

Synthesis of novel 1,4-naphthoquinones possessing indole scaffolds using $\text{In}(\text{OTf})_3$ under solvent-free conditions

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Content

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Acquisition Parameter

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	180.0 Vpp	Set Divert Valve	Waste

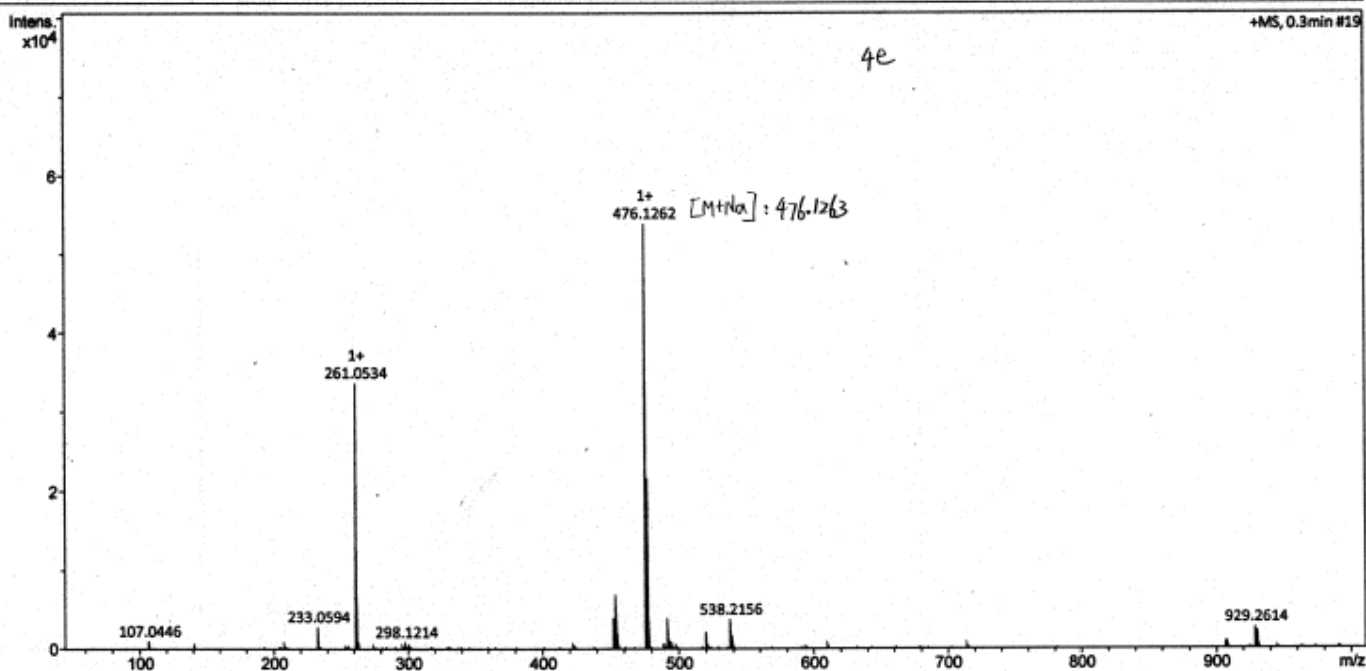


Figure S1 HRMS of 4a

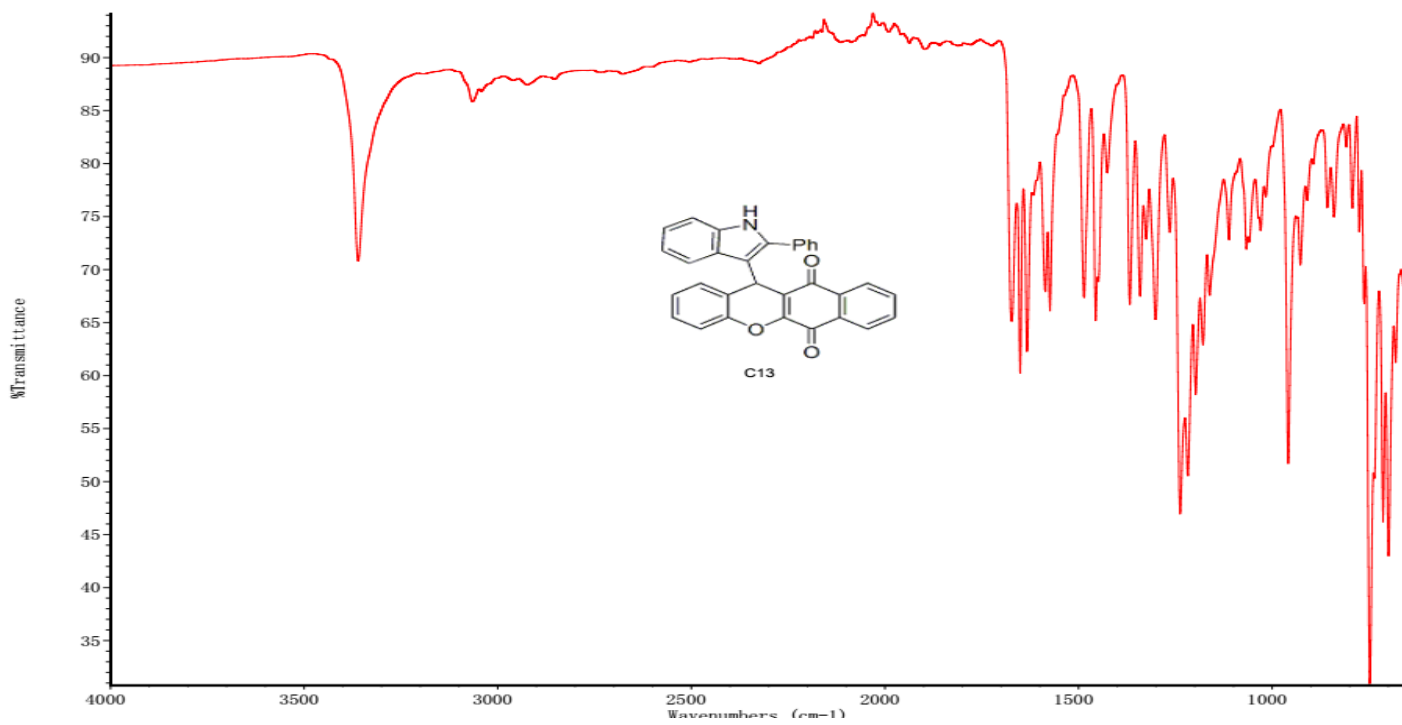


Figure S2 IR of 4a

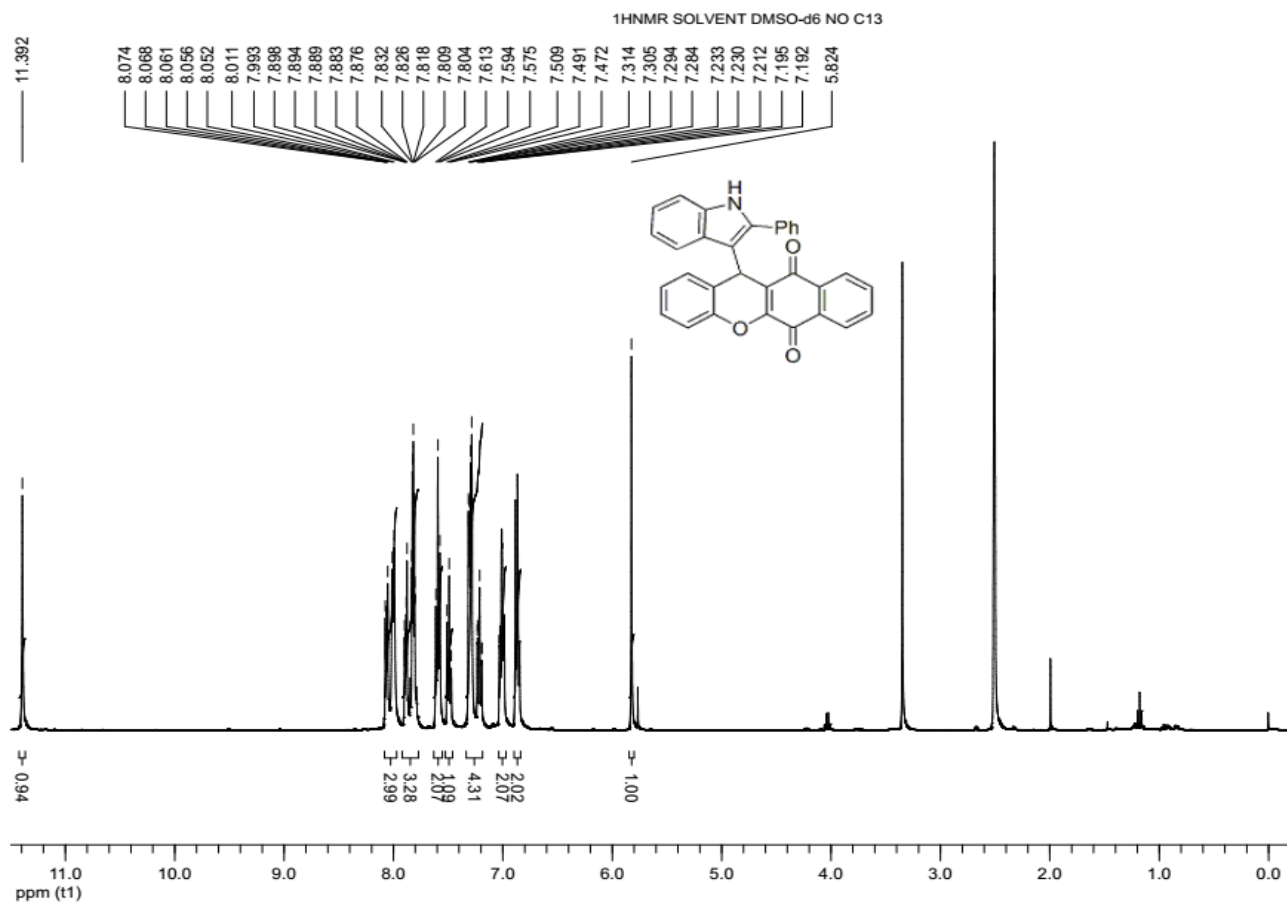


Figure S3 ^1H NMR of 4a

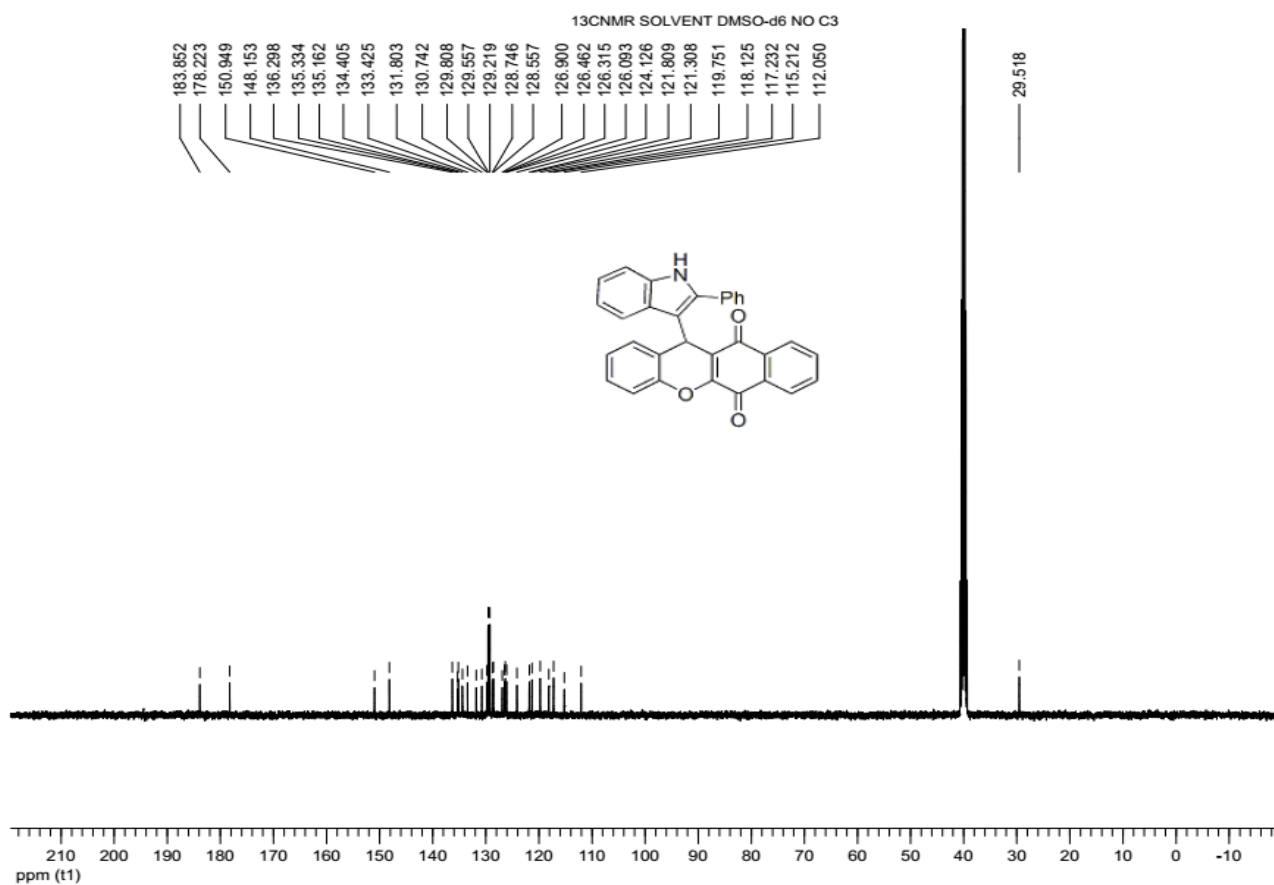


Figure S4 ^{13}C NMR of 4a

Acquisition Parameter					
Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	0.3 Bar
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Scan End	1000 m/z	Set Collision Cell RF	600.0 Vpp	Set Divert Valve	Waste

