

Synthesis and biological evaluation of novel 1,2-naphthoquinones possessing tetrazolo[1,5-*a*]pyrimidine scaffolds as potent antitumor agents

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Content

Copy of IR, ¹H NMR, ¹³C NMR and HRMS.....2-60

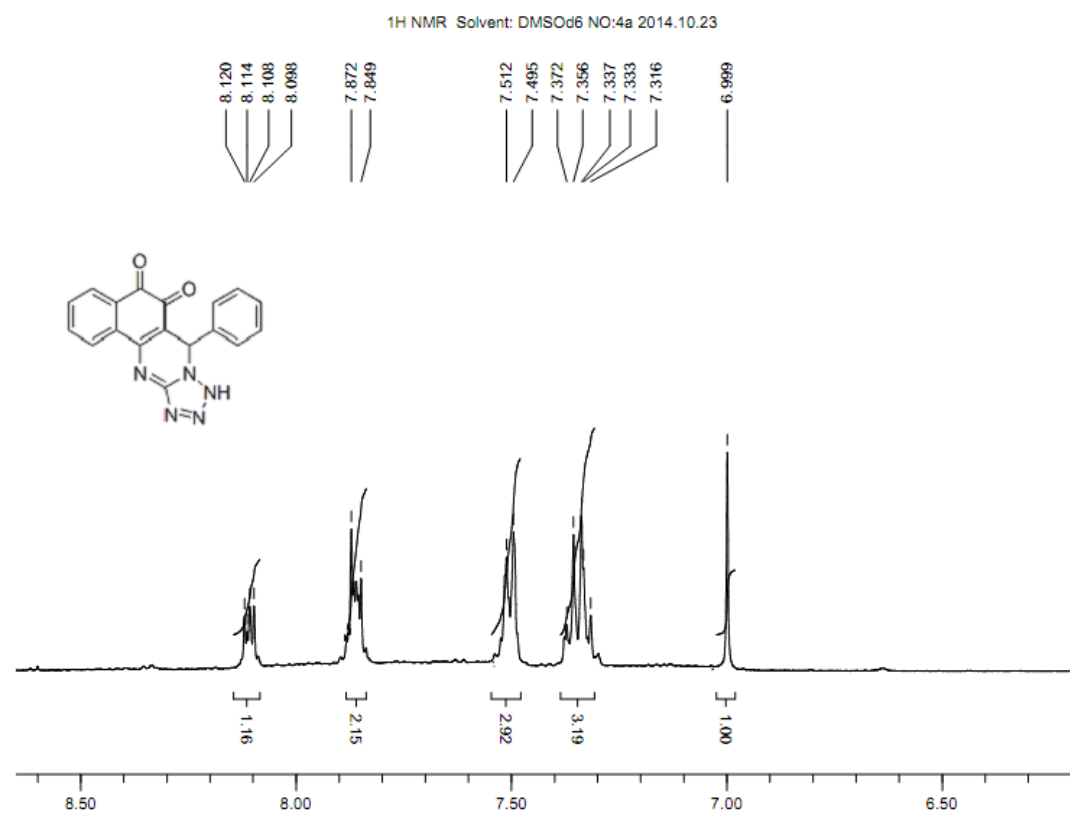
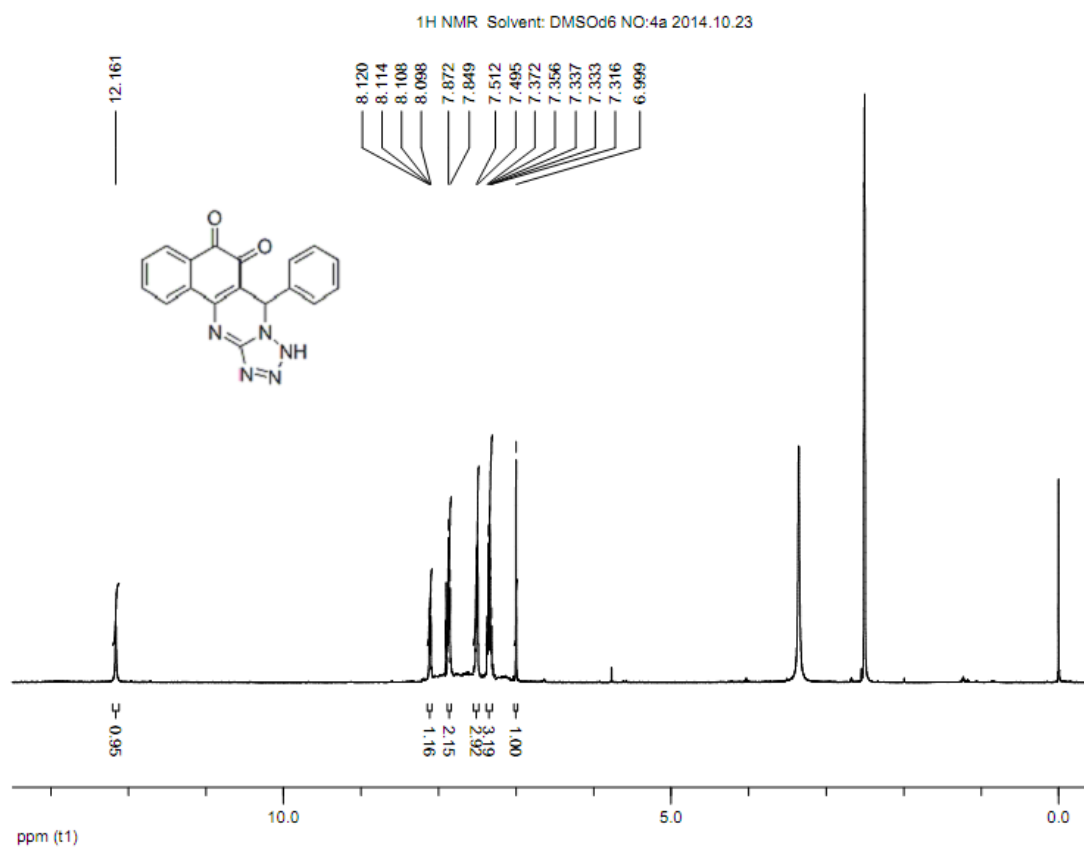


Figure 1 ¹H NMR of 4a

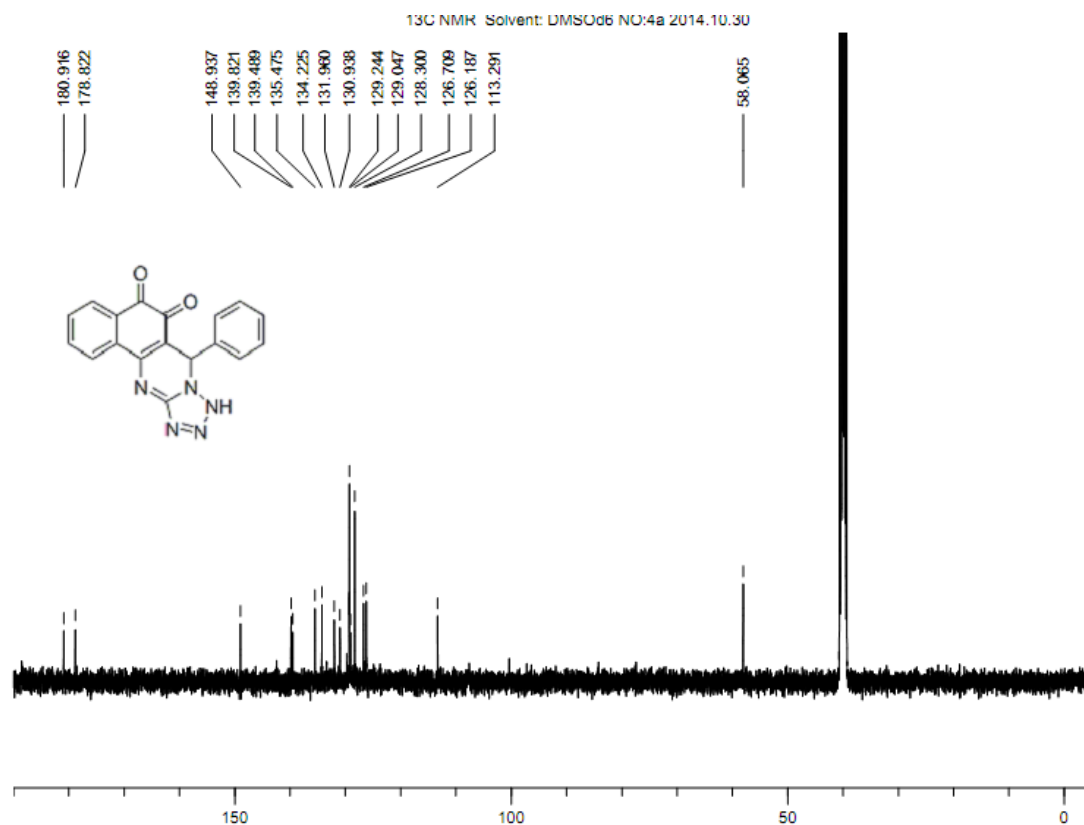


Figure 2 ^{13}C NMR of 4a

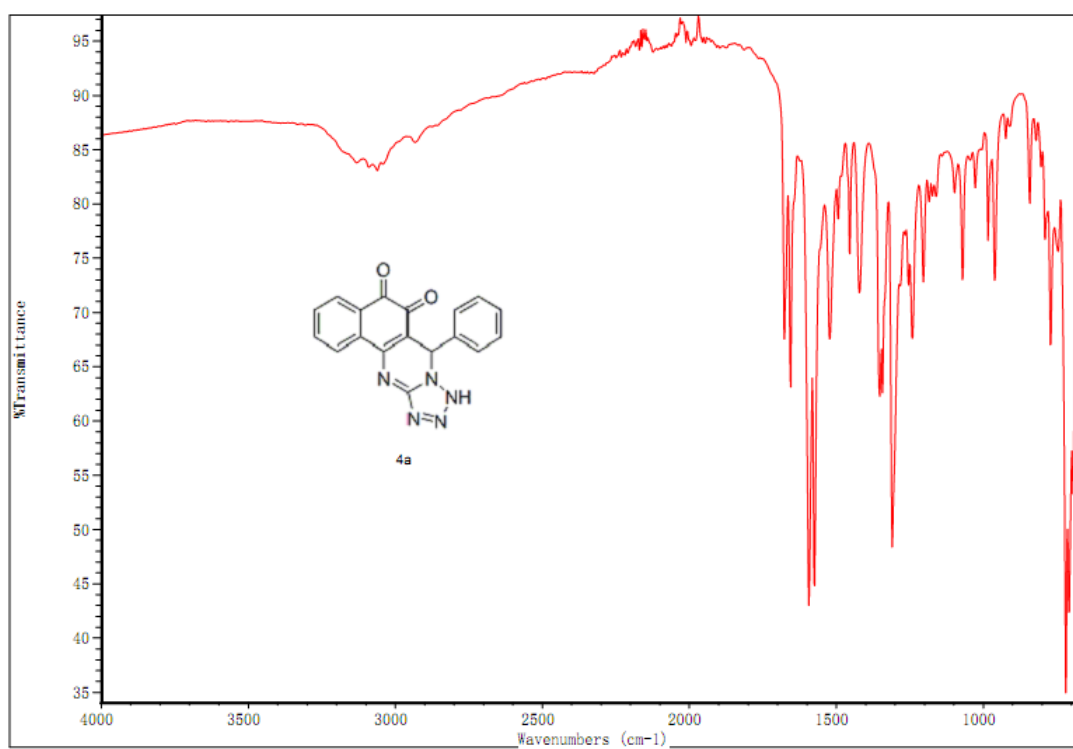


Figure 3 IR of 4a

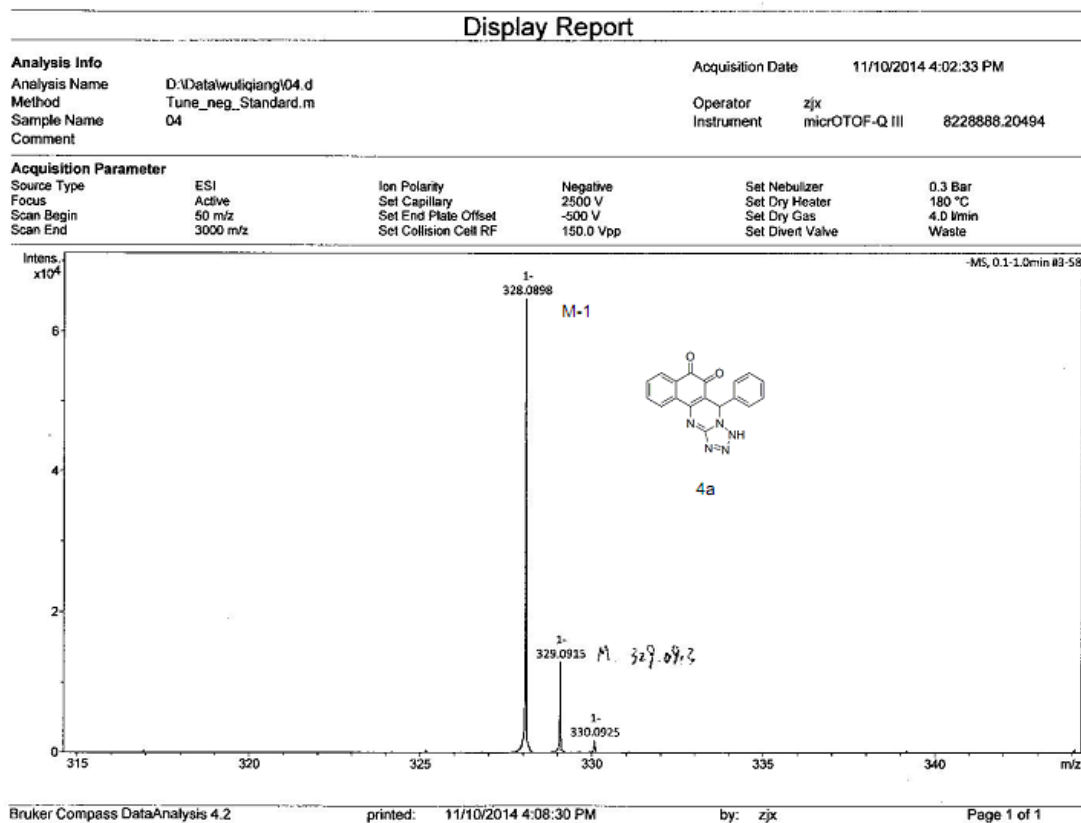


Figure 4 HRMS of **4a**

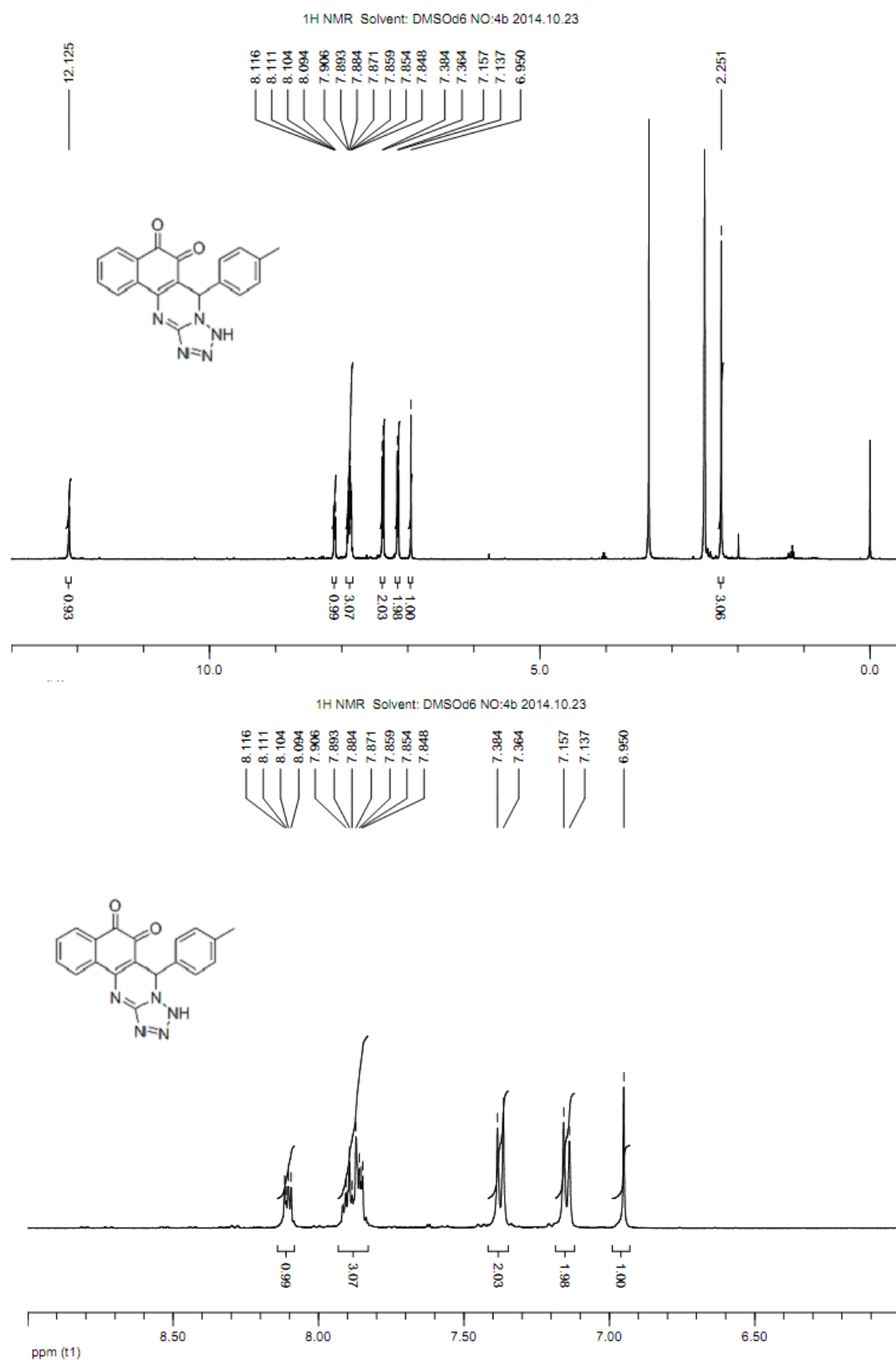


Figure 5 ^1H NMR of 4b

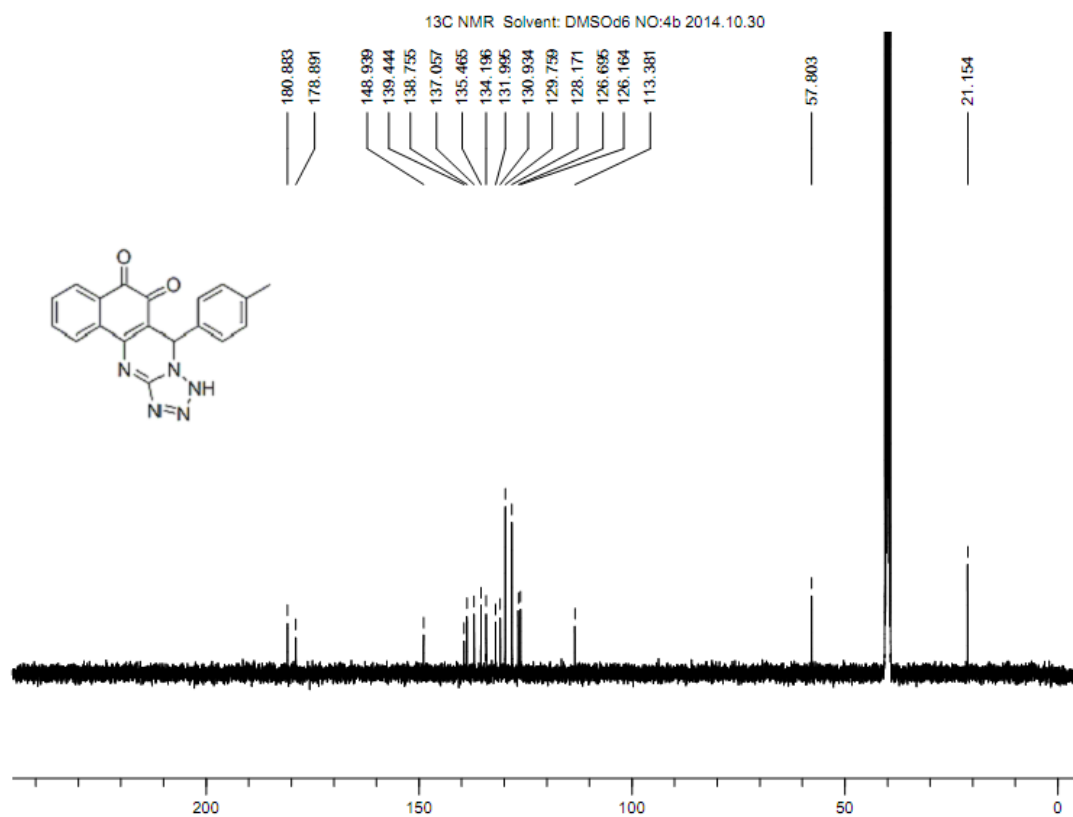


Figure 6 ¹³C NMR of 4b

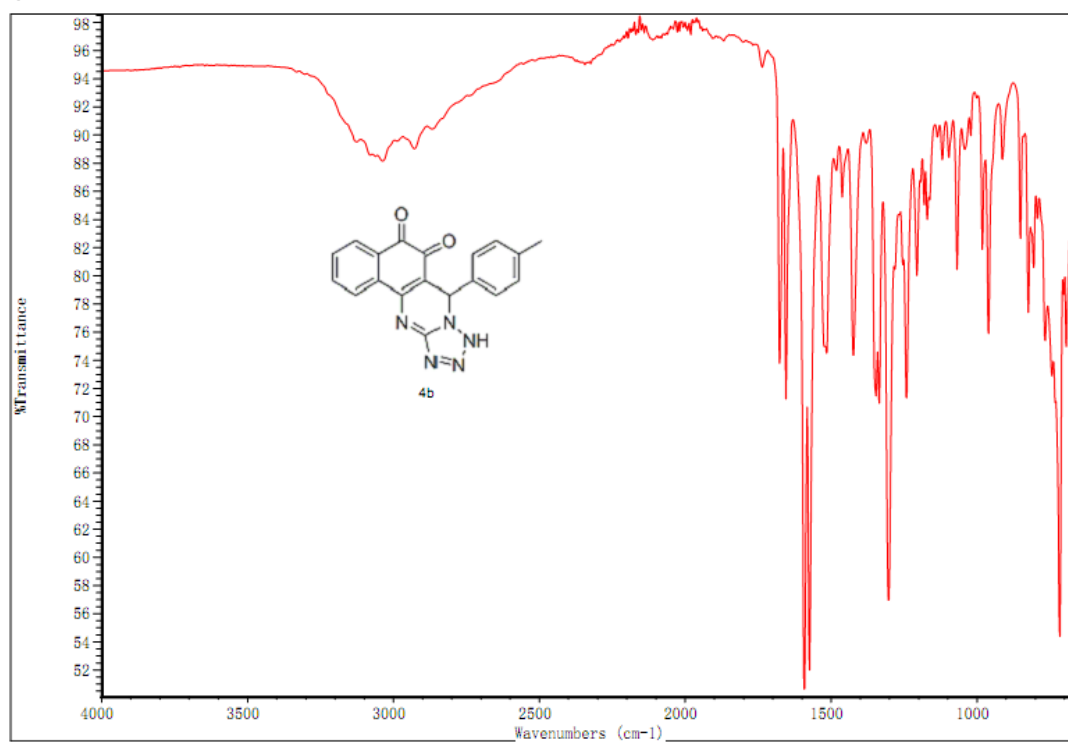


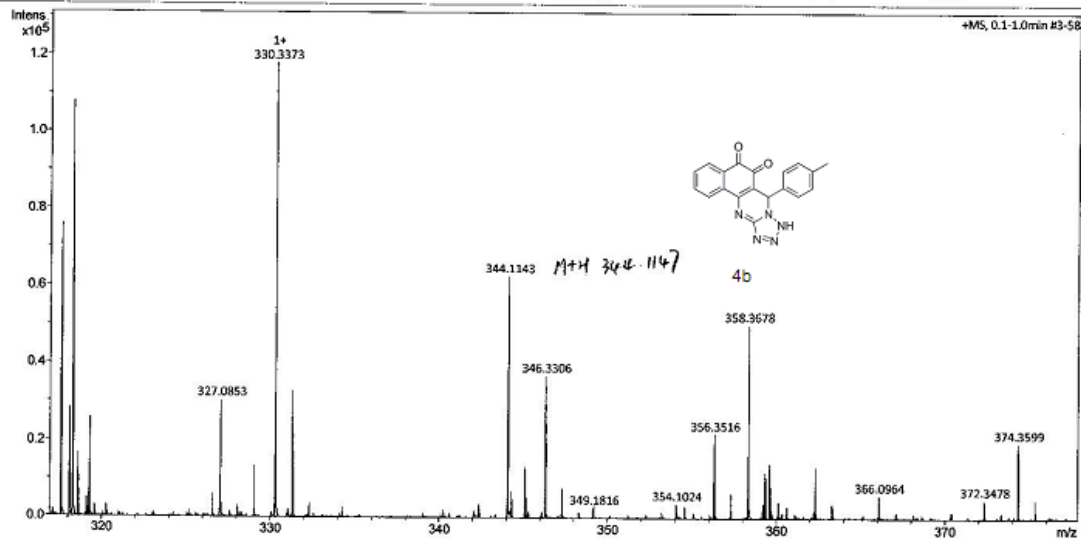
Figure 7 IR of 4b

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Method	Tune_pos_Standard.m	Instrument	micrOTOF-Q III
Sample Name	016		8226888.20494
Comment			

Acquisition Parameter

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	0.3 Bar
Focus	Active	Set Capillary	4500 V	Set Dry Heater	200 °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



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Figure 8 HRMS of 4b

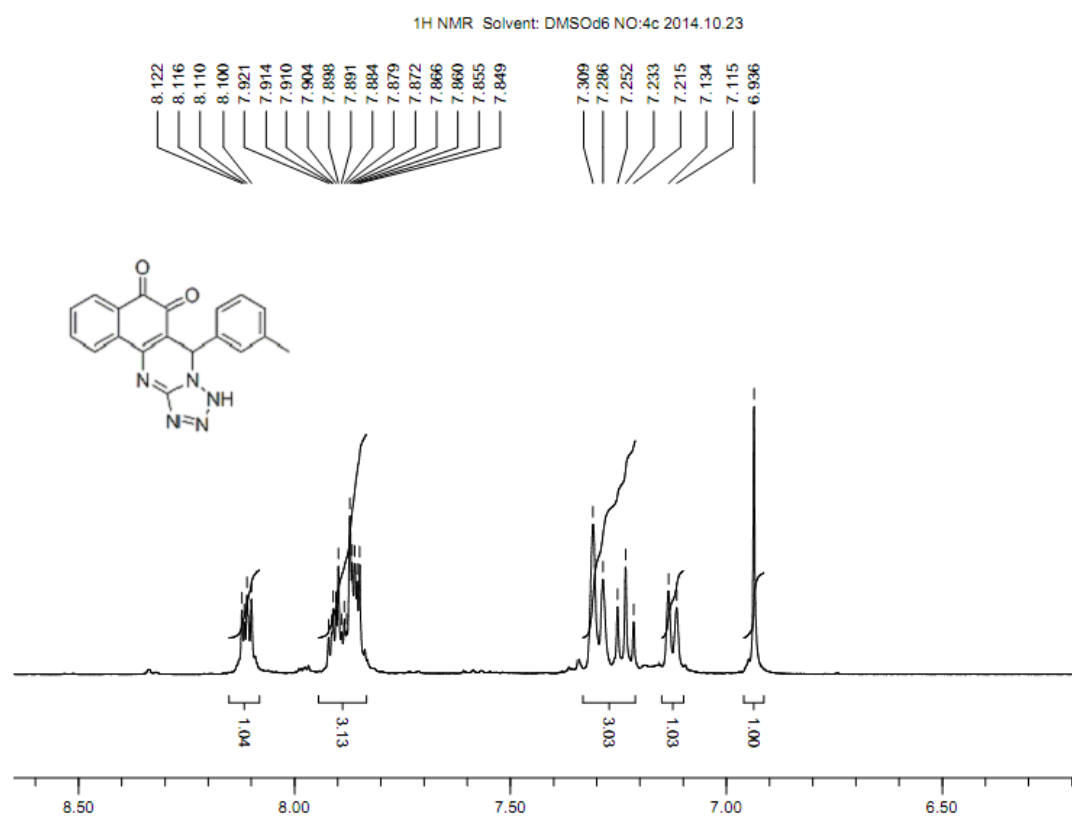
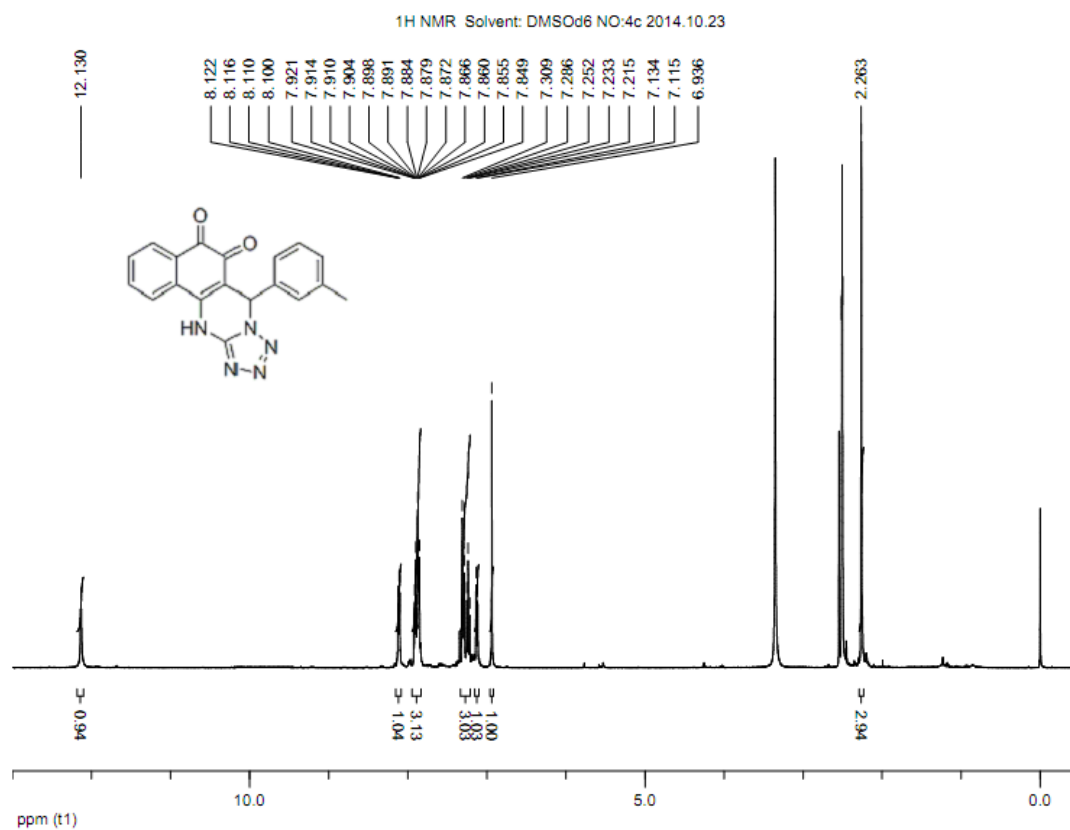


