

Supporting information

Synthesis, antimalarial activity, and target binding of dibenzazepine-tethered isoxazolines

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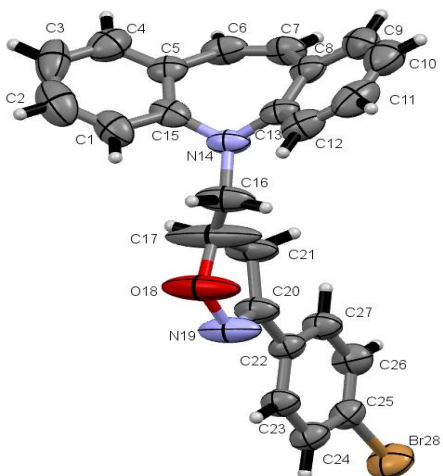
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Table S1 Docking results of dibenzazepine derivatives with PfA-M1

Compound	Docking score (kcal/mol)
6a	-5.37
6b	-4.17
6c	-5.93
6d	-6.68
6e	-5.48
6f	-5.72
6g	-6.20
6h	-3.75
6i	-6.29
6j	-8.06
6k	-7.90
8a	-6.16
8b	-5.98
8c	-7.40
8d	-7.04
8e	-6.16
8f	-6.88
8g	-6.09
8h	-5.36
8i	-3.61
8j	-6.99
8k	-7.80

Figure S1 ORTEP diagrammatic representation of the crystal structure of compound **6d**



The compound **6d** crystallizes in monoclinic space group $P2_1/c$. The lattice parameters are, $a=18.750(2)$ Å, $b=6.8019(9)$ Å, $c=15.436(2)$ Å and $\beta=94.233(7)^\circ$. The final residual value, $R1$ is 0.0845. The packing of the molecule is stabilized with the C-H... π and C-Br... π short contacts. The short bond lengths $N14-C13 = 1.438(9)$ Å and $N14-C15 = 1.422(9)$ Å indicate π -electron delocalization in the ring. As a result there is a difference in the bond length of $C5-C6 = 1.459(9)$ Å and $C7-C8 = 1.440(9)$ Å.

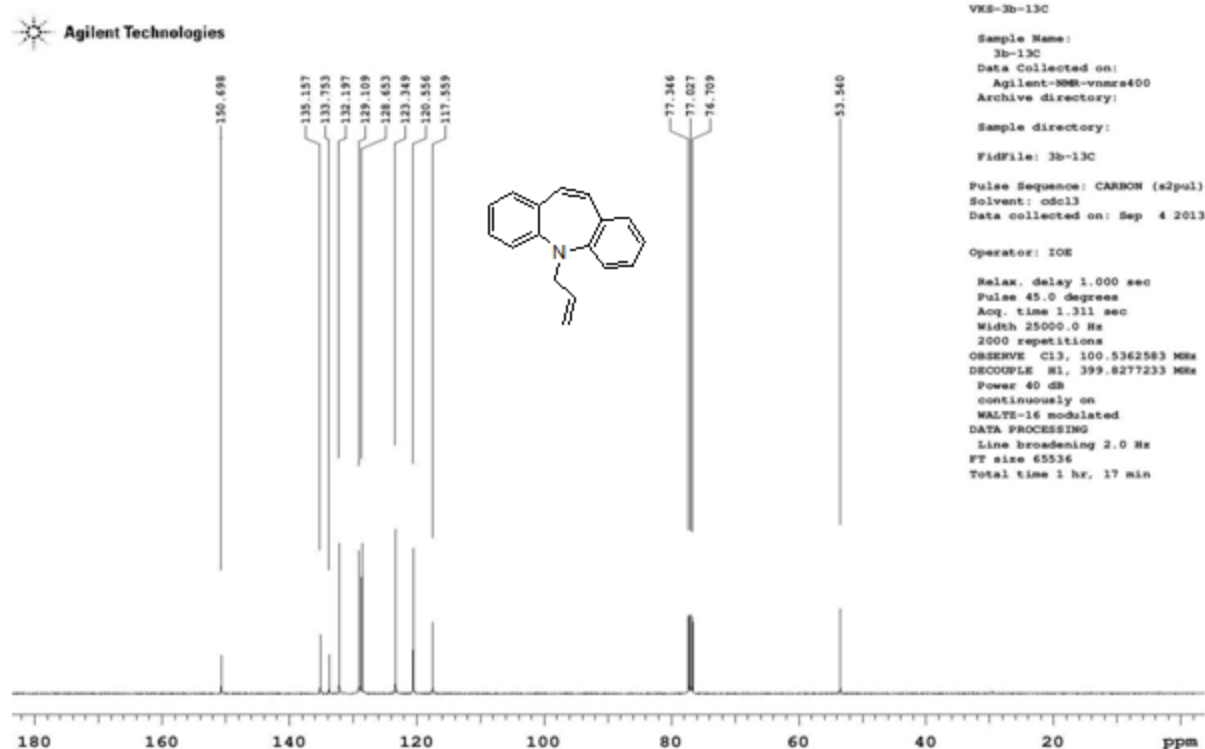
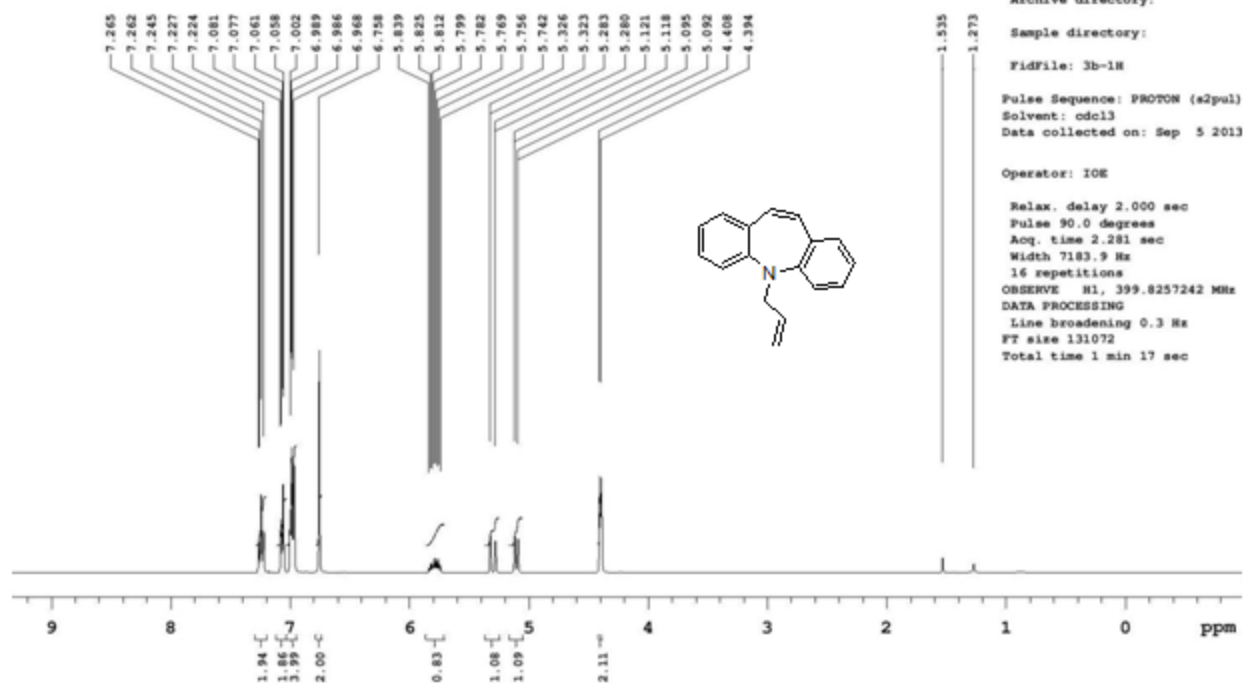
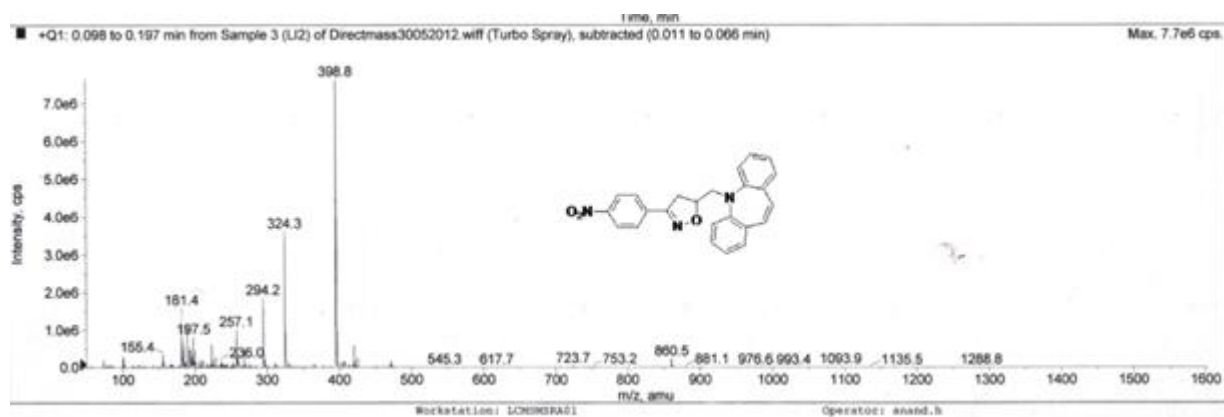
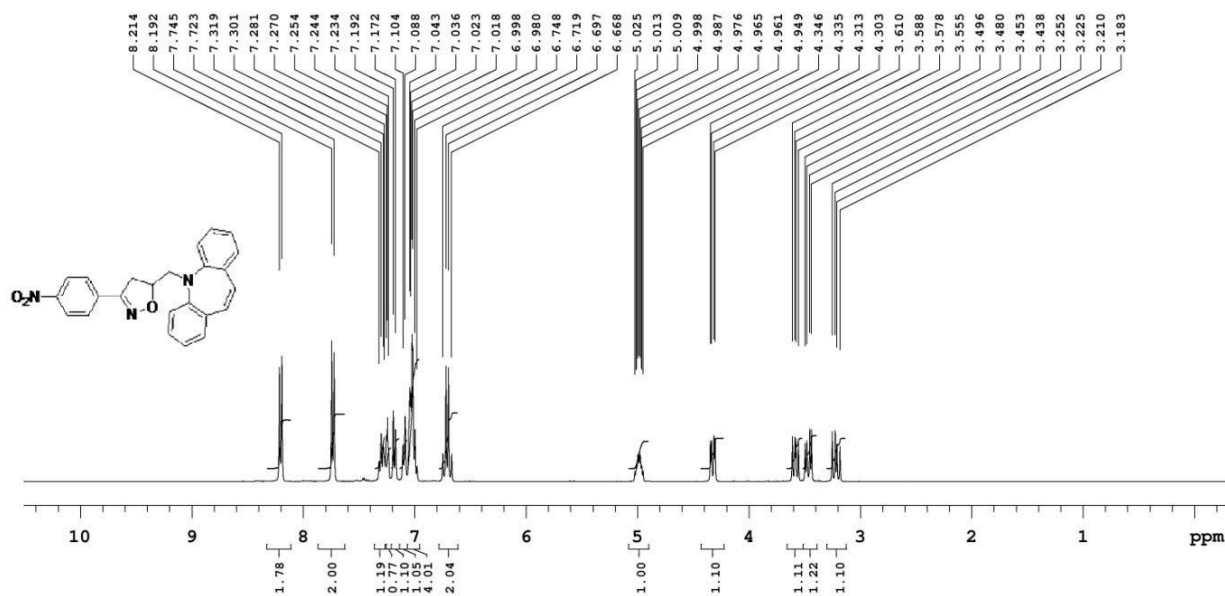


Figure S2 ^1H and ^{13}C NMR spectra of 5-(prop-2-yn-1-yl)-5H-dibenzo[b,f]azepine2



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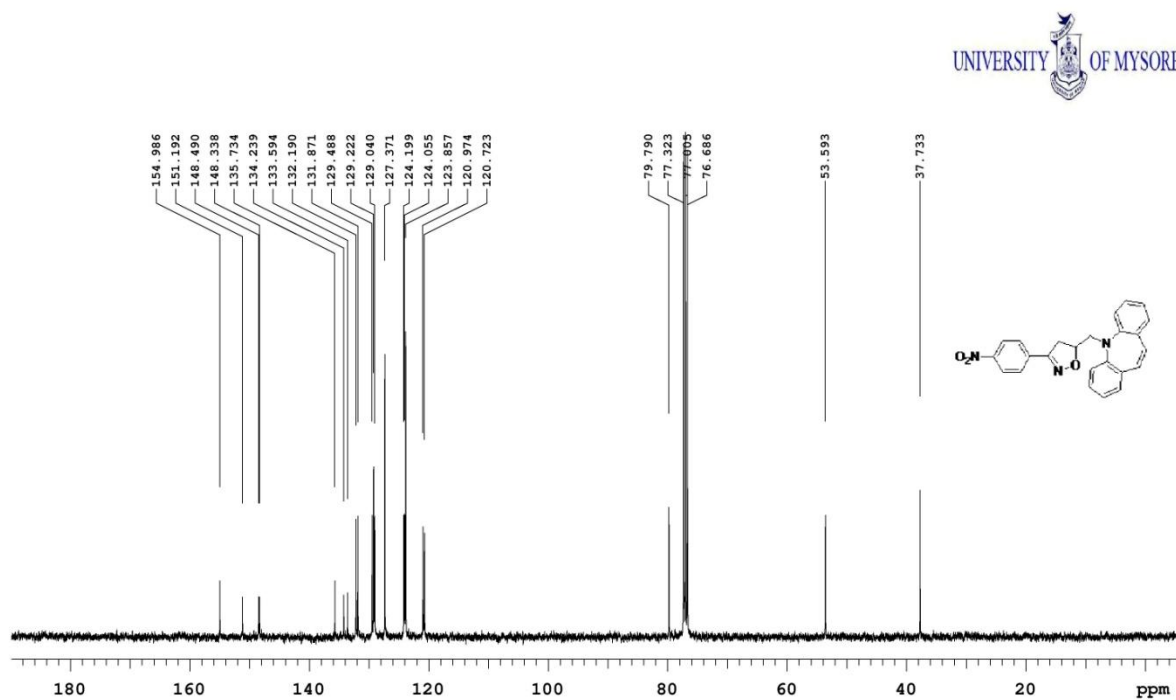
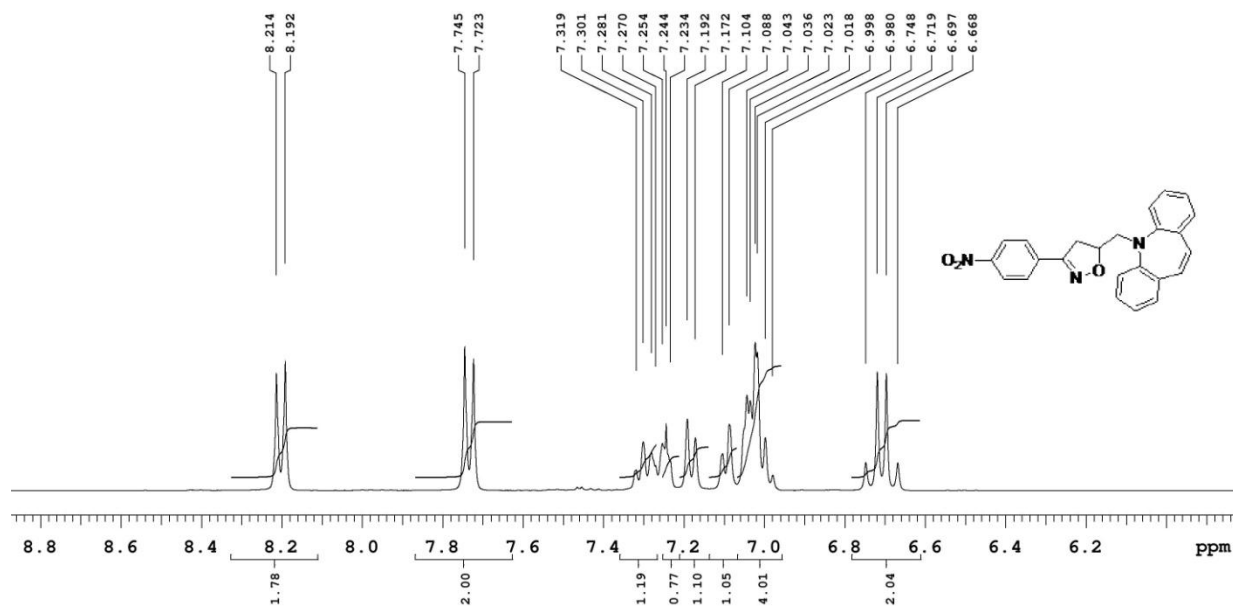
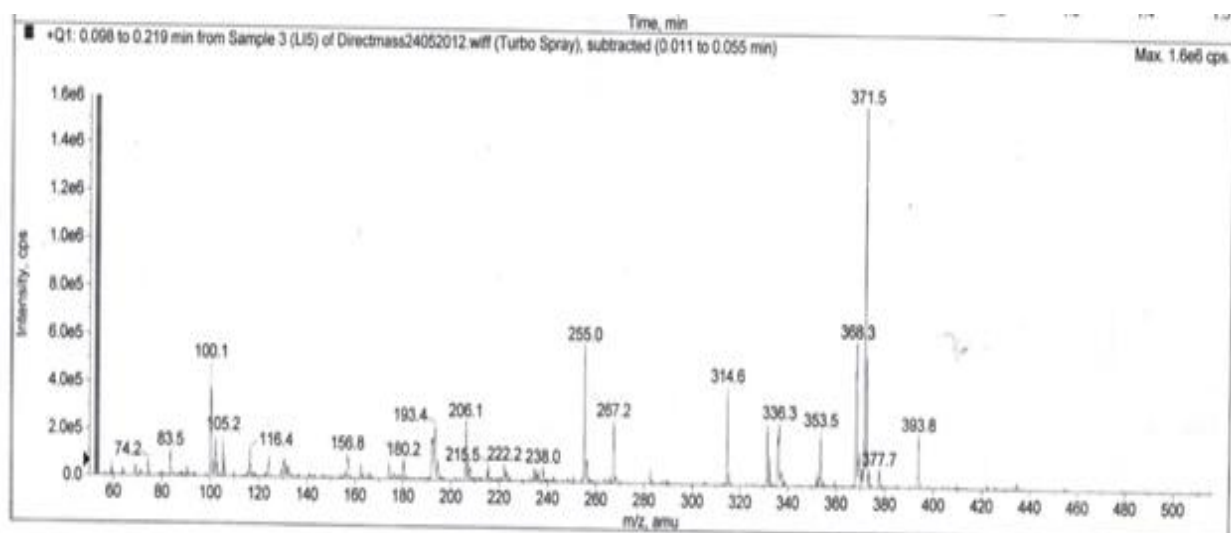
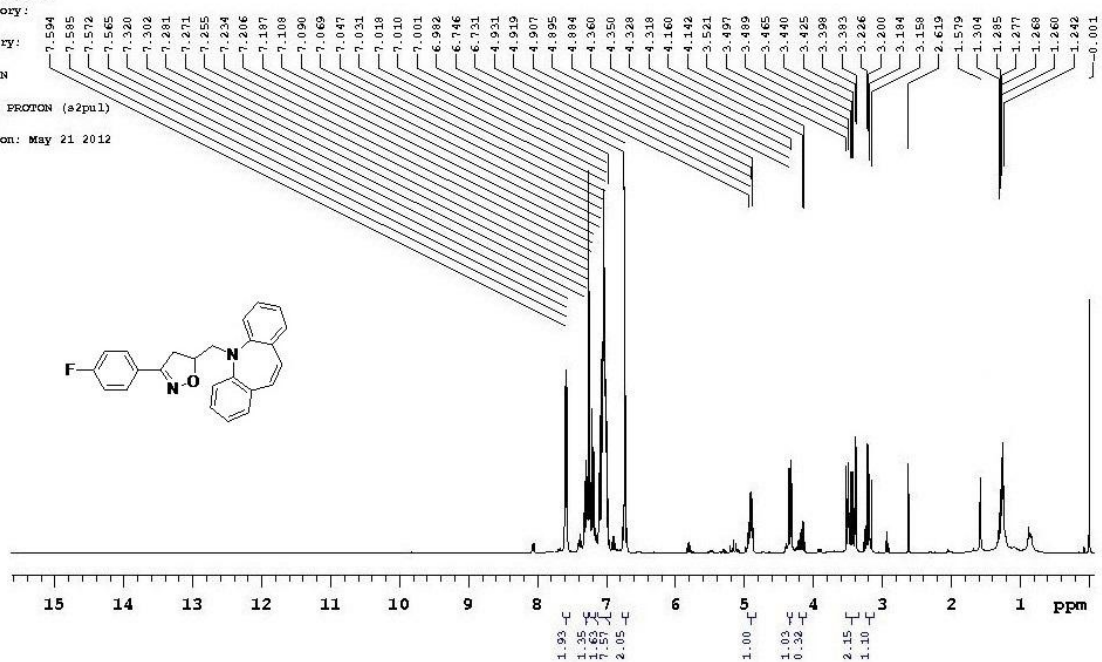


Figure S3 MASS, ¹H and ¹³C NMR spectra of compound 6a



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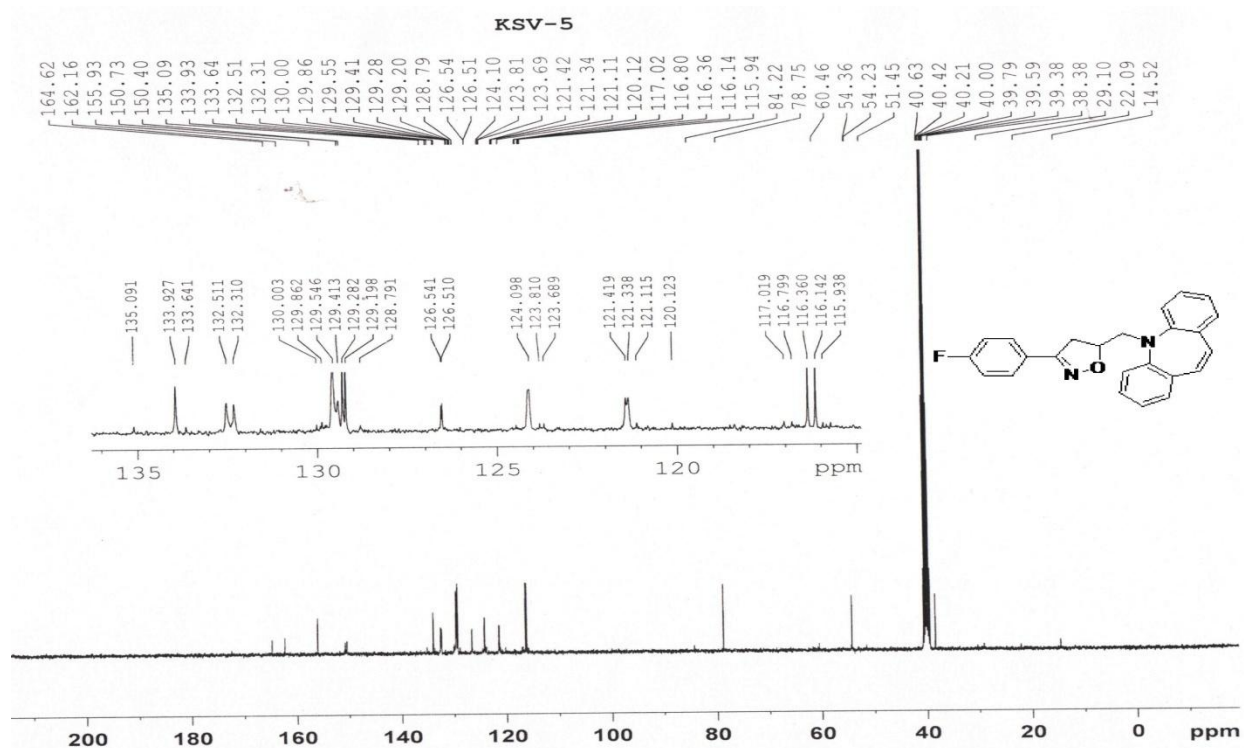
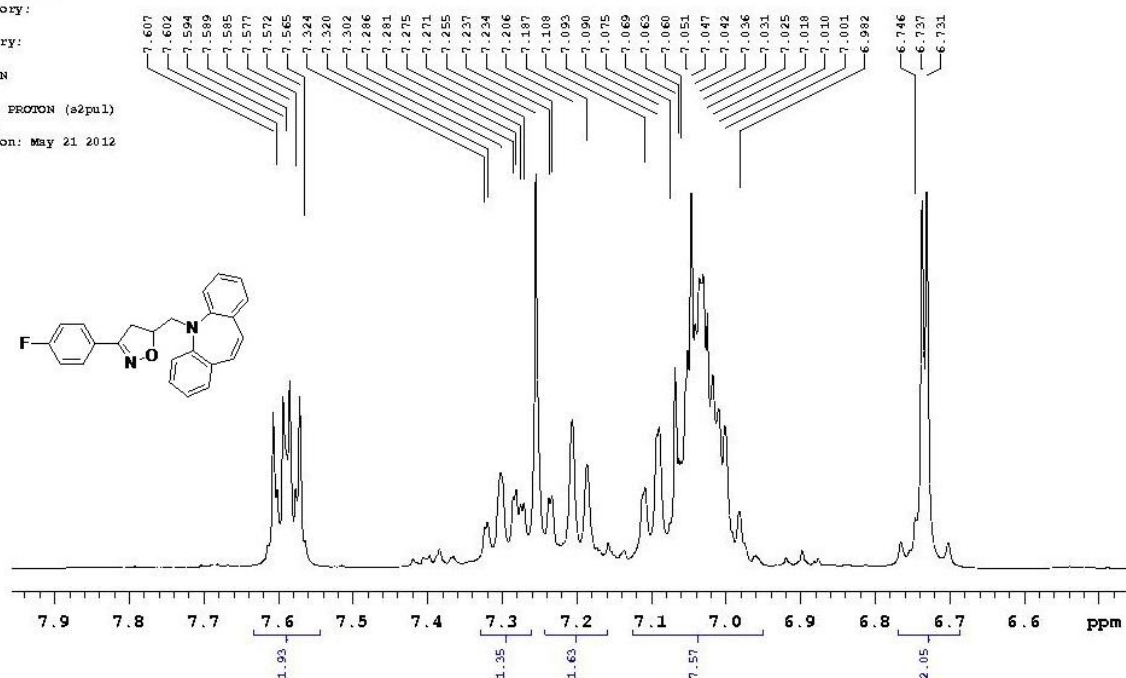
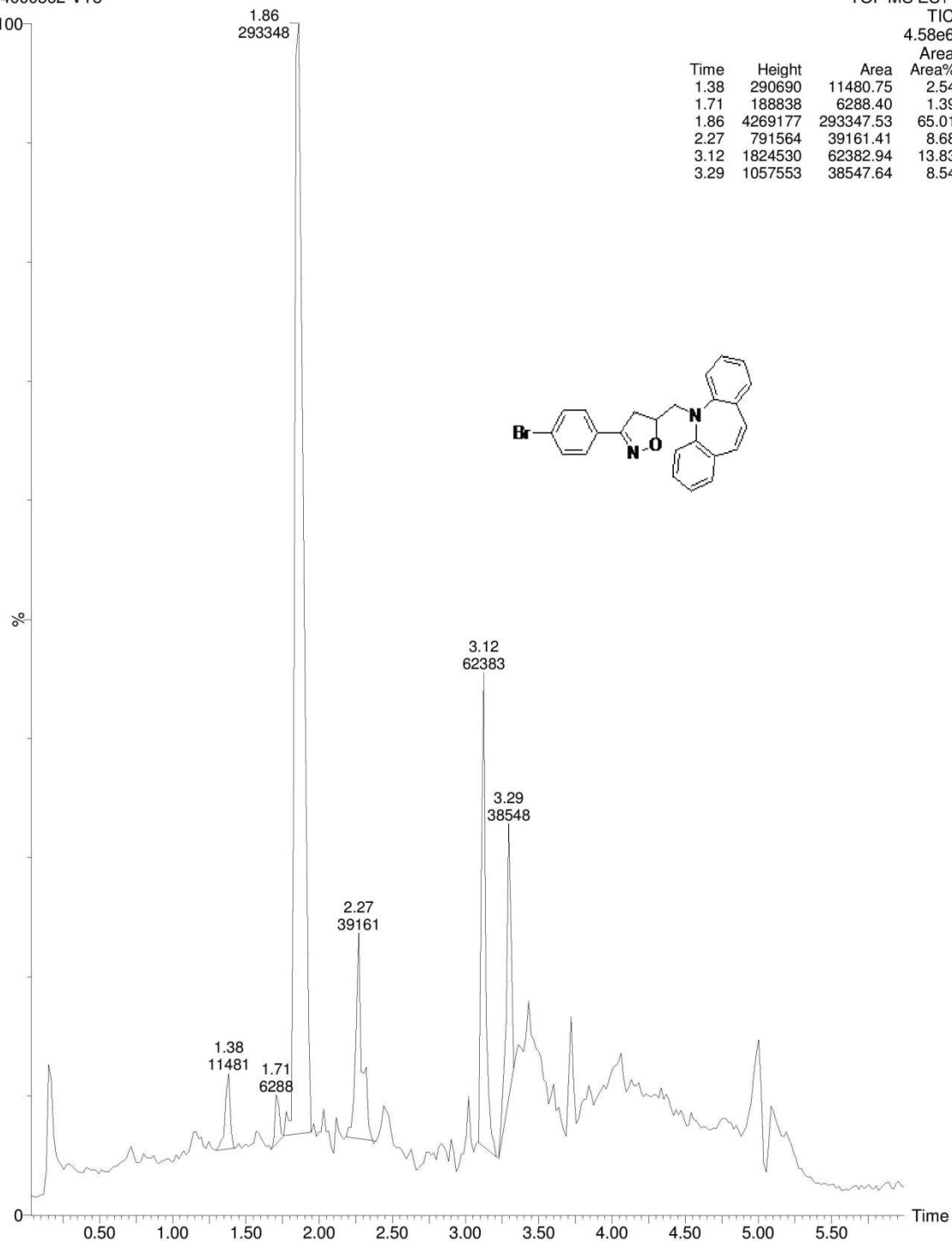


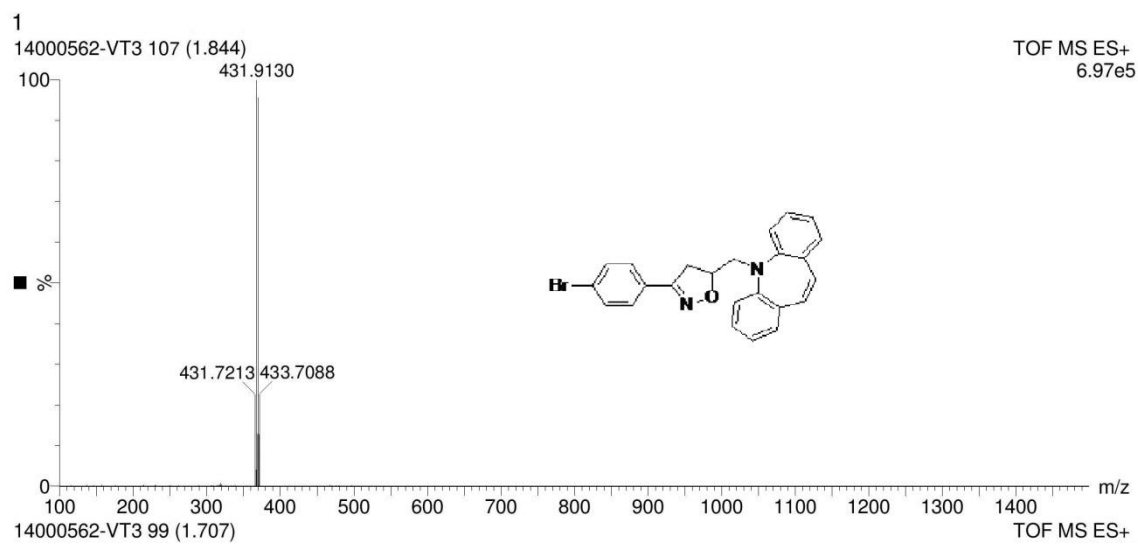
Figure S4 MASS, ¹H and ¹³C NMR spectra of compound 6b

