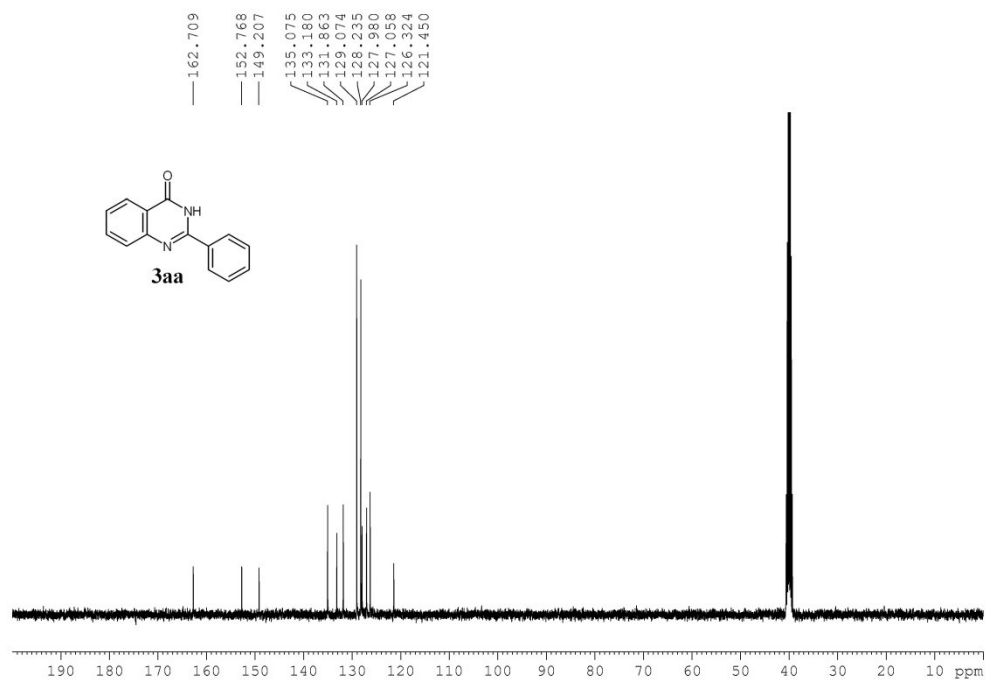
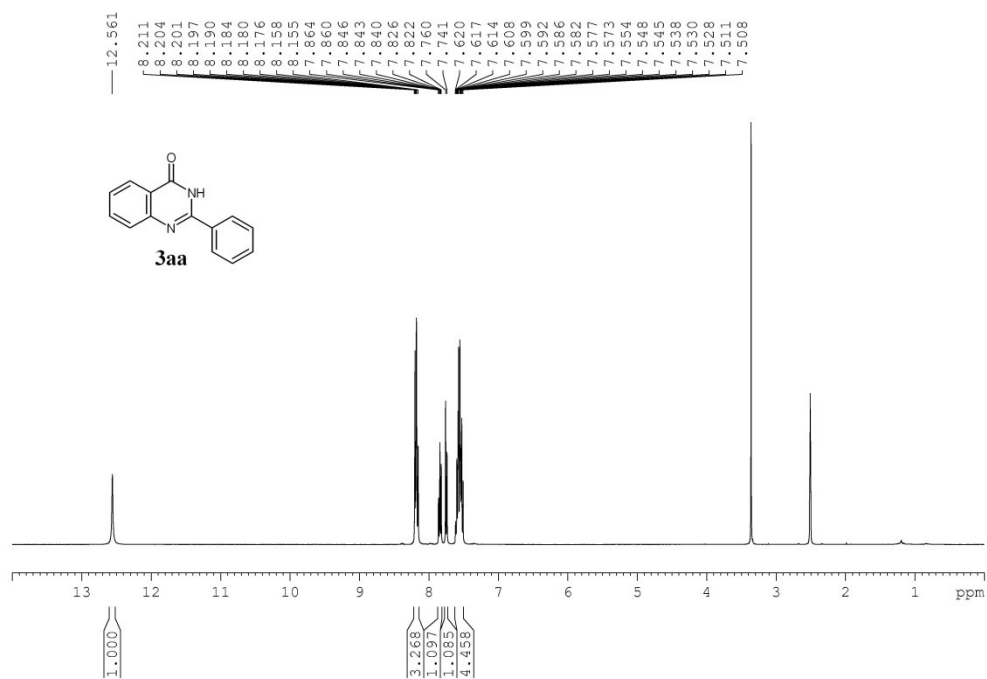


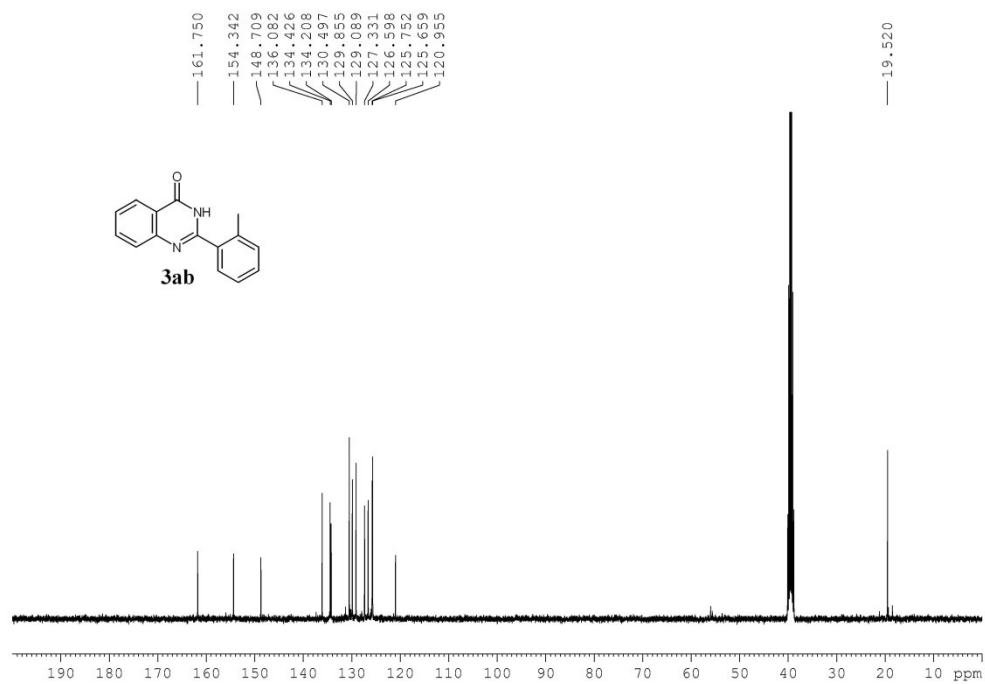
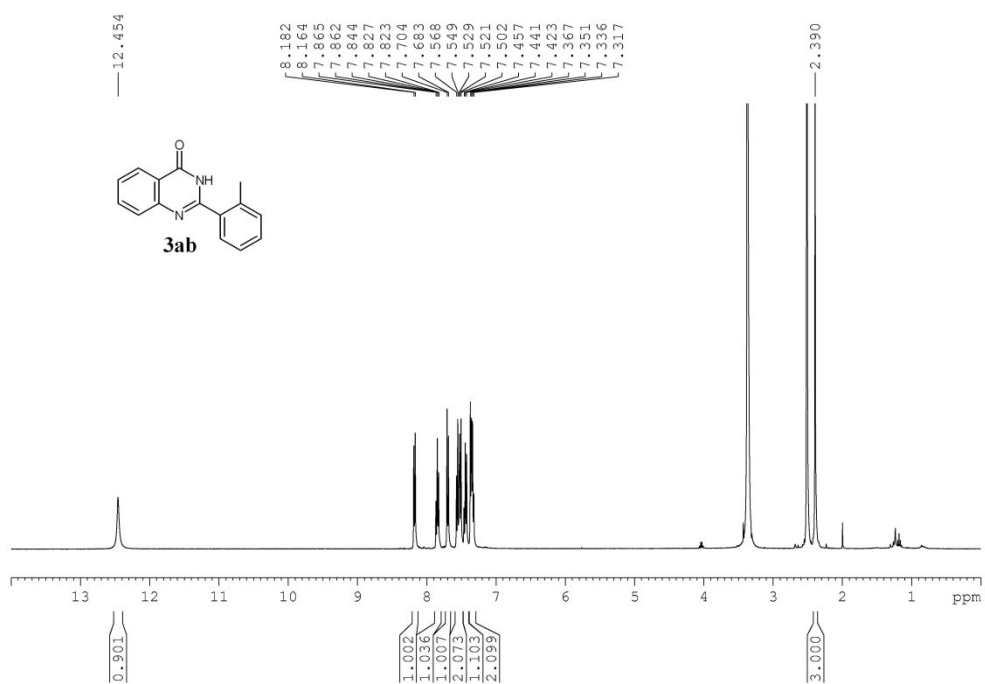
**3-Methyl-2-(2-thienyl)-4(3H)-quinazolinone (3ii)<sup>5</sup>:** White solid; 63% yield (30.5 mg); mp 235-238 °C; TLC (PE: EA=3:1 to 4:1) R<sub>f</sub> = 0.40. <sup>1</sup>H NMR (400 MHz, DMSO-*d*<sub>6</sub>) δ 8.17-8.11 (m, 1H), 7.87 (d, *J* = 5.1 Hz, 1H), 7.84-7.77 (m, 2H), 7.65 (d, *J* = 8.1 Hz, 1H), 7.52 (m, 1H), 7.25 (m, 7.26-7.23, 1H), 3.70 (s, 3H). <sup>13</sup>C NMR (101 MHz, DMSO-*d*<sub>6</sub>) δ 162.2, 150.5, 147.2, 137.6, 135.0, 131.4, 131.0, 128.3, 127.4, 127.3, 126.7, 119.9, 34.2.

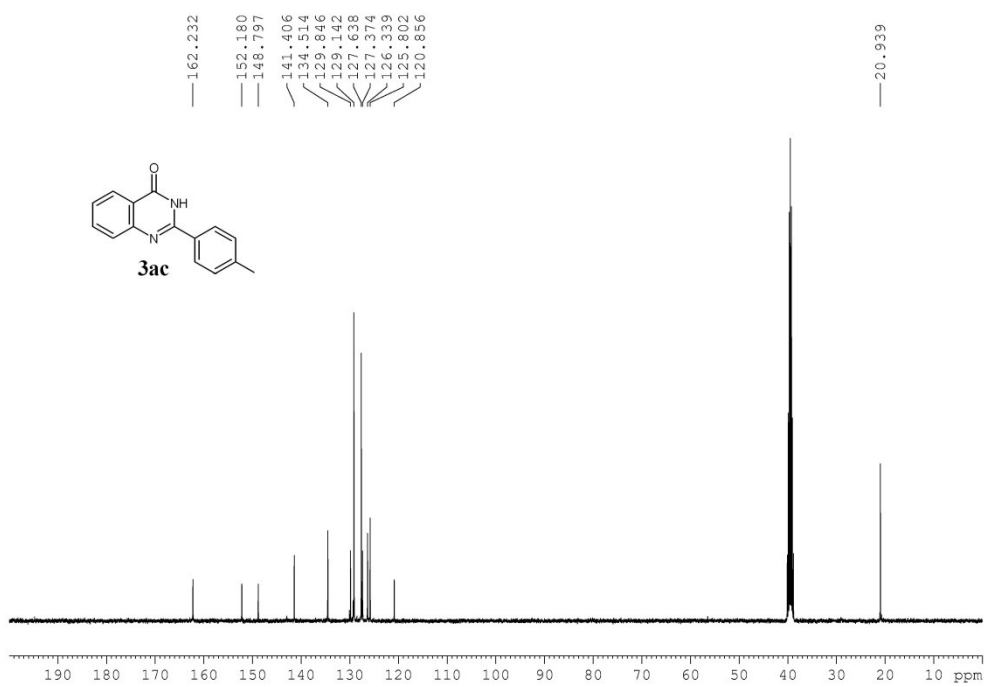
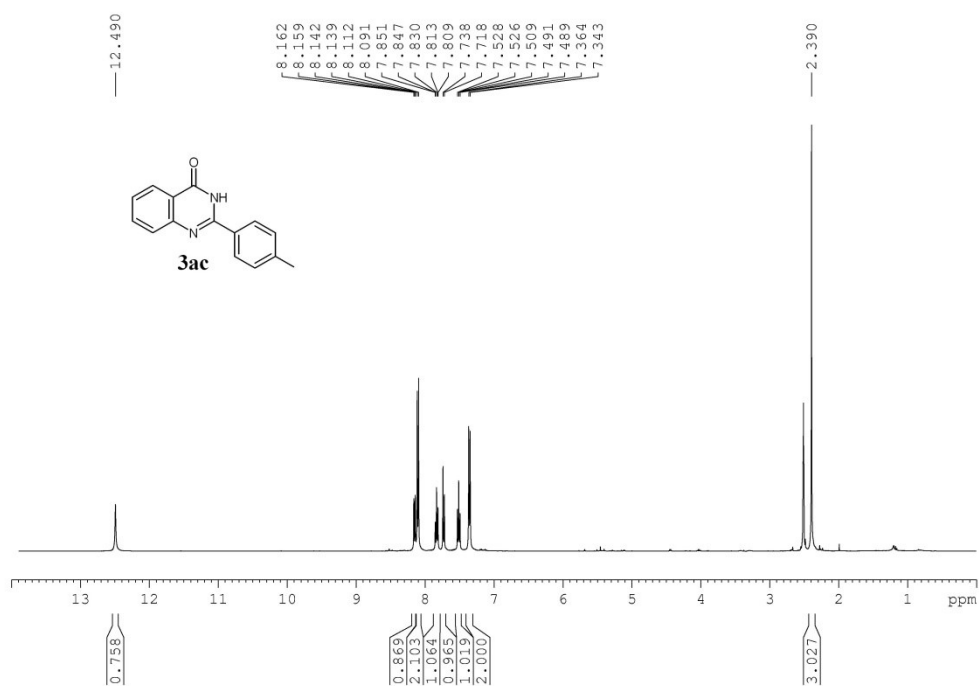


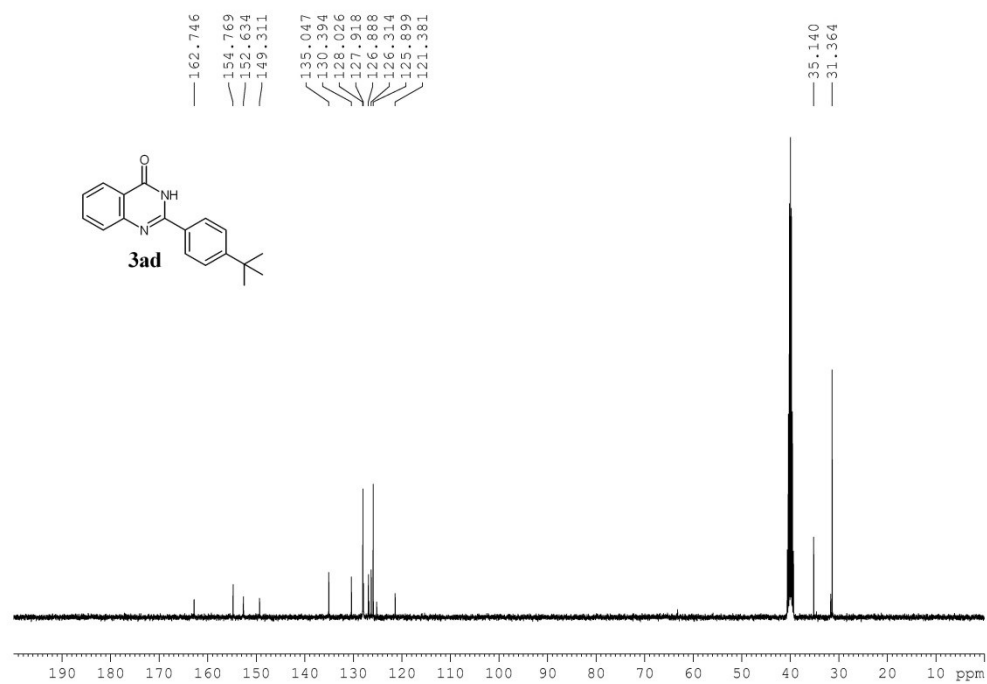
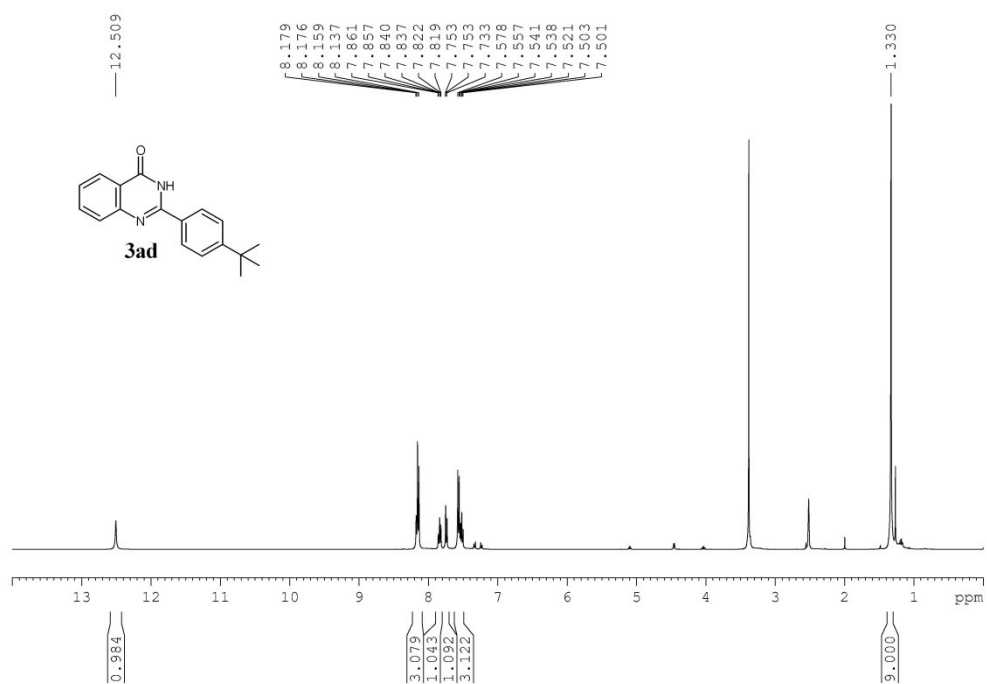
**2-Phenyl-2,3-dihydroquinazolin-4(1H)-one (4aa)<sup>3</sup>**: White solid; TLC (PE: EA=3:1),  $R_f = 0.30$ .  $^1\text{H}$  NMR (400 MHz,  $\text{DMSO-}d_6$ )  $\delta$  8.32 (s, 1H), 7.63 (dd,  $J = 7.8, 1.6$  Hz, 1H), 7.52-7.50 (d, 7.58 Hz, 2H), 7.39 (m, 7.42-7.34, 3H), 7.26 (t,  $J = 7.62$  Hz, 1H), 7.14 (s, 1H), 6.77 (d,  $J = 7.9$  Hz, 1H), 6.69 (td,  $J = 7.4, 1.1$  Hz, 1H), 5.77 (s, 1H).  $^{13}\text{C}$  NMR (101 MHz,  $\text{DMSO-}d_6$ )  $\delta$  164.1, 148.3, 142.1, 133.8, 128.9, 128.8, 127.8, 127.3, 117.6, 115.4, 114.9, 67.0.

## 5. Copies of $^1\text{H}$ , $^{13}\text{C}$ , $^{19}\text{F}$ NMR Spectra for the Products

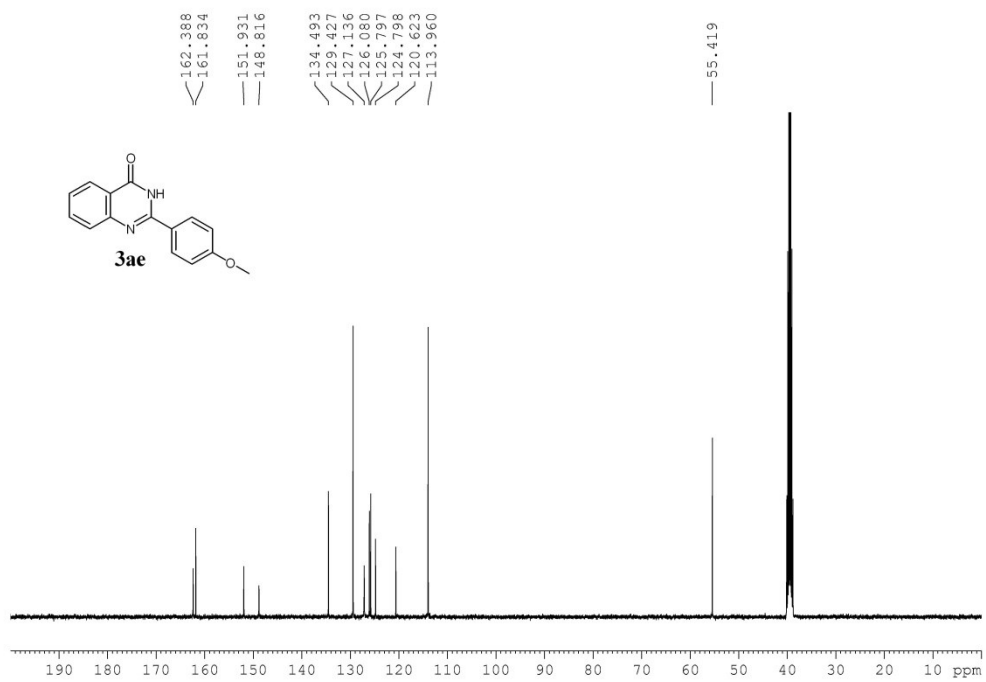
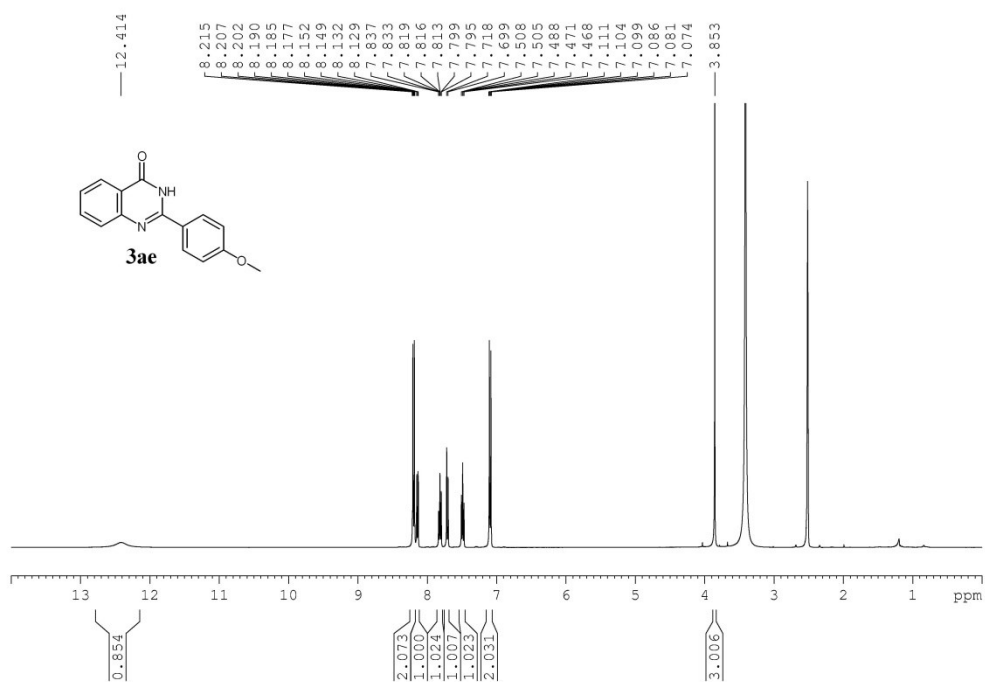


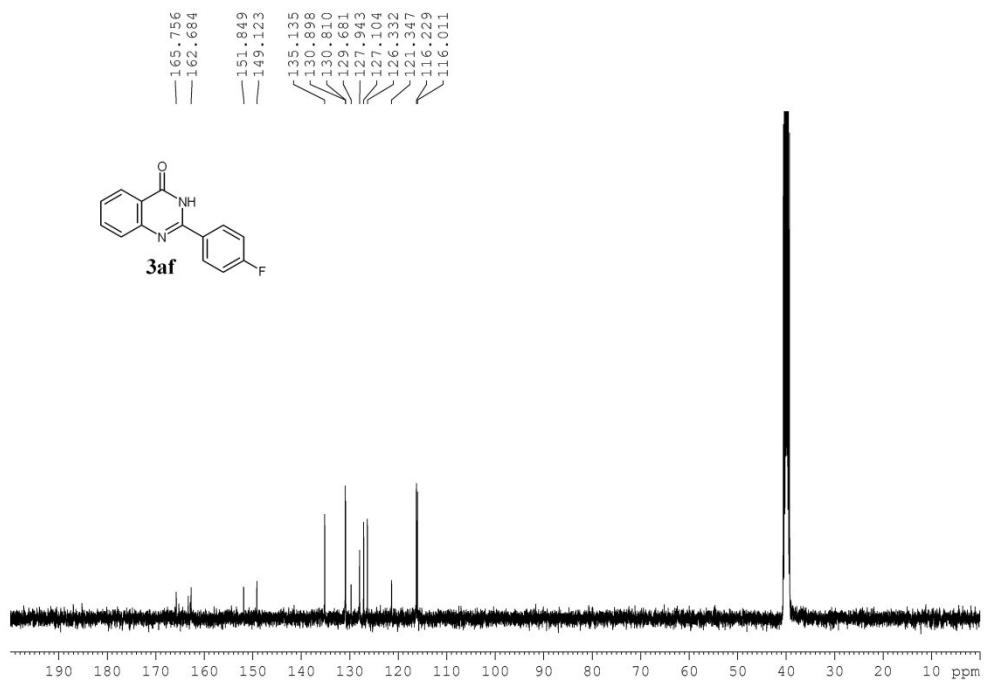
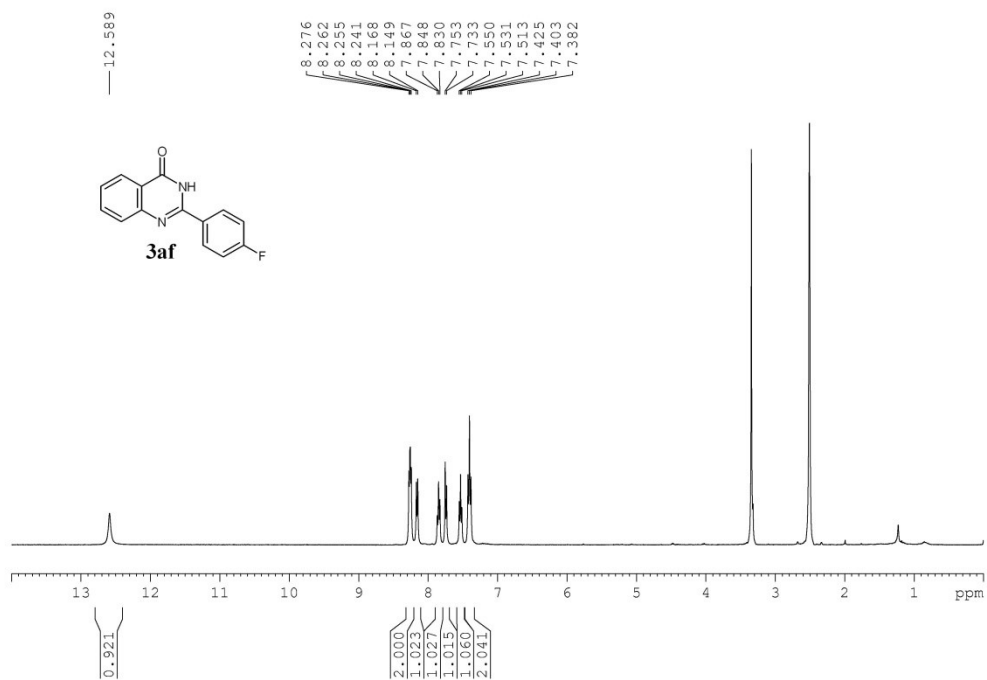


