

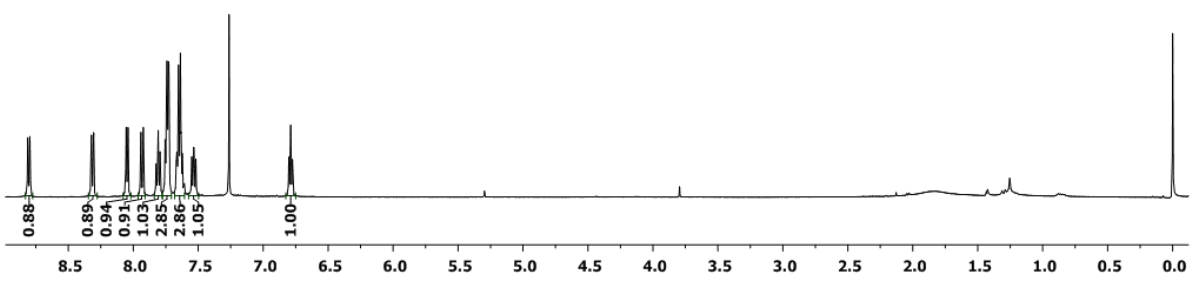
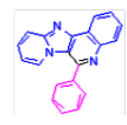
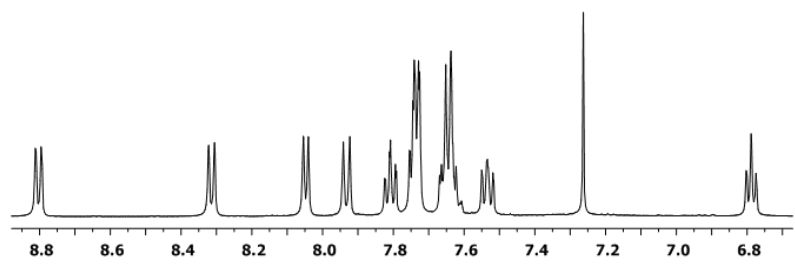
## Supporting information

### **Molecular iodine-catalysed oxidative CO-C(alkyl) bond cleavage of aryl/heteroaryl alkyl ketones: An efficient strategy to access fused polyheterocycles**

Geeta Sai Mani,<sup>a</sup> Ayanampudi Venkata Subba Rao,<sup>b</sup> Yellaiah Tangella,<sup>b</sup> Satish sunkari,<sup>b</sup>  
Faria Sultana,<sup>b</sup> Hari Krishna Namballa,<sup>a</sup> Nagula Shankaraiah<sup>a,\*</sup> and Ahmed Kamal<sup>\*a,b,c</sup>

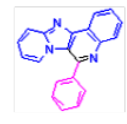
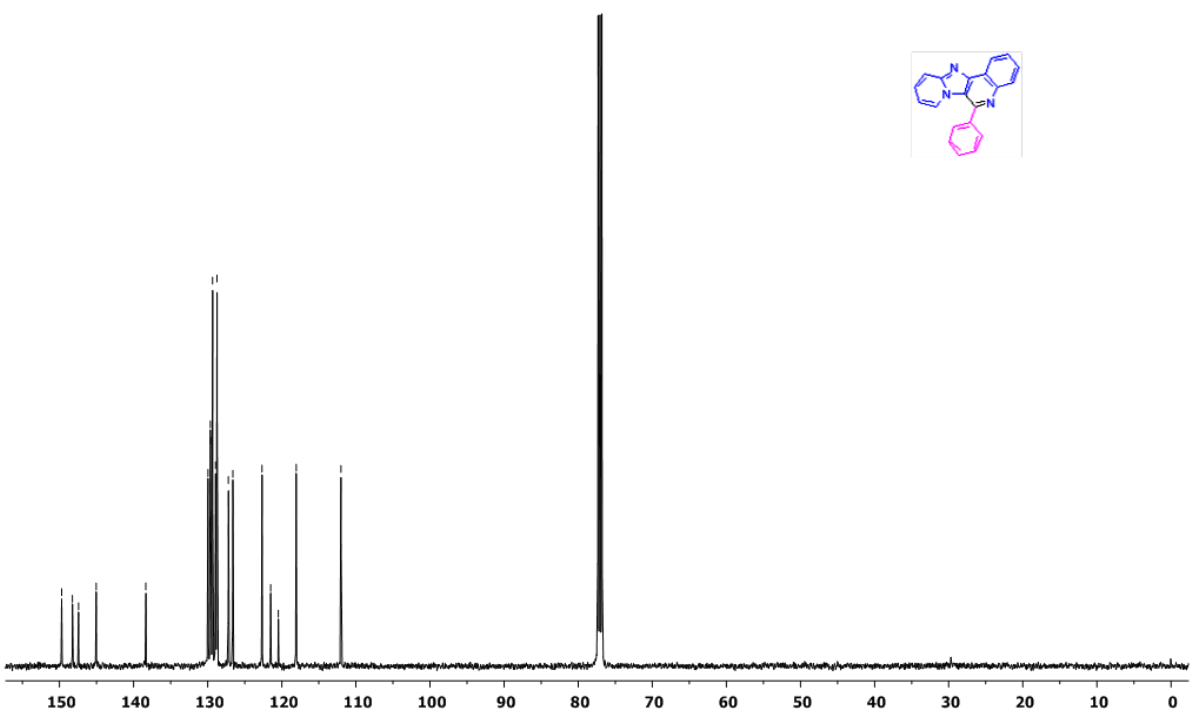
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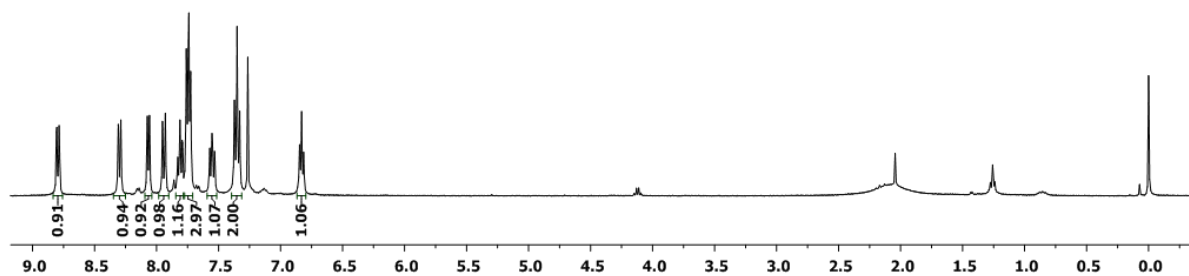
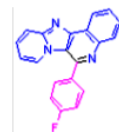
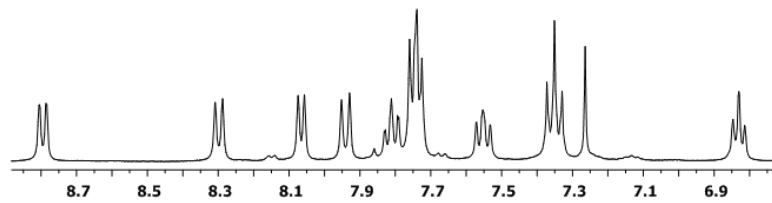


<sup>1</sup>H NMR spectrum of compound 4a

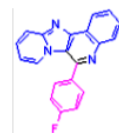
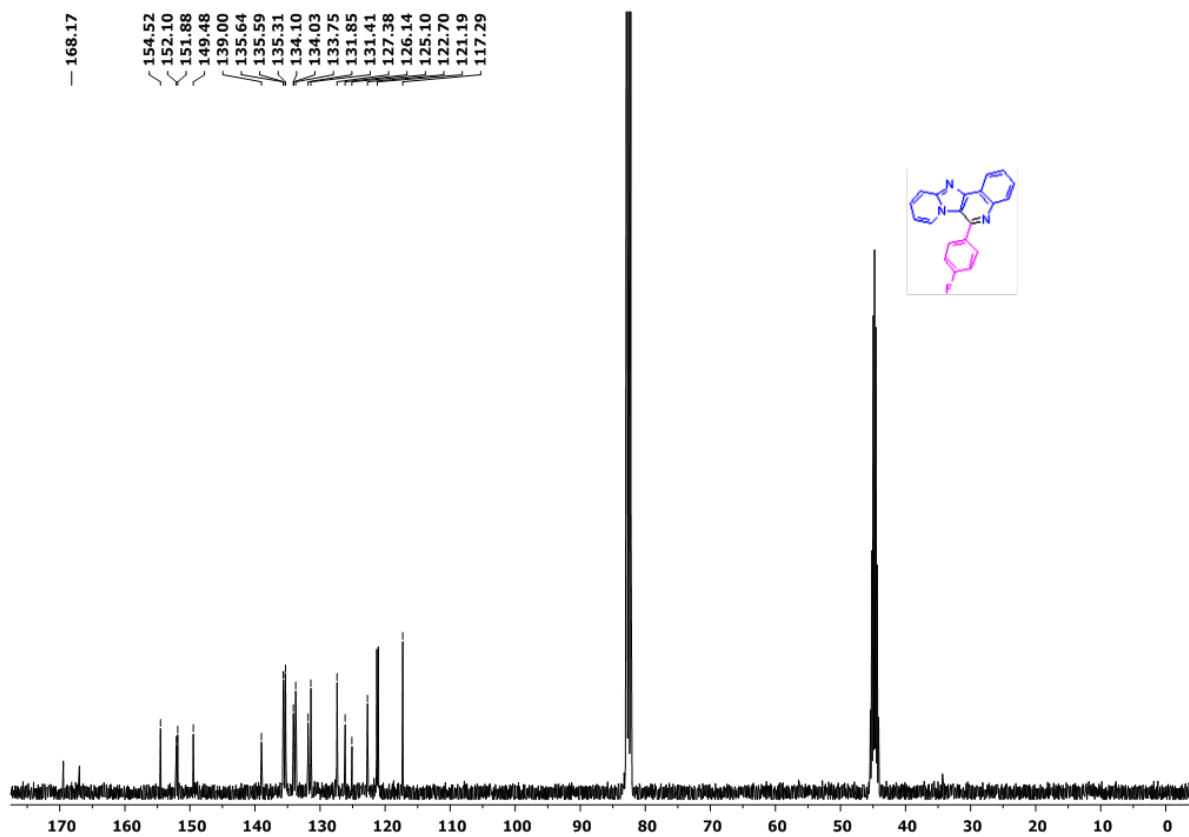
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- 148.25
- 147.43
- 145.05
- 138.35
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- 129.34
- 128.94
- 128.74
- 126.61
- 122.67
- 119.89



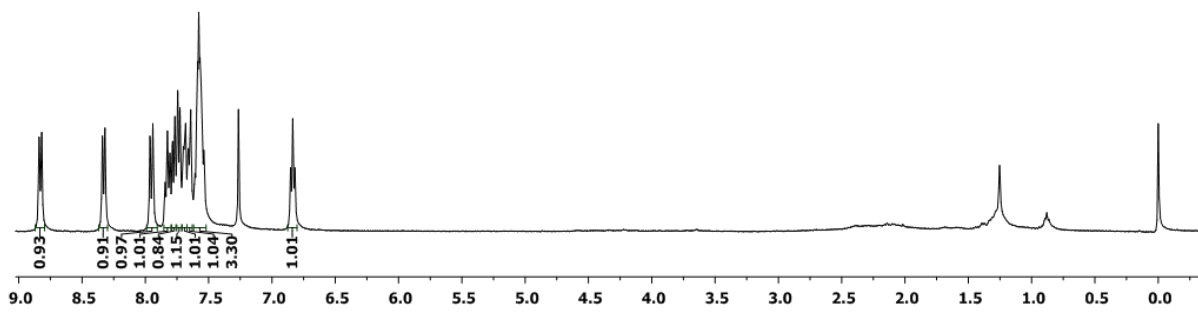
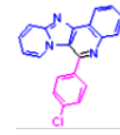
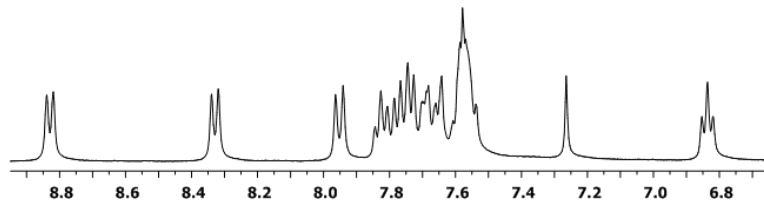
<sup>13</sup>C NMR spectrum of compound 4a



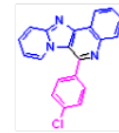
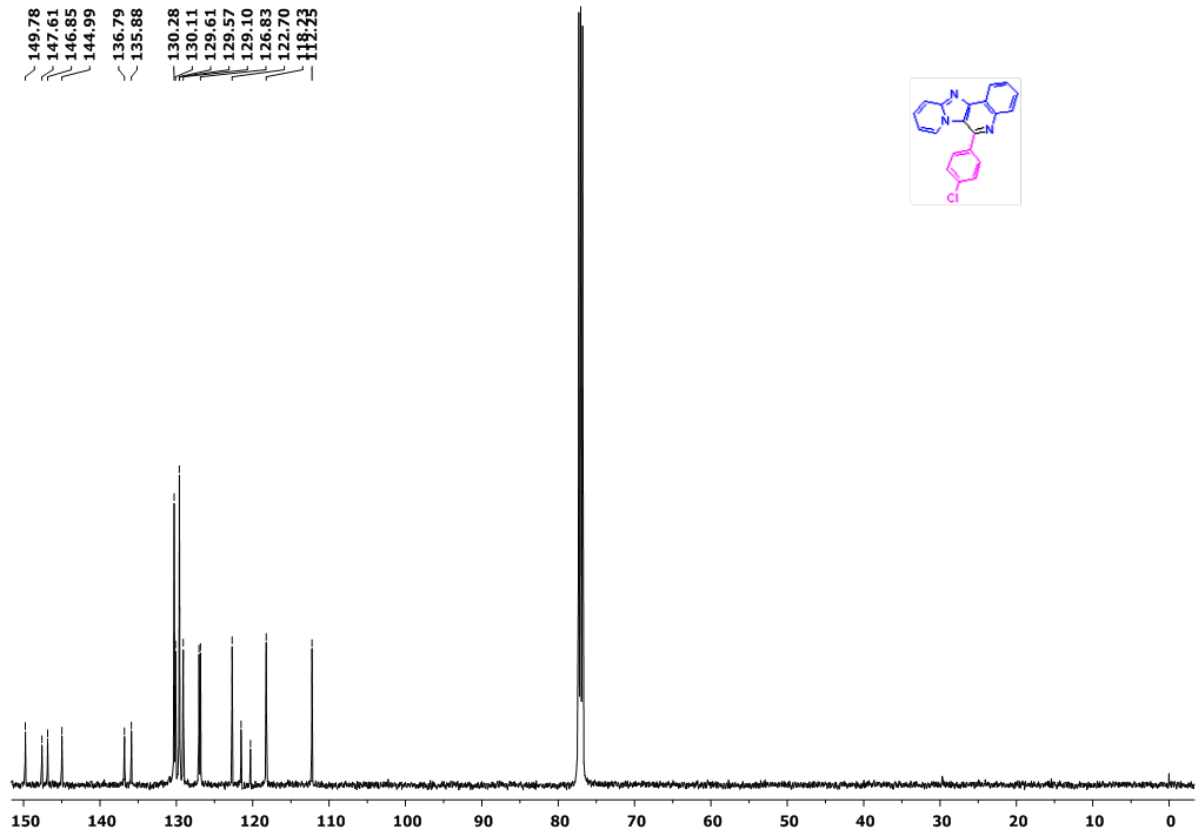
<sup>1</sup>H NMR spectrum of compound 4b



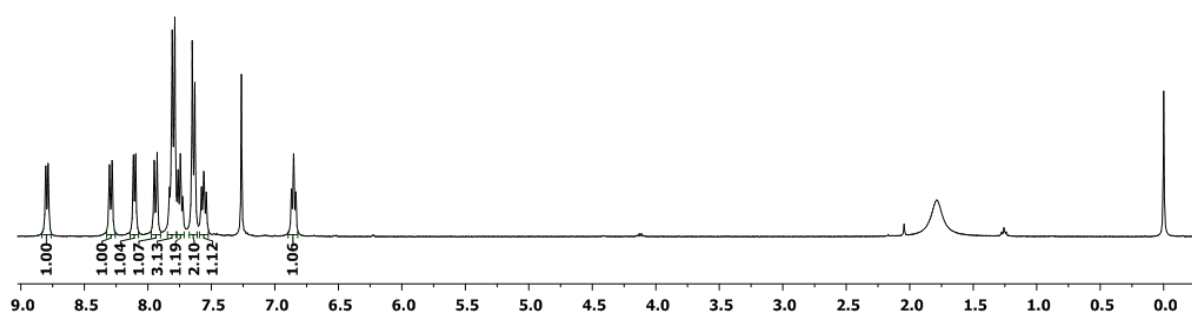
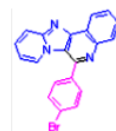
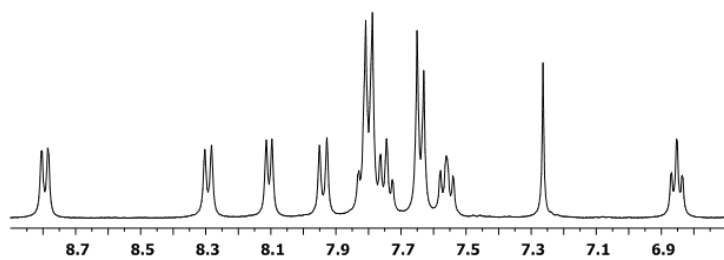
<sup>13</sup>C NMR spectrum of compound 4b



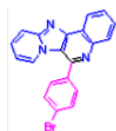
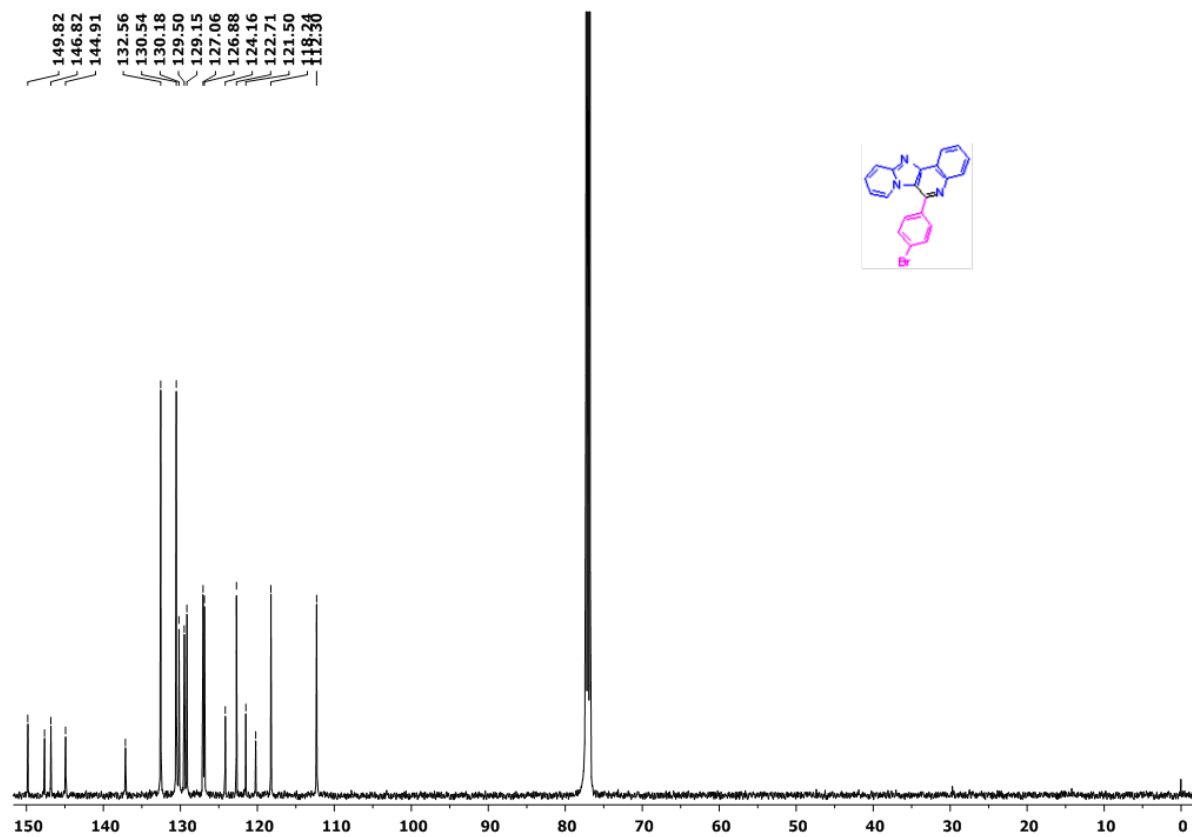
$^1\text{H}$  NMR spectrum of compound **4c**



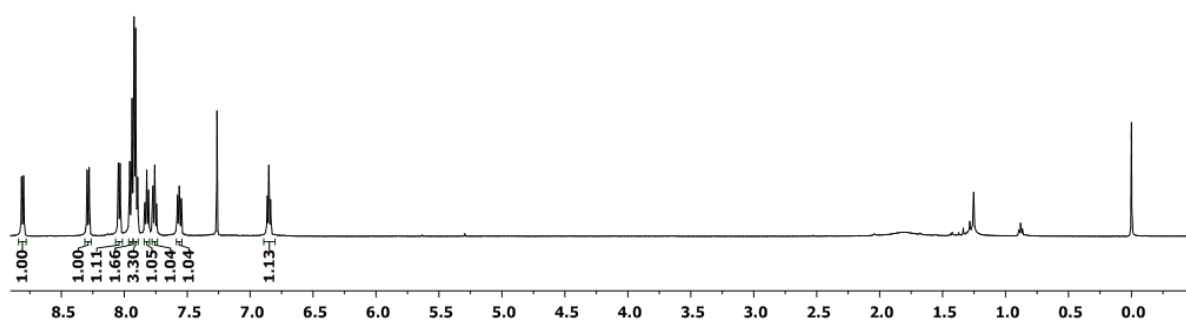
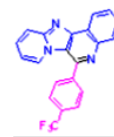
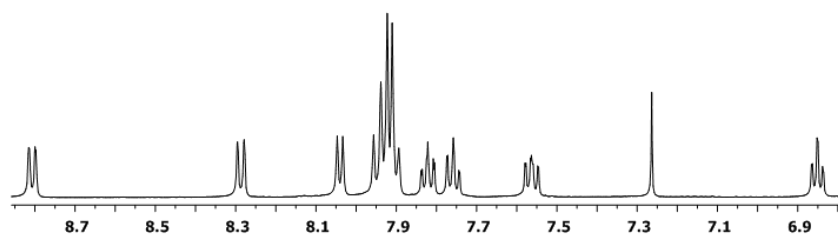
$^{13}\text{C}$  NMR spectrum of compound **4c**



