

## Quinoline-Sulfonamides as a Multi-targeting Neurotherapeutic for Cognitive Decline: In-vitro, In-silico studies and ADME evaluation of Monoamine Oxidases and Cholinesterases Inhibitors

Saquib Jalil<sup>1,2</sup>, Zahid hussain<sup>1</sup>, Syed Mobashir Ali Abid<sup>1,2</sup>, Abdul Hameed,<sup>4</sup> Jamshed Iqbal<sup>1,2,3</sup>

<sup>1</sup>Centre for Advanced Drug Research, Department of Pharmacy COMSATS University Islamabad, Abbottabad Campus, Abbottabad-22060, Pakistan

<sup>2</sup>Department of Pharmacy COMSATS University Islamabad, Abbottabad Campus, Abbottabad. 22060, Pakistan

<sup>3</sup>Department of Chemistry, COMSATS University Islamabad, Abbottabad Campus, Abbottabad 22060, Pakistan

<sup>4</sup>Department of Chemistry, University of Sahiwal, Sahiwal, 57000, Pakistan

### List of Figures

<b>Figure 1:</b> <sup>1</sup> HNMR of compound <b>a1</b> .....	4
<b>Figure 2:</b> <sup>13</sup> CNMR of compound <b>a1</b> .....	5
<b>Figure 3:</b> <sup>1</sup> HNMR of compound <b>a2</b> .....	5
<b>Figure 4:</b> <sup>13</sup> CNMR of compound <b>a2</b> .....	6
<b>Figure 5:</b> <sup>1</sup> HNMR of compound <b>a3</b> .....	6
<b>Figure 6:</b> <sup>13</sup> CNMR of compound <b>a3</b> .....	7
<b>Figure 7:</b> <sup>1</sup> HNMR of compound <b>a4</b> .....	7
<b>Figure 8:</b> <sup>13</sup> CNMR of compound <b>a4</b> .....	8
<b>Figure 9:</b> <sup>1</sup> HNMR of compound <b>a5</b> .....	9
<b>Figure 10:</b> <sup>13</sup> CNMR of compound <b>a5</b> .....	9
<b>Figure 11:</b> <sup>1</sup> HNMR of compound <b>a6</b> .....	10
<b>Figure 12:</b> <sup>13</sup> CNMR of compound <b>a6</b> .....	10
<b>Figure 13:</b> <sup>1</sup> HNMR of compound <b>a8</b> .....	11
<b>Figure 14:</b> <sup>13</sup> CNMR of compound <b>a8</b> .....	11
<b>Figure 15:</b> <sup>1</sup> NMR of compound <b>a9</b> .....	12
<b>Figure 16:</b> <sup>13</sup> CNMR of compound <b>a9</b> .....	12
<b>Figure 17:</b> <sup>1</sup> HNMR of compound <b>a10</b> .....	13
<b>Figure 18:</b> <sup>13</sup> CNMR of compound <b>10</b> .....	13
<b>Figure 19:</b> <sup>1</sup> HNMR of compound <b>a11</b> .....	14
<b>Figure 20:</b> <sup>13</sup> CNMR of compound <b>a11</b> .....	14
<b>Figure 21:</b> <sup>1</sup> HNMR of compound <b>a12</b> .....	15

<b>Figure 22:</b> $^{13}\text{C}$ NMR of compound <b>a12</b> .....	15
<b>Figure 23:</b> $^1\text{H}$ NMR of compound <b>a14</b> .....	16
<b>Figure 24:</b> $^{13}\text{C}$ NMR of compound <b>a14</b> .....	16
<b>Figure 25:</b> $^1\text{H}$ NMR of compound <b>a15</b> .....	17
<b>Figure 26:</b> $^{13}\text{C}$ NMR of compound <b>a15</b> .....	18
<b>Figure 27:</b> $^1\text{H}$ NMR of compound <b>a16</b> .....	18
<b>Figure 28:</b> $^{13}\text{C}$ NMR of compound <b>a16</b> .....	19
<b>Figure 29:</b> $^1\text{H}$ NMR of compound <b>a17</b> .....	20
<b>Figure 30:</b> $^{13}\text{C}$ NMR of compound <b>a17</b> .....	20
<b>Figure 31:</b> $^1\text{H}$ NMR of compound <b>a18</b> .....	21
<b>Figure 32:</b> $^{13}\text{C}$ NMR of compound <b>a18</b> .....	21
<b>Figure 33:</b> FTIR graph of compound <b>a1</b> .....	22
<b>Figure 34:</b> FTIR graph of compound <b>a2</b> .....	22
<b>Figure 35:</b> FTIR graph of compound <b>a3</b> .....	23
<b>Figure 36:</b> FTIR graph of compound <b>a4</b> .....	23
<b>Figure 37:</b> FTIR graph of compound <b>a5</b> .....	24
<b>Figure 38:</b> FTIR graph of compound <b>a6</b> .....	24
<b>Figure 39:</b> FTIR graph of compound <b>a7</b> .....	25
<b>Figure 40:</b> FTIR graph of compound <b>a8</b> .....	25
<b>Figure 41:</b> FTIR graph of compound <b>a9</b> .....	26
<b>Figure 42:</b> FTIR graph of compound <b>a10</b> .....	26
<b>Figure 43:</b> FTIR graph of compound <b>a11</b> .....	27
<b>Figure 44:</b> FTIR graph of compound <b>a12</b> .....	28
<b>Figure 45:</b> FTIR graph of compound <b>a13</b> .....	28
<b>Figure 46:</b> FTIR graph of compound <b>a14</b> .....	29
<b>Figure 47:</b> FTIR graph of compound <b>a15</b> .....	29
<b>Figure 48:</b> FTIR graph of compound <b>a16</b> .....	30
<b>Figure 49:</b> FTIR graph of compound <b>a17</b> .....	30
<b>Figure 50:</b> FTIR graph of compound <b>a18</b> .....	31
<b>Figure 51:</b> Chromatogram of compound <b>a5</b> .....	32
<b>Figure 52:</b> Chromatogram of compound <b>a3</b> .....	33
<b>Figure 53:</b> Chromatogram of compound <b>a4</b> .....	34

<b>Figure 54:</b> 2d interaction of compound <b>a5</b> left side MAO-A (a) and <b>a12</b> right side MAO-B (b).....	45
<b>Figure 55:</b> 2d interaction of compound <b>a11</b> left side AChE (c) and <b>a6</b> right side BChE (d).....	45

### **List of Tables**

<b>Table 1:</b> The docking scores of synthesized compounds on MAO-A, MAO-B, AChE, and BChE.....	34
<b>Table 2:</b> IC <sub>50</sub> values of synthesized compounds against monoamine oxidase.....	35
<b>Table 3:</b> IC <sub>50</sub> values of synthesized compounds against AChE and BChE .....	39

