

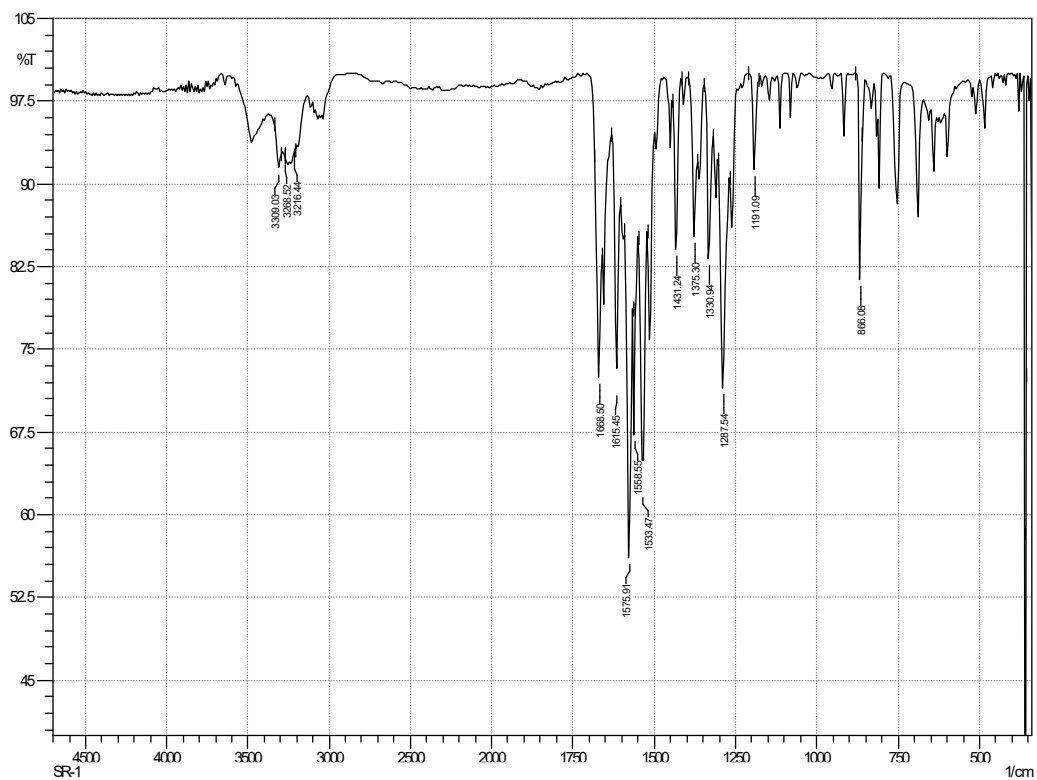
**Quinoline-based Schiff's base as possible antidiabetic agents: Ligand-based pharmacophore modeling, 3D QSAR, docking, and molecular dynamic simulations study**

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**Affiliation(s):**

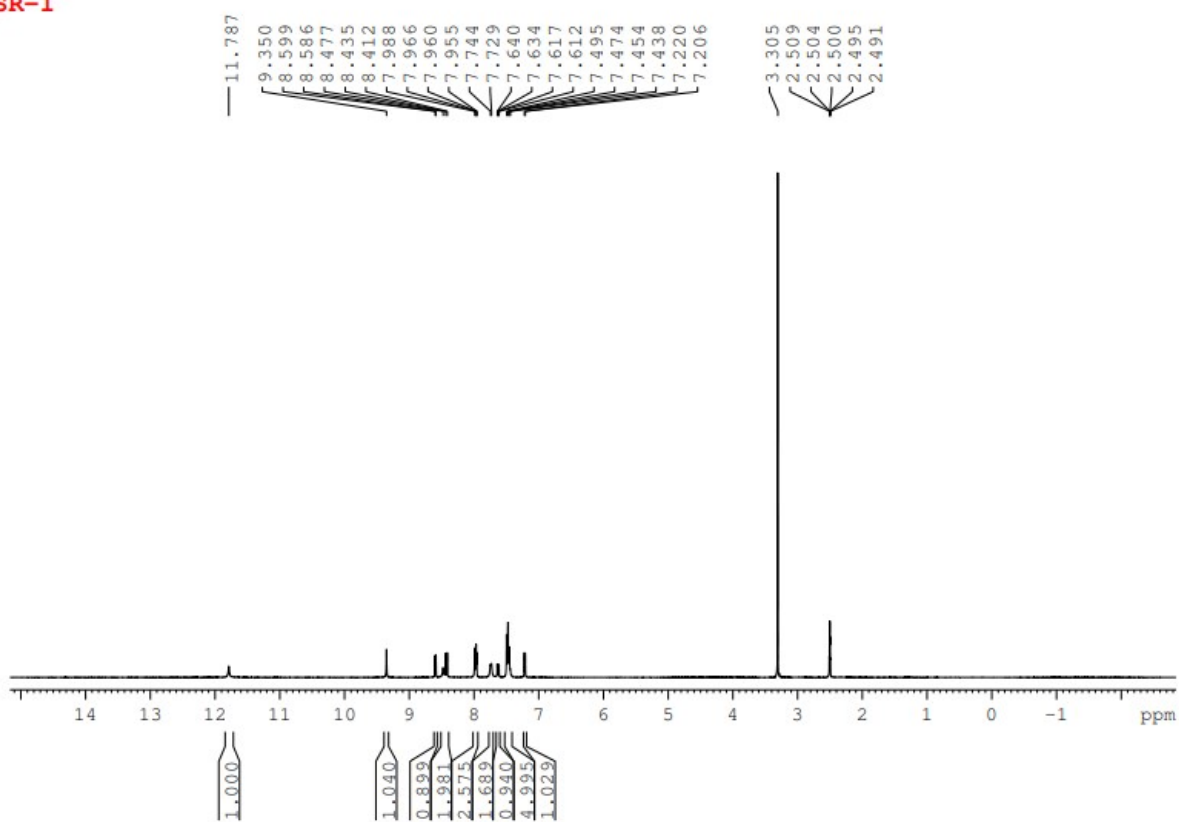
<sup>a</sup>Department of Pharmaceutical Chemistry, KLE College of Pharmacy, Belagavi, KLE Academy of Higher education and Research, Belagavi - 590 010, Karnataka, India

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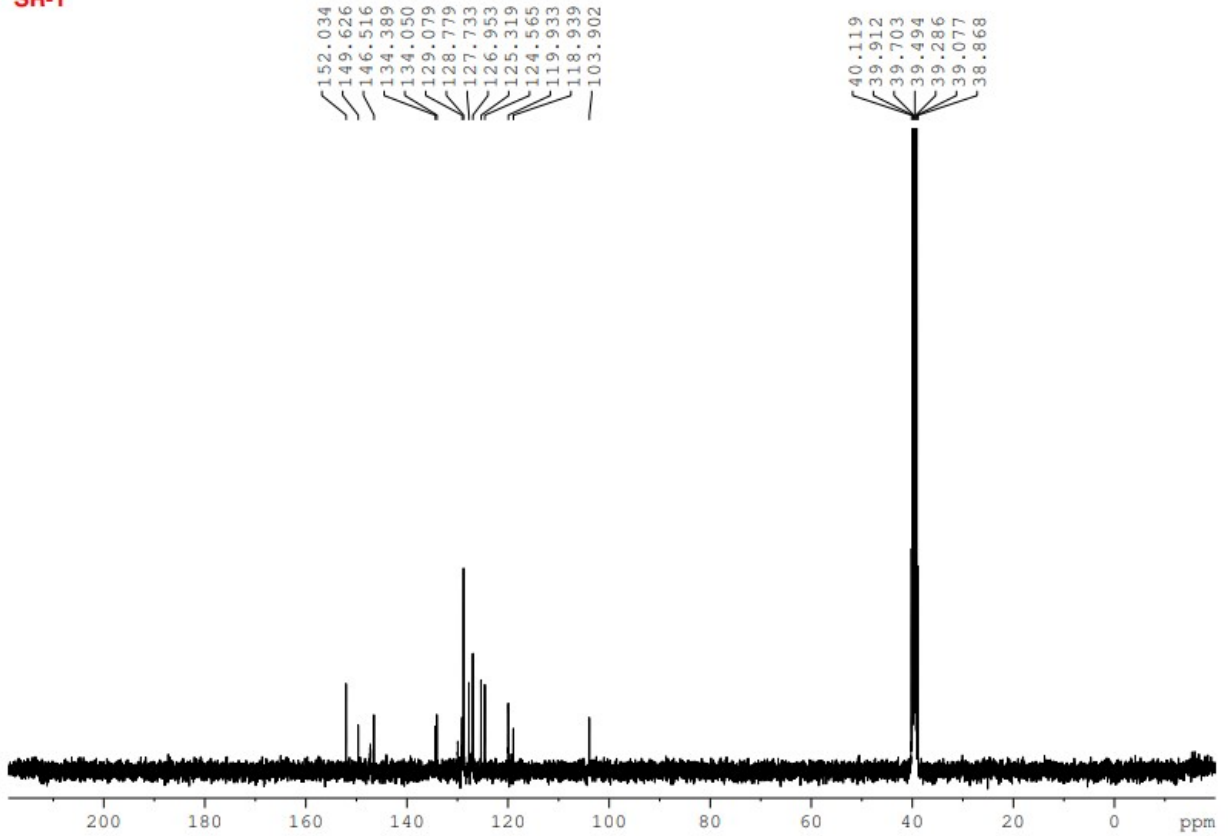
FTIR (KBr, cm<sup>-1</sup>) spectra of compound 6a

SR-1



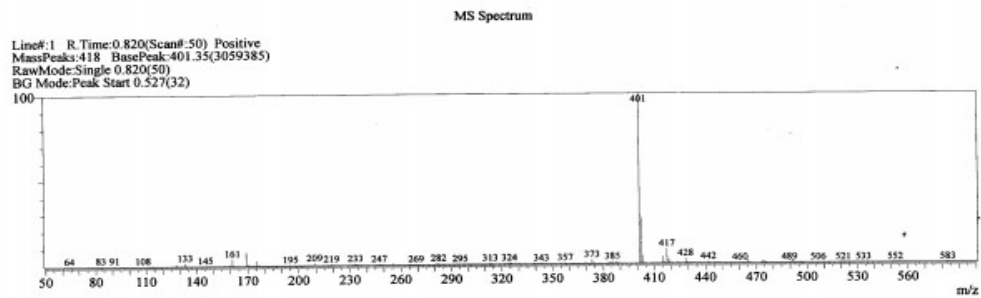
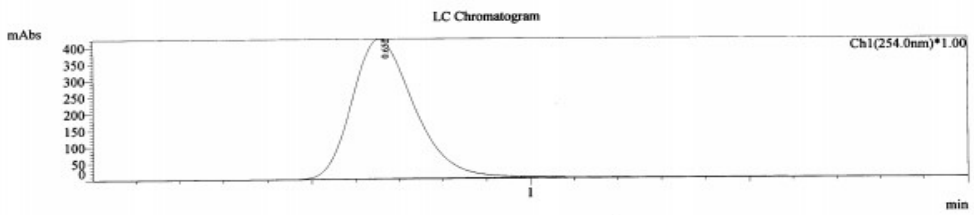
<sup>1</sup>H NMR (400 MHz, δ, ppm) spectra of compound 6a

SR-1



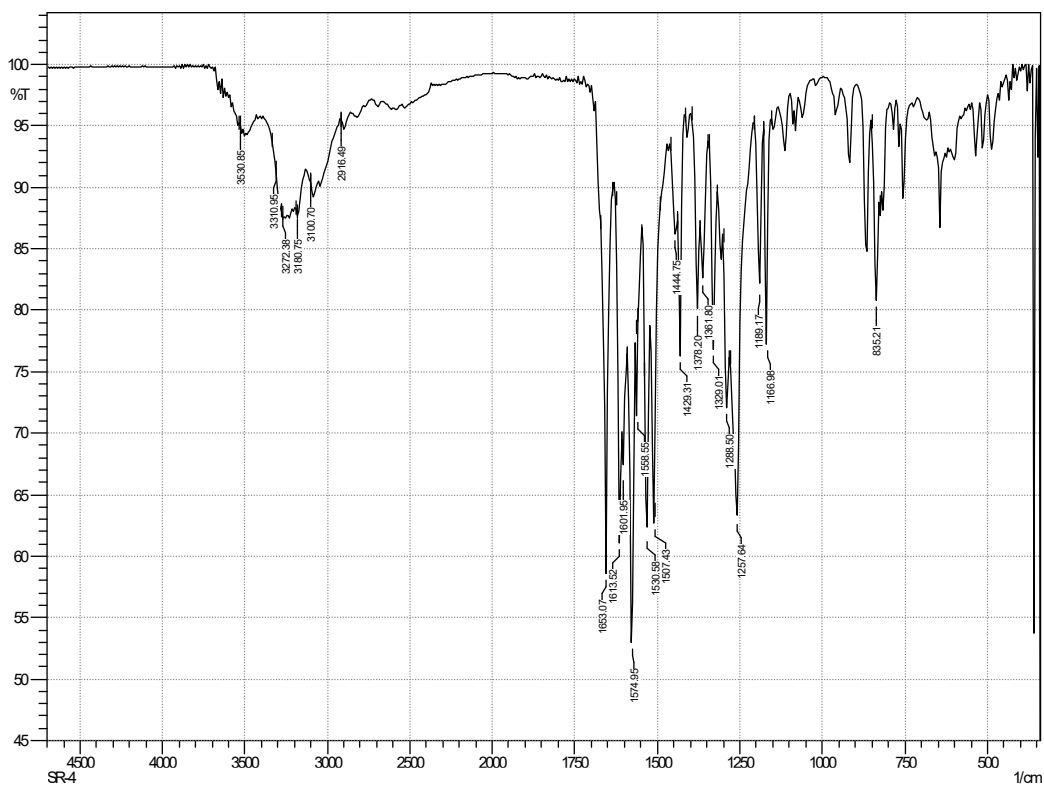
<sup>13</sup>C NMR (400 MHz, δ, ppm) spectra of compound 6a