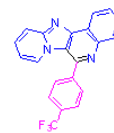
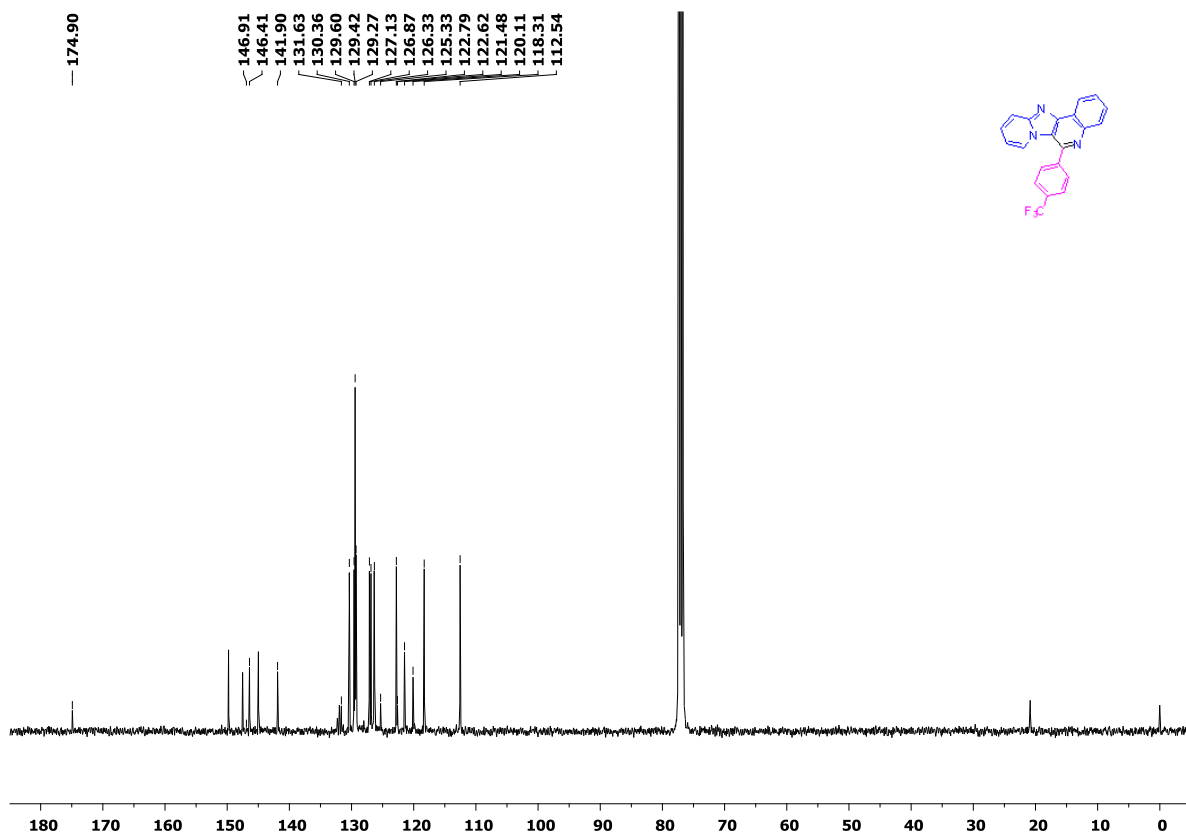
$^1\text{H}$  NMR spectrum of compound **4d**



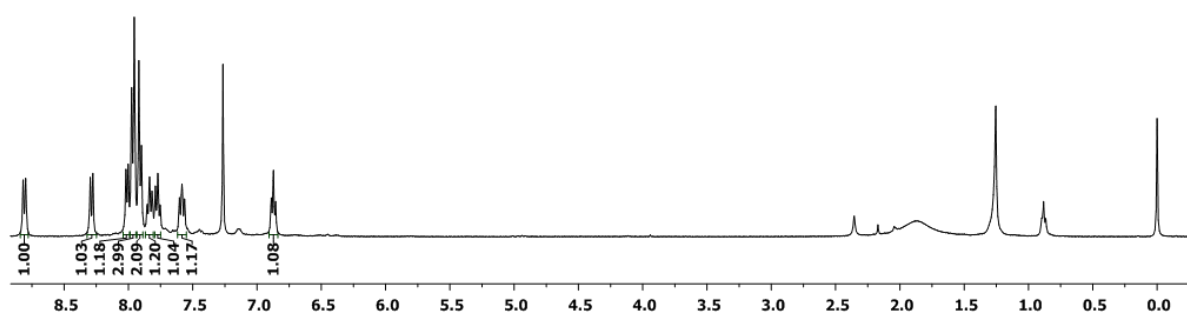
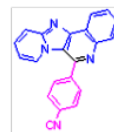
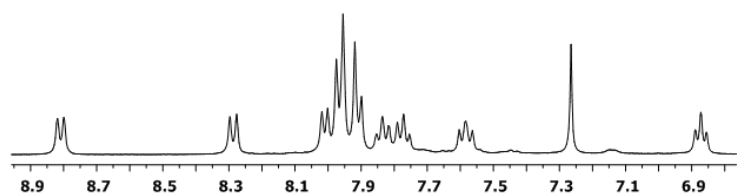
$^{13}\text{C}$  NMR spectrum of compound **4d**



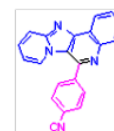
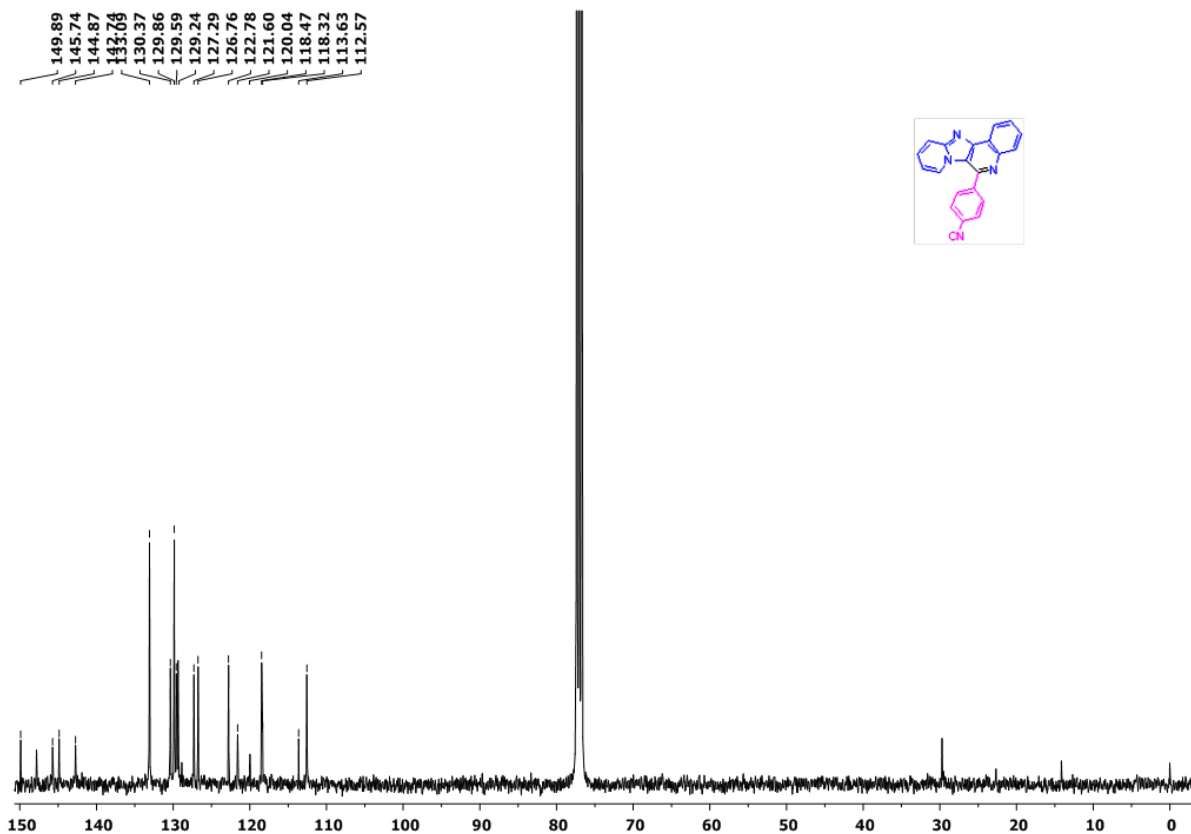
<sup>1</sup>H NMR spectrum of compound 4e



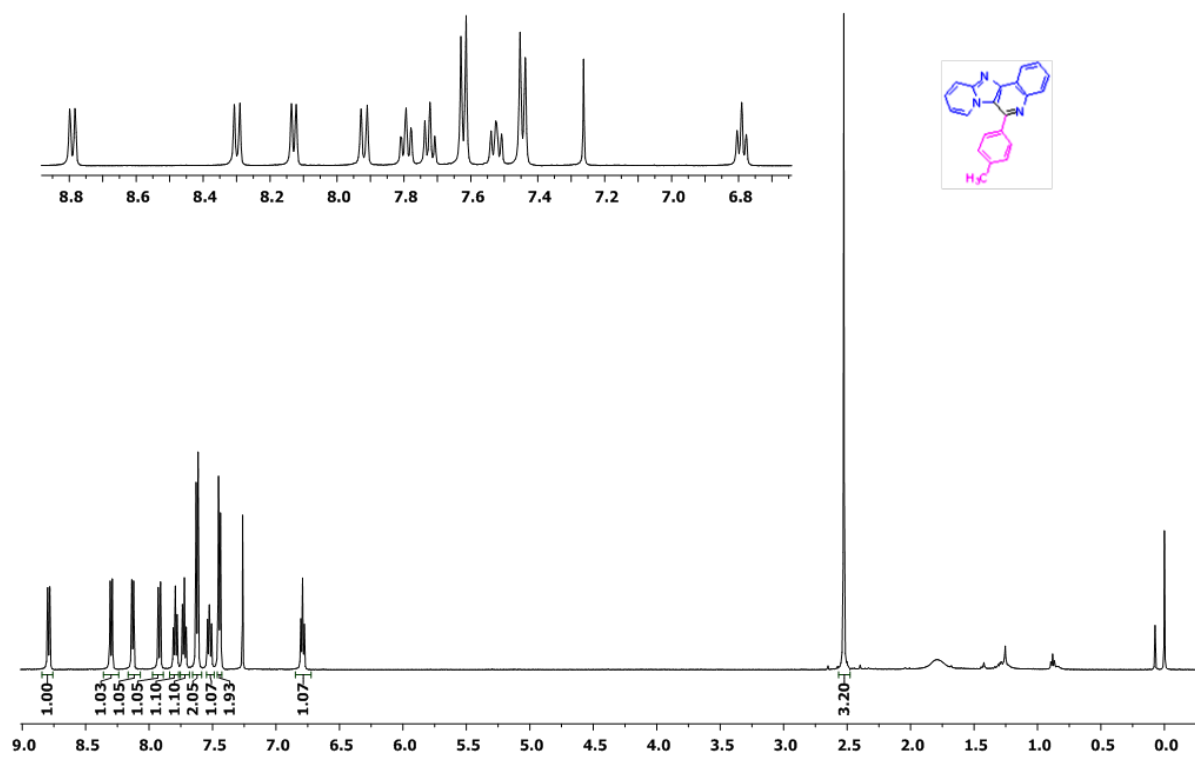
<sup>13</sup>C NMR spectrum of compound 4e



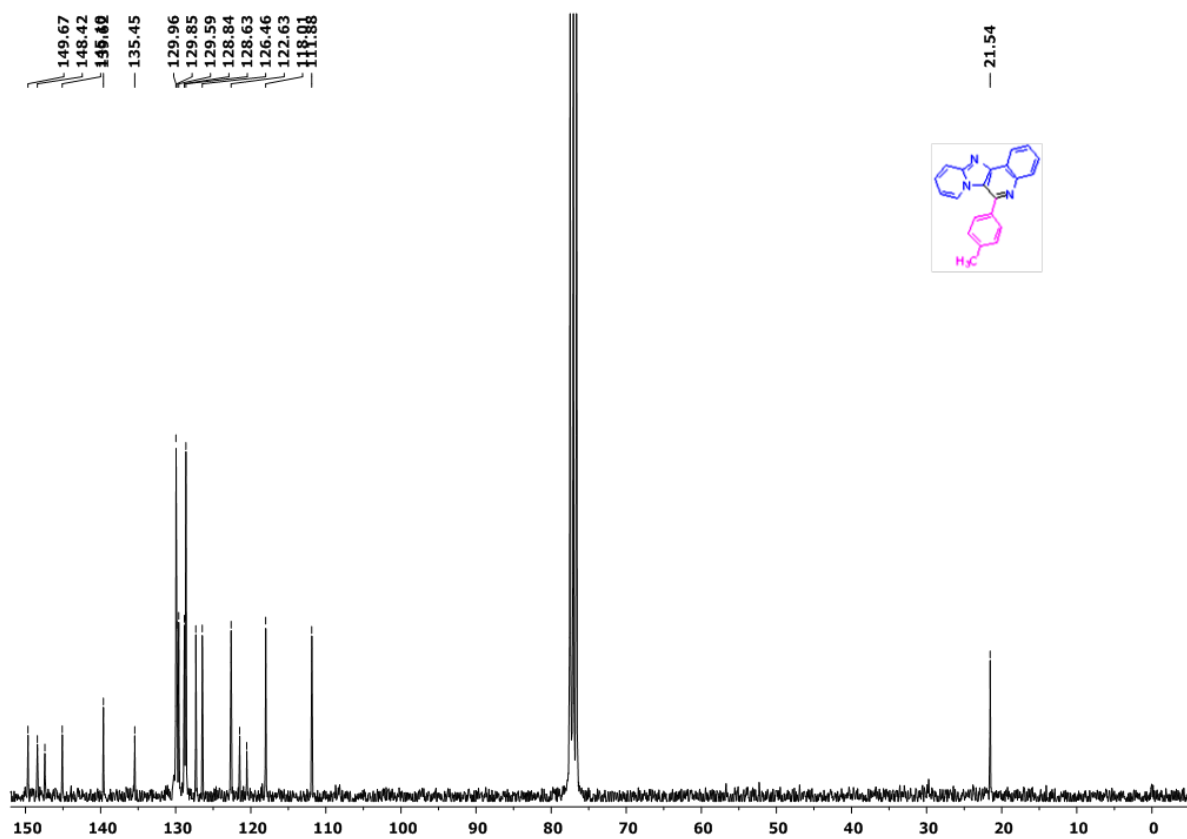
<sup>1</sup>H NMR spectrum of compound **4f**



<sup>13</sup>C NMR spectrum of compound **4f**

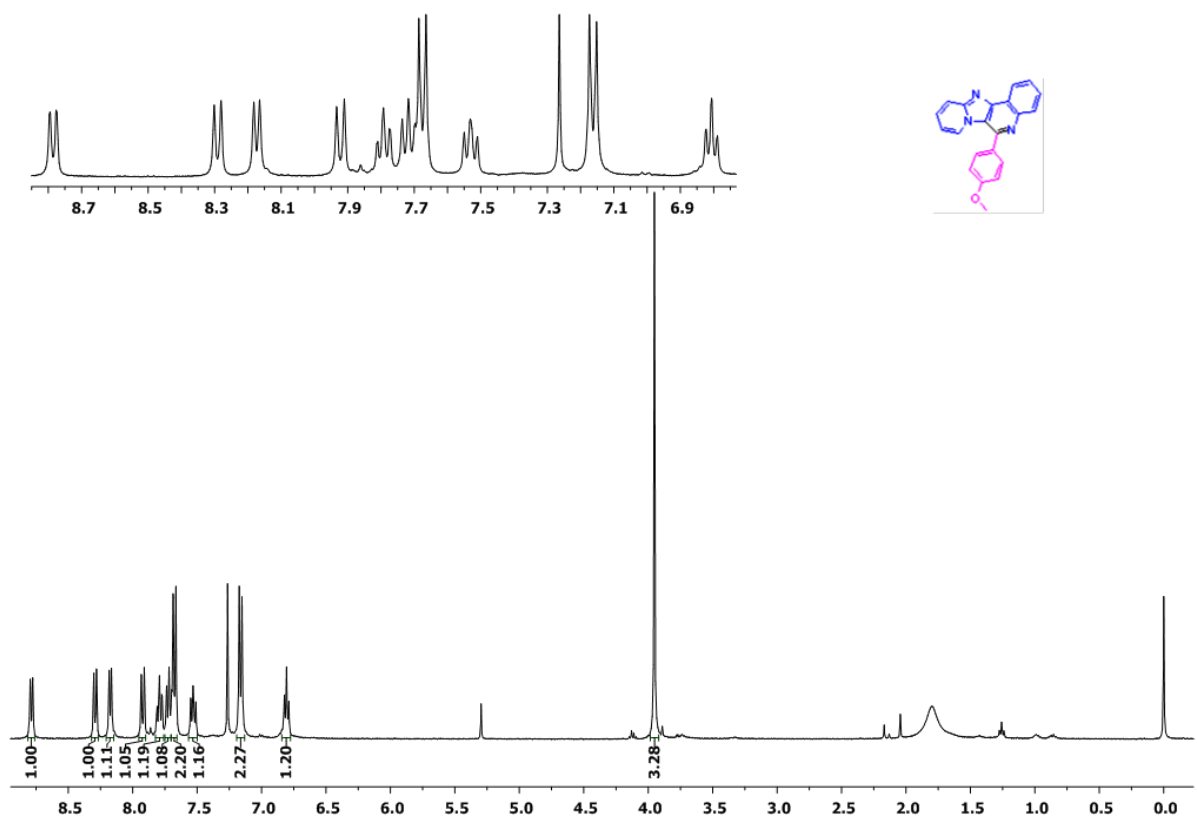


<sup>1</sup>H NMR spectrum of compound **4g**

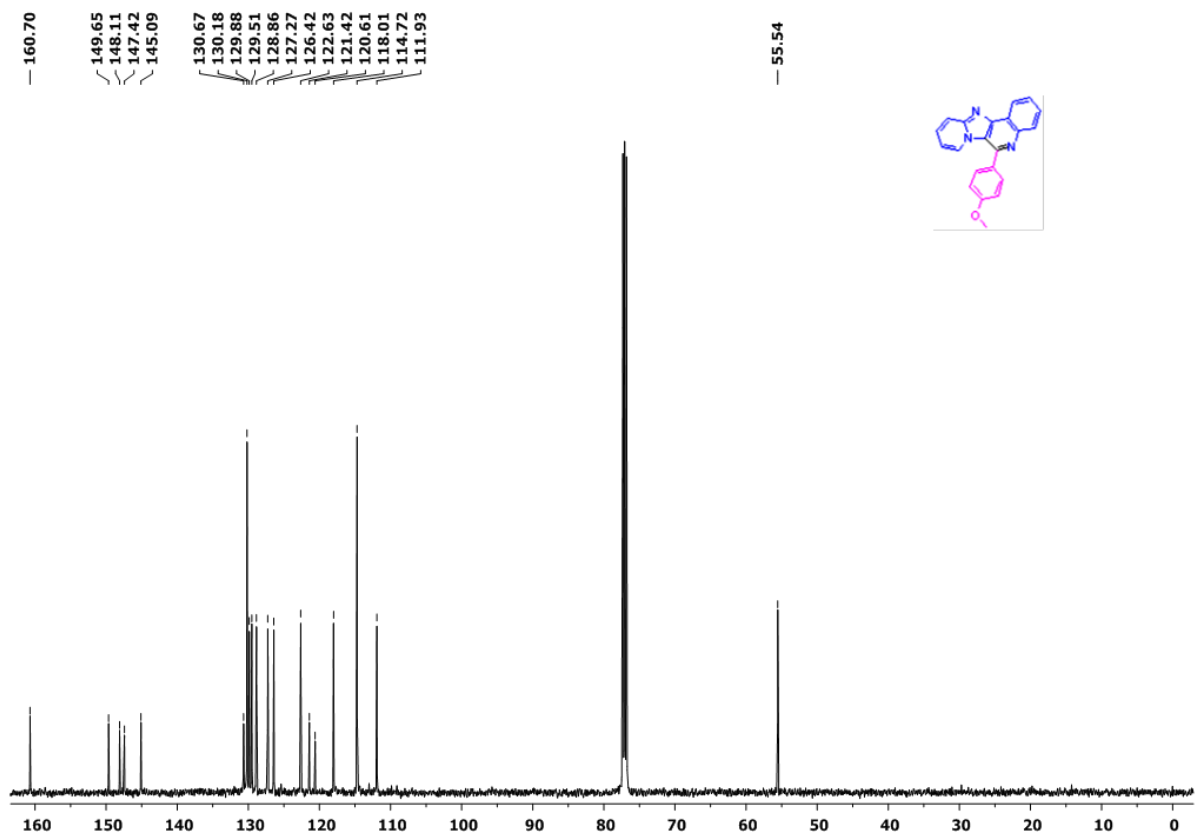


<sup>13</sup>C NMR spectrum of compound **4g**

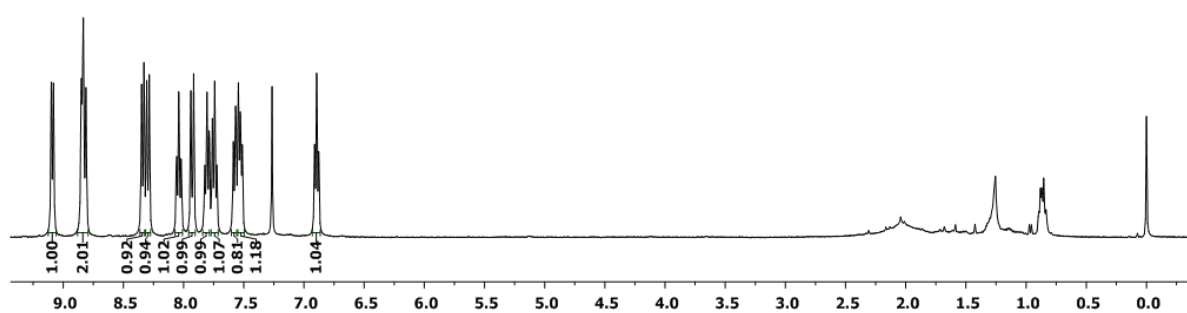
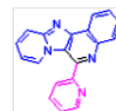
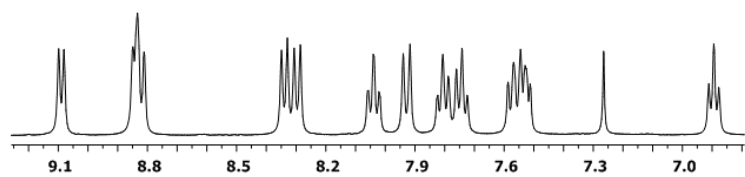