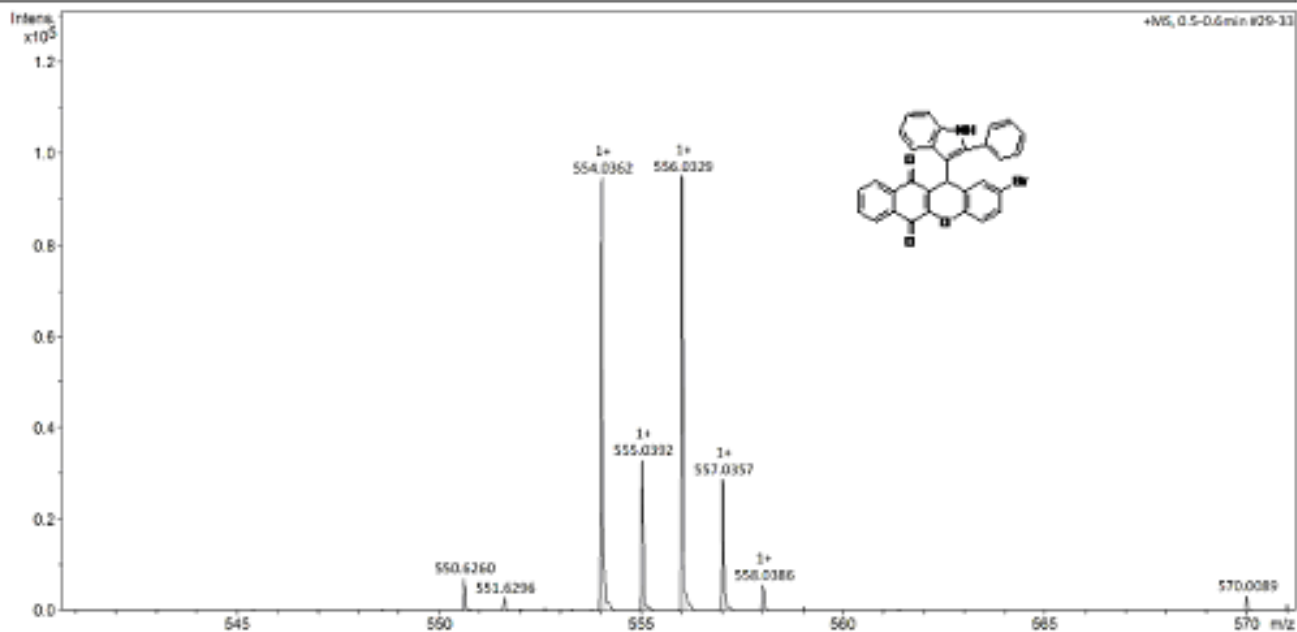


Figure S5 HRMS of 4b

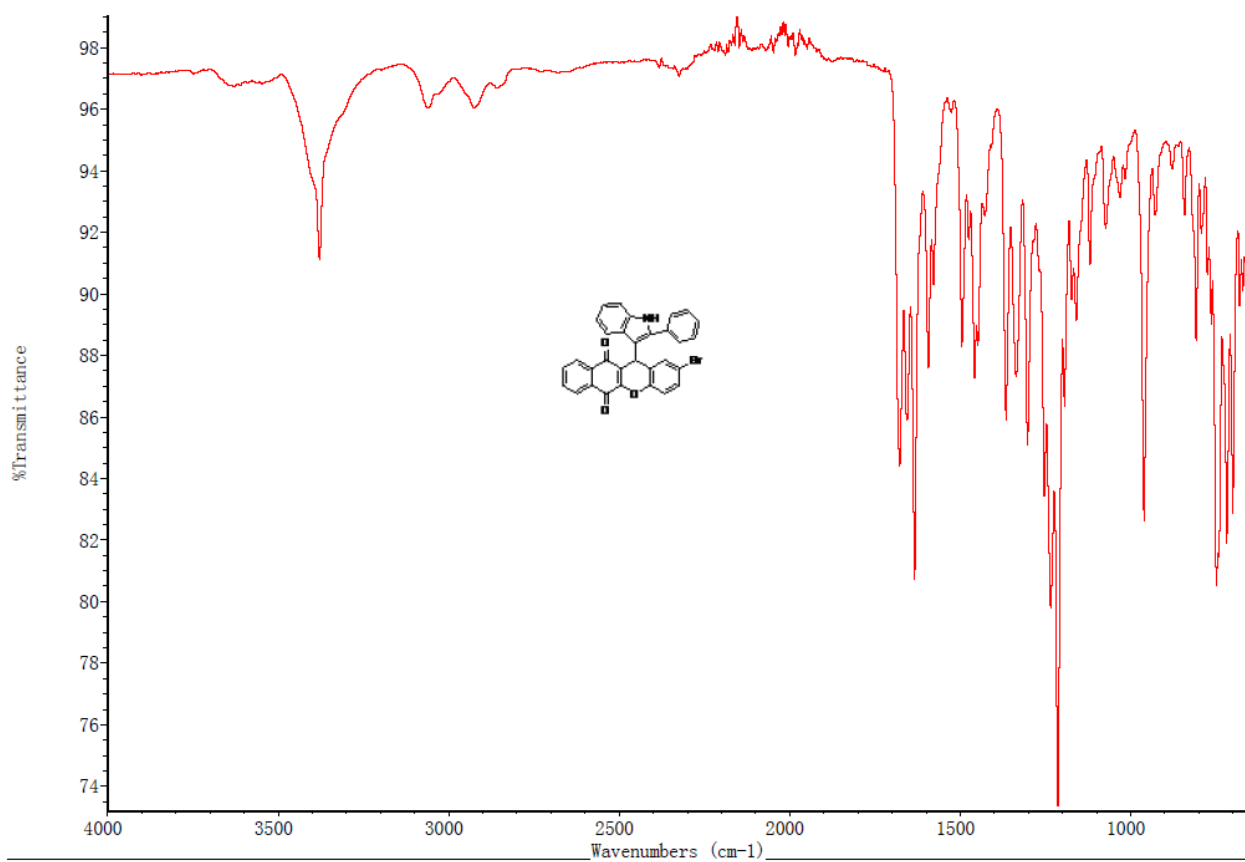


Figure S6 IR of 4b

1H NMR SOLVENT DMSO-d6 NO D1

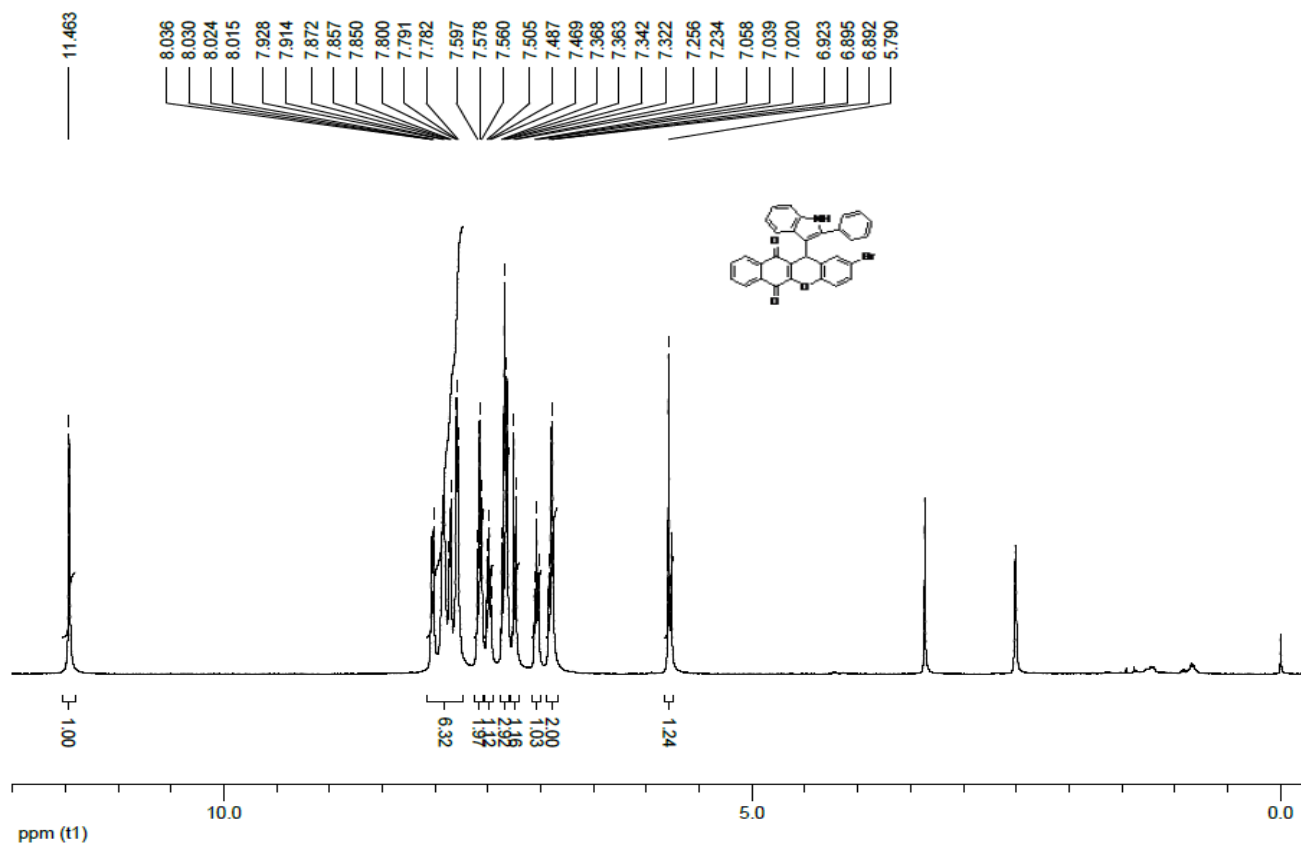


Figure S7 1H NMR of 4b

13C NMR SOLVENT DMSO-d6 NO D1

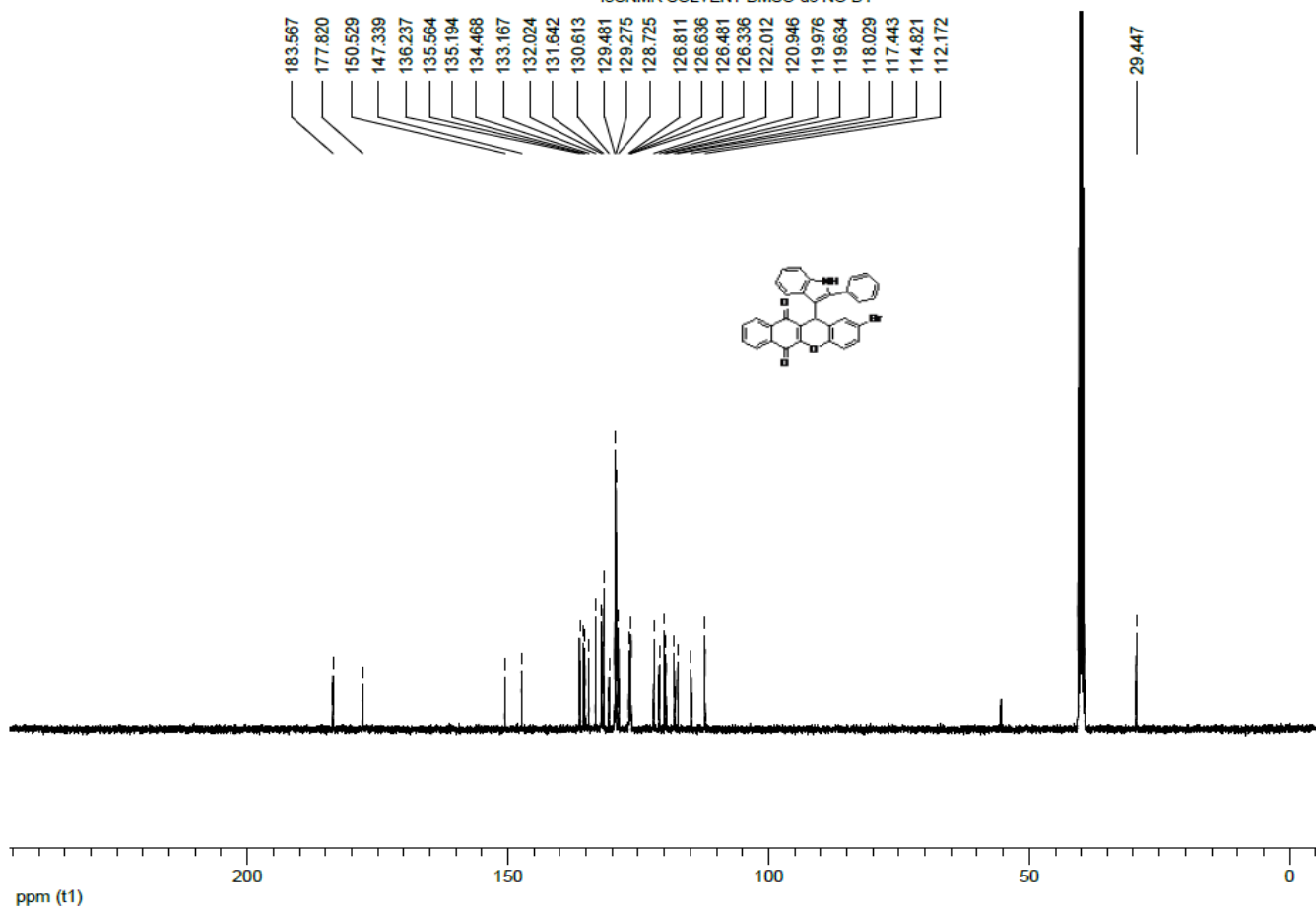


Figure S8 13C NMR of 4b

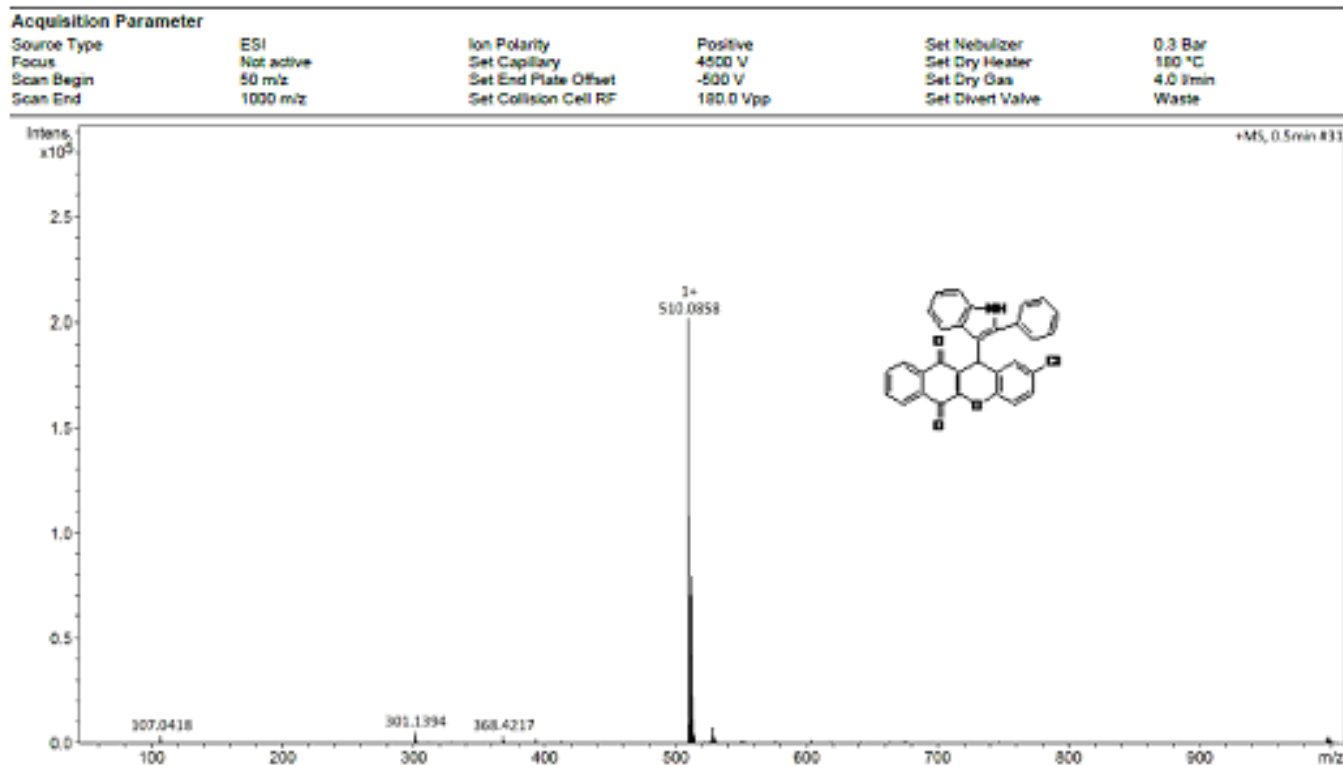


Figure S9 HRMS of 4c

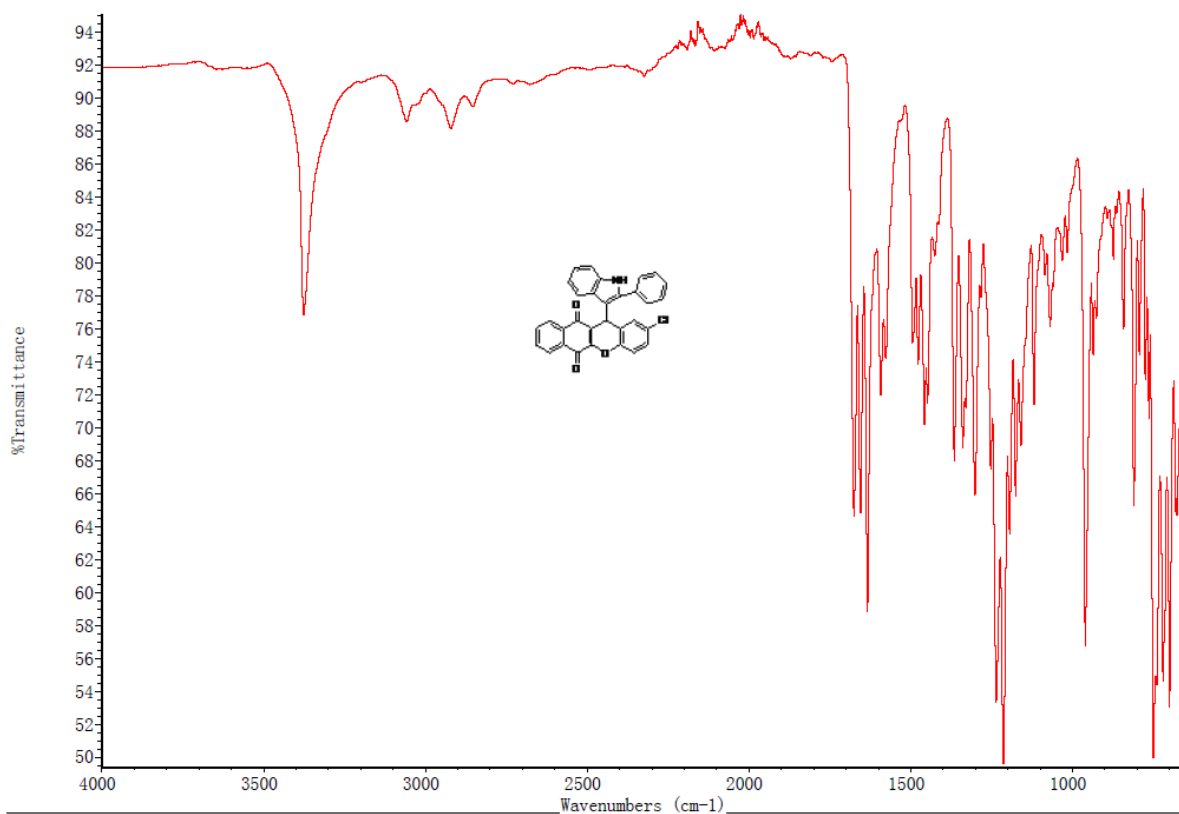


Figure S10 IR of 4c

1H NMR SOLVENT DMSO-d6 NO D2

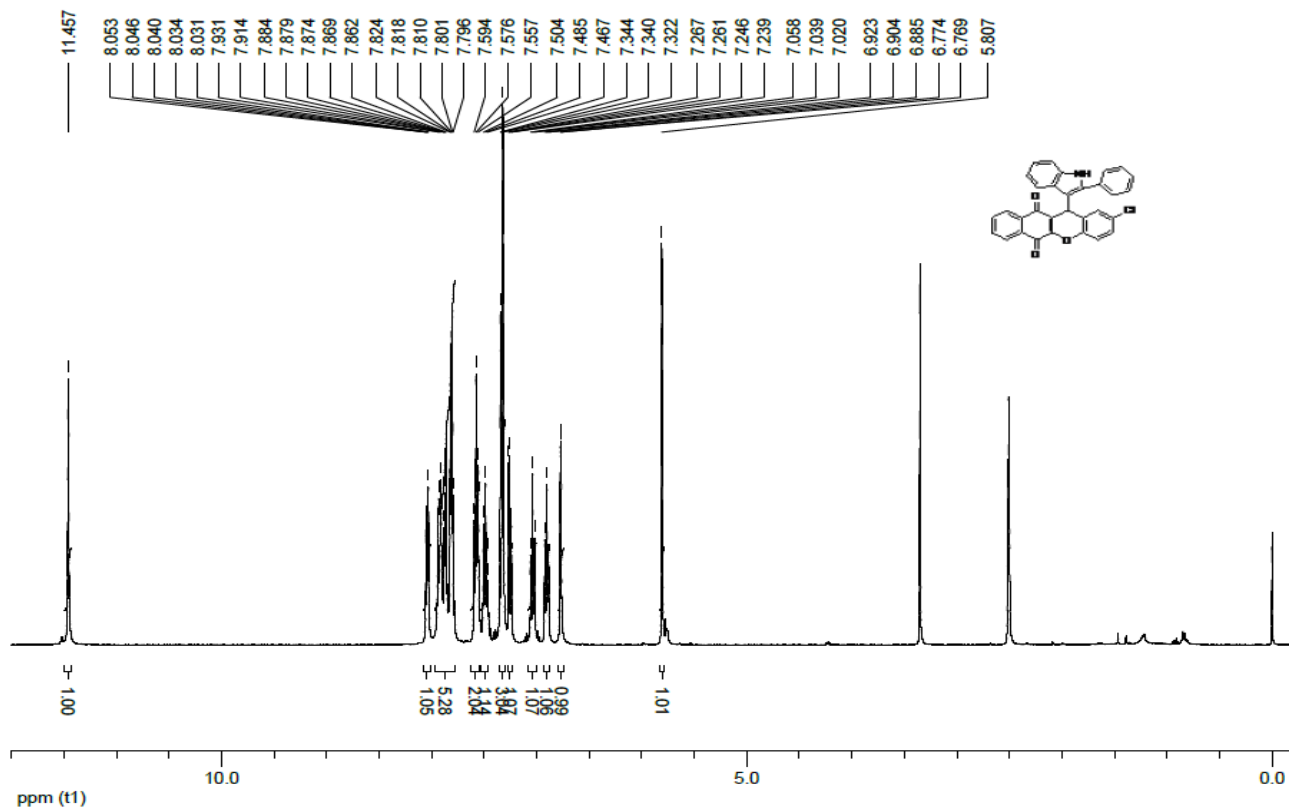


Figure S11 1H NMR of 4c

13C NMR SOLVENT DMSO-d6 NO D2

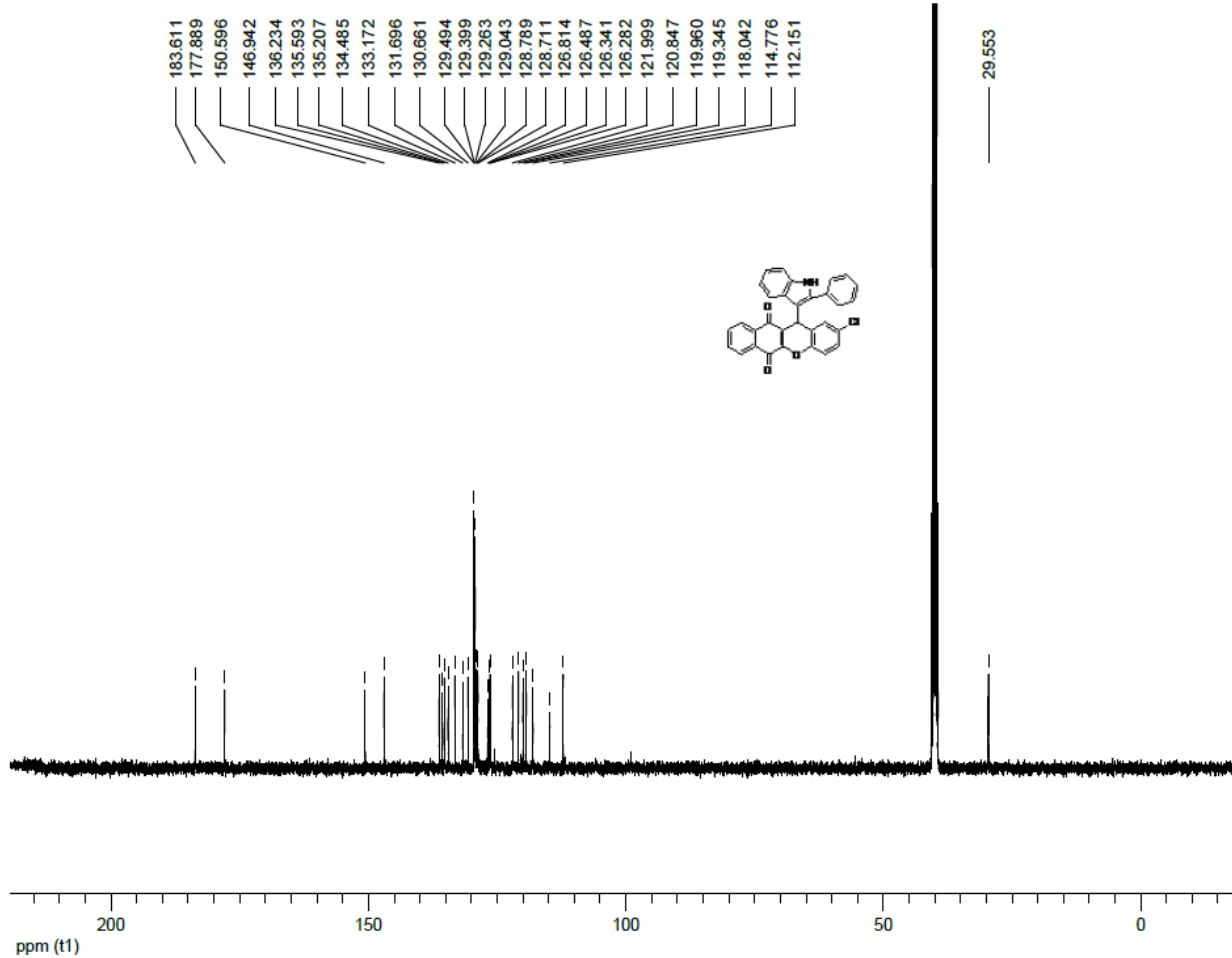
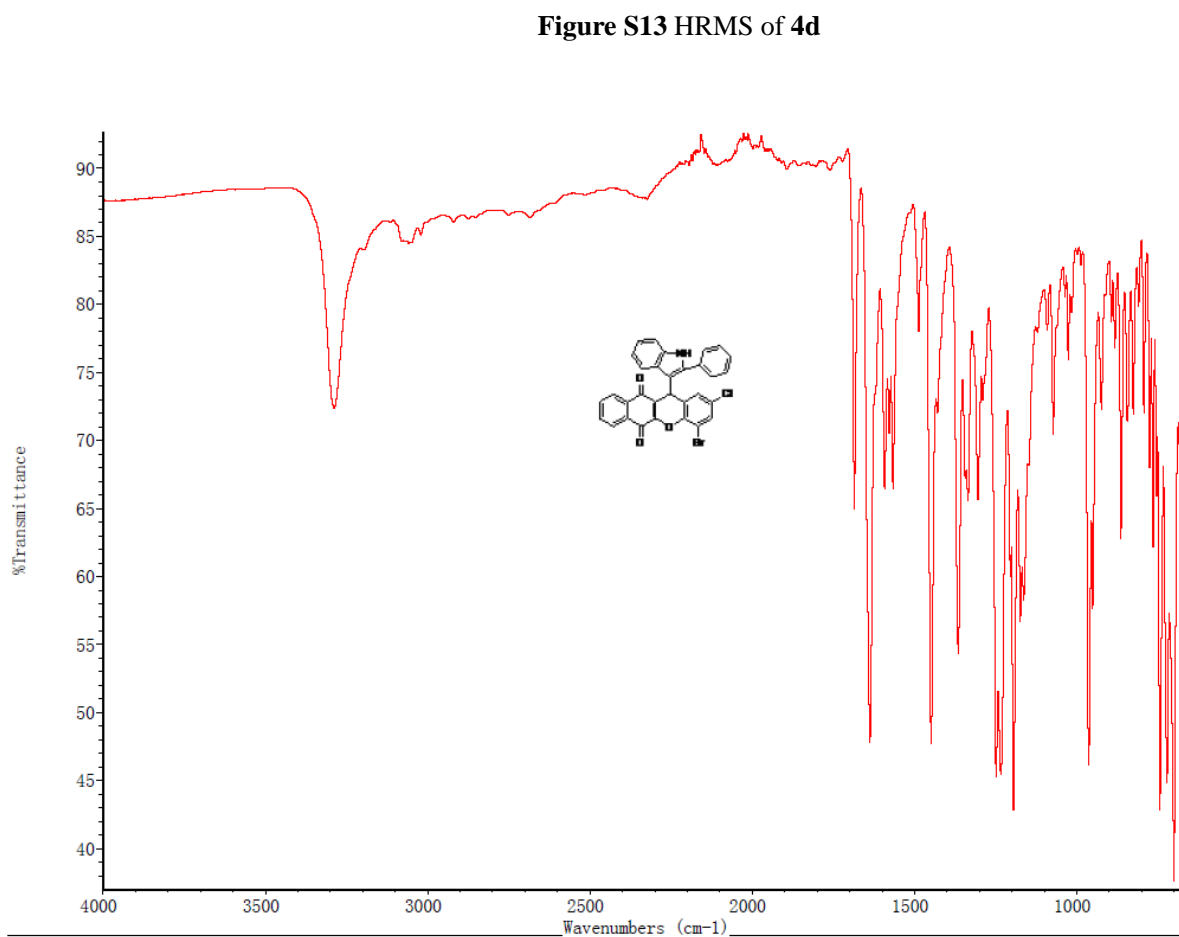
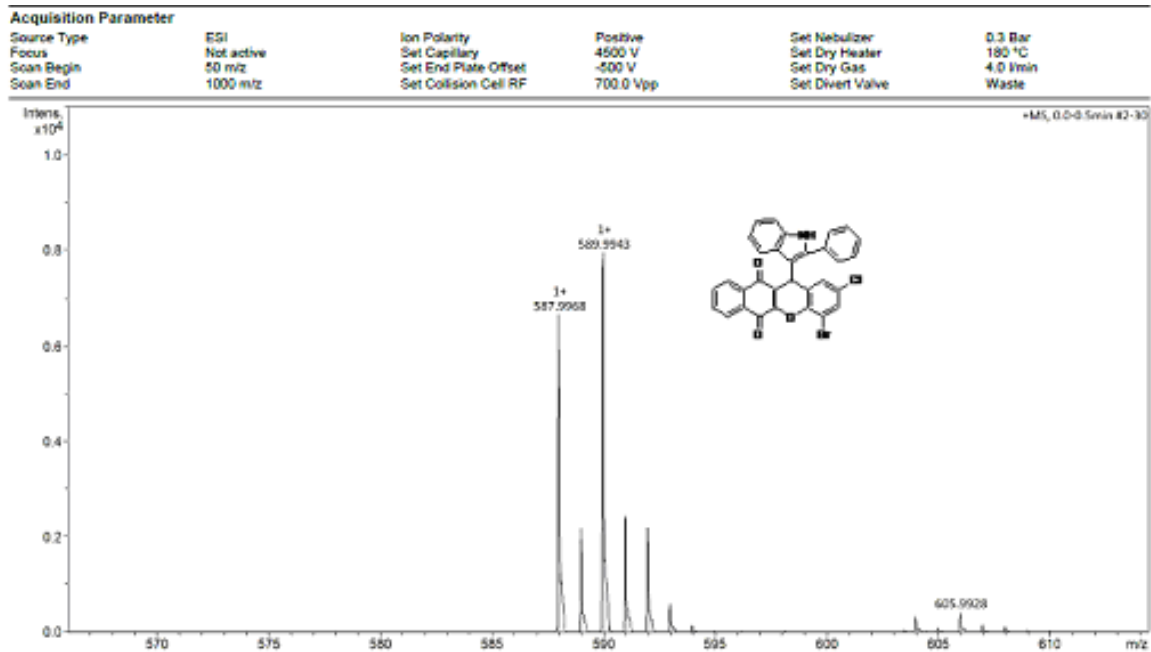