Figure 9 ^1H NMR of 4c

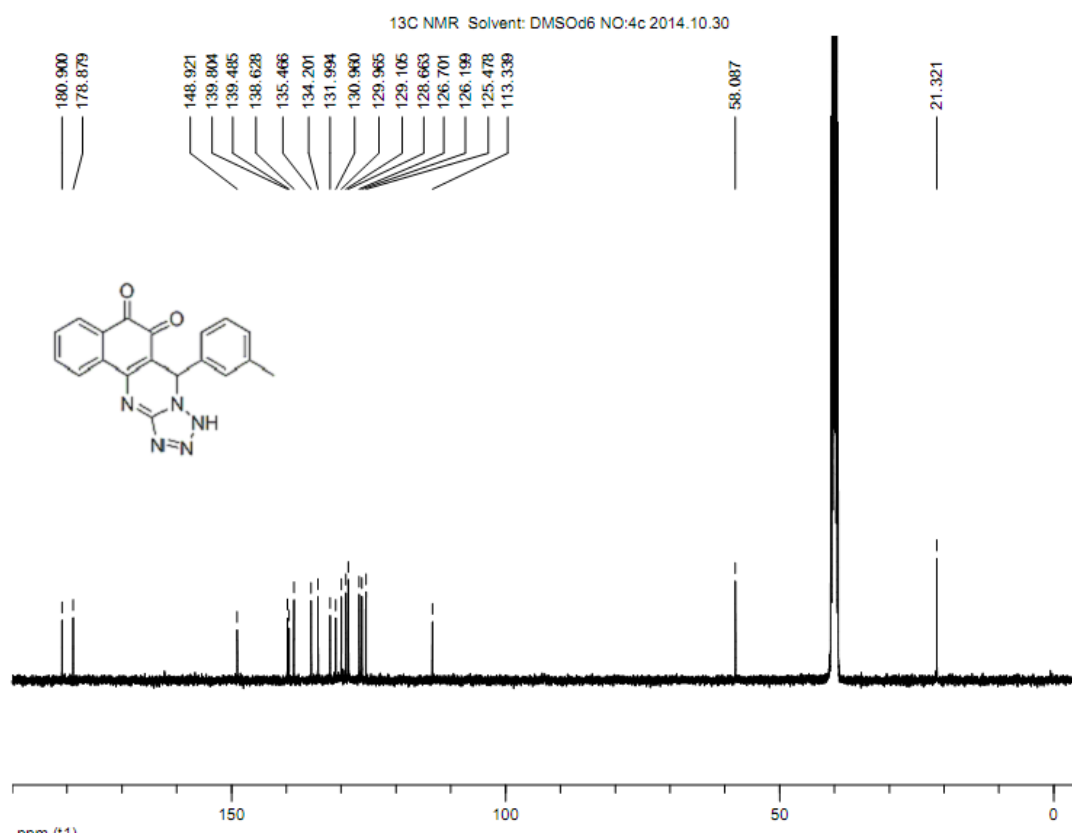


Figure 10 ¹³C NMR of 4c

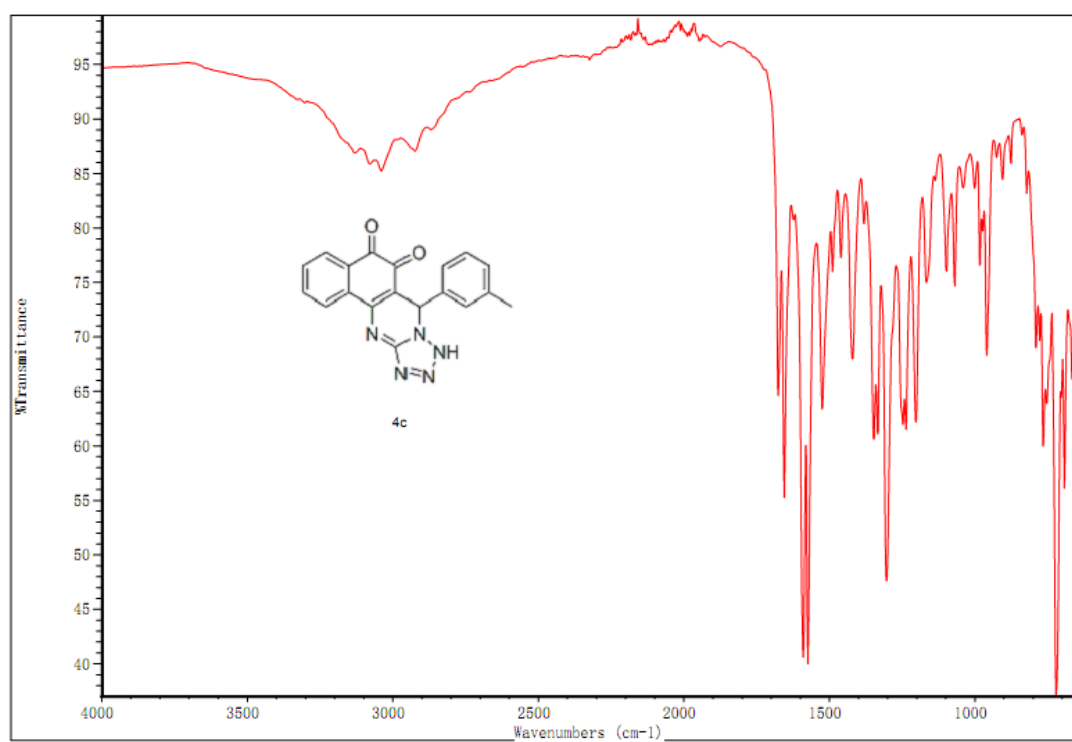


Figure 11 IR of 4c

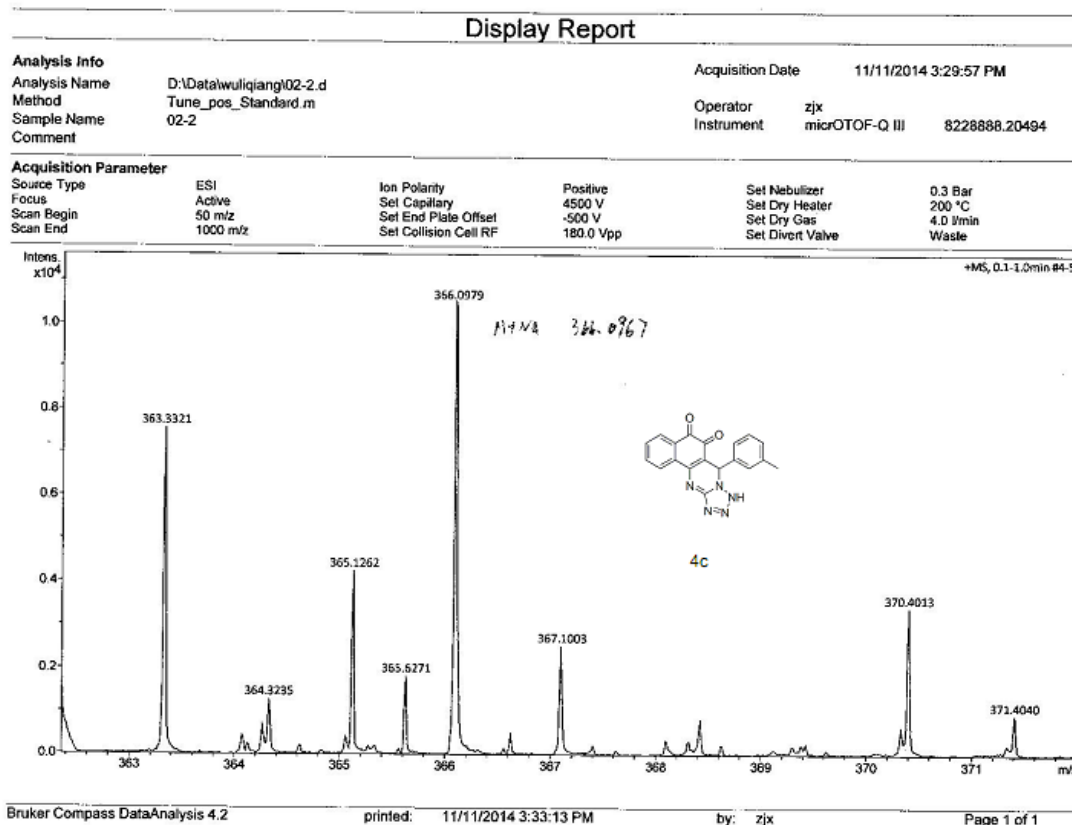


Figure 12 HRMS of **4c**

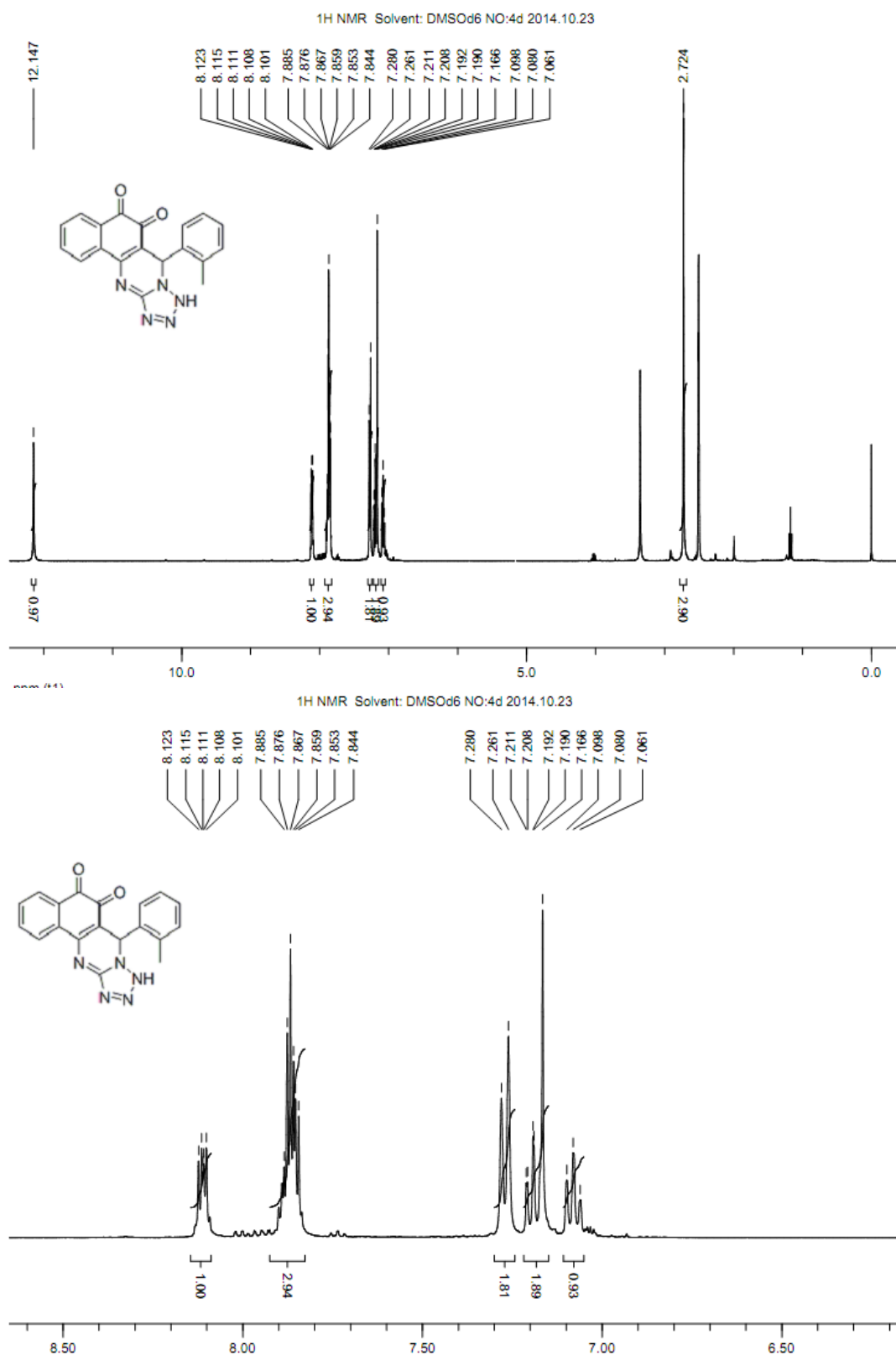


Figure 13 ^1H NMR of 4d

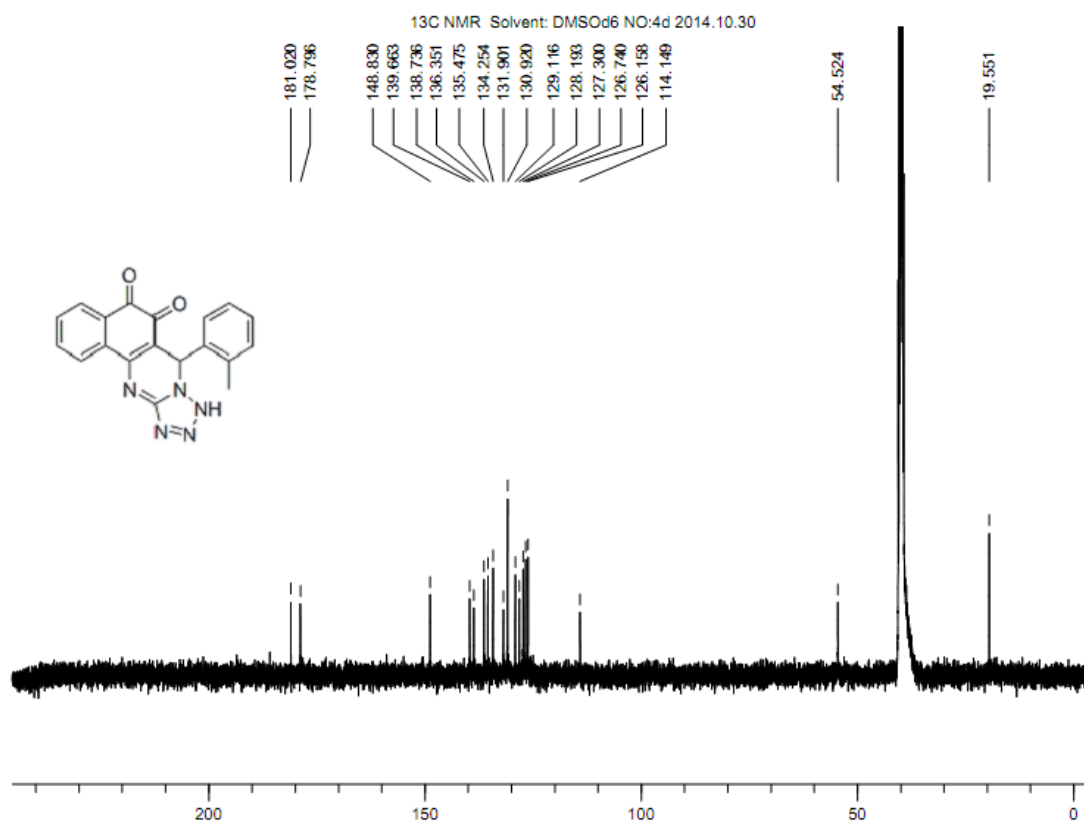


Figure 14 ¹³C NMR of 4d

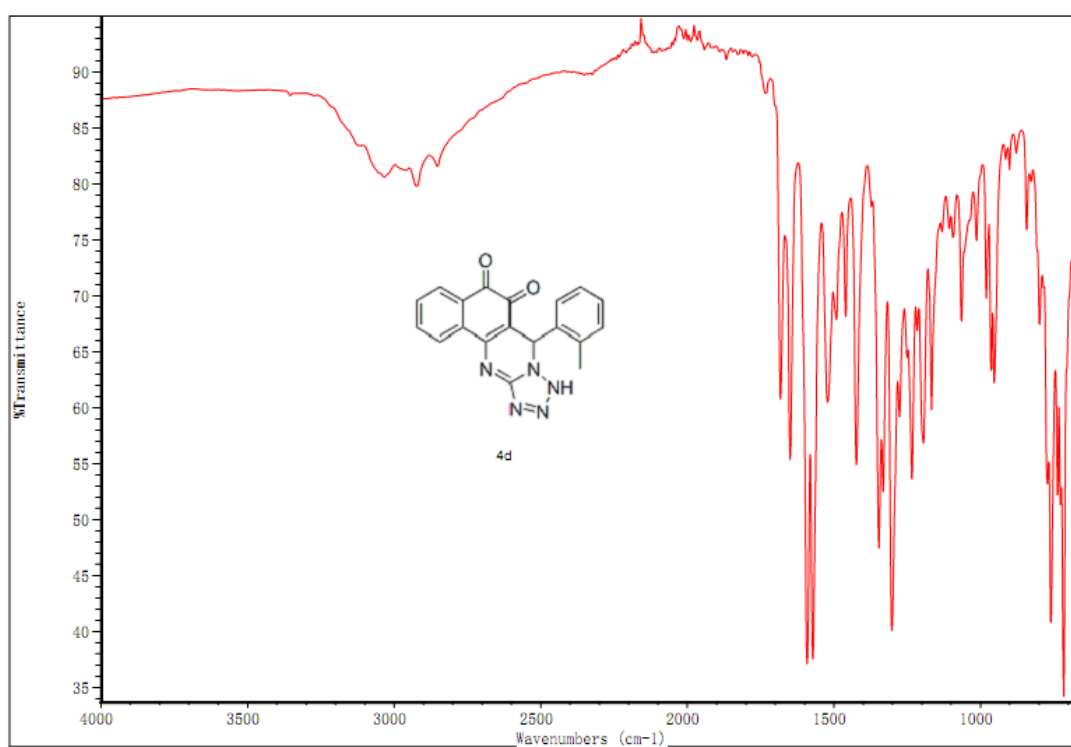
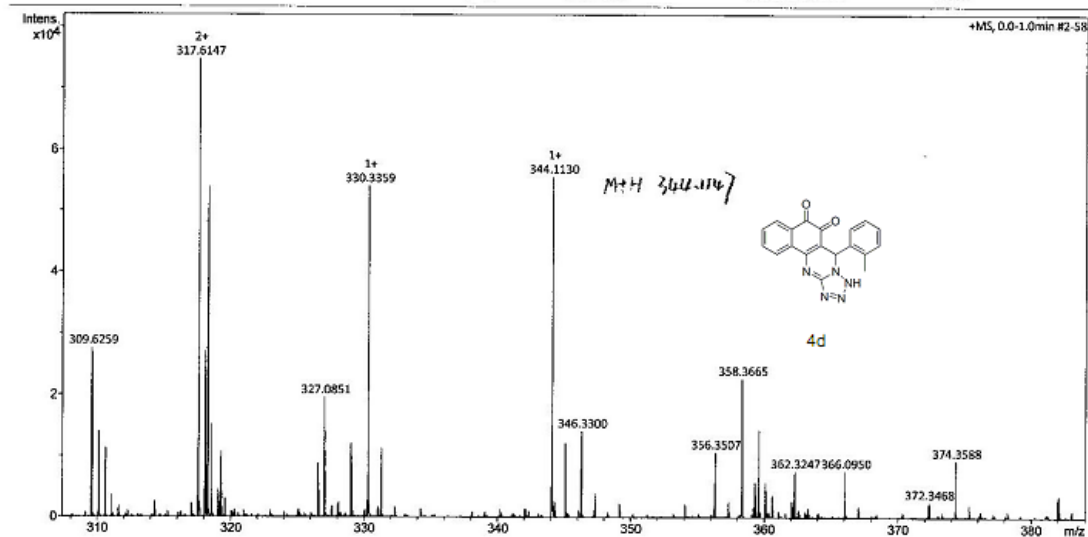


Figure 15 IR of 4d

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Method	Tune_pos_Standard.m	Instrument	micrOTOF-Q III
Sample Name	013		8228888.20494
Comment			

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



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Figure 16 HRMS of **4d**

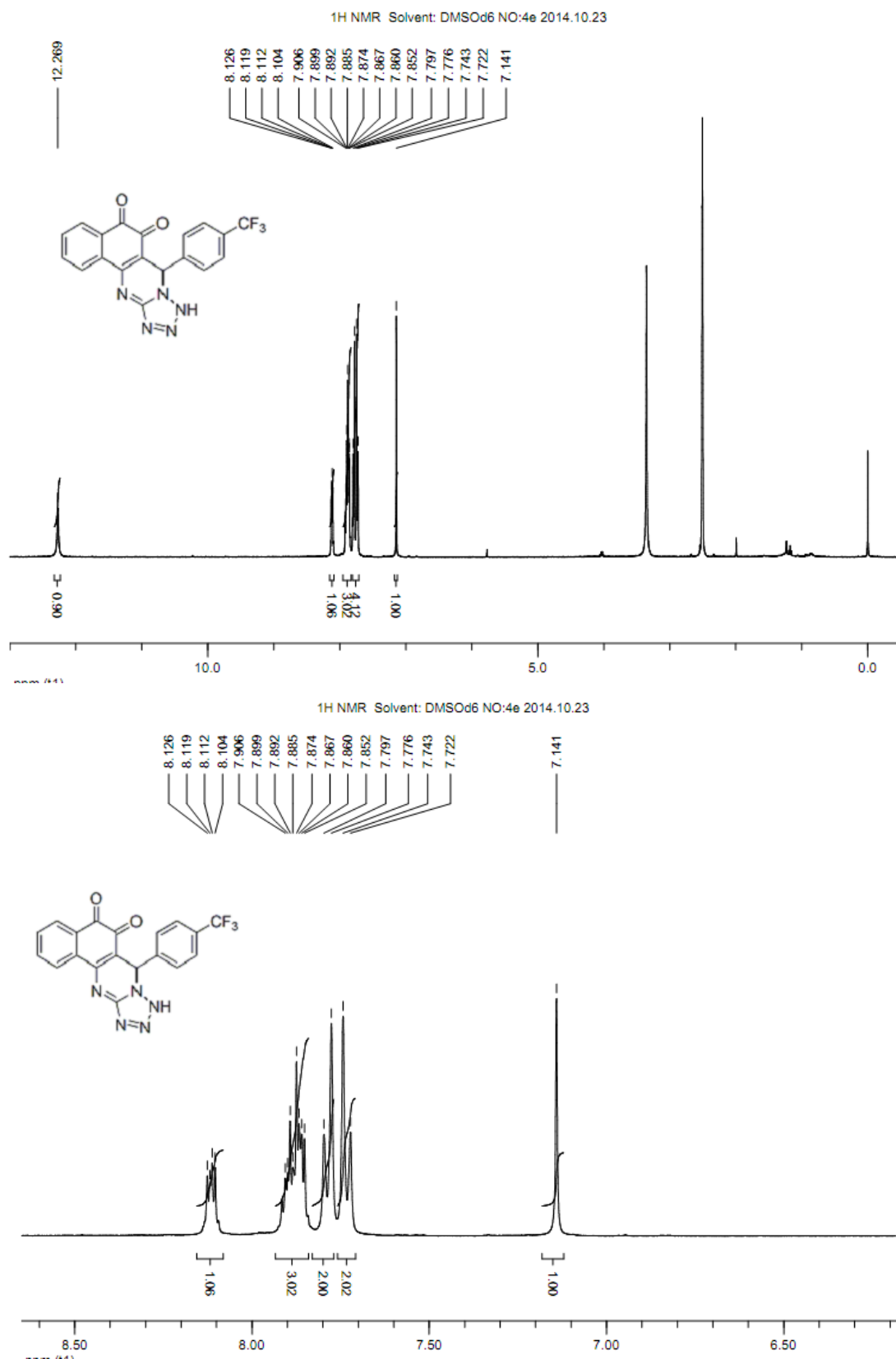


Figure 17 ¹H NMR of 4e

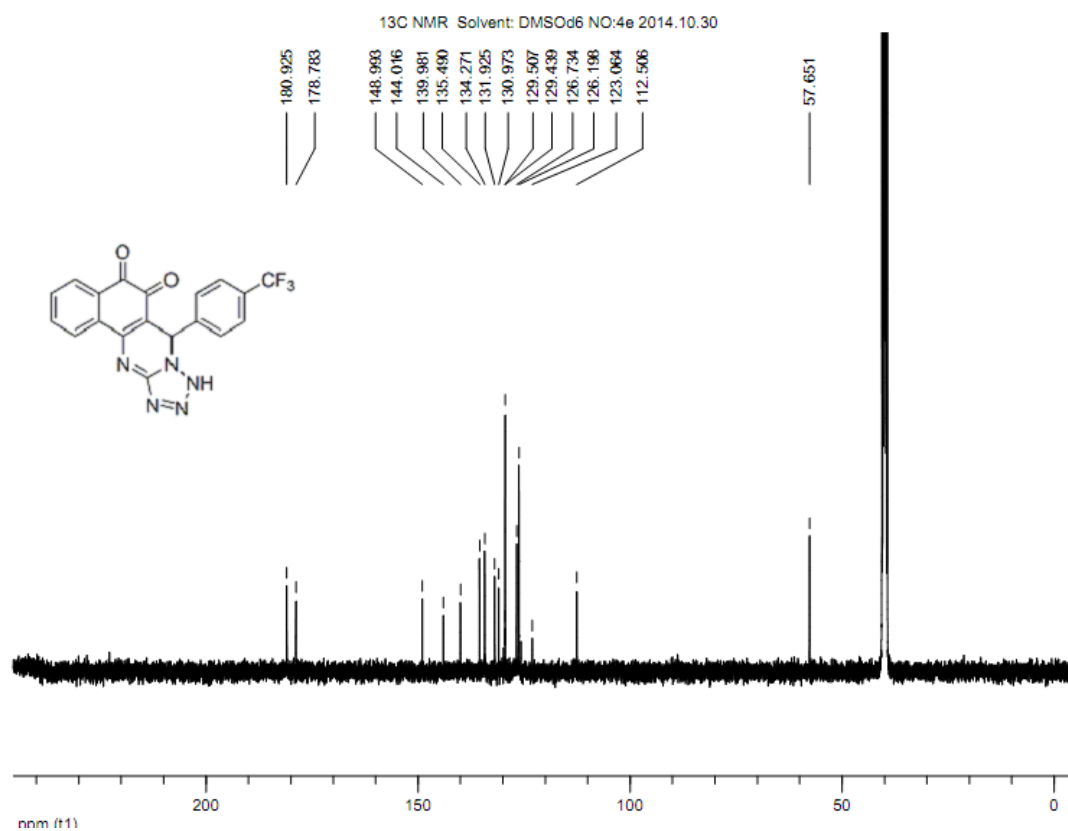


Figure 18 ¹³C NMR of 4e

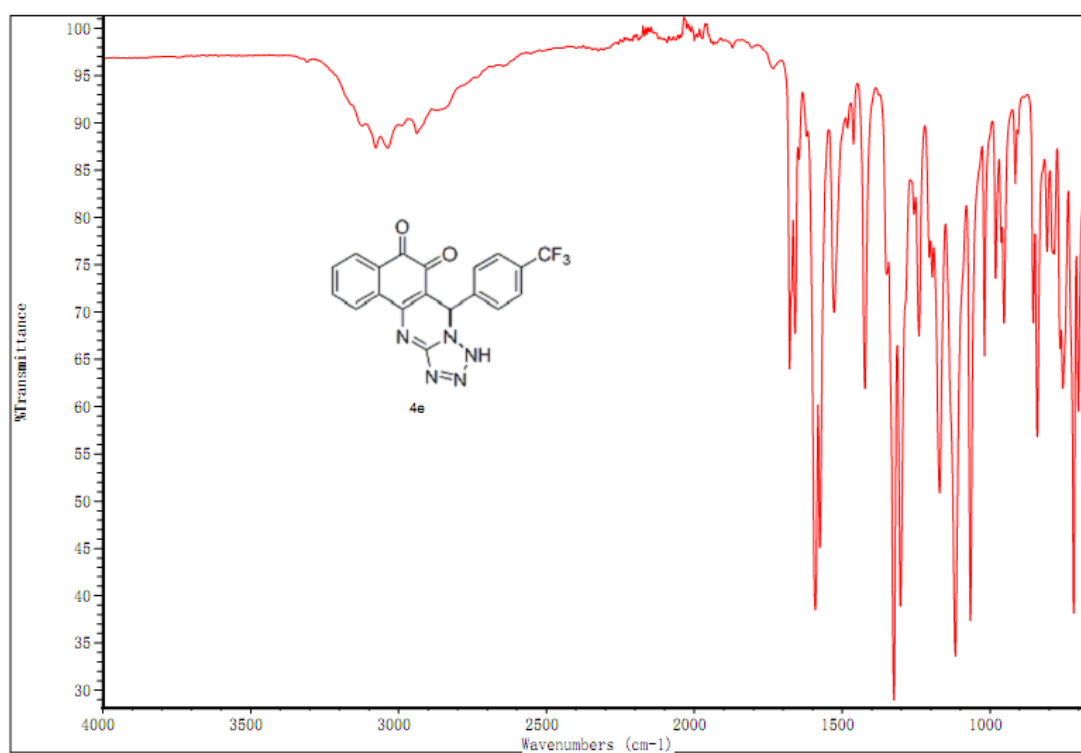


Figure 19 IR of 4e

Display Report

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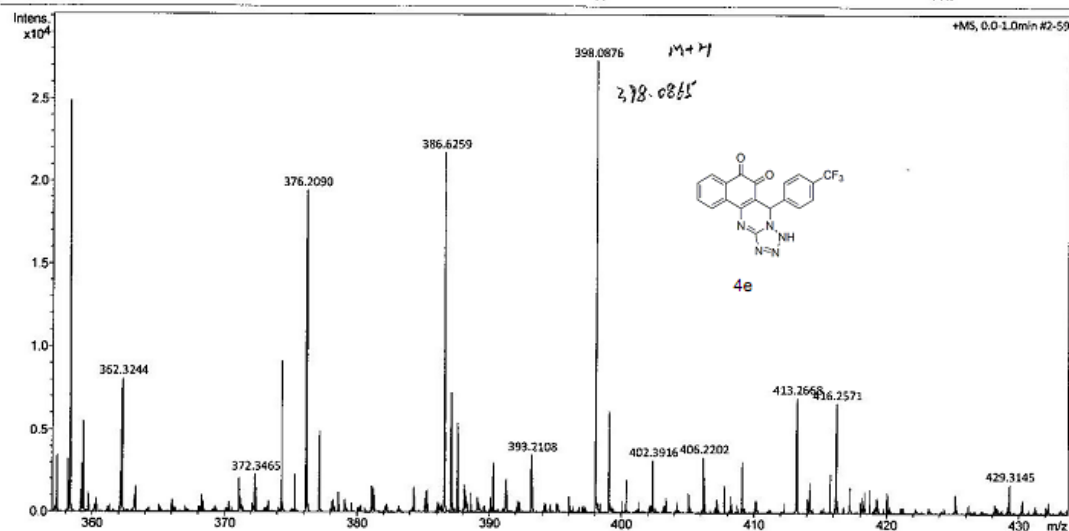
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Method Tune_pos_Standard.m
Sample Name 07
Comment

Acquisition Date 11/10/2014 4:21:17 PM

Operator zjx
Instrument micrOTOF-Q III 8228888.20494

Acquisition Parameter

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	0.3 Bar
Focus	Active	Set Capillary	4500 V	Set Dry Heater	200 °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