<sup>1</sup>H NMR spectrum of compound **4h**

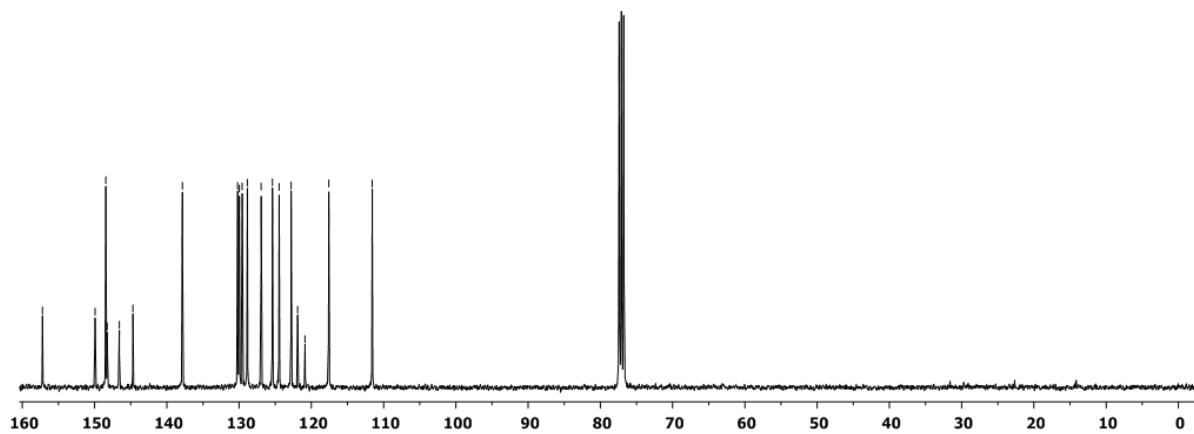
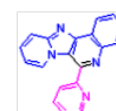


<sup>13</sup>C NMR spectrum of compound **4h**

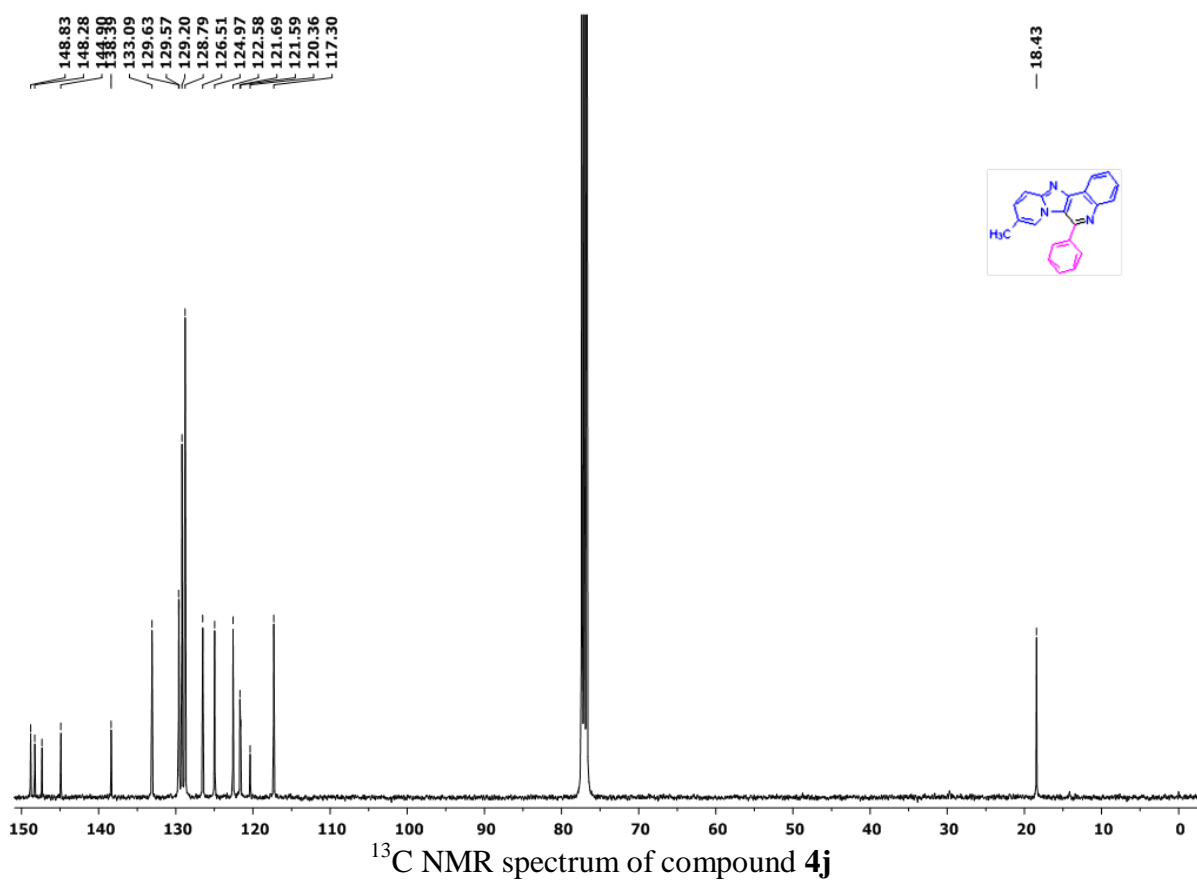
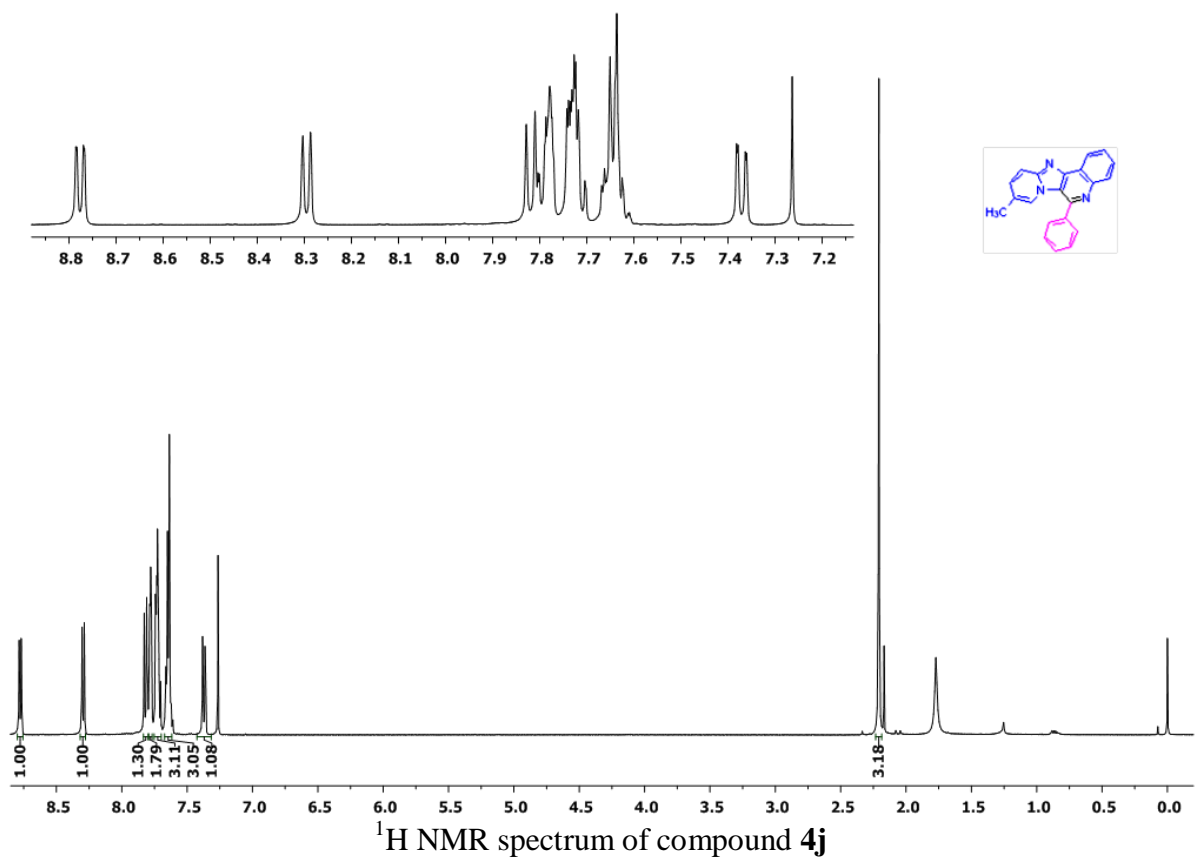


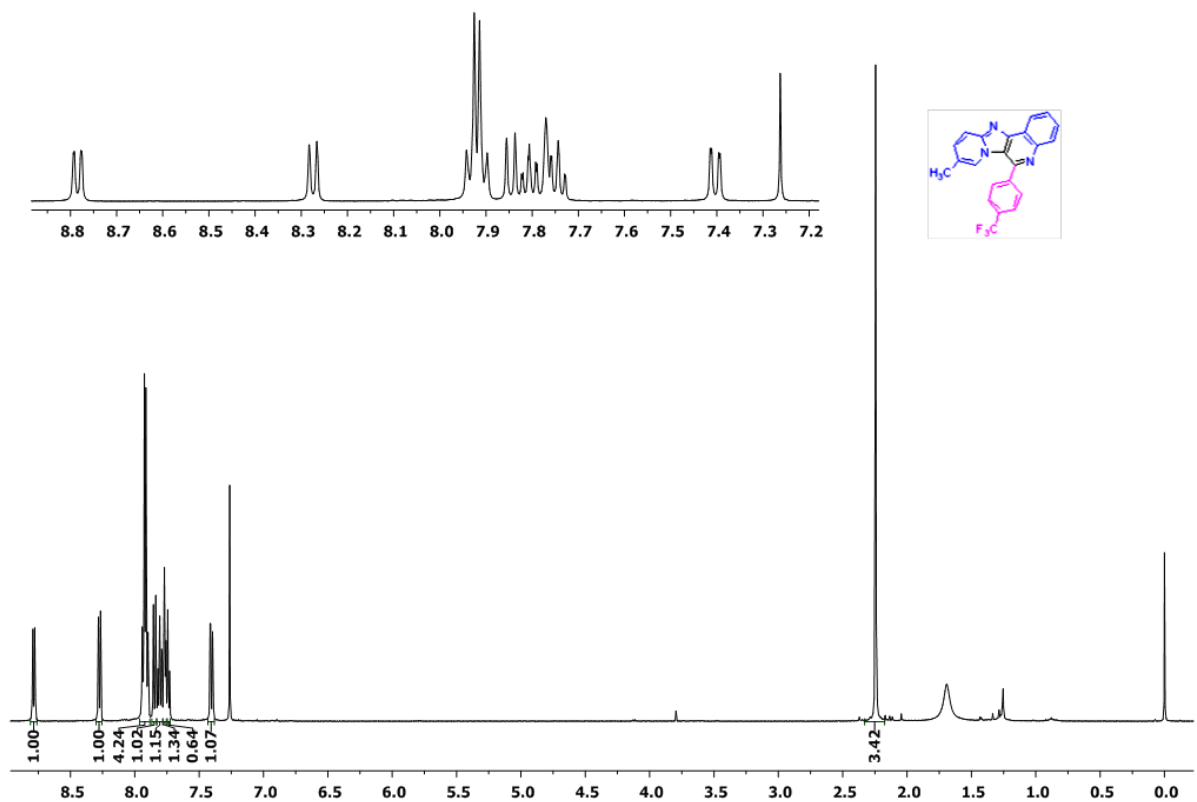
<sup>1</sup>H NMR spectrum of compound 4i

157.22  
 149.93  
 148.45  
 148.26  
 146.58  
 144.69  
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 130.21  
 129.97  
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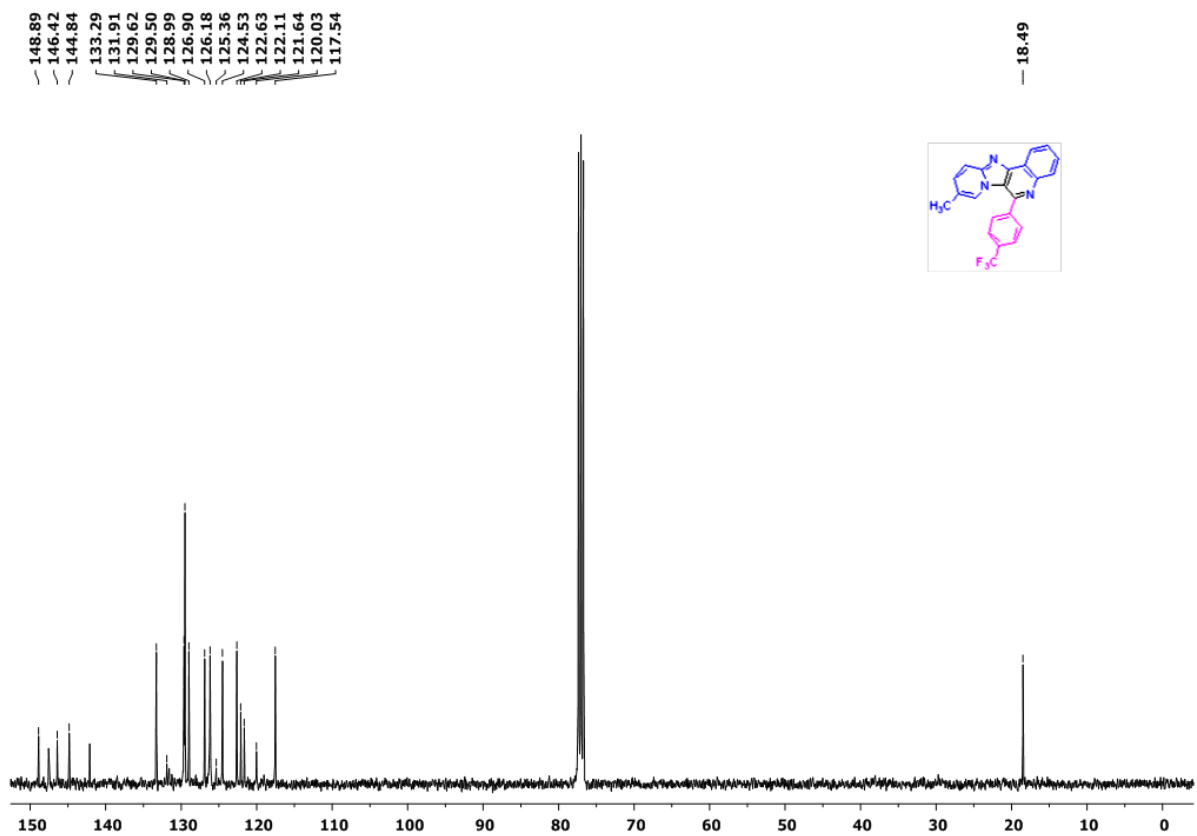


<sup>13</sup>C NMR spectrum of compound 4i

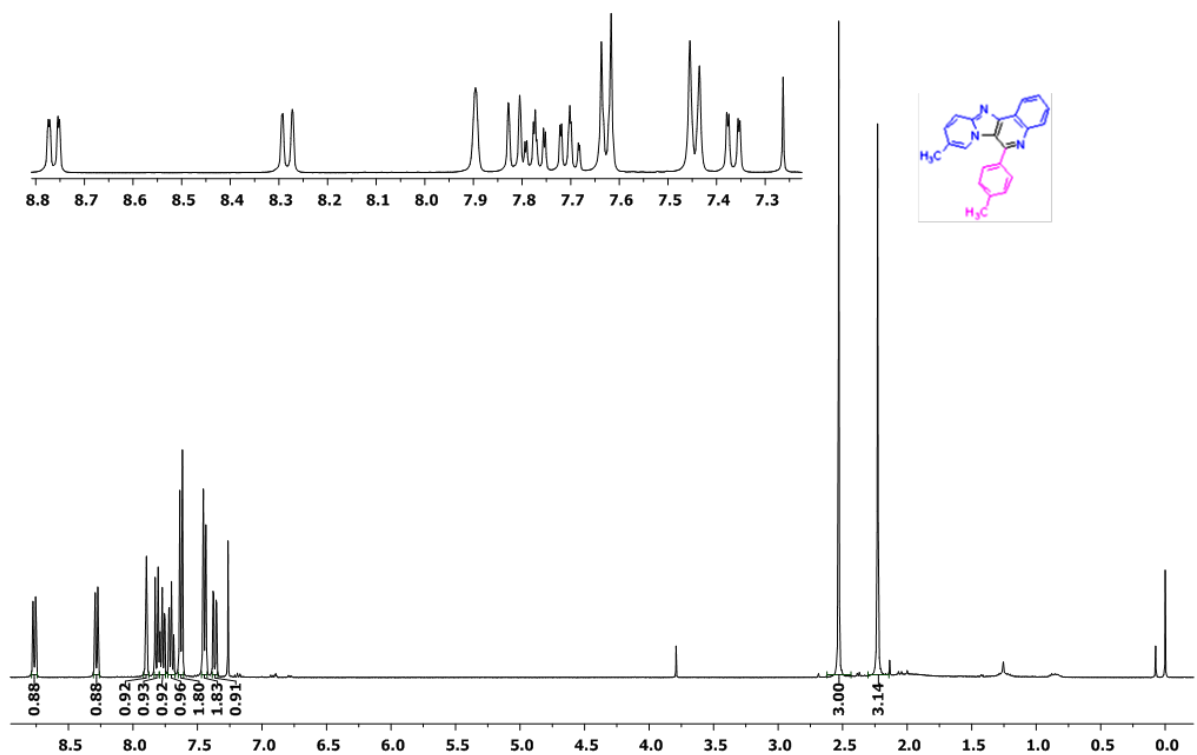




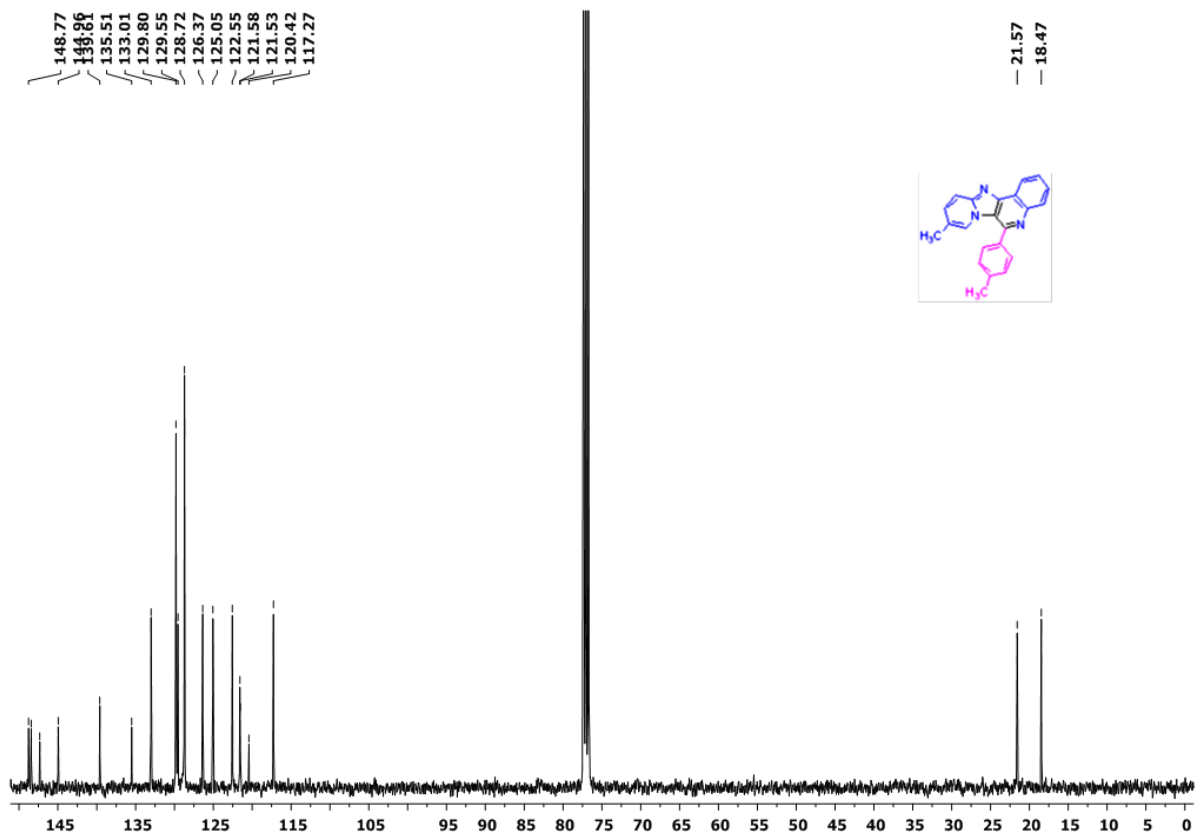
<sup>1</sup>H NMR spectrum of compound **4k**