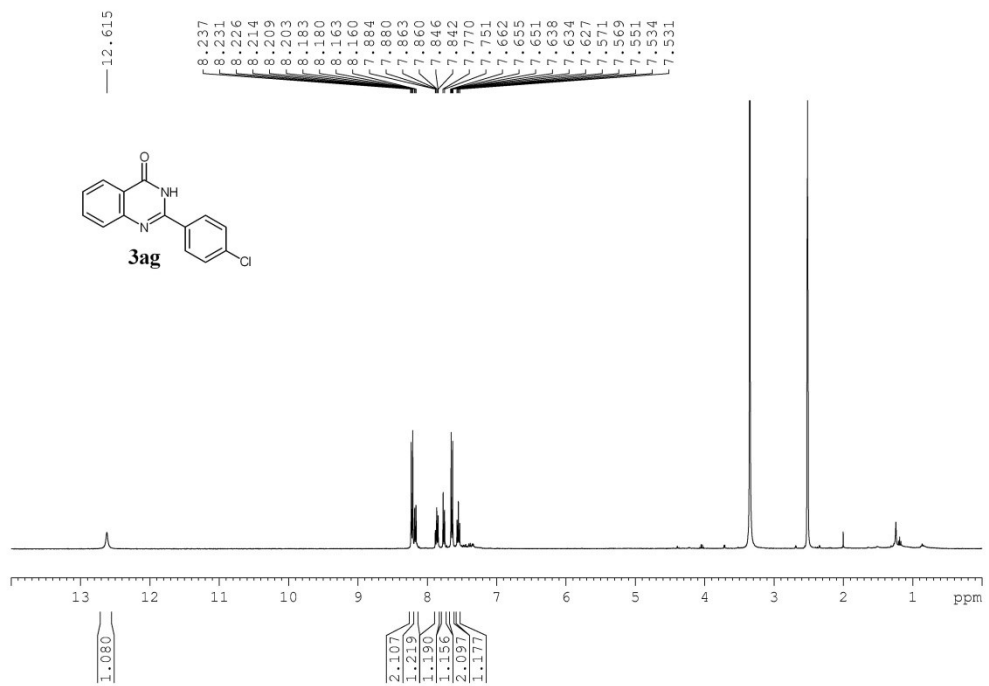
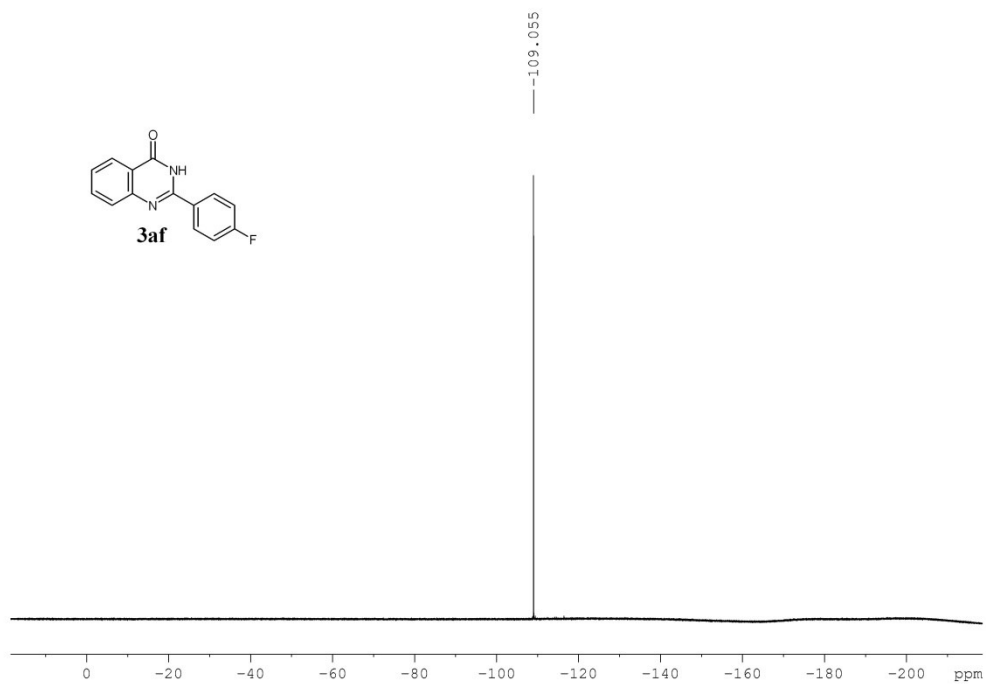


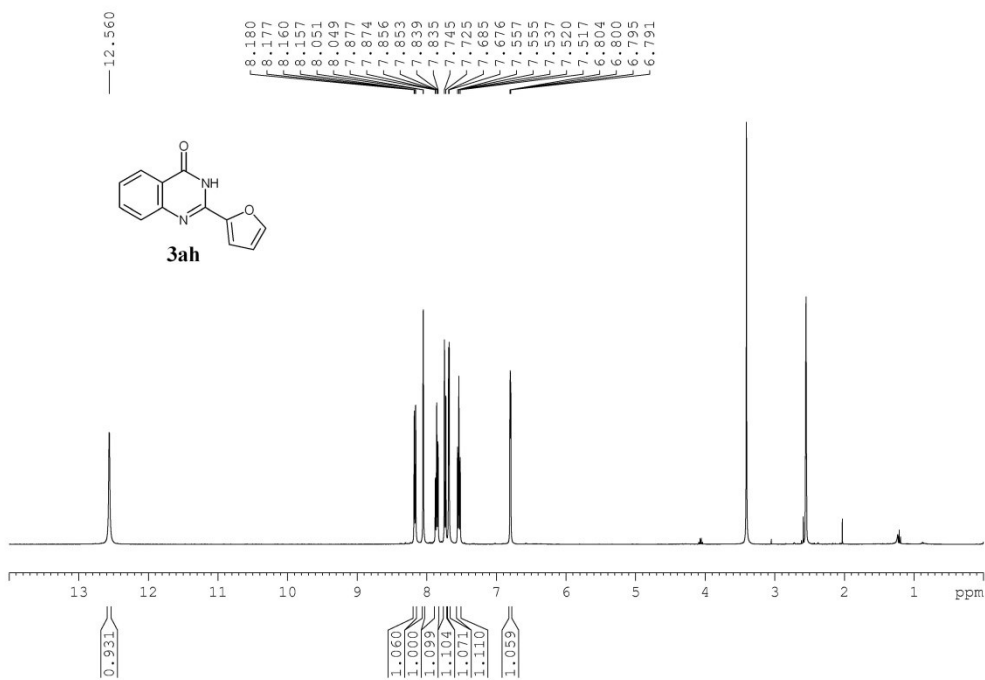
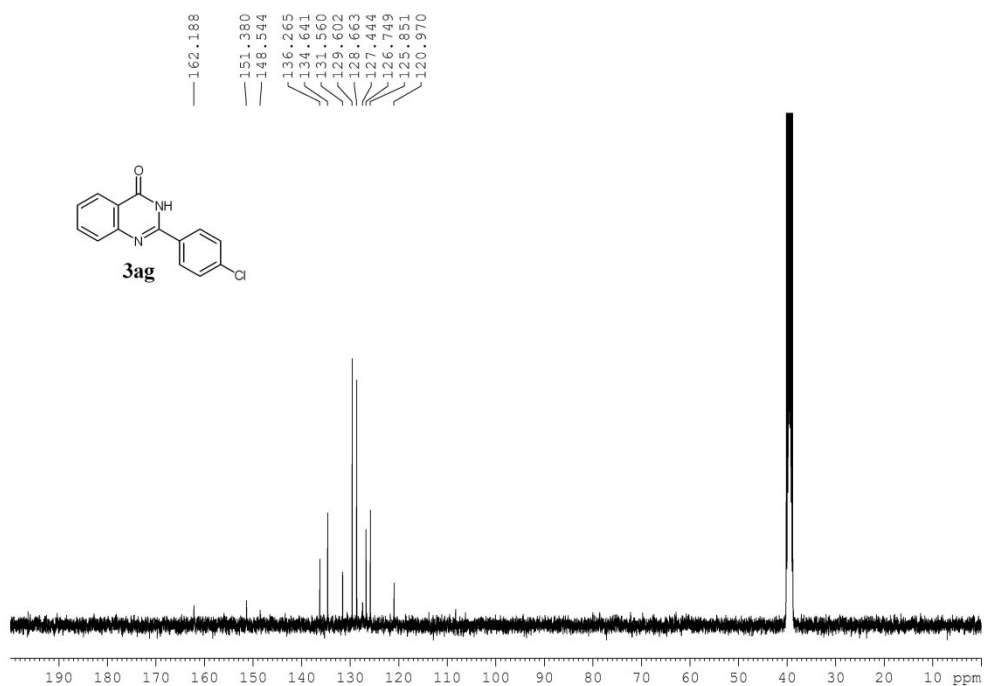


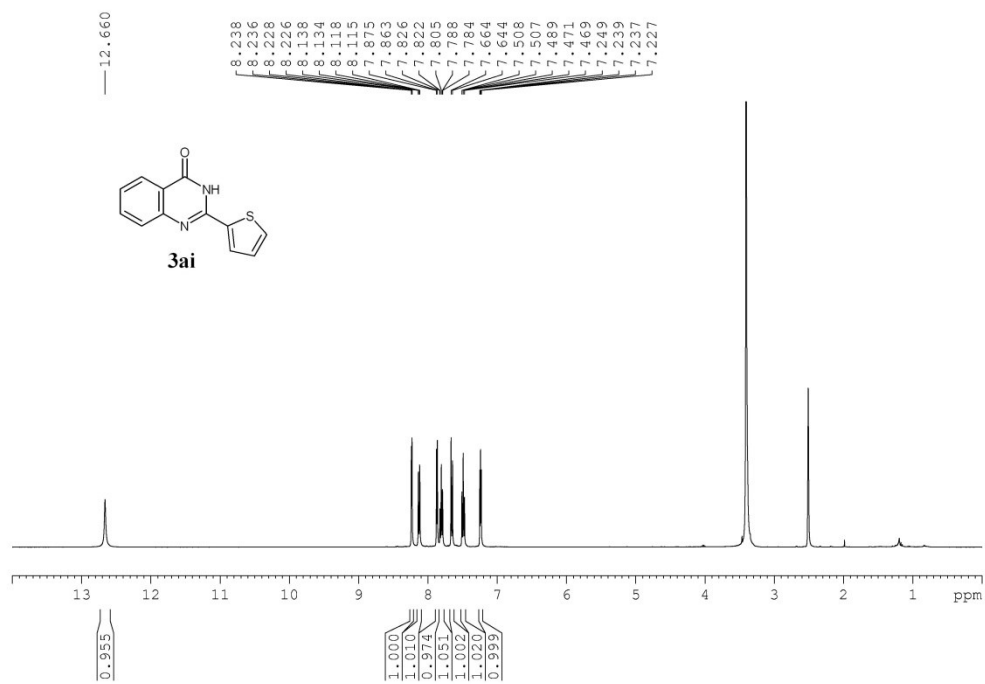
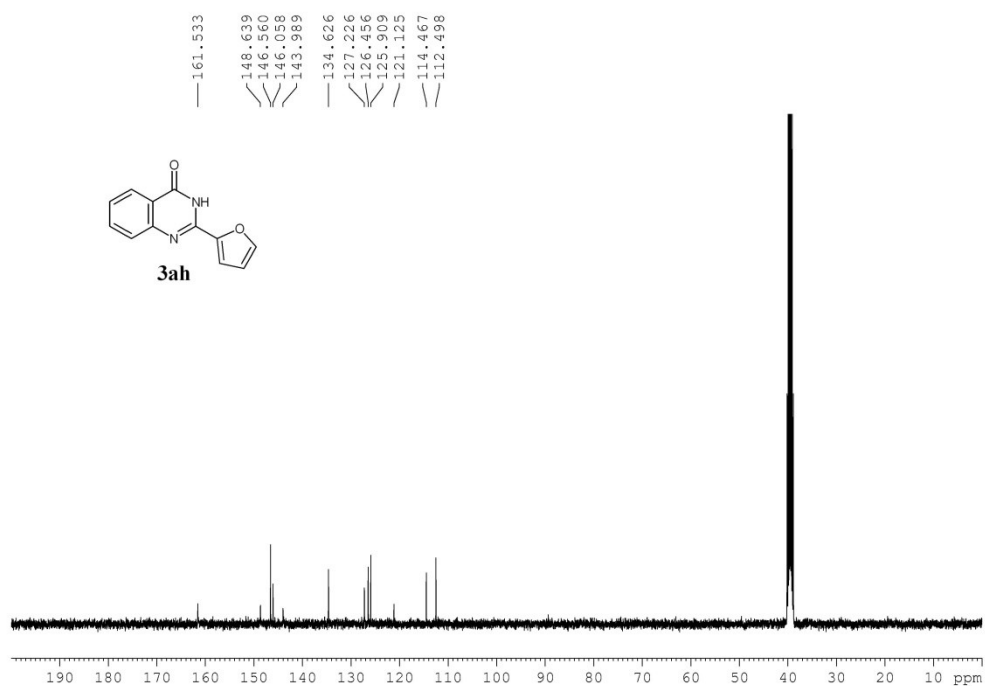


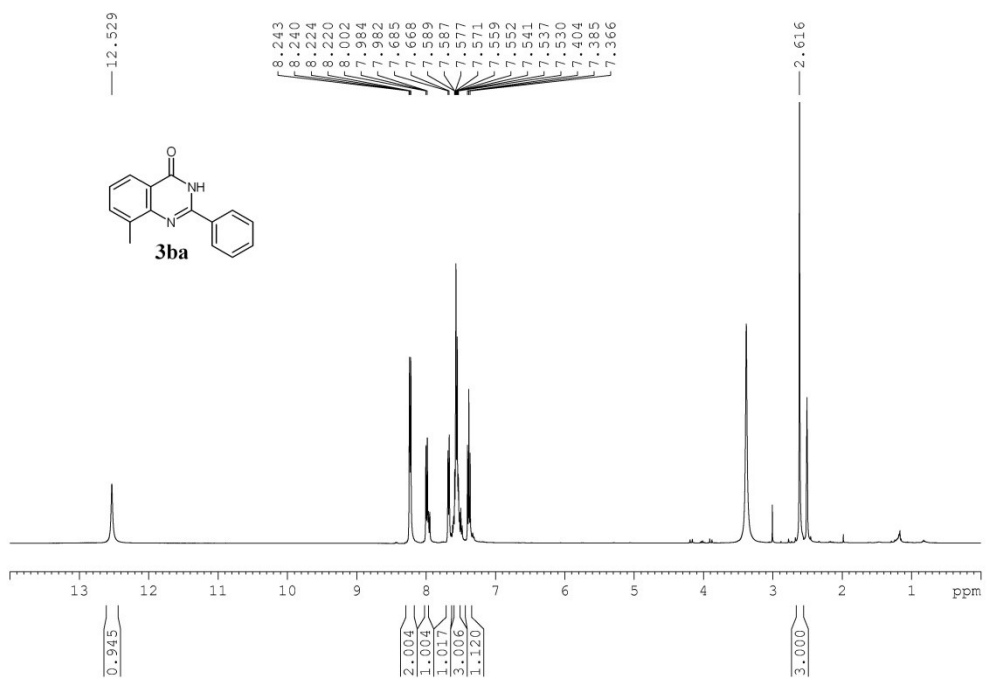
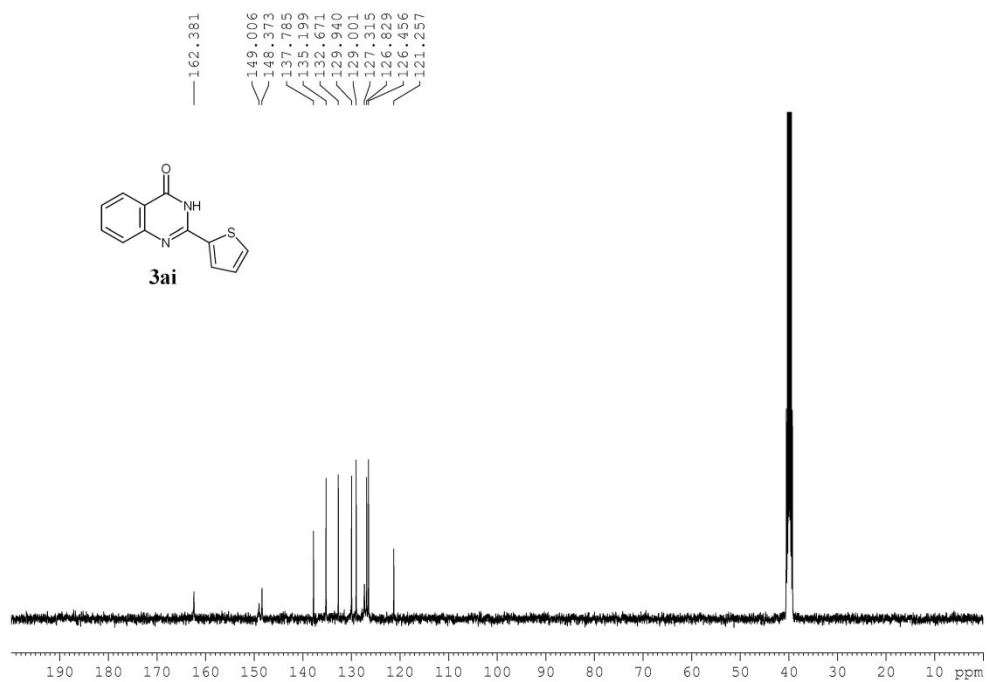


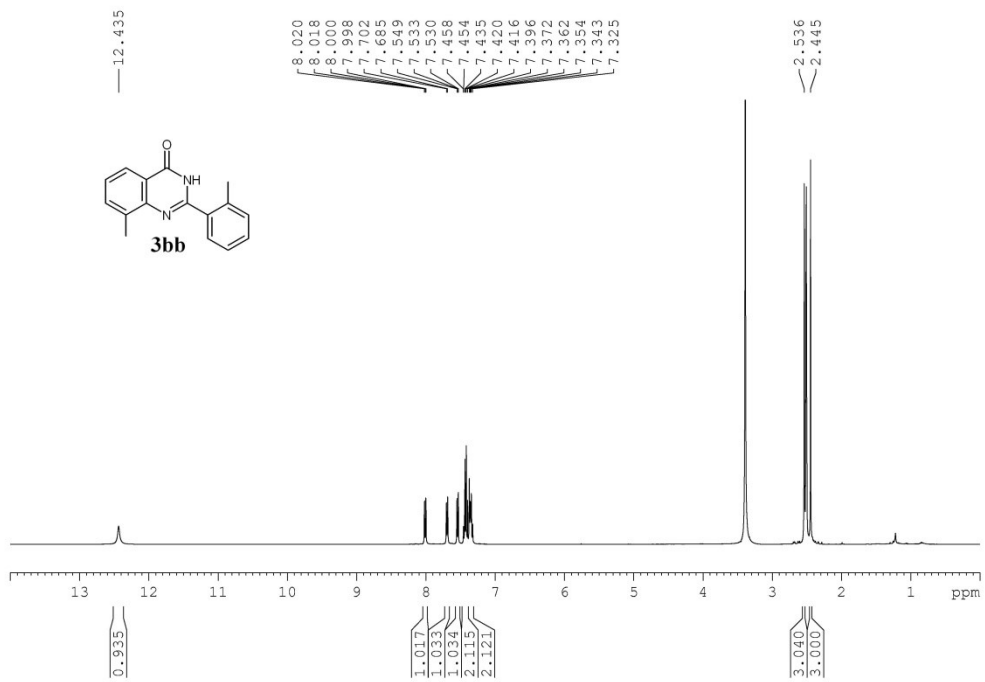
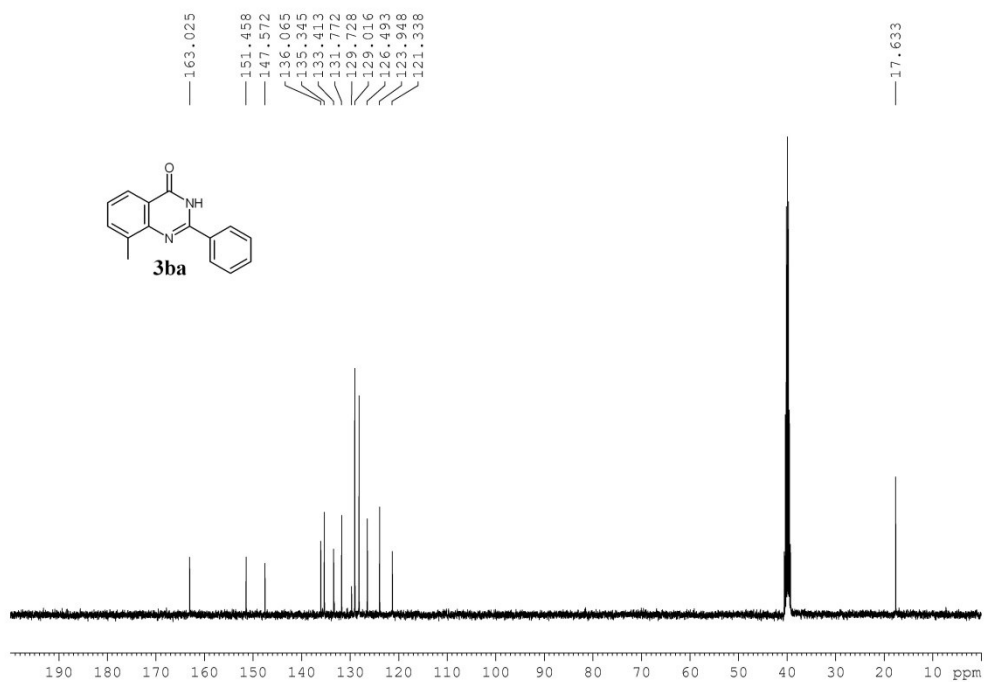


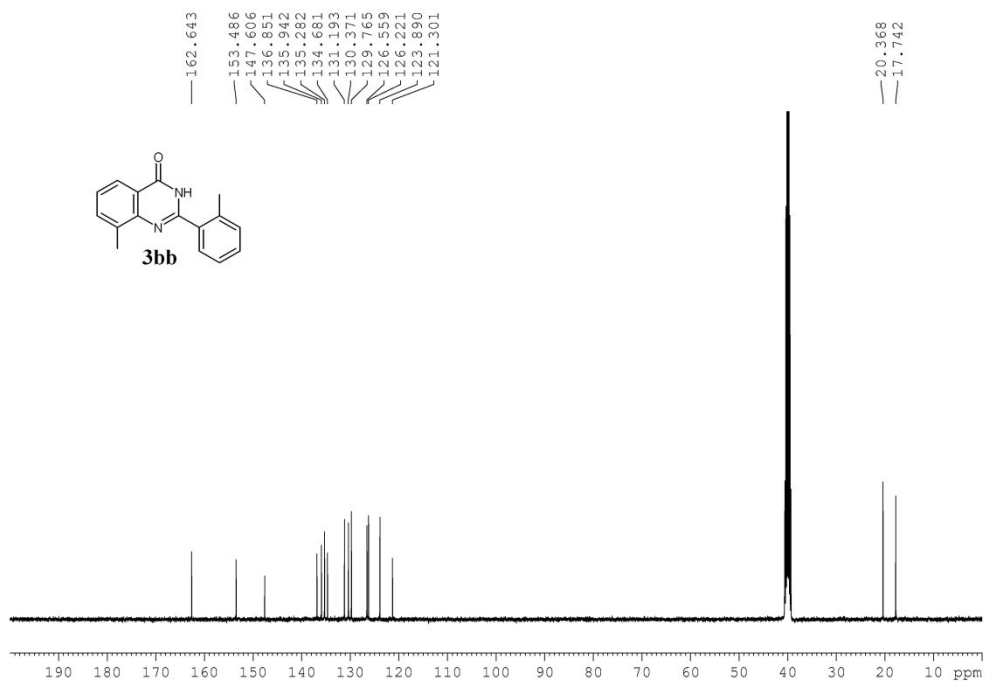




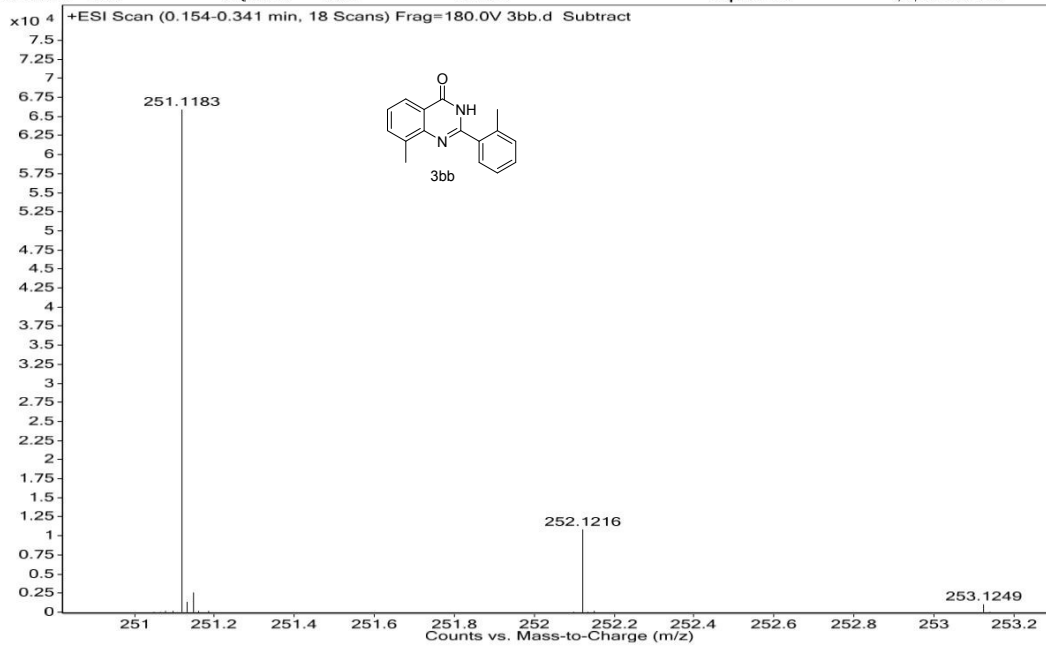




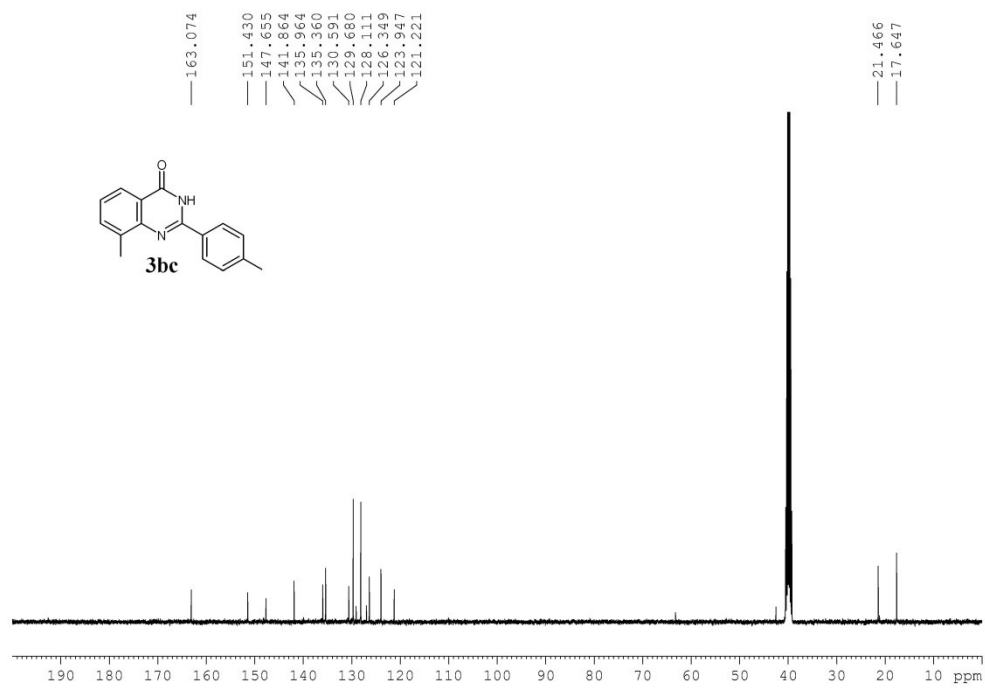
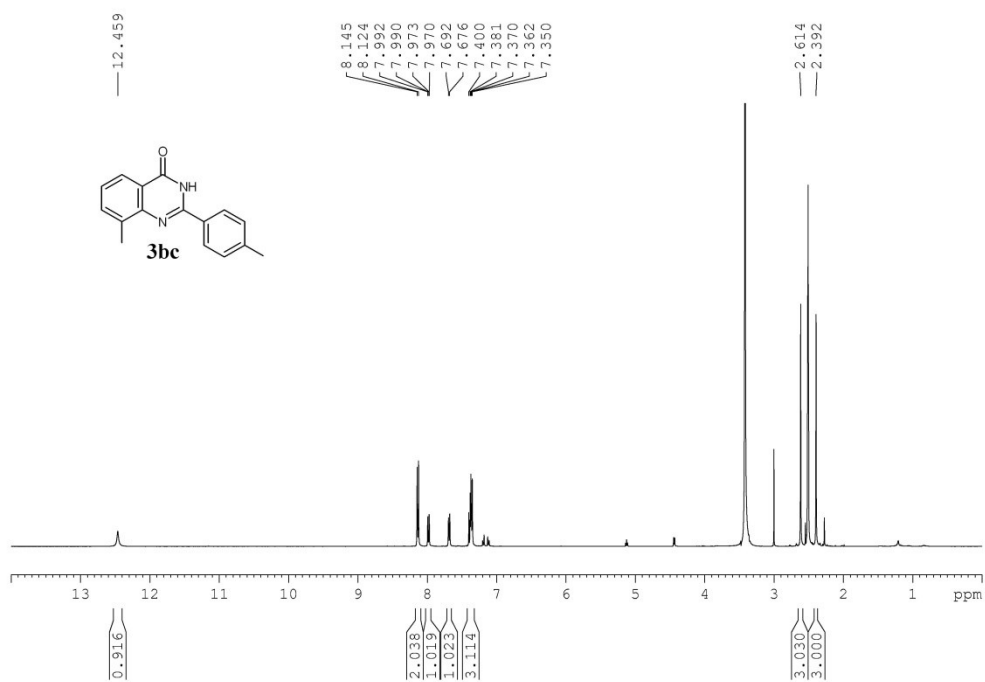