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Inj. Volume : 5.000  
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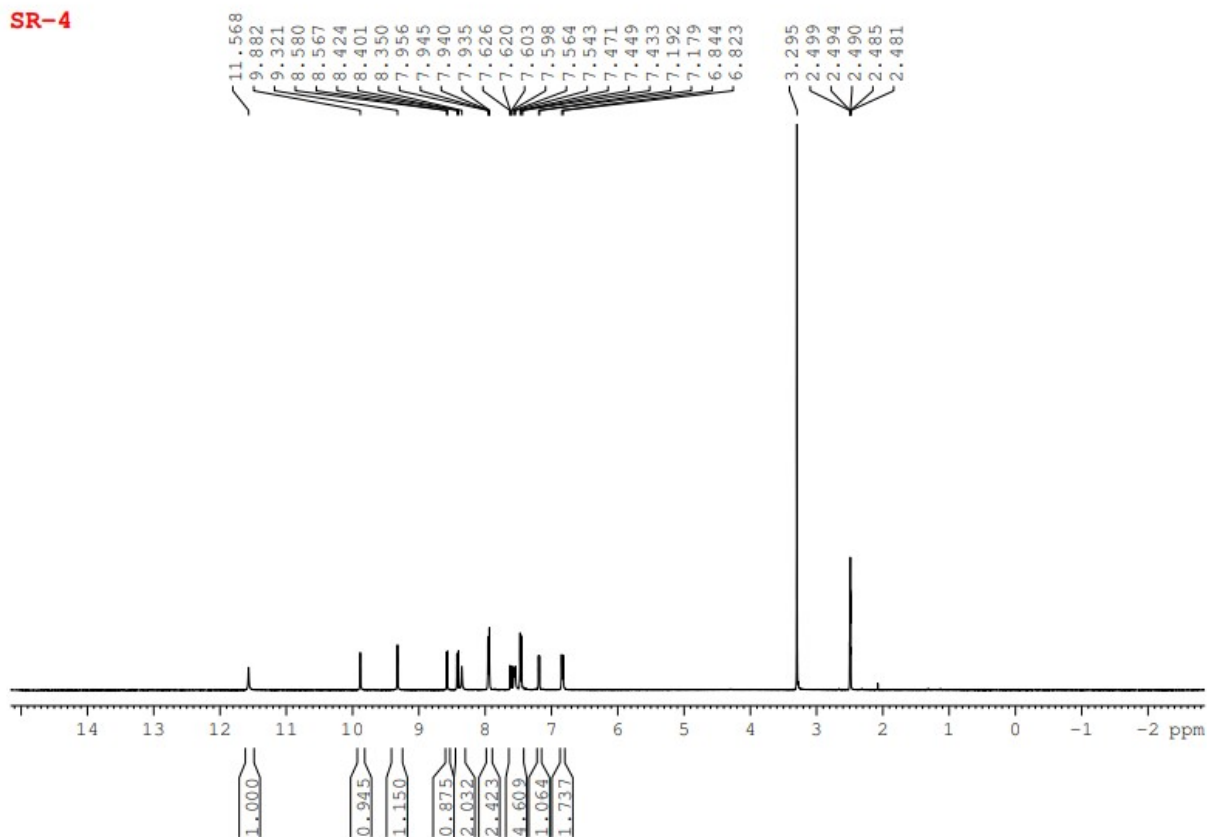
Peak#	R.Time	I.Time	F.Time	Area	Height	A/H	Mark	%Total	Name	Base m/z	Base Int.
1	0.820	0.527	1.093	80256286	4955872	16.19		100.00		401.35	3059385
				80256286	4955872			100.00			

LC-MS spectra of compound 6a



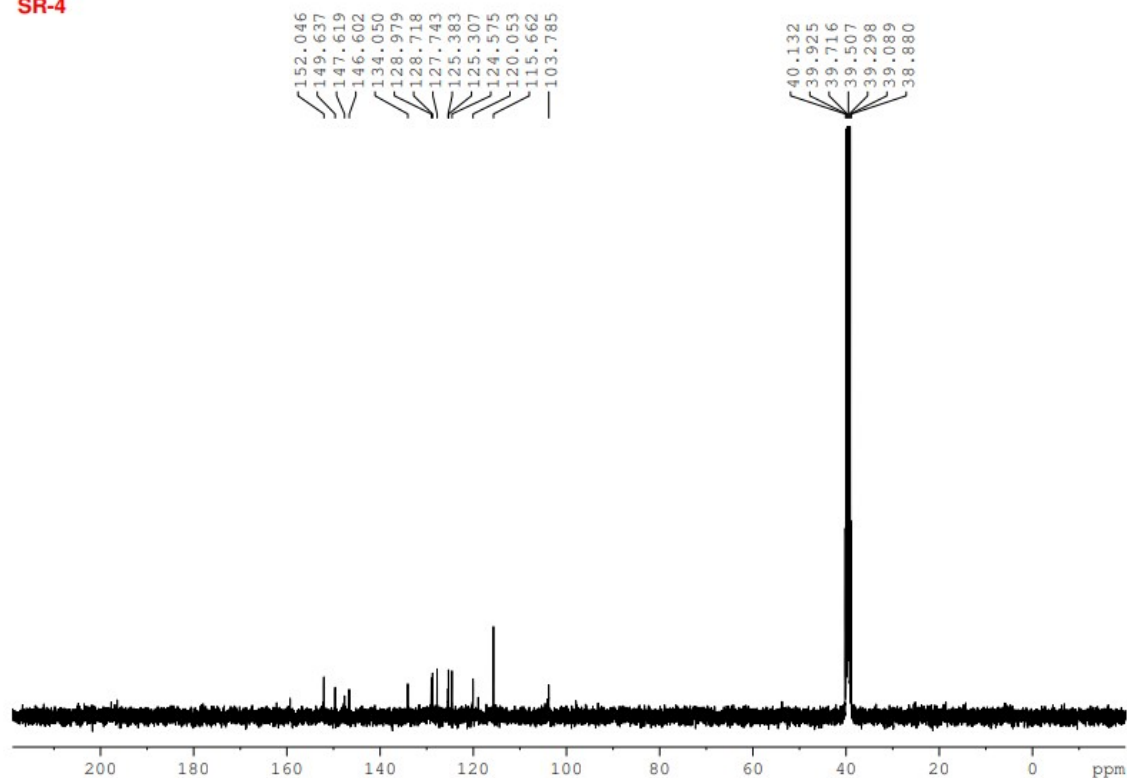
FTIR (KBr, cm<sup>-1</sup>) spectra of compound 6b

SR-4



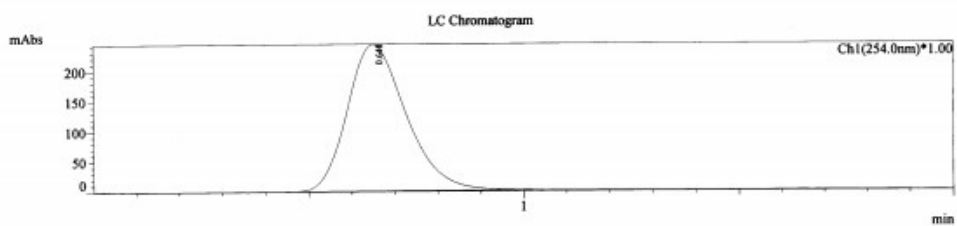
<sup>1</sup>H NMR (400 MHz, δ, ppm) spectra of compound 6b

SR-4



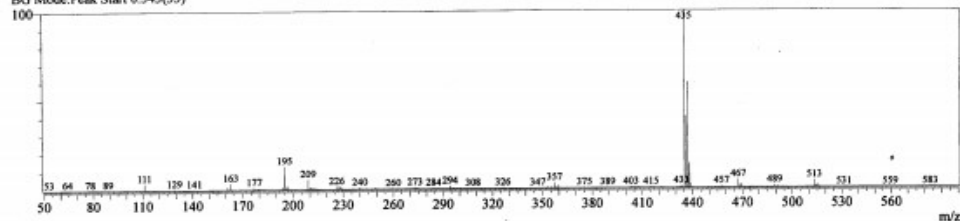
<sup>13</sup>C NMR (400 MHz, δ, ppm) spectra of compound 6b

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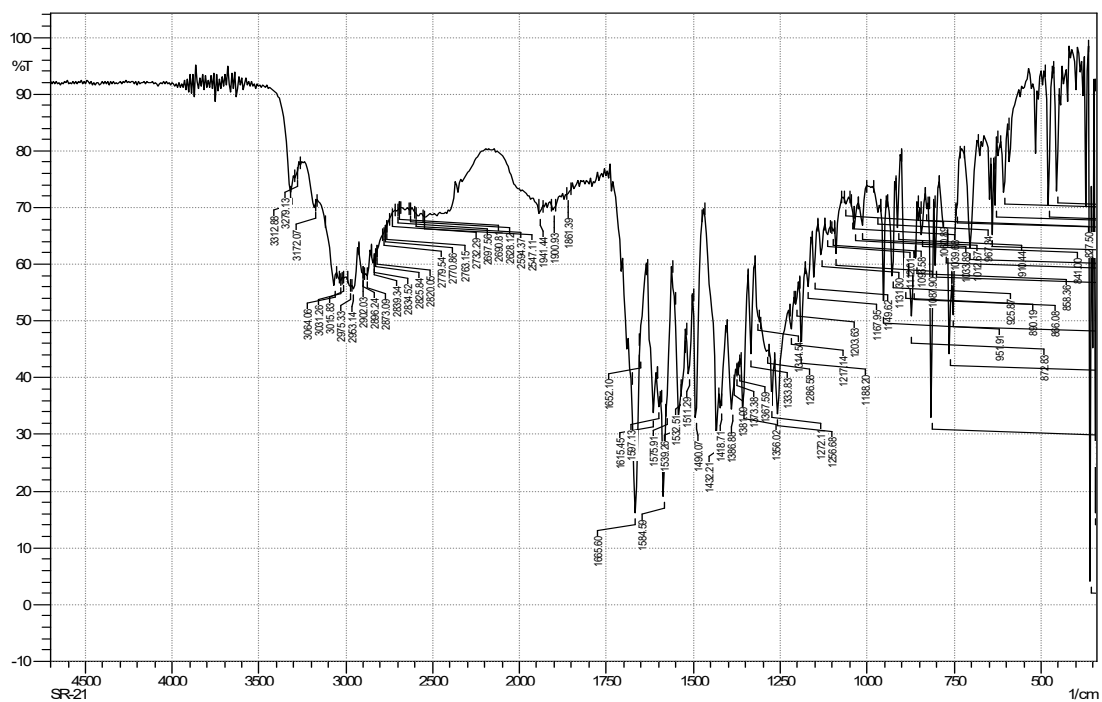
MS Spectrum

Line# 1 R.Time: 0.744(Scan#: 45) Positive  
MassPeaks: 443 BasePeak: 435.30(11504669)  
RawMode: Single 0.744(45)  
BG Mode: Peak Start 0.543(33)

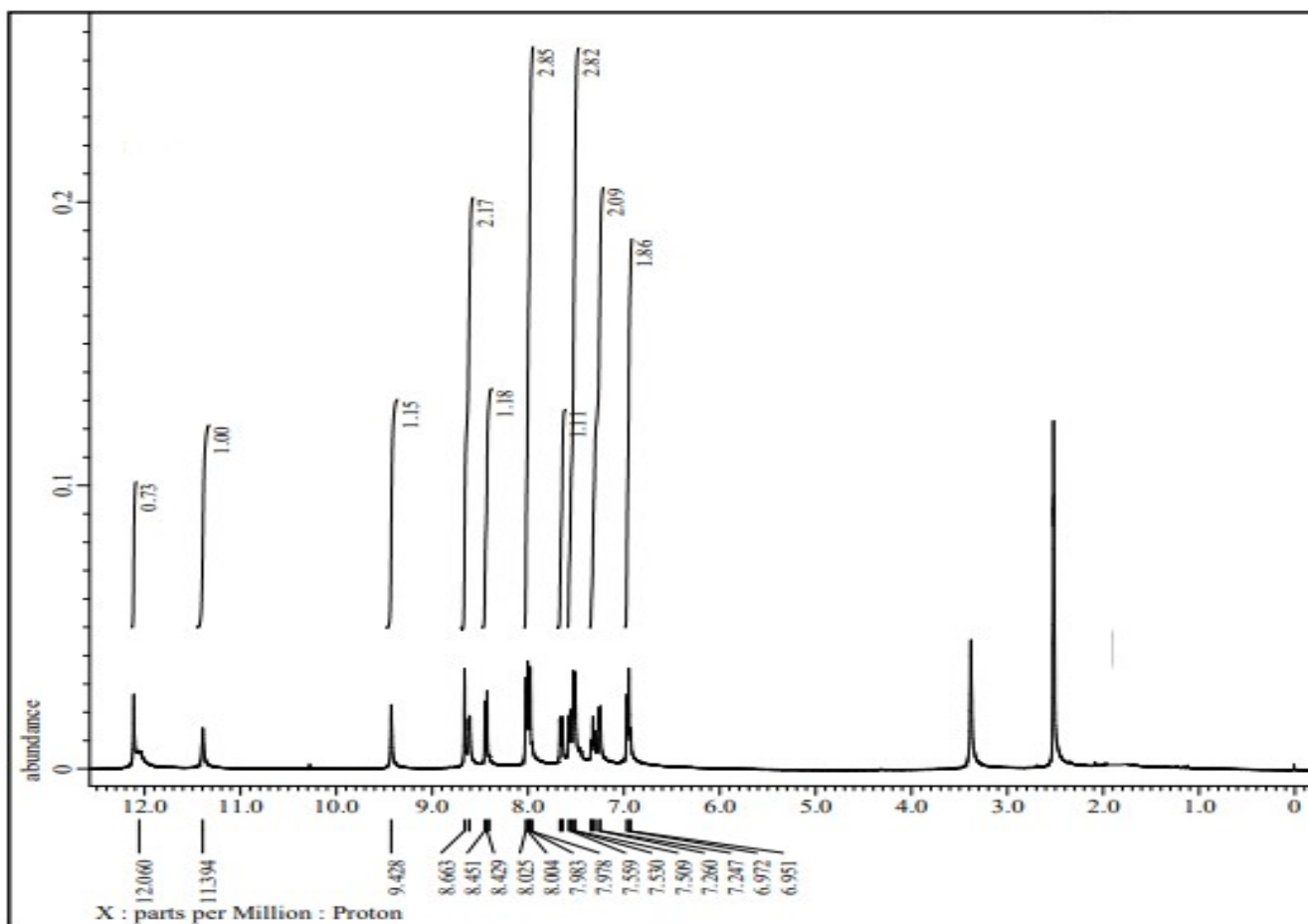


Peak#	R.Time	I.Time	F.Time	Area	Height	A/H	Mark	%Total	Name	Base m/z	Base Int.
1	0.744	0.543	1.043	361513168	22896170	15.78		100.00		435.30	11504669
				361513168	22896170			100.00			