## Supporting Information

### 1.1 $^1\text{H}$ NMR, $^{13}\text{C}$ NMR Spectra of the synthesized compounds

#### Compound a1

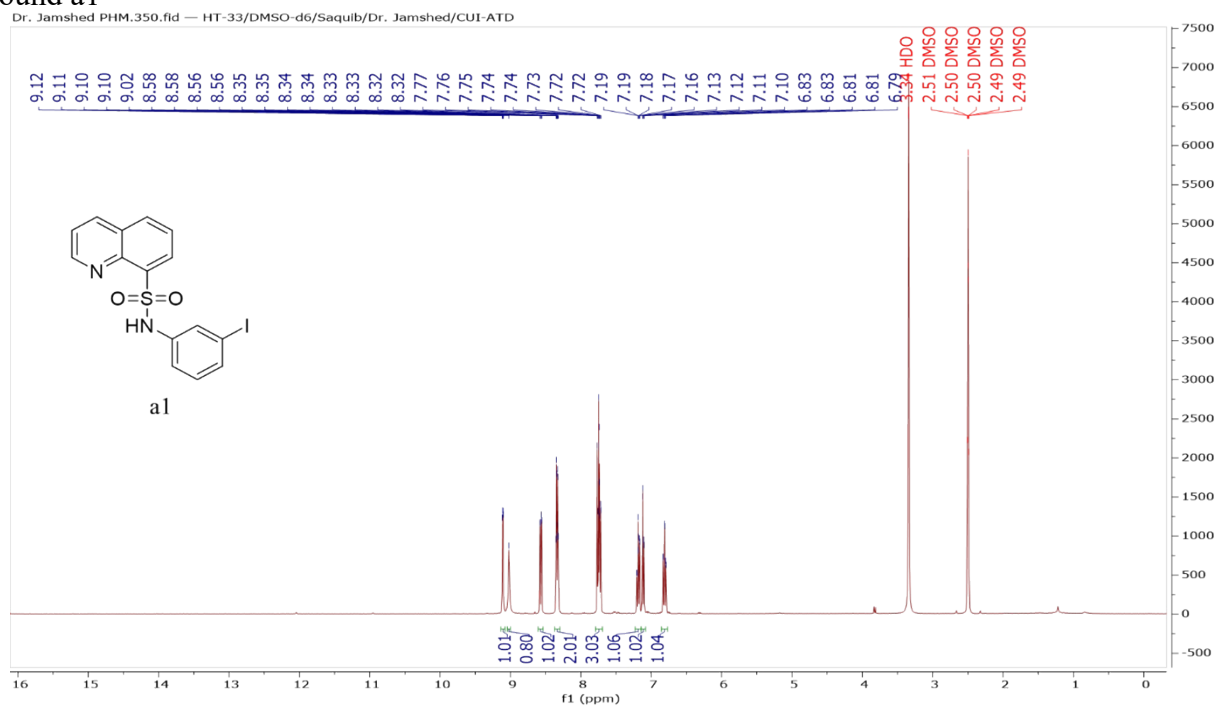


Figure 1:  $^1\text{H}$ NMR of compound a1

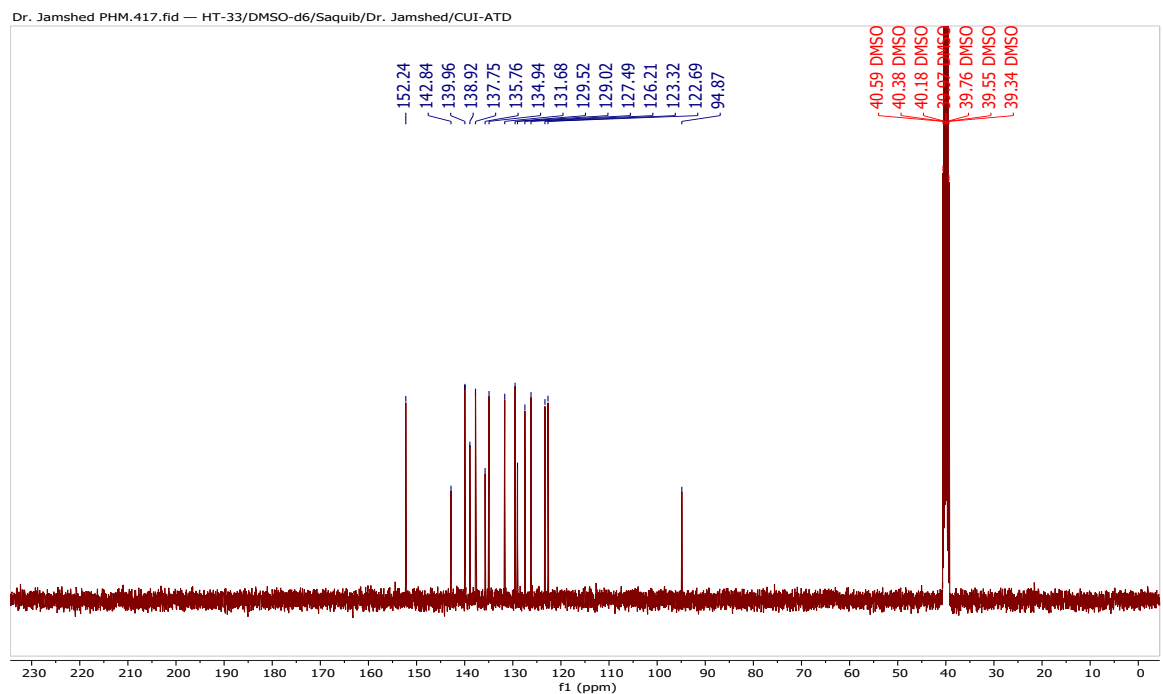


Figure 2:  $^{13}\text{C}$ NMR of compound a1

# Compound a2

Dr. Jamshed PHM.351.fid — HT-34/DMSO-d6/Saqib/Dr. Jamshed/CUI-ATD

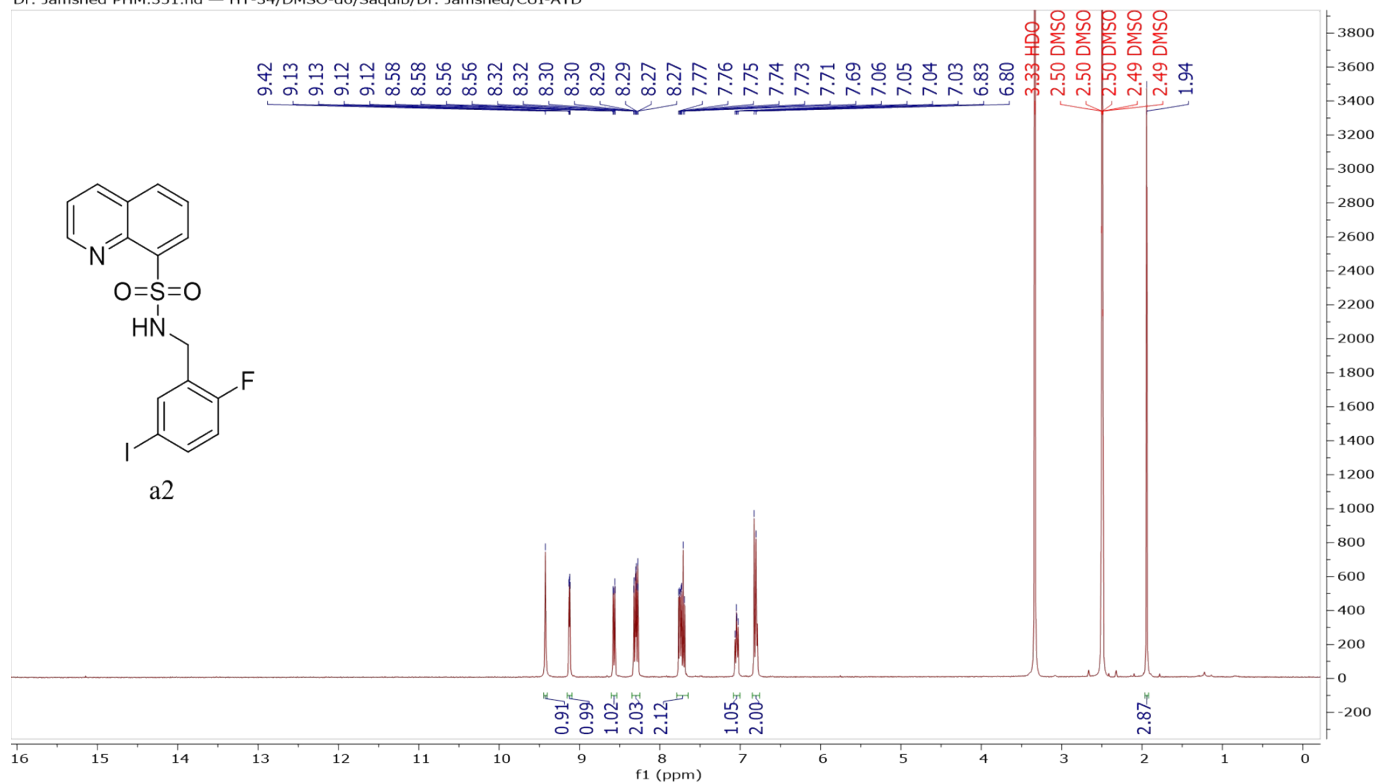


Figure 3: <sup>1</sup>H NMR of compound a2

Dr. Jamshed PHM.418.fid — HT-34/DMSO-d6/Saqib/Dr. Jamshed/CUI-ATD

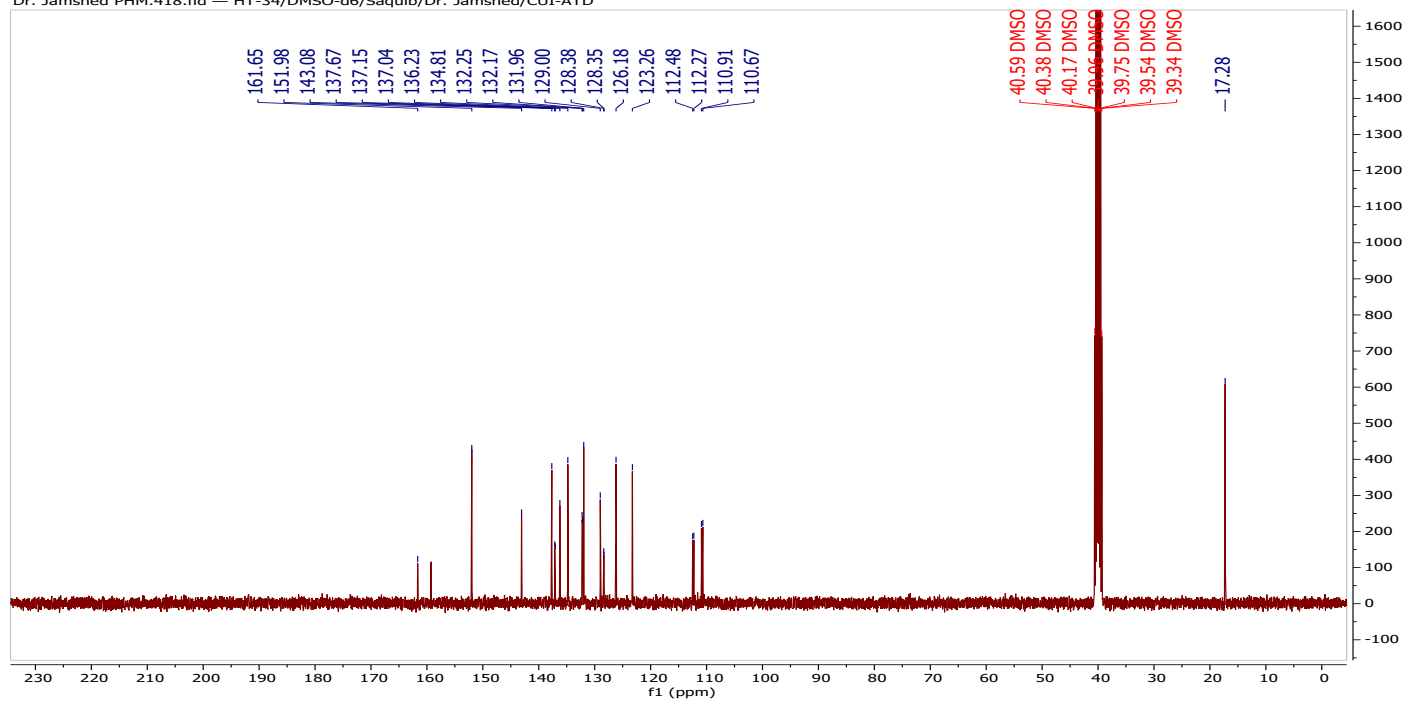


Figure 4: <sup>13</sup>C NMR of compound a2

# Compound a3

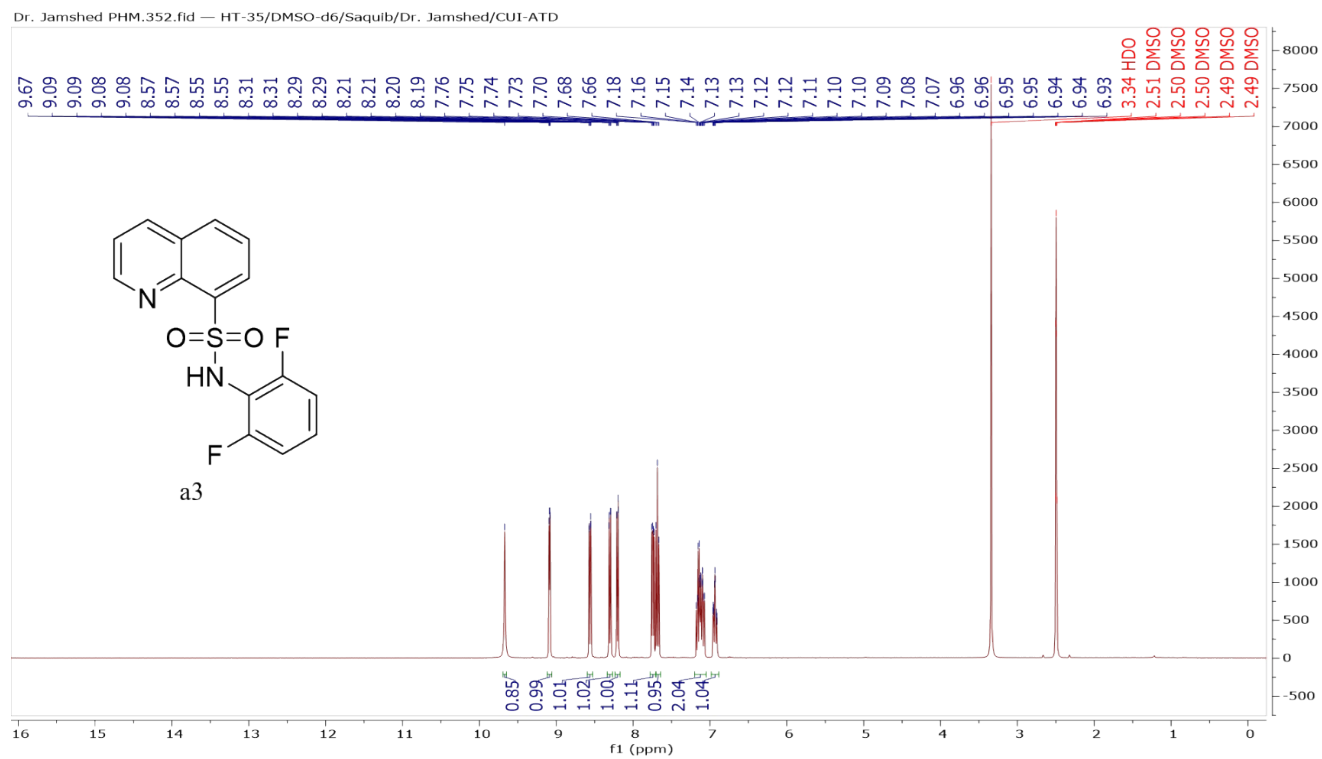


Figure 5: <sup>1</sup>H NMR of compound a3

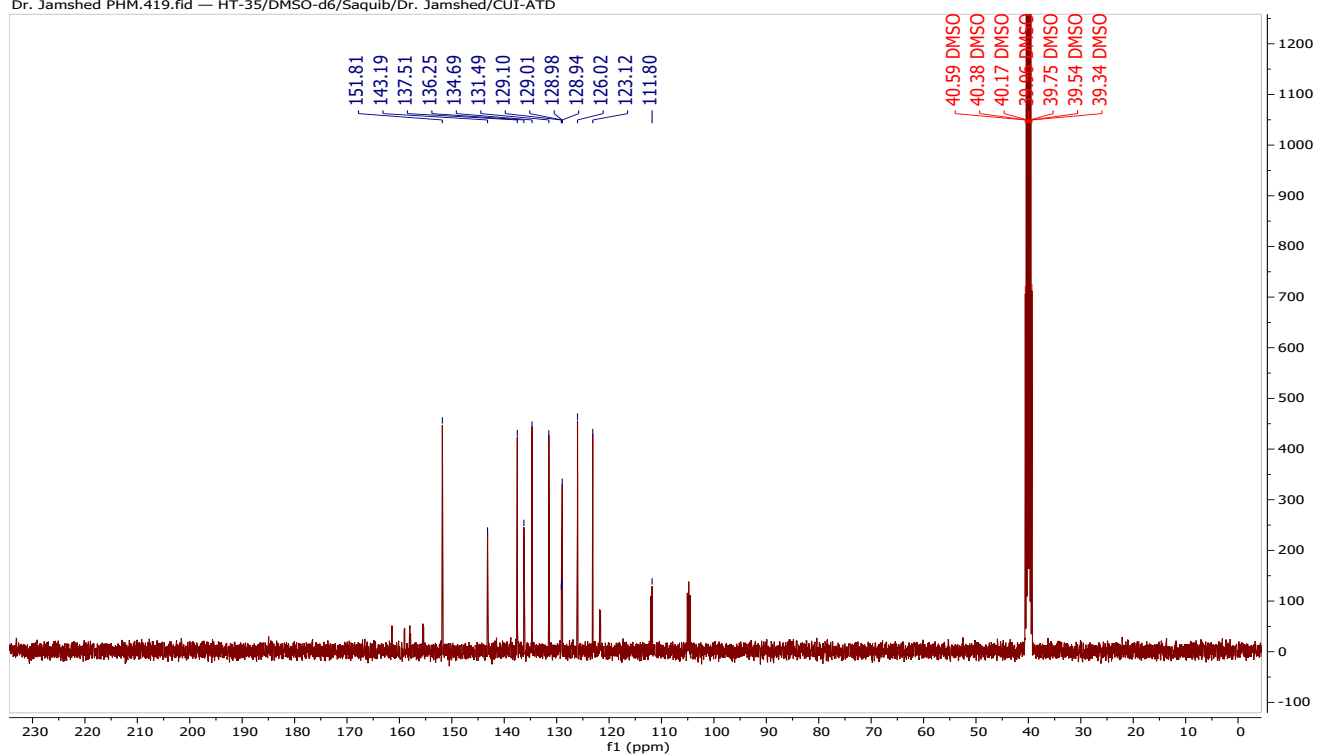


Figure 6: <sup>13</sup>CNMR of compound a3

Compound a4

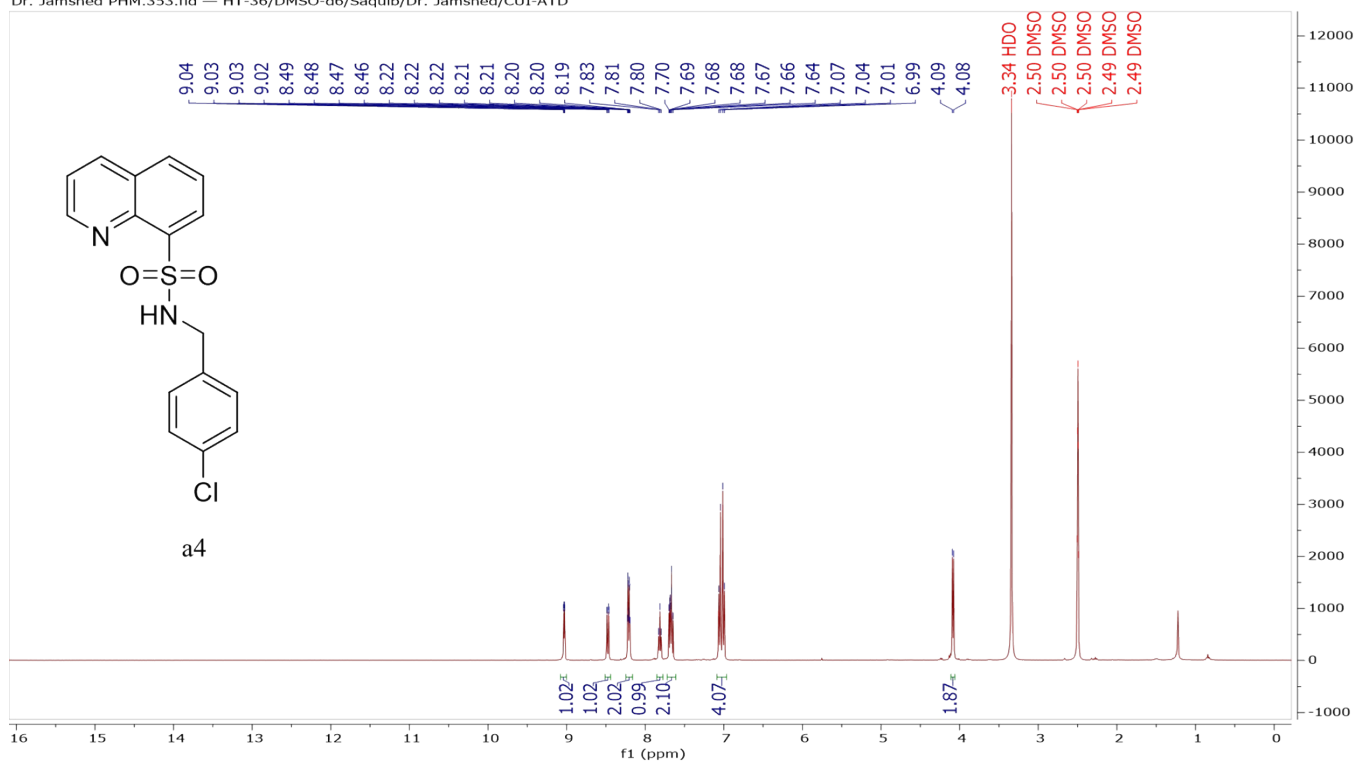


Figure 7: <sup>1</sup>HNMR of compound a4

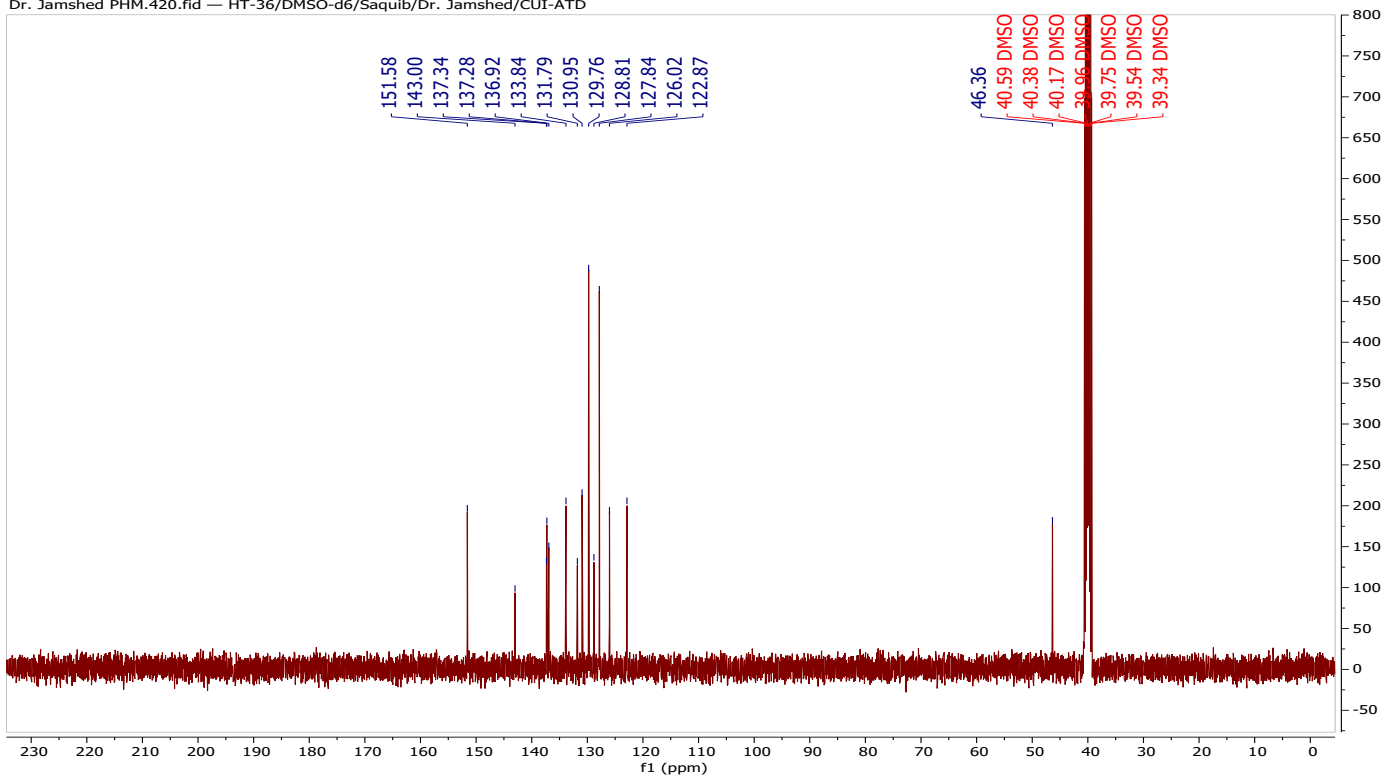


Figure 8: <sup>13</sup>CNMR of compound a4

Compound a5



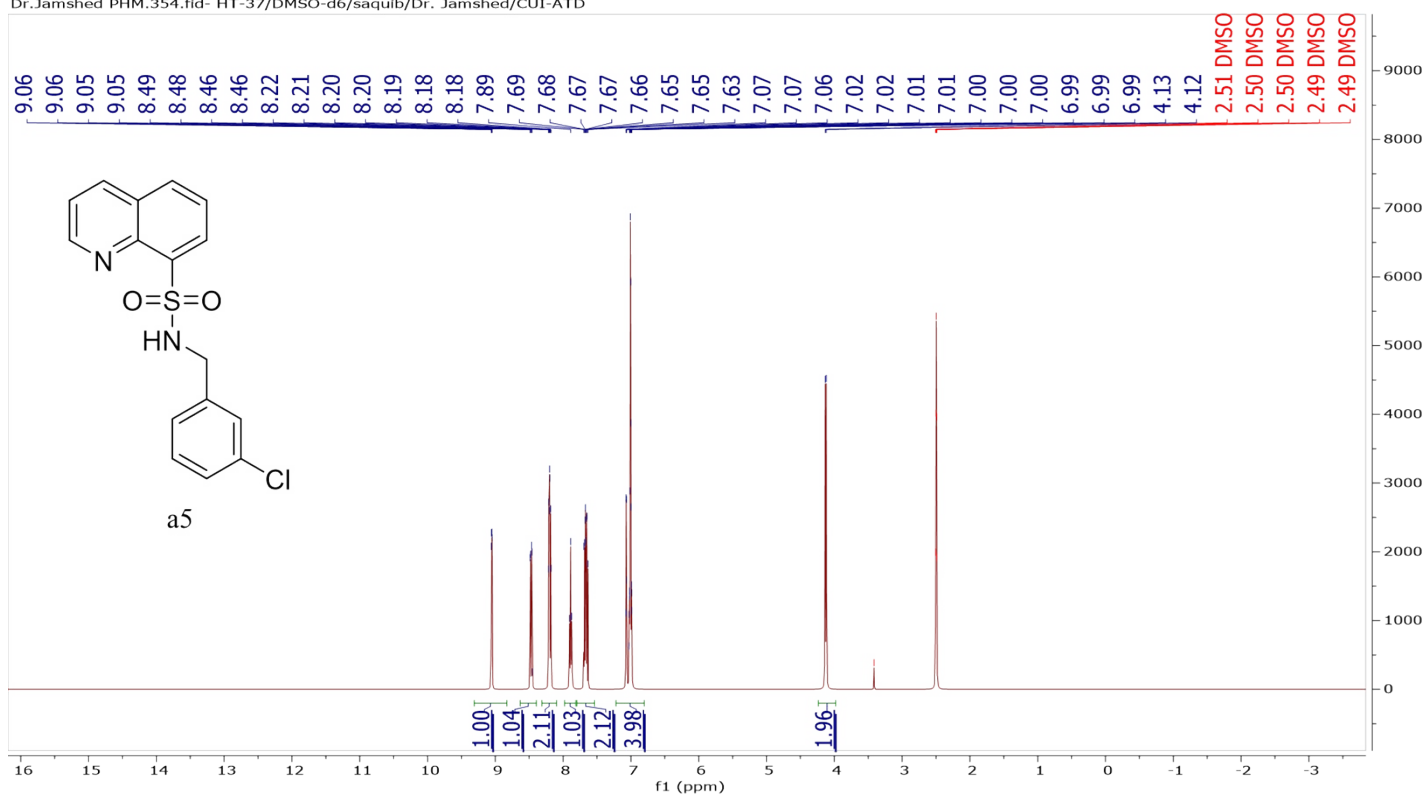


Figure 9: <sup>1</sup>H NMR of compound a5