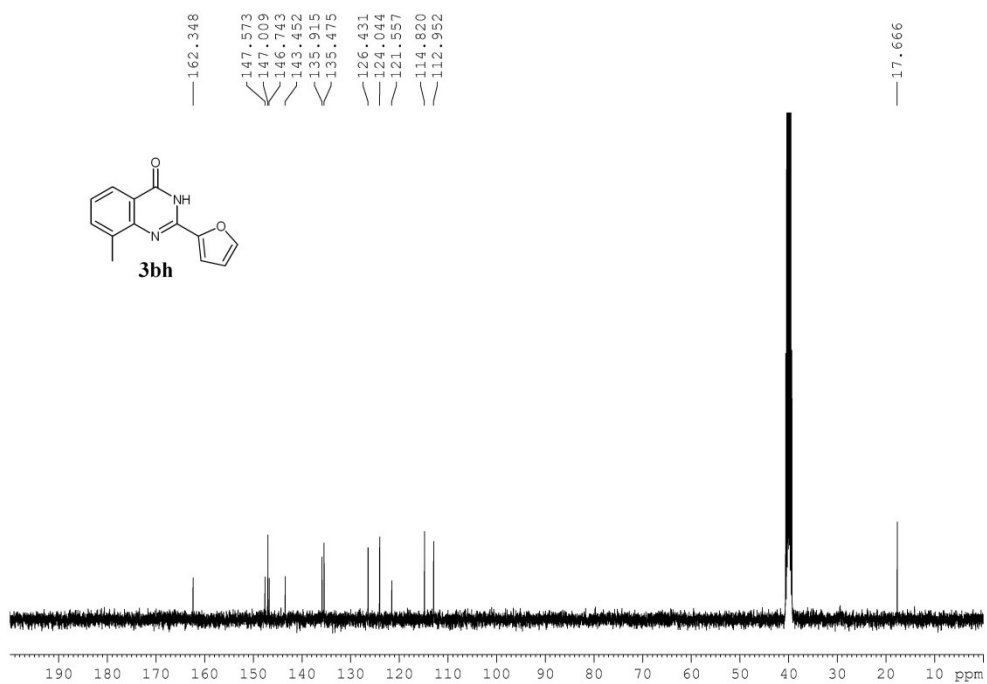
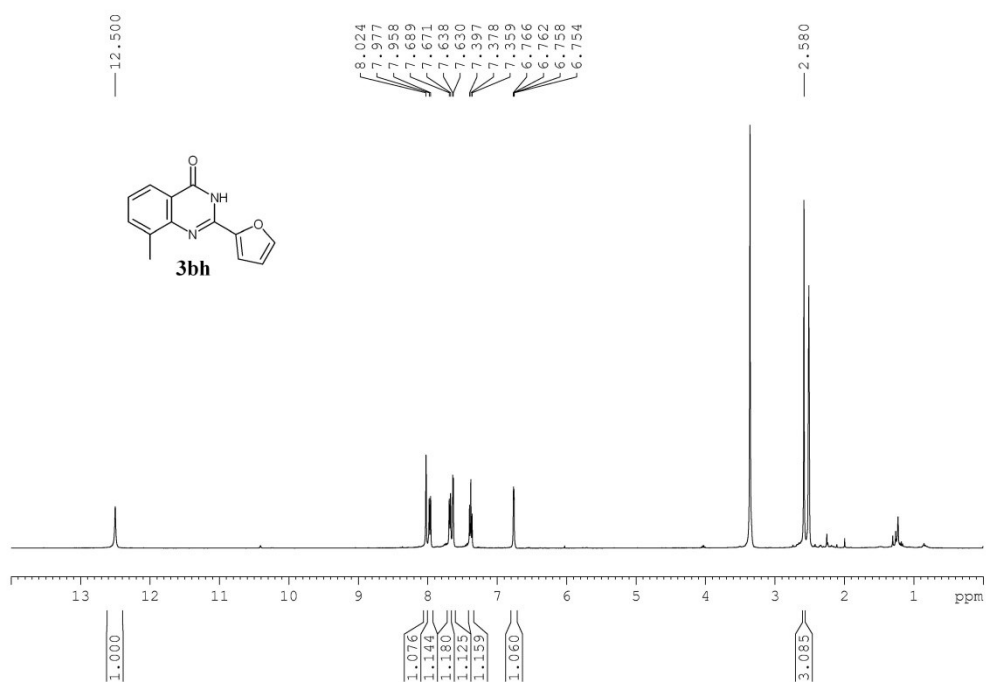


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Inj Vol	InjPosition	Sample Type	IRM Calibration Status
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Data Filename	ACQ Method	Comment	Acquired Time
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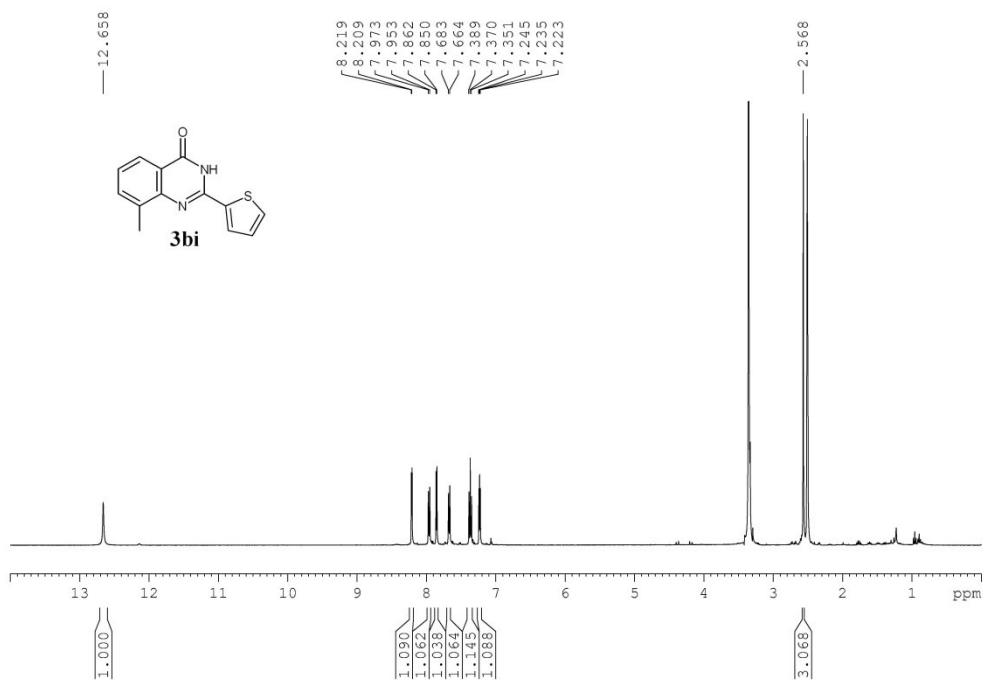
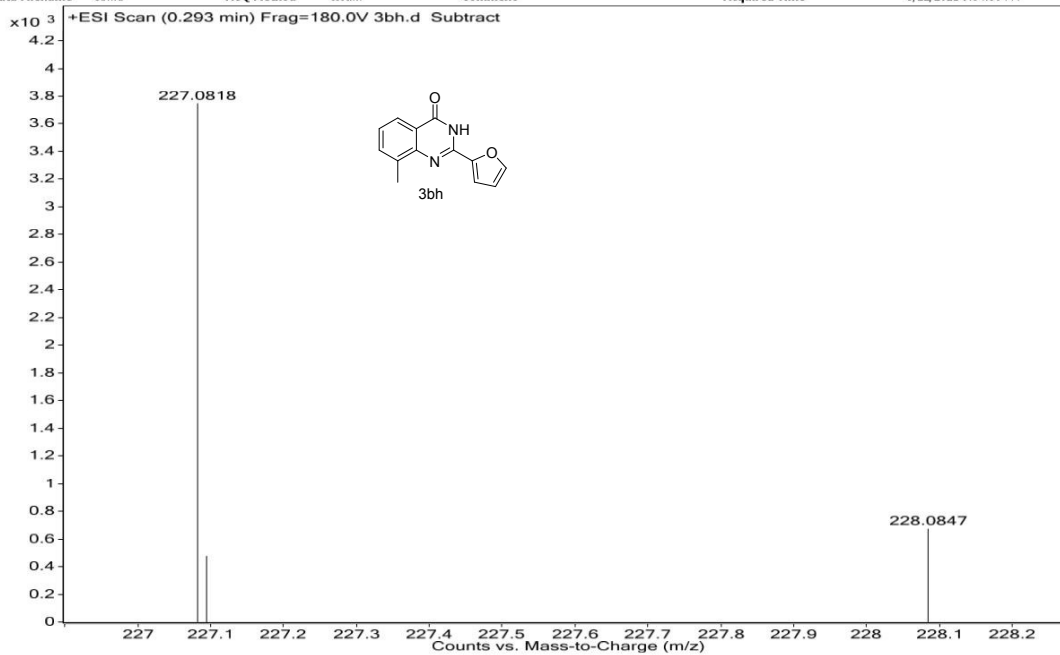


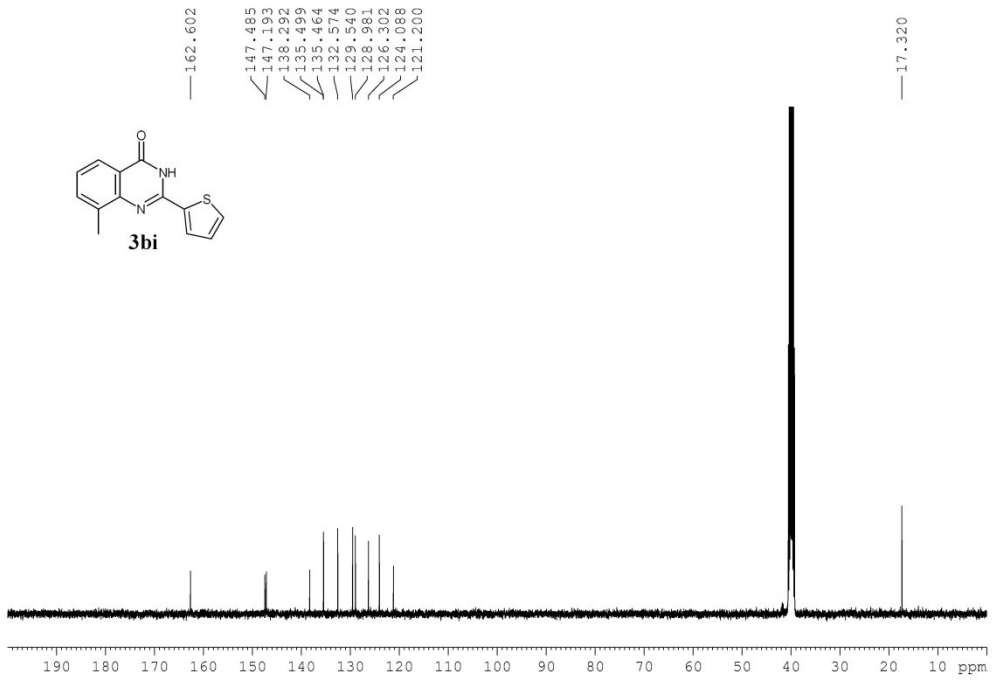




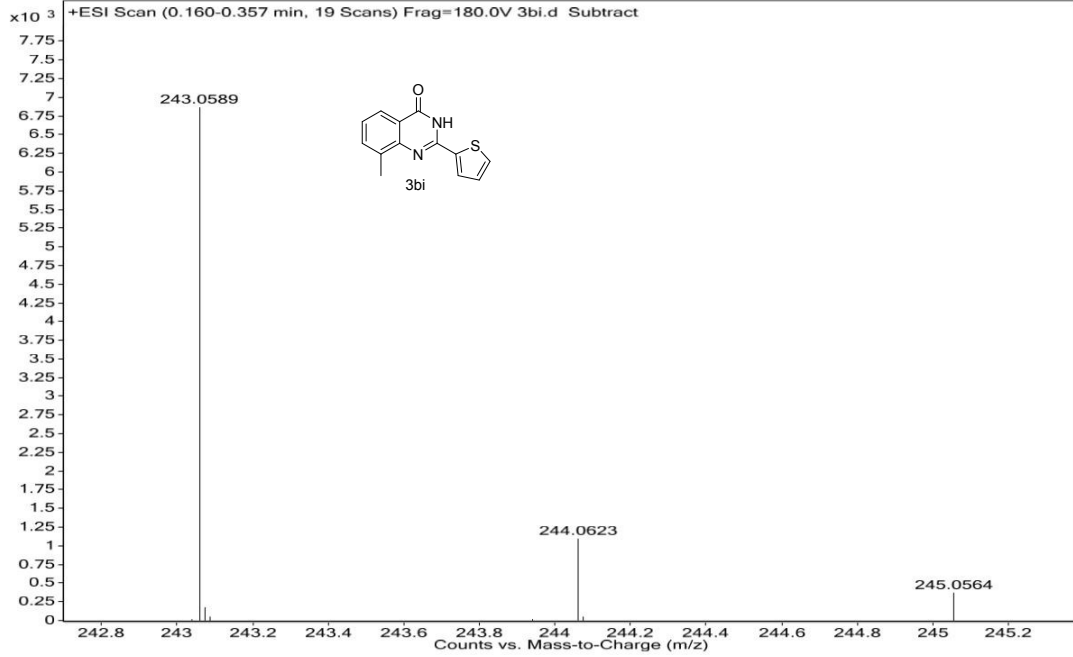


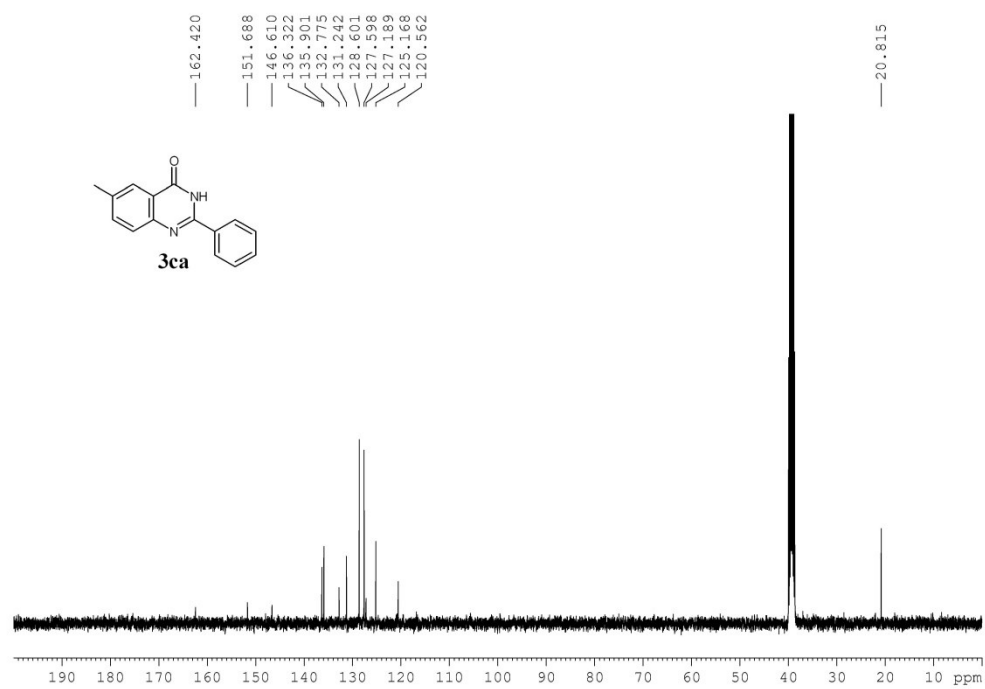
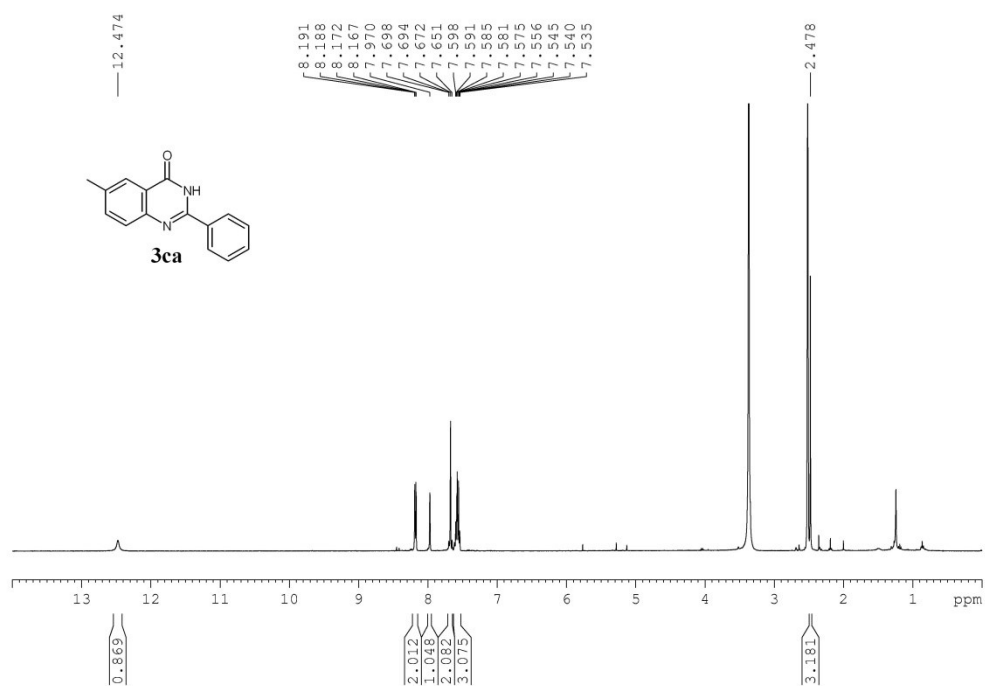
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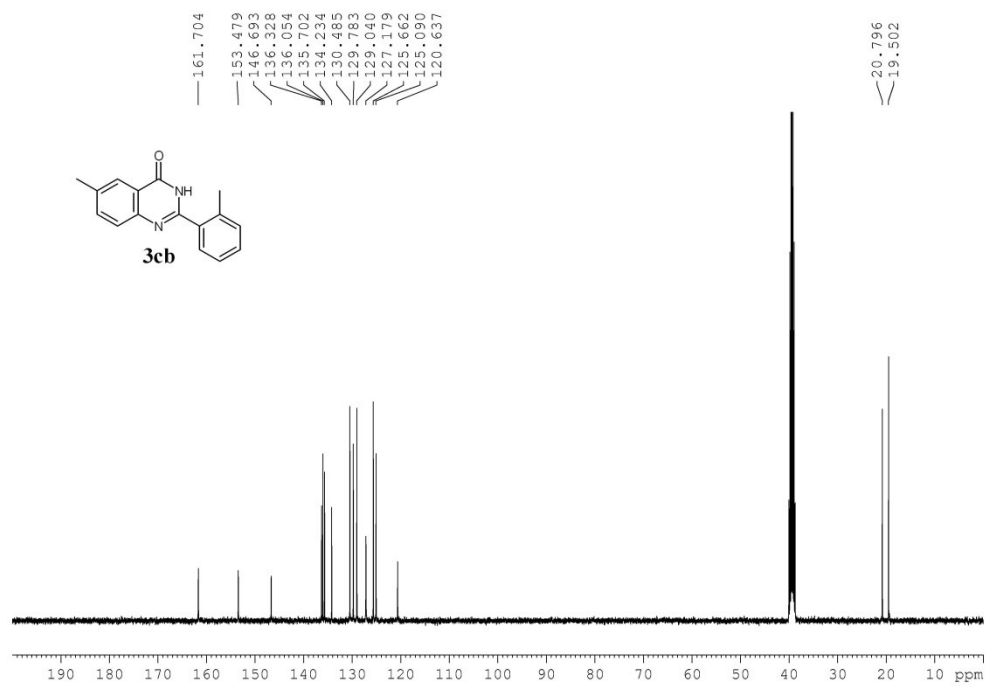
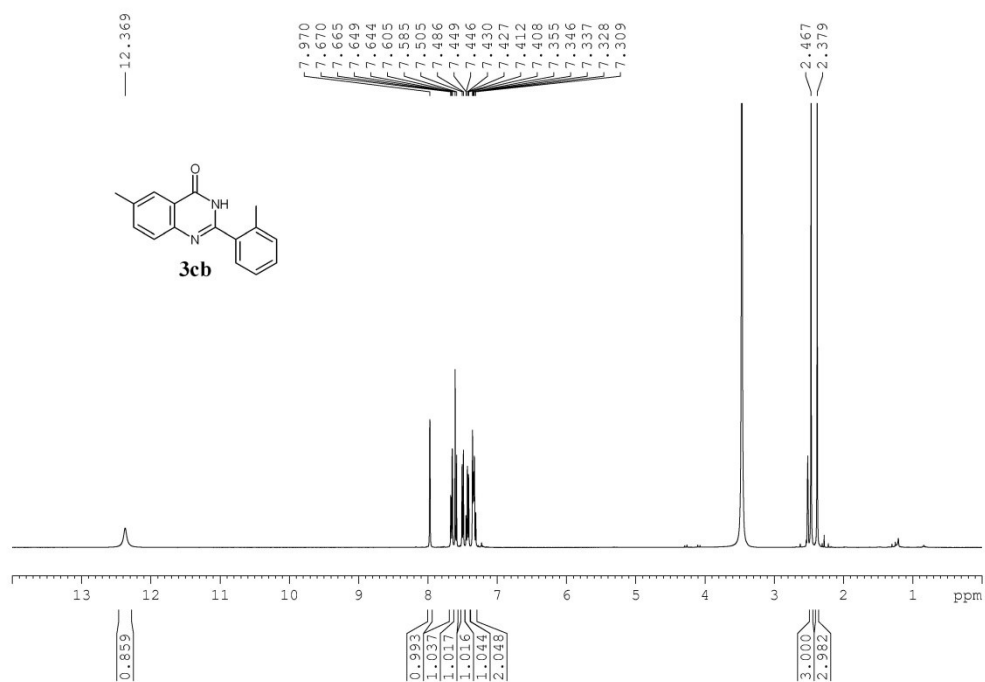


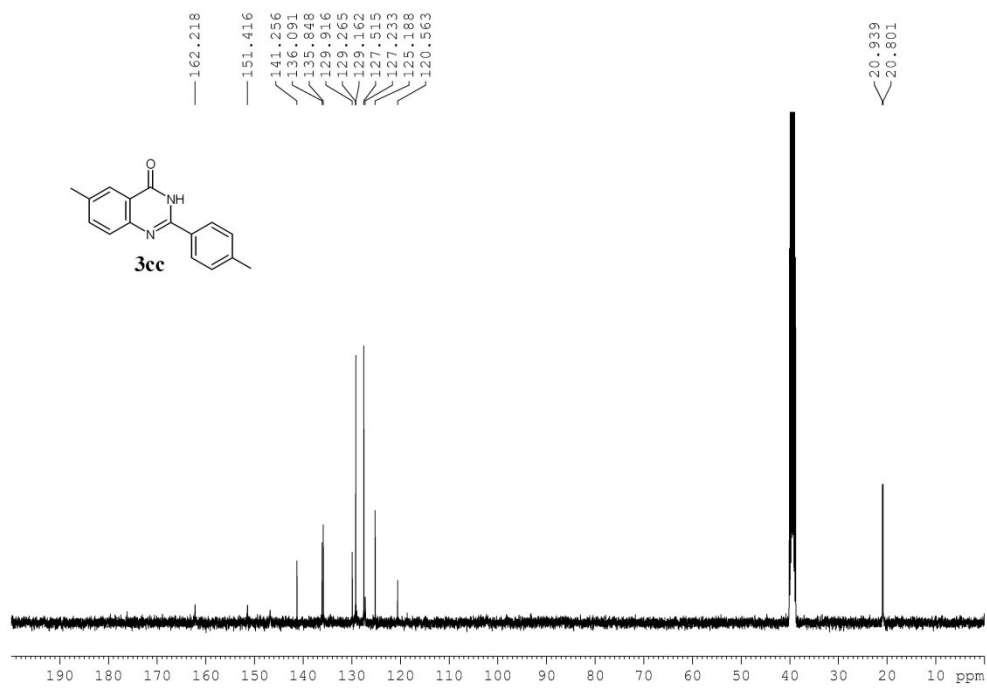
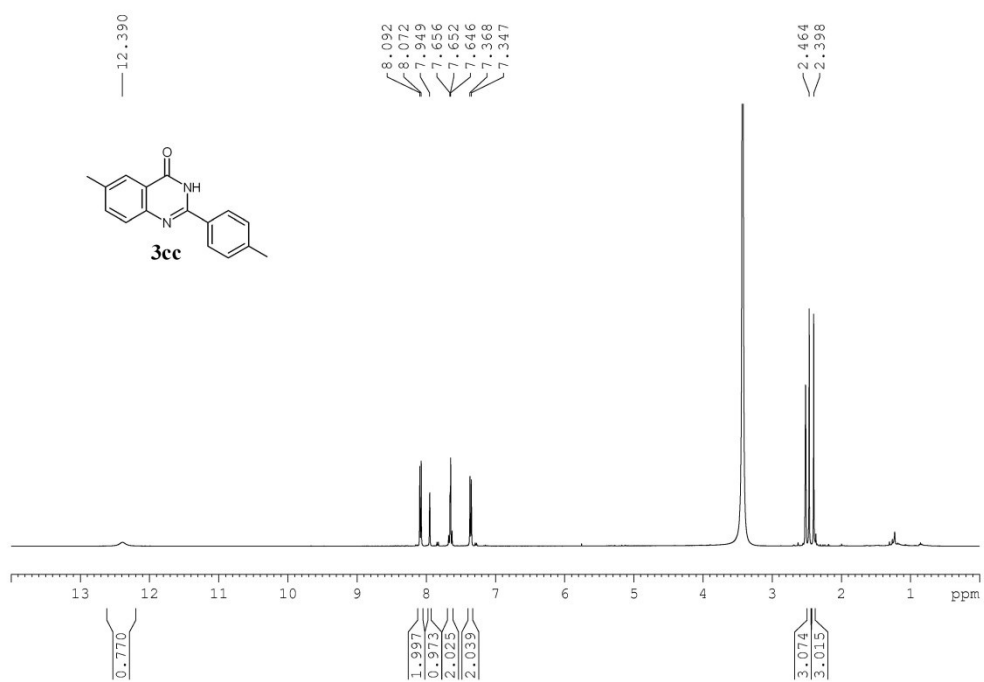