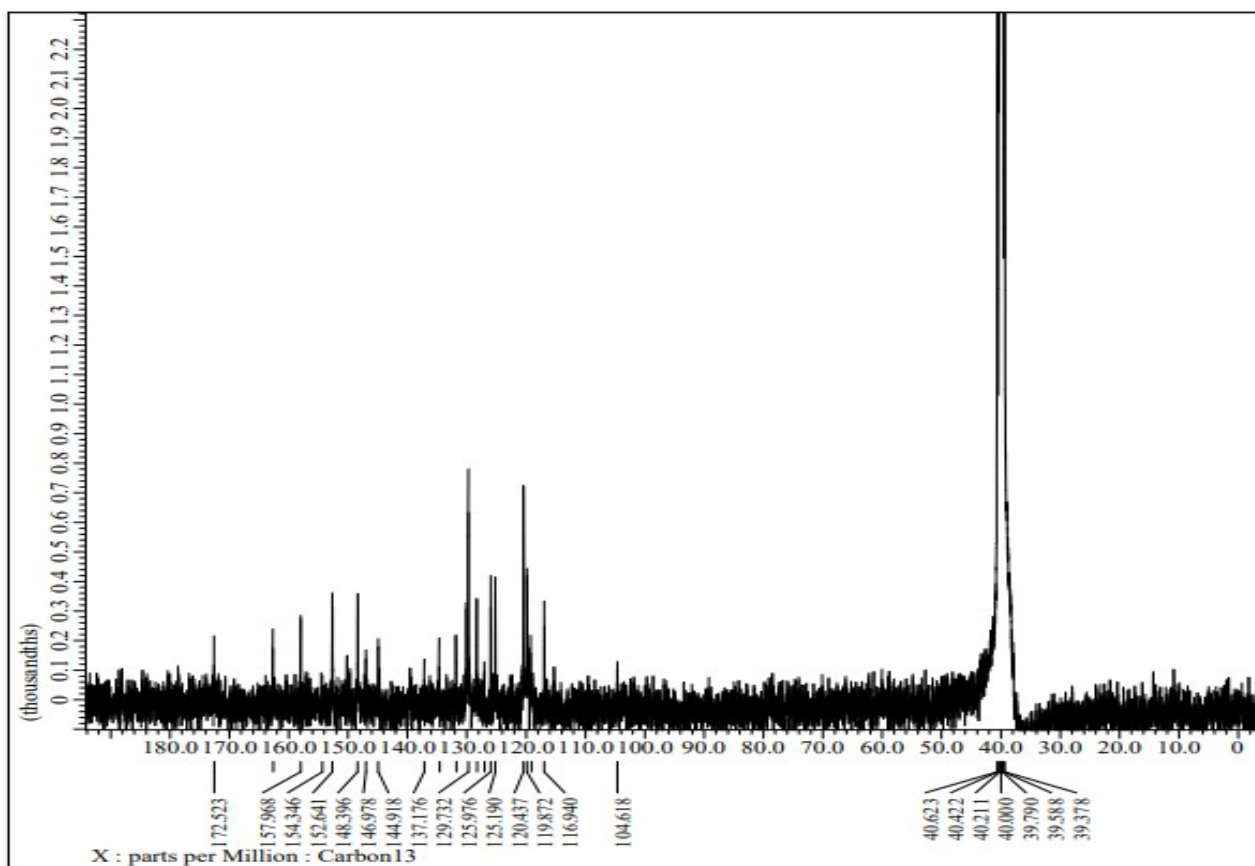
LC-MS spectra of compound 6b



FTIR (KBr,  $\text{cm}^{-1}$ ) spectra of compound 6c

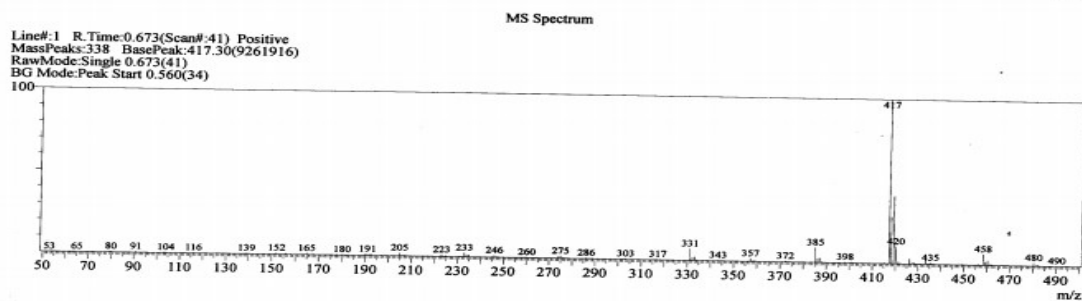
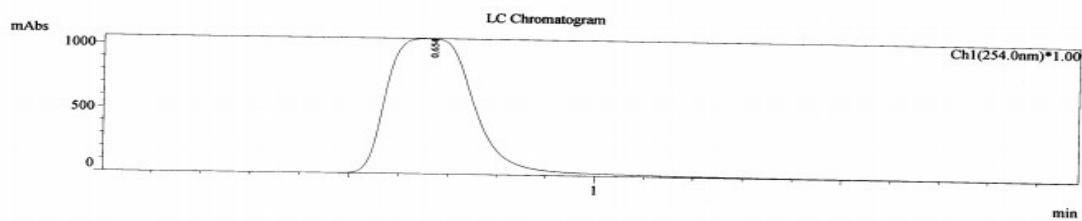


$^1\text{H}$  NMR (400 MHz,  $\delta$ , ppm) spectra of compound 6c



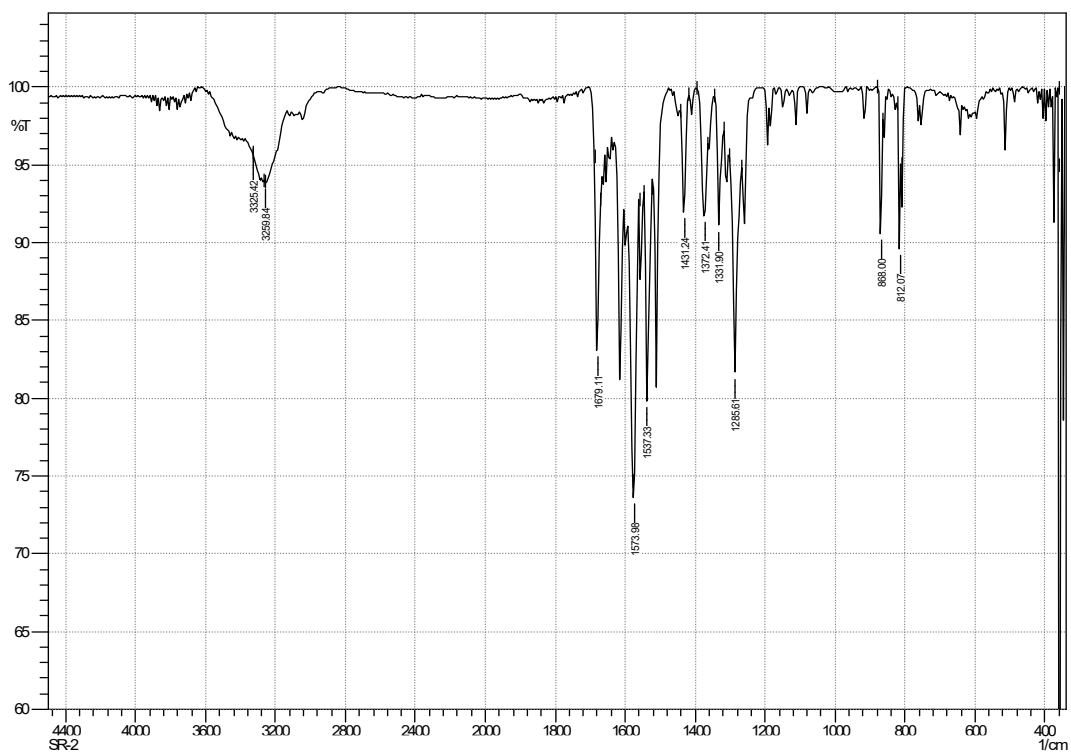
<sup>13</sup>C NMR (400 MHz, δ, ppm) spectra of compound 6c

User : Admin  
 Sample : SR-21  
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 Method Name : C:\LCMSsolution\User\Method\vesi.qlm



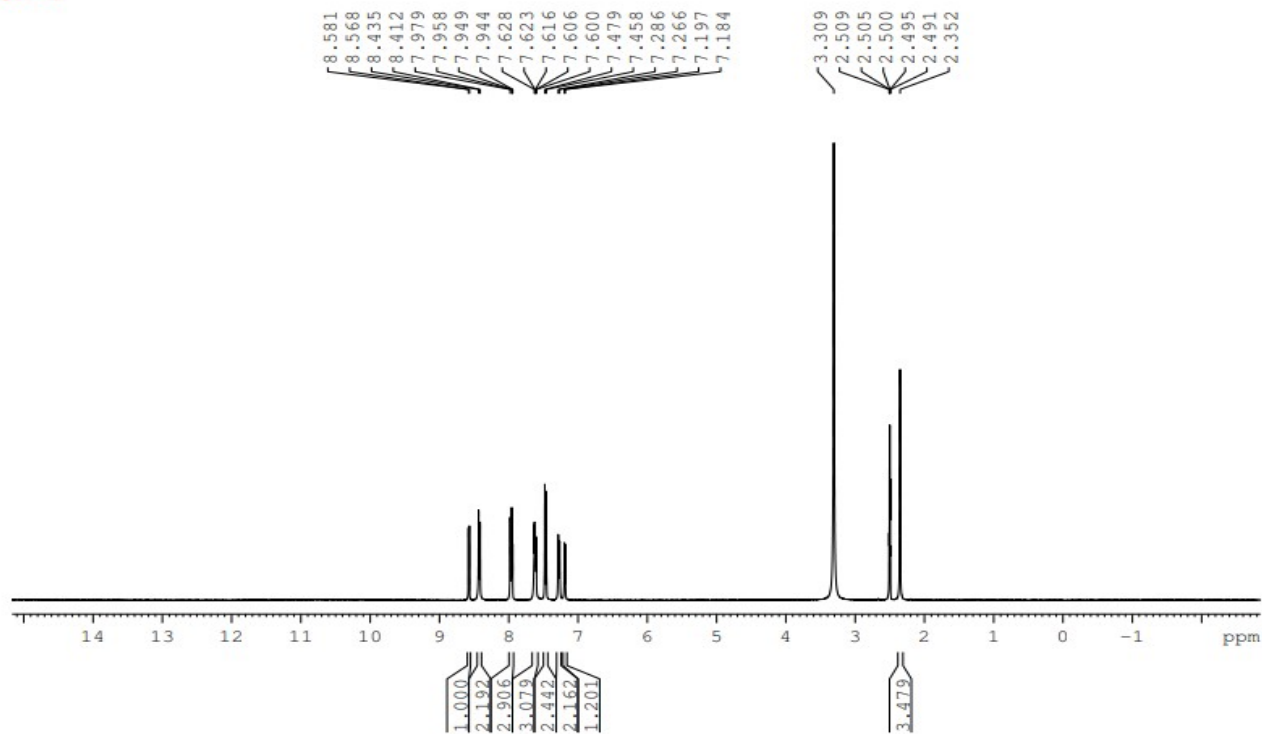
Peak#	R.Time	I.Time	F.Time	Area	Height	A/H	Mark	%Total	Name	Base m/z	Base Int.
1	0.673	0.560	1.043	147710890	13955548	10.58		100.00		417.30	9261916

LC-MS spectra of compound 6c



FTIR (KBr, cm<sup>-1</sup>) spectra of compound 6d

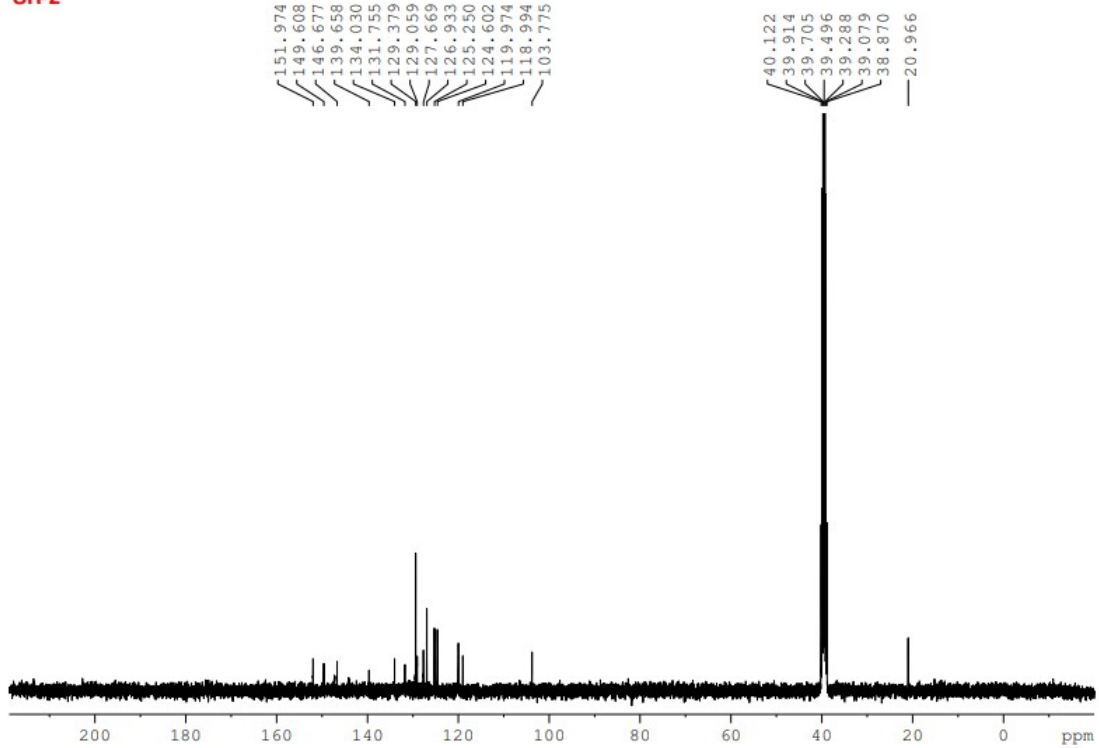
SR-2



<sup>1</sup>H NMR (400 MHz, δ, ppm) spectra of compound 6d

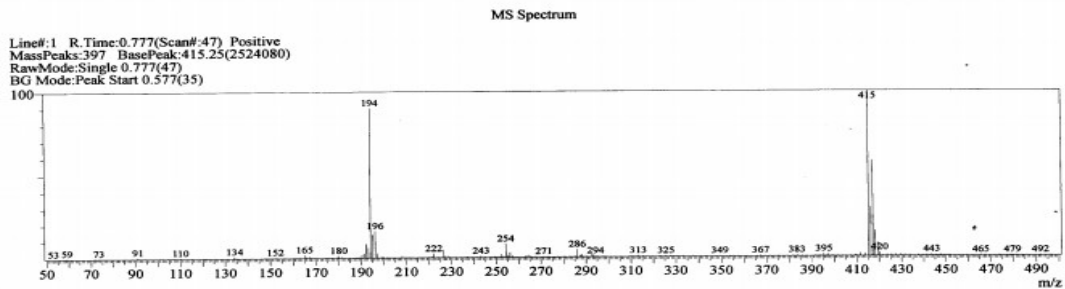
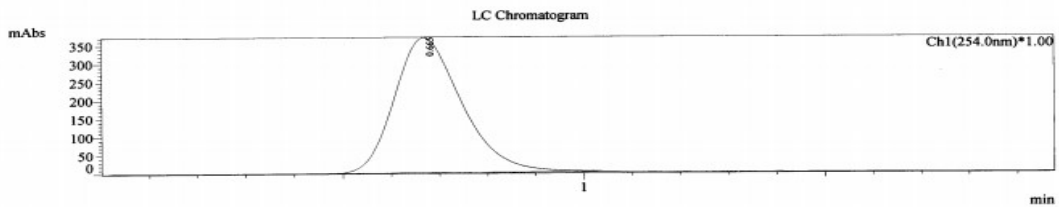