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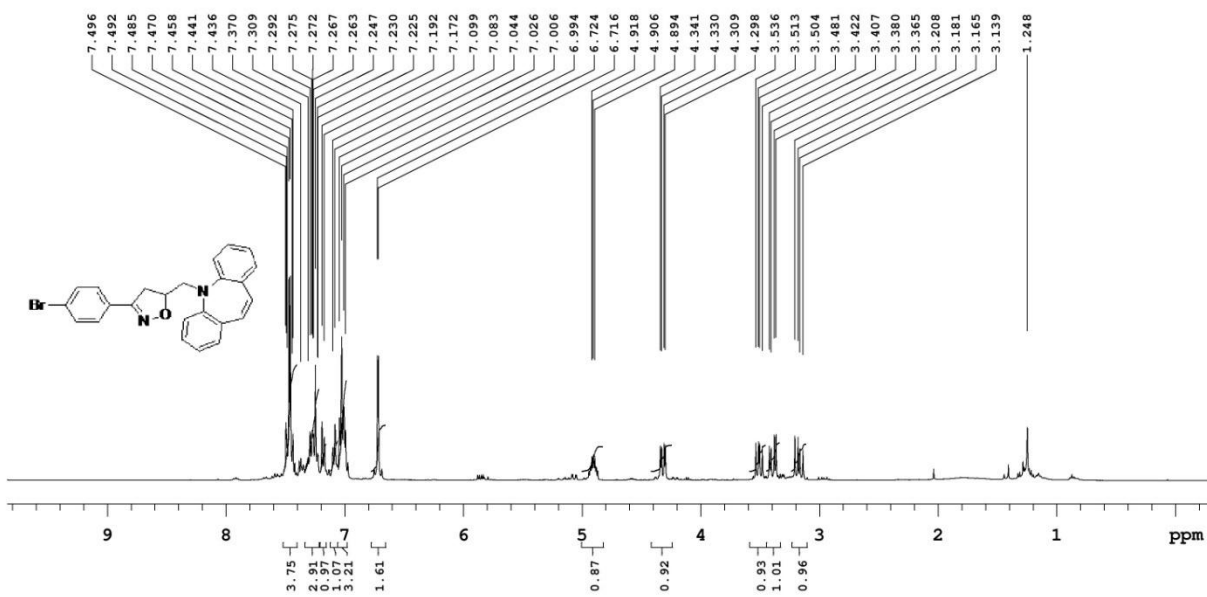
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2.27	791564	39161.41	8.68
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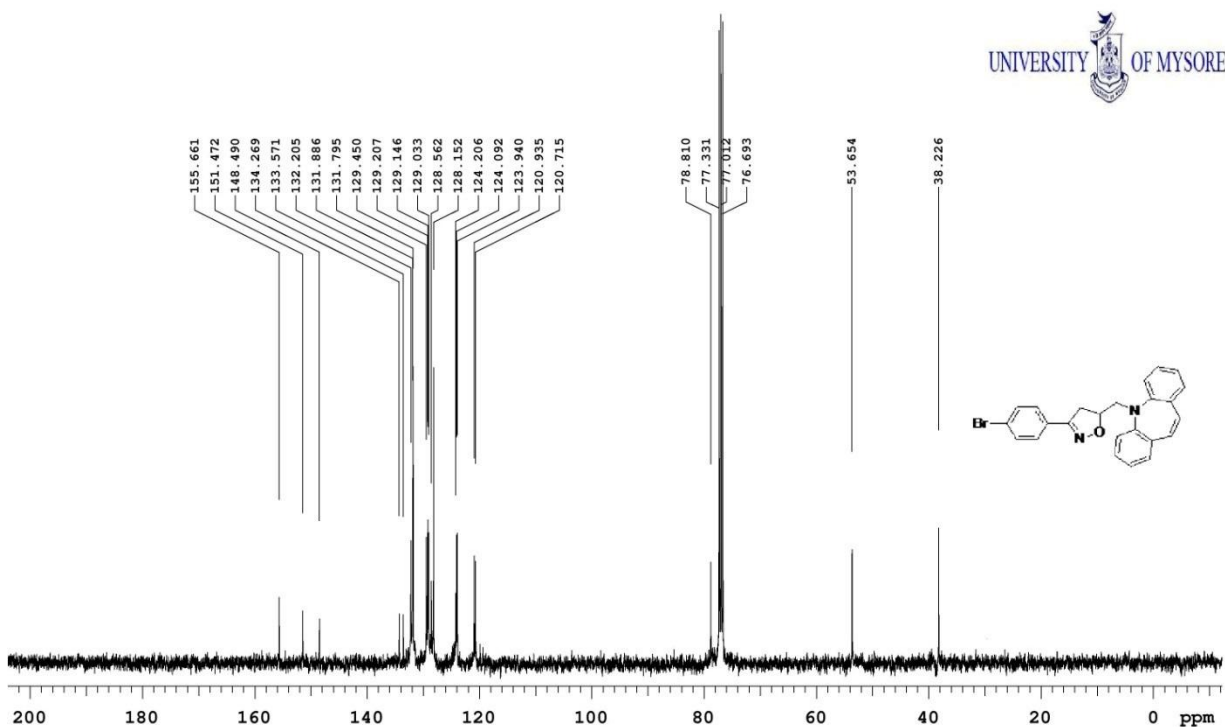
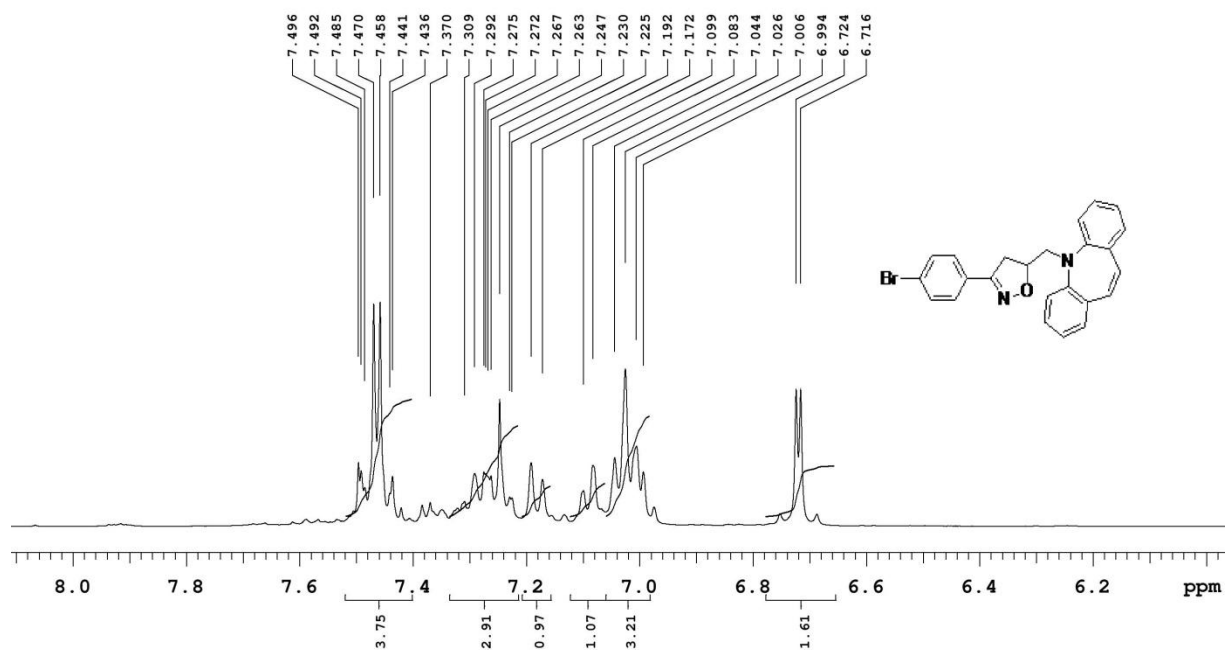
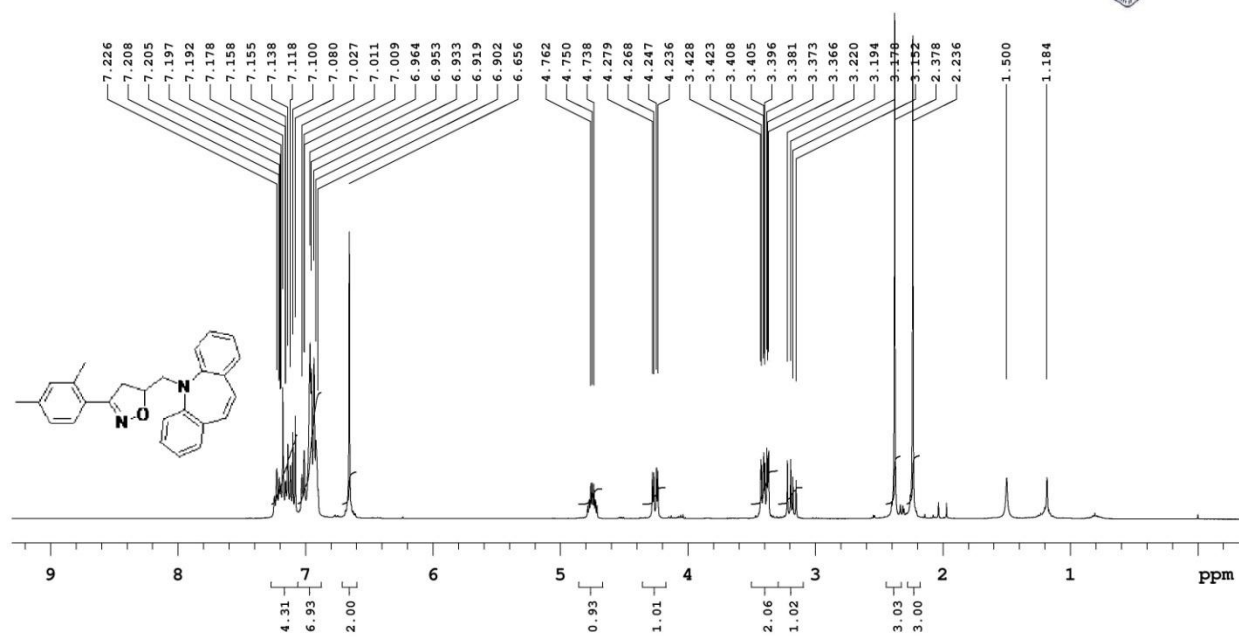
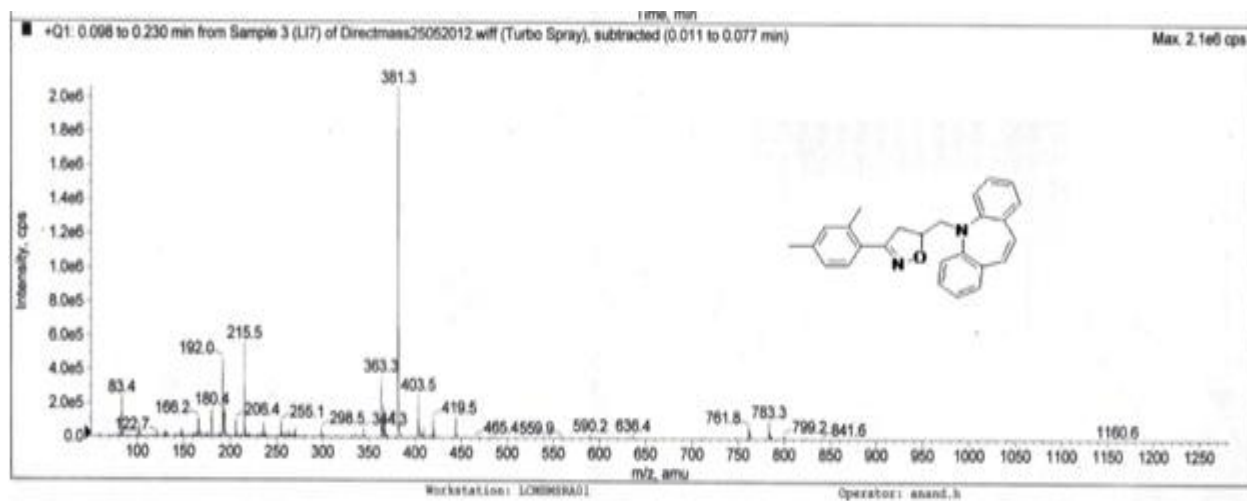


Figure S6 MASS, ¹H and ¹³C NMR spectra of compound **6d**



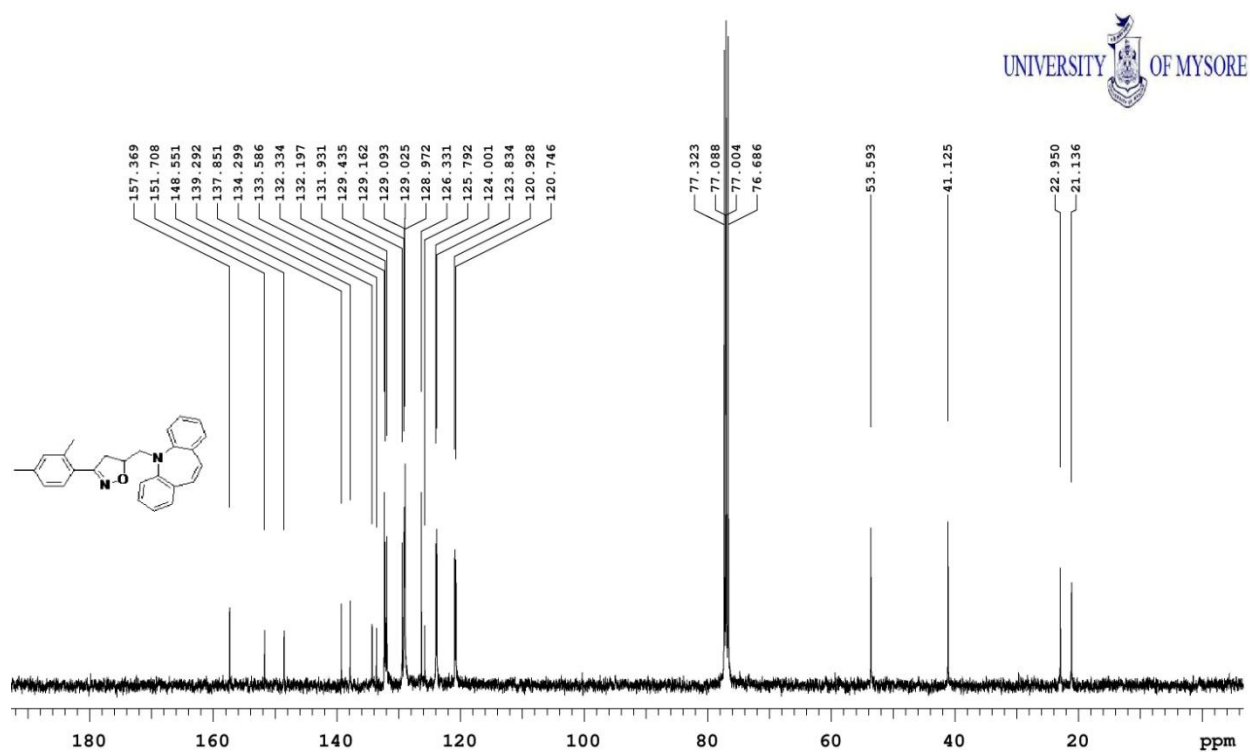
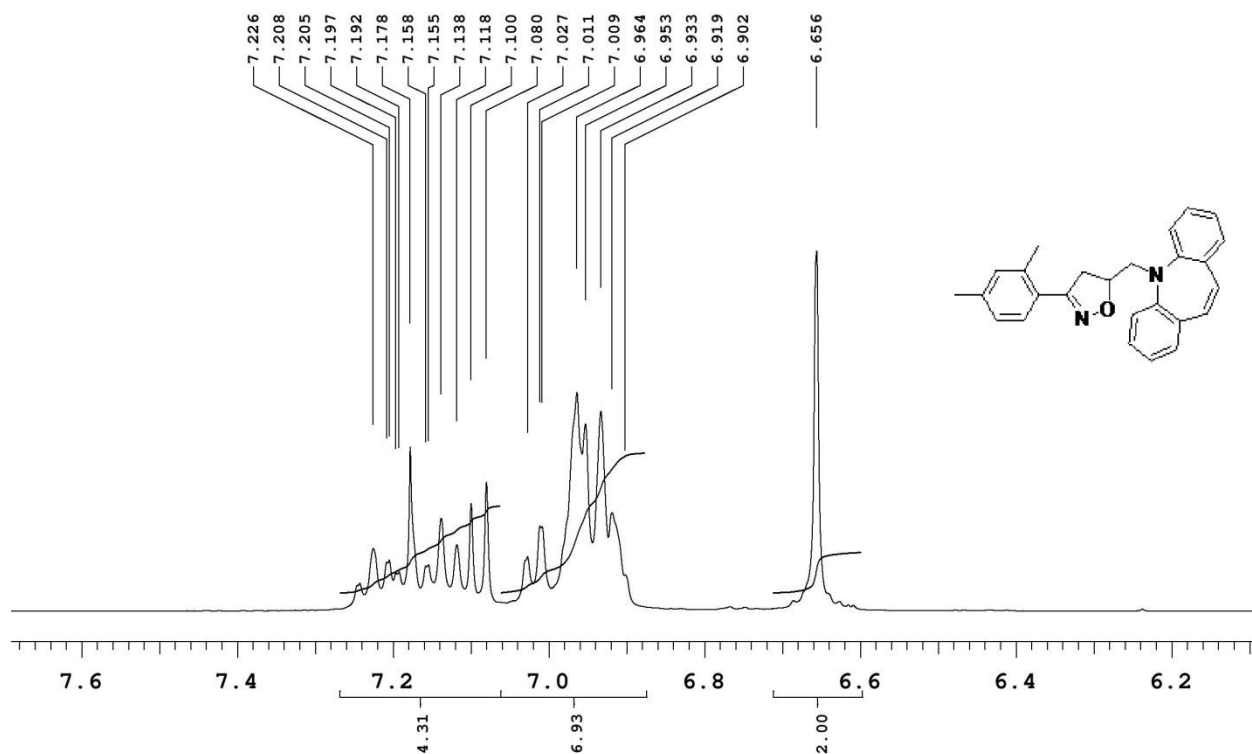
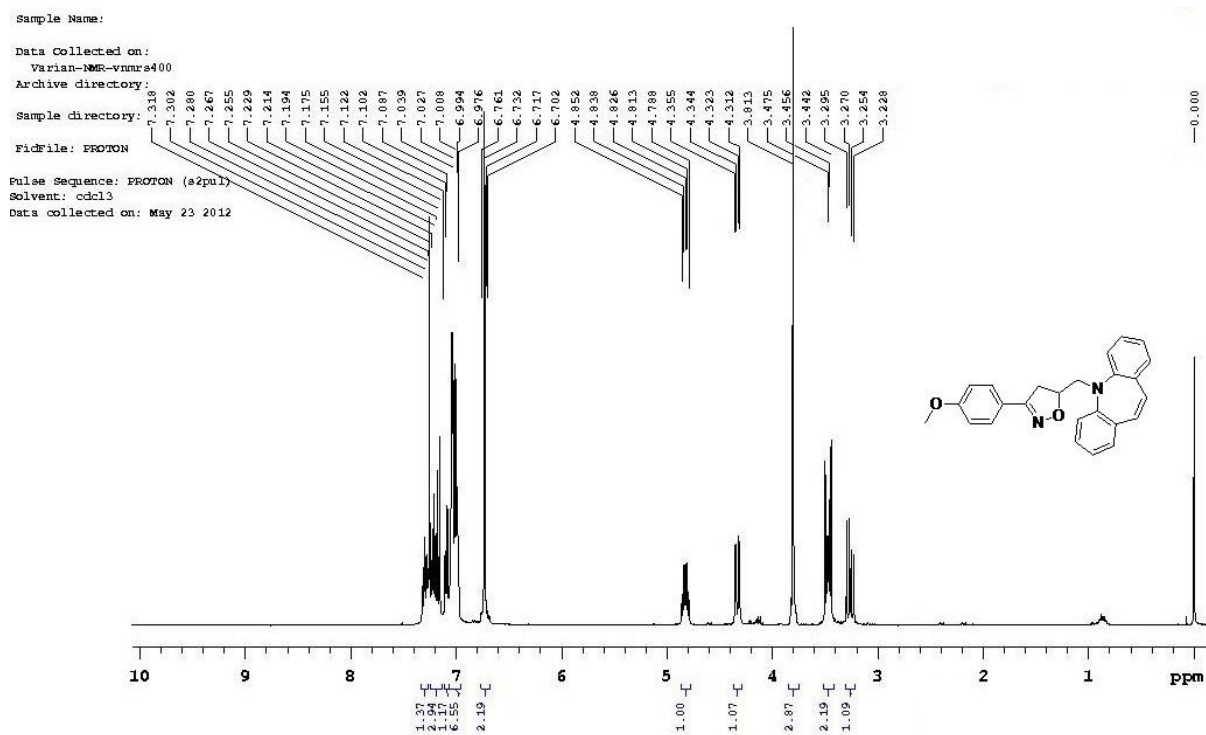
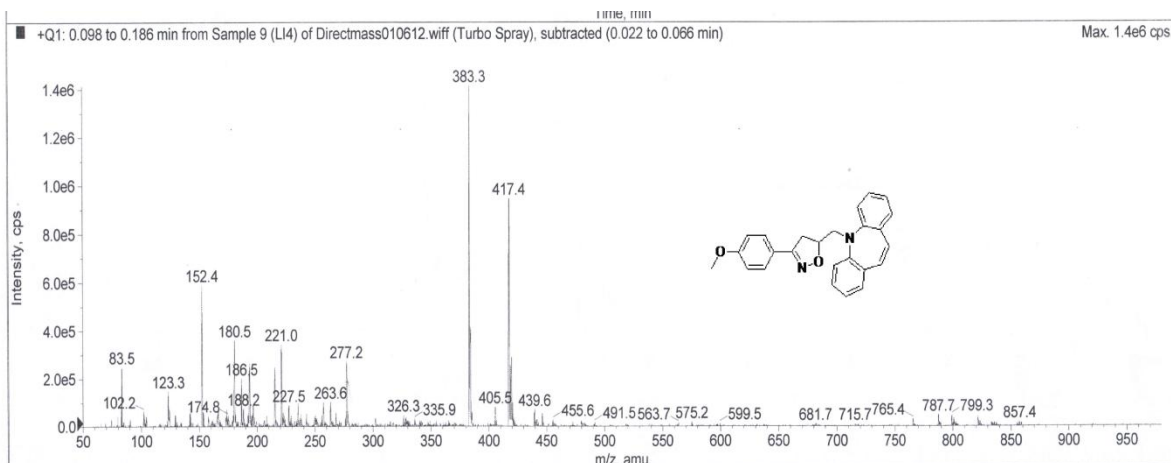
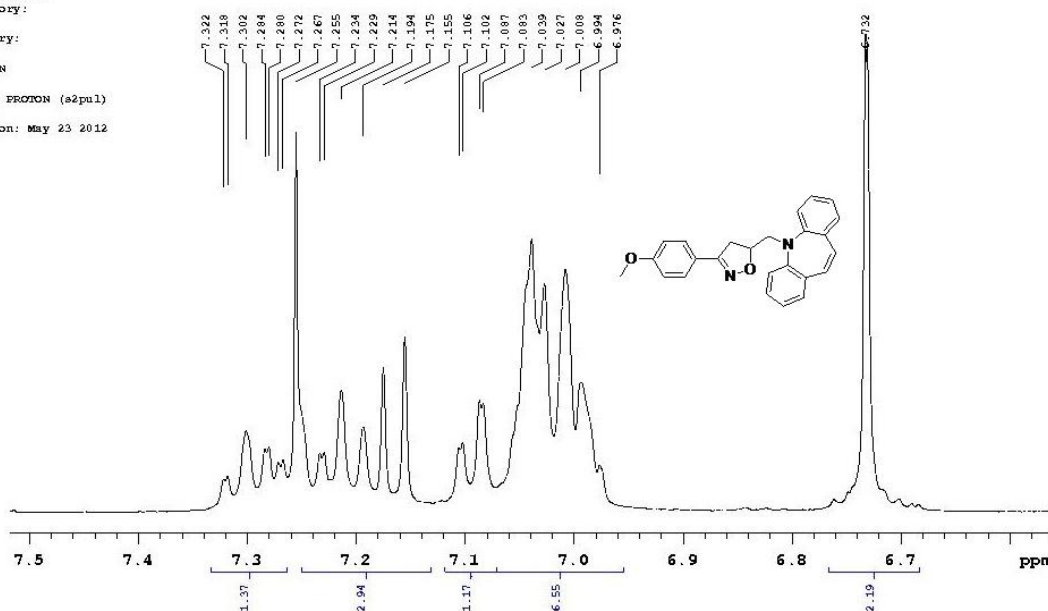


Figure S7 MASS, ¹H and ¹³C NMR spectra of compound **6e**



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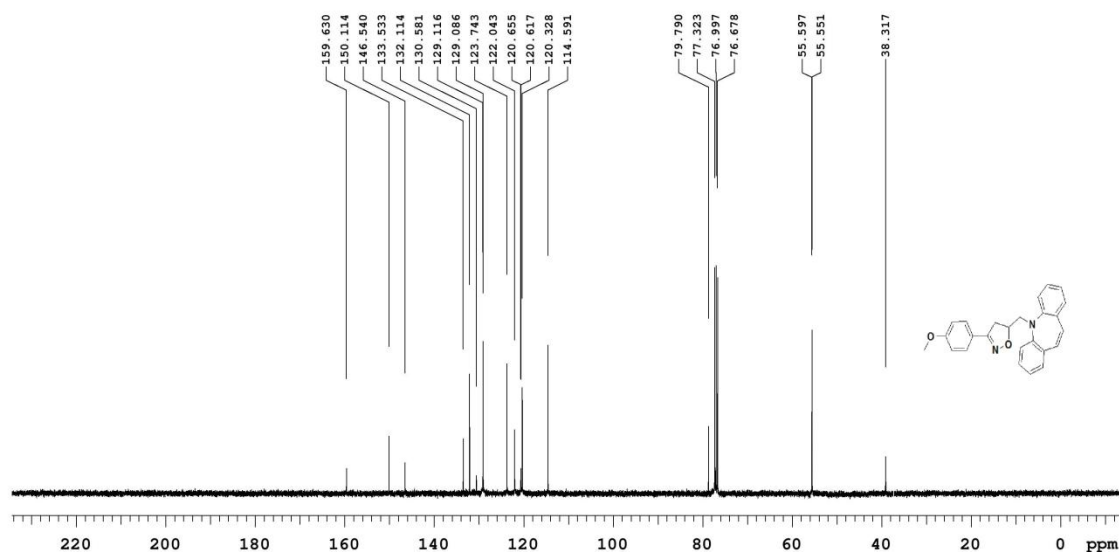
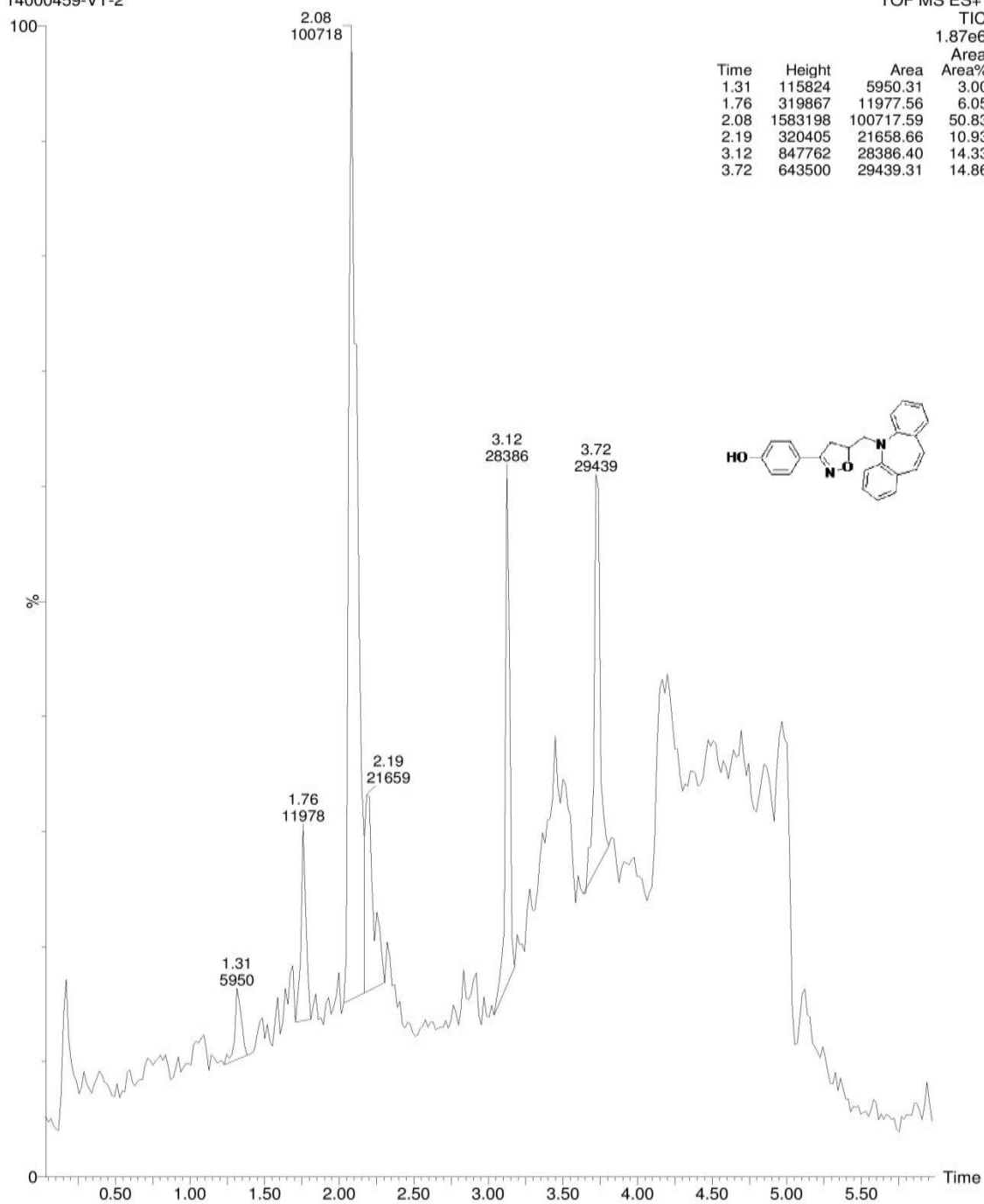
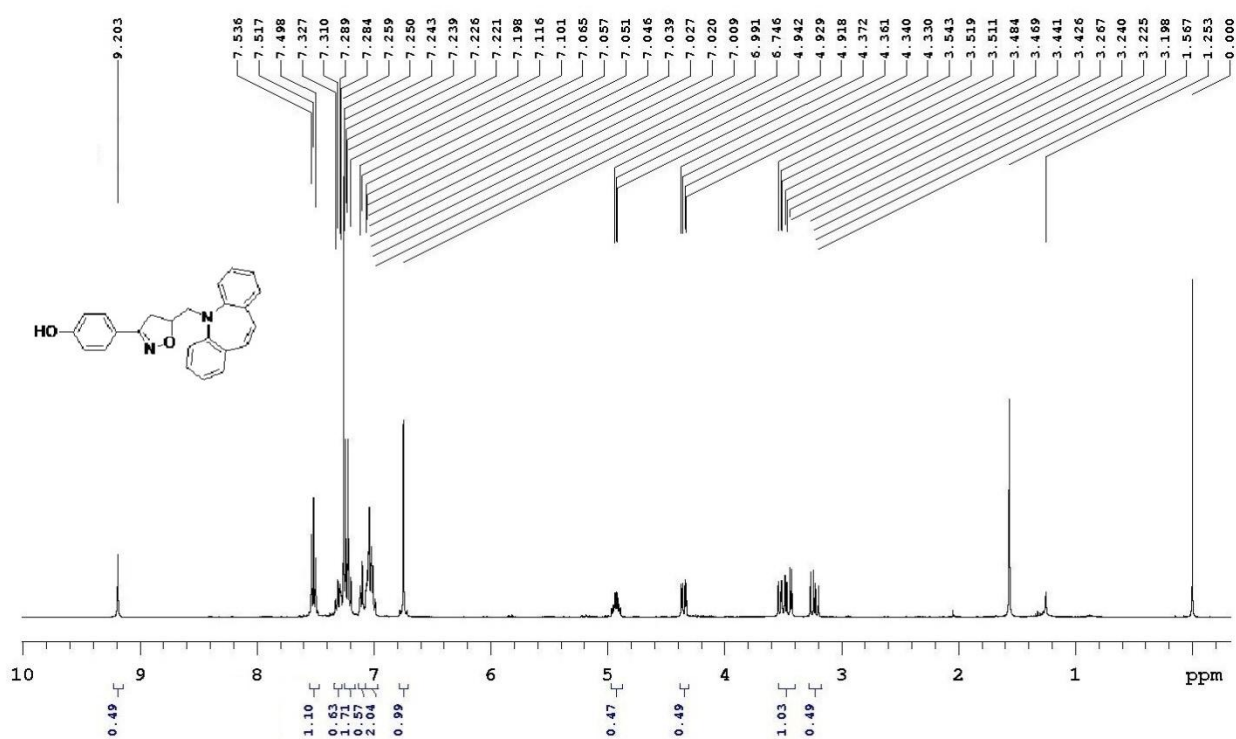
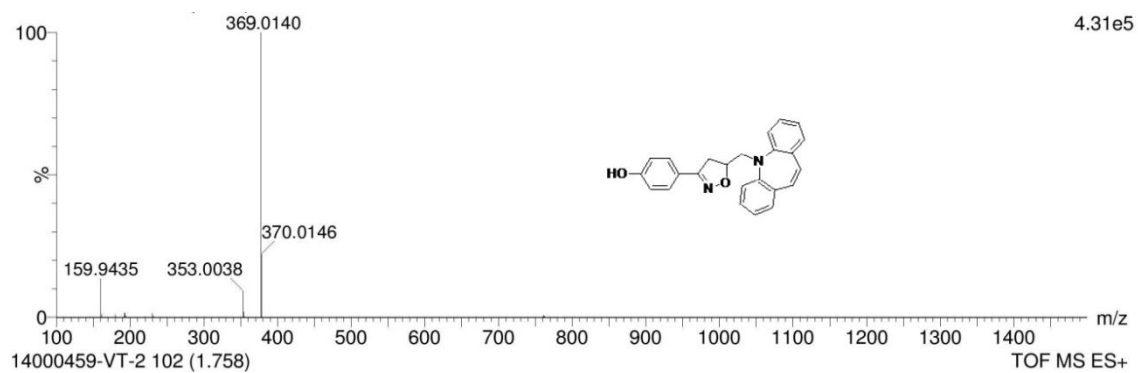


