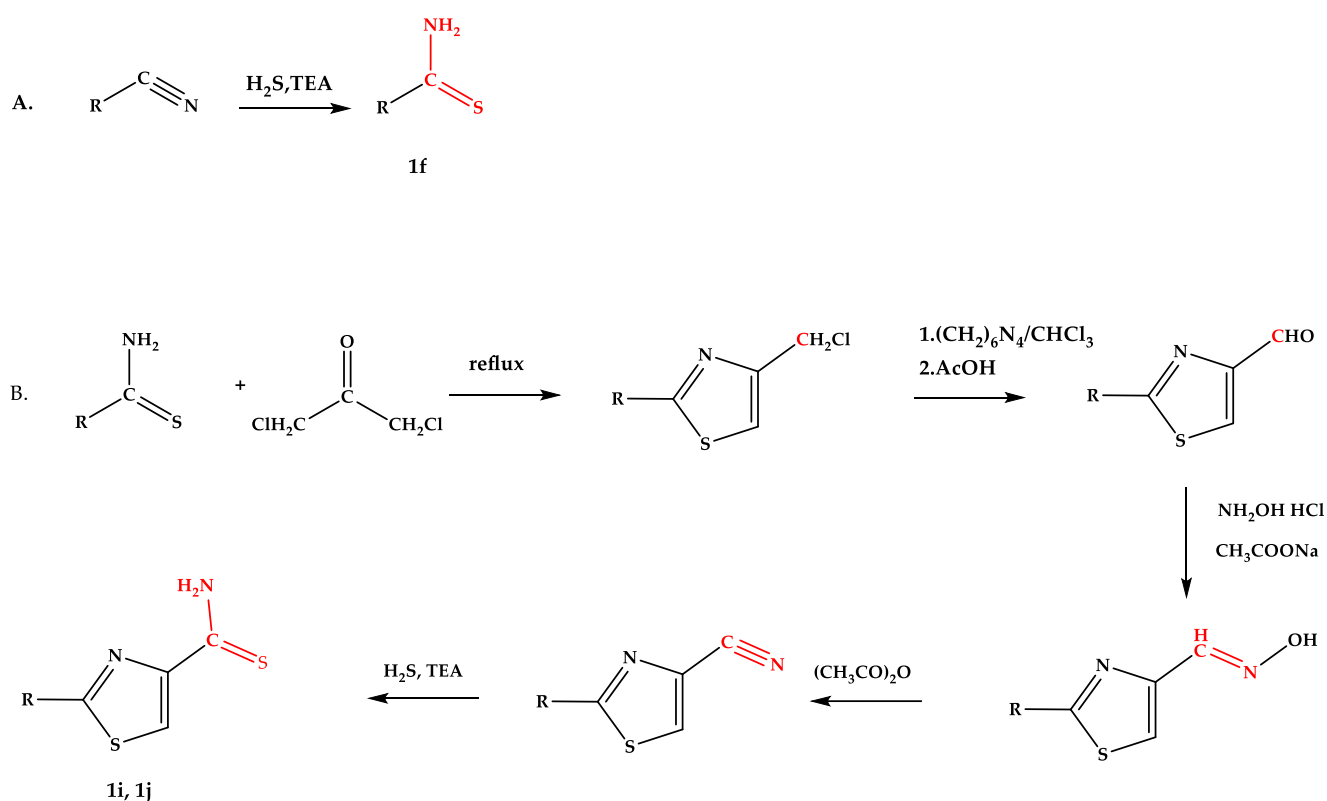


# Supplementary Material: Synthesis, cytotoxicity and antioxidant activity of new compounds with thiazolyl-polyphenolic structure

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## 1. Schemes

1.1 The synthesis route for obtention of intermediate thioamides **1f**, **1i** and **1j**, reported in our group previous reports