Figure S12 13C NMR of 4c



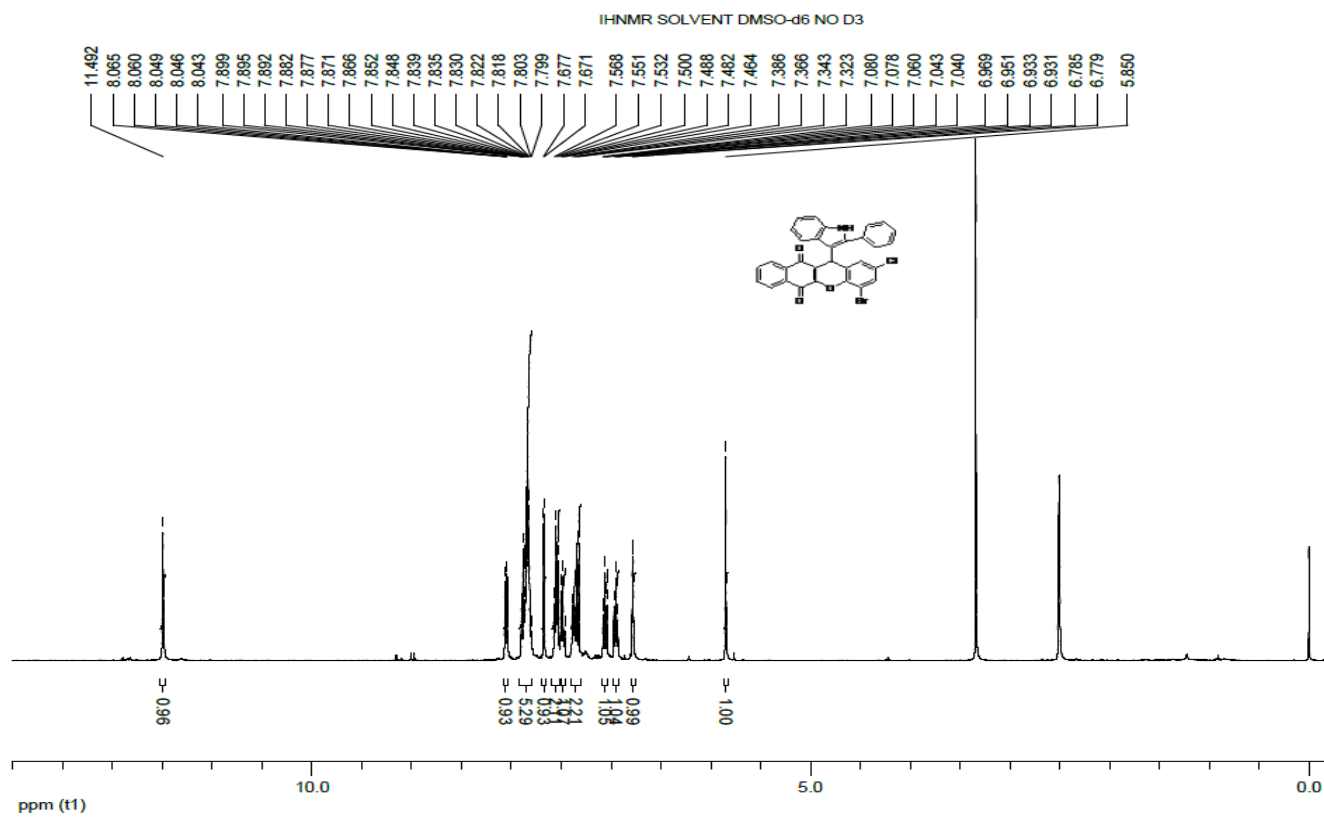


Figure S15 1H NMR of 4d

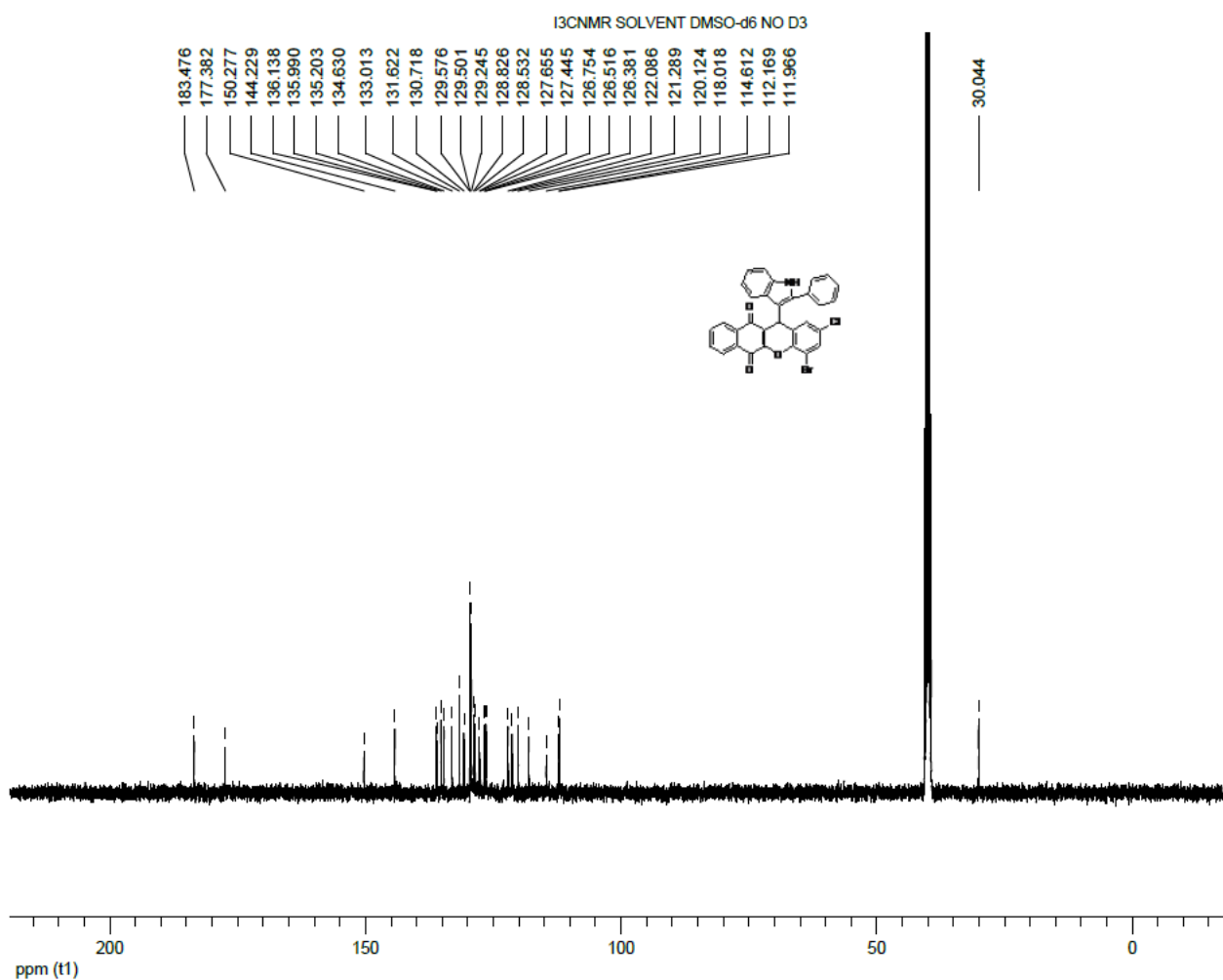


Figure S16 13C NMR of 4d

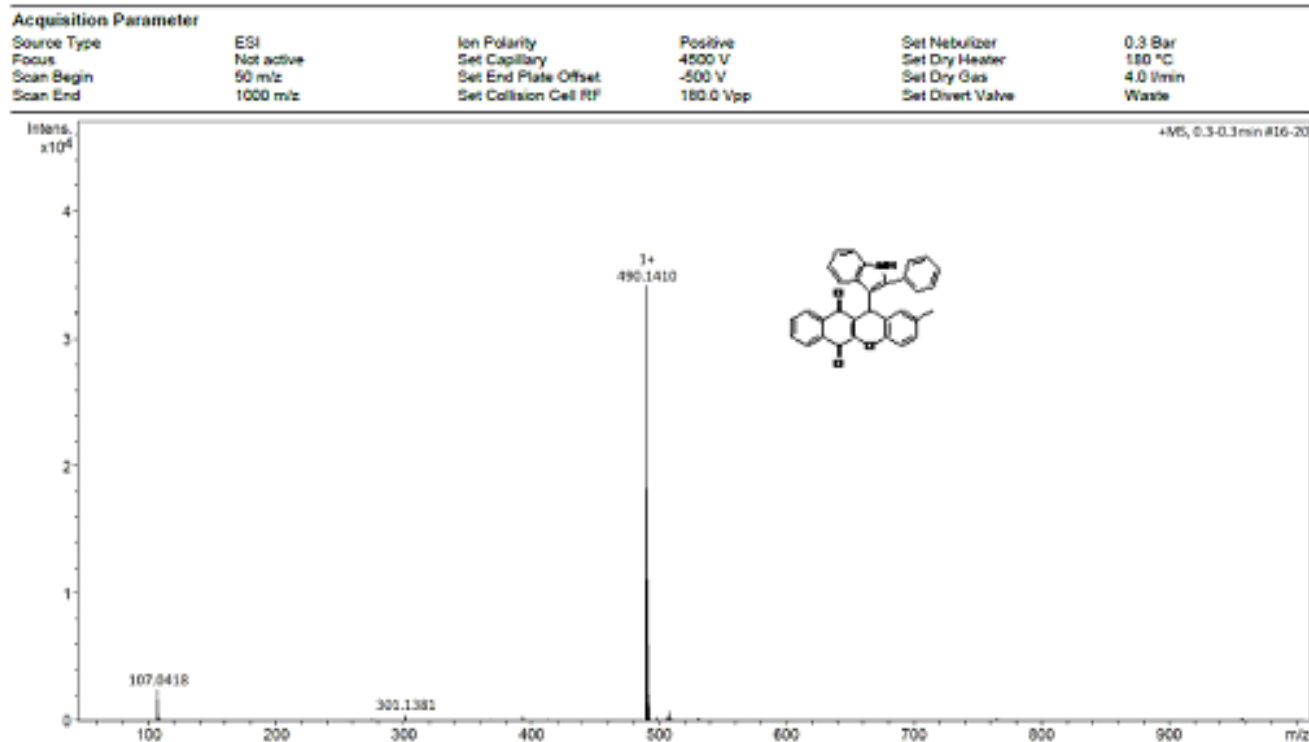


Figure S17 HRMS of 4e

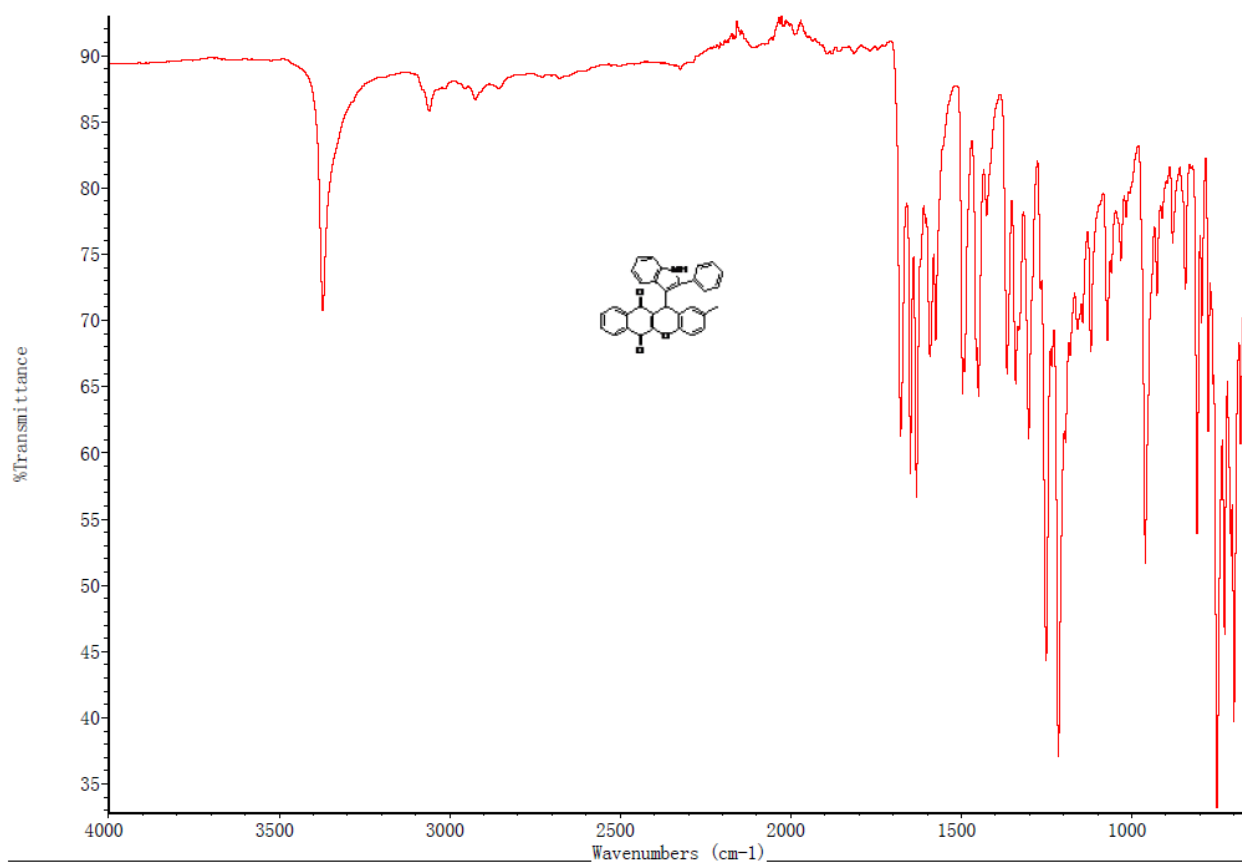


Figure S18 IR of 4e

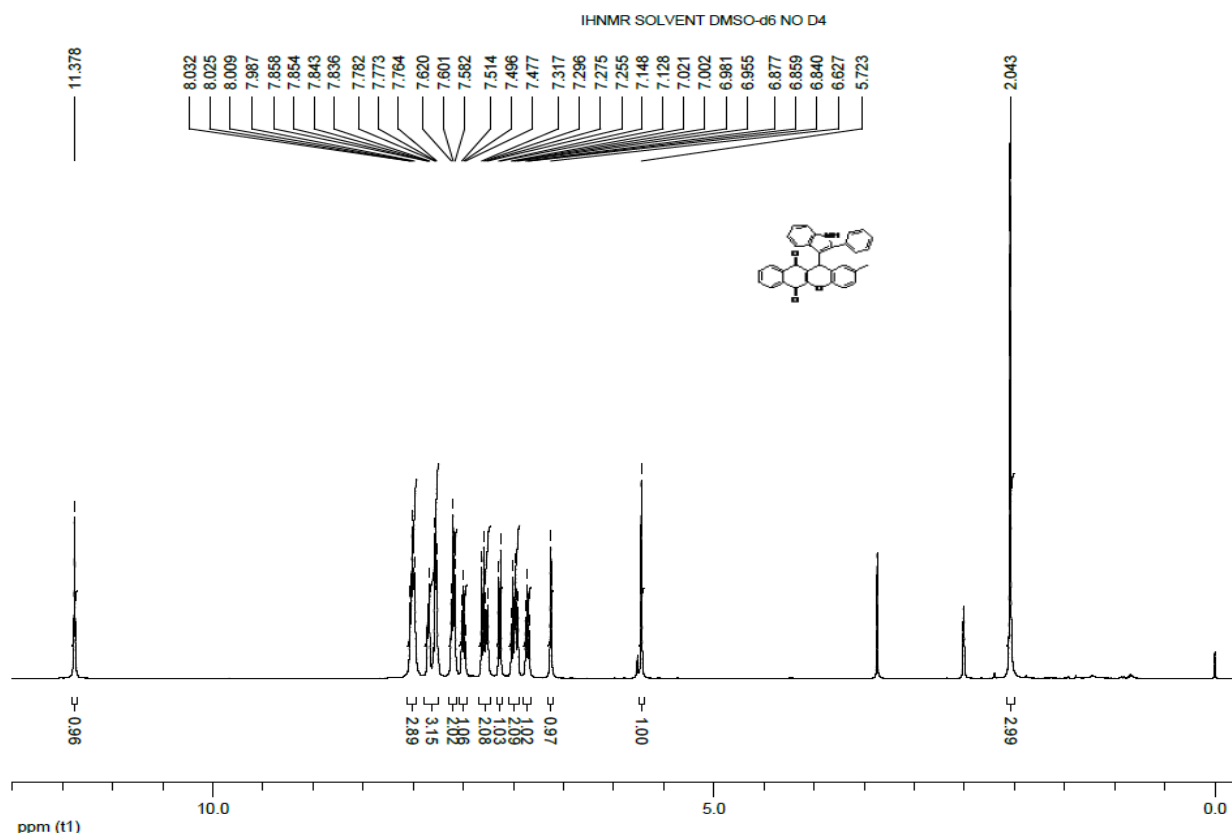


Figure S19 1H NMR of 4e

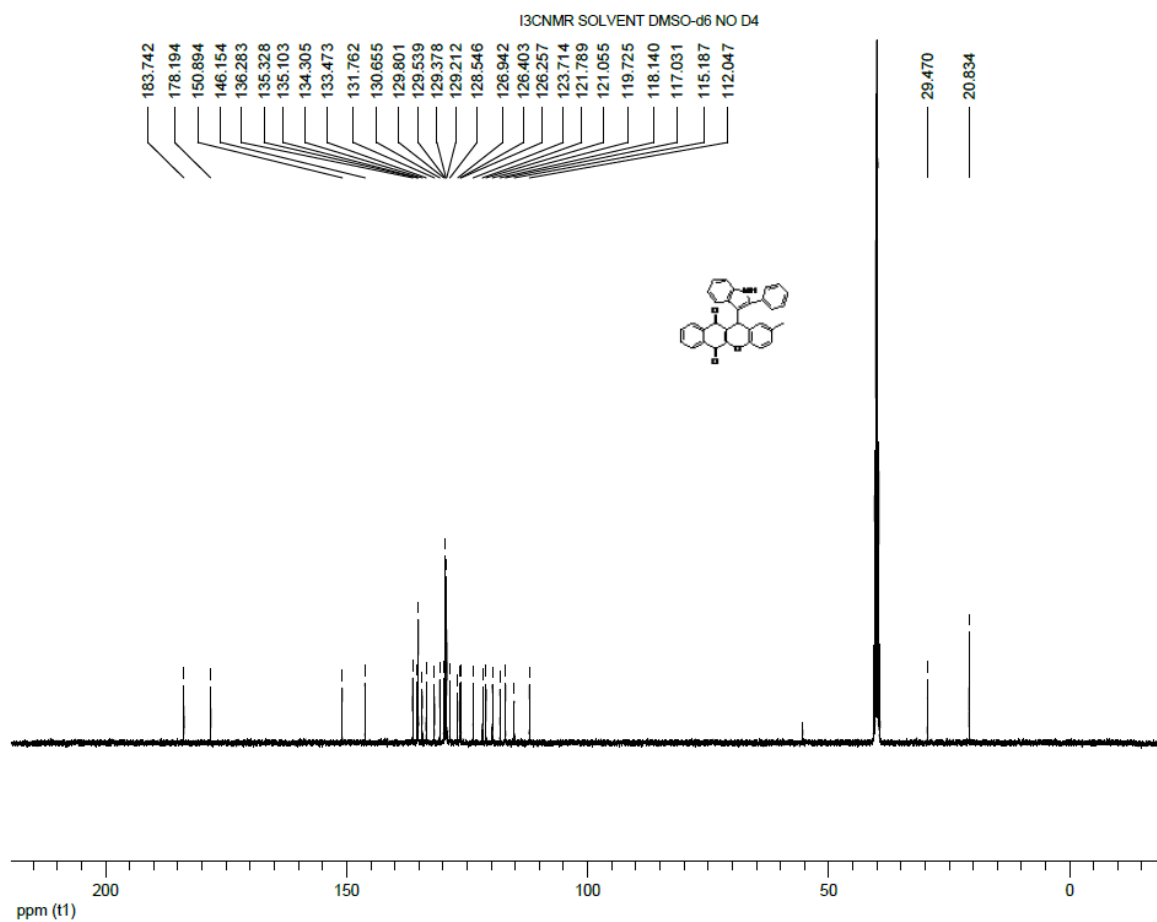
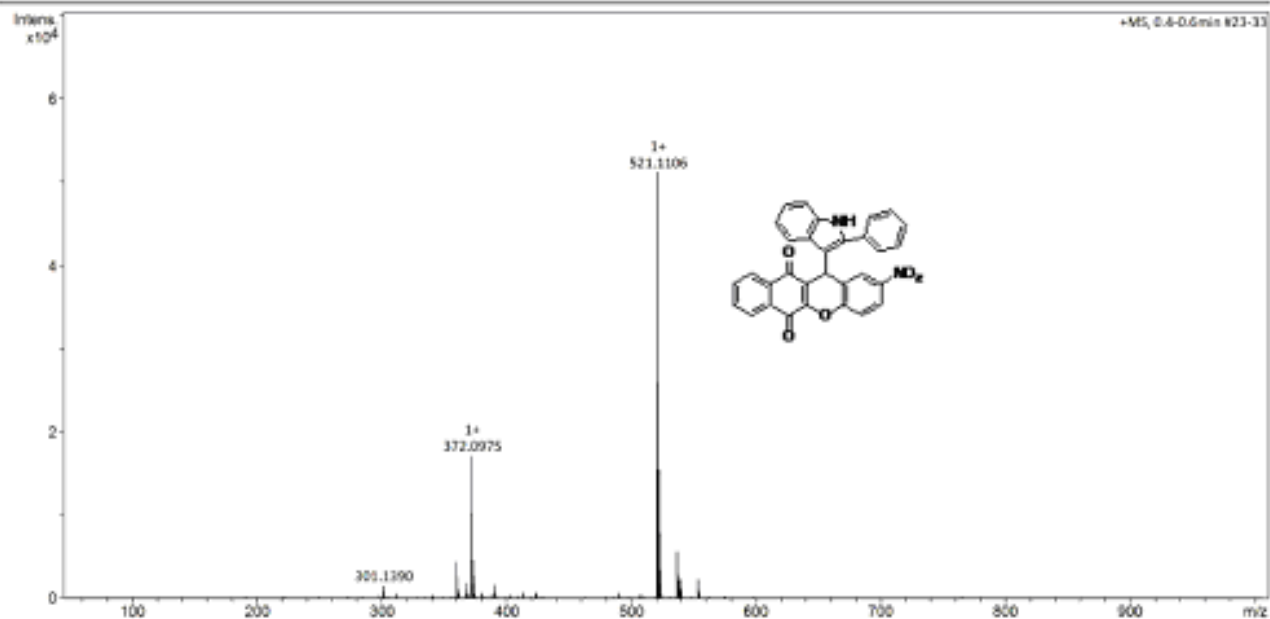
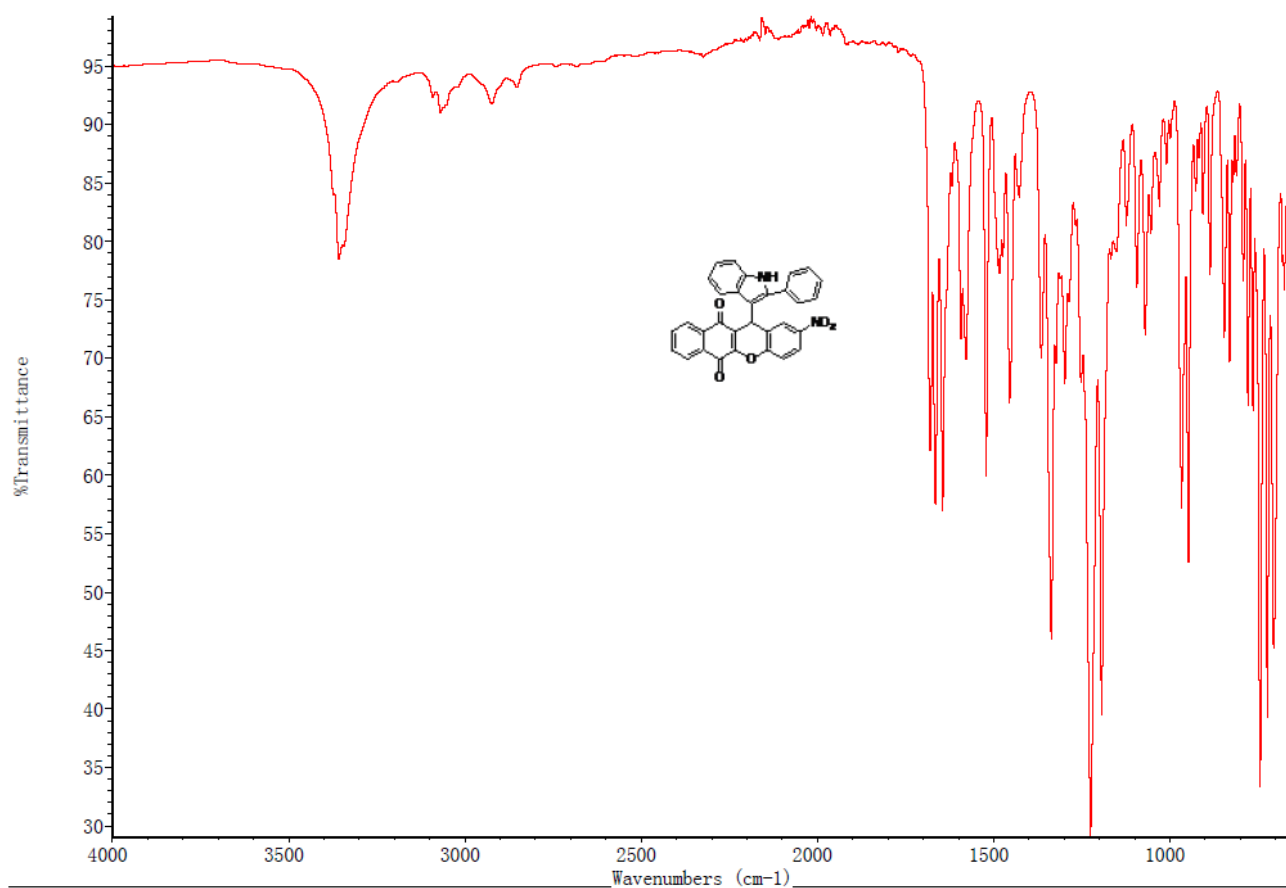


Figure S20 13C NMR of 4e

Acquisition Parameter

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	350.0 Vpp	Set Divert Valve	Waste

**Figure S21 HRMS of 4f****Figure S22 IR of 4f**

Acquisition Parameter						
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	280.0 Vpp	Set Divert Valve	Waste	