Figure S8 Mass, ^1H and ^{13}C NMR spectra of compound 6f

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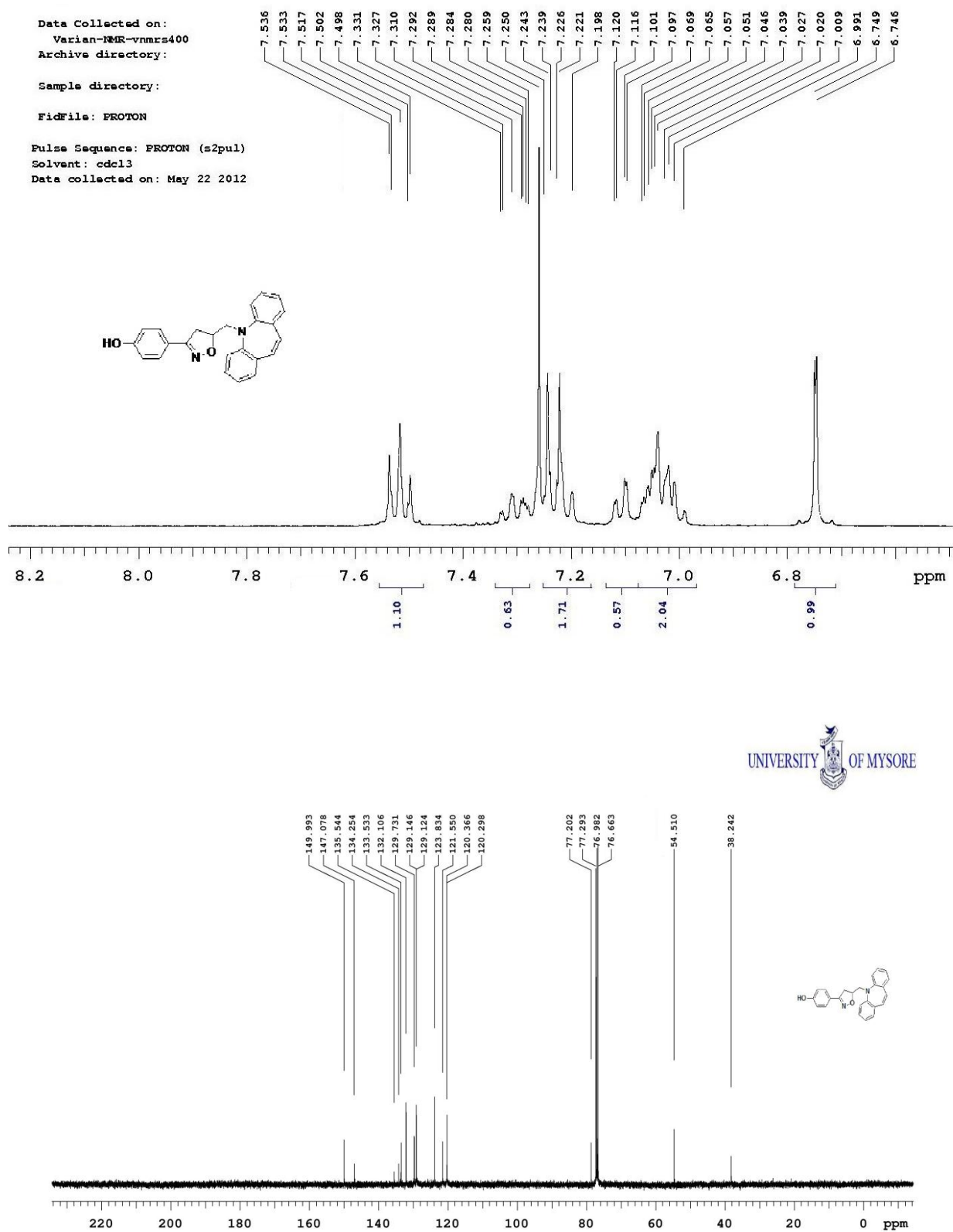
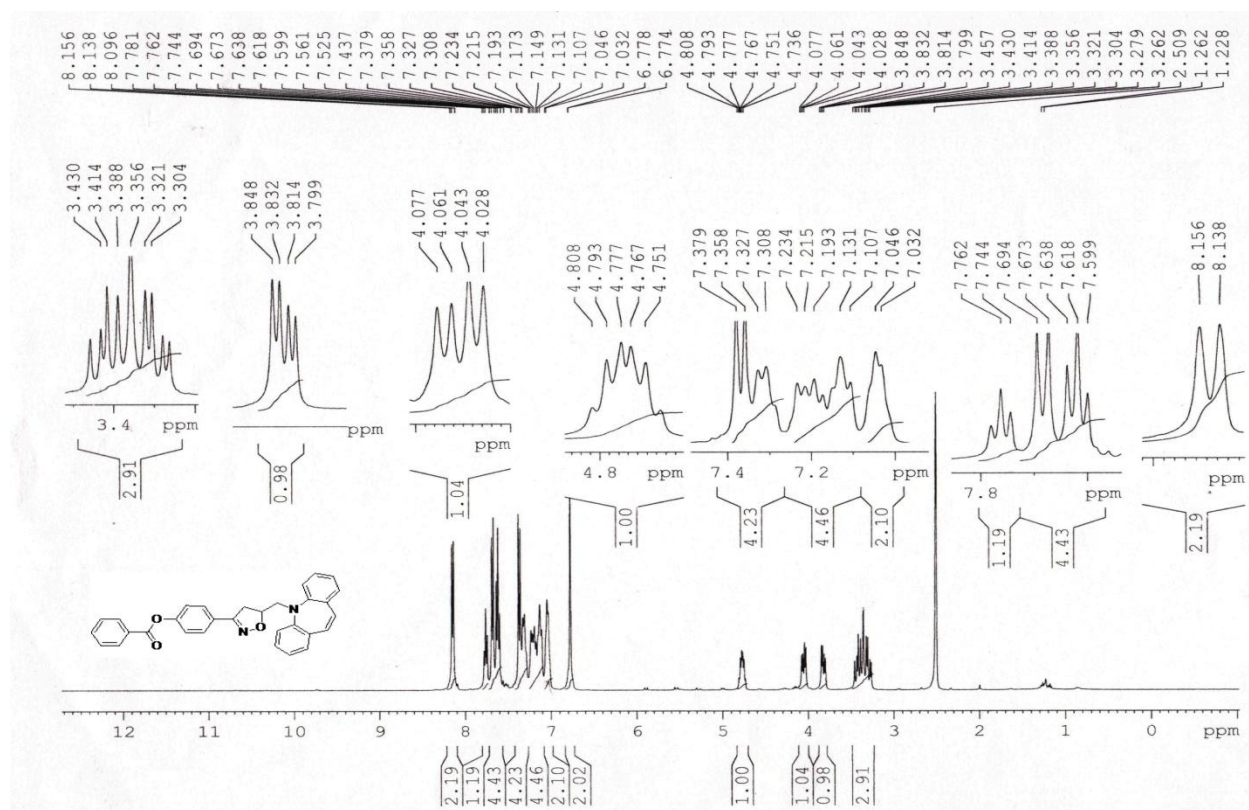
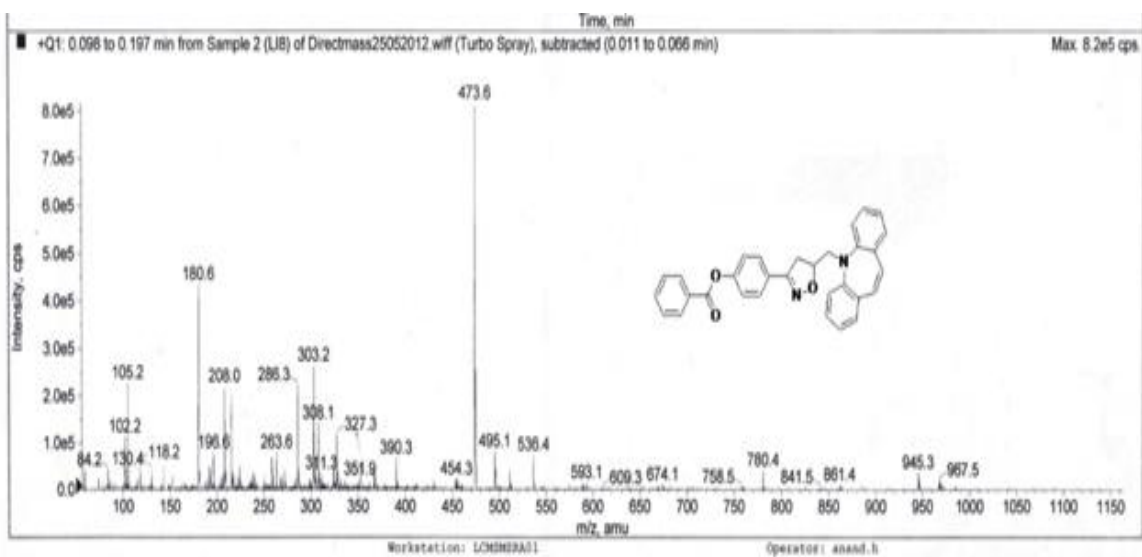


Figure S9 Mass, ¹H and ¹³C NMR spectra of compound 6g



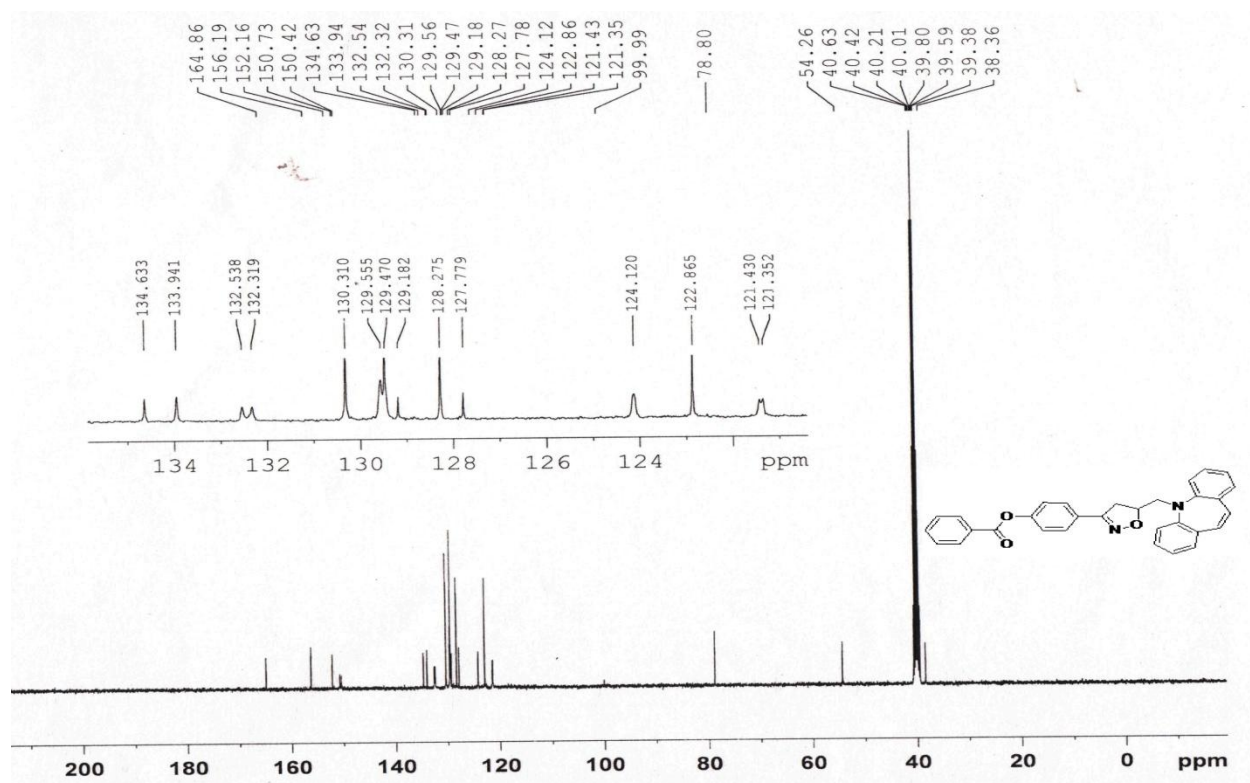
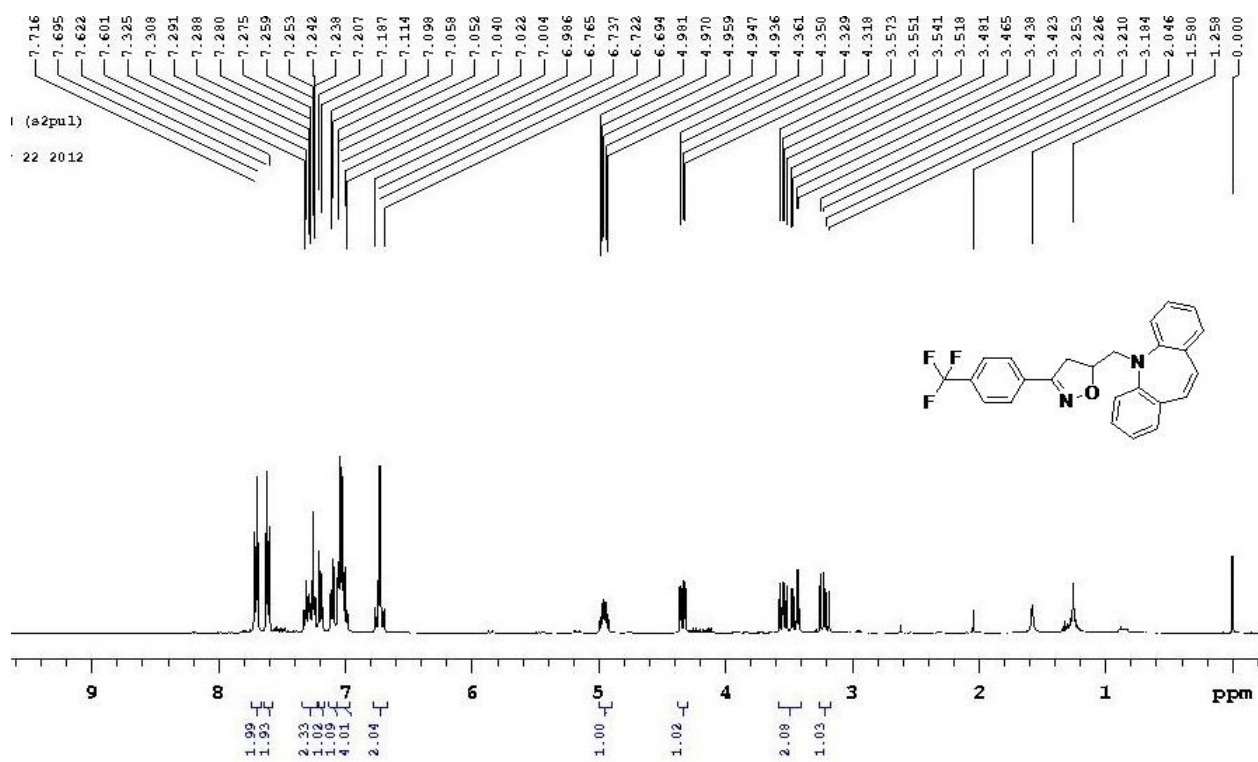
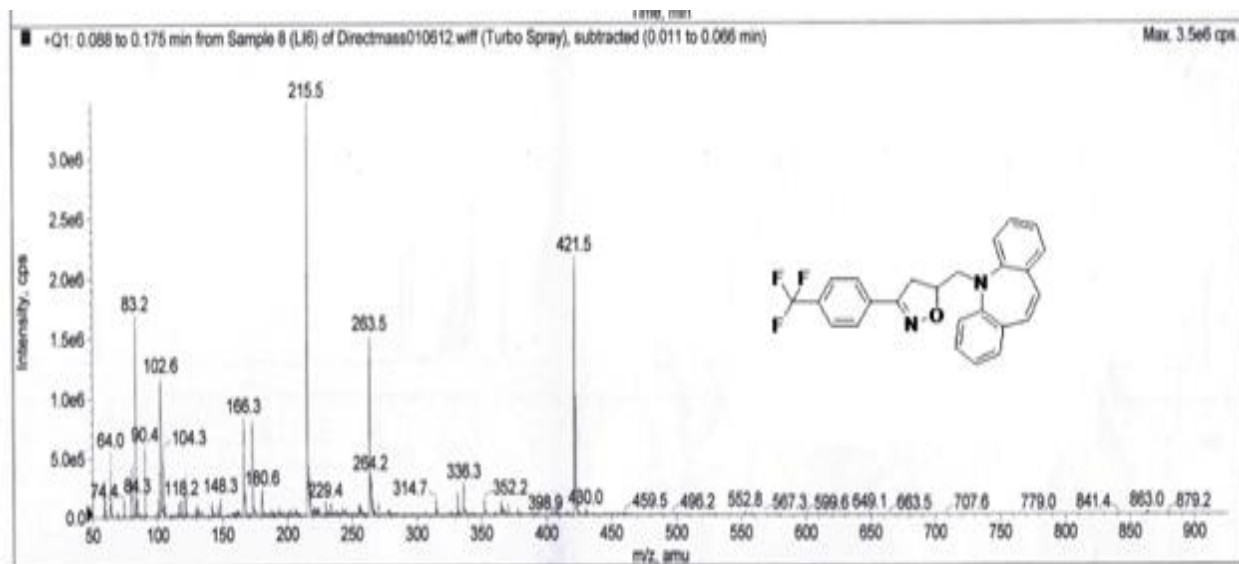


Figure S10 Mass, ¹H and ¹³C NMR spectra of compound **6h**



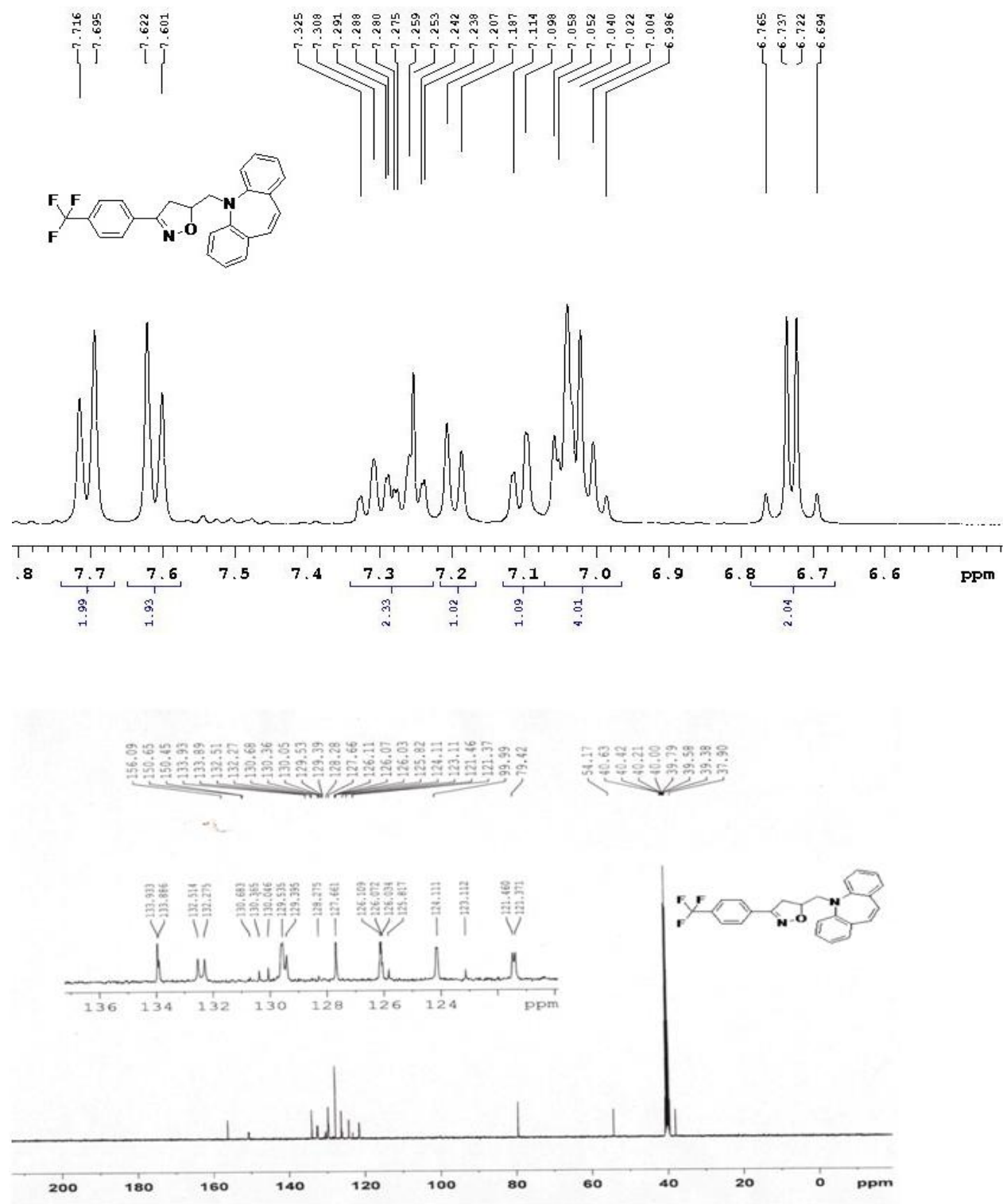
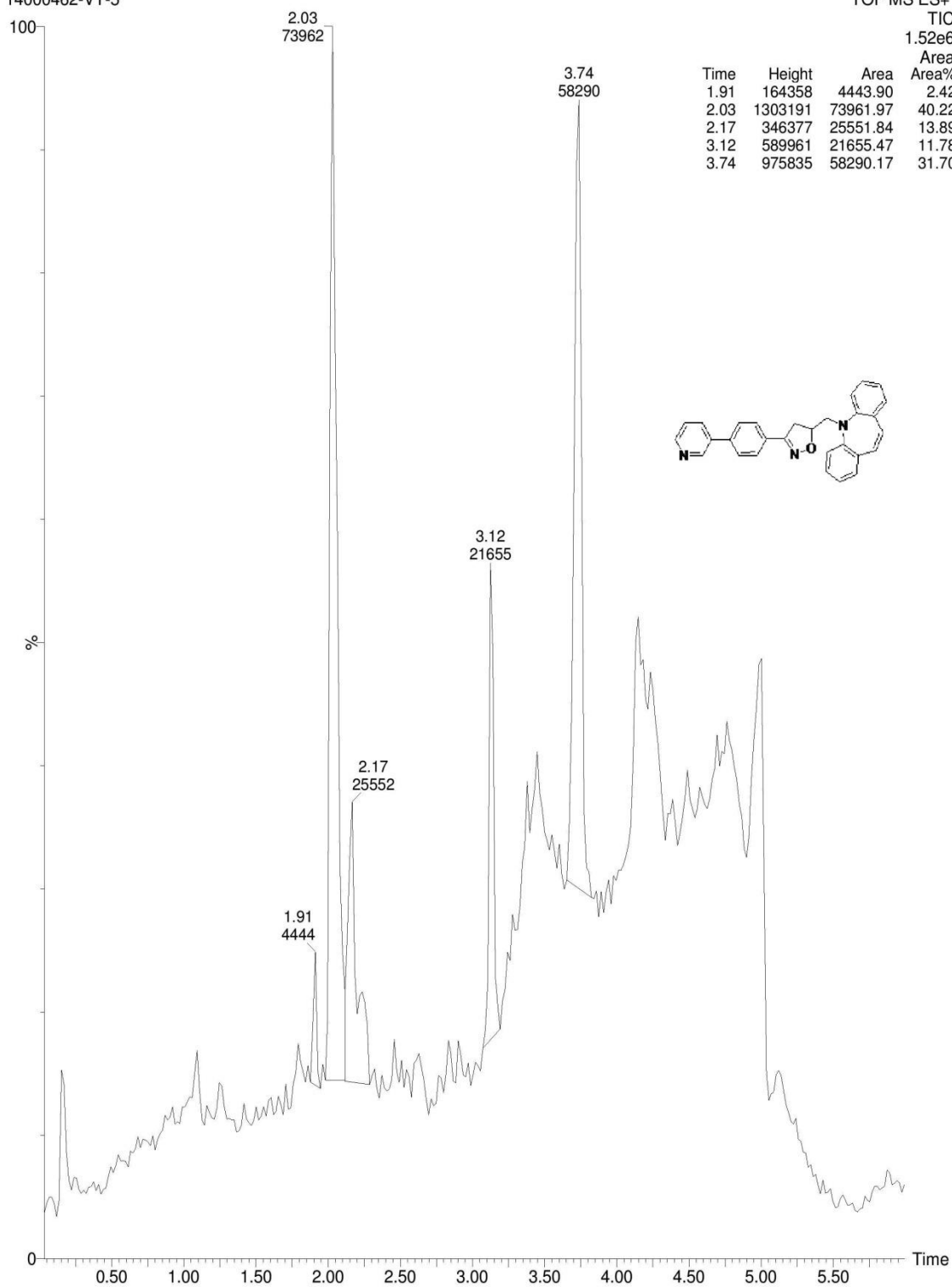
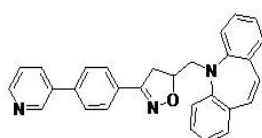
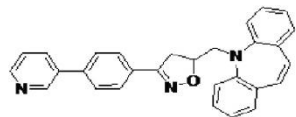


Figure S11 Mass, ¹H and ¹³C NMR spectra of compound 6i

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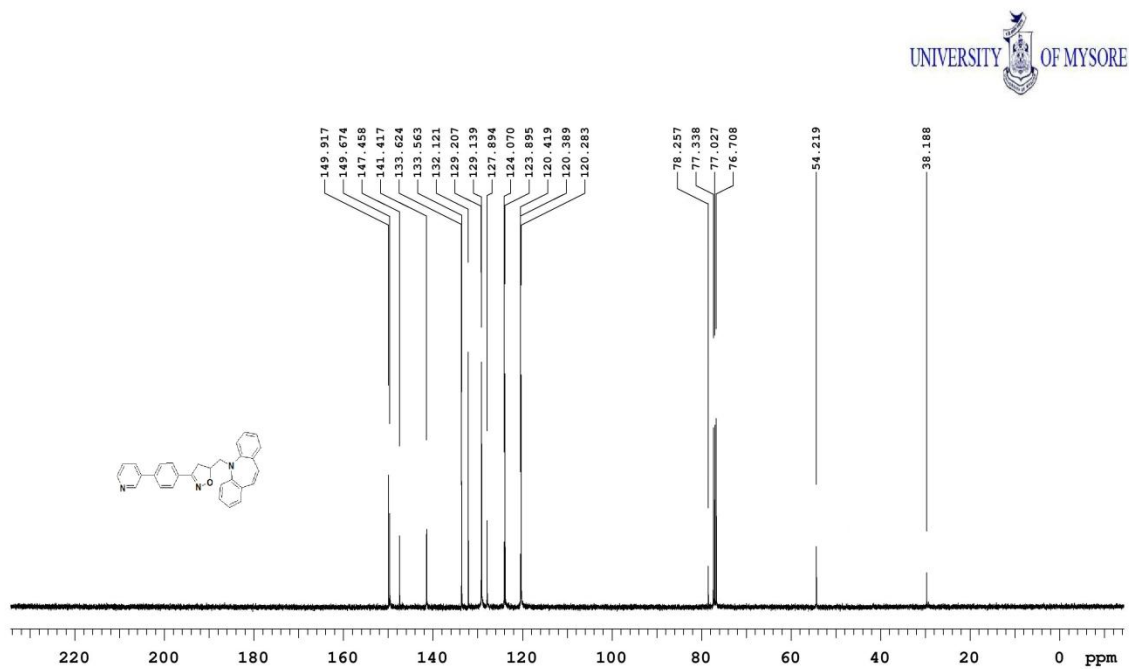
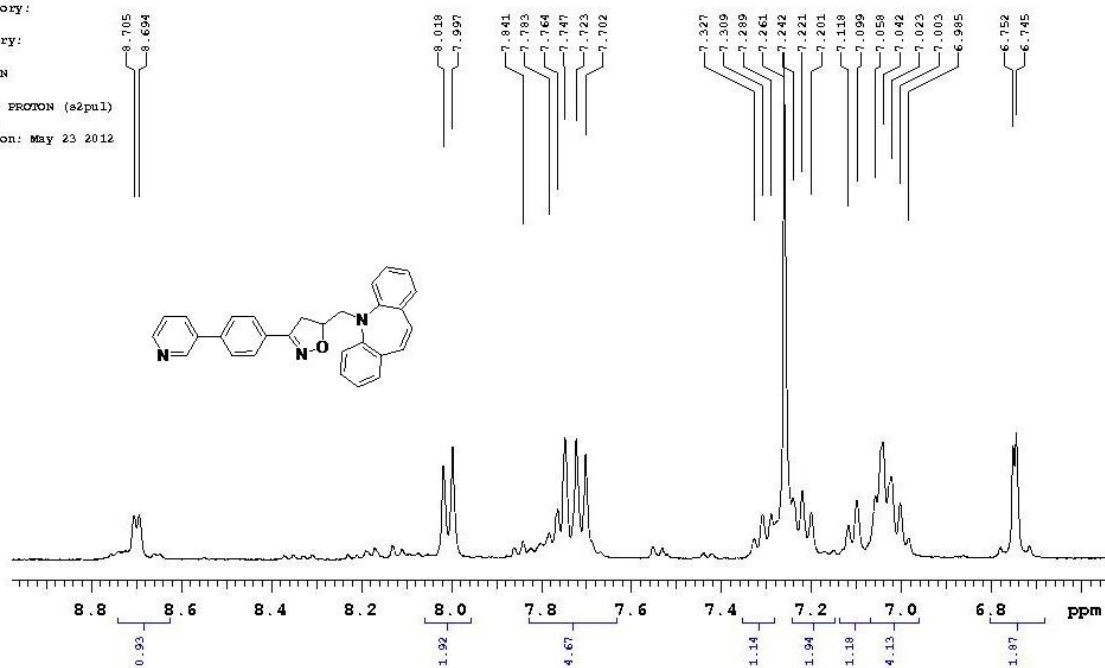
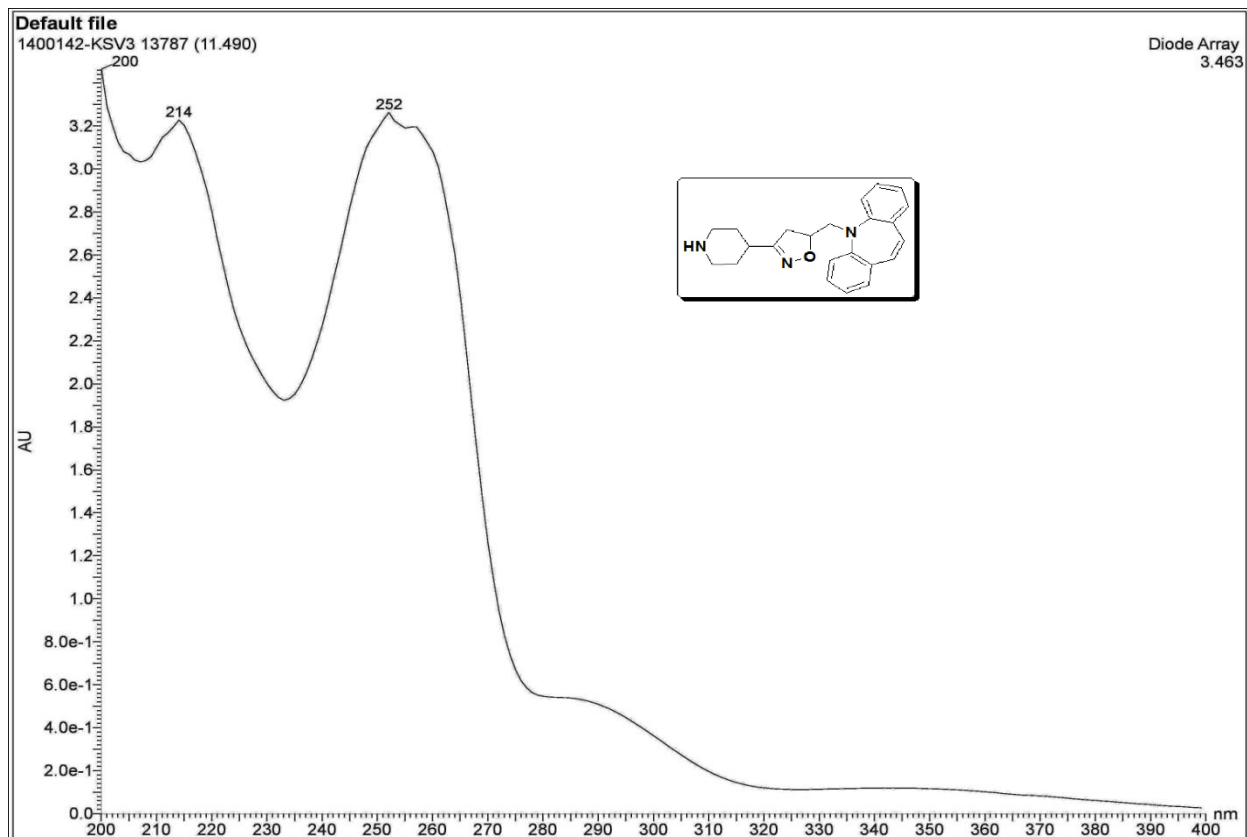
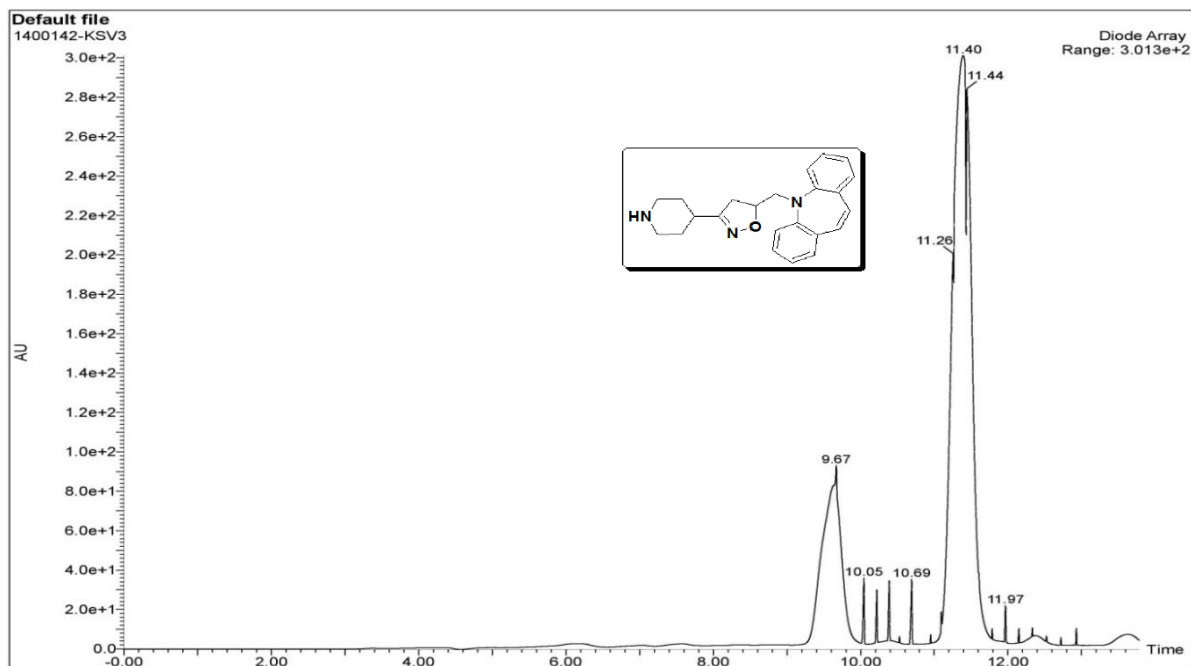
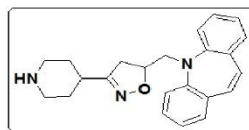
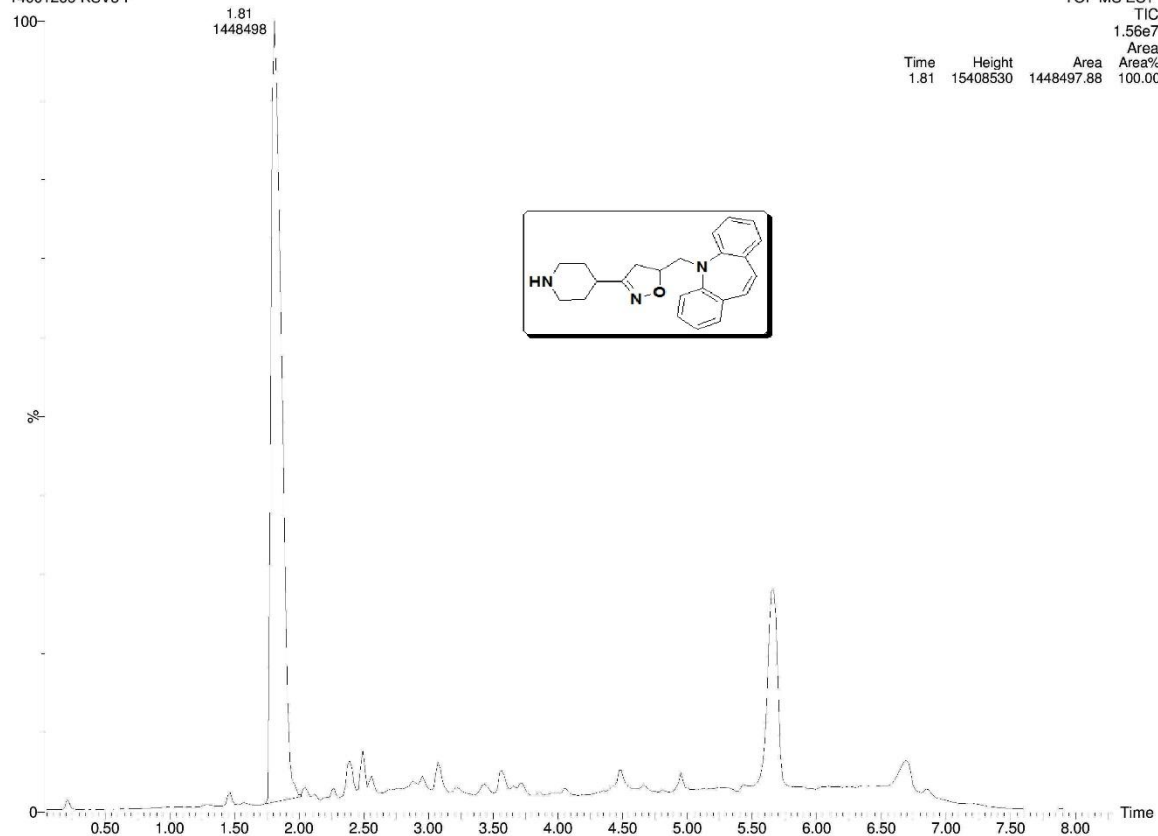