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Figure 20 HRMS of 4e

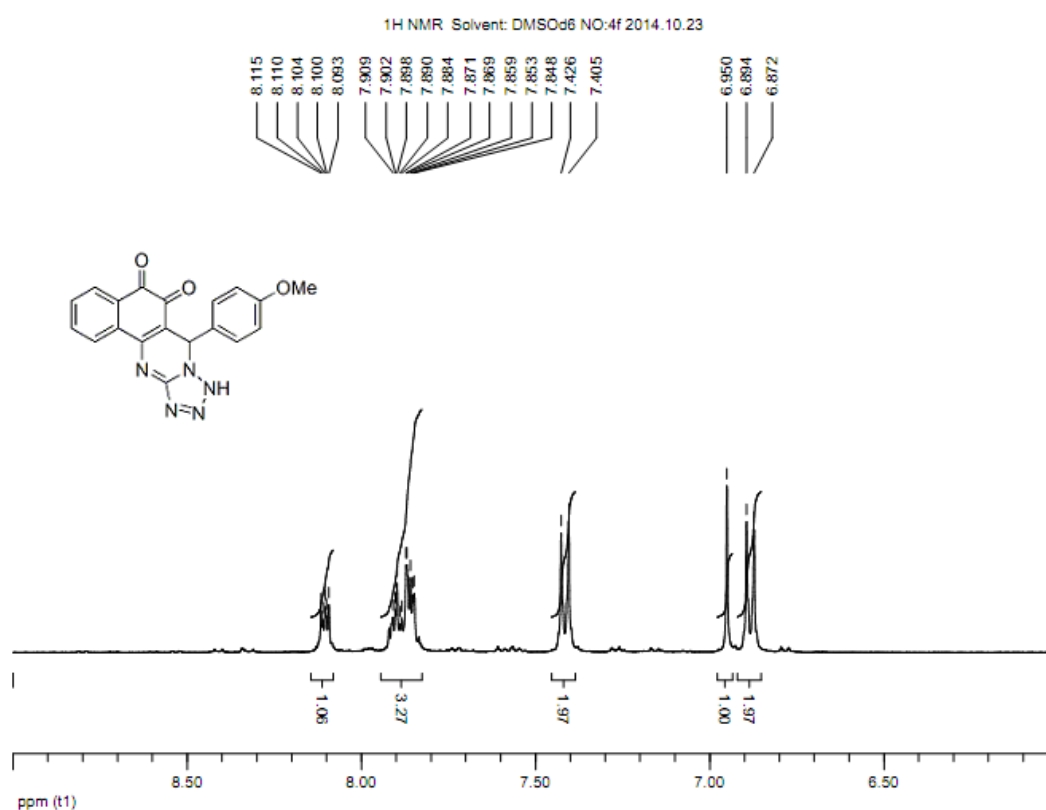
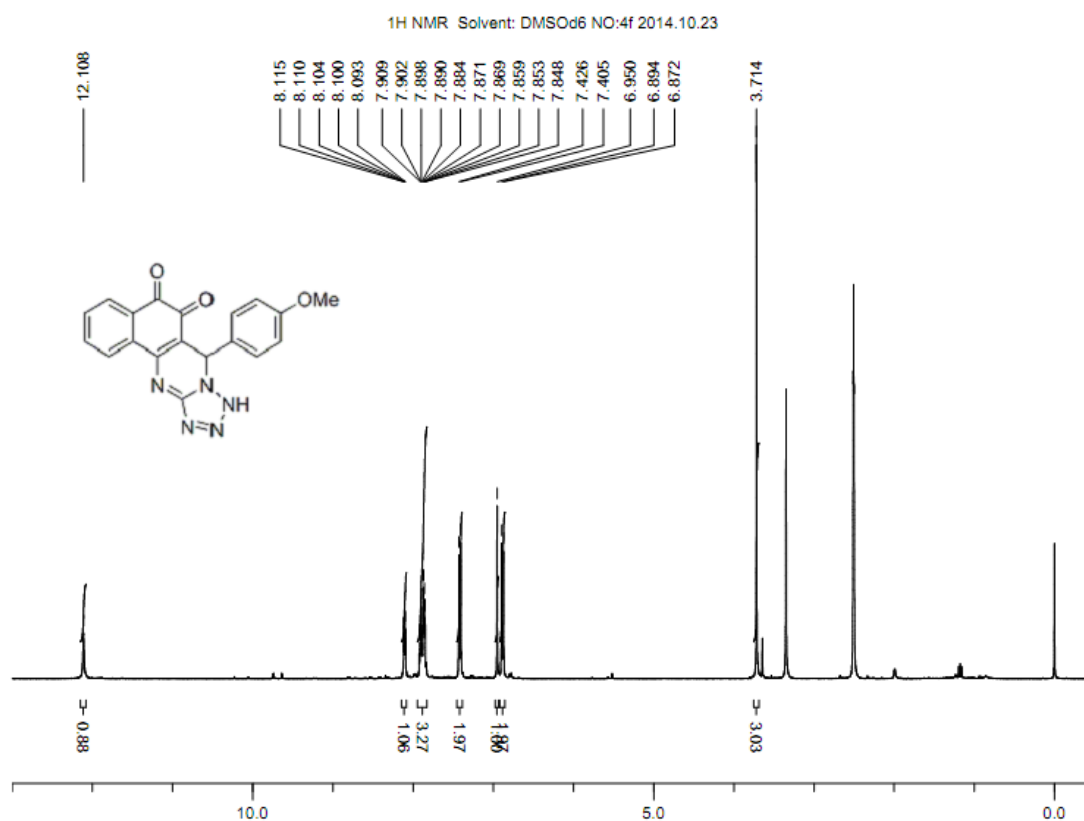


Figure 21 ^1H NMR of 4f

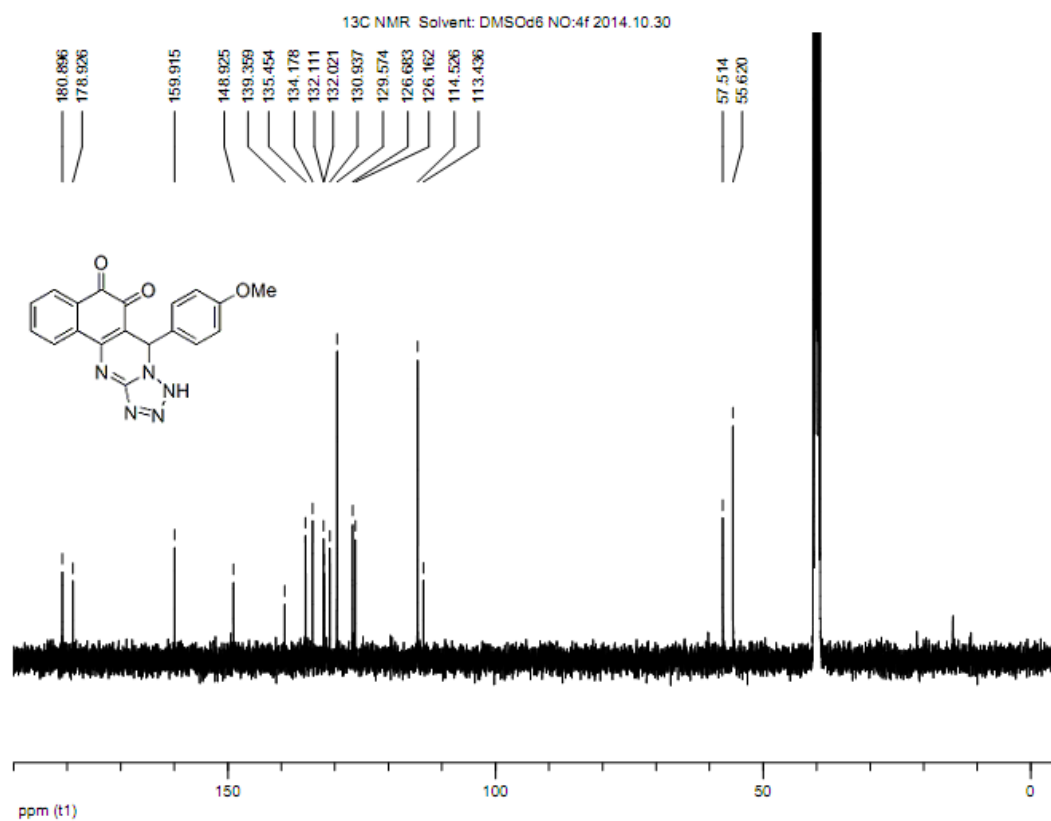


Figure 22 ¹³C NMR of 4f

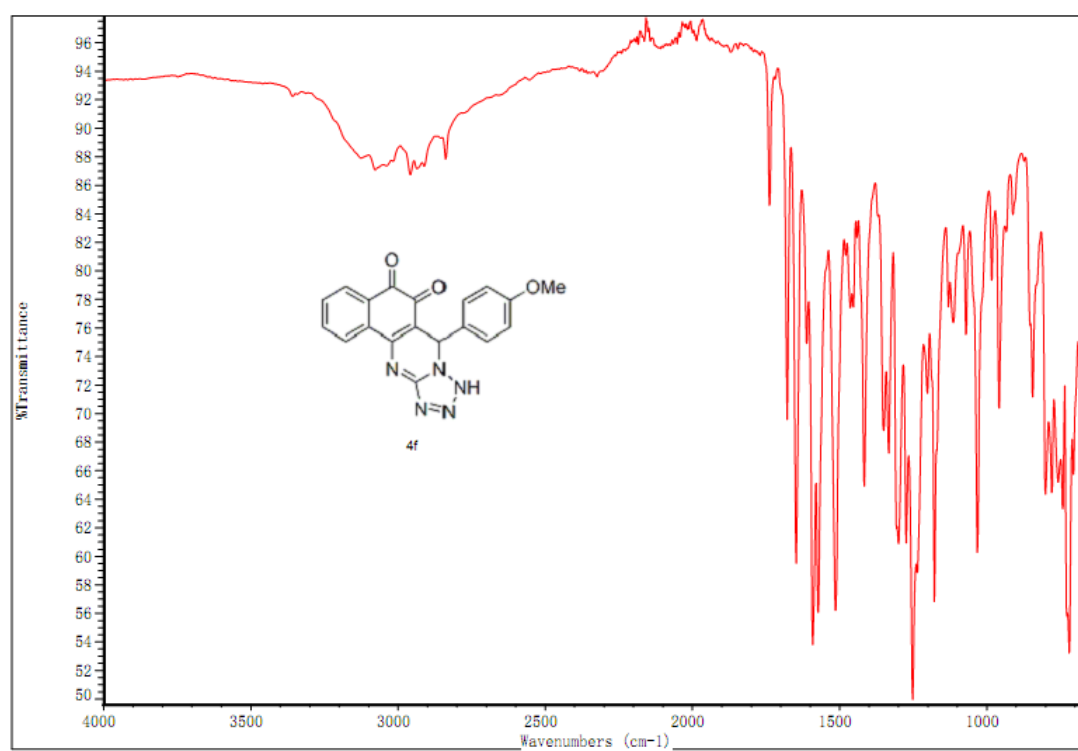


Figure 23 IR of 4f

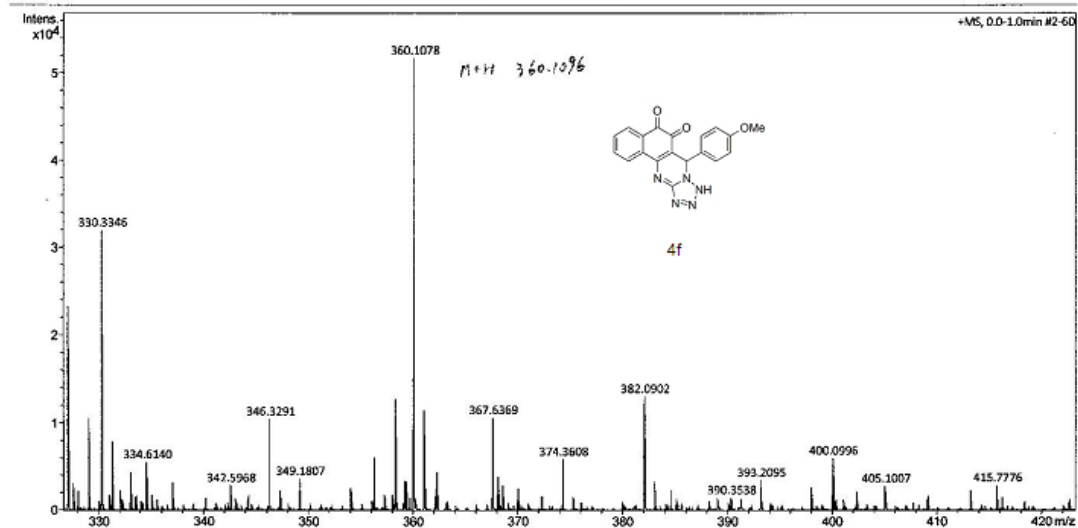
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 Sample Name 8
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 Operator zjx
 Instrument micrOTOF-Q III 6228888.20494

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	180.0 Vpp	Set Divert Valve	Waste



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Figure 24 HRMS of 4f

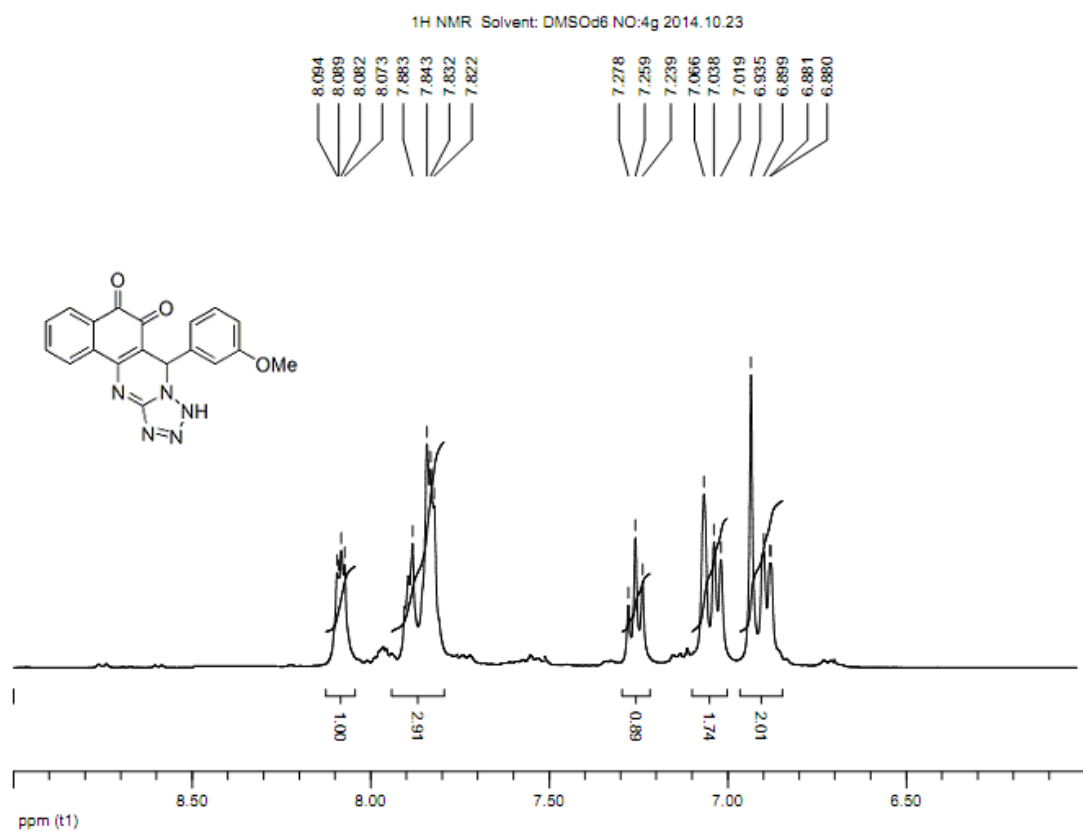
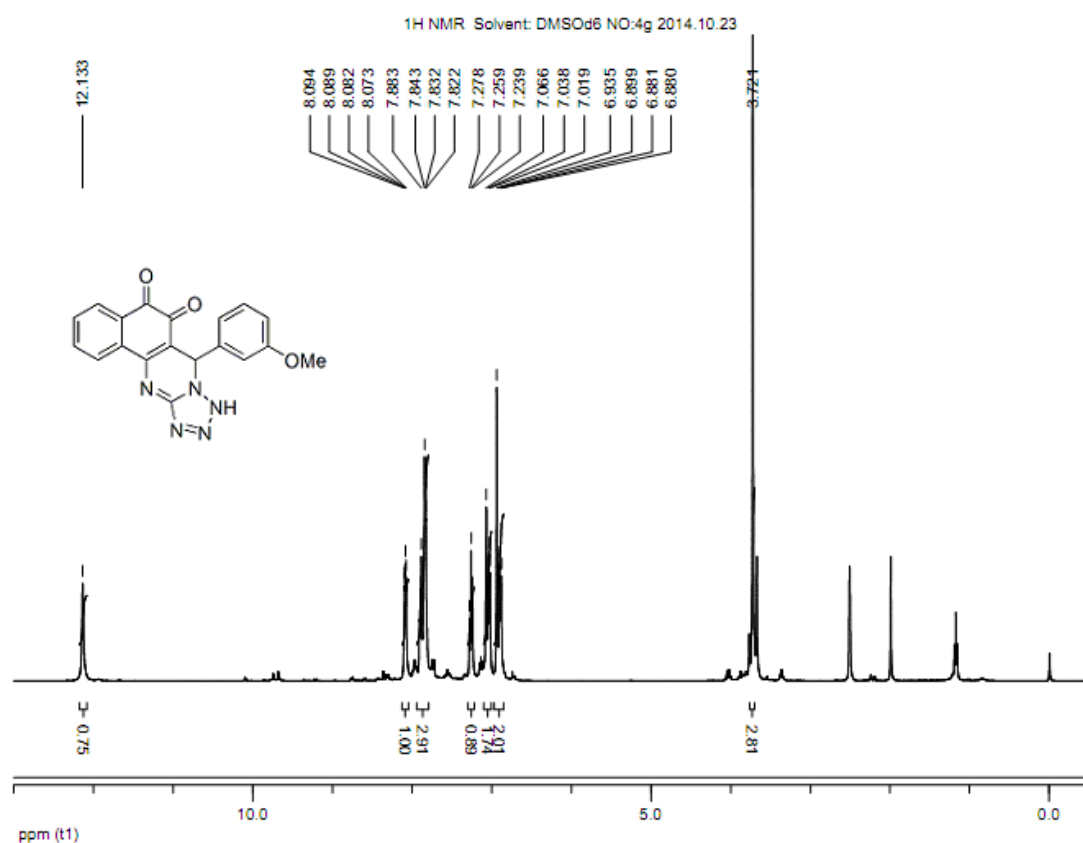


Figure 25 ^1H NMR of 4g

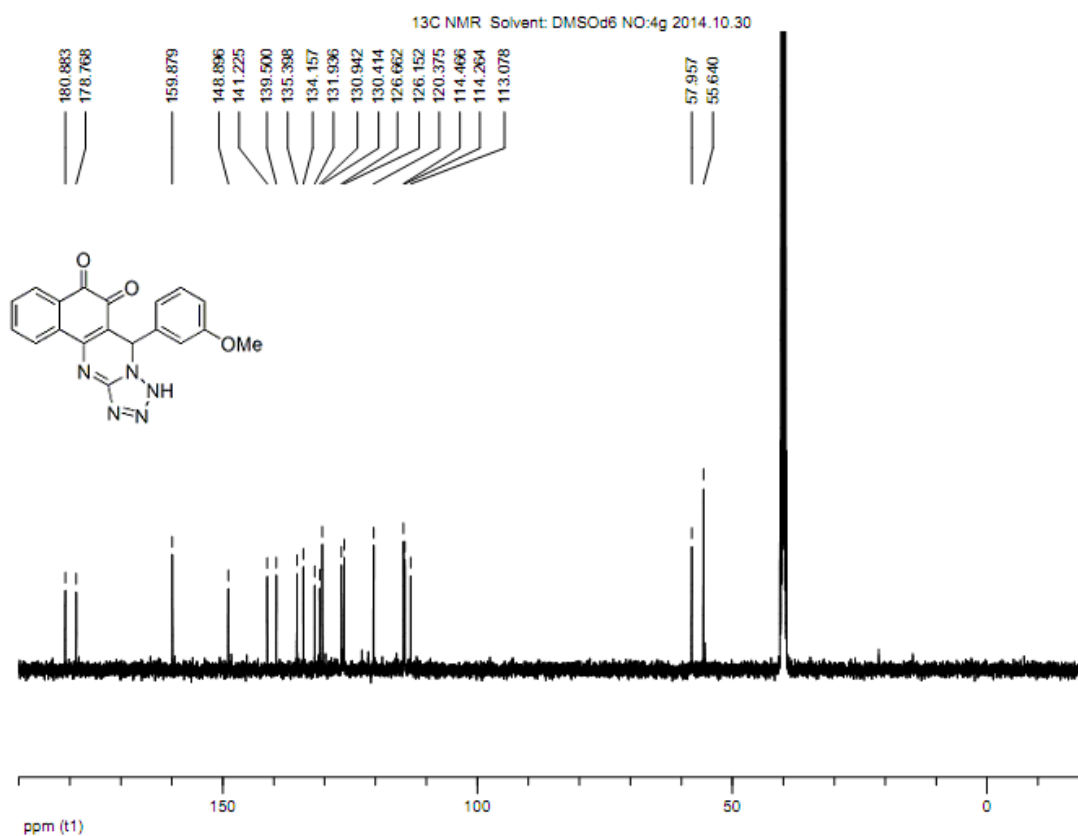


Figure 26 ¹³C NMR of 4g

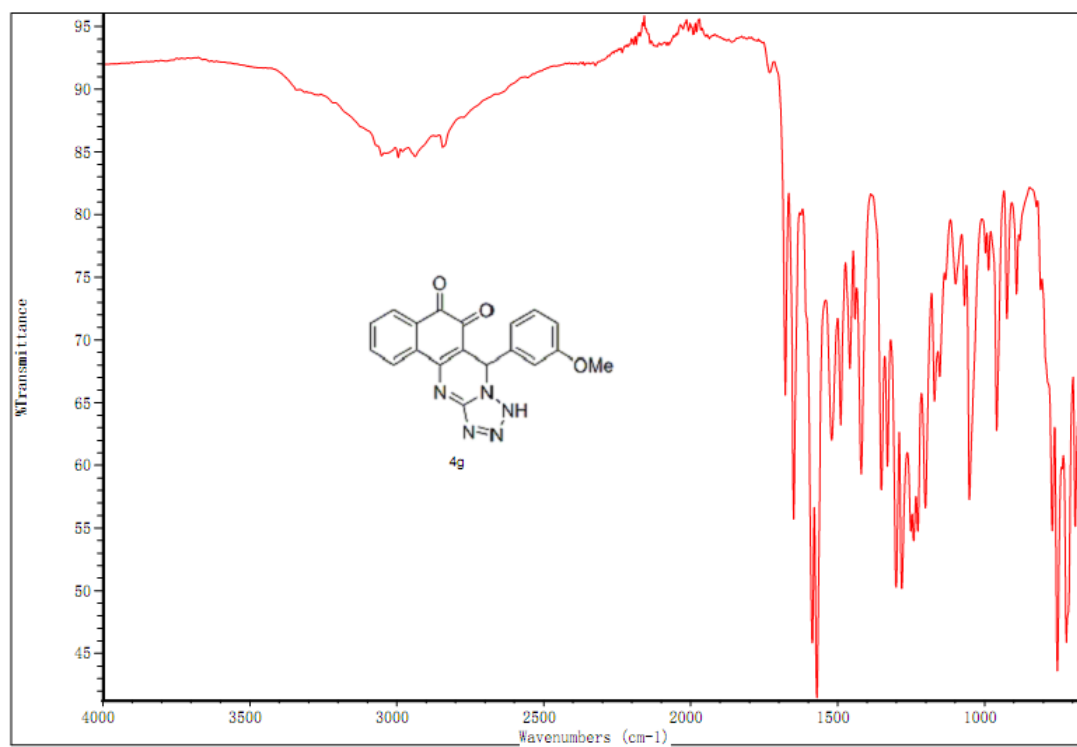
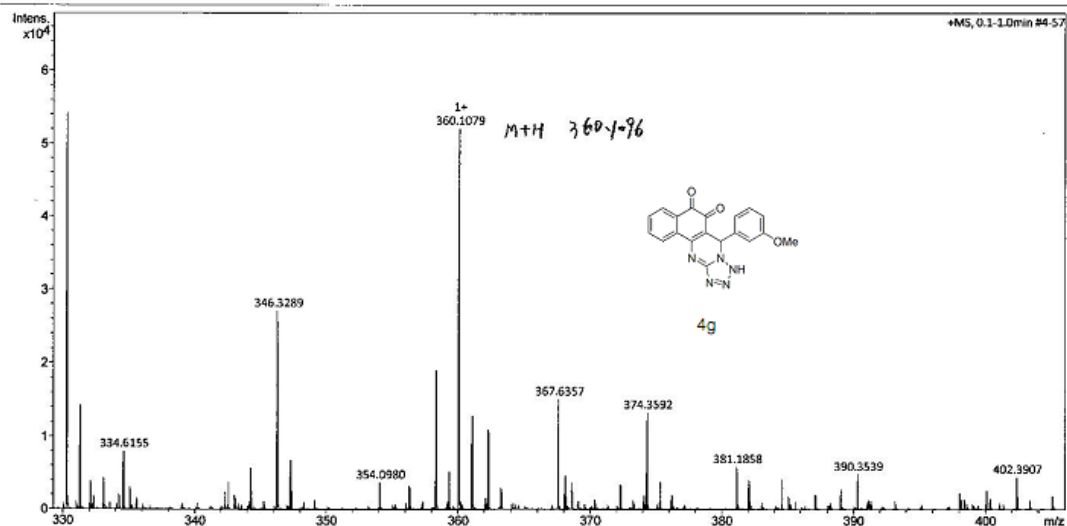


Figure 27 IR of 4g

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Method	Tune_pos_Standard.m	Instrument	microTOF-Q III		
Sample Name	025a		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	180.0 Vpp	Set Divert Valve	Waste



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Figure 28 HRMS of 4g

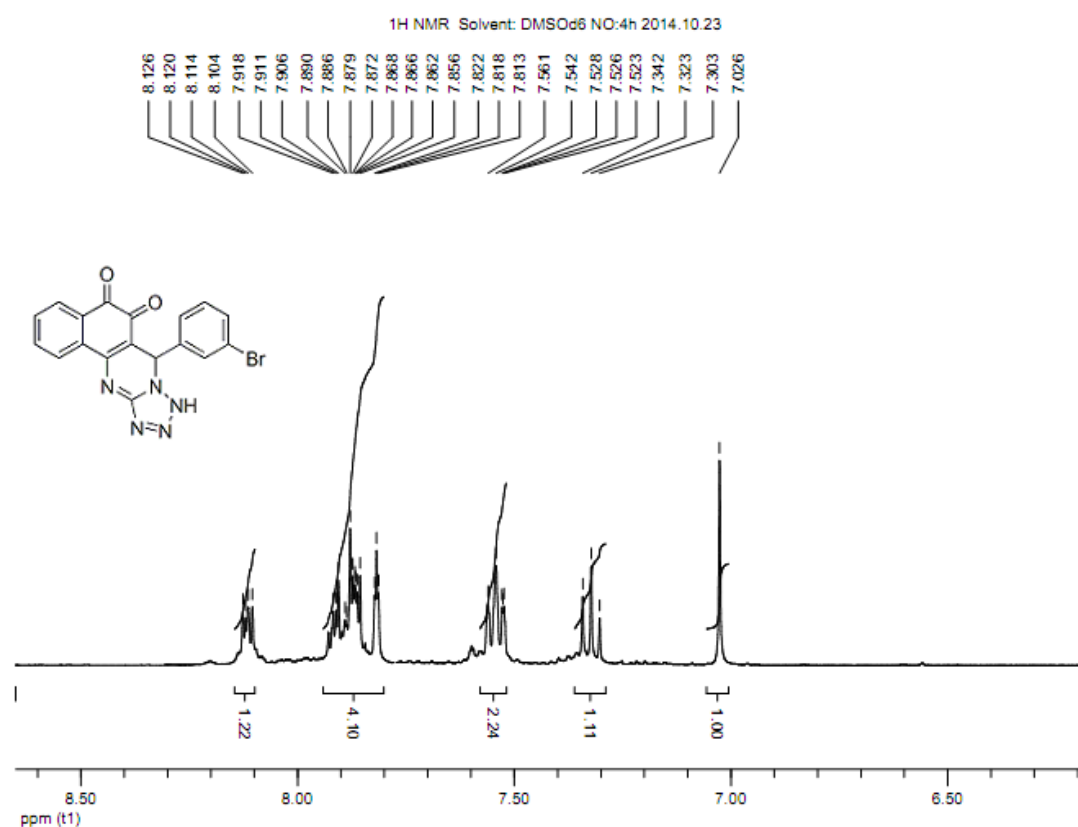
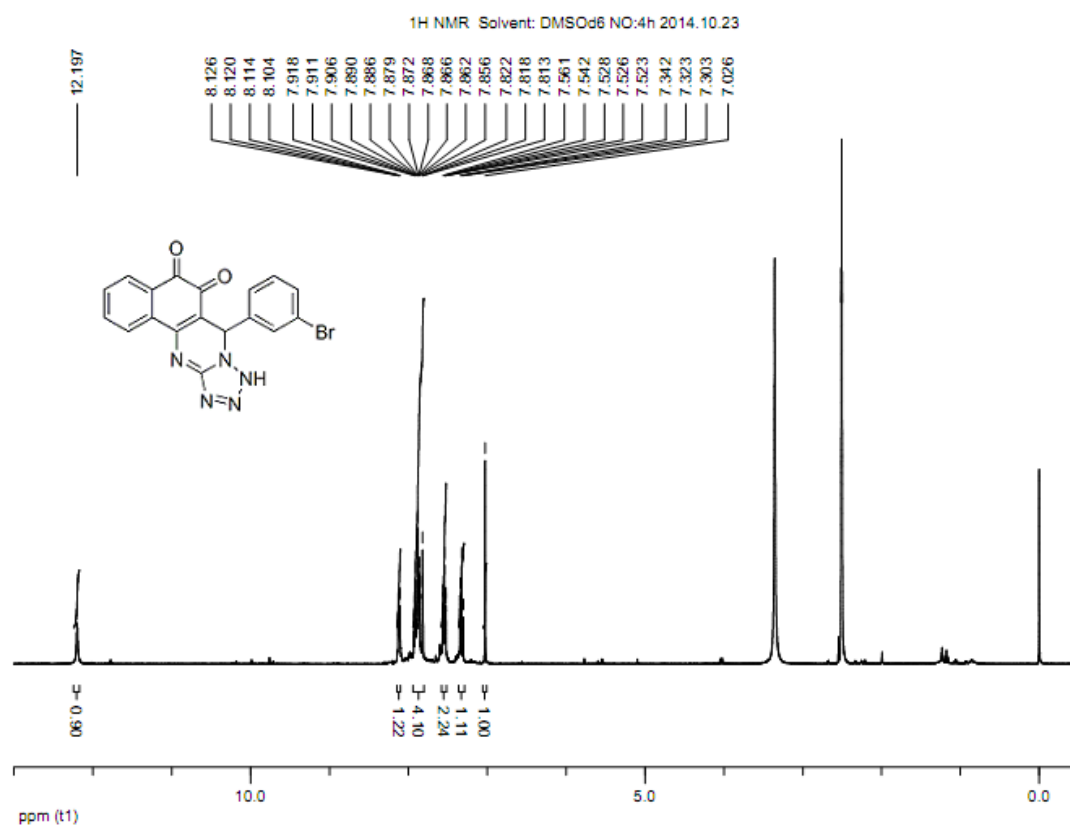