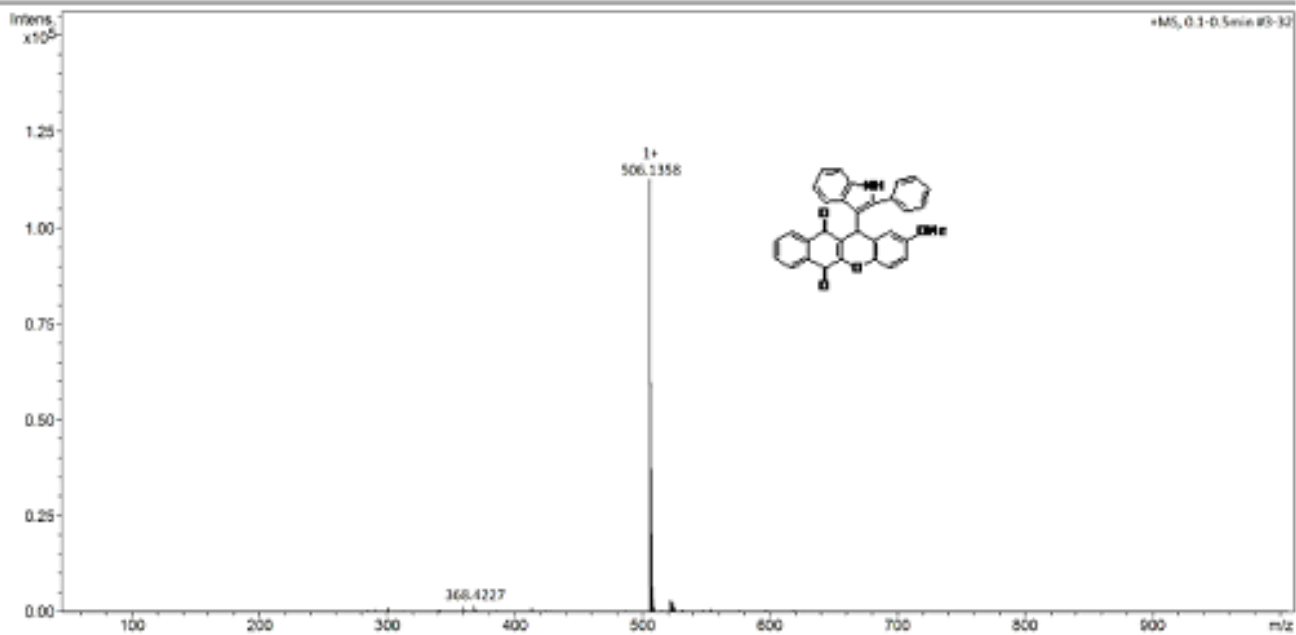


Figure S25 HRMS of 4g

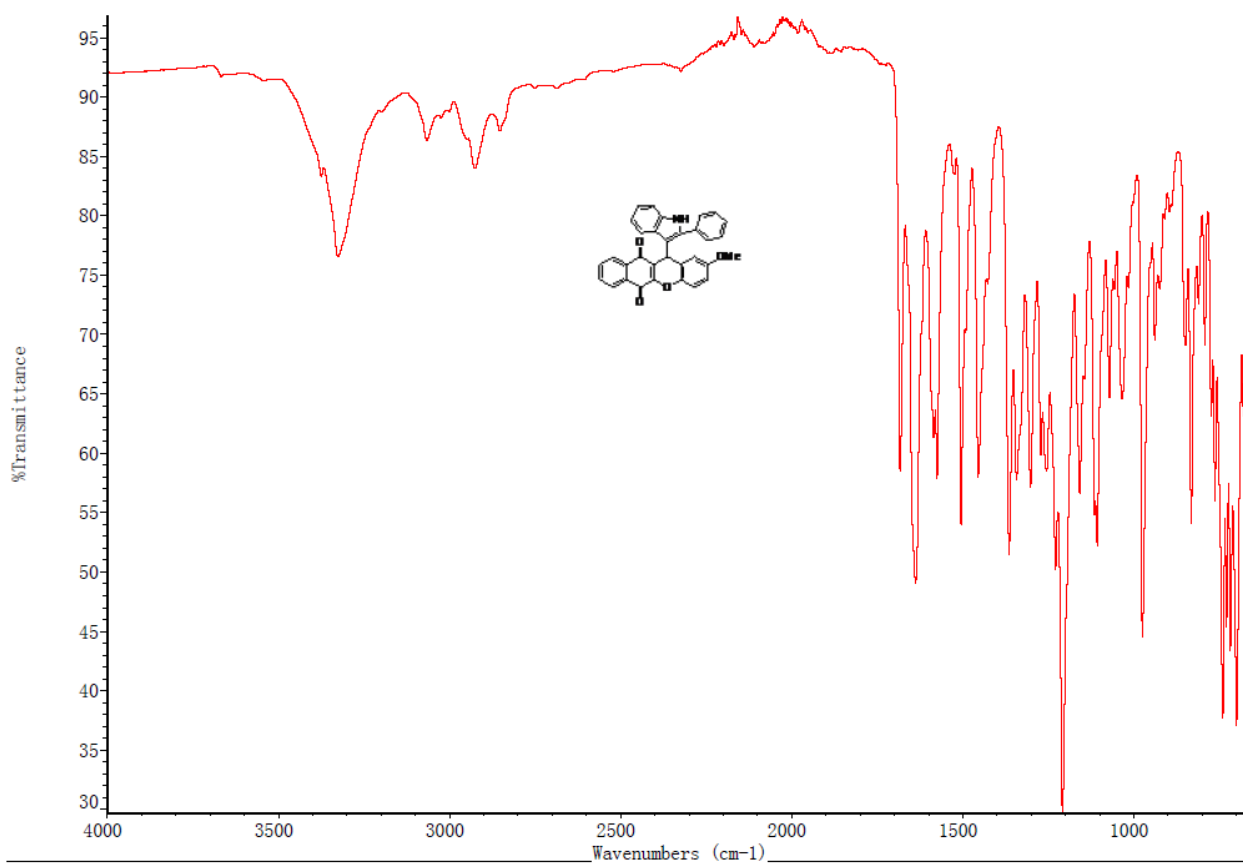


Figure S26 IR of 4g

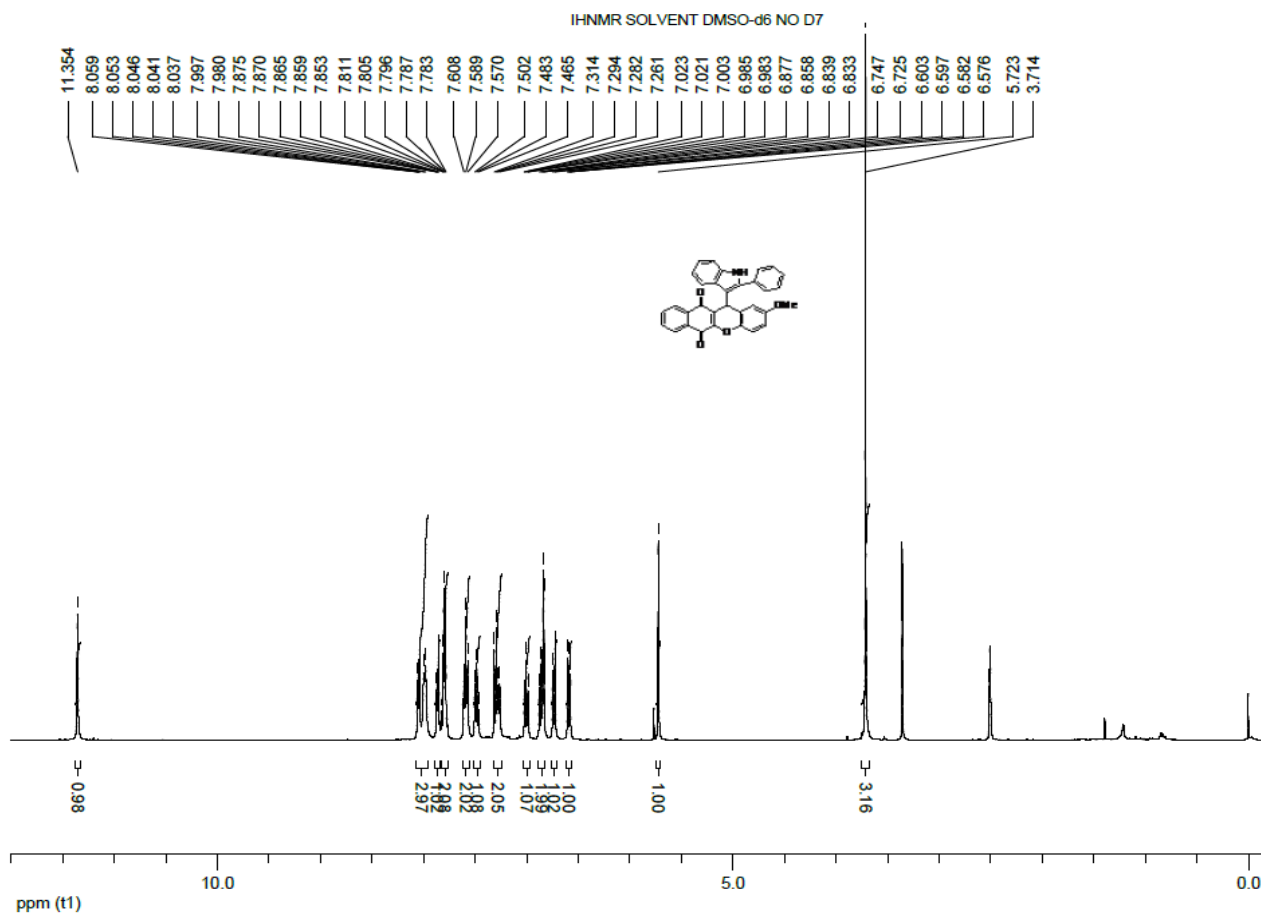


Figure S27 ¹H NMR of 4g

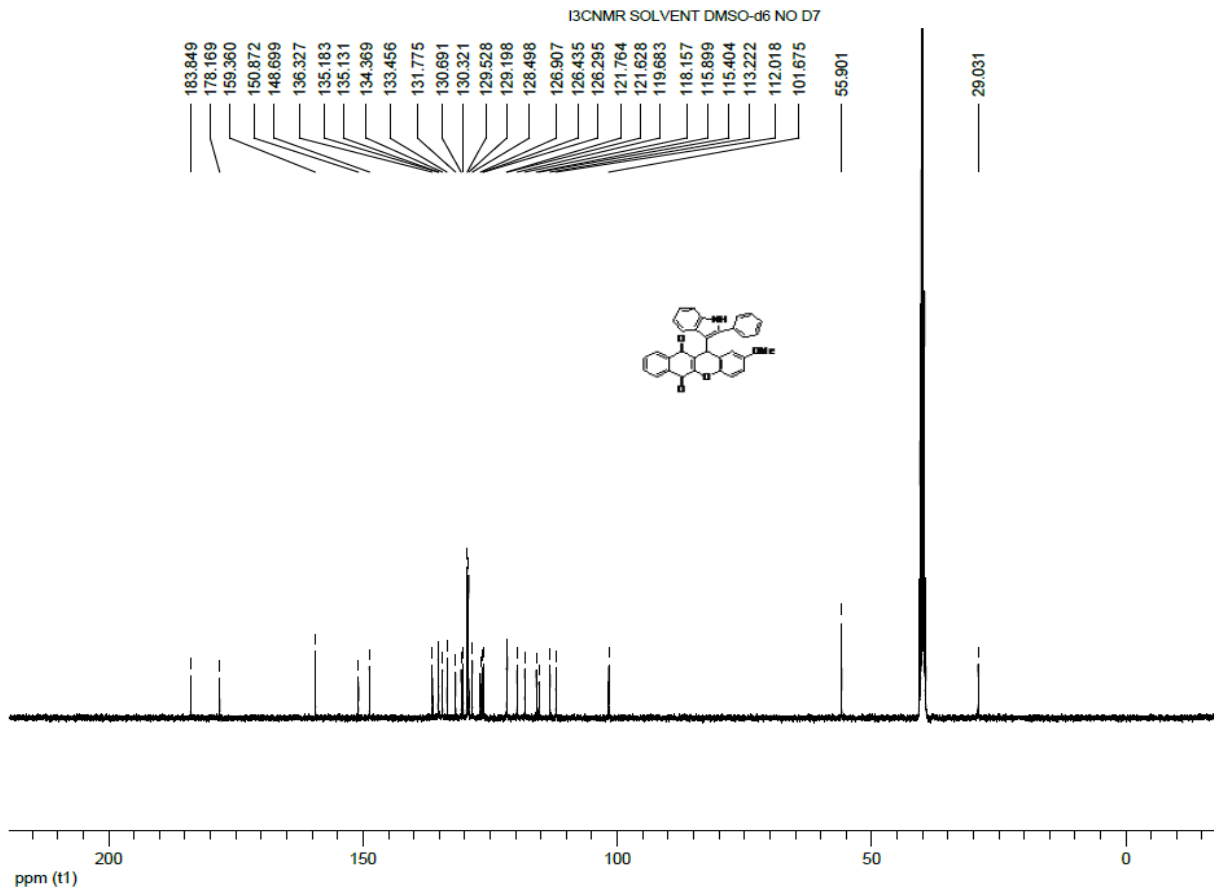
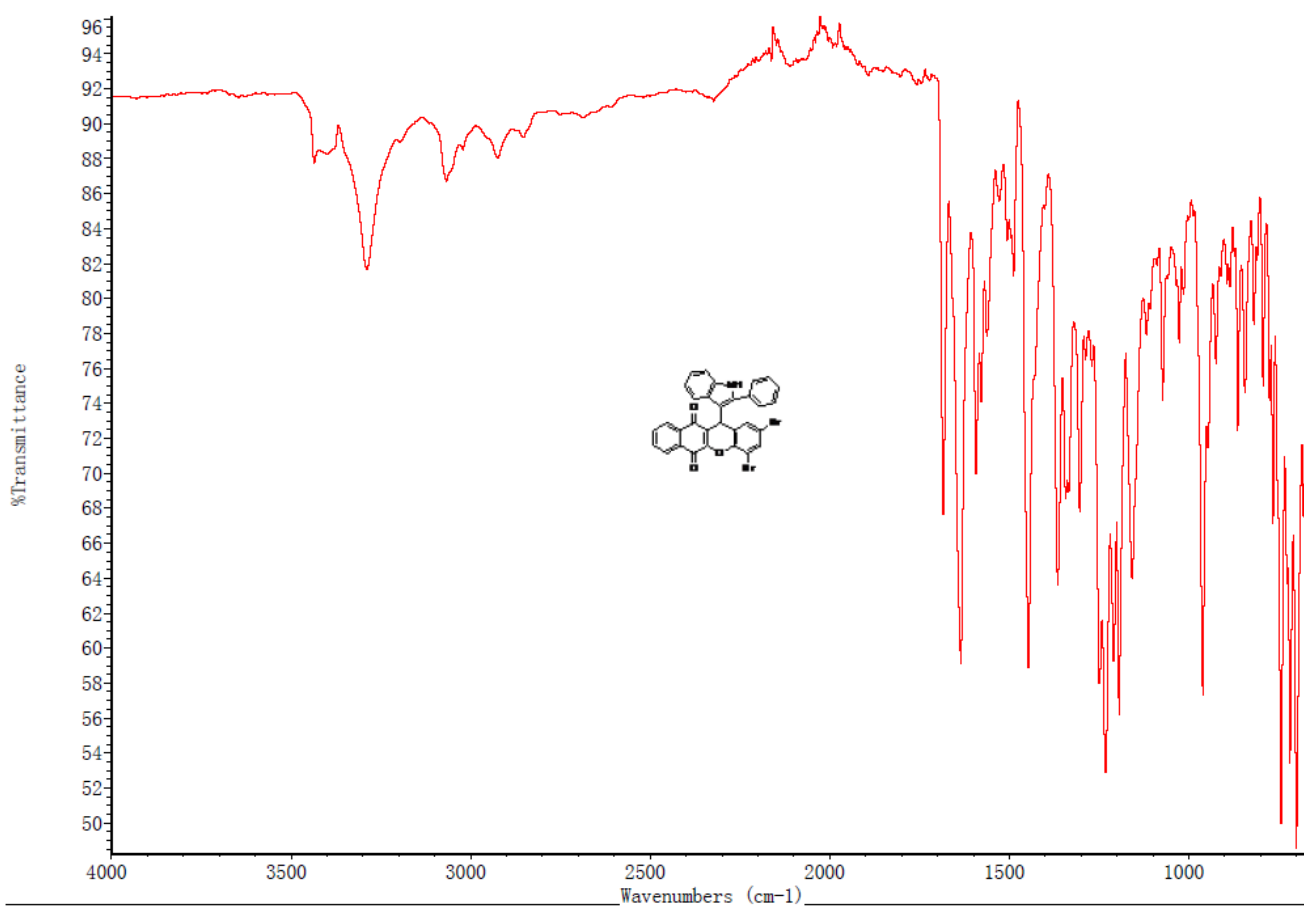
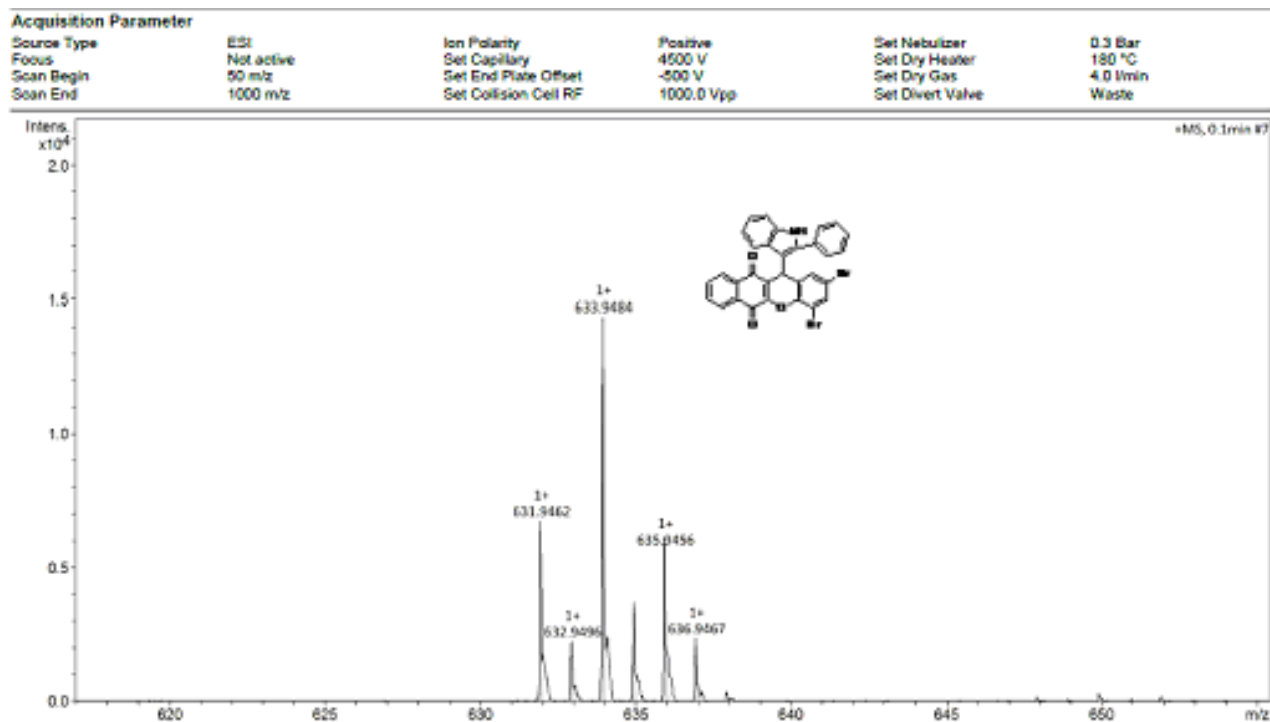


Figure S28 ¹³C NMR of 4g



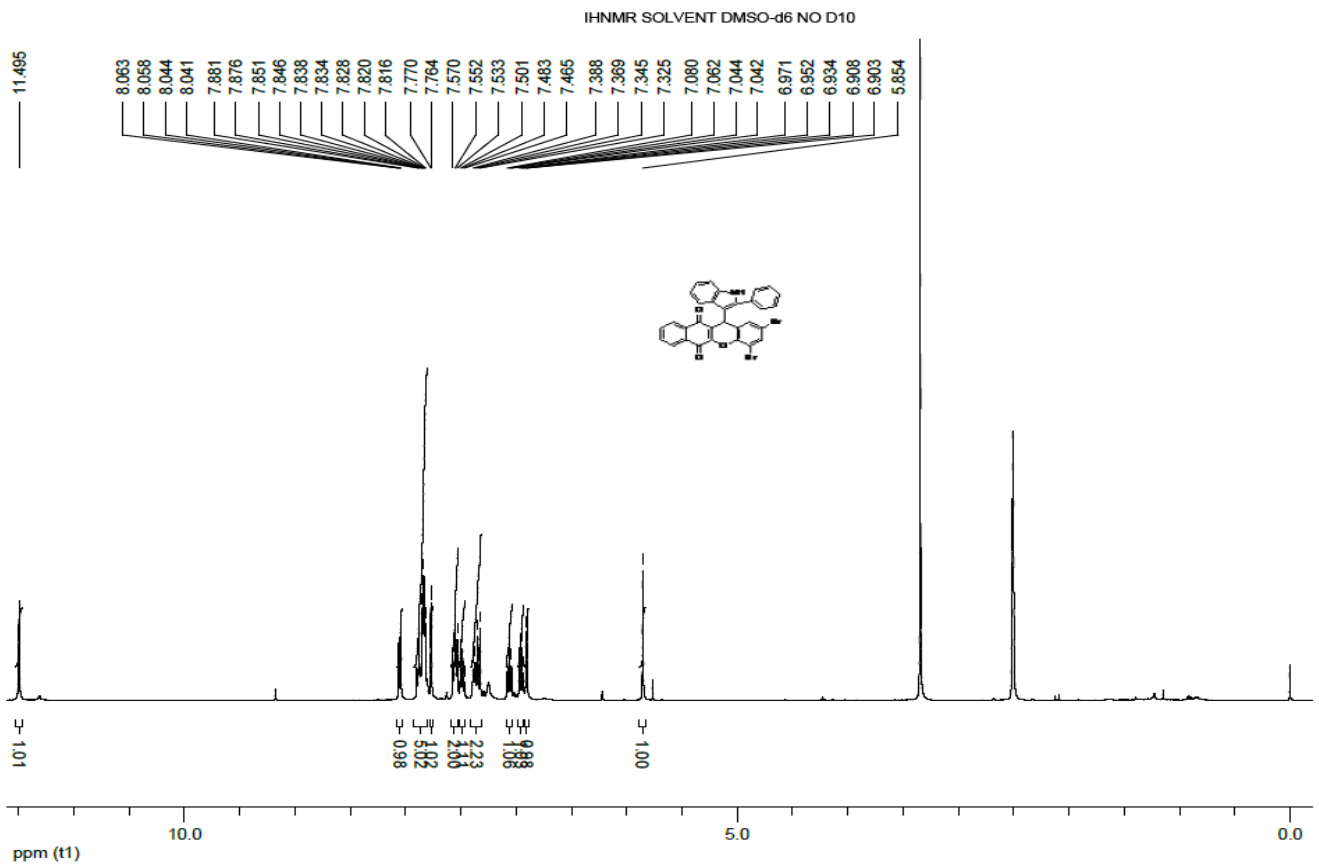


Figure S31 1H NMR of 4h

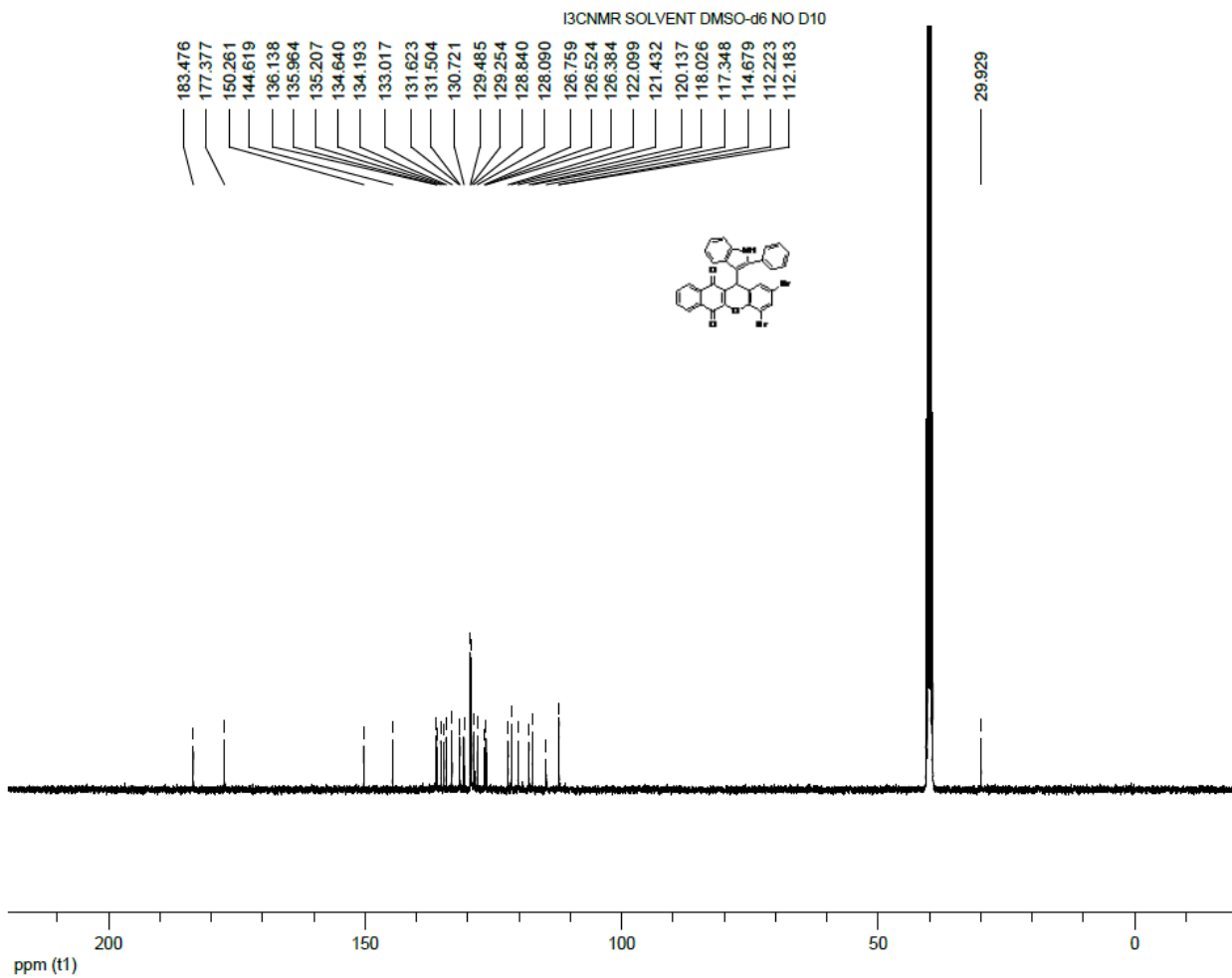


Figure S32 13C NMR of 4h

Acquisition Parameter					
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	600.0 Vpp	Set Divert Valve	Waste

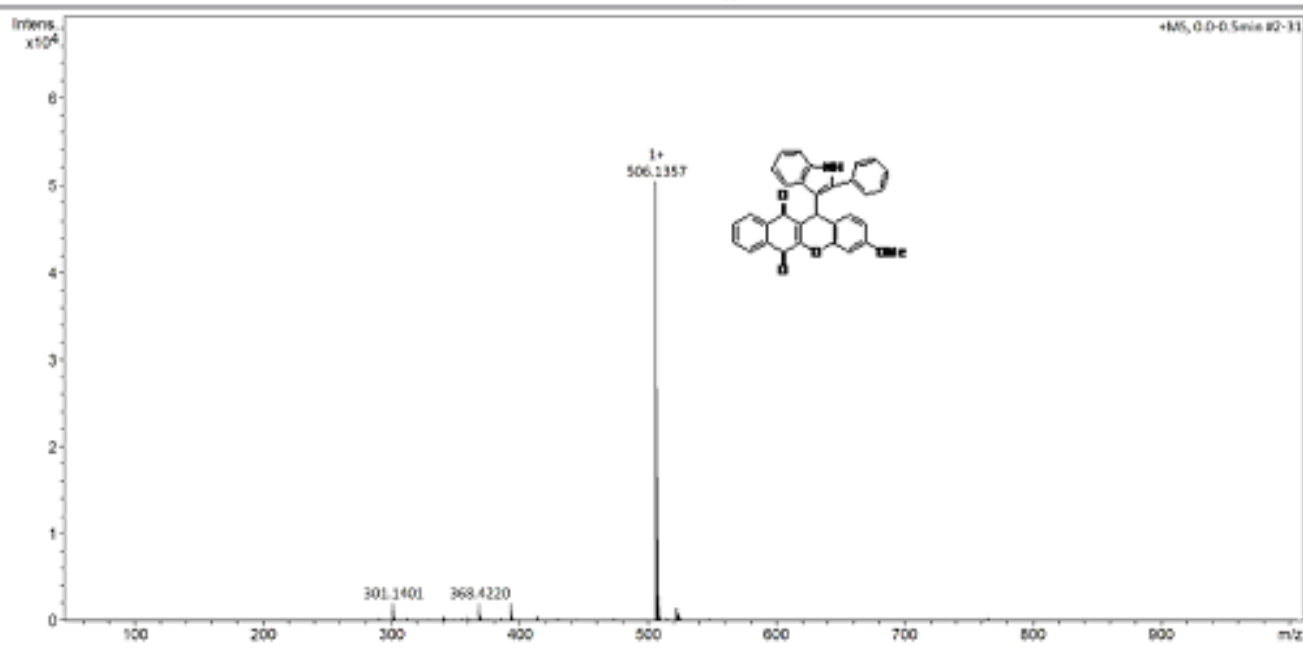


Figure S33 HRMS of 4i

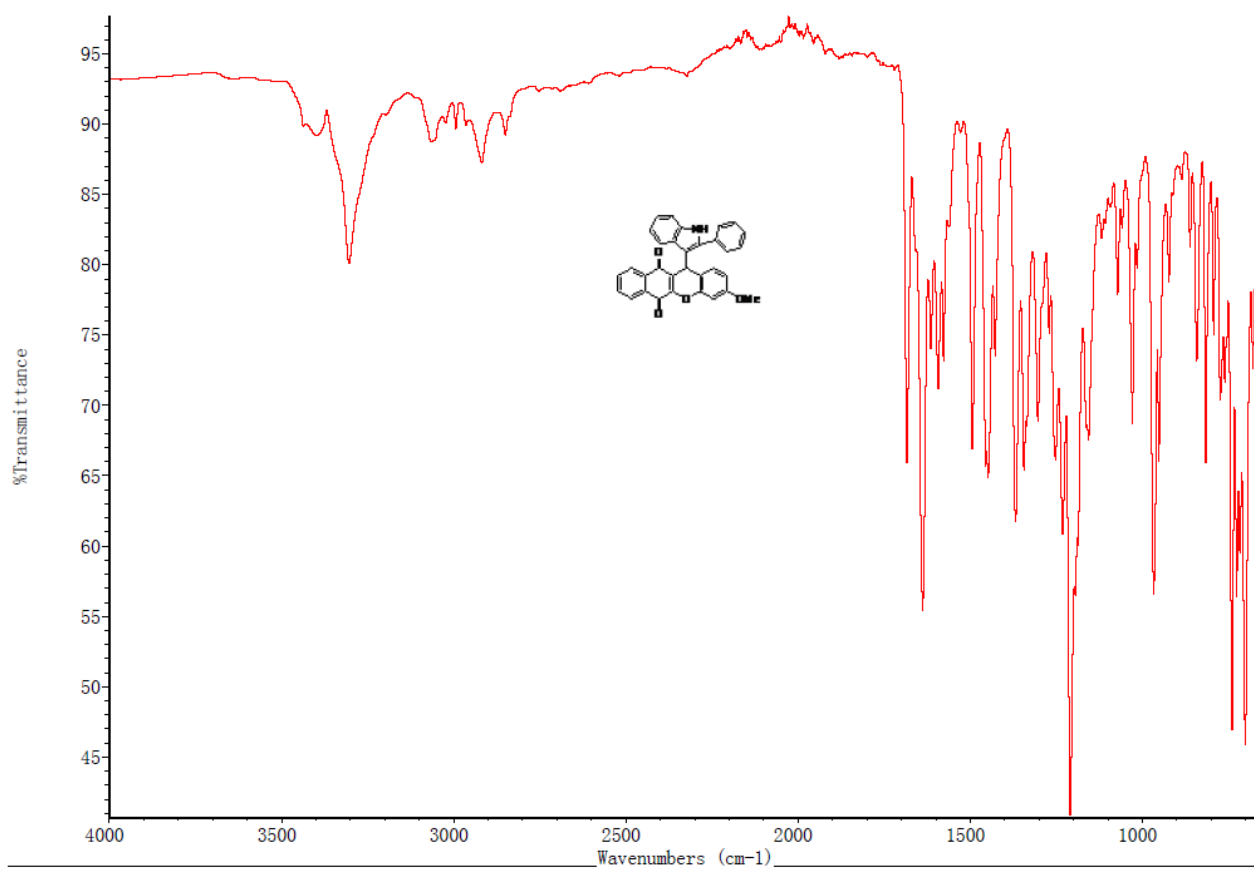


Figure S34 IR of 4i

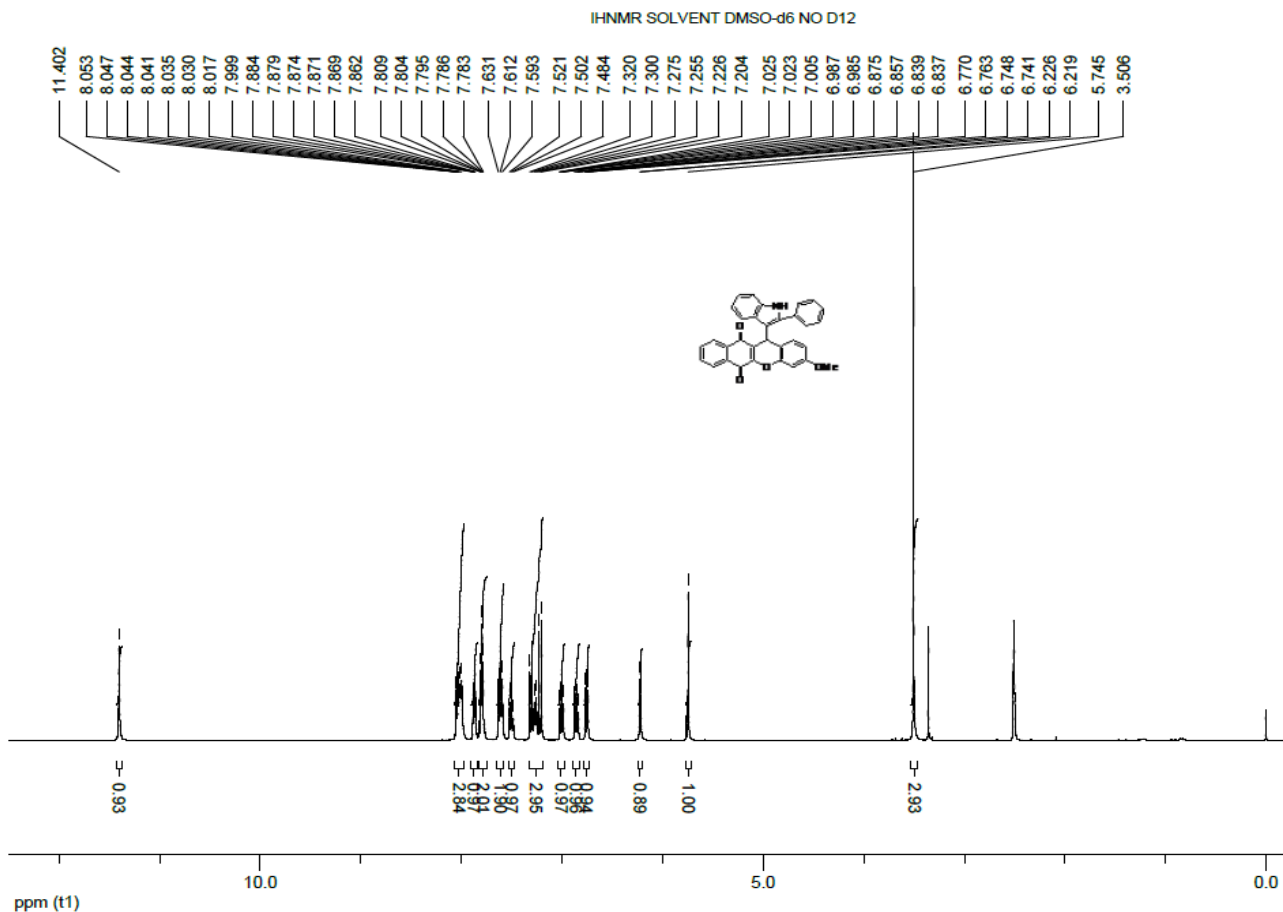


Figure S35 1H NMR of **4i**

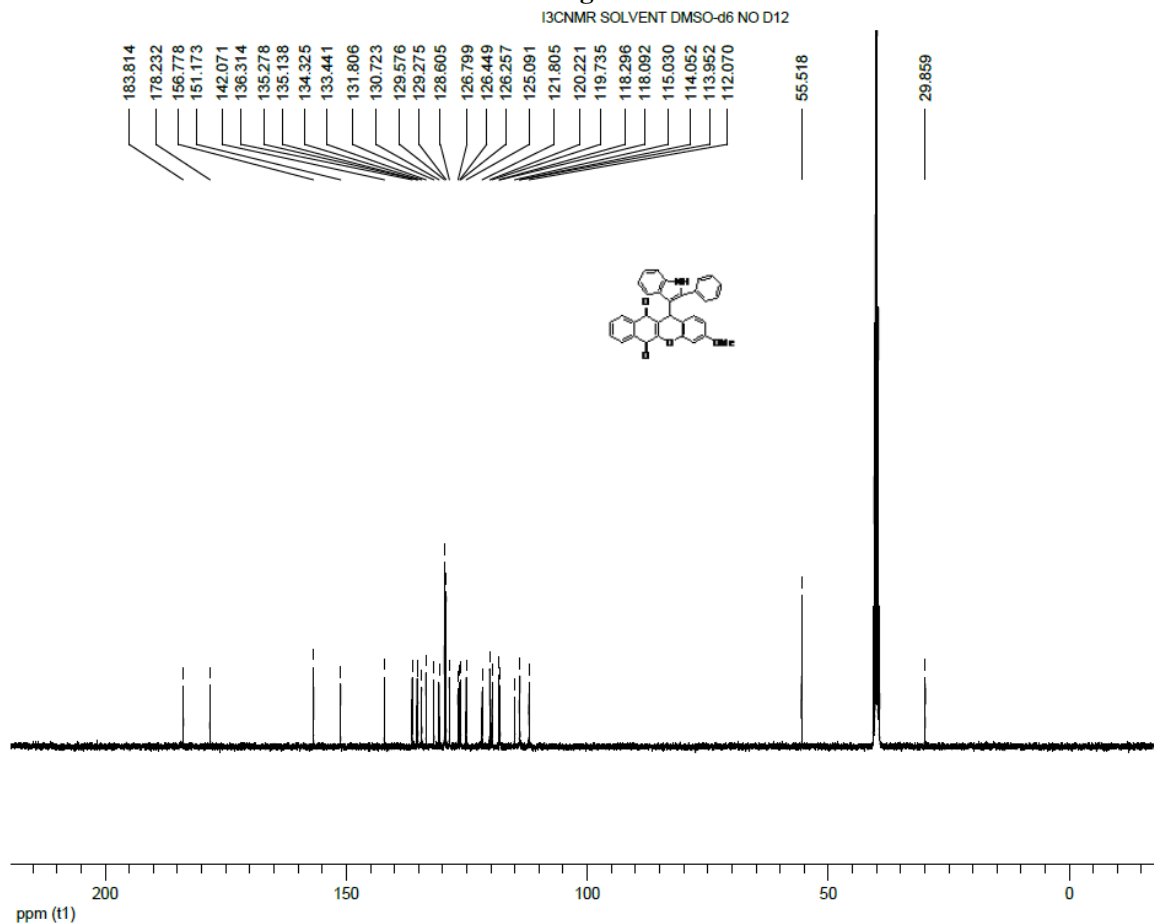


Figure S36 13C NMR of **4i**

Acquisition Parameter					
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	180.0 Vpp	Set Divert Valve	Waste