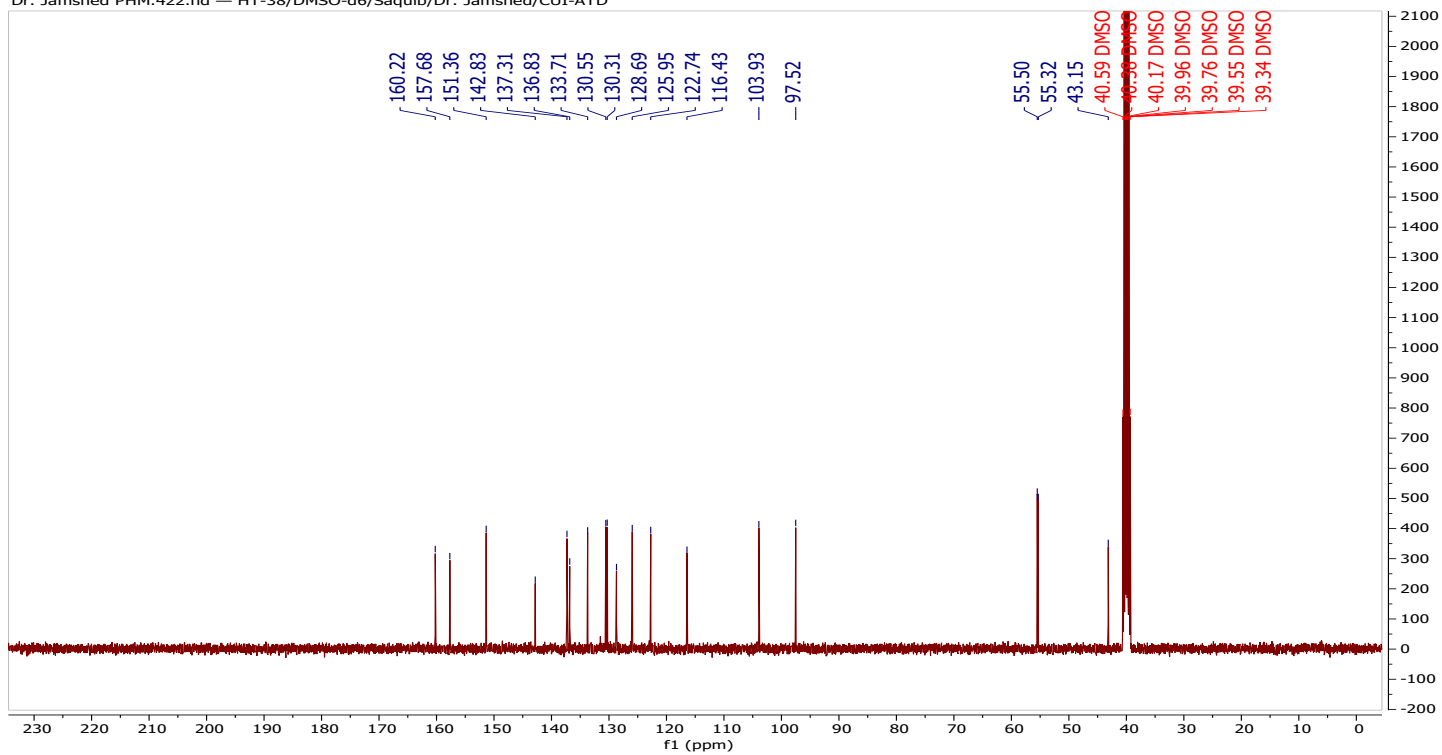


Figure 10: <sup>13</sup>C NMR of compound a5

# Compound a6

Dr. Jamshed PHM.355.fid- HT-38/DMSO-d6/Saqib/Dr. Jamshed/CUI-ATD

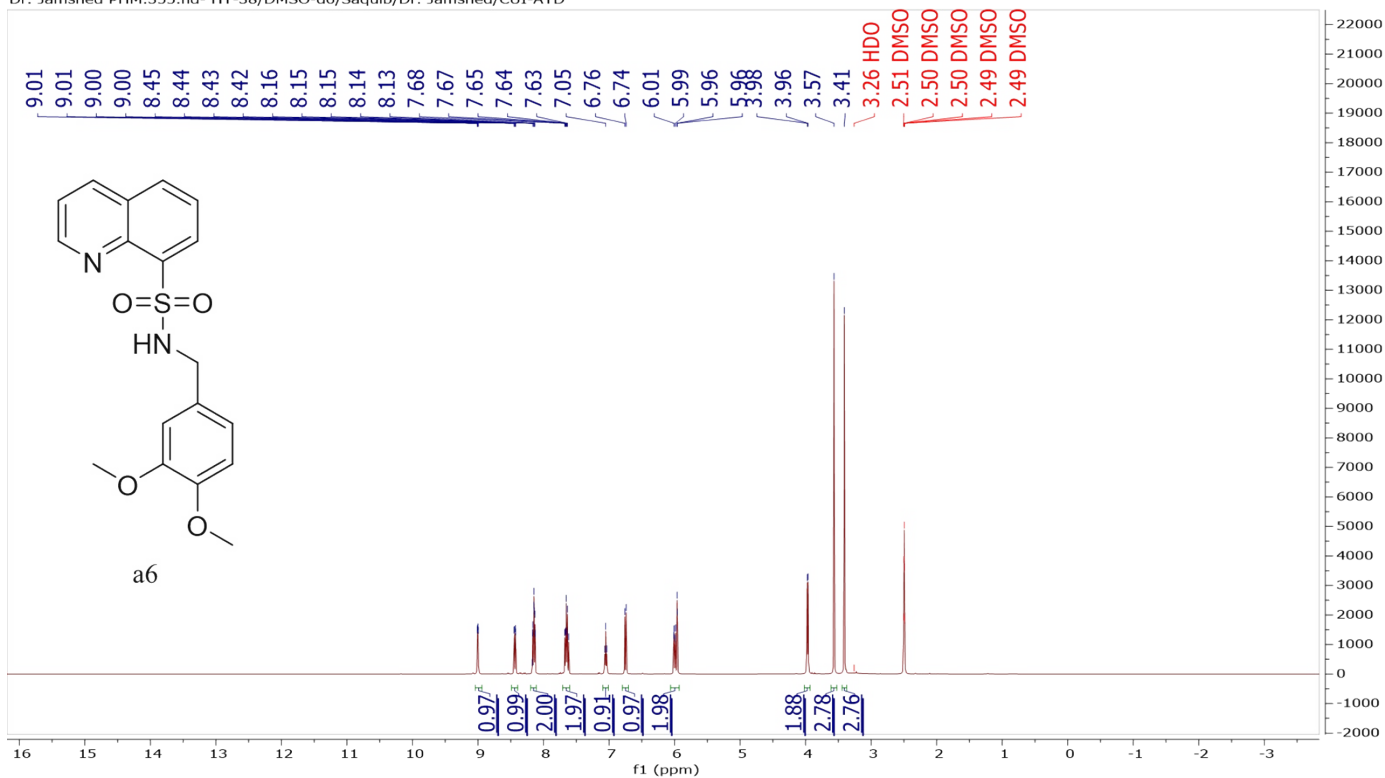


Figure 11: <sup>1</sup>H NMR of compound a6

Dr. Jamshed PHM.422.fid — HT-38/DMSO-d6/Saqib/Dr. Jamshed/CUI-ATD

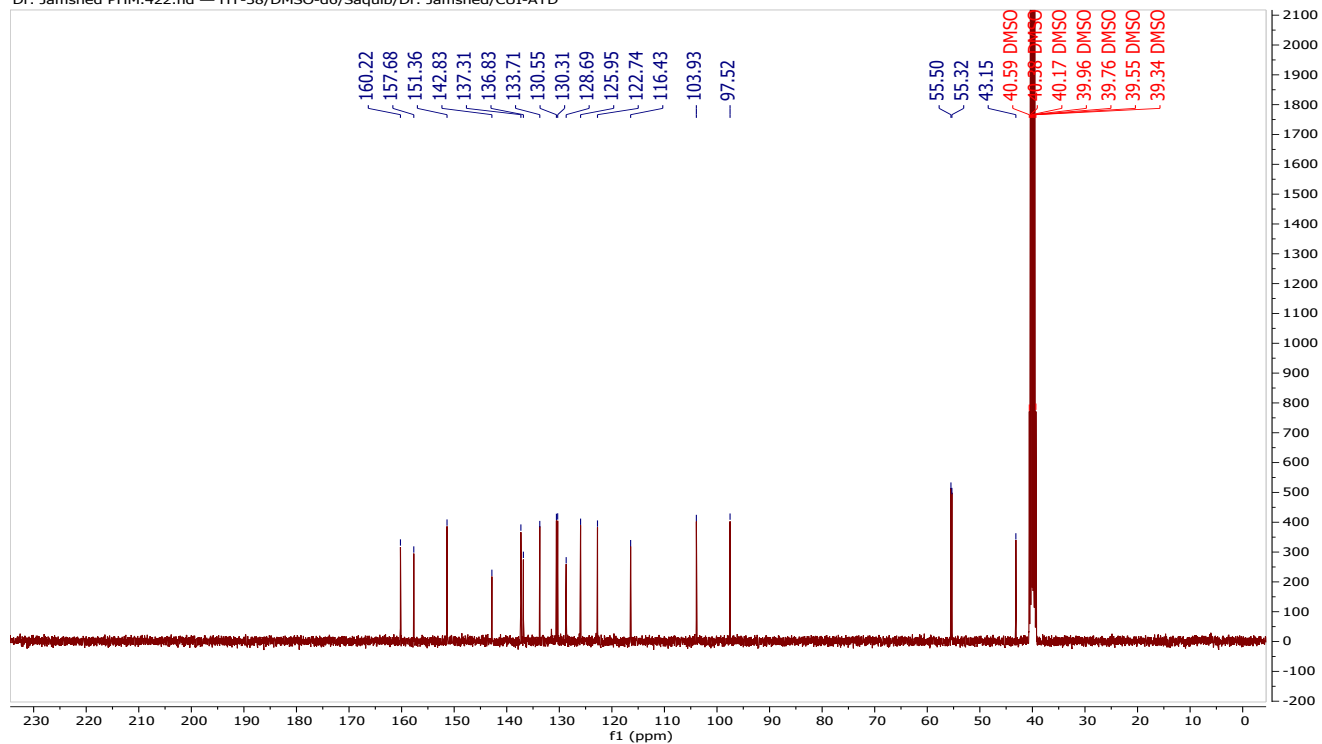


Figure 12: <sup>13</sup>C NMR of compound a6

# Compound a8

Dr. Jamshed PHM.443.fid — HT-42/DMSO-d6/Saqib/Dr. Jamshed Iqbal/CUI-ATD

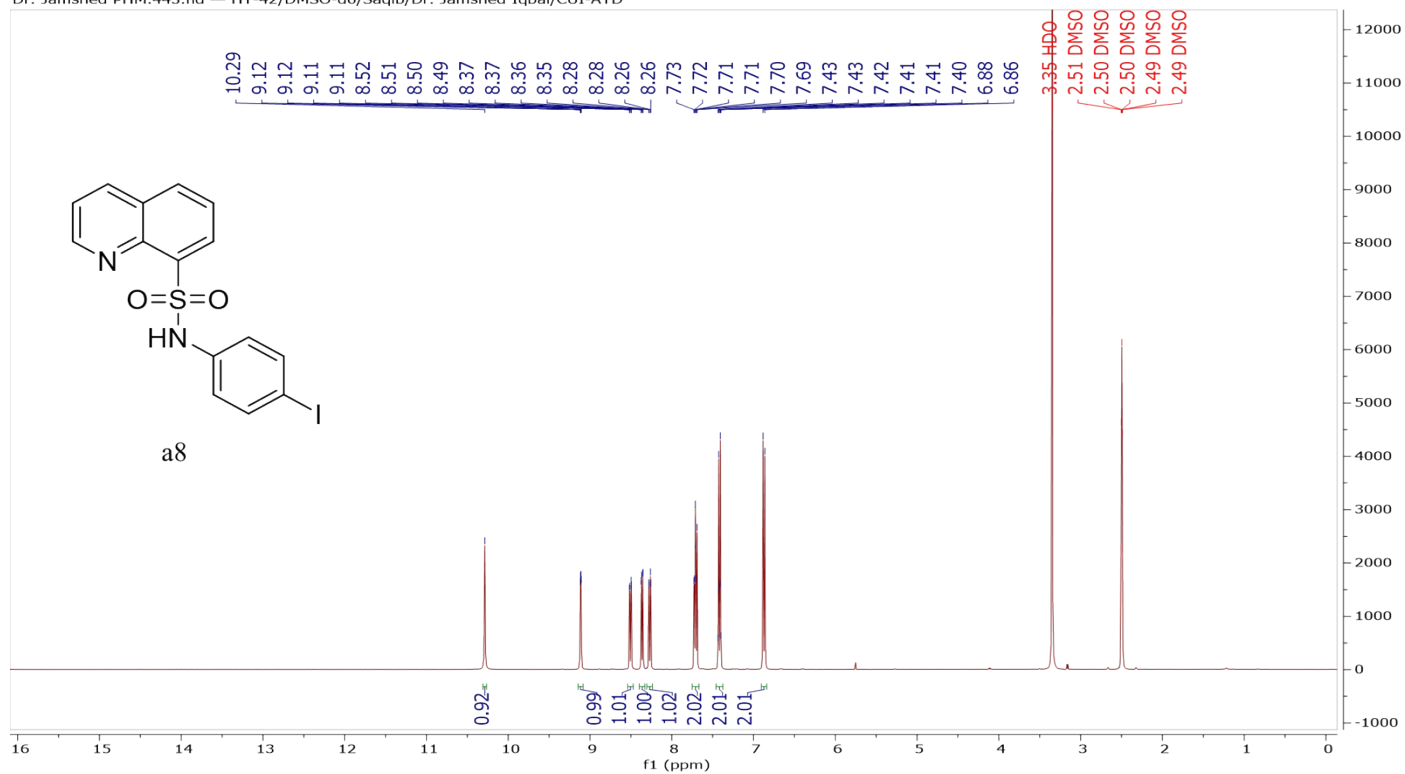


Figure 13: <sup>1</sup>H NMR of compound a8

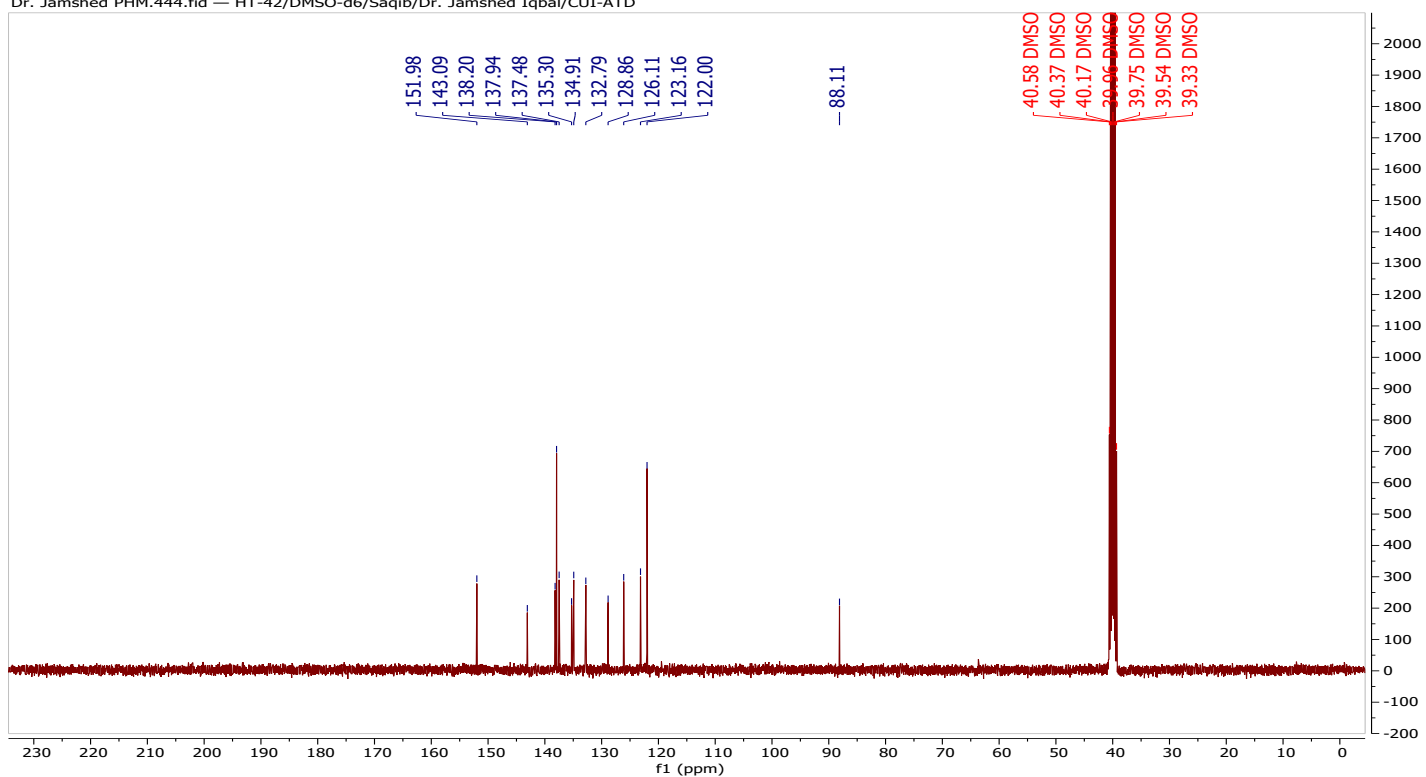


Figure 14:  $^{13}\text{C}$ NMR of compound a8

### Compound a9

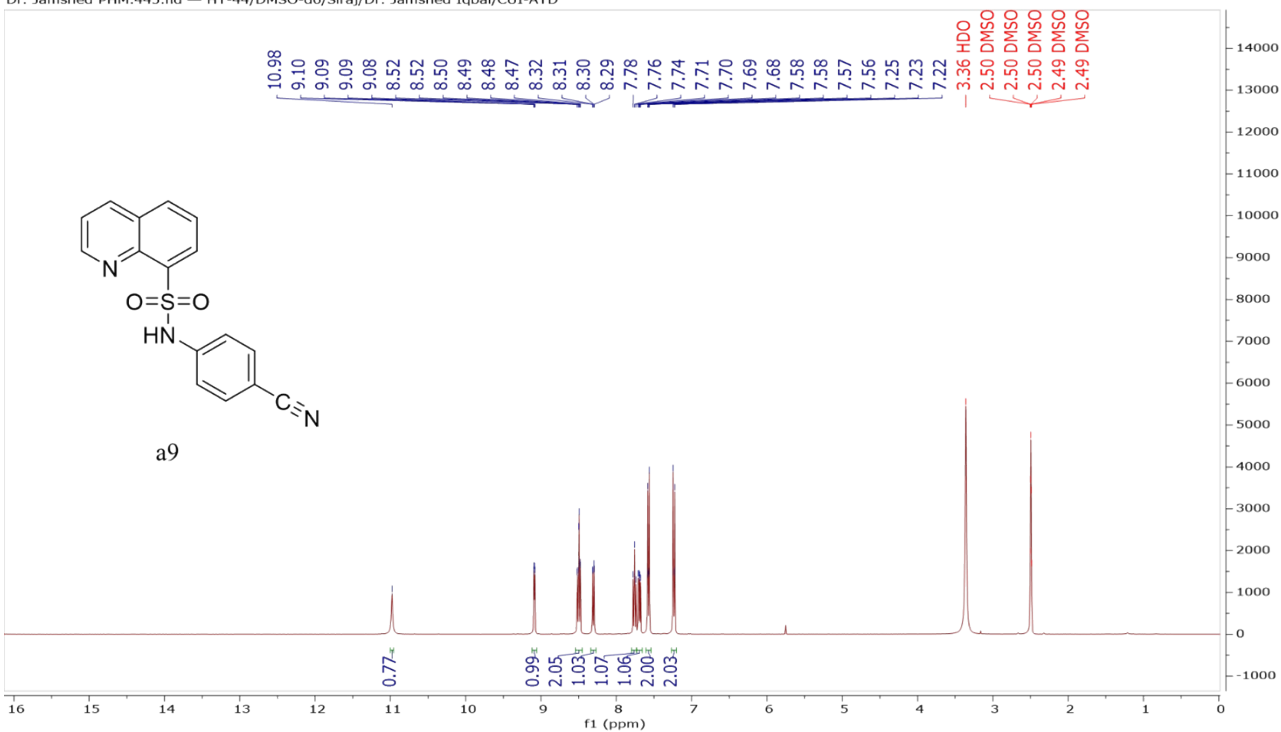


Figure 15:  $^1\text{H}$ NMR of compound a9

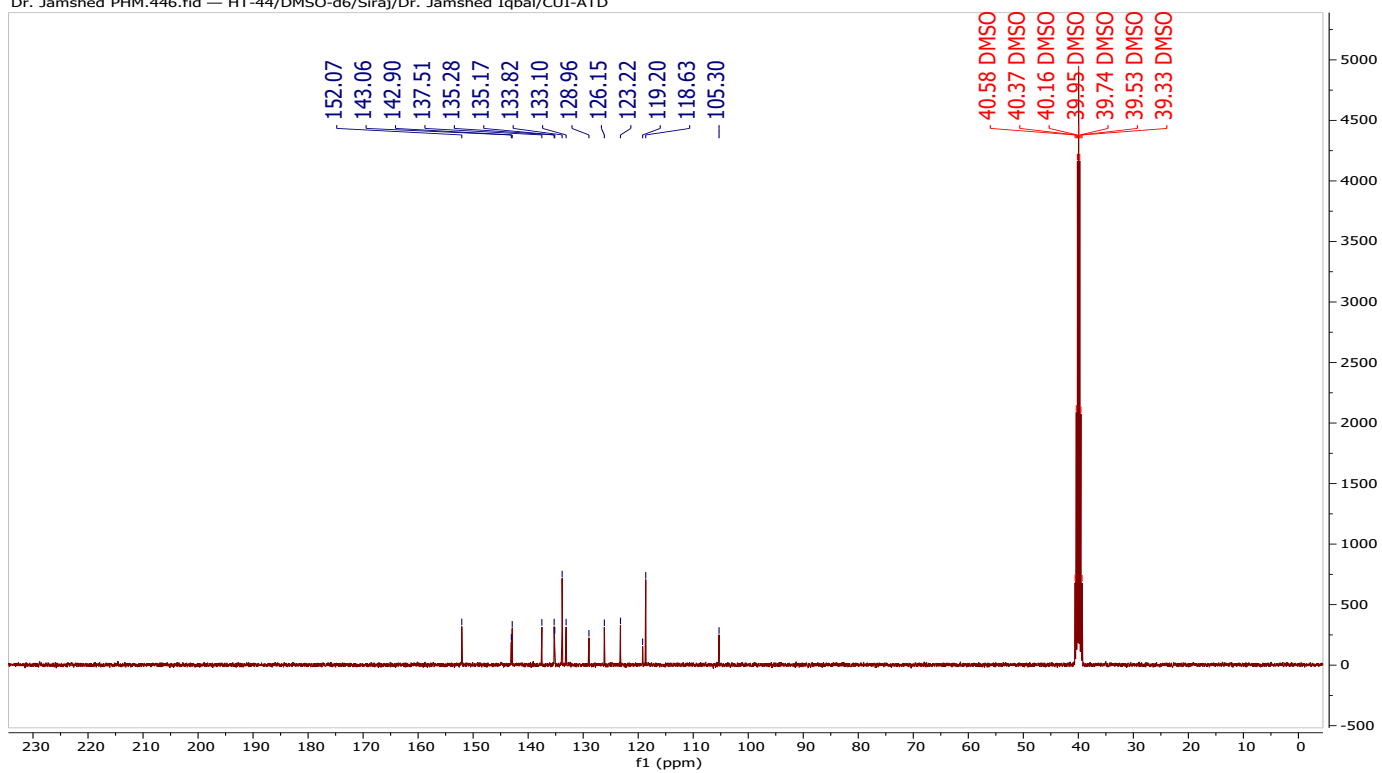


Figure 16:  $^{13}\text{C}$ NMR of compound a9

Compound a10

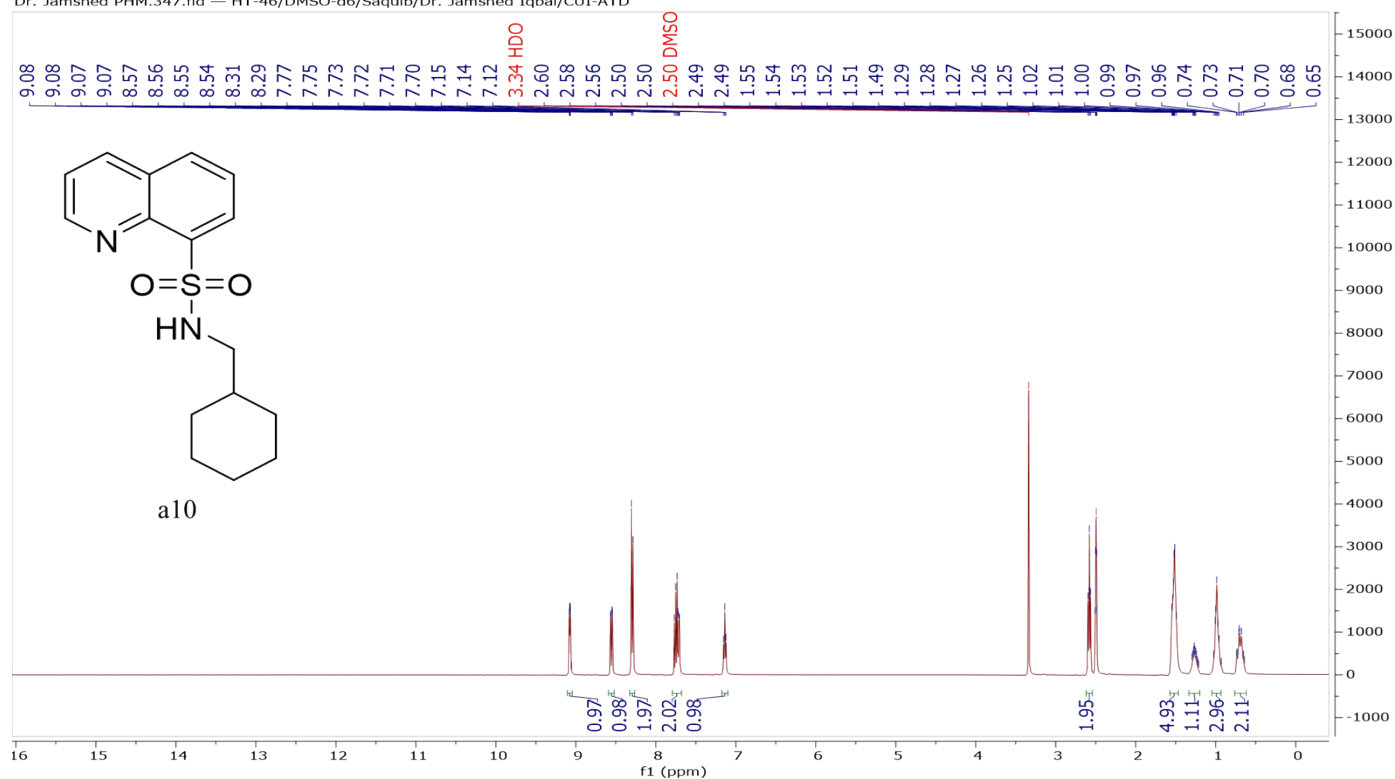


Figure 17: <sup>1</sup>H NMR of compound a10

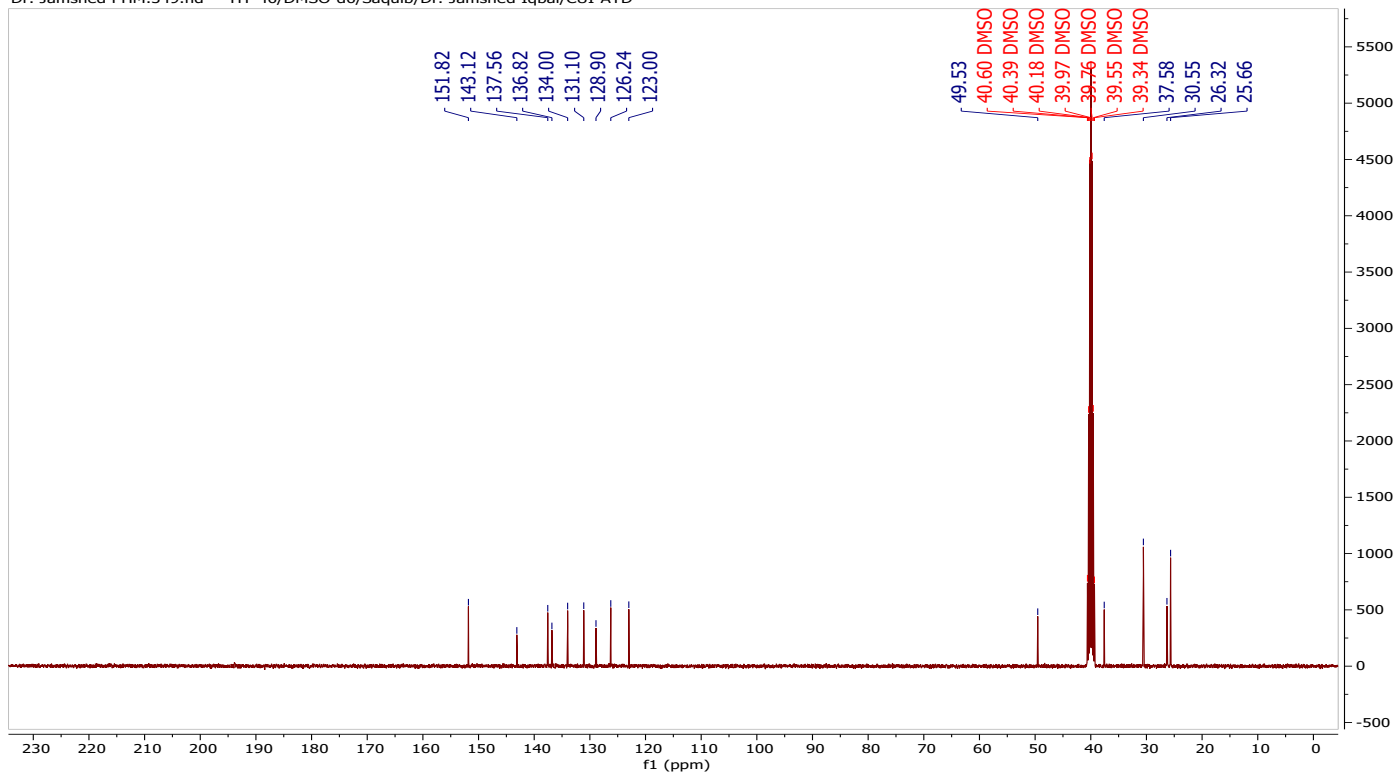
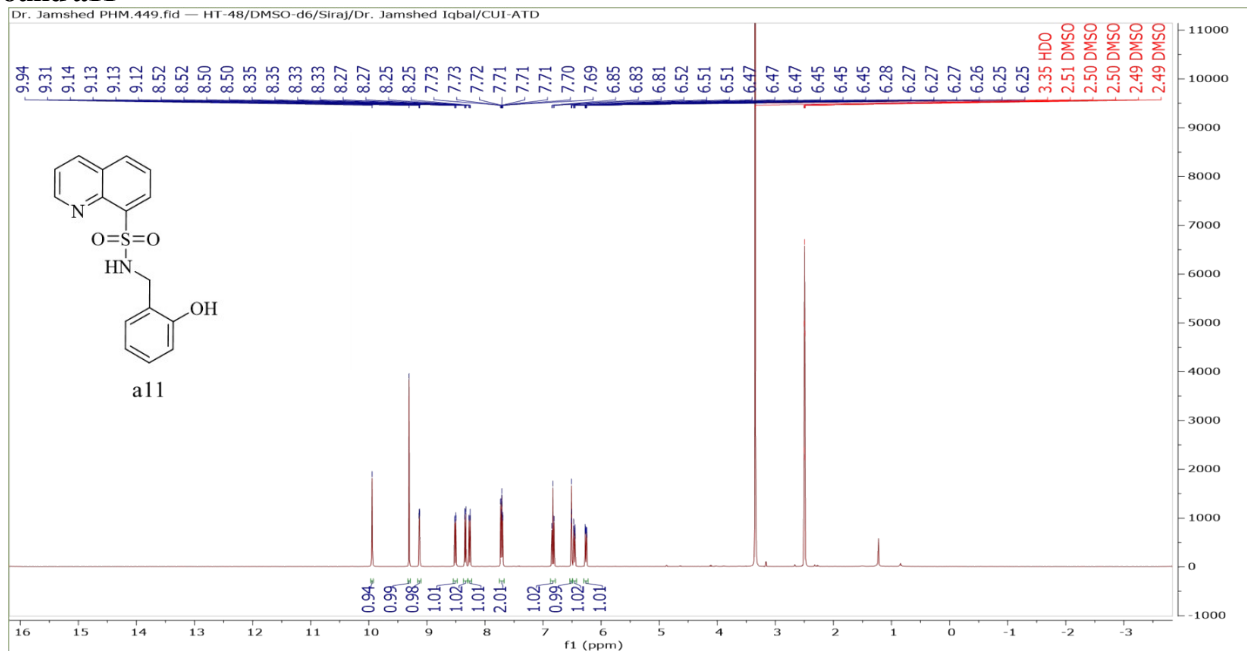