SR-2



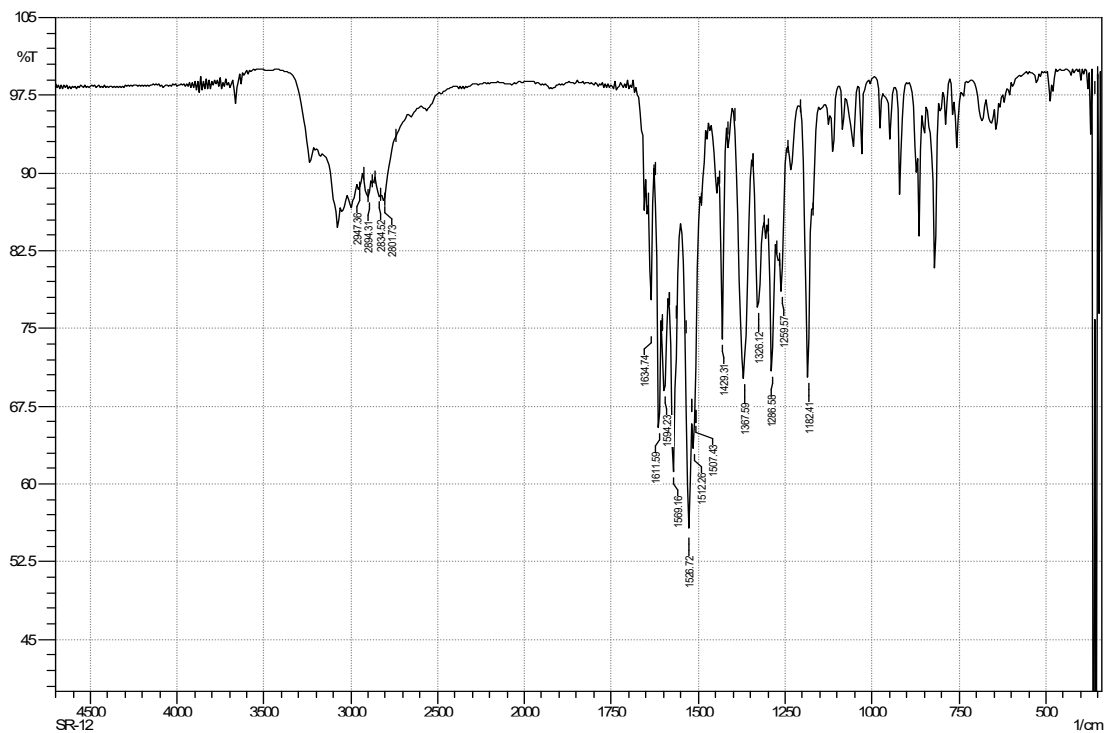
### <sup>13</sup>C NMR (400 MHz, δ, ppm) spectra of compound 6d

User : Admin  
Sample : SR-2  
Inj. Volume : 5.000  
Data Name : D:\lcms-data-c\SR-2-APCI-POS1.qld  
Method Name : C:\LCMSsolution\User\Method\esi.qlm

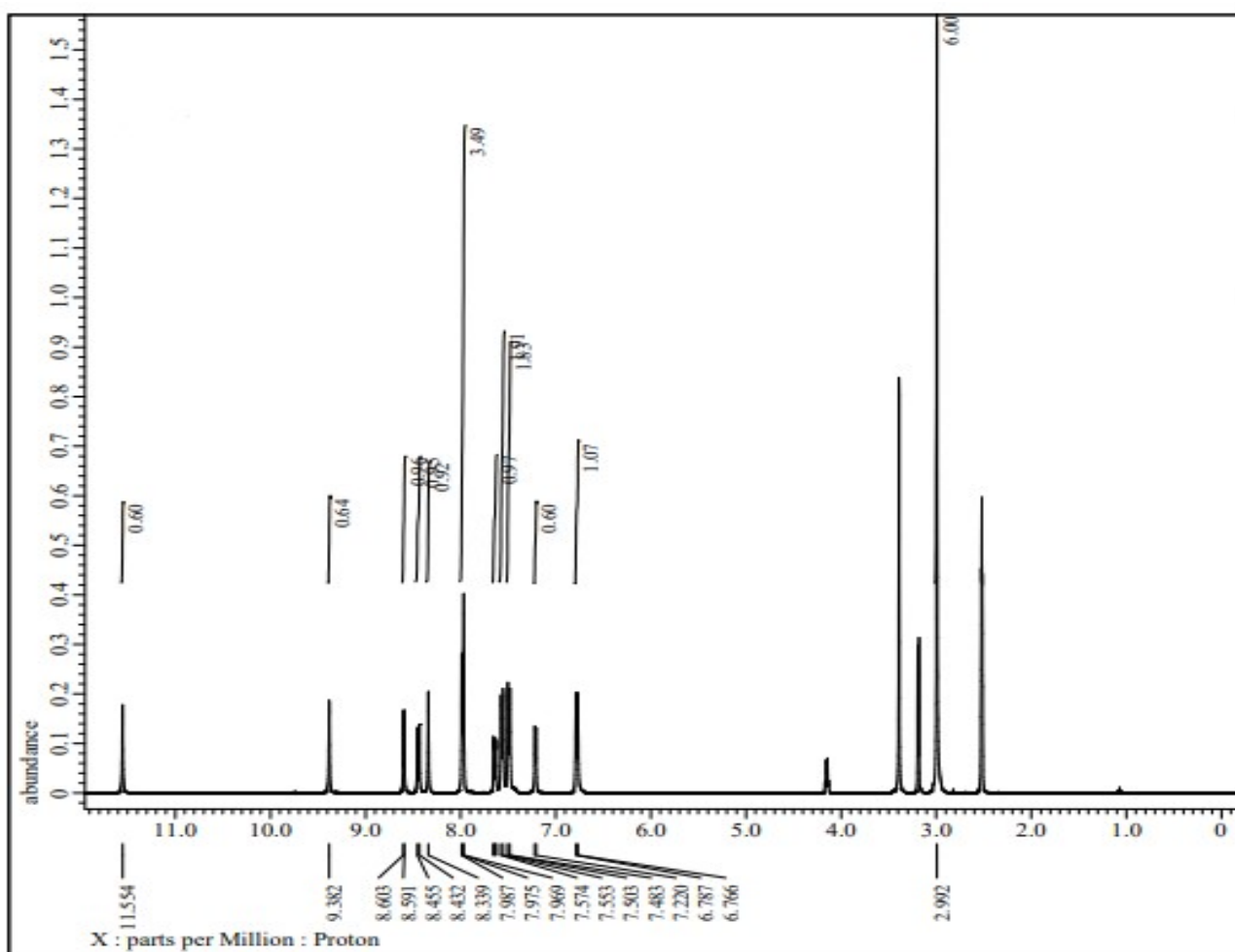


Peak#	R.Time	LTime	F.Time	Area	Height	A/H	Mark	%Total	Name	Base m/z	Base Int.
1	0.777	0.577	1.043	145448674	12323758	11.80		100.00		415.25	2524080

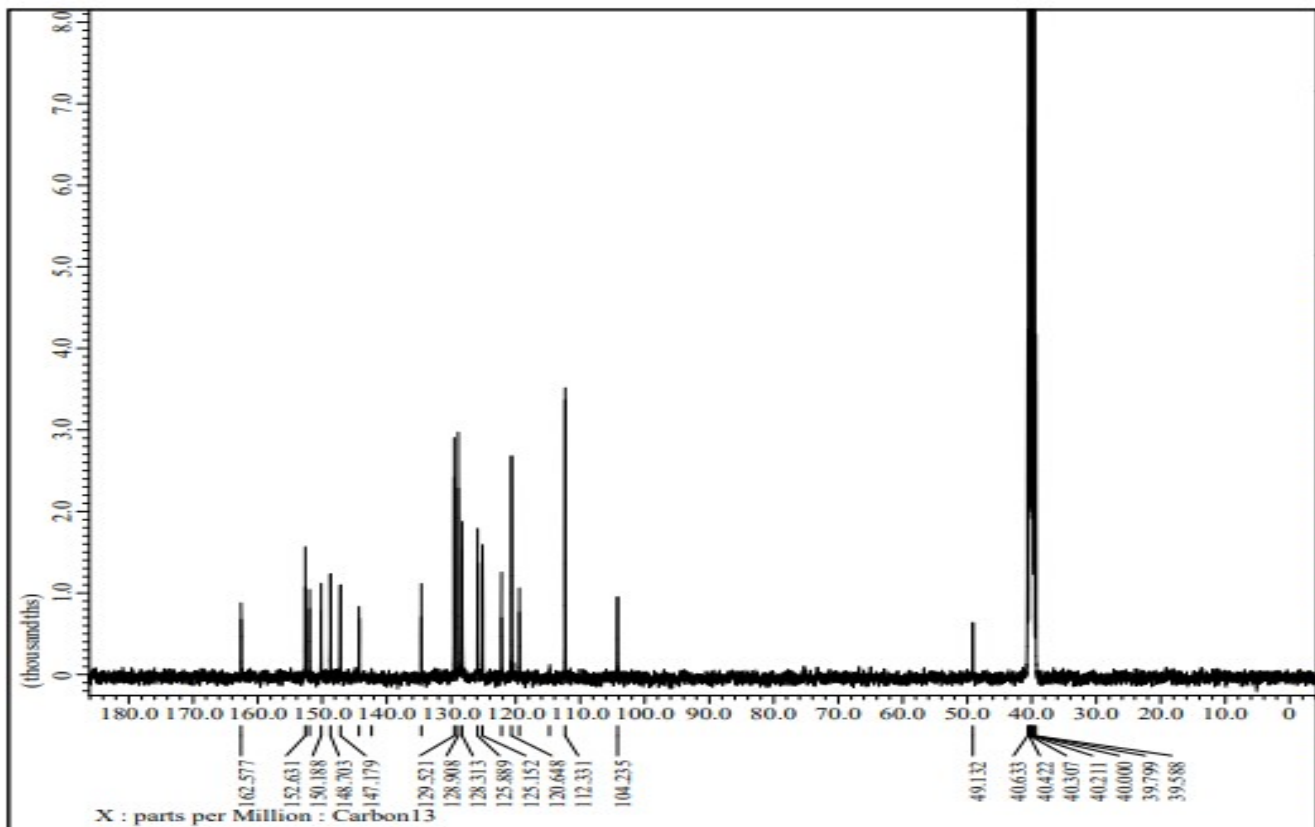
### LC-MS spectra of compound 6d



FTIR (KBr,  $\text{cm}^{-1}$ ) spectra of compound 6e

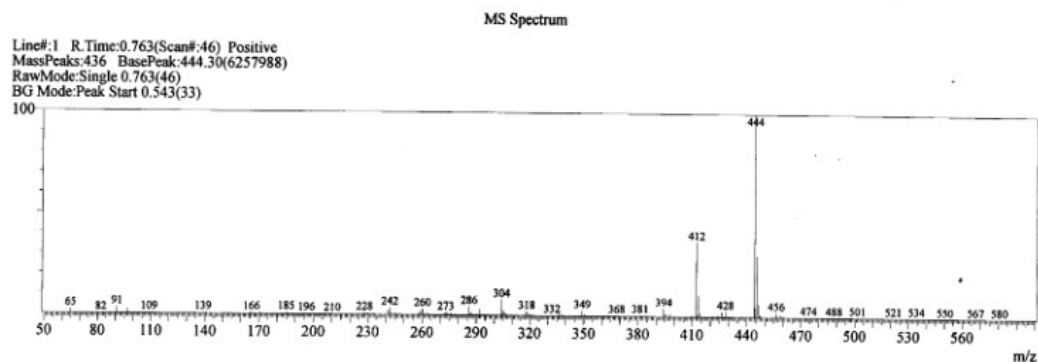
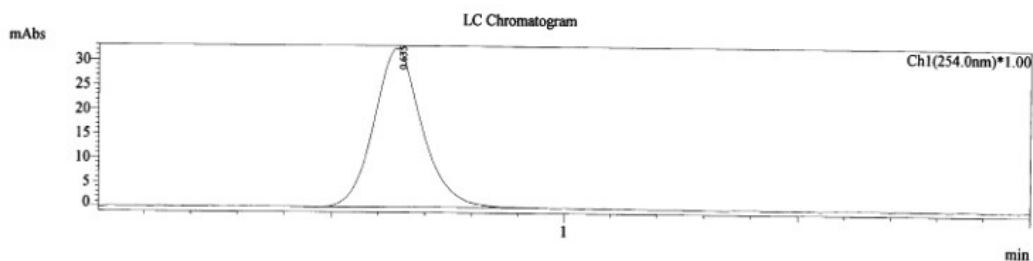


$^1\text{H}$  NMR (400 MHz,  $\delta$ , ppm) spectra of compound 6e

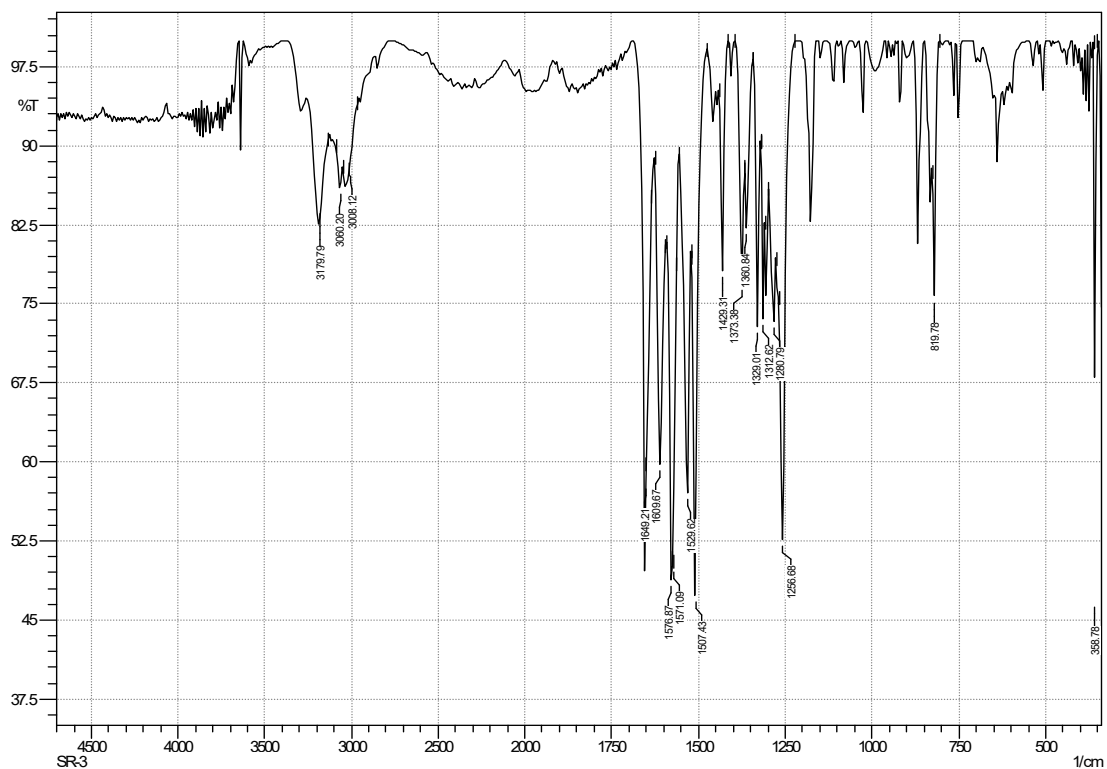


$^{13}\text{C}$  NMR (400 MHz,  $\delta$ , ppm) spectra of compound 6e

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 Sample : SR-12  
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 Method Name : C:\LCMSsolution\User\Method\esi.qlm