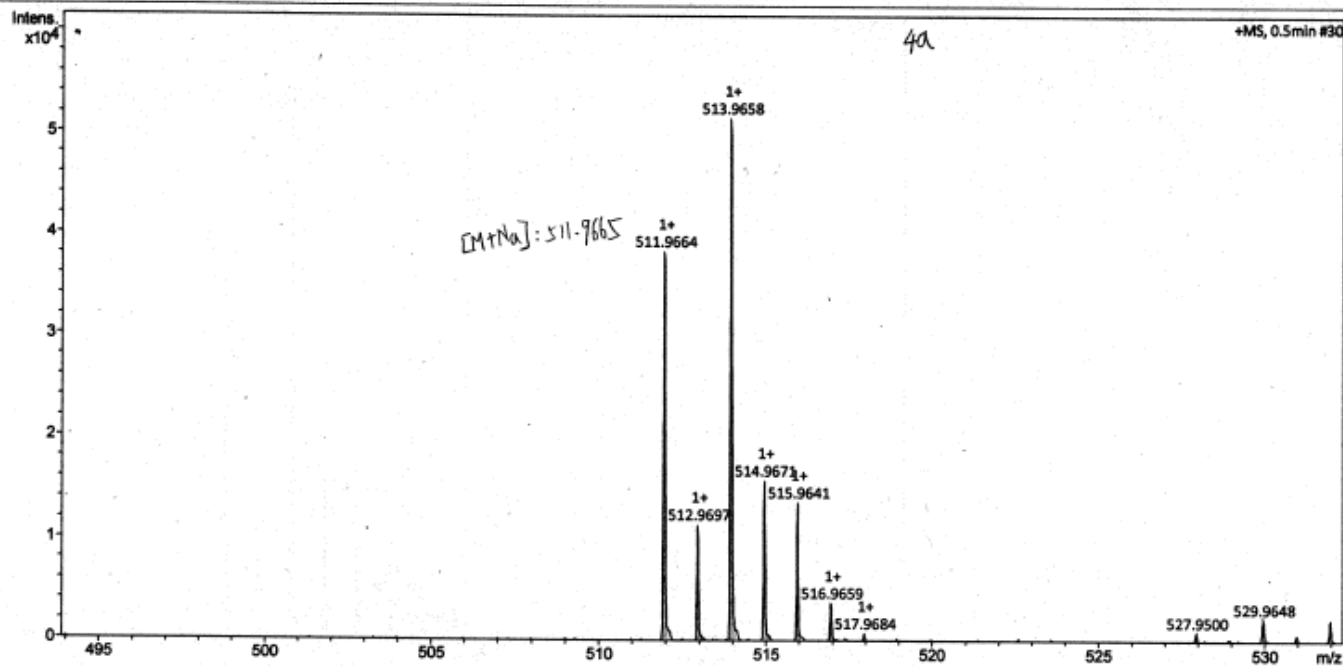


Figure S37 HRMS of 4j

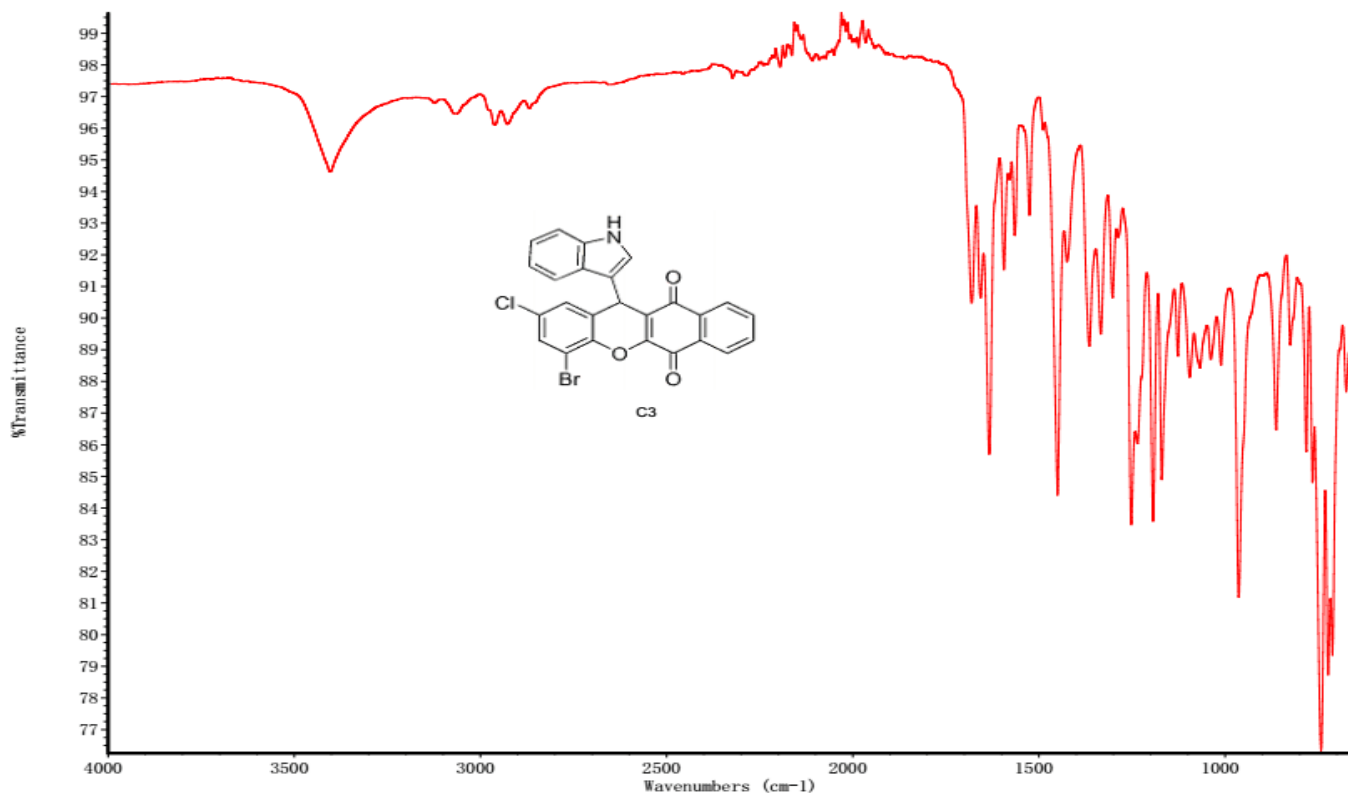


Figure S38 IR of 4j

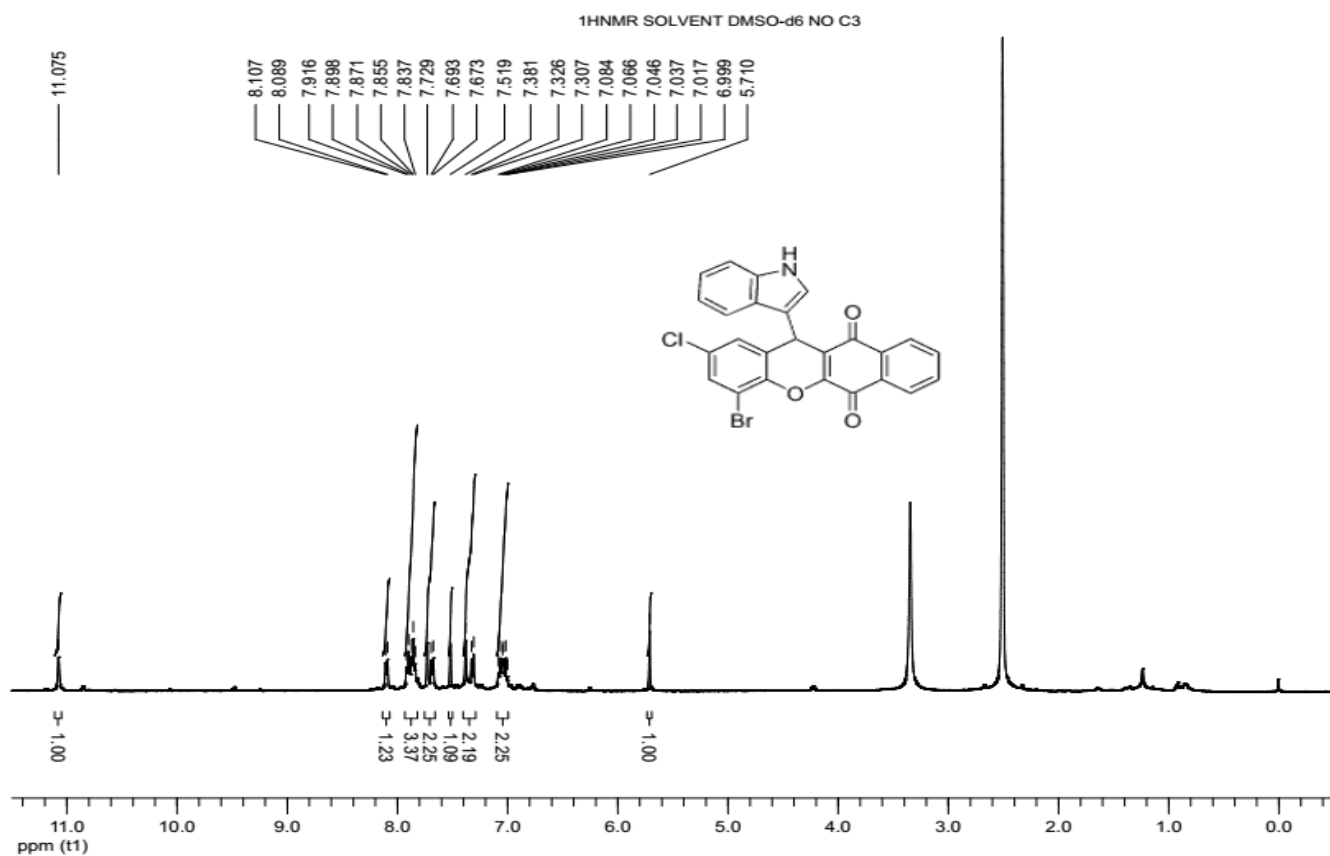


Figure S39 ¹H NMR of 4j

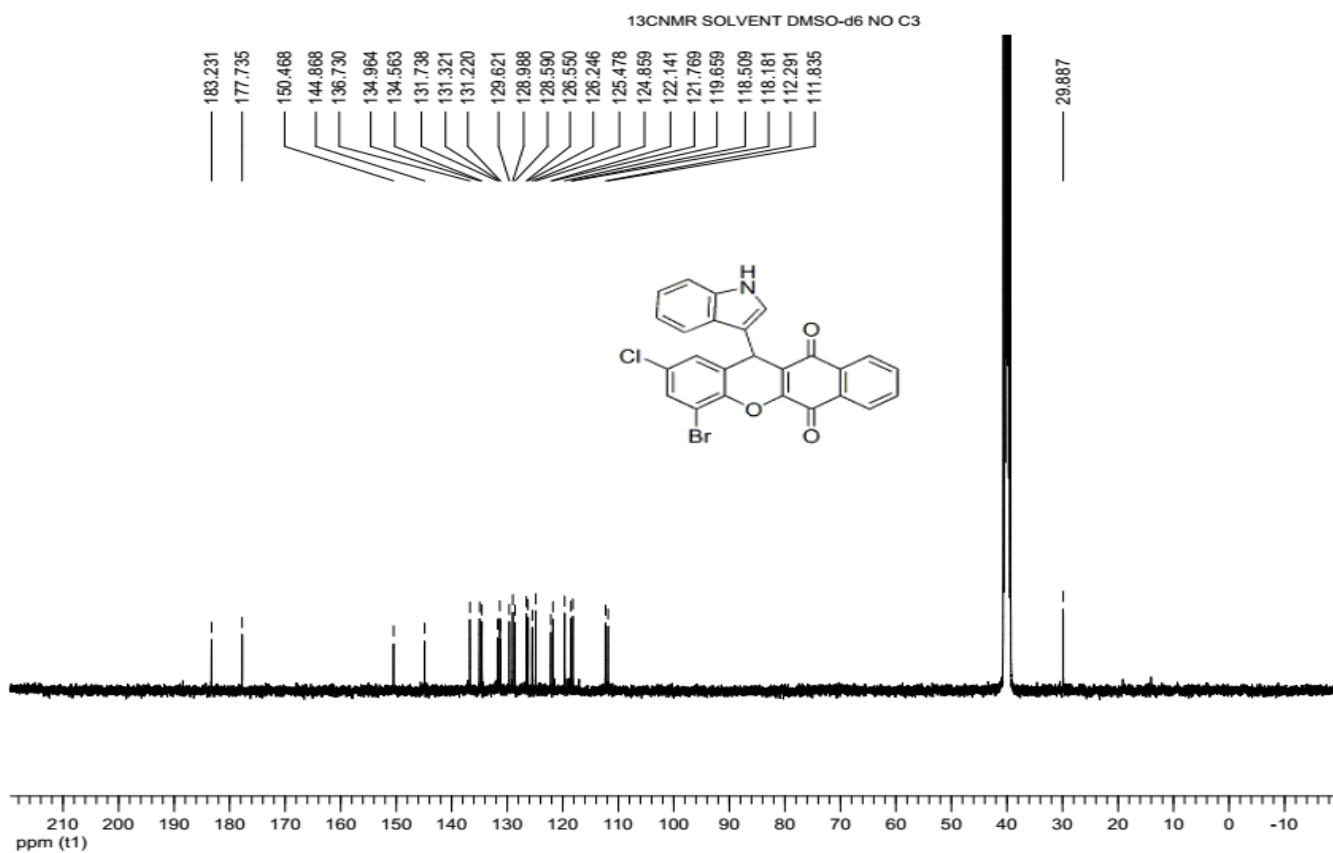


Figure S40 ¹³C NMR 4j

Acquisition Parameter

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	180.0 Vpp	Set Divert Valve	Waste

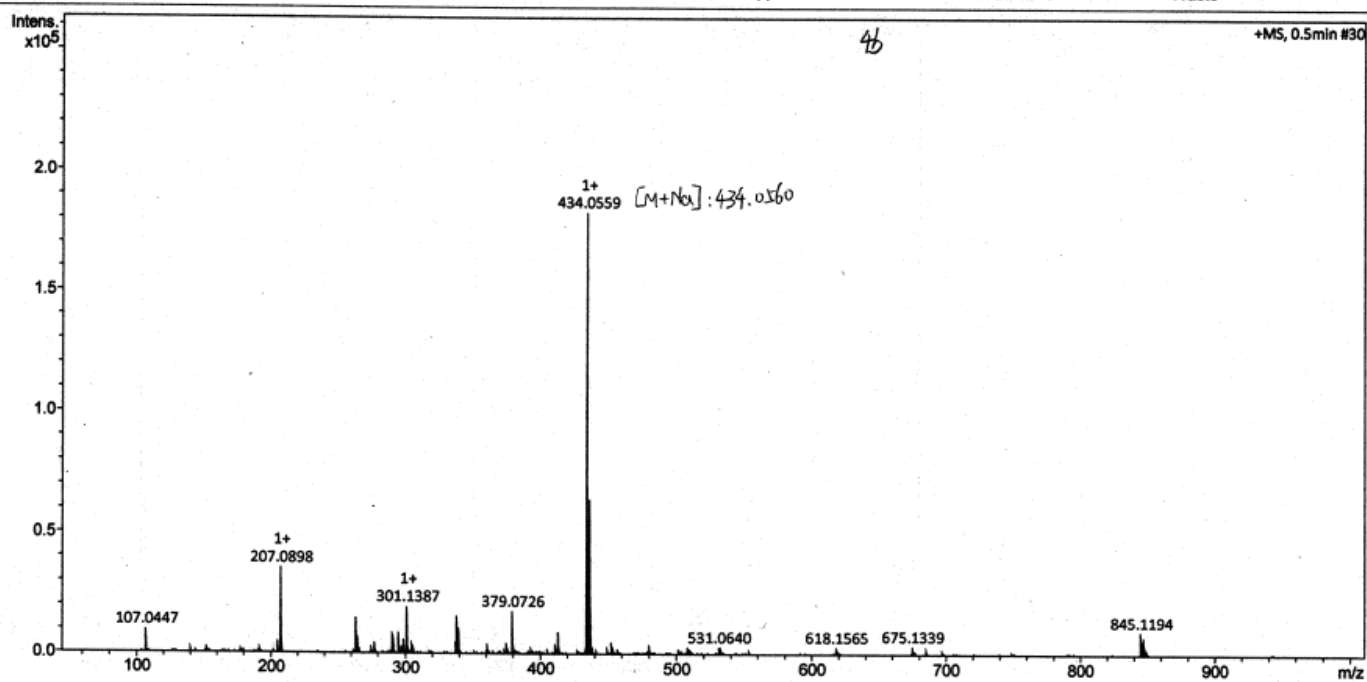


Figure S41 HRMS of 4k

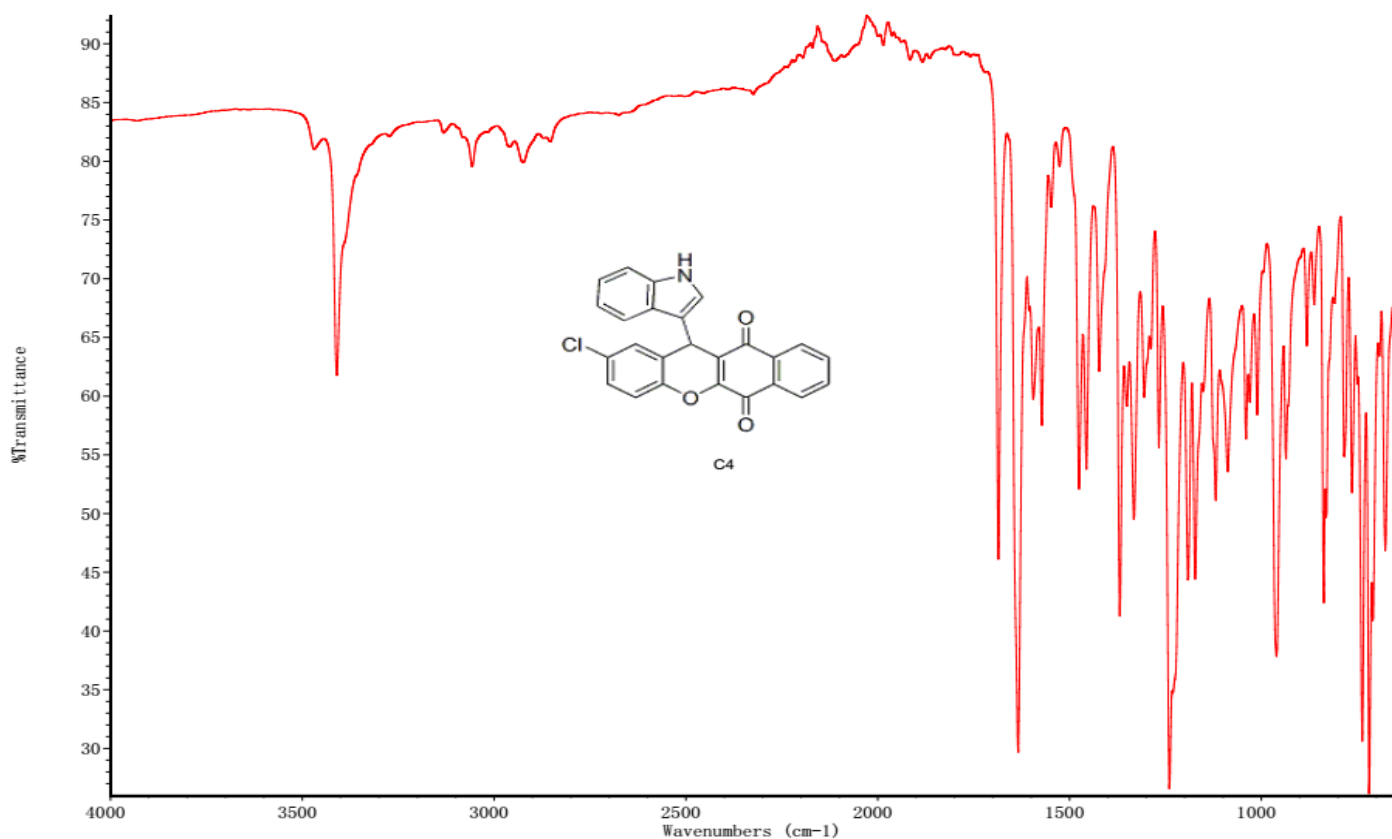


Figure S42 IR of 4k

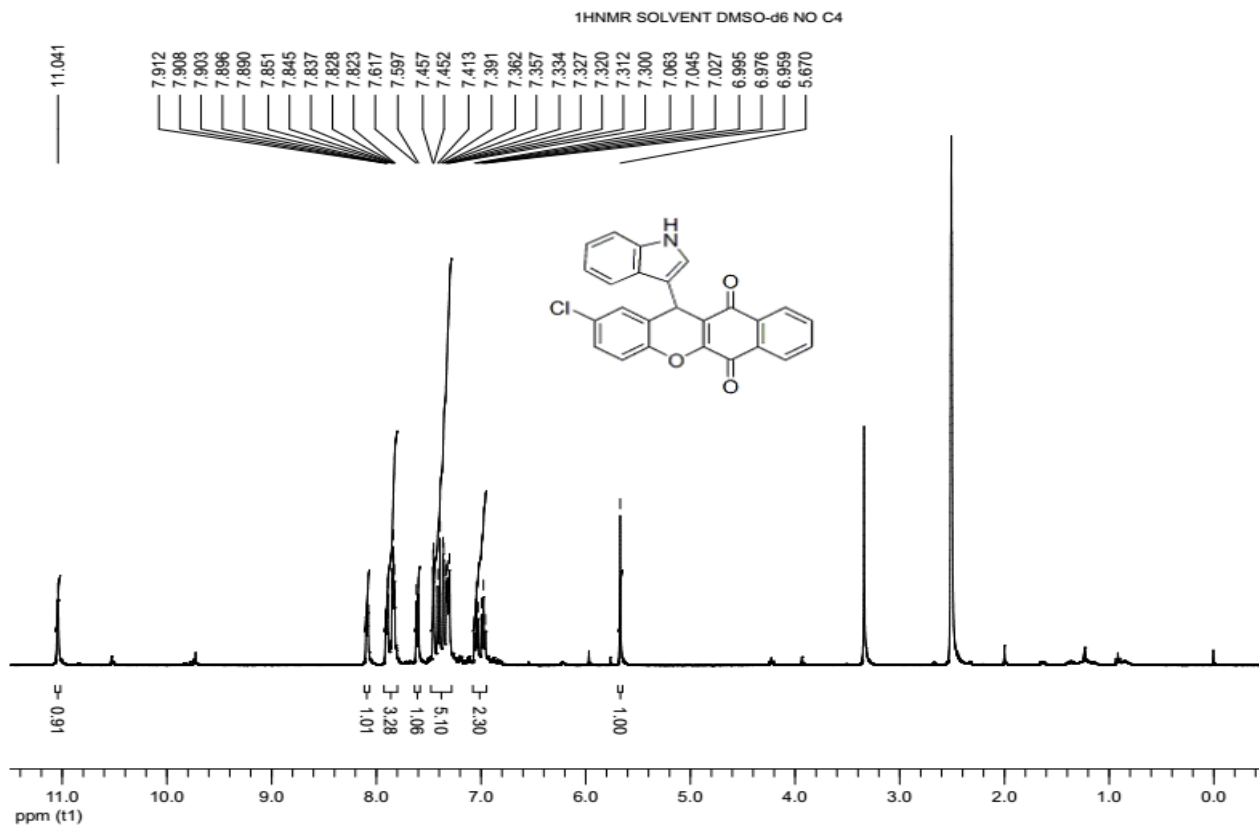


Figure S43 ^1H NMR of 4k

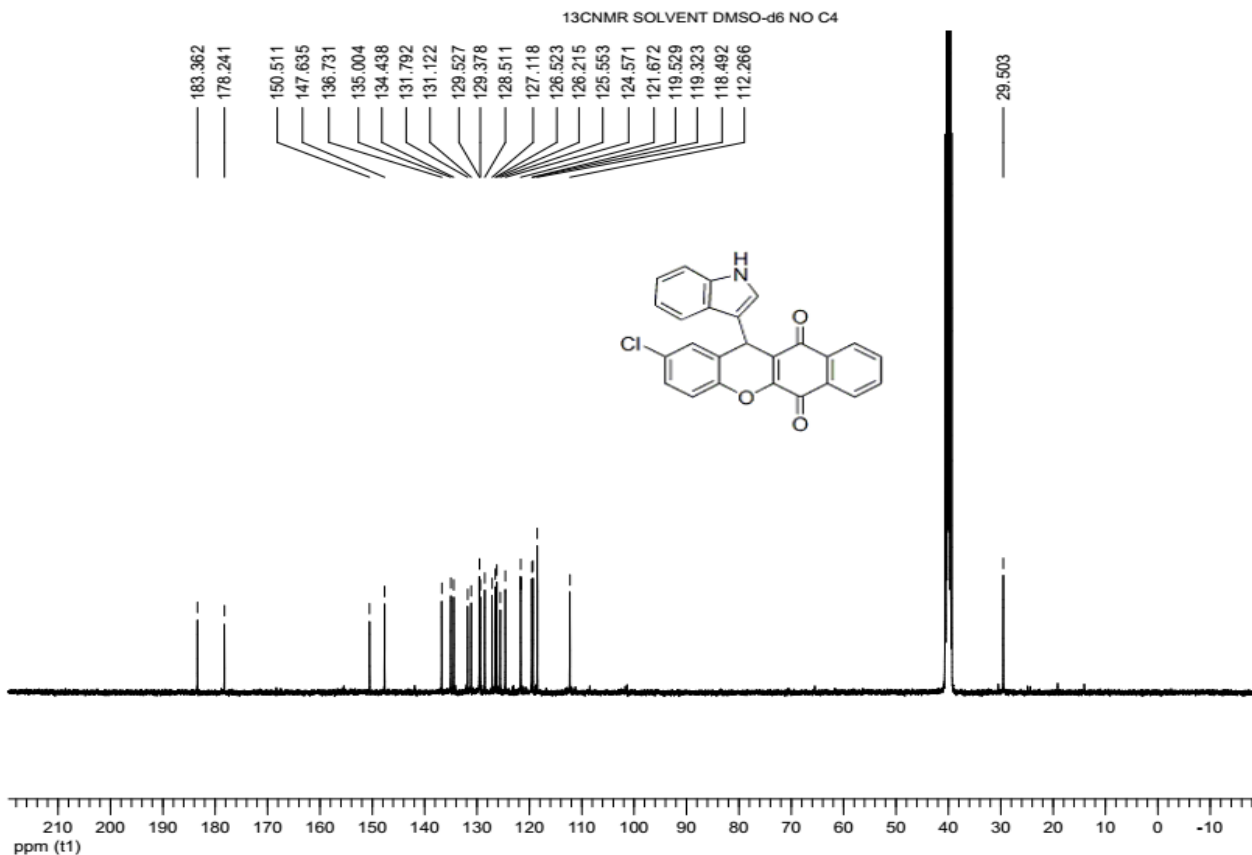


Figure S44 ^{13}C NMR of 4k

Acquisition Parameter					
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	180.0 Vpp	Set Divert Valve	Waste