Figure 29 ¹H NMR of 4h

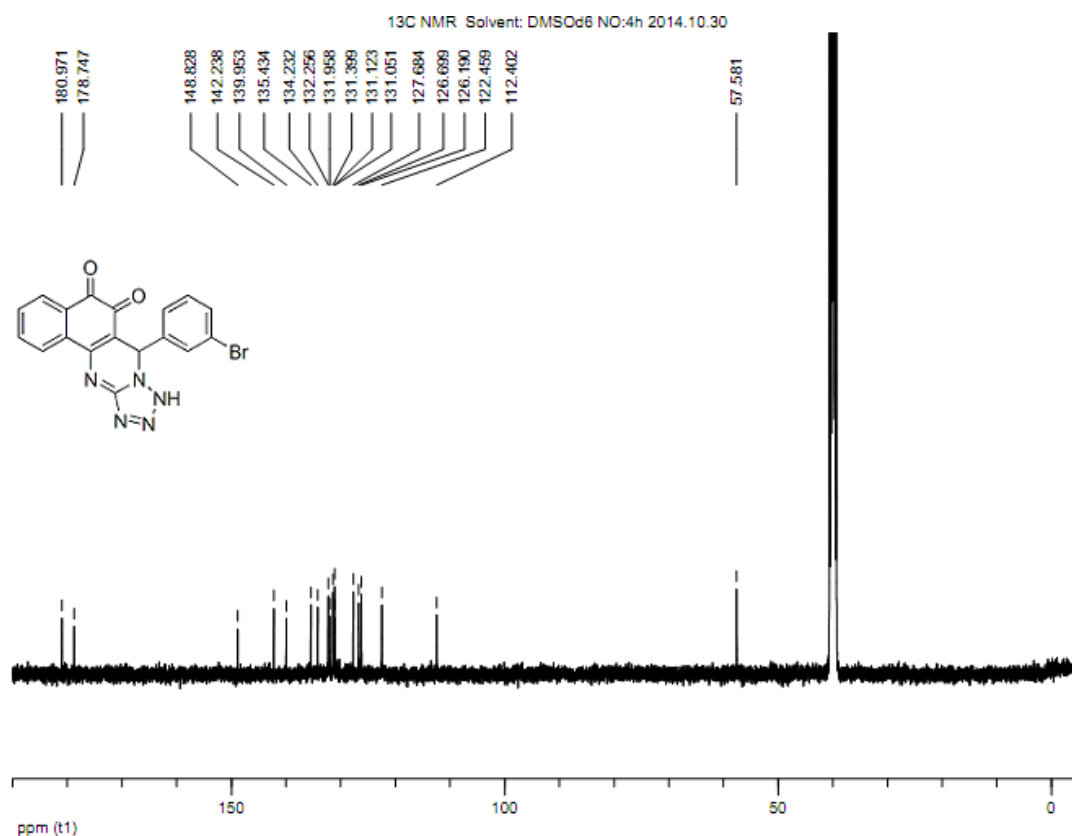


Figure 30 ^{13}C NMR of 4h

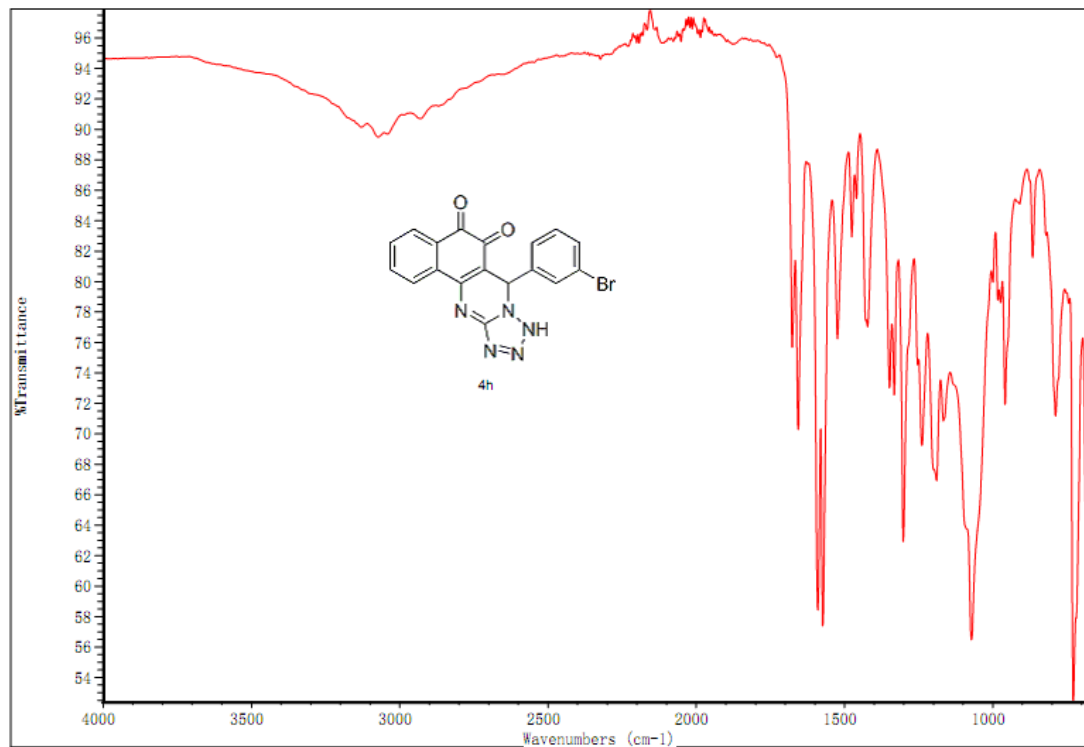
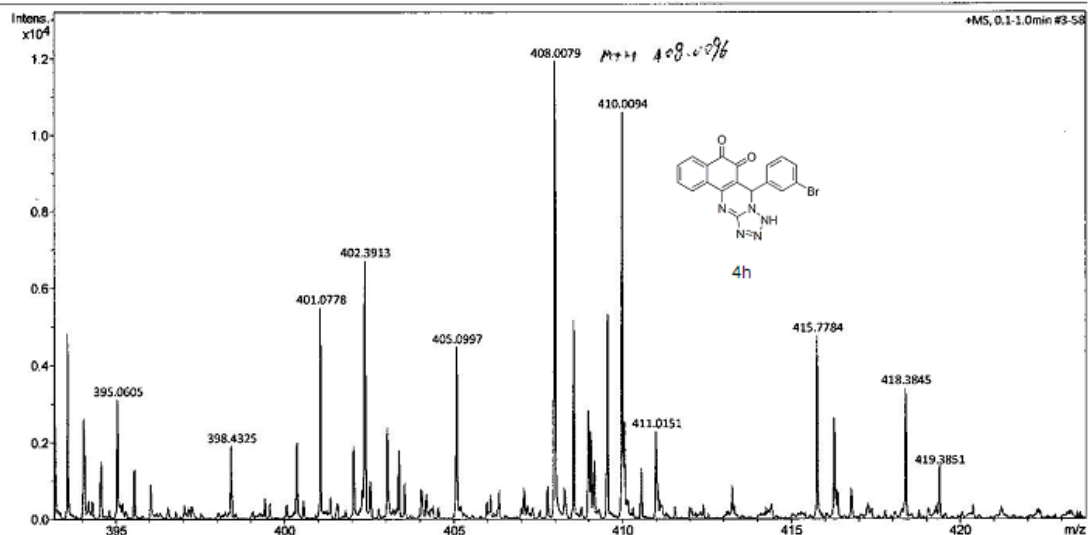


Figure 31 IR of 4h

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Analysis Name	D:\Data\wuliqiang\9.d	Operator	zjx
Method	Tune_pos_Standard.m	Instrument	micrOTOF-Q III
Sample Name	9		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	180.0 Vpp	Set Divert Valve	Waste



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Figure 32 HRMS of 4h

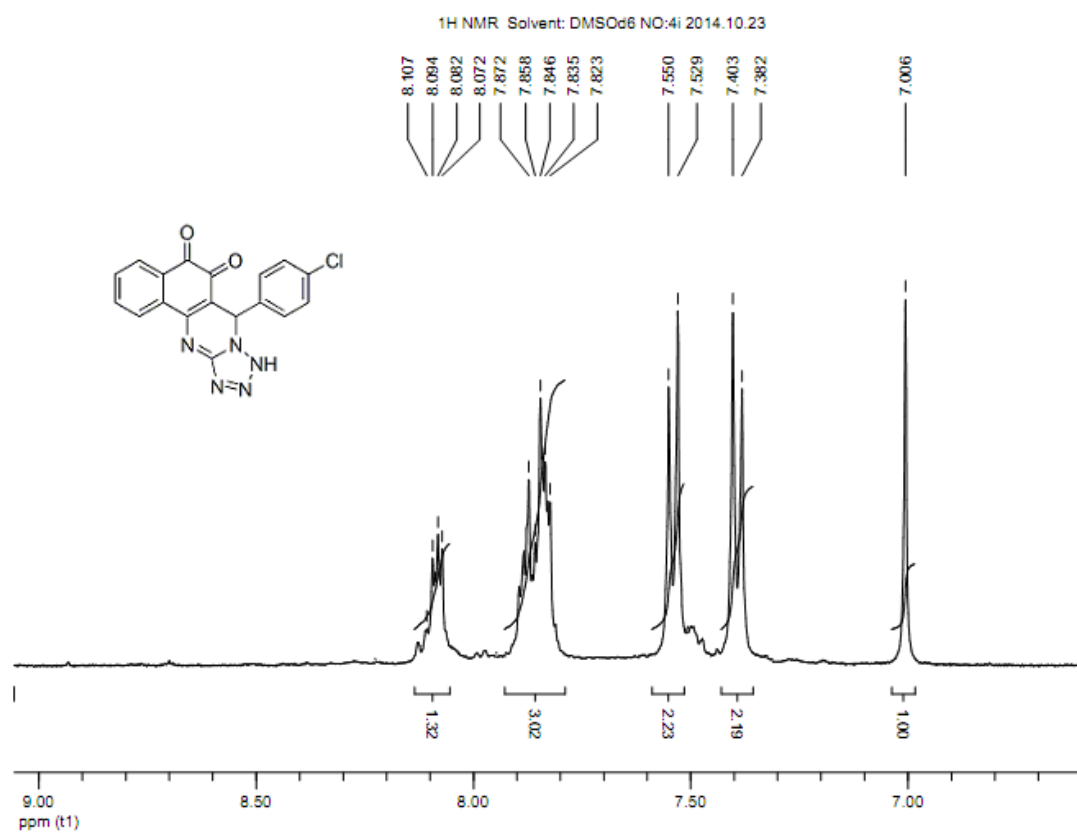
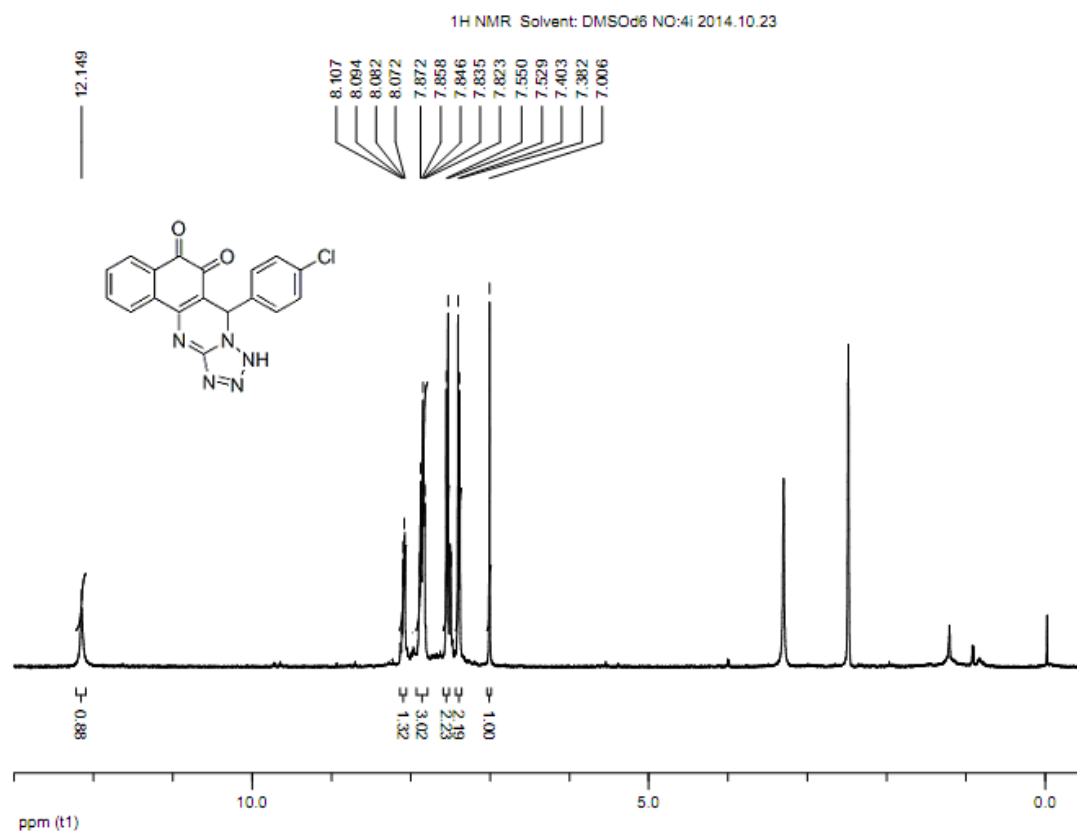


Figure 33 ¹H NMR of 4i

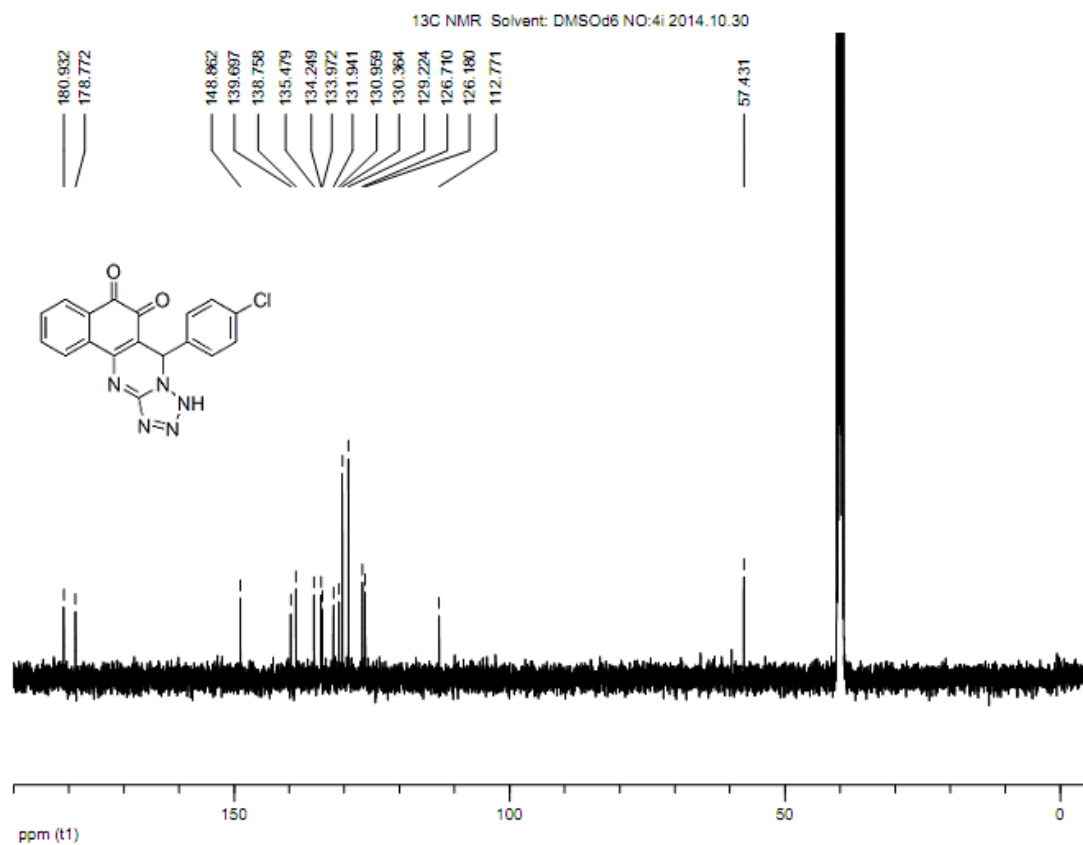


Figure 34 ¹³C NMR of 4i

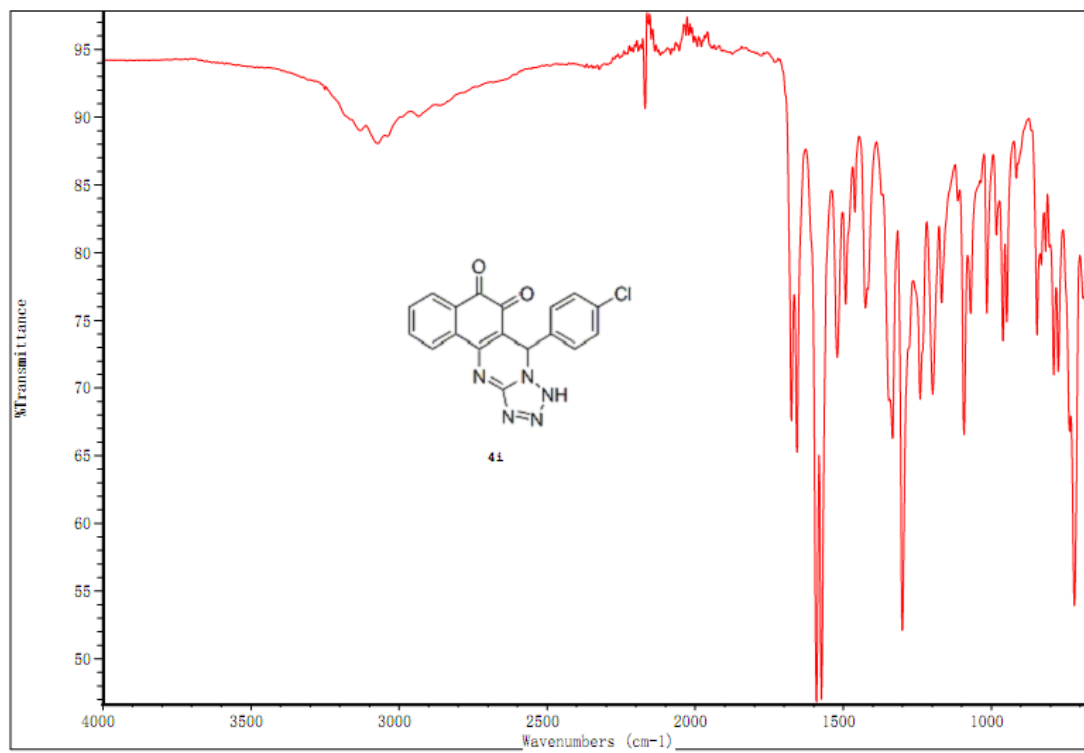
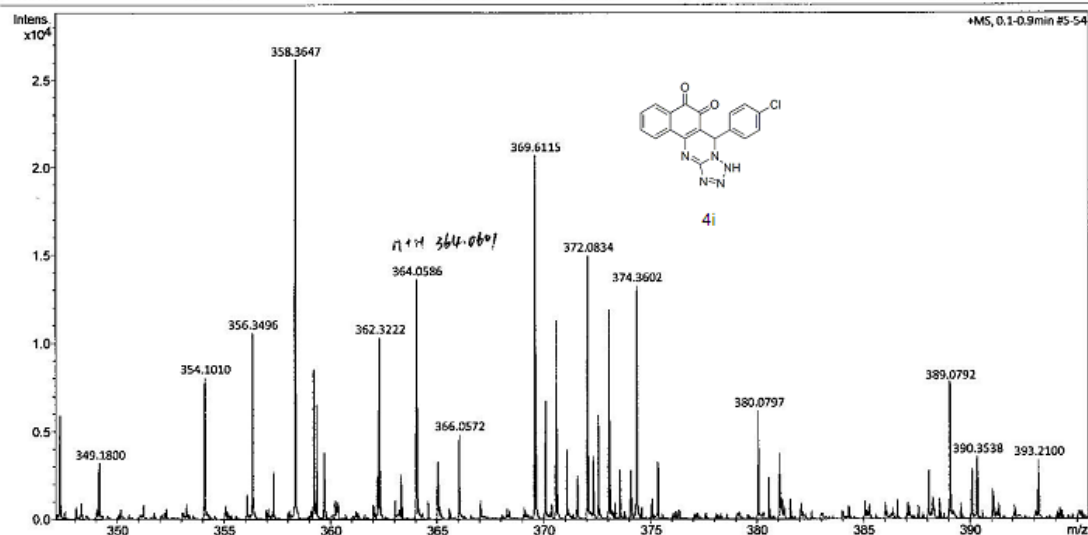


Figure 35 IR of 4i

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Method	Tune_pos_Standard.m	Instrument	micrOTOF-Q III
Sample Name	11		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	180.0 Vpp	Set Divert Valve	Waste



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Figure 36 HRMS of **4i**

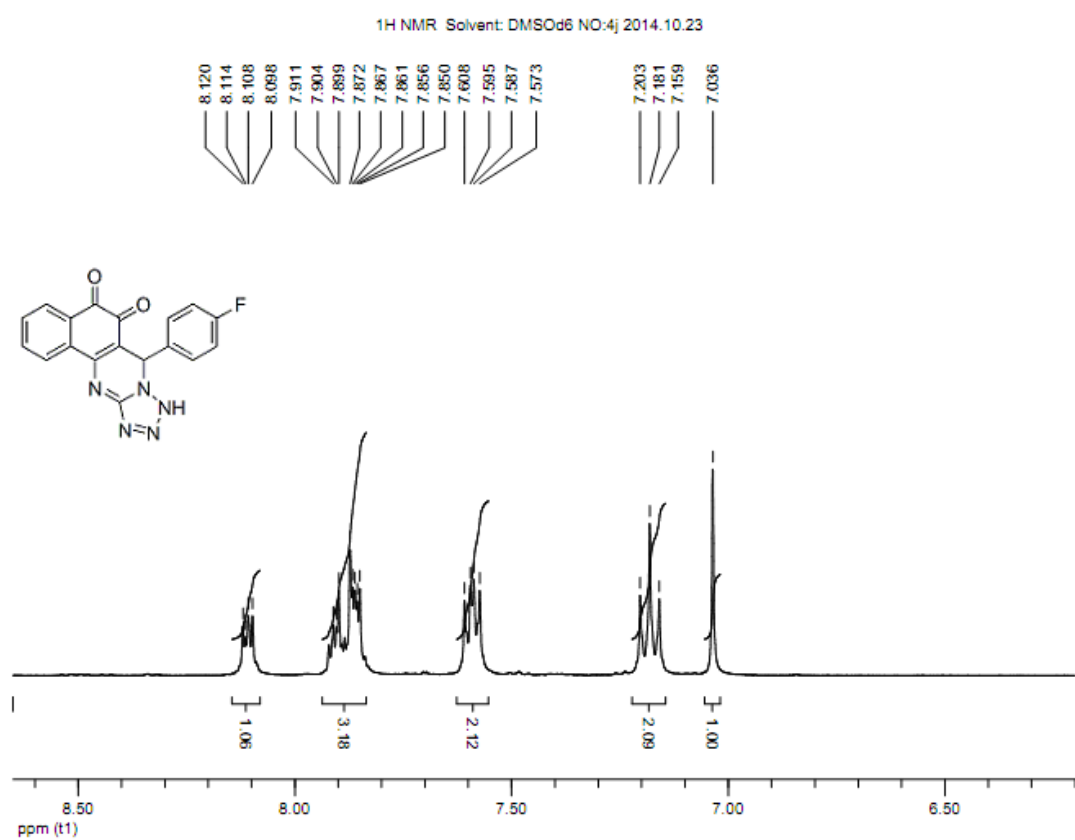
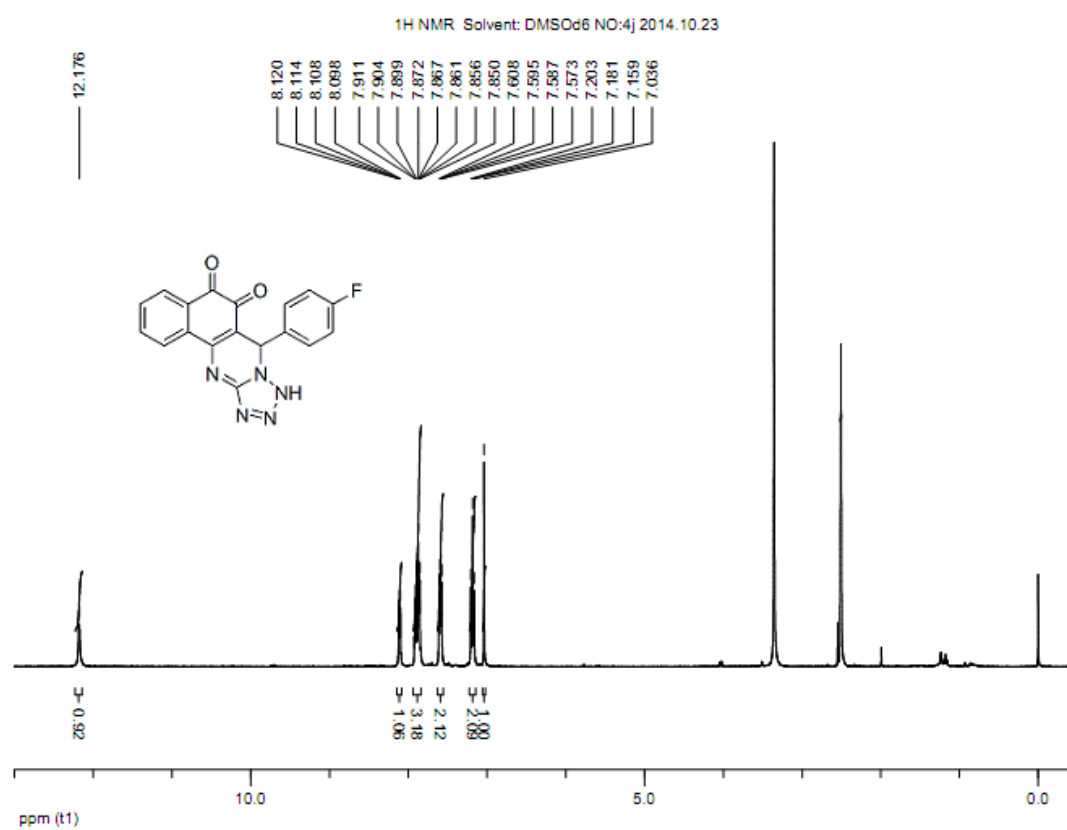


Figure 37 ¹H NMR of 4j

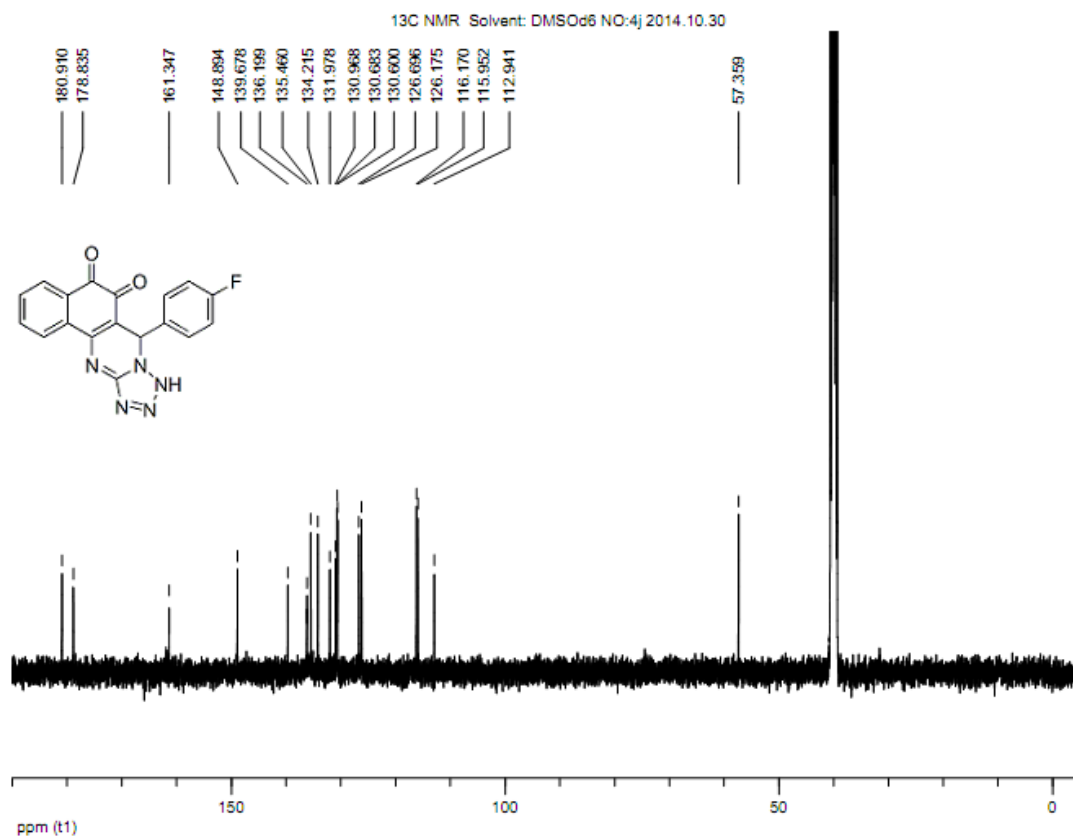


Figure 38 ¹³C NMR of 4j

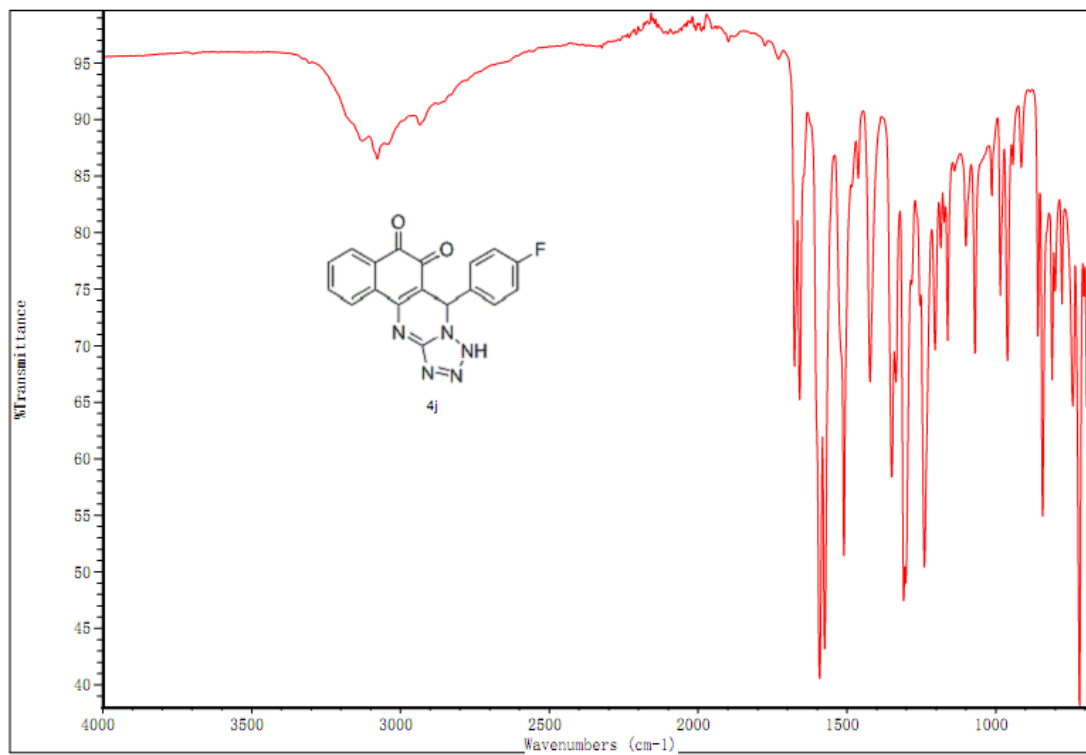


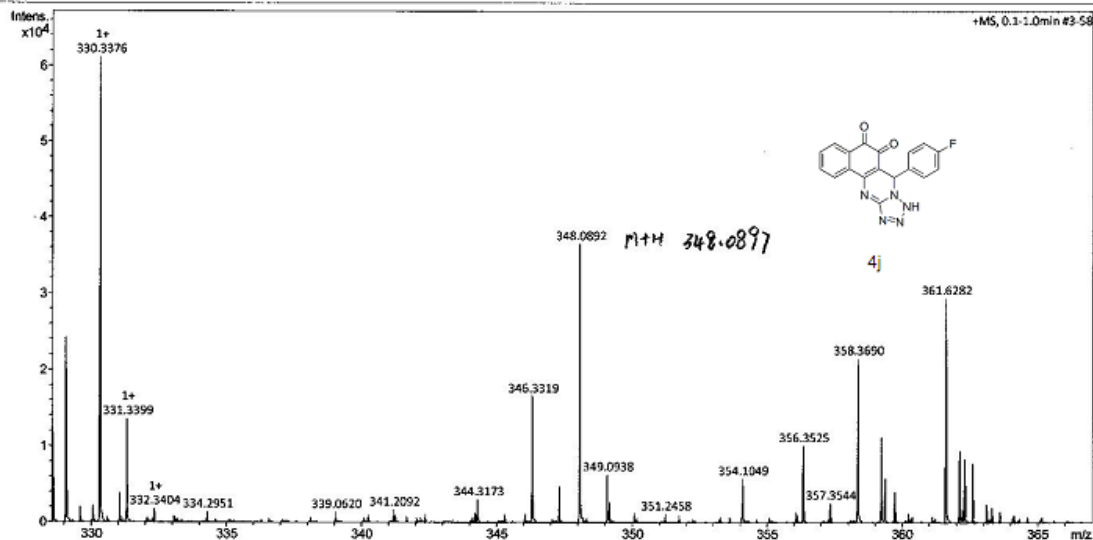
Figure 39 IR of 4j

Display Report

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Method	Tune_pos_Standard.m	Instrument	micrOTOF-Q III
Sample Name	021		8228888.20494
Comment			

Acquisition Parameter

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	0.3 Bar
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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	180.0 Vpp	Set Divert Valve	Waste