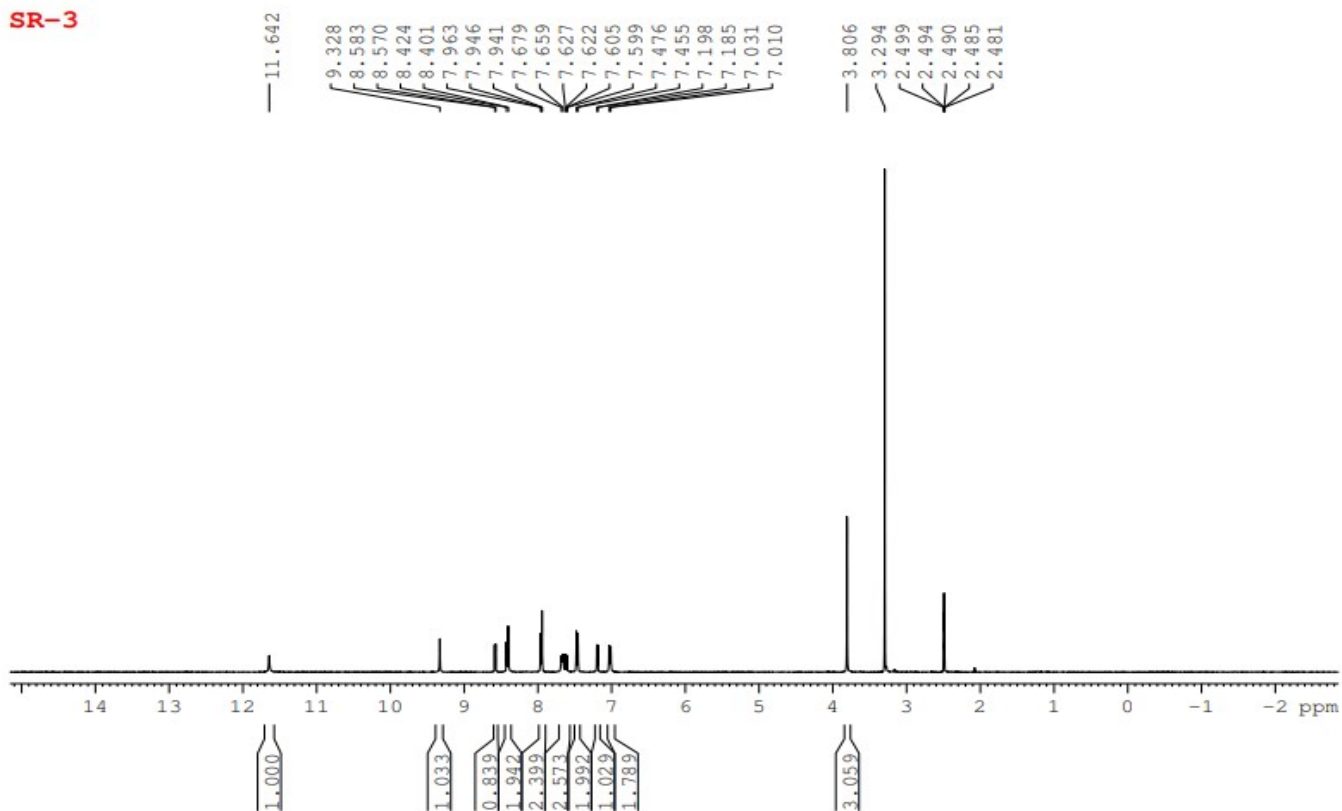


LC-MS spectra of compound 6e



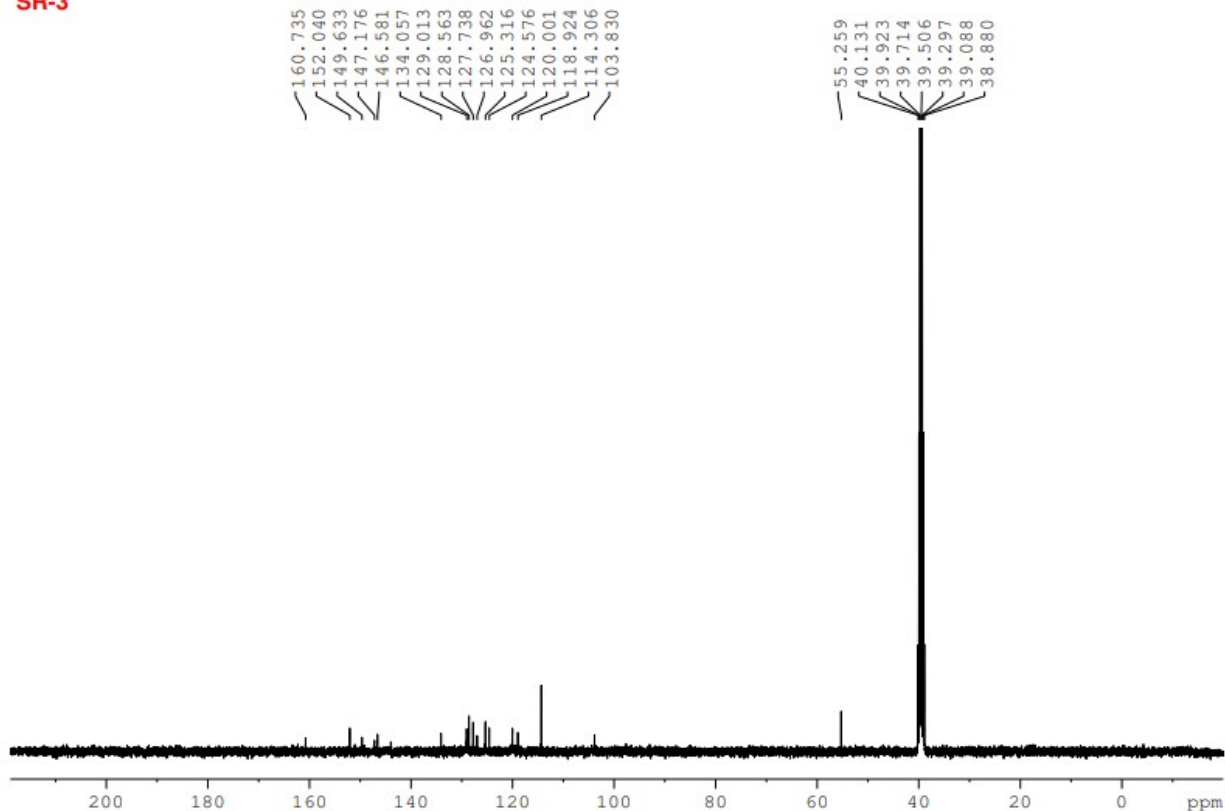
FTIR (KBr,  $\text{cm}^{-1}$ ) spectra of compound 6f

SR-3



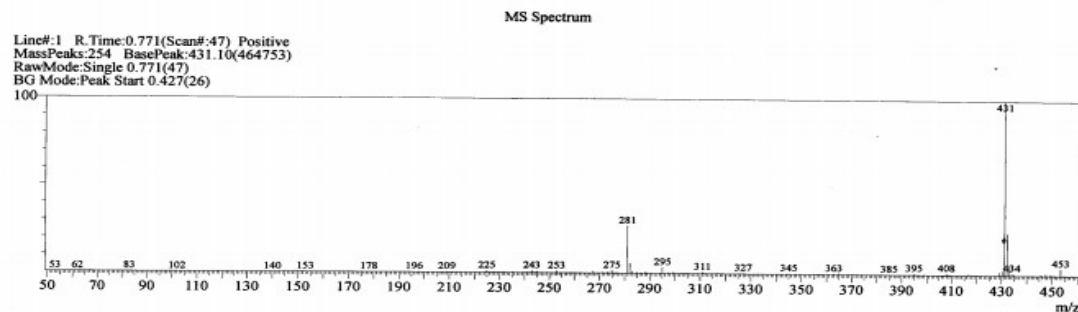
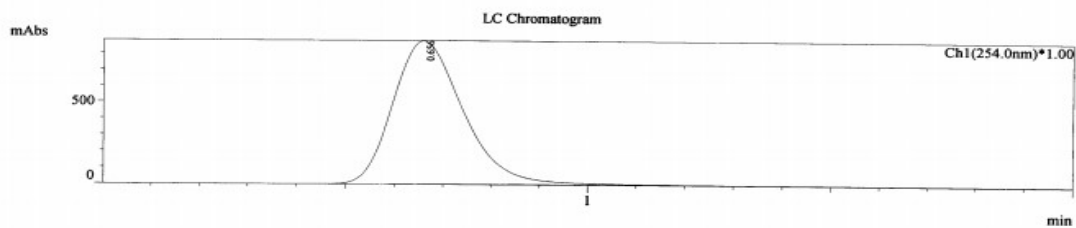
$^1\text{H}$  NMR (400 MHz,  $\delta$ , ppm) spectra of compound 6f

SR-3



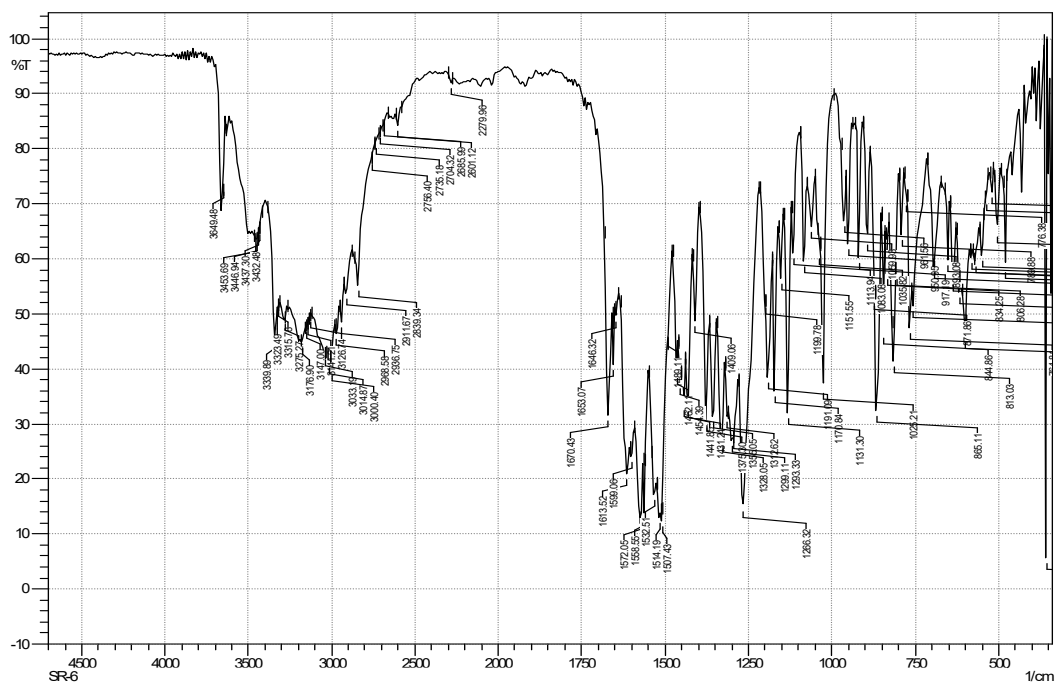
<sup>13</sup>C NMR (400 MHz, δ, ppm) spectra of compound 6f

User : Admin  
 Sample : SR-3  
 Inj. Volume : 5.000  
 Data Name : D:\lcms-data-c\SR-3-APCI-POS1.qld  
 Method Name : C:\LCMSsolution\User\Method\esi.qlm

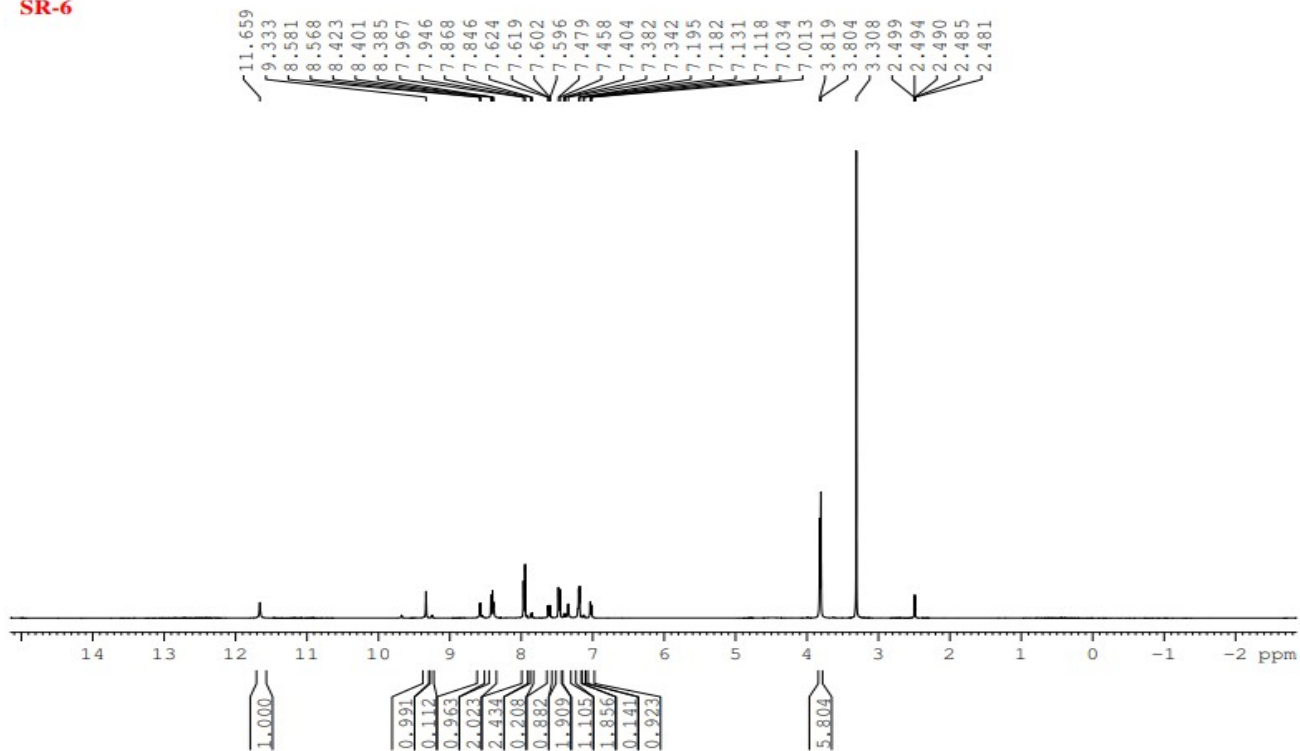


Peak#	R.Time	I.Time	F.Time	Area	Height	A/H	Mark	%Total	Name	Base m/z	Base Int.
1	0.771	0.427	1.460	42640671	1373942	31.03		100.00		431.10	464753
				42640671	1373942			100.00			

