

# **Synthesis and antitumor activity evaluation of novel substituted 5*H*-benzo[*i*][1,3,4]thiadiazolo[3,2-*a*]quinazoline-6,7-diones**

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## **Content**

**Copy of UV-vis, IR, <sup>1</sup>H NMR, <sup>13</sup>C NMR and HRMS.....2-**

**44**

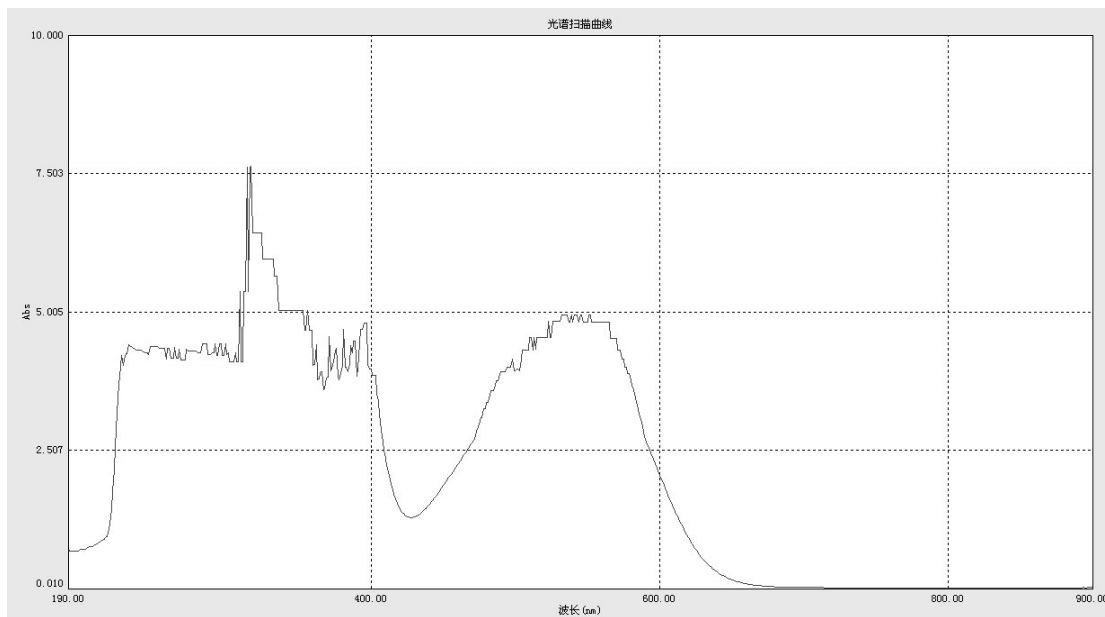


Figure 1 UV-vis of 4a

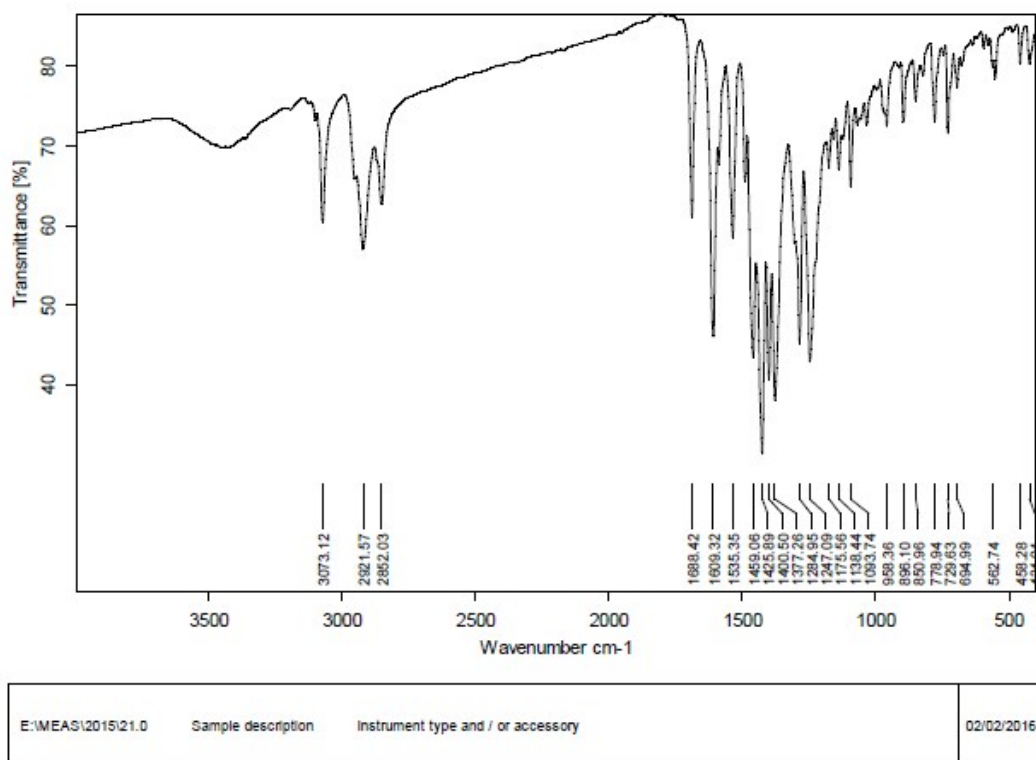


Figure 2 IR of 4a

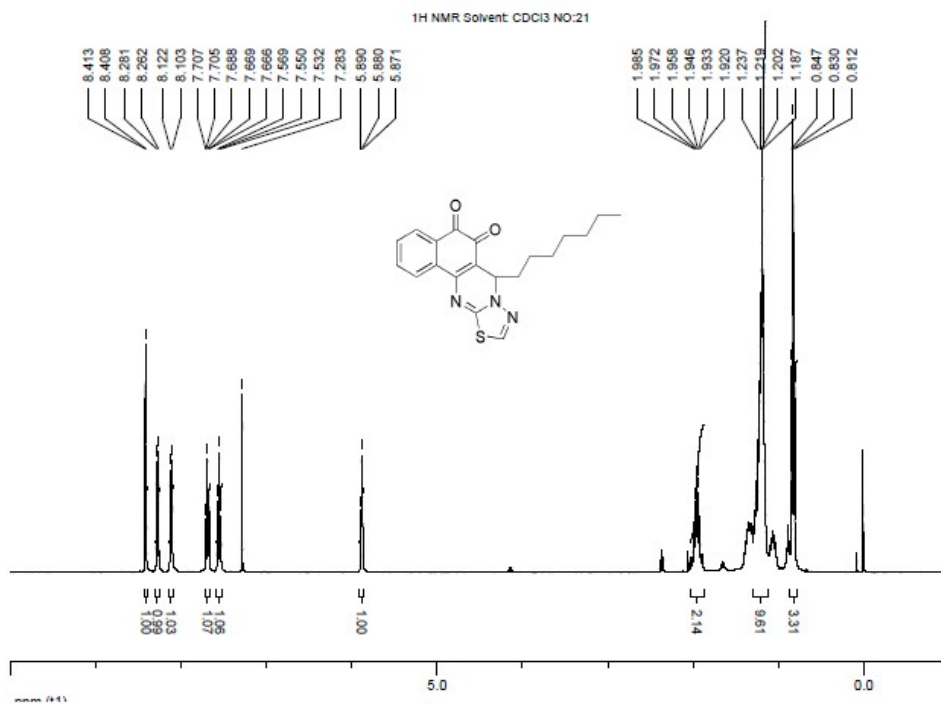


Figure 3  $^1\text{H}$  NMR of 4a

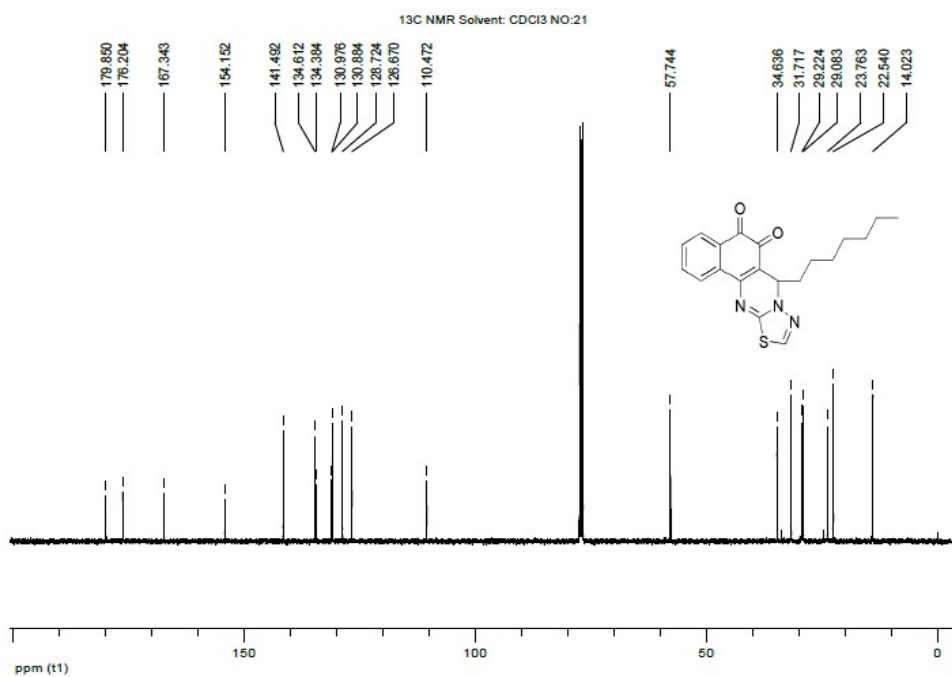
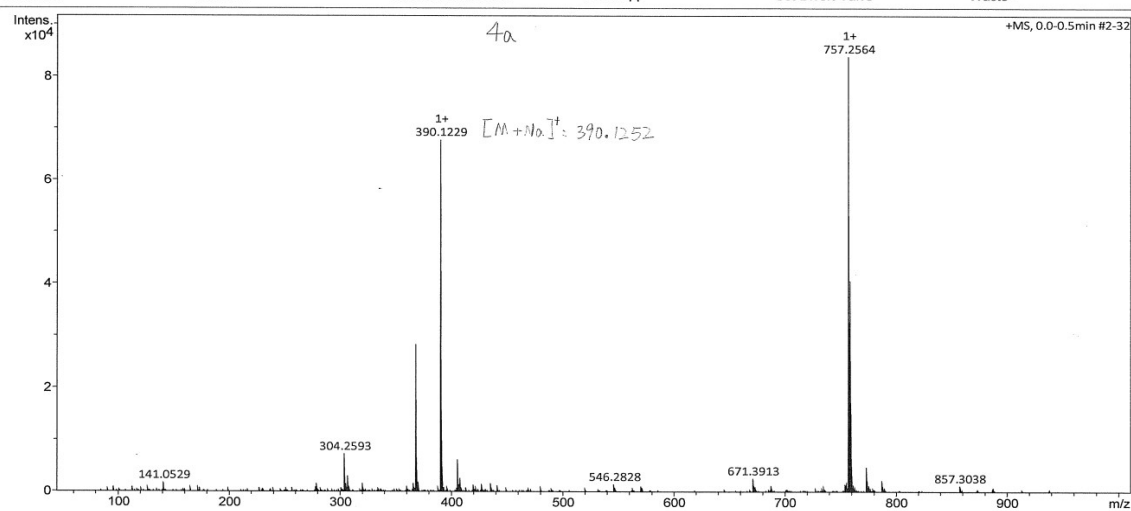


Figure 4  $^{13}\text{C}$  NMR of 4a

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Sample Name	w-21	Instrument	micrOTOF-Q III 8228888.20494		
Comment					
Acquisition Parameter					
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Scan Begin	50 m/z	Set End Plate Offset	-500 V	Set Dry Gas	4.0 l/min
Scan End	1000 m/z	Set Collision Cell RF	120.0 Vpp	Set Divert Valve	Waste