Figure 18: <sup>13</sup>C NMR of compound 10

# Compound a11



80

Figure 19: <sup>1</sup>H NMR of compound a11

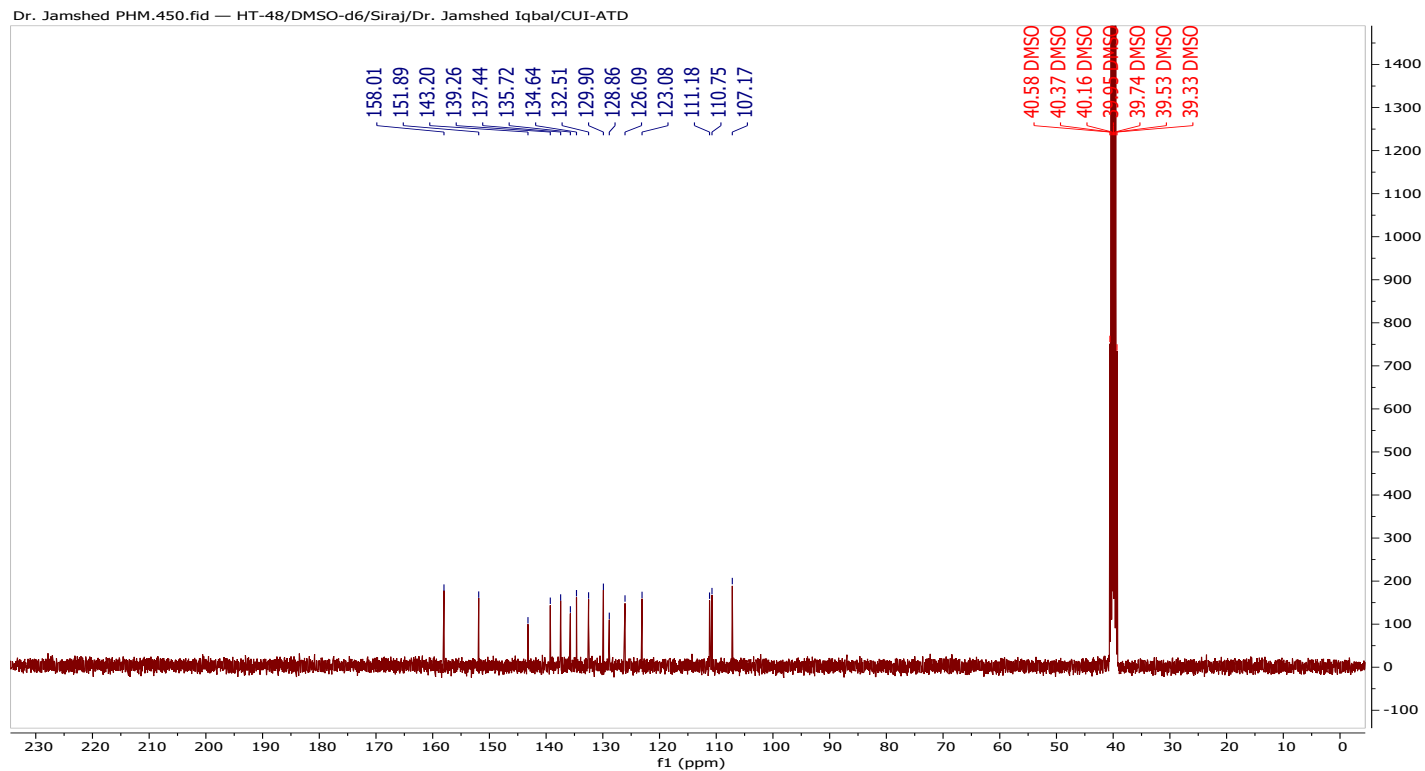


Figure 20: <sup>13</sup>C NMR of compound a11

# Compound a12

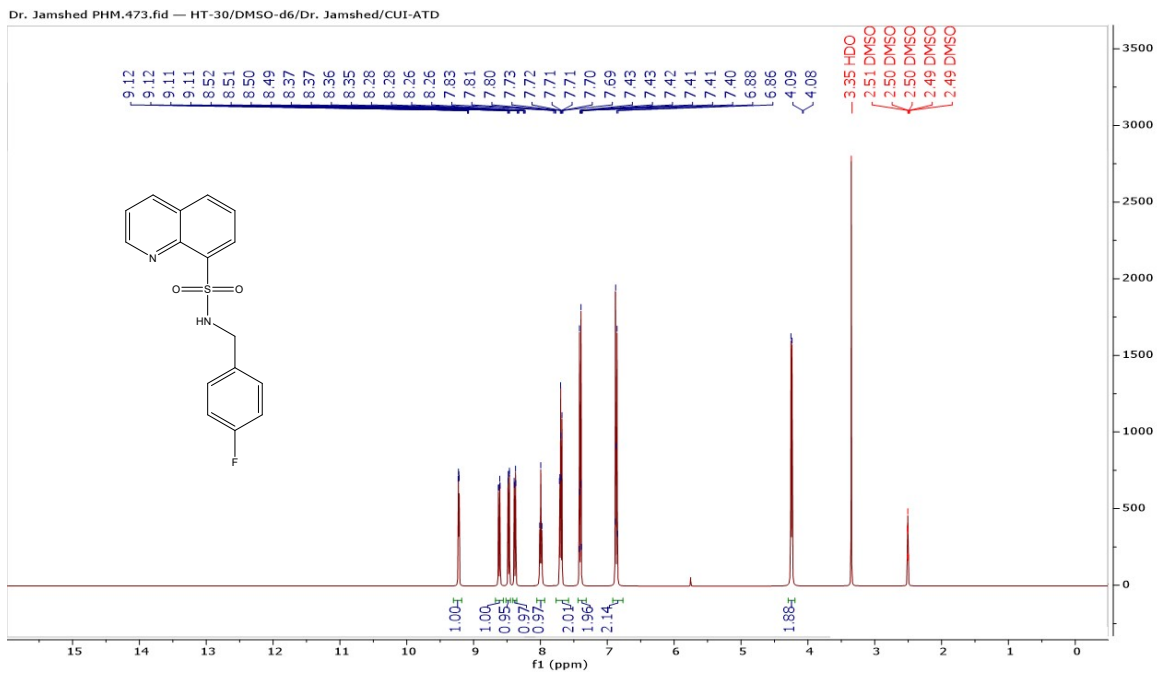


Figure 21:  $^1\text{H}$ NMR of compound a12

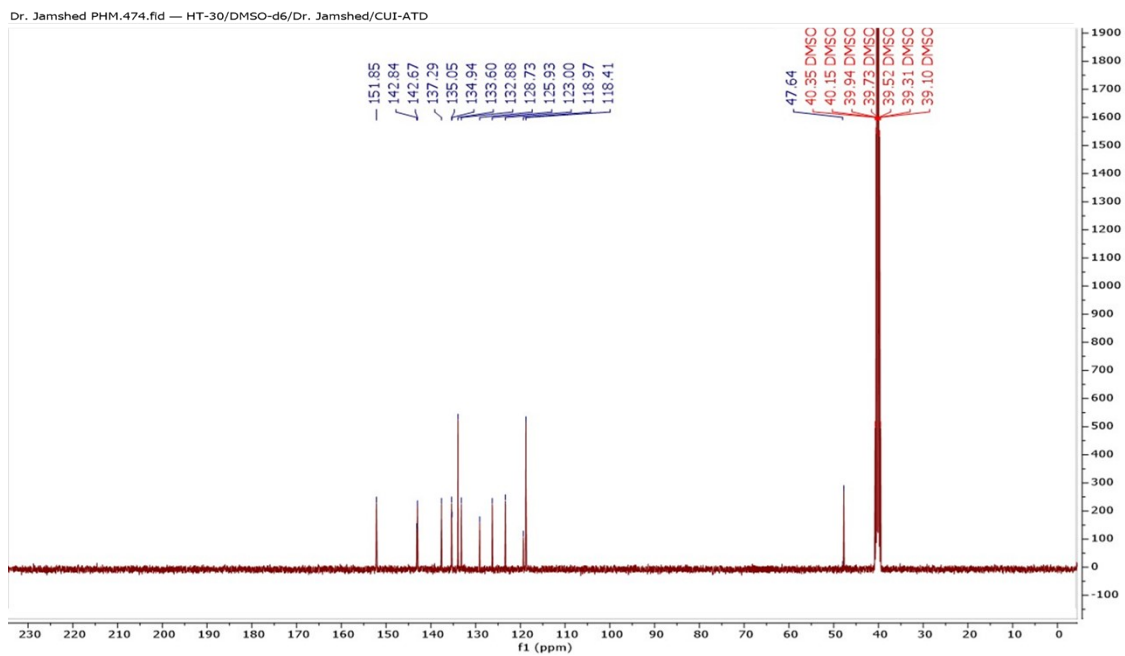


Figure 22:  $^{13}\text{C}$ NMR of compound a12



# Compound a14

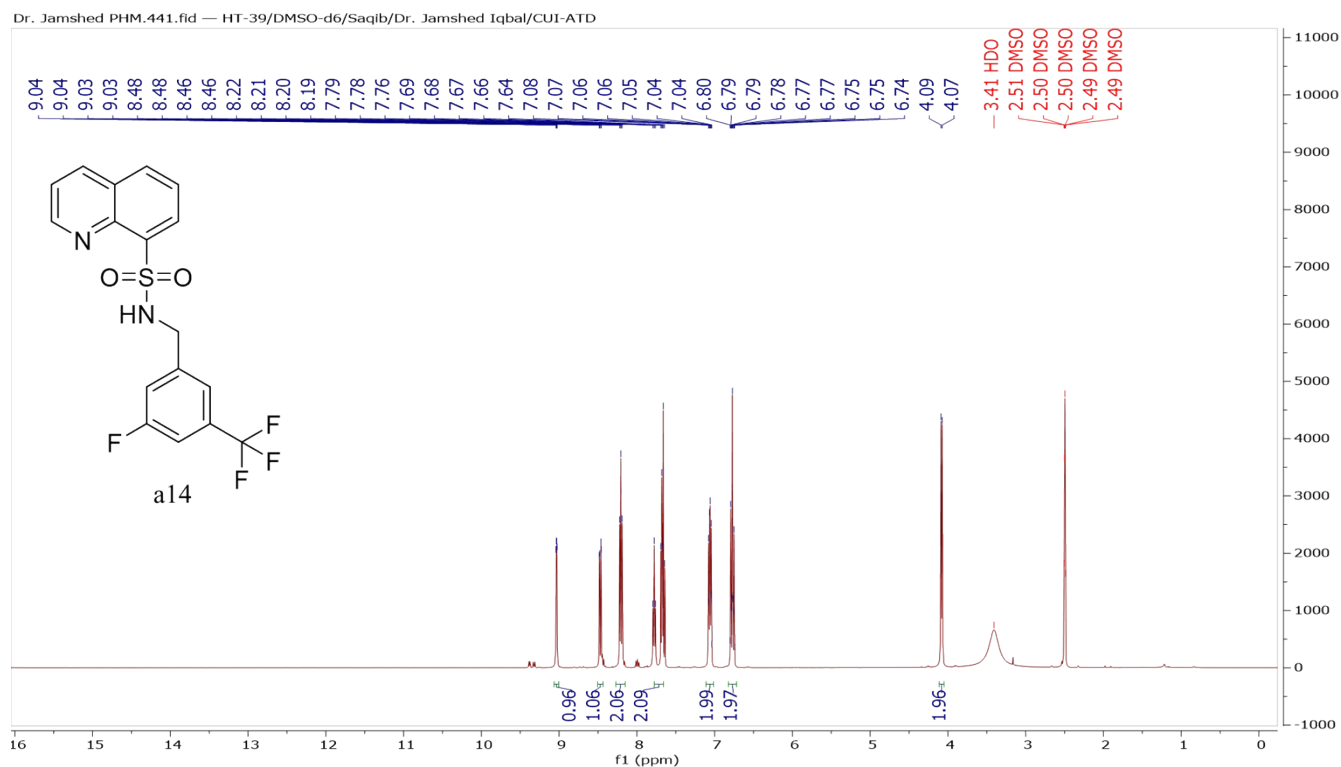


Figure 23: <sup>1</sup>H NMR of compound a14

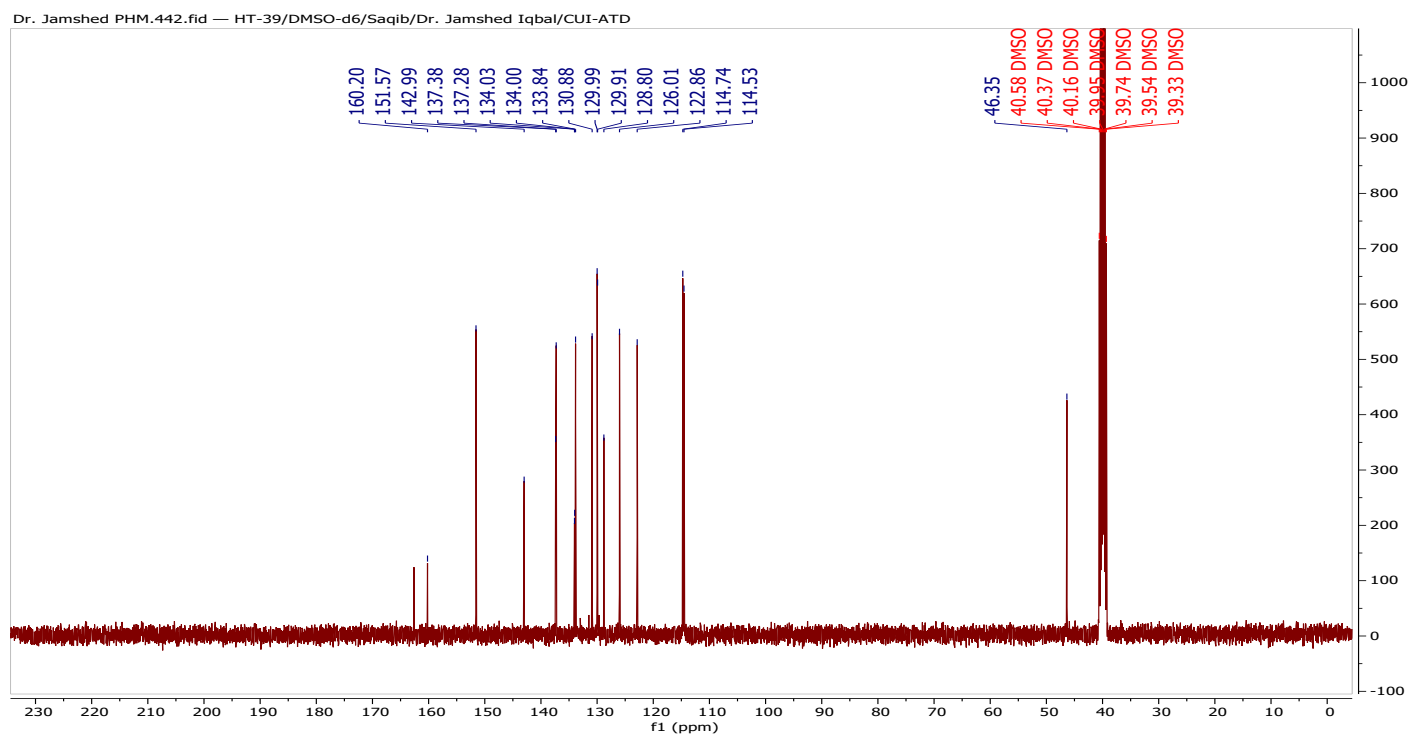


Figure 24: <sup>13</sup>C NMR of compound a14

# Compound a15

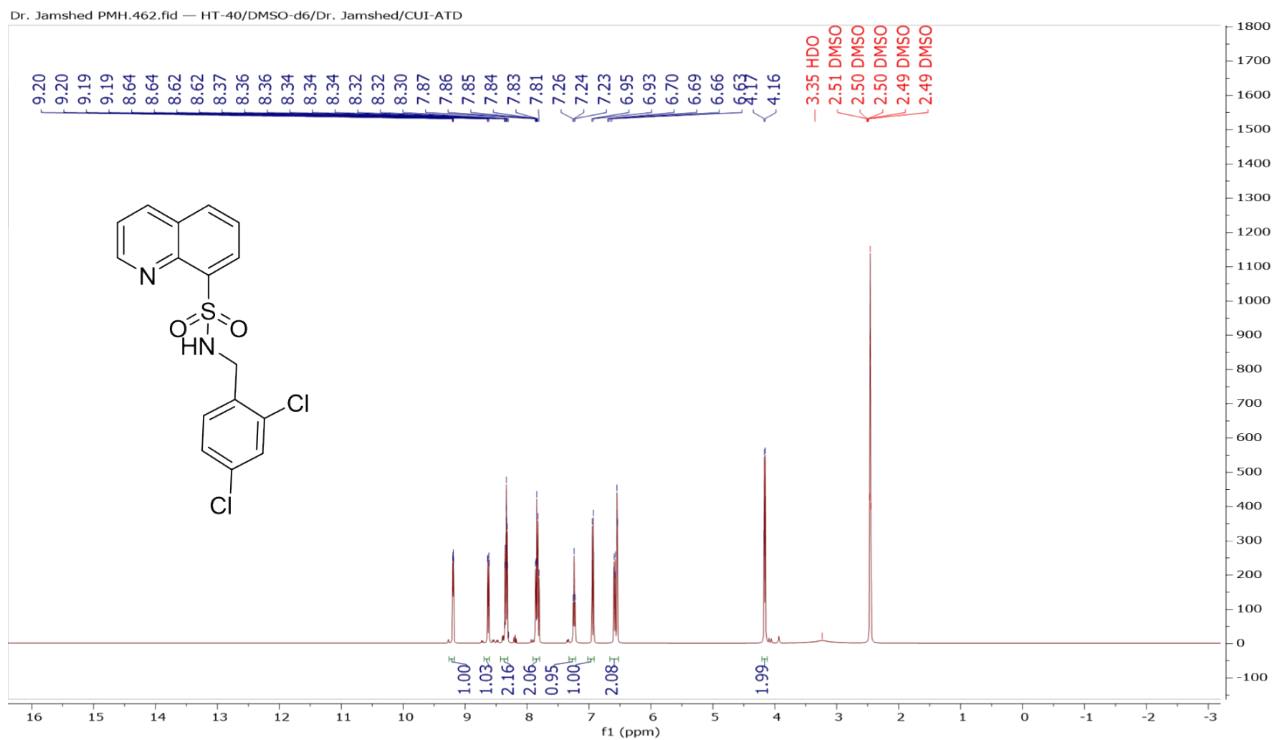


Figure 25: <sup>1</sup>H NMR of compound a15

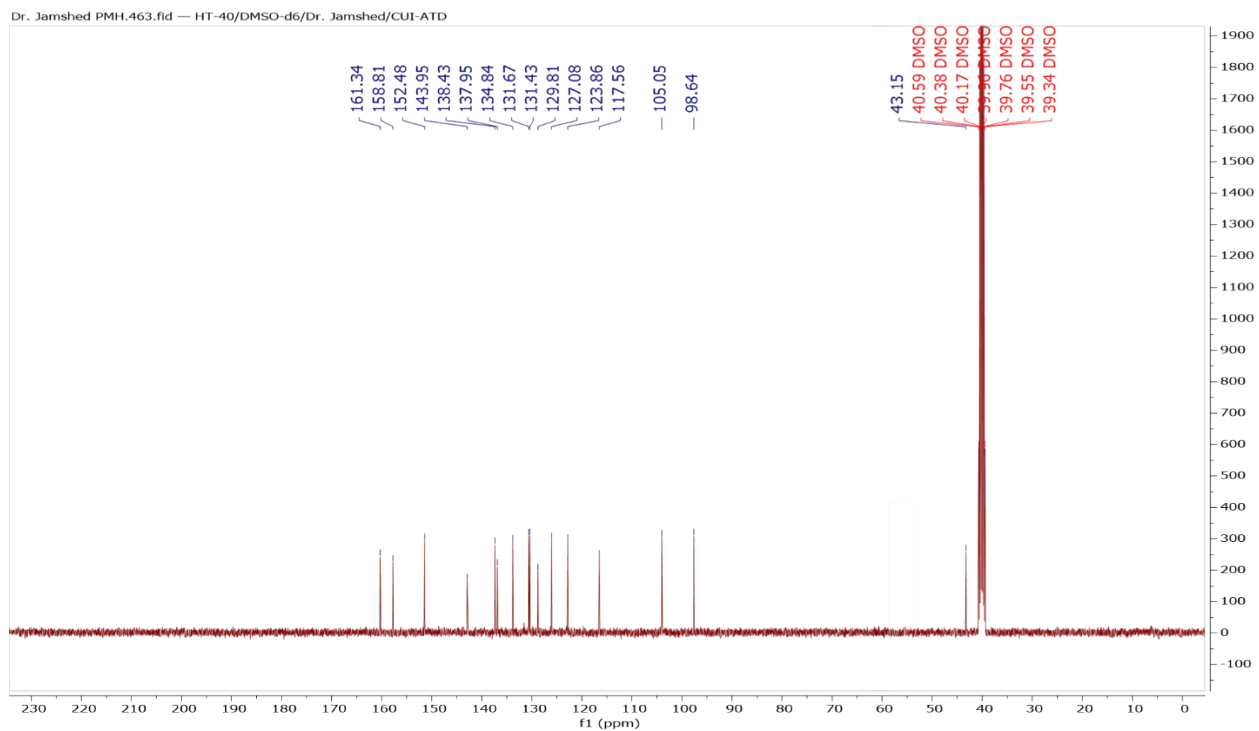


Figure 26:  $^{13}\text{C}$ NMR of compound a15