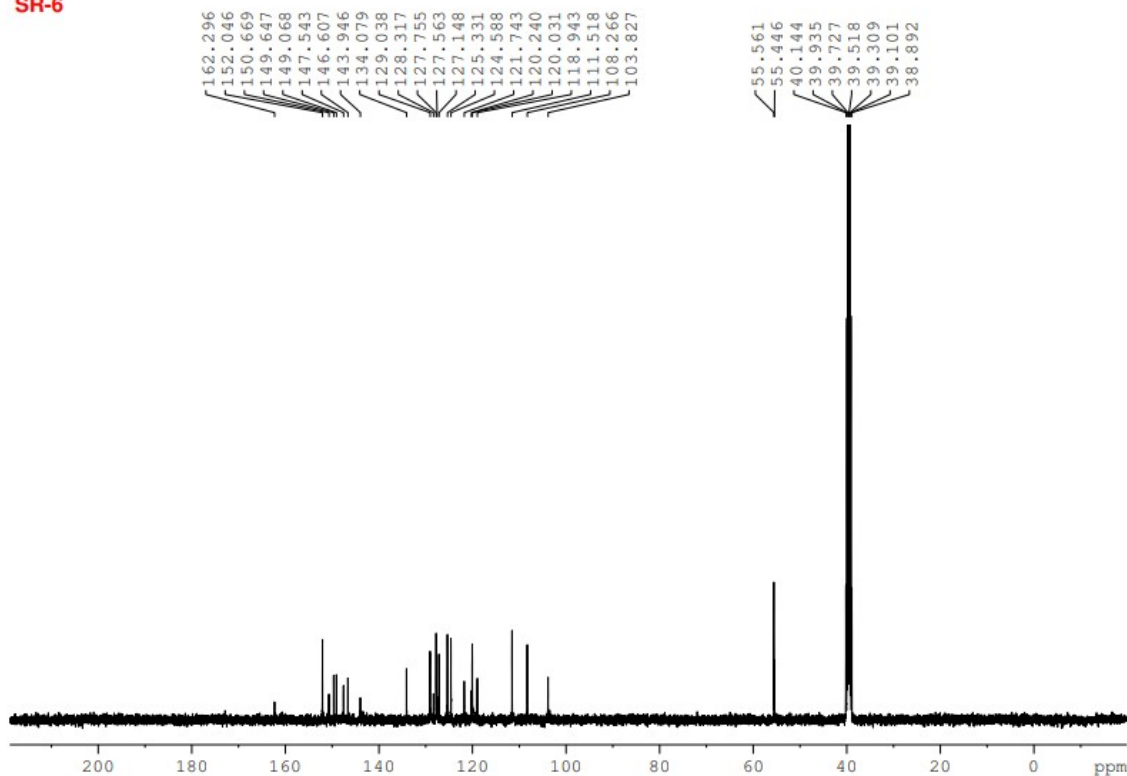
LC-MS spectra of compound 6f



SR-6

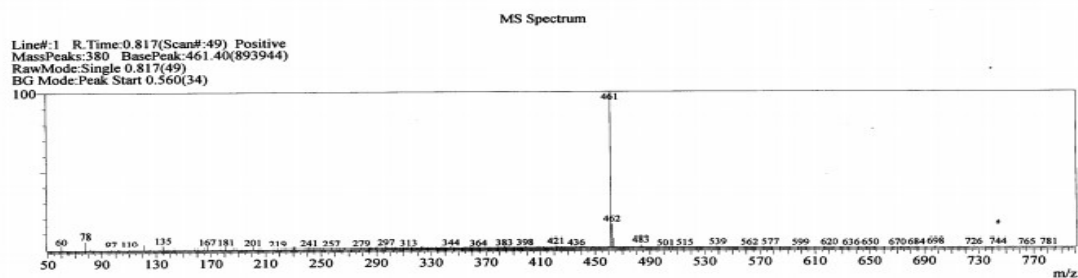
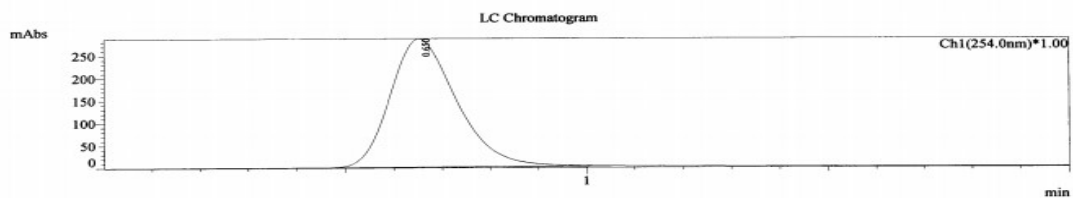


SR-6



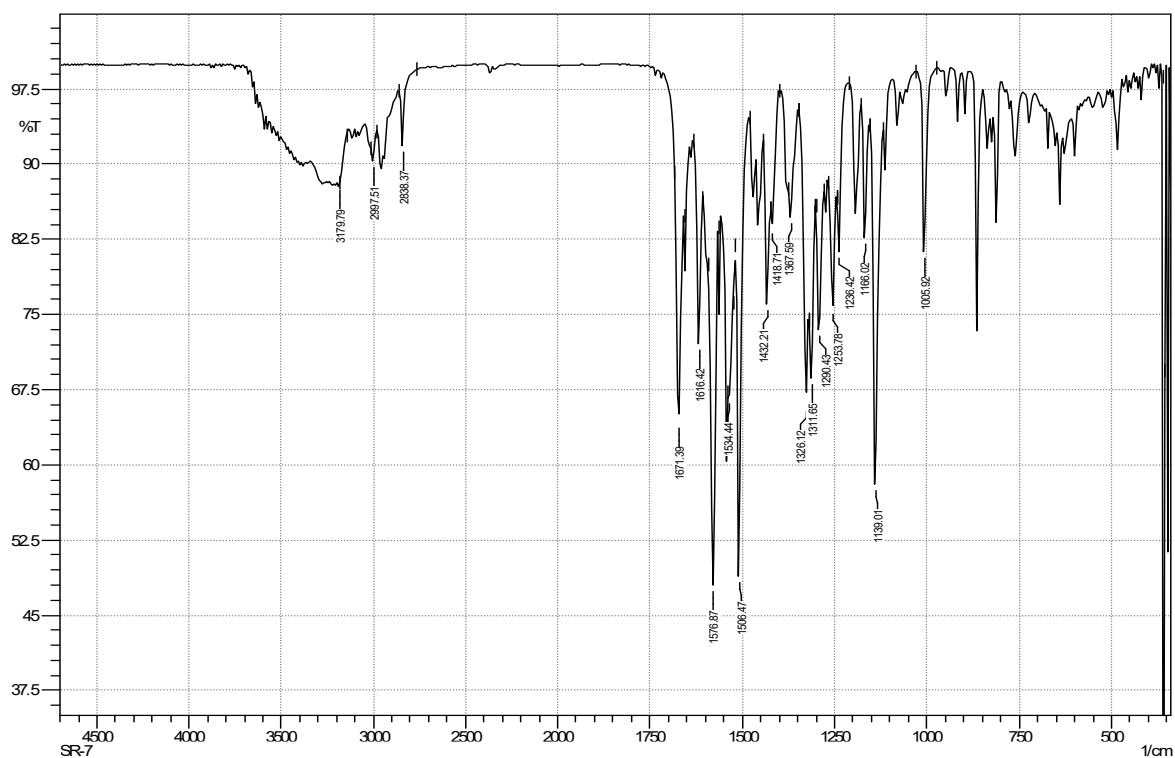
<sup>13</sup>C NMR (400 MHz, δ, ppm) spectra of compound 6g

User : Admin  
 Sample : SR-6  
 Inj. Volume : 5.000  
 Data Name : D:\lcms-data-c\SR-6-APCI-POS1.qld  
 Method Name : C:\LCMSsolution\User\Method\esi.qlm



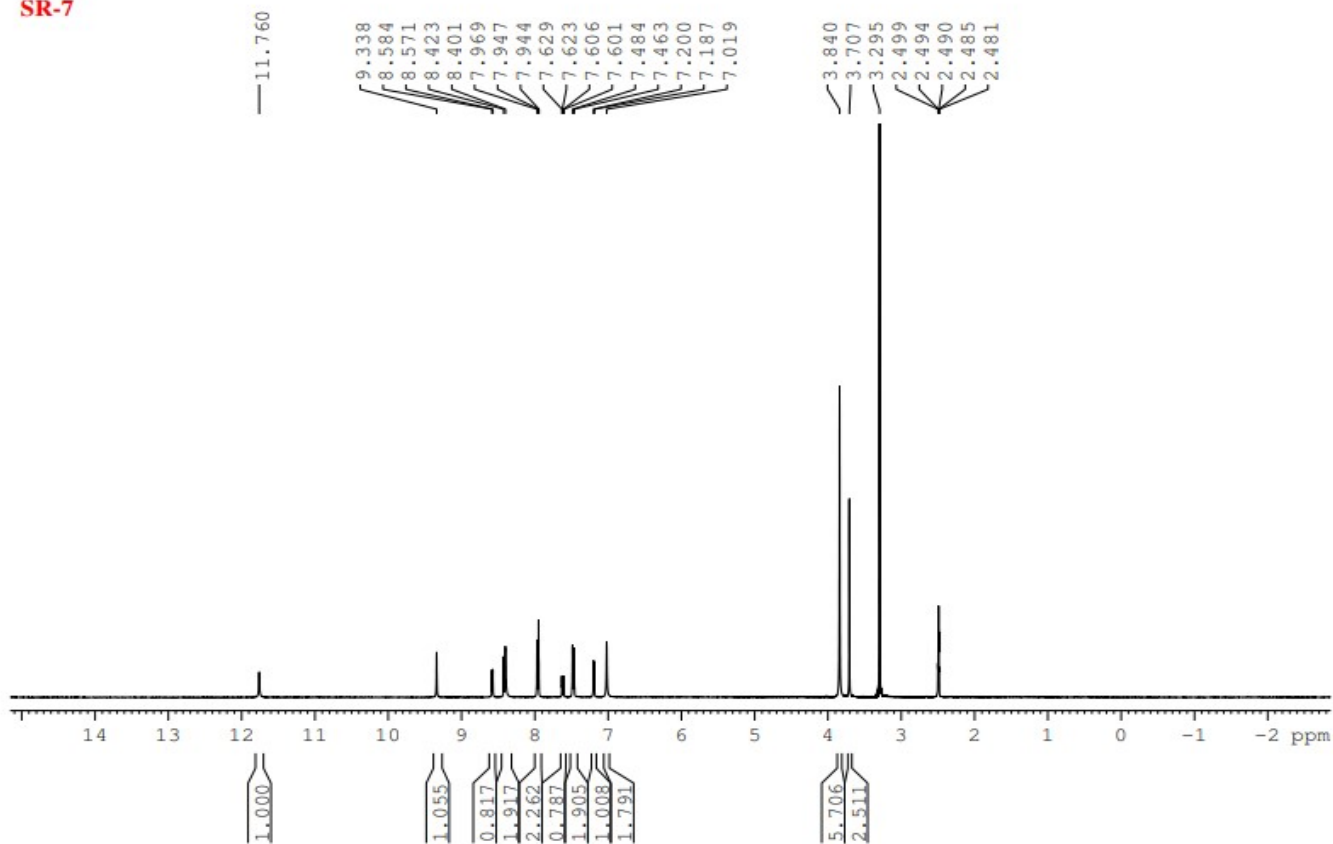
Peak#	R.Time	I.Time	F.Time	Area	Height	A/H	Mark	%Total	Name	Base m/z	Base Int.
1	0.817	0.560	1.143	20378433	1393488	14.62		100.00		461.40	893944
				20378433	1393488			100.00			

LC-MS spectra of compound 6g



FTIR (KBr,  $\text{cm}^{-1}$ ) spectra of compound 6h

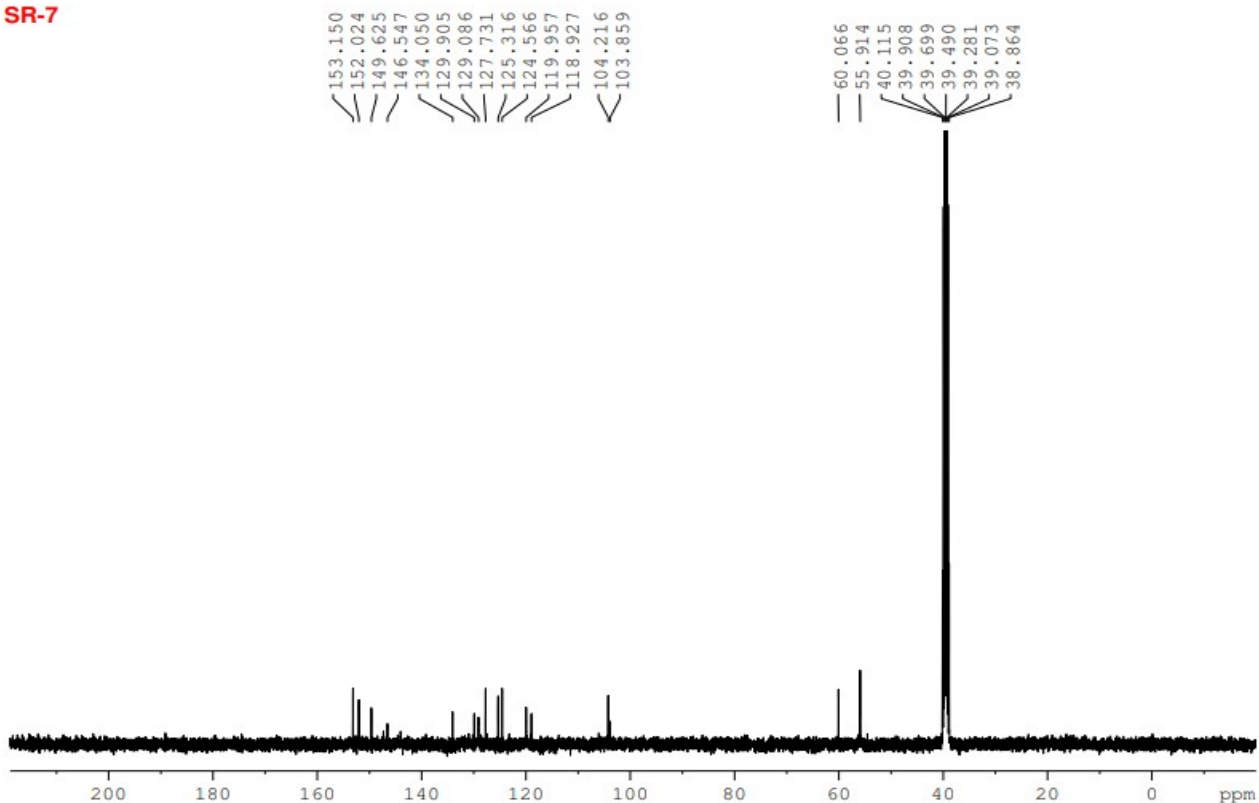
SR-7



$^1\text{H}$  NMR (400 MHz,  $\delta$ , ppm) spectra of compound 6h

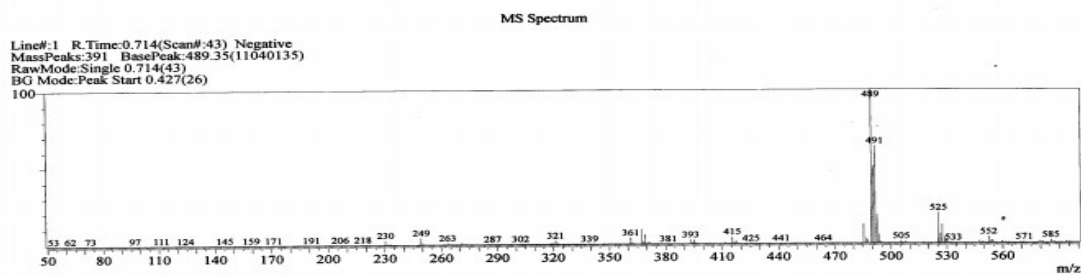
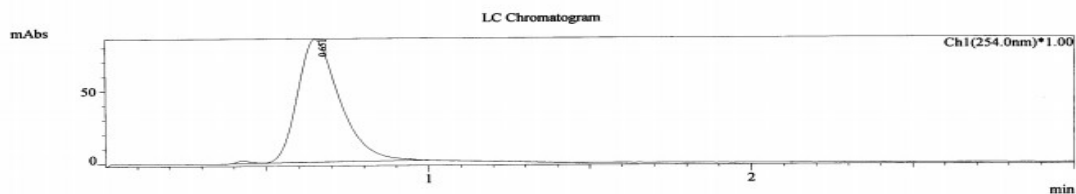