**Scheme S1.** Synthesis of the thioamides **1f** (A) and **1i-j** (B), according to our group previous reports [18-20]

## 2.Figures

### 2.1 The IR spectra

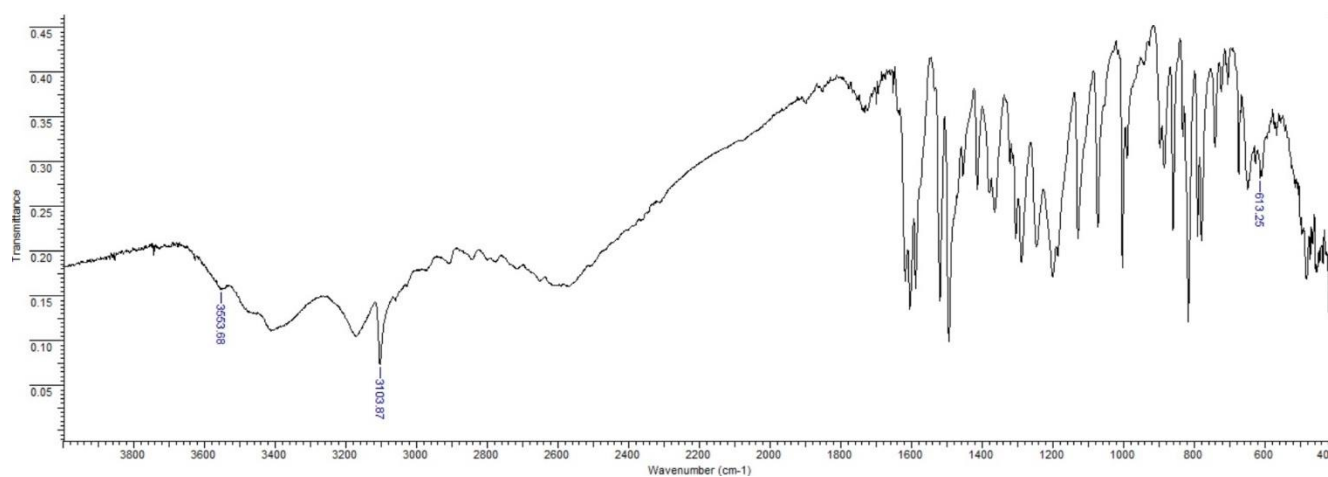


Figure S1. The IR spectrum for the compound 3d

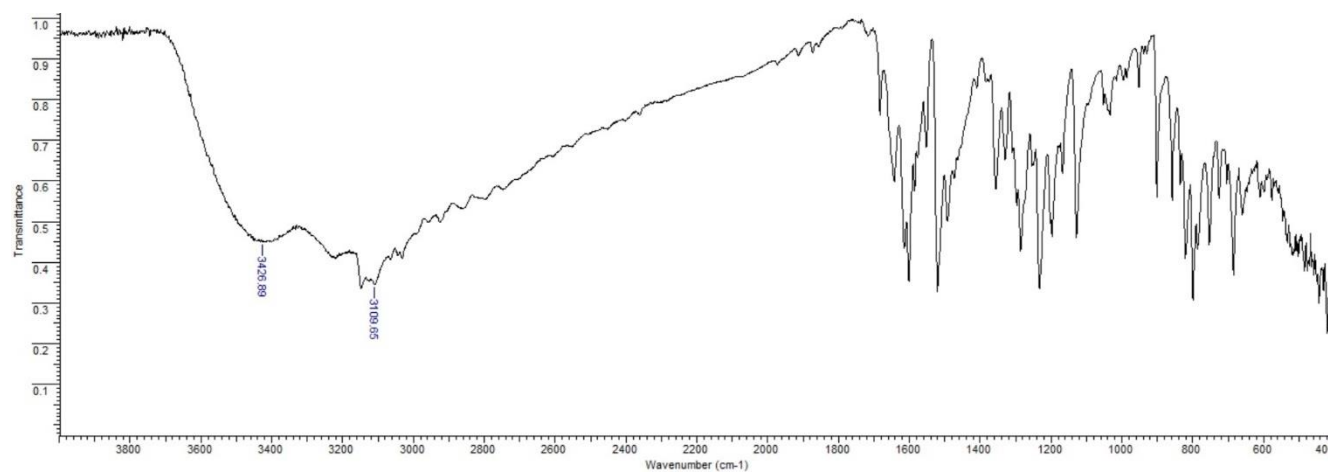


Figure S2. The IR spectrum for the compound 3e

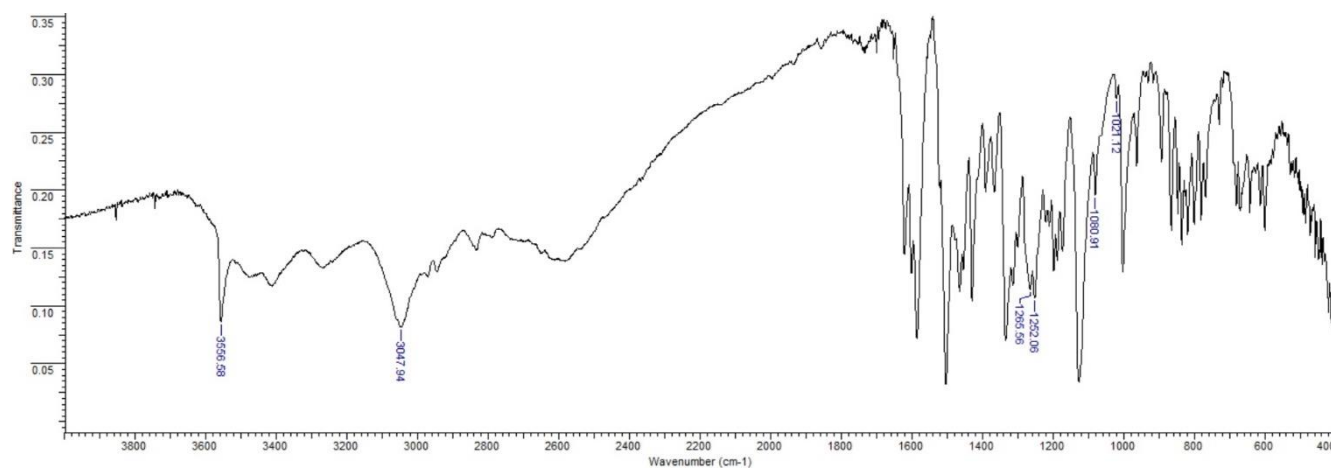
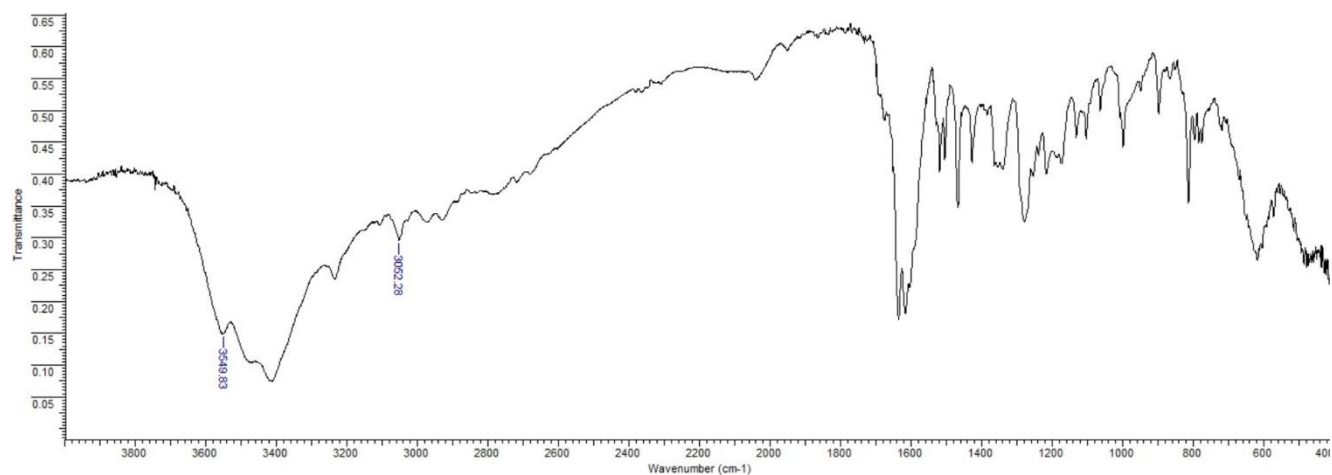
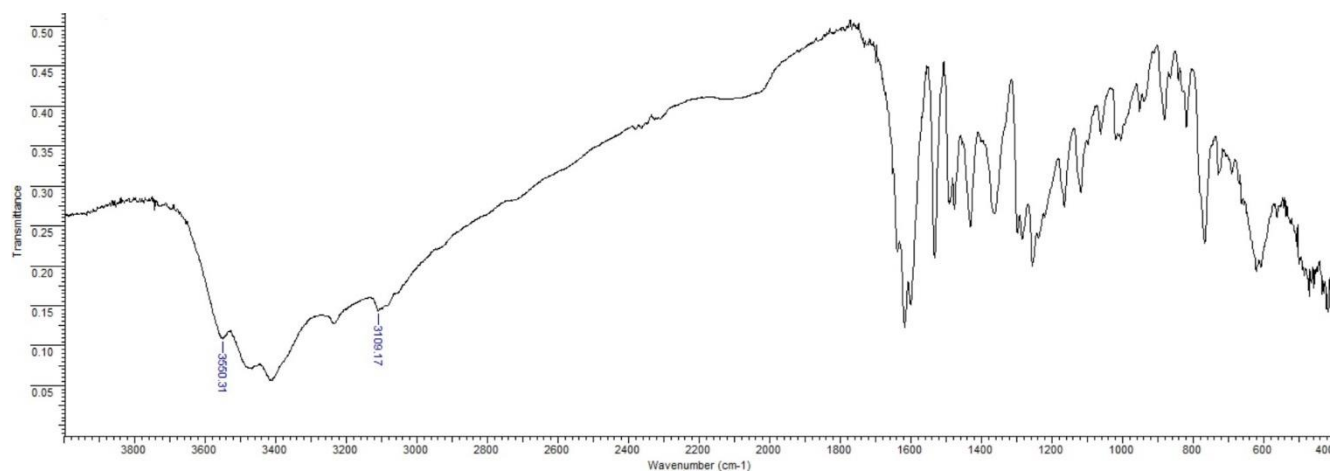


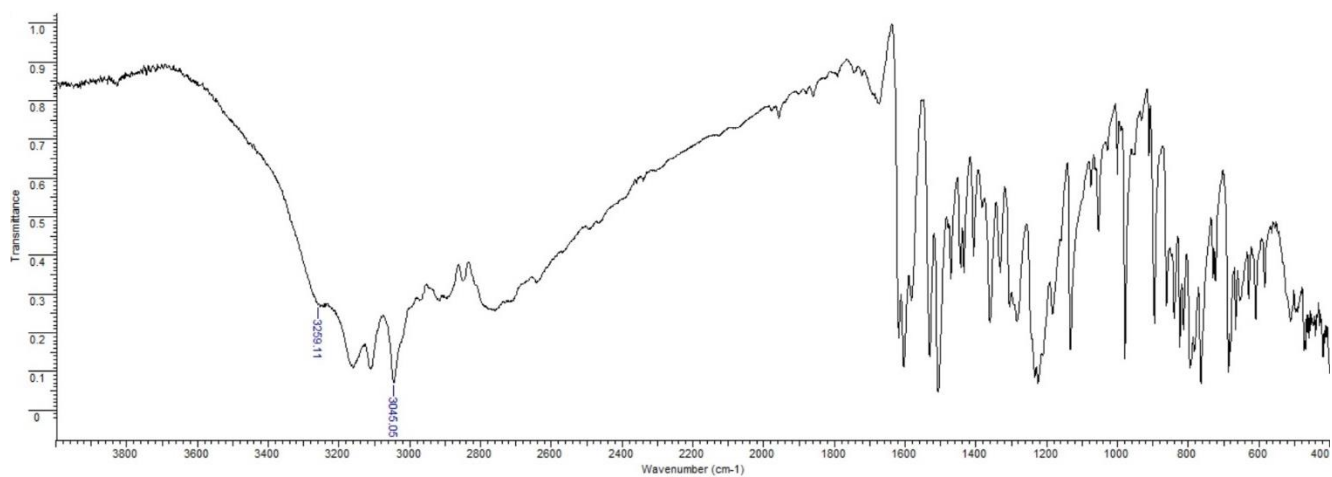
Figure S3. The IR spectrum for the compound 3f



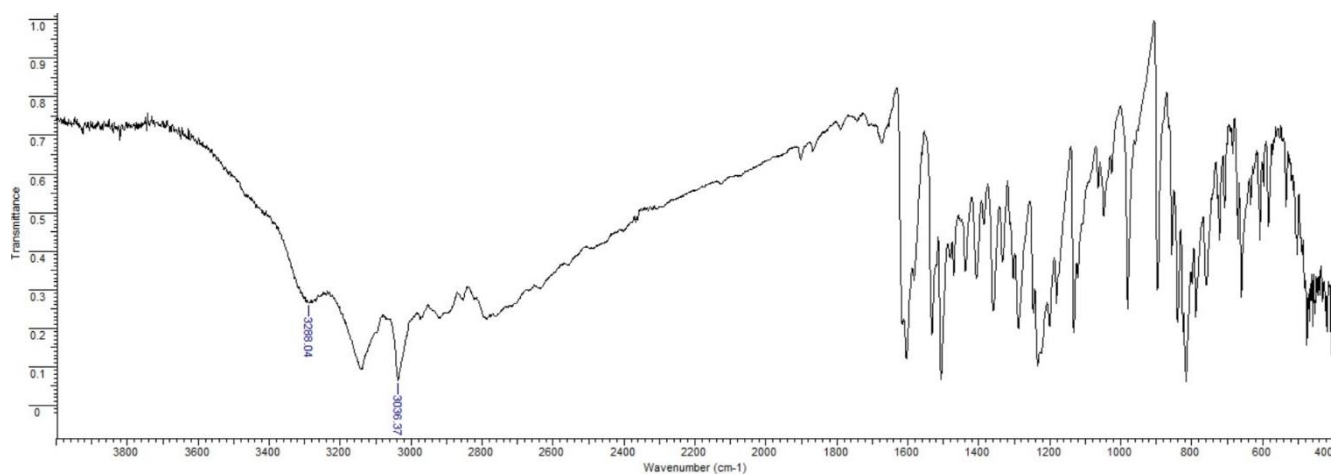
**Figure S4.** The IR spectrum for the compound **3g**