Compound a16

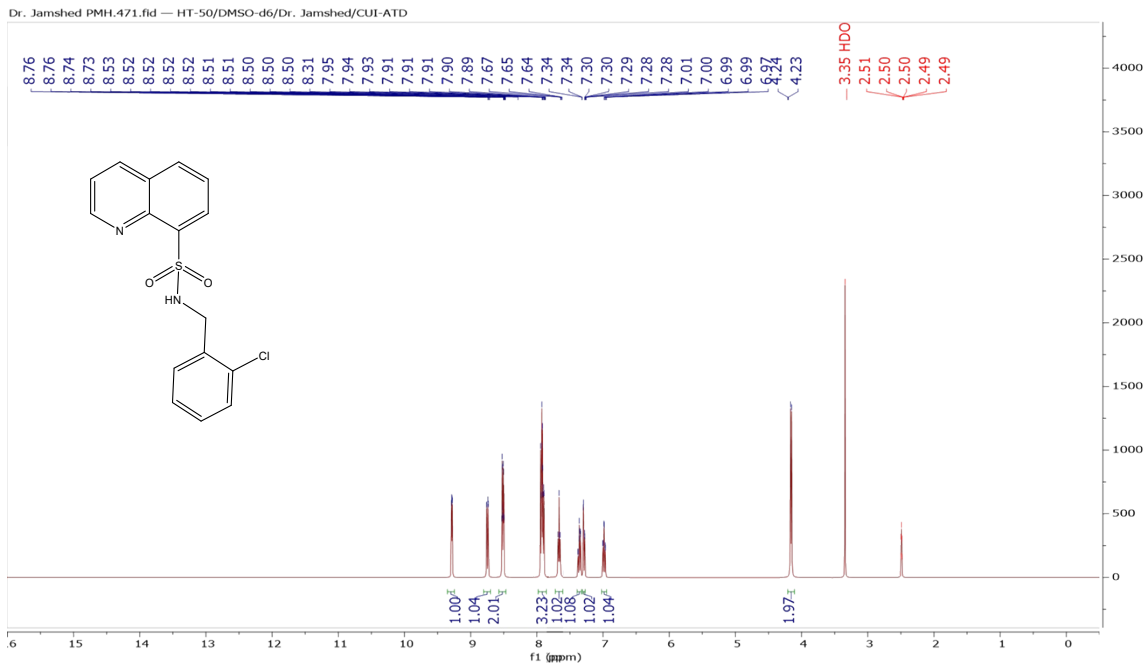


Figure 27:  $^1\text{H}$ NMR of compound a16

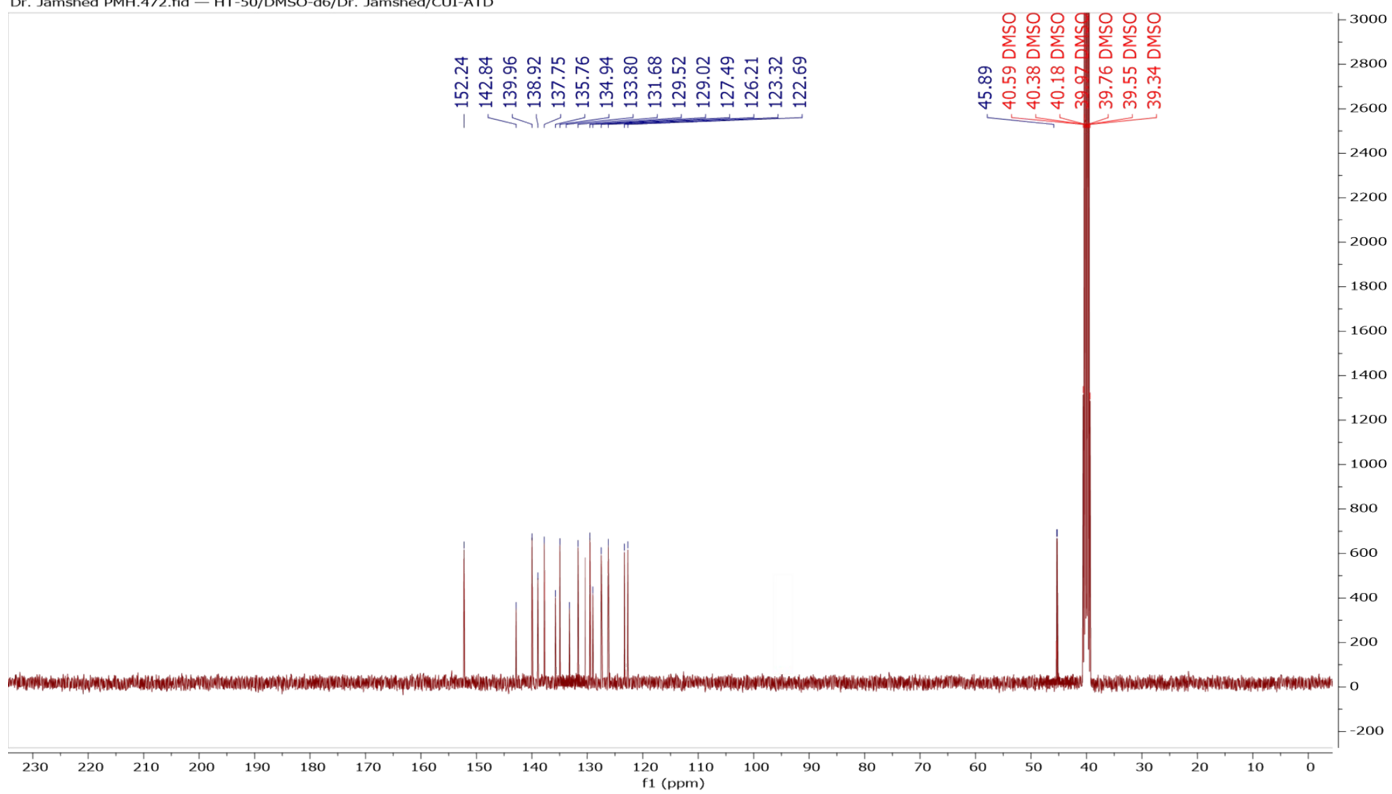


Figure 28: <sup>13</sup>CNMR of compound a16

**Compound a17**

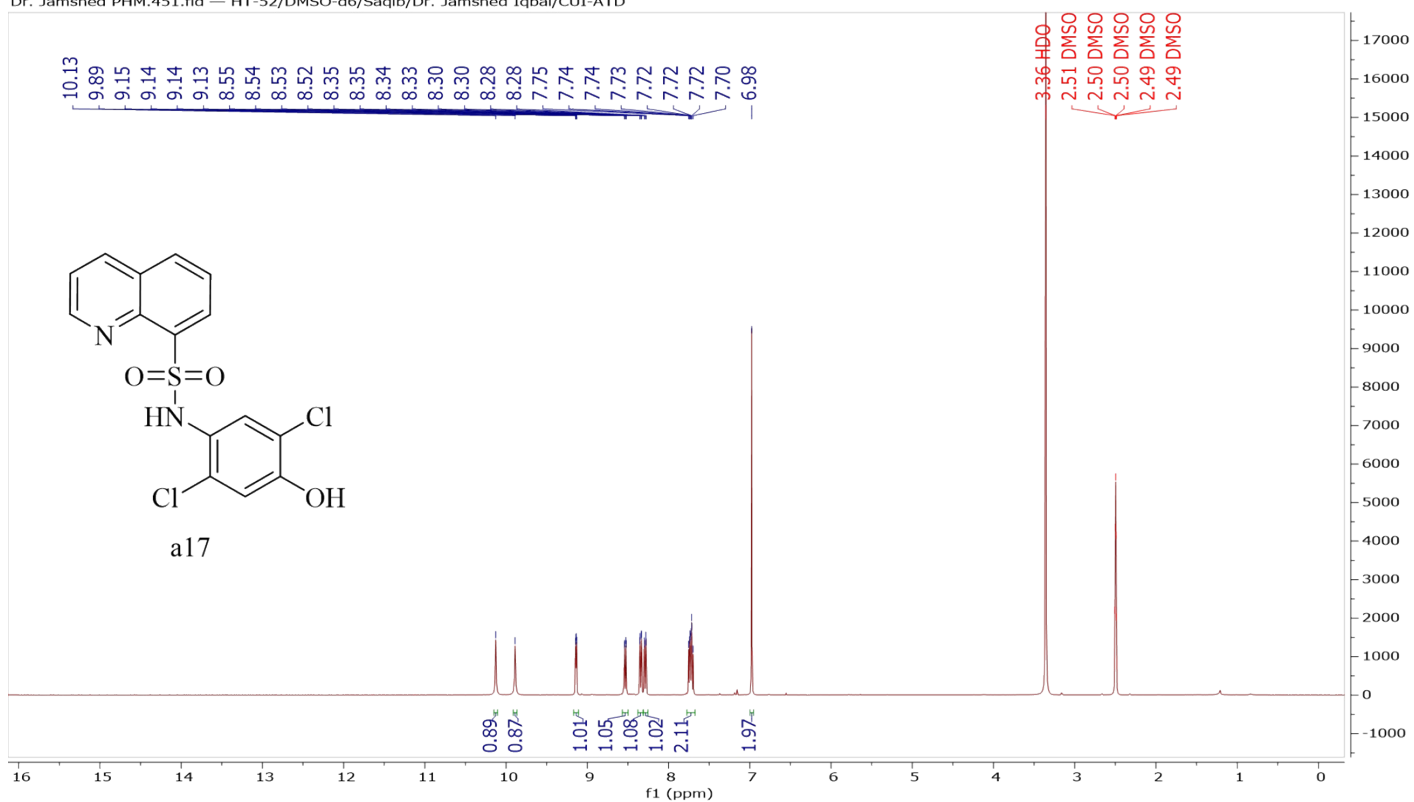


Figure 29: <sup>1</sup>H NMR of compound **a17**

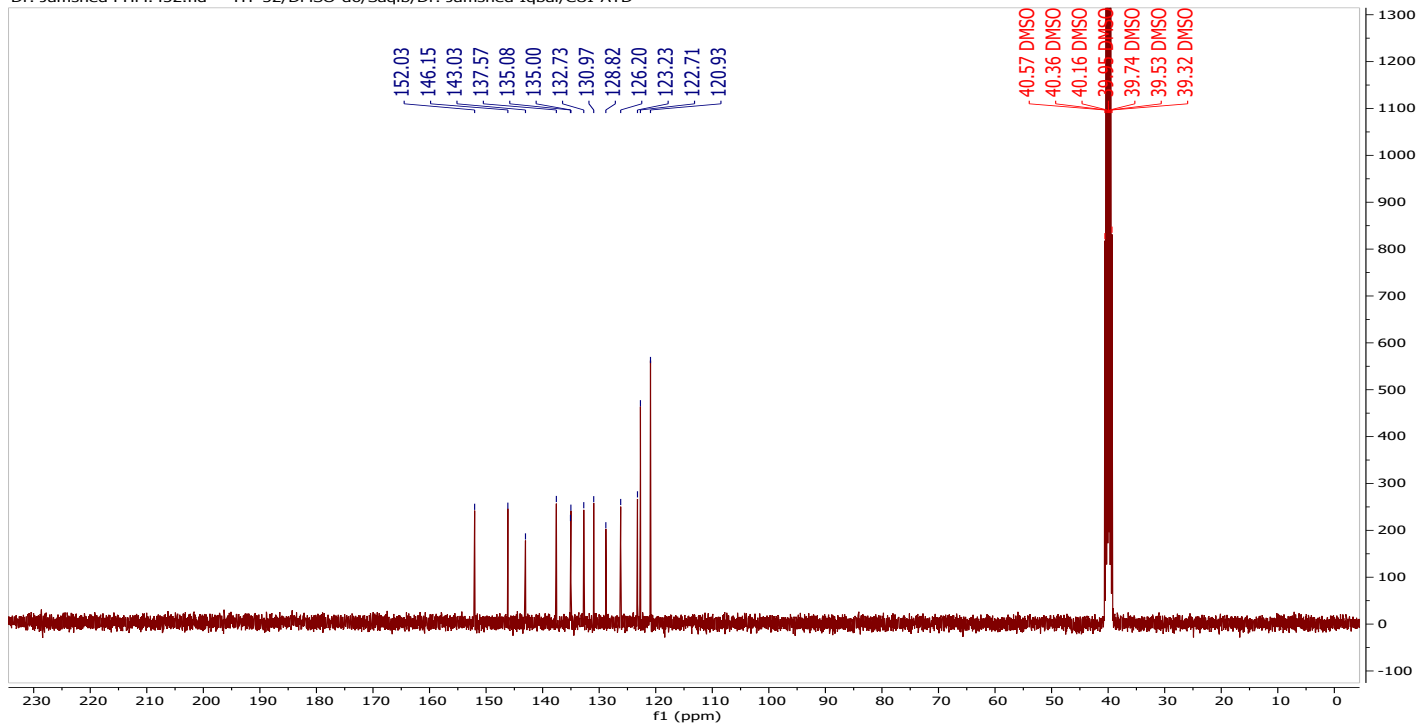


Figure 30: <sup>13</sup>C NMR of compound **a17**

# Compound 18

Dr. Jamshed PMH.467.fid — HT-49/DMSO-d6/Dr. Jamshed/CUI-ATD

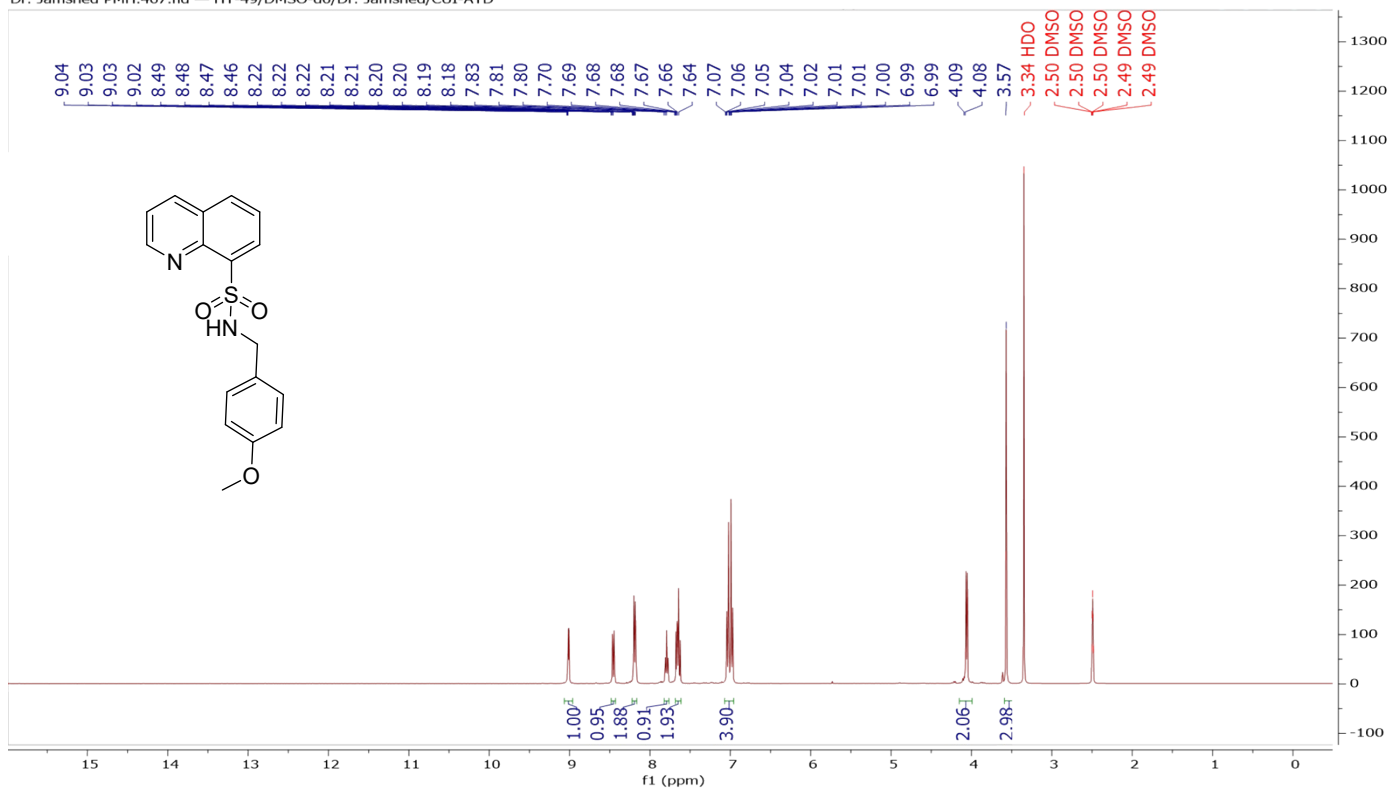


Figure 31:  $^1\text{H}$ NMR of compound a18

Dr. Jamshed PMH.468.fid — HT-49/DMSO-d6/Dr. Jamshed/CUI-ATD

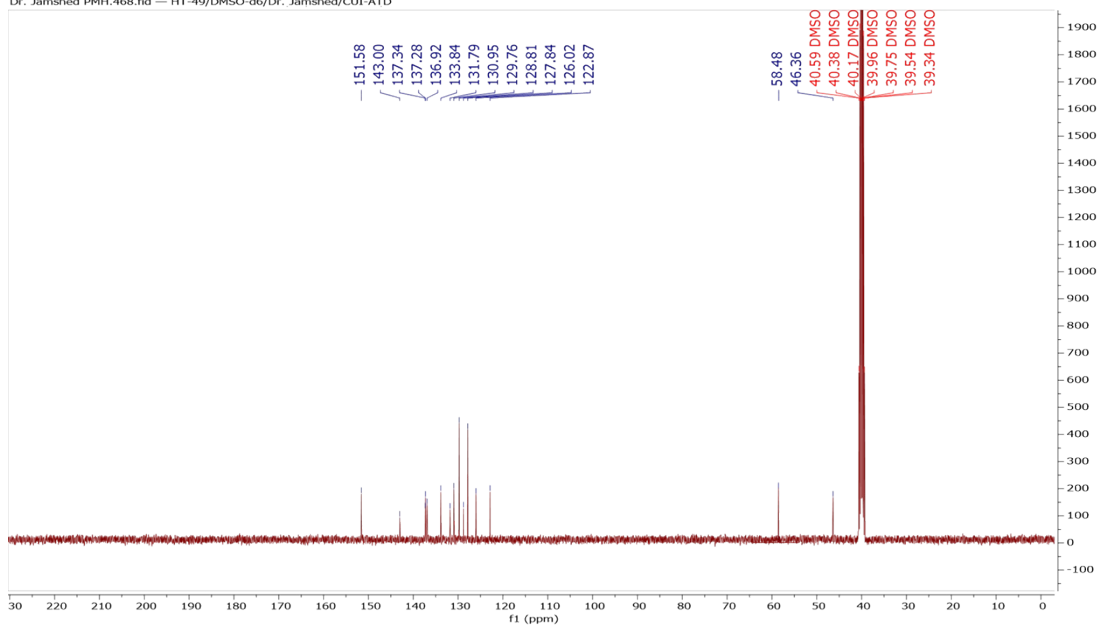
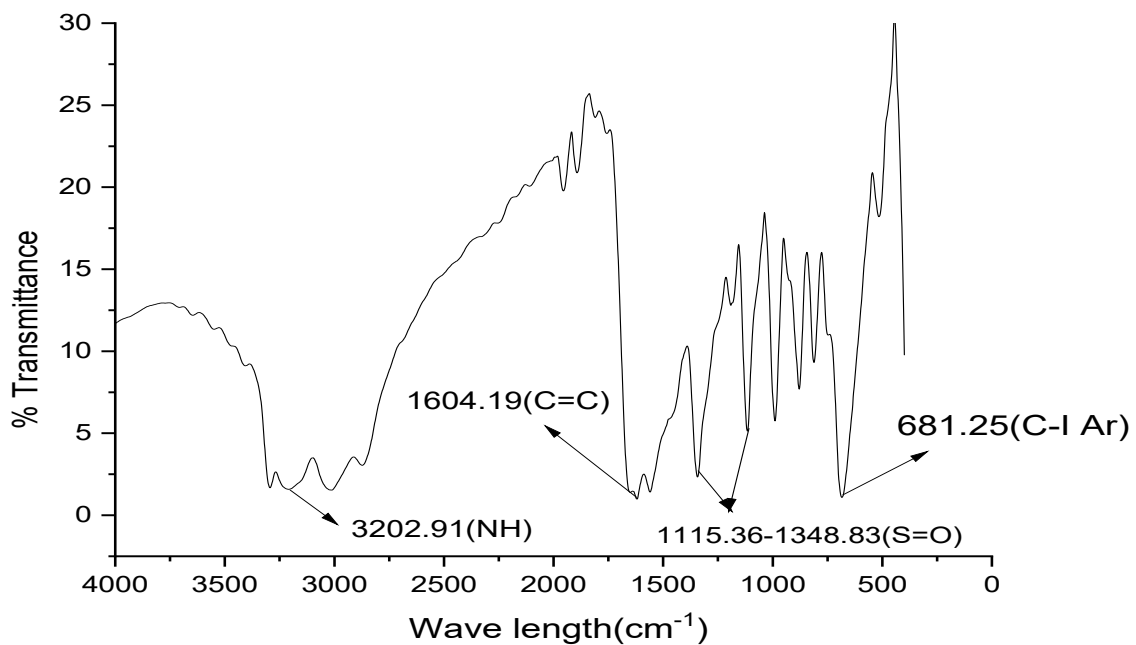
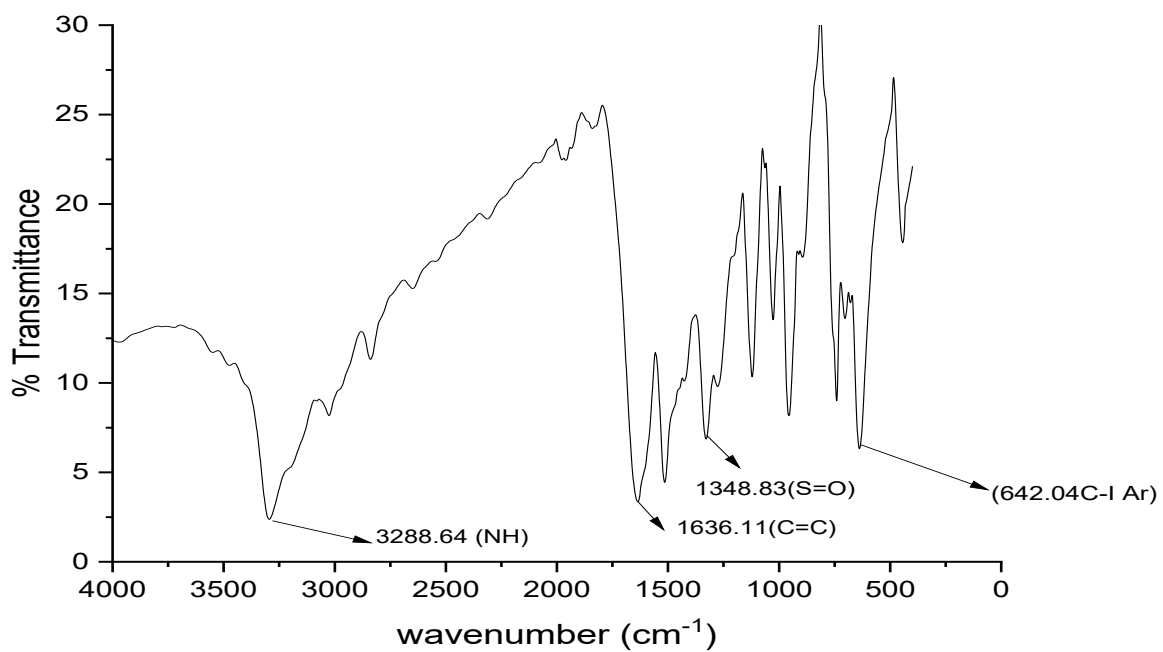