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Figure 5 HRMC of 4a

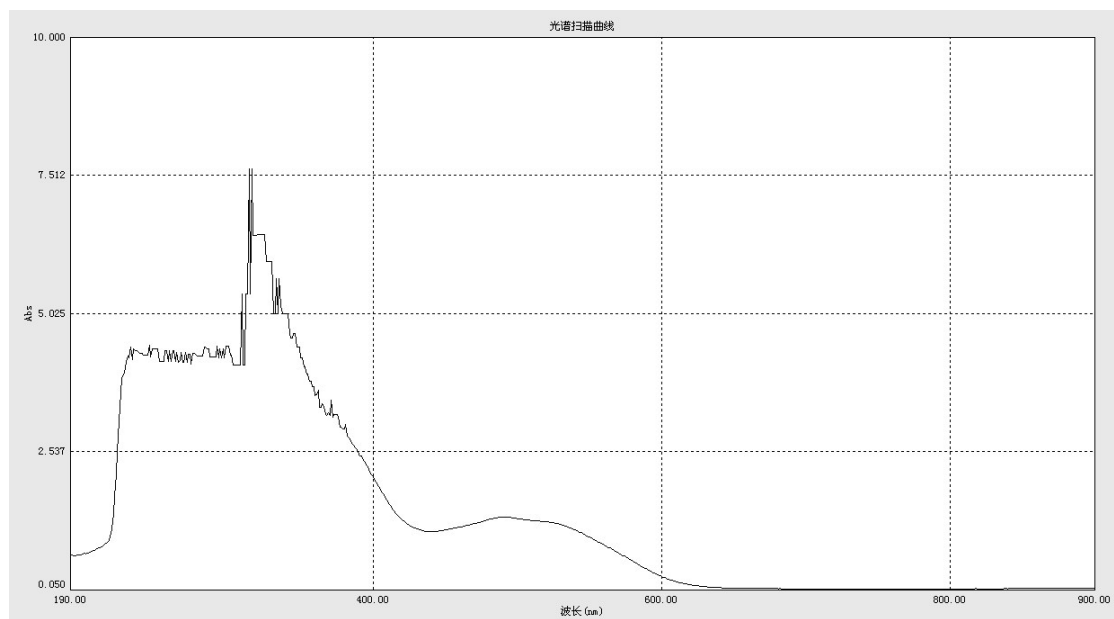


Figure 6 UV-vis of 4b

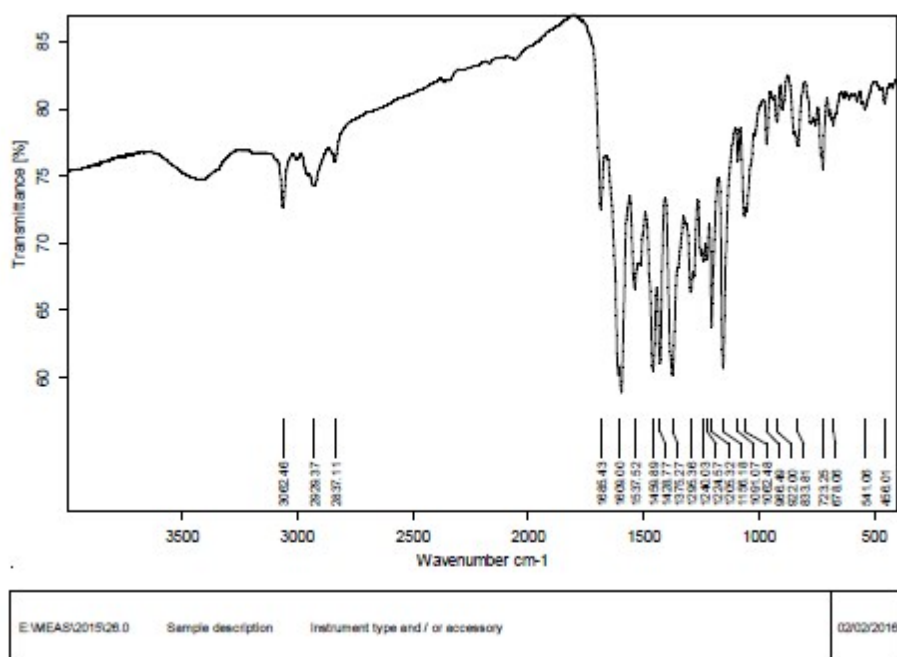


Figure 7 IR of 4b

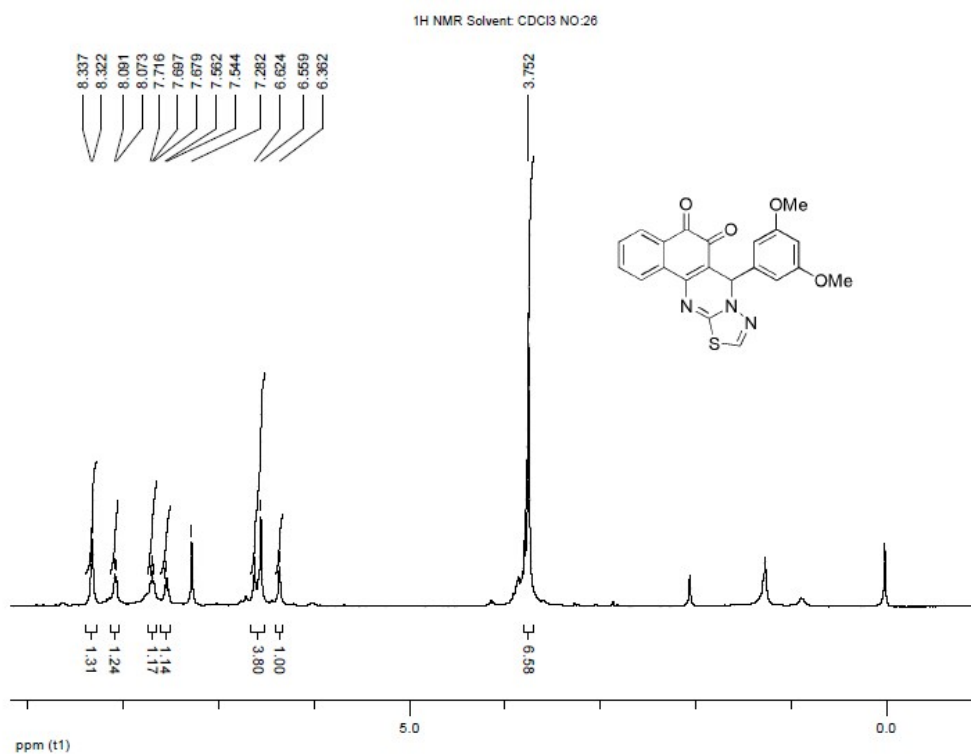


Figure 8 <sup>1</sup>H NMR of 4b

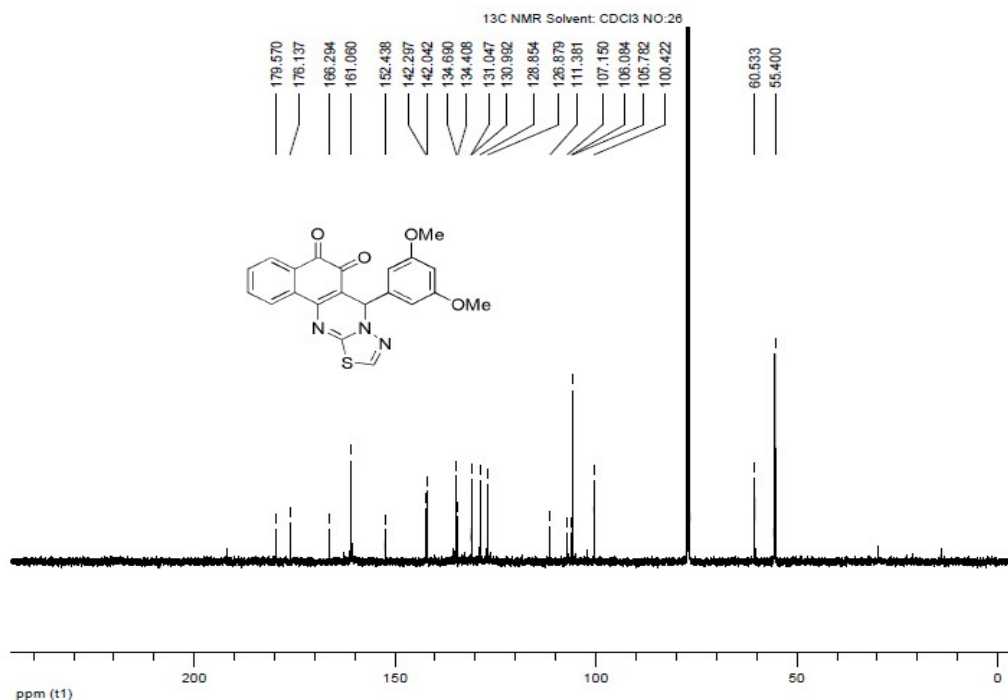


Figure 9  $^{13}\text{C}$  NMR of 4b

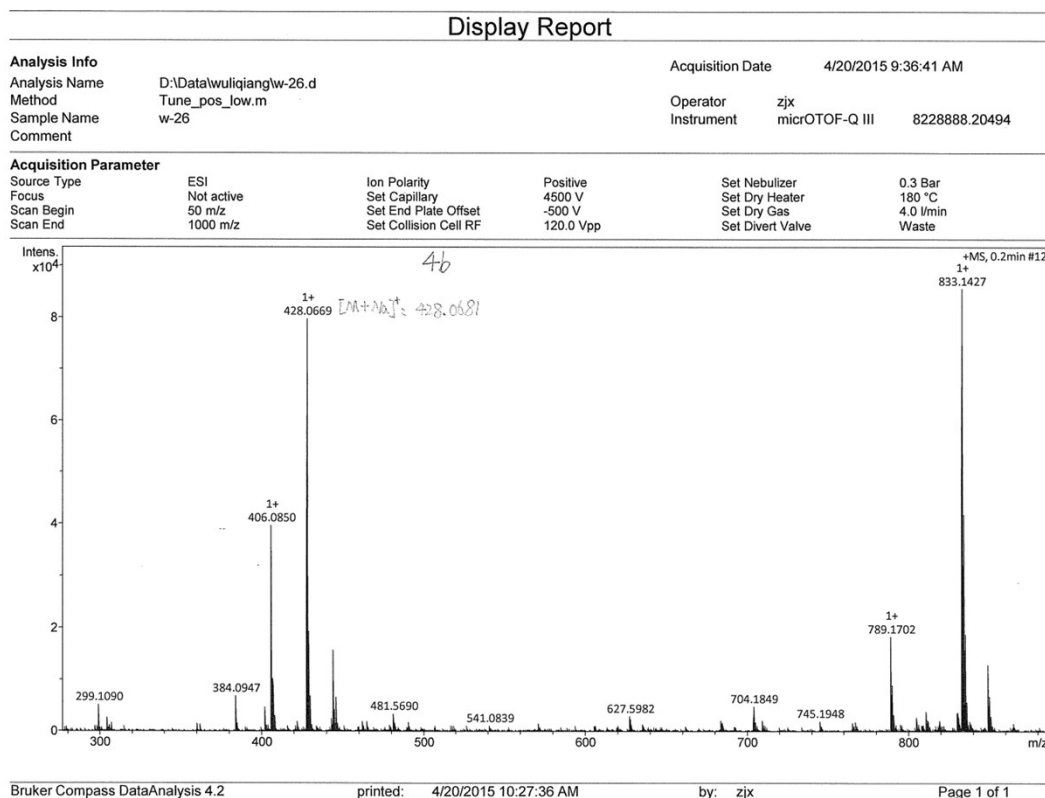


Figure 10 HRMS of 4b

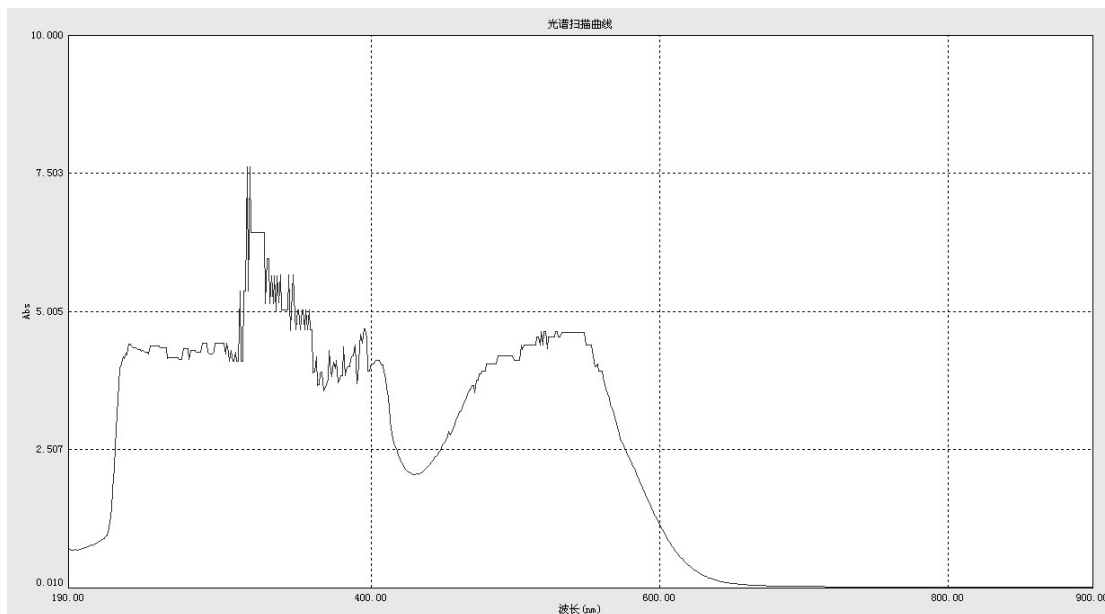


Figure 11 UV-vis of 4c

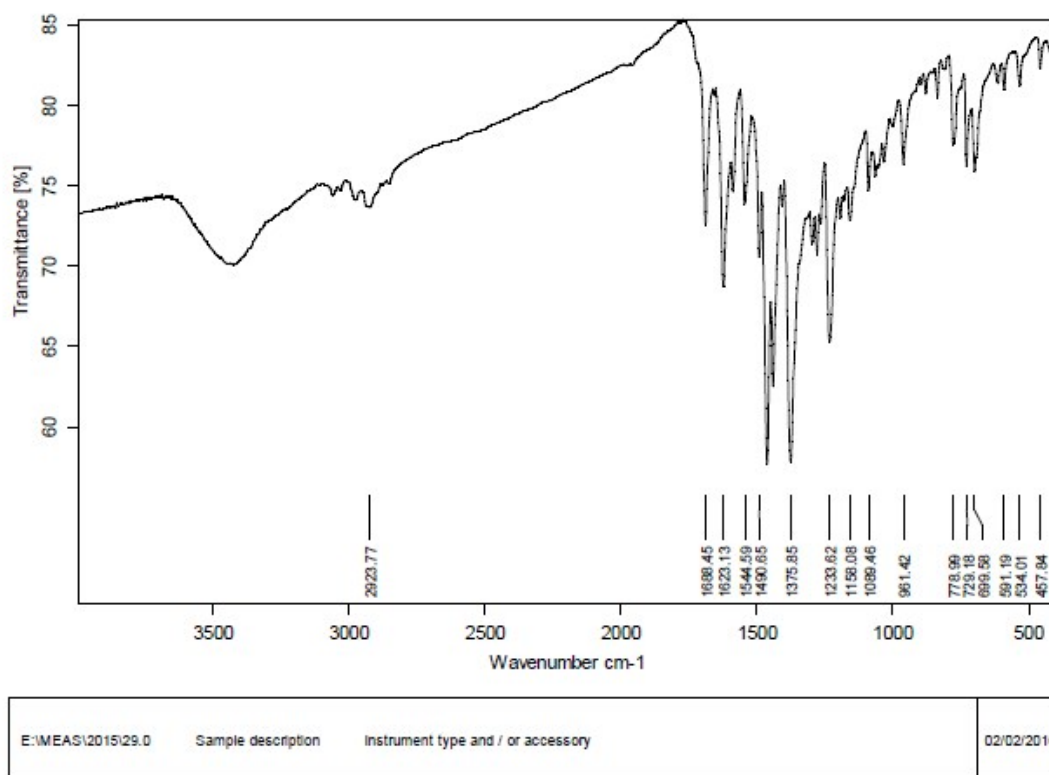


Figure 12 IR of 4c

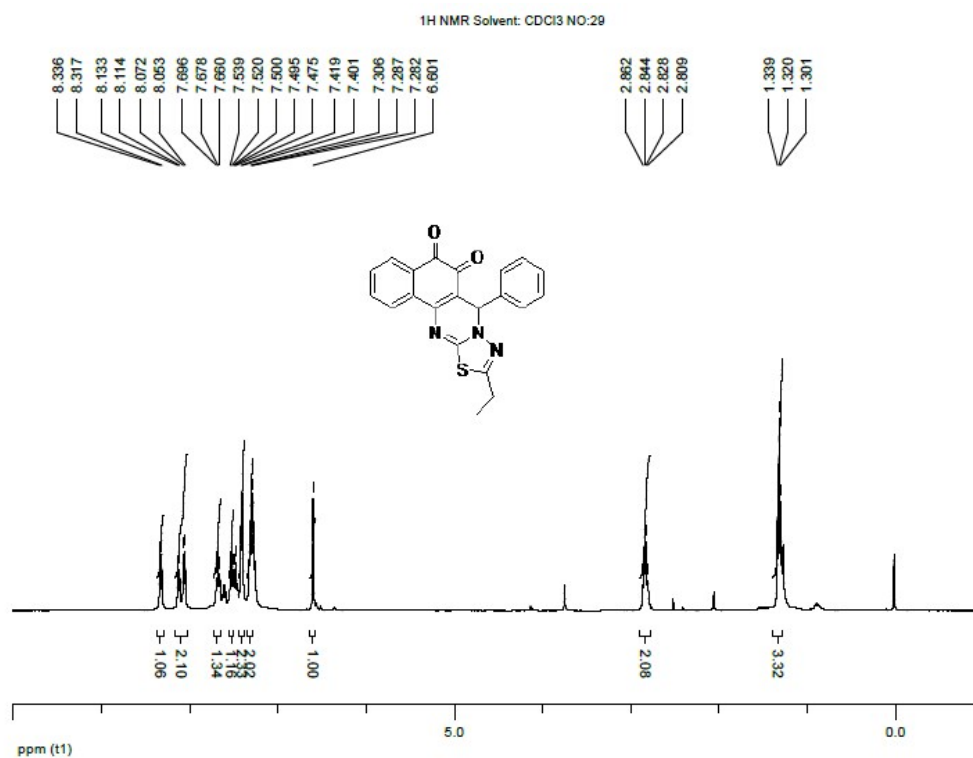


Figure 13  $^1\text{H}$  NMR of 4c

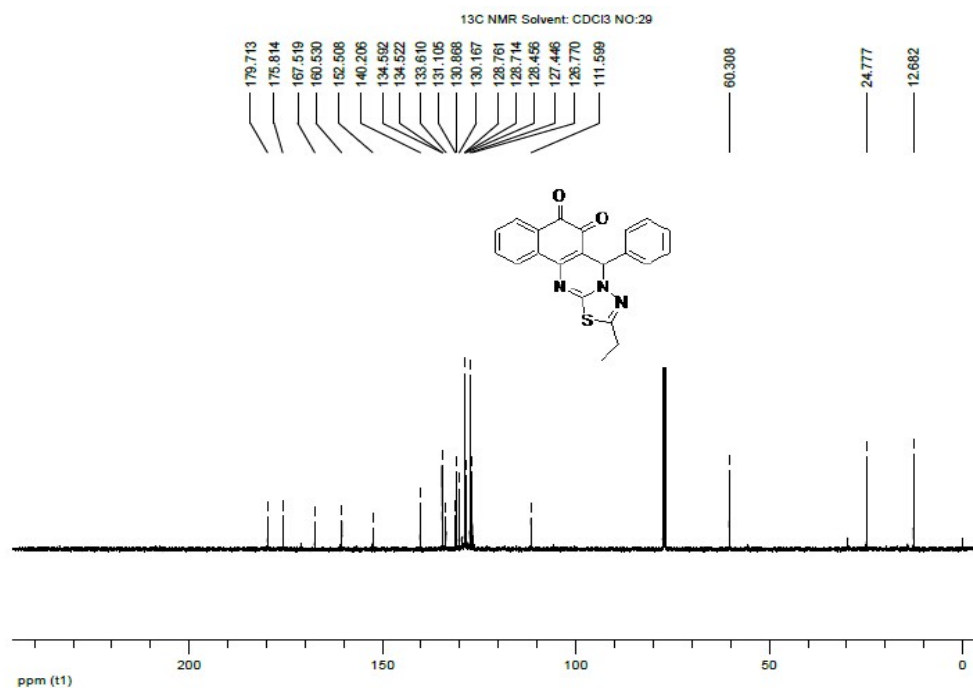


Figure 14  $^{13}\text{C}$  NMR of 4c



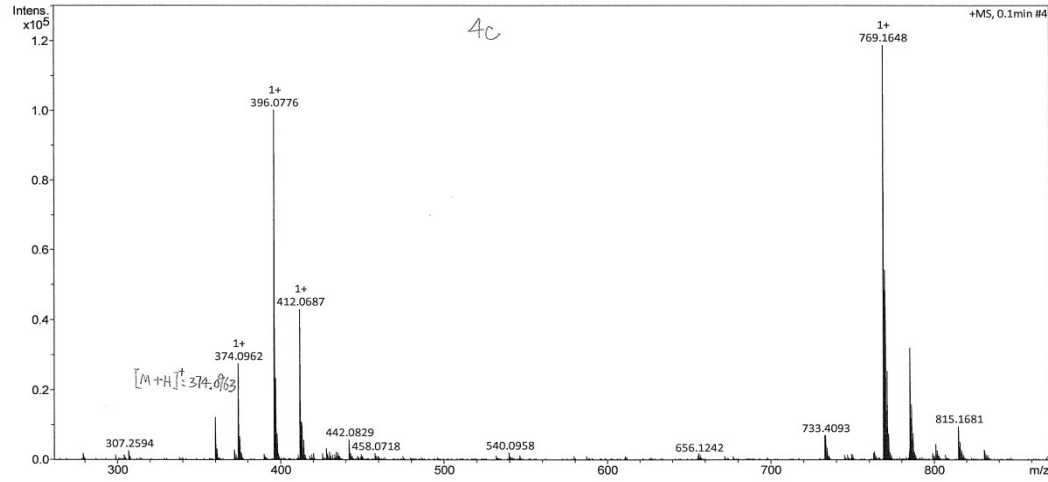
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Method: Tune\_pos\_low.m  
Sample Name: w-29  
Comment:

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Operator: zjx  
Instrument: micrOTOF-Q III 8228888.20494

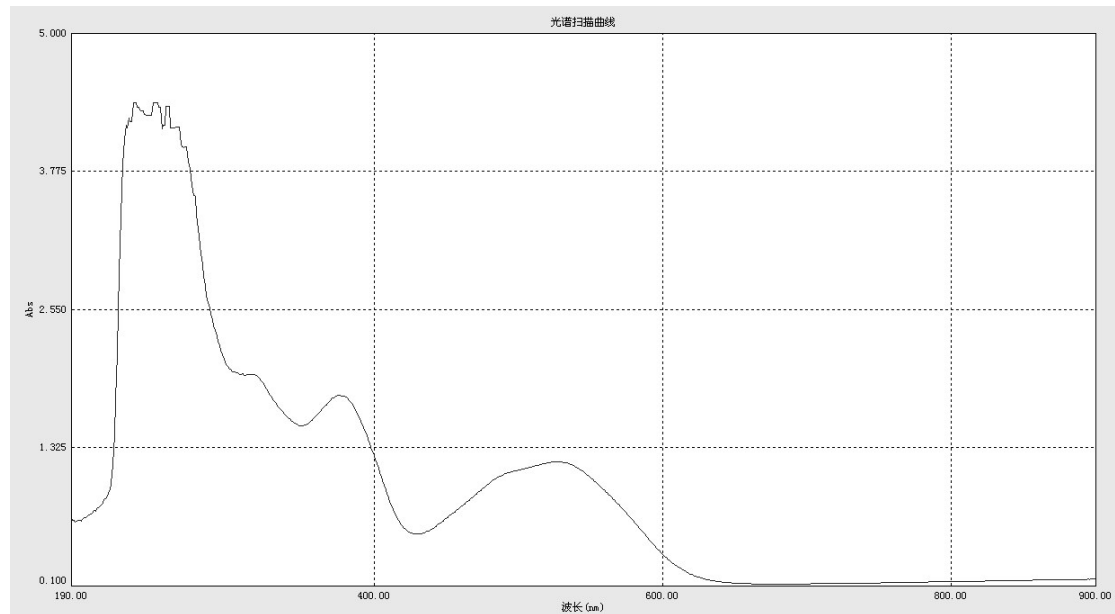
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Scan Begin	50 m/z	Set End Plate Offset	-500 V	Set Dry Gas	4.0 l/min
Scan End	1000 m/z	Set Collision Cell RF	120.0 Vpp	Set Divert Valve	Waste



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**Figure 15** HRMS of **4c**