Figure S12 Mass, ¹H and ¹³C NMR spectra of compound 6j



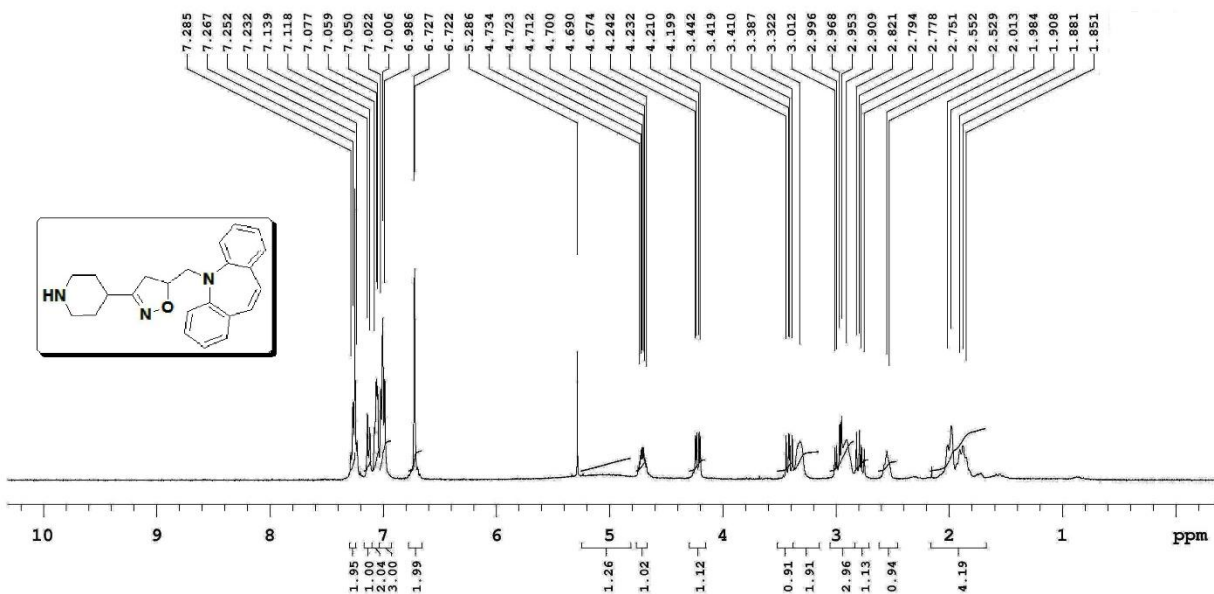
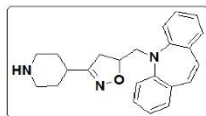
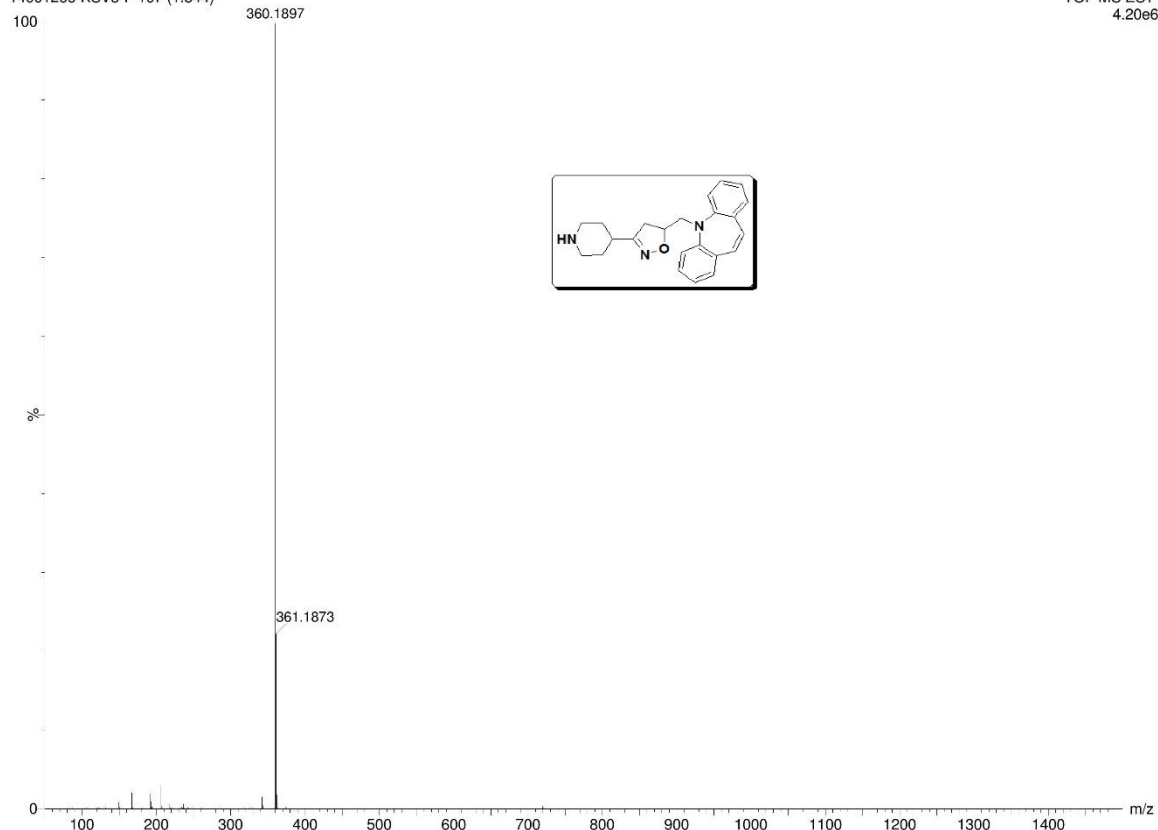
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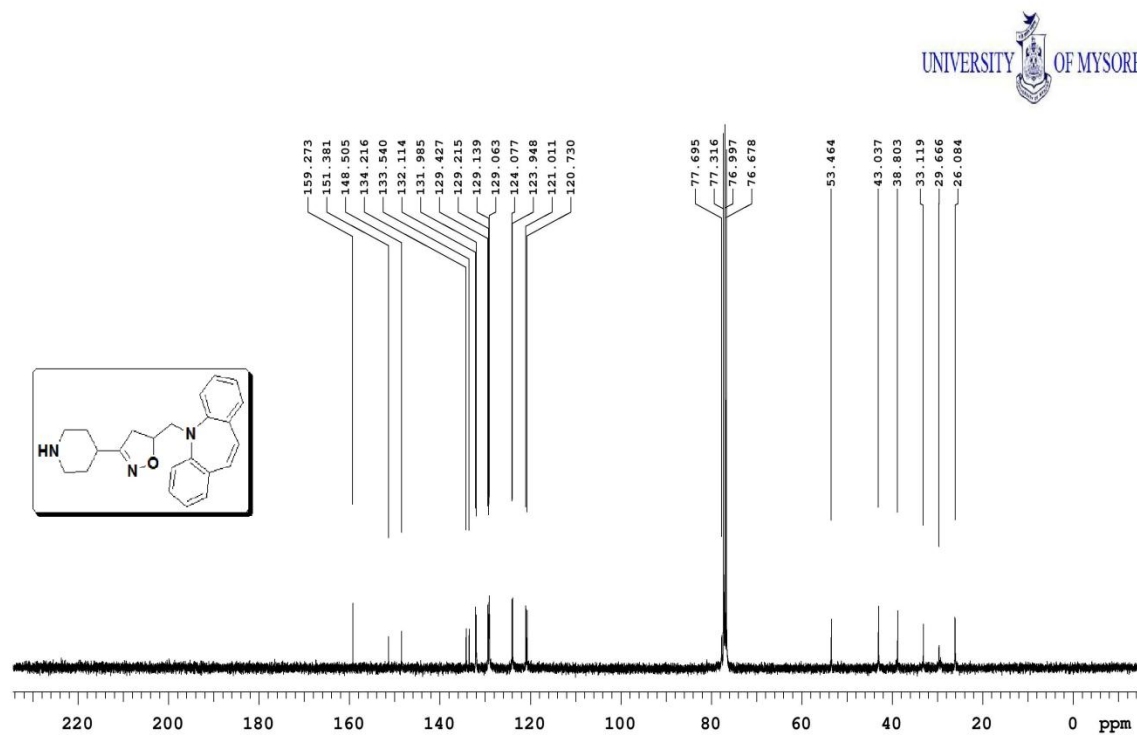
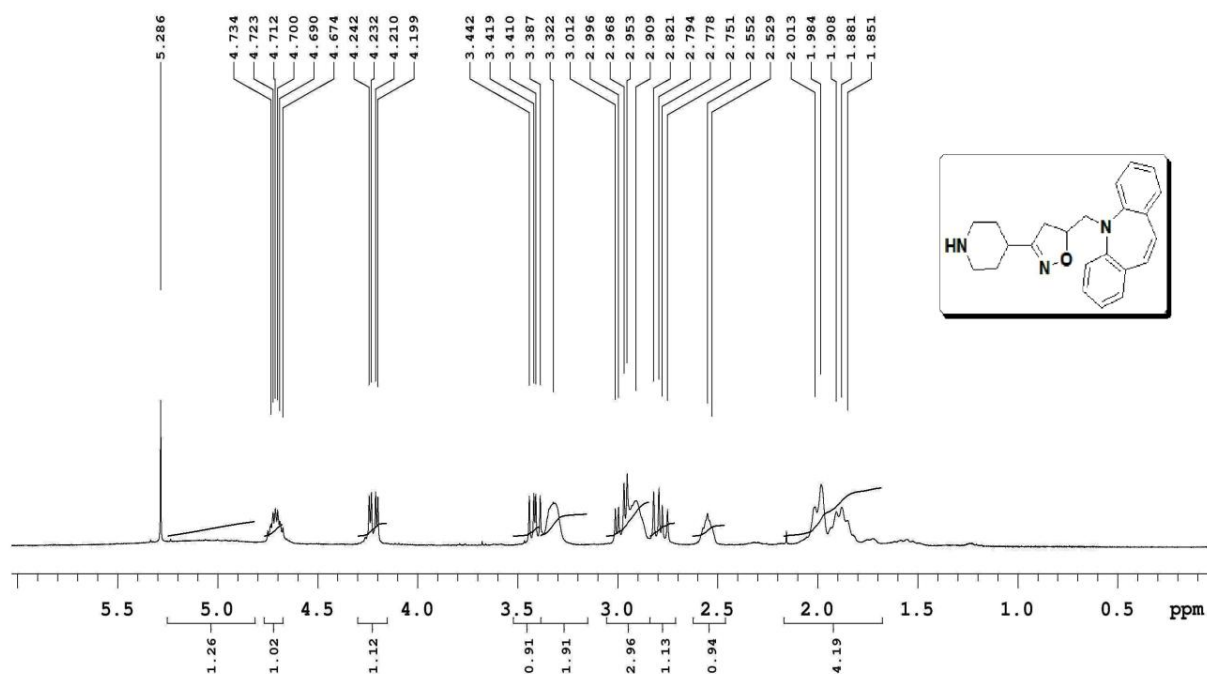
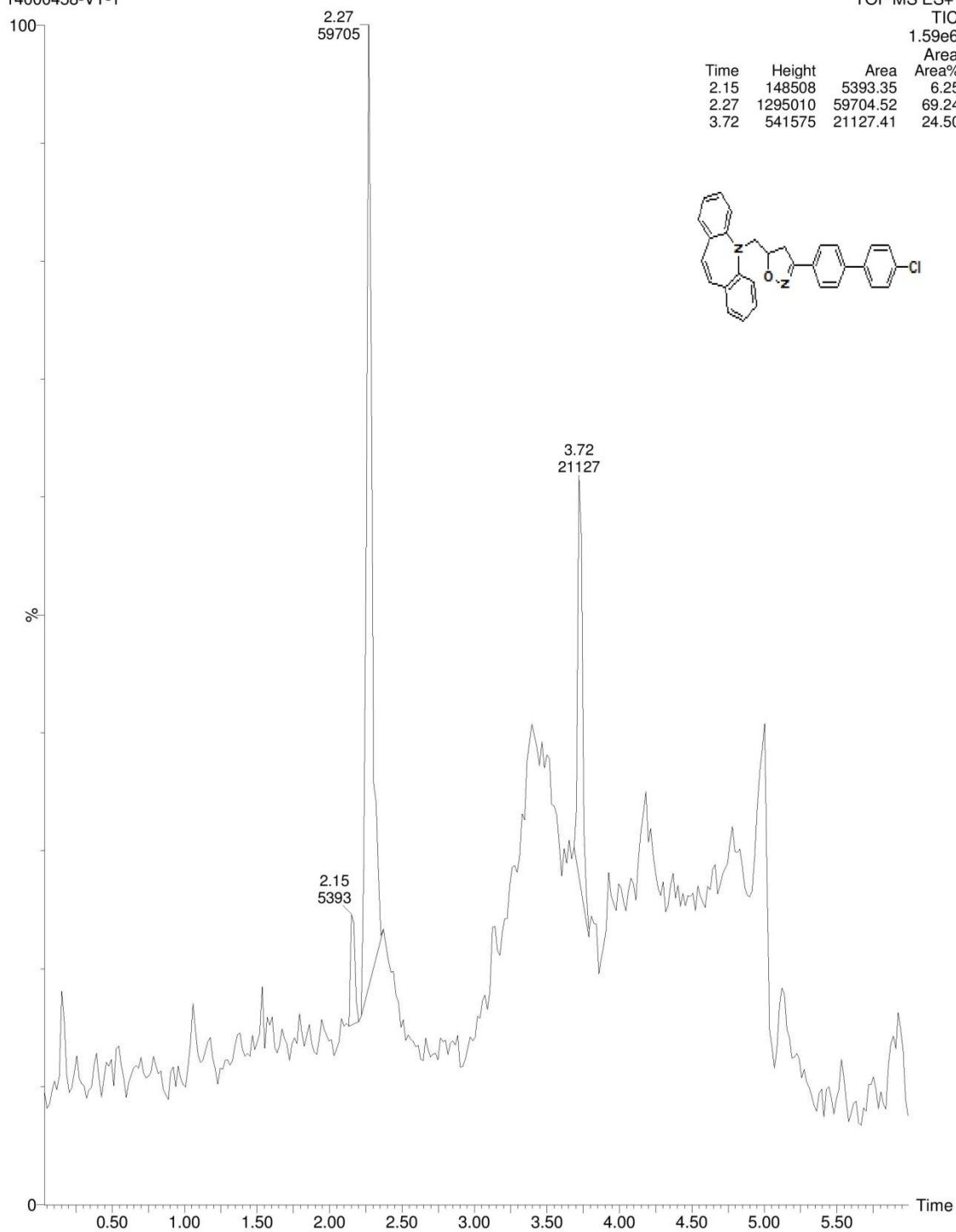
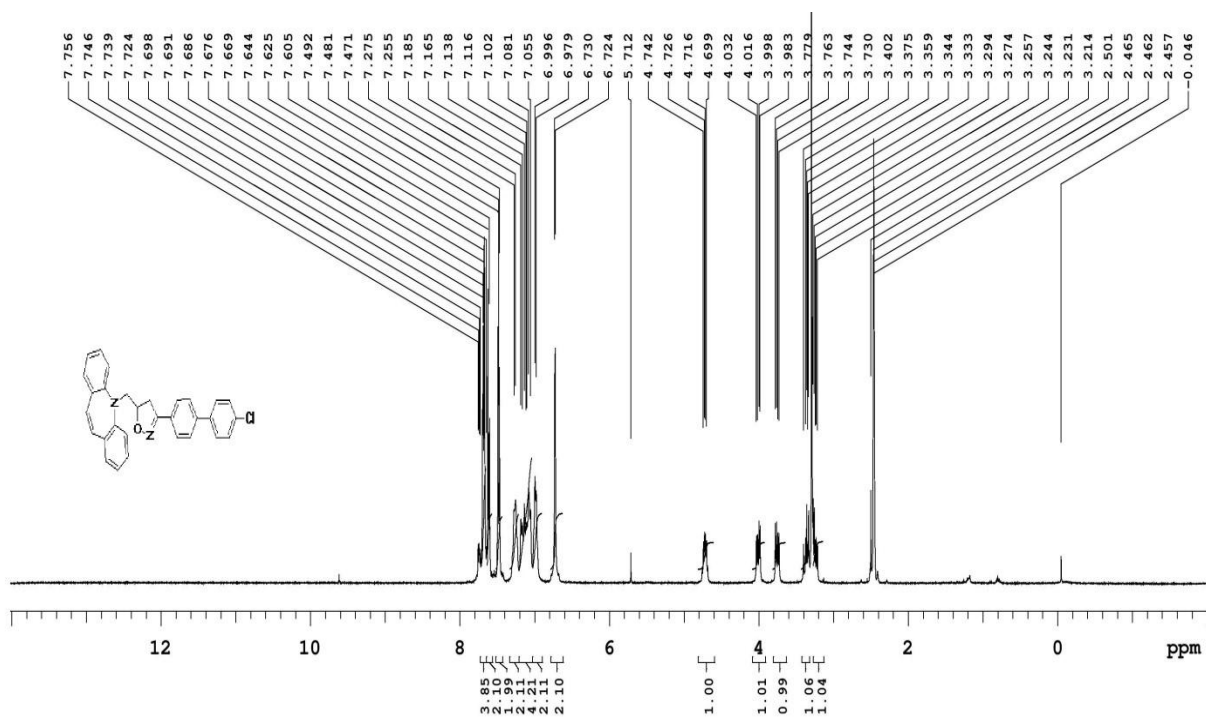
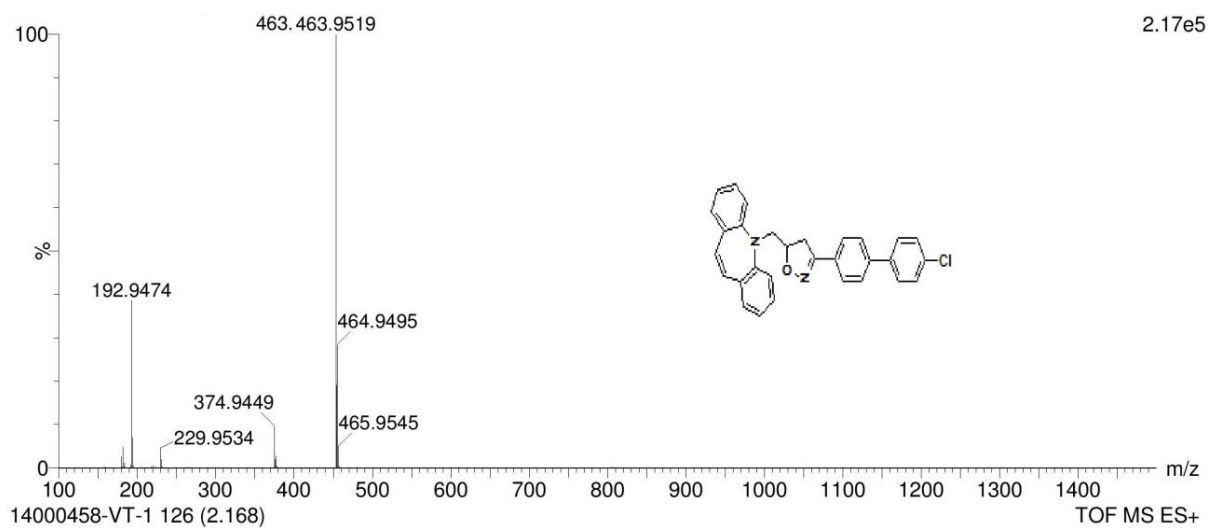


Figure S13 HPLC, Mass, ¹H and ¹³C NMR spectra of compound **6k**

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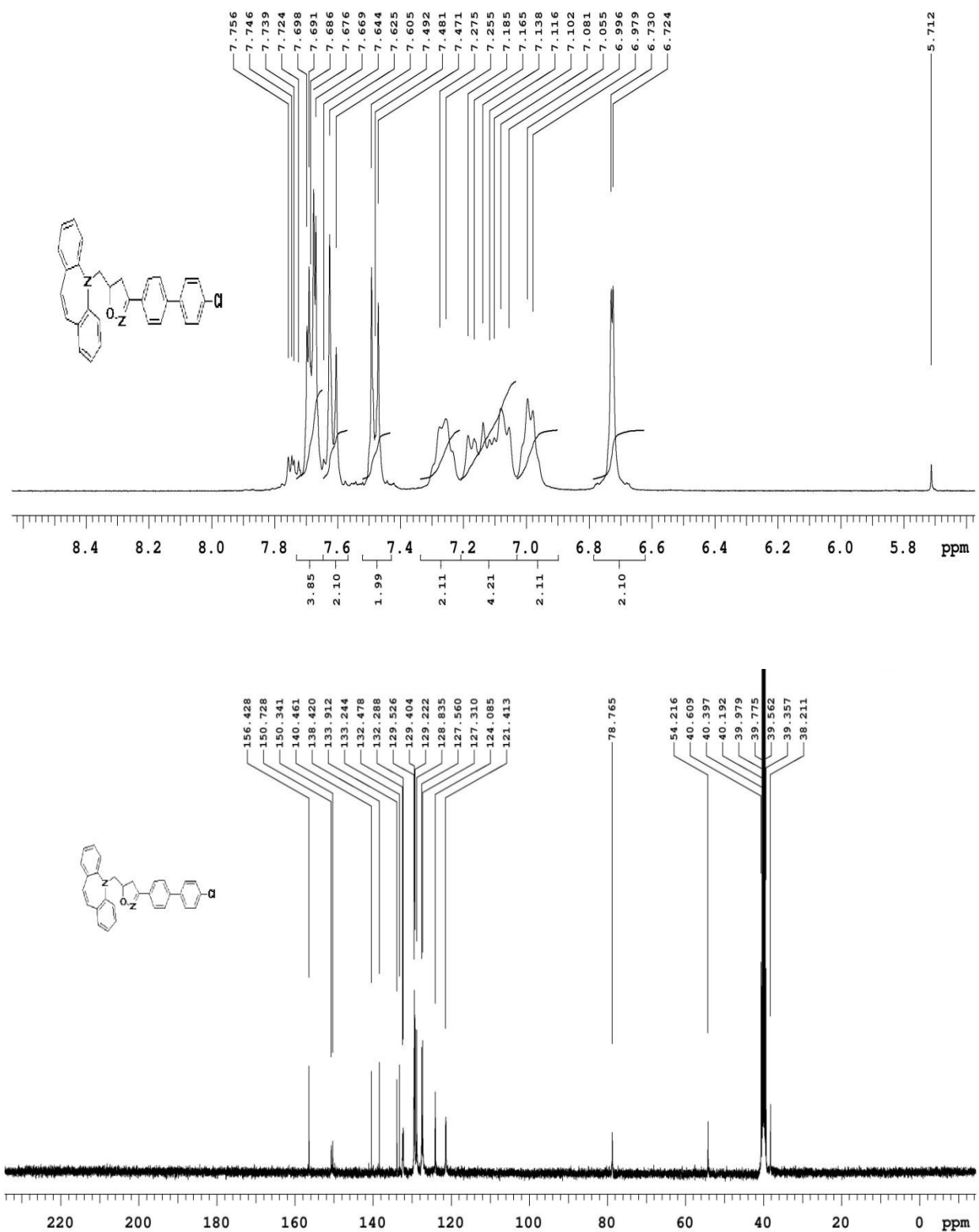
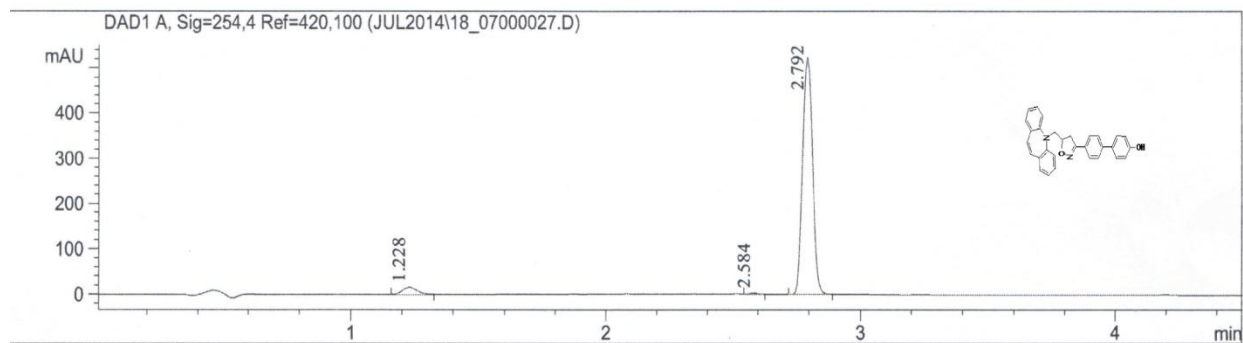
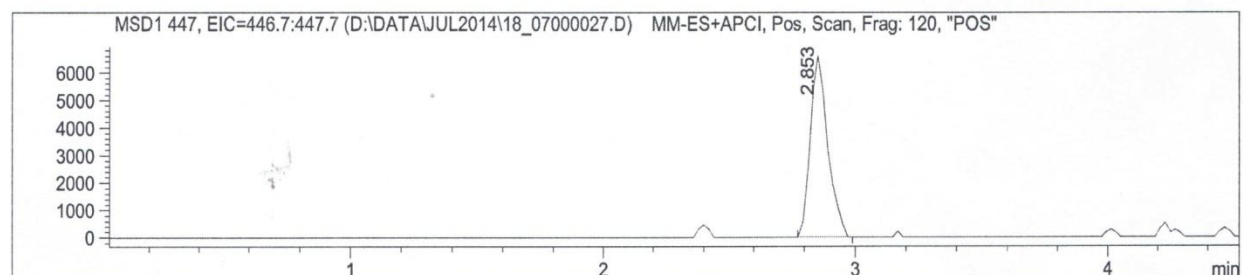
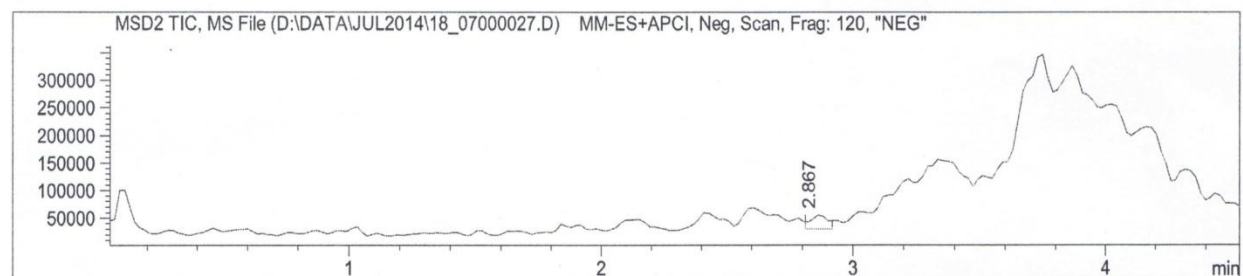
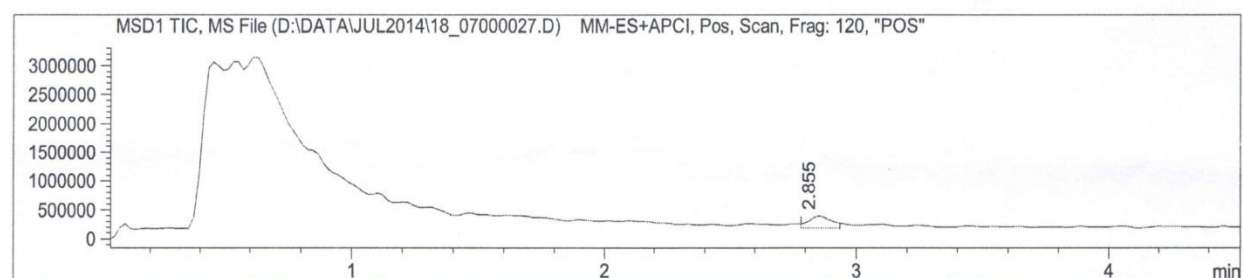
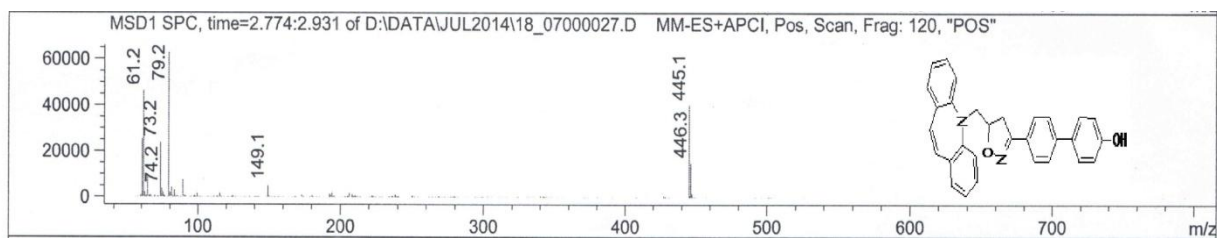


Figure S14 Mass, ¹H and ¹³C NMR spectra of compound 8a



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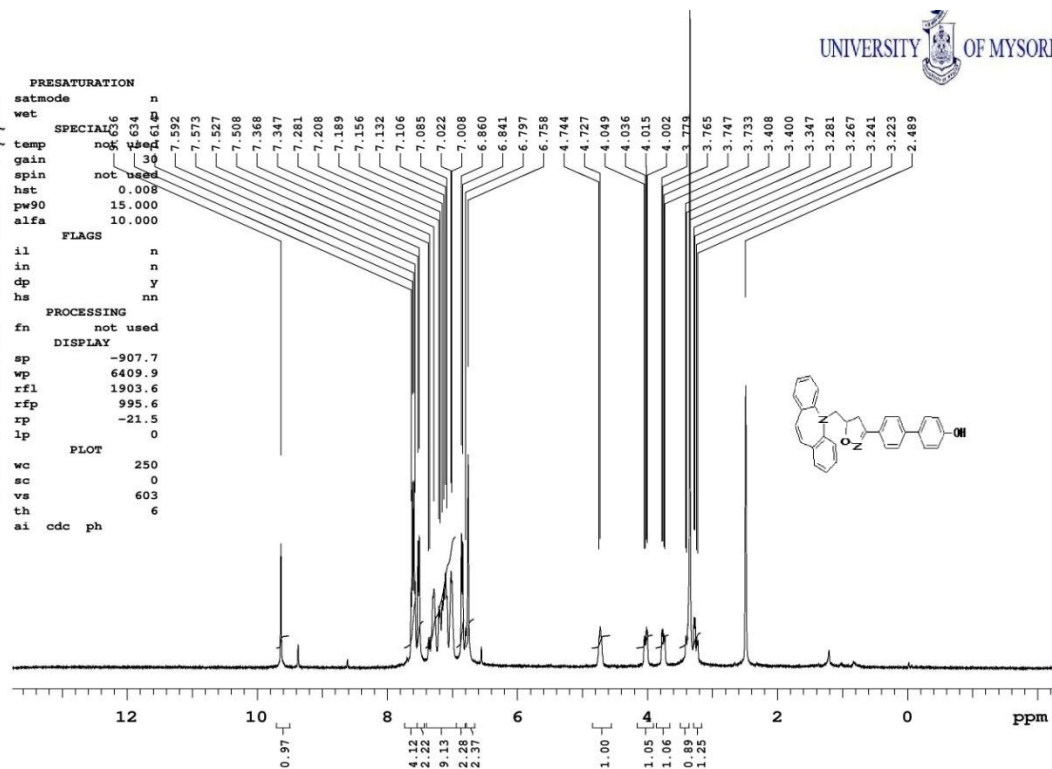