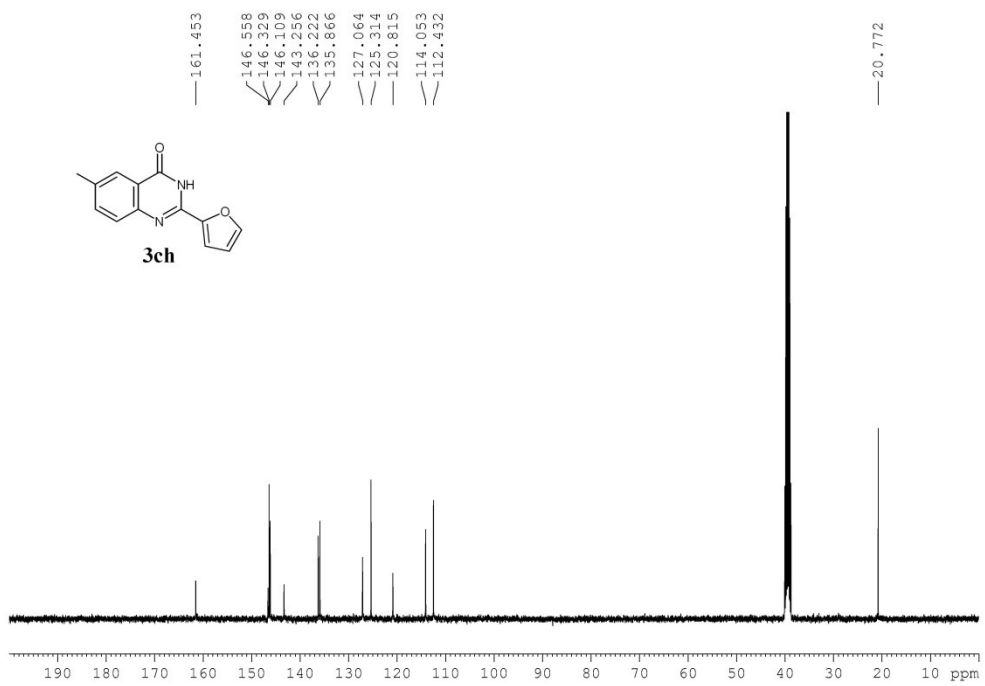
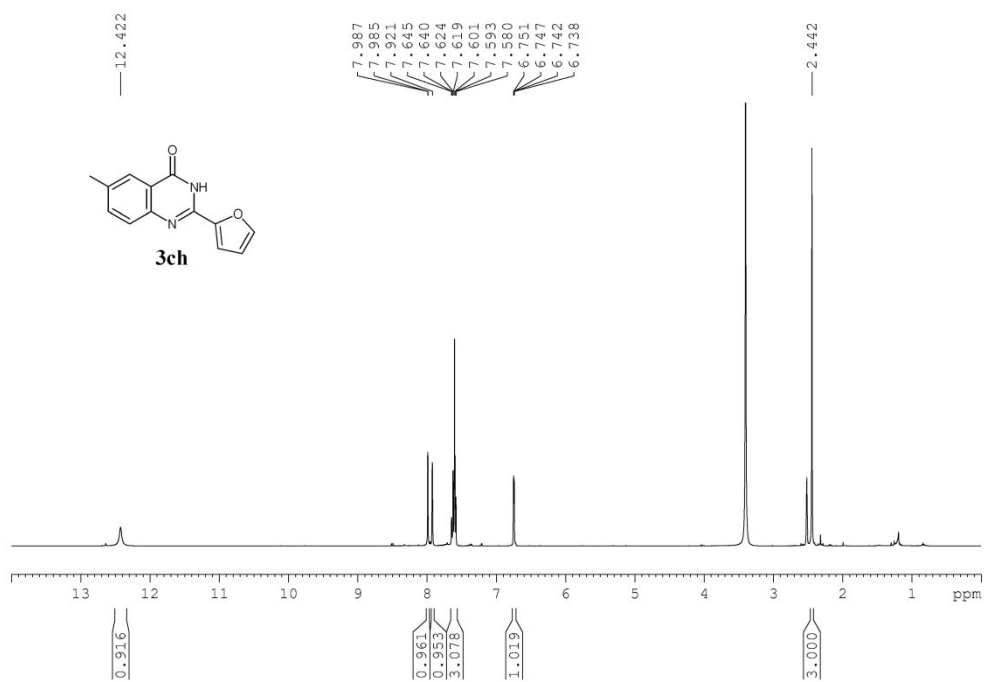
Sample Name	3bi	Position	P1-B4	Instrument Name	Instrument 1	User Name	
Inj Vol	0.5	InjPosition		SampleType	Sample	IRM Calibration Status	All Ions Missed
Data Filename	3bi.d	ACQ Method	test.m	Comment		Acquired Time	3/22/2021 10:09:13 PM



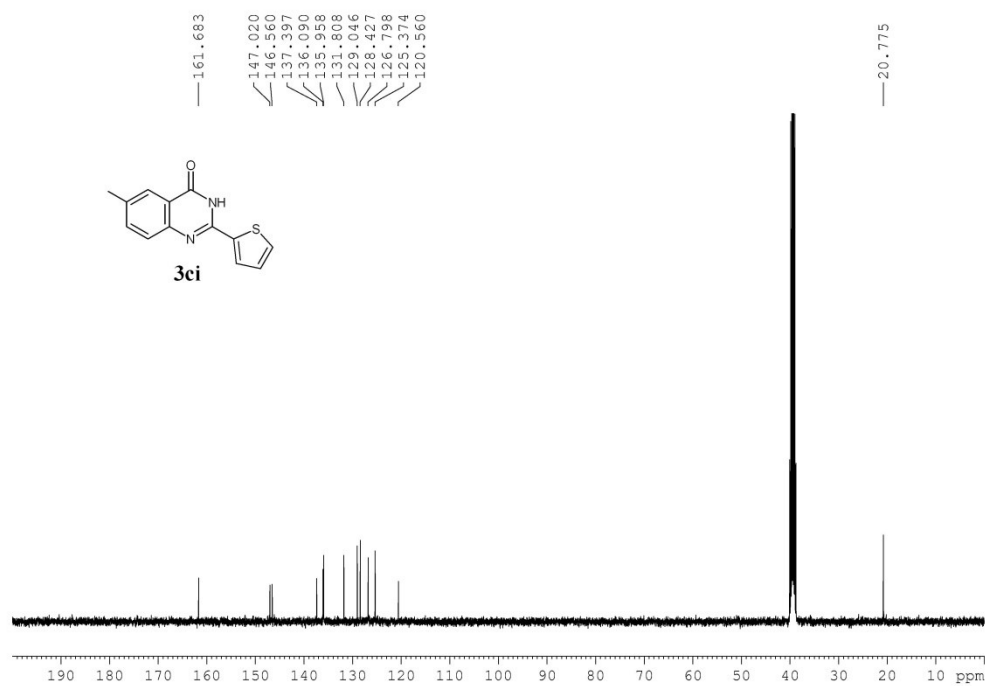
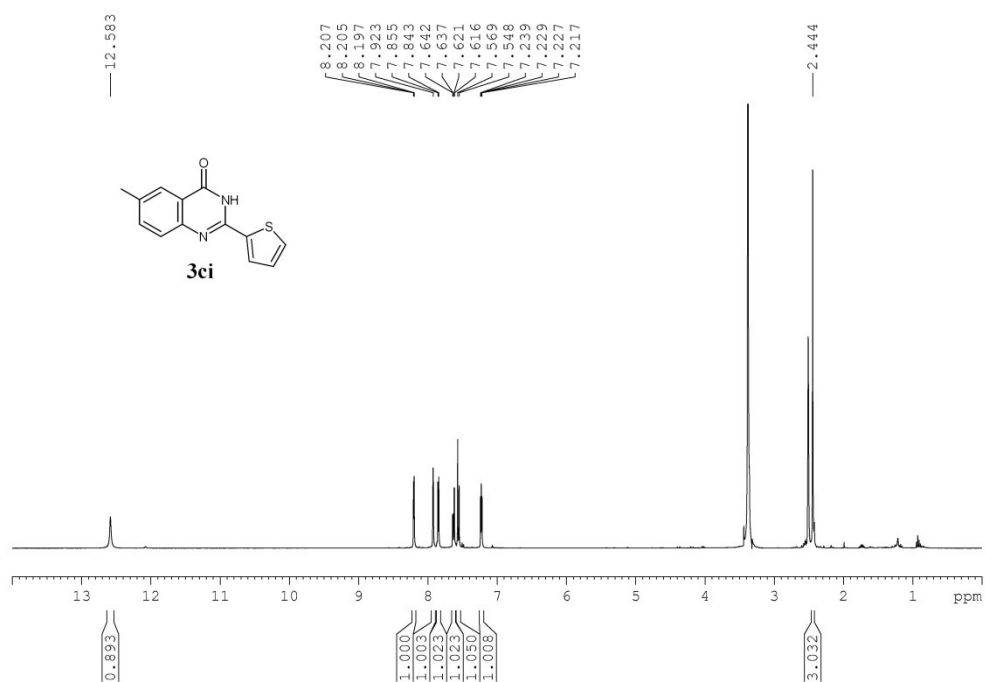


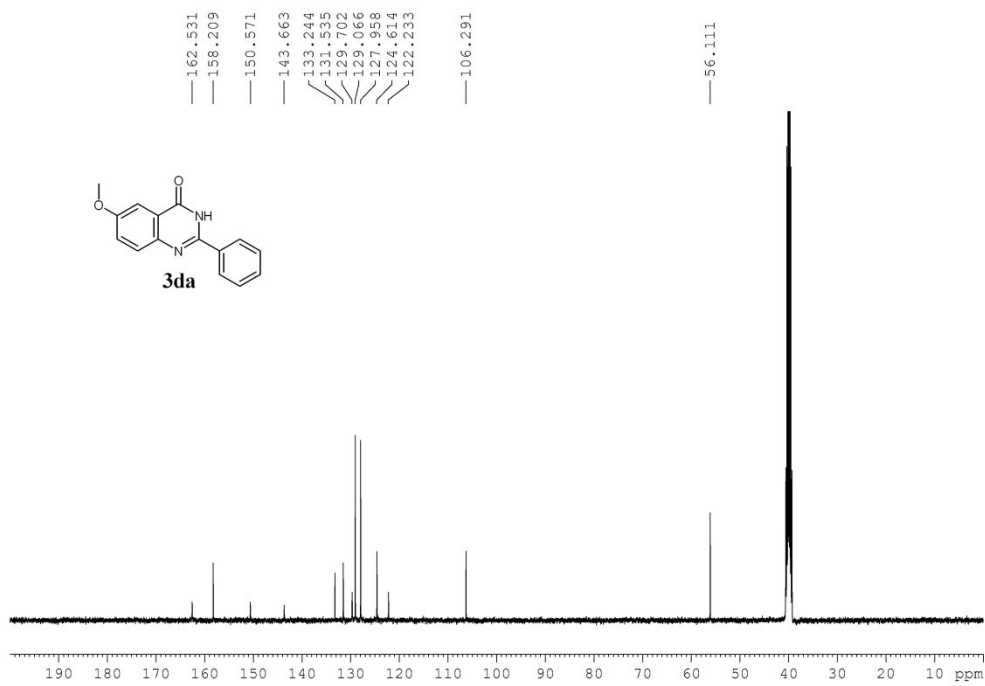
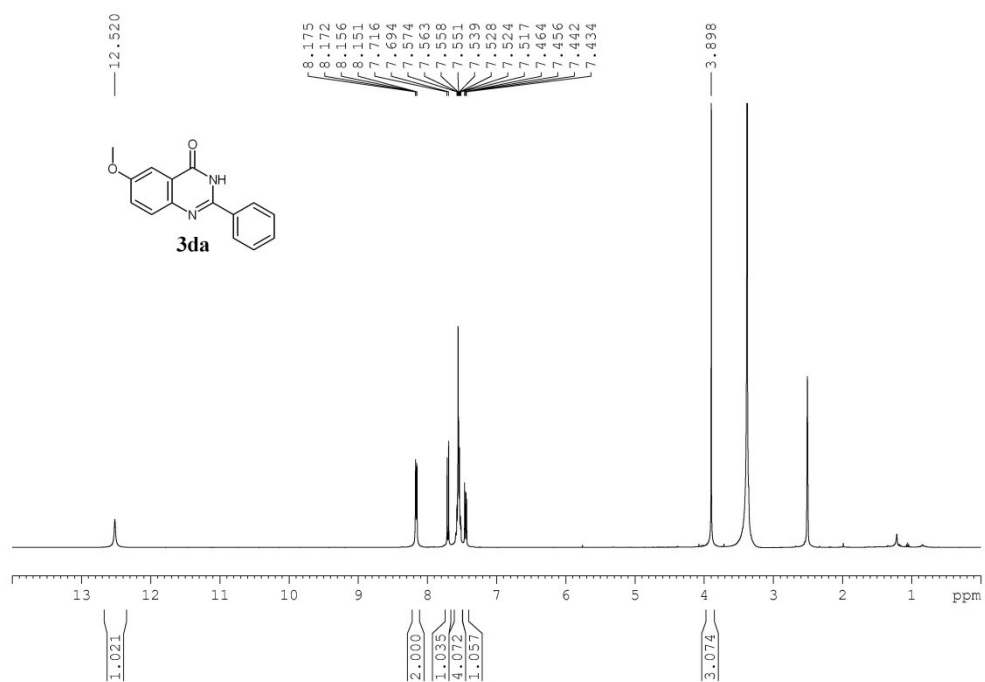


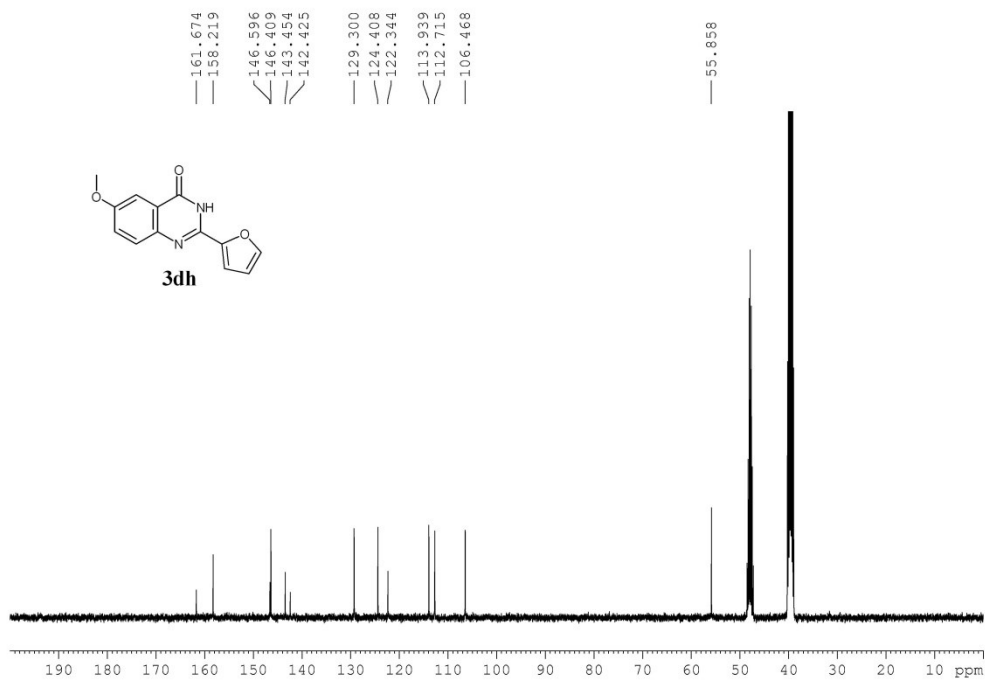
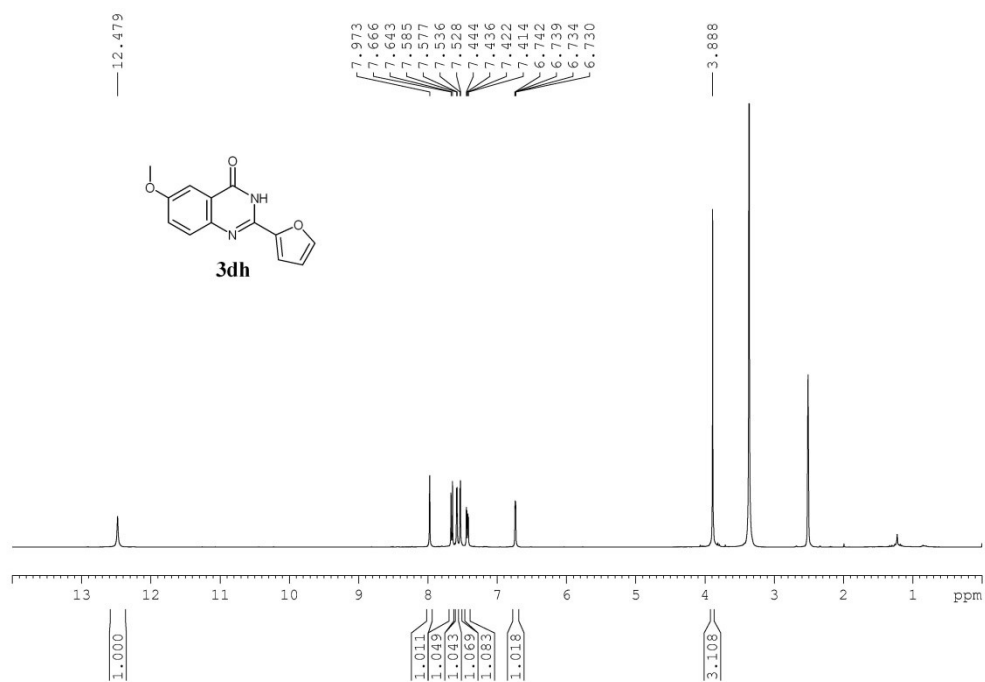




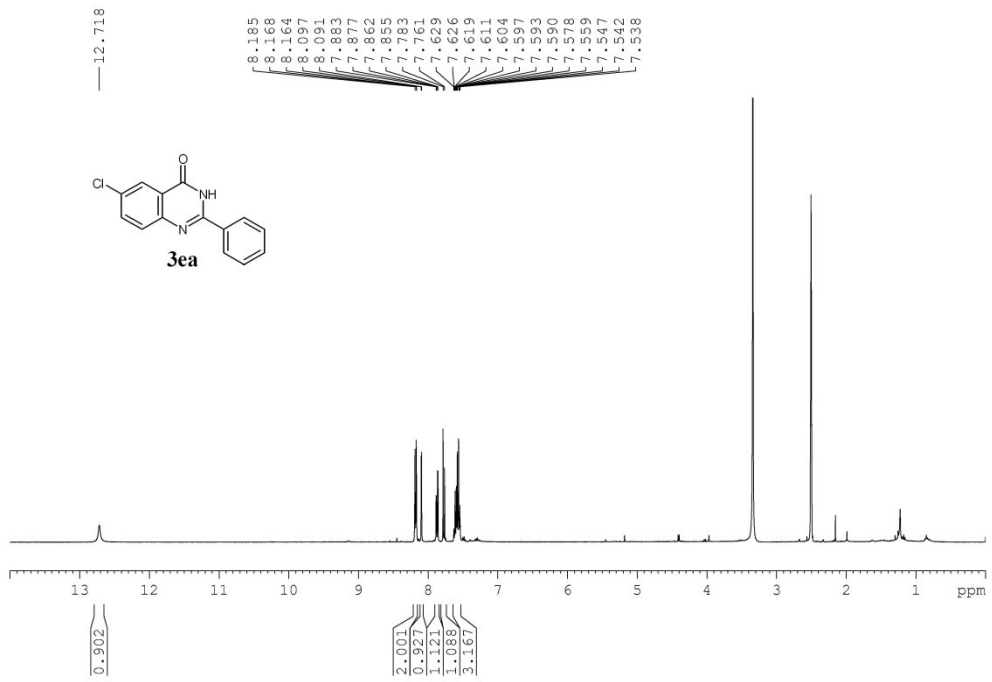
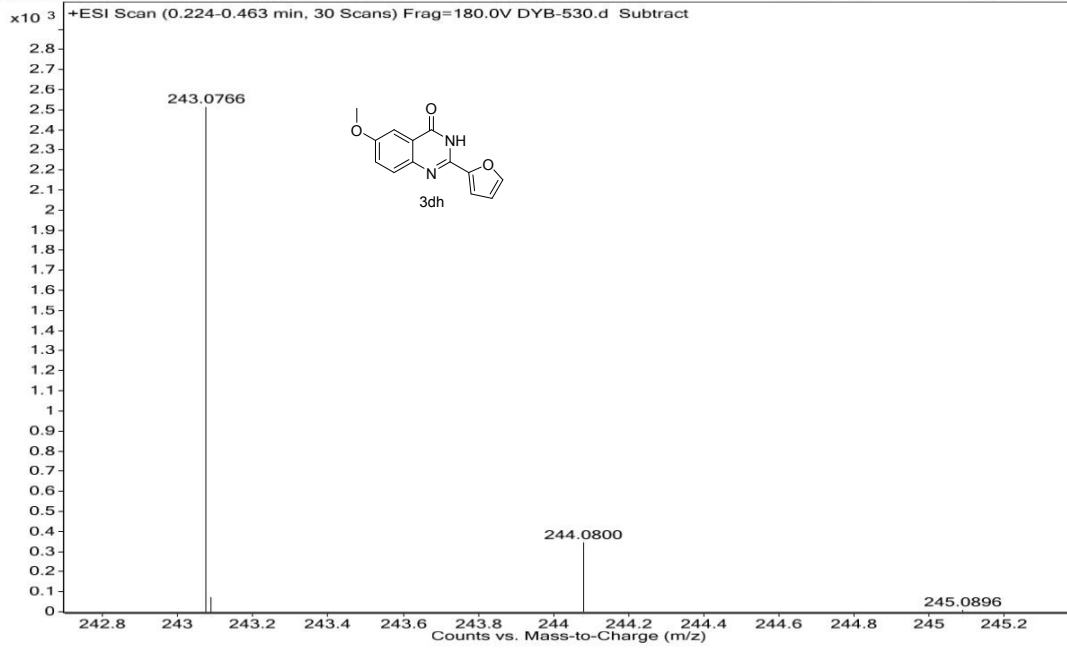


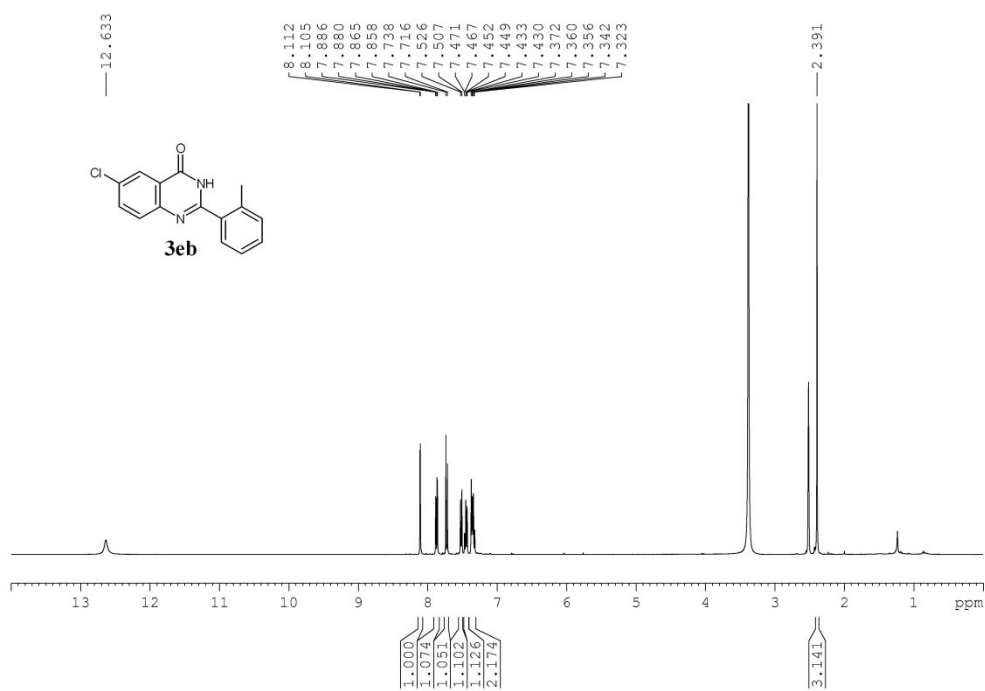
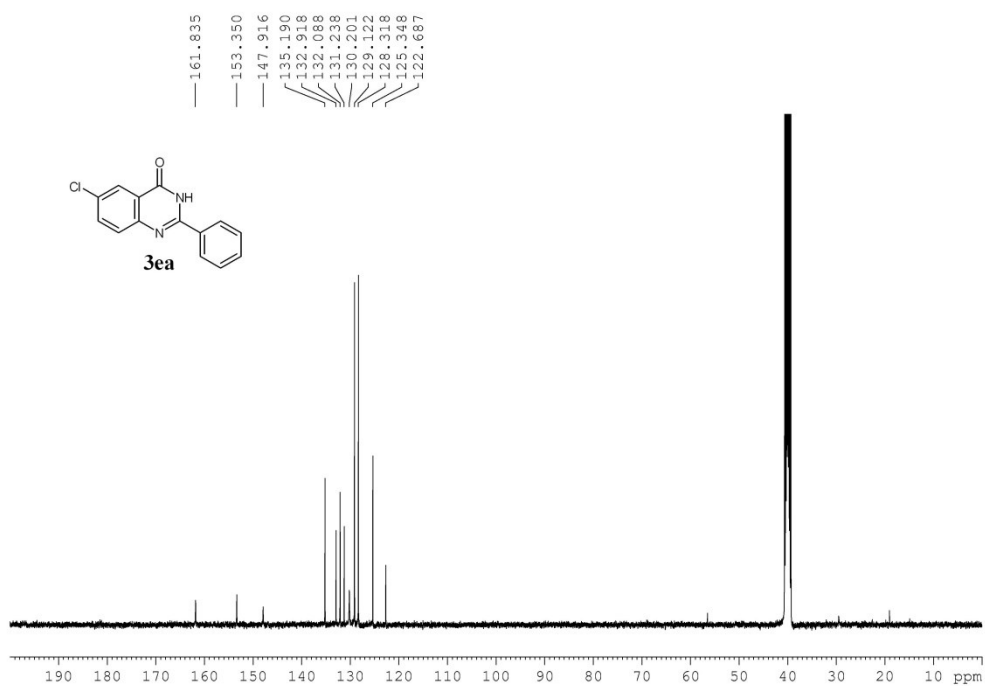


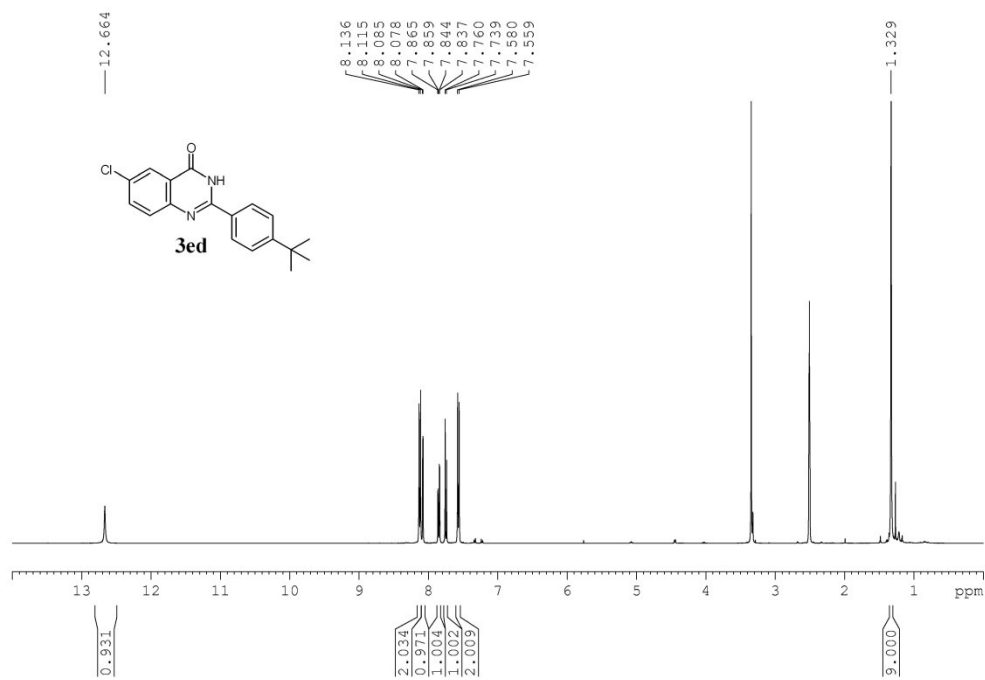
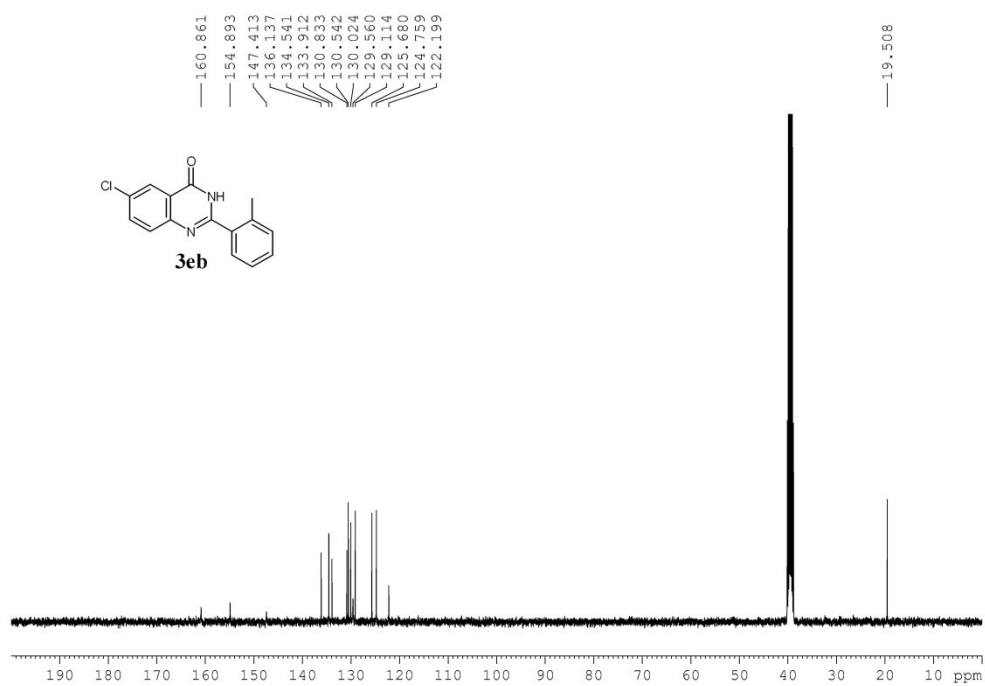