**Figure 16** UV-vis of **4d**

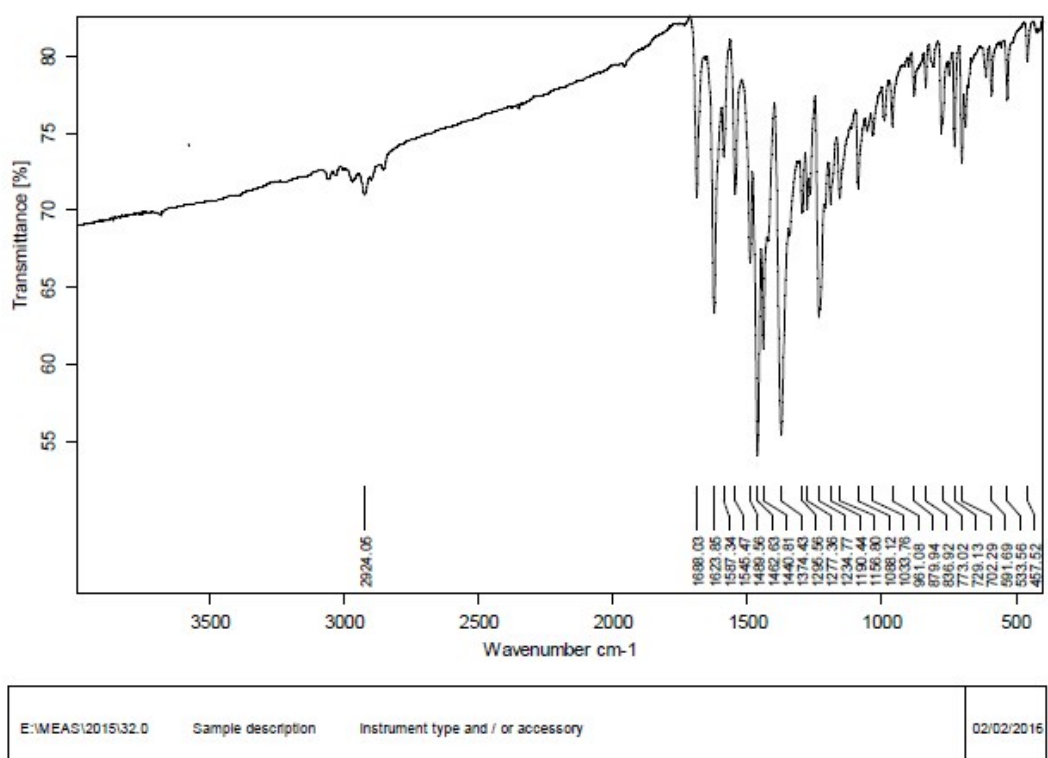


Figure 17 IR of 4d

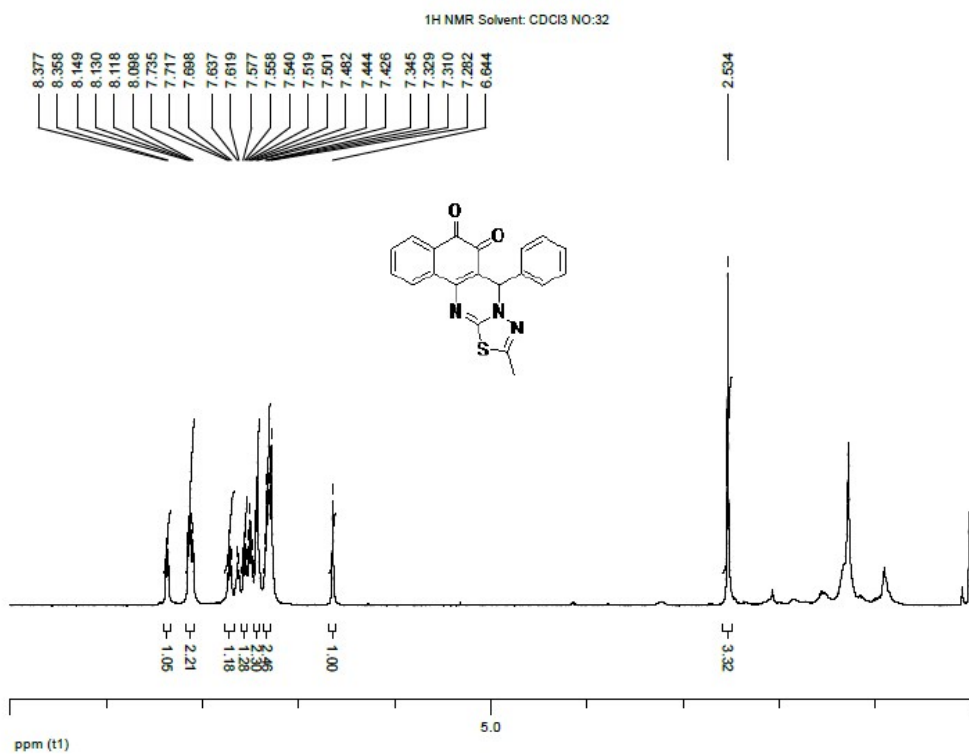


Figure 18 <sup>1</sup>H NMR of 4d

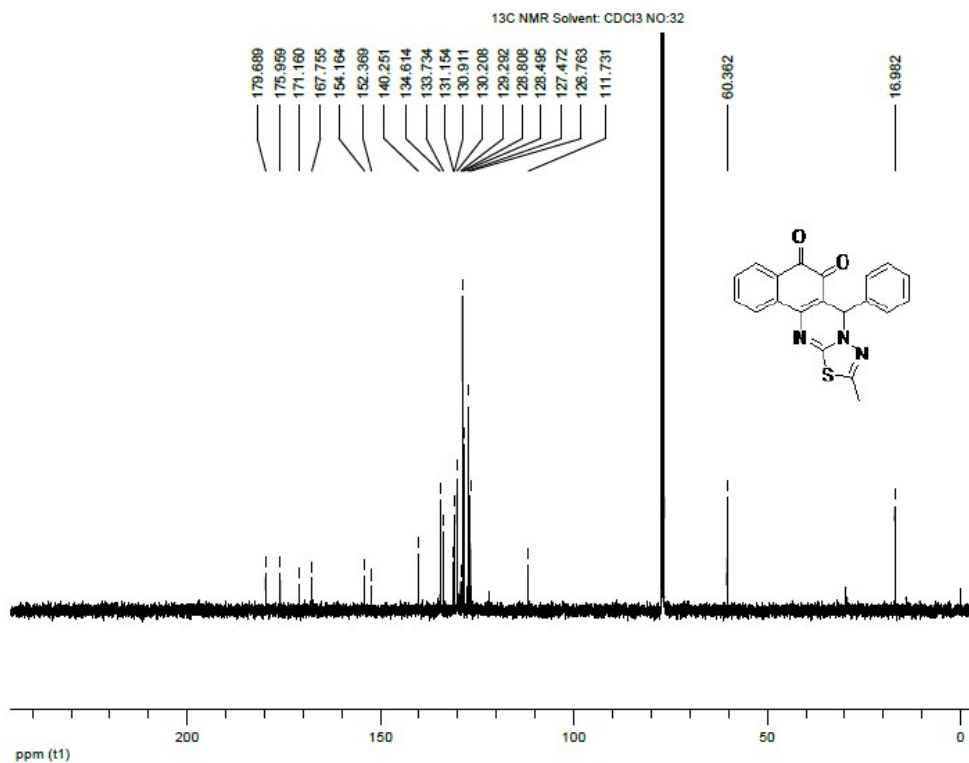


Figure 19  $^{13}\text{C}$  NMR of 4d

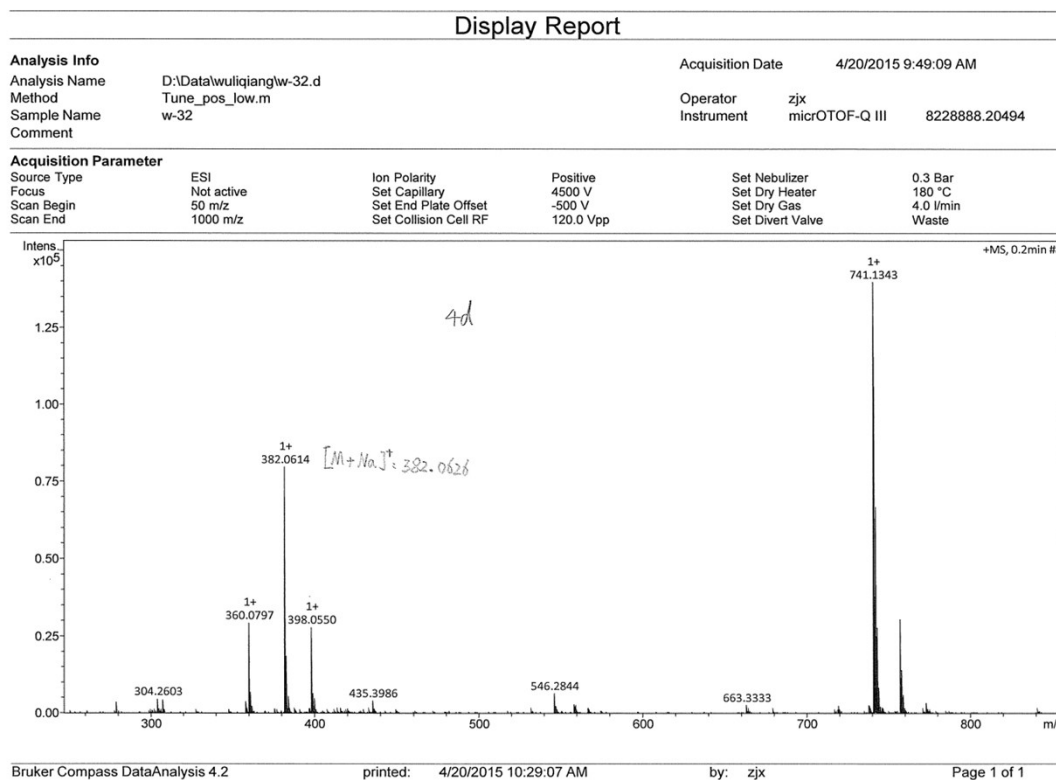


Figure 20 HRMS of 4d

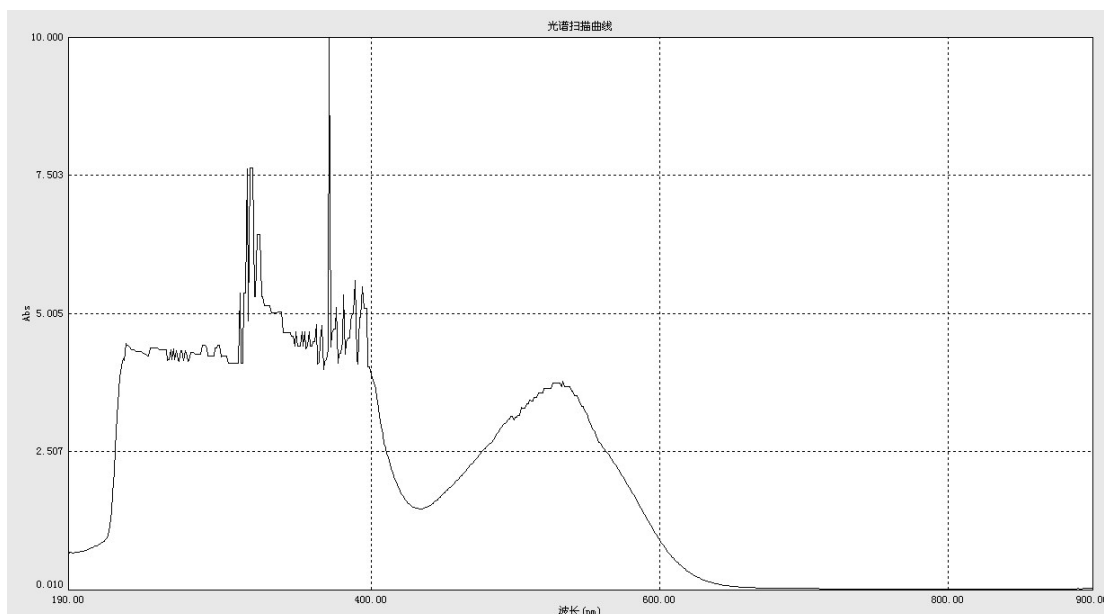


Figure 21 UV-vis of 4e

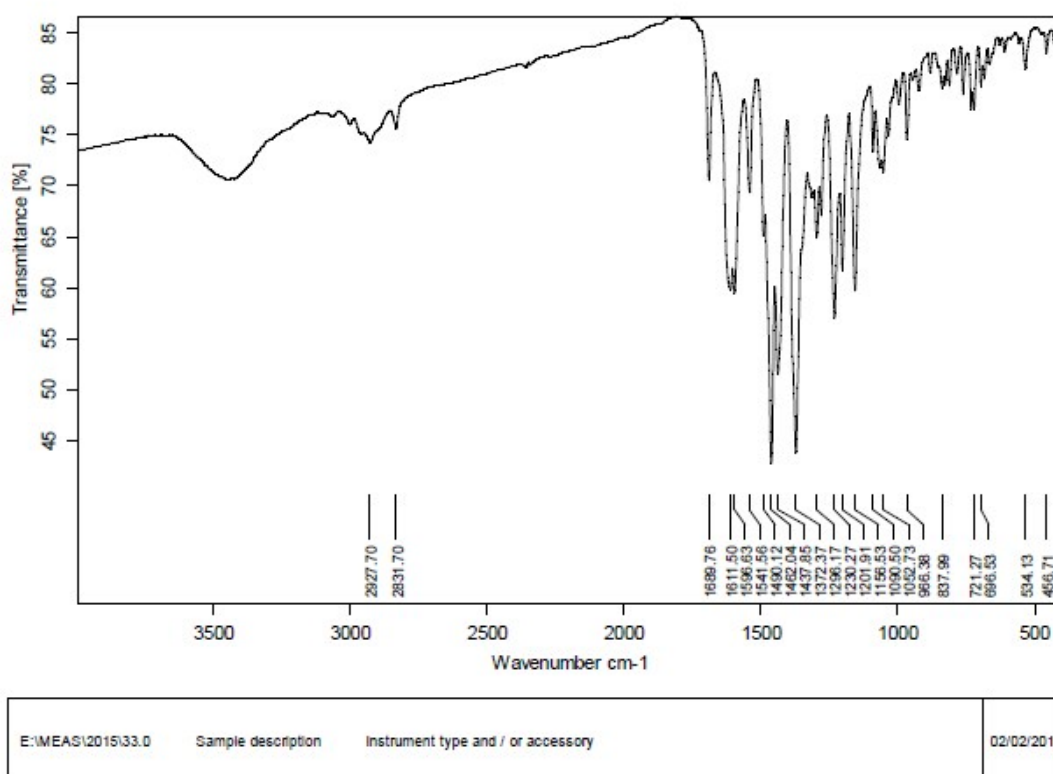


Figure 22 IR of 4e

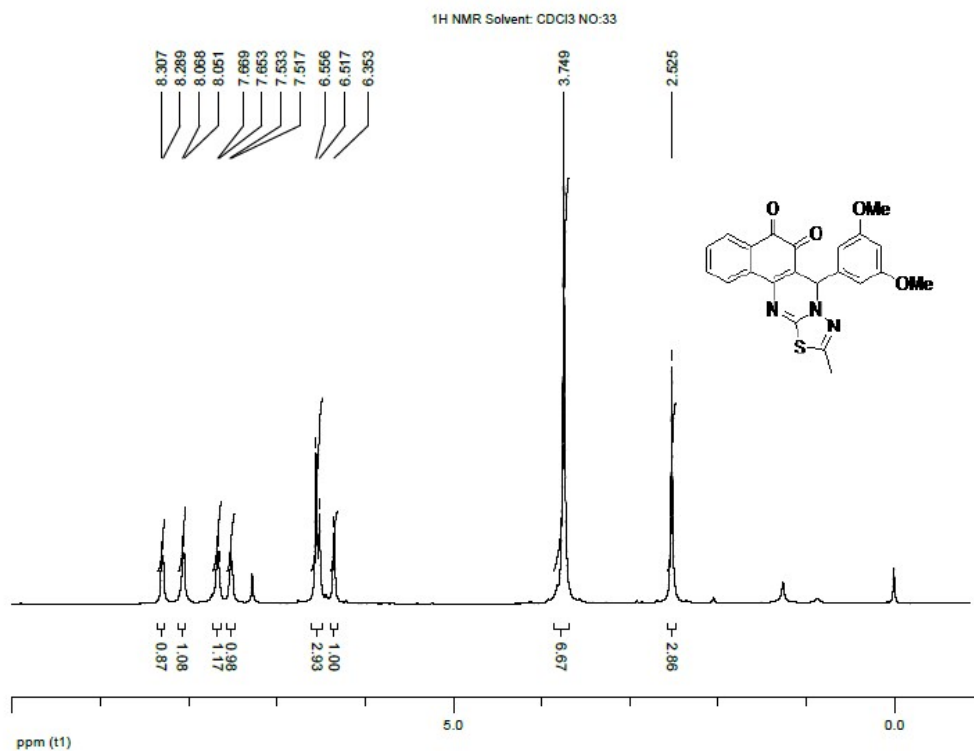


Figure 23  $^1\text{H}$  NMR of 4e

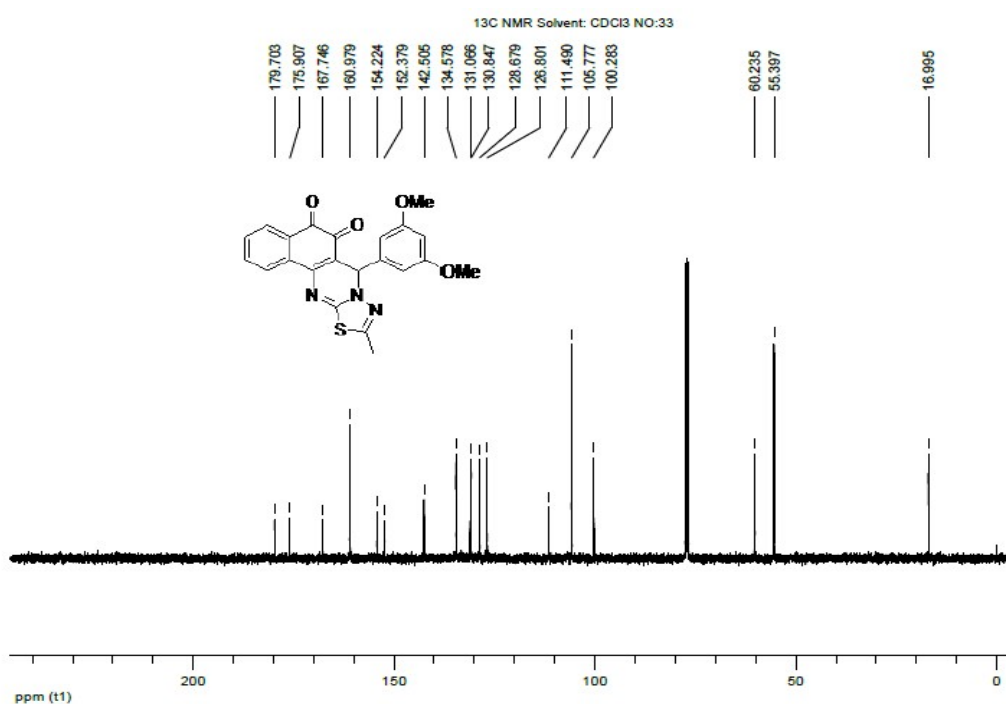
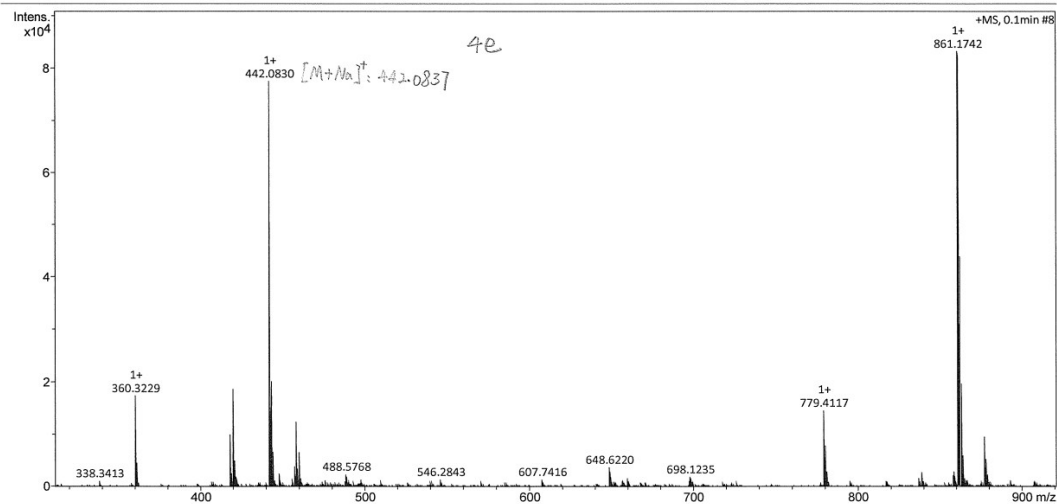


Figure 24  $^{13}\text{C}$  NMR of 4e

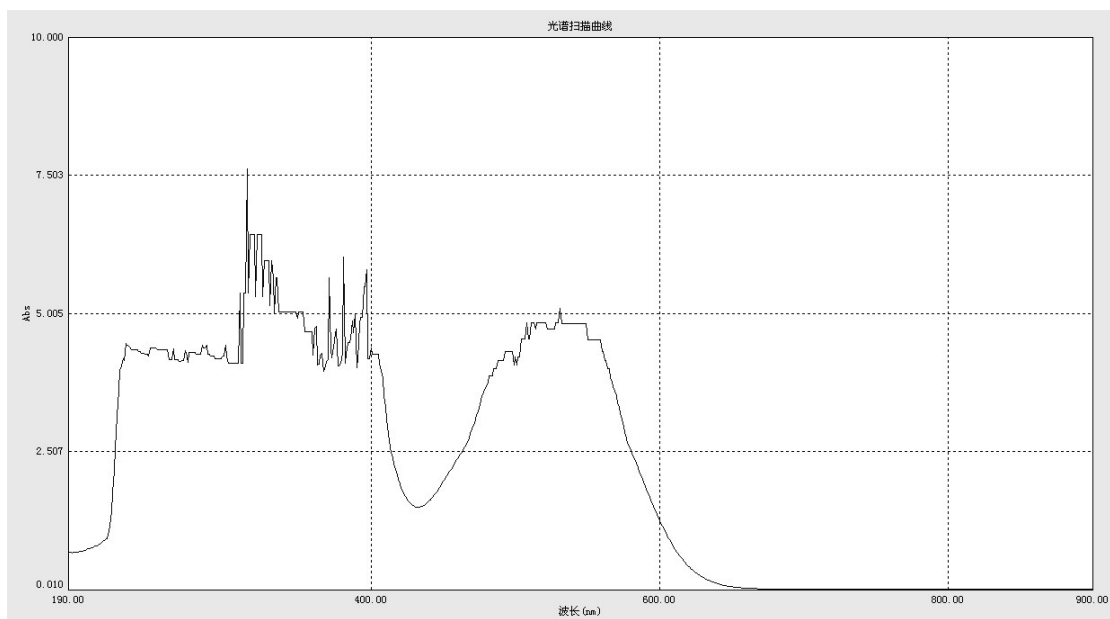
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Sample Name	w-33		8228888.20494		
Comment					
<b>Acquisition Parameter</b>					
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Focus	Not active	Set Capillary	4500 V	Set Dry Heater	180 °C
Scan Begin	50 m/z	Set End Plate Offset	-500 V	Set Dry Gas	4.0 l/min
Scan End	1000 m/z	Set Collision Cell RF	120.0 Vpp	Set Divert Valve	Waste



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**Figure 25** HRMS of **4e**



**Figure 26** UV-vis of **4f**

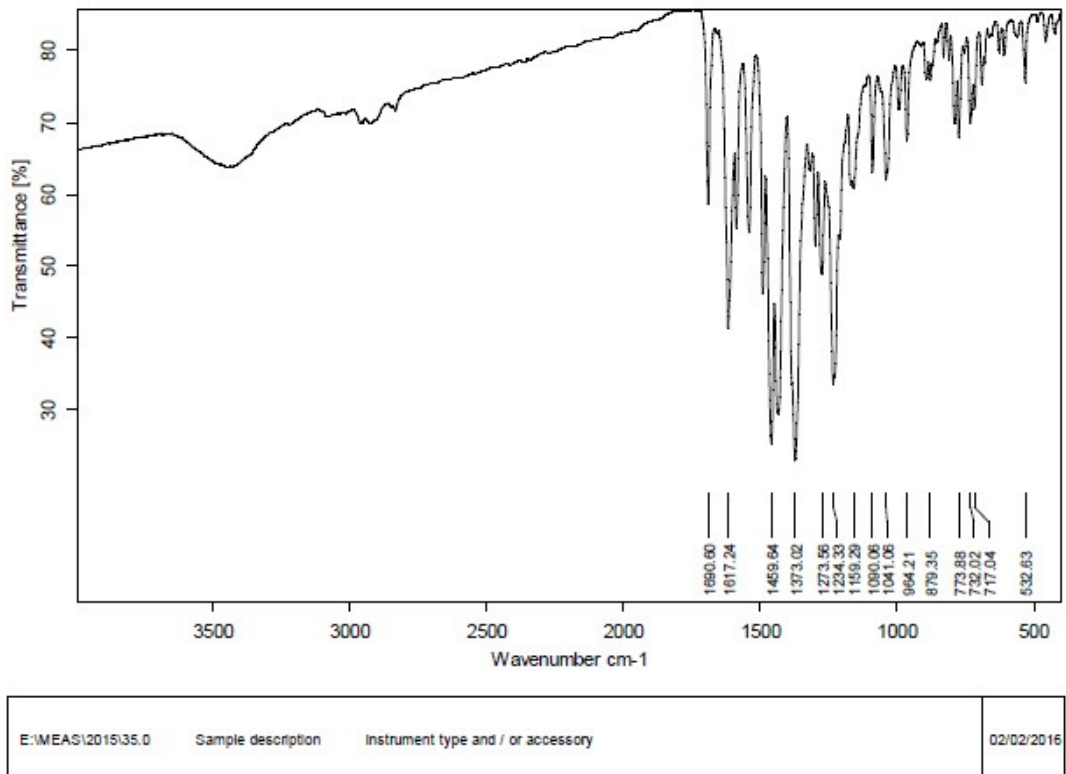


Figure 27 IR of 4f

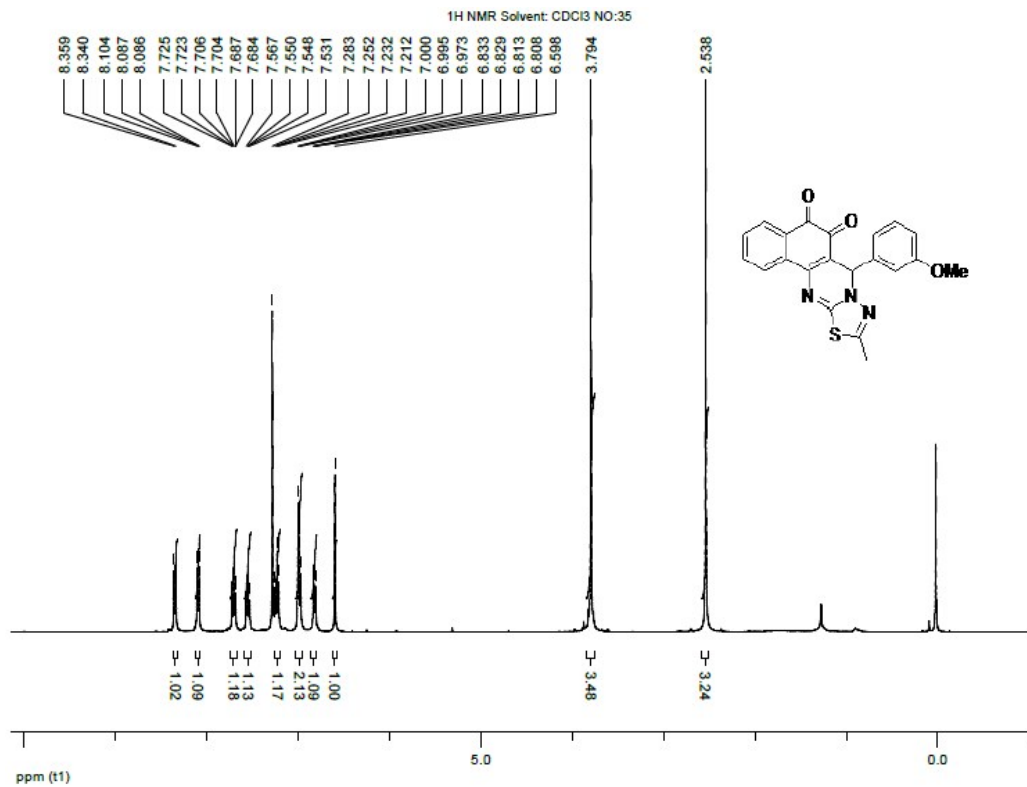


Figure 28 <sup>1</sup>H NMR of 4f

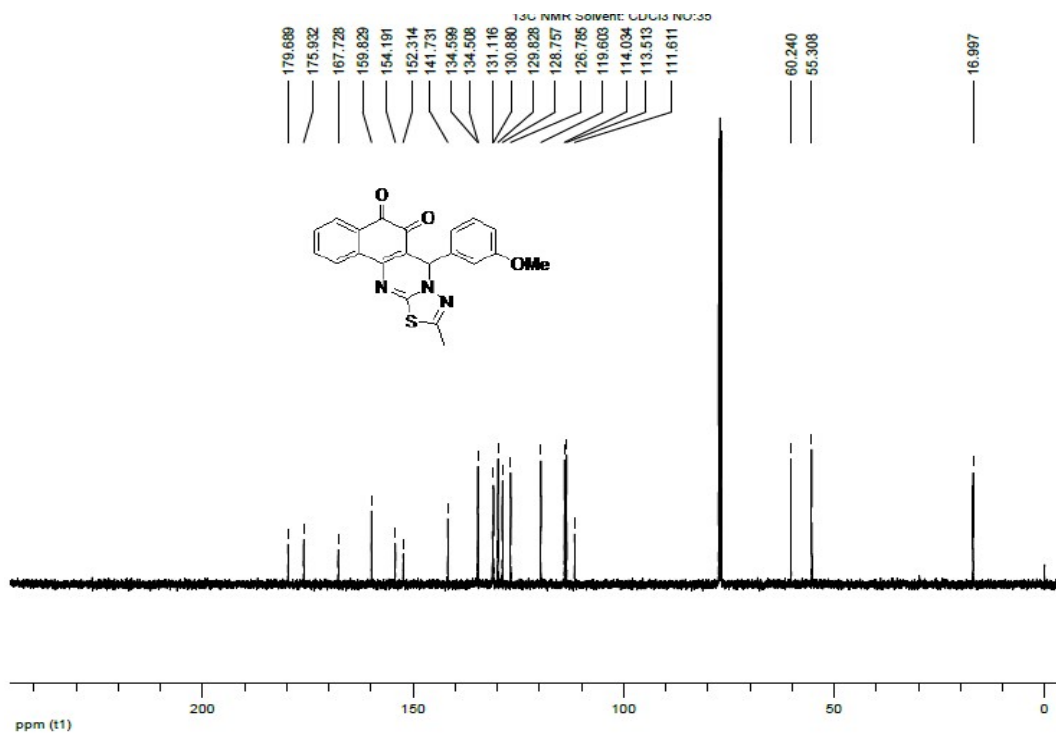
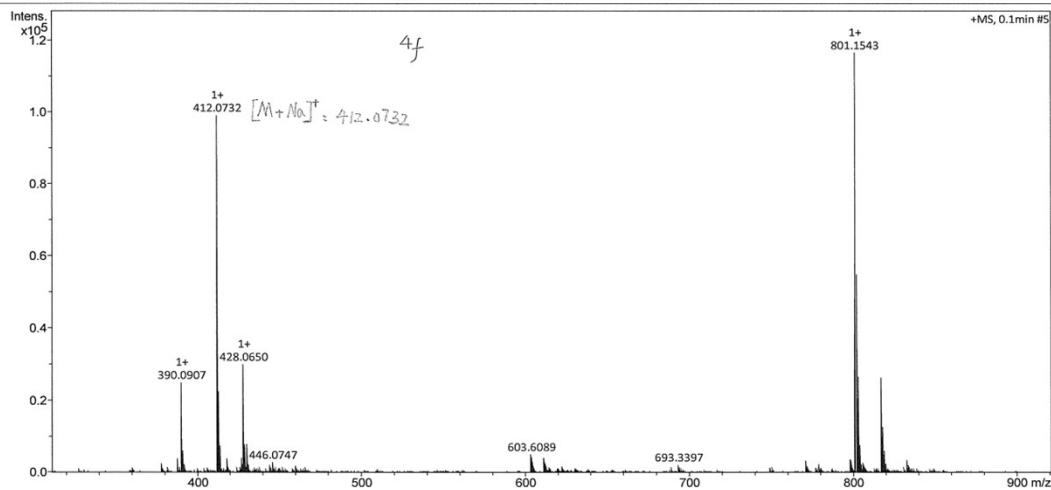


Figure 29 <sup>13</sup>C NMR of 4f

Display Report

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Comment			

Acquisition Parameter			
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		Set Nebulizer	0.3 Bar
		Set Dry Heater	180 °C
		Set Dry Gas	4.0 l/min
		Set Divert Valve	Waste



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Figure 30 HRMS of 4f



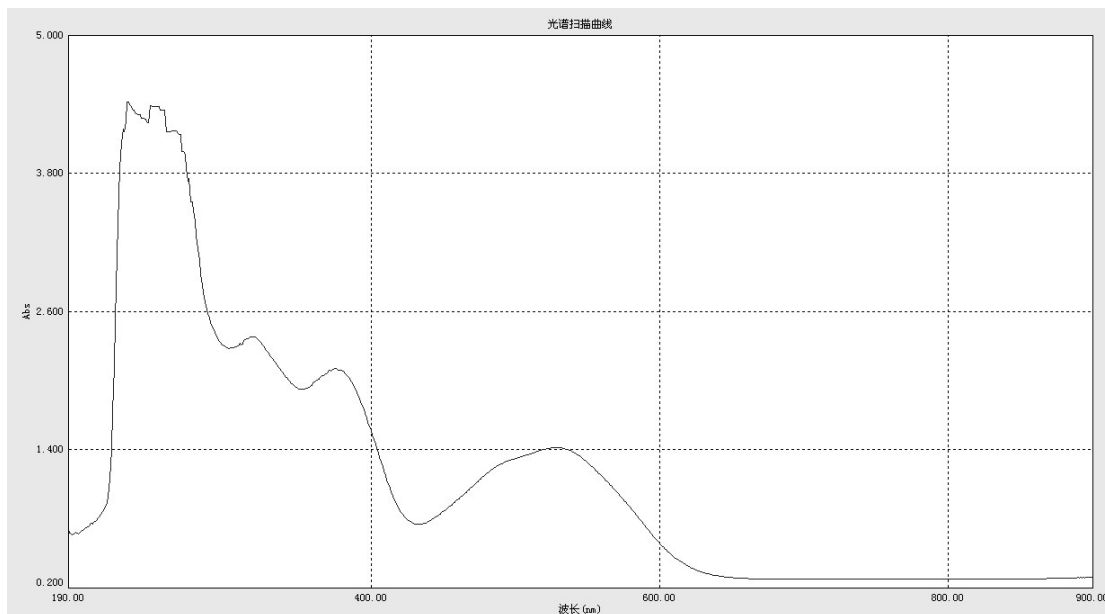


Figure 31 UV-vis of 4g

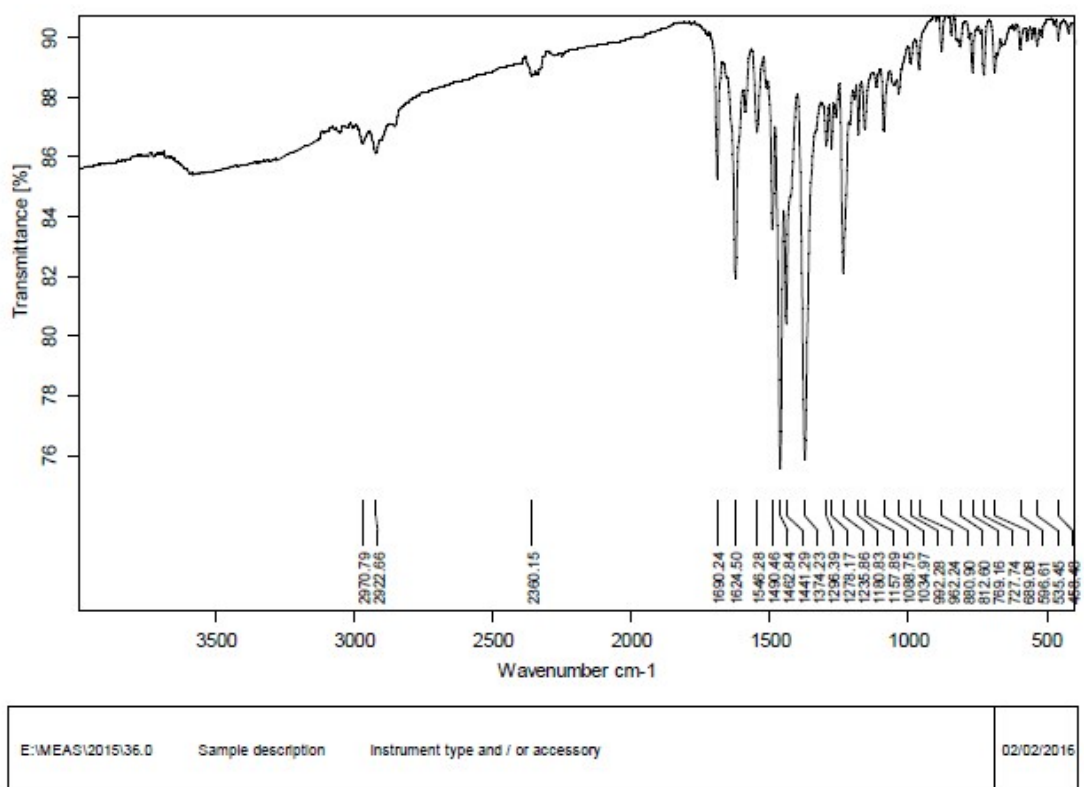


Figure 32 IR of 4g

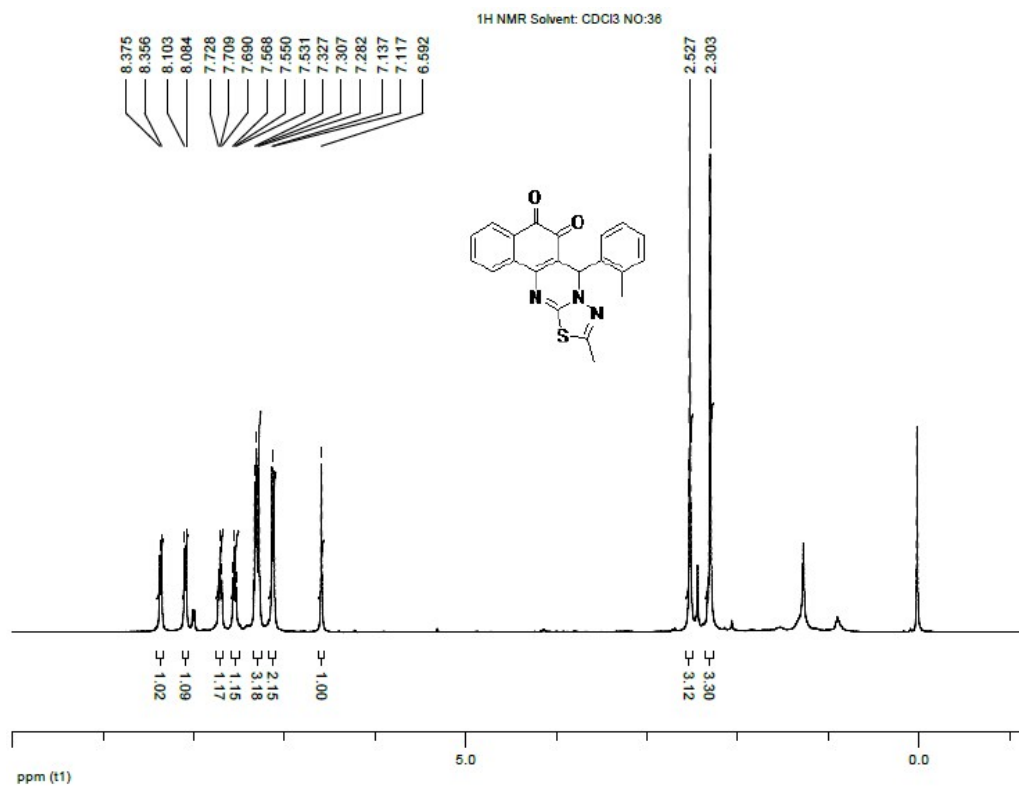


Figure 33 <sup>1</sup>H NMR of 4g

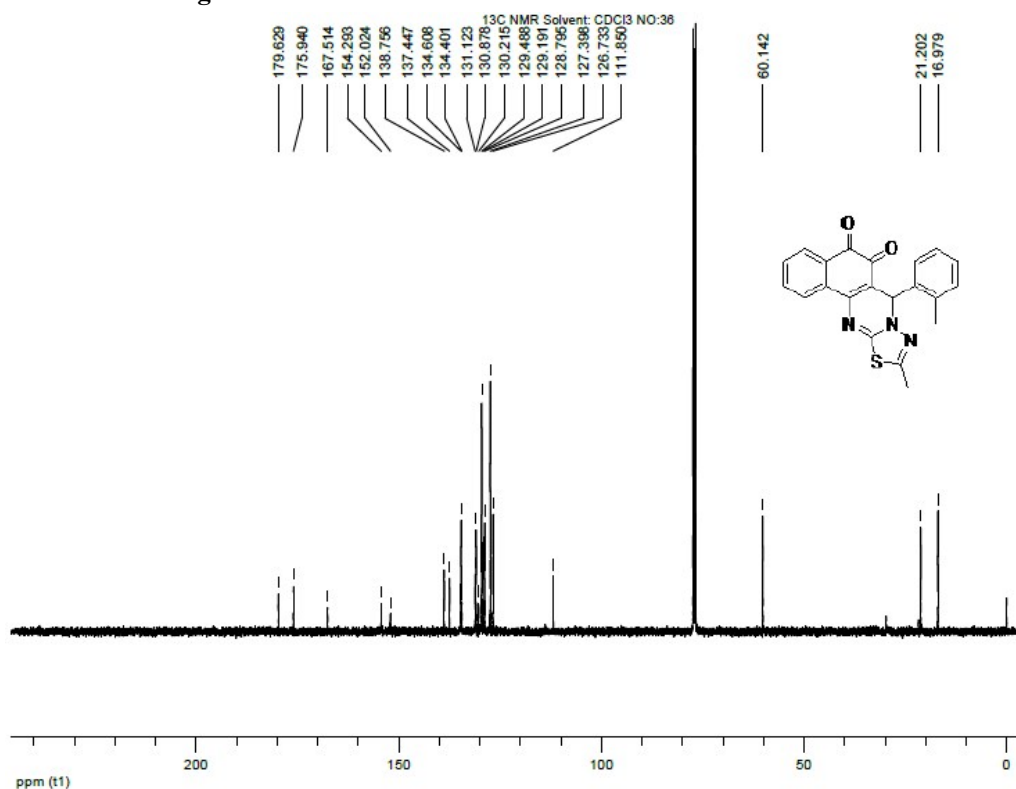
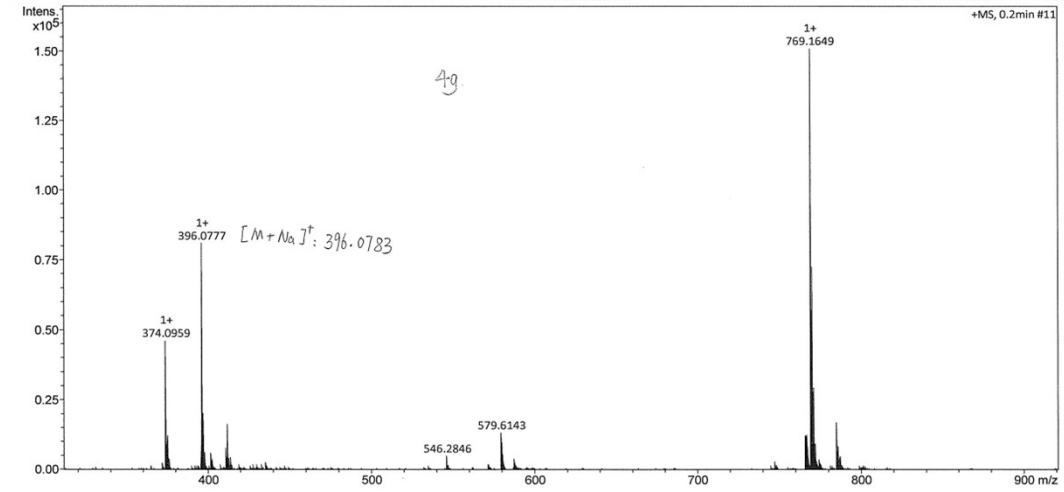