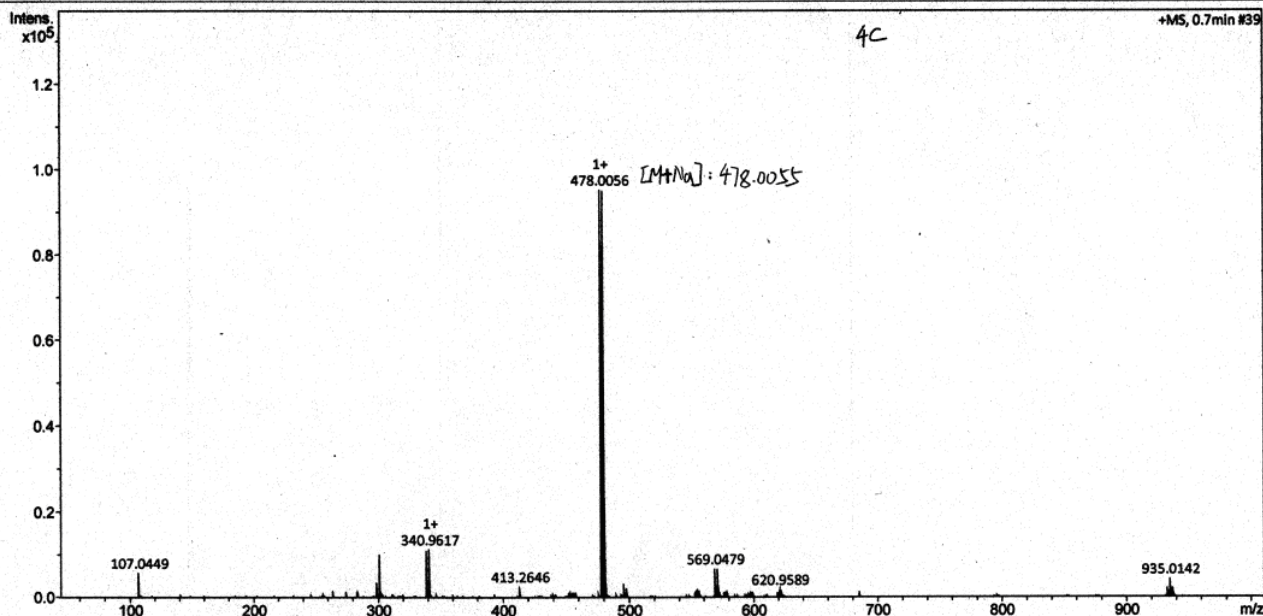


Figure S45 HRMS of 4I

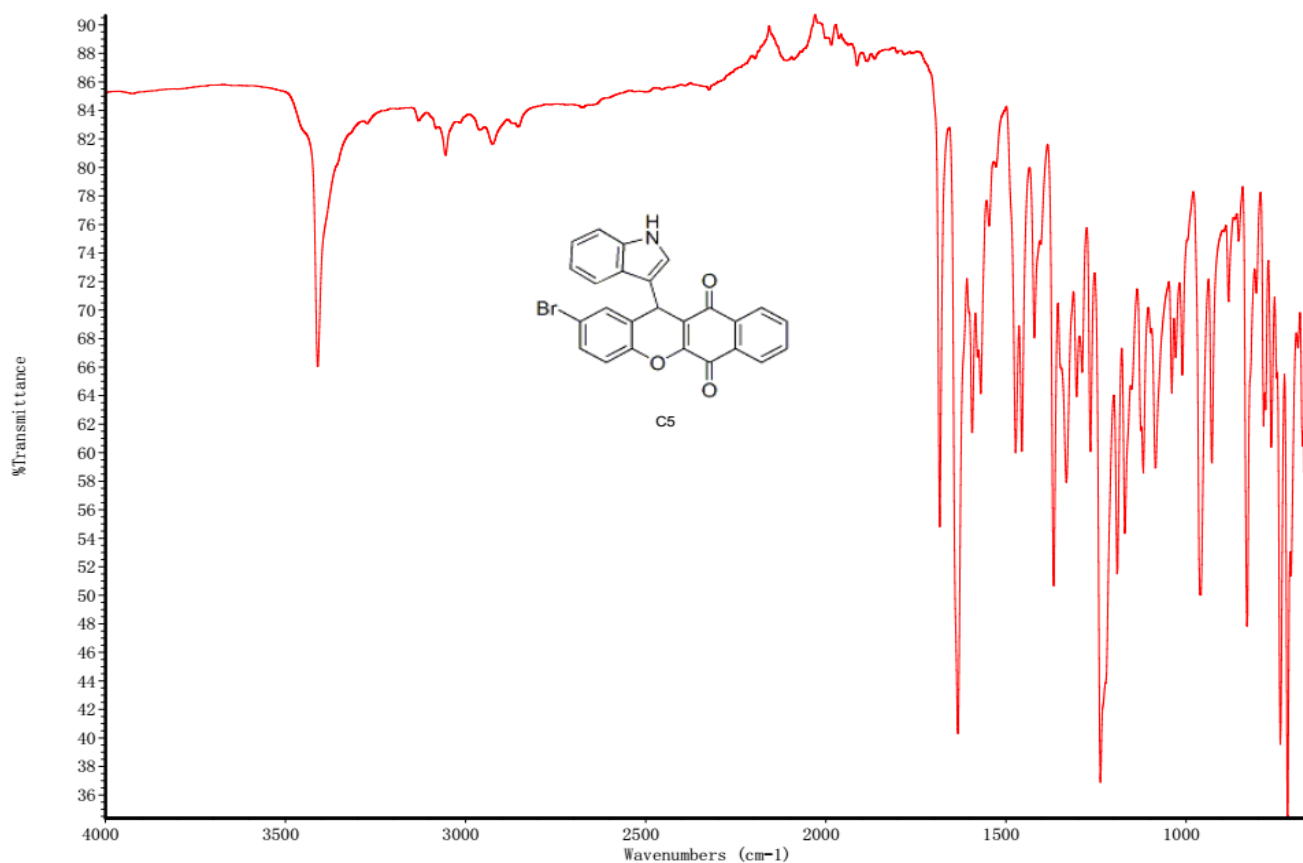


Figure S46 IR of 4I

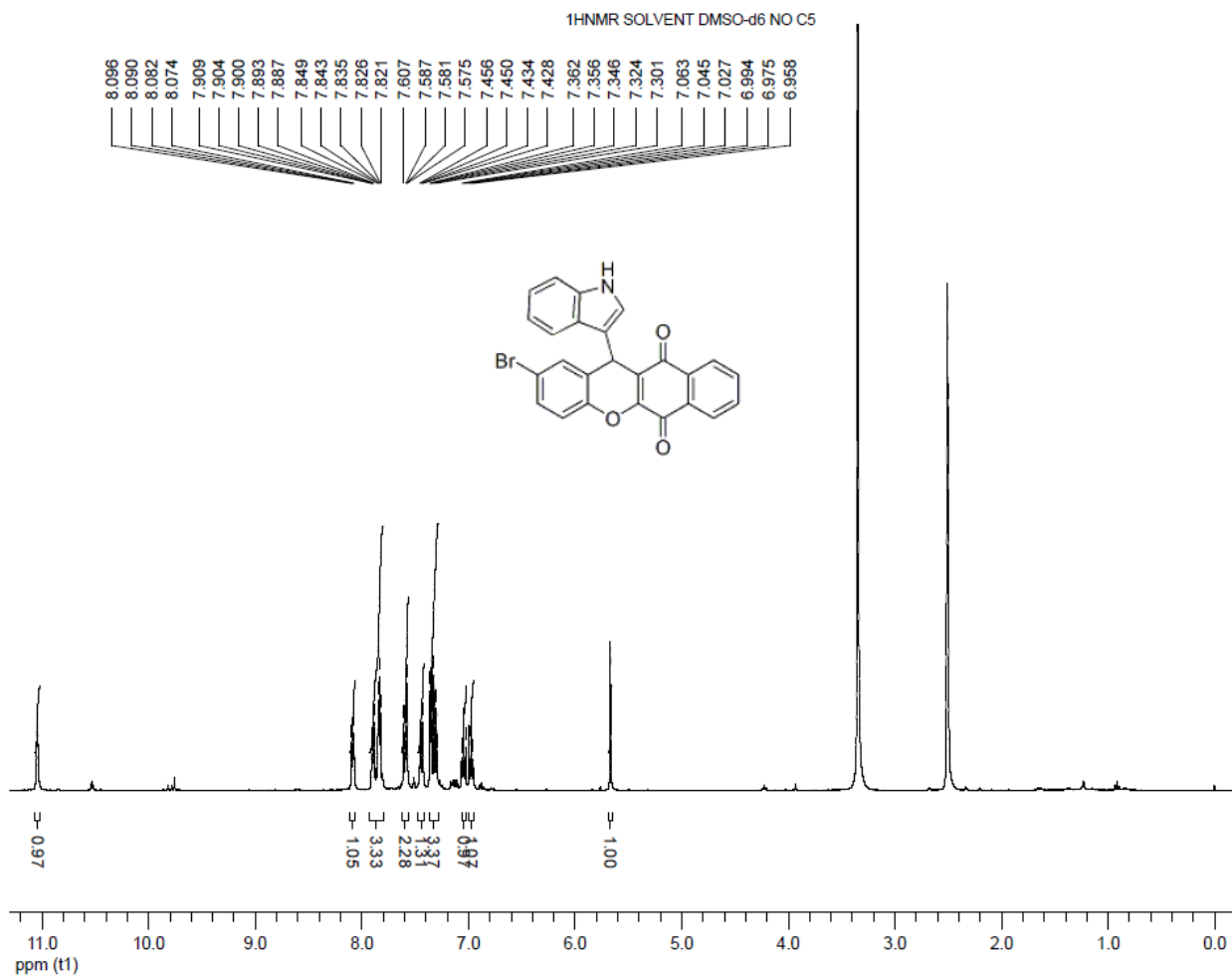


Figure S47 ¹H NMR of 4l

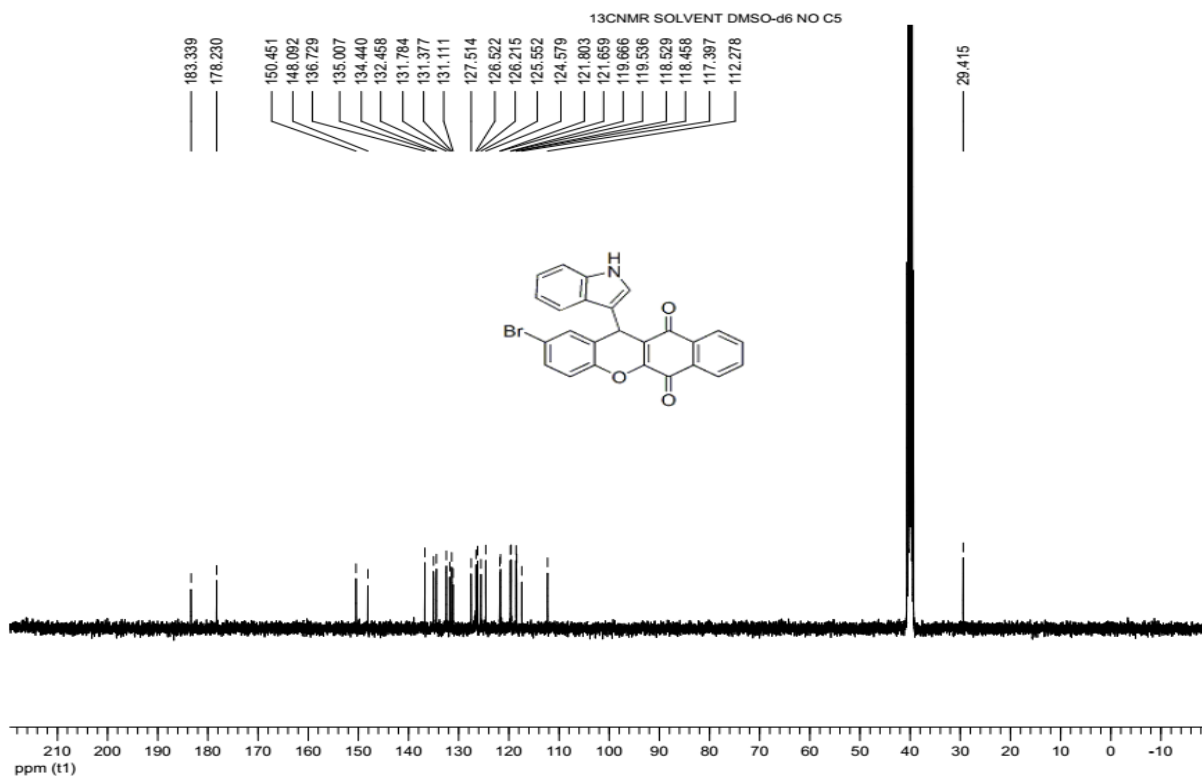
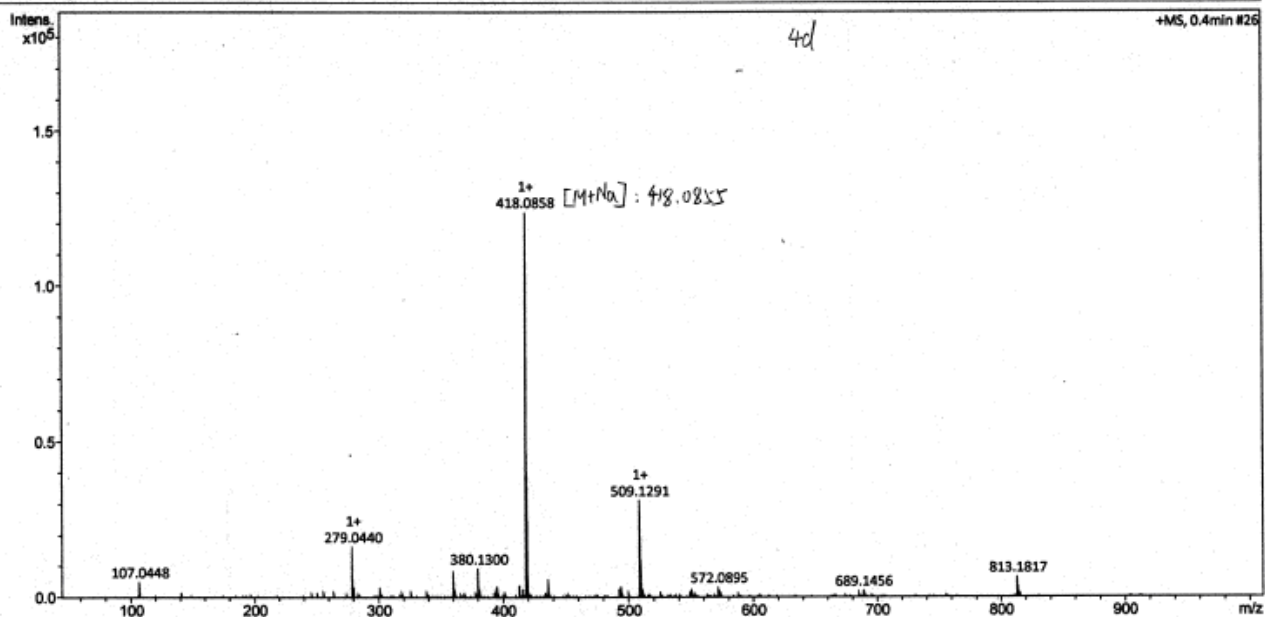
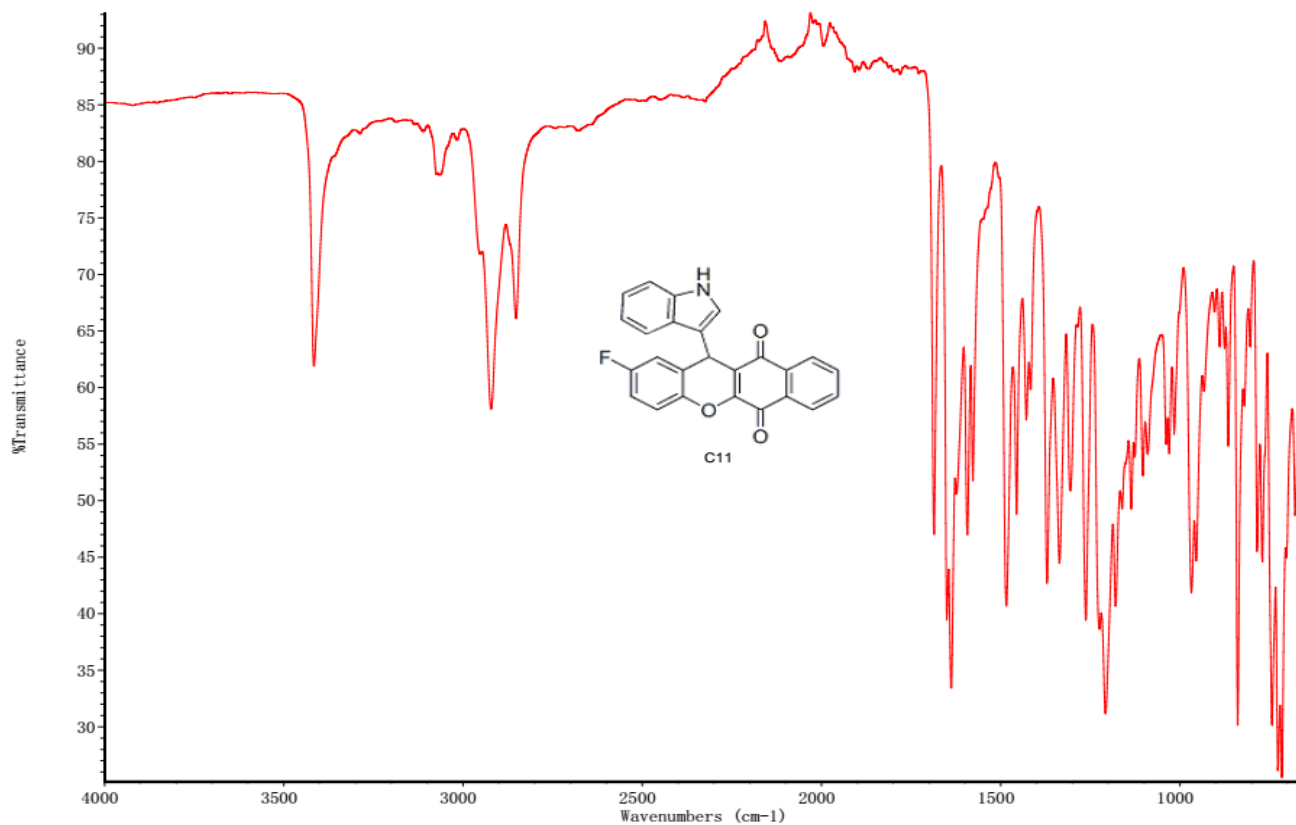
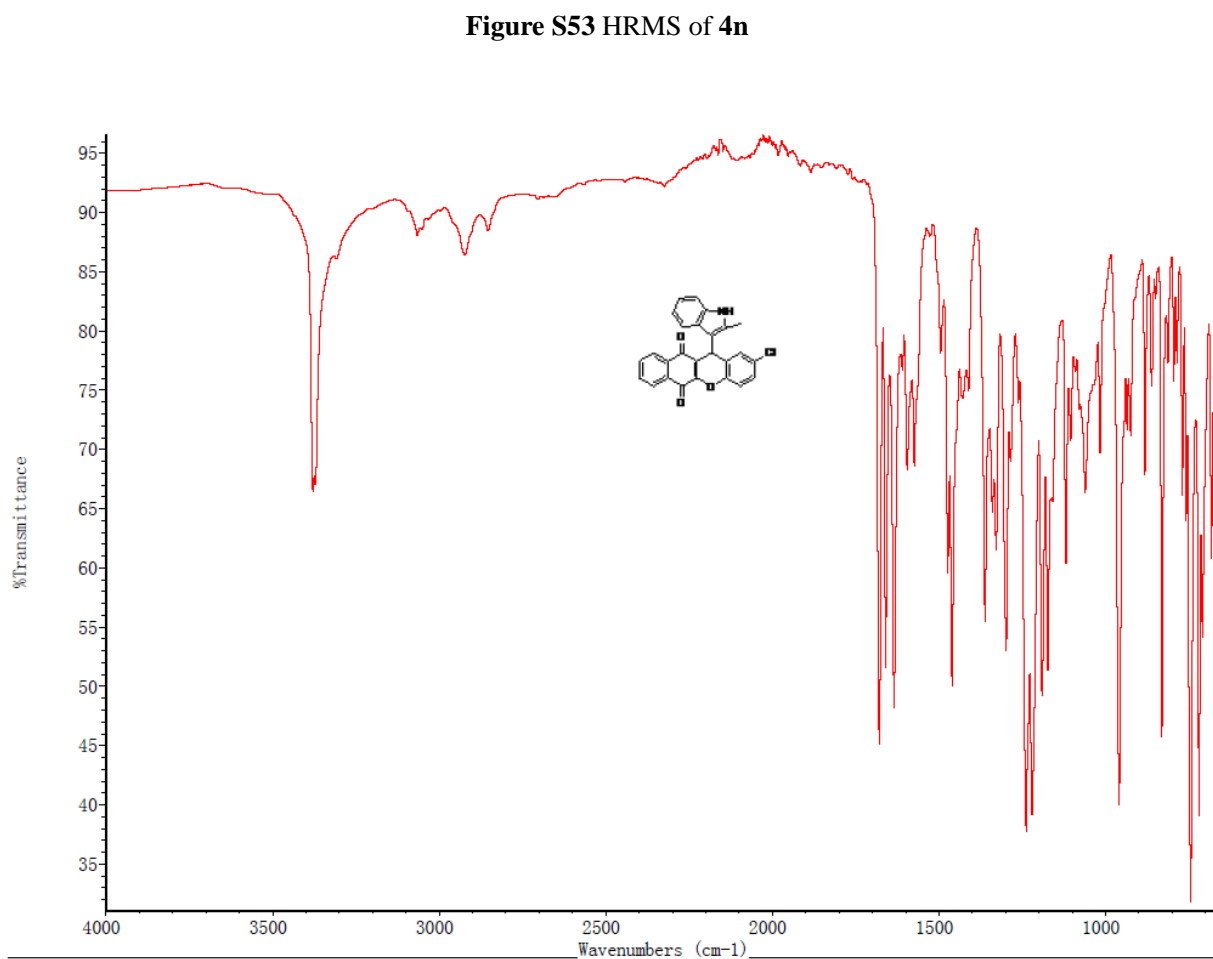
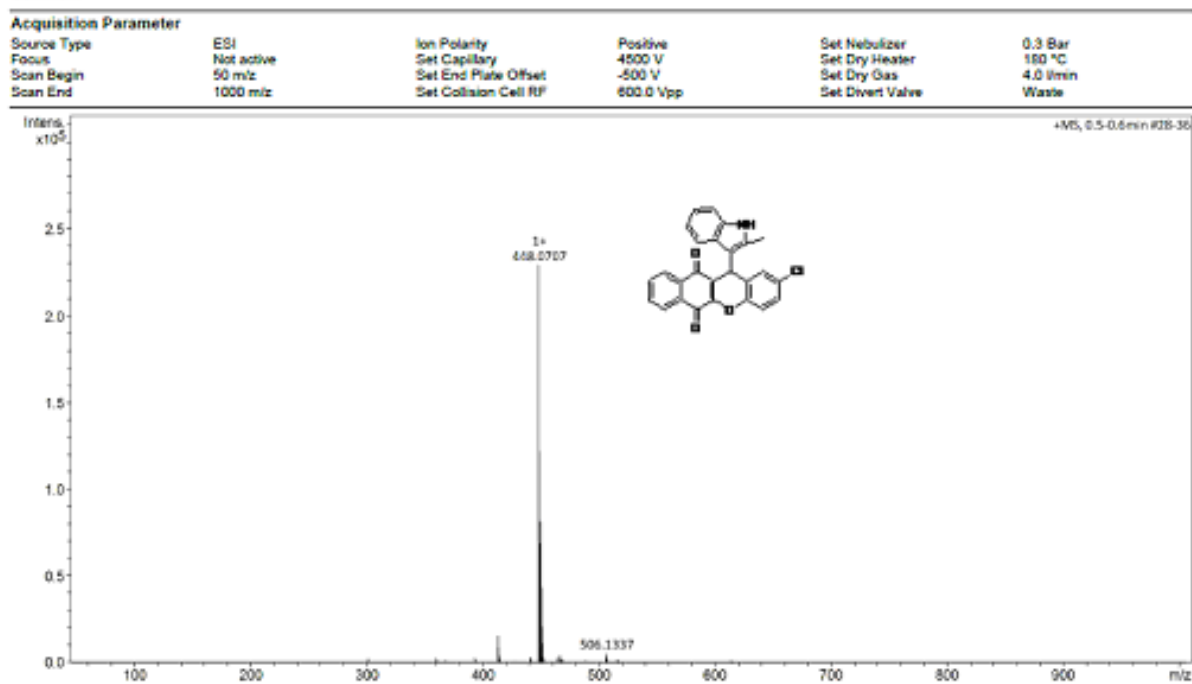


Figure S48 ¹³C NMR of 4l

Acquisition Parameter

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	180.0 Vpp	Set Divert Valve	Waste