**Figure S5.** The IR spectrum for the compound **3h**

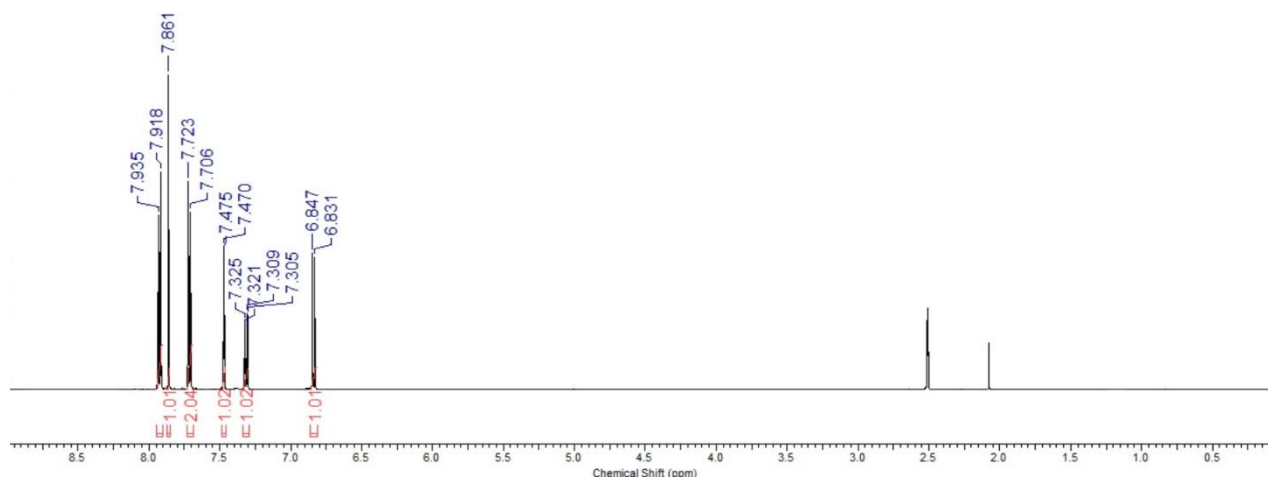


**Figure S6.** The IR spectrum for the compound **3i**

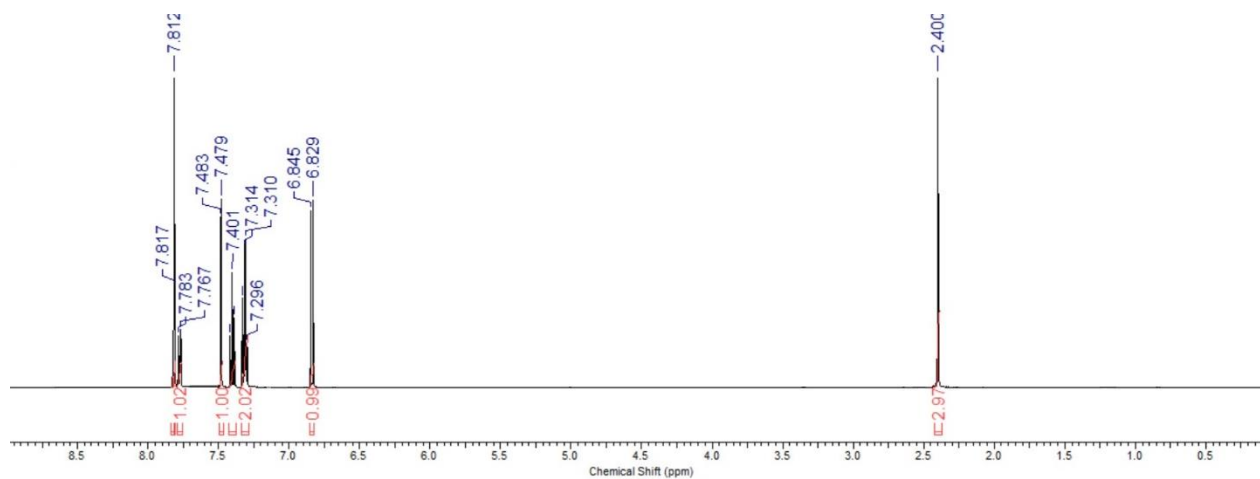


**Figure S7.** The IR spectrum for the compound **3j**

## 2.2 The $^1\text{H}$ -NMR spectra



**Figure S8.** The  $^1\text{H}$ -NMR spectrum for the compound **3d**



**Figure S9.** The  $^1\text{H}$ -NMR spectrum for the compound **3e**

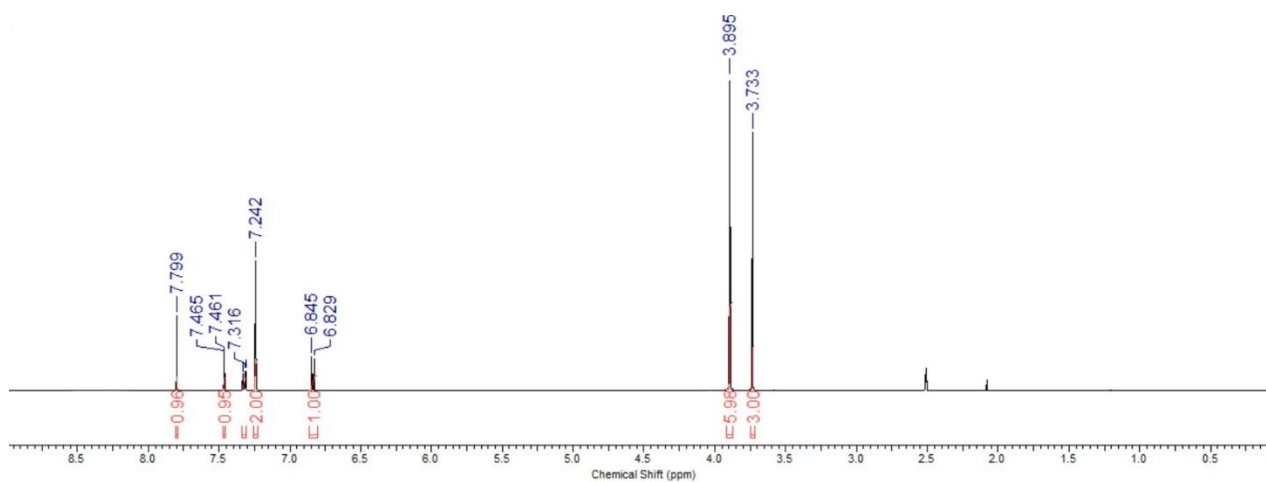


Figure S10. The  $^1\text{H}$ -NMR spectrum for the compound **3f**