Figure 34 <sup>13</sup>C NMR of 4g

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Sample Name: w-36  
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Operator: zjx  
Instrument: micrOTOF-Q III 8228888.20494

**Acquisition Parameter**  
Source Type: ESI  
Focus: Not active  
Scan Begin: 50 m/z  
Scan End: 1000 m/z  
Ion Polarity: Positive  
Set Capillary: 4500 V  
Set End Plate Offset: -500 V  
Set Collision Cell RF: 120.0 Vpp  
Set Nebulizer: 0.3 Bar  
Set Dry Heater: 180 °C  
Set Dry Gas: 4.0 l/min  
Set Divert Valve: Waste



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Figure 35 HRMS of 4g

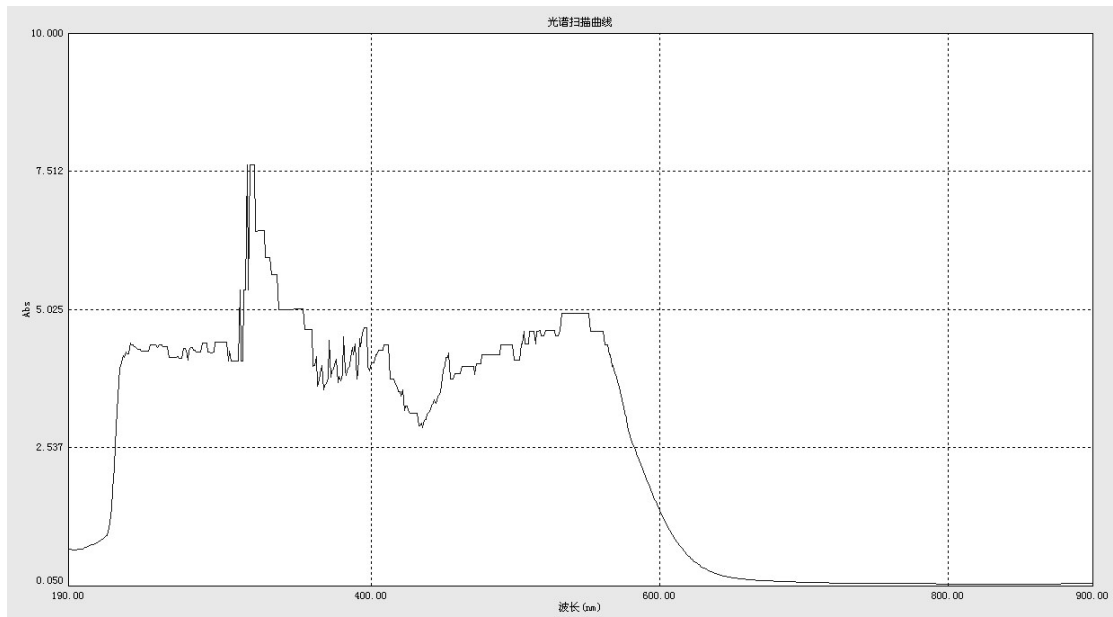


Figure 36 UV-vis of 4h

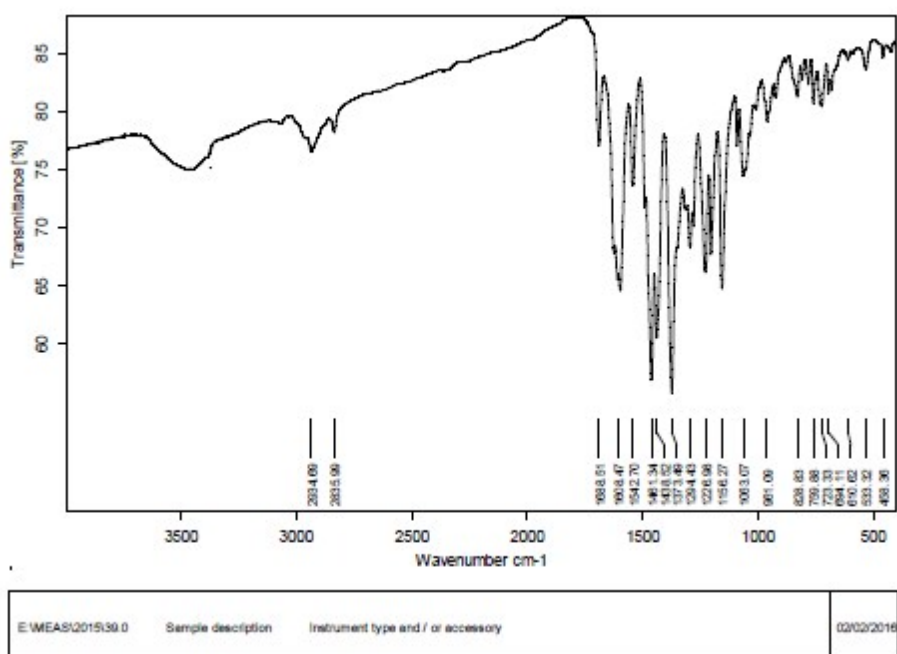


Figure 37 IR of 4h

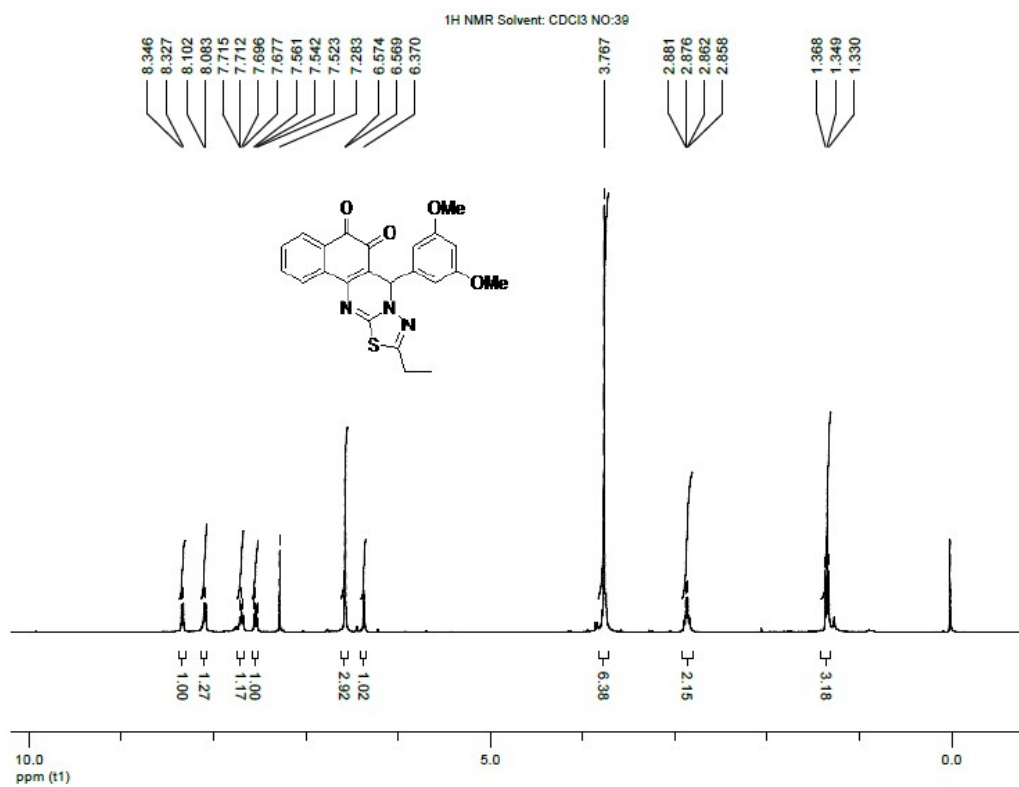


Figure 38 <sup>1</sup>H NMR of 4h

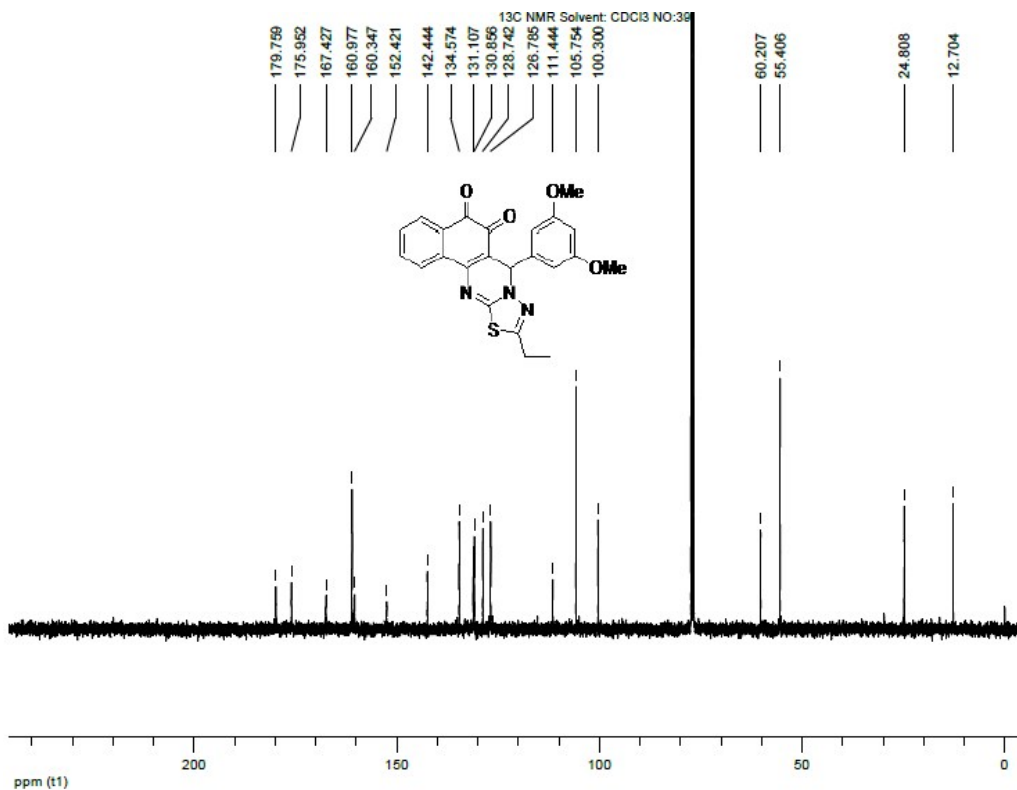


Figure 39 <sup>13</sup>C NMR of 4h

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Sample Name	w-39				
Comment					
Acquisition Parameter					
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Scan End	1000 m/z	Set Collision Cell RF	120.0 Vpp	Set Divert Valve	Waste

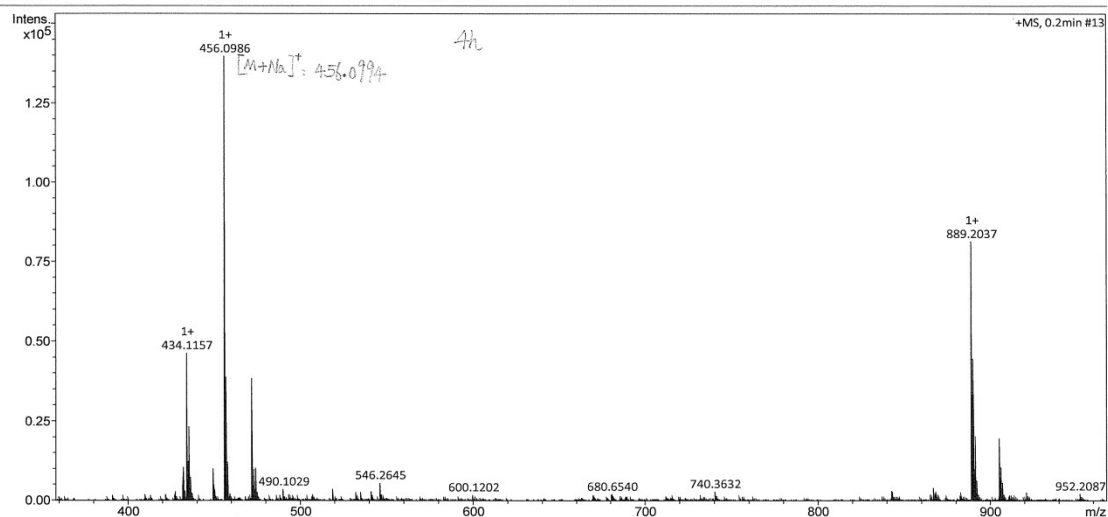


Figure 40 HRMS of 4h

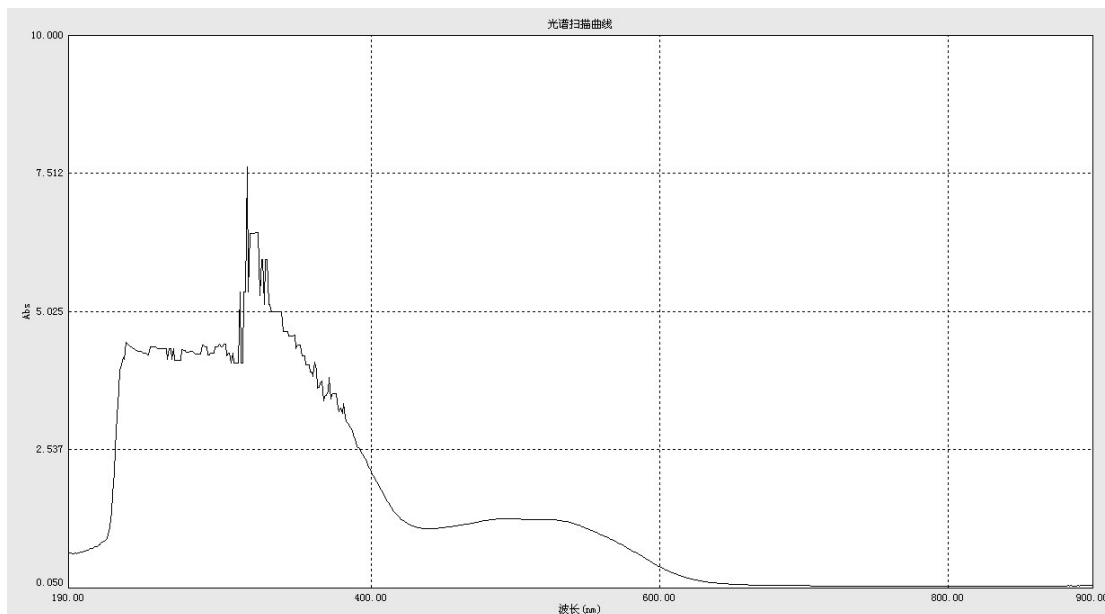


Figure 41 UV-vis of 4i

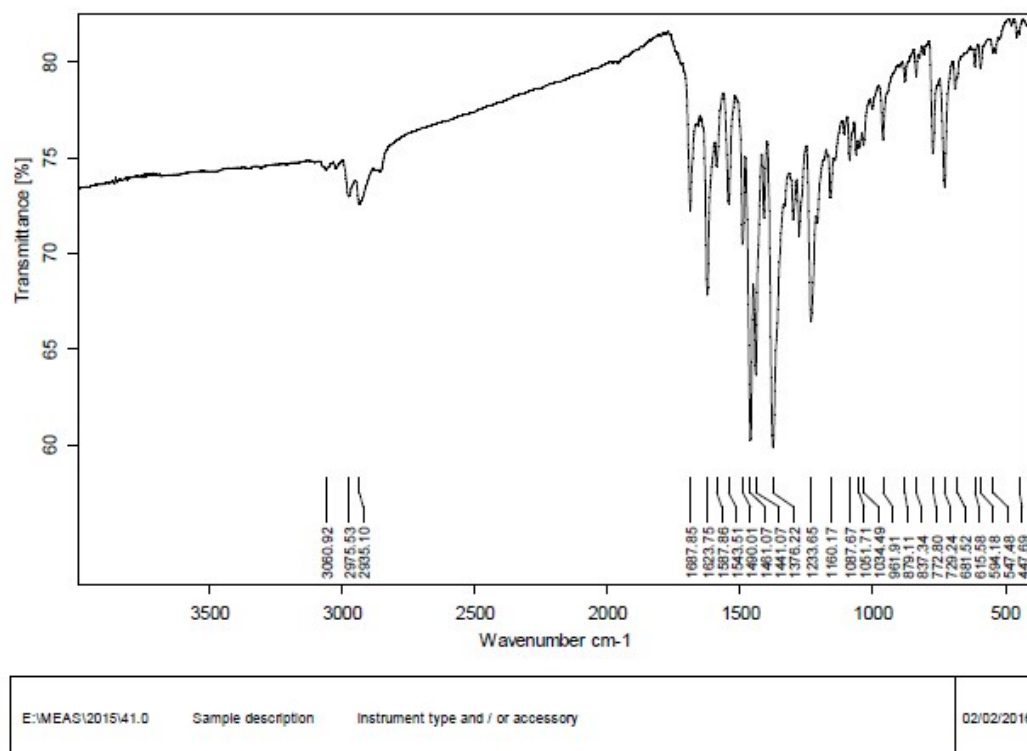


Figure 42 IR of 4i

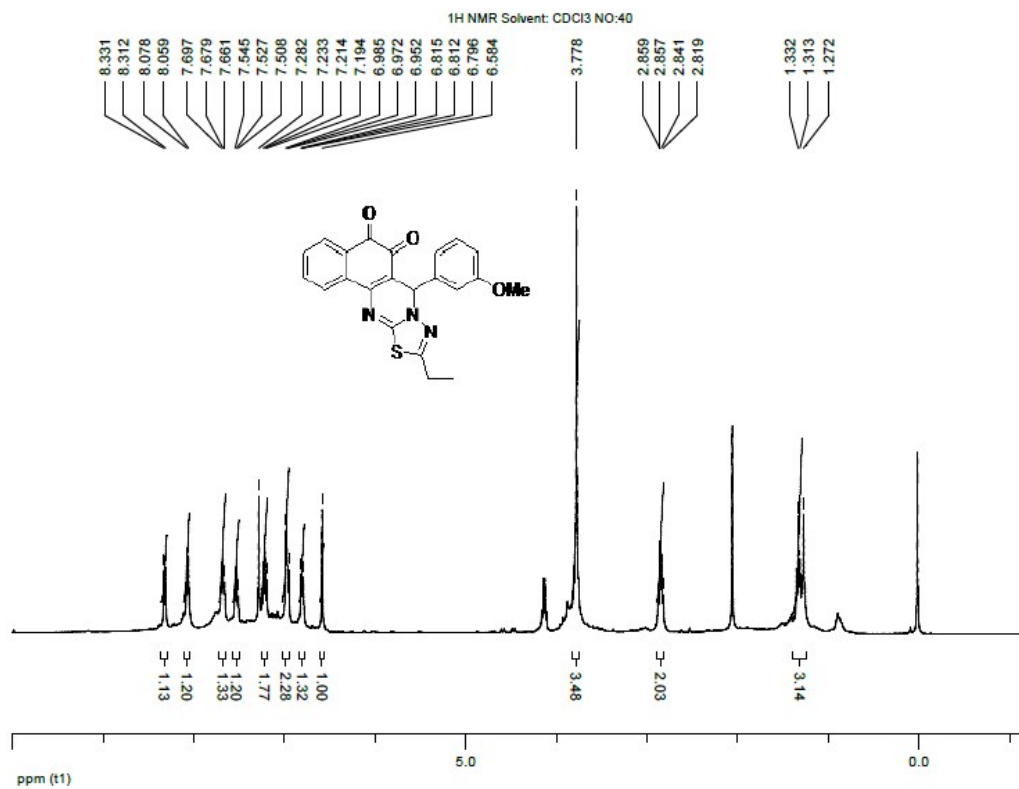


Figure 43  $^1\text{H}$  NMR of 4i

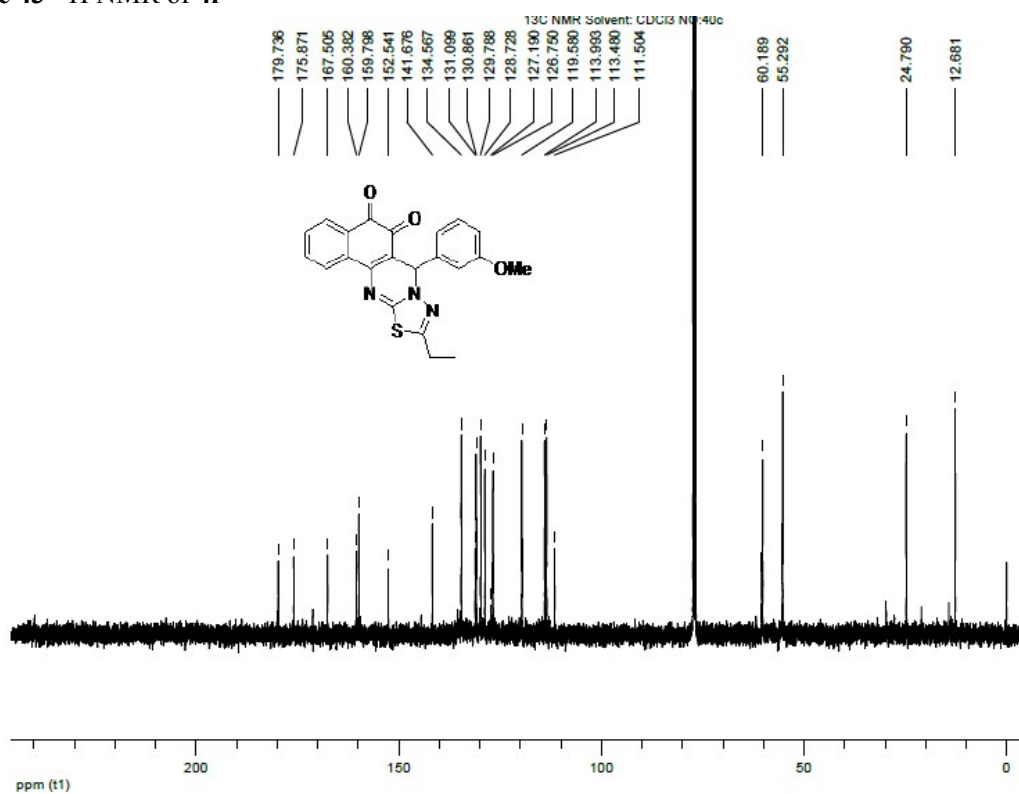
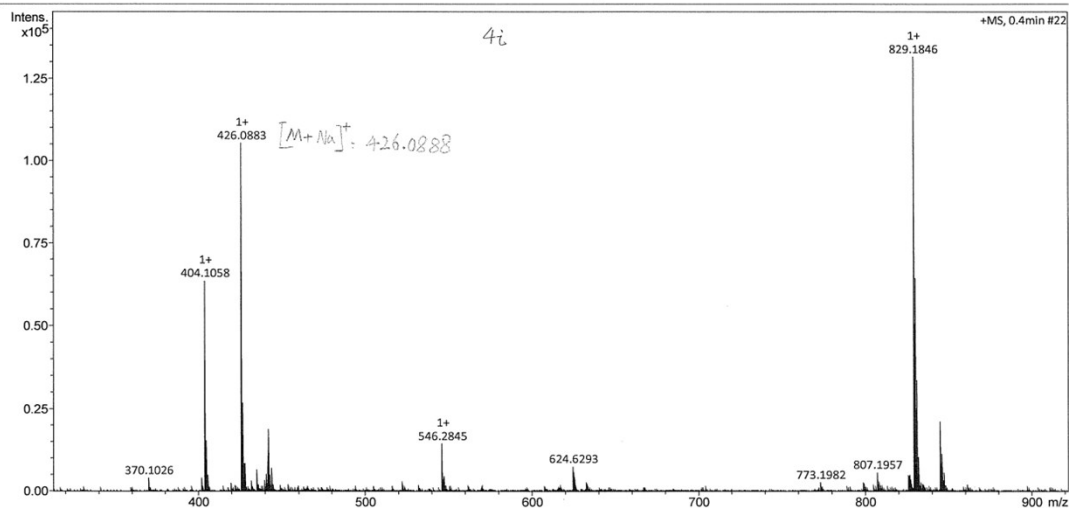