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Figure 40 HRMS of 4j

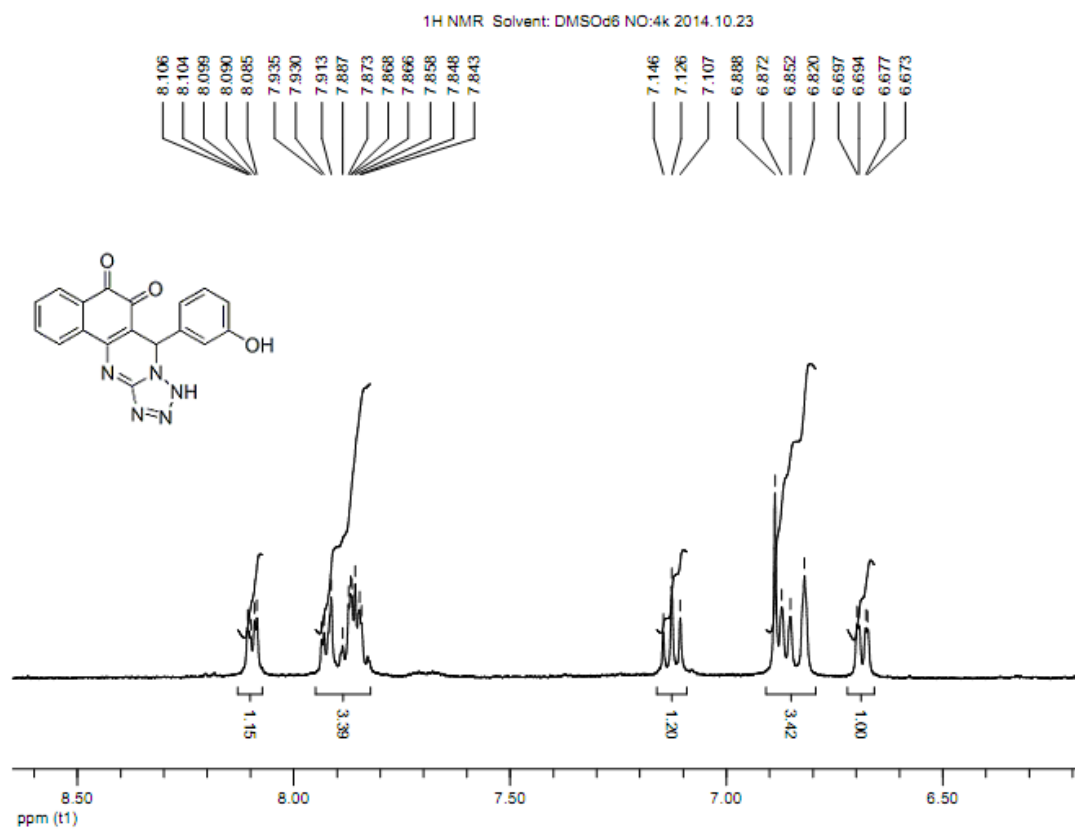
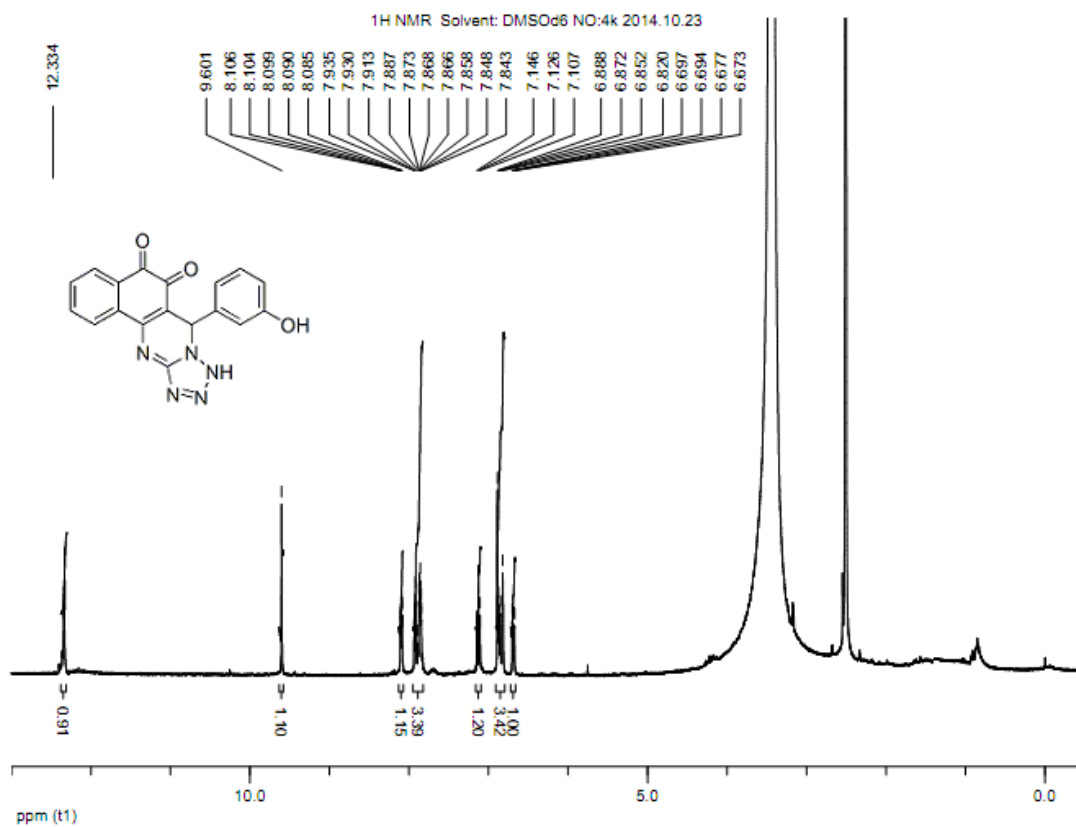


Figure 41 ¹H NMR of 4k

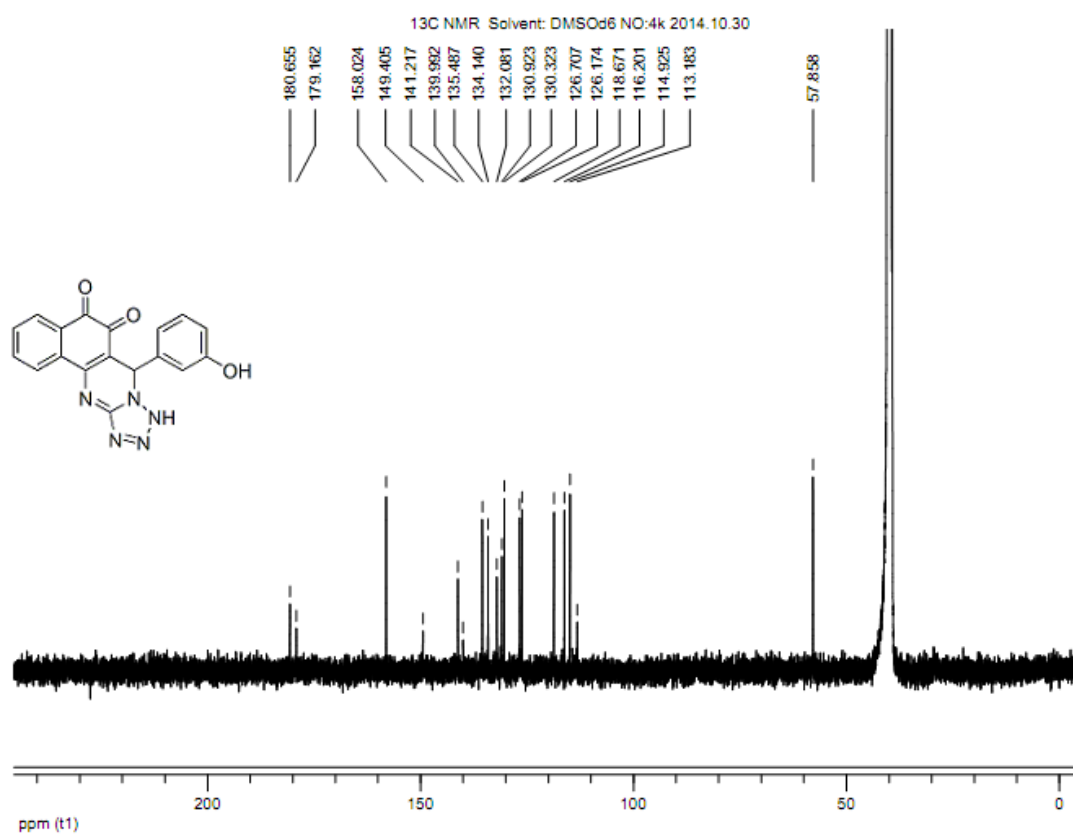


Figure 42 ¹³C NMR of 4k

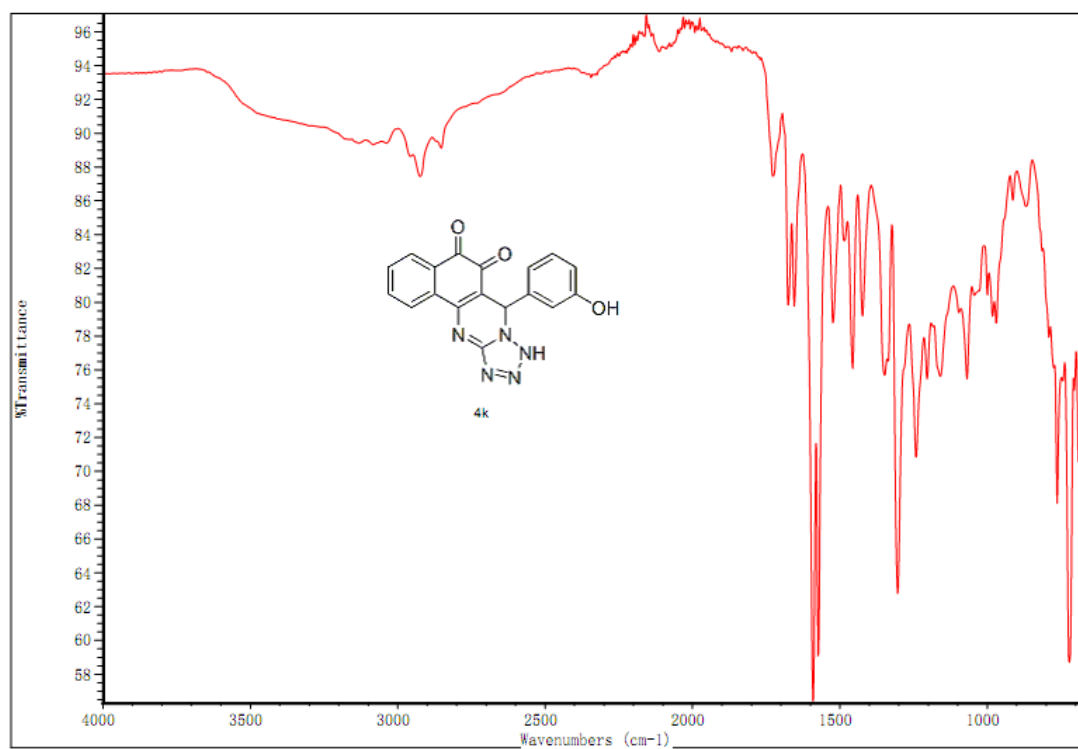
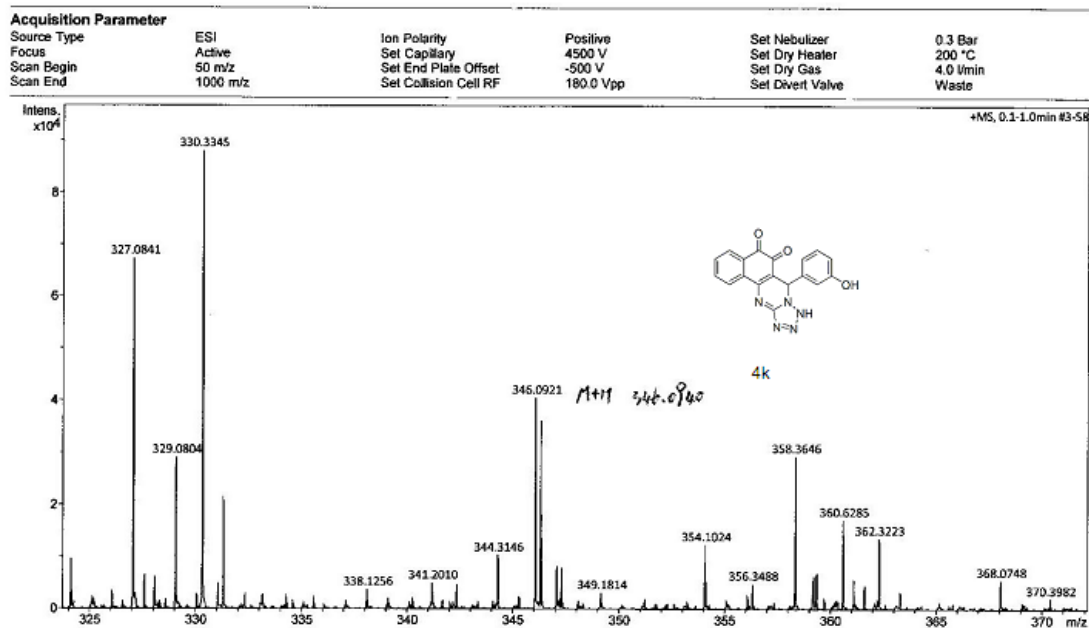


Figure 43 IR of 4k

Display Report

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Method	Tune_pos_Standard.m	Instrument	micrOTOF-Q III
Sample Name	15		8228888.20494
Comment			



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Figure 44 HRMS of **4k**

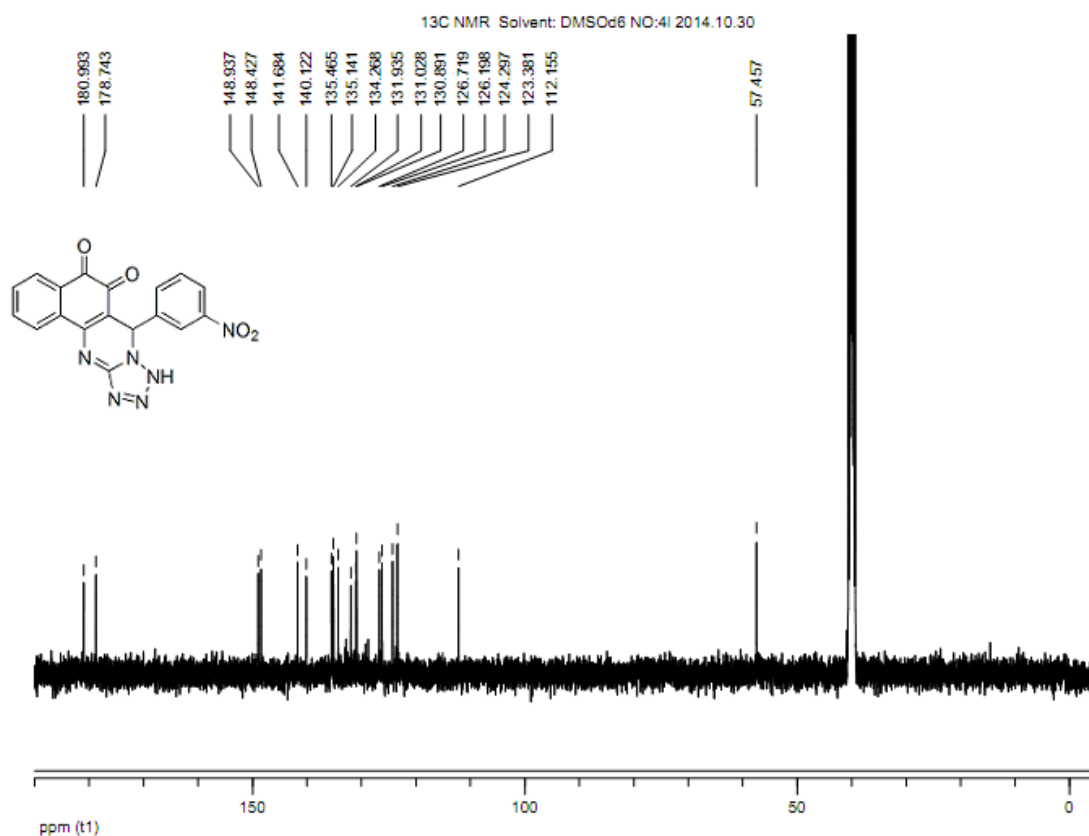


Figure 46 ¹³C NMR of 41

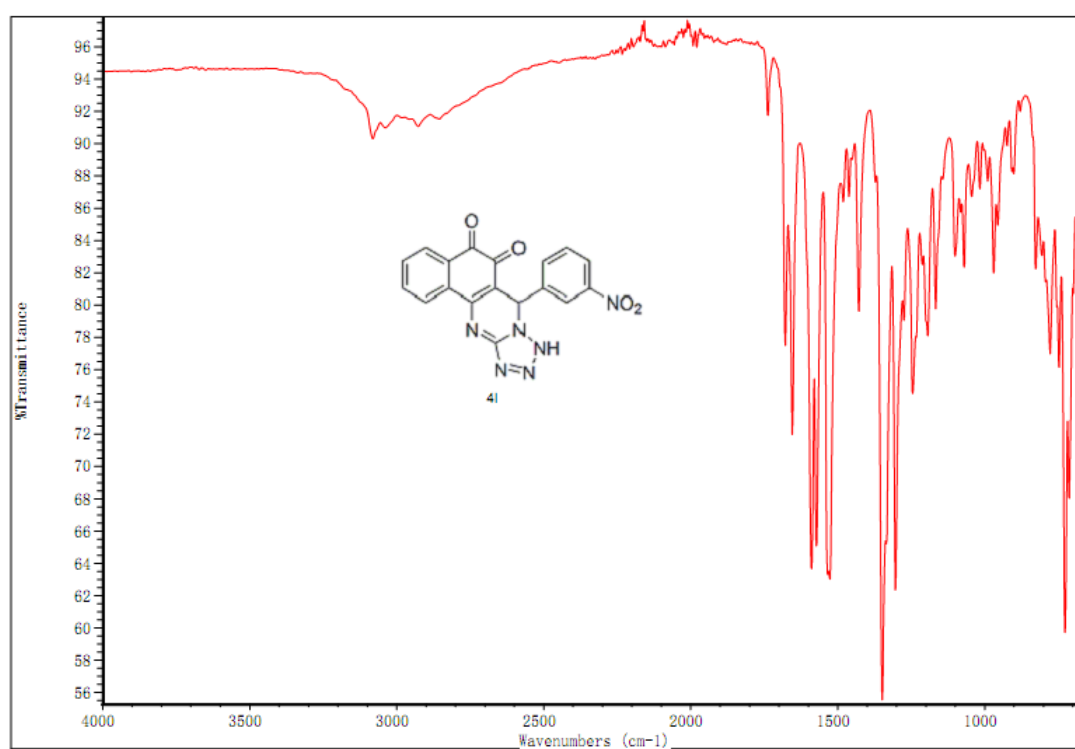


Figure 47 IR of 41

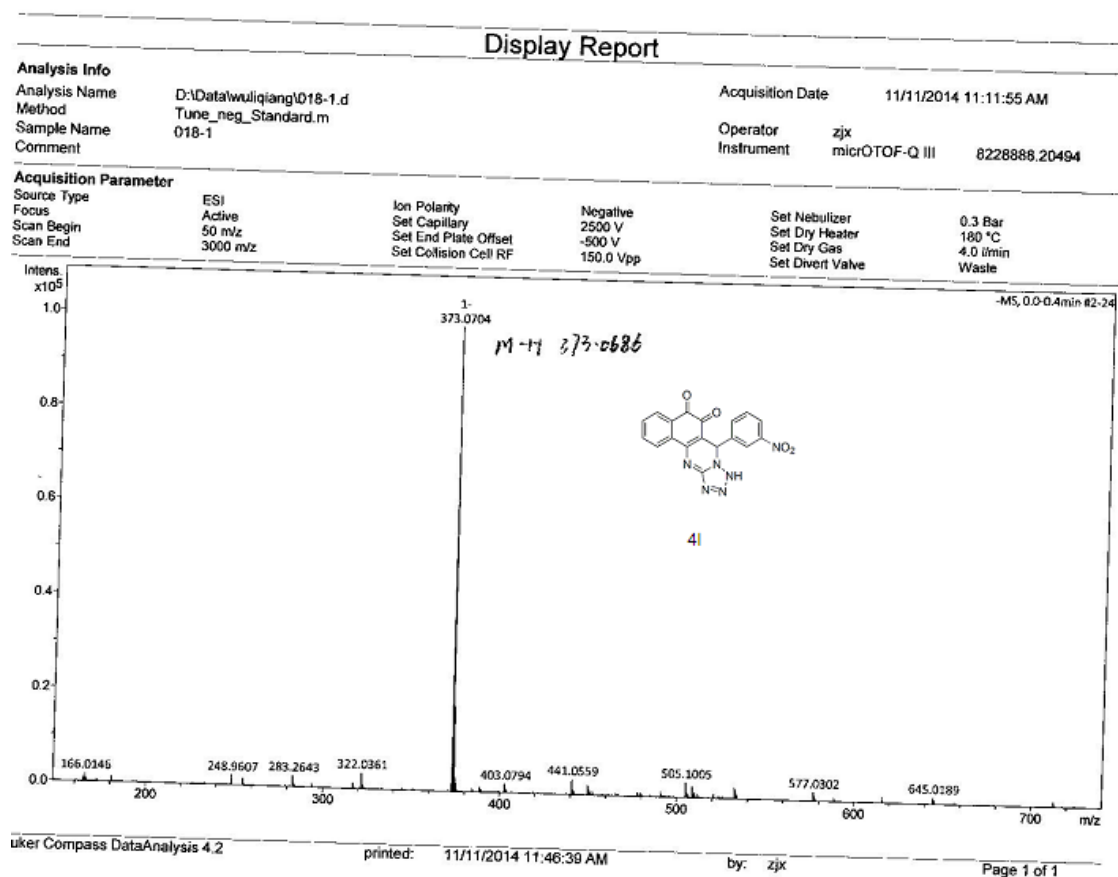


Figure 48 HRMS of **4I**

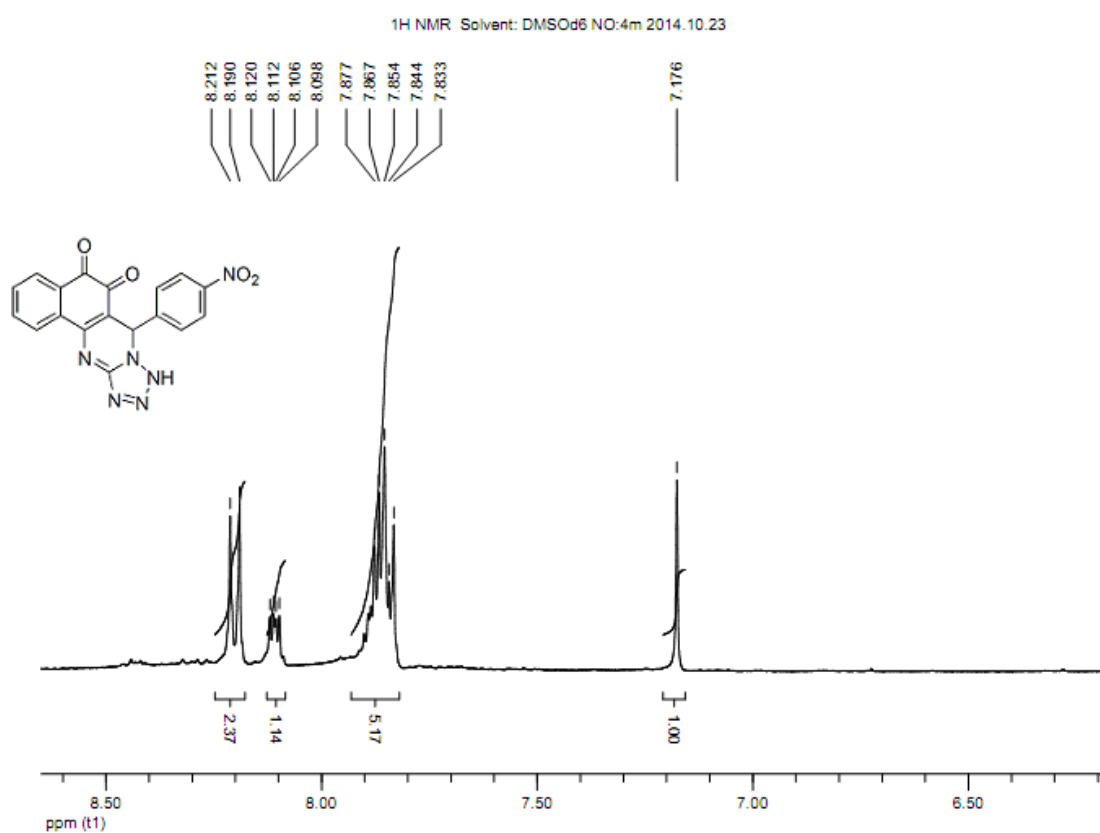
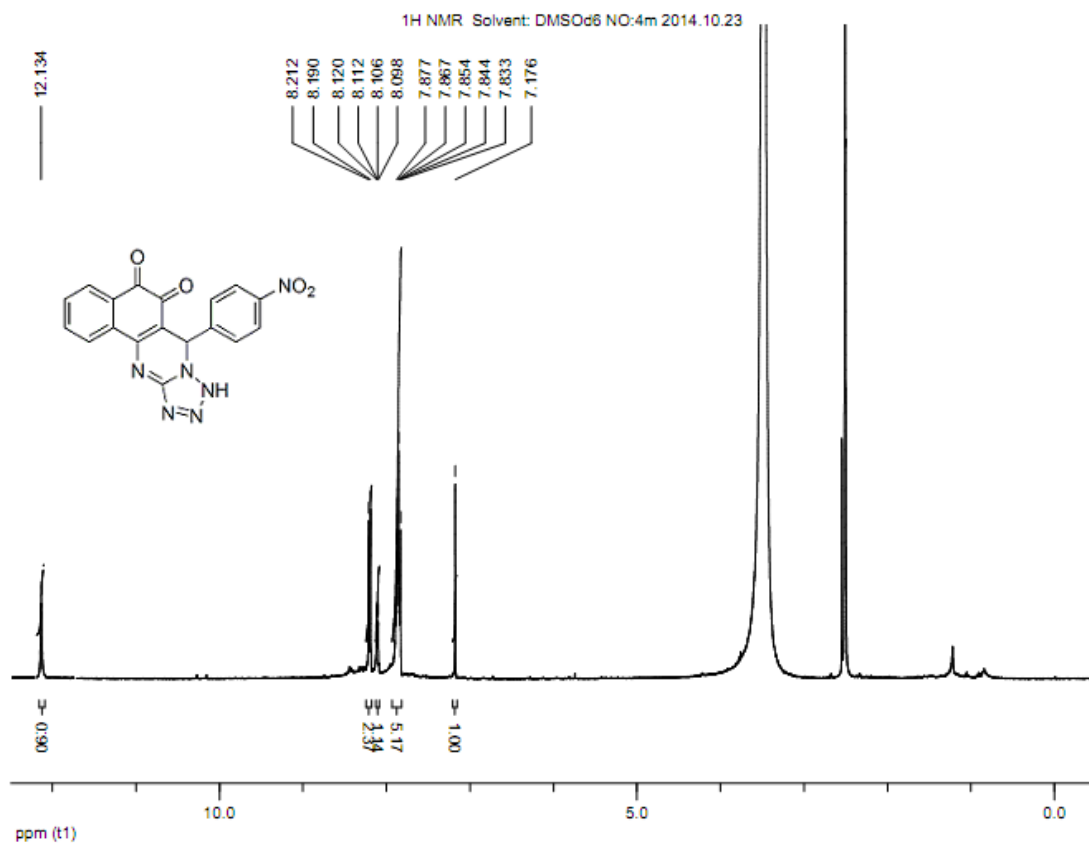


Figure 49 ^1H NMR of 4m

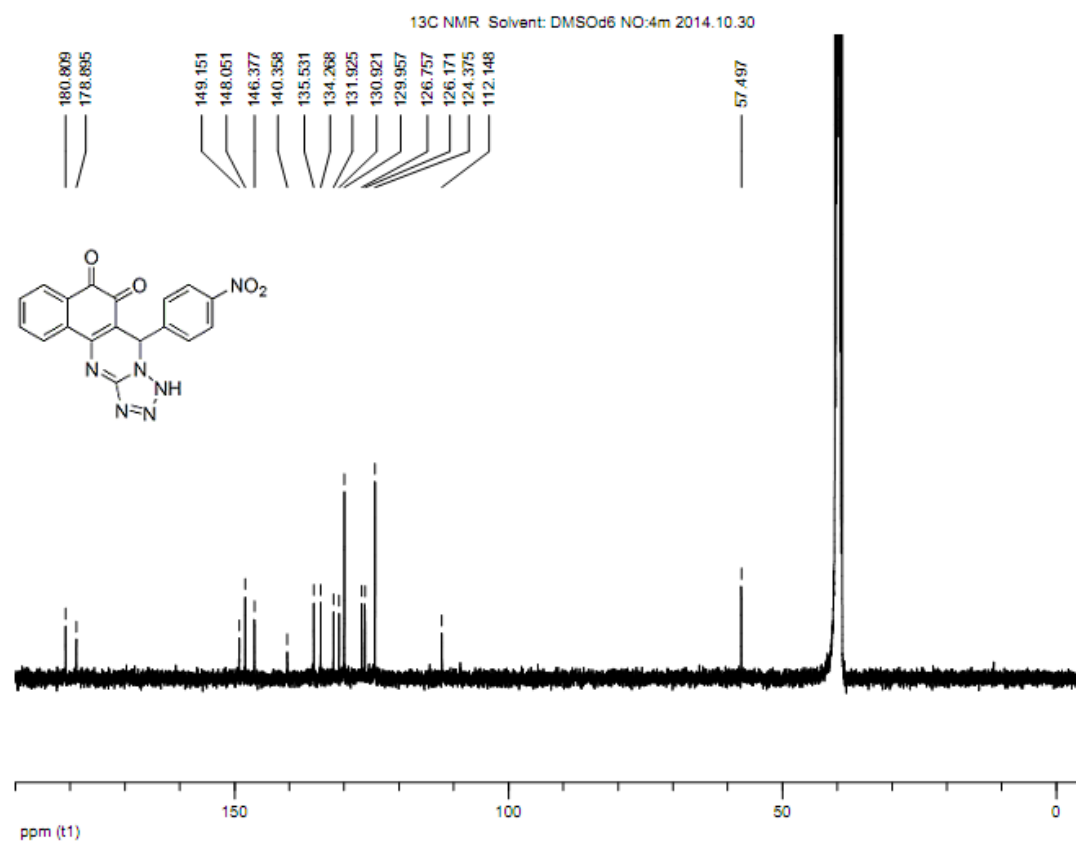


Figure 50 ¹³C NMR of 4m

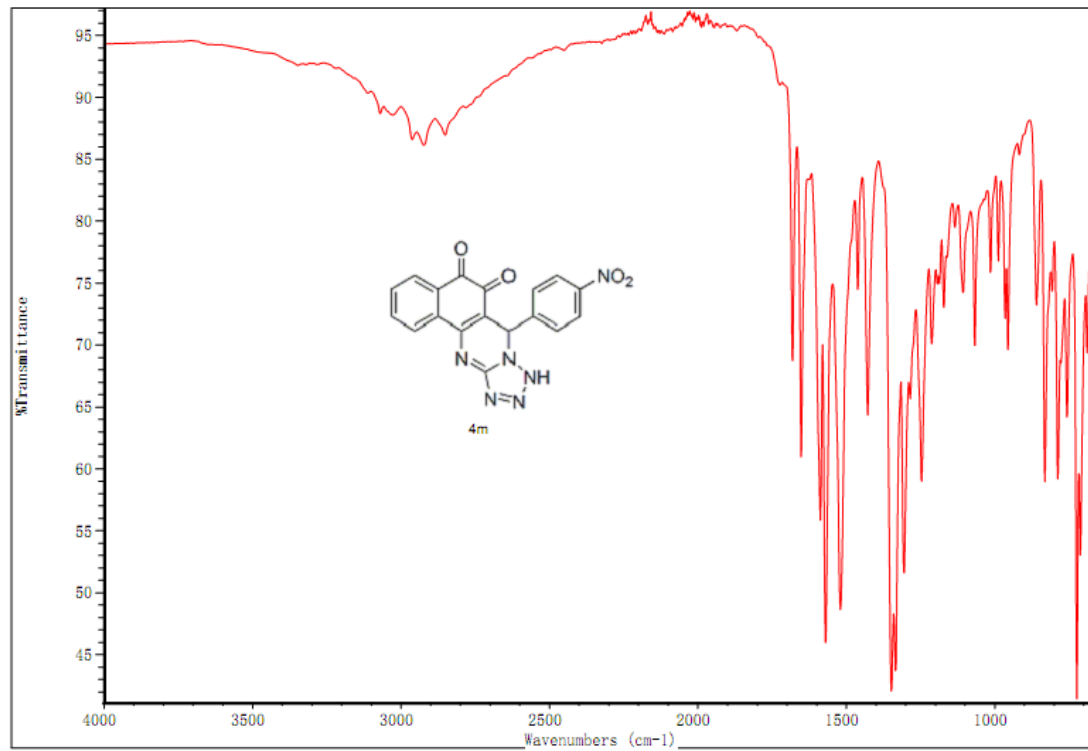


Figure 51 IR of 4m

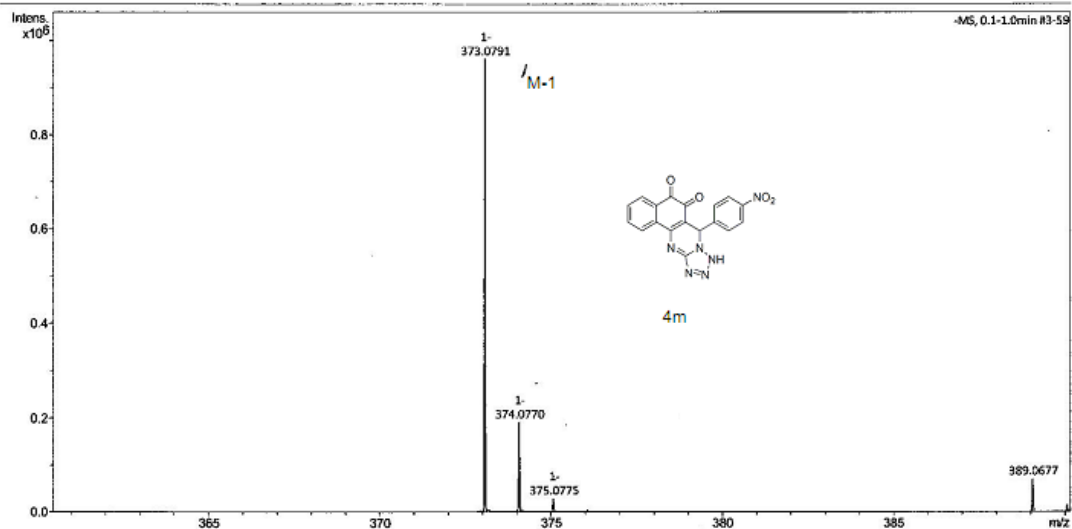
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 Method Tune_neg_Standard.m
 Sample Name 20-neg
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 Operator zjx
 Instrument micrOTOF-Q III 6228888.20494