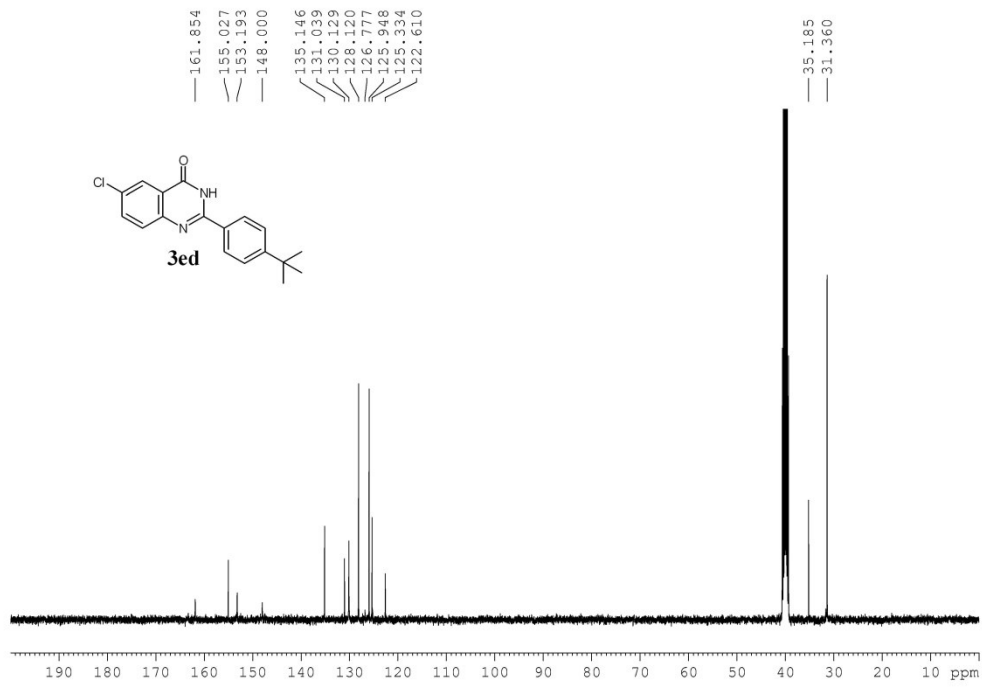


Sample Name	DYB-530	Position	P1-B9	Instrument Name	Instrument 1	User Name	
Inj Vol	0.2	InjPosition		SampleType	Sample	IRM Calibration Status	All Ions Missed
Data Filename	DYB-530.d	ACQ Method	test.m	Comment		Acquired Time	12/26/2020 9:30:41 AM

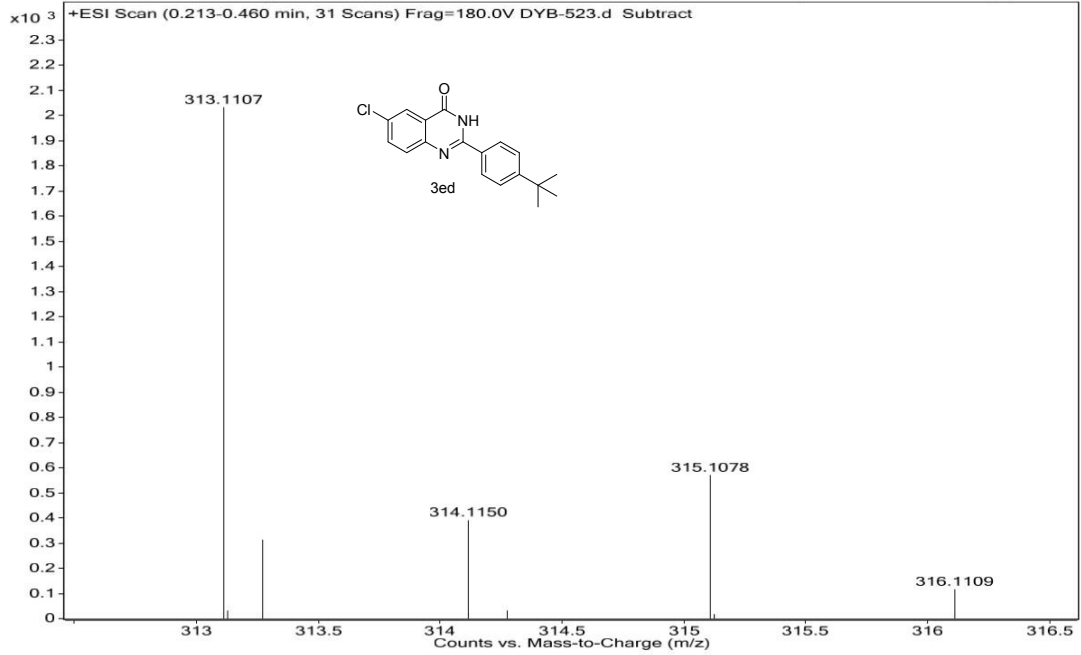


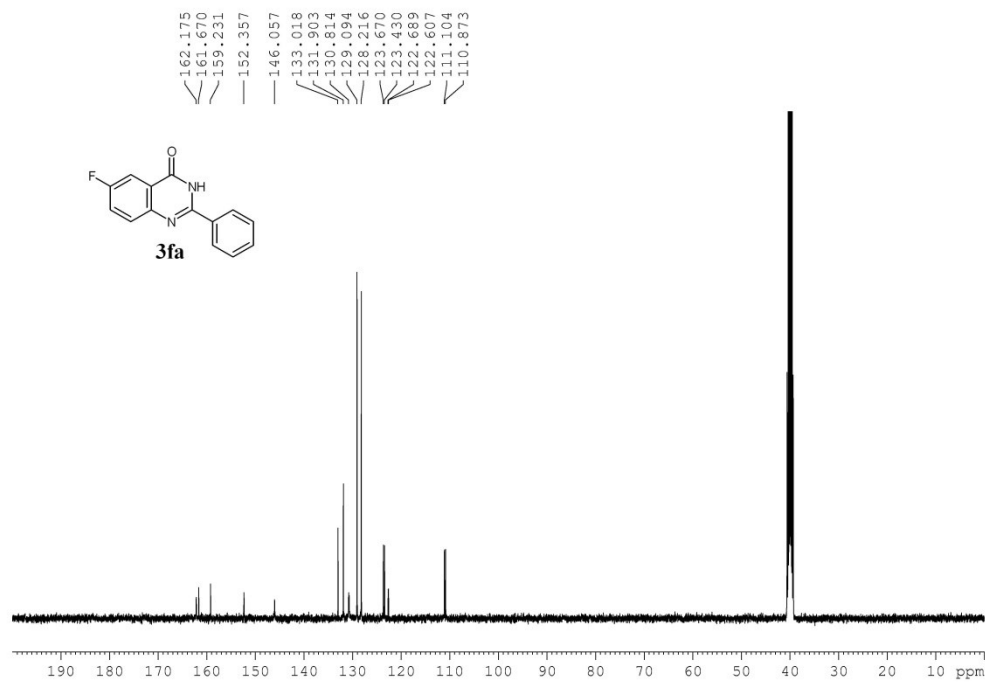
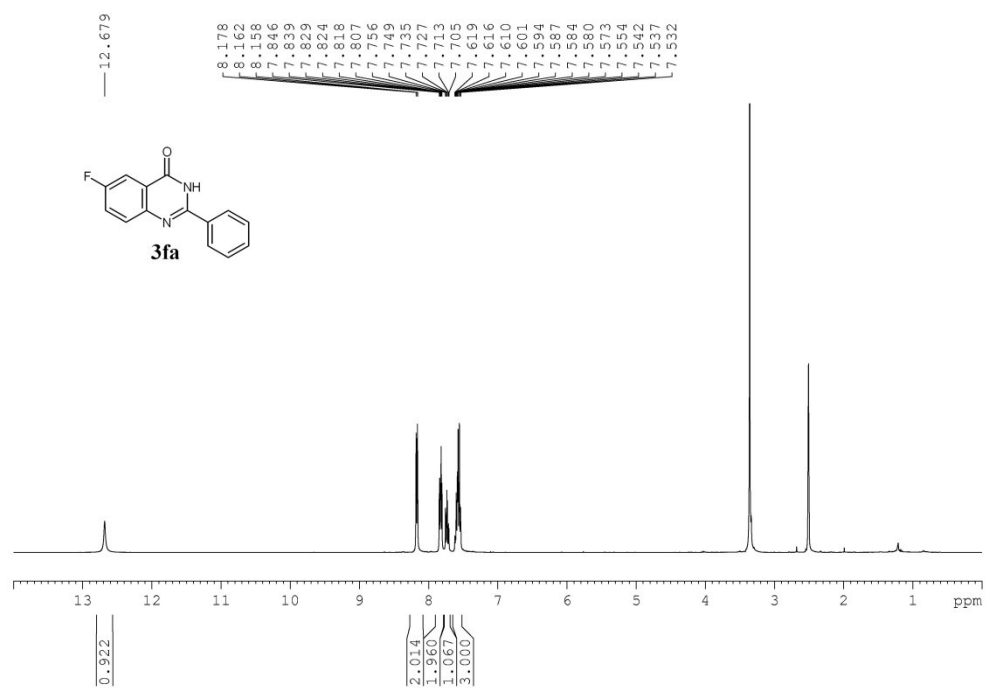




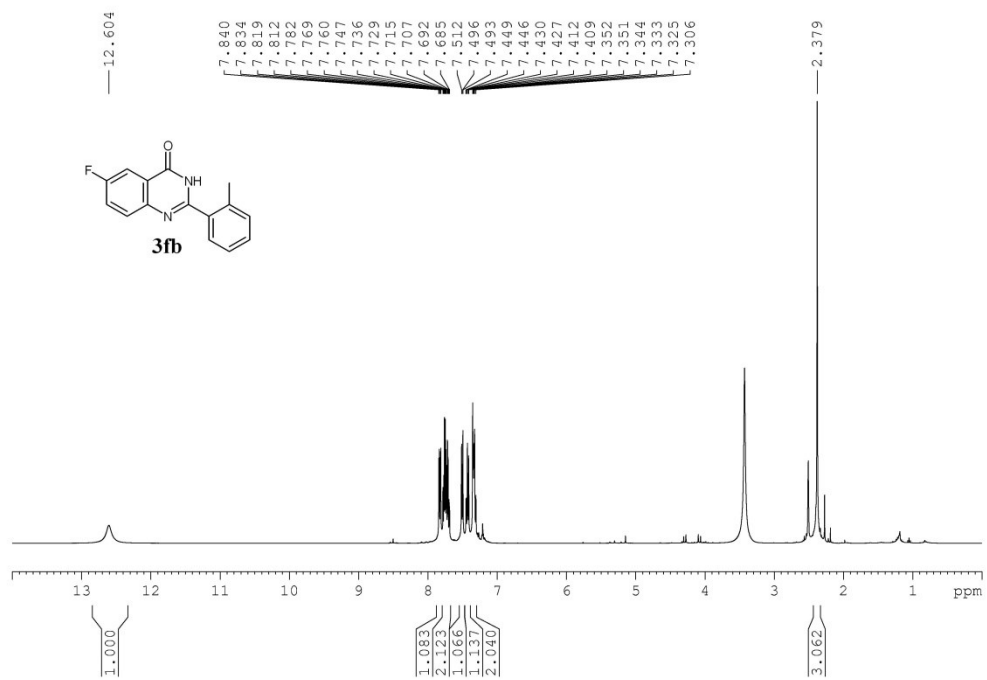
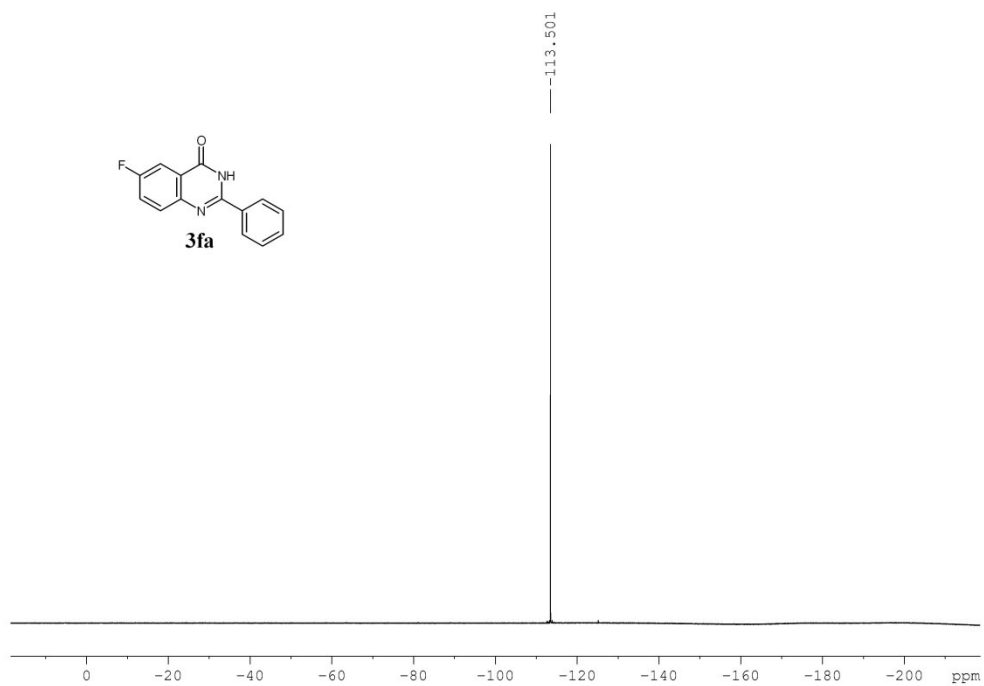


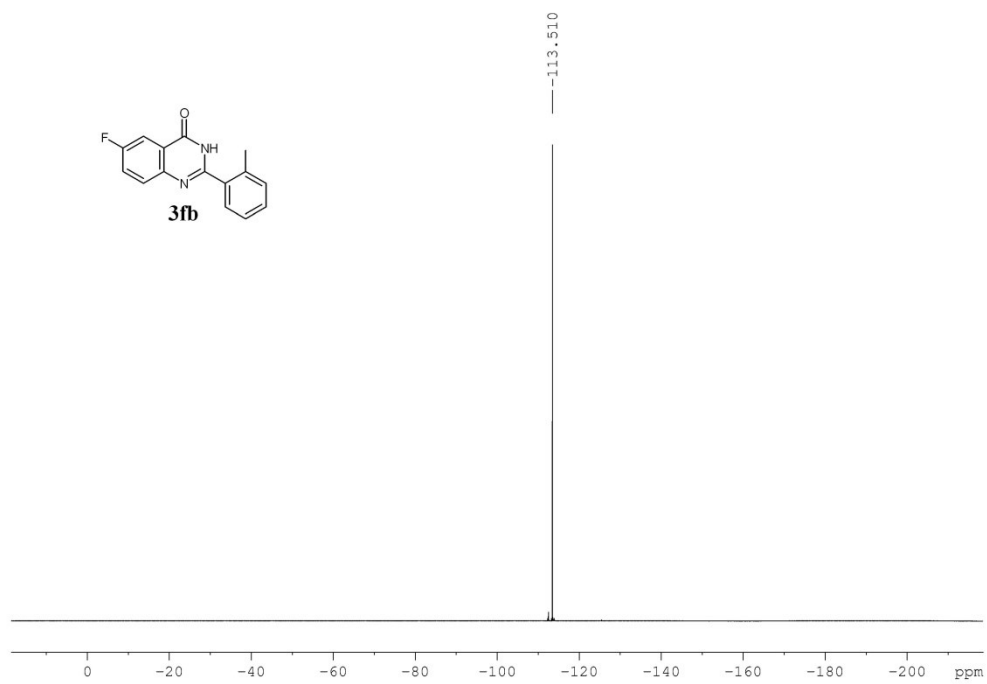
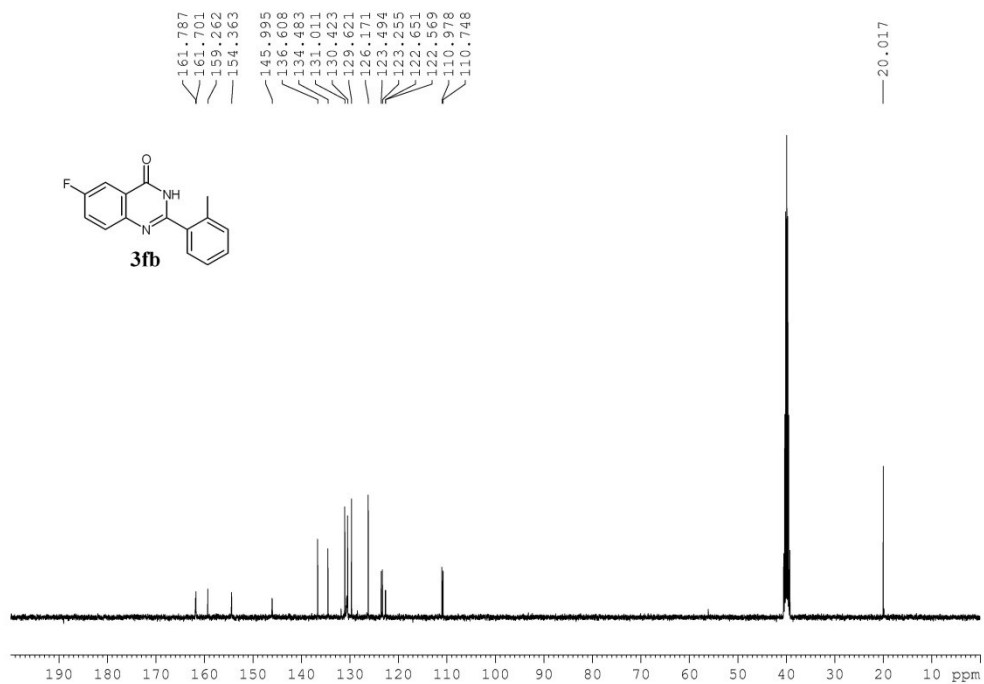
Sample Name	DYB-523	Position	P1-B8	Instrument Name	Instrument 1	User Name	
Inj Vol	0.2	InjPosition		SampleType	Sample	IRM Calibration Status	All Ions Missed
Data Filename	DYB-523.d	ACQ Method	test.m	Comment		Acquired Time	12/26/2020 9:29:25 AM



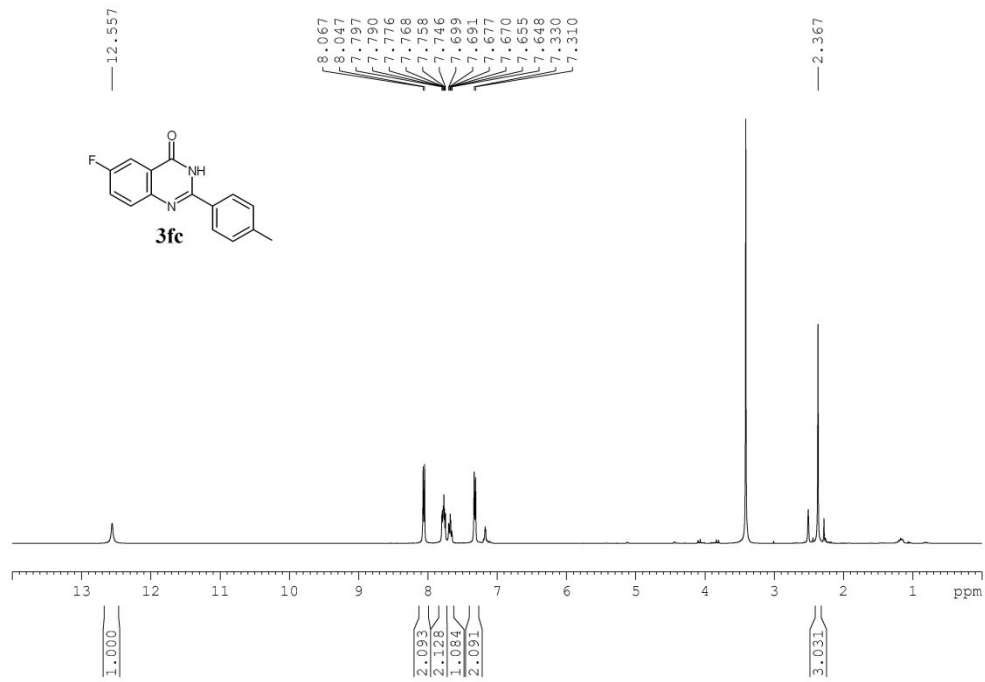
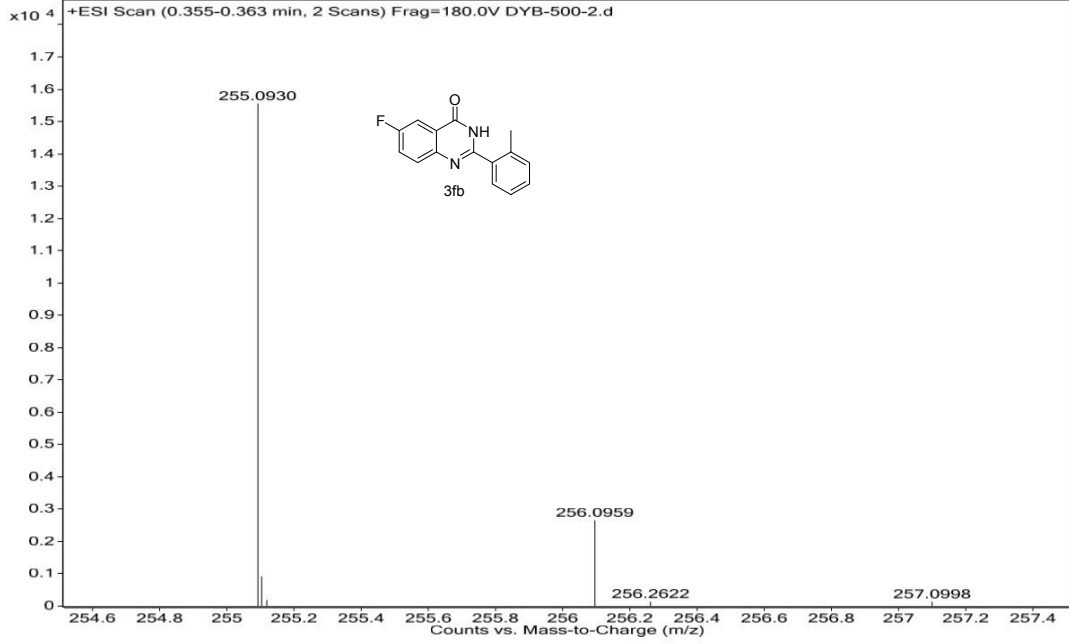


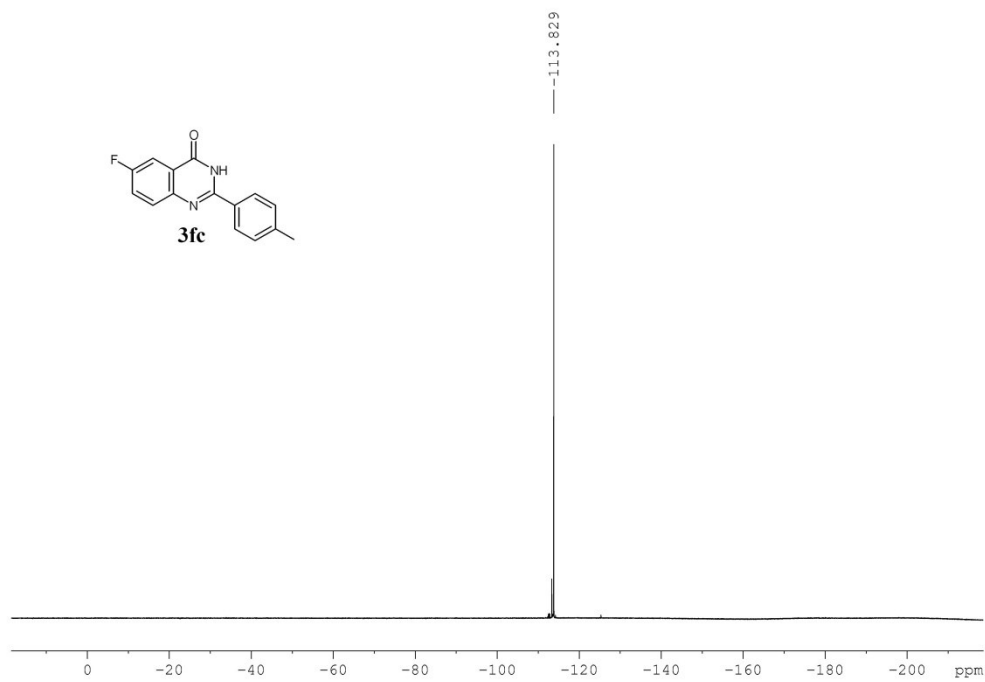
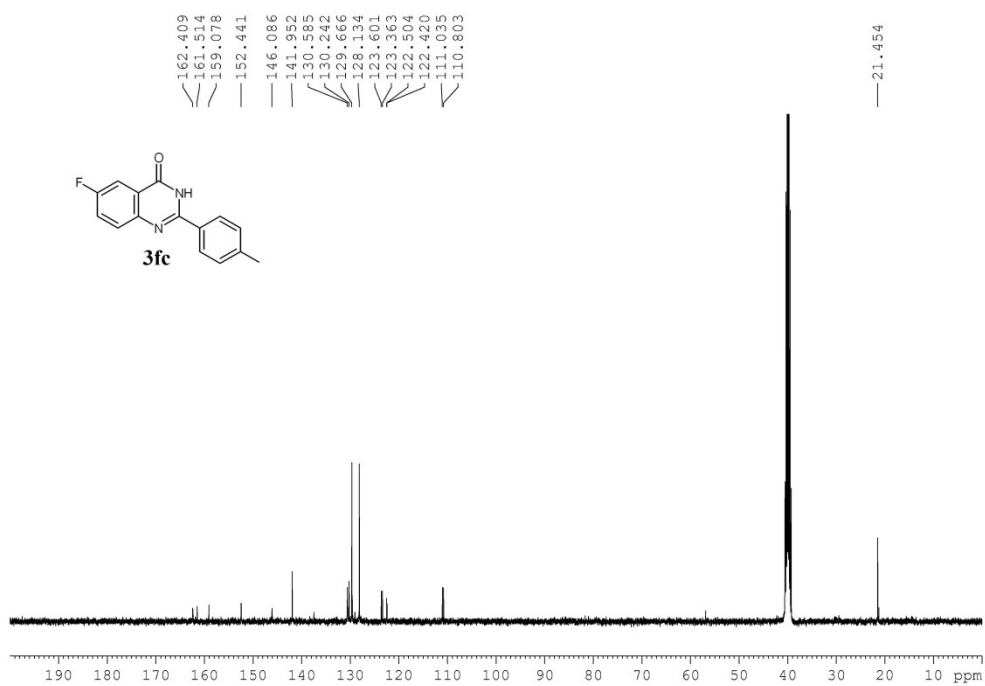