SR-7



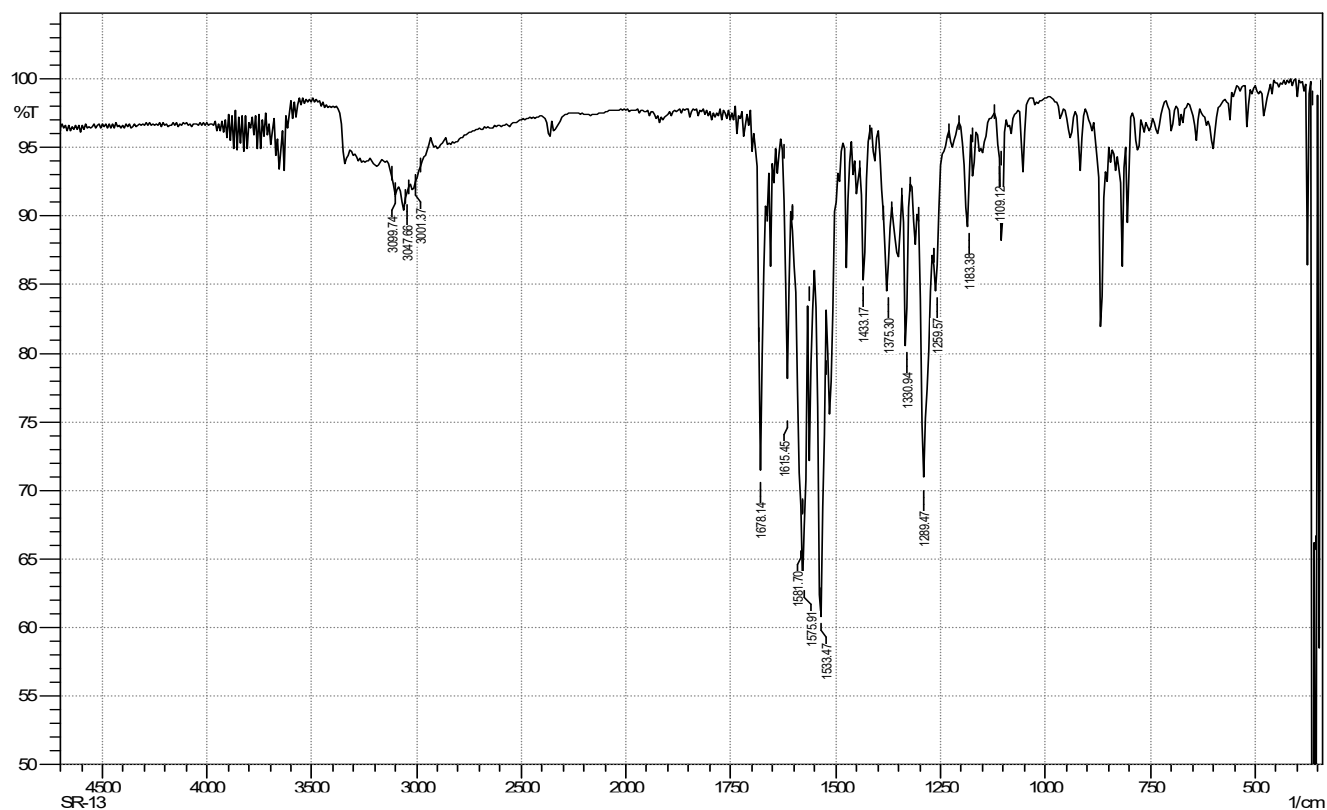
$^{13}\text{C}$  NMR (400 MHz,  $\delta$ , ppm) spectra of compound 6h

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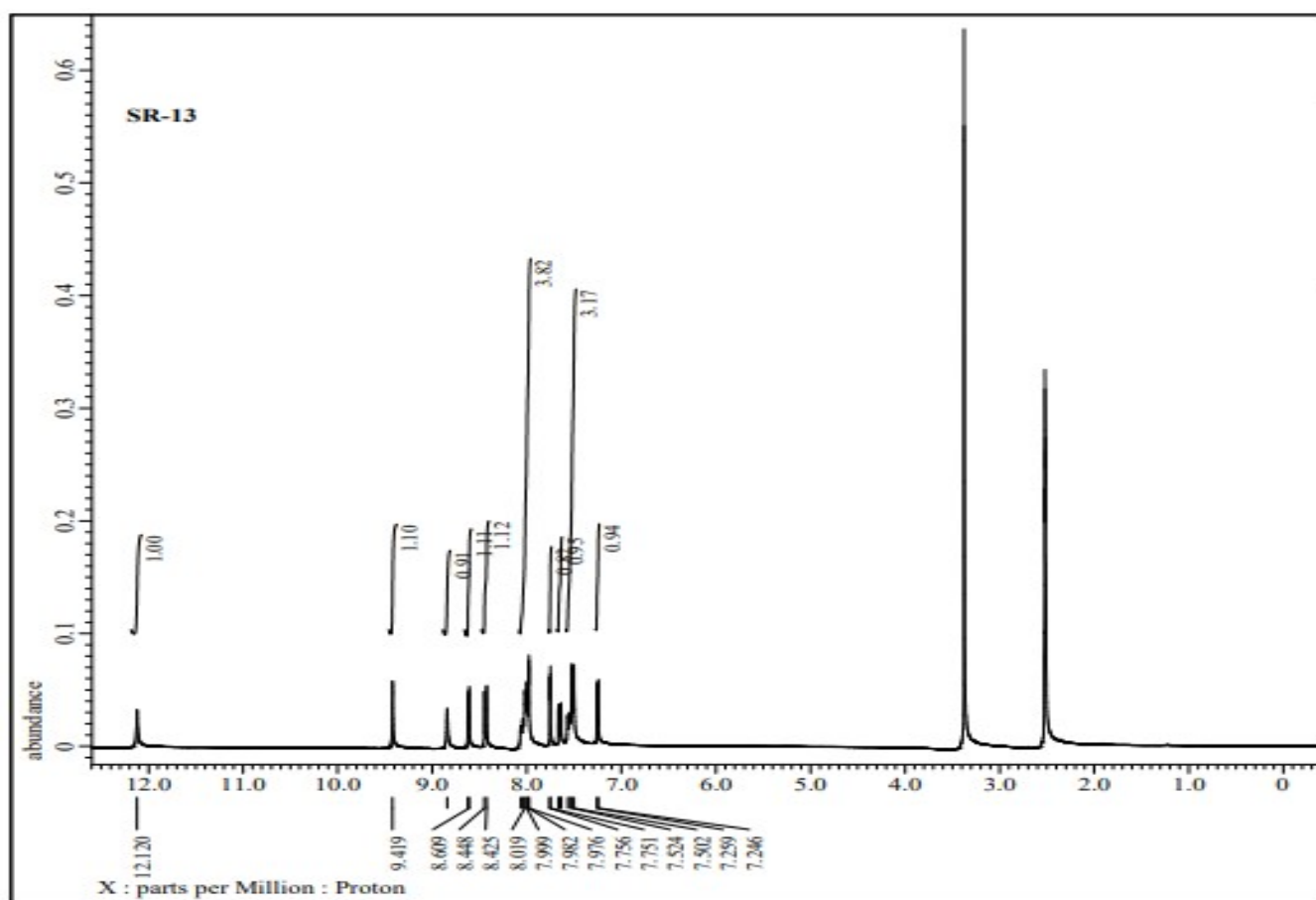


Peak#	R.Time	I.Time	F.Time	Area	Height	A/H	Mark	%Total	Name	Base m/z	Base Int.
1	0.714	0.427	1.043	817424646	43634230	18.73		100.00		489.35	11040135

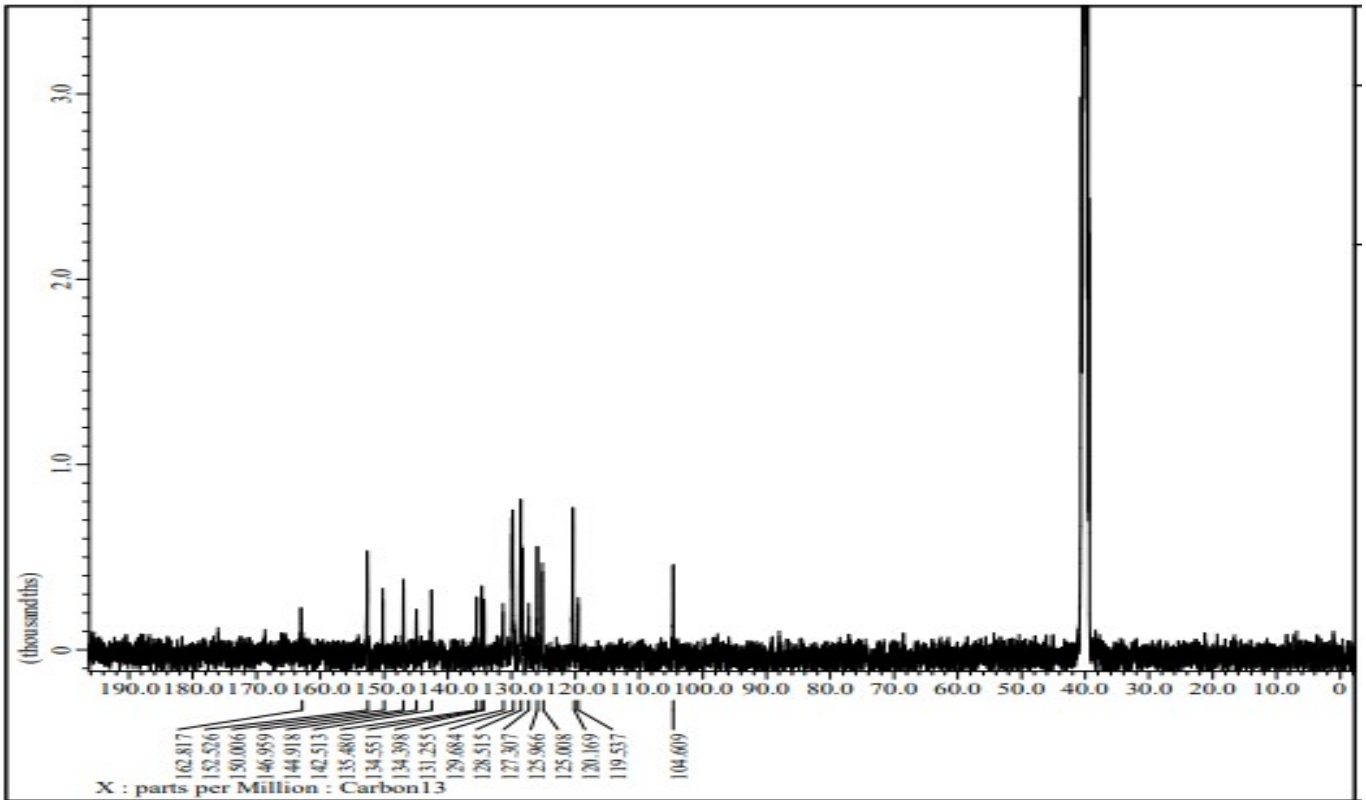
LC-MS spectra of compound 6h



FTIR (KBr,  $\text{cm}^{-1}$ ) spectra of compound 6i

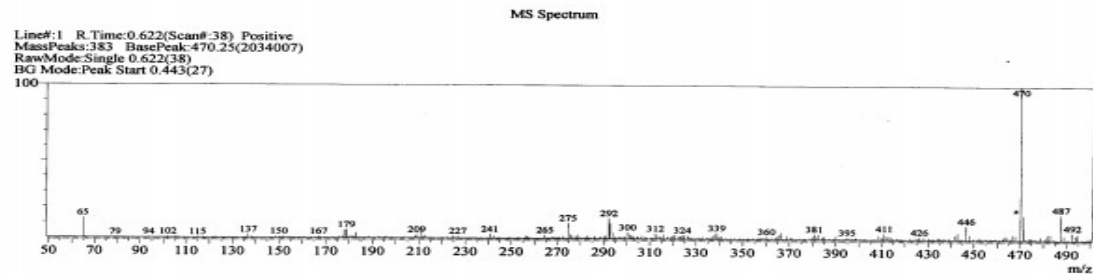
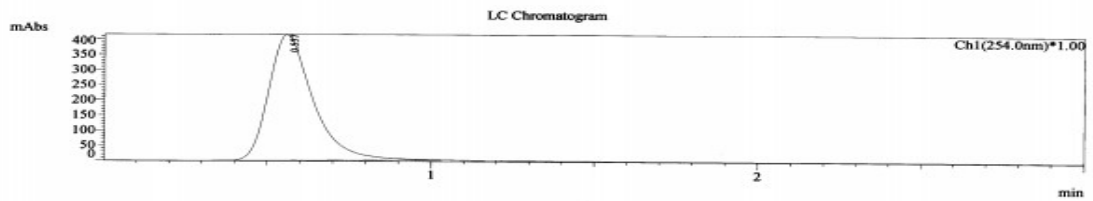


<sup>1</sup>H NMR (400 MHz, δ, ppm) spectra of compound 6i



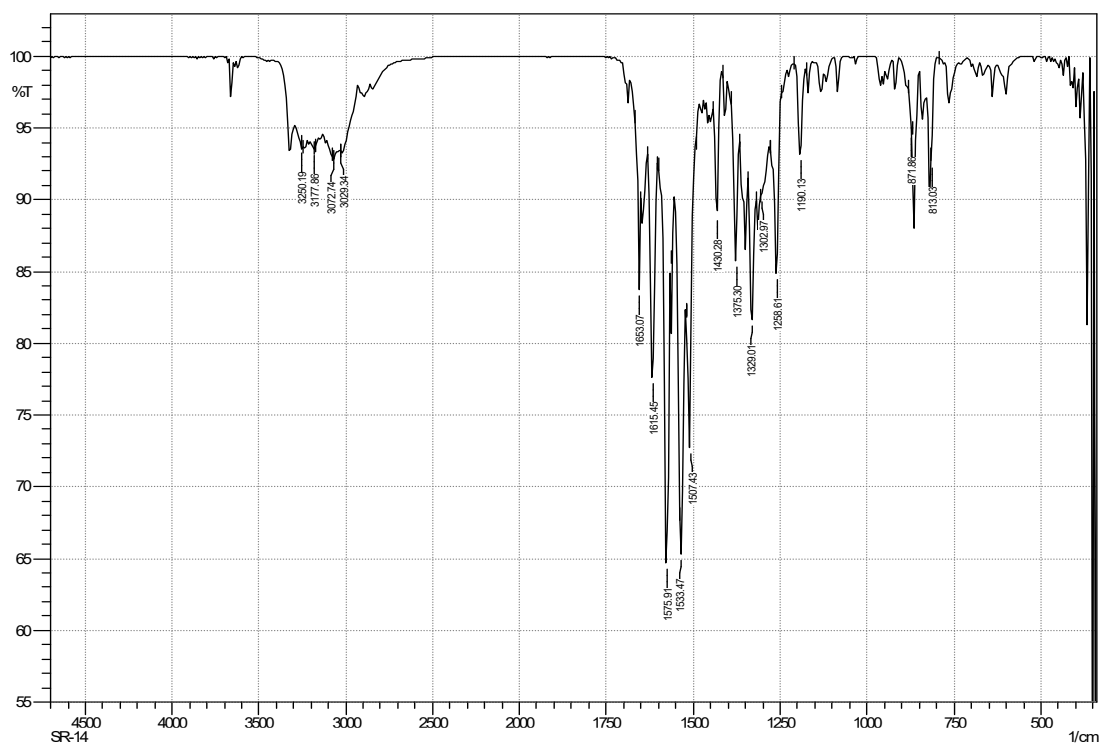
<sup>13</sup>C NMR (400 MHz, δ, ppm) spectra of compound 6i