Acquisition Parameter

Source Type	ESI	Ion Polarity	Negative	Set Nebulizer	0.3 Bar
Focus	Active	Set Capillary	2500 V	Set Dry Heater	180 °C
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Scan End	3000 m/z	Set Collision Cell RF	150.0 Vpp	Set Divert Valve	Waste



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Figure 52 HRMS of 4m

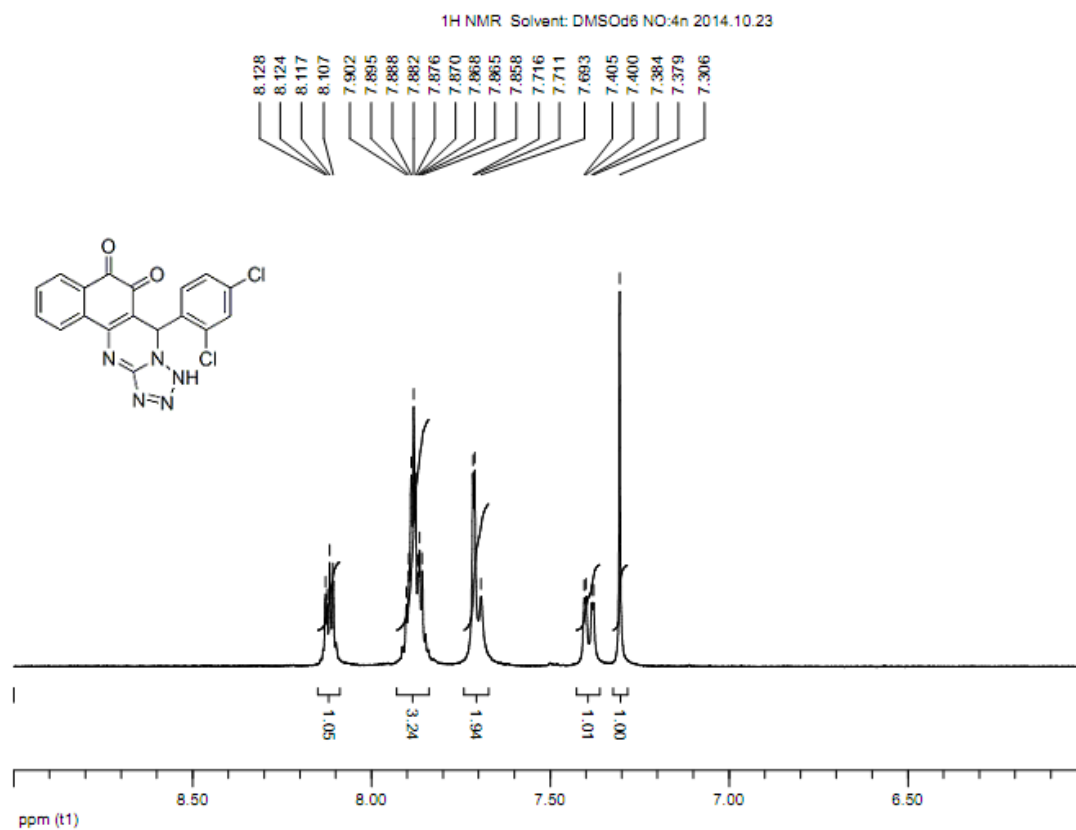
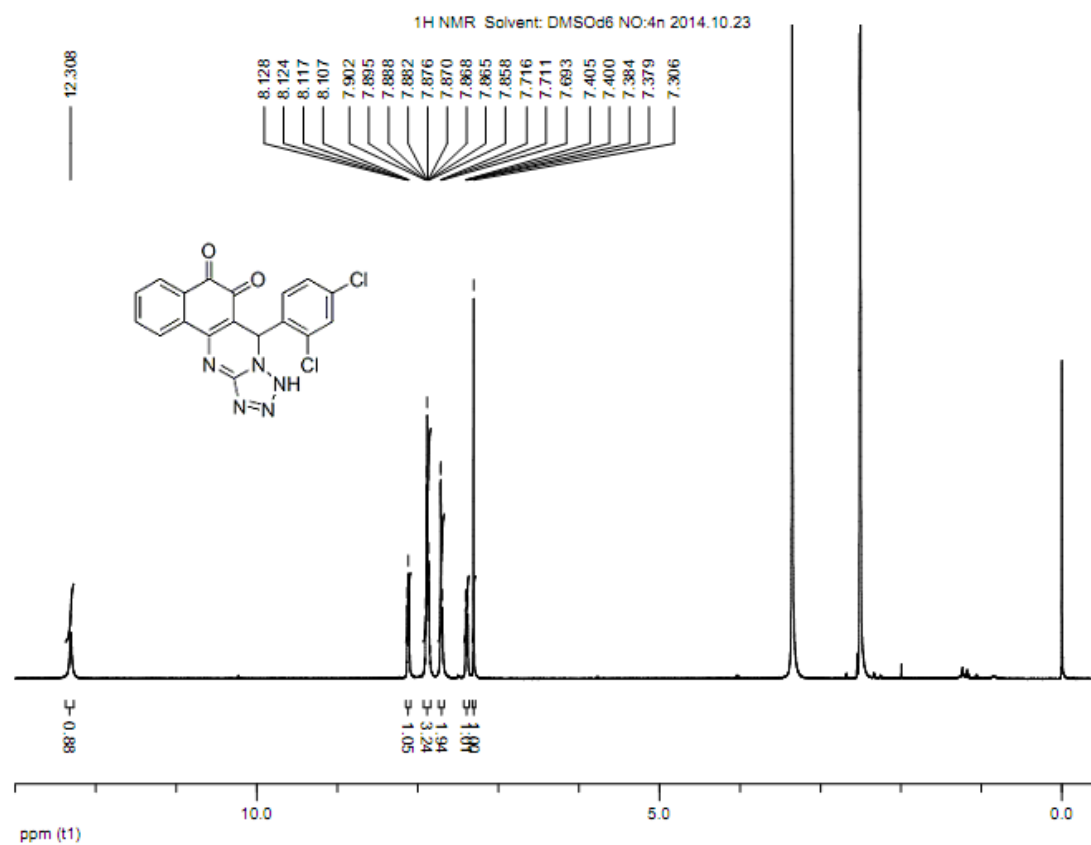


Figure 53 ^1H NMR of 4n

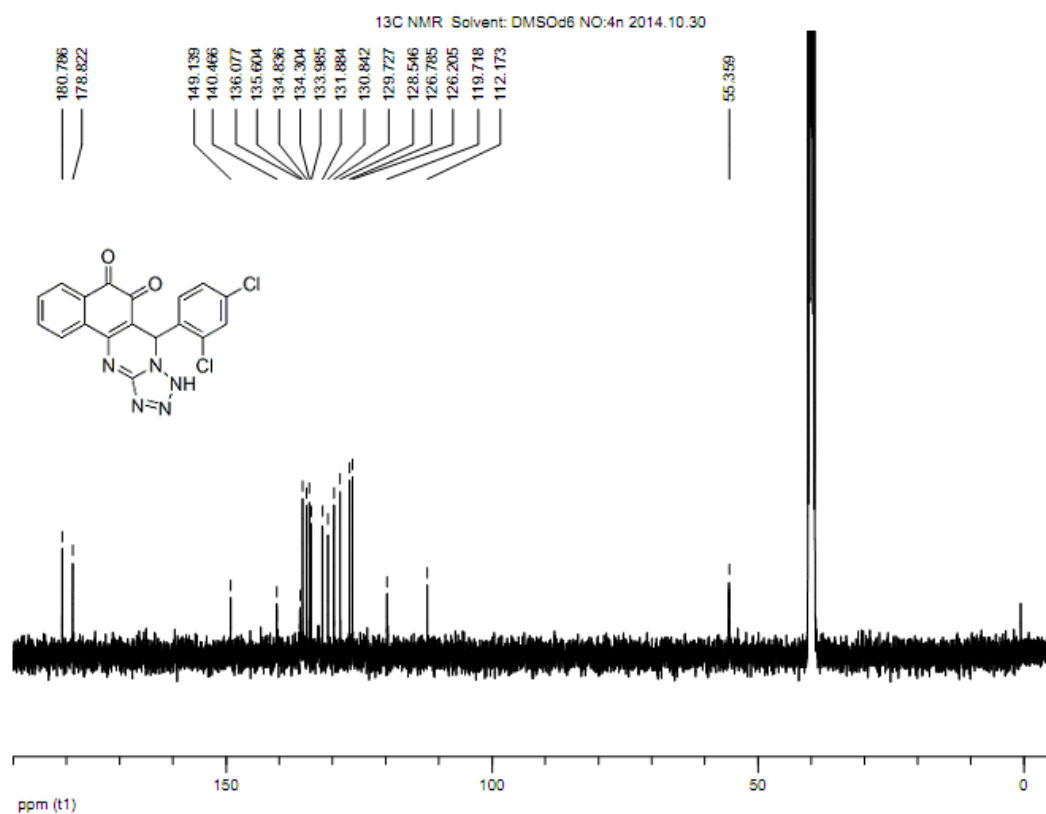


Figure 54 ^{13}C NMR of 4n

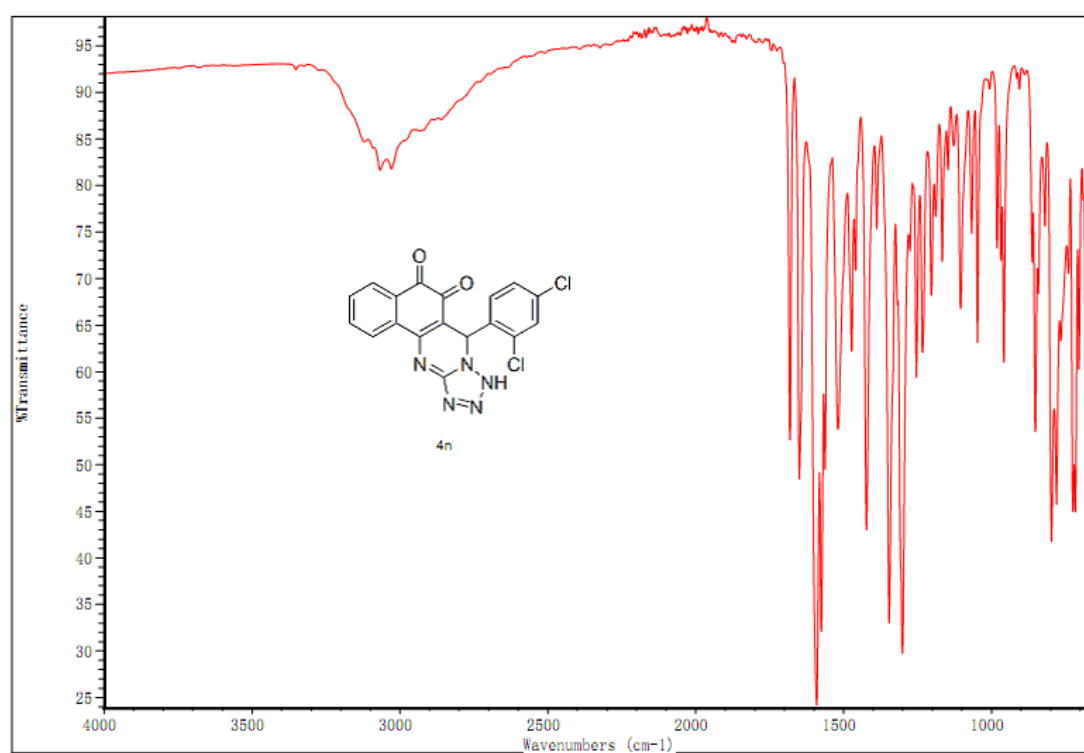


Figure 55 IR of 4n

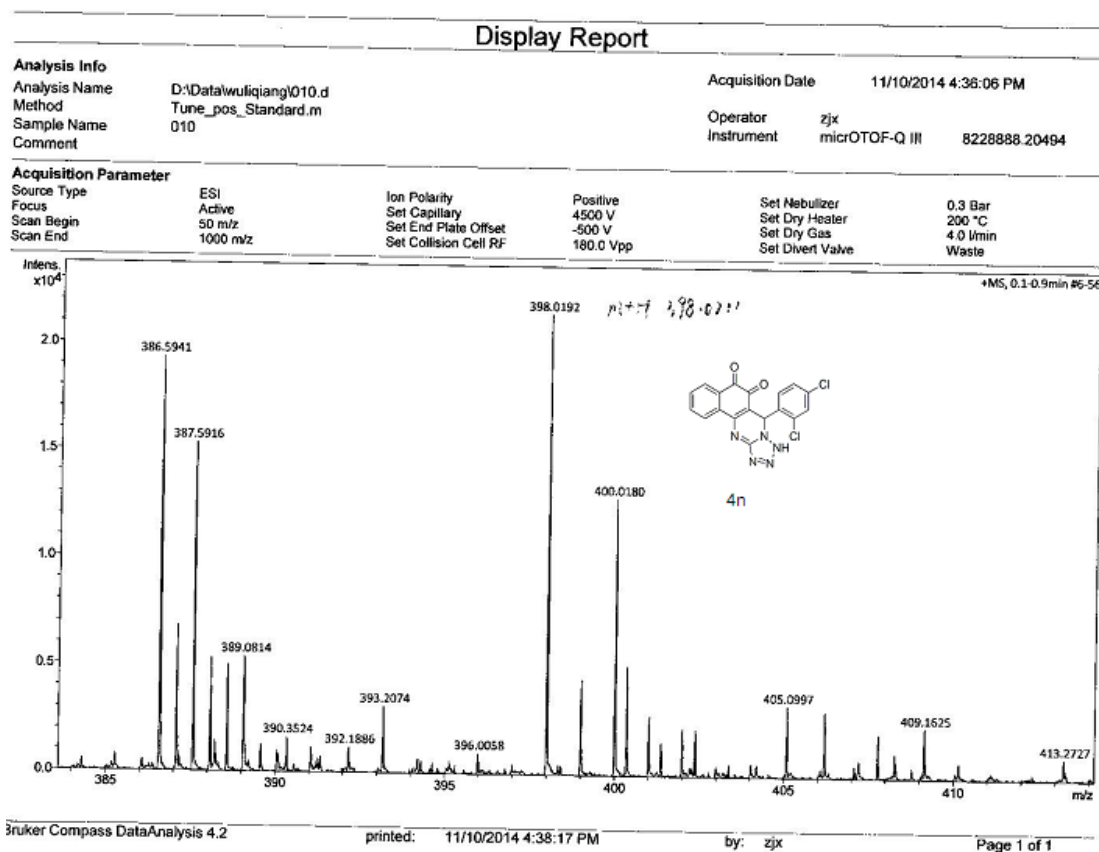


Figure 56 HRMS of **4n**

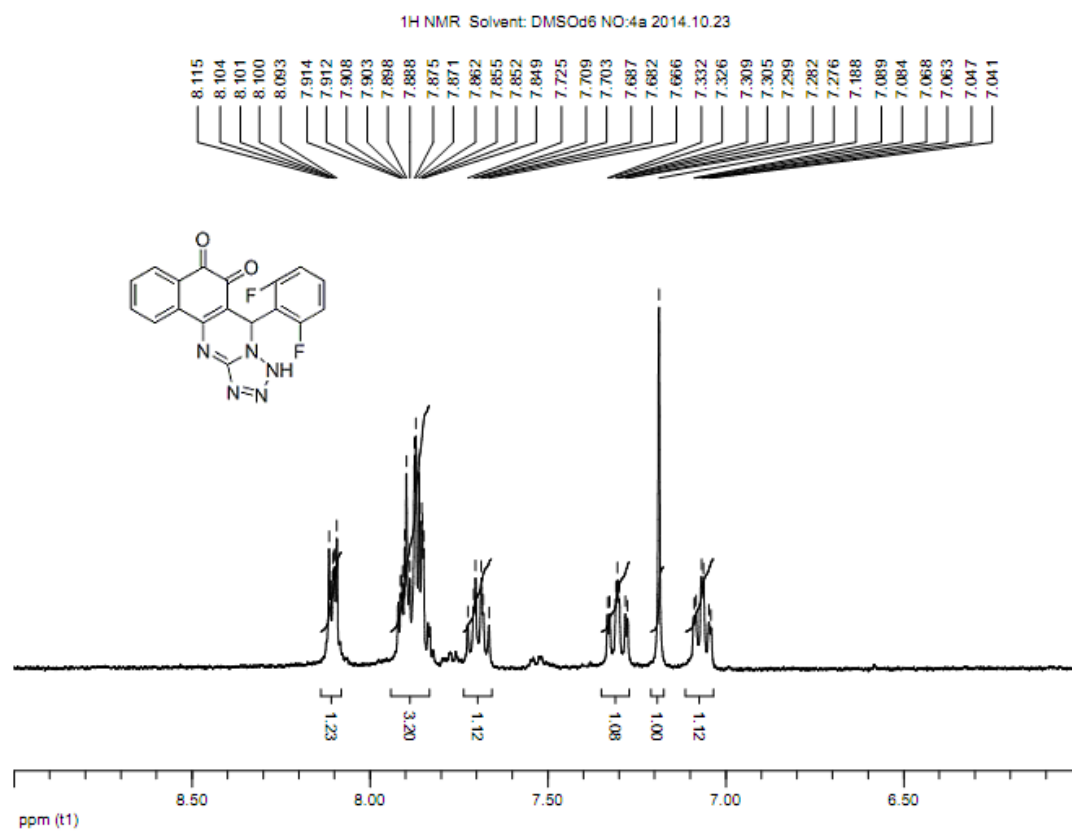
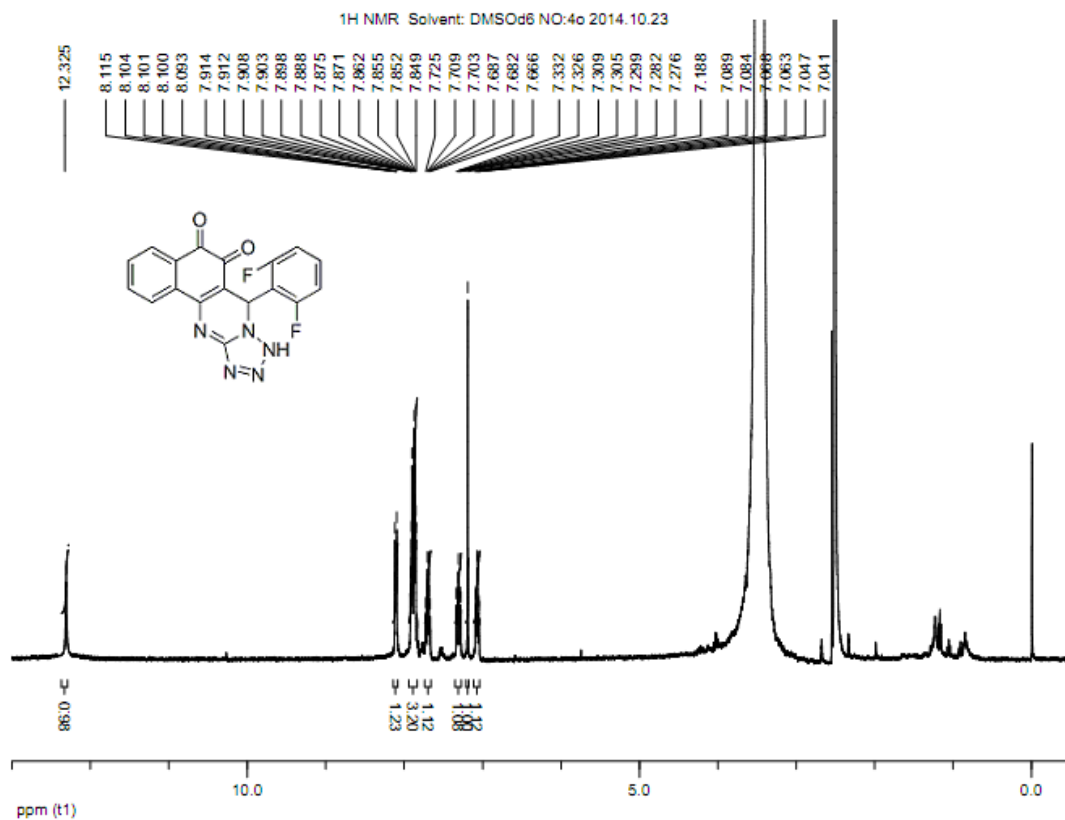


Figure S7 ¹H NMR of 4o

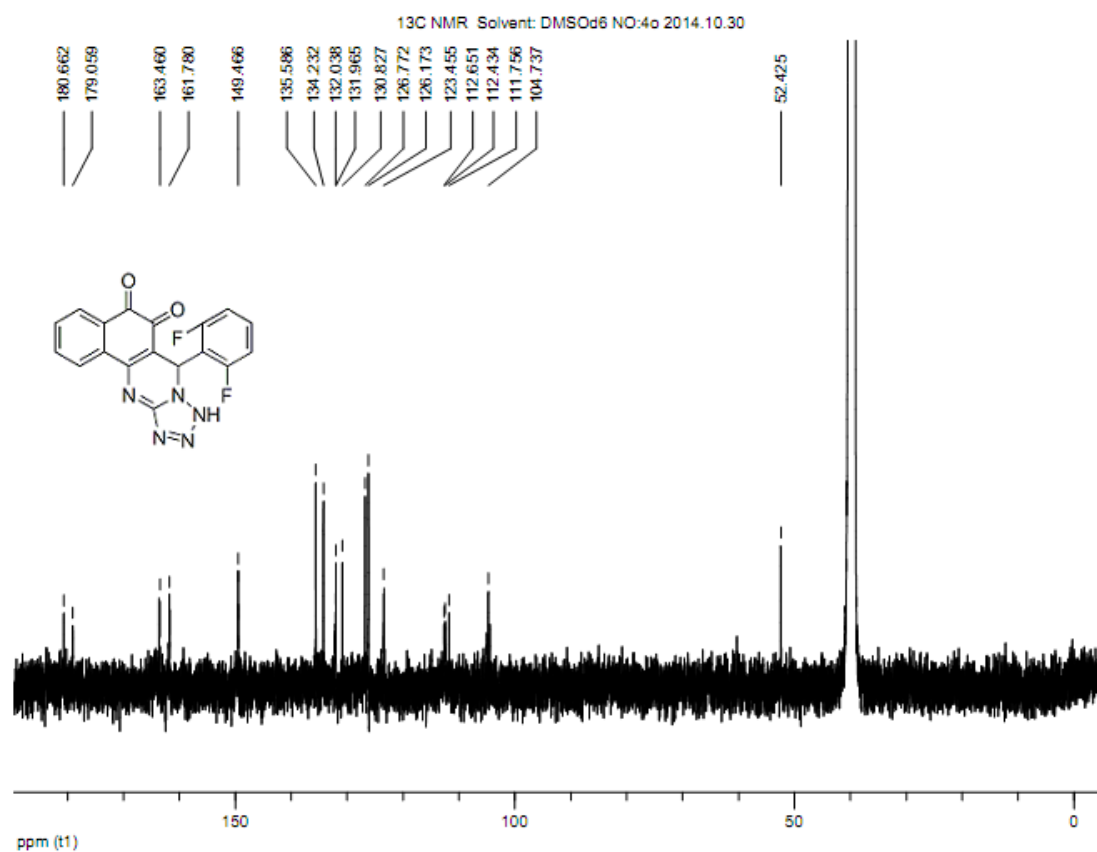


Figure 58 ¹³C NMR of 4o

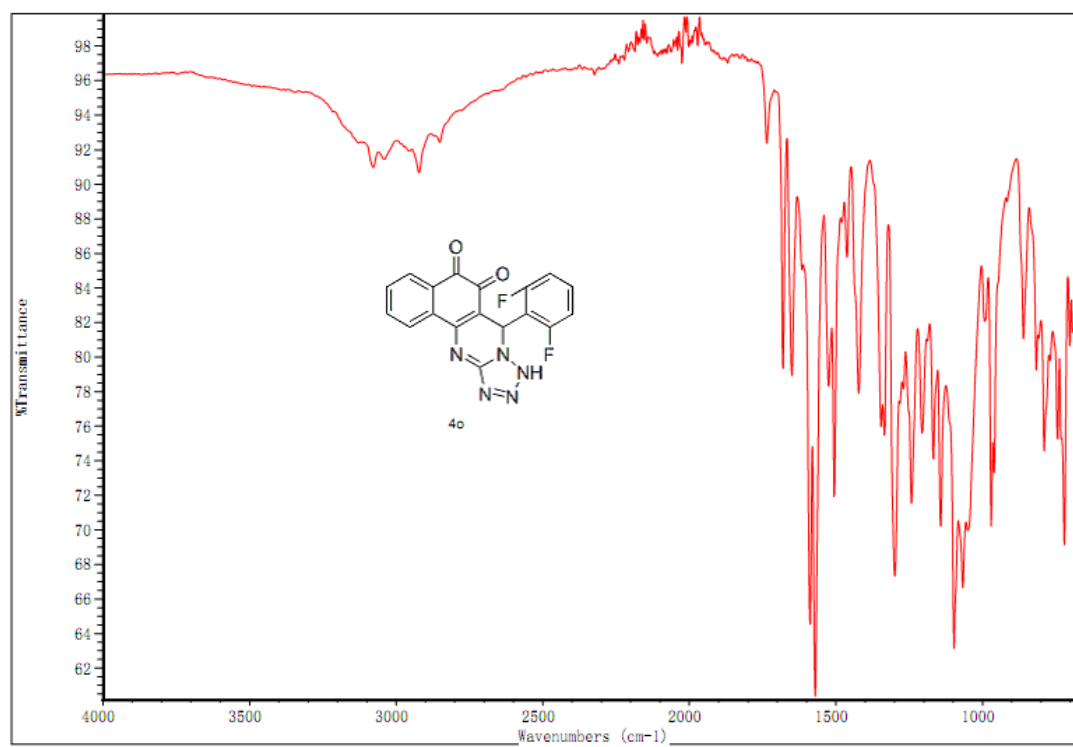


Figure 59 IR of 4o

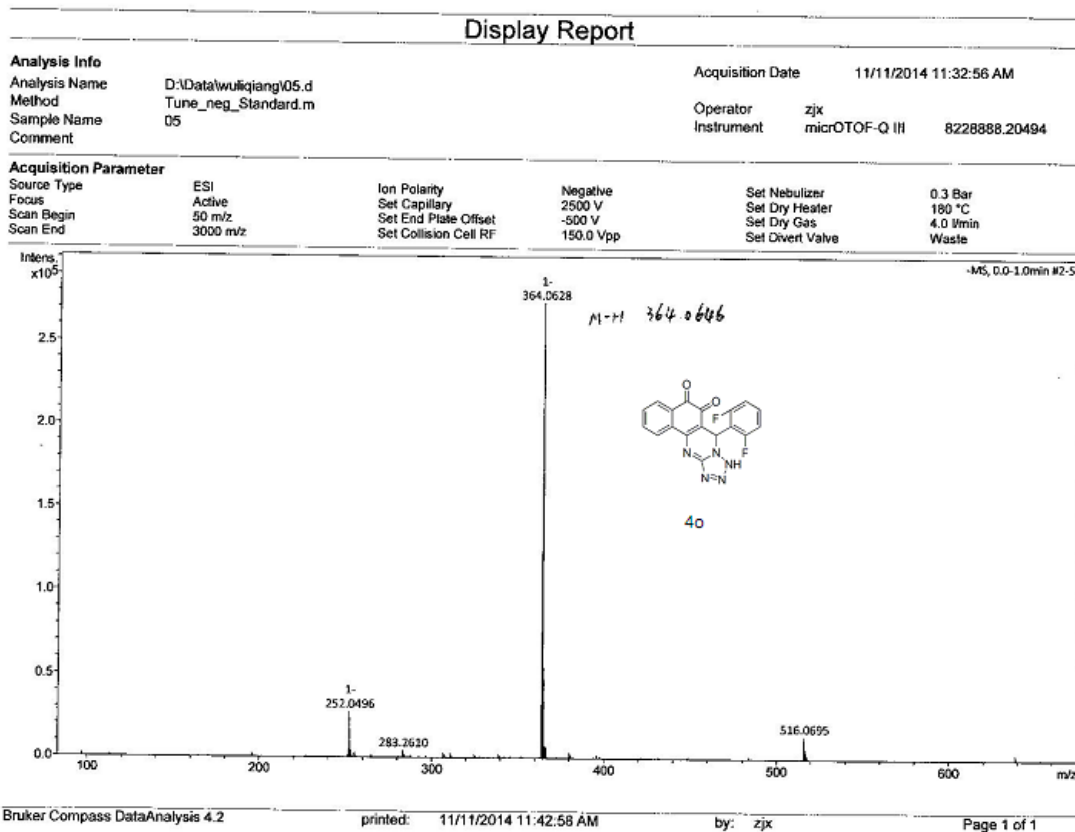


Figure 60 HRMS of **4o**

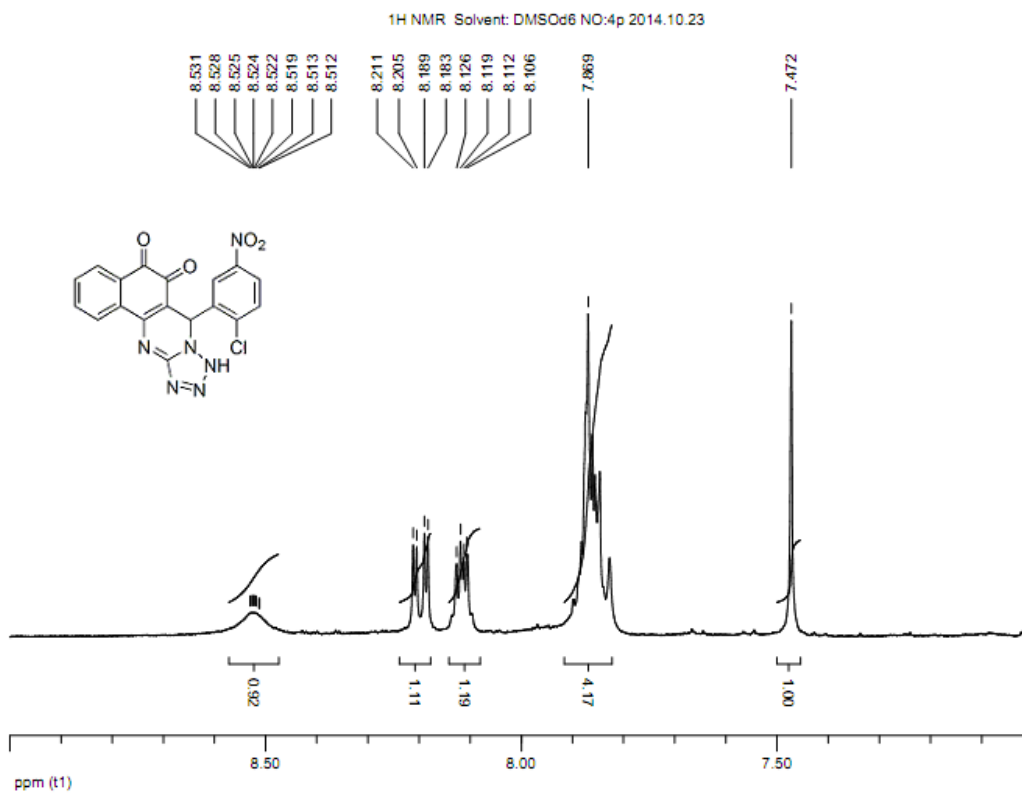
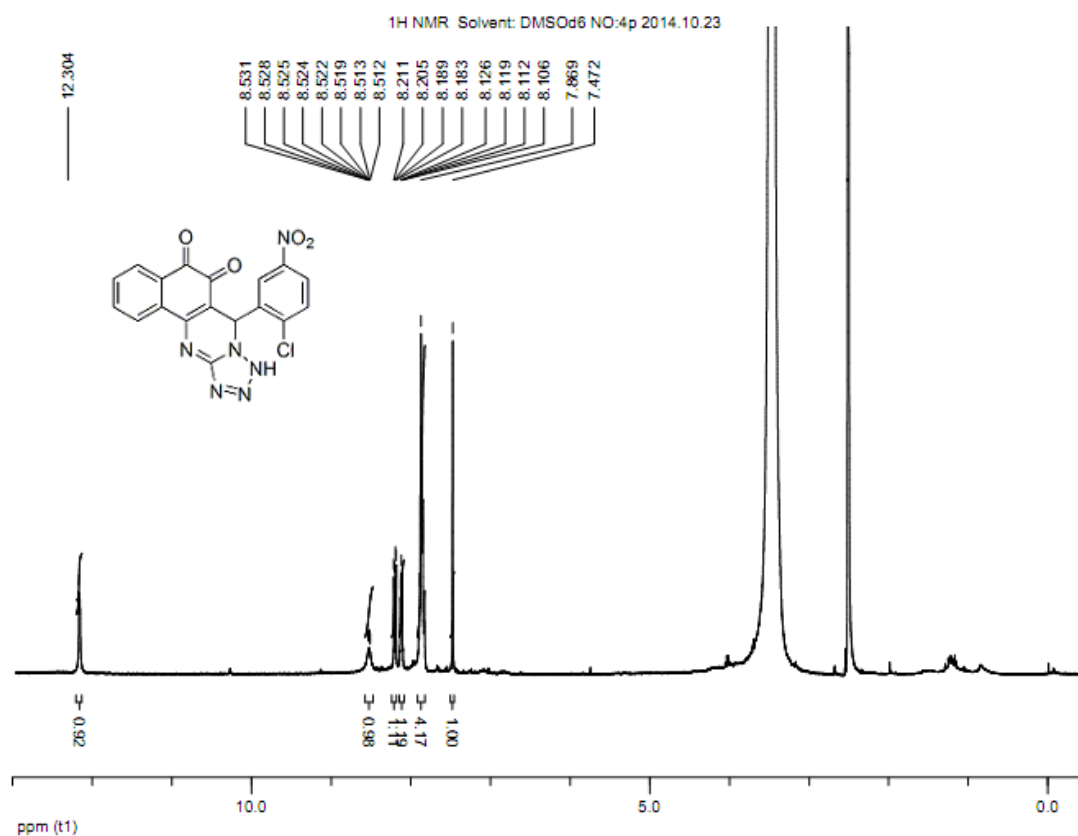