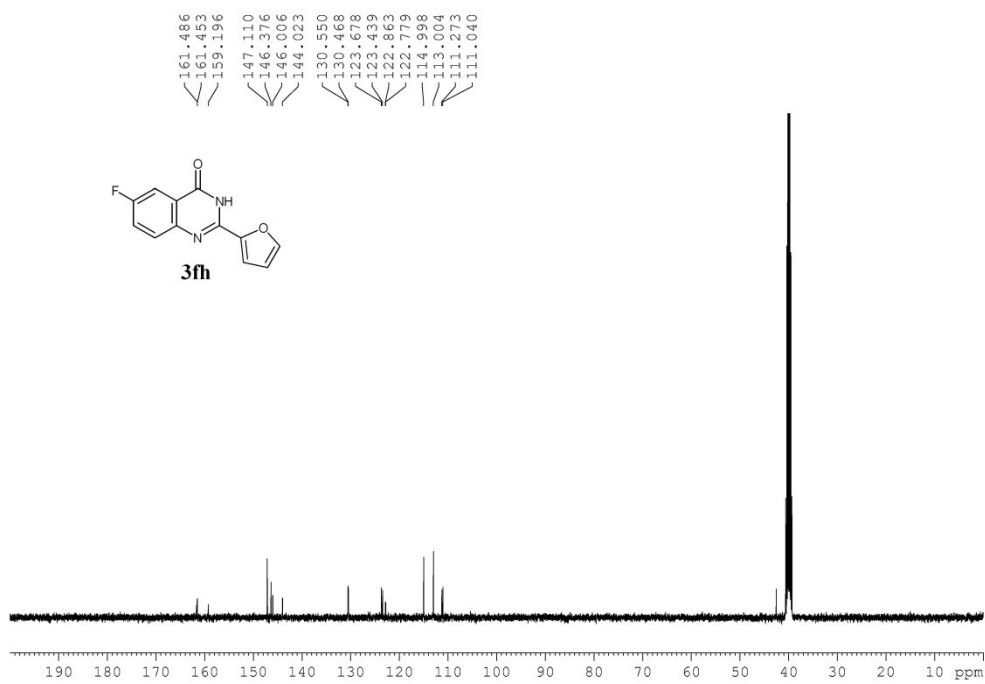
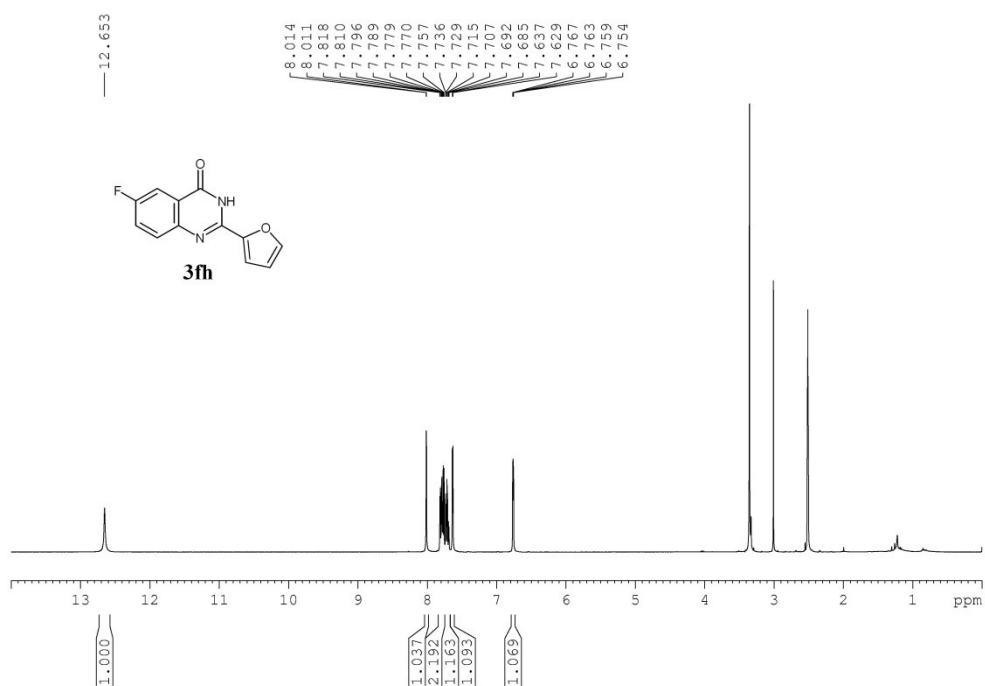


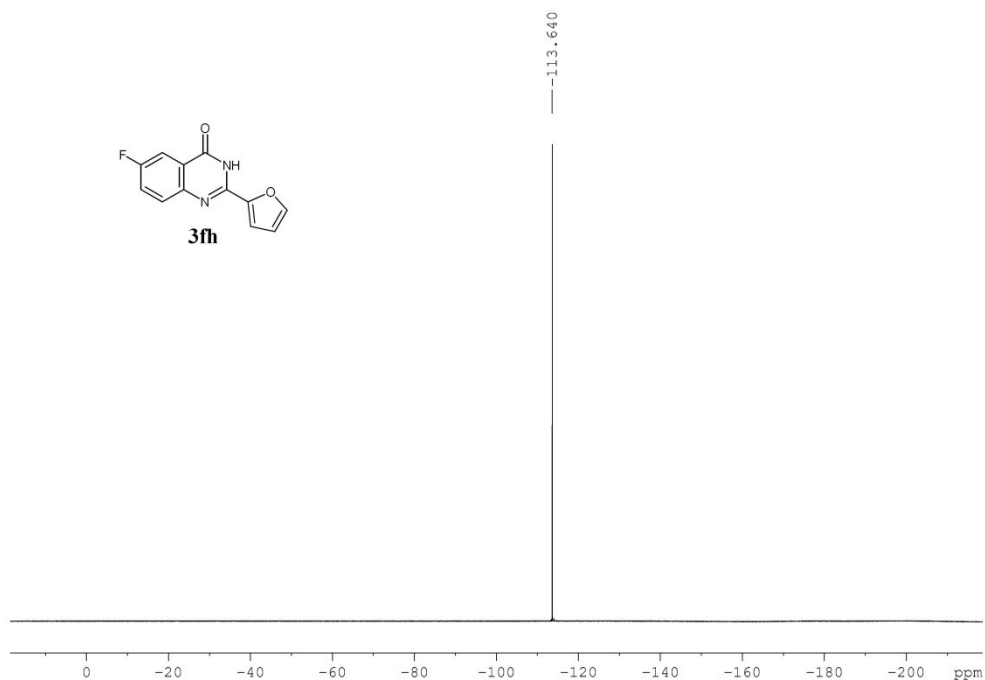


Sample Name	DYB-500-2	Position	P1-C2	Instrument Name	Instrument 1	User Name	
Inj Vol	0.8	InjPosition		SampleType	Sample	IRM Calibration Status	All Ions Missed
Data Filename	DYB-500-2.d	ACQ Method	test.m	Comment		Acquired Time	12/8/2020 3:03:40 PM

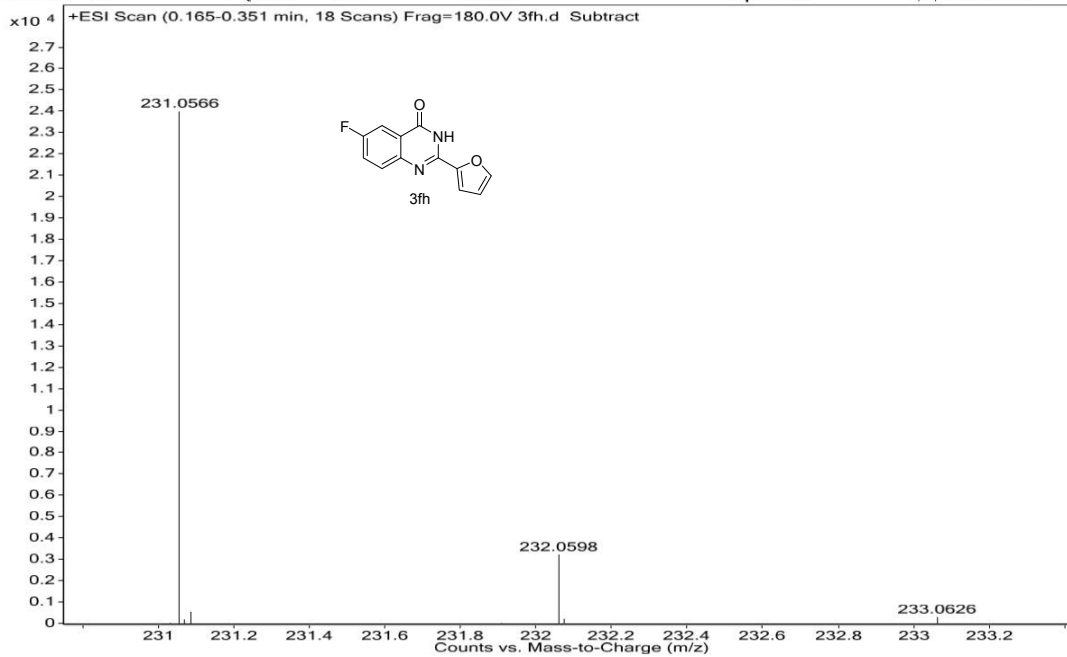


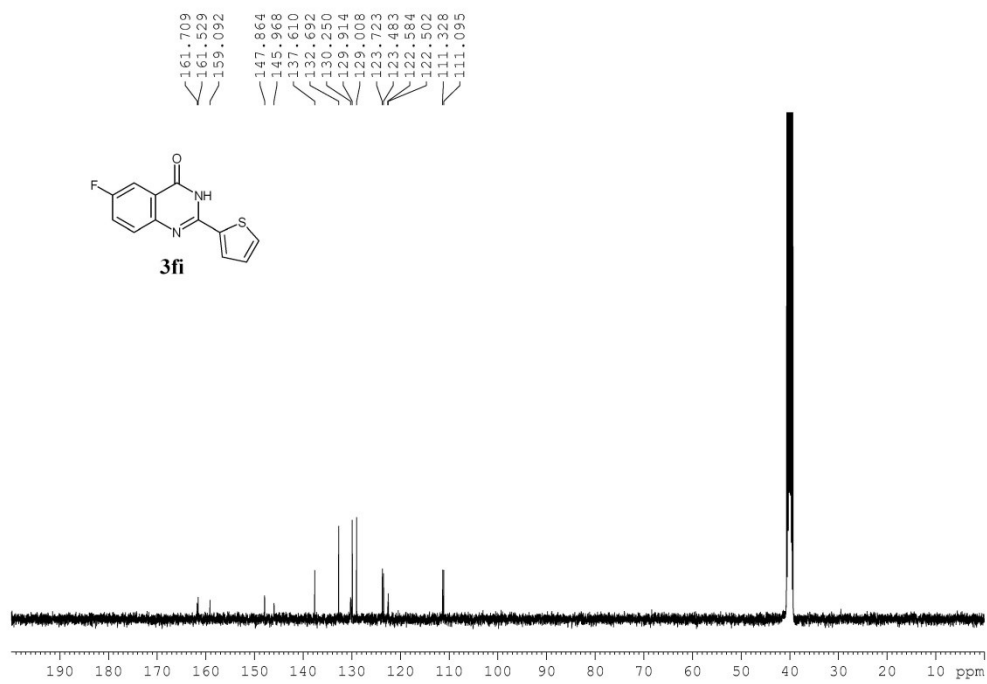
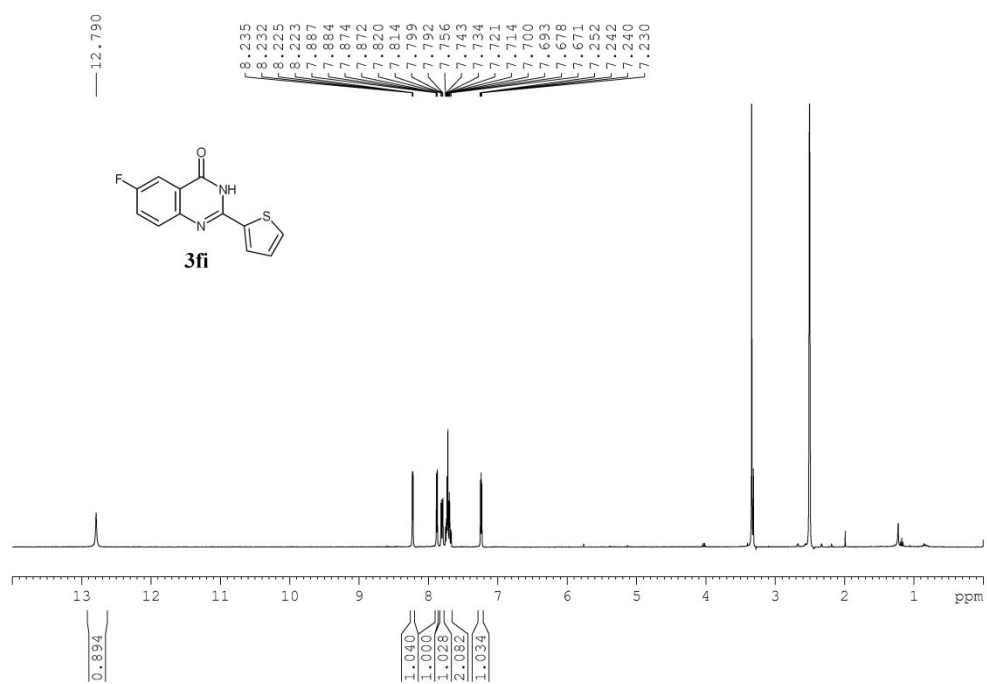


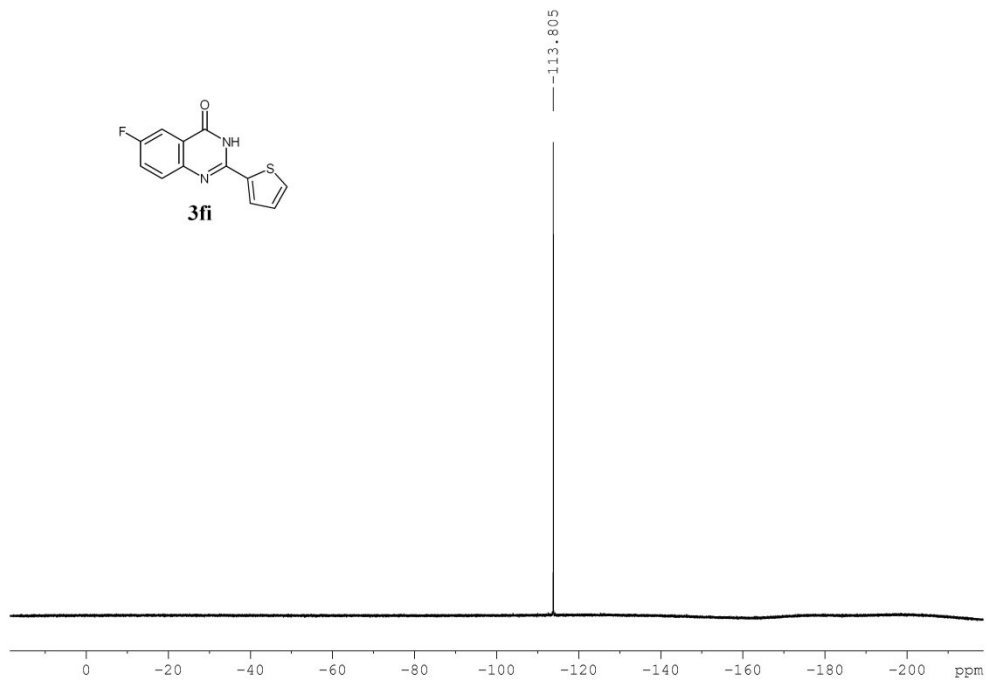




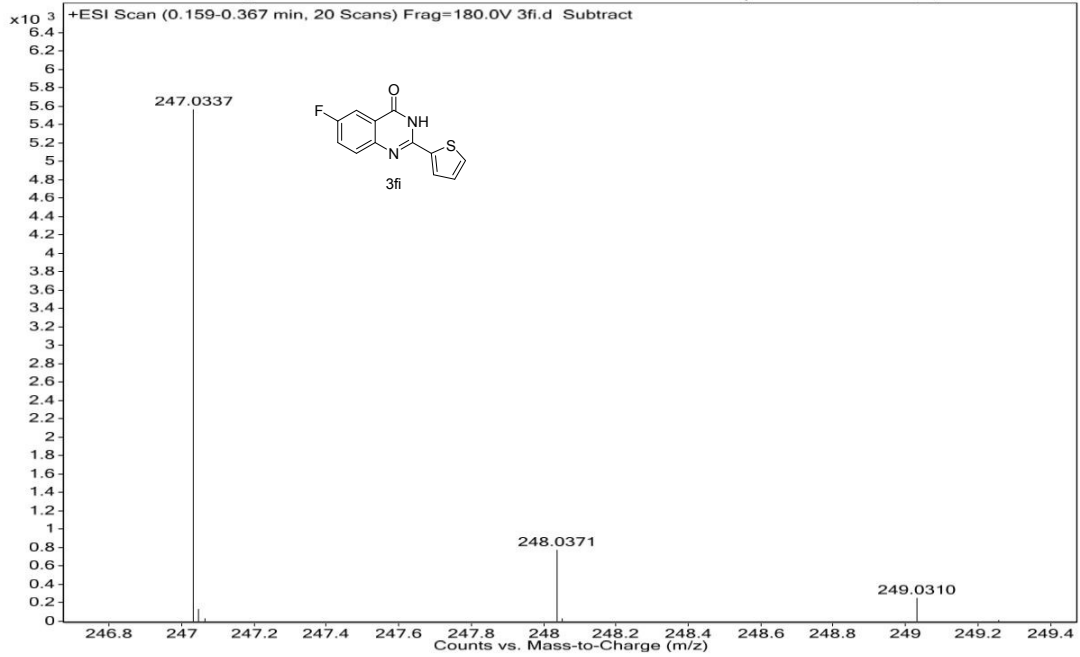
Sample Name	3fh	Position	P1-B5	Instrument Name	Instrument 1	User Name	
Inj Vol	0.5	InjPosition		SampleType	Sample	IRM Calibration Status	All Ions Missed
Data Filename	3fh.d	ACQ Method	test.m	Comment		Acquired Time	3/22/2021 10:10:31 PM



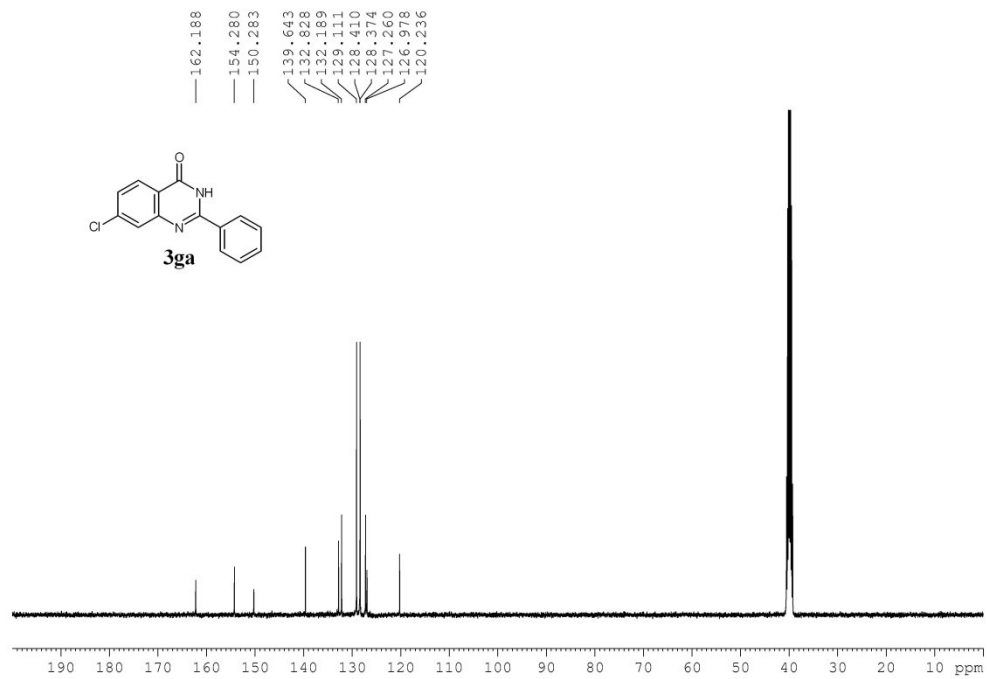
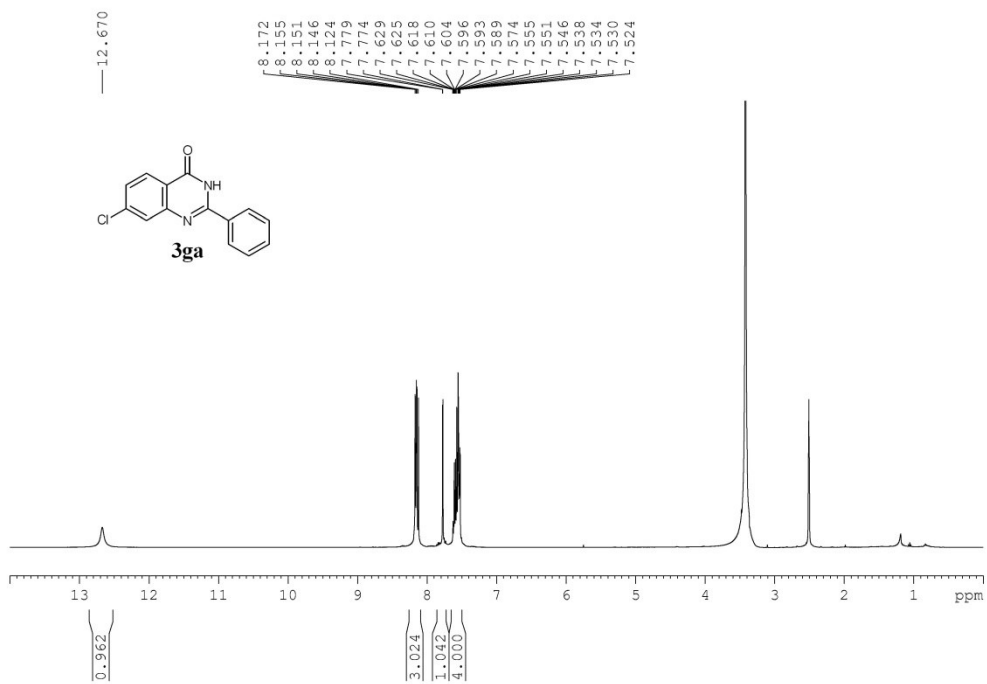


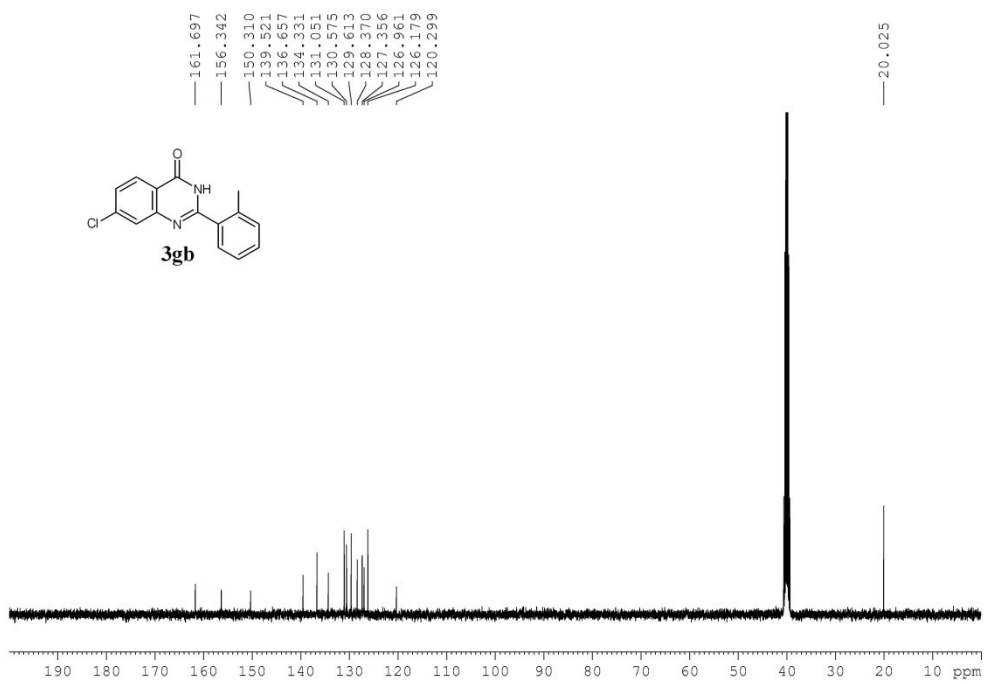
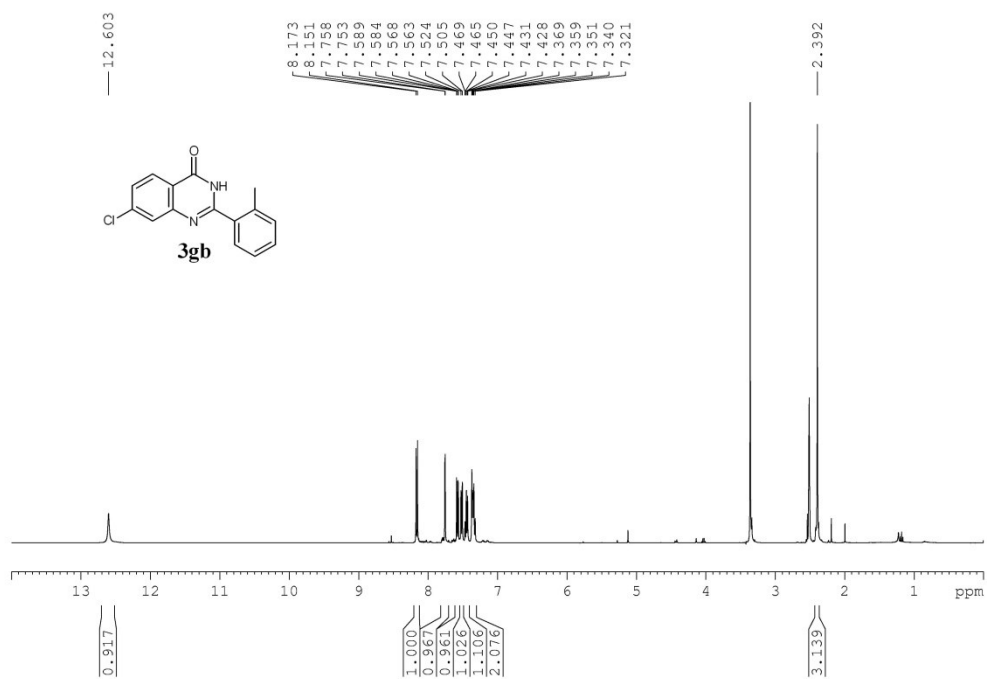


Sample Name	3fi	Position	P1-B6	Instrument Name	Instrument 1	User Name	
Inj Vol	0.5	InjPosition		SampleType	Sample	IRM Calibration Status	All Ions Missed
Data Filename	3fi.d	ACQ Method	test.m	Comment		Acquired Time	3/22/2021 10:11:48 PM

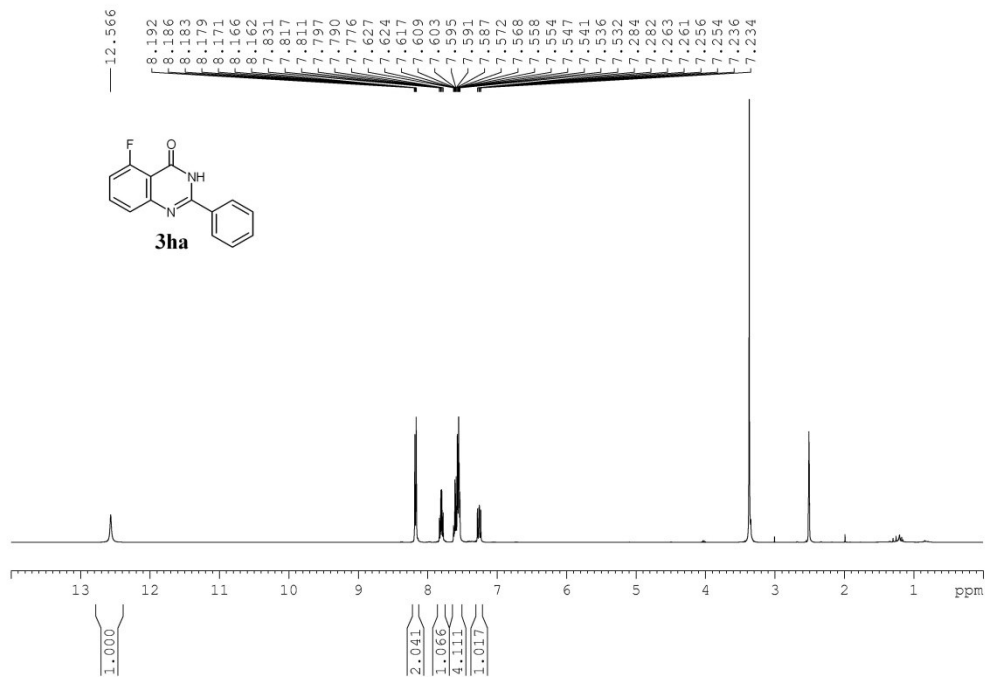
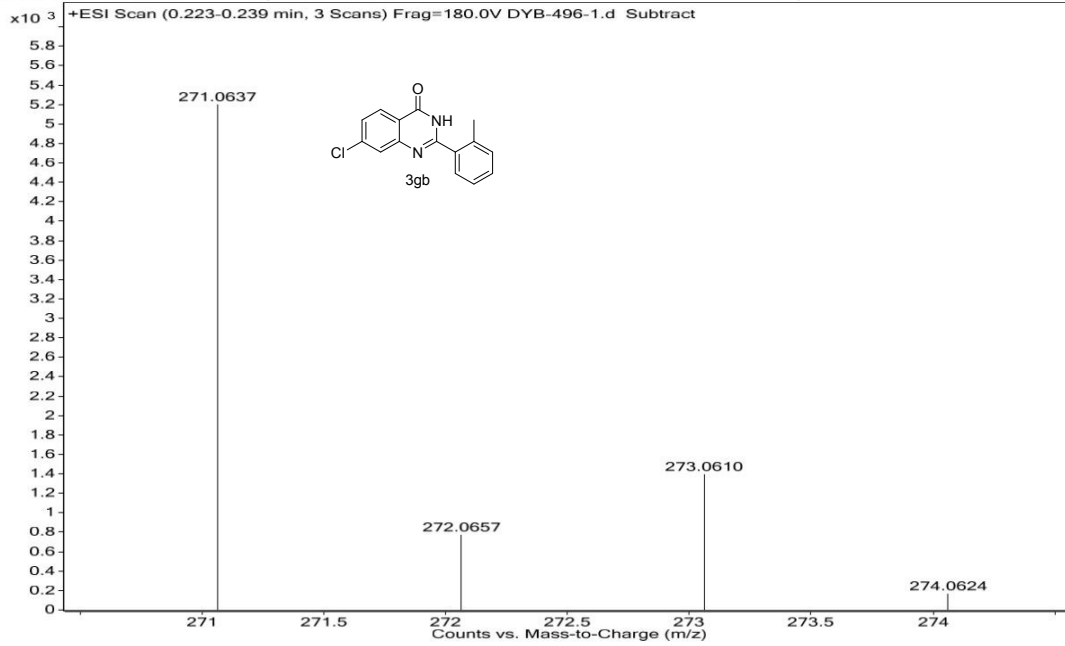