**Figure S49 HRMS of 4m****Figure S50 IR of 4m**



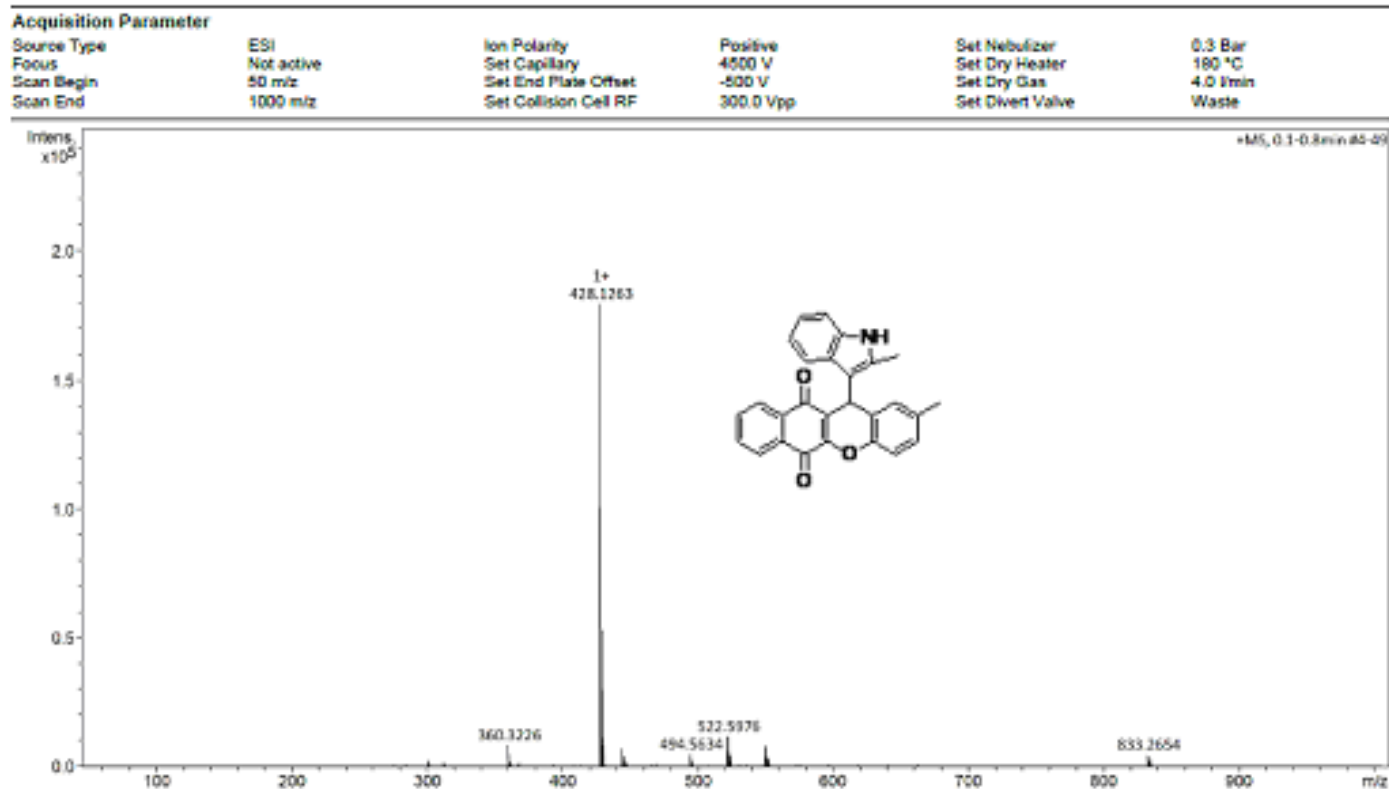


Figure S57 HRMS of **4o**

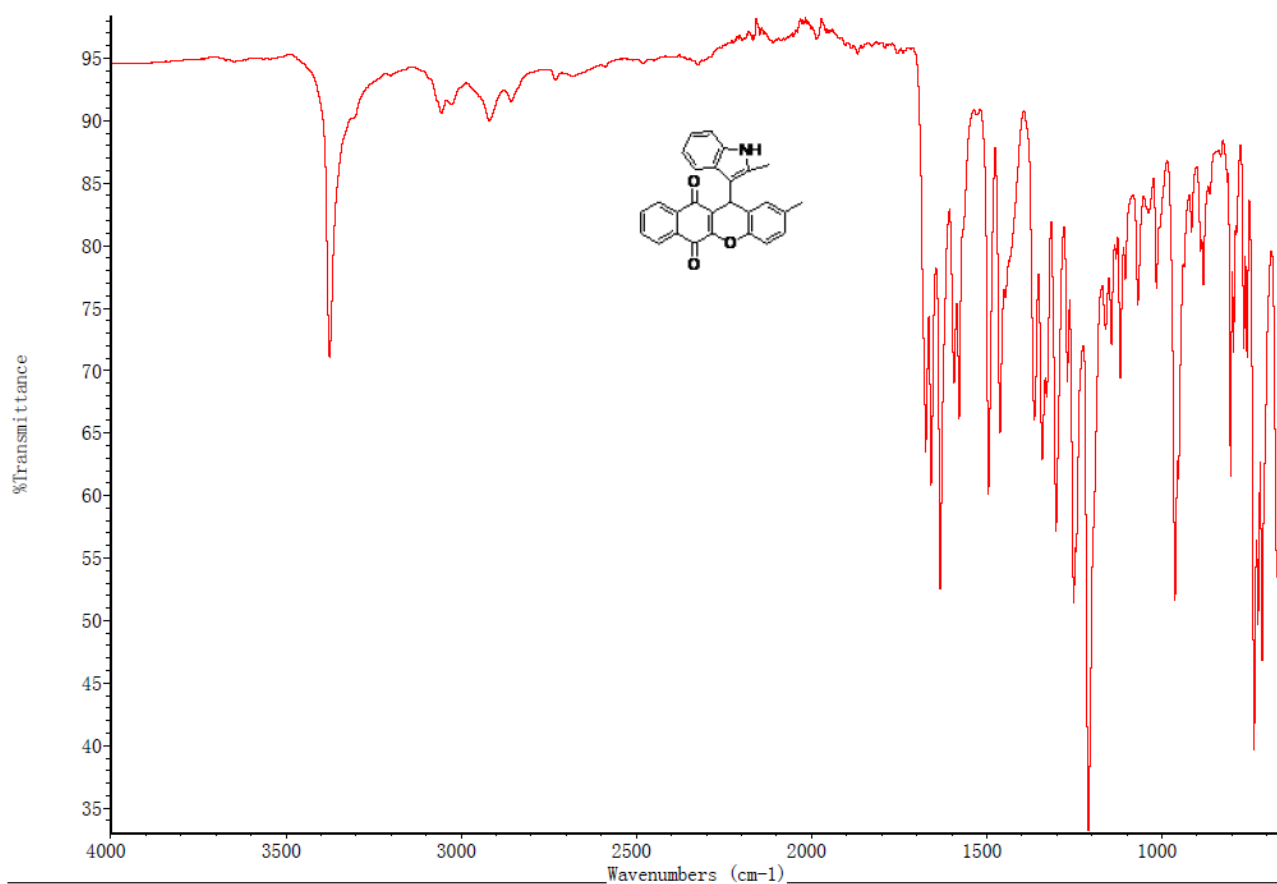


Figure S58 IR of **4o**

1H NMR SOLVENT DMSO-d6 NO D4X

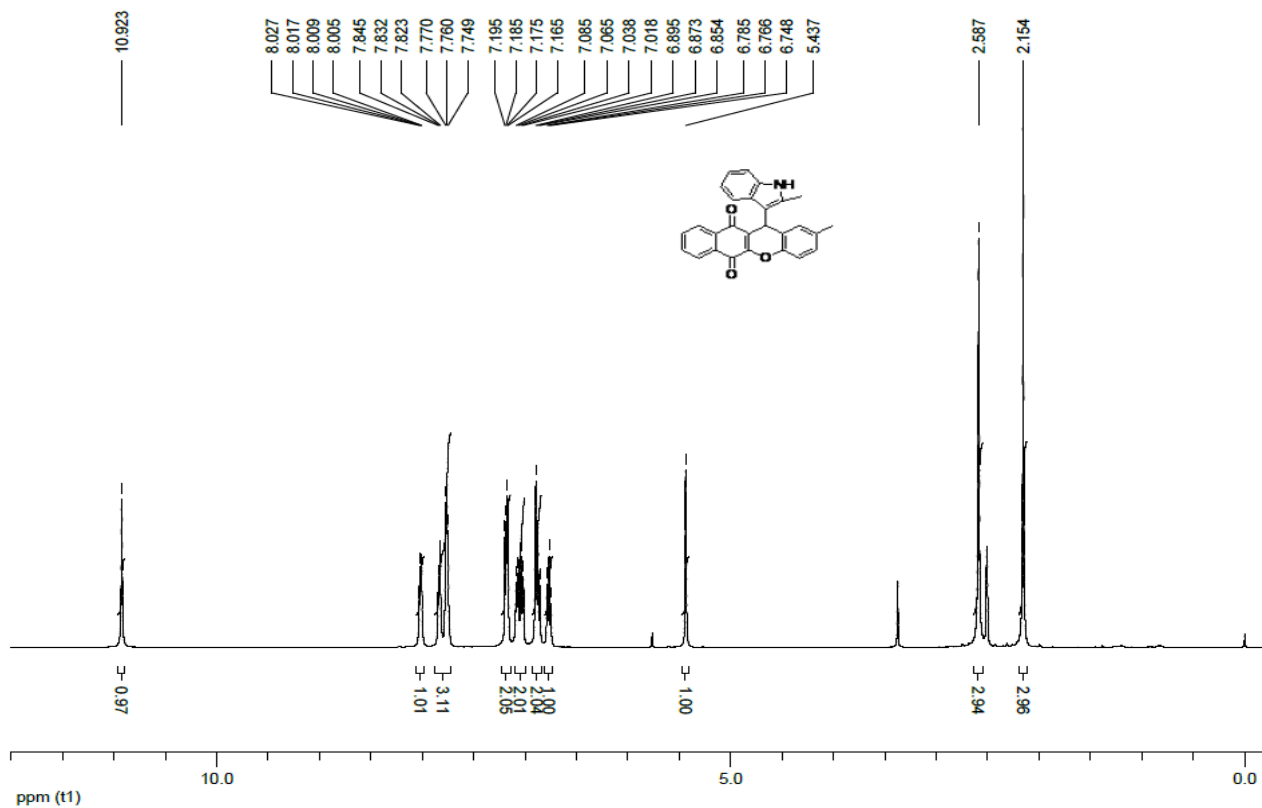


Figure S59 ¹H NMR of 4o

13C NMR SOLVENT DMSO-d6 NO D4X

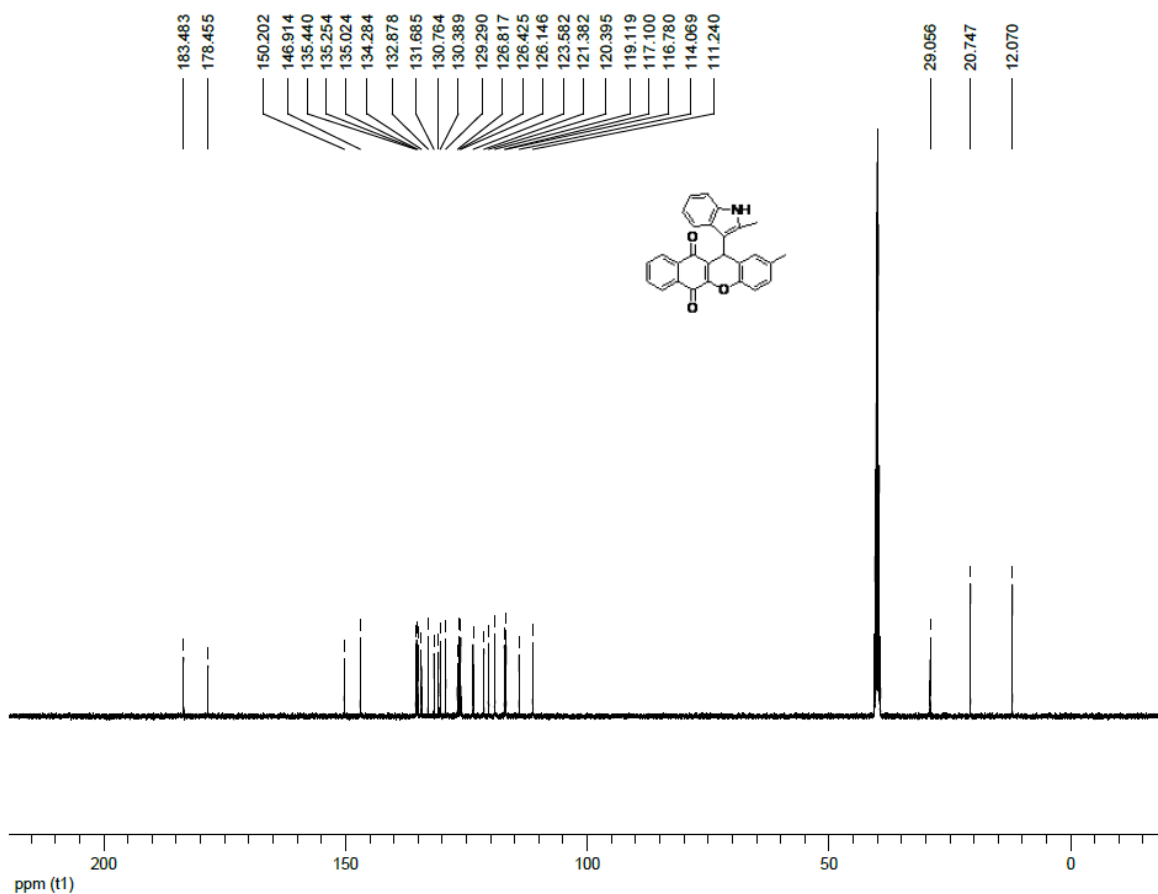
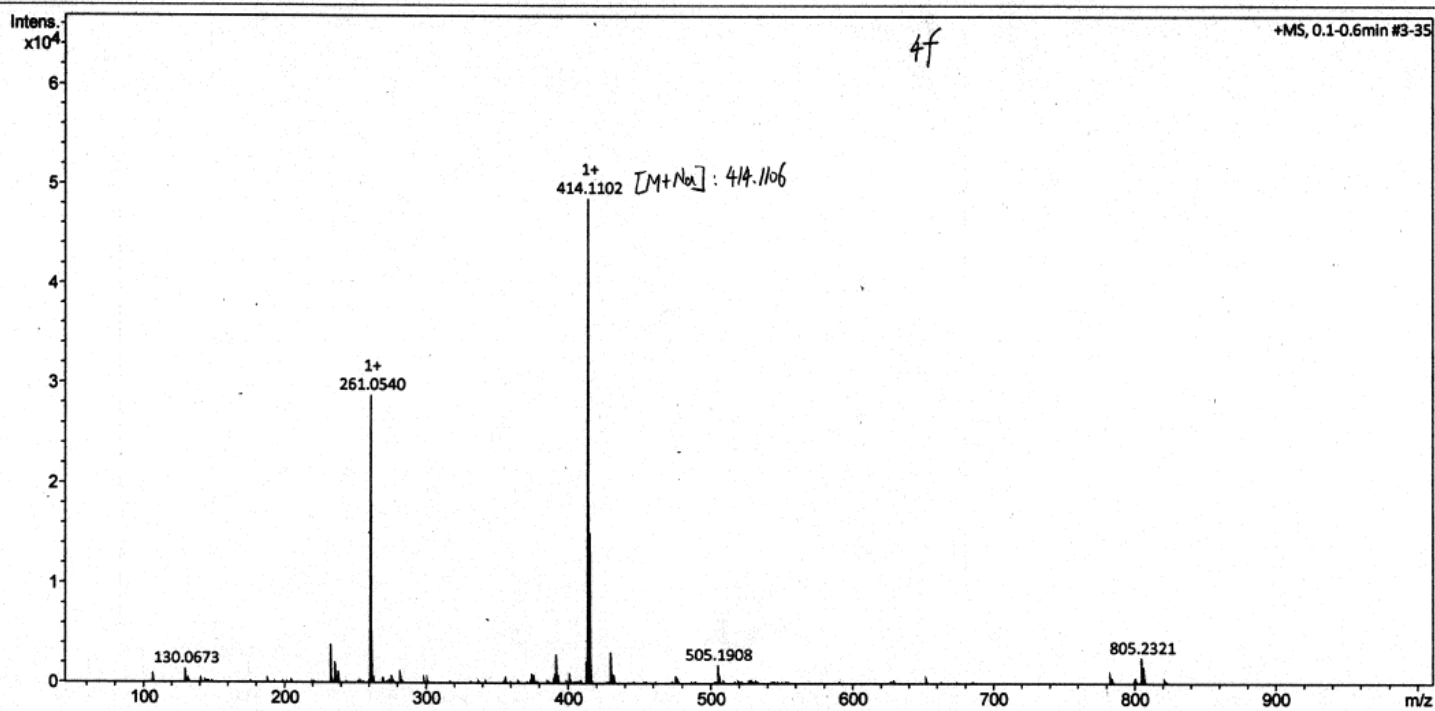
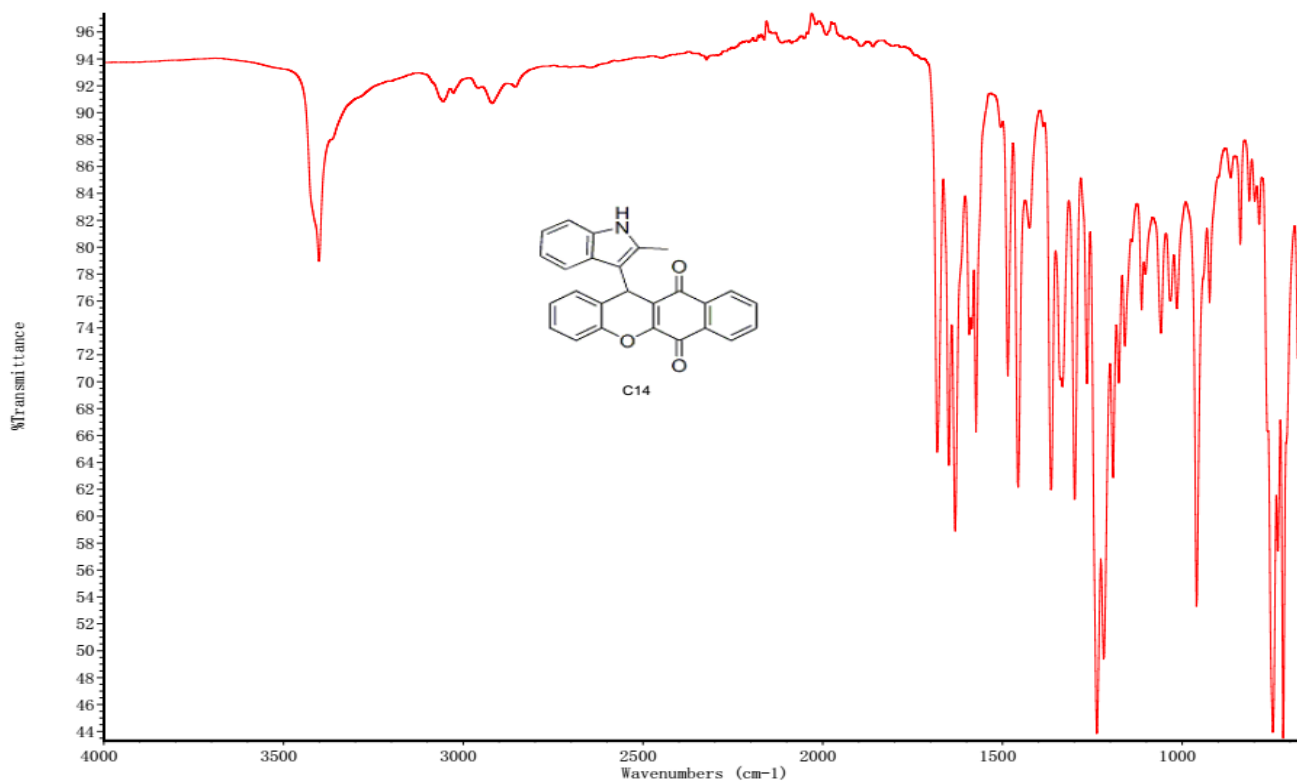


Figure S60 ¹³C NMR of 4o

Acquisition Parameter

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	180.0 Vpp	Set Divert Valve	Waste

**Figure S61 HRMS of 4p****Figure S62 IR of 4p**

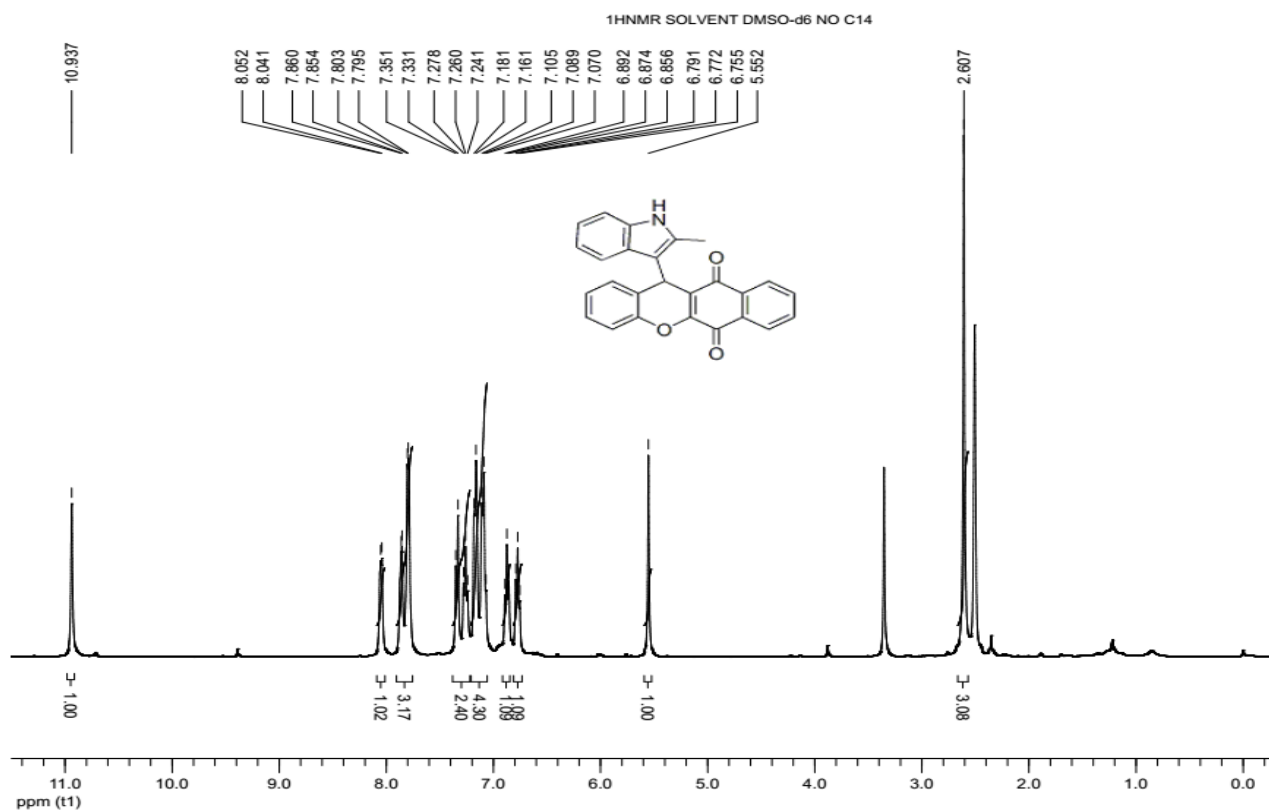


Figure S63 ^1H NMR of 4p

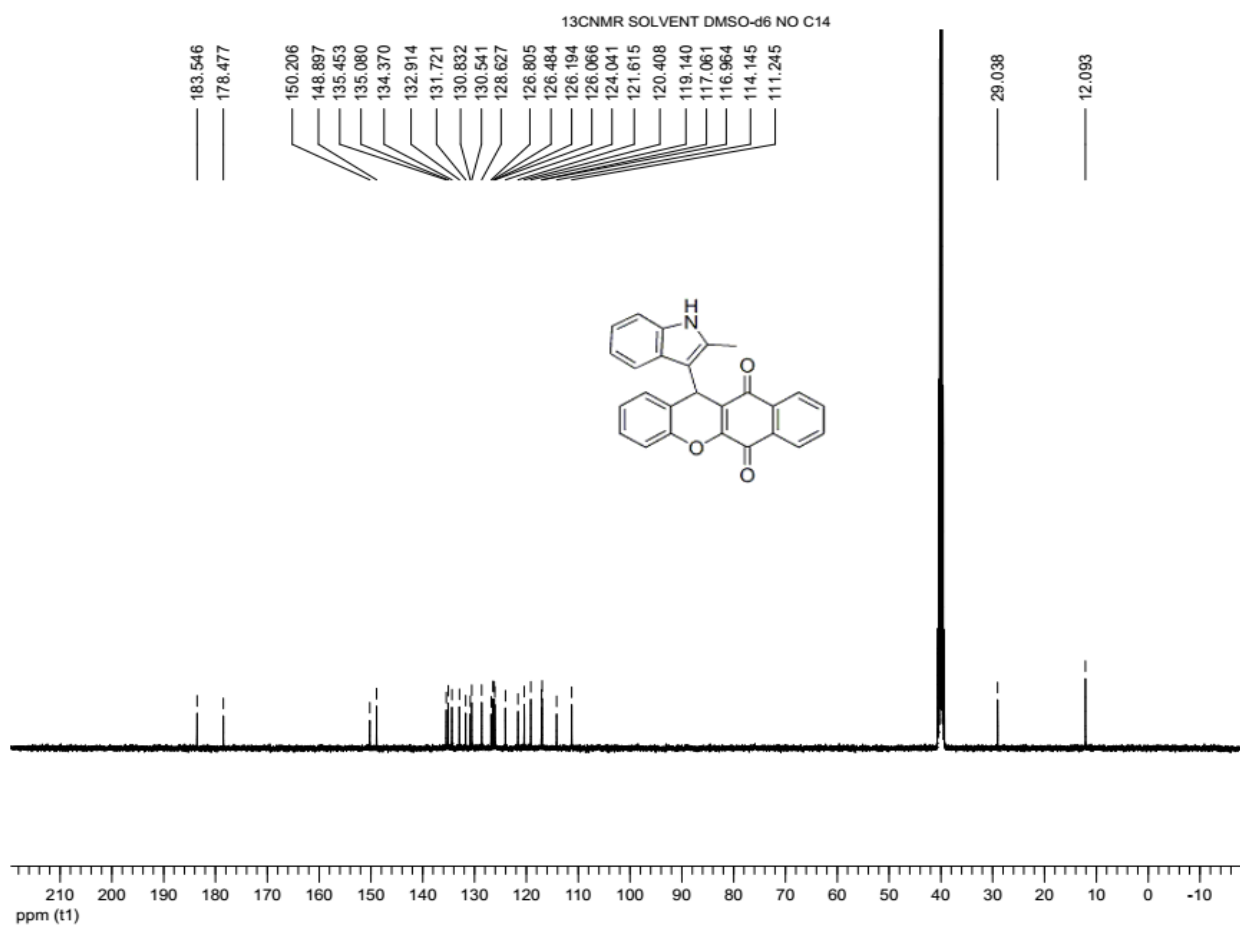
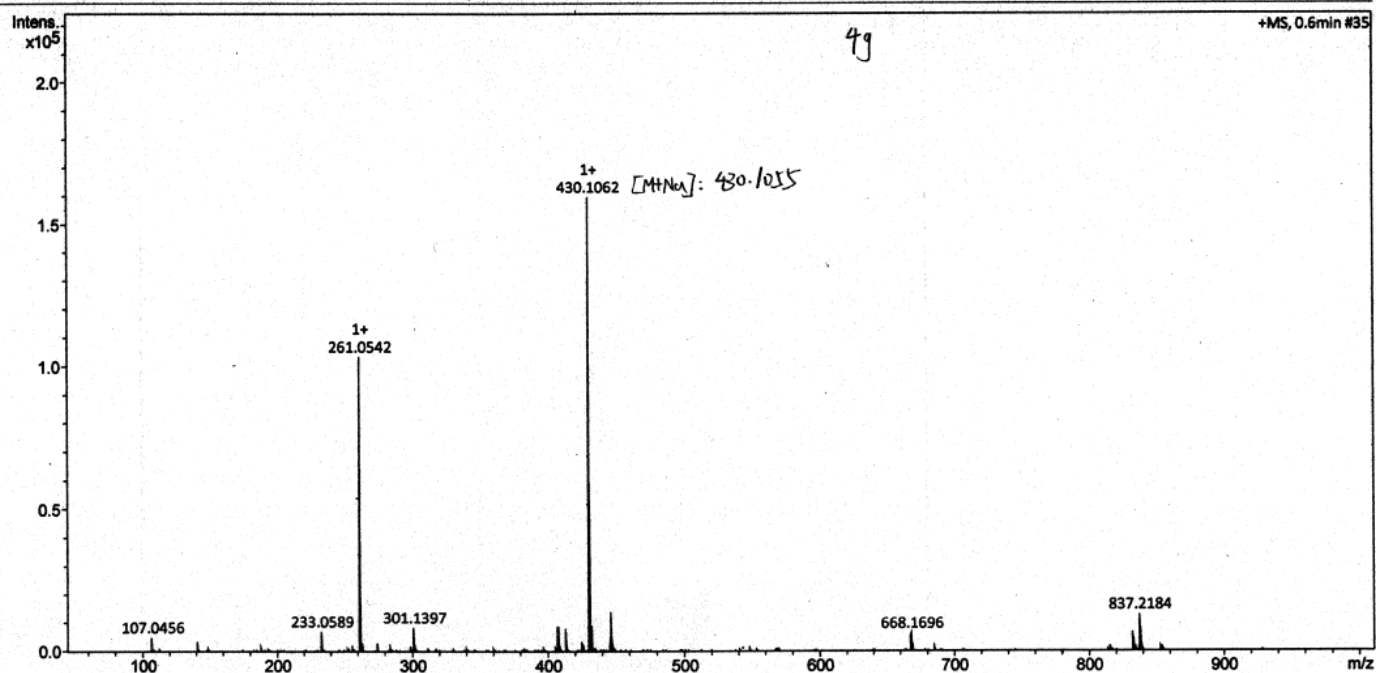
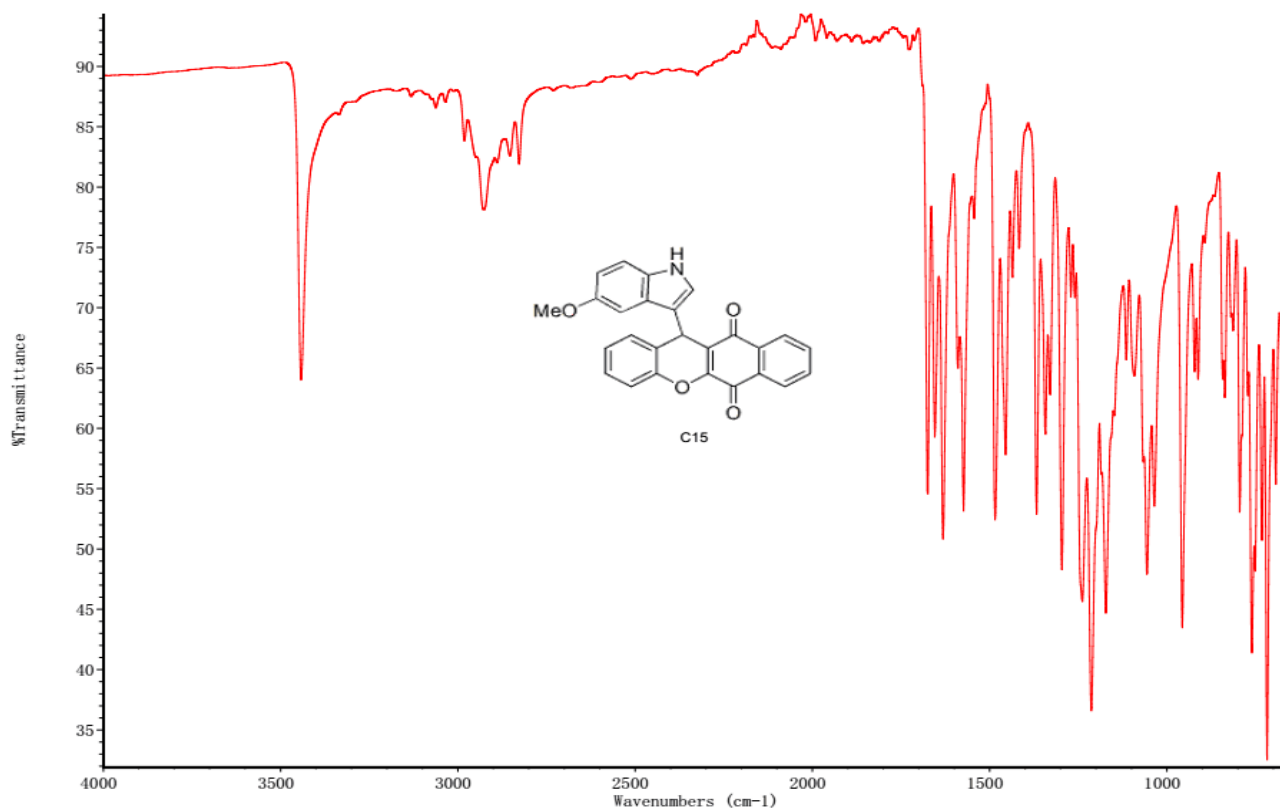