Figure 61 ¹H NMR of 4p

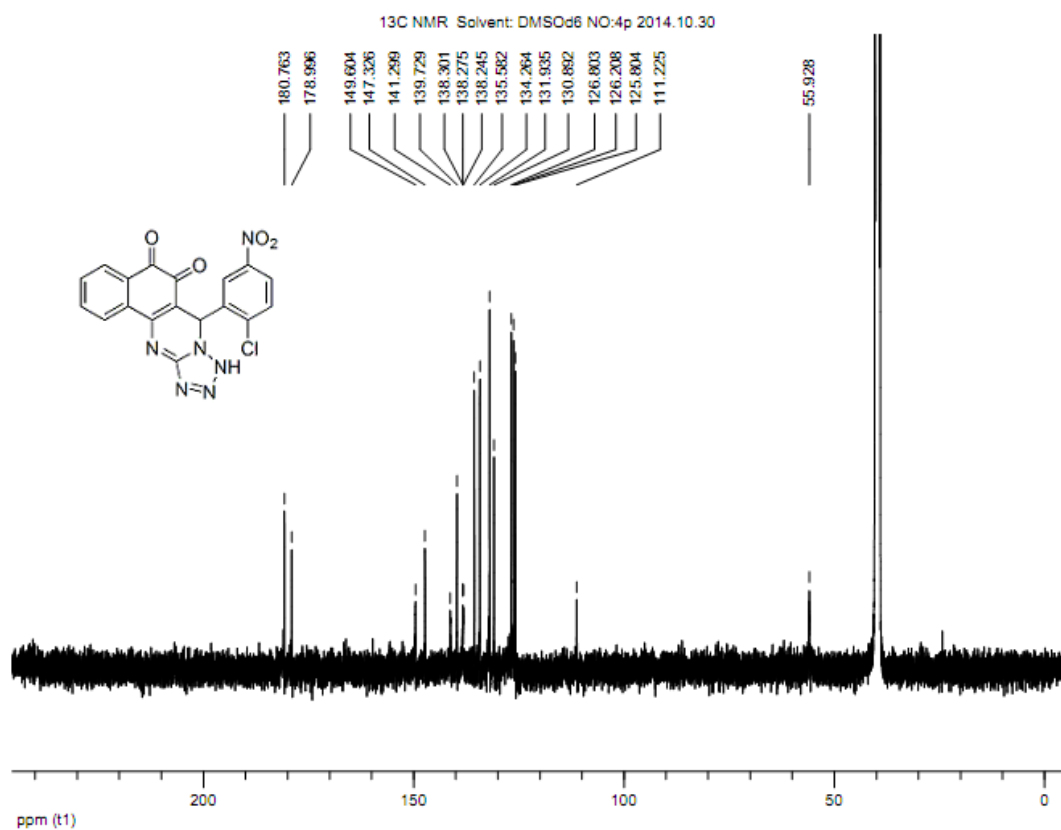


Figure 62 ¹³C NMR of 4p

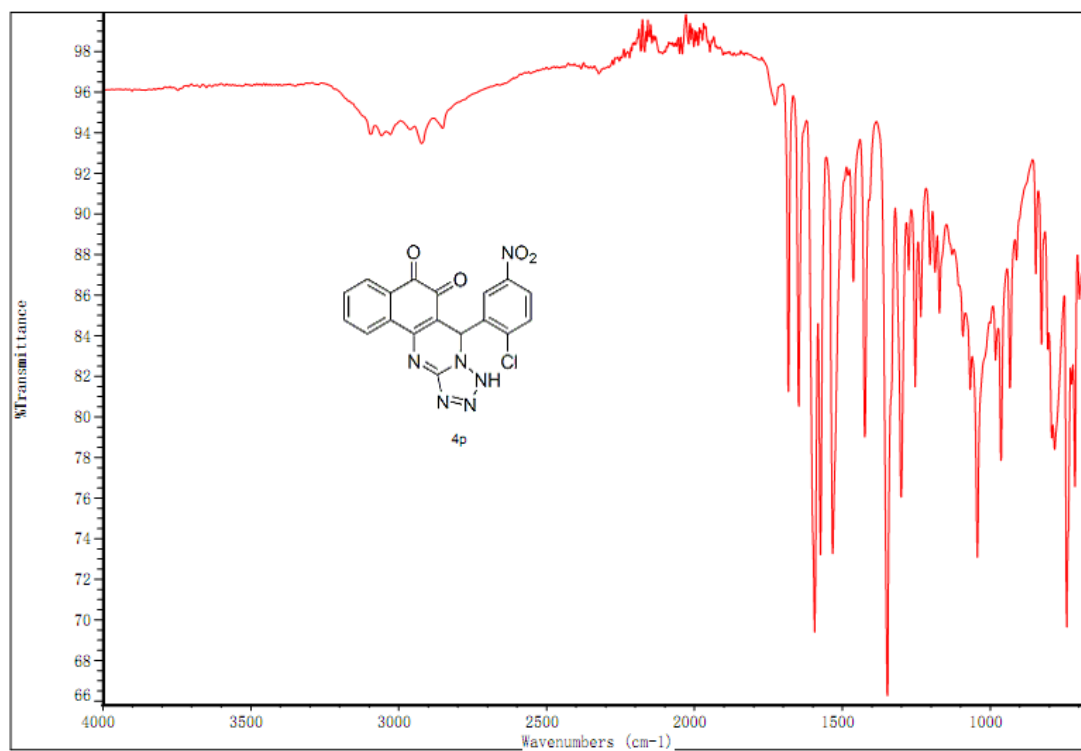
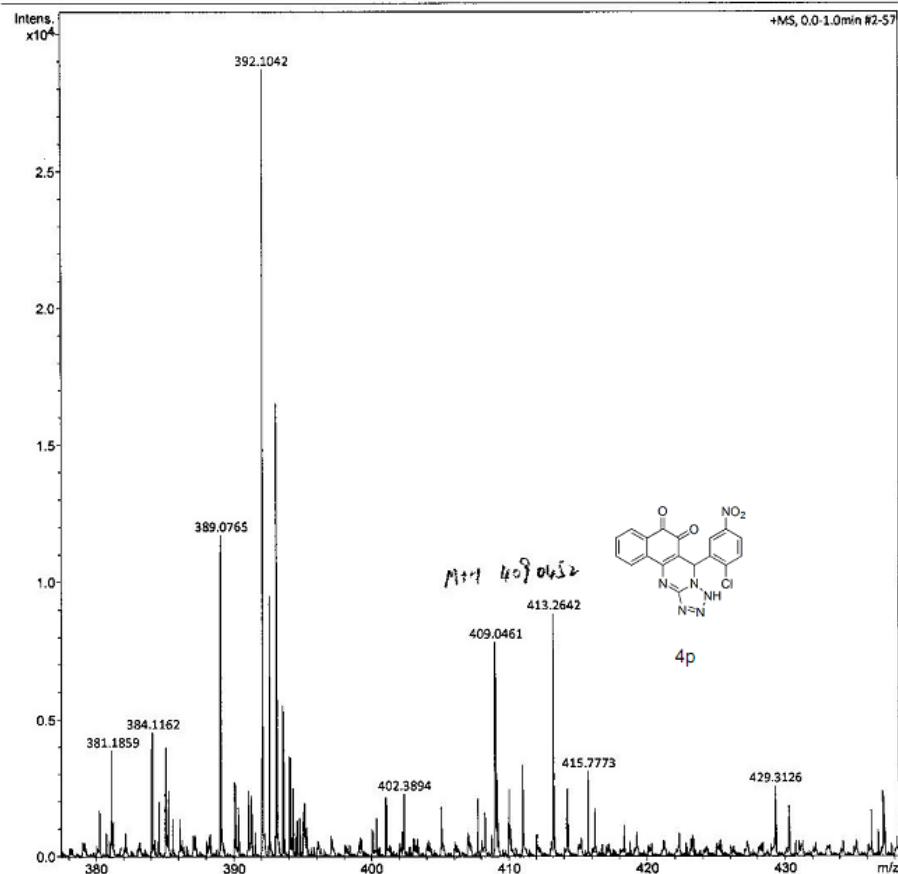


Figure 63 IR of 4p

Display Report

Analysis Info		Acquisition Date	11/6/2014 9:31:18 AM
Analysis Name	D:\Data\wuliqiang\6-meoh.d	Operator	zjx
Method	Tune_pos_Standard.m	Instrument	microTOF-Q III 8228888.20494
Sample Name	6-meoh		
Comment			

Acquisition Parameter			
Source Type	ESI	Ion Polarity	Positive
Focus	Active	Set Capillary	4500 V
Scan Begin	50 m/z	Set End Plate Offset	-500 V
Scan End	1000 m/z	Set Collision Cell RF	180.0 Vpp
		Set Nebulizer	0.3 Bar
		Set Dry Heater	200 °C
		Set Dry Gas	4.0 l/min
		Set Divert Valve	Waste



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 by: zjx
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Figure 64 HRMS of **4p**

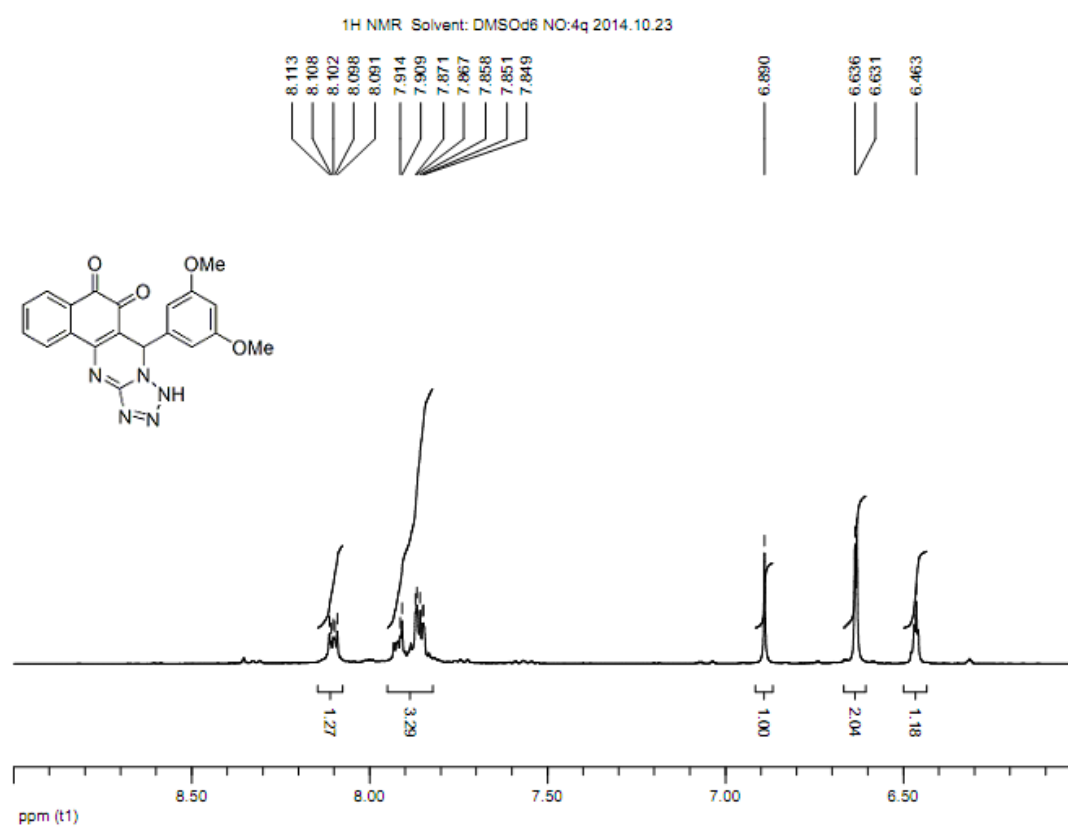
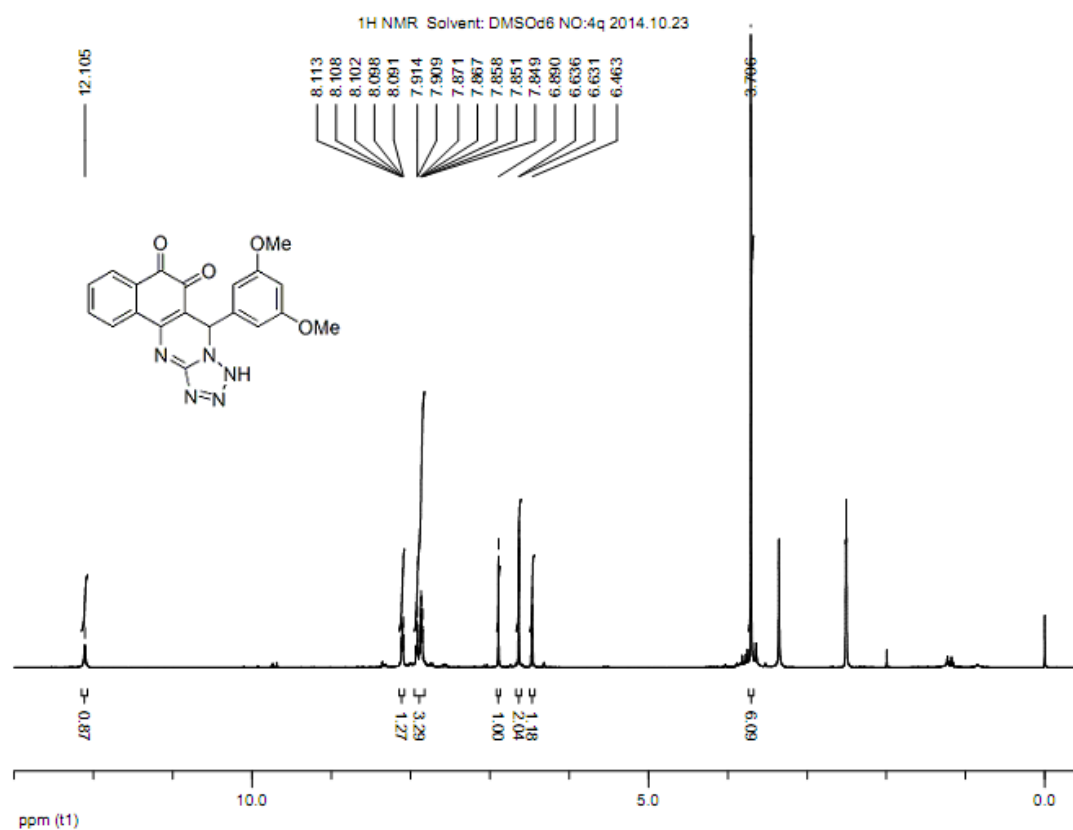


Figure 65 ^1H NMR of 4q

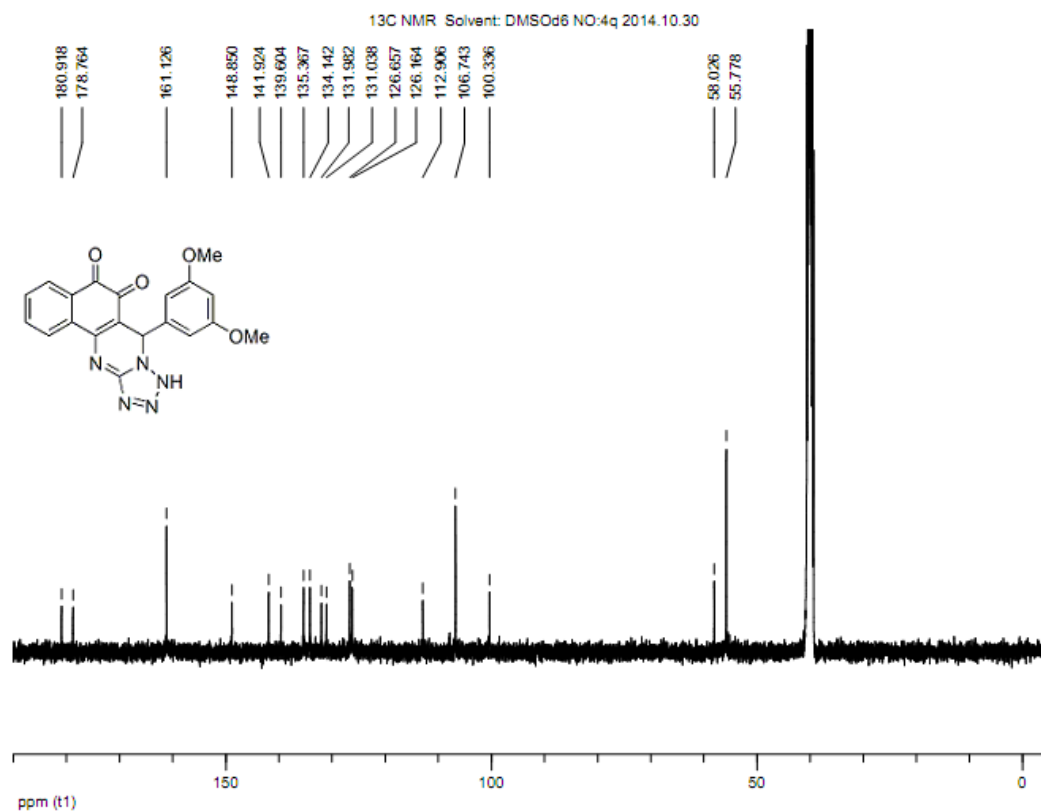


Figure 66 ¹³C NMR of 4q

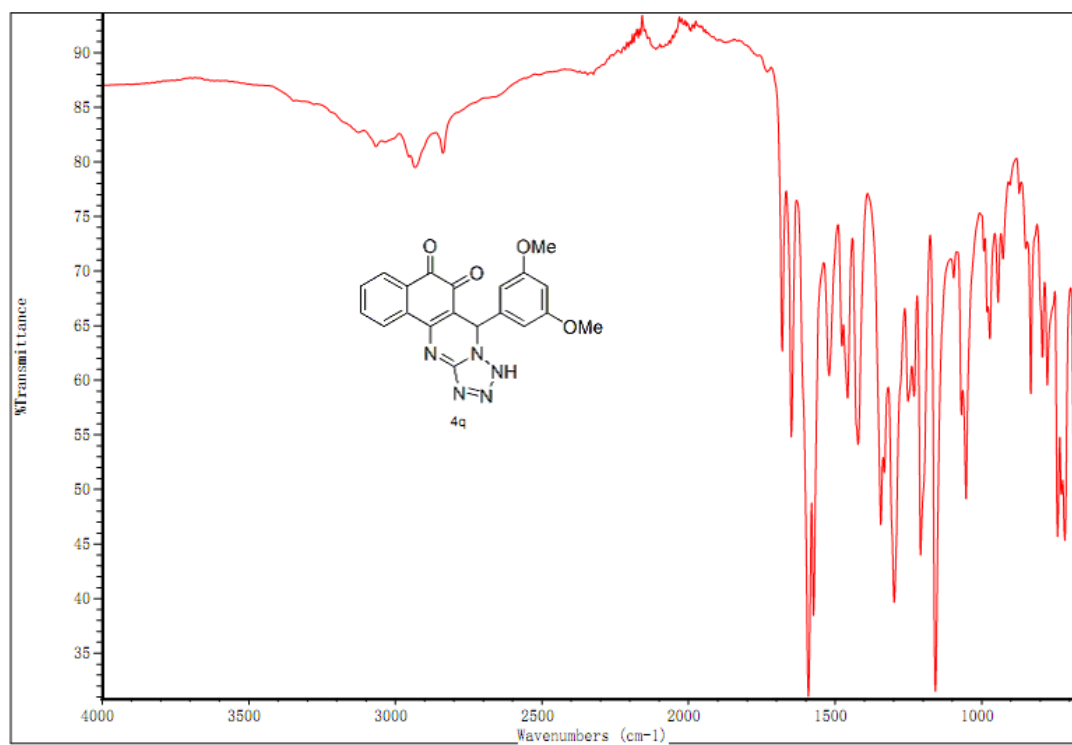


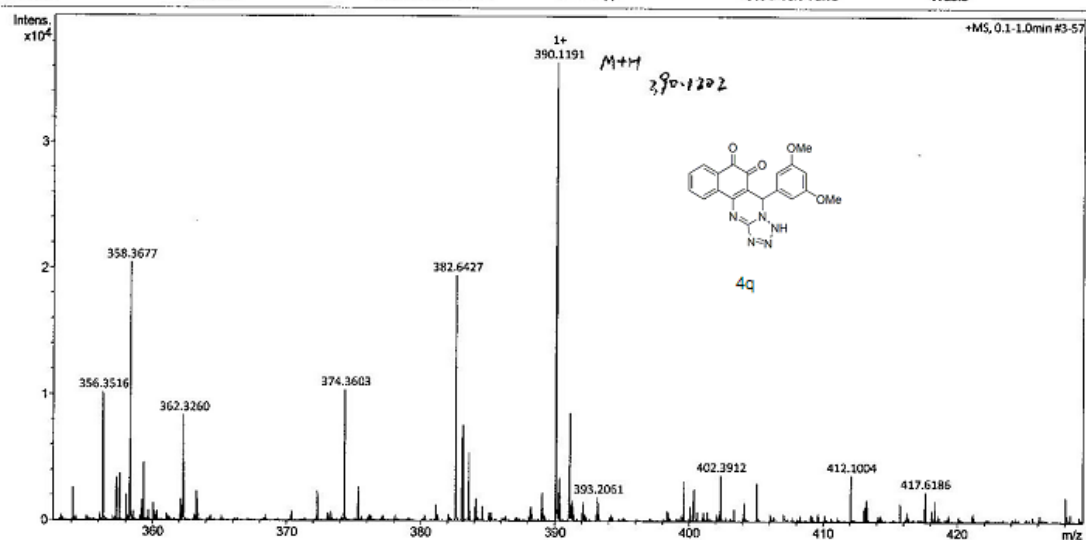
Figure 67 IR of 4q

Display Report

Analysis Info		Acquisition Date 11/10/2014 5:08:59 PM	
Analysis Name	D:\Data\wuliqiang\014-2.d	Operator	zjx
Method	Tune_pos_Standard.m	Instrument	micrOTOF-Q III
Sample Name	014-2		8228888.20494
Comment			

Acquisition Parameter

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	0.3 Bar
Focus	Active	Set Capillary	4500 V	Set Dry Heater	200 °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



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printed: 11/10/2014 5:10:42 PM

by: zjx

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Figure 68 HRMS of **4q**

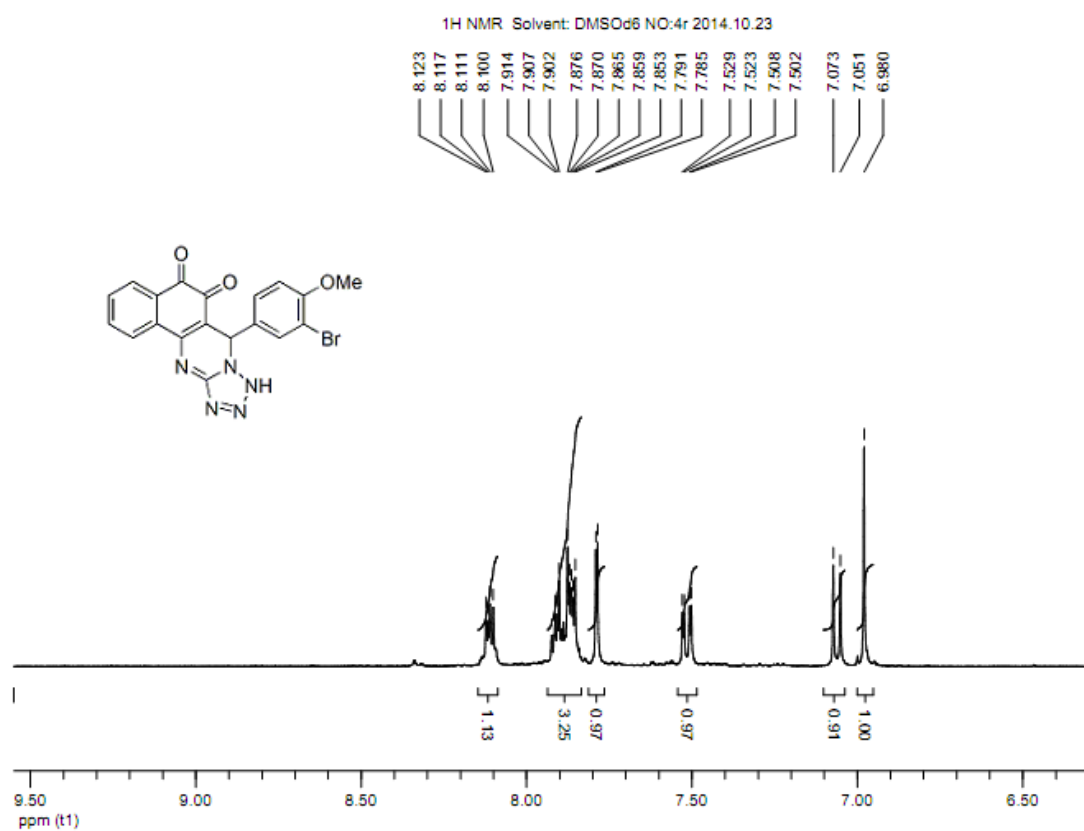
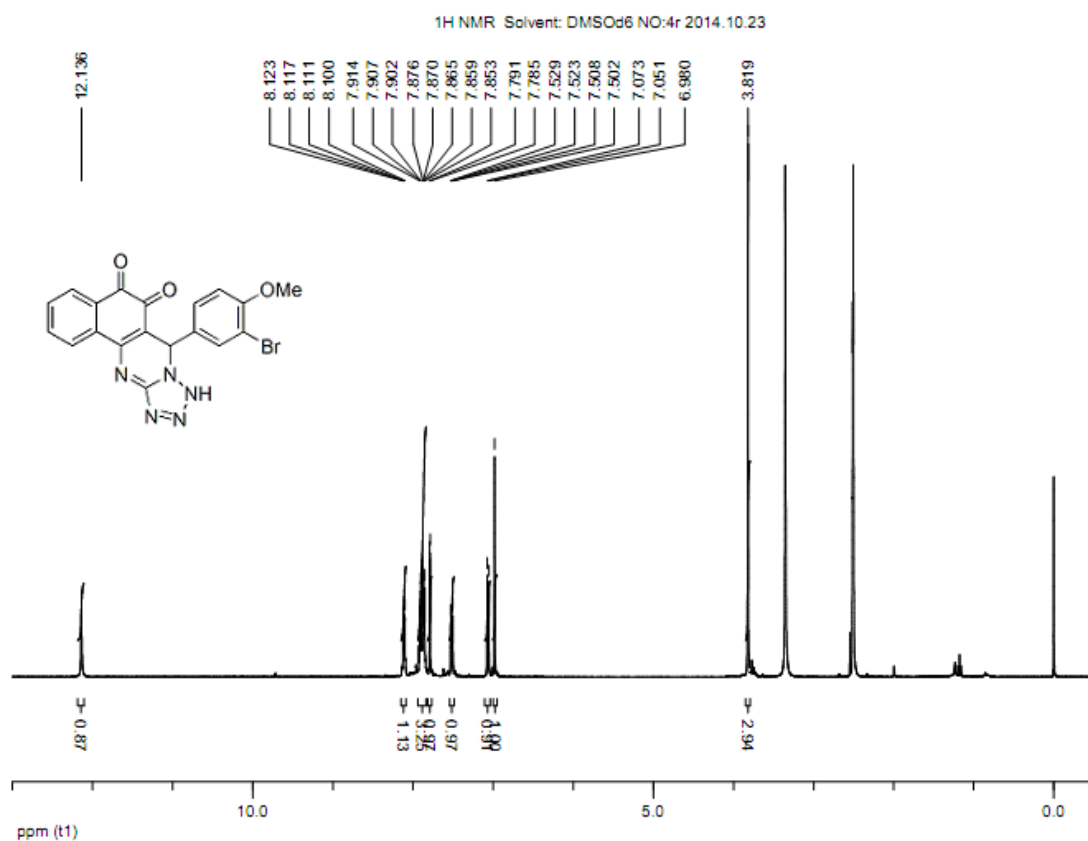