Figure 44  $^{13}\text{C}$  NMR of 4i

## Display Report

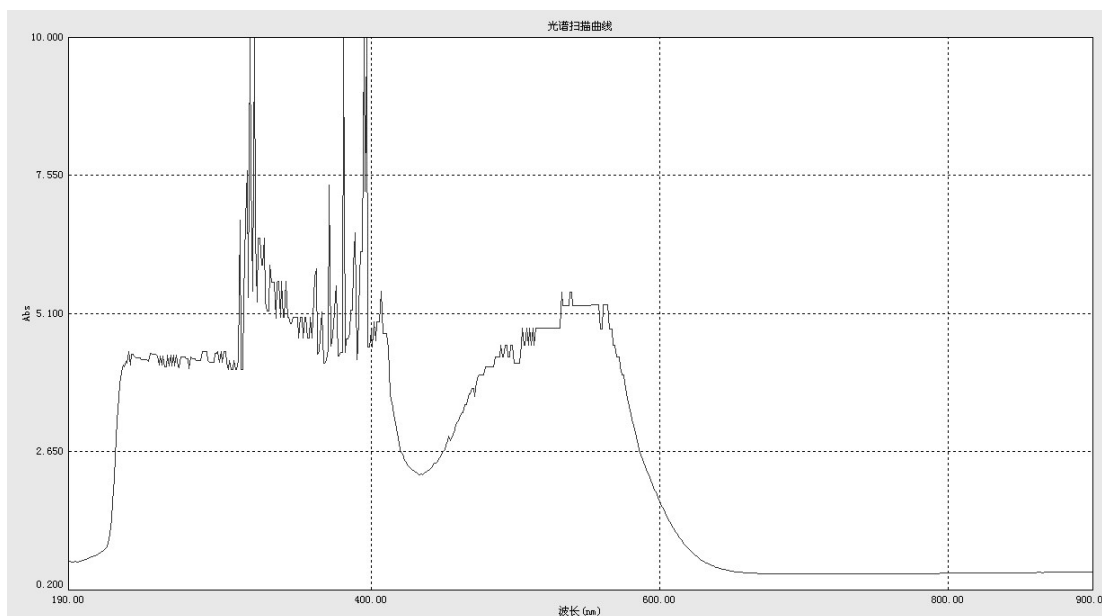
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Scan End	1000 m/z	Set Collision Cell RF	120.0 Vpp	Set Divert Valve	Waste



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**Figure 45** HRMS of 4i



**Figure 46** UV-vis of 4j



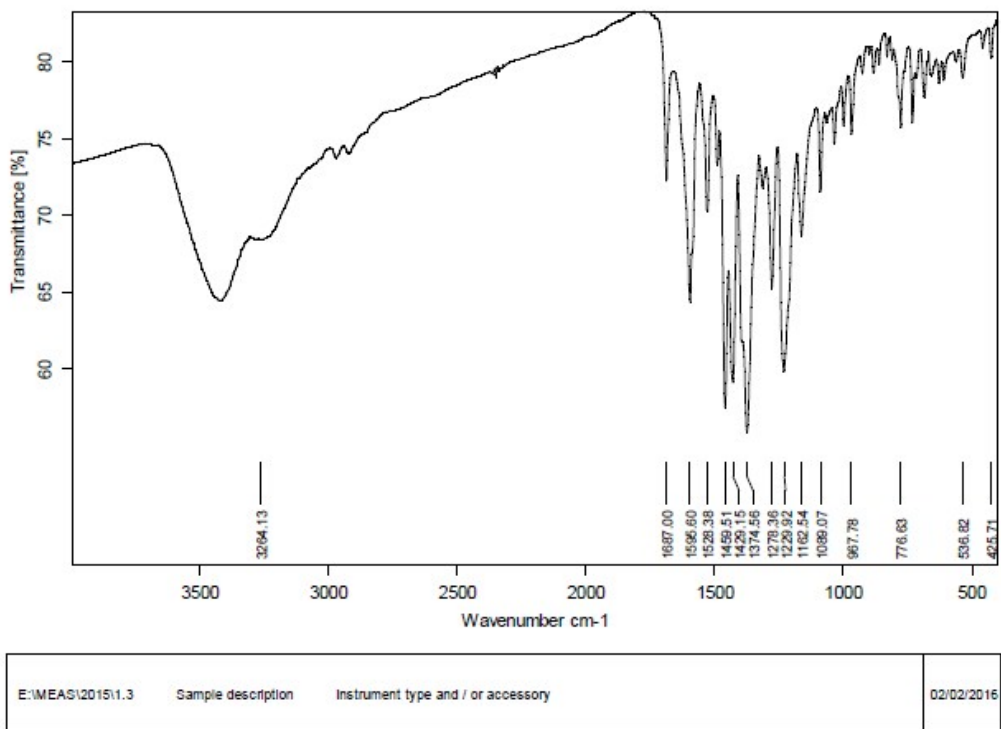


Figure 47 IR of 4j

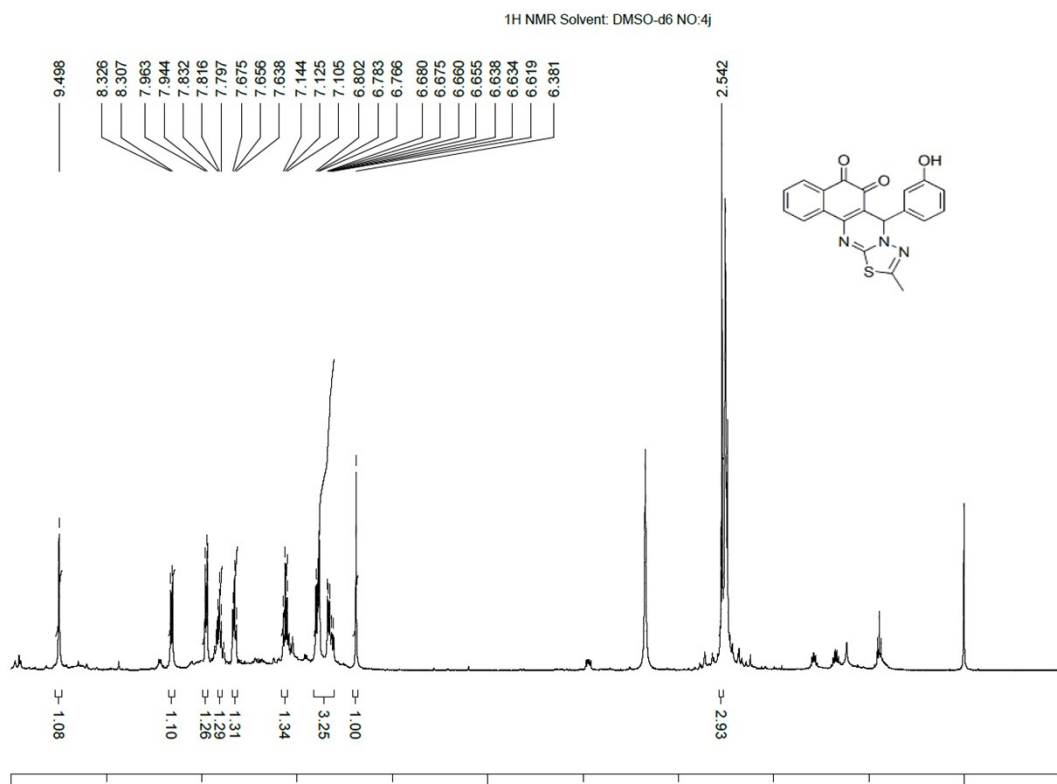


Figure 48 <sup>1</sup>H NMR of 4j

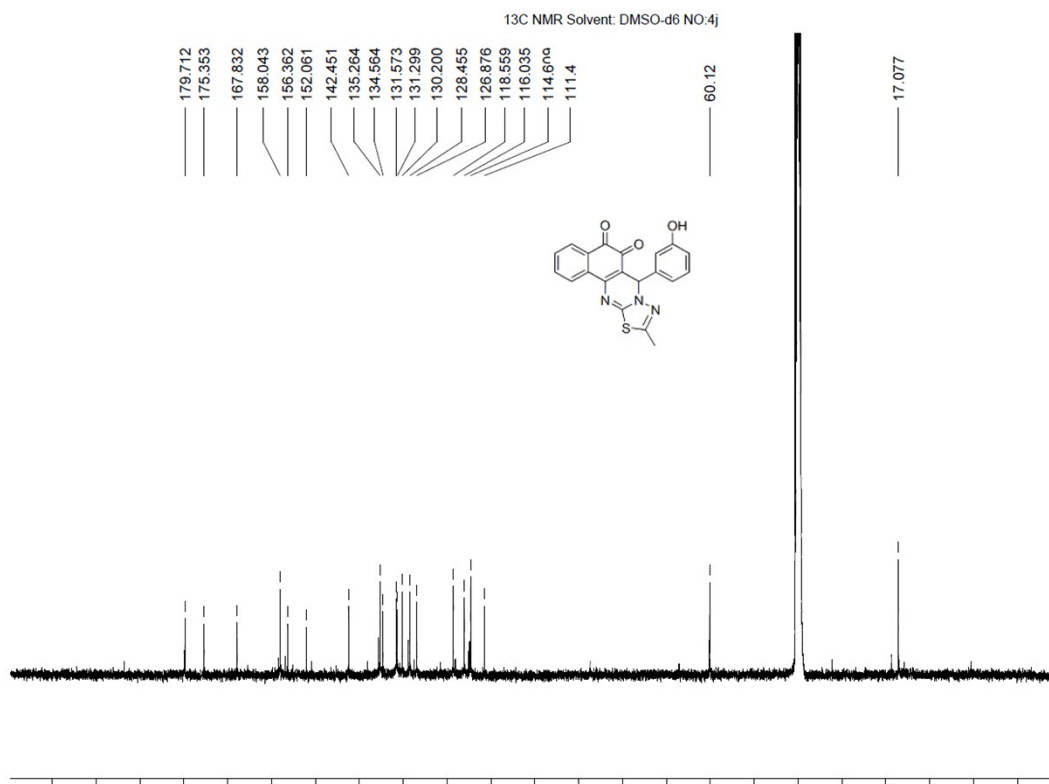


Figure 49 <sup>13</sup>C NMR of 4j

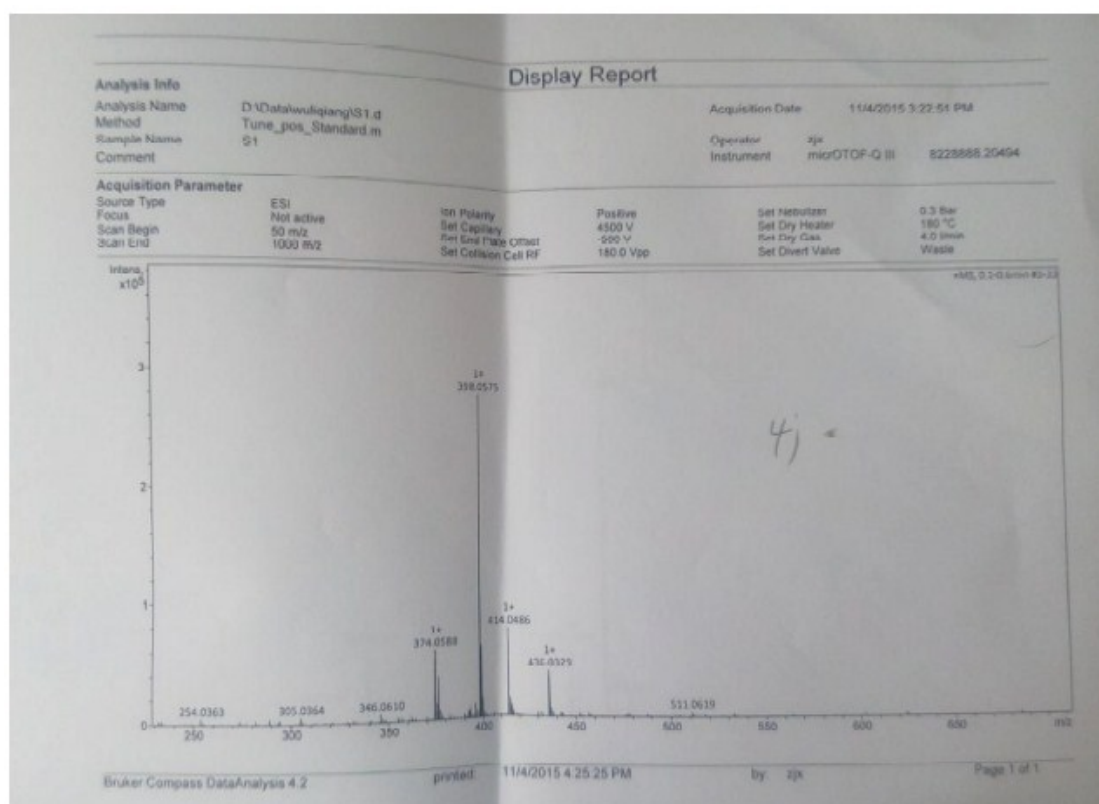


Figure 50 HRMS of 4j

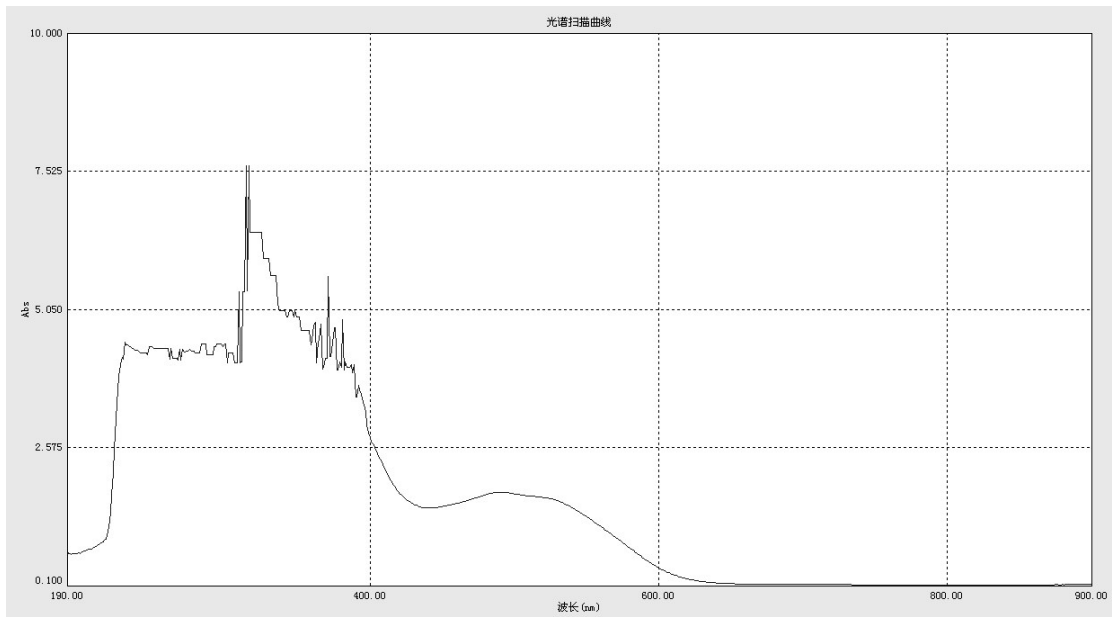


Figure 51 UV-vis of 4k

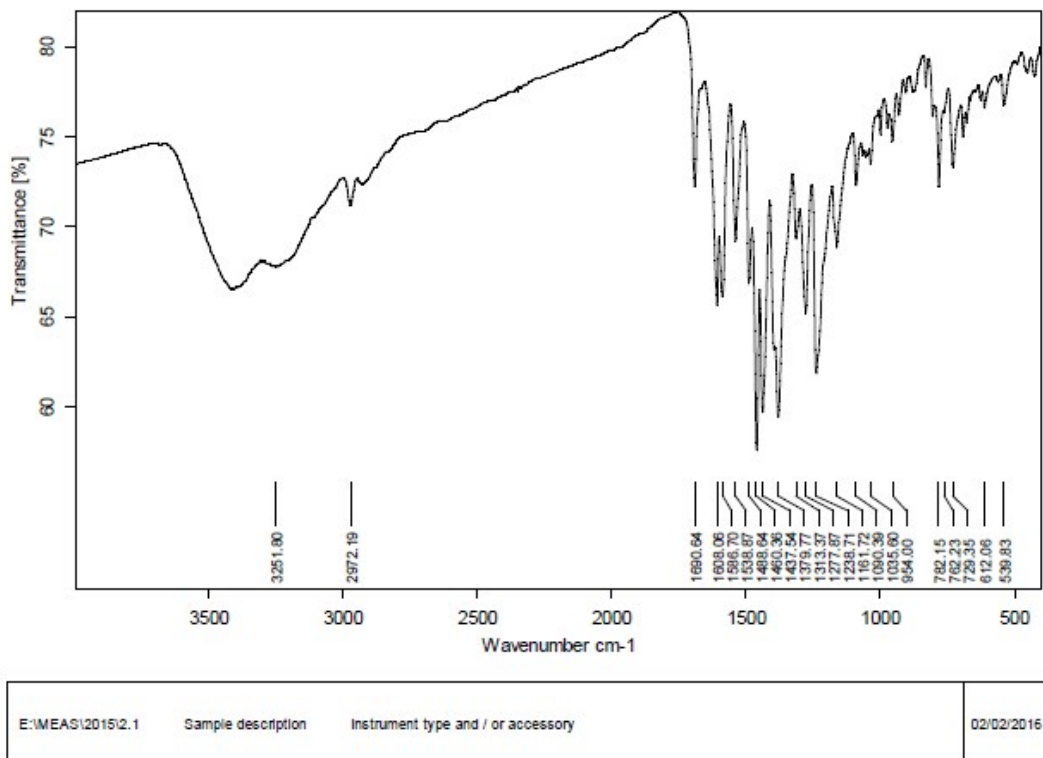


Figure 52 IRof 4k

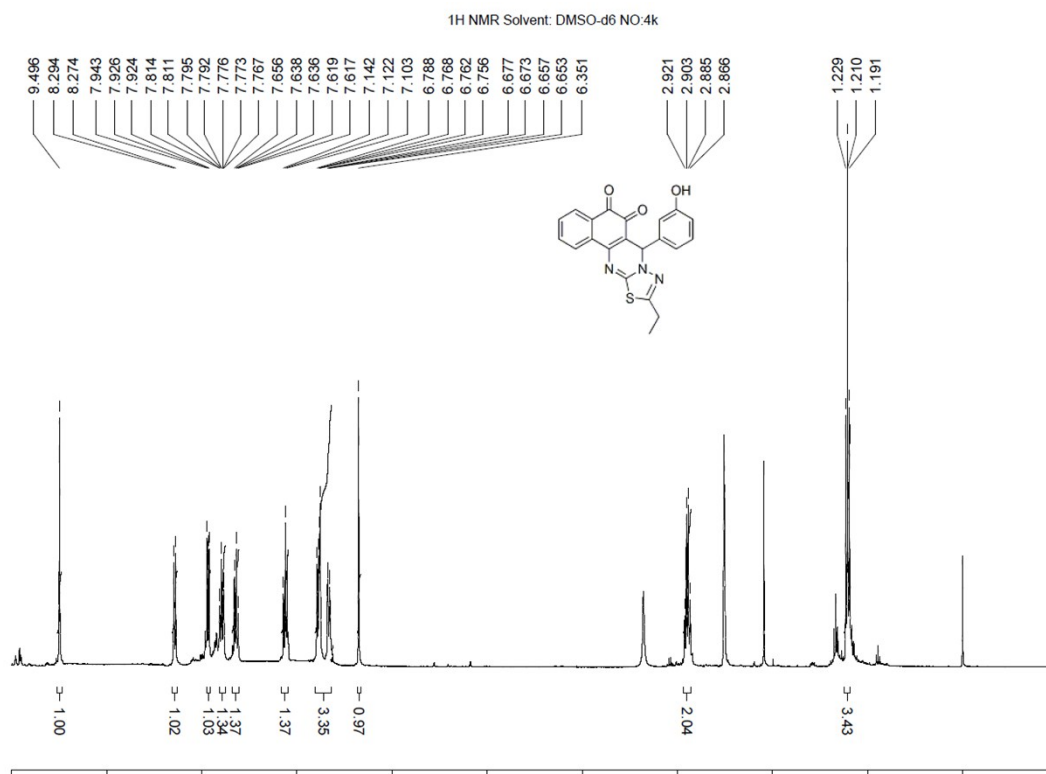


Figure 53 <sup>1</sup>H NMR of 4k

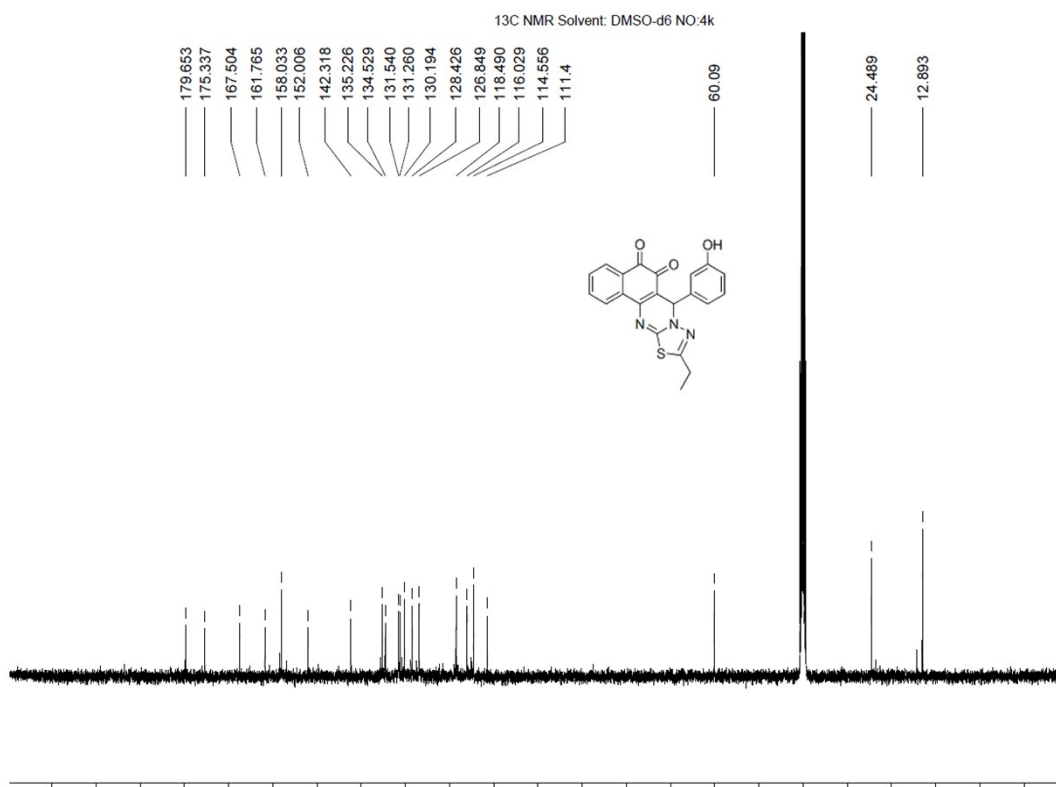
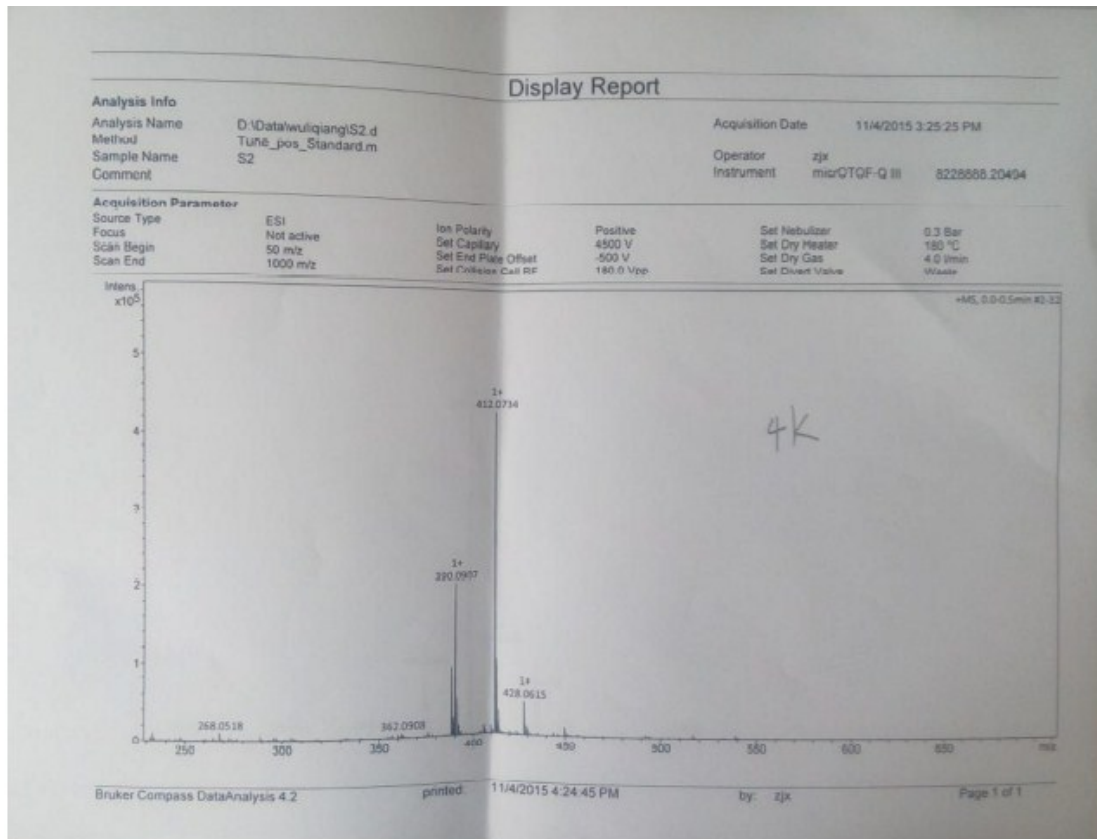
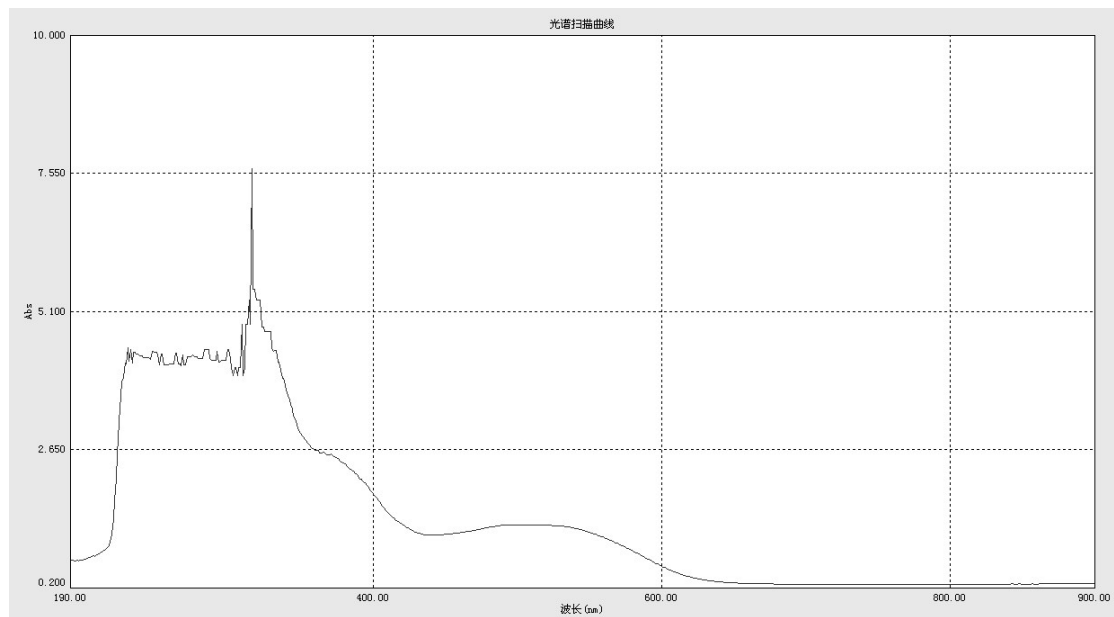