Figure S64 ^{13}C NMR of 4p

Acquisition Parameter

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	180.0 Vpp	Set Divert Valve	Waste

**Figure S65 HMRS of 4q****Figure S66 IR of 4q**

Acquisition Parameter

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 Vmin
Scan End	1000 m/z	Set Collision Cell RF	180.0 Vpp	Set Divert Valve	Waste

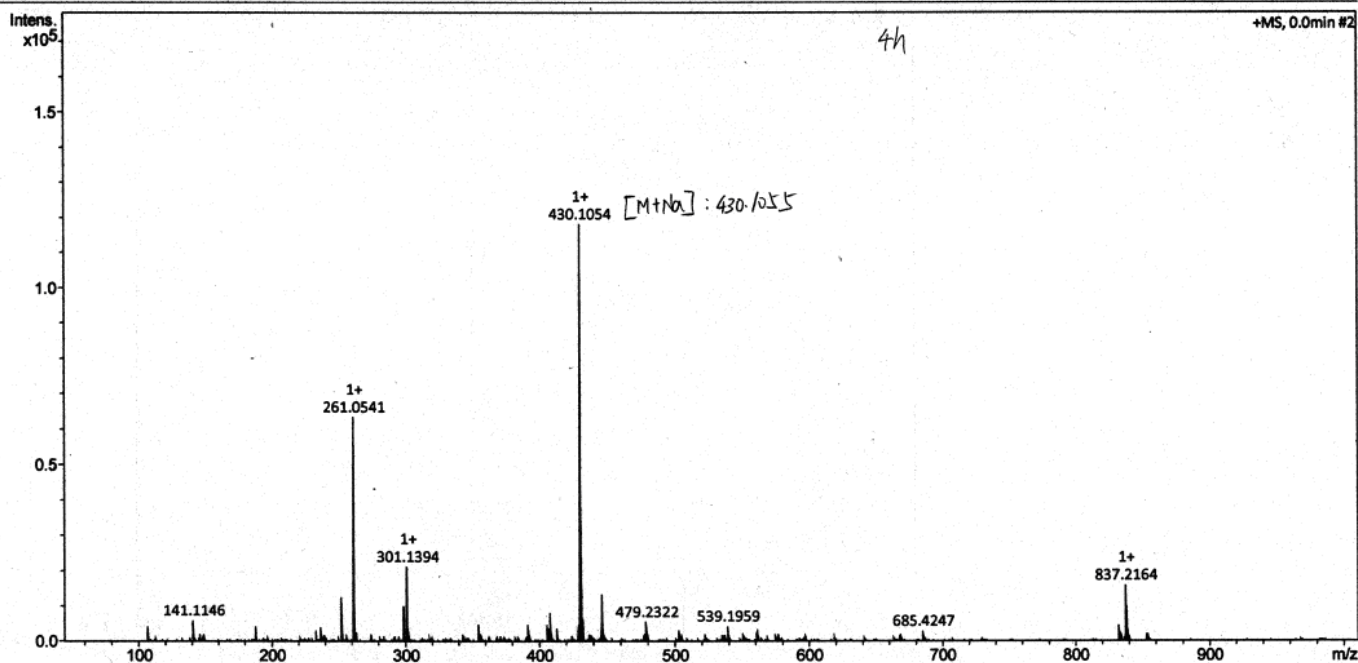


Figure S69 HRMS of 4r

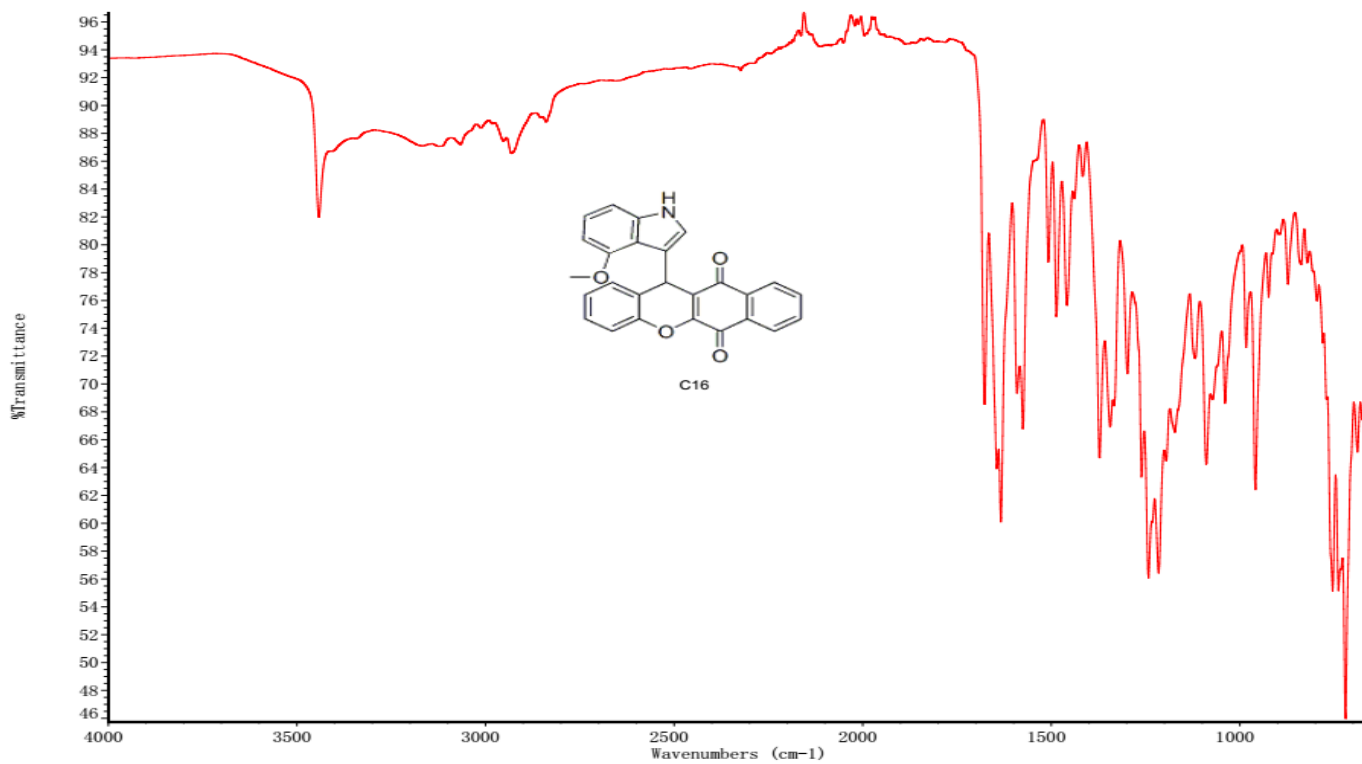


Figure S70 IR of 4r

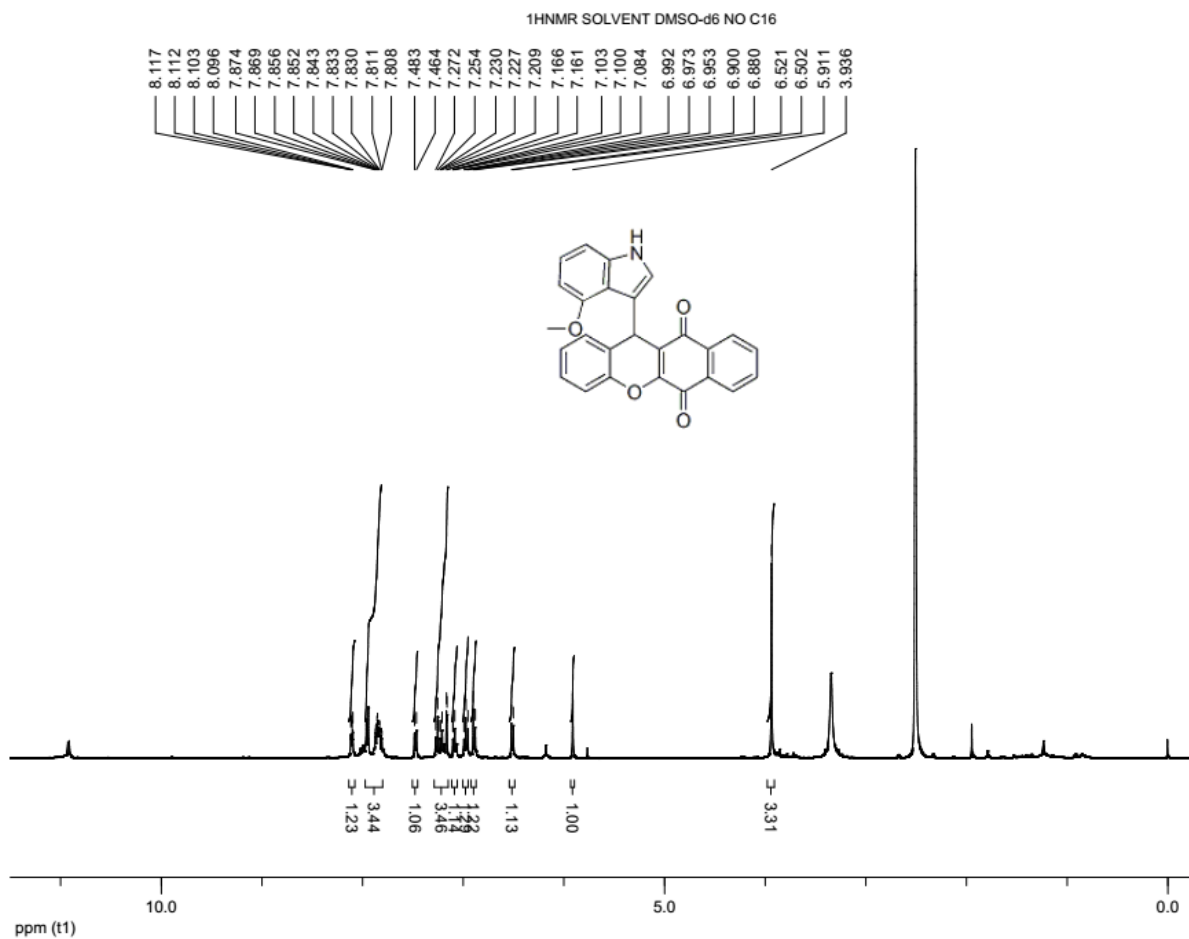


Figure S71 ¹H NMR of 4r

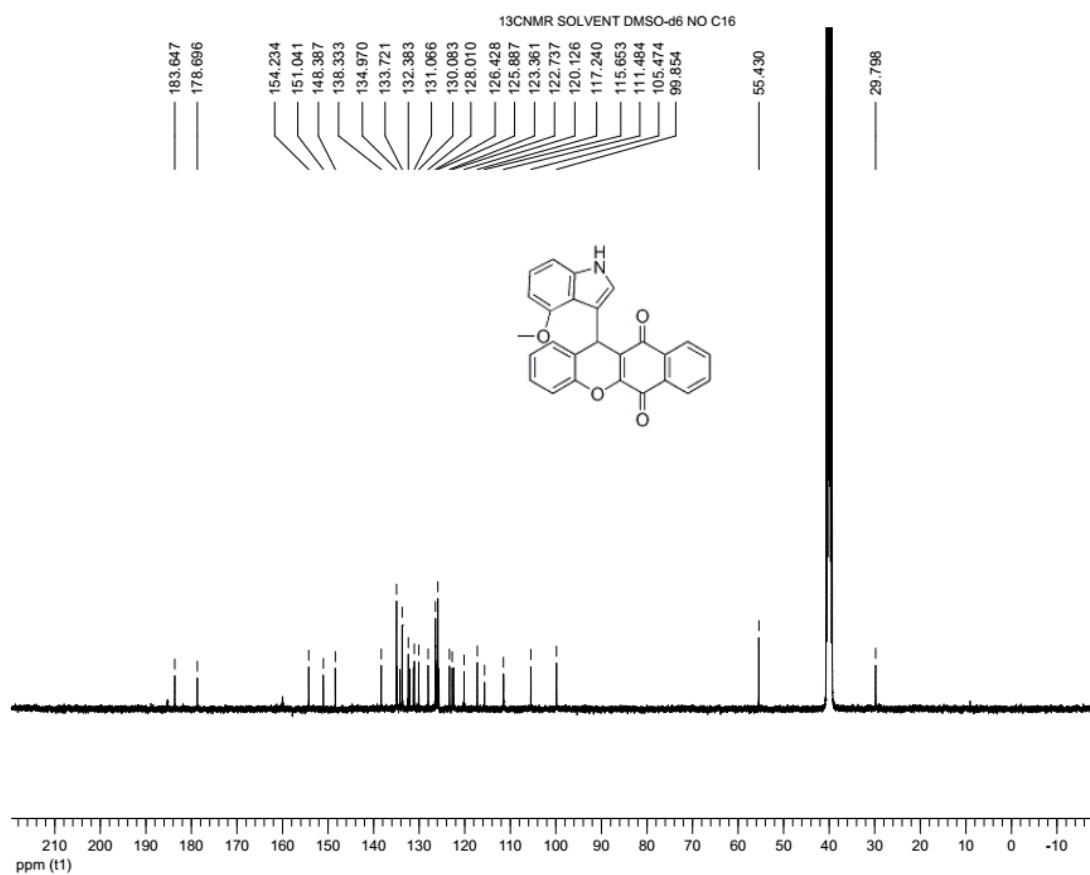


Figure S72 ¹³C NMR of 4r

Acquisition Parameter

Source Type

ESI

Focus

Not active

Scan Begin

50 m/z

Scan End

1000 m/z

Ion Polarity

Set Capillary

Set End Plate Offset

Set Collision Cell RF

Positive

4500 V

-500 V

180.0 Vpp

Set Nebulizer

Set Dry Heater

Set Dry Gas

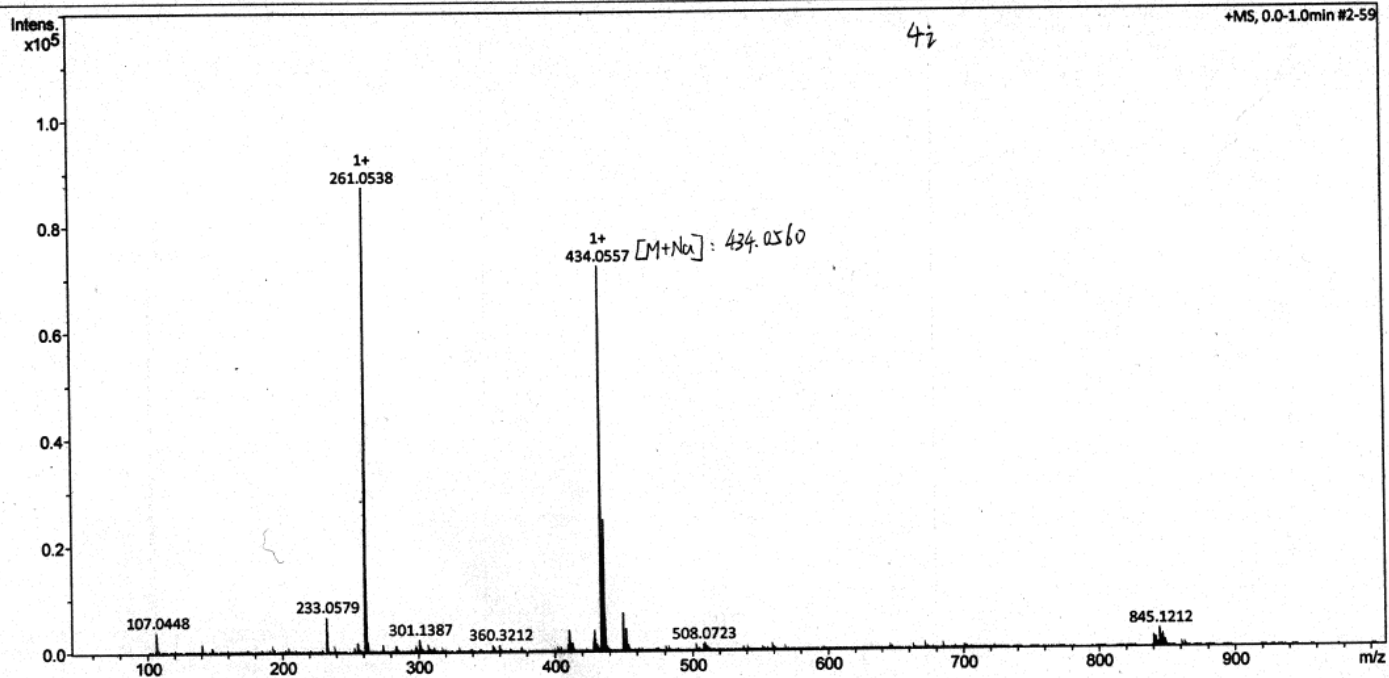
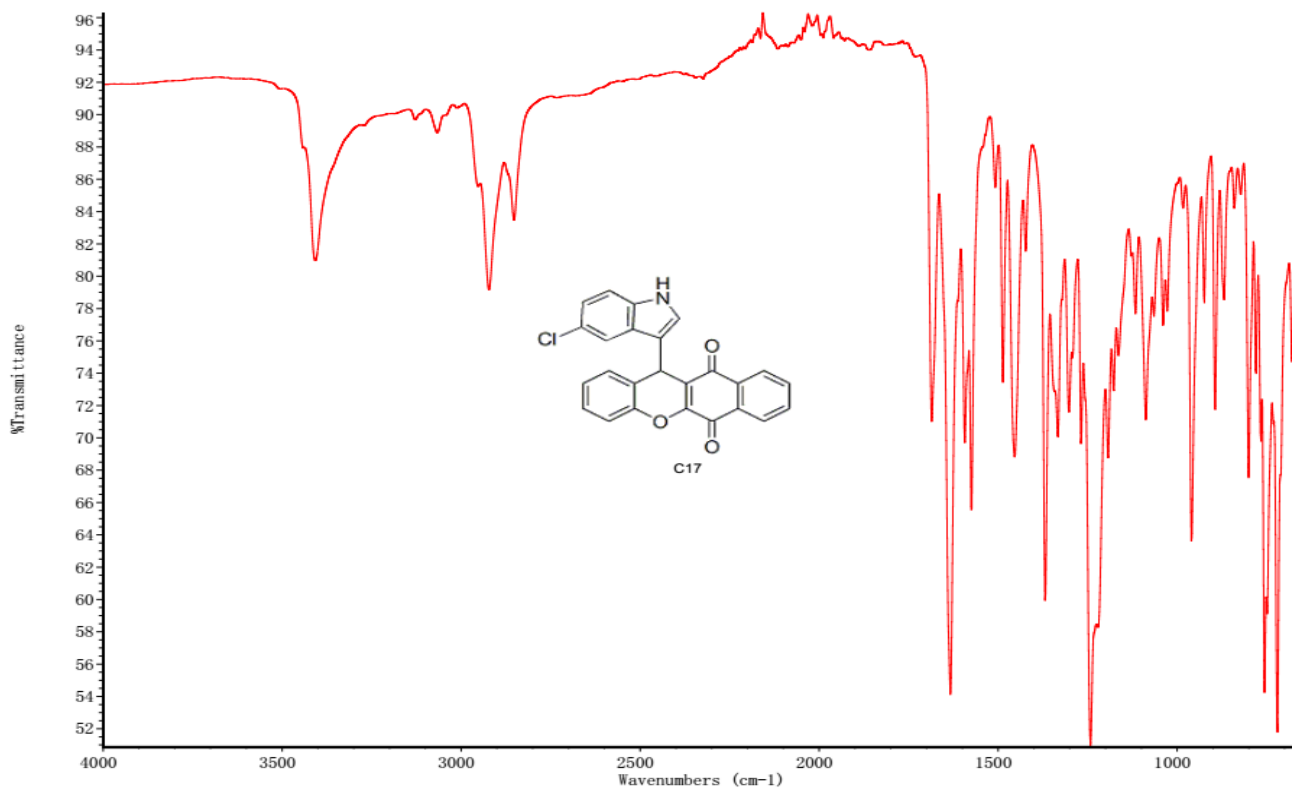
Set Divert Valve

0.3 Bar

180 °C

4.0 l/min

Waste

**Figure S73** HMRS of 4s**Figure S74** IR of 4s

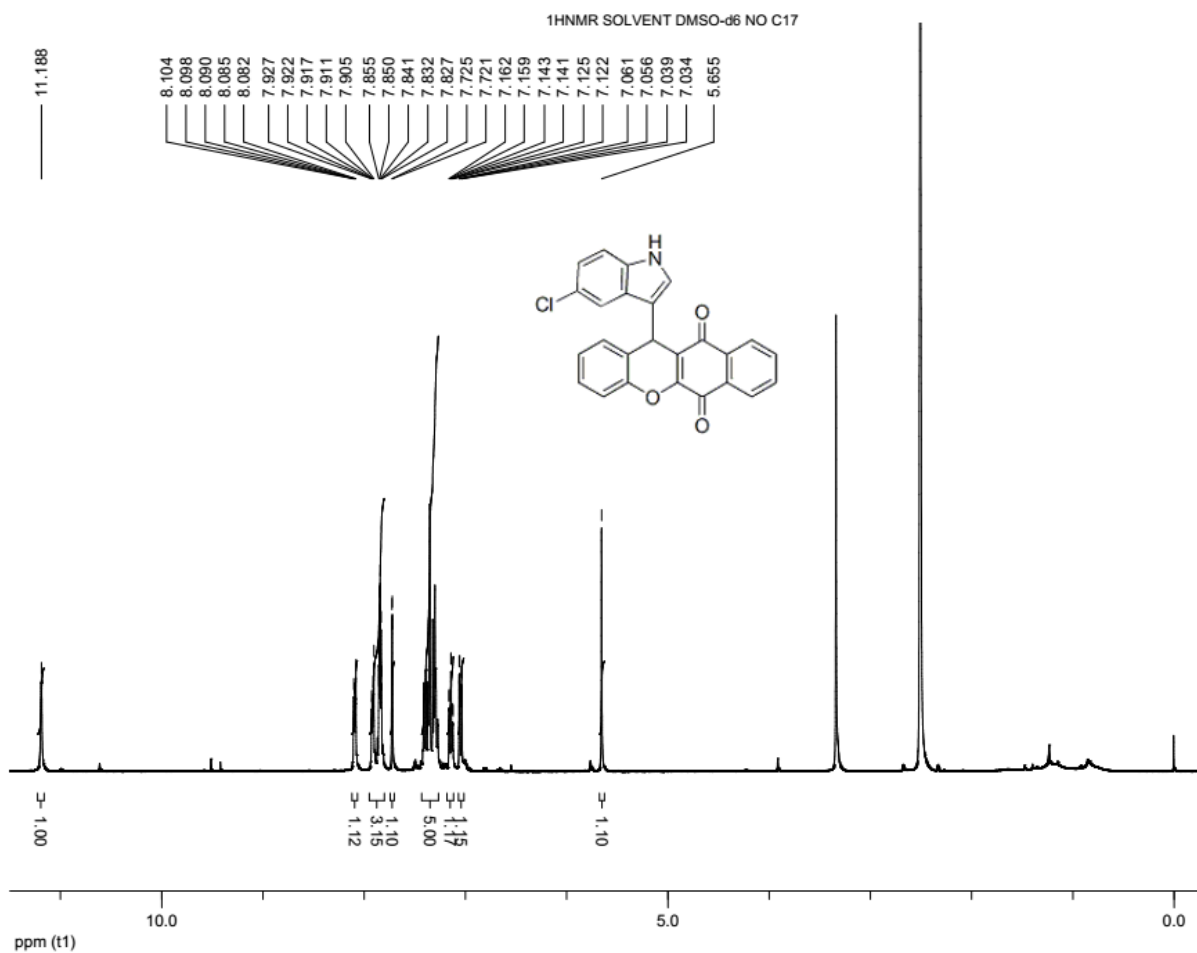


Figure S75 ¹H NMR of 4s

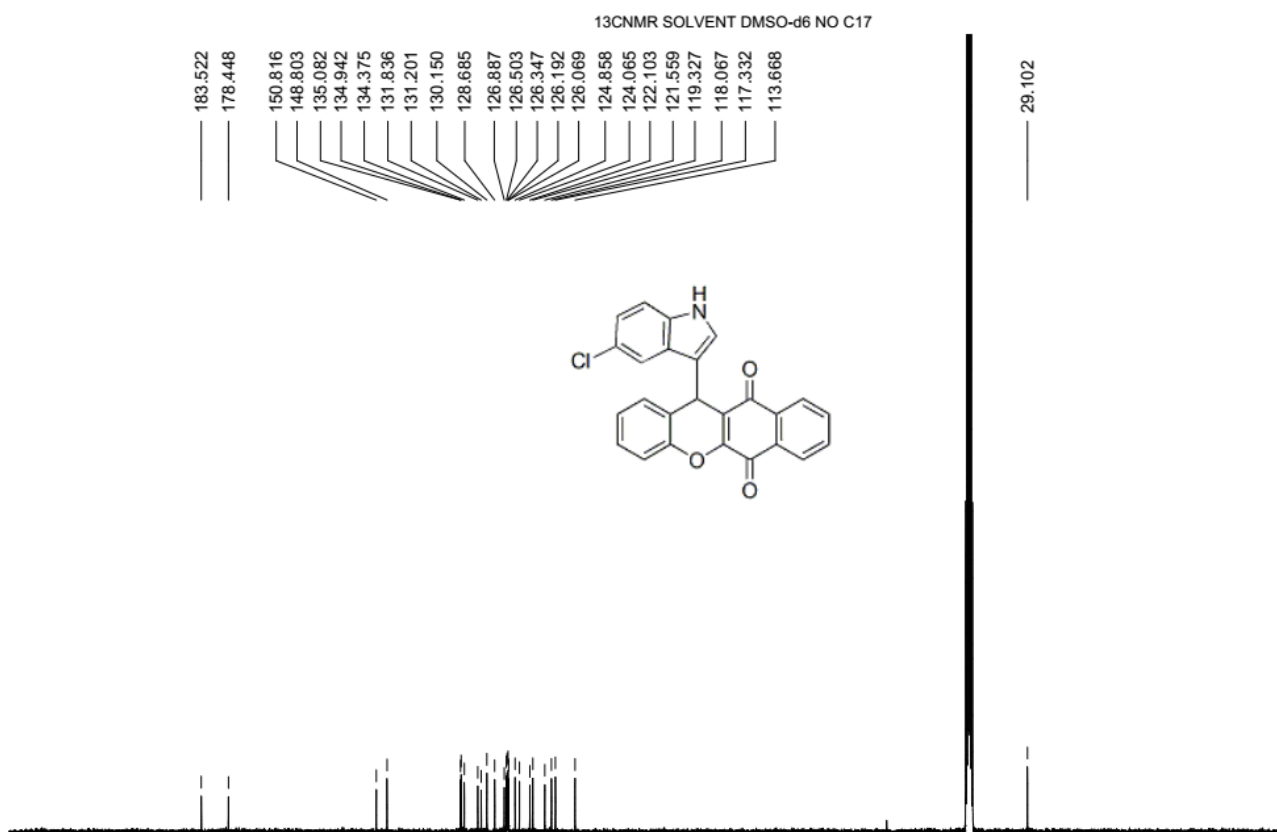


Figure S76 ¹³C NMR of 4s