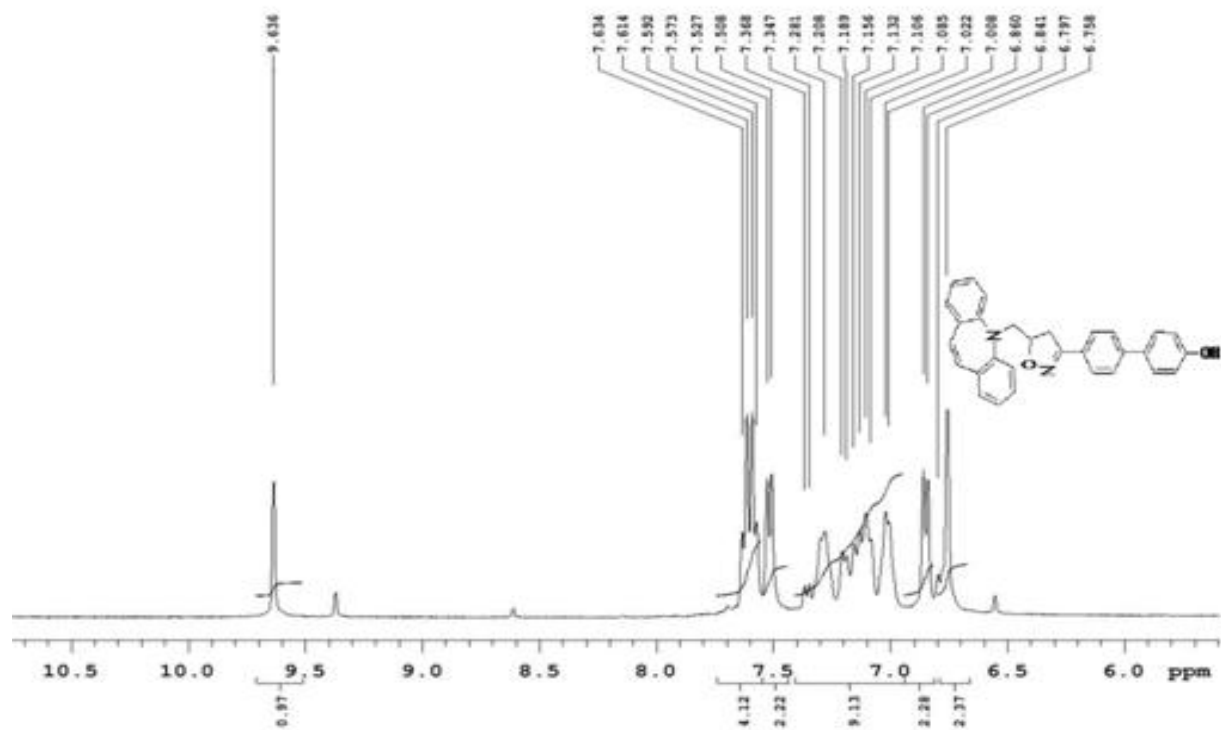
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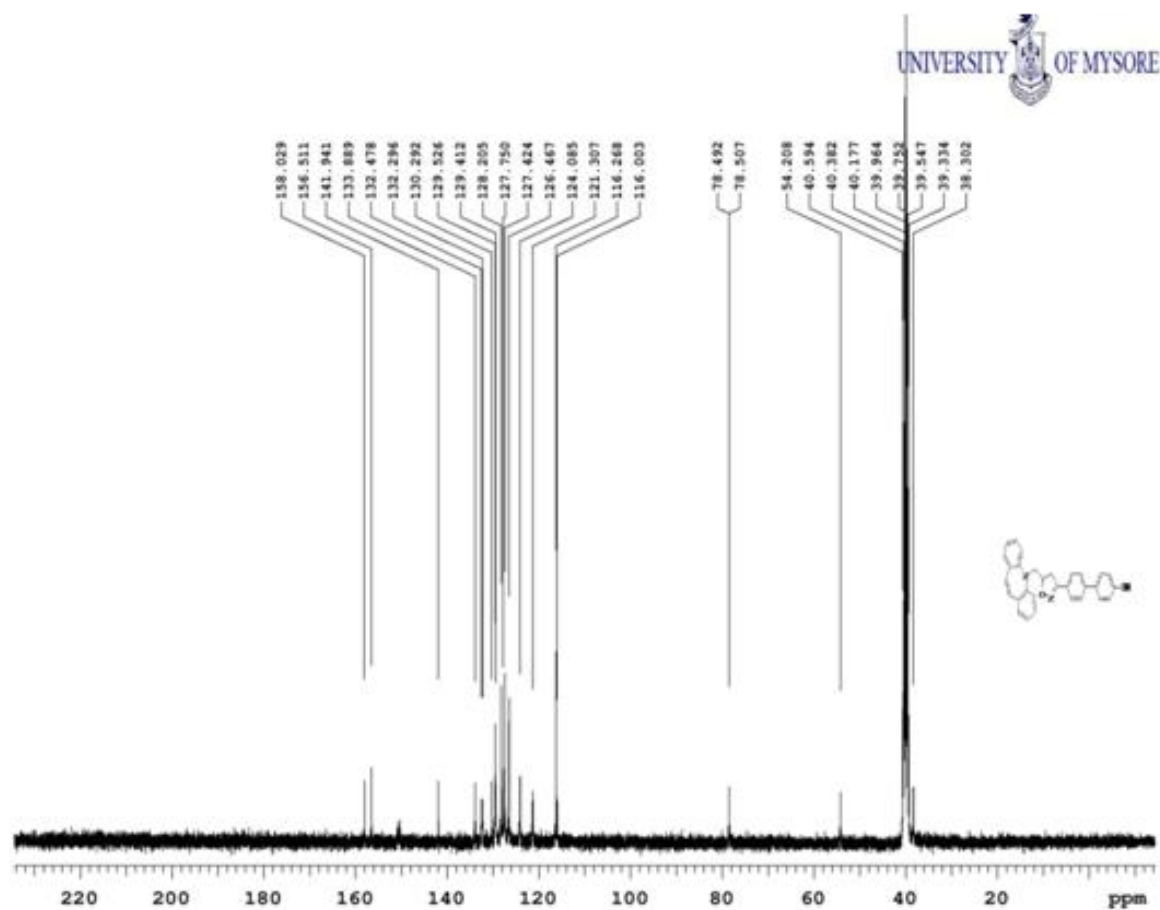
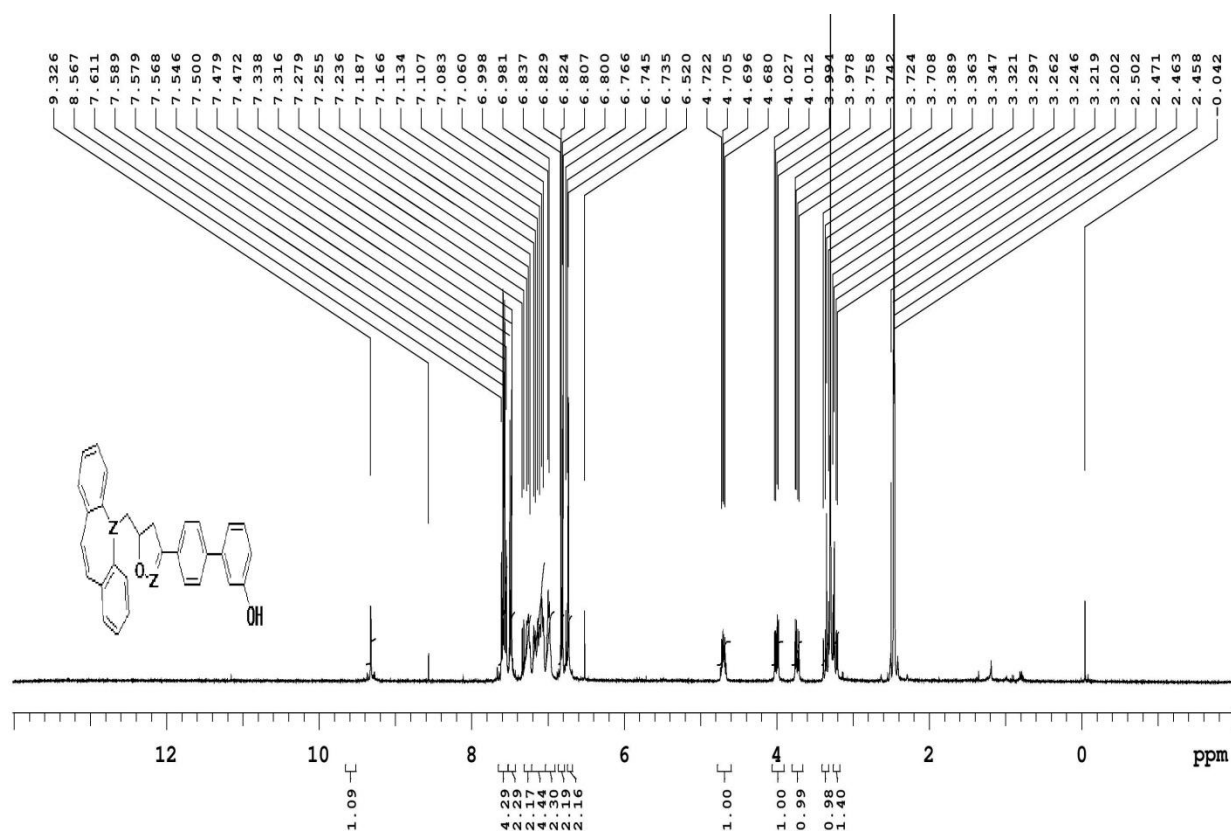
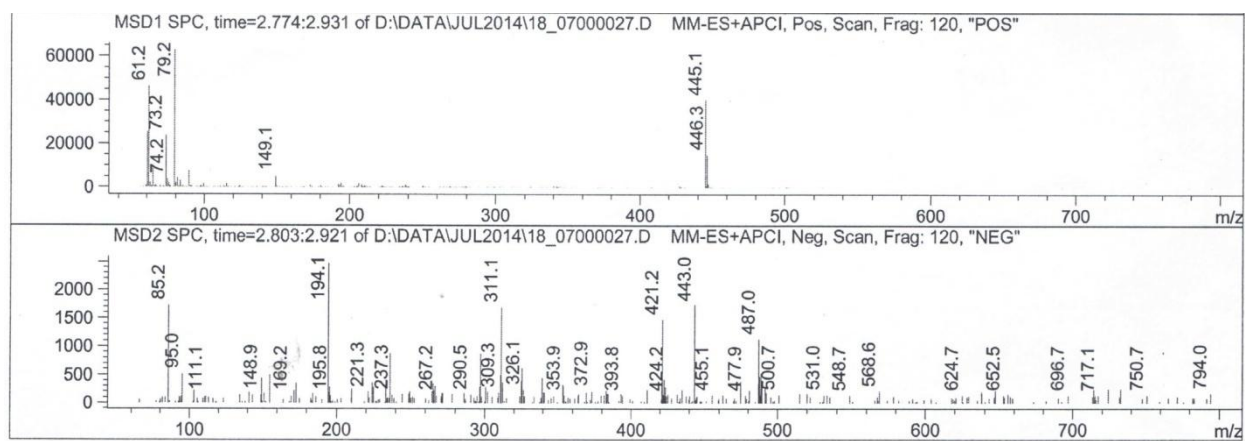


Figure S15 Mass, ¹H and ¹³C NMR spectra of compound **8b**



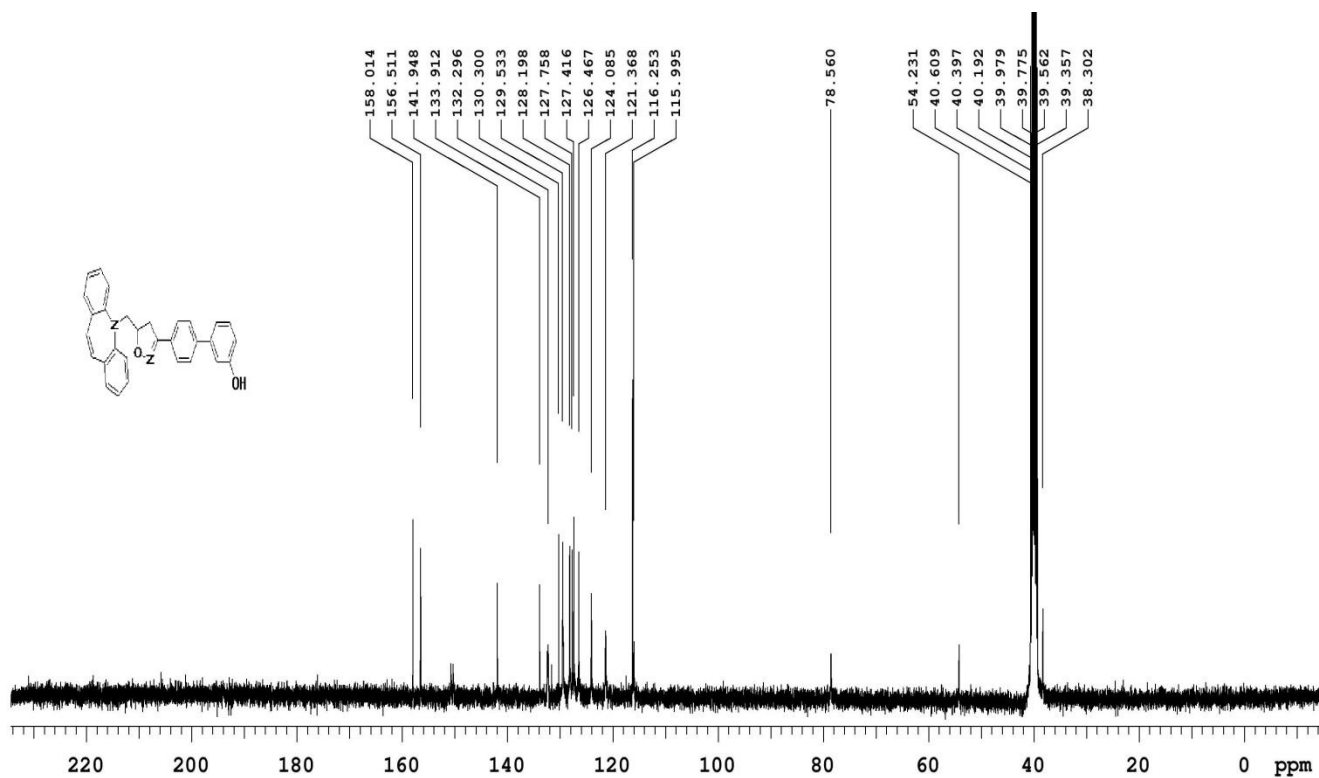
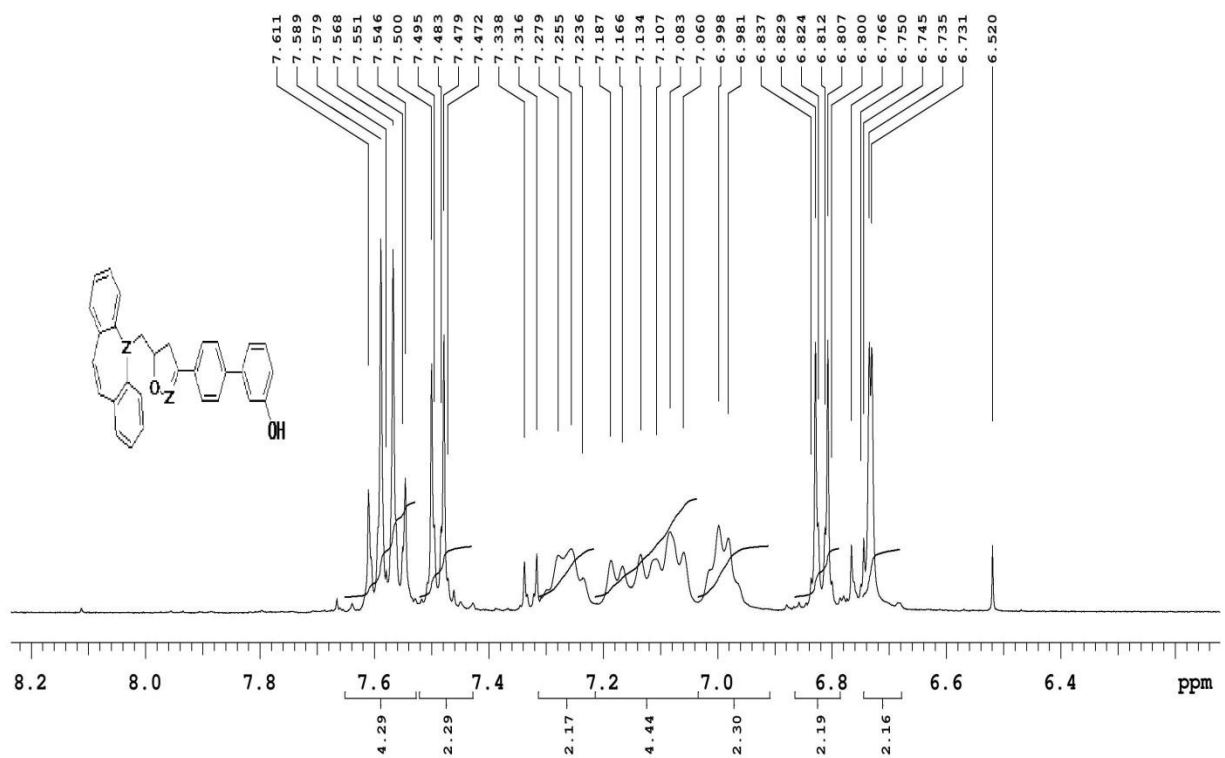
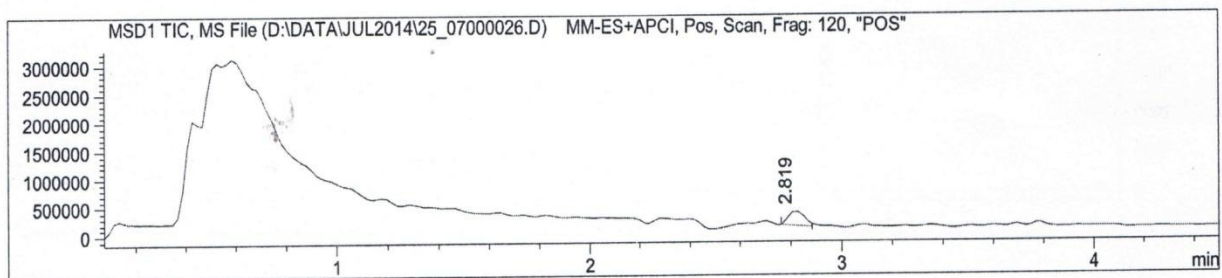
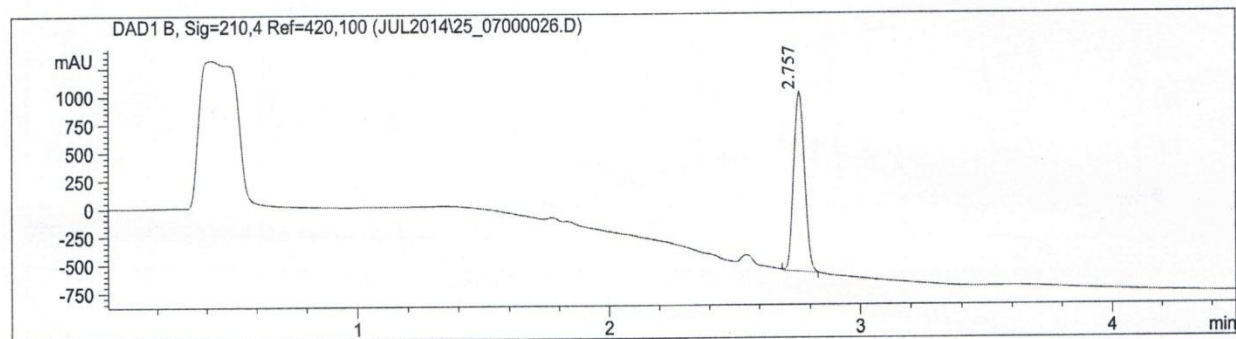
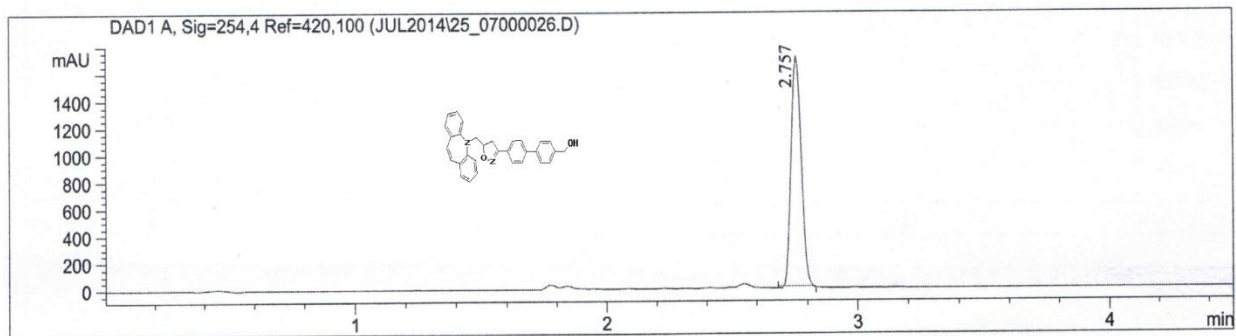
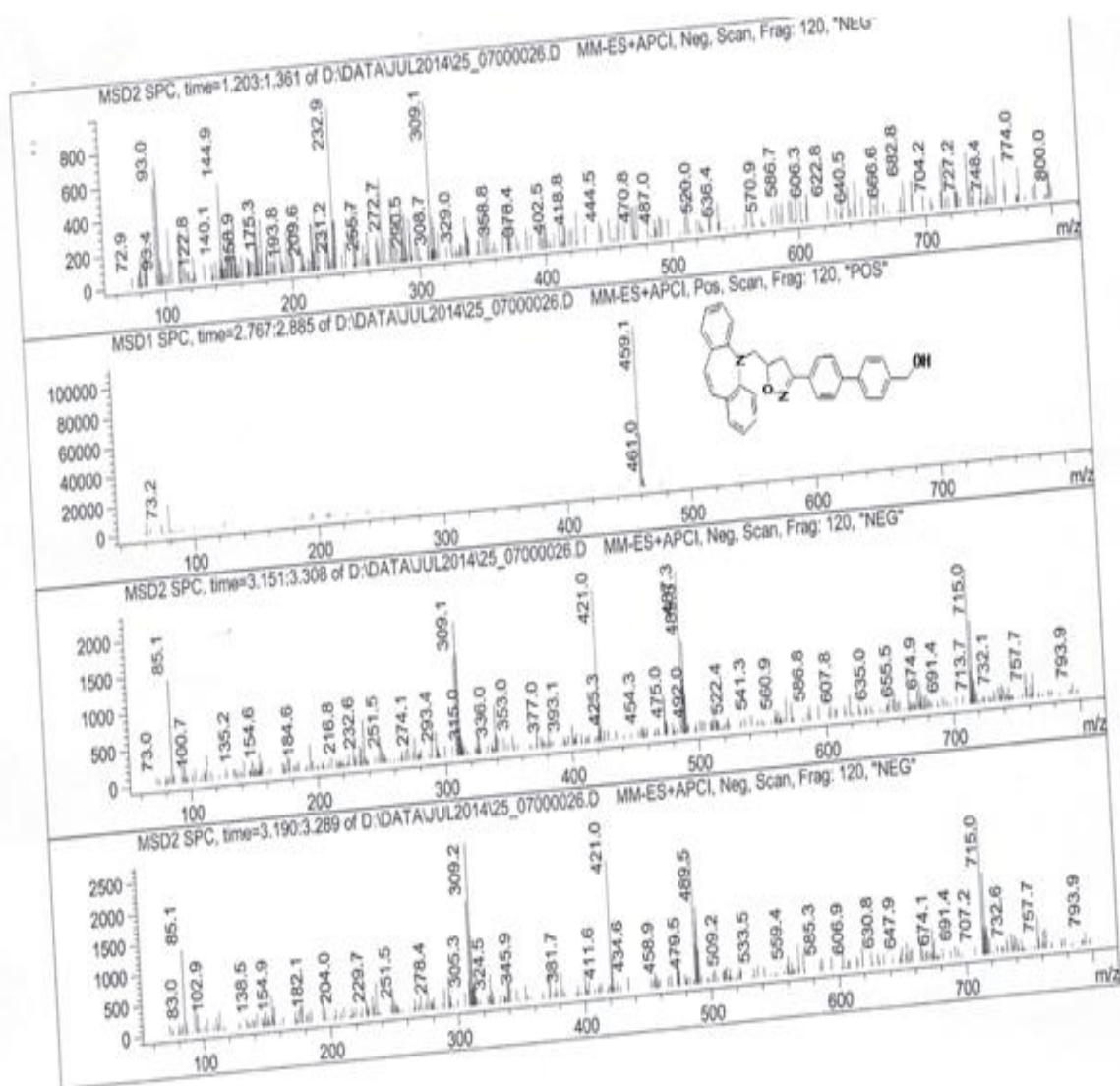
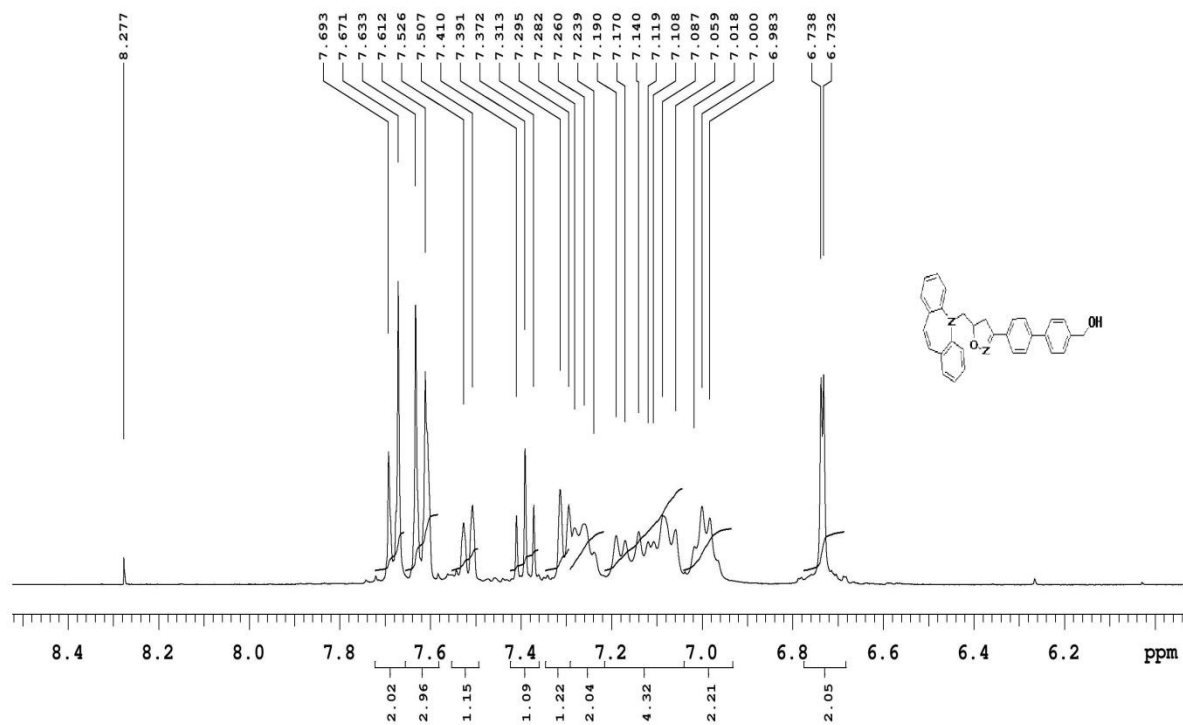
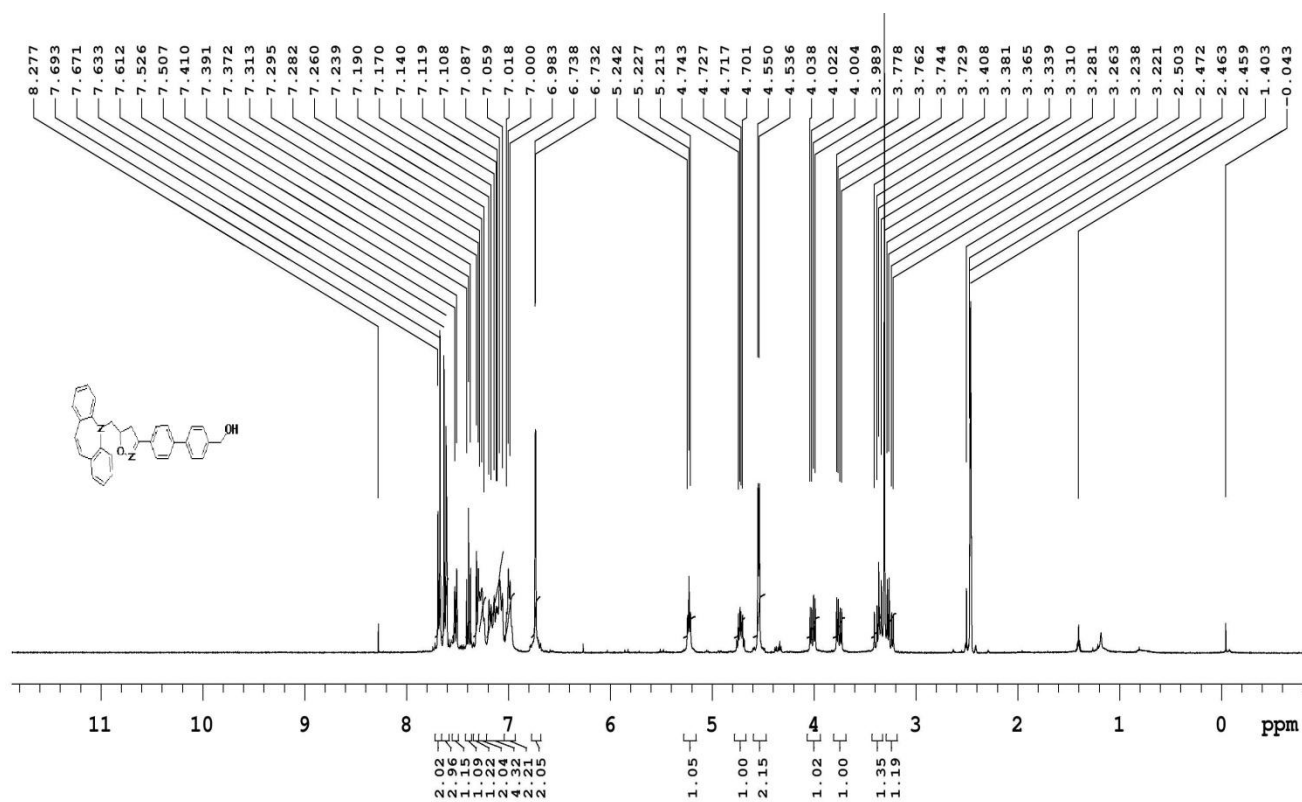


Figure S16 Mass, ¹H and ¹³C NMR spectra of compound **8c**







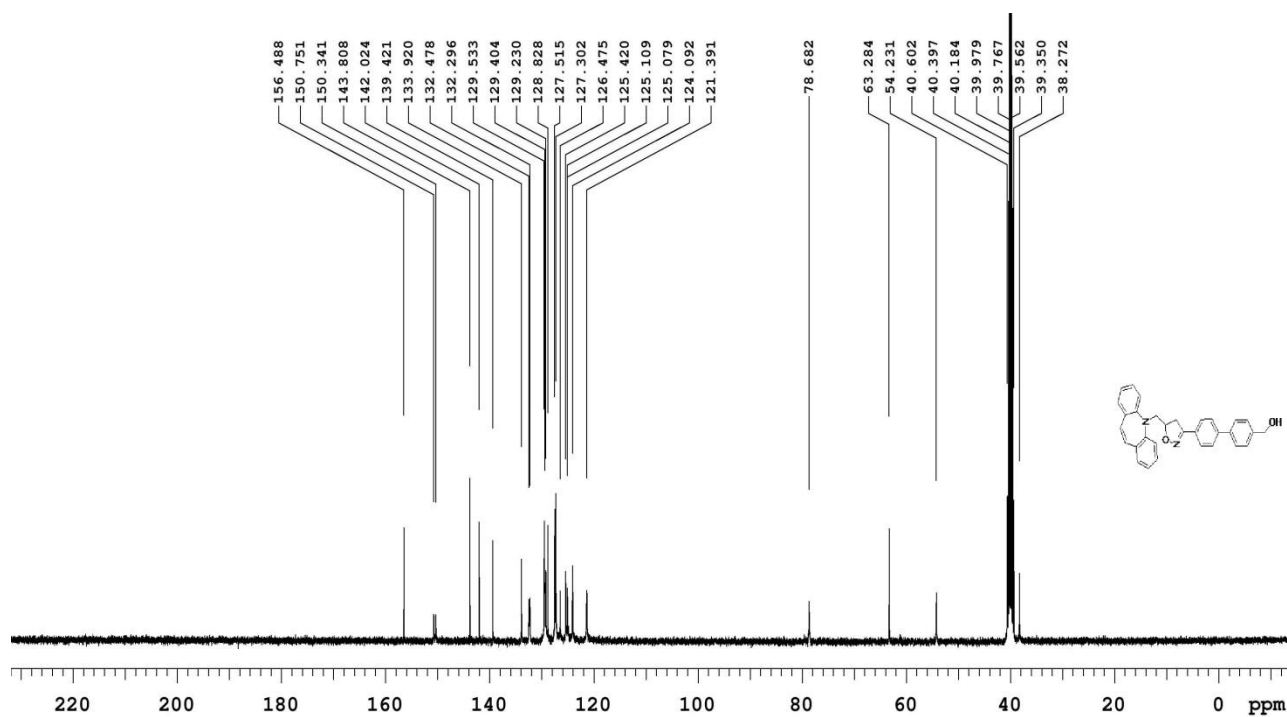
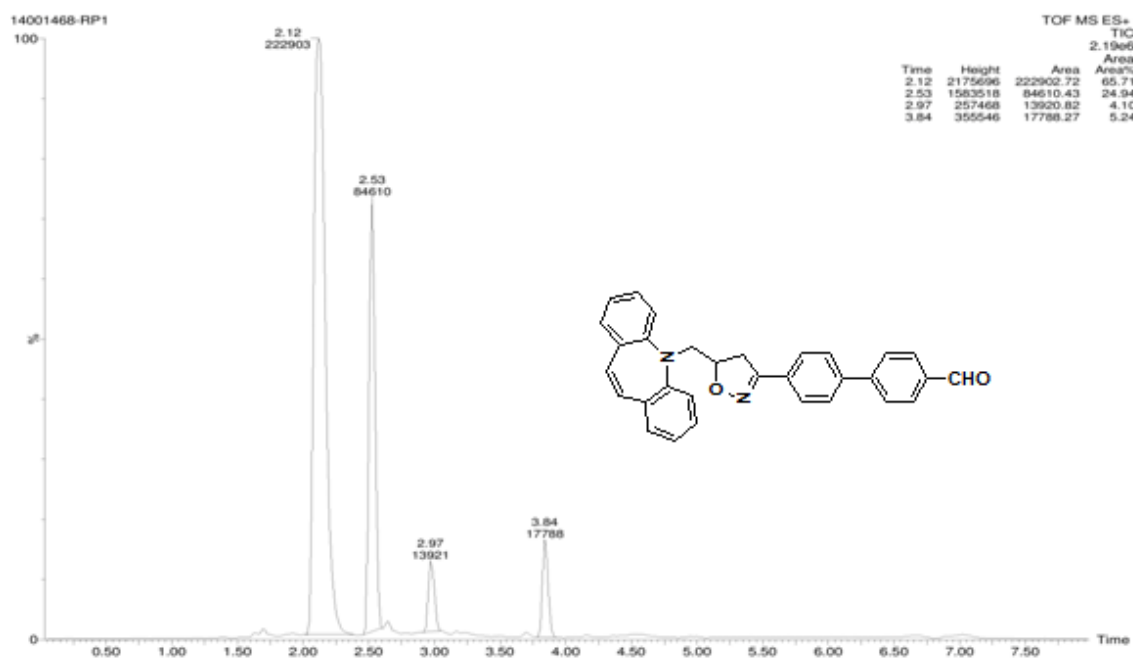
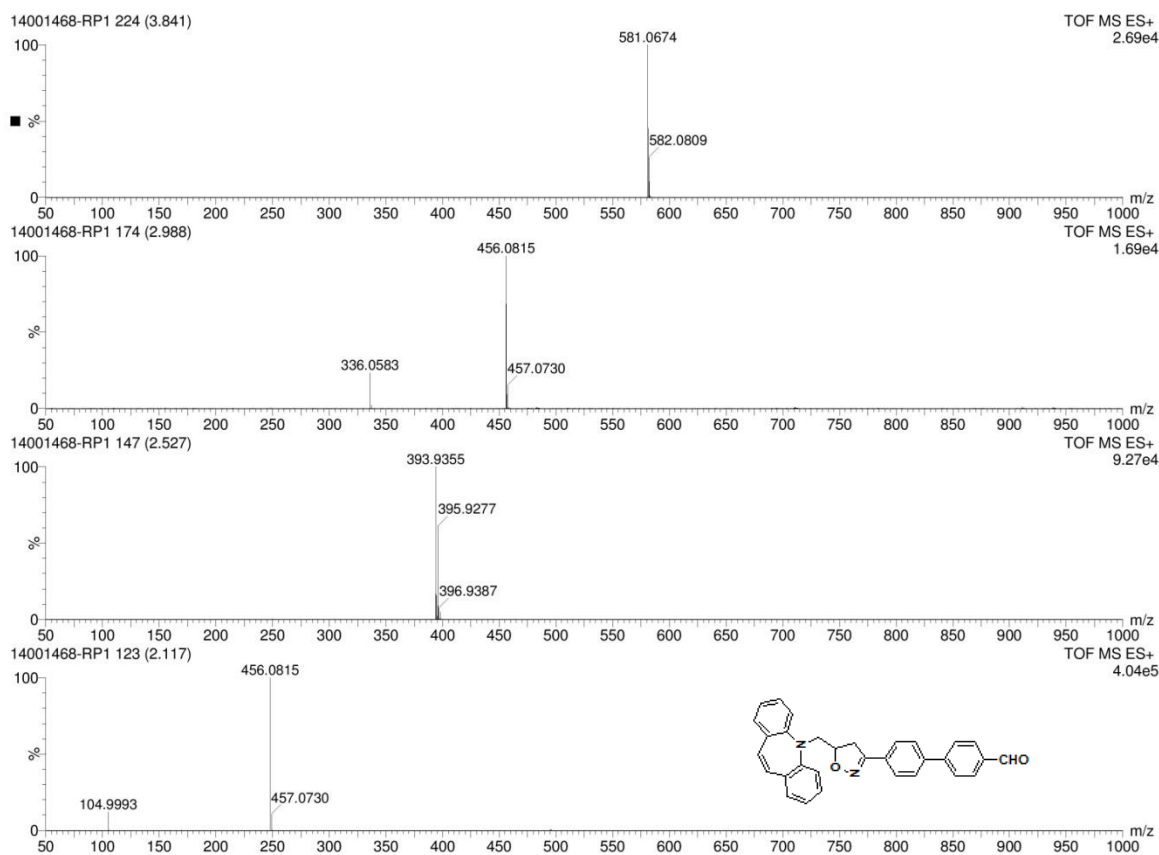