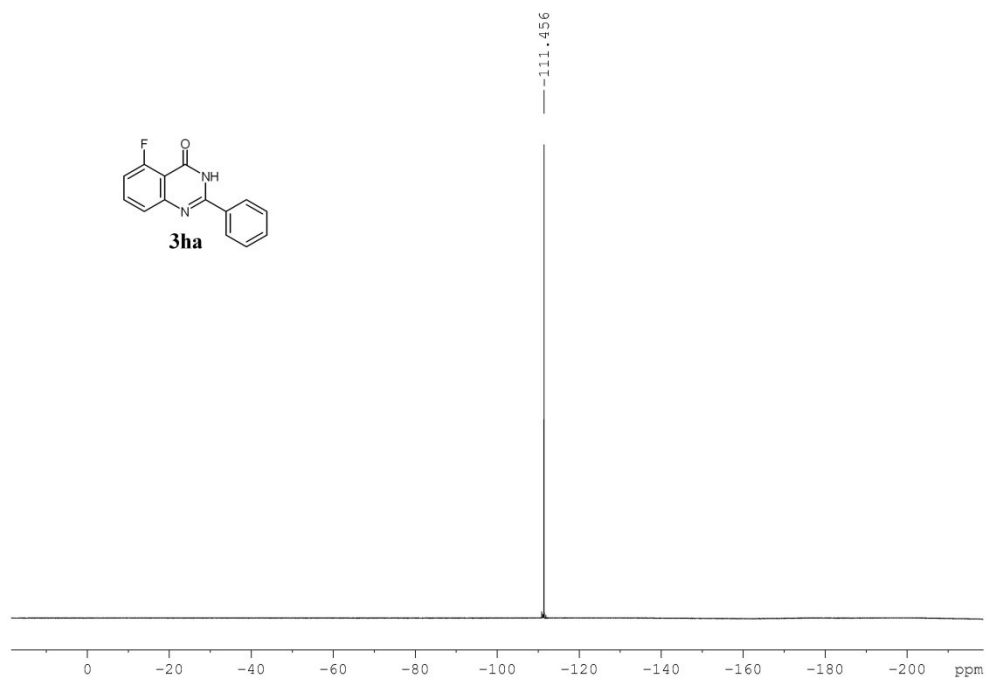
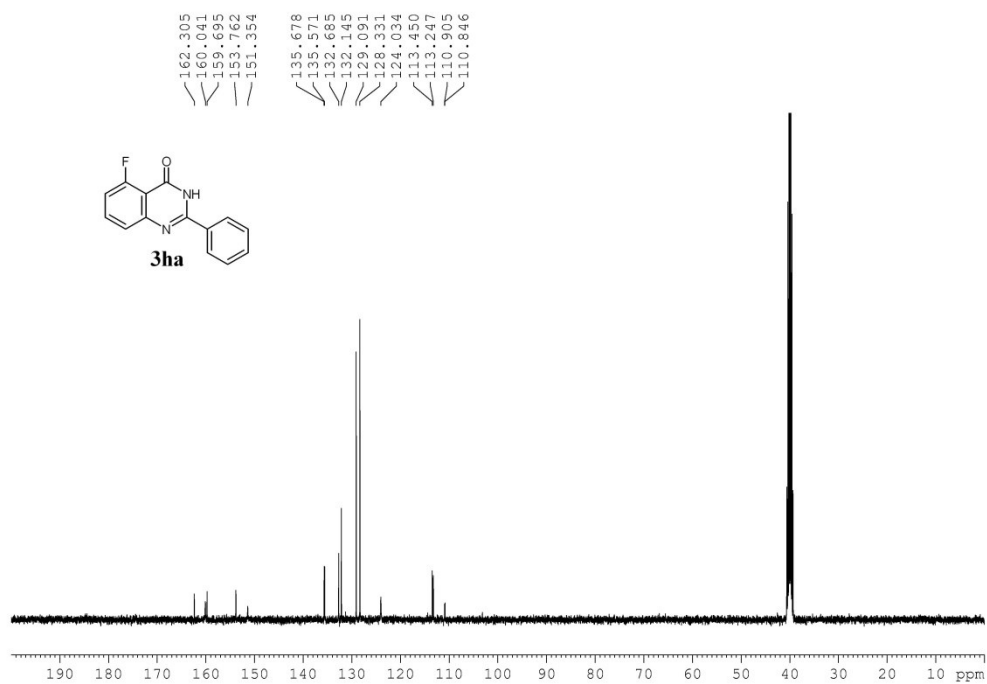


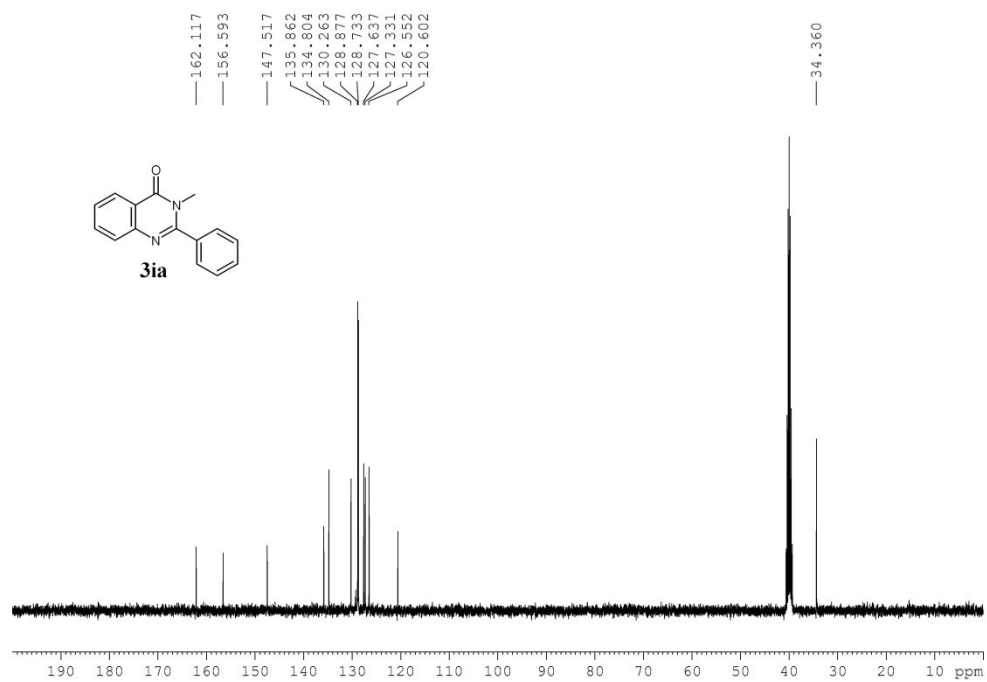
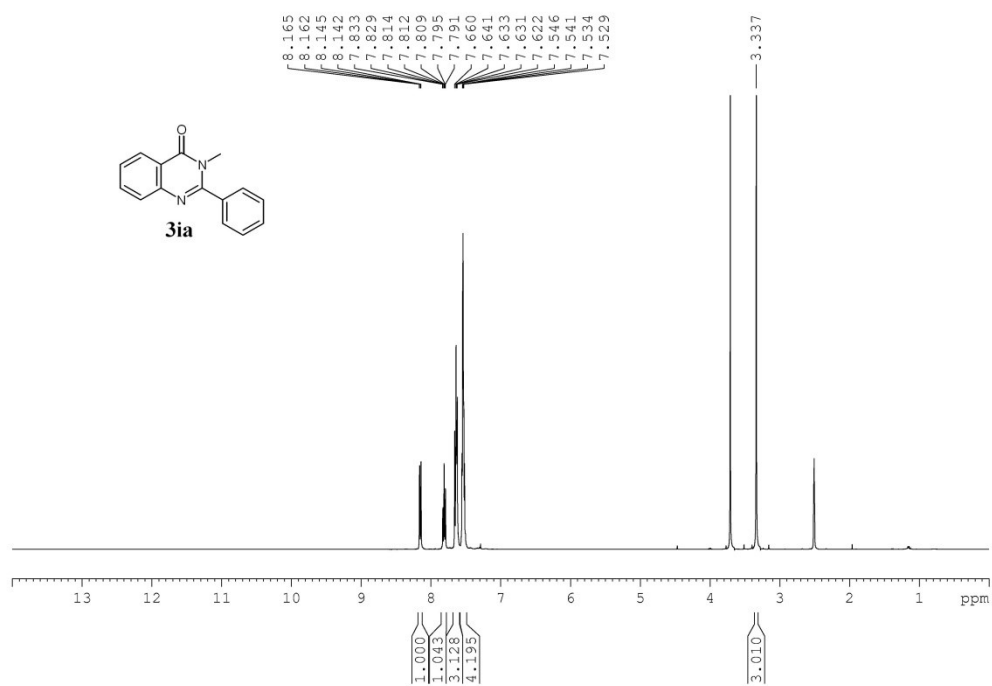


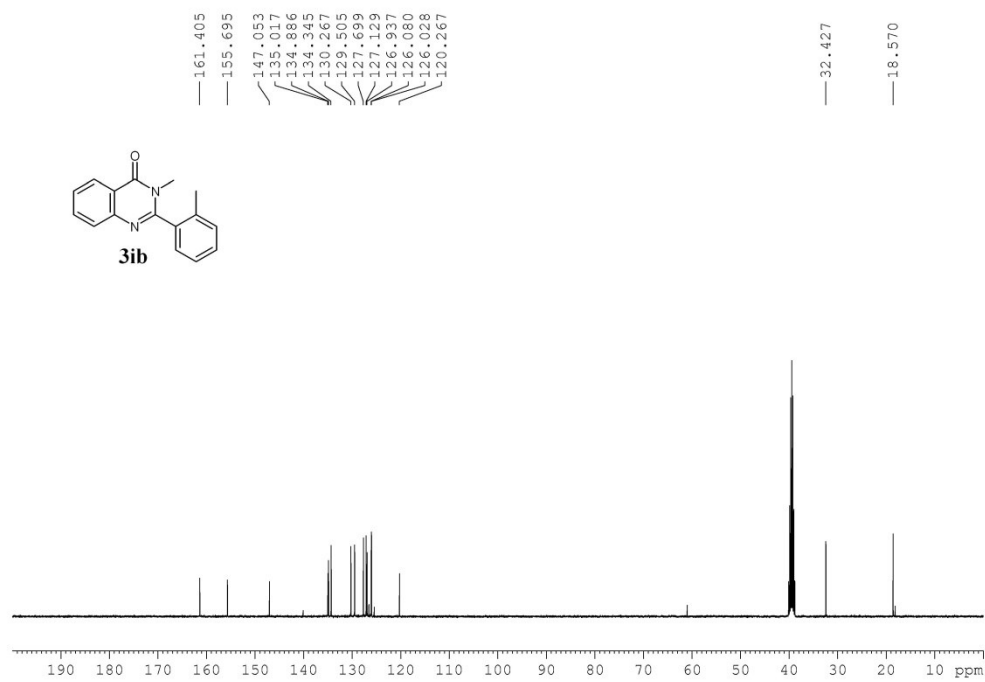
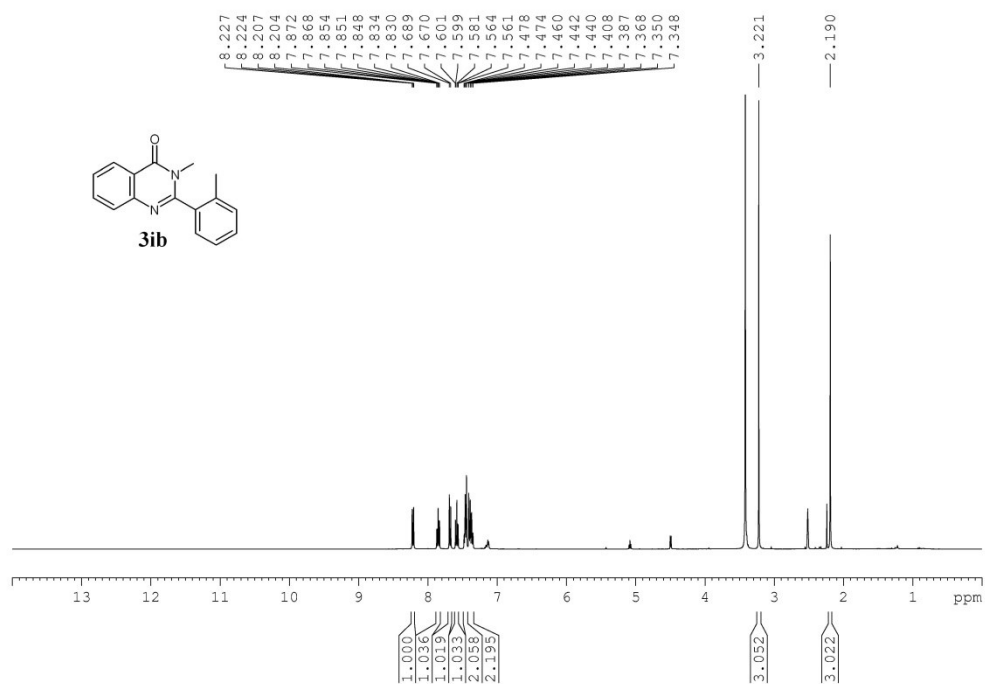


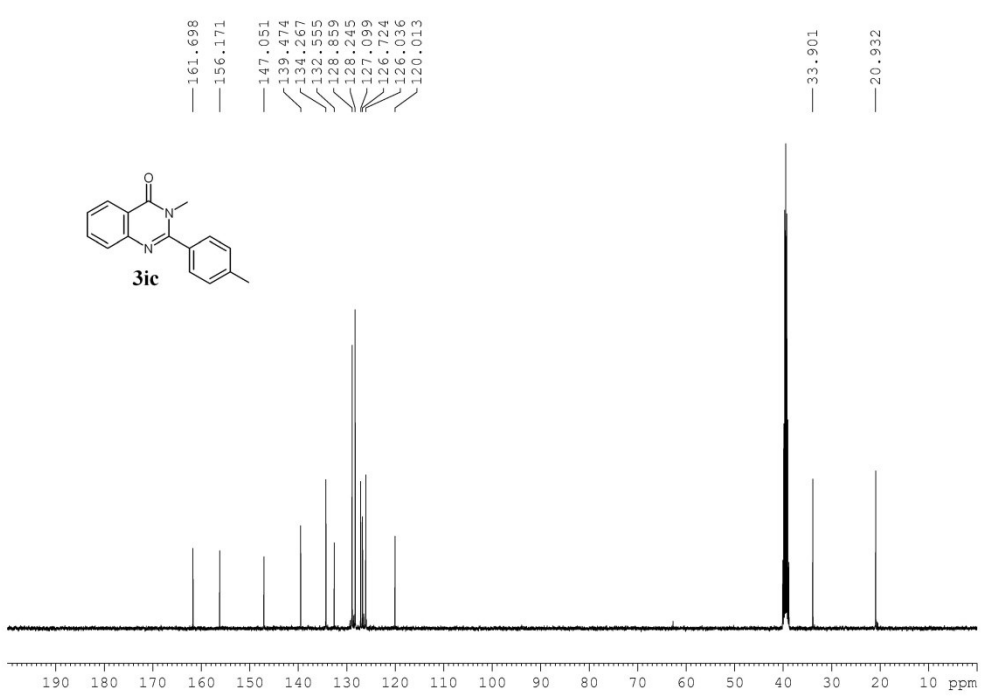
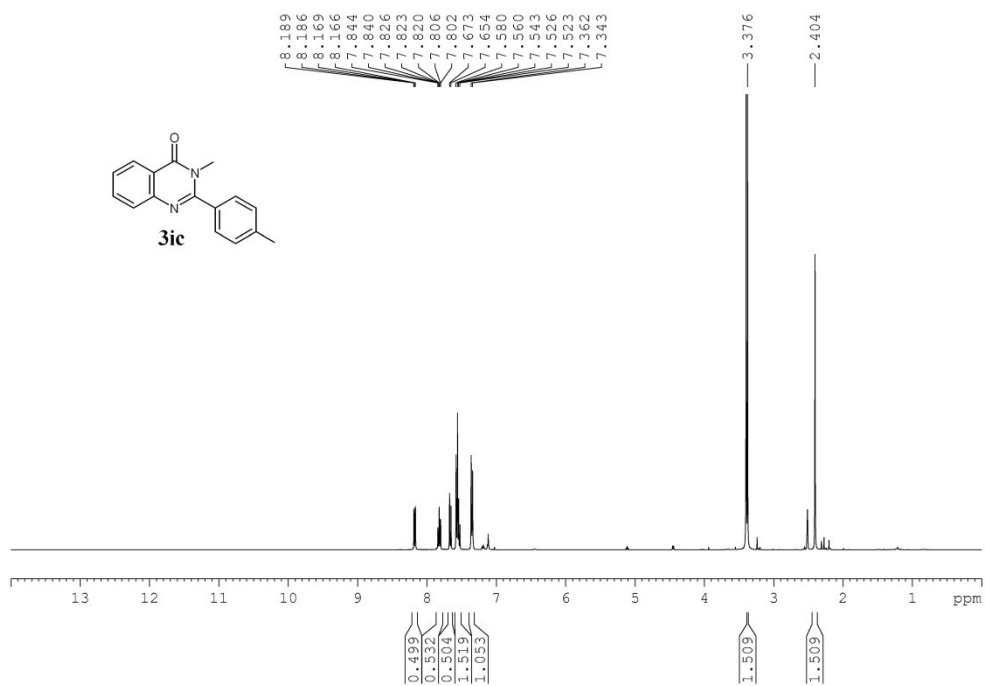
Sample Name	DYB-496-1	Position	P1-C3	Instrument Name	Instrument 1	User Name	
Inj Vol	0.2	InjPosition		SampleType	Sample	IRM Calibration Status	All Ions Missed
Data Filename	DYB-496-1.d	ACQ Method	test.m	Comment		Acquired Time	12/8/2020 2:53:48 PM

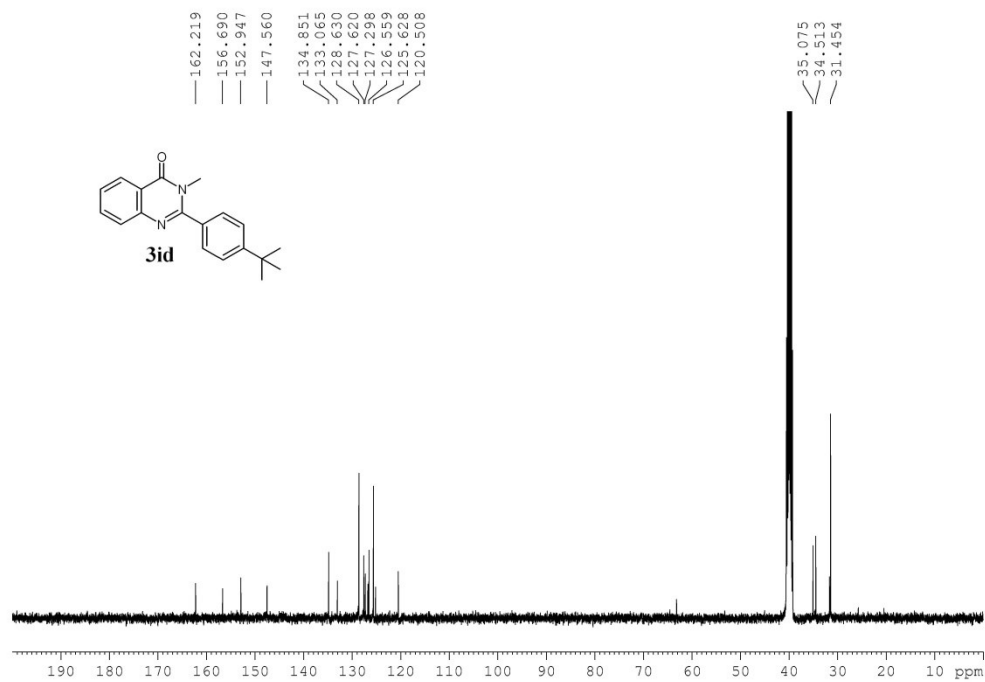
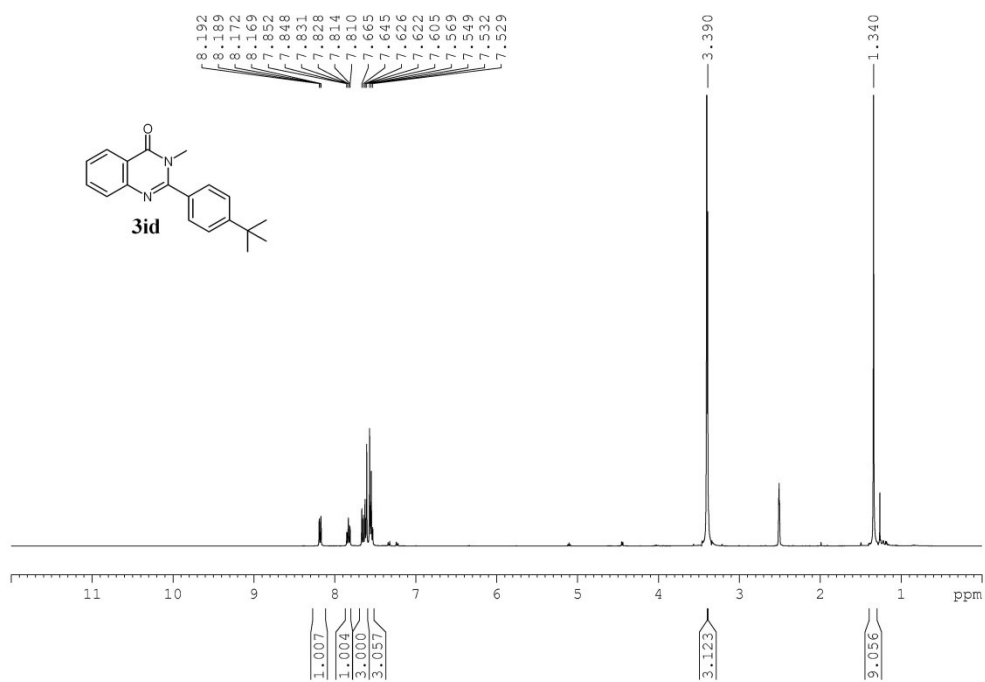




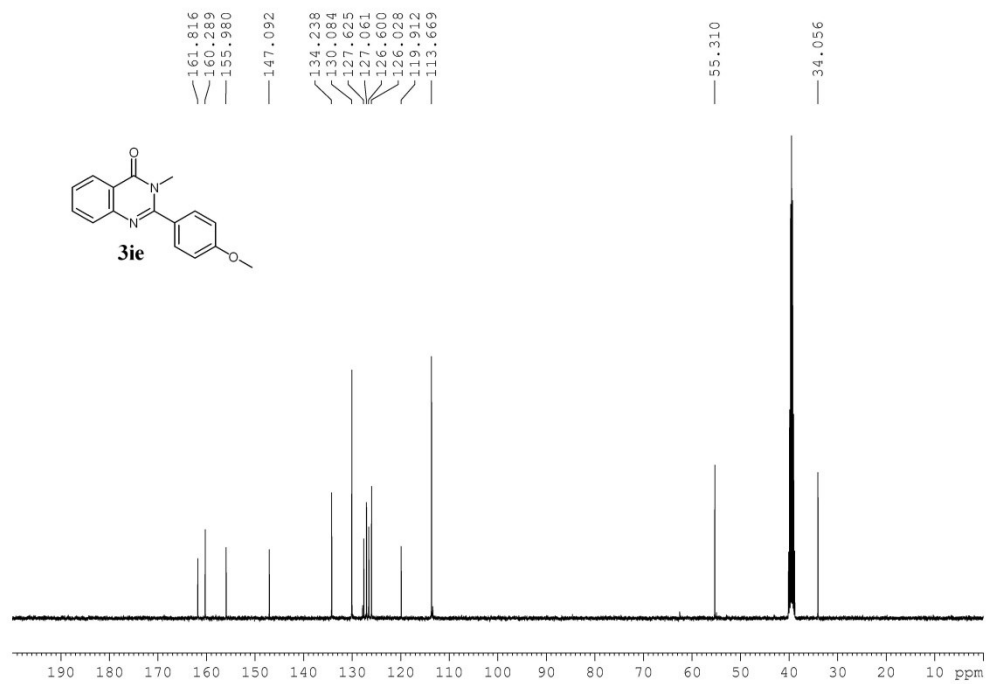
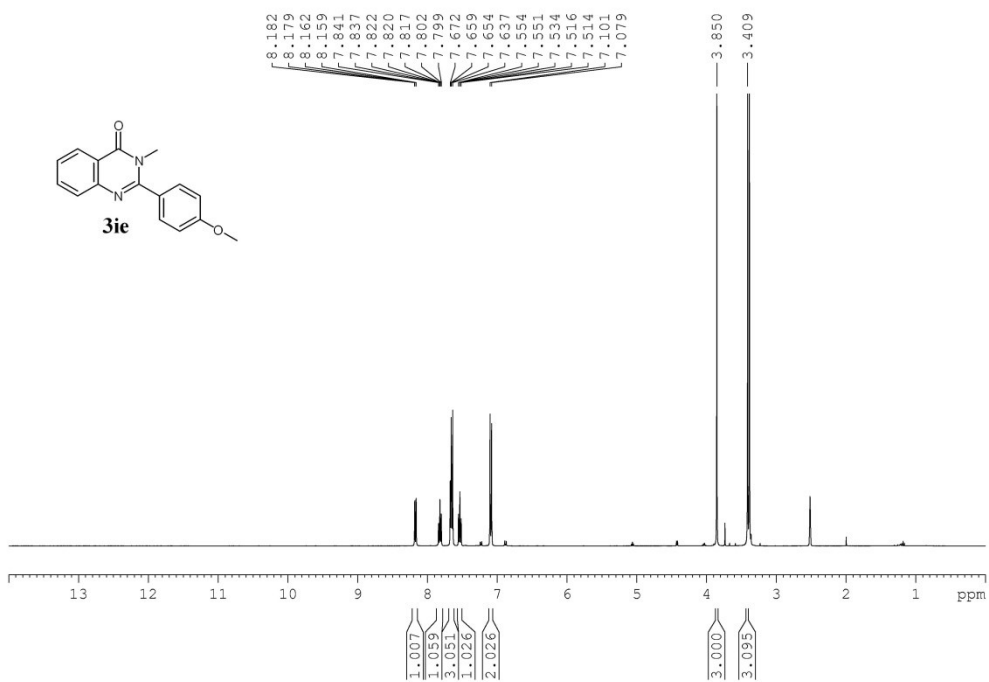