Figure 69 ^1H NMR of 4r

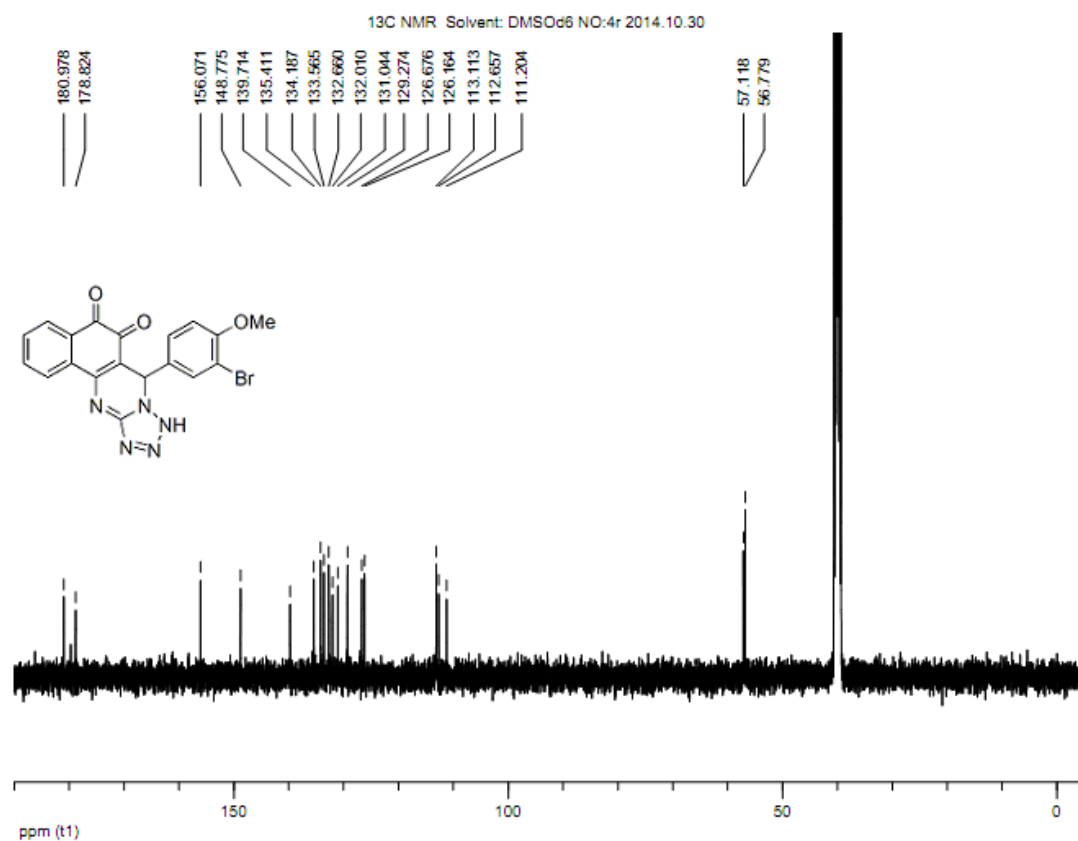


Figure 70 ¹³C NMR of 4r

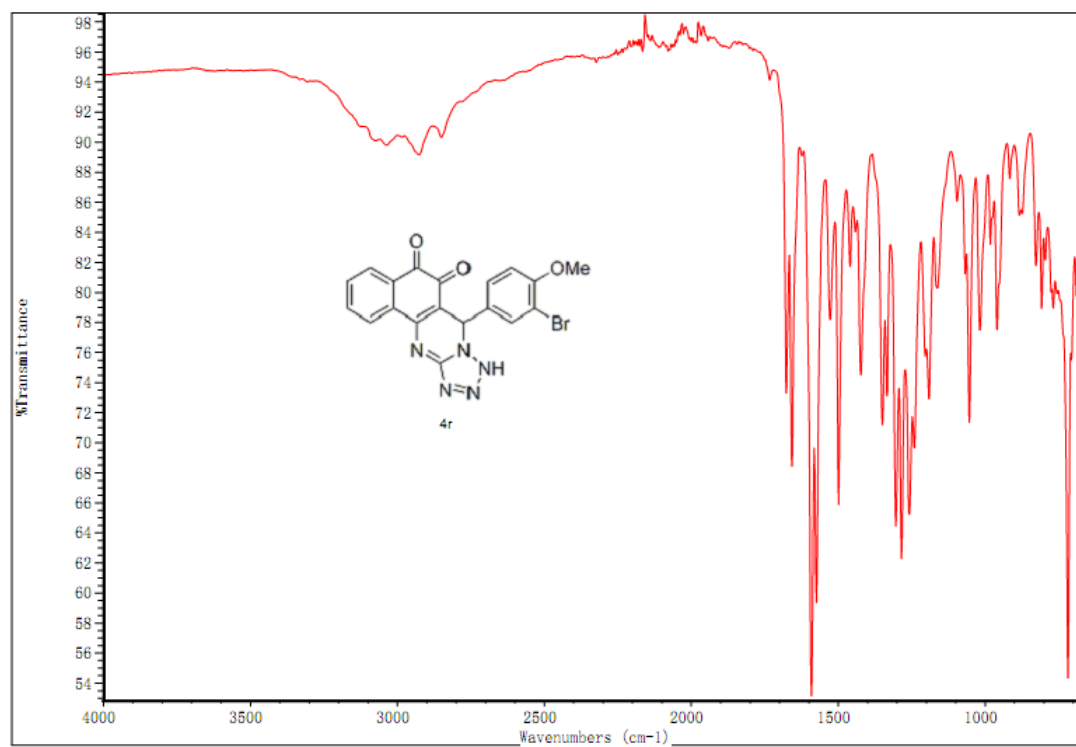


Figure 71 IR of 4r

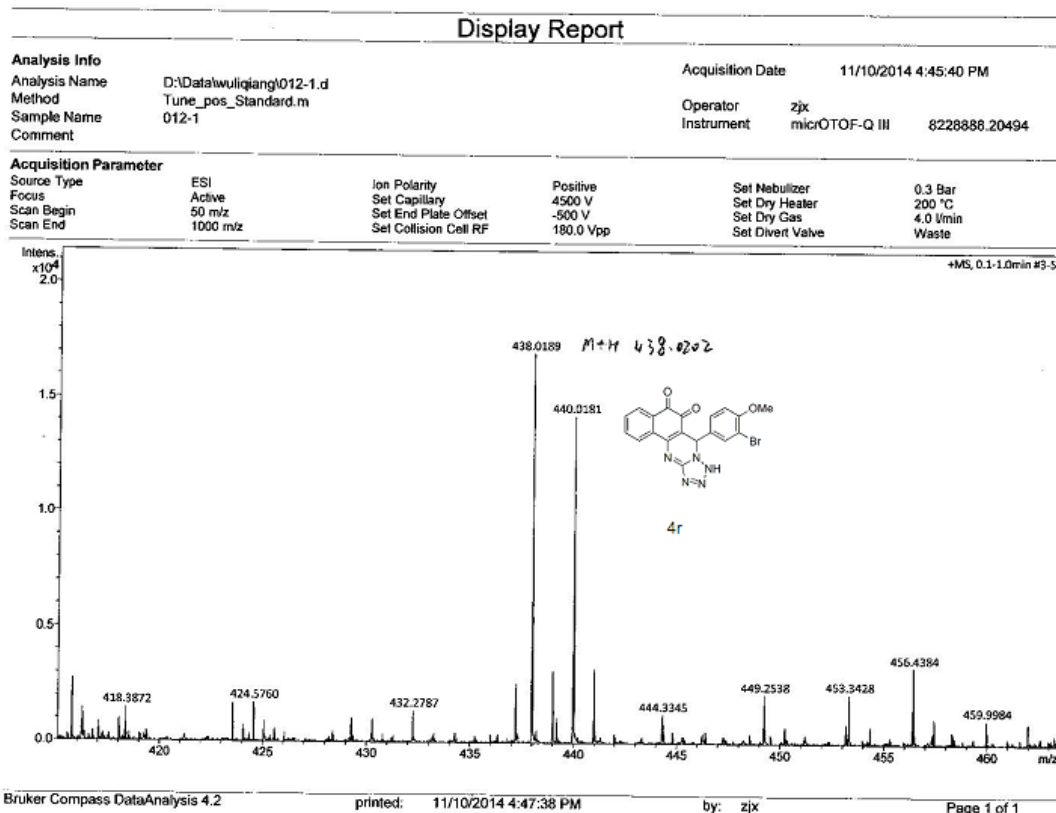


Figure 72 HRMS of **4r**

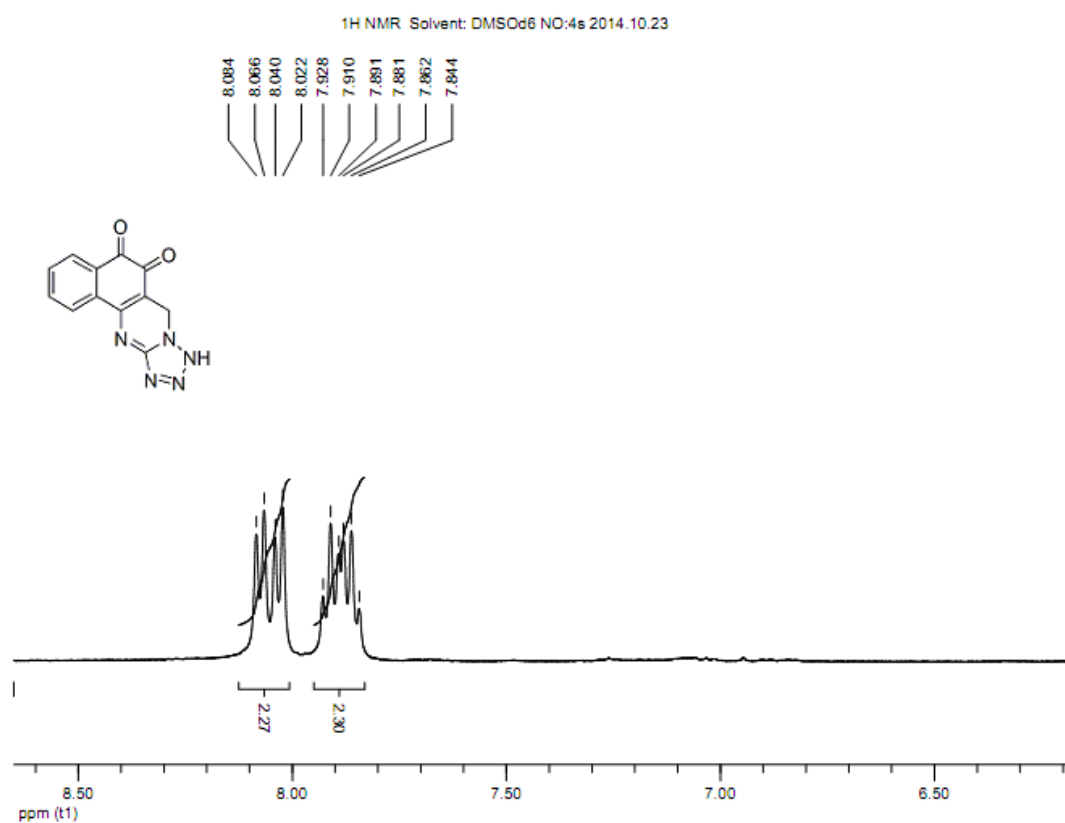
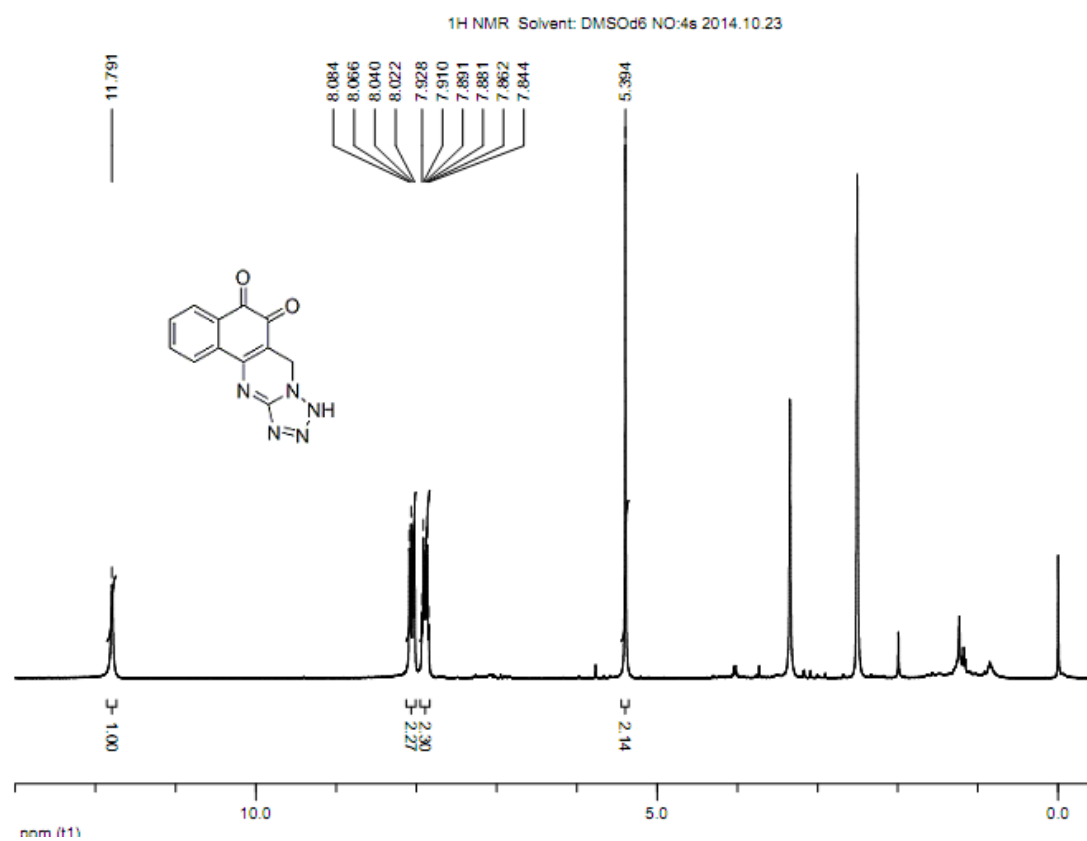


Figure 73 ^1H NMR of 4s

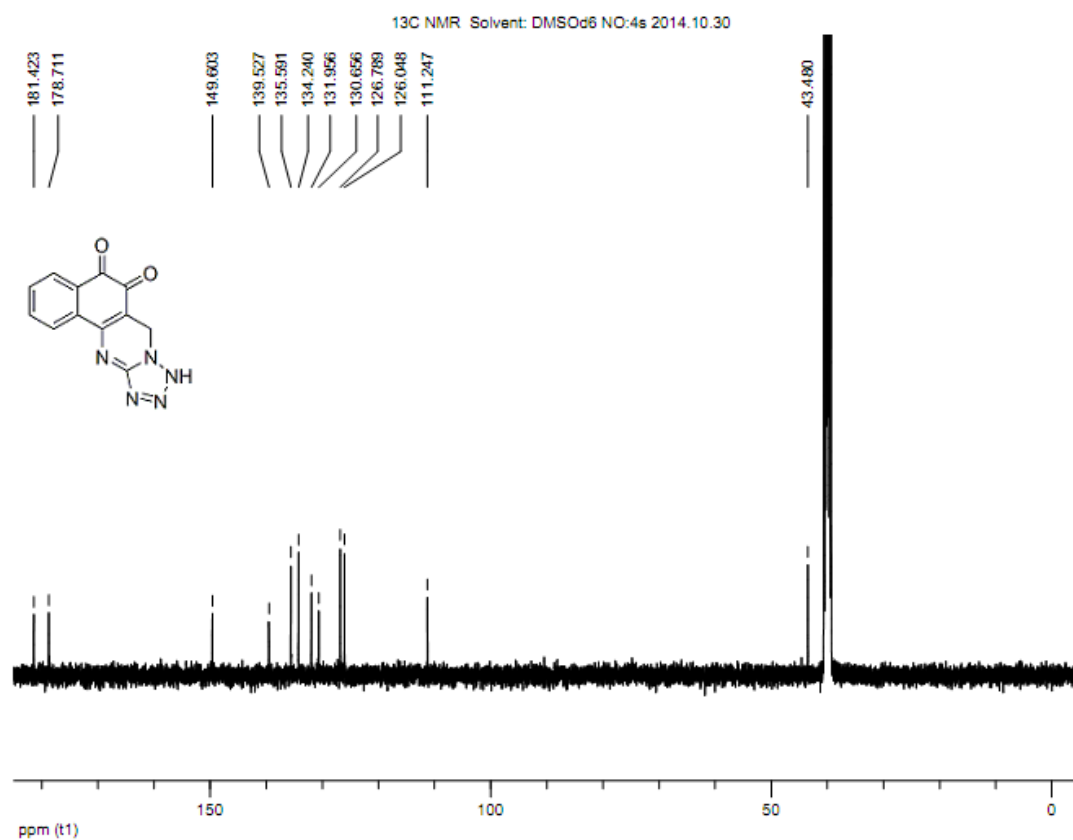


Figure 74 ¹³C NMR of 4s

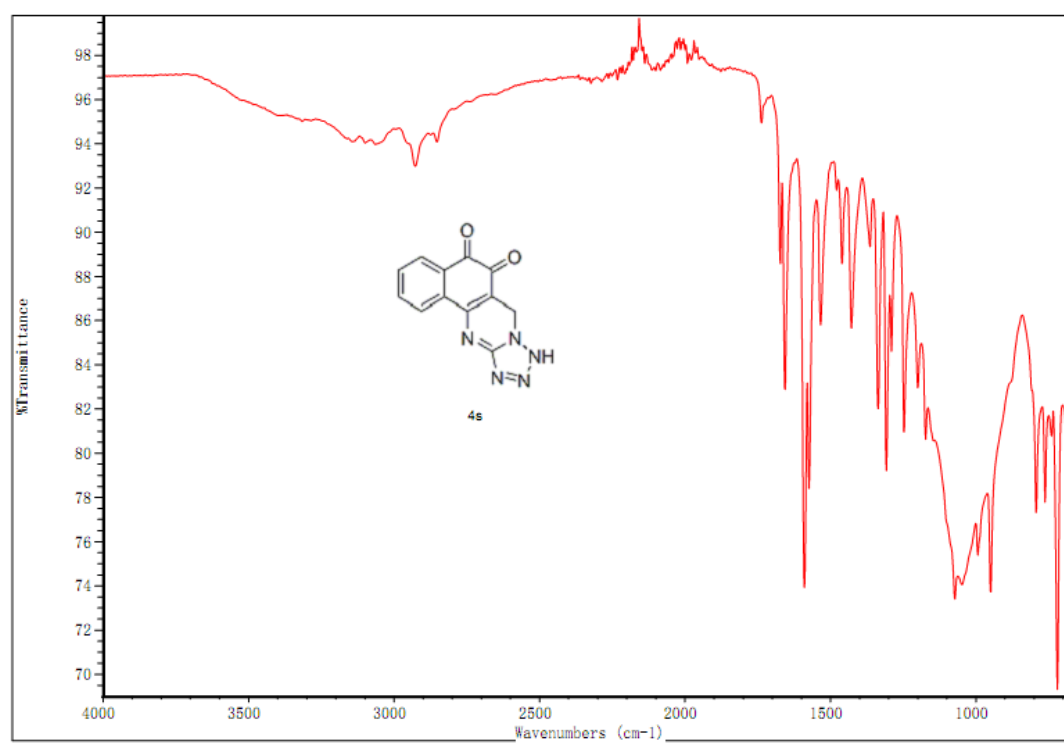


Figure 75 IR of 4s

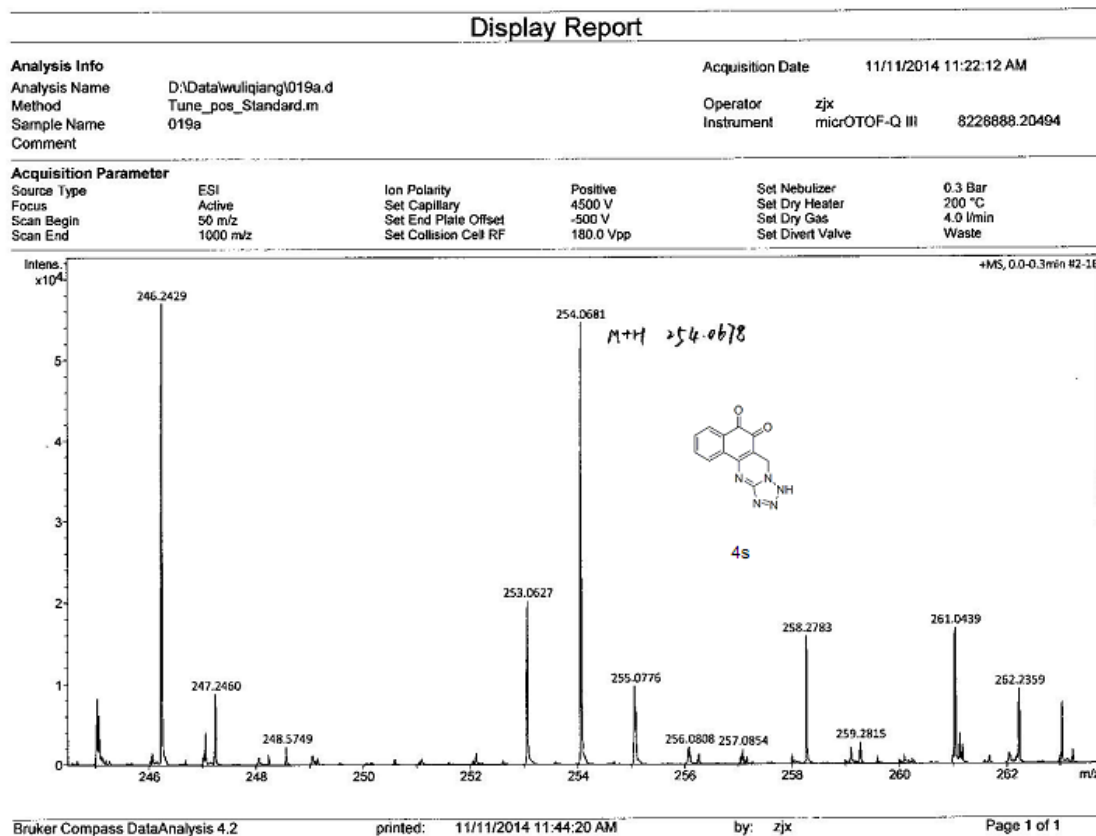


Figure 76 HRMS of **4s**

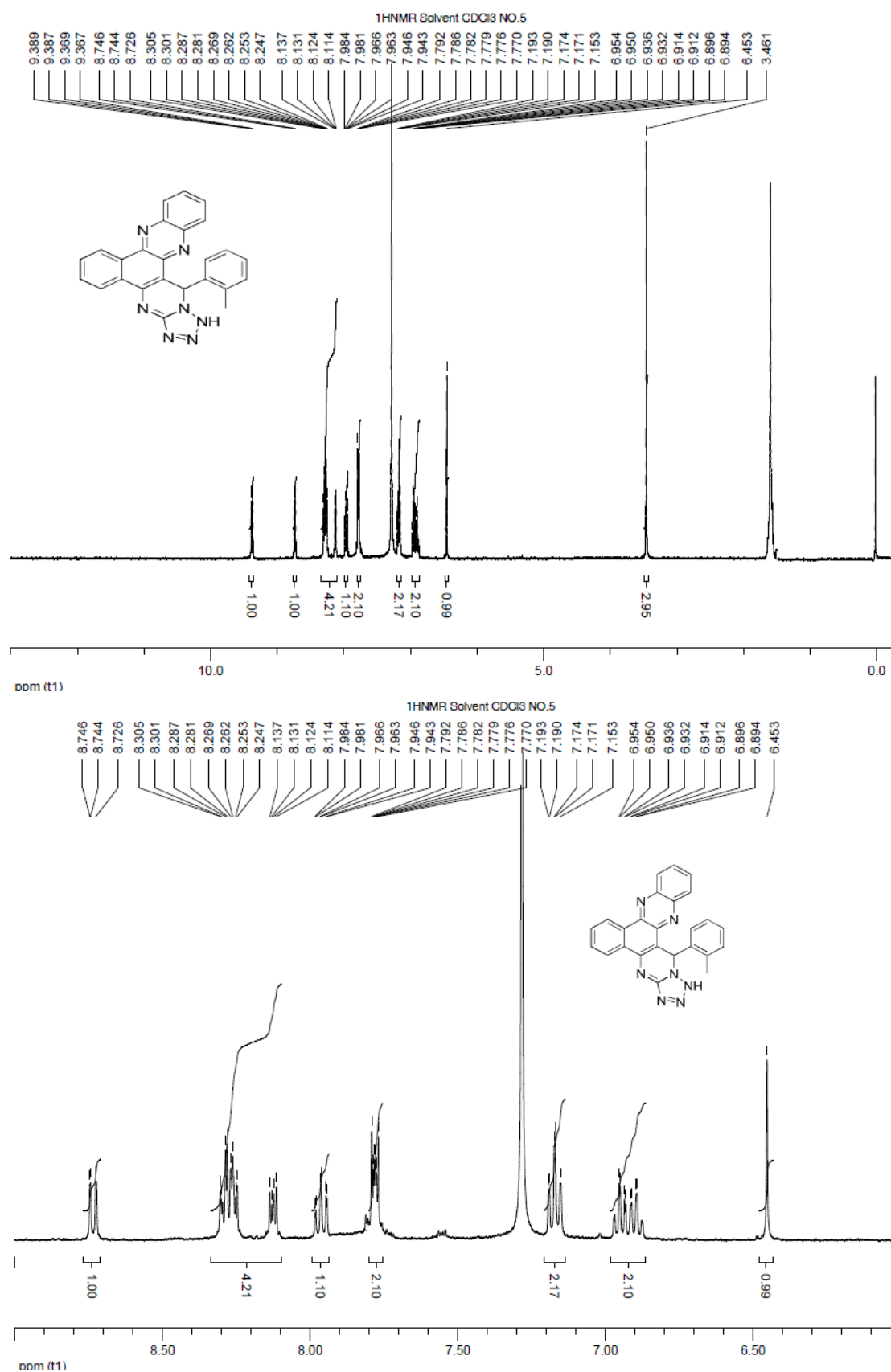


Figure 77 ¹H NMR of **5**

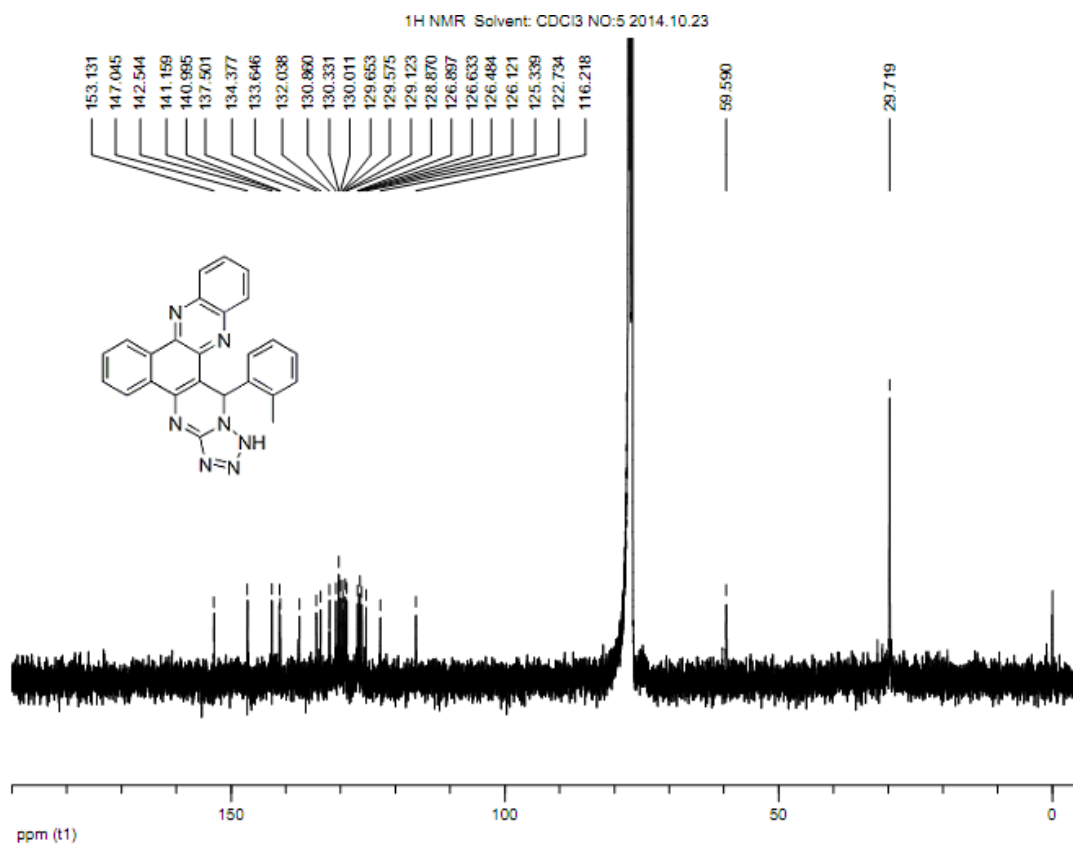


Figure 78 ^{13}C NMR of 5

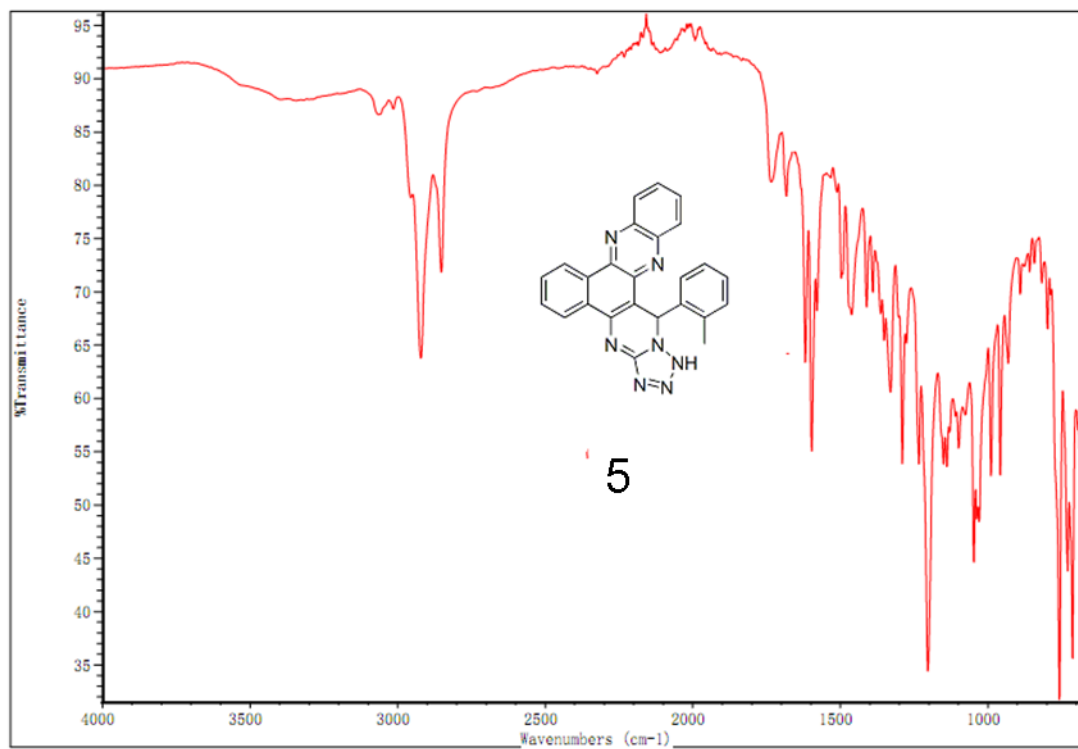


Figure 79 IR of 5