Figure S17 Mass, ¹H and ¹³C NMR spectra of compound **8d**







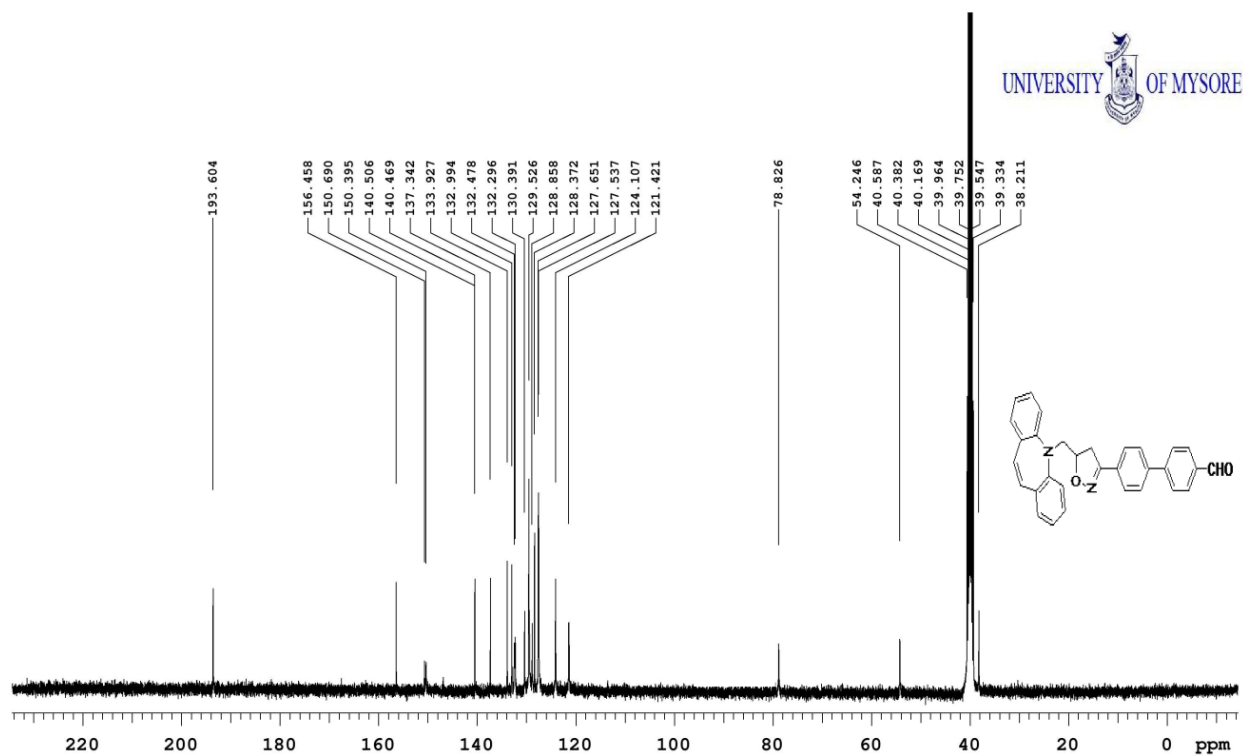
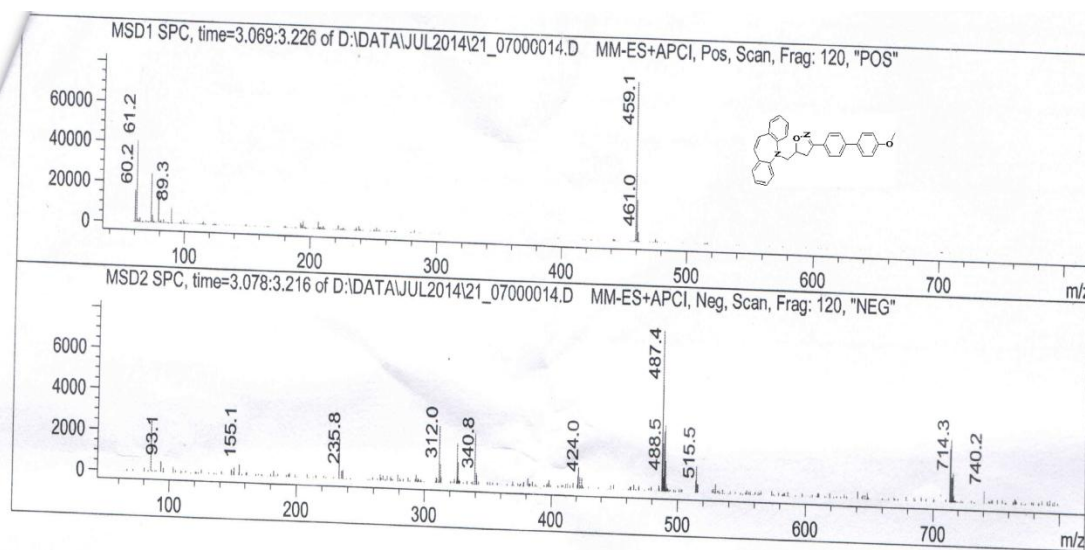
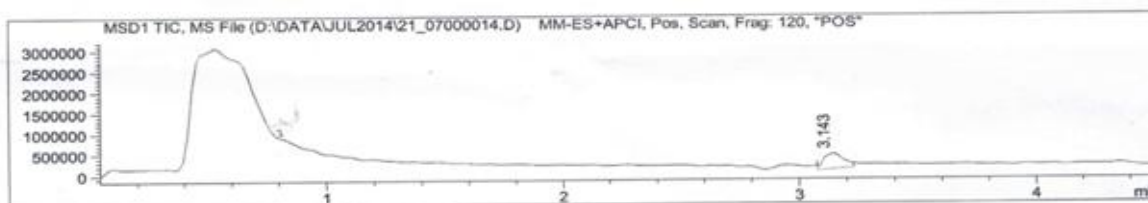
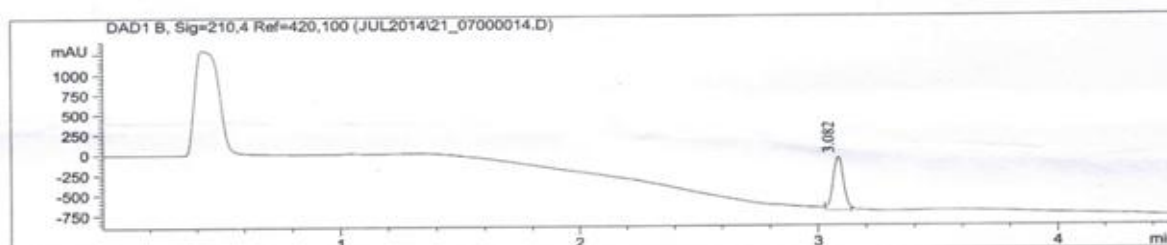
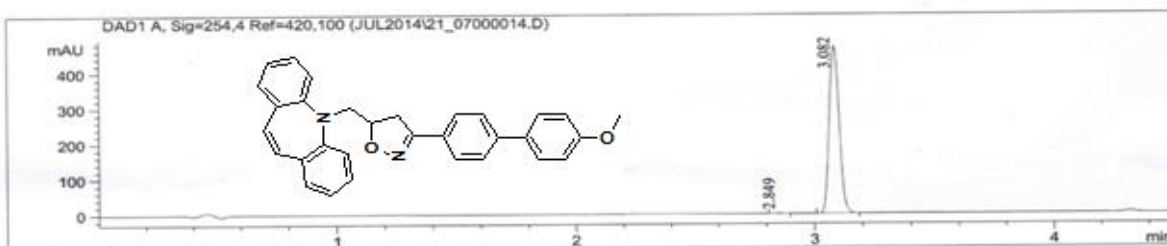
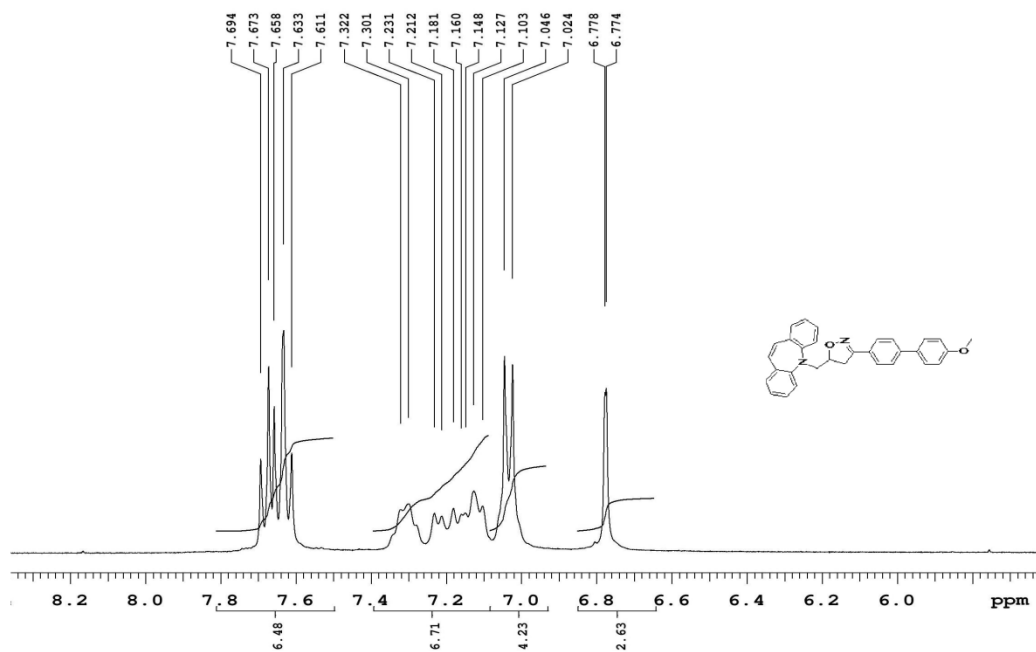
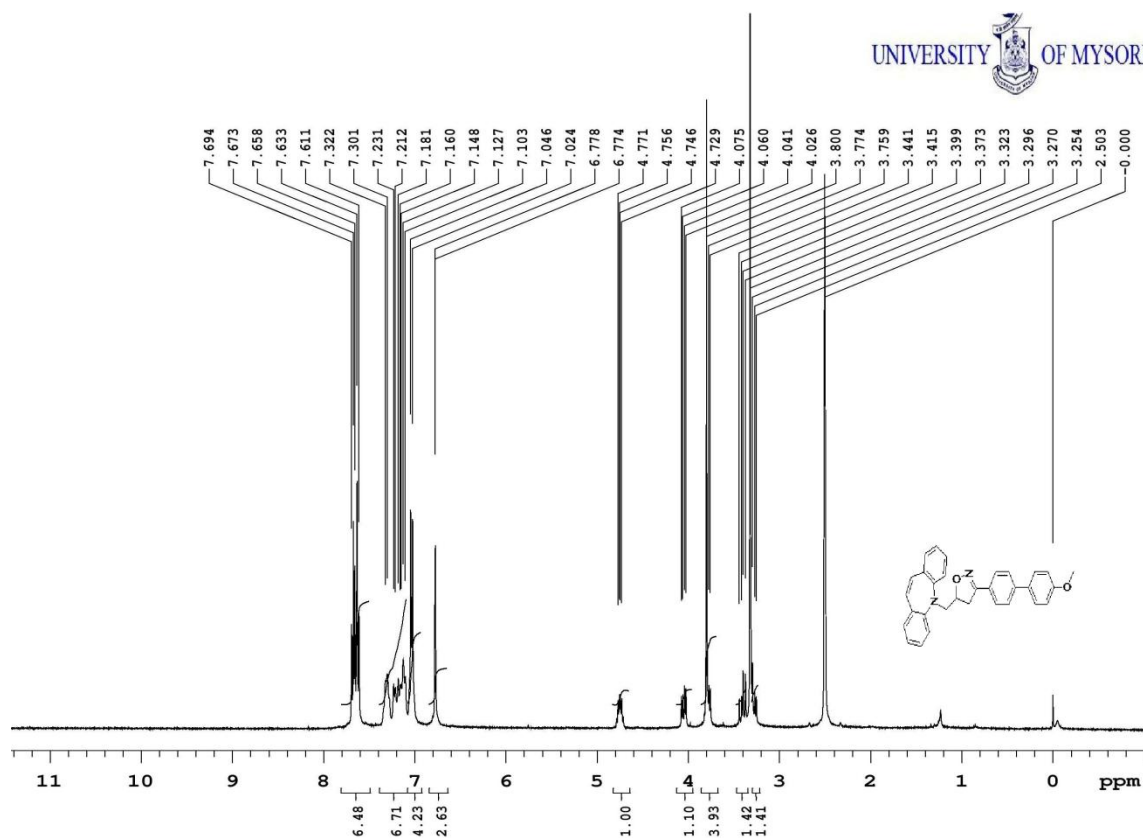


Figure S18 Mass, ¹H and ¹³C NMR spectra of compound **8e**





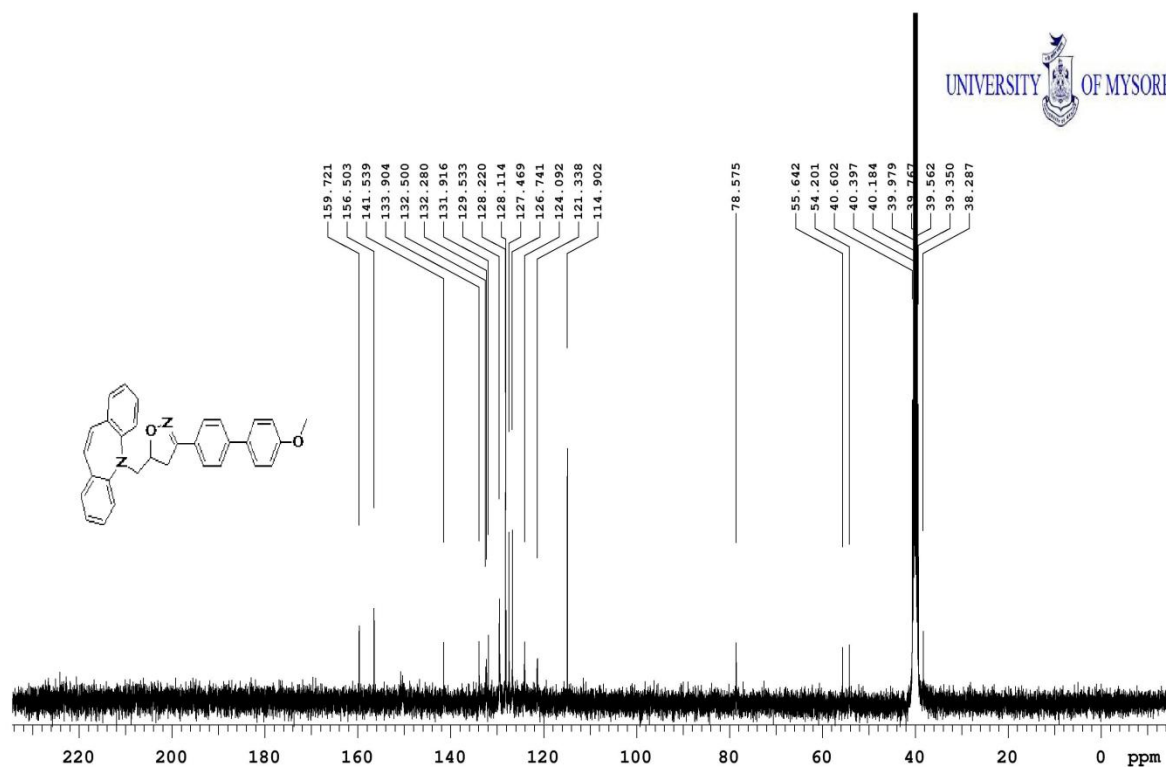
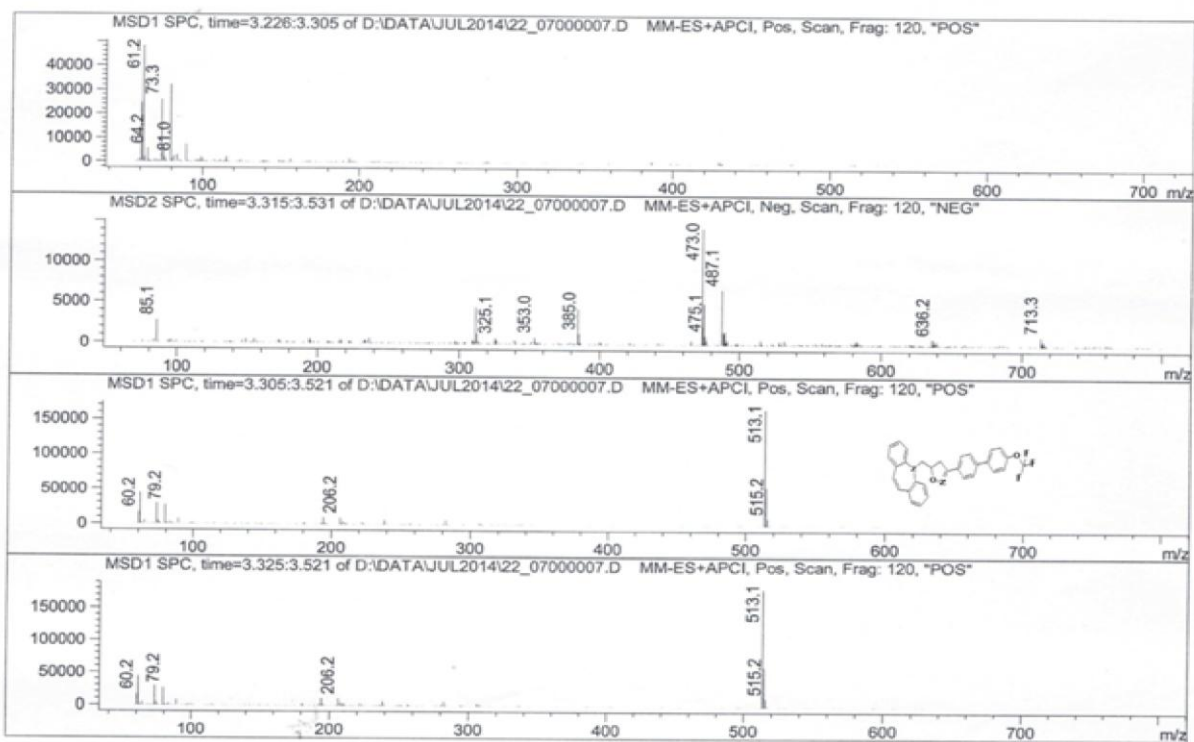
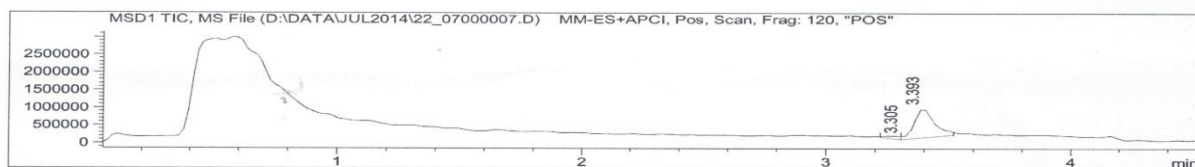
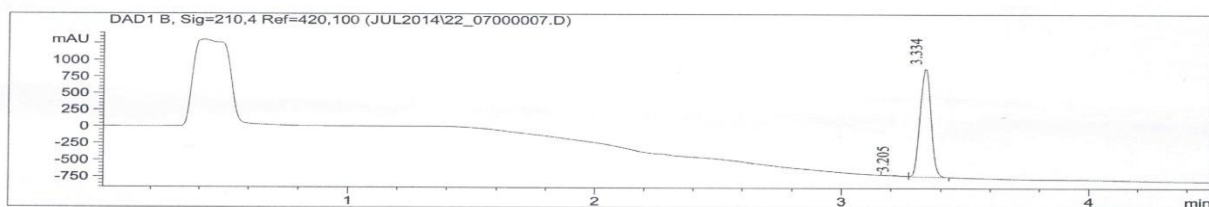
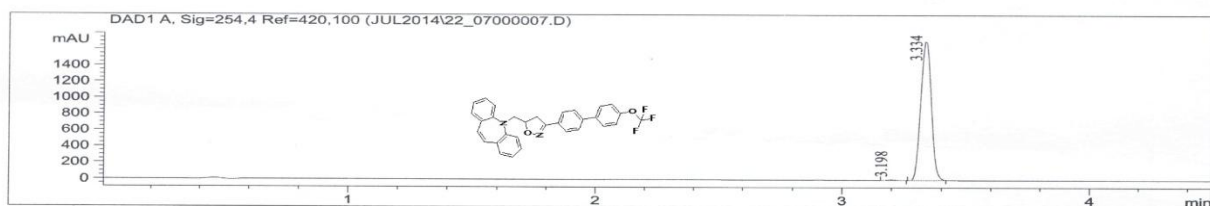
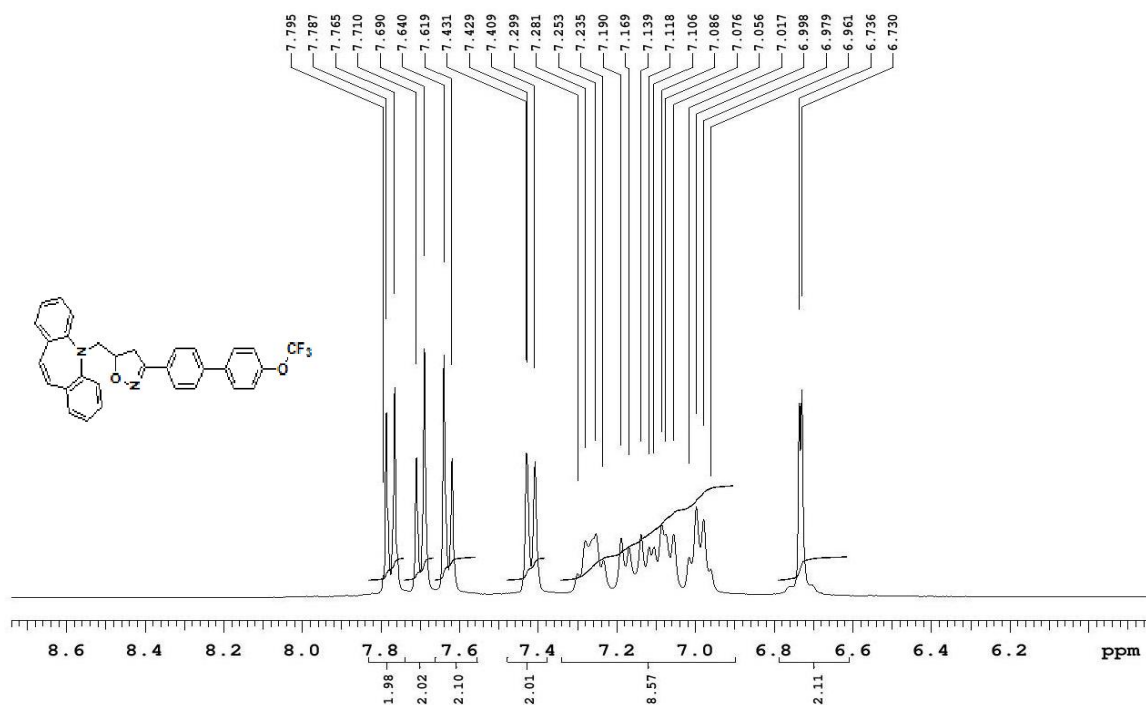
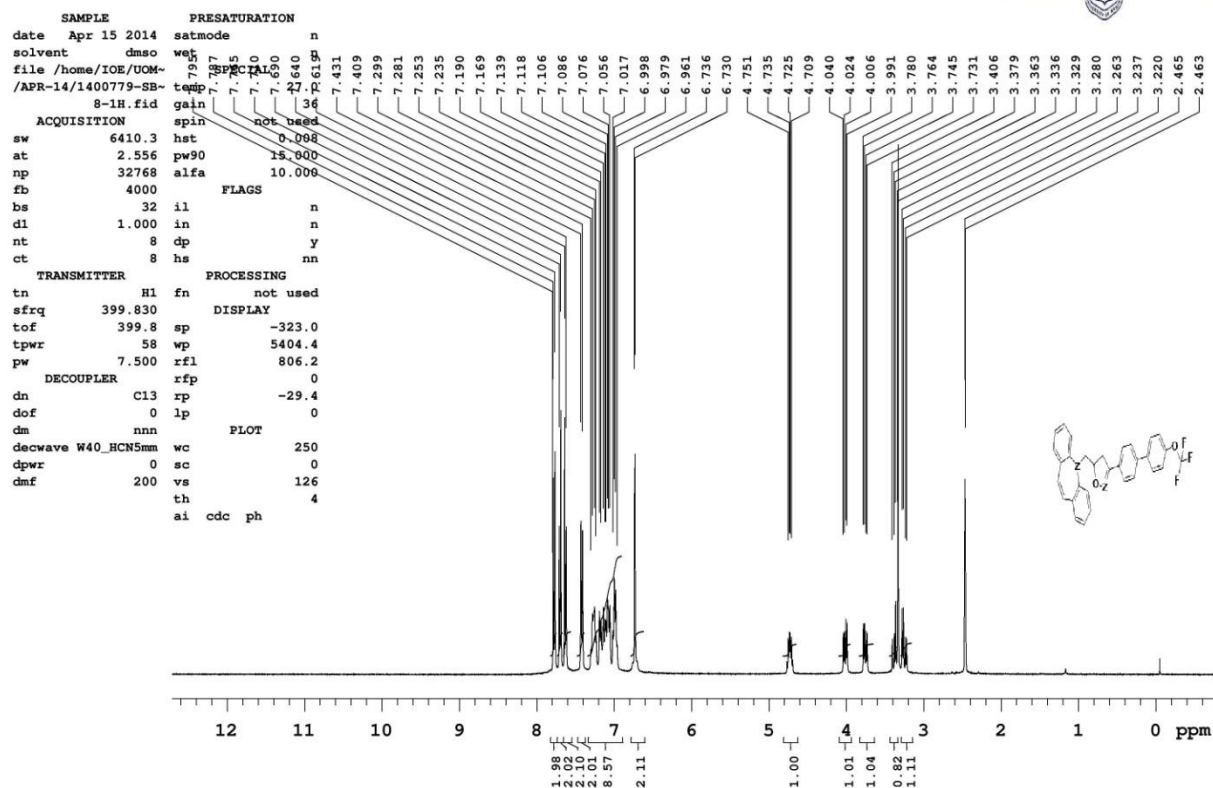


Figure S19 Mass, ^1H and ^{13}C NMR spectra of compound **8f**



1400779-SBS-1H

expl1 PROTON



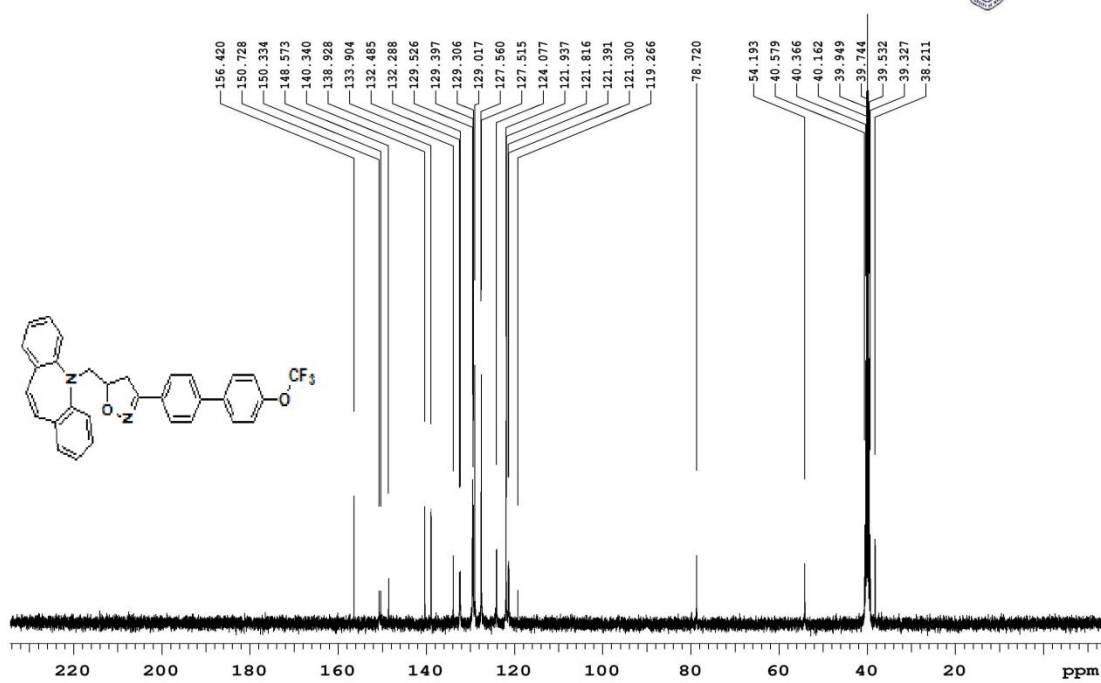
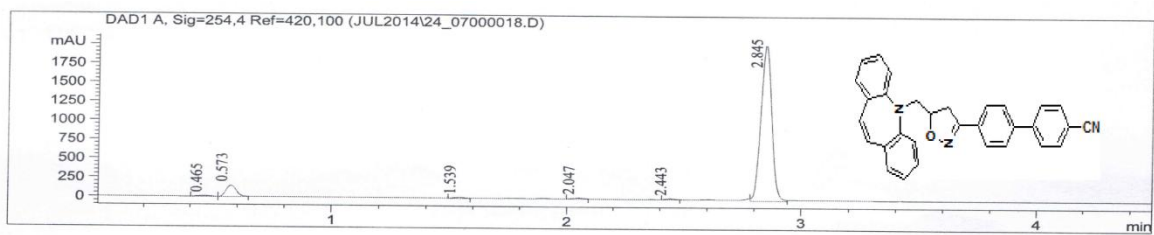
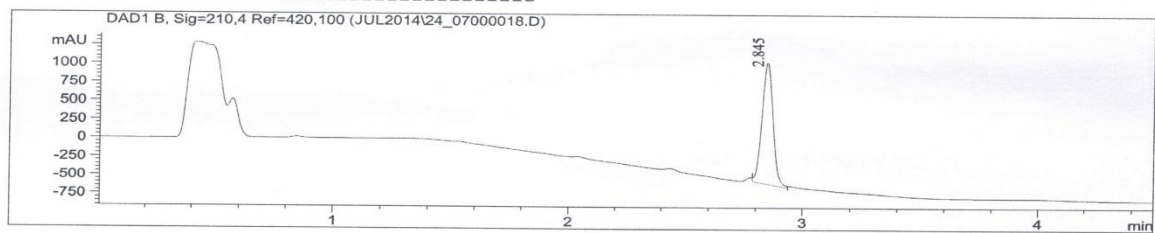