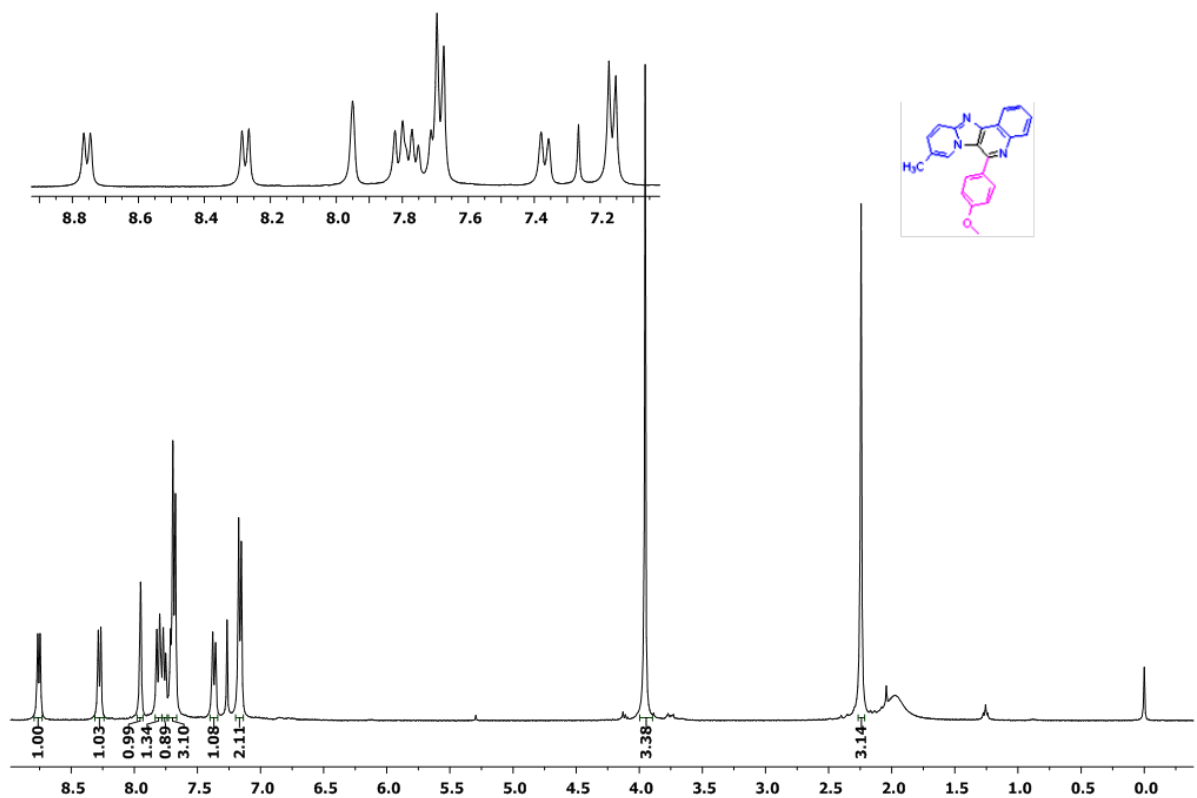
<sup>13</sup>C NMR spectrum of compound **4k**



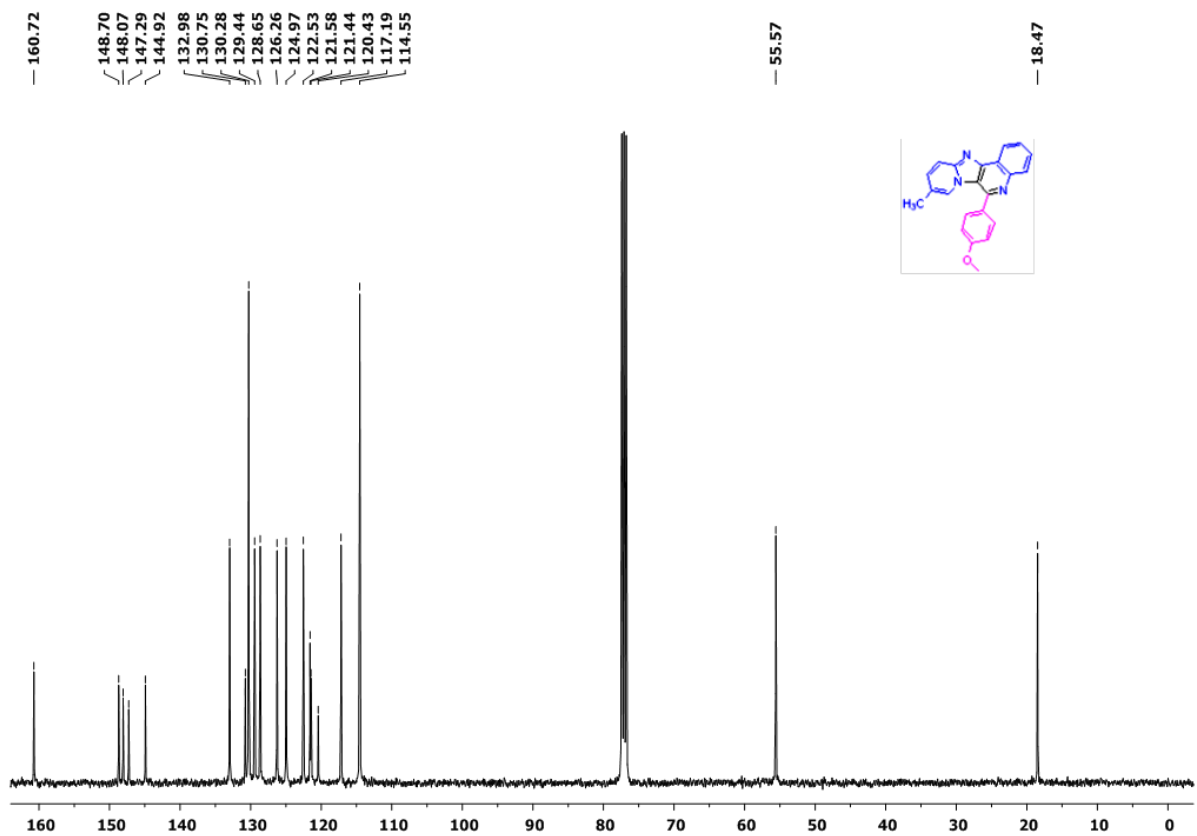
$^1\text{H}$  NMR spectrum of compound **41**



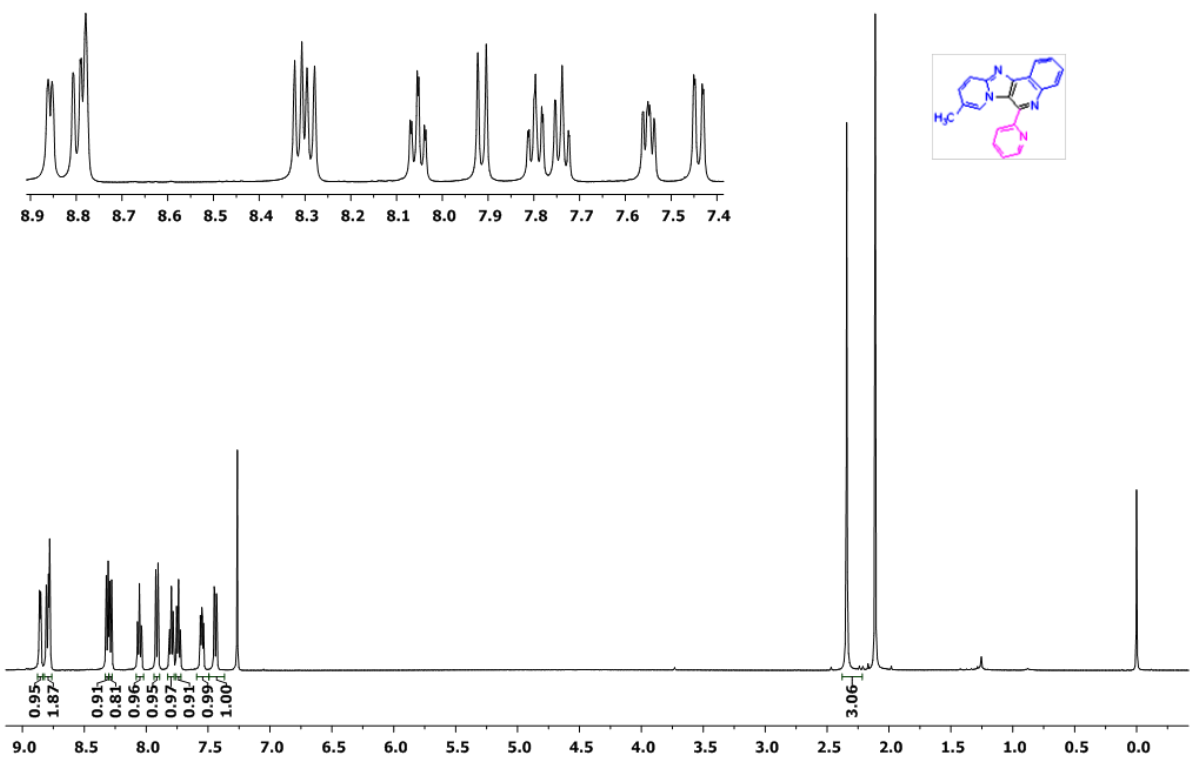
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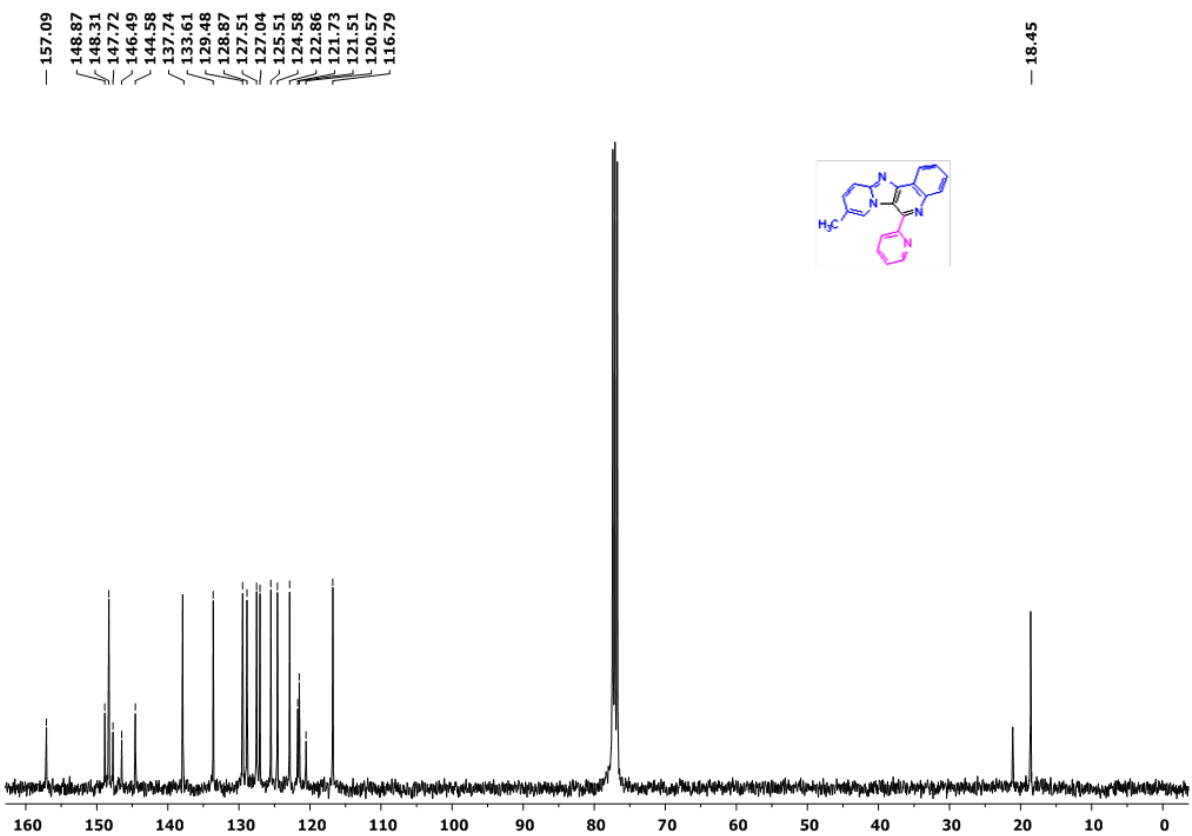
$^1\text{H}$  NMR spectrum of compound **4m**



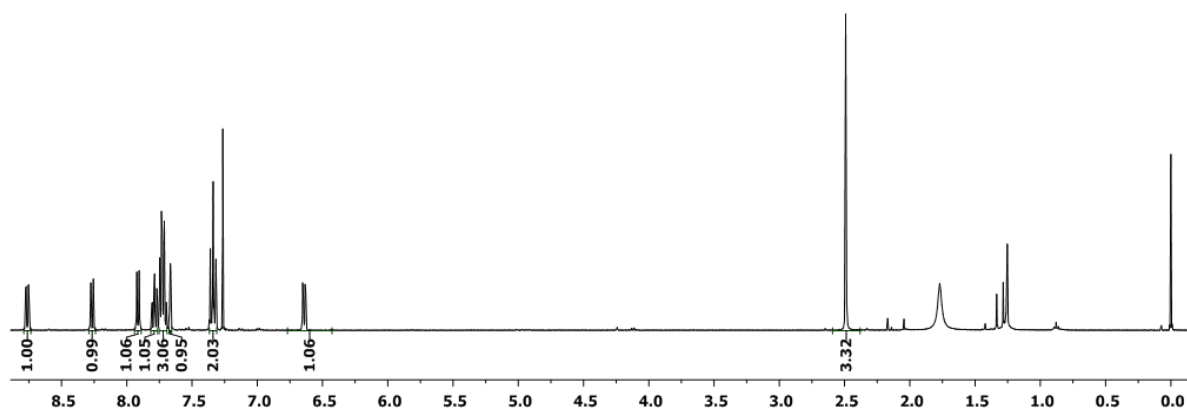
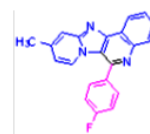
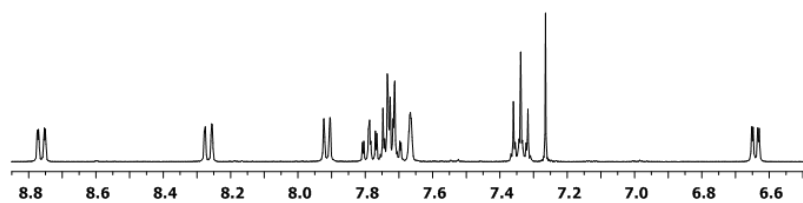
$^{13}\text{C}$  NMR spectrum of compound **4m**



$^1\text{H}$  NMR spectrum of compound **4n**



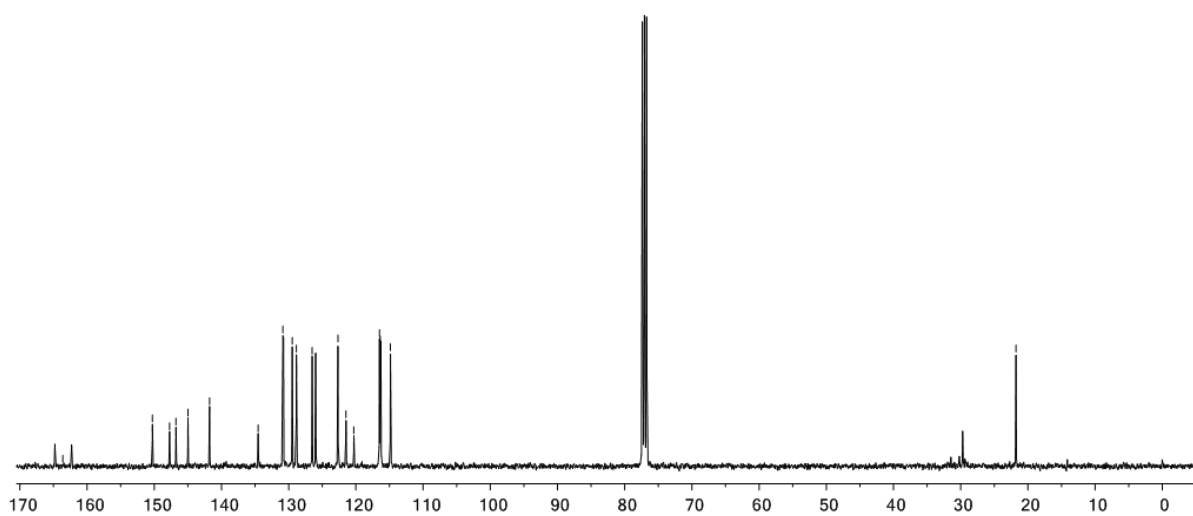
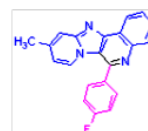
$^{13}\text{C}$  NMR spectrum of compound **4n**



<sup>1</sup>H NMR spectrum of compound **4o**

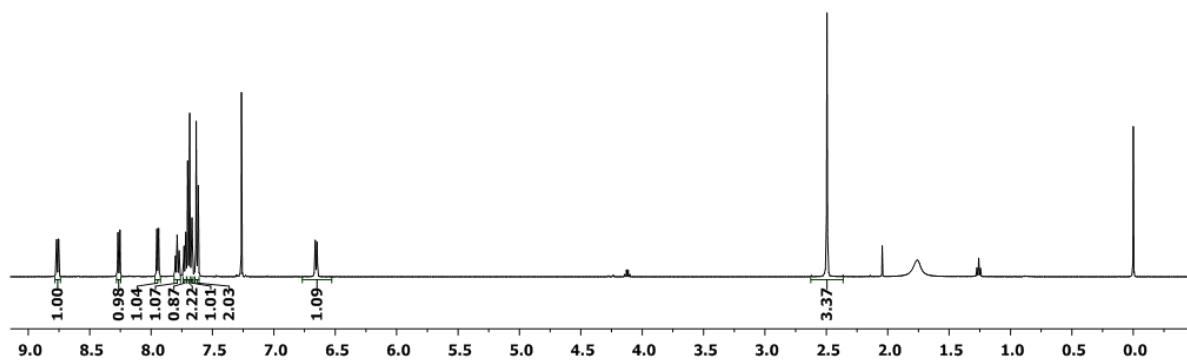
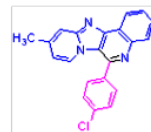
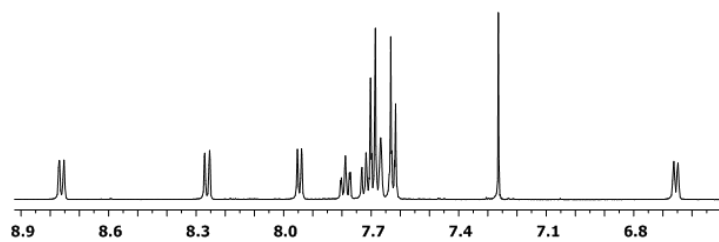
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 — 150.27  
 — 147.72  
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 — 130.86  
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 — 128.86  
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 — 122.67  
 — 121.47  
 — 120.30  
 — 116.49  
 — 116.37  
 — 114.86

— 21.78

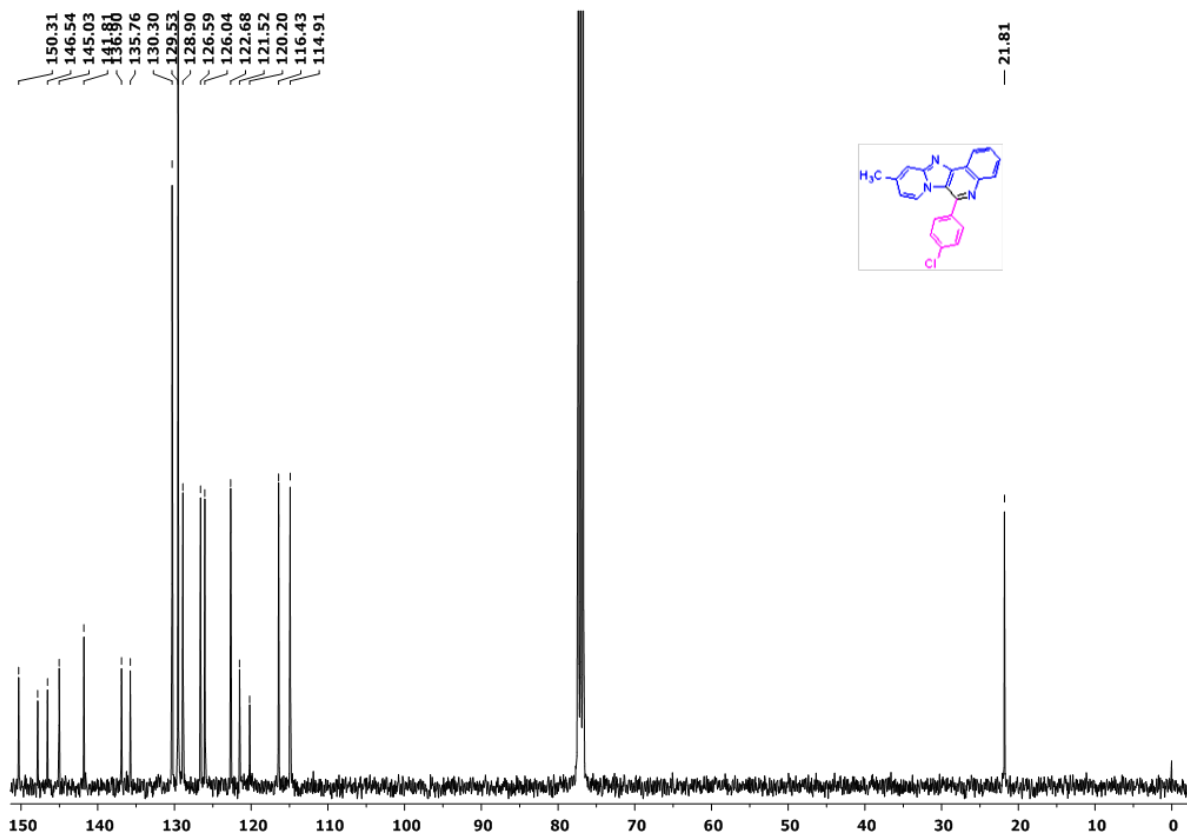


<sup>13</sup>C NMR spectrum of compound **4o**

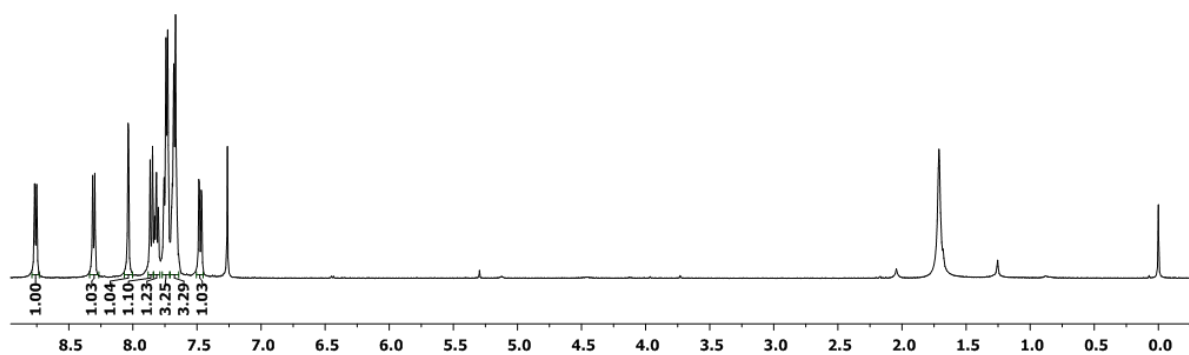
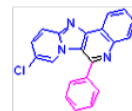
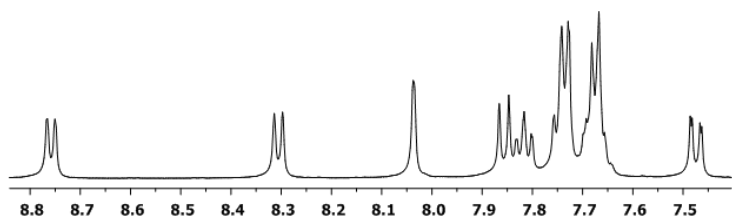