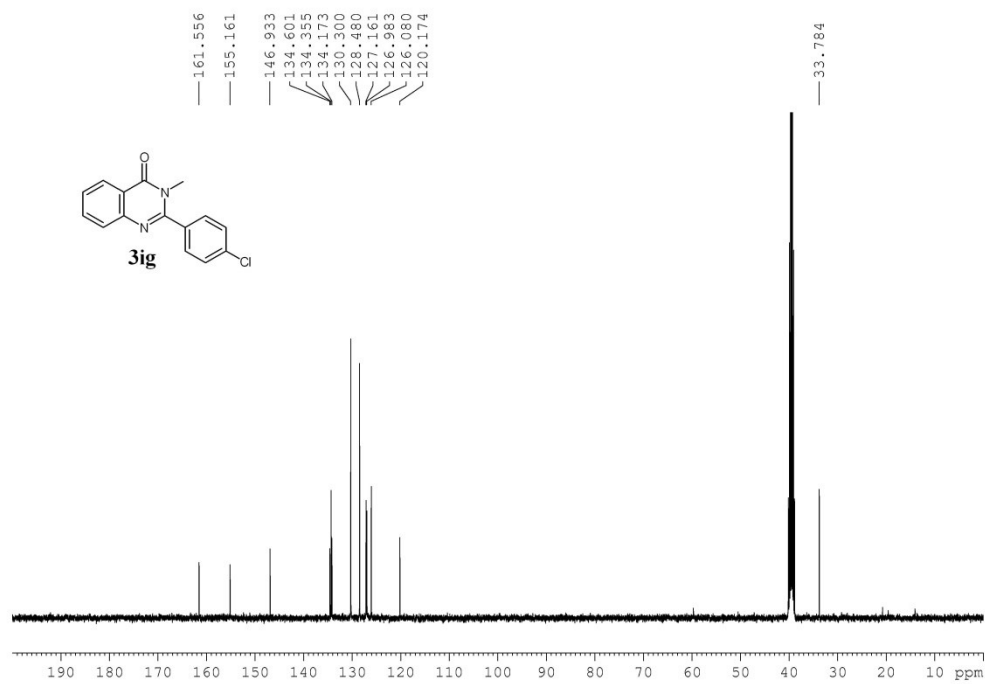
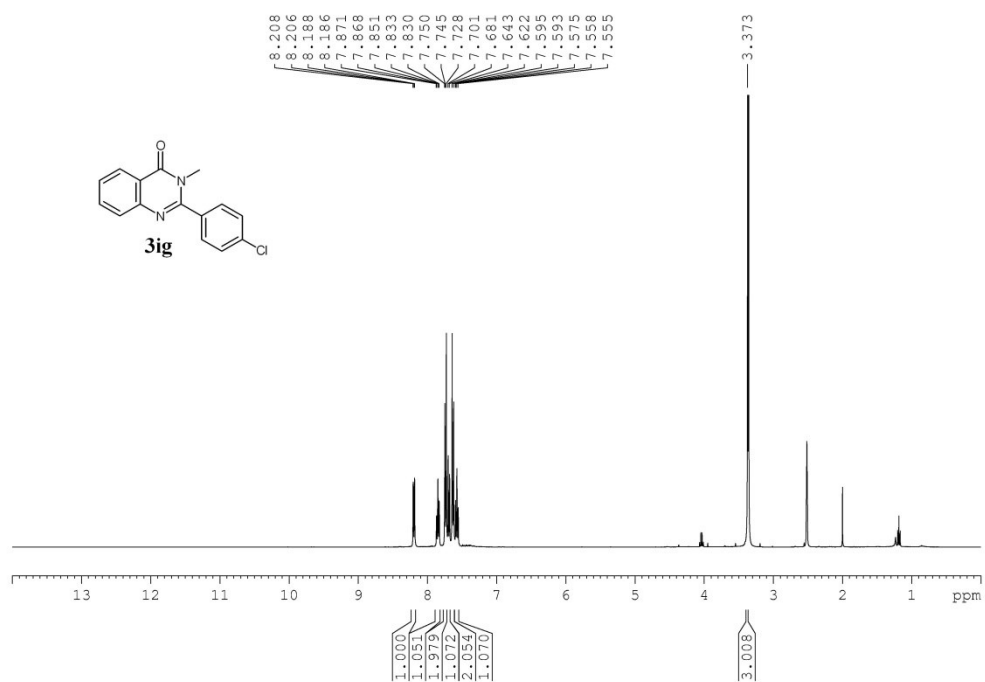


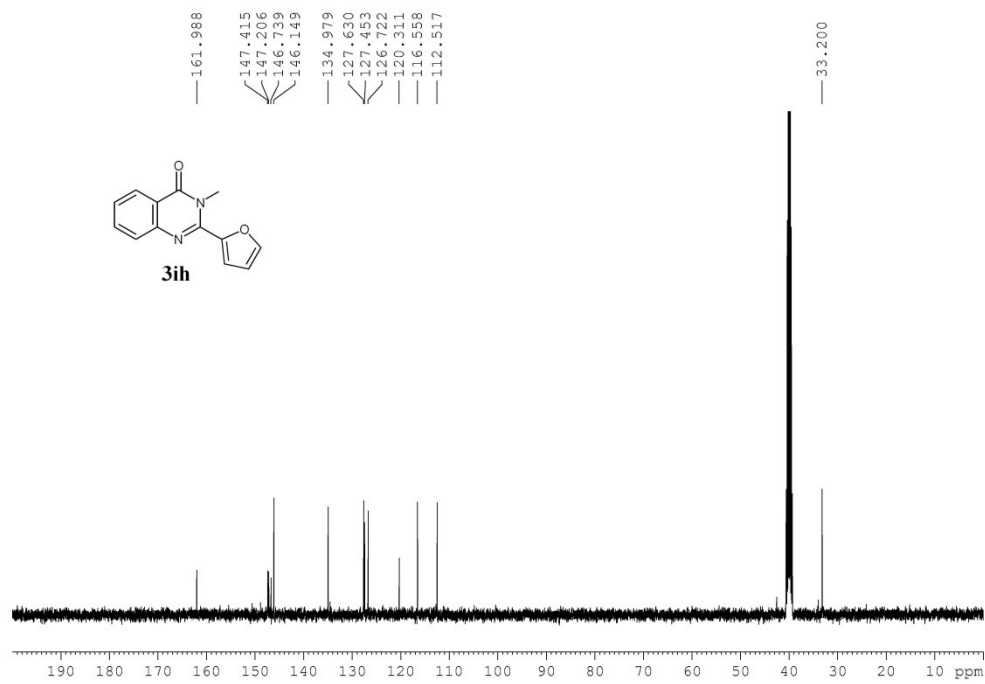
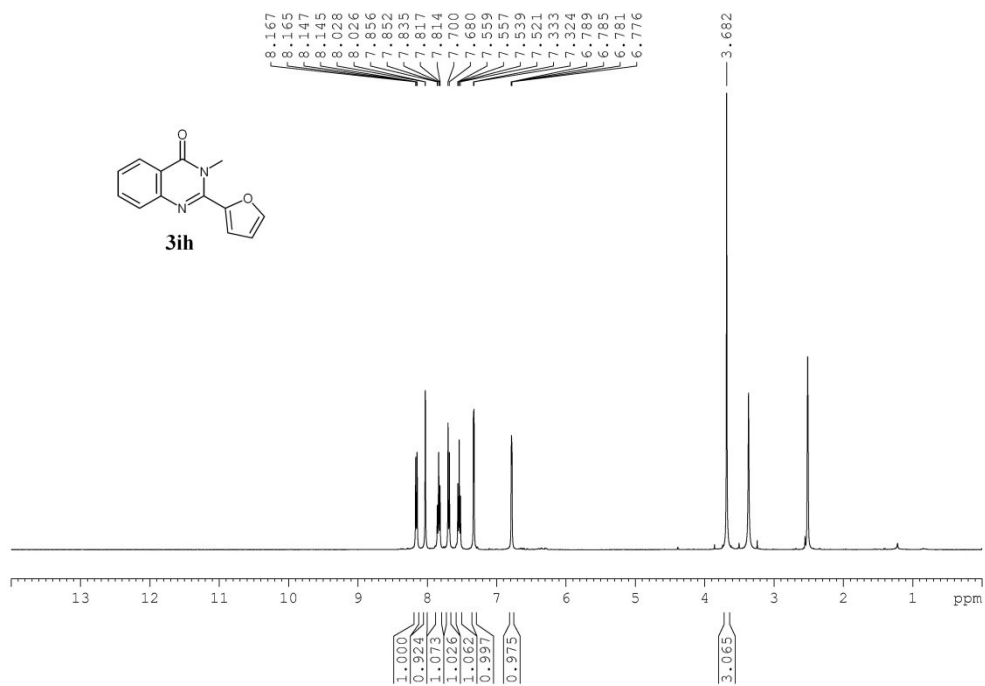


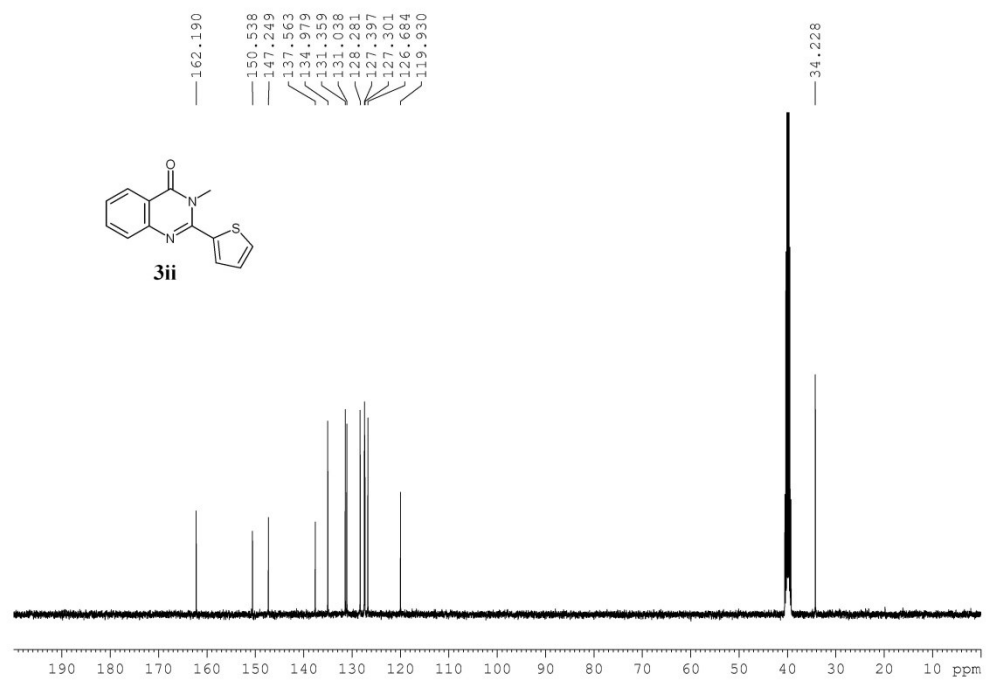
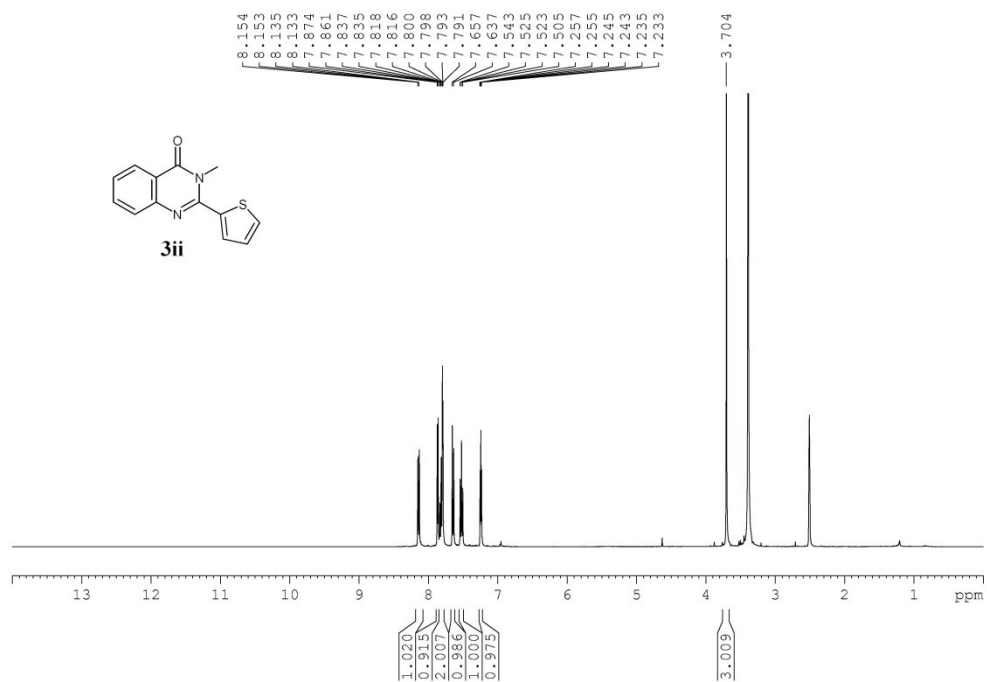


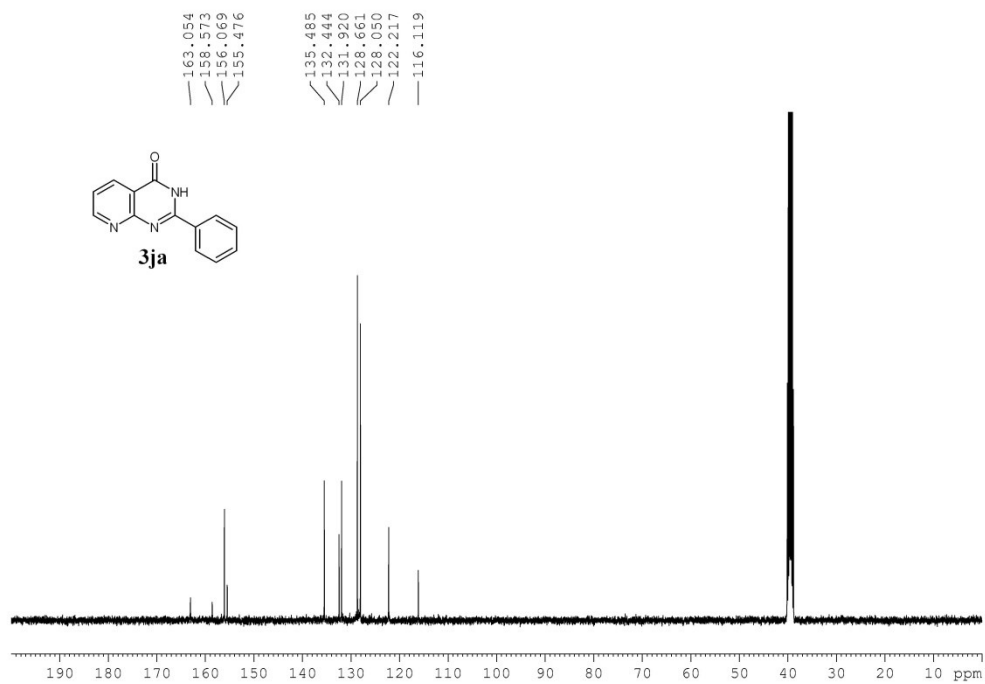
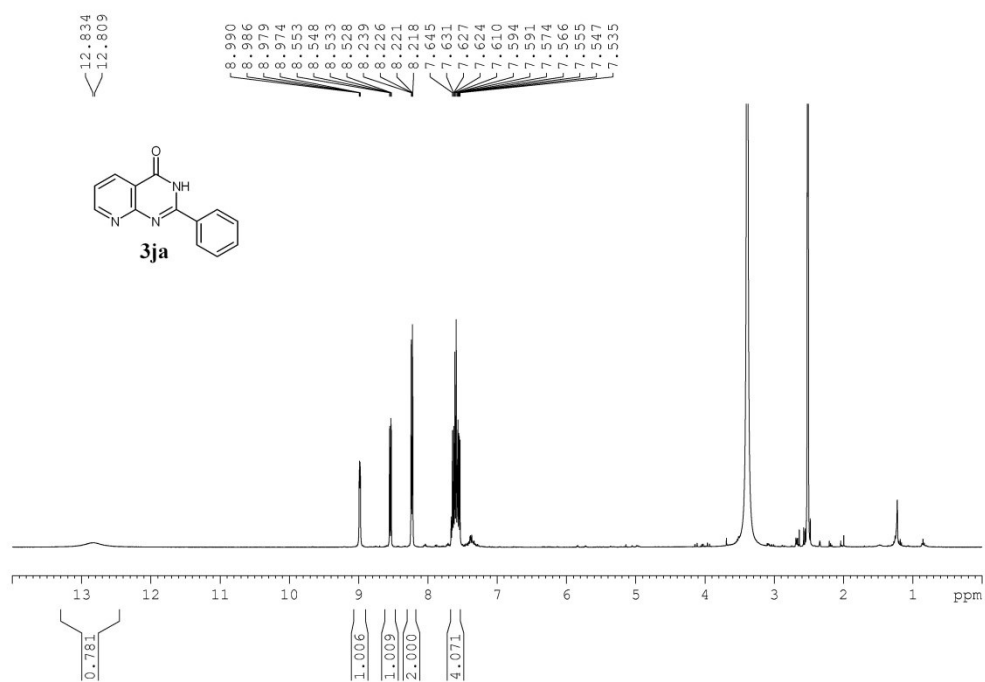


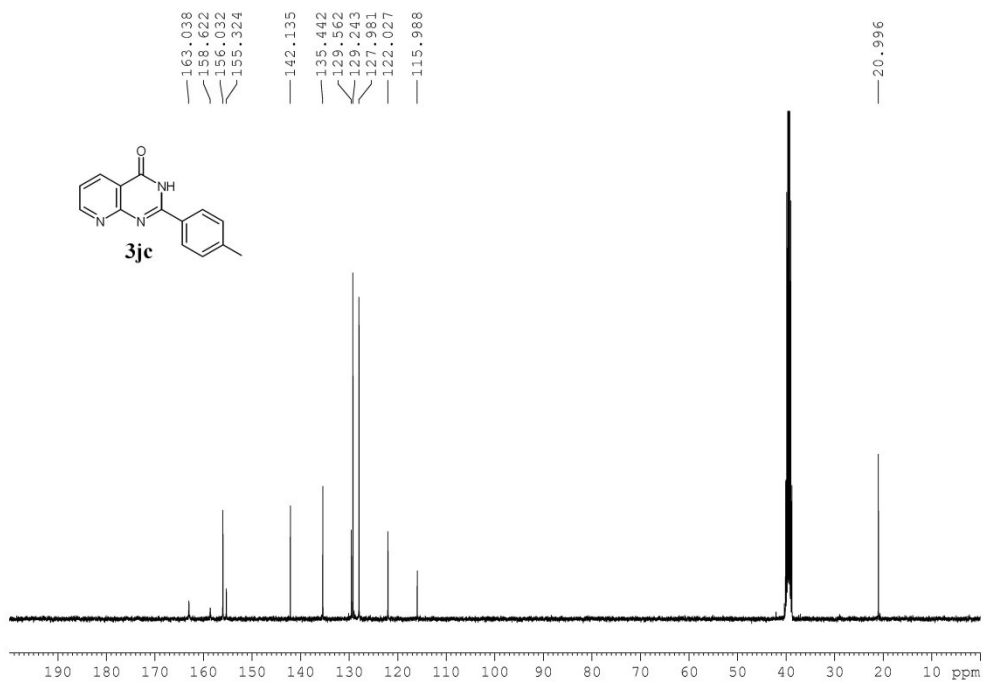
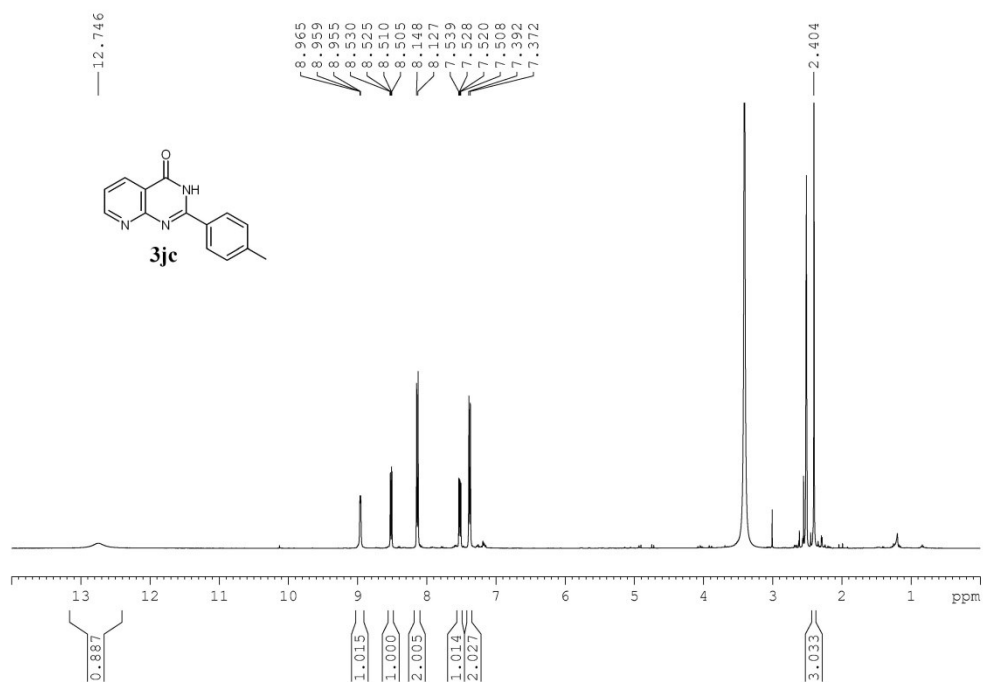


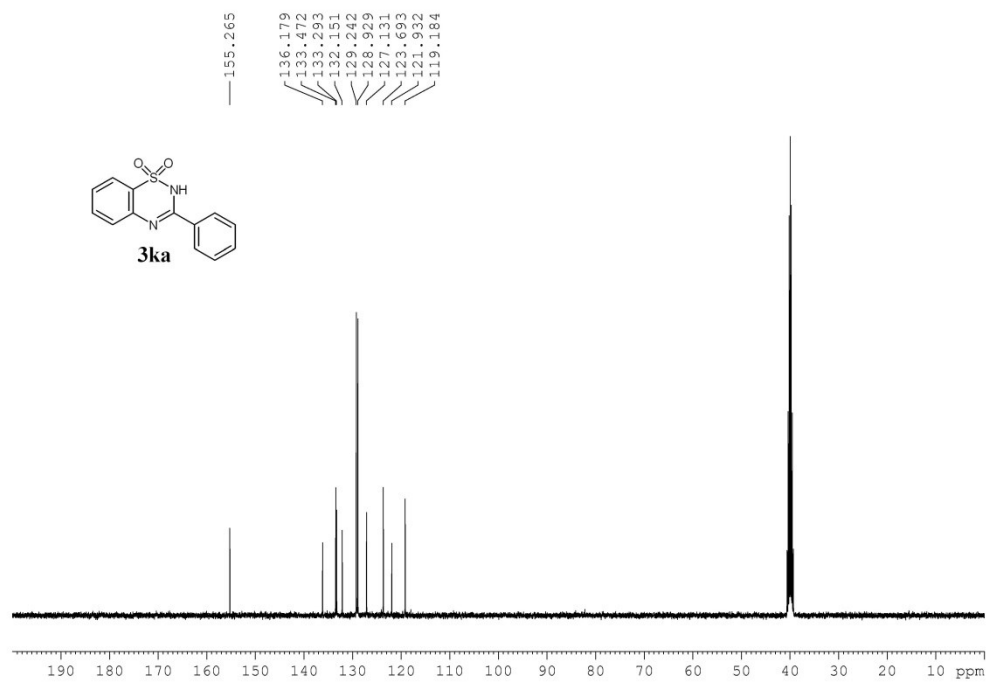
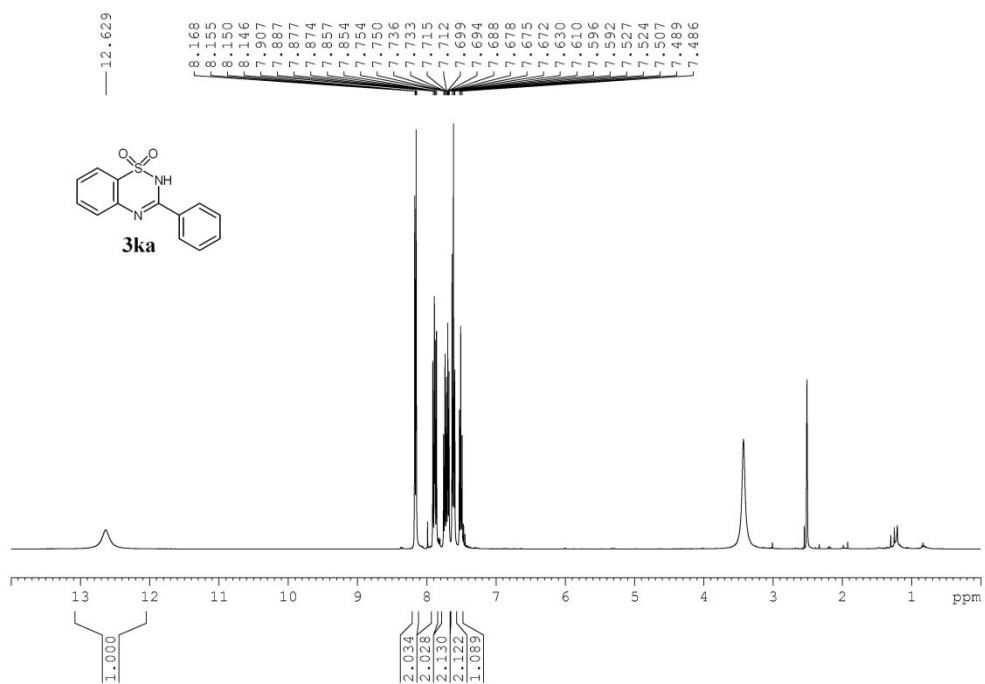


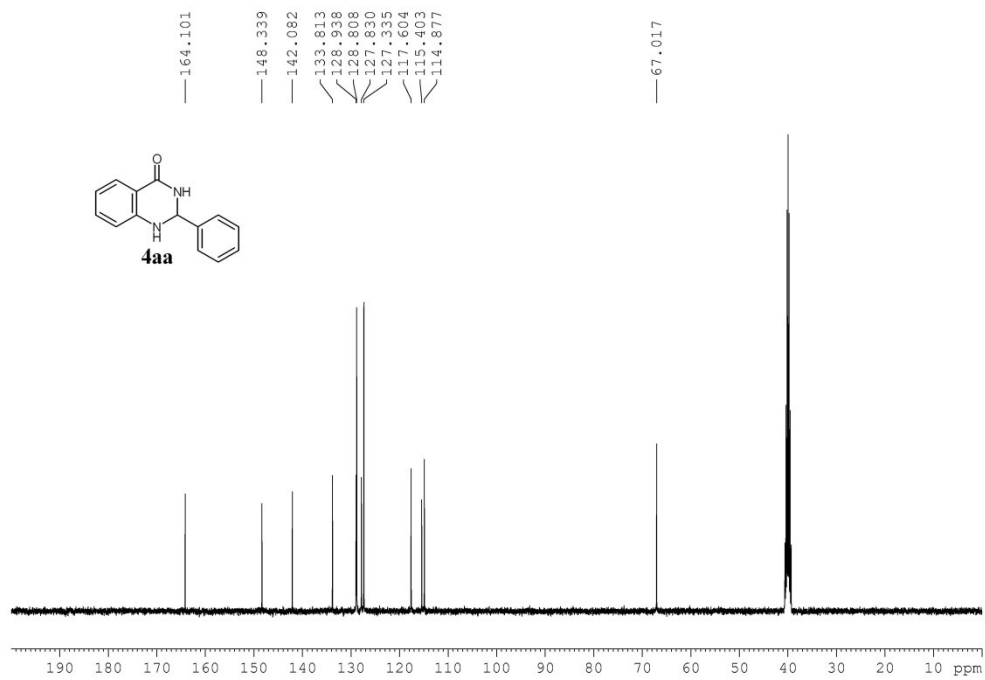
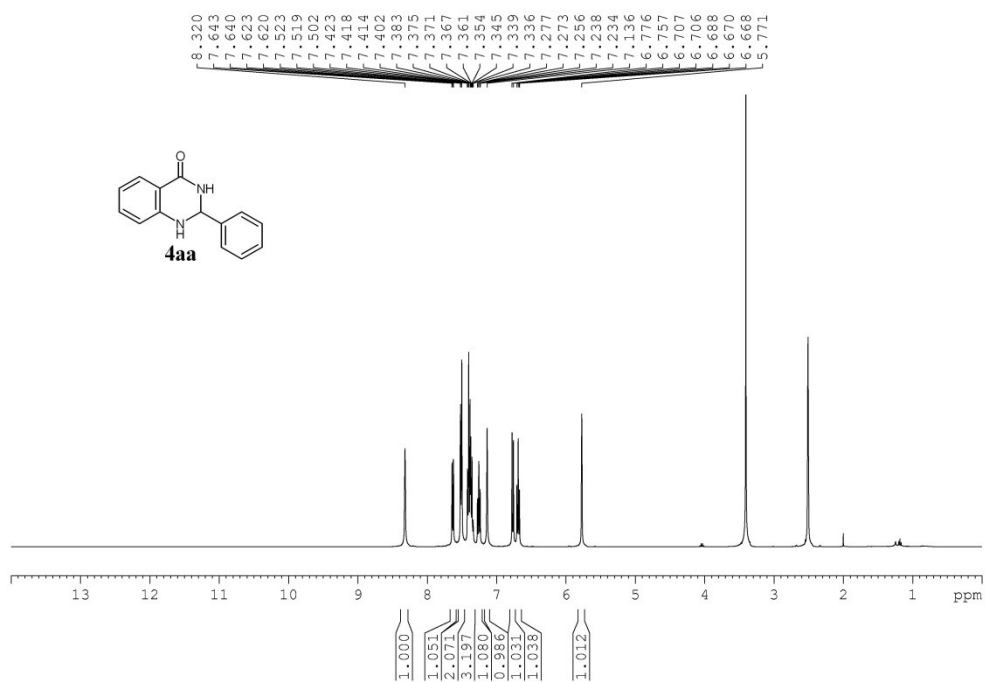














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