Figure 32:  $^{13}\text{C}$ NMR of compound a18

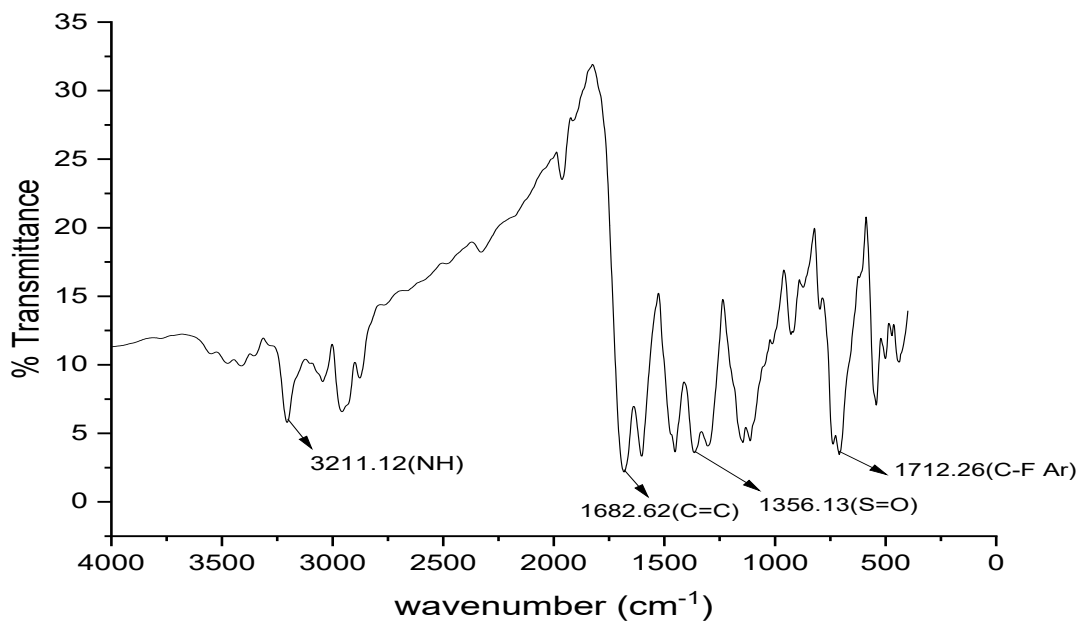
## 1.2 FTIR analysis



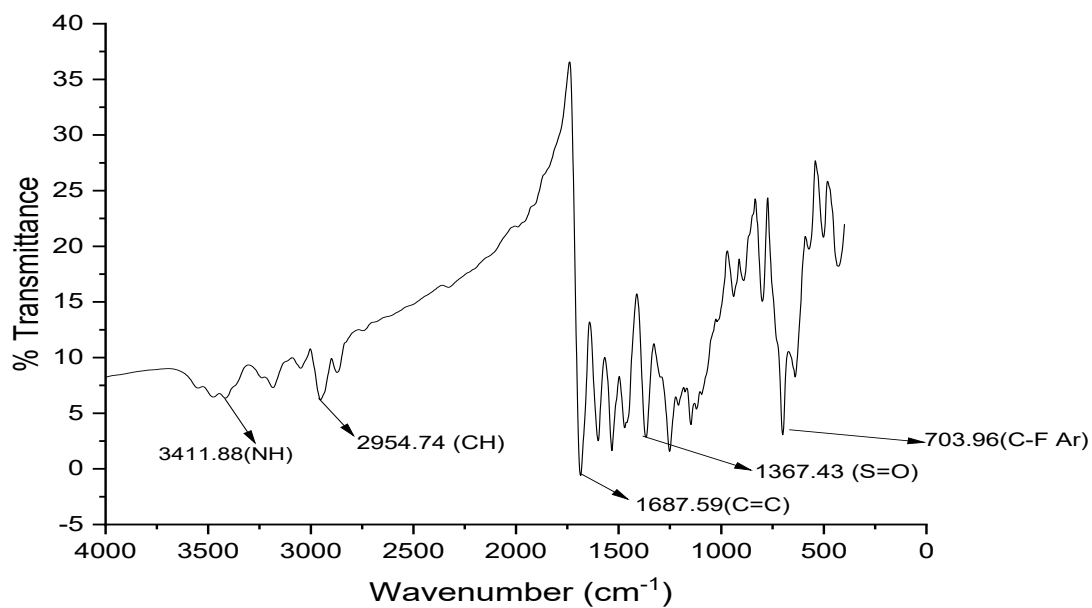
**Figure 33:** FTIR graph of compound a1



**Figure 34:** FTIR graph of compound a2

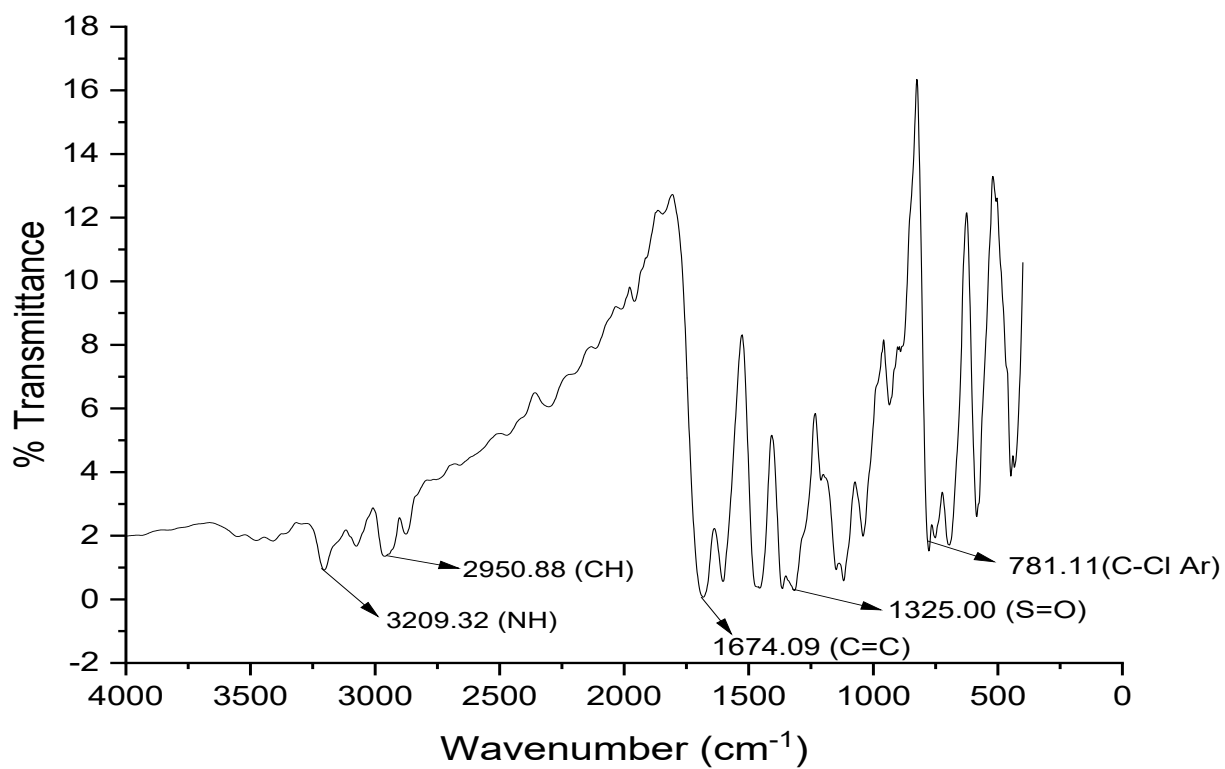


**Figure 35: FTIR graph of compound a3**

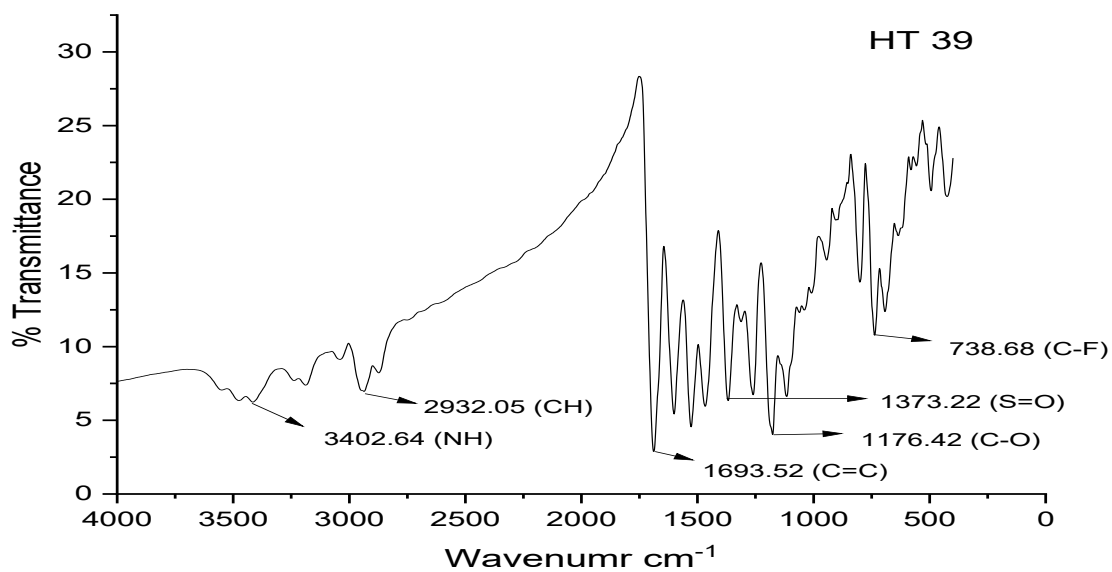


**Figure 36: FTIR graph of compound a4**

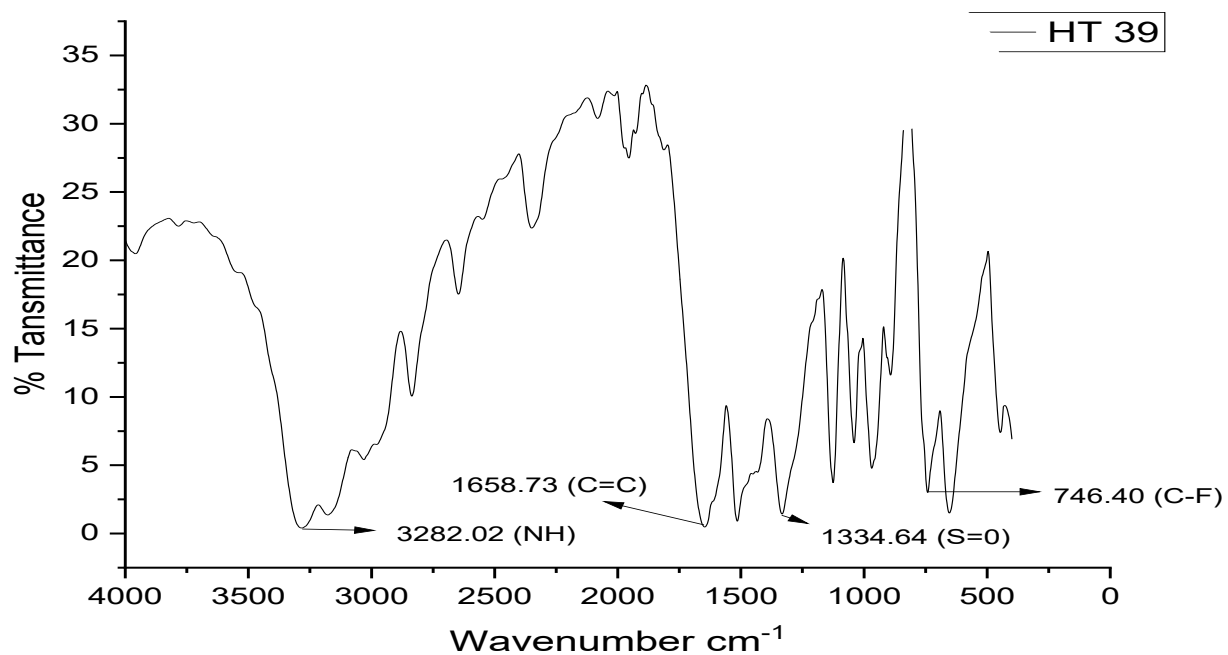




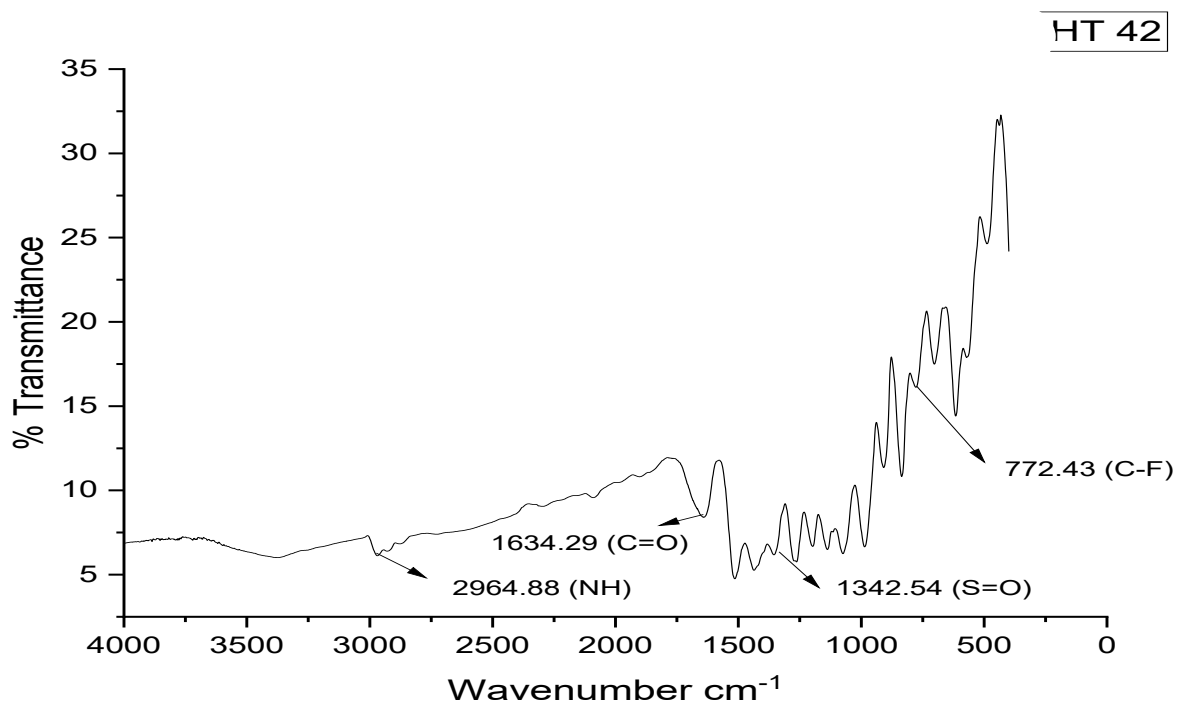
**Figure 37:** FTIR graph of compound a5



**Figure 38:** FTIR graph of compound a6



**Figure 39:** FTIR graph of compound a7



**Figure 40:** FTIR graph of compound a8

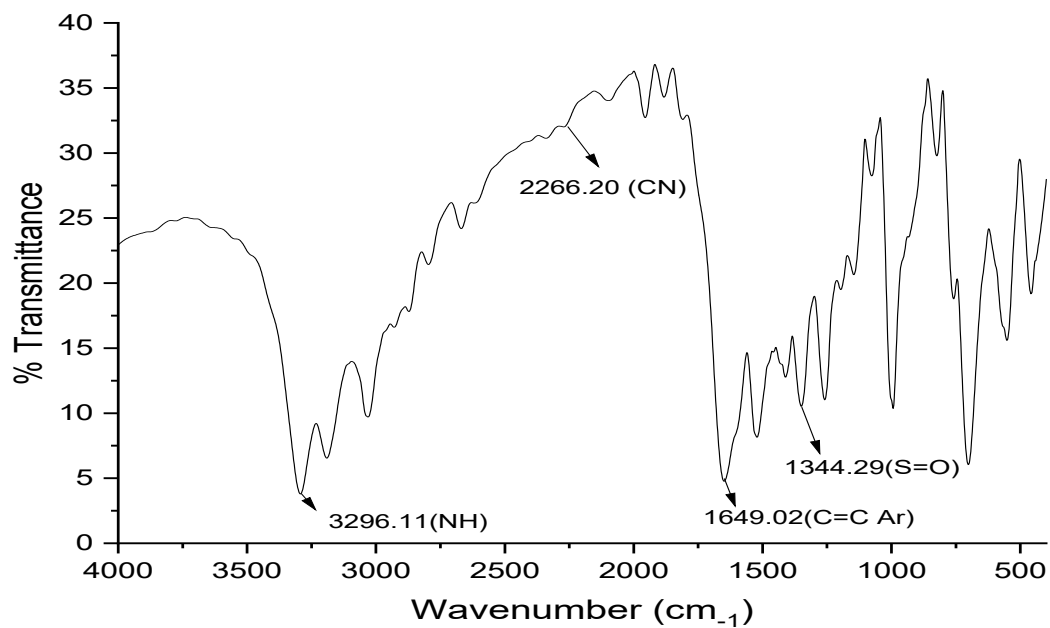


Figure 41 :FTIR graph of compound a9

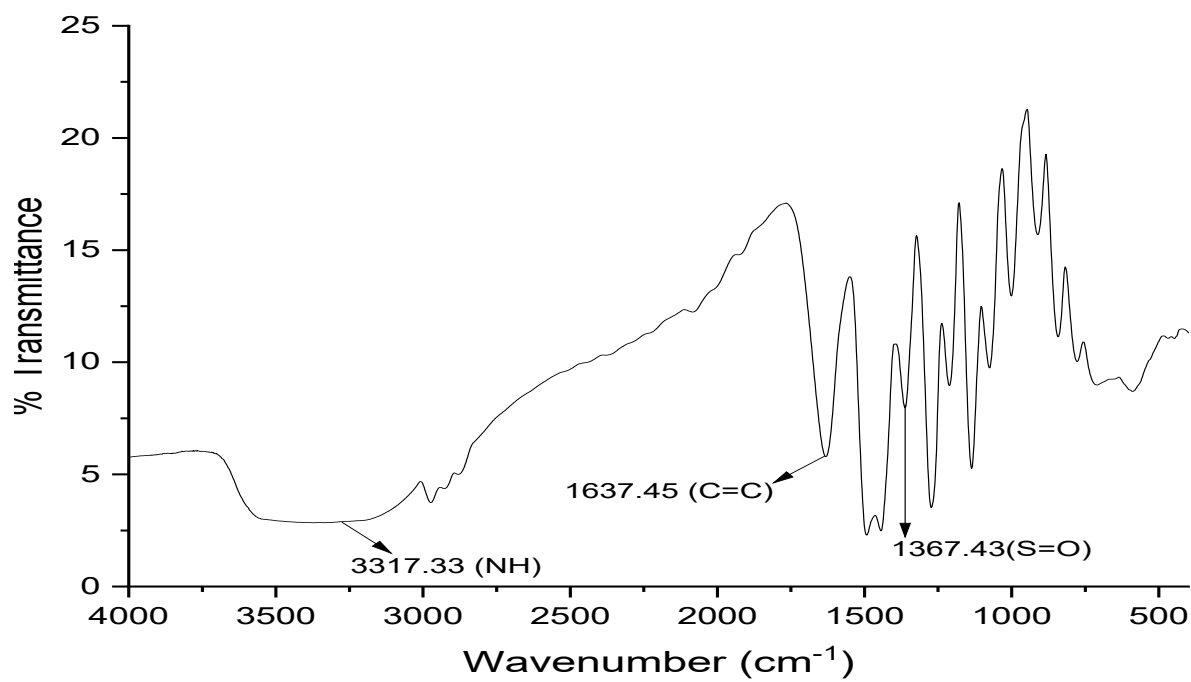
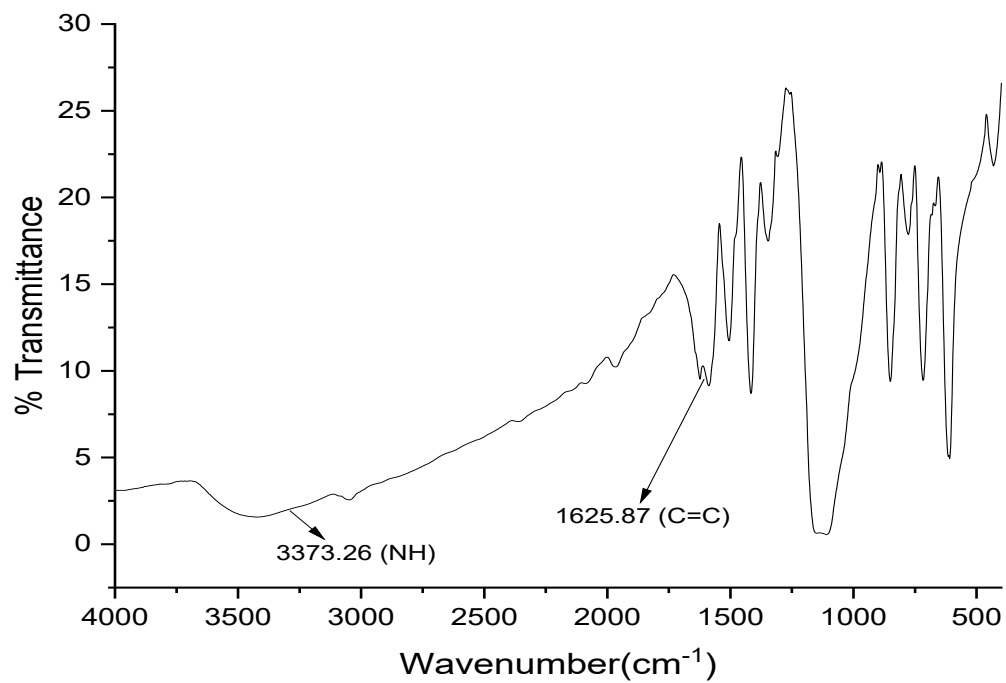