<sup>1</sup>H NMR spectrum of compound **4p**

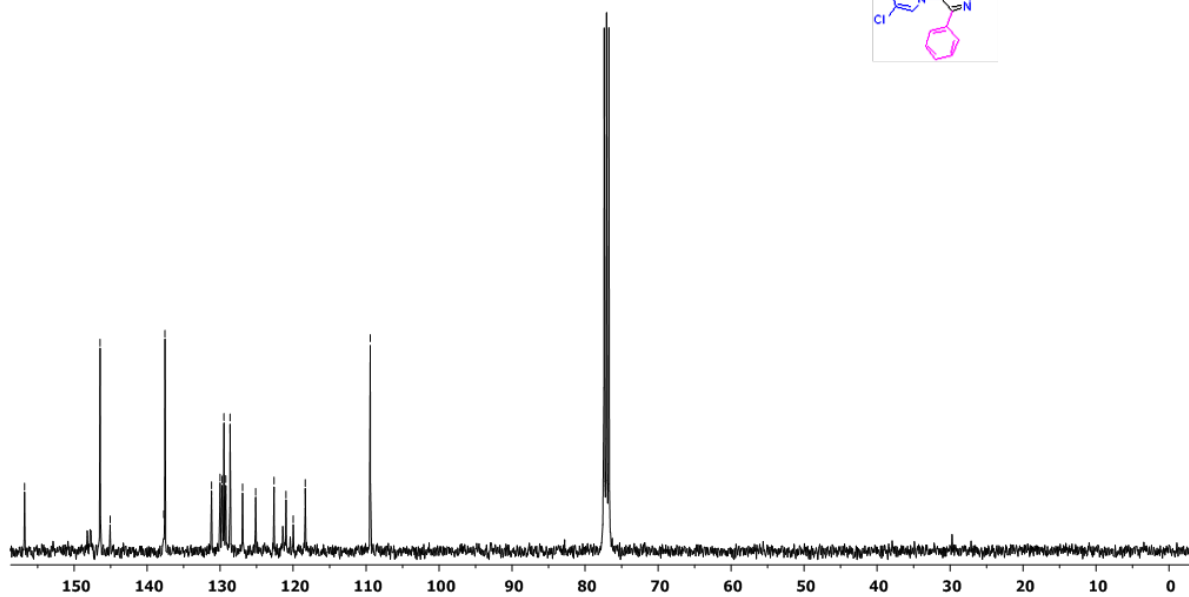
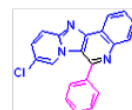


<sup>13</sup>C NMR spectrum of compound **4p**

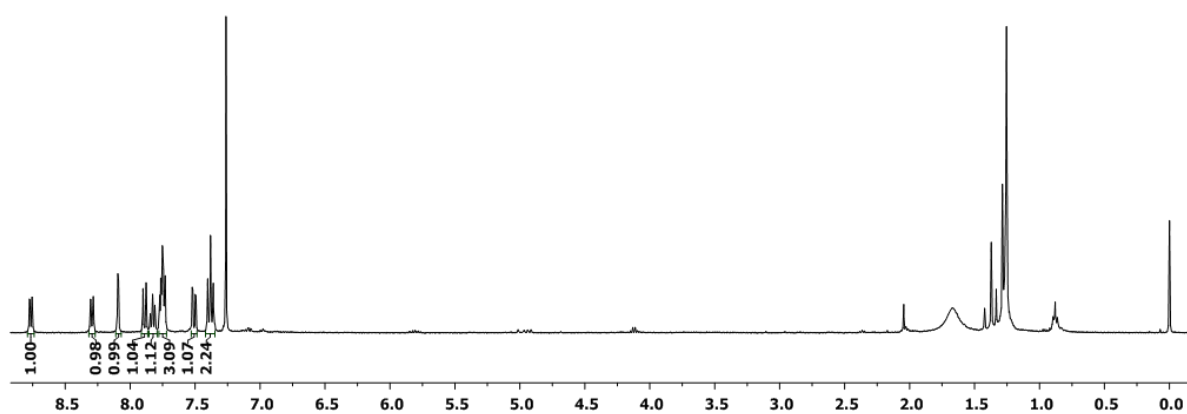
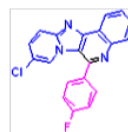
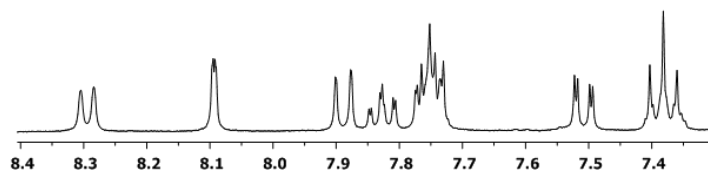


<sup>1</sup>H NMR spectrum of compound 4q

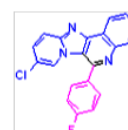
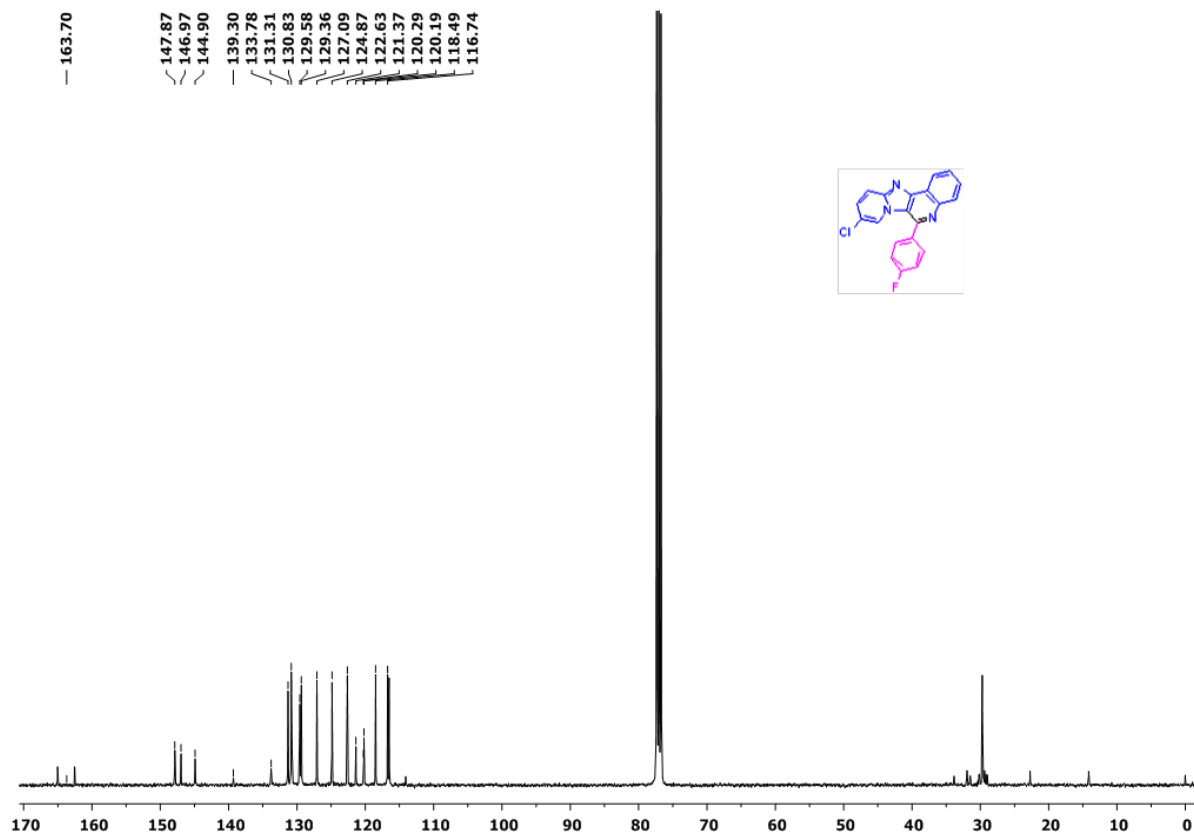
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122.62  
118.34



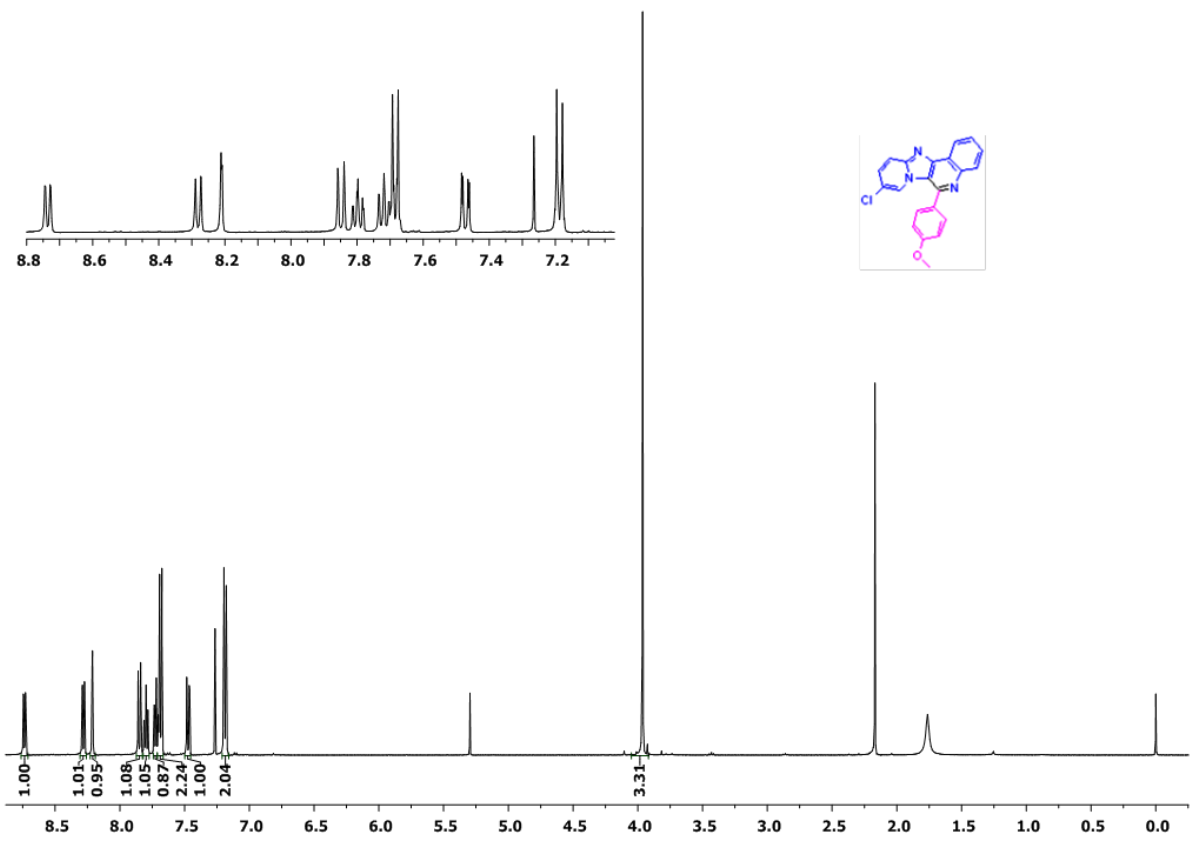
<sup>13</sup>C NMR spectrum of compound 4q



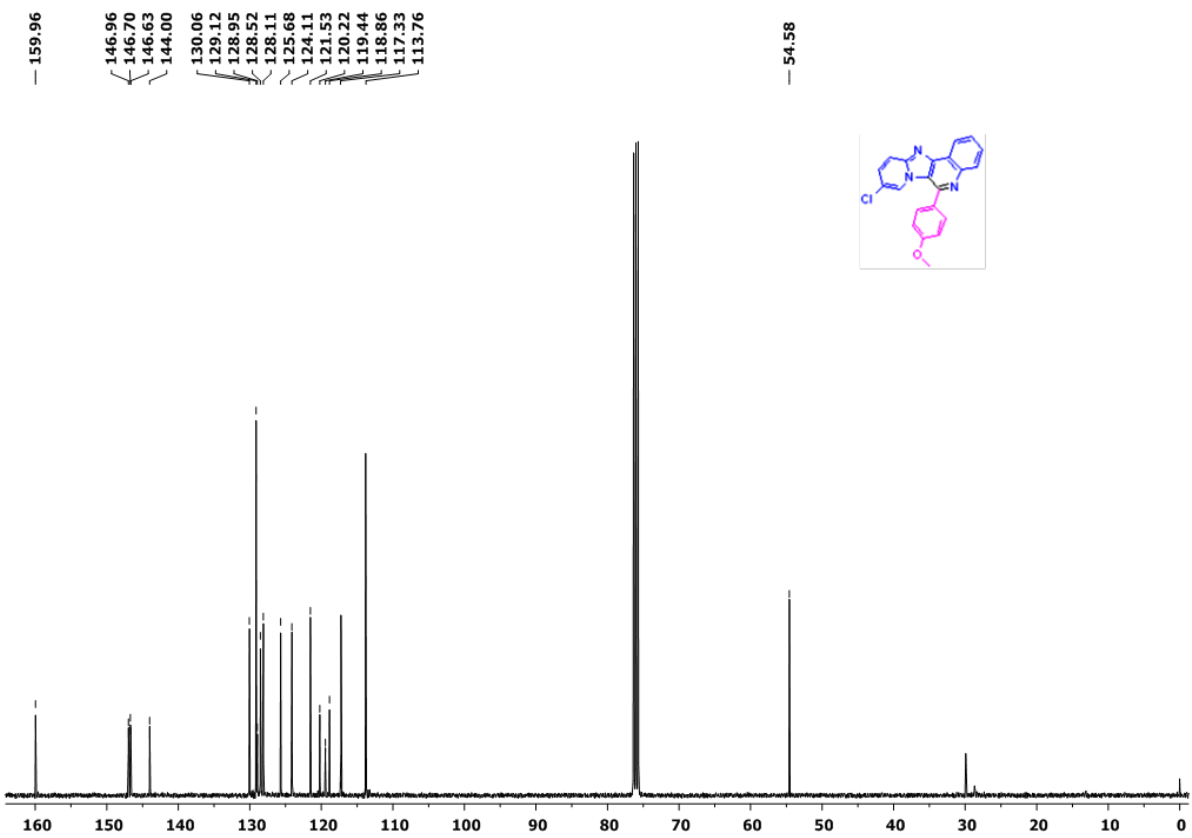
<sup>1</sup>H NMR spectrum of compound 4r



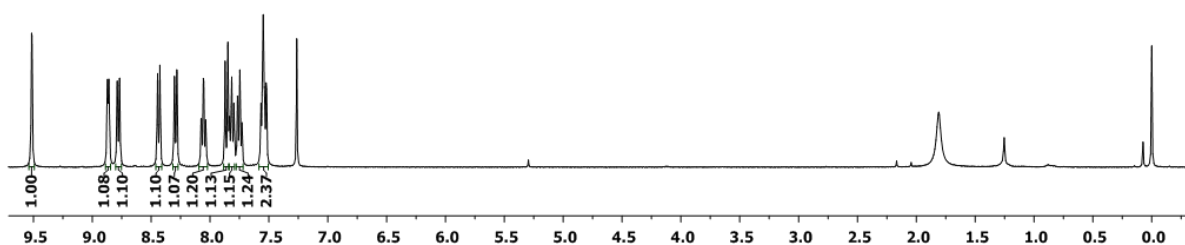
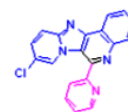
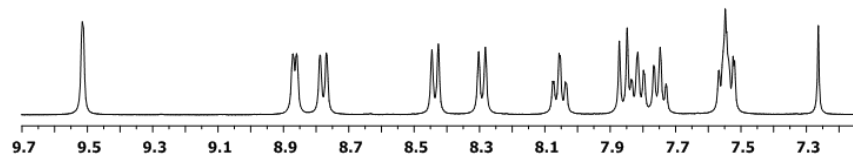
<sup>13</sup>C NMR spectrum of compound 4r



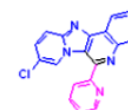
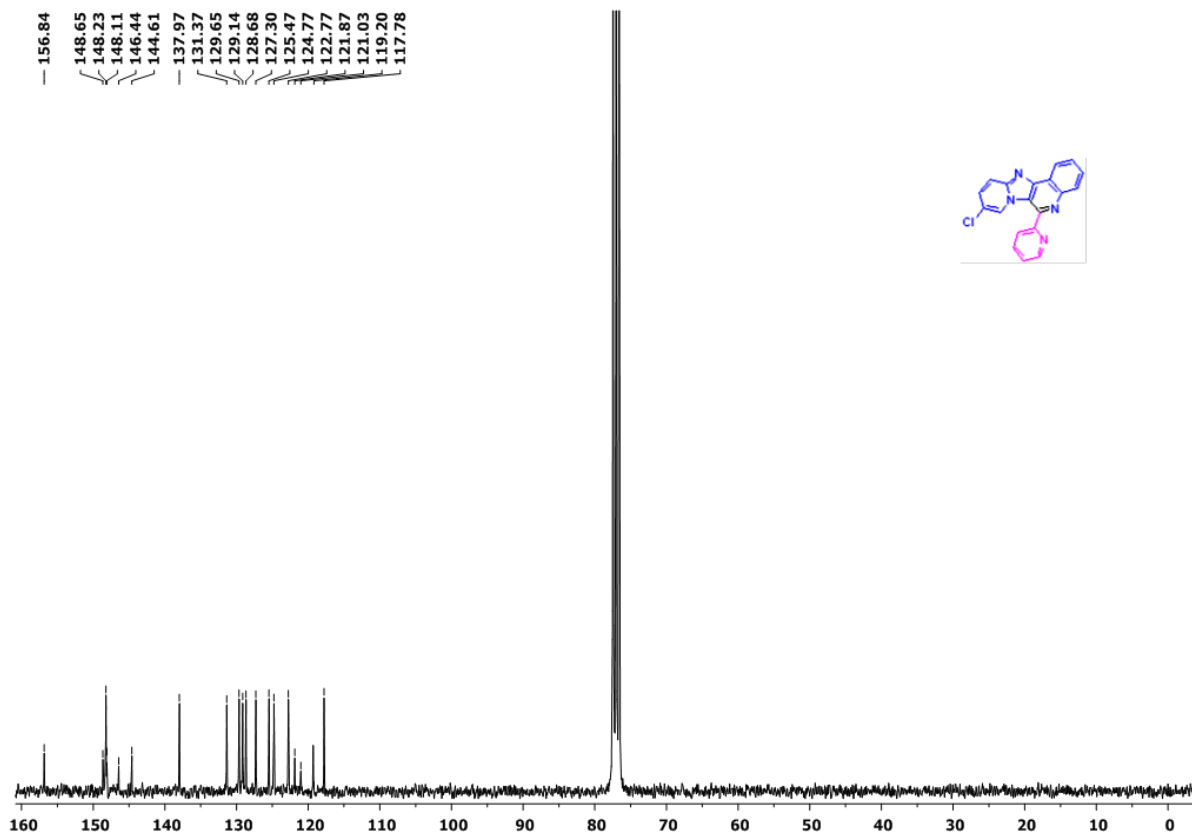
$^1\text{H}$  NMR spectrum of compound **4s**



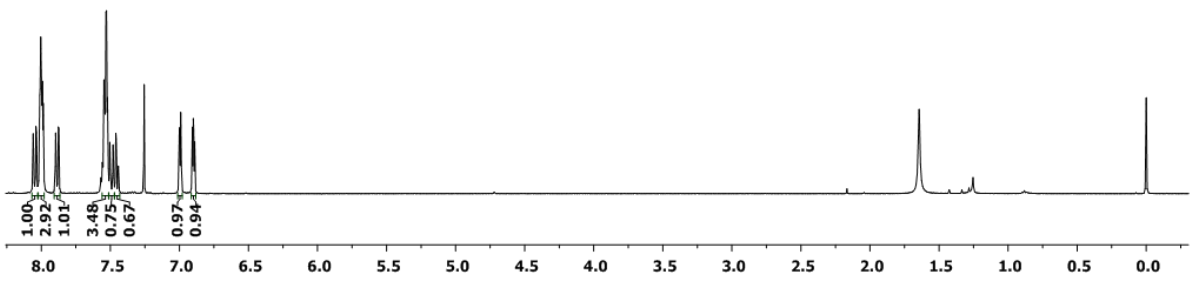
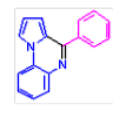
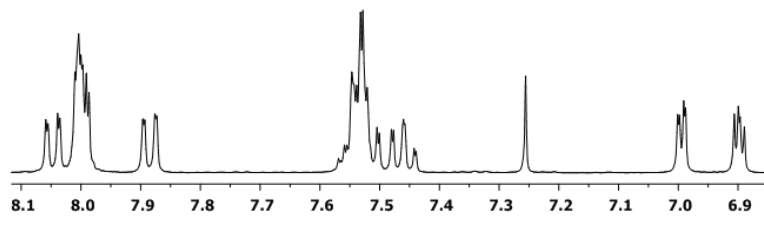
$^{13}\text{C}$  NMR spectrum of compound **4s**



<sup>1</sup>H NMR spectrum of compound **4t**

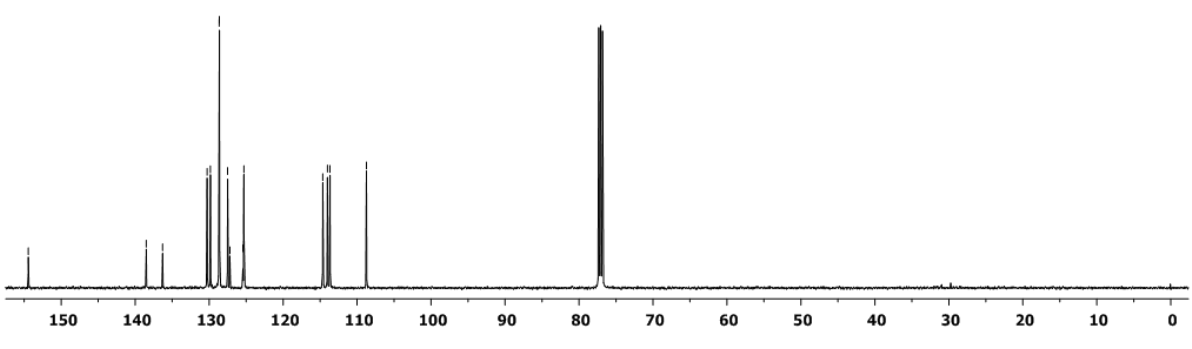
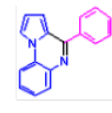