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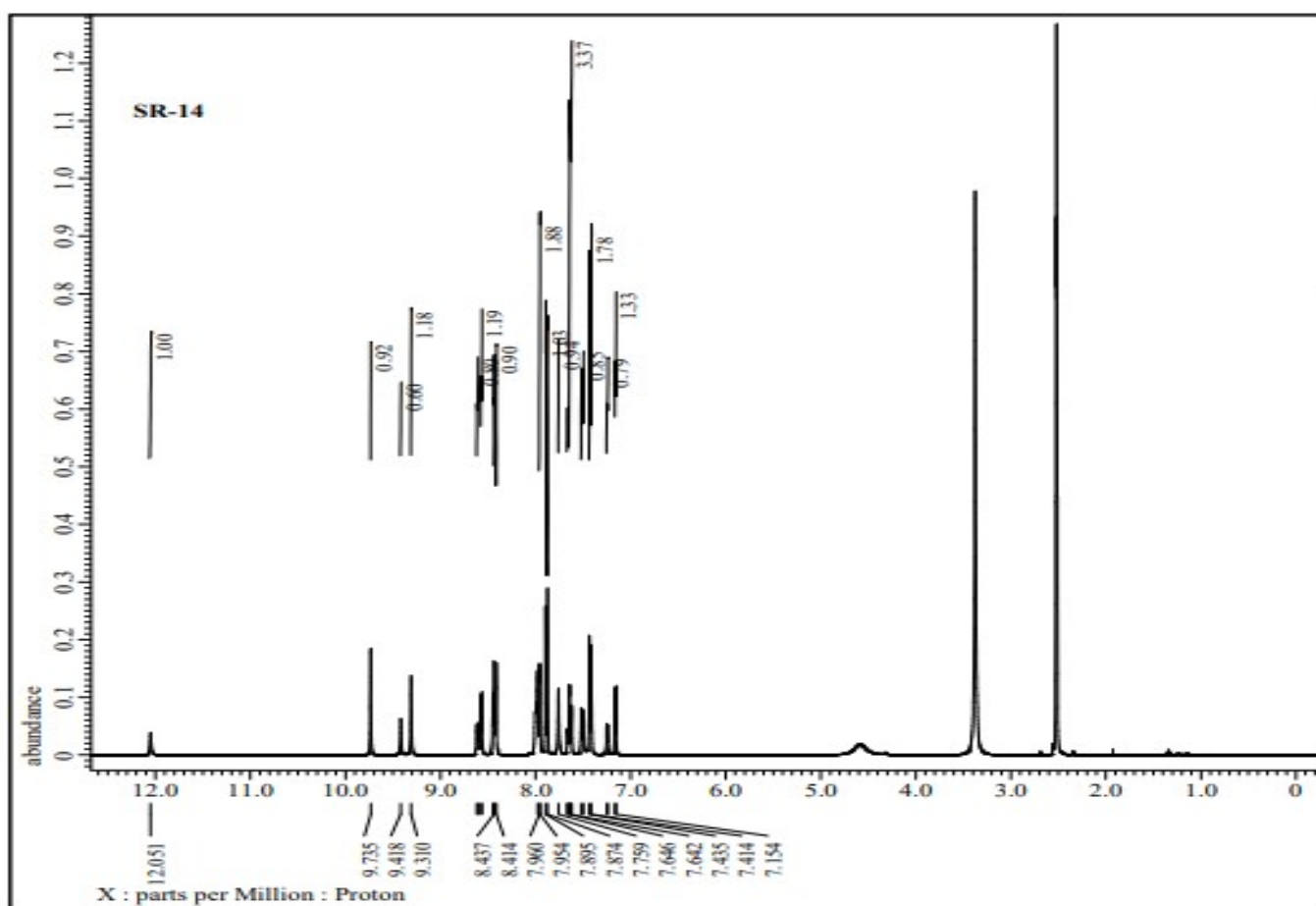


Peak#	R.Time	I.Time	F.Time	Area	Height	A/H	Mark	%Total	Name	Base m/z	Base Int.
1	0.622	0.443	0.843	237171585	25460835	9.31		100.00		470.25	2034007
				237171585	25460835			100.00			

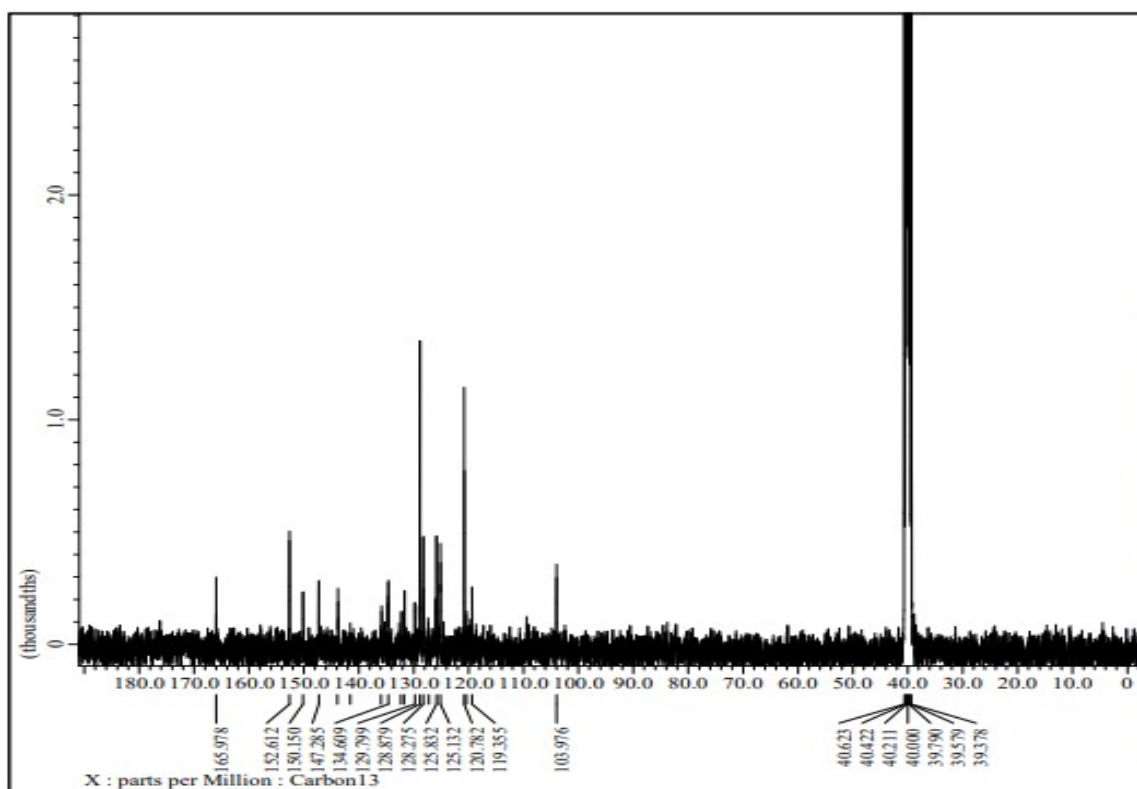
LC-MS spectra of compound 6i



FTIR (KBr, cm<sup>-1</sup>) spectra of compound 6j

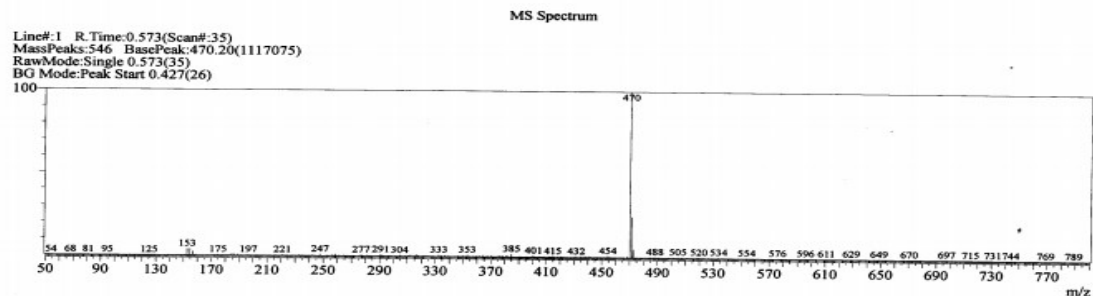
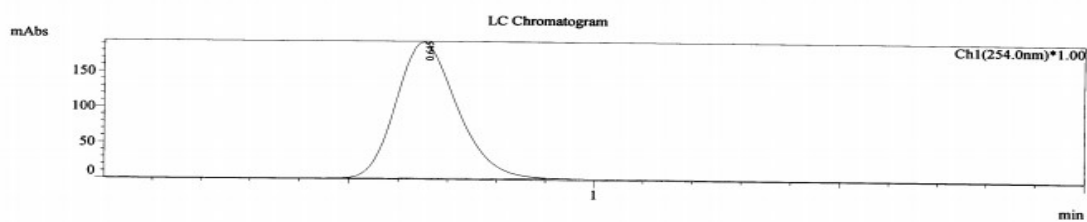


<sup>1</sup>H NMR (400 MHz, δ, ppm) spectra of compound 6j



<sup>13</sup>C NMR (400 MHz, δ, ppm) spectra of compound 6j

User : Admin  
 Sample : SR-14  
 Inj. Volume : 5.000  
 Data Name : D:\lcms-data1-c\SR-14-APCI-POS1.qld  
 Method Name : C:\LCMSsolution\User\Method\esi.qlm



Line# 1 R.Time:0.573(Scan#:35)  
 MassPeaks:546 BasePeak:470.20(1117075)  
 RawMode:Single 0.573(35)  
 BG Mode:Peak Start 0.427(26)

Peak#	R.Time	I.Time	F.Time	Area	Height	A/H	Mark	%Total	Name	Base m/z	Base Int.
1	0.573	0.427	0.960	22193071	1990096	11.15		100.00		470.20	1117075

LC-MS spectra of compound 6j

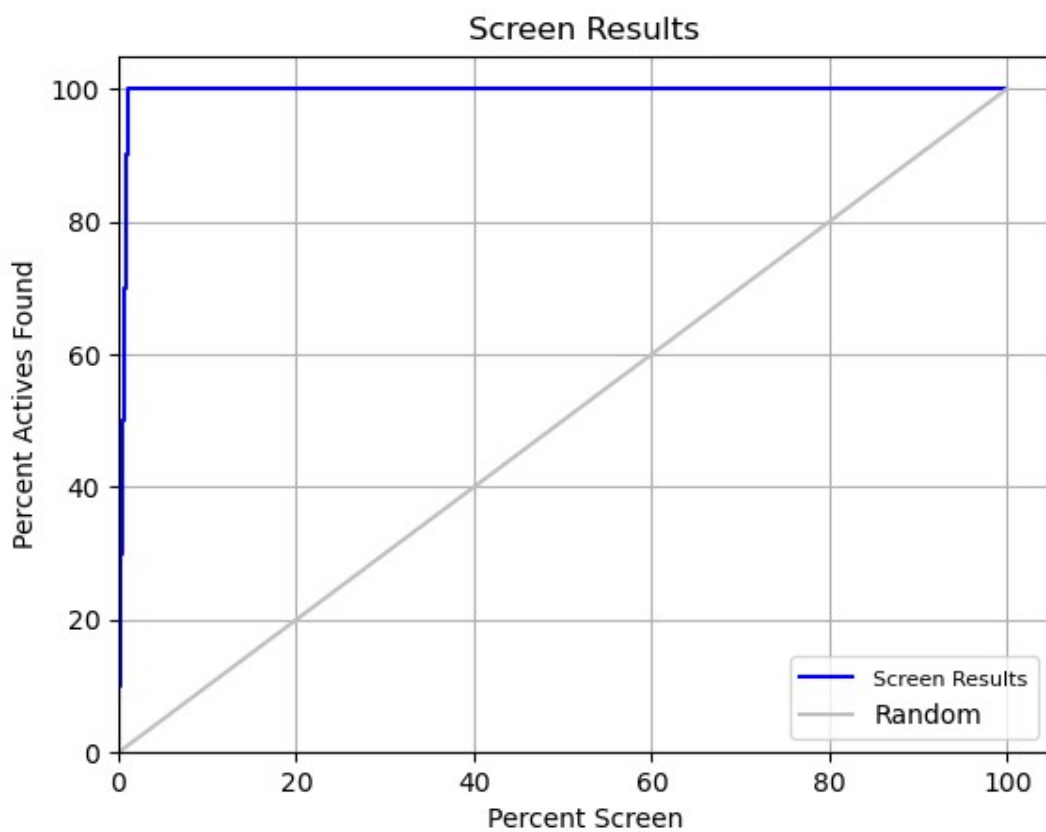
<b>Title</b>	<b>Survival Score</b>	<b>Site Score</b>	<b>Vector Score</b>	<b>Volume Score</b>	<b>BEDROC Score</b>	<b>PhaseHypoScore</b>
AADRR_1	5.069738	0.991397	0.955287	0.73662	0.98377	1.287982
AADRR_3	4.905304	0.813427	0.8755	0.715986	0.99262	1.286918
ADRR_2	4.84413	0.995019	0.941394	0.735339	0.987352	1.278046
AADRR_5	4.711901	0.723739	0.815888	0.631069	0.988926	1.271614
AAARR_2	4.739191	0.728928	0.8424	0.635954	0.973156	1.257552
AAADR_2	4.63441	0.823841	0.908019	0.715564	0.97829	1.256364
ADRR_1	4.87274	0.992516	0.944214	0.736519	0.962434	1.254762
AADR_2	4.6006	0.992794	0.952345	0.736964	0.973126	1.249136
AARR_3	4.602119	0.690675	0.957448	0.729225	0.863529	1.139626
AARR_2	4.724841	0.790252	0.964125	0.751729	0.842105	1.125588
ARRR_2	4.674086	0.685647	0.966347	0.716074	0.67823	0.958646

**Table. S1:** Total generated hypothesis.

<b>Title</b>	<b>Fitness</b>
6a	2.593529
6d	2.591902
6c	2.590907
6b	2.587568
6f	2.58324
6h	2.583012
6e	2.575609
6j	2.571411
6i	2.565869
6g	2.565004
schrod_417623	1.983863
schrod_540219	1.980556
schrod_801249	1.980008
schrod_652409	1.972778
schrod_666306	1.960321
schrod_262504	1.940985
schrod_277226	1.940023
schrod_441781	1.927018
schrod_704471	1.919194
6m	1.918694
schrod_795607	1.918697

schrod_459822	1.915985
schrod_650568	1.9158
schrod_614928	1.9154

**Table S2:** Top 10 identified molecules by pharmacophore based screening of designed molecules and Decoy set ligands.



**Fig.S1:** Enrichment analysis plot of pharmacophore based screening.