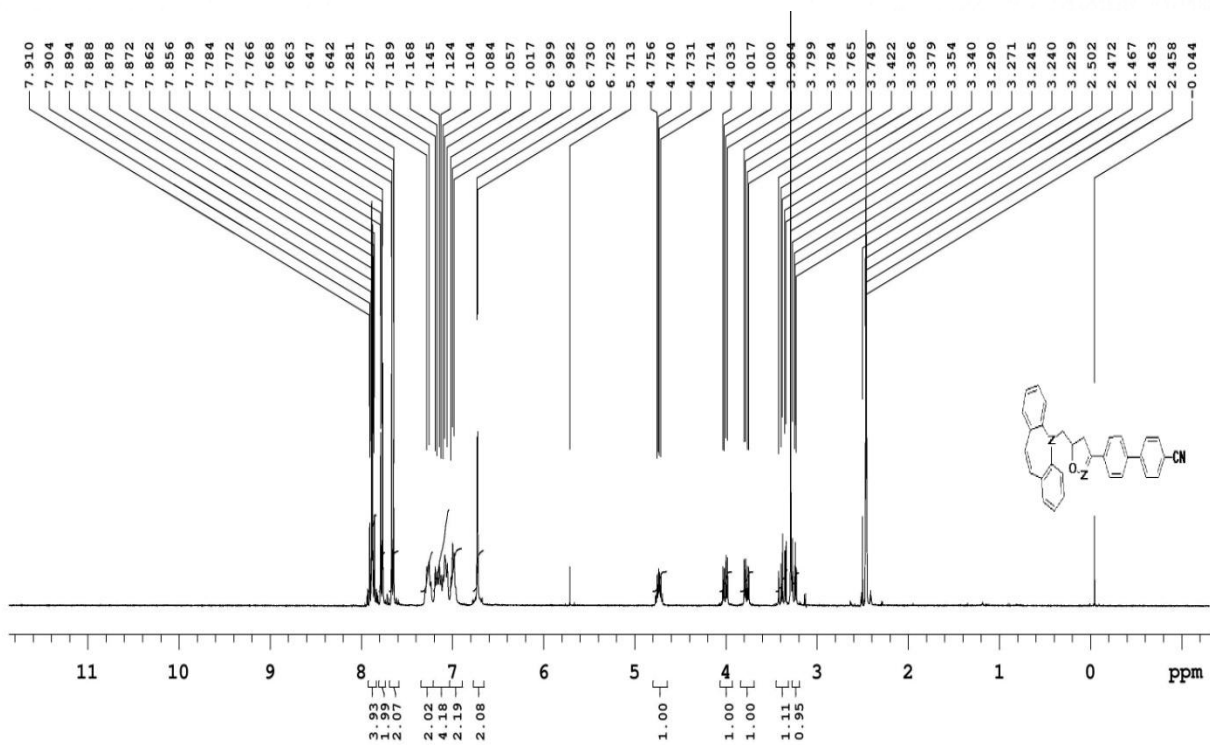
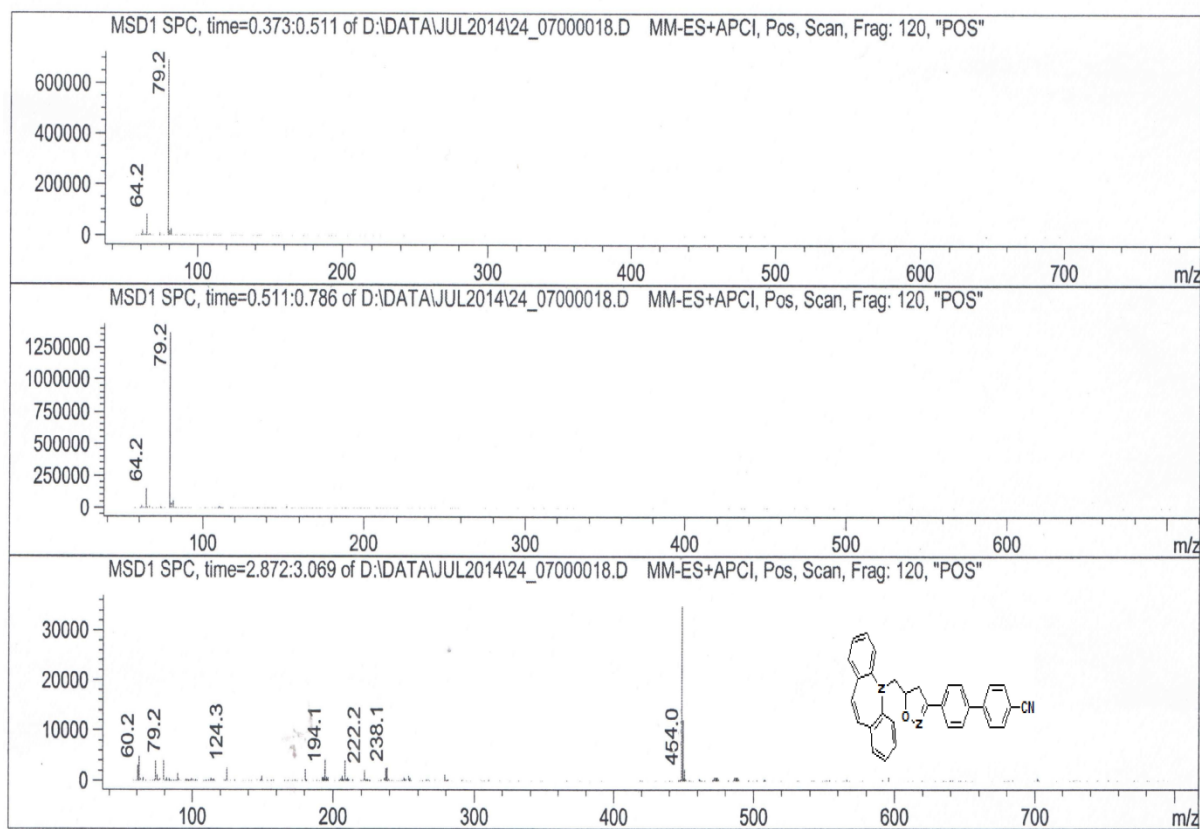
Figure S20 Mass, ¹H and ¹³C NMR spectra of compound **8g**

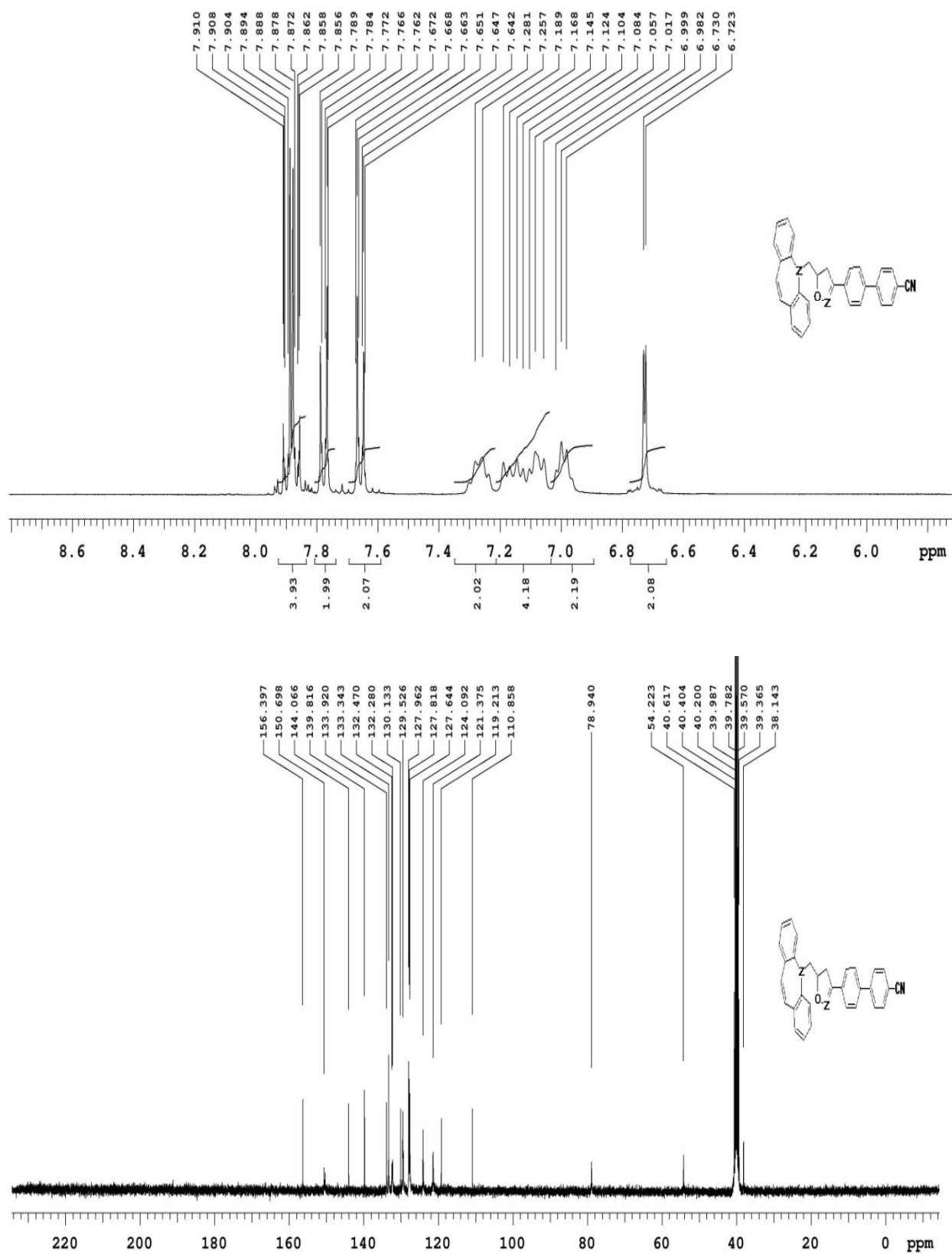


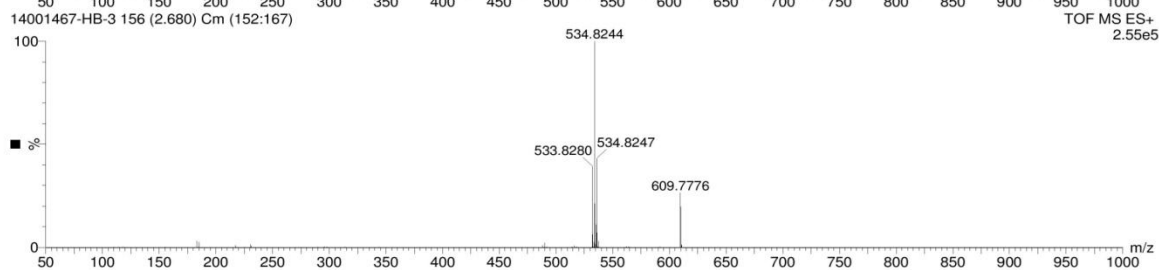
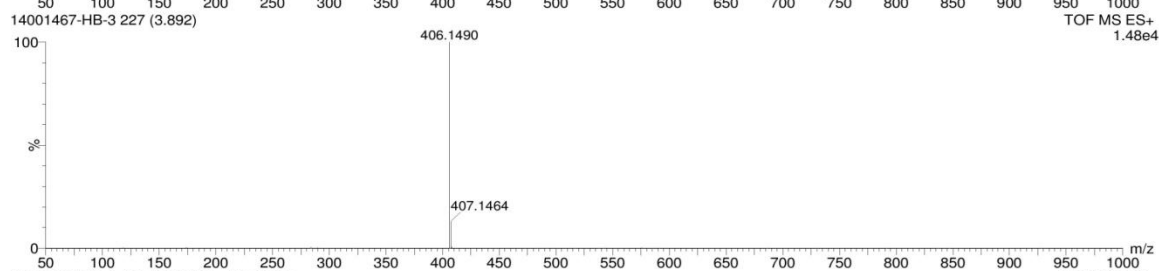
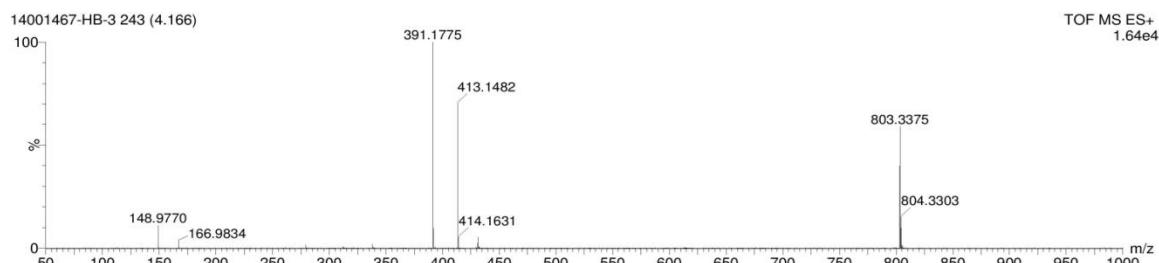
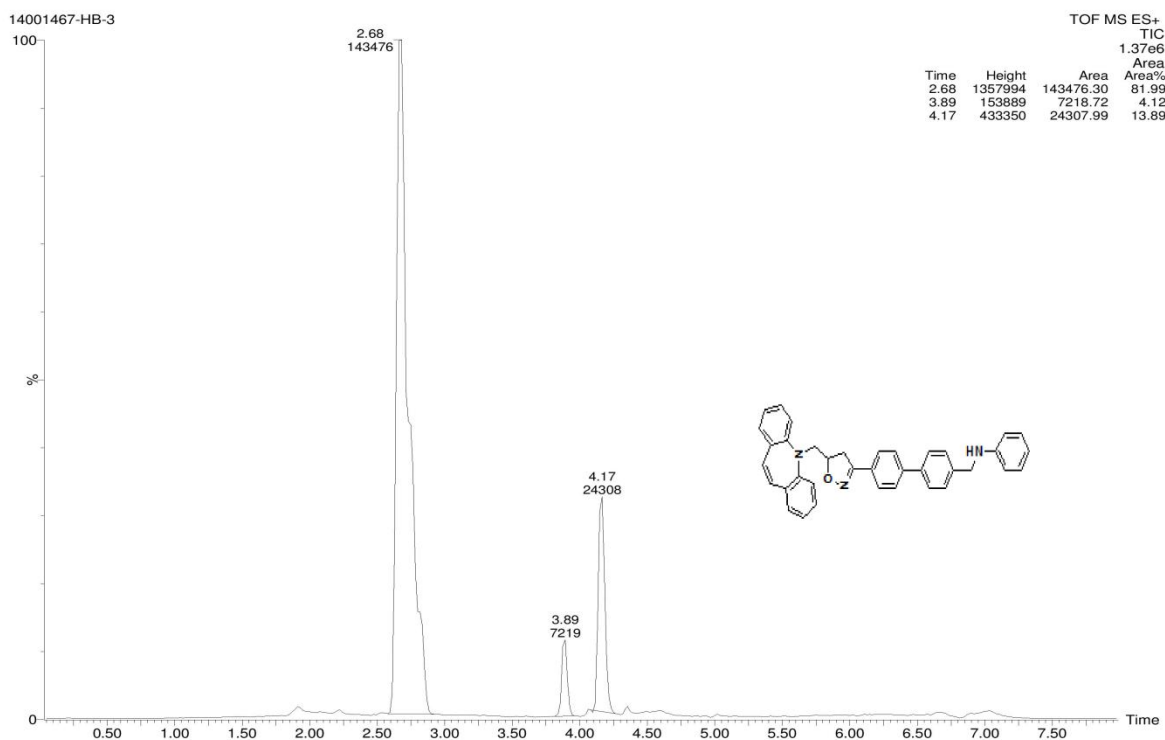
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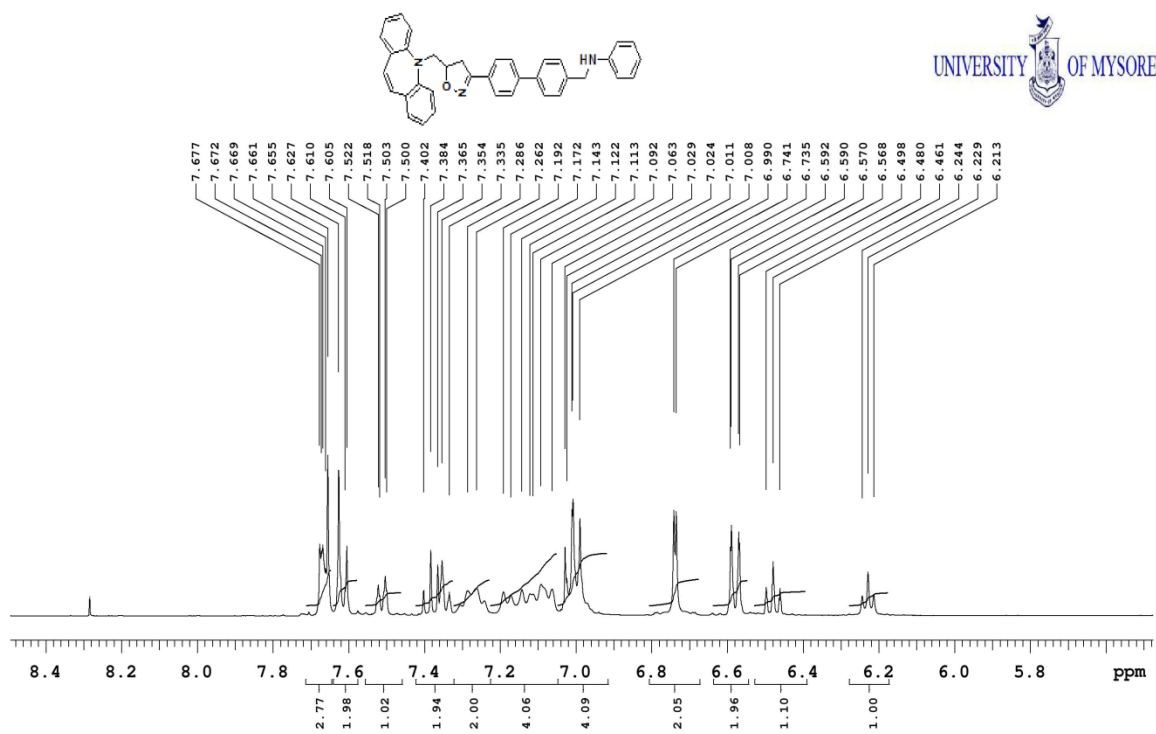
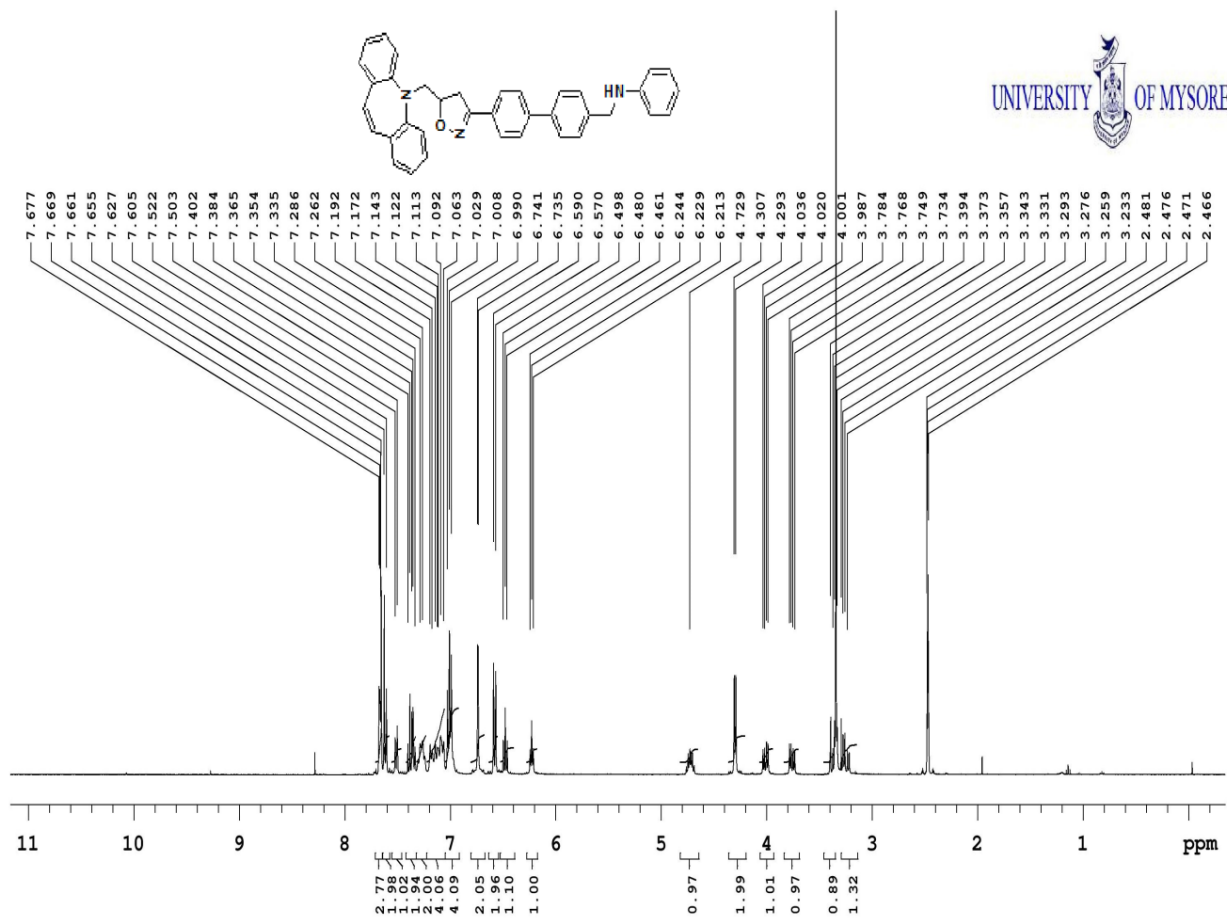


Peak No	RT min	Area	Area %
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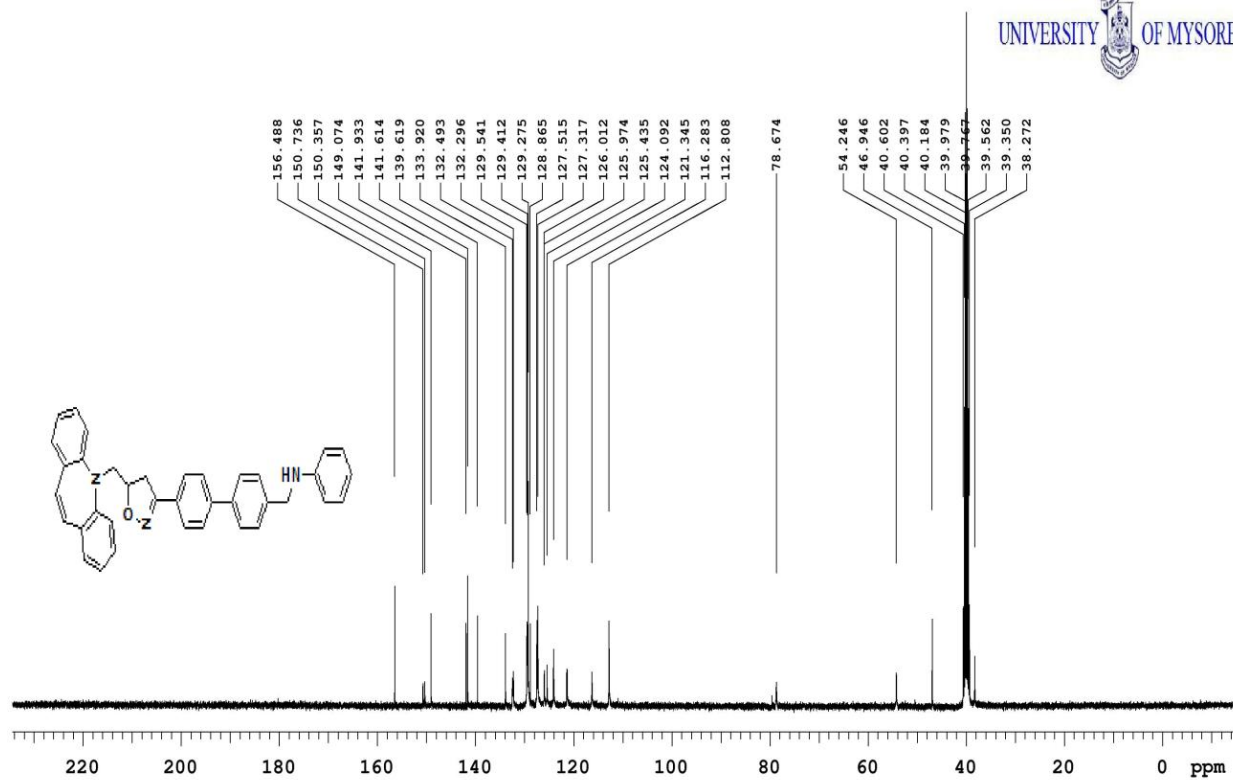
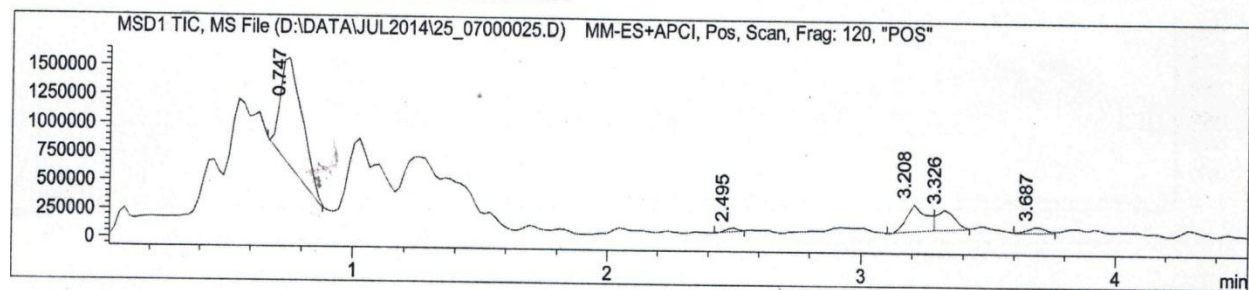
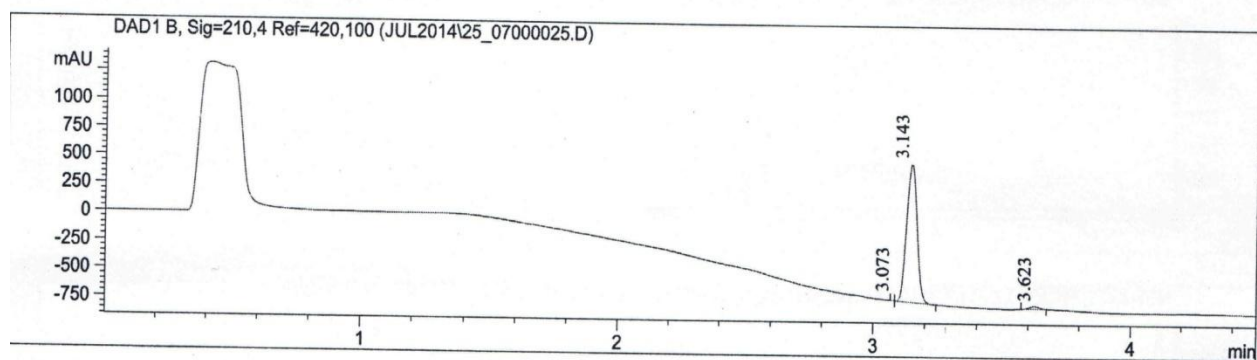
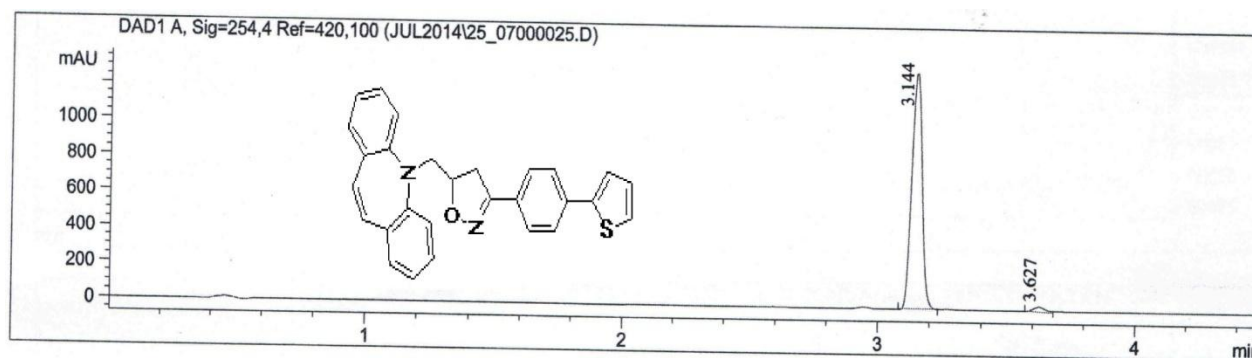
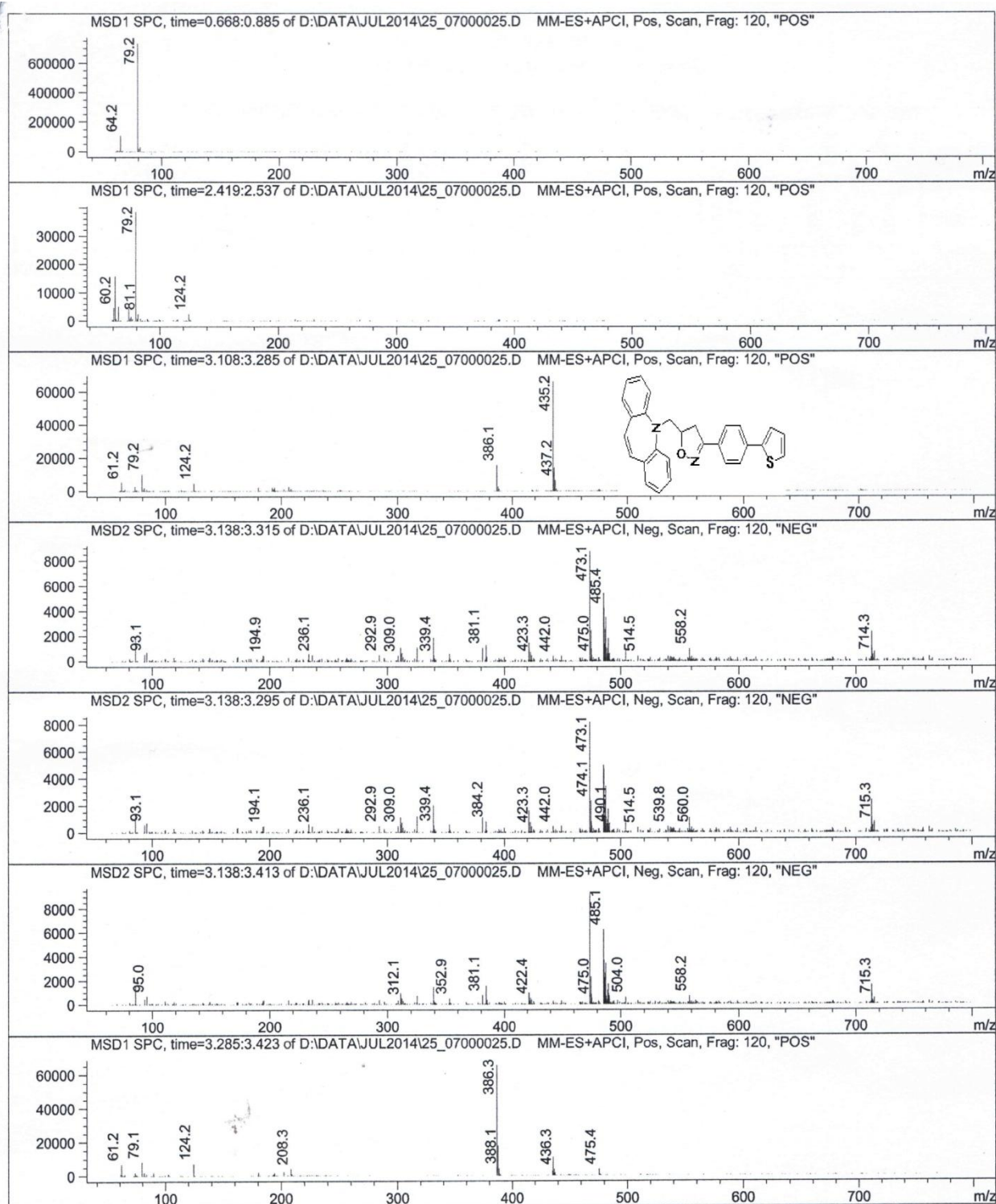
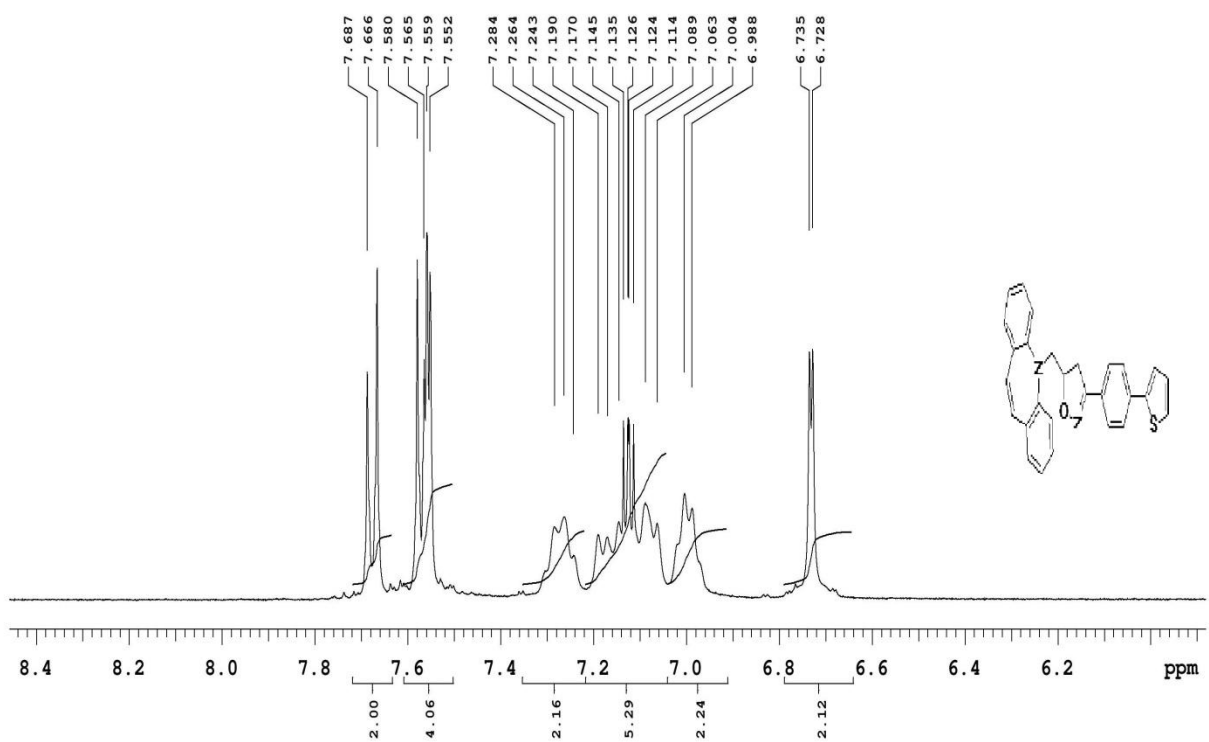
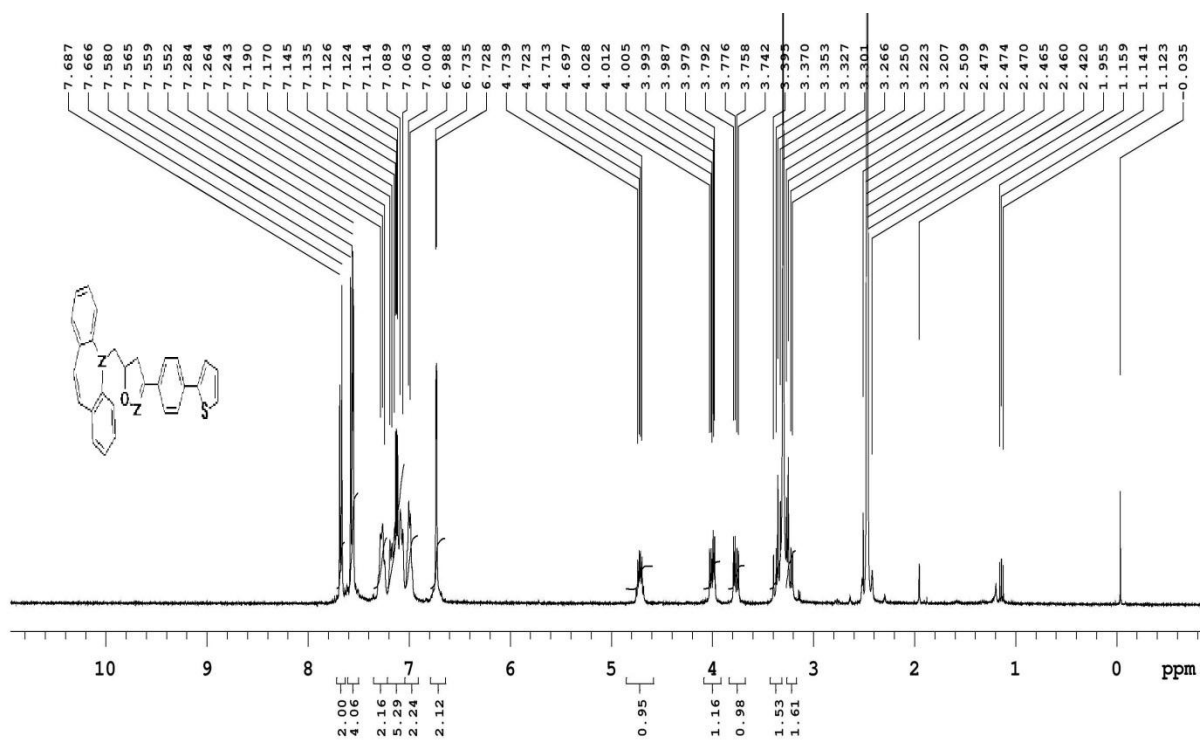