<sup>13</sup>C NMR spectrum of compound **4t**

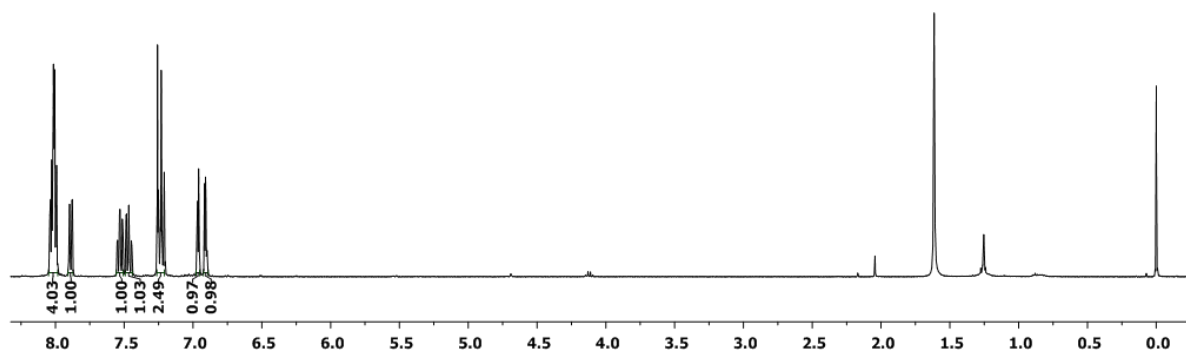
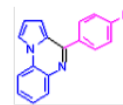
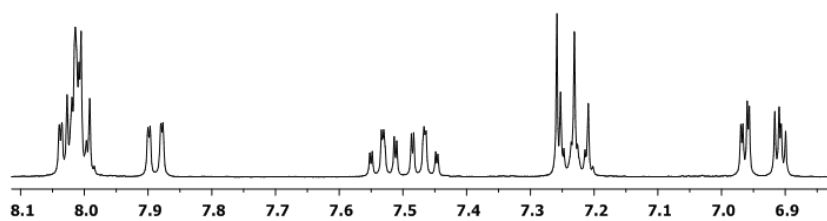


<sup>1</sup>H NMR spectrum of compound **6a**

- 154.45
- 138.50
- 136.30
- 130.28
- 129.83
- 128.65
- 128.62
- 127.50
- 125.43
- 124.31
- 117.64
- 114.01
- 113.66
- 108.74

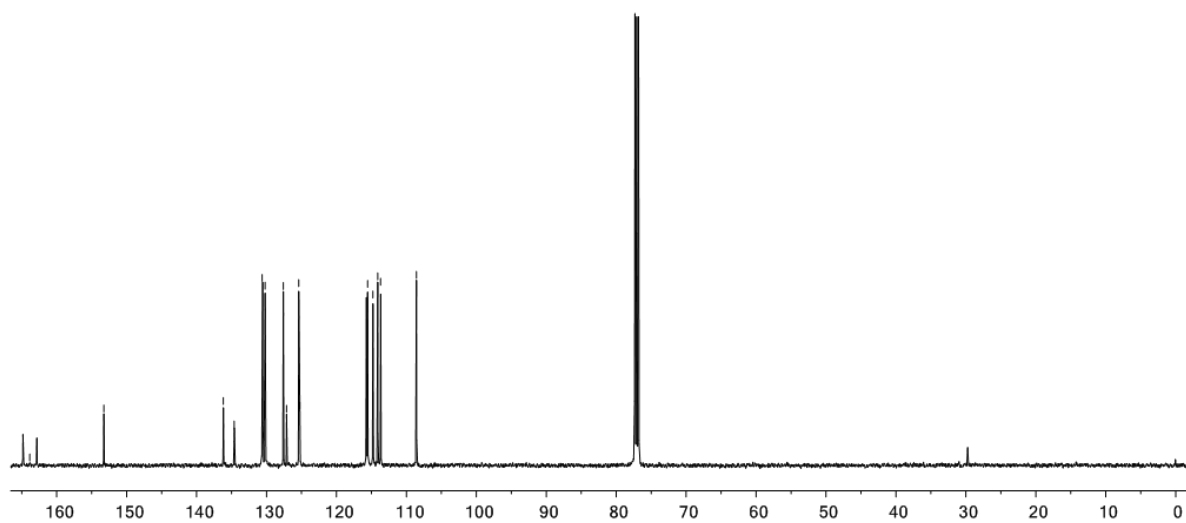
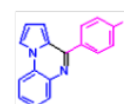


<sup>13</sup>C NMR spectrum of compound **6a**

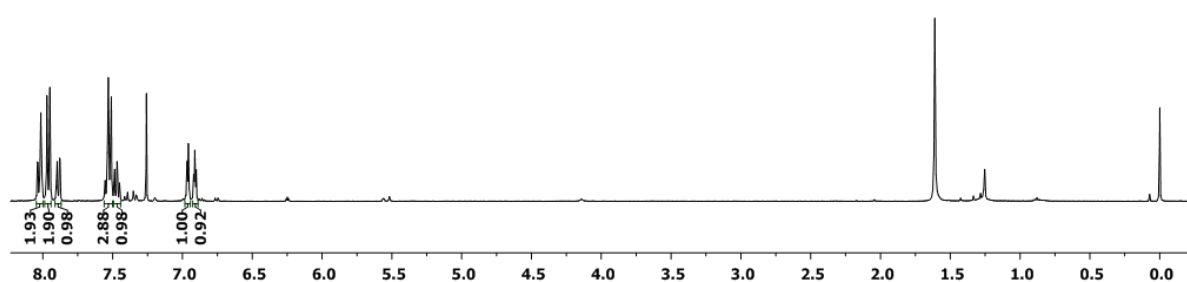
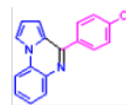
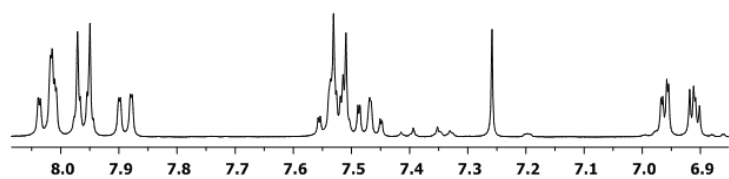


$^1\text{H}$  NMR spectrum of compound **6b**

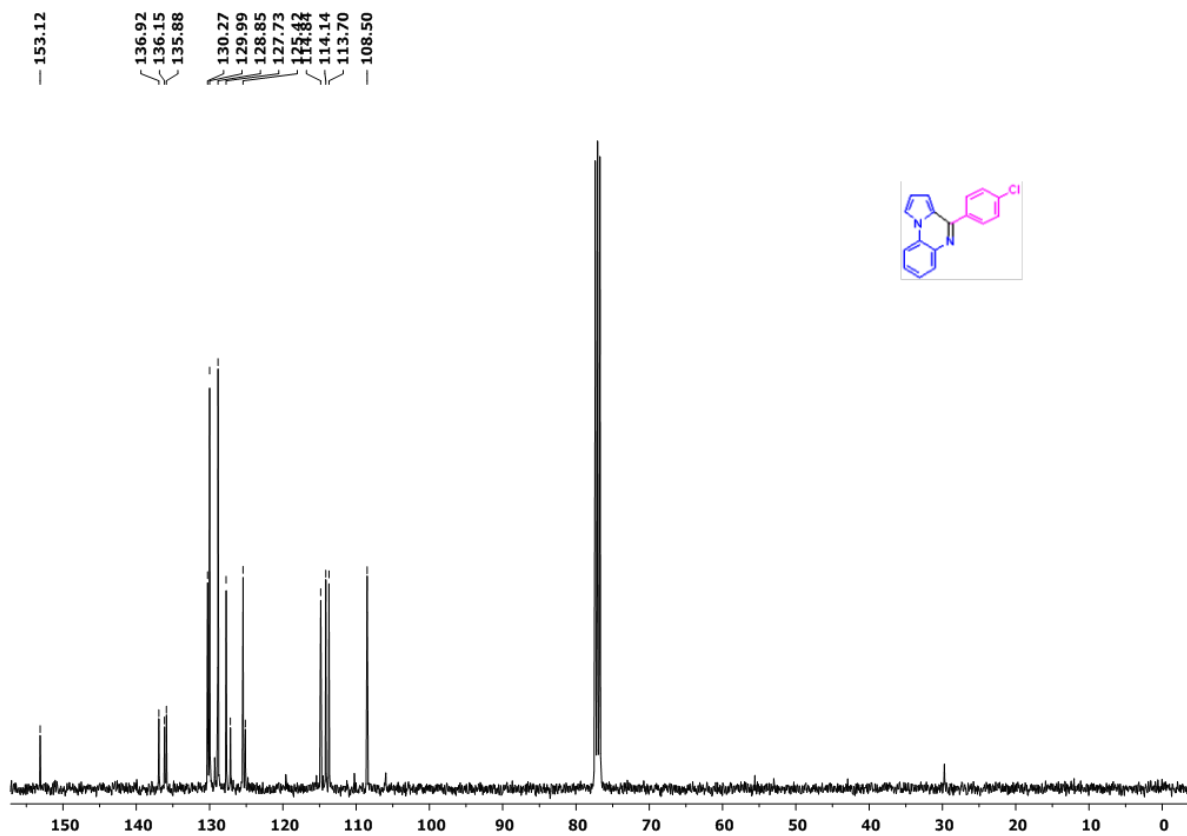
$-\text{163.85}$   
 $-\text{153.26}$   
 $\text{136.17}$   
 $\text{134.63}$   
 $\text{130.62}$   
 $\text{130.21}$   
 $\text{127.61}$   
 $\text{127.14}$   
 $\text{125.39}$   
 $\text{125.24}$   
 $\text{115.55}$   
 $\text{114.79}$   
 $\text{114.09}$   
 $\text{113.69}$   
 $\text{108.57}$



$^{13}\text{C}$  NMR spectrum of compound **6b**

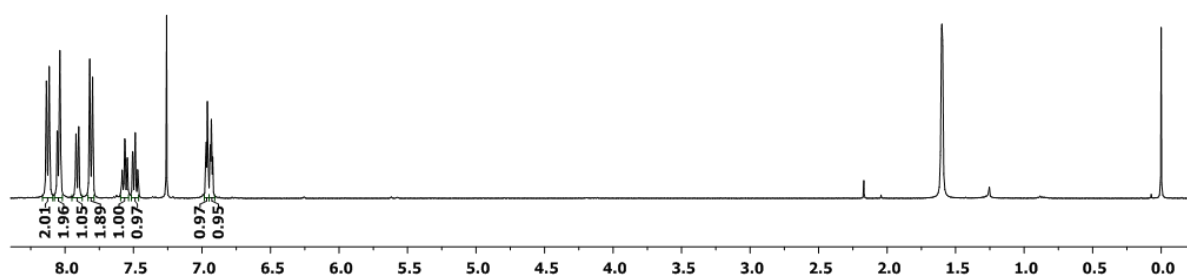
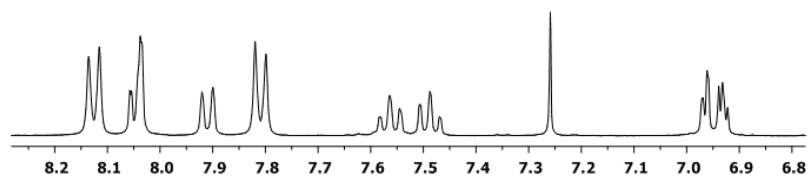


<sup>1</sup>H NMR spectrum of compound **6c**



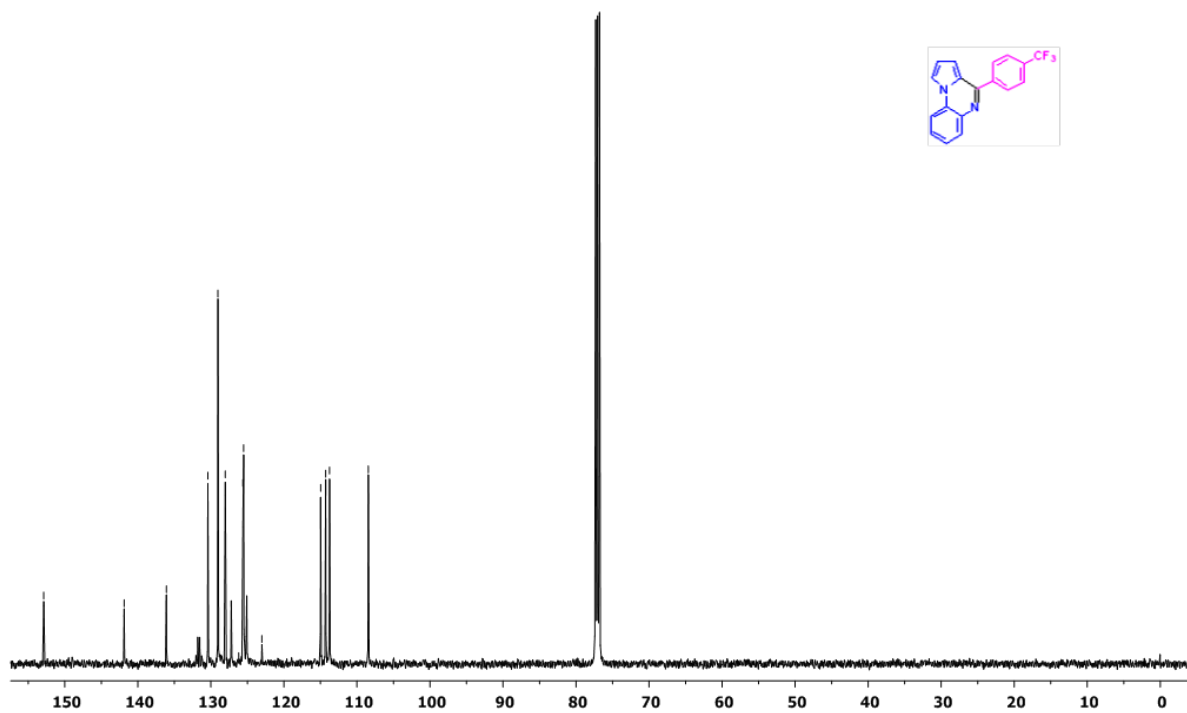
<sup>13</sup>C NMR spectrum of compound **6c**



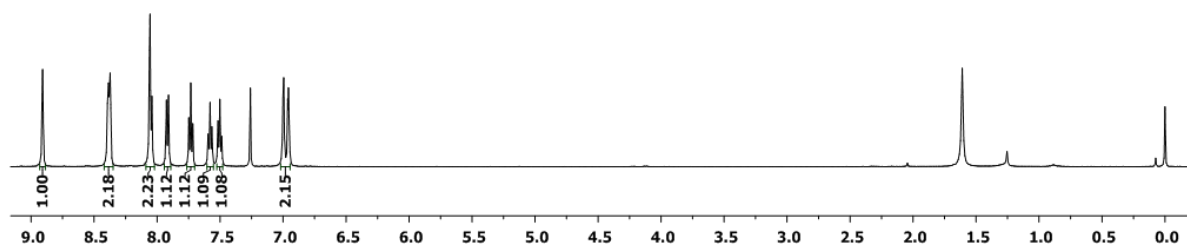
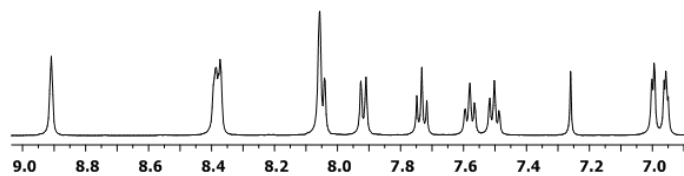


$^1\text{H}$  NMR spectrum of compound **6d**

— 152.88  
 — 141.88  
 — 136.09  
 — 130.42  
 — 129.04  
 — 128.03  
 — 126.18  
 — 125.61  
 — 125.51  
 — 117.97  
 — 114.28  
 — 113.75  
 — 108.44

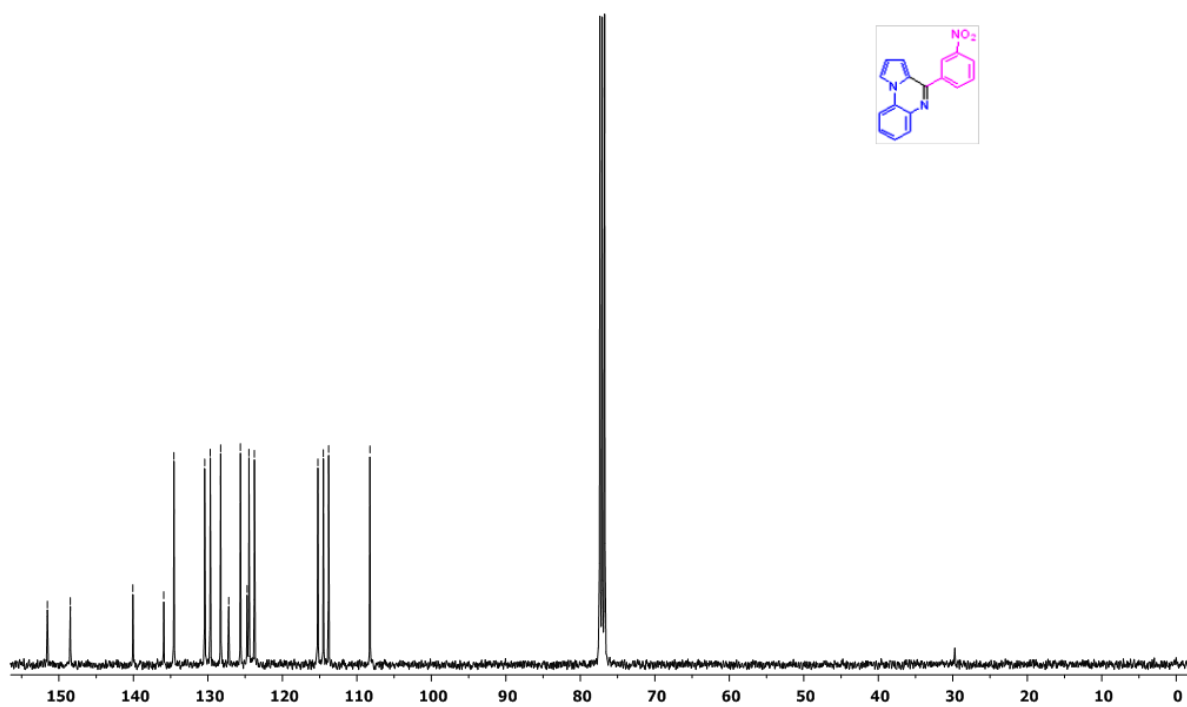


$^{13}\text{C}$  NMR spectrum of compound **6d**

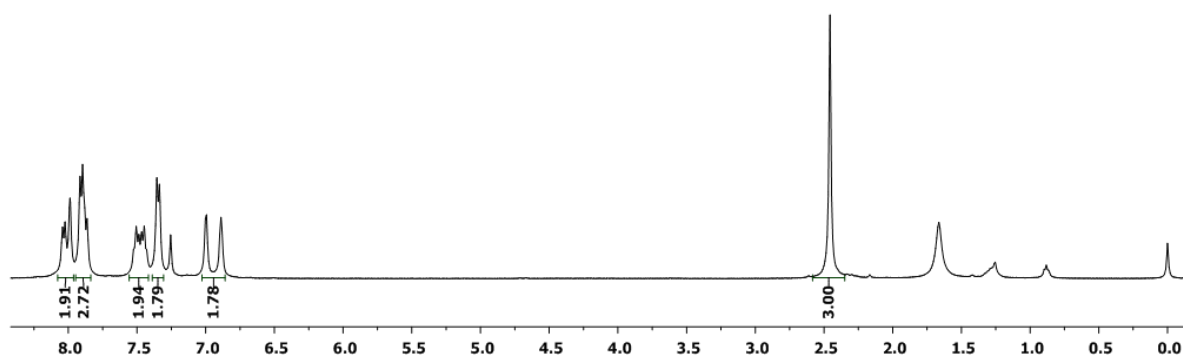
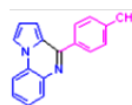
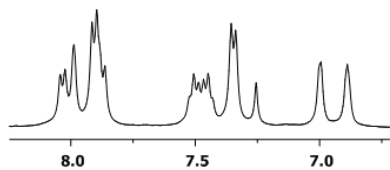


$^1\text{H}$  NMR spectrum of compound **6e**

Chemical structure of compound **6e** is shown in the top right corner: O=[N+]([O-])c1ccc(cc1)C2=NC3=CC=CC=C3N=C2



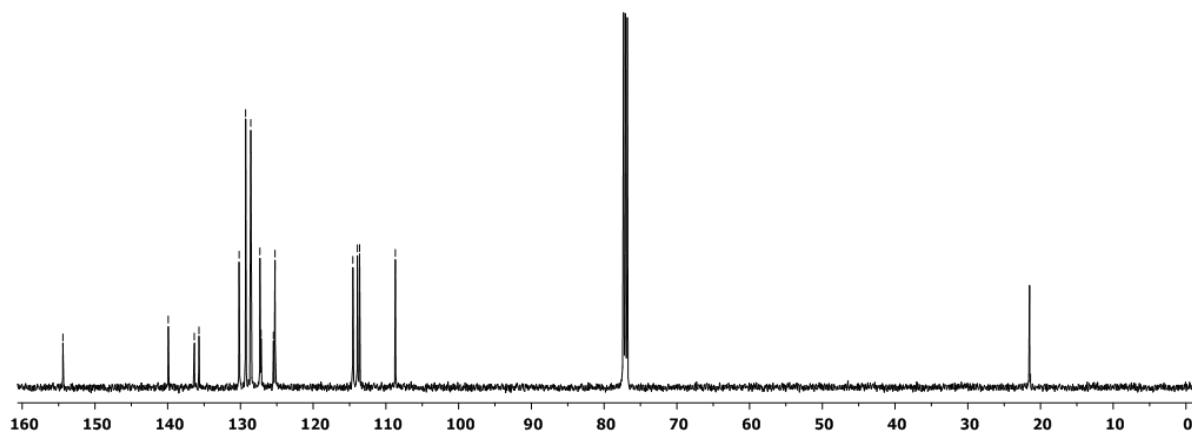
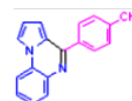
$^{13}\text{C}$  NMR spectrum of compound **6e**