Figure 54 <sup>13</sup>C NMR of 4k



**Figure 55** HRMS of 4k



**Figure 56** UV-vis of 4l

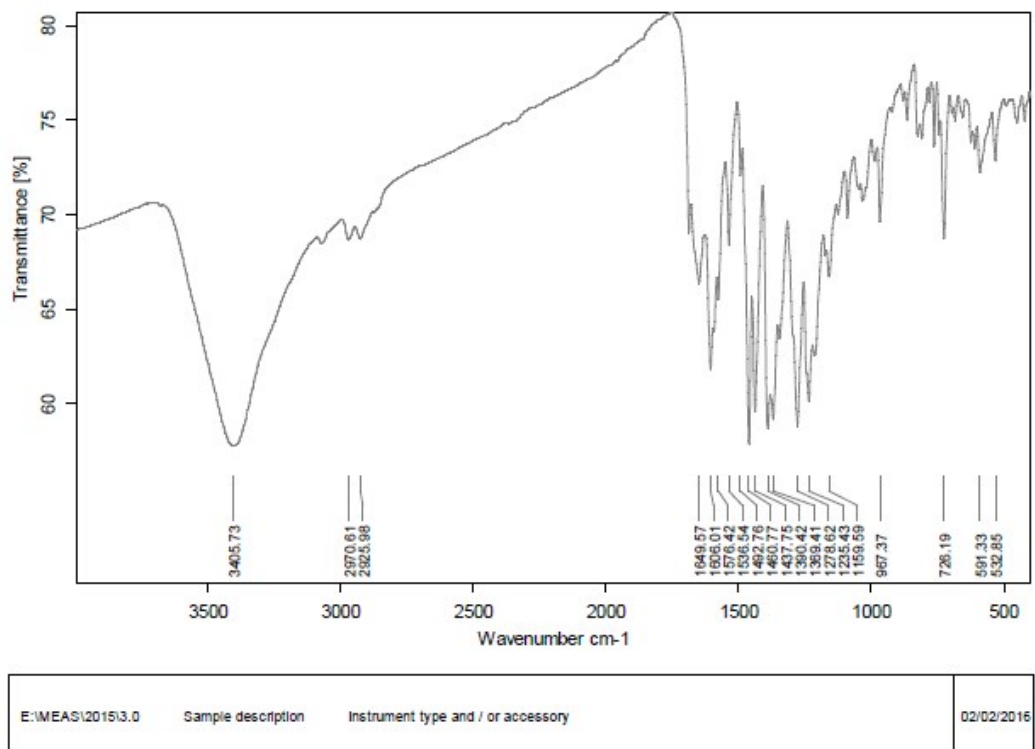


Figure 57 IR of 41

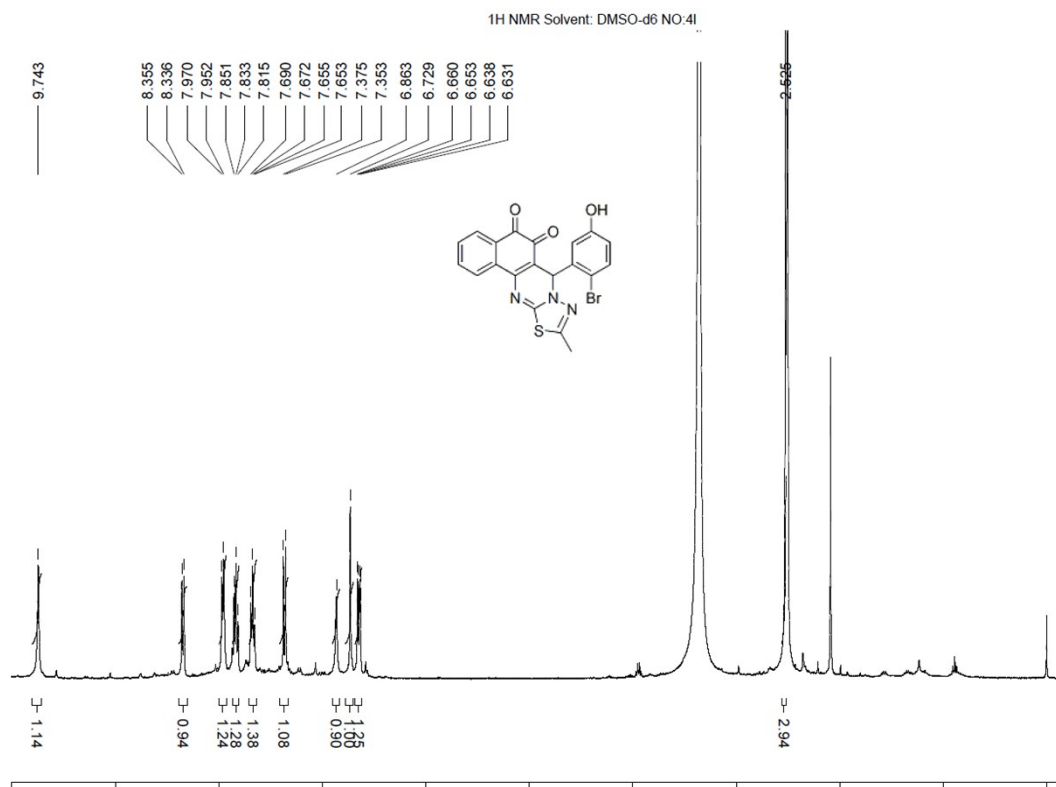


Figure 58 <sup>1</sup>H NMR of 41

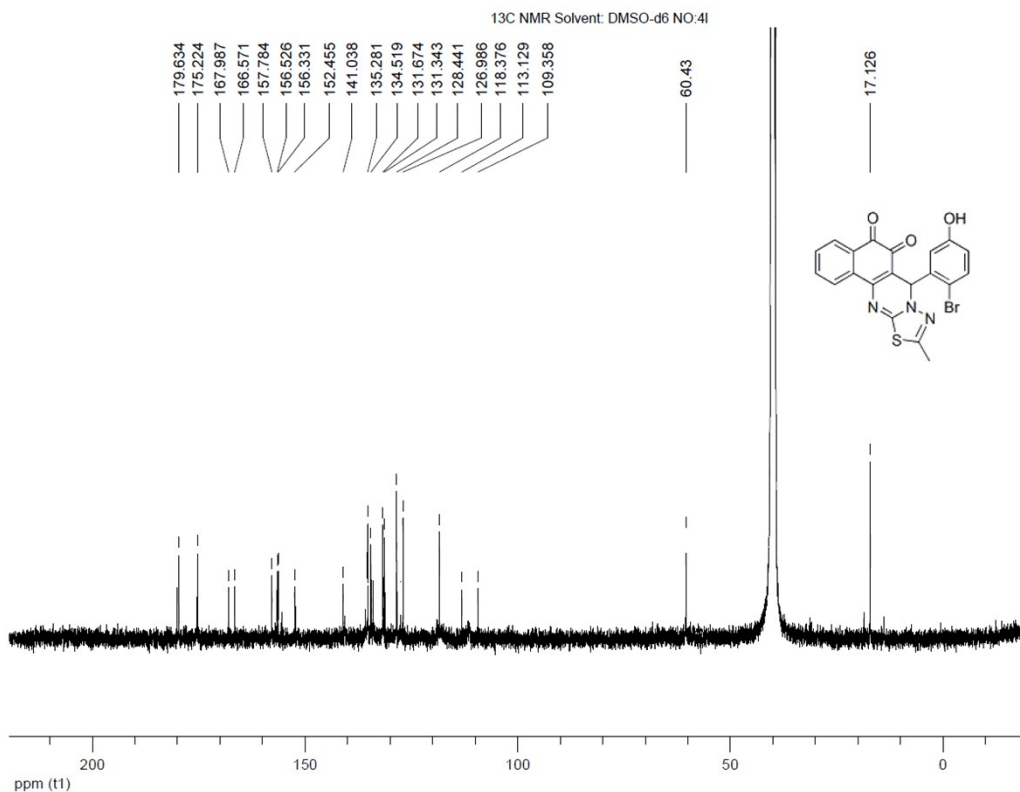


Figure 59 <sup>13</sup>C NMR of 4l

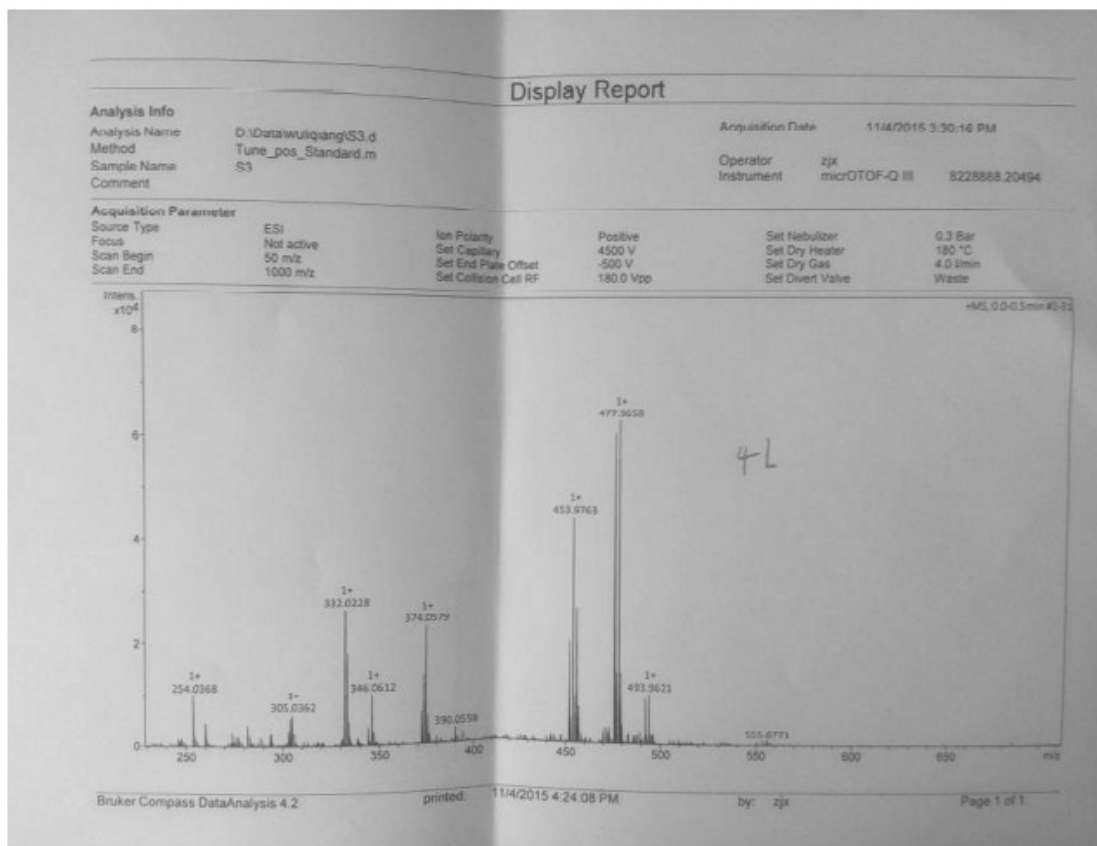


Figure 60 HRMS of 4l

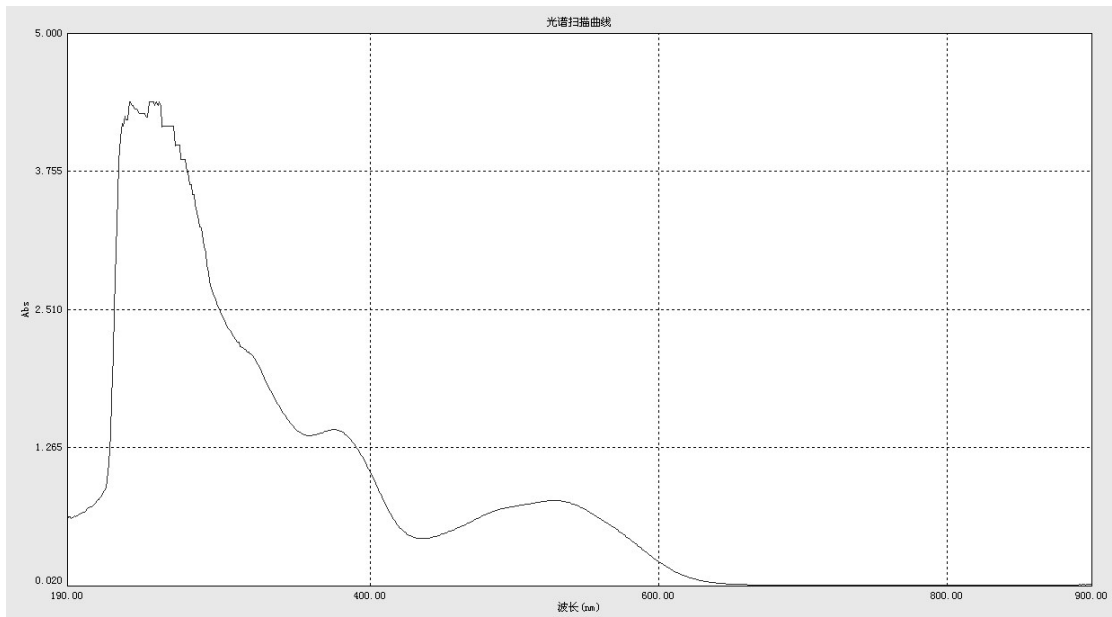


Figure 61 UV-vis of 4m

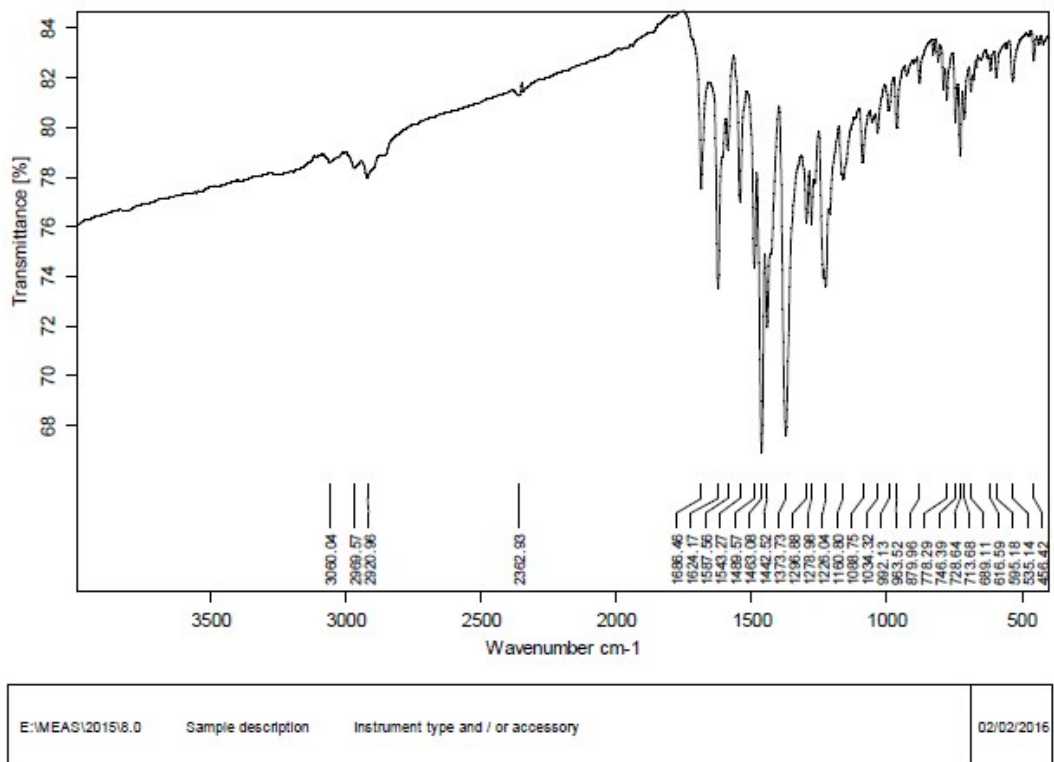


Figure 62 IR of 4m



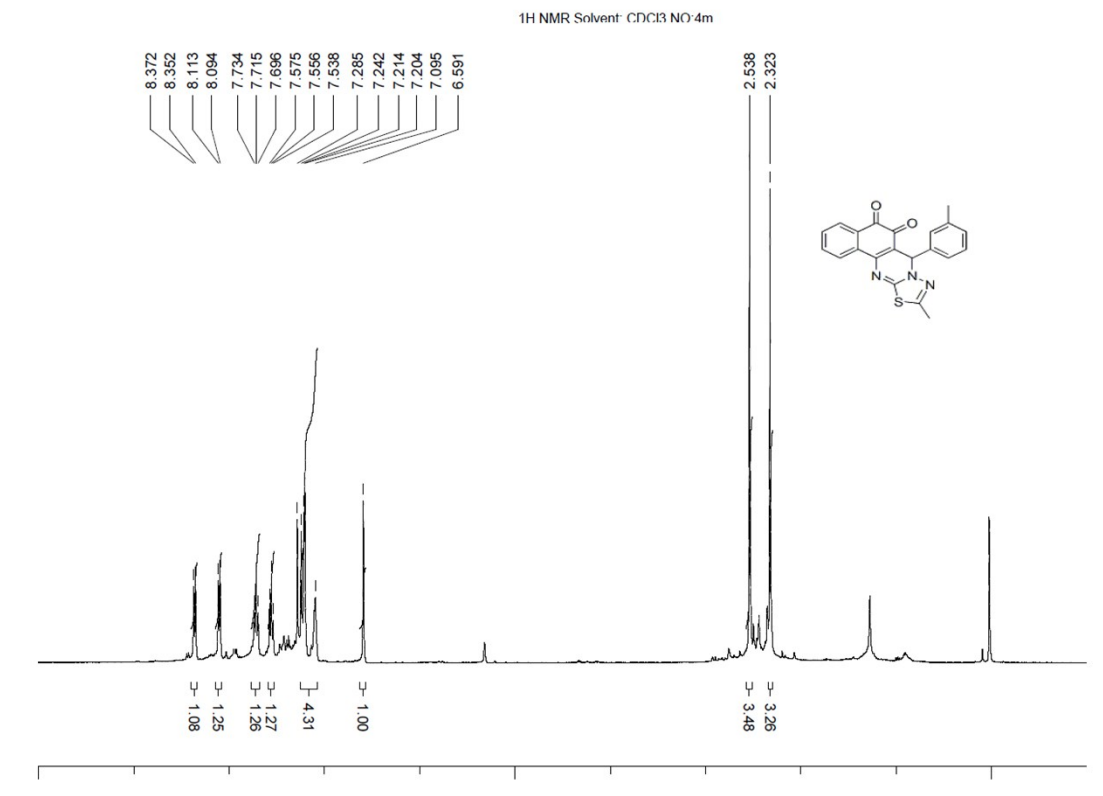


Figure 63  $^1\text{H}$  NMR of 4m

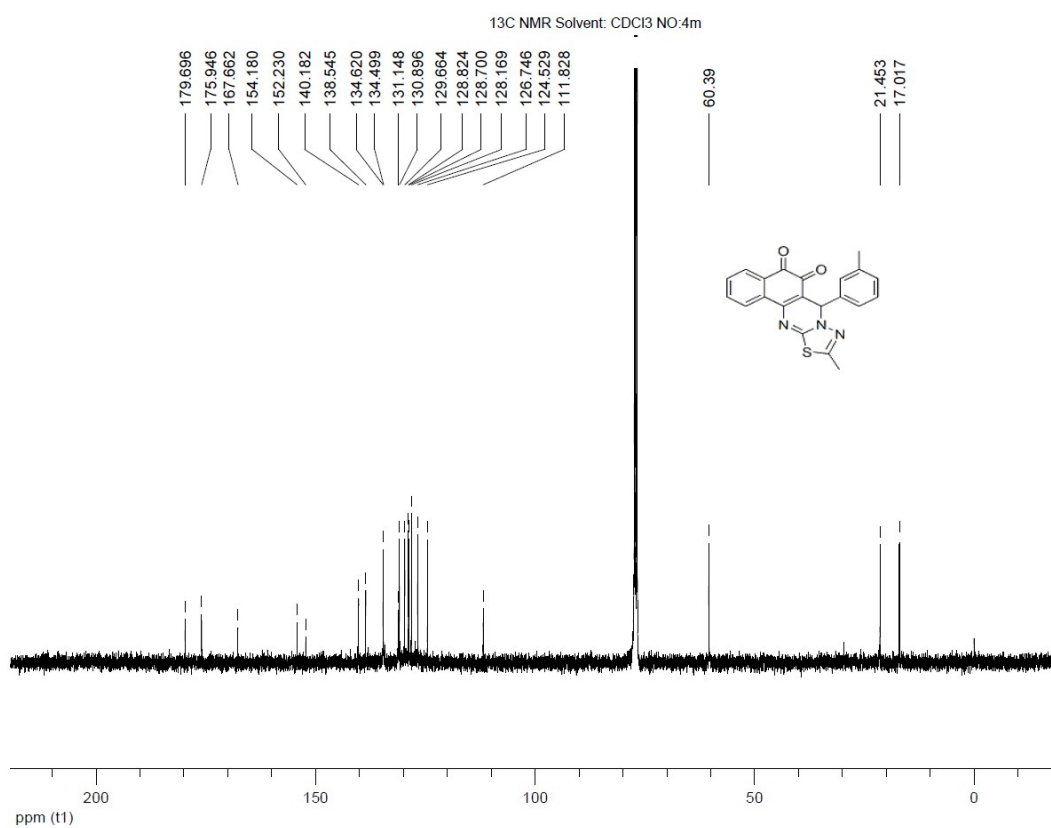
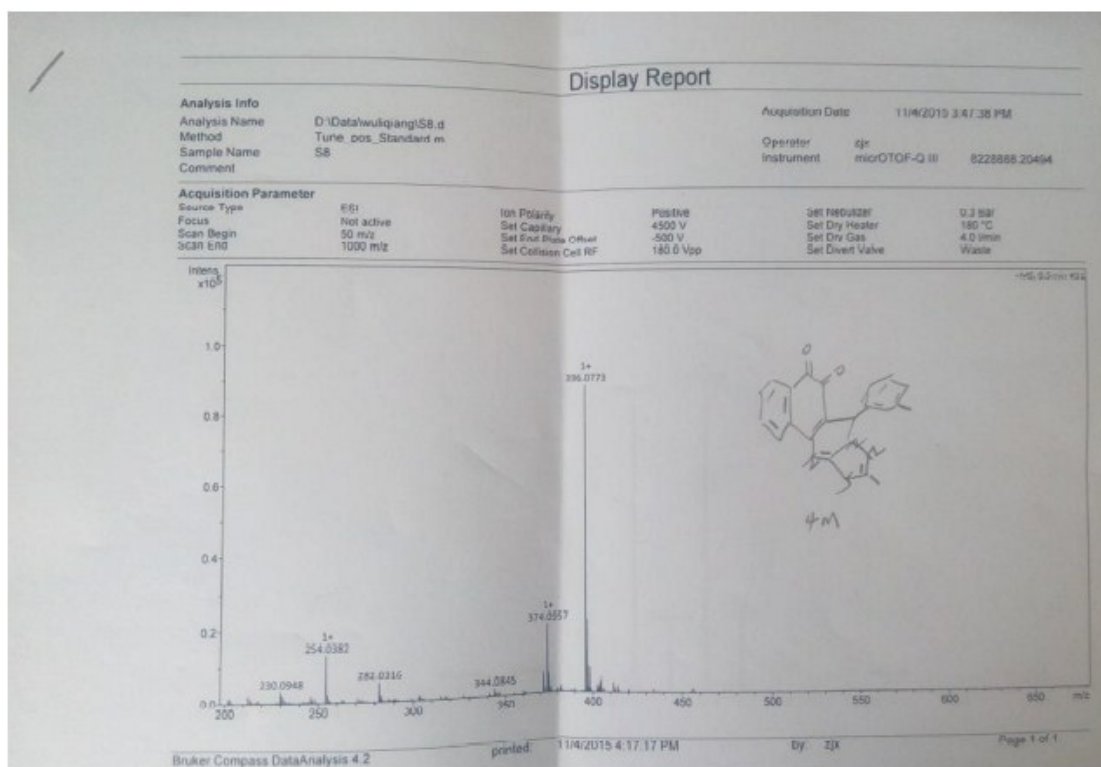
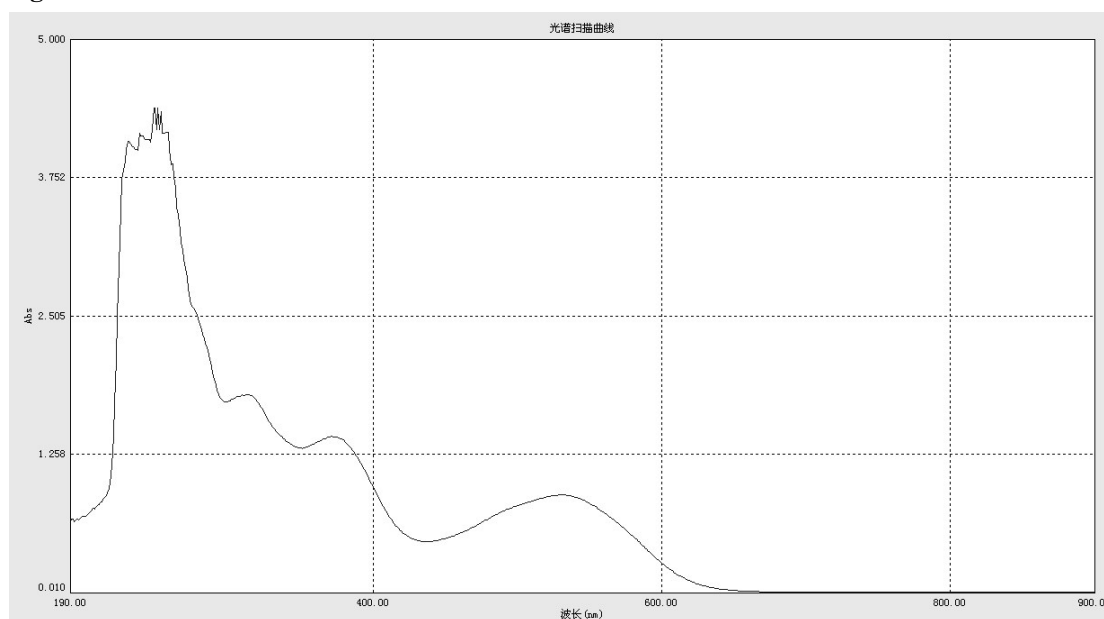