Figure S22 Mass, ^1H and ^{13}C NMR spectra of compound **8i**







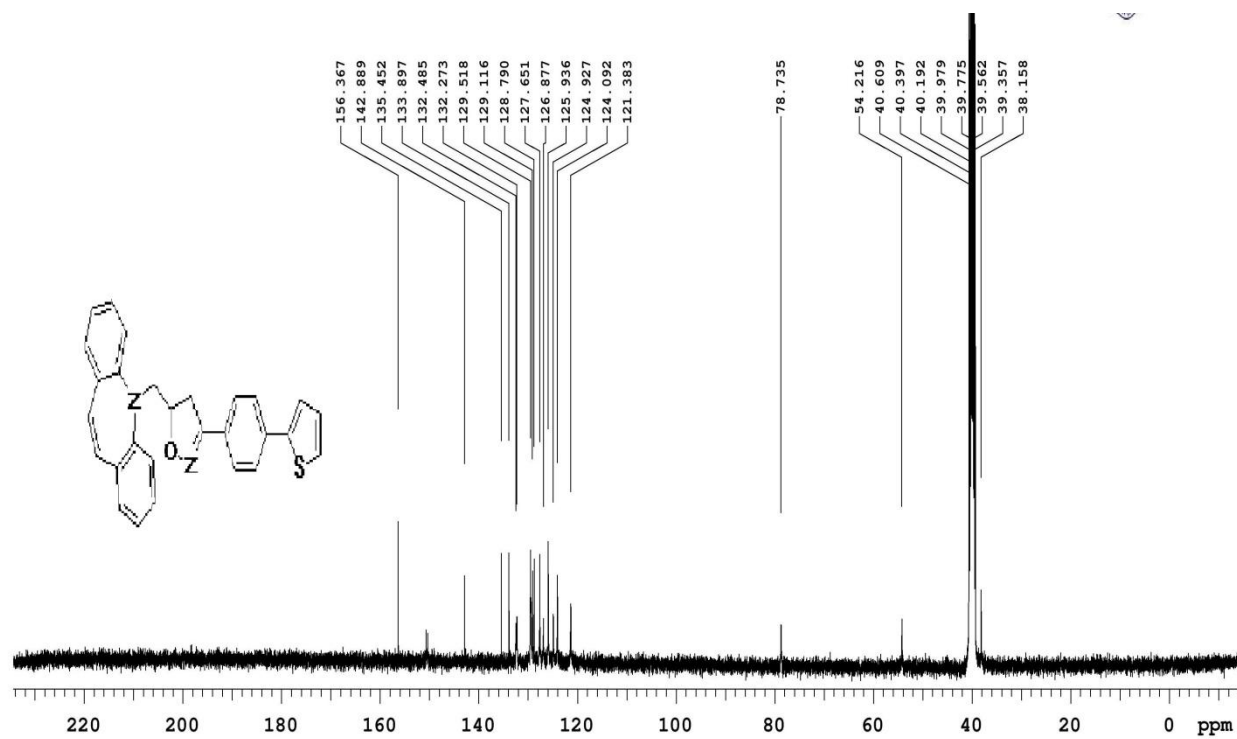
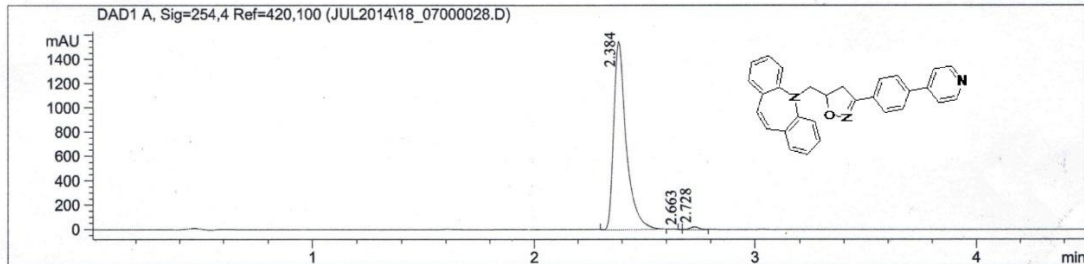


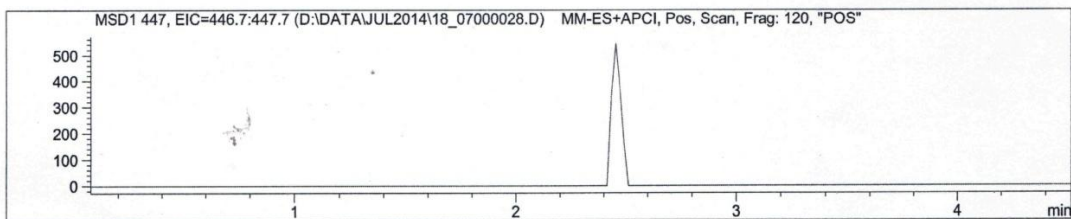
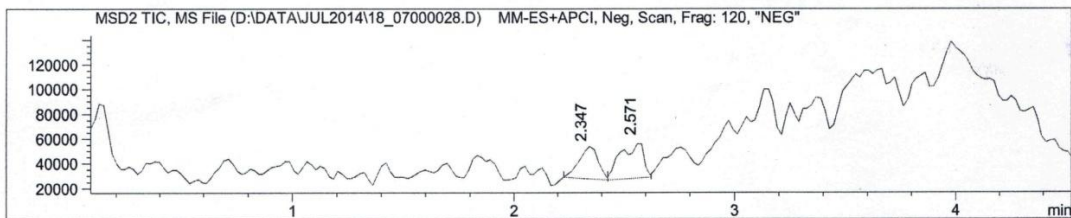
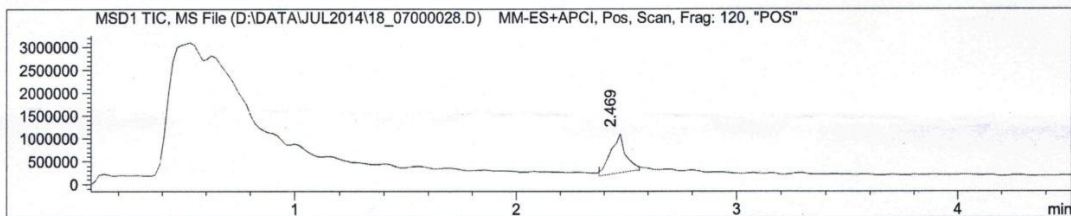
Figure S23 Mass, ^1H and ^{13}C NMR spectra of compound **8j**

LC-MS REPORT
Connexios Life Sciences Pvt Ltd

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Injection Date : Fri, Jul.18. 2014 , 5:45:54 PM
Sample Name : 88/287 B



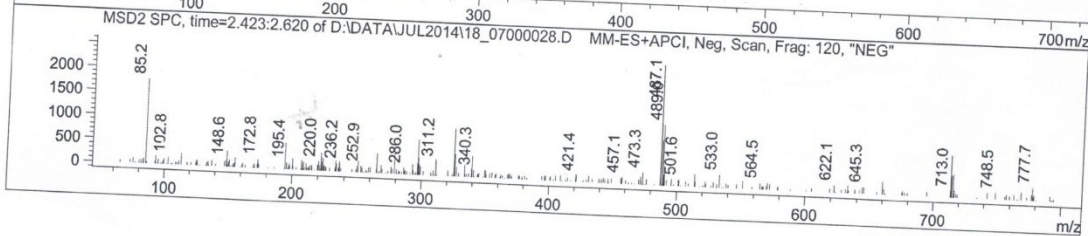
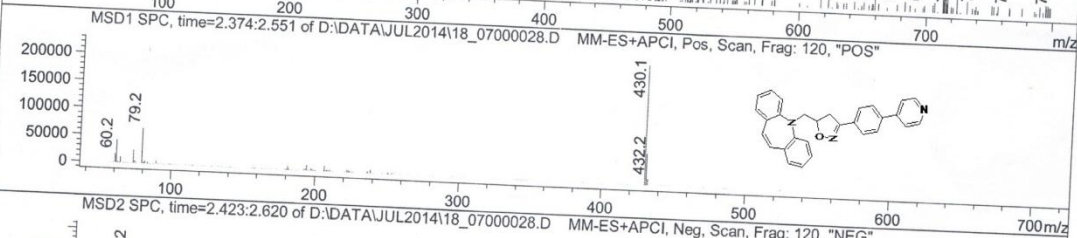
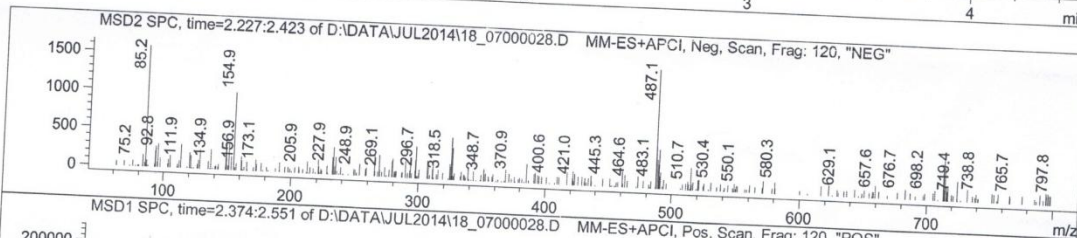
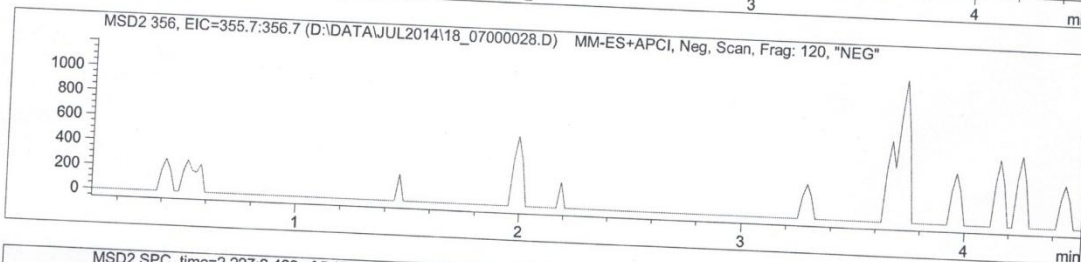
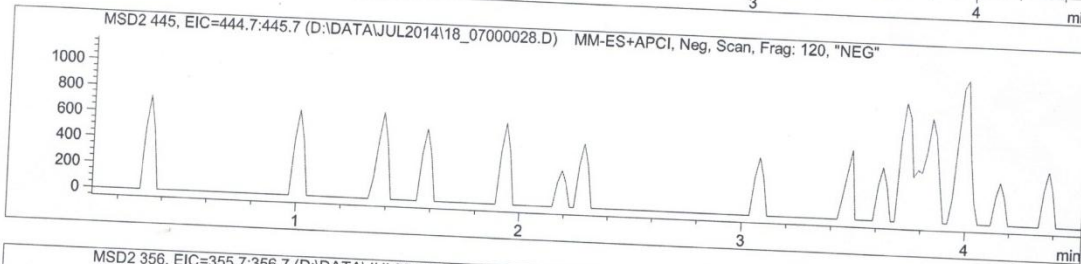
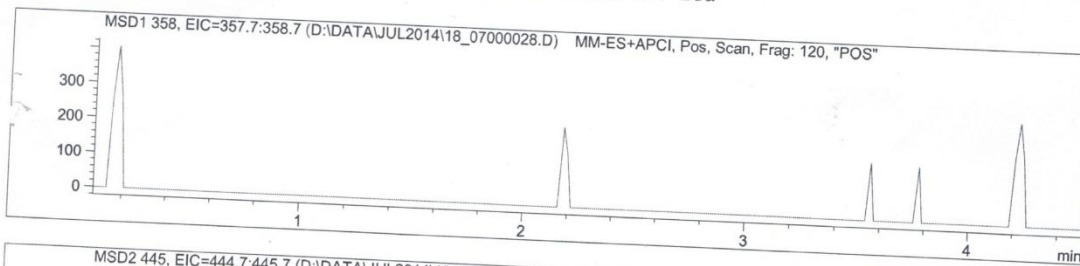
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Analysed by: Jeyakumar
Instrument code: CON/LCMS/001
7/18/2014 5:54:05 PM

Page 1 of 2

LC-MS REPORT
Connexios Life Sciences Pvt Ltd

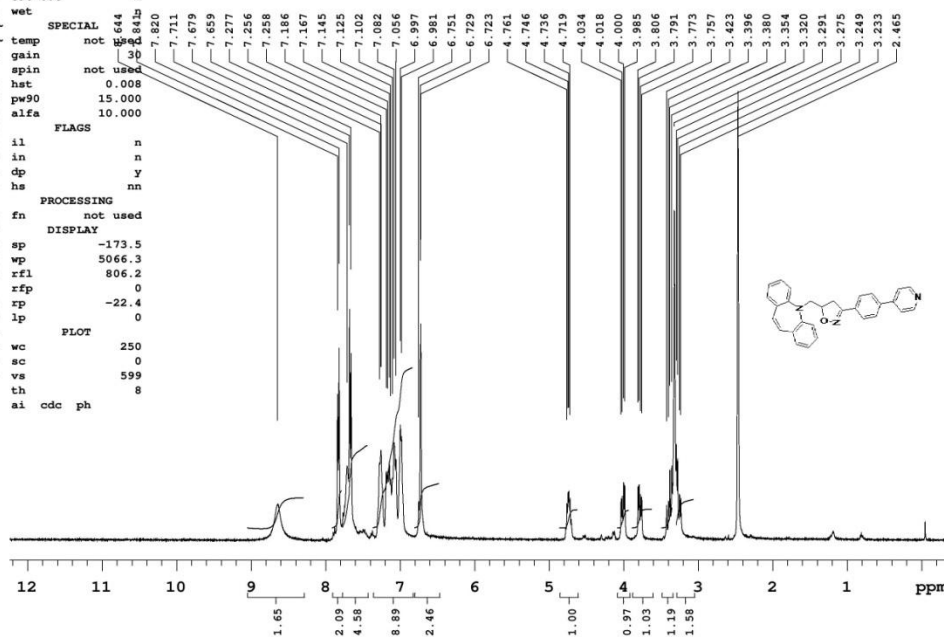


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1400756-SB1-1H

expl1 PROTON

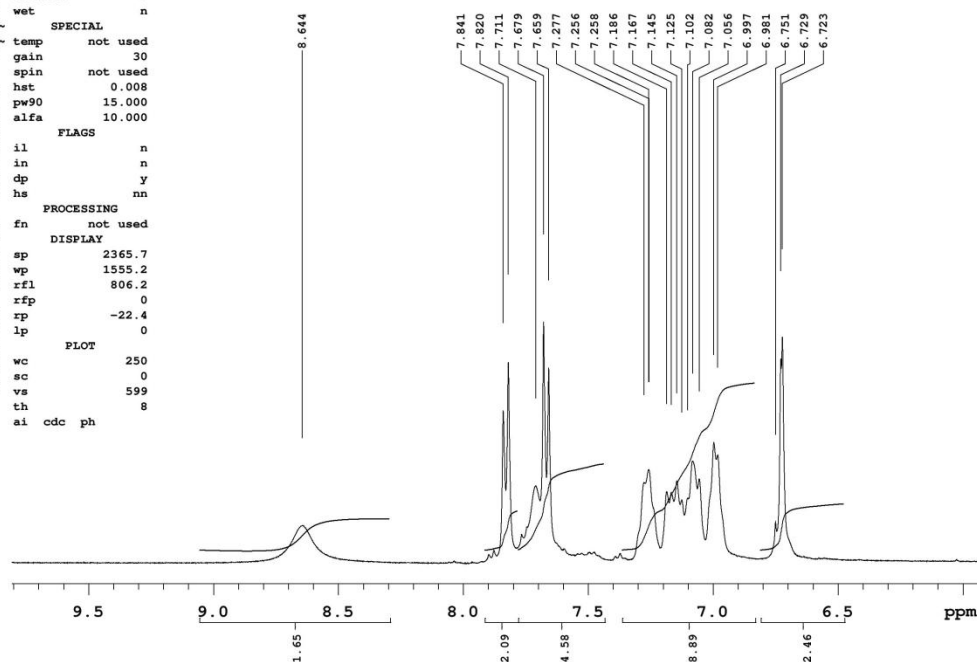
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 at 2.556 pw90 15.000
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 fb 4000
 bs 2 il
 dl 1.000 in
 nt 8 dp
 ct 8 hs
 TRANSMITTER PROCESSING
 tn H1 fn not used
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 tof 399.8 sp -173.5
 tpwr 58 wp 5066.3
 pw 7.500 rfl 806.2
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 dn C13 rp -22.4
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 ai cdc ph 8



1400756-SB1-1H

expl1 PROTON

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 bs 2 il
 dl 1.000 in
 nt 8 dp
 ct 8 hs
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1400757-SB1-13C

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bs 64
dl 1.000
nt 2048
ct 384
TRANSMITTER
tn C13
sfrq 100.548
tof 1530.9
tpwr 57
pw 5.000
DECOUPLER
dn H1
dof 0
dm yyy
decwave w
dpwr 40
dmf 10000

PRESATURATION
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wet
SPECIAL
temp not
gain 1.50
spin not used
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dp y
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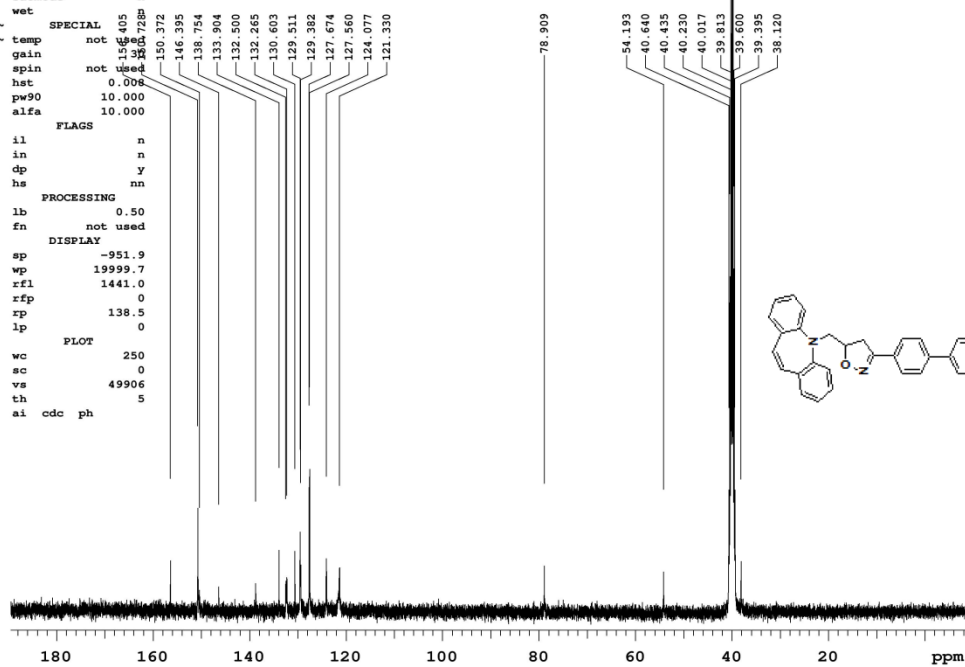
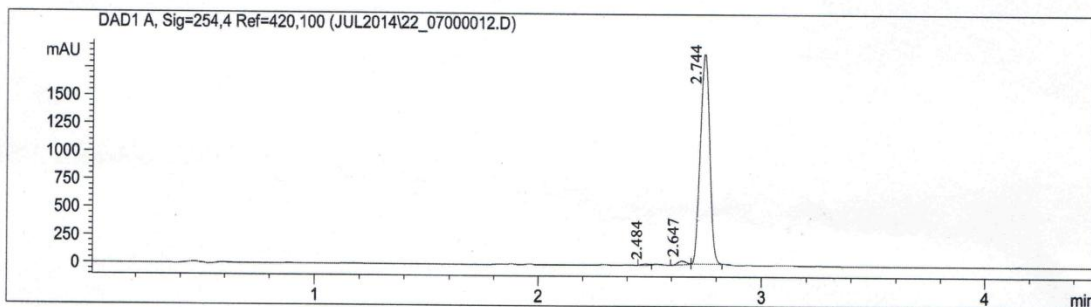
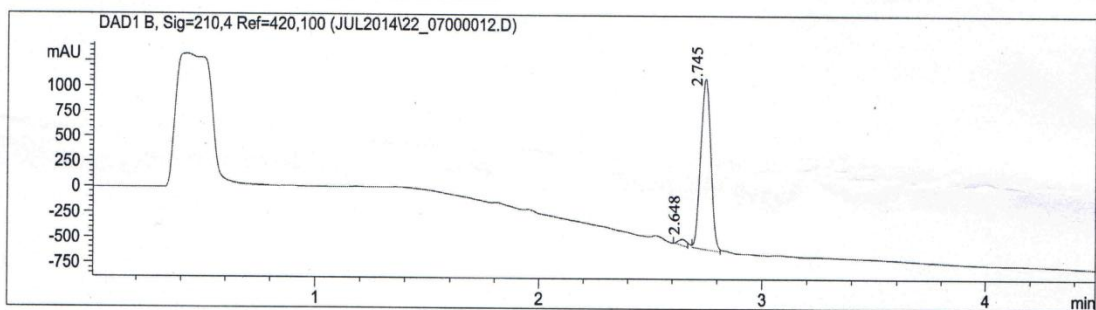
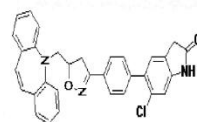


Figure S24 Mass, ^1H and ^{13}C NMR spectra of compound 8k

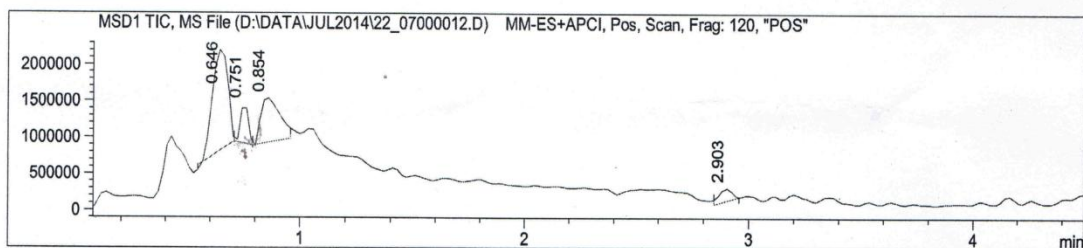
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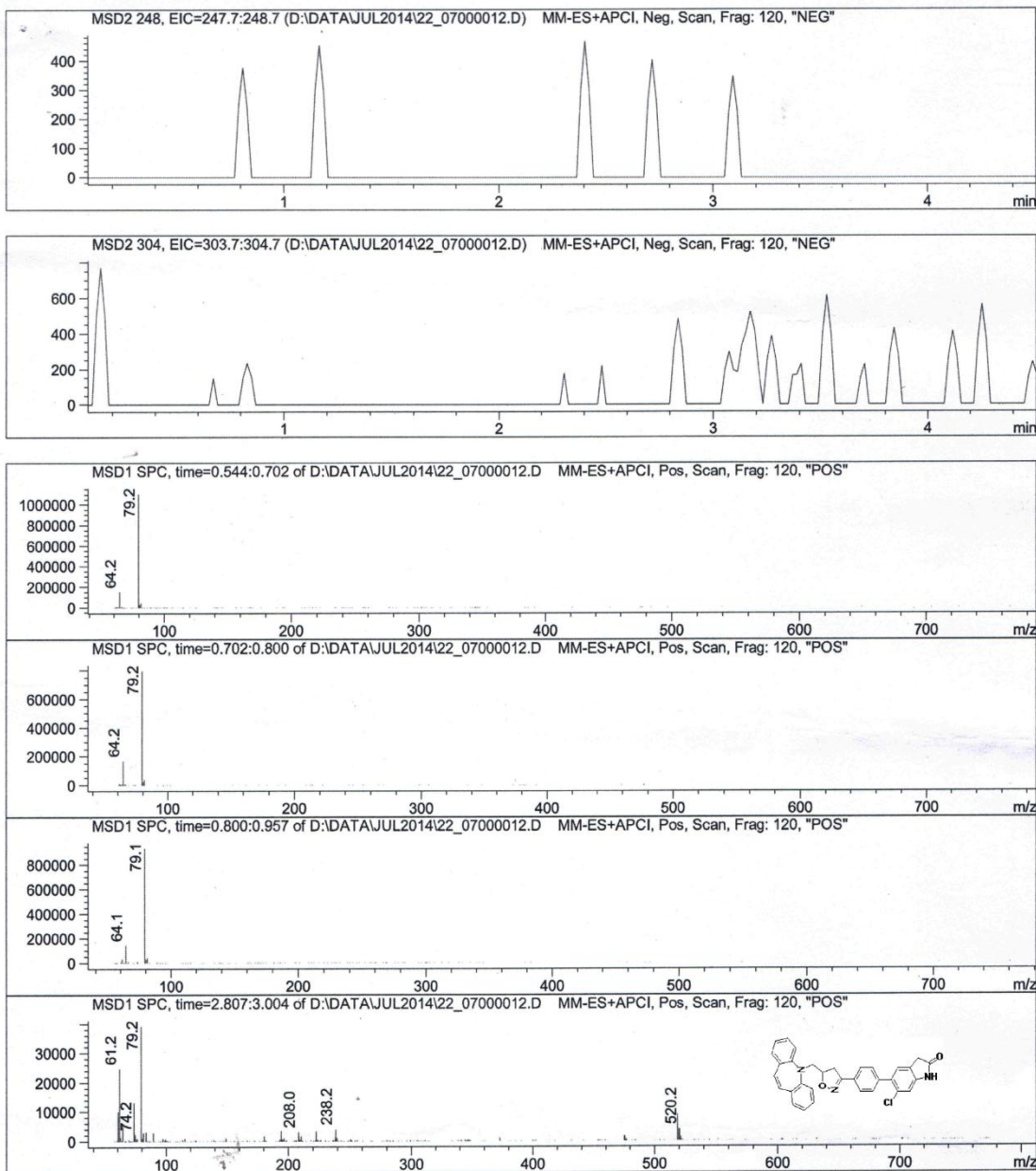


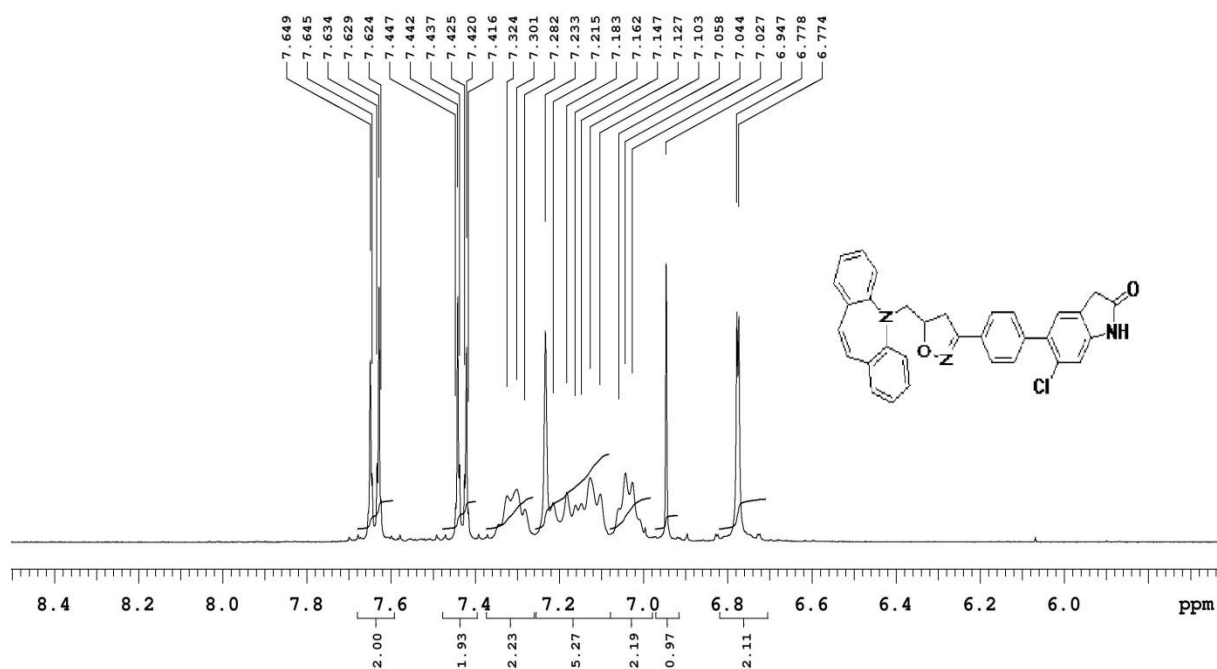
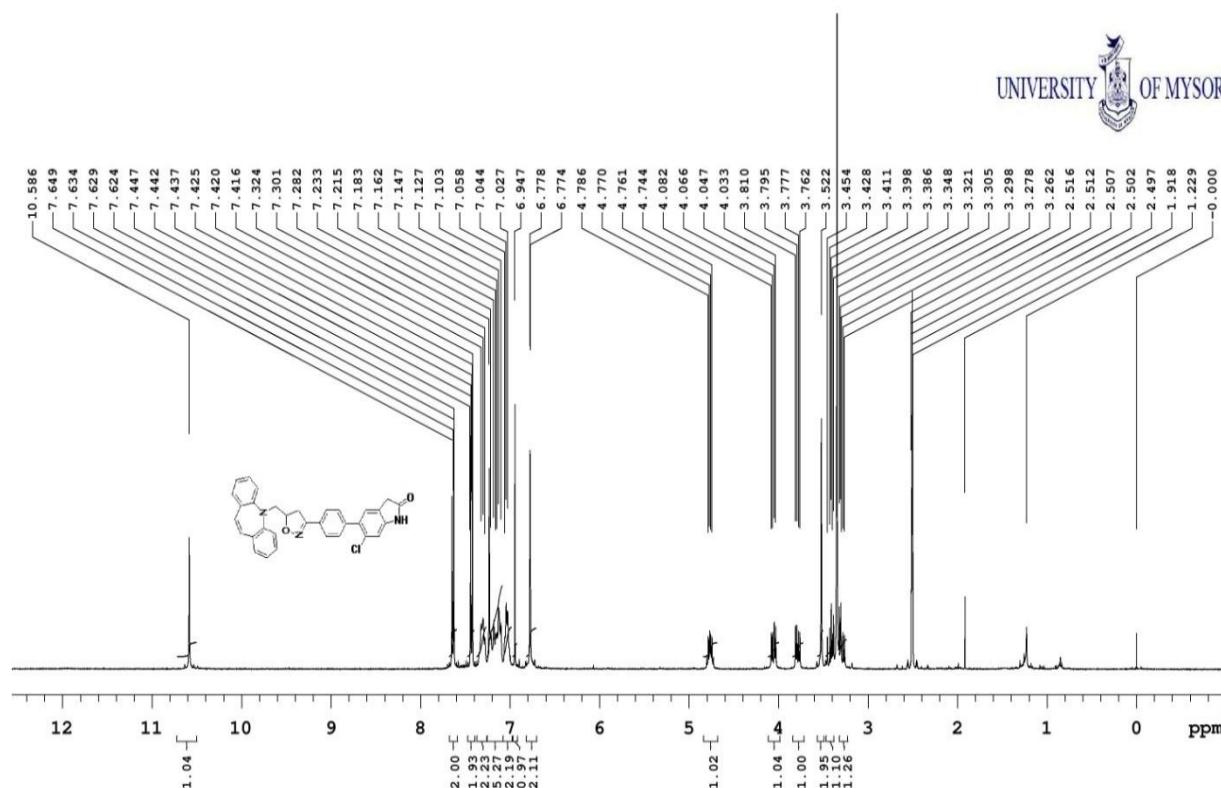
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Peak No	RT min	Area	Area %
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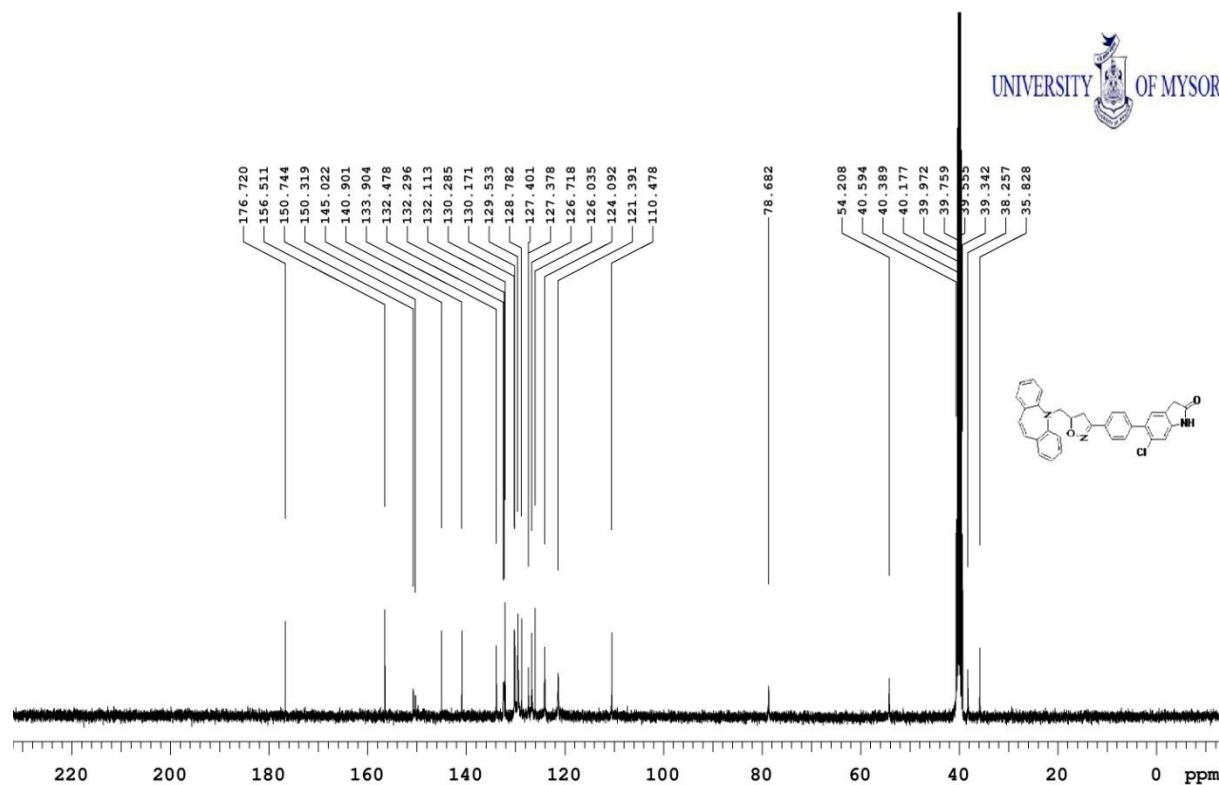


Figure S25 Mass, ¹H and ¹³C NMR spectra of compound **8l**