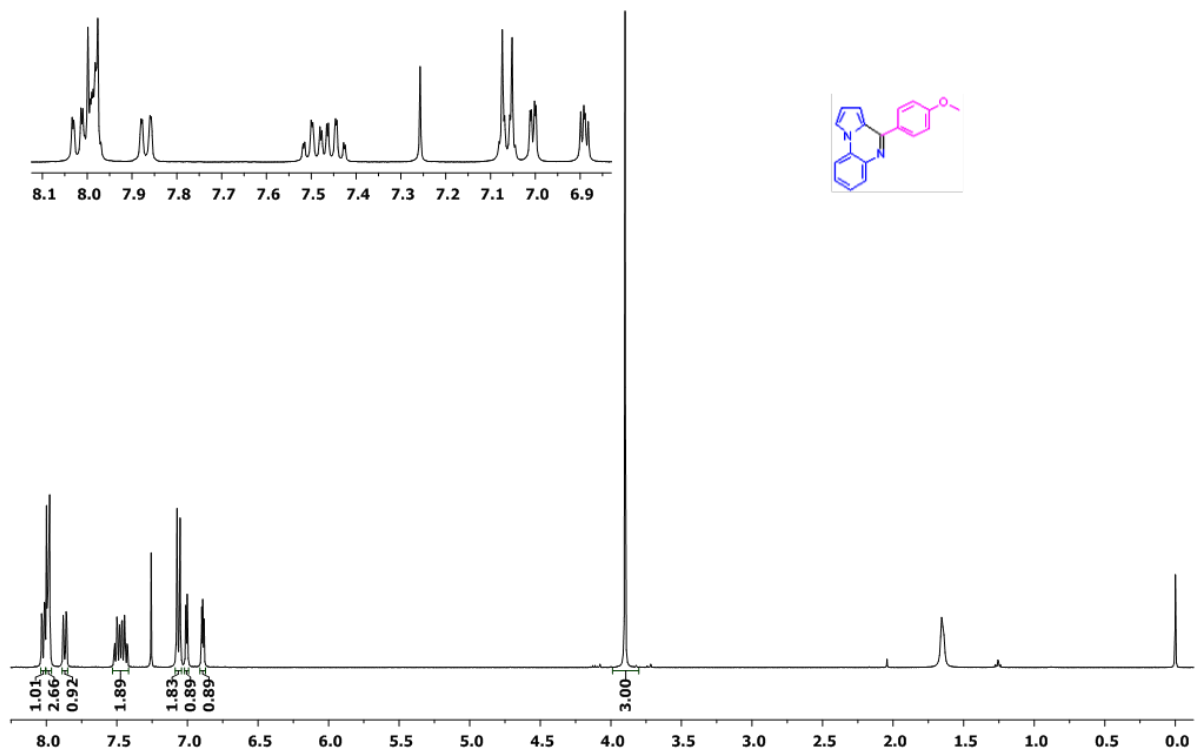
$^1\text{H}$  NMR spectrum of compound **6f**

— 154.41  
 — 139.92  
 — 136.34  
 — 135.71  
 — 130.19  
 — 129.29  
 — 128.58  
 — 127.32  
 — 127.17  
 — 118.53  
 — 118.53  
 — 113.92  
 — 113.63  
 — 108.71

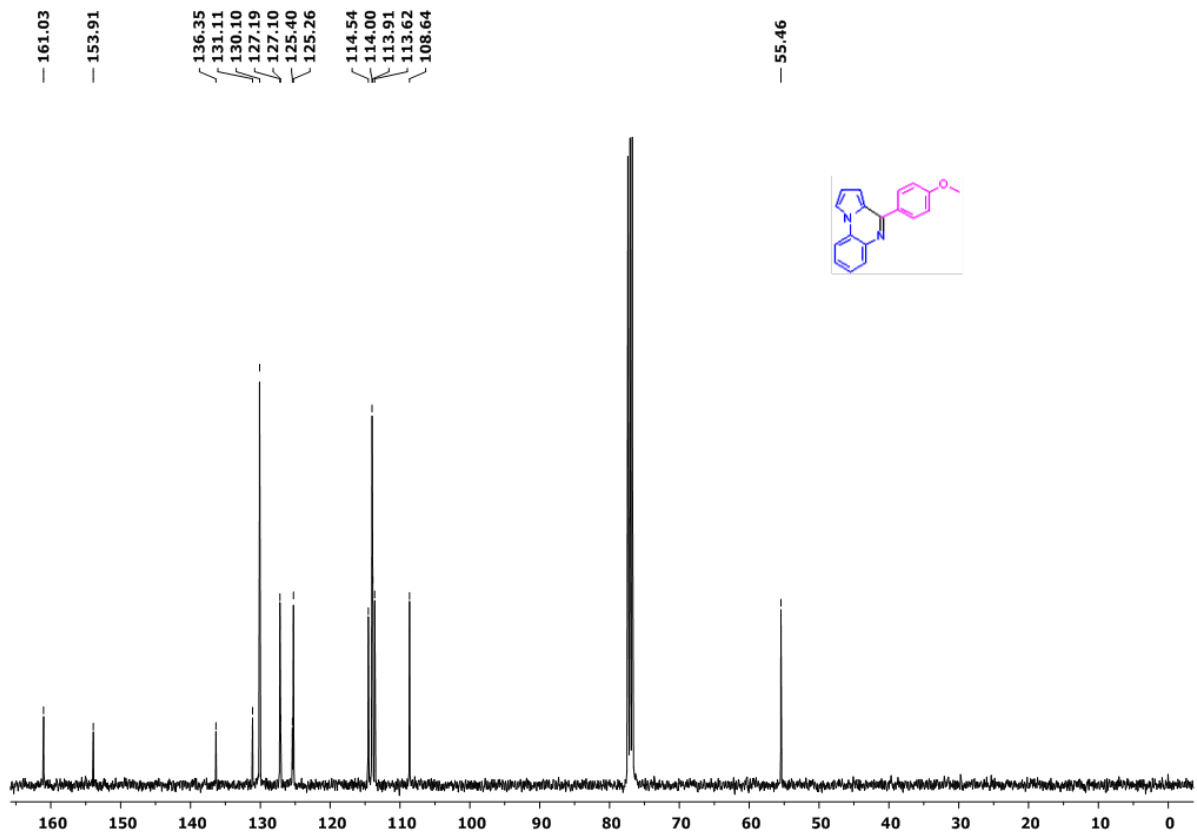
— 21.37



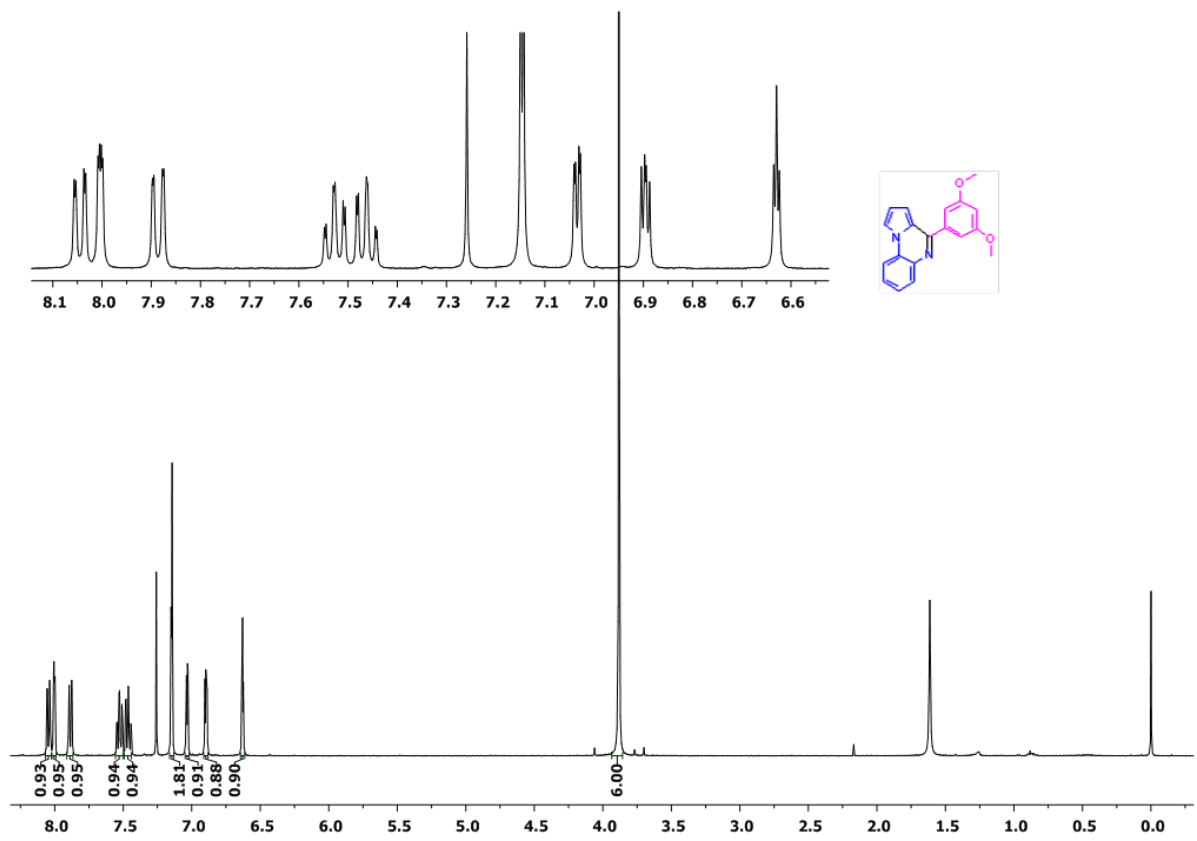
$^{13}\text{C}$  NMR spectrum of compound **6f**



$^1\text{H NMR}$  spectrum of compound **6g**



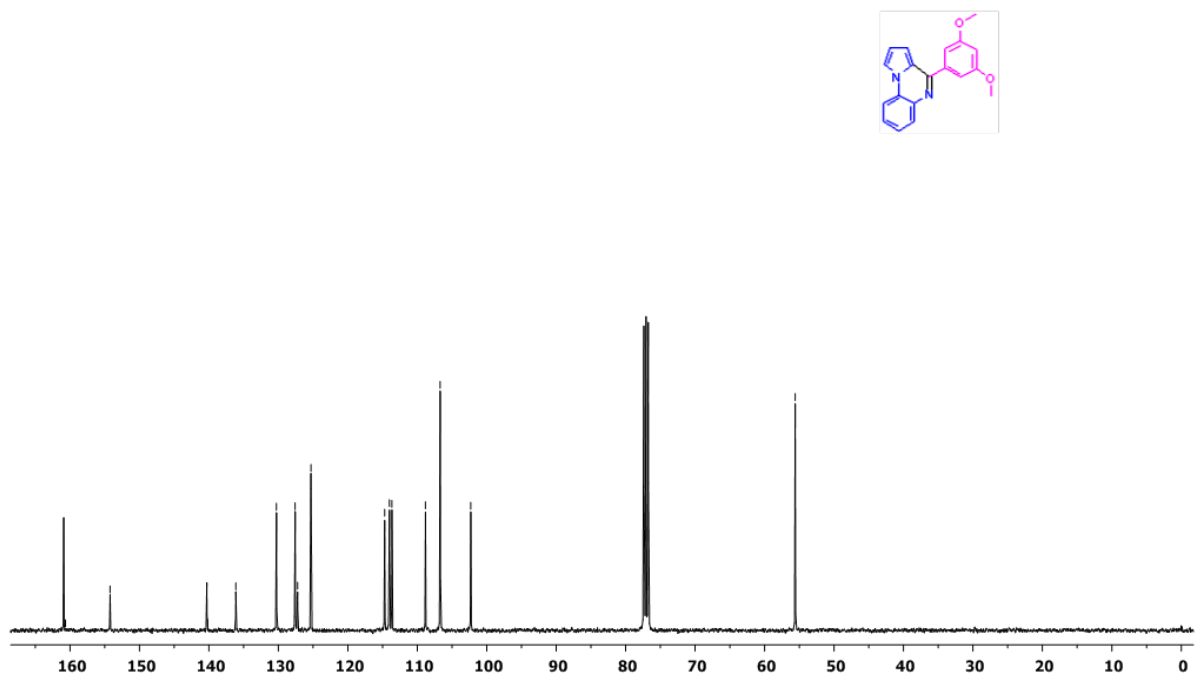
$^{13}\text{C NMR}$  spectrum of compound **6g**



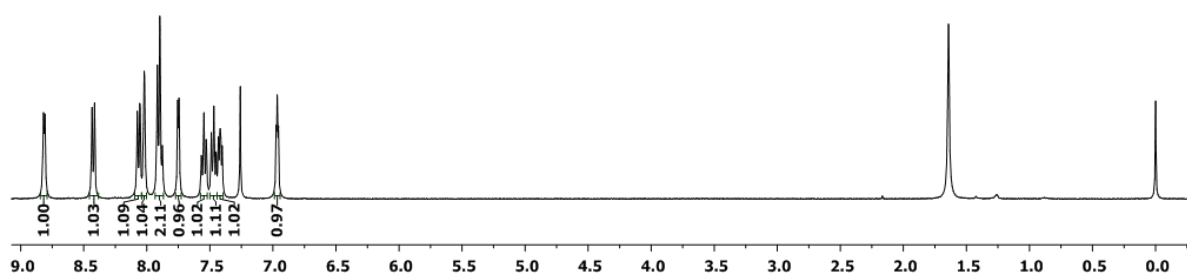
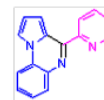
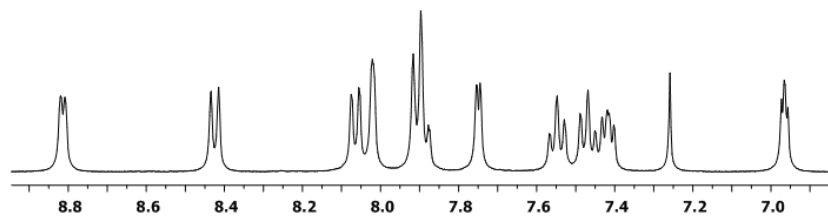
<sup>1</sup>H NMR spectrum of compound **6h**

Chemical shift values (ppm) for the <sup>13</sup>C NMR spectrum of compound **6h**:

160.64	154.23	140.20	136.13	130.28	127.59	127.24	125.32	114.71	114.01	113.65	108.82	106.70	102.30	55.60
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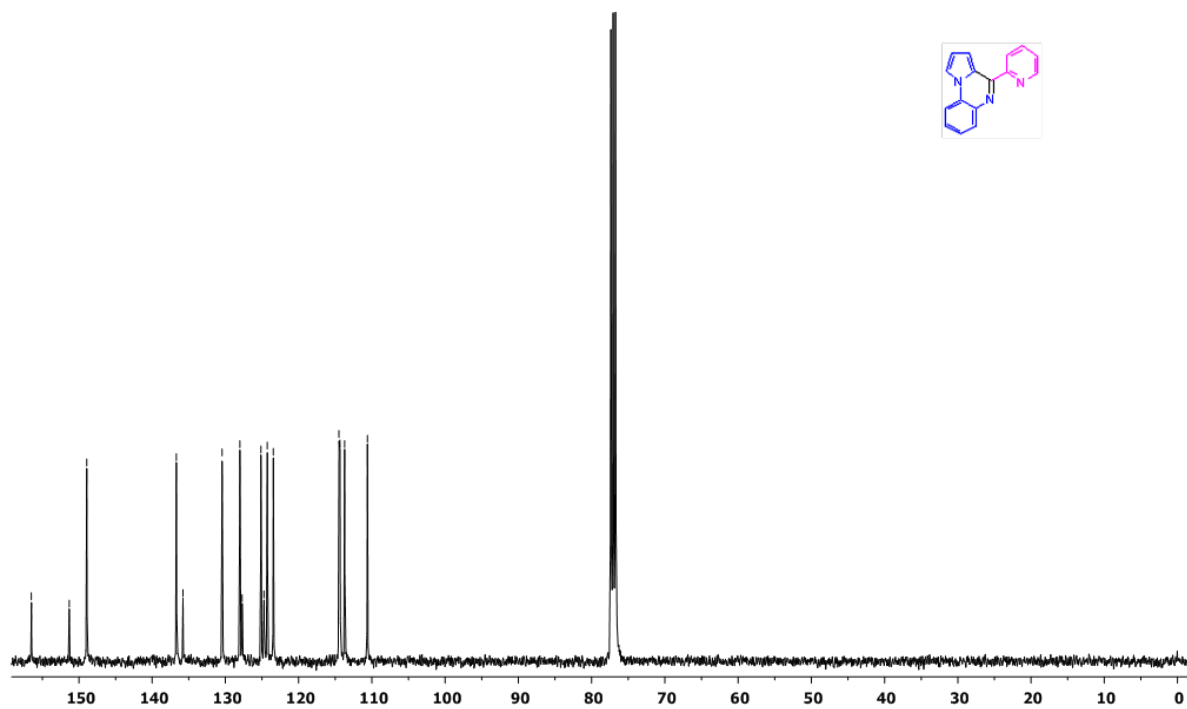


<sup>13</sup>C NMR spectrum of compound **6h**

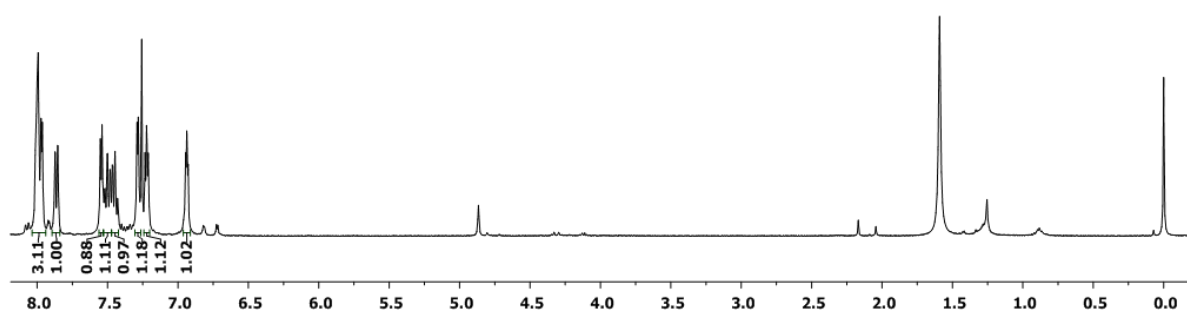
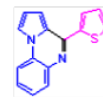
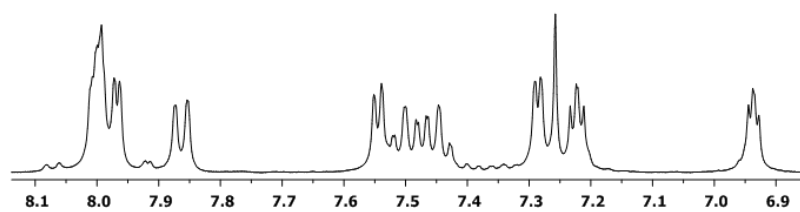


$^1\text{H}$  NMR spectrum of compound **6i**

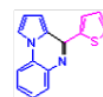
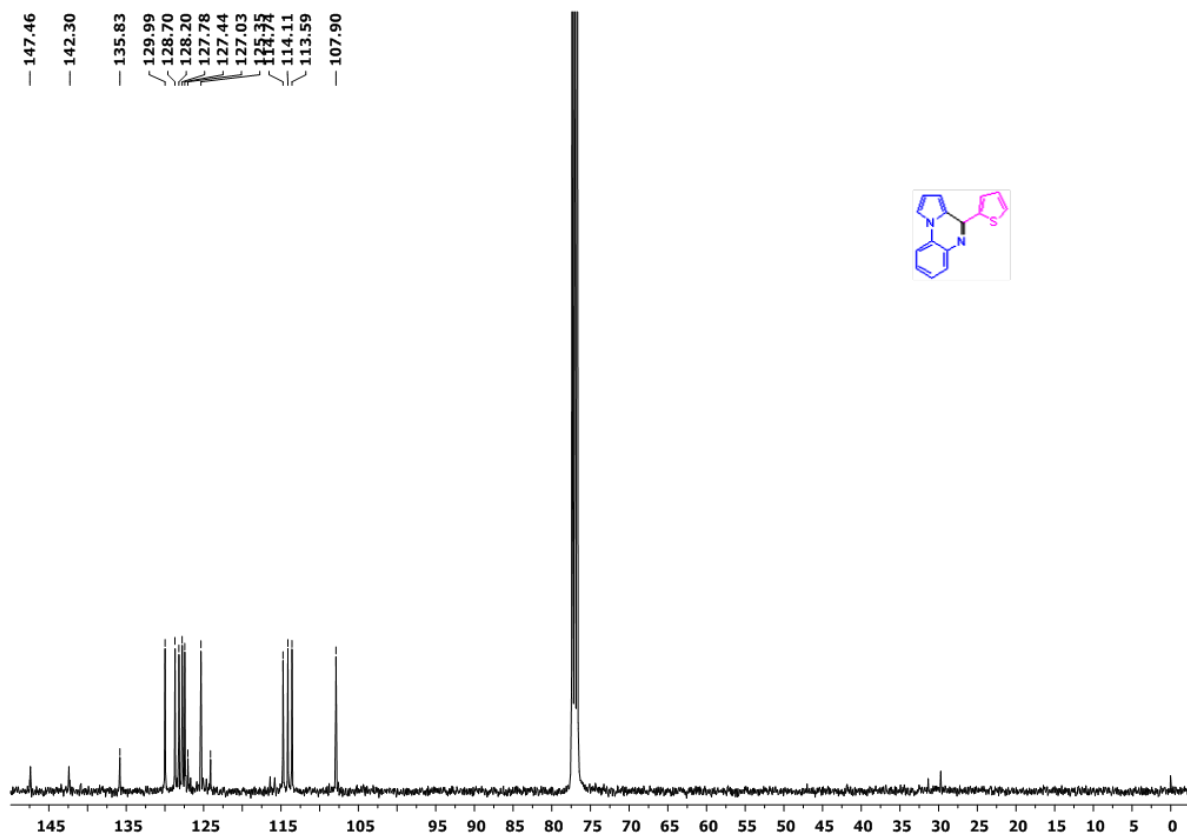
— 156.49  
 — 151.32  
 — 148.93  
 — 136.70  
 — 135.79  
 — 130.45  
 — 128.03  
 — 125.16  
 — 124.73  
 — 124.28  
 — 122.56  
 — 122.56  
 — 114.36  
 — 113.72  
 — 110.61



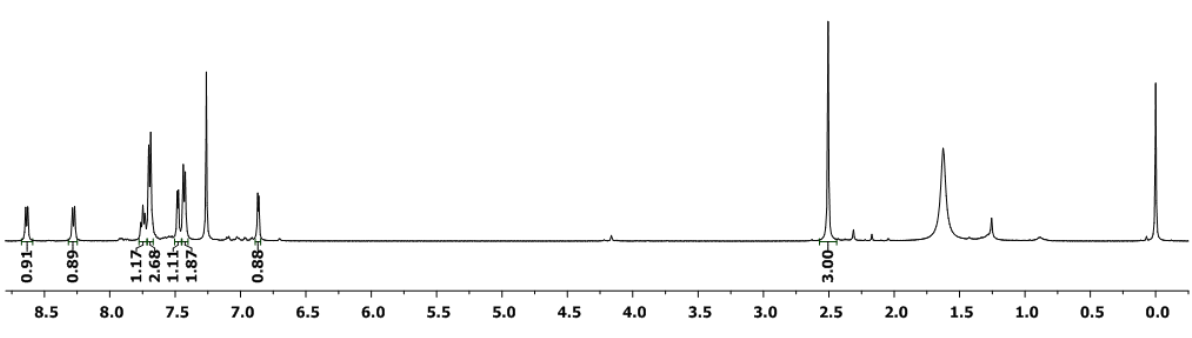
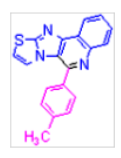
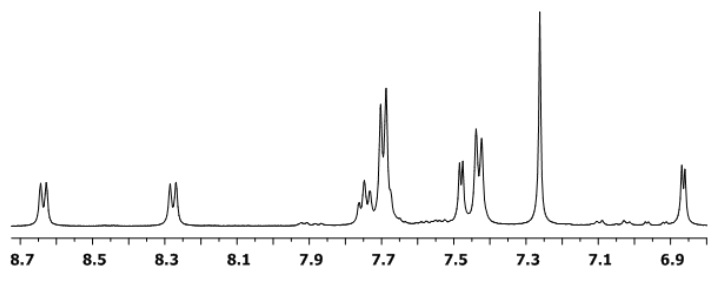
$^{13}\text{C}$  NMR spectrum of compound **6i**



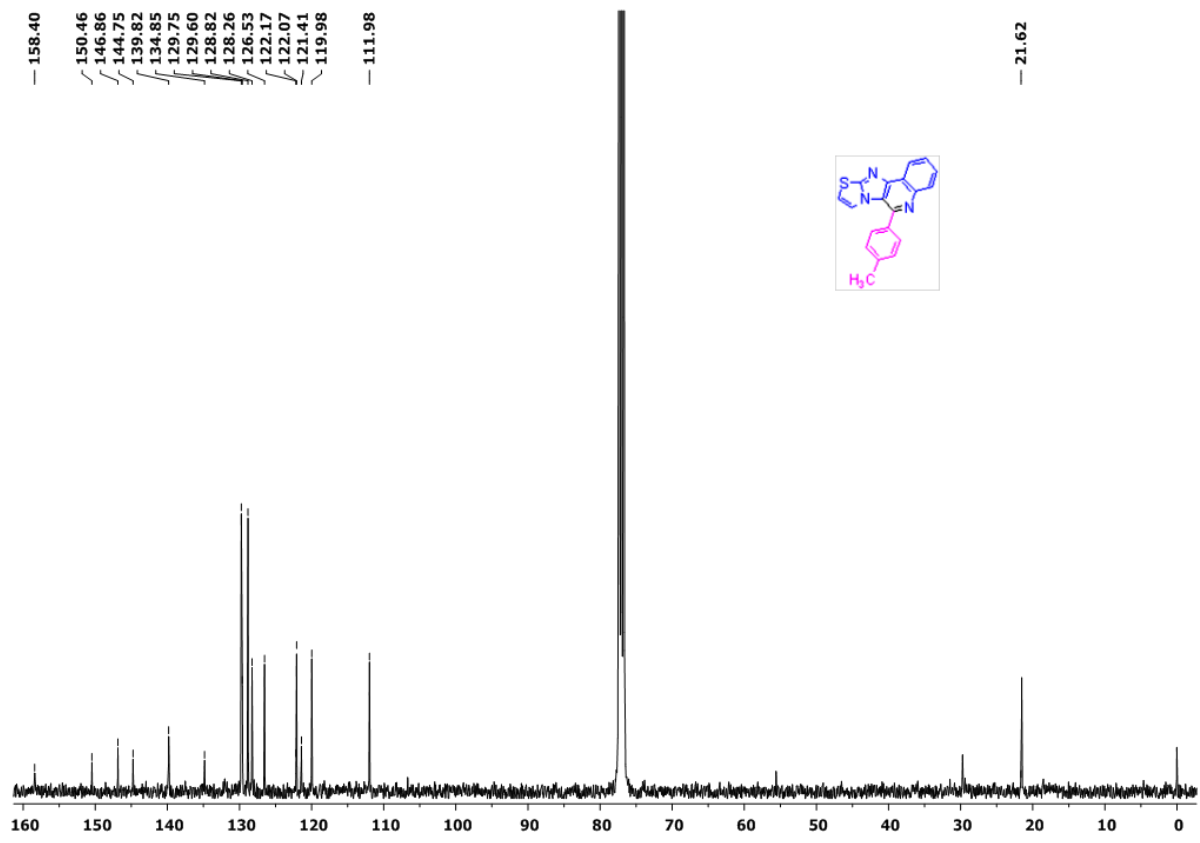
<sup>1</sup>H NMR spectrum of compound **6j**



<sup>13</sup>C NMR spectrum of compound **6j**

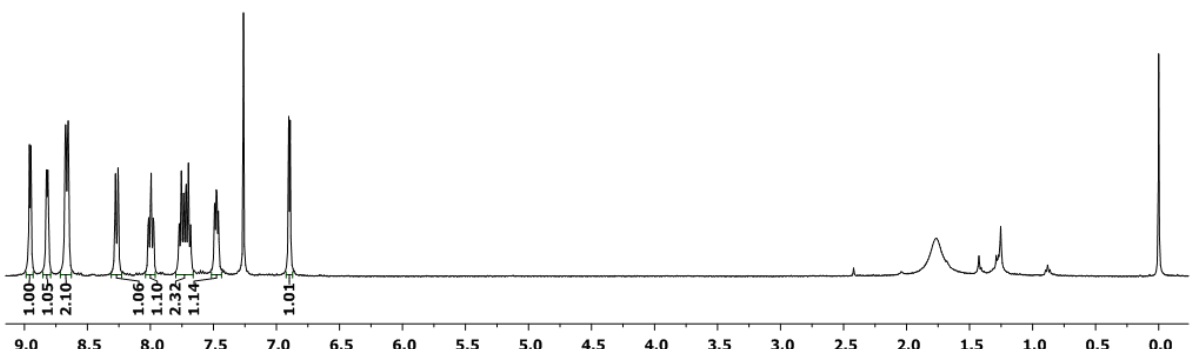
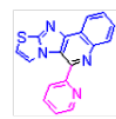
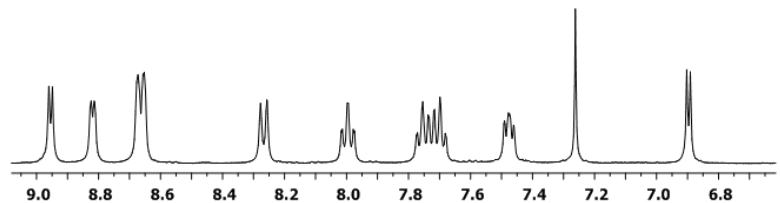


<sup>1</sup>H NMR spectrum of compound **8a**



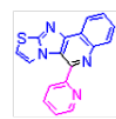
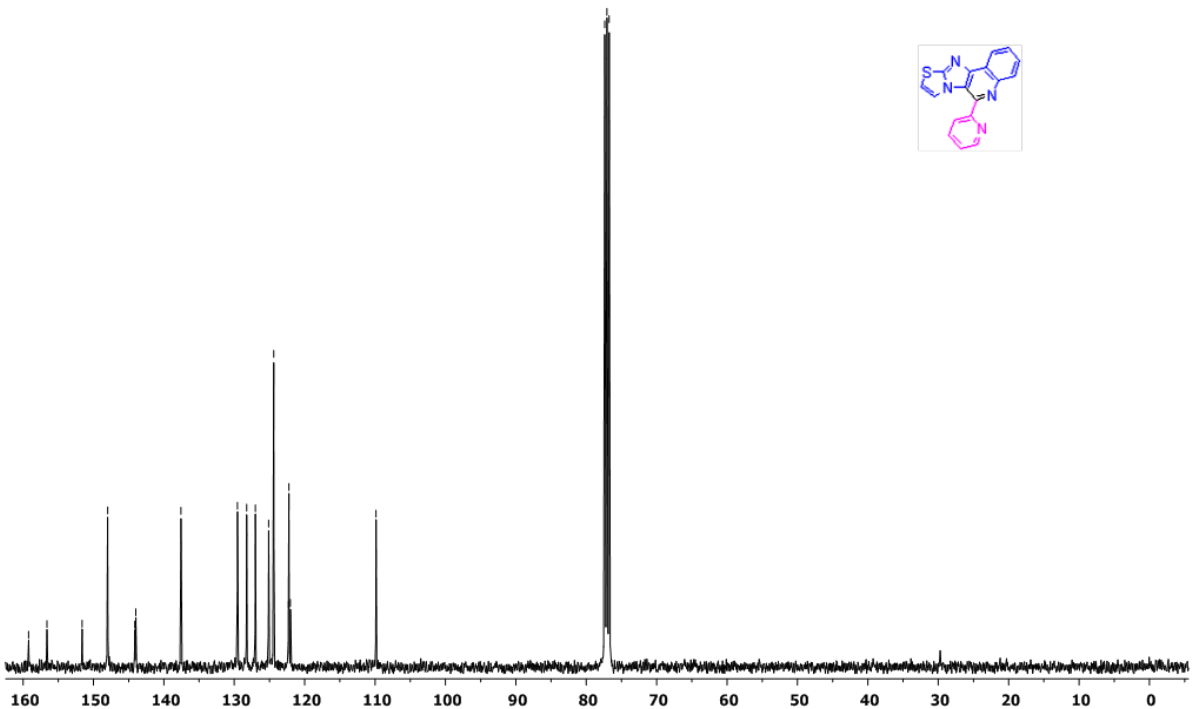
<sup>13</sup>C NMR spectrum of compound **8a**



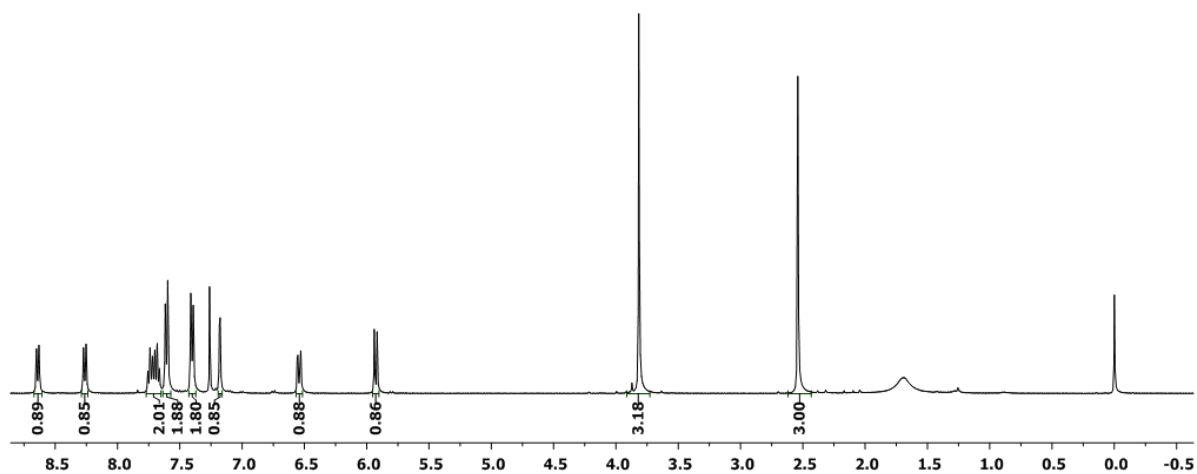
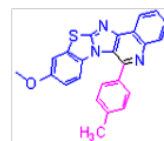
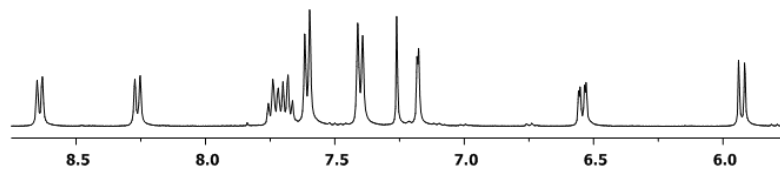


<sup>1</sup>H NMR spectrum of compound **8b**

- ~ 159.21
- ~ 156.61
- ~ 151.62
- ~ 147.99
- ~ 144.13
- ~ 143.98
- 137.57
- 129.54
- 128.24
- 127.01
- 125.12
- 124.39
- 122.30
- 122.24
- 122.02
- 109.86
- 77.38
- 77.06
- 76.74



<sup>13</sup>C NMR spectrum of compound **8b**

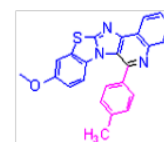
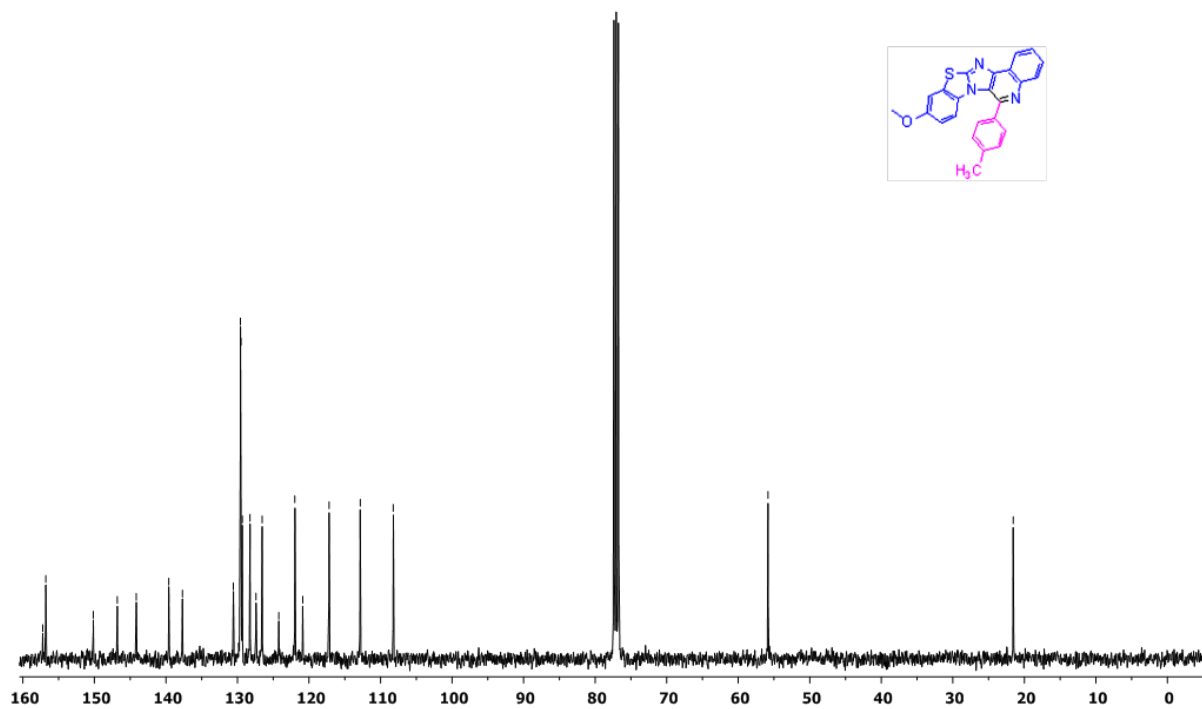


<sup>1</sup>H NMR spectrum of compound **8c**

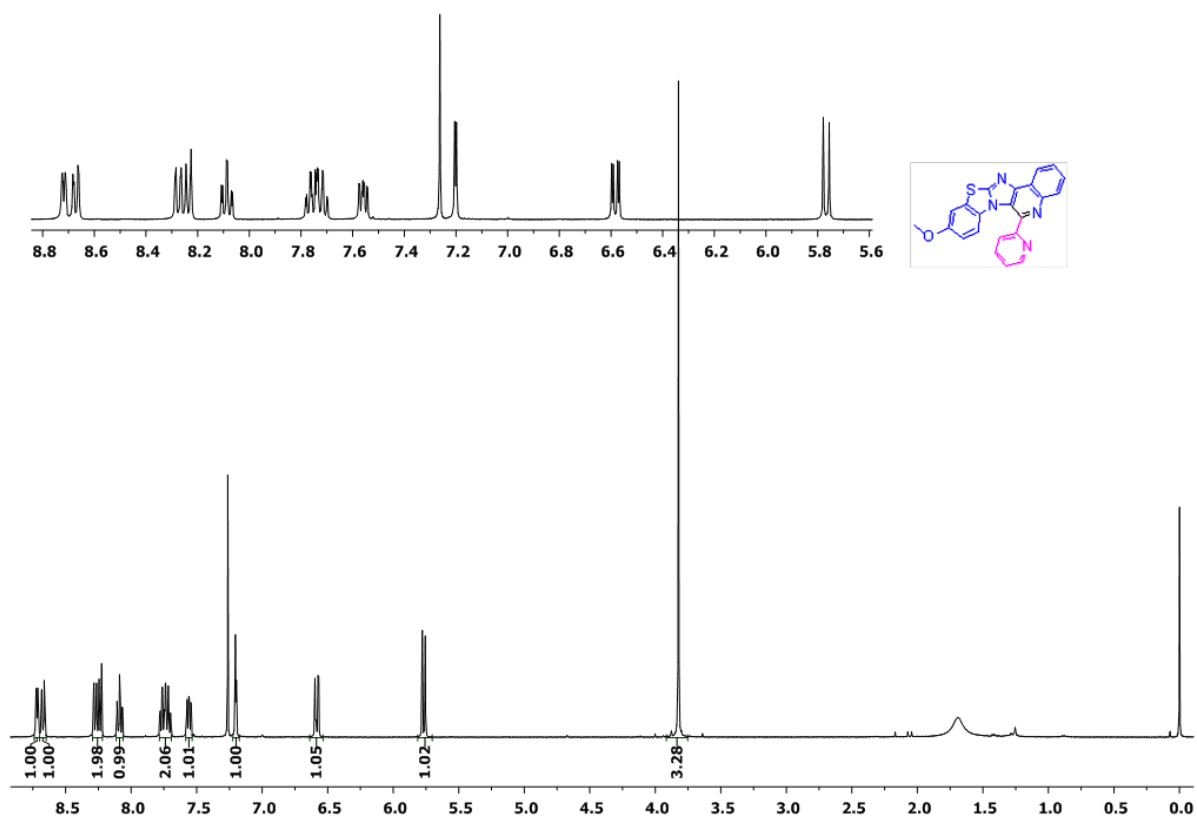
157.24  
156.80  
150.16  
146.79  
144.14  
139.61  
137.70  
130.57  
129.58  
129.50  
129.33  
128.25  
127.41  
126.55  
124.23  
121.97  
120.88  
117.20  
112.84  
108.22

55.84

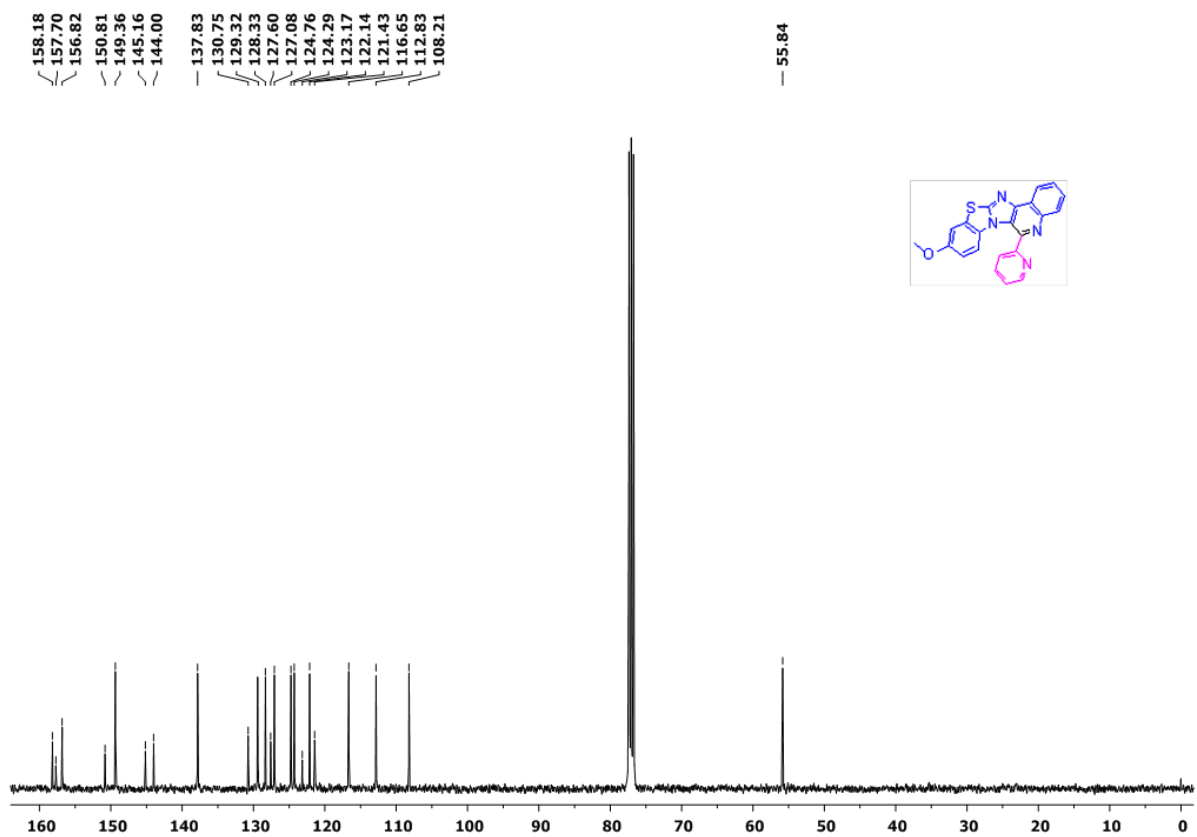
21.56



<sup>13</sup>C NMR spectrum of compound **8c**



$^1\text{H}$  NMR spectrum of compound **8d**



$^{13}\text{C}$  NMR spectrum of compound **8d**