Figure 64  $^{13}\text{C}$  NMR of 4m



**Figure 65** HRMS of **4m**



**Figure 66** UV-vis of **4n**

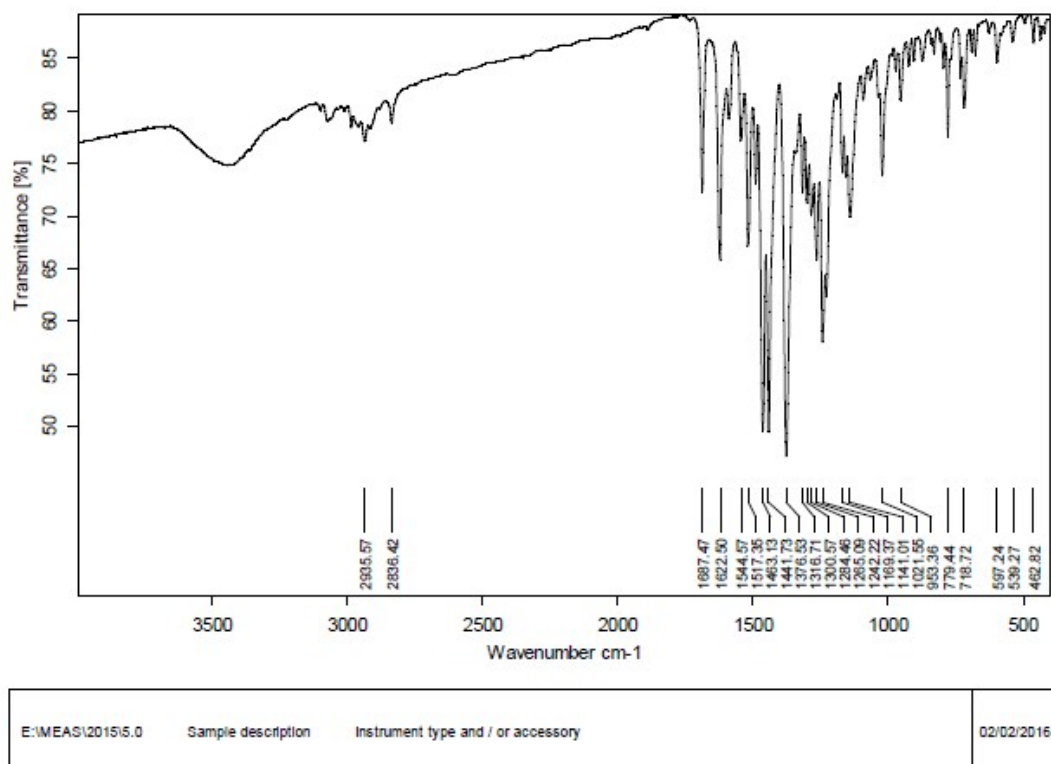


Figure 67 IR of 4n

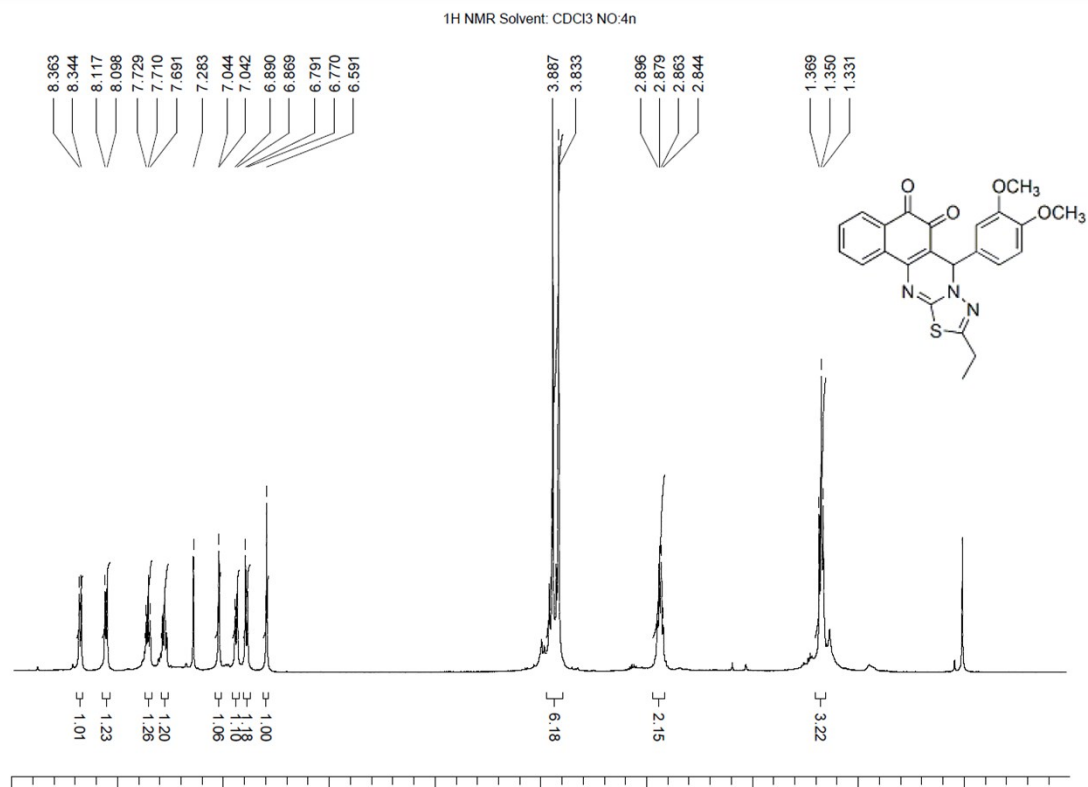


Figure 68 <sup>1</sup>H NMR of 4n

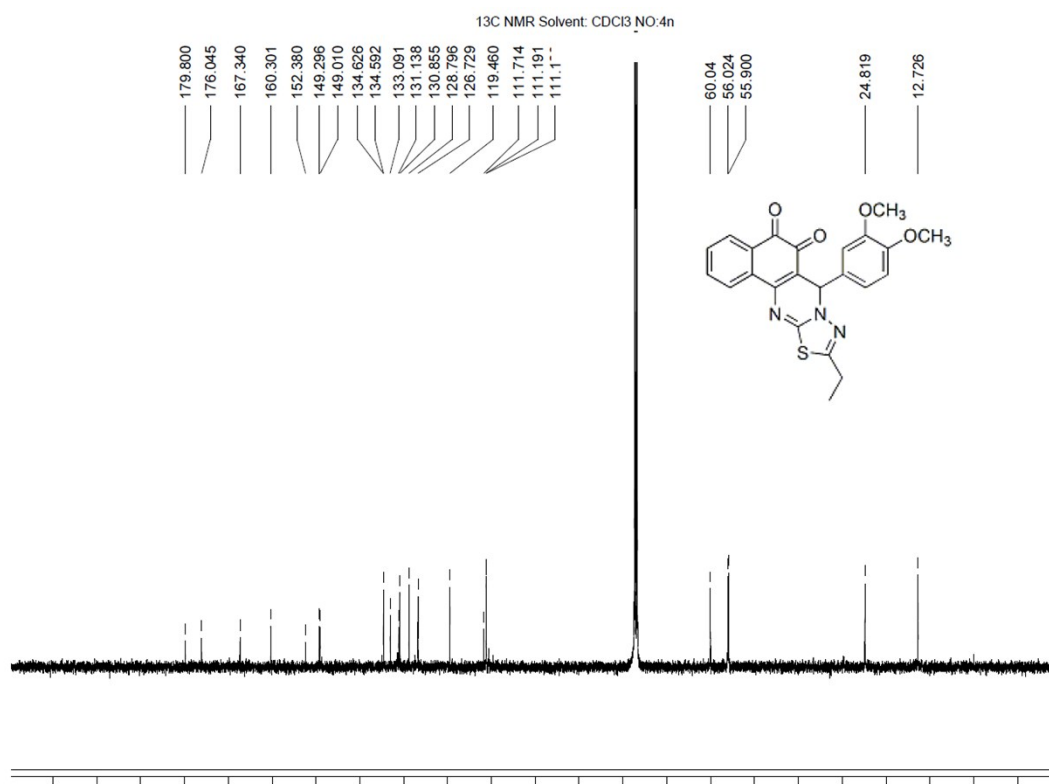


Figure 69  $^{13}\text{C}$  NMR of 4n

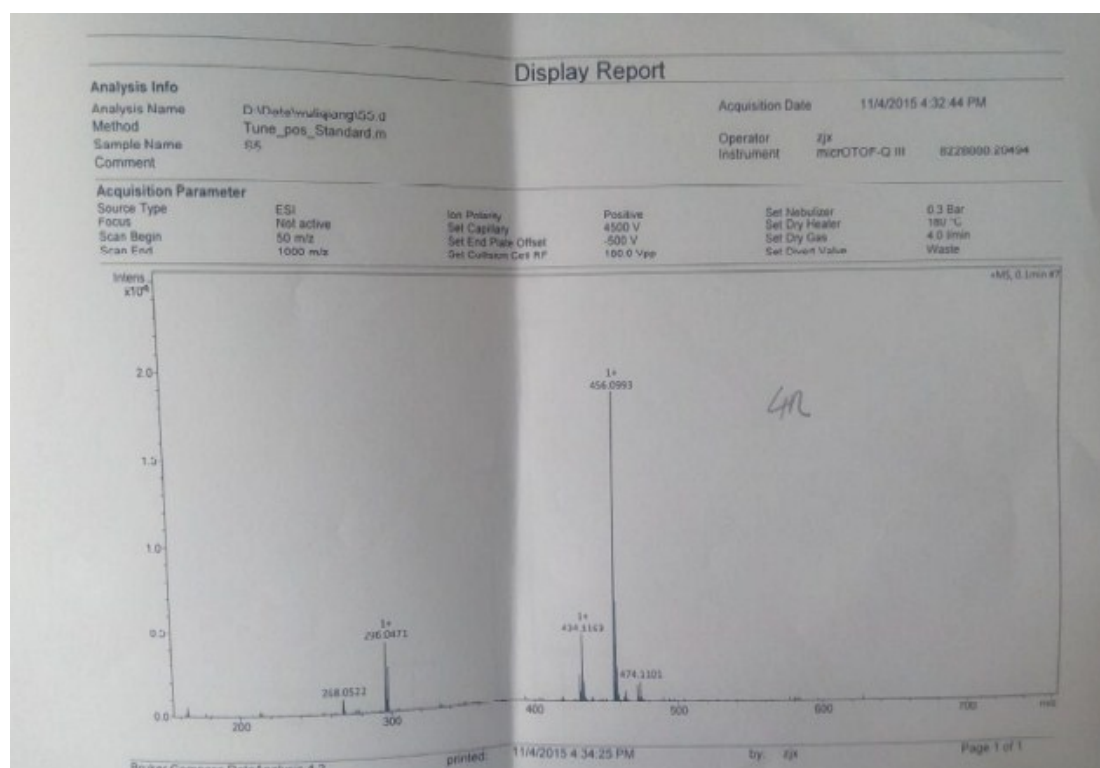


Figure 70 HRMS of 4n

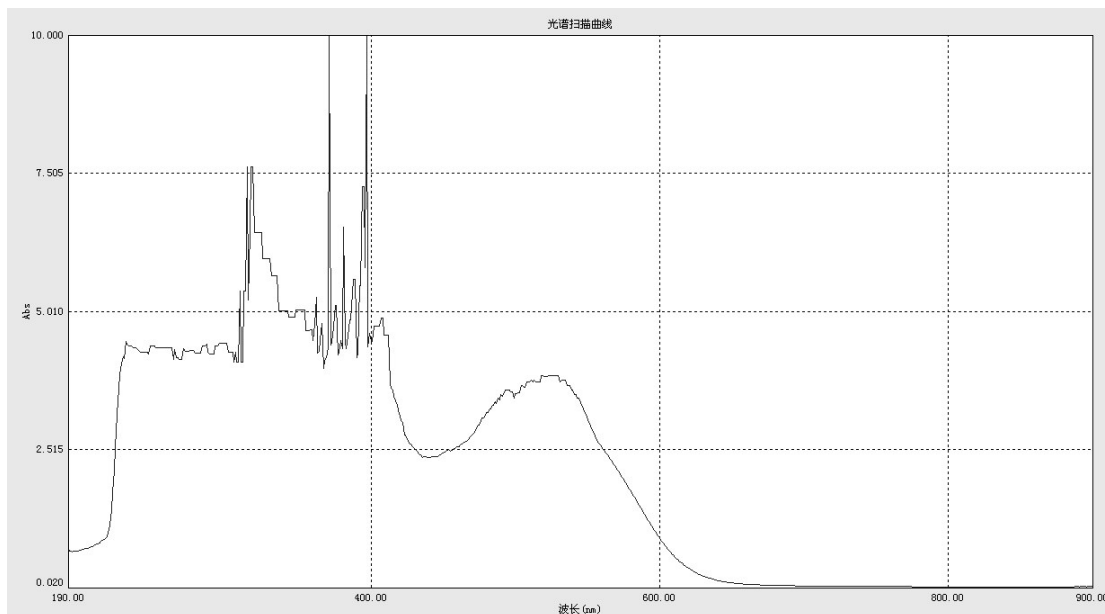


Figure 71 UV-vis of 4o

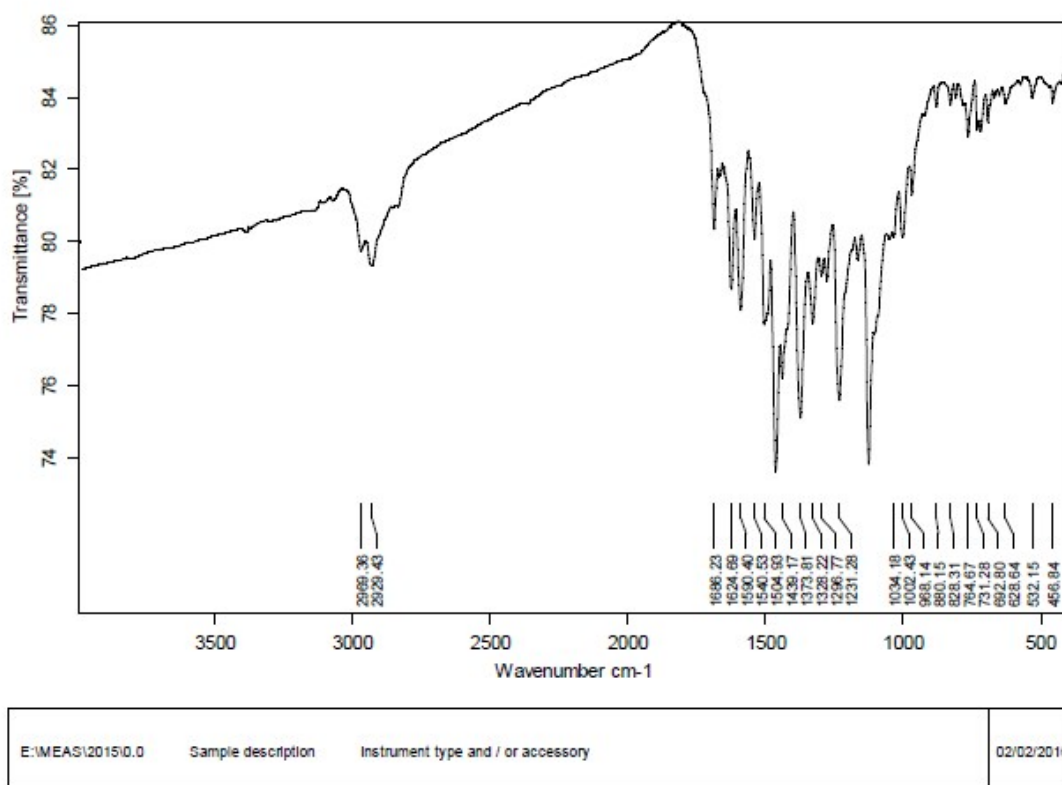


Figure 72 IR of 4o

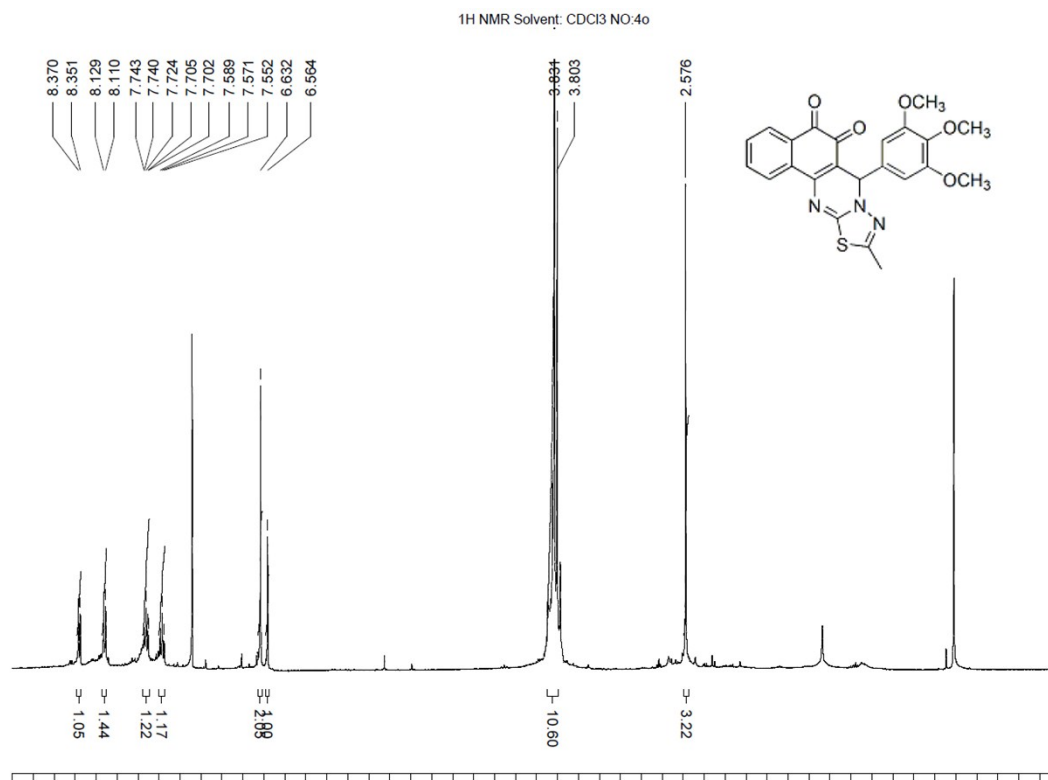


Figure 73  $^1\text{H}$  NMR of 4o

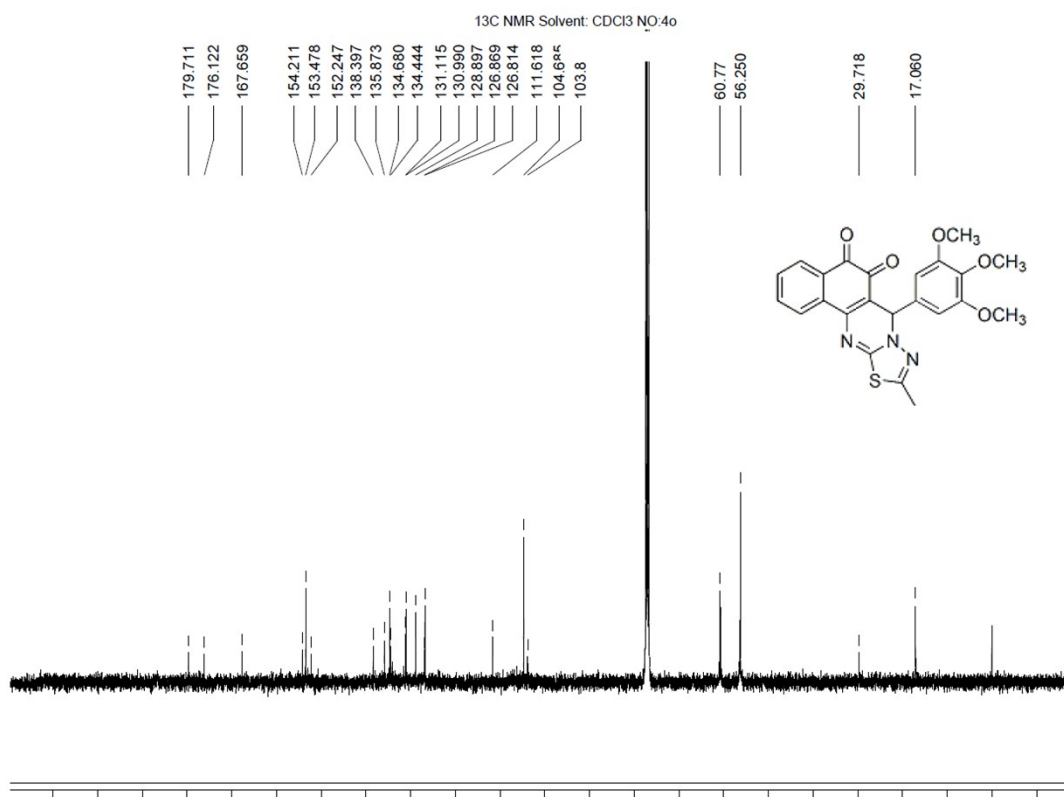
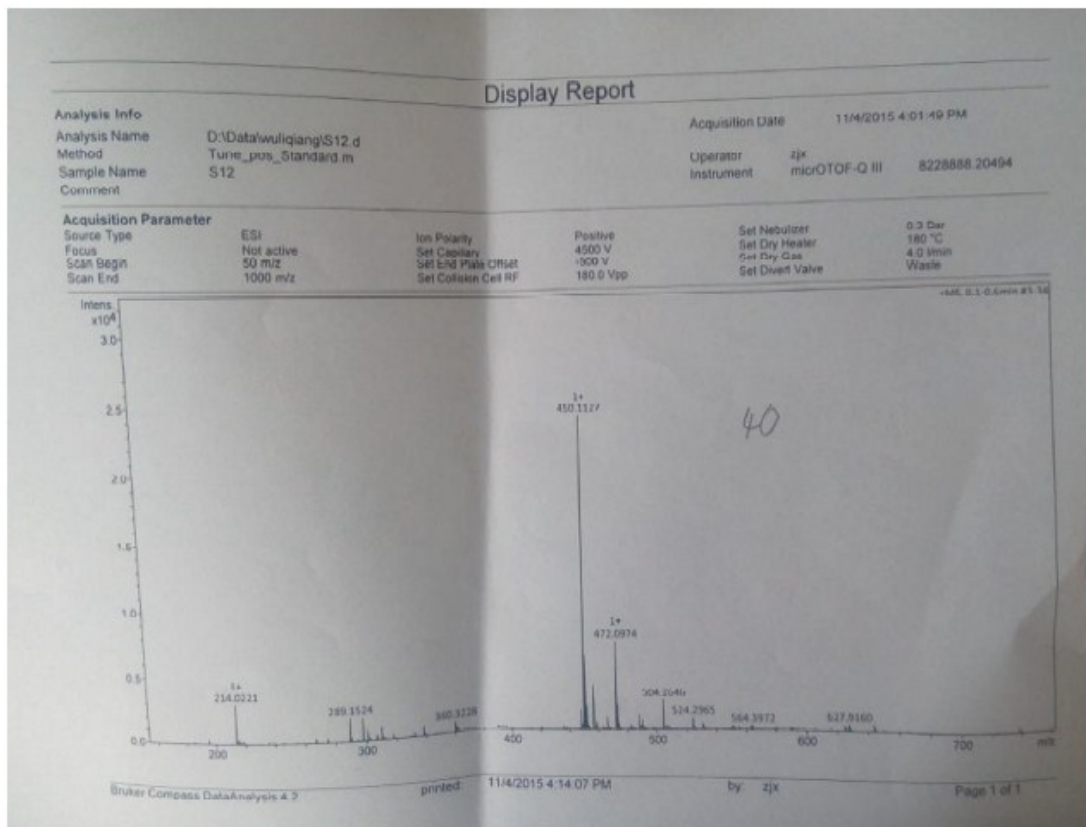
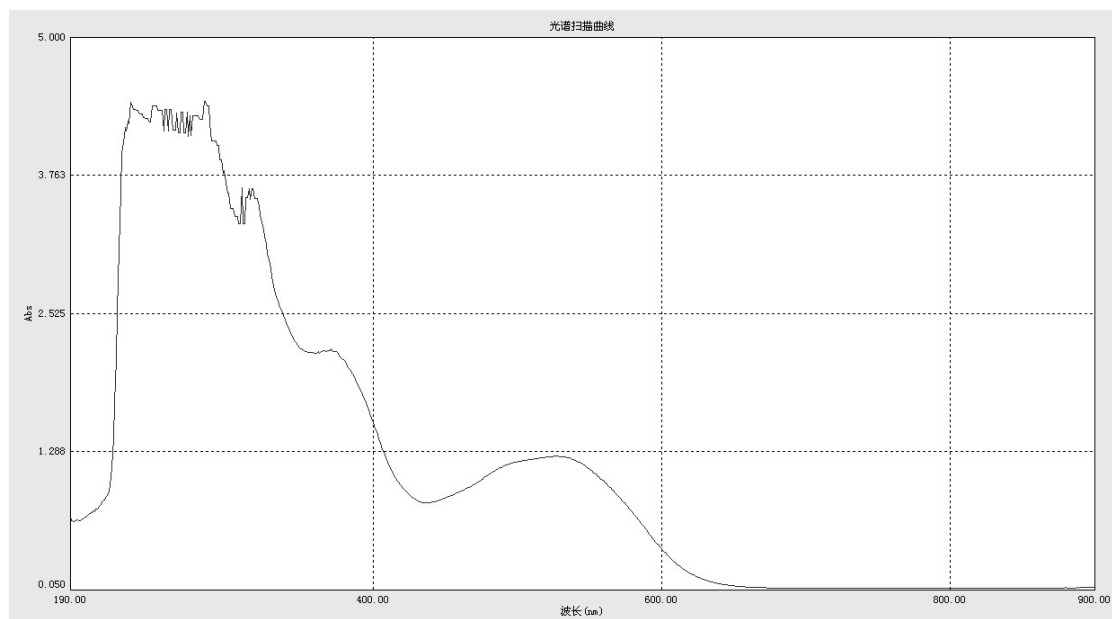