Figure 42: FTIR graph of compound a10



**Figure 43:** FTIR graph of compound **a11**

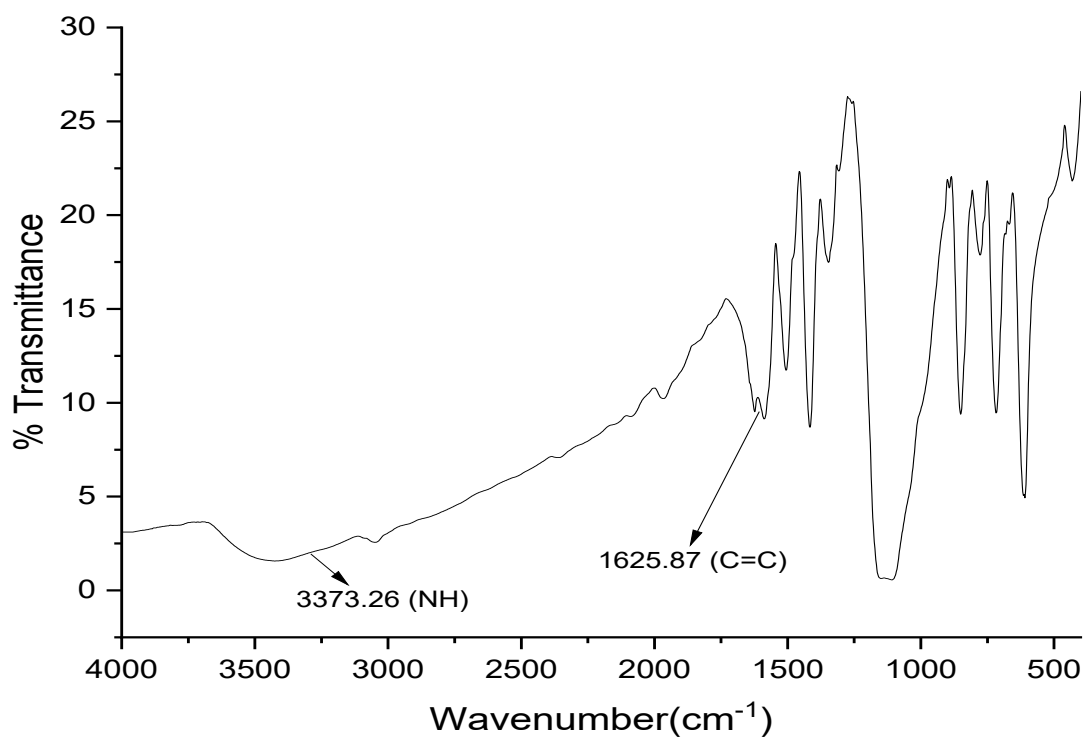


Figure 44: FTIR graph of compound **a12**

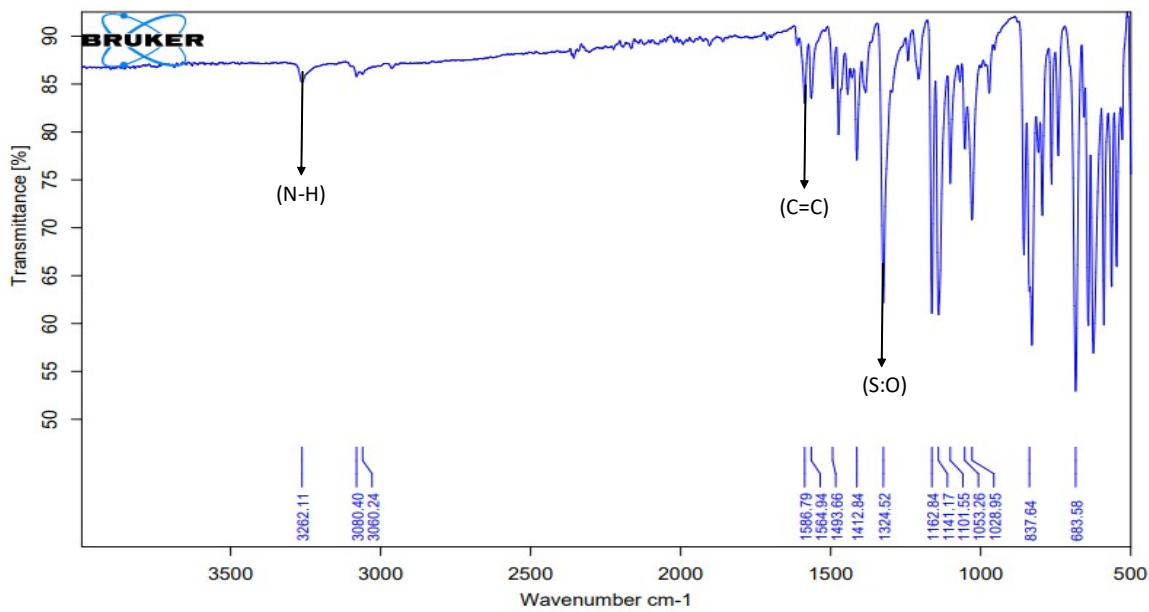


Figure 45: FTIR graph of compound **a13**

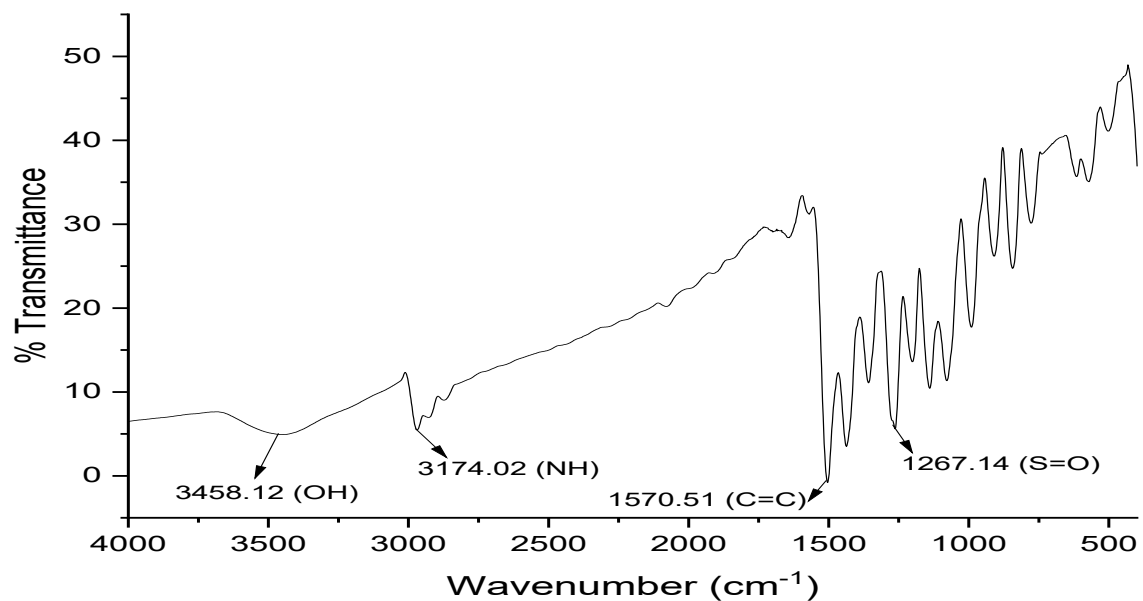


Figure 46: FTIR graph of compound a14

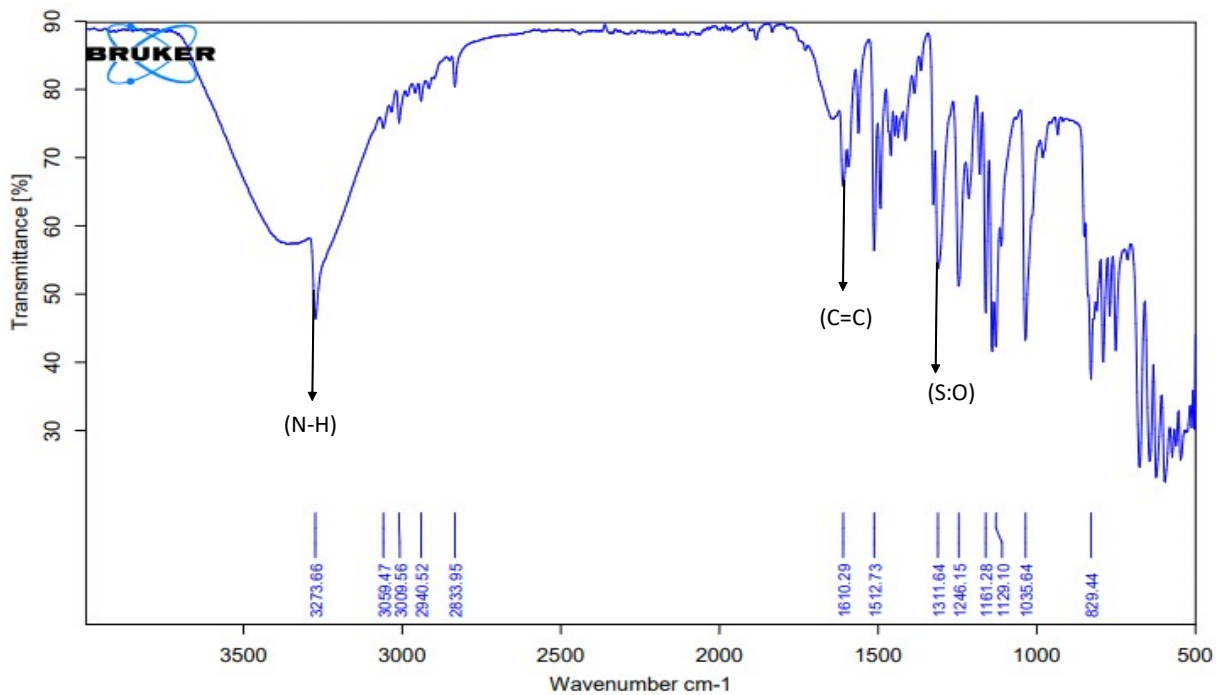


Figure 47: FTIR graph of compound a15

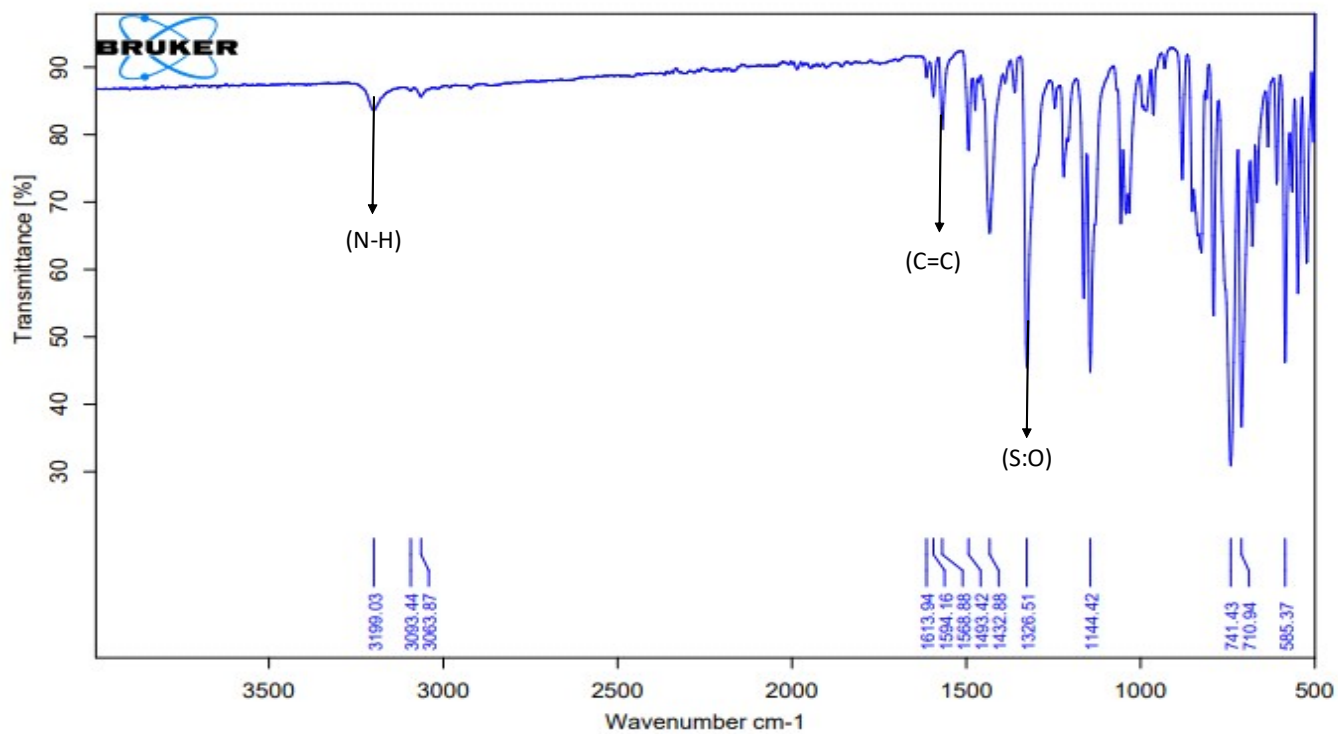


Figure 48: FTIR graph of compound a16

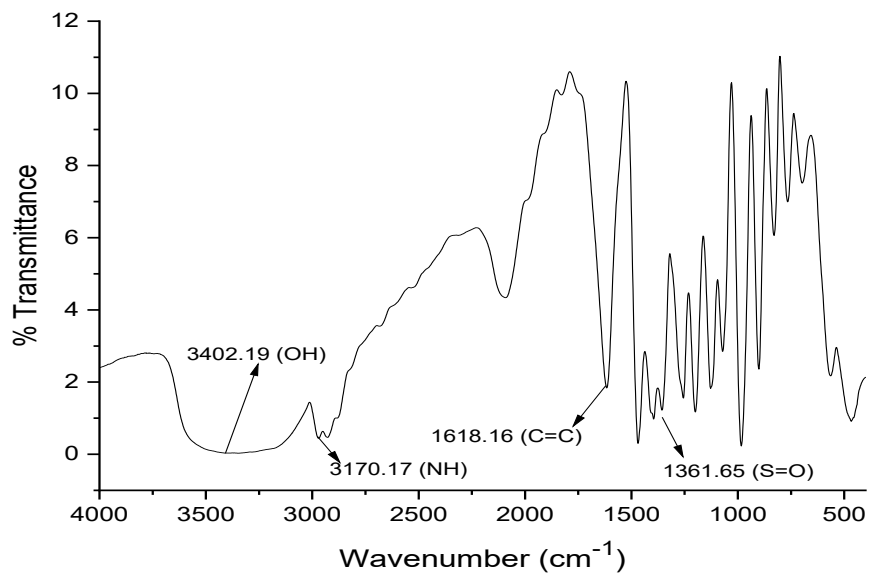


Figure 49: FTIR graph of compound a17

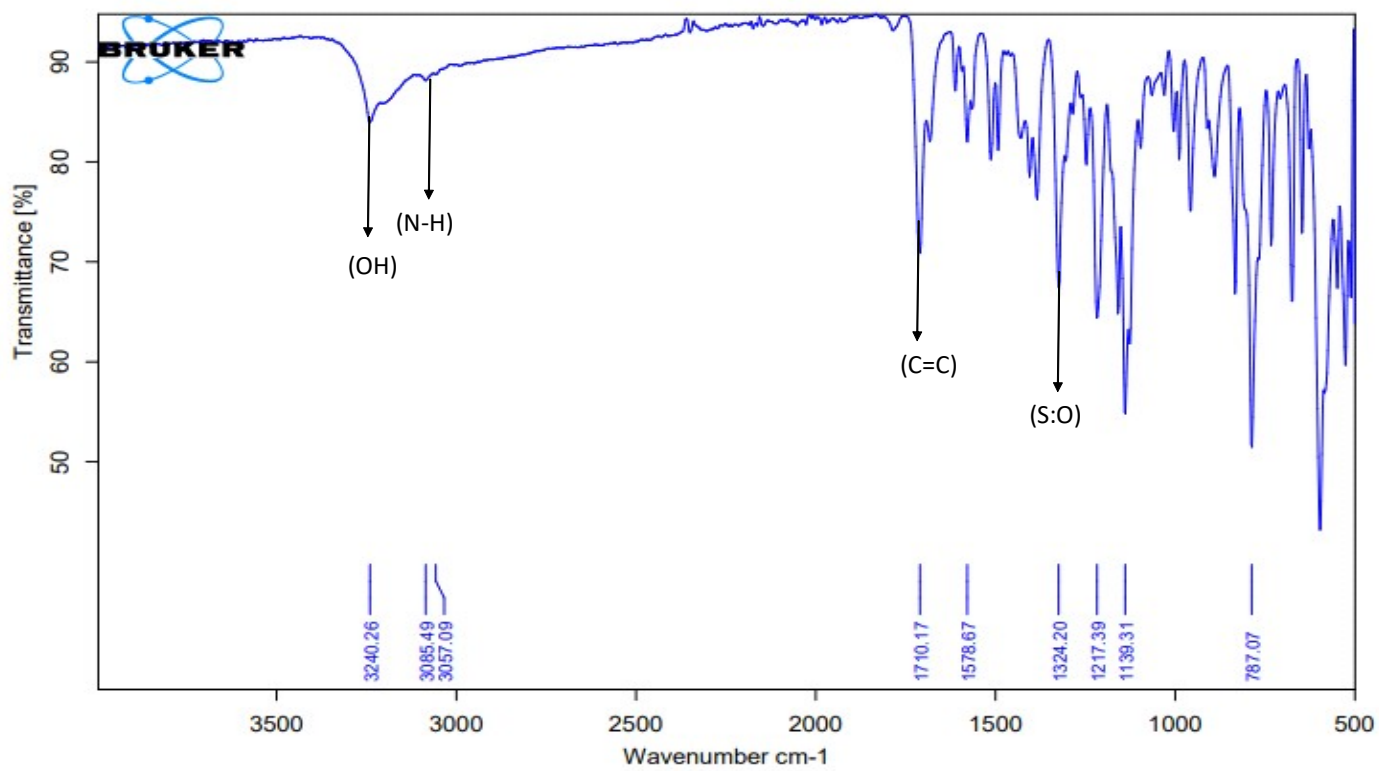


Figure 50: FTIR graph of compound a18



# HPLC Chromatogram



SHIMADZU  
LabSolutions

## Analysis Report

### <Sample Information>

Sample Name	: Saqib HT37-1 by Zubair	Sample Type	: Unknown
Sample ID	: SHT37-1-1Z	Acquired by	: System Administrator
Data Filename	: Saqib HT37-1by Zubair Data1.lcd	Processed by	: System Administrator
Method Filename	: Saqib HT35-1 by Zubair.lcm		
Batch Filename	:		
Vial #	: 1-1		
Injection Volume	: 20 uL		
Date Acquired	: 10-Jan-24 7:21:03 PM		
Date Processed	: 10-Jan-24 7:31:14 PM		

### <Chromatogram>

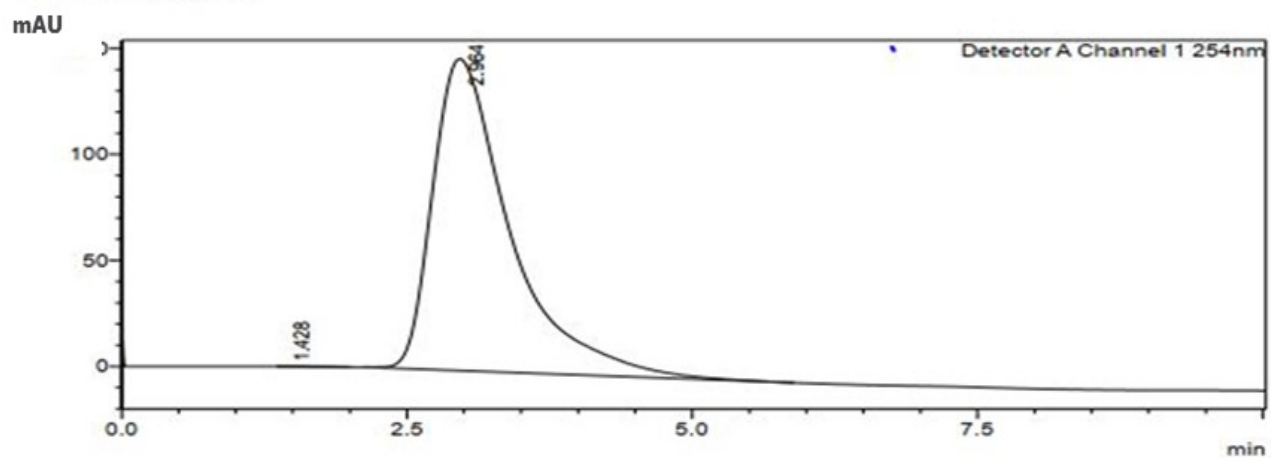


Figure 51: Chromatogram of compound a5

## <Sample Information>

Sample Name	: Saqib HT35-1 by Zubair	Sample Type	: Unknown
Sample ID	: SHT35-1Z	Acquired by	: System Administrator
Data Filename	: Saqib HT35-1 by Zubair Data1.lcd	Processed by	: System Administrator
Method Filename	: Saqib HT35-1 by Zubair.lcm		
Batch Filename	:		
Vial #	: 1-1		
Injection Volume	: 20 uL		
Date Acquired	: 10-Jan-24 3:04:44 PM		
Date Processed	: 10-Jan-24 3:19:56 PM		

## <Chromatogram>

mAU

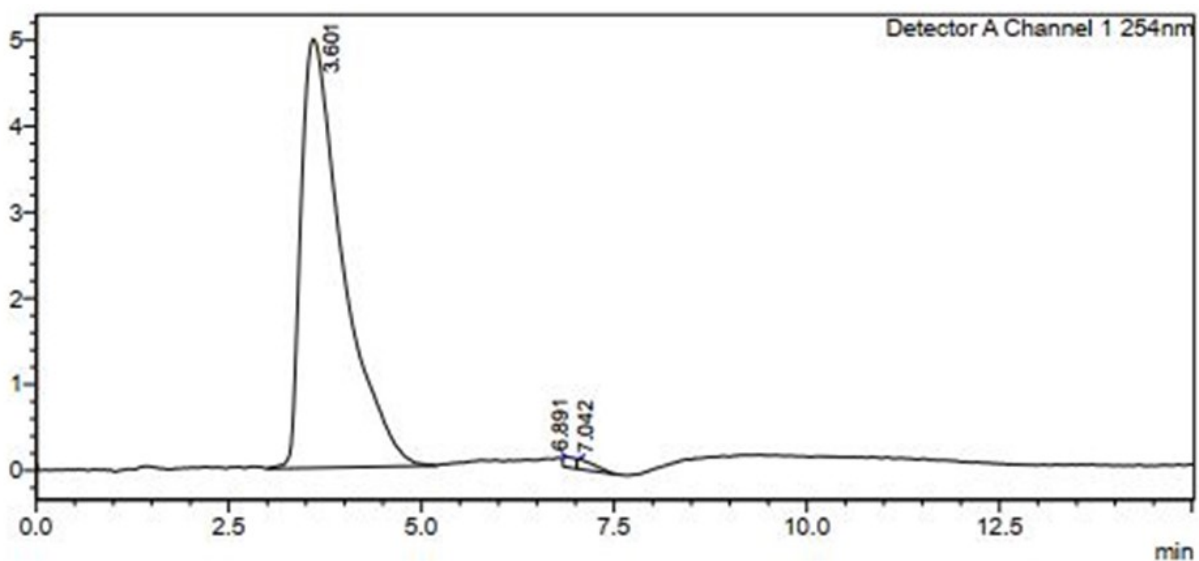


Figure 52: Chromatogram of compound a3



SHIMADZU

LabSolutions

# Analysis Report

## <Sample Information>

Sample Name	: Saqlb HT36-1 by Zubair	Sample Type	: Unknown
Sample ID	: SHT36-1Z		
Data Filename	: Saqlb HT36-1 by Zubair Data1.lcd		
Method Filename	: Saqlb Sample by zubair HT35.lcm		
Batch Filename	:		
Vial #	: 1-1		
Injection Volume	: 20 uL	Acquired by	: System Administrator
Date Acquired	: 10-Jan-24 4:03:15 PM	Processed by	: System Administrator
Date Processed	: 10-Jan-24 4:33:27 PM		

## <Chromatogram>

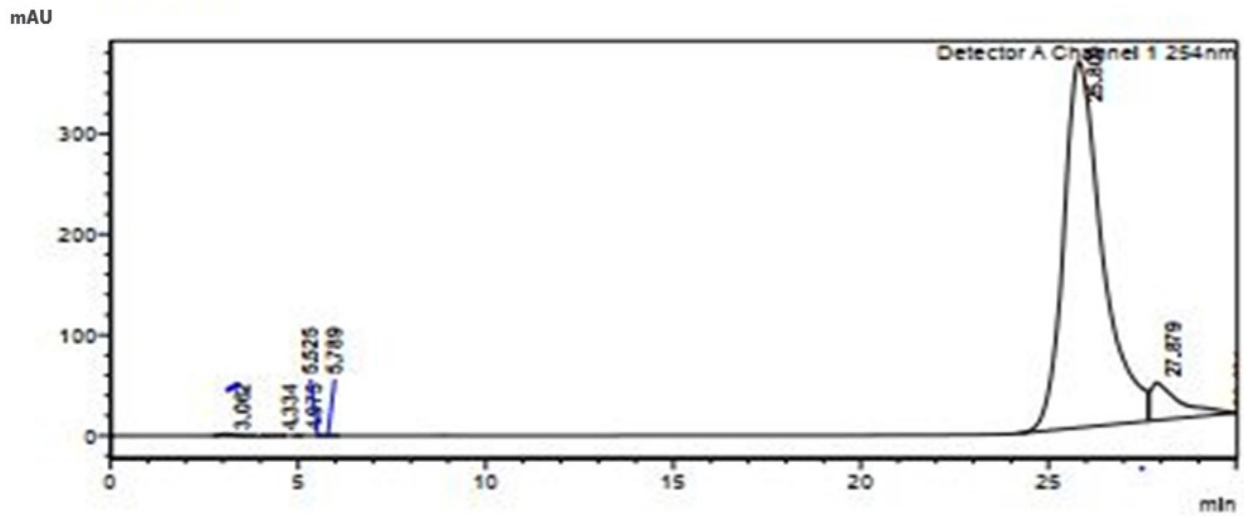


Figure 53: Chromatogram of compound a4

**Table 1:** The docking scores of synthesized compounds on MAO-A, MAO-B, AChE, and BChE

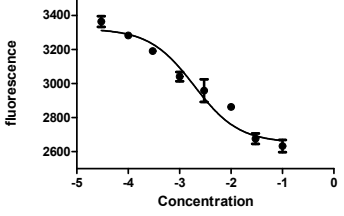
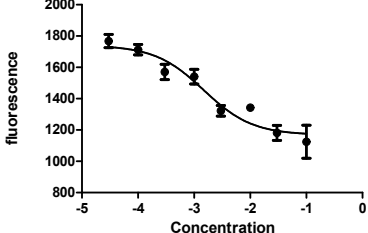
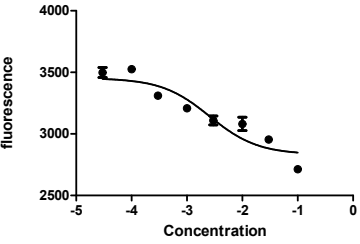
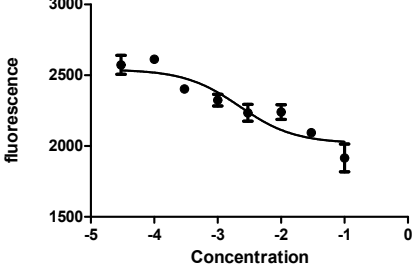
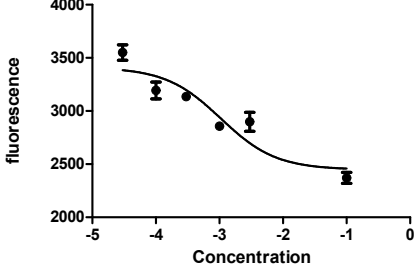
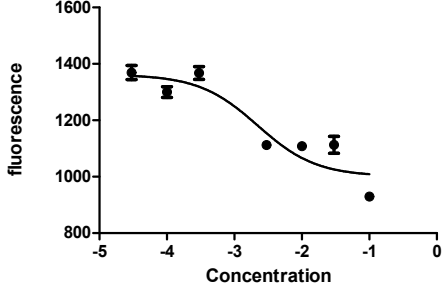
Molecule	MAO A	MAO A	AChE	BChE
	S value (kcal/mol)			
<b>a1.</b>	-8.76	-9.87	-8.18	-3.18
<b>a2.</b>	-8.50	-8.73	-7.43	-4.88
<b>a3.</b>	-8.55	-9.65	-7.03	-3.70
<b>a4.</b>	-8.62	-9.94	-8.18	-4.02
<b>a5.</b>	-10.40	-9.73	-5.78	-4.84
<b>a6.</b>	-9.26	-9.57	-7.46	-7.68
<b>a7.</b>	-8.79	-7.48	-3.57	-3.88
<b>a8.</b>	-8.51	-9.59	-2.97	-3.55
<b>a9.</b>	-8.58	-9.88	-4.15	-2.48
<b>a10.</b>	-8.36	-9.41	-7.13	-2.58
<b>a11.</b>	-9.36	-10.52	-8.88	-6.48
<b>a12.</b>	-7.39	-10.57	-7.38	-6.59
<b>a13.</b>	-8.76	-10.07	-6.59	-3.08
<b>a14.</b>	-9.23	-9.49	-7.01	-6.89
<b>a15.</b>	-9.41	-8.43	-7.98	-2.88
<b>a16.</b>	-7.54	-7.93	-7.81	-4.36
<b>a17.</b>	-8.90	-8.19	-6.20	-3.31
<b>a18.</b>	-8.54	-8.60	-7.32	-5.38

**Table 2:** IC<sub>50</sub> values of synthesized compounds against monoamine oxidase

Code	Graph	Graph
a1		
a2		
a3		
a4		
a5		

a6	<p>Graph a6: fluorescence vs Concentration. The y-axis ranges from 2500 to 3500, and the x-axis from -5 to 0. The data shows a decreasing trend from approximately 3300 at concentration -4.5 to 2600 at concentration -1.</p>	<p>Graph a6: fluorescence vs Concentration. The y-axis ranges from 1000 to 1800, and the x-axis from -5 to 0. The data shows a decreasing trend from approximately 1550 at concentration -4.5 to 1200 at concentration -1.</p>
a7	<p>Graph a7: fluorescence vs Concentration. The y-axis ranges from 0 to 4000, and the x-axis from -5 to 0. The data shows a decreasing trend from approximately 3400 at concentration -4.5 to 2000 at concentration -1.</p>	<p>Graph a7: fluorescence vs Concentration. The y-axis ranges from 1000 to 2500, and the x-axis from -5 to 0. The data shows a decreasing trend from approximately 2100 at concentration -4.5 to 1400 at concentration -1.</p>
a8	<p>Graph a8: fluorescence vs Concentration. The y-axis ranges from 0 to 3000, and the x-axis from -5 to 0. The data shows a decreasing trend from approximately 2500 at concentration -4.5 to 1400 at concentration -1.</p>	<p>Graph a8: fluorescence vs Concentration. The y-axis ranges from 1000 to 3000, and the x-axis from -5 to 0. The data shows a decreasing trend from approximately 2400 at concentration -4.5 to 1600 at concentration -1.</p>
a9	<p>Graph a9: fluorescence vs Concentration. The y-axis ranges from 0 to 2000, and the x-axis from -5 to 0. The data shows a decreasing trend from approximately 1600 at concentration -4.5 to 900 at concentration -1.</p>	<p>Graph a9: fluorescence vs Concentration. The y-axis ranges from 1800 to 3000, and the x-axis from -5 to 0. The data shows a decreasing trend from approximately 2500 at concentration -4.5 to 1900 at concentration -1.</p>
a10	<p>Graph a10: fluorescence vs Concentration. The y-axis ranges from 1500 to 3000, and the x-axis from -5 to 0. The data shows a decreasing trend from approximately 2600 at concentration -4.5 to 1900 at concentration -1.</p>	<p>Graph a10: fluorescence vs Concentration. The y-axis ranges from 1800 to 2800, and the x-axis from -5 to 0. The data shows a decreasing trend from approximately 2350 at concentration -4.5 to 2000 at concentration -1.</p>

a11		
a12		
a13		
a14		
a15		

a16	 <table border="1"><caption>Data for a16 (left column)</caption><thead><tr><th>Concentration</th><th>Fluorescence</th></tr></thead><tbody><tr><td>-5</td><td>3350</td></tr><tr><td>-4</td><td>3300</td></tr><tr><td>-3</td><td>3050</td></tr><tr><td>-2</td><td>2850</td></tr><tr><td>-1</td><td>2650</td></tr></tbody></table>	Concentration	Fluorescence	-5	3350	-4	3300	-3	3050	-2	2850	-1	2650	 <table border="1"><caption>Data for a16 (right column)</caption><thead><tr><th>Concentration</th><th>Fluorescence</th></tr></thead><tbody><tr><td>-5</td><td>1750</td></tr><tr><td>-4</td><td>1700</td></tr><tr><td>-3</td><td>1550</td></tr><tr><td>-2</td><td>1350</td></tr><tr><td>-1</td><td>1150</td></tr></tbody></table>	Concentration	Fluorescence	-5	1750	-4	1700	-3	1550	-2	1350	-1	1150
Concentration	Fluorescence																									
-5	3350																									
-4	3300																									
-3	3050																									
-2	2850																									
-1	2650																									
Concentration	Fluorescence																									
-5	1750																									
-4	1700																									
-3	1550																									
-2	1350																									
-1	1150																									
a17	 <table border="1"><caption>Data for a17 (left column)</caption><thead><tr><th>Concentration</th><th>Fluorescence</th></tr></thead><tbody><tr><td>-5</td><td>3500</td></tr><tr><td>-4</td><td>3500</td></tr><tr><td>-3</td><td>3200</td></tr><tr><td>-2</td><td>3050</td></tr><tr><td>-1</td><td>2750</td></tr></tbody></table>	Concentration	Fluorescence	-5	3500	-4	3500	-3	3200	-2	3050	-1	2750	 <table border="1"><caption>Data for a17 (right column)</caption><thead><tr><th>Concentration</th><th>Fluorescence</th></tr></thead><tbody><tr><td>-5</td><td>2550</td></tr><tr><td>-4</td><td>2600</td></tr><tr><td>-3</td><td>2300</td></tr><tr><td>-2</td><td>2200</td></tr><tr><td>-1</td><td>1900</td></tr></tbody></table>	Concentration	Fluorescence	-5	2550	-4	2600	-3	2300	-2	2200	-1	1900
Concentration	Fluorescence																									
-5	3500																									
-4	3500																									
-3	3200																									
-2	3050																									
-1	2750																									
Concentration	Fluorescence																									
-5	2550																									
-4	2600																									
-3	2300																									
-2	2200																									
-1	1900																									
a18	 <table border="1"><caption>Data for a18 (left column)</caption><thead><tr><th>Concentration</th><th>Fluorescence</th></tr></thead><tbody><tr><td>-5</td><td>3500</td></tr><tr><td>-4</td><td>3200</td></tr><tr><td>-3</td><td>2850</td></tr><tr><td>-2</td><td>2900</td></tr><tr><td>-1</td><td>2400</td></tr></tbody></table>	Concentration	Fluorescence	-5	3500	-4	3200	-3	2850	-2	2900	-1	2400	 <table border="1"><caption>Data for a18 (right column)</caption><thead><tr><th>Concentration</th><th>Fluorescence</th></tr></thead><tbody><tr><td>-5</td><td>1350</td></tr><tr><td>-4</td><td>1300</td></tr><tr><td>-3</td><td>1350</td></tr><tr><td>-2</td><td>1100</td></tr><tr><td>-1</td><td>950</td></tr></tbody></table>	Concentration	Fluorescence	-5	1350	-4	1300	-3	1350	-2	1100	-1	950
Concentration	Fluorescence																									
-5	3500																									
-4	3200																									
-3	2850																									
-2	2900																									
-1	2400																									
Concentration	Fluorescence																									
-5	1350																									
-4	1300																									
-3	1350																									
-2	1100																									
-1	950																									

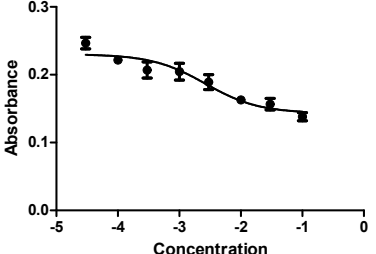
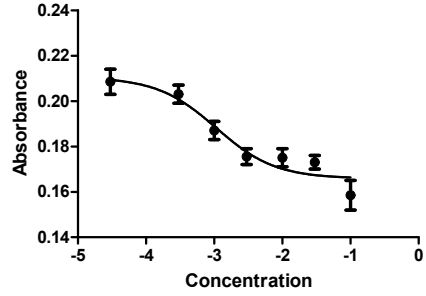
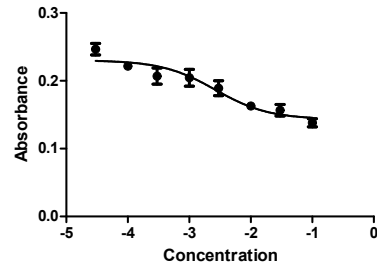


**Table 3:** IC<sub>50</sub> values of synthesized compounds against AChE and BChE

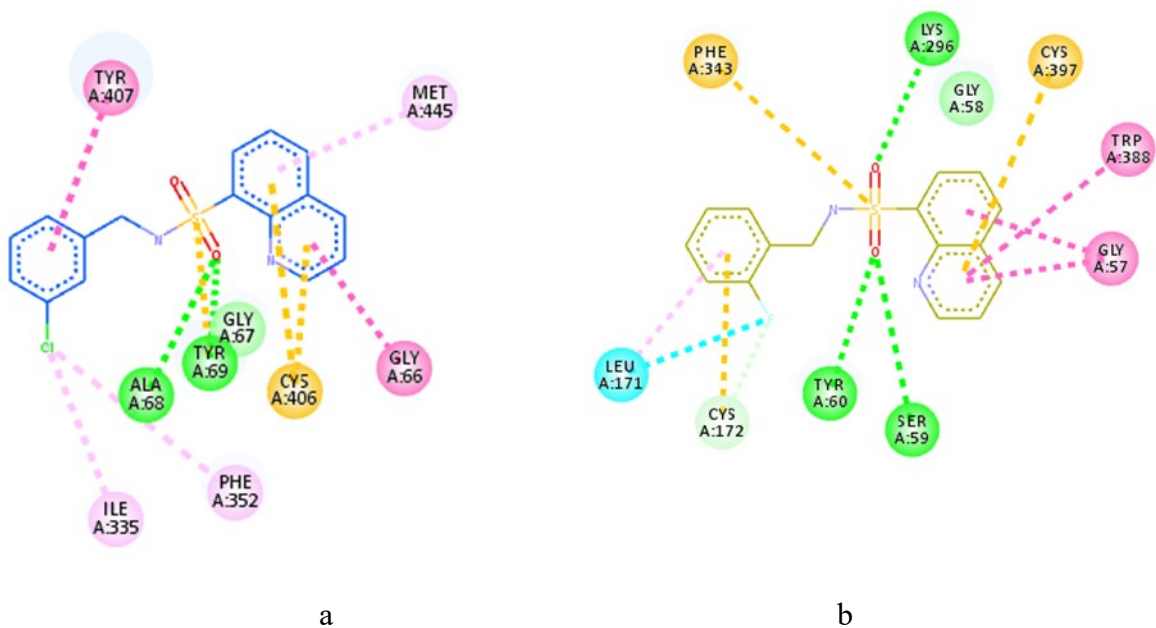
Code	AChE	BChE
a1		
a2		
a3		
a4		
a5		

a6		
a7		
a8		
a9		
a10		
a11		

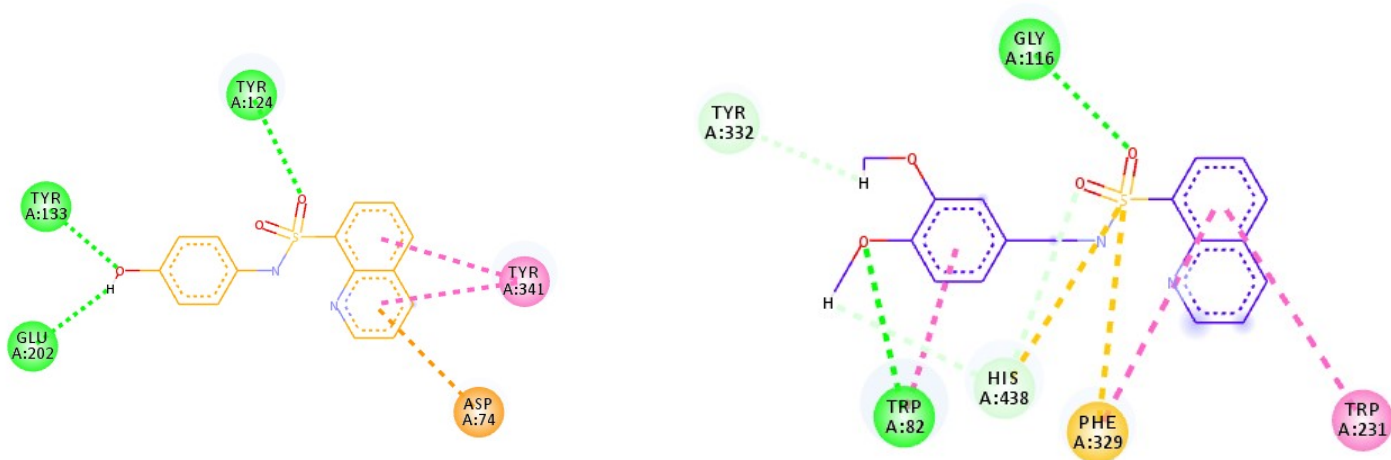
a12		
a13		
a14		
a15		
a16		

a17	 <p>A line graph showing Absorbance on the y-axis (ranging from 0.0 to 0.3) versus Concentration on the x-axis (ranging from -5 to 0). The data points, represented by black squares with vertical error bars, show a decreasing trend from approximately 0.25 at concentration -4.5 to 0.14 at concentration -1. A smooth curve is fitted to the data points.</p> <table border="1"><thead><tr><th>Concentration</th><th>Absorbance</th></tr></thead><tbody><tr><td>-4.5</td><td>0.25</td></tr><tr><td>-4.0</td><td>0.22</td></tr><tr><td>-3.5</td><td>0.20</td></tr><tr><td>-3.0</td><td>0.19</td></tr><tr><td>-2.5</td><td>0.18</td></tr><tr><td>-2.0</td><td>0.16</td></tr><tr><td>-1.5</td><td>0.15</td></tr><tr><td>-1.0</td><td>0.14</td></tr></tbody></table>	Concentration	Absorbance	-4.5	0.25	-4.0	0.22	-3.5	0.20	-3.0	0.19	-2.5	0.18	-2.0	0.16	-1.5	0.15	-1.0	0.14																			
Concentration	Absorbance																																					
-4.5	0.25																																					
-4.0	0.22																																					
-3.5	0.20																																					
-3.0	0.19																																					
-2.5	0.18																																					
-2.0	0.16																																					
-1.5	0.15																																					
-1.0	0.14																																					
a18	 <p>A line graph showing Absorbance on the y-axis (ranging from 0.14 to 0.24) versus Concentration on the x-axis (ranging from -5 to 0). The data points, represented by black squares with vertical error bars, show a decreasing trend from approximately 0.21 at concentration -4.5 to 0.15 at concentration -1. A smooth curve is fitted to the data points.</p> <table border="1"><thead><tr><th>Concentration</th><th>Absorbance</th></tr></thead><tbody><tr><td>-4.5</td><td>0.21</td></tr><tr><td>-4.0</td><td>0.20</td></tr><tr><td>-3.5</td><td>0.19</td></tr><tr><td>-3.0</td><td>0.18</td></tr><tr><td>-2.5</td><td>0.17</td></tr><tr><td>-2.0</td><td>0.17</td></tr><tr><td>-1.5</td><td>0.17</td></tr><tr><td>-1.0</td><td>0.15</td></tr></tbody></table>	Concentration	Absorbance	-4.5	0.21	-4.0	0.20	-3.5	0.19	-3.0	0.18	-2.5	0.17	-2.0	0.17	-1.5	0.17	-1.0	0.15	 <p>A line graph showing Absorbance on the y-axis (ranging from 0.0 to 0.3) versus Concentration on the x-axis (ranging from -5 to 0). The data points, represented by black squares with vertical error bars, show a decreasing trend from approximately 0.25 at concentration -4.5 to 0.14 at concentration -1. A smooth curve is fitted to the data points.</p> <table border="1"><thead><tr><th>Concentration</th><th>Absorbance</th></tr></thead><tbody><tr><td>-4.5</td><td>0.25</td></tr><tr><td>-4.0</td><td>0.22</td></tr><tr><td>-3.5</td><td>0.20</td></tr><tr><td>-3.0</td><td>0.19</td></tr><tr><td>-2.5</td><td>0.18</td></tr><tr><td>-2.0</td><td>0.16</td></tr><tr><td>-1.5</td><td>0.15</td></tr><tr><td>-1.0</td><td>0.14</td></tr></tbody></table>	Concentration	Absorbance	-4.5	0.25	-4.0	0.22	-3.5	0.20	-3.0	0.19	-2.5	0.18	-2.0	0.16	-1.5	0.15	-1.0	0.14
Concentration	Absorbance																																					
-4.5	0.21																																					
-4.0	0.20																																					
-3.5	0.19																																					
-3.0	0.18																																					
-2.5	0.17																																					
-2.0	0.17																																					
-1.5	0.17																																					
-1.0	0.15																																					
Concentration	Absorbance																																					
-4.5	0.25																																					
-4.0	0.22																																					
-3.5	0.20																																					
-3.0	0.19																																					
-2.5	0.18																																					
-2.0	0.16																																					
-1.5	0.15																																					
-1.0	0.14																																					

## 2D interaction of potent compounds



**Figure 54:** 2D interaction of compound **a5** left side MAO-A (a) and **a12** right side MAO-B (b)



**Figure 55:** 2D interaction of compound **a11** left side AChE (c) and **a6** right side BChE (d)