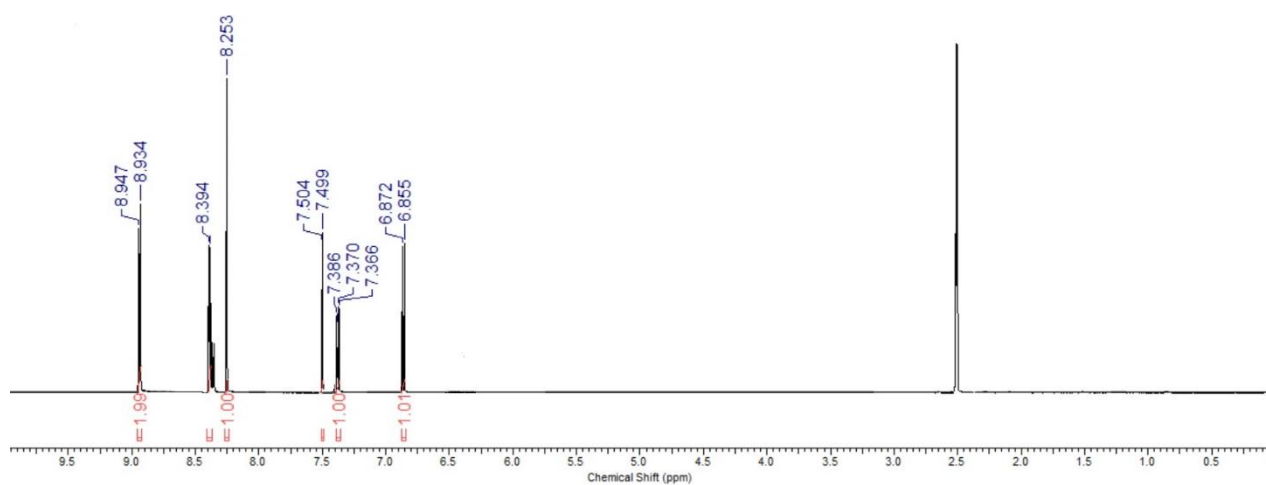


Figure S11. The  $^1\text{H}$ -NMR spectrum for the compound **3g**

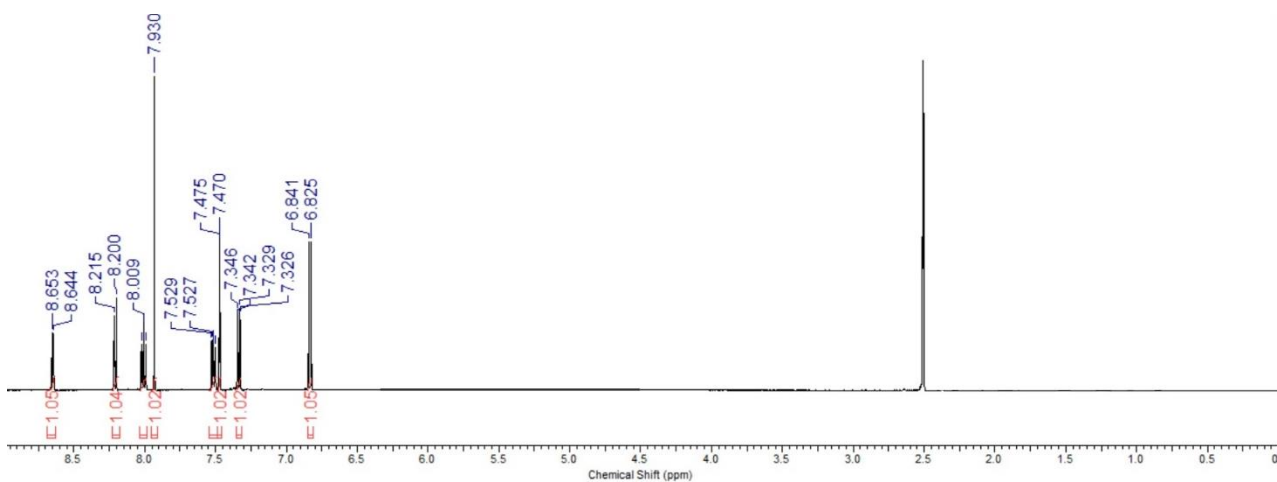


Figure S12. The  $^1\text{H}$ -NMR spectrum for the compound **3h**

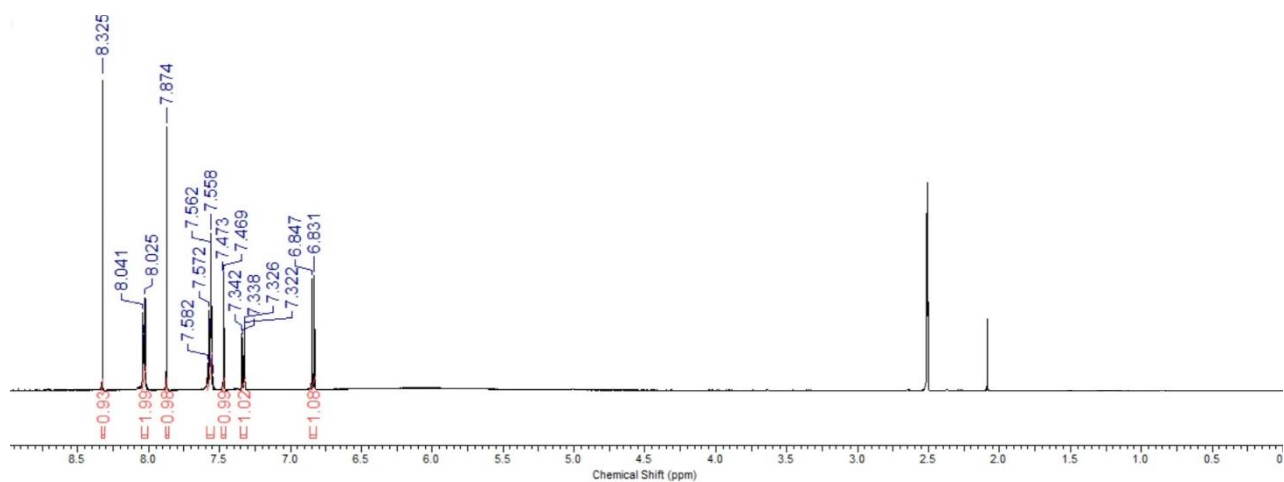


Figure S13. The  $^1\text{H}$ -NMR spectrum for the compound **3i**

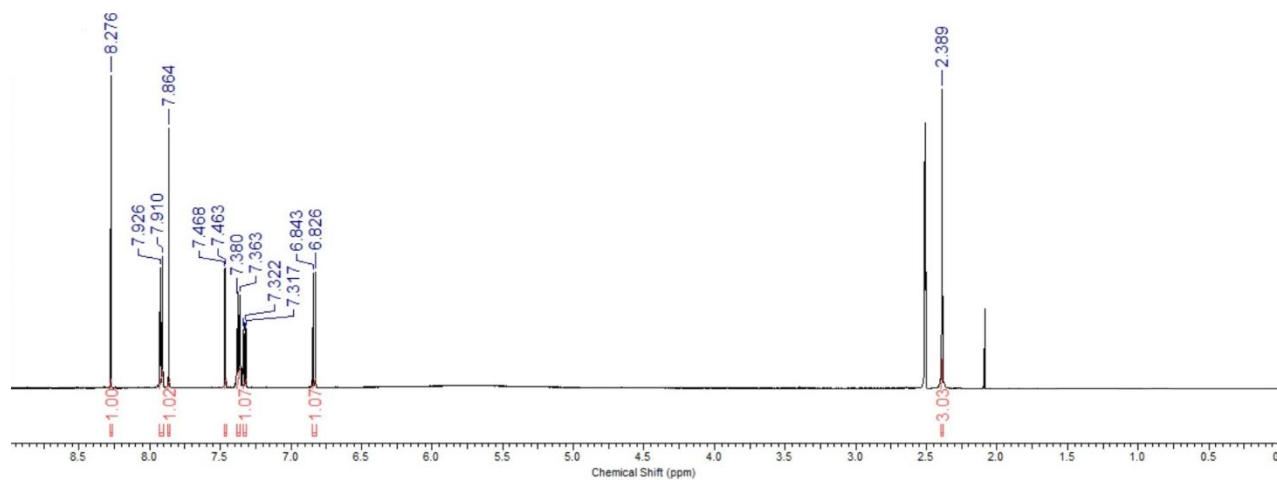


Figure S14. The  $^1\text{H}$ -NMR spectrum for the compound **3j**

### 2.3 The $^{13}\text{C}$ -NMR spectra

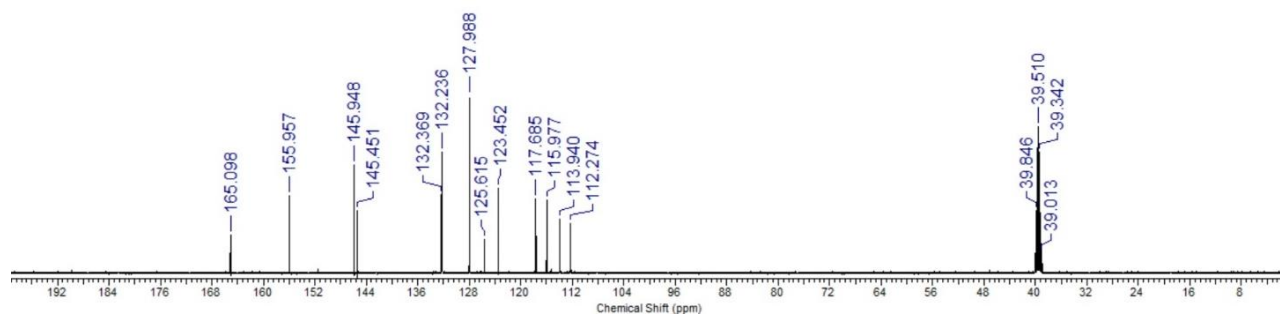


Figure S15. The  $^{13}\text{C}$ -NMR spectrum for the compound **3d**

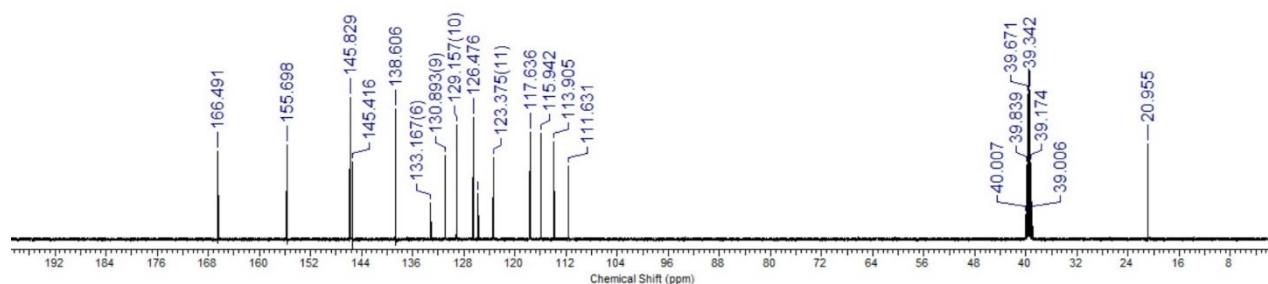


Figure S16. The <sup>13</sup>C-NMR spectrum for the compound 3e

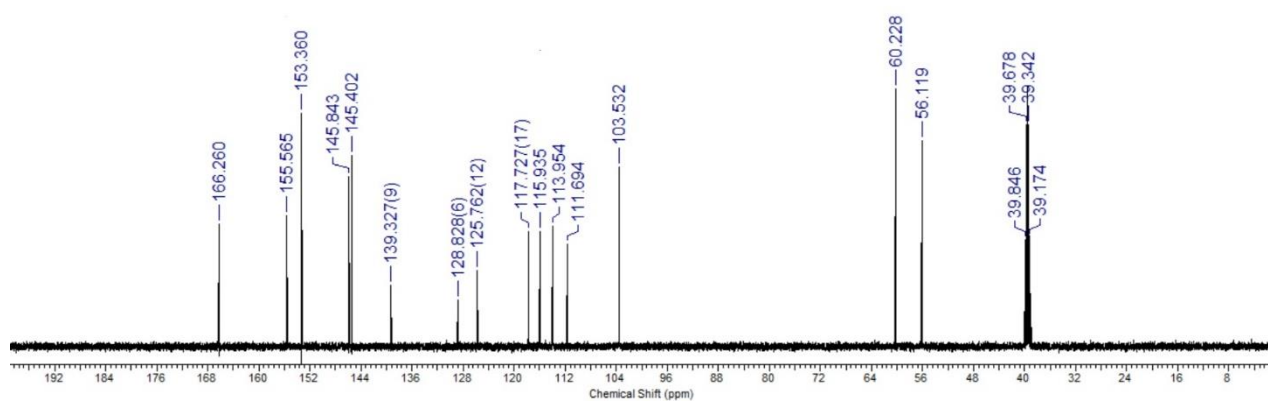


Figure S17. The <sup>13</sup>C-NMR spectrum for the compound 3f

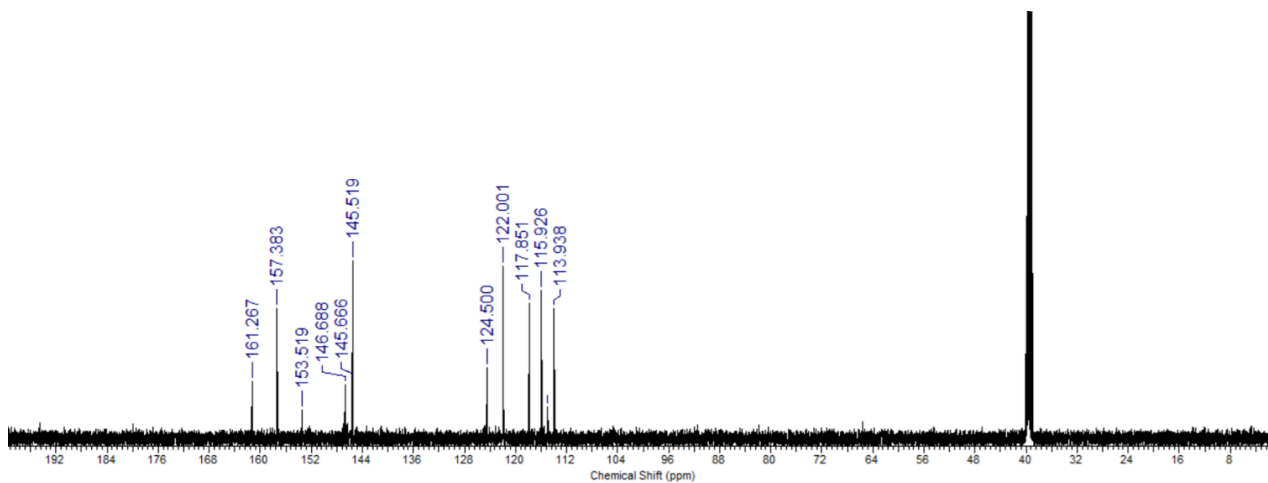


Figure S18. The <sup>13</sup>C-NMR spectrum for the compound 3g

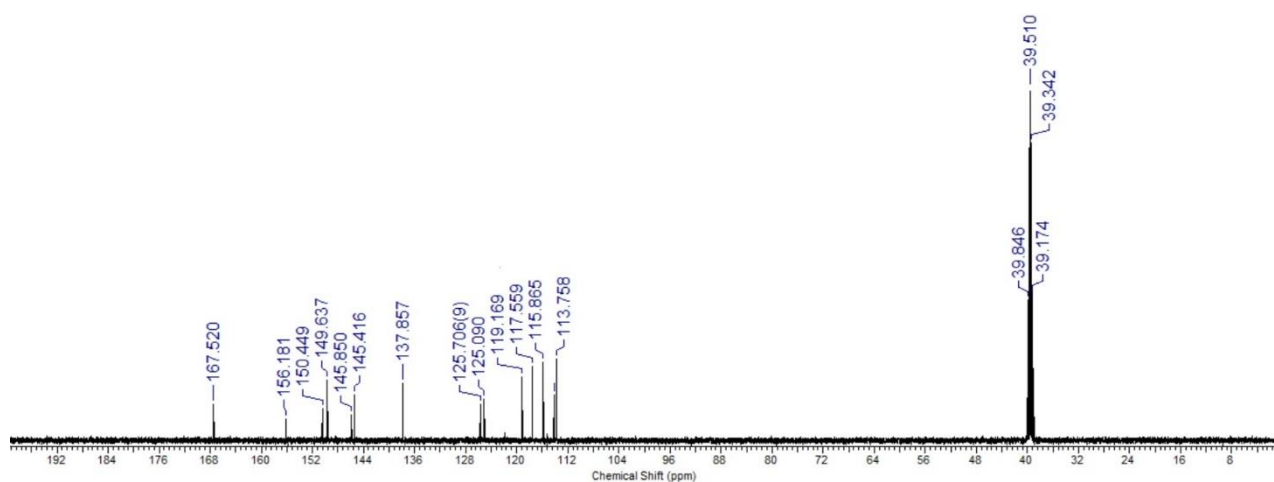


Figure S19. The <sup>13</sup>C-NMR spectrum for the compound 3h

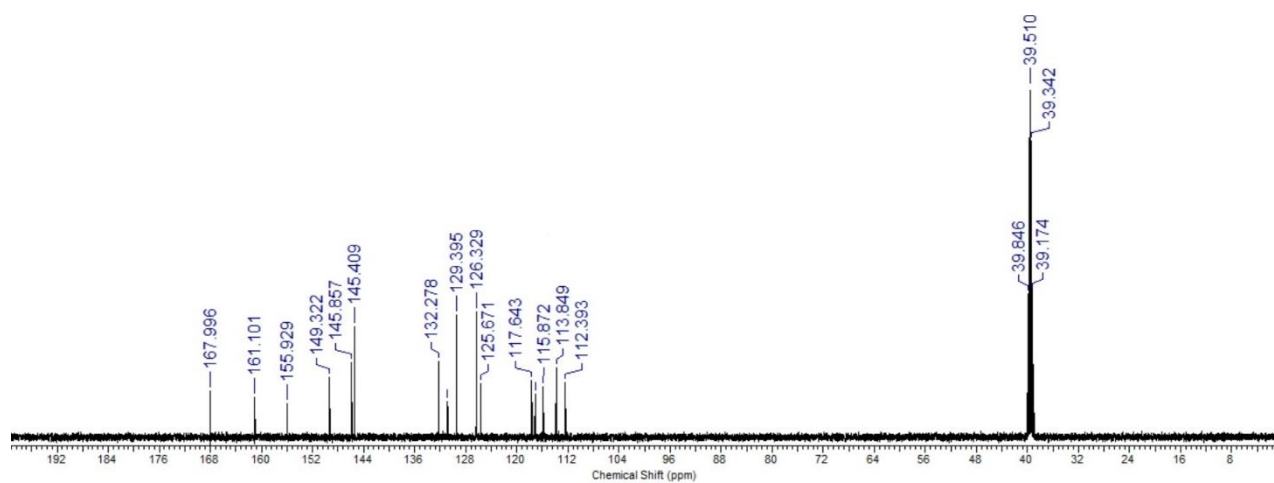


Figure S20. The <sup>13</sup>C-NMR spectrum for the compound 3i

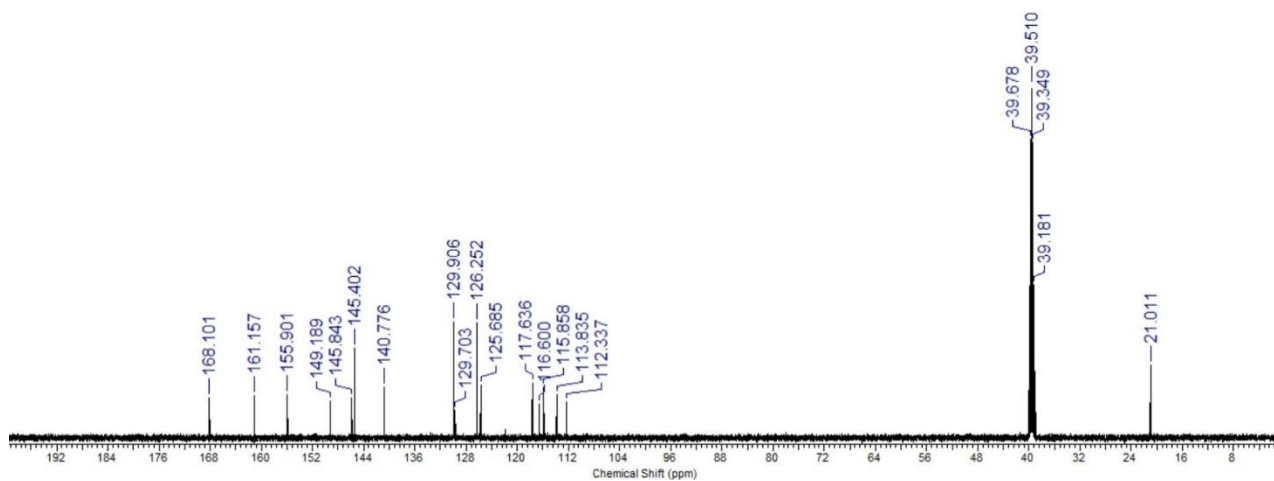


Figure S21. The <sup>13</sup>C-NMR spectrum for the compound 3j



## 2.4 The MS spectra

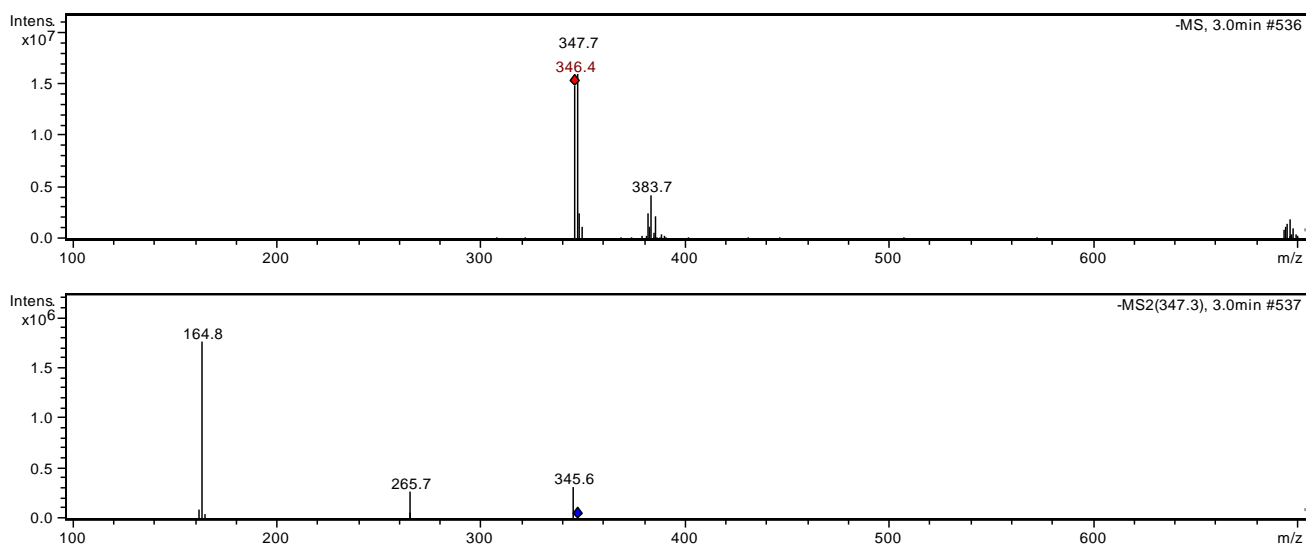


Figure S22. The MS spectrum for the compound 3d.

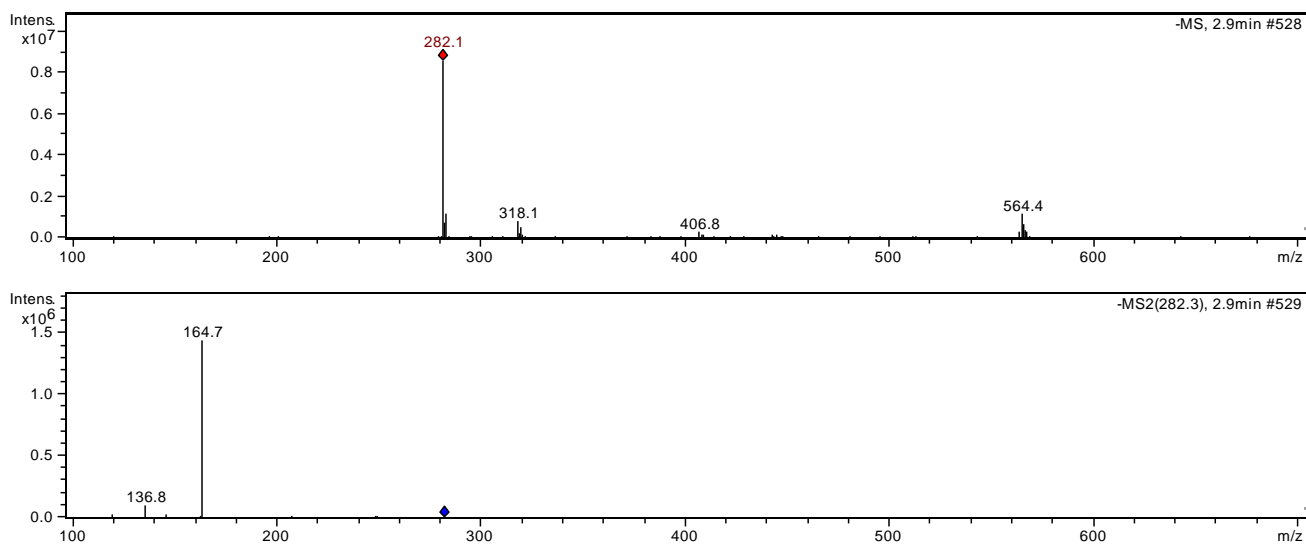


Figure S23. The MS spectrum for the compound 3e.

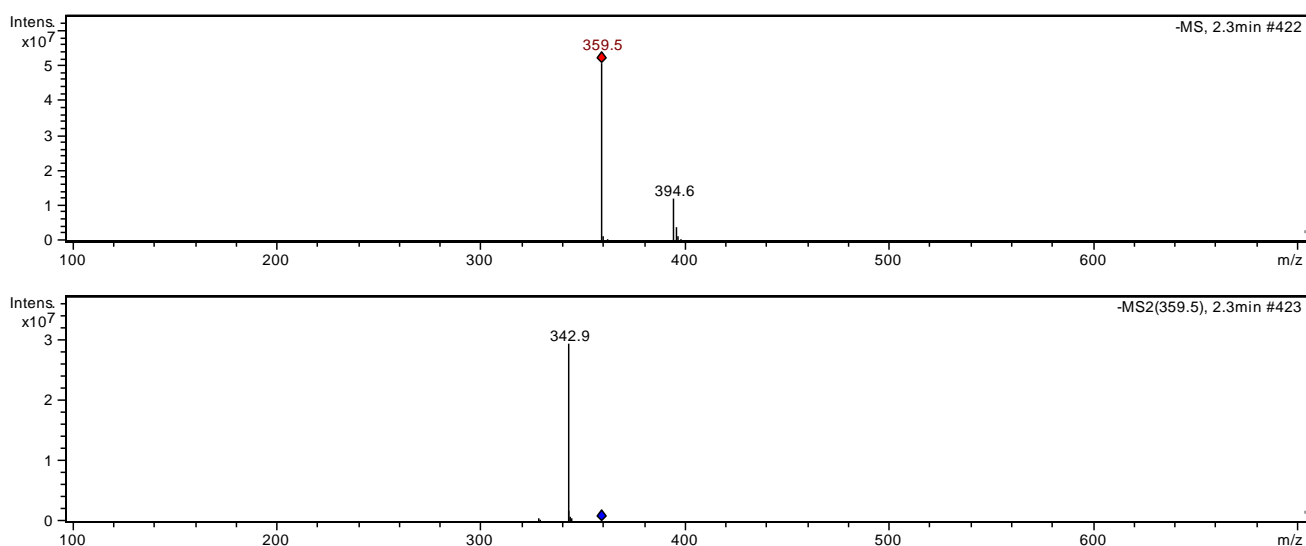


Figure S24. The MS spectrum for the compound 3f.

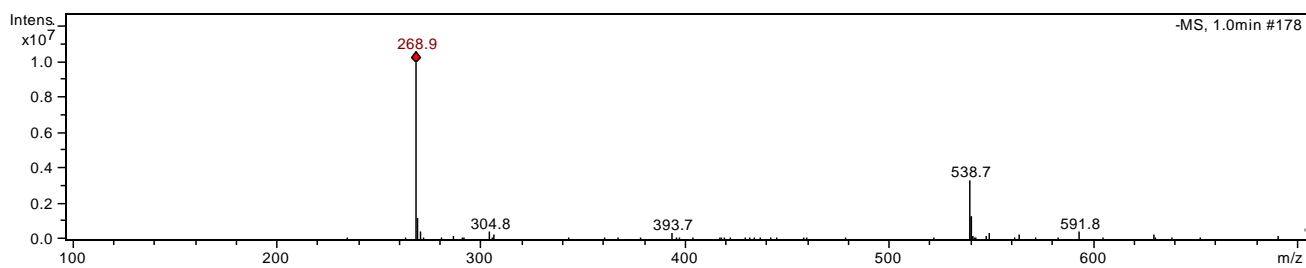


Figure S25. The MS spectrum for the compound 3g

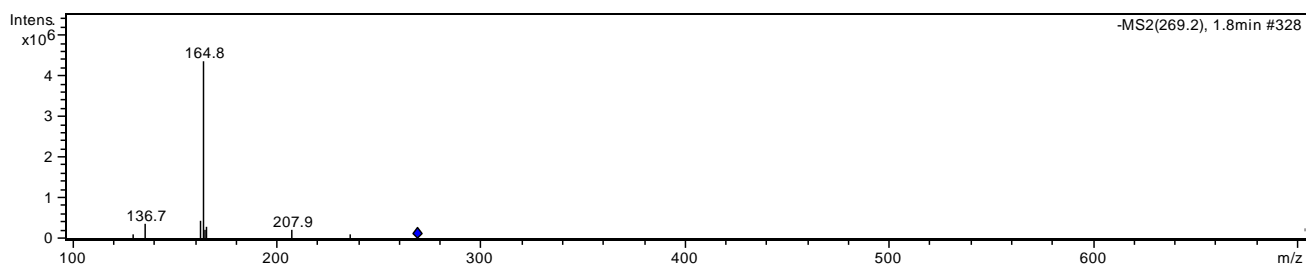
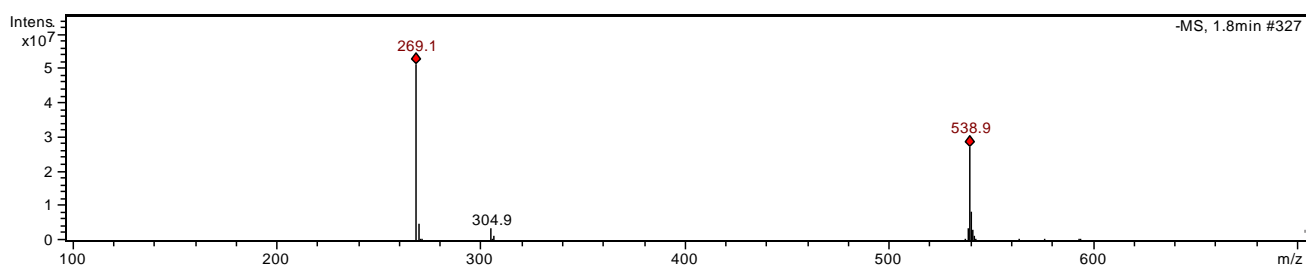
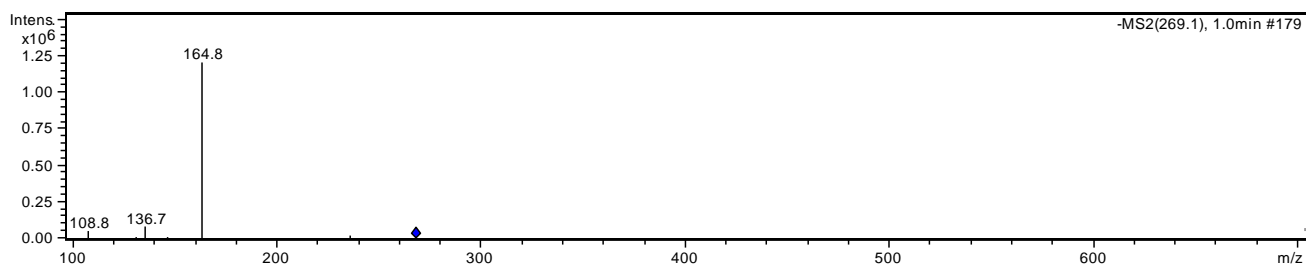


Figure S26. The MS spectrum for the compound 3h

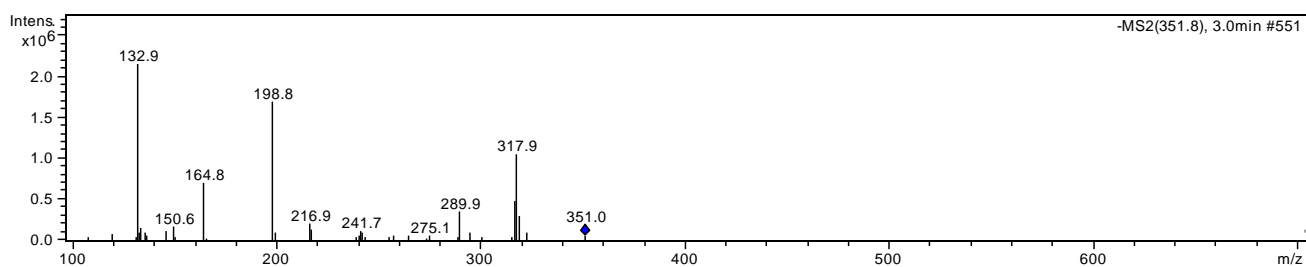
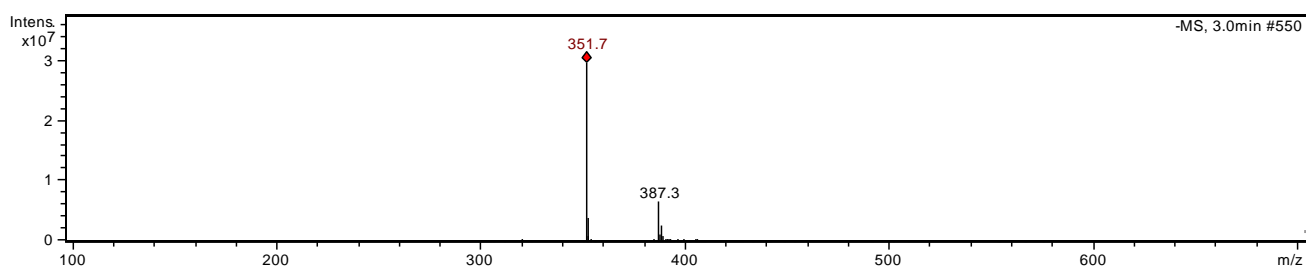
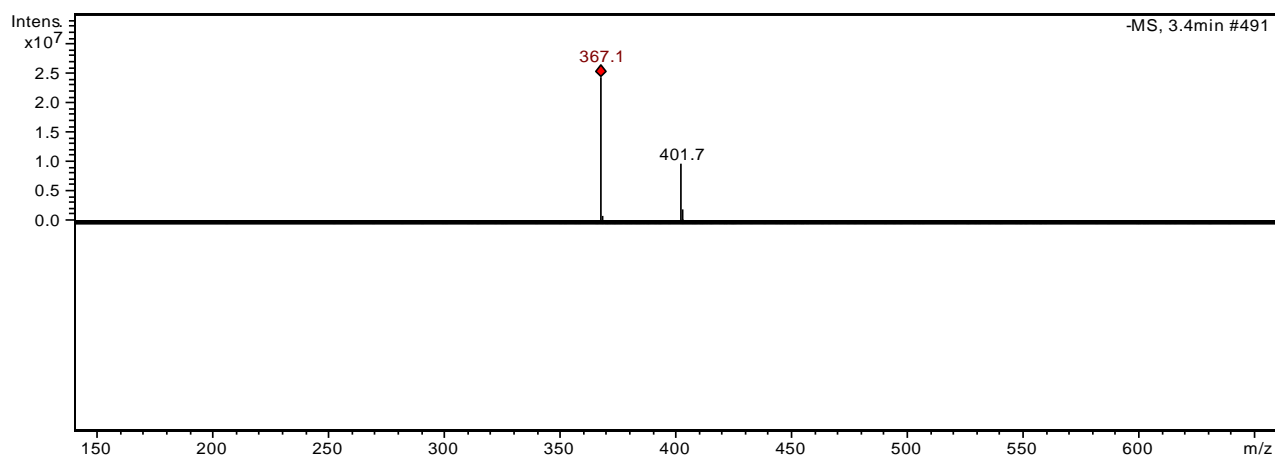


Figure S27. The MS spectrum for the compound 3i

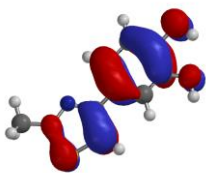
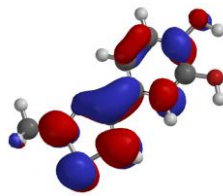
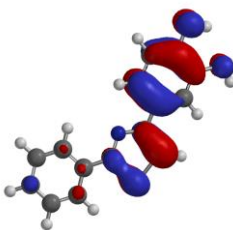
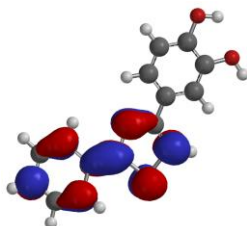
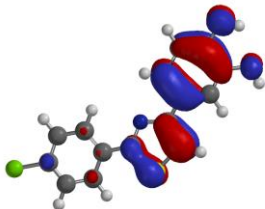
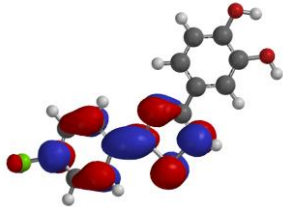


**Figure S28.** The MS spectrum for the compound **3j**

### 3. Tables

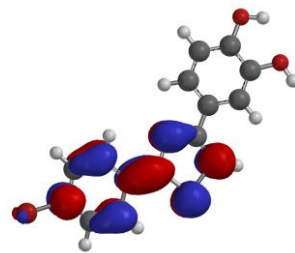
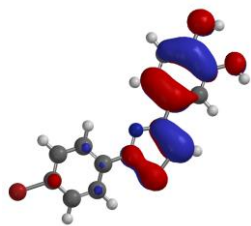
#### 3.1. The depiction of HOMO and LUMO and the depiction of the spin density maps of compounds **3a-j**

**Table S1.** The depiction of HOMO and LUMO of the compounds **3a-j**

Compound	HOMO	LUMO
<b>3a</b>		
<b>3b</b>		
<b>3c</b>		

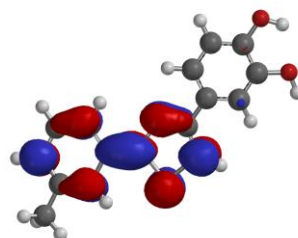
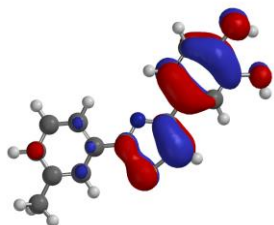
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3d



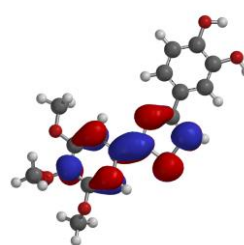
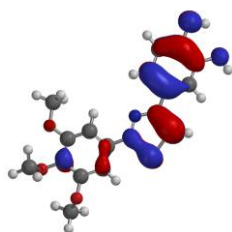
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3e



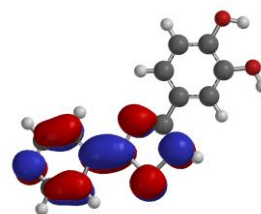
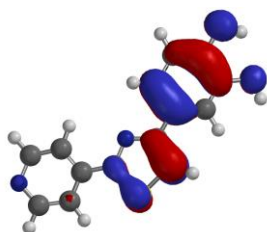
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3f



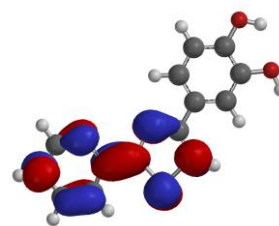
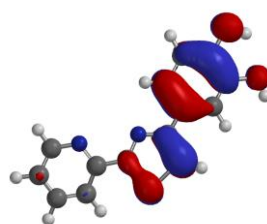
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3g



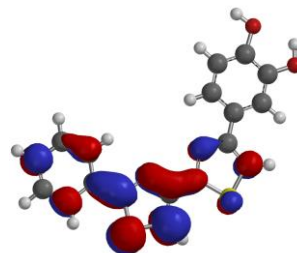
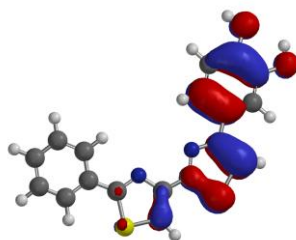
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3h

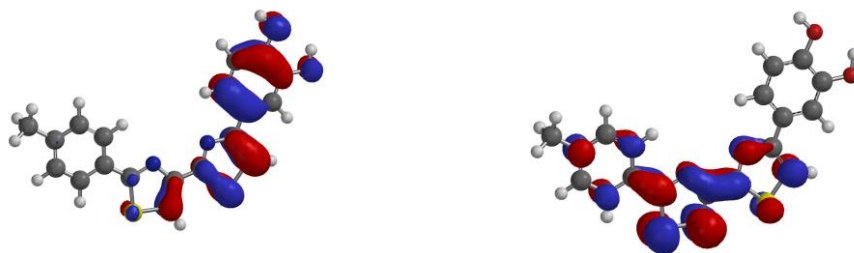


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3i



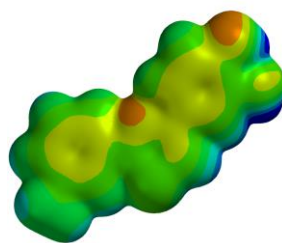
3j



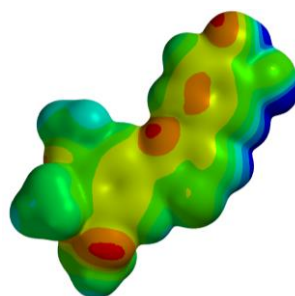
**Table S2.** The electrostatic potential maps of the compounds **3a-j**

Compound	EPM
3a	
3b	
3c	
3d	

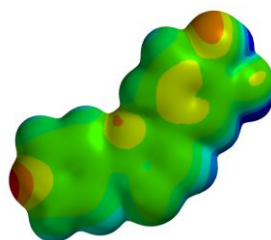
3e



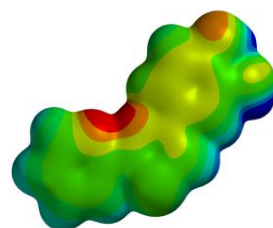
3f



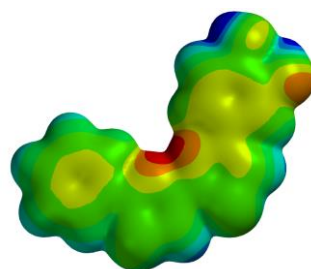
3g



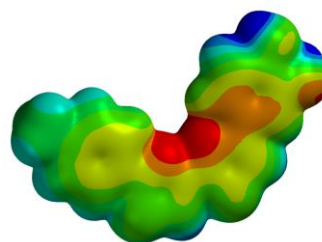
3h



3i



3j



### 3.2. Thermodynamic data computed for compounds **3a-j**

**Table S3.** Thermodynamic data computed for compounds **3a-j** in vacuum (T=298.15K, P=1atm)

Compound	ZPE (kJ/mol)	S <sup>0</sup> (J/mol*K)	H <sup>0</sup> (au)	G <sup>0</sup> (au)	Cv (J/mol*K)
<b>3a</b>	430.48	430.48	-989.67923	-989.737123	212.70
<b>3b</b>	563.64	563.64	-1181.36434	-1181.429950	271.52
<b>3c</b>	539.60	539.60	-1640.96879	-1641.036220	287.48
<b>3d</b>	538.18	538.18	-3754.65427	-3754.722470	288.95
<b>3e</b>	632.32	632.32	-1220.65350	-1220.723420	289.16
<b>3f</b>	806.99	806.99	-1524.81570	-1524.899090	390.98
<b>3g</b>	534.26	534.26	-1197.41177	-1197.476640	226.56
<b>3h</b>	534.03	534.03	-1197.40757	-1197.482550	226.76
<b>3i</b>	652.13	652.13	-1749.18372	-1749.259180	341.99

**Table S4.** Thermodynamic data computed for compounds **3a-j** in nonpolar solvent (T=298.15K, P=1atm)

Compound	ZPE (kJ/mol)	S <sup>0</sup> (J/mol*K)	H <sup>0</sup> (au)	G <sup>0</sup> (au)	Cv (J/mol*K)
<b>3a</b>	430.14	440.16	-989.69427	-989.75210	212.69
<b>3b</b>	563.56	487.32	-1181.38043	-1181.44601	271.42
<b>3c</b>	539.82	506.61	-1640.98501	-1641.05229	287.10
<b>3d</b>	537.86	514.85	-3754.67074	-3754.73895	289.09
<b>3e</b>	632.18	512.77	-1220.67588	-1220.73960	288.98
<b>3f</b>	807.57	602.21	-1524.83600	-1524.91916	390.39
<b>3g</b>	534.24	485.69	-1197.42978	-1197.49464	266.47
<b>3h</b>	534.19	485.05	-1197.43010	-1197.49977	266.59
<b>3i</b>	652.63	550.82	-1749.21055	-1749.27902	341.51

**Table S5.** Thermodynamic data computed for compounds **3a