Figure 74  $^{13}\text{C}$  NMR of 4o



**Figure 75** HRMS of **4o**



**Figure 76** UV-vis of **4p**

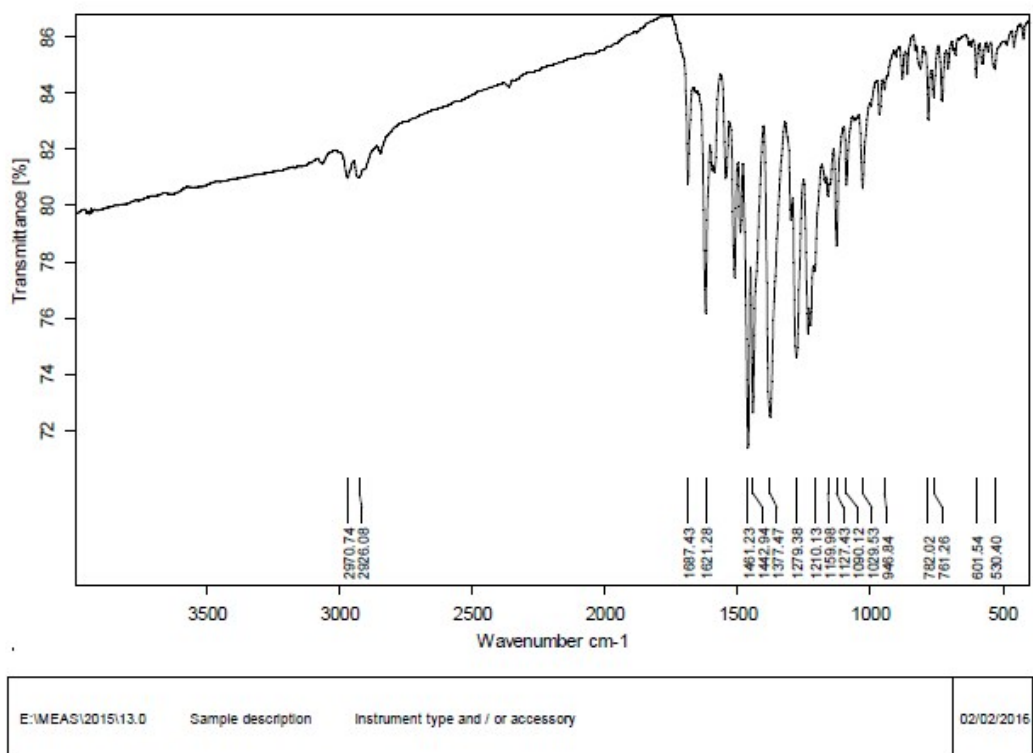


Figure 77 IR of 4p

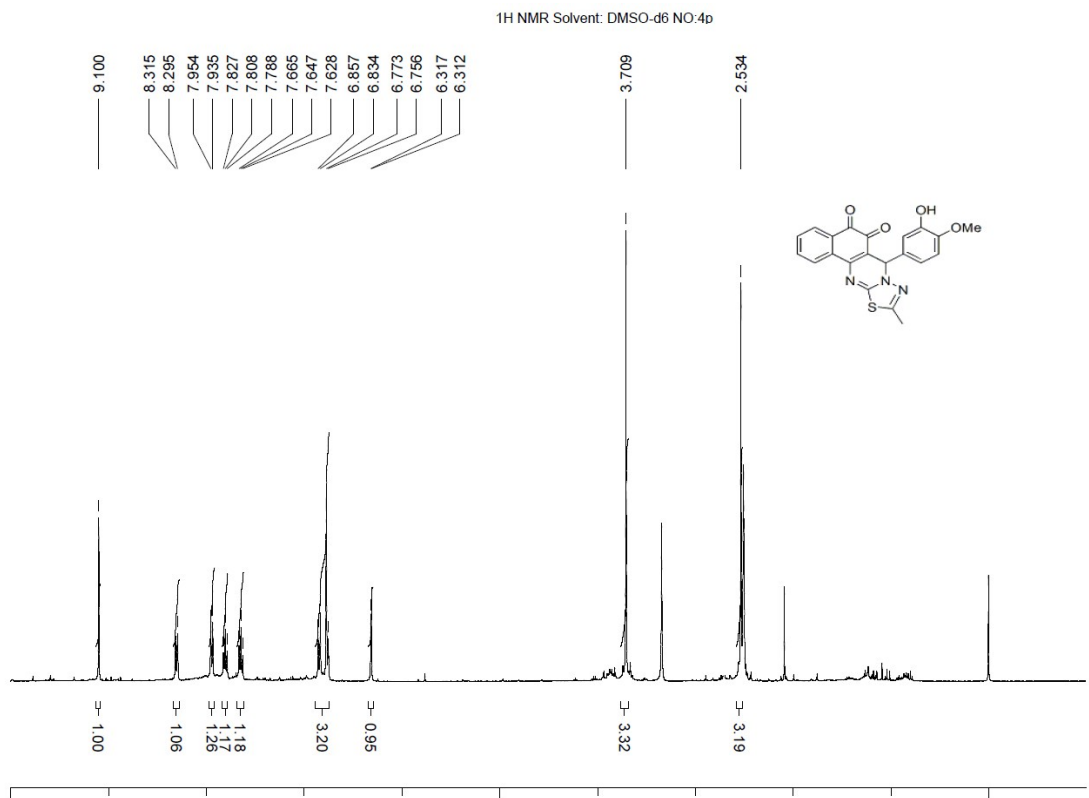


Figure 78 <sup>1</sup>H NMR of 4p



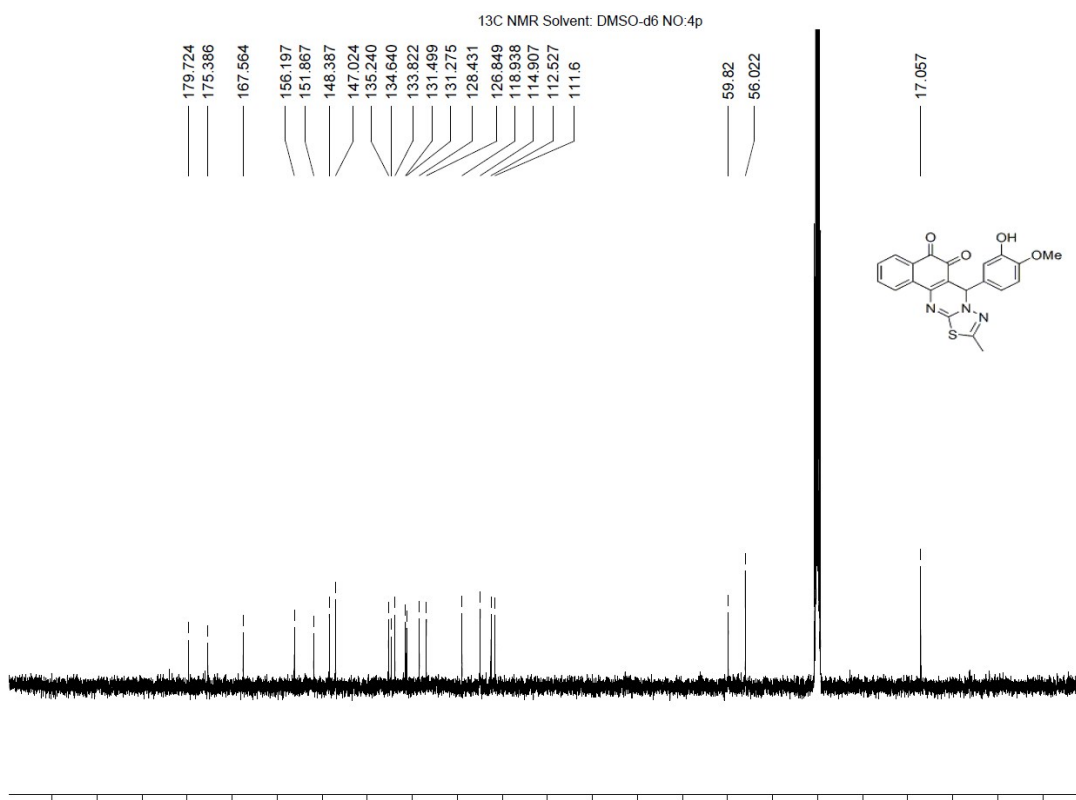


Figure 79 <sup>13</sup>C NMR of 4p

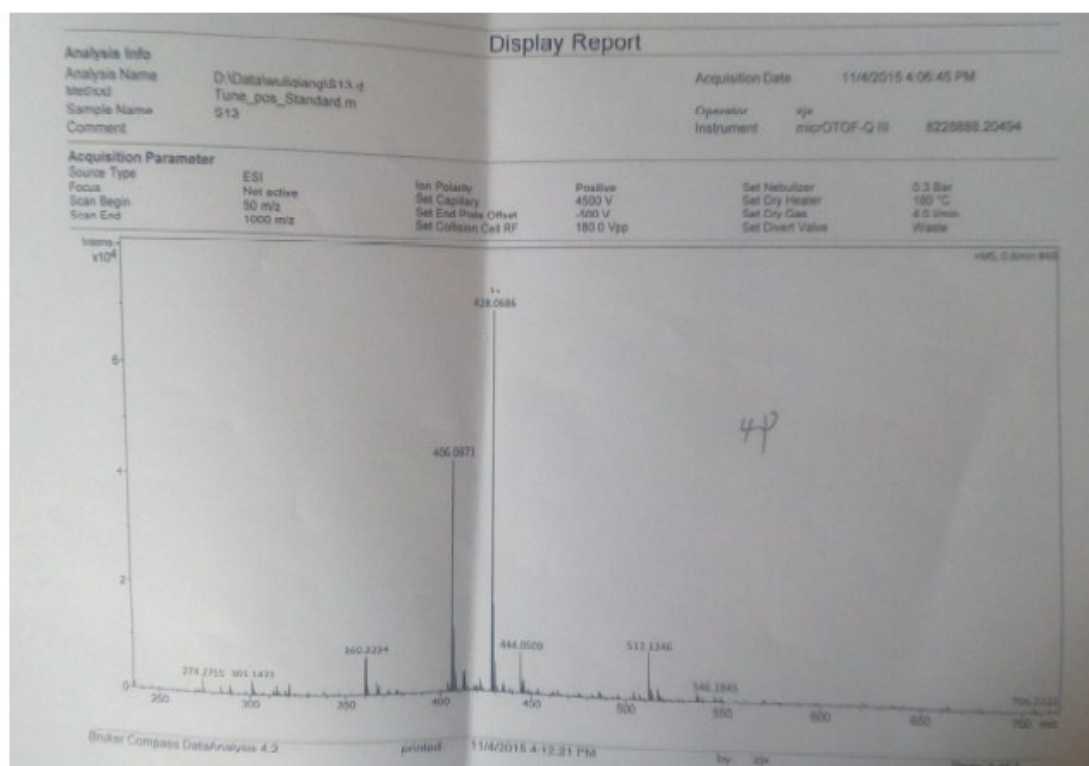


Figure 80 HRMS of 4p

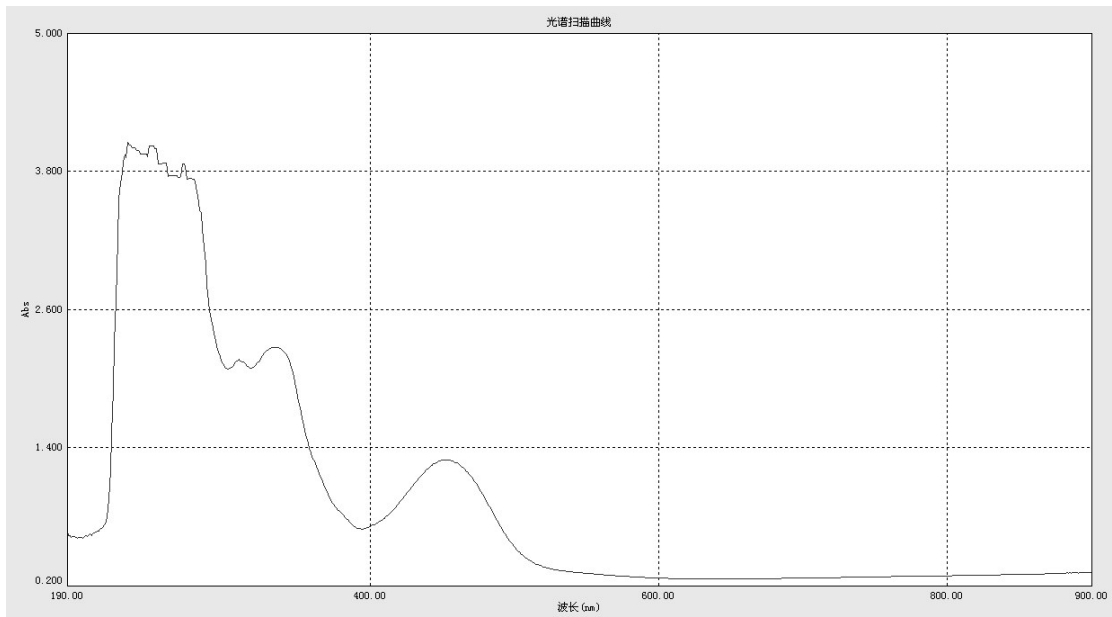


Figure 81 UV-vis of 5

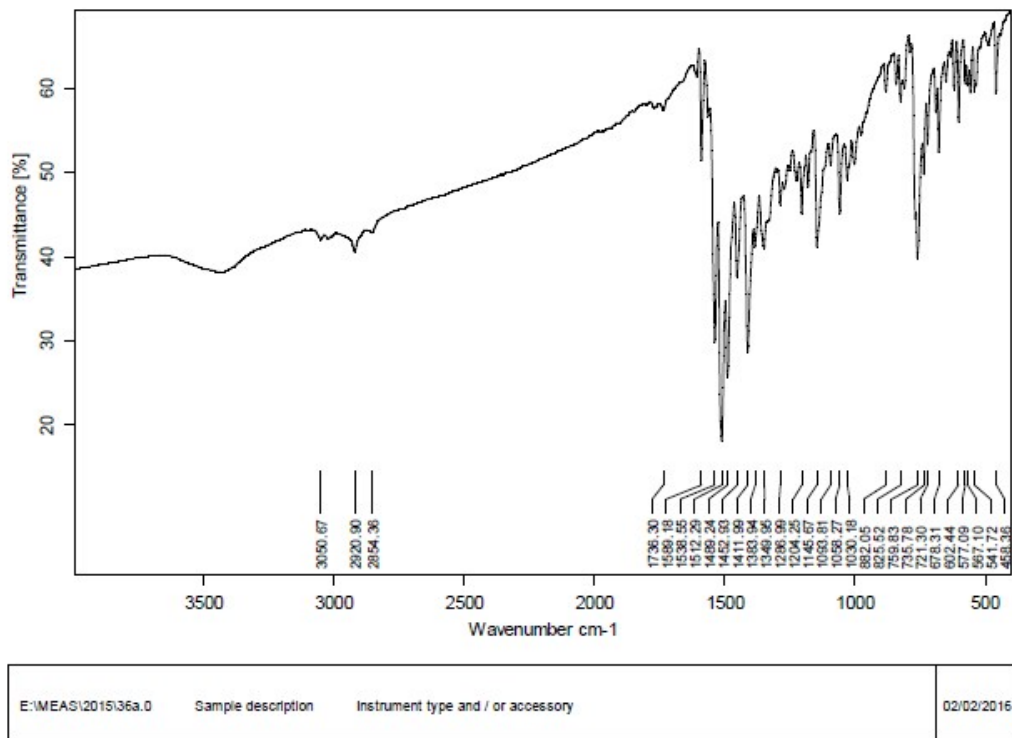


Figure 82 IR of 5

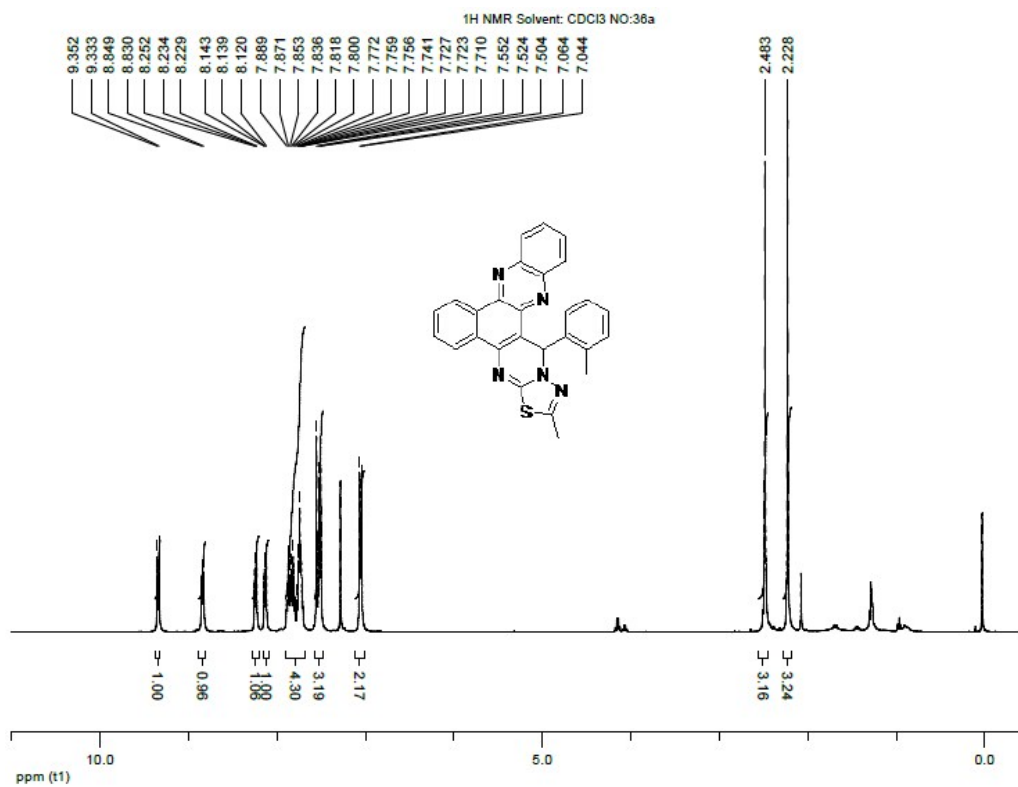


Figure 83 <sup>1</sup>H NMR of 5

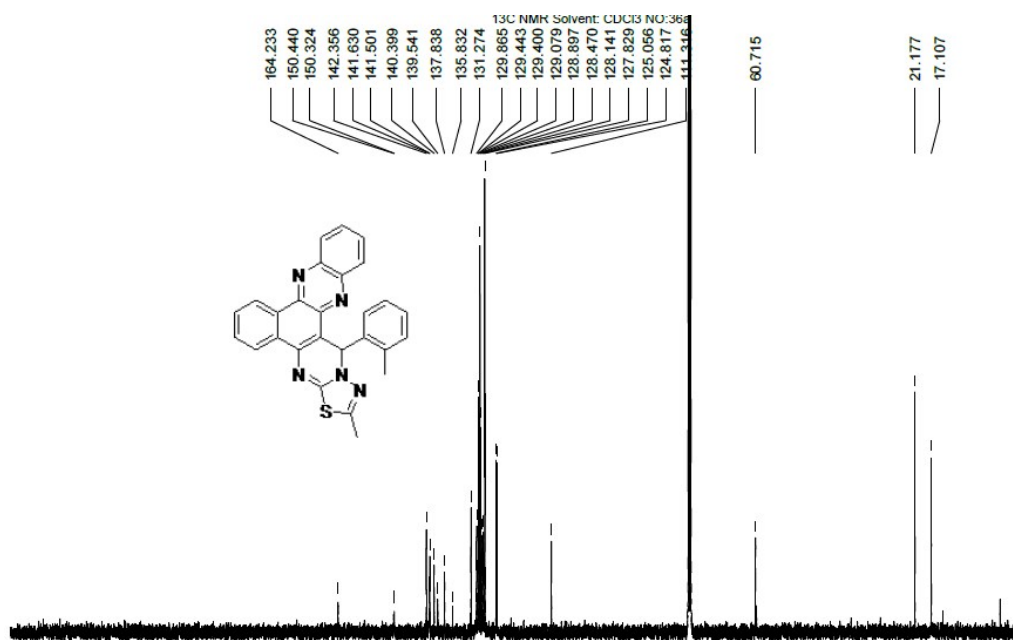


Figure 84 HRMS of 5

### Display Report

<b>Analysis Info</b>		Acquisition Date		4/20/2015 9:57:58 AM	
Analysis Name	D:\Data\wuliqiang\w-36a.d	Operator	zjx		
Method	Tune_pos_low.m	Instrument	micrOTOF-Q III	8228888.20494	
Sample Name	w-36a				
Comment					
<b>Acquisition Parameter</b>					
Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	0.3 Bar
Focus	Not active	Set Capillary	4500 V	Set Dry Heater	180 °C
Scan Begin	50 m/z	Set End Plate Offset	-500 V	Set Dry Gas	4.0 l/min
Scan End	1000 m/z	Set Collision Cell RF	120.0 Vpp	Set Divert Valve	Waste

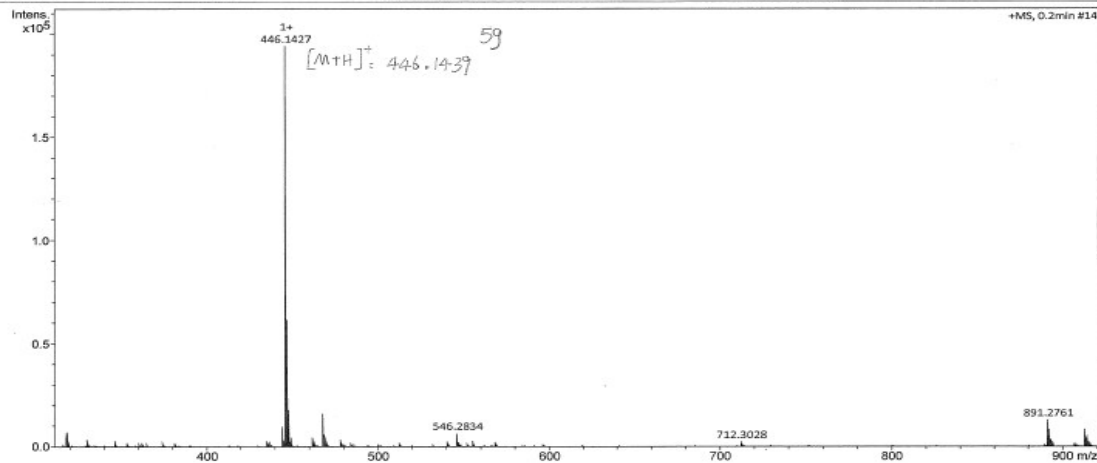


Figure 85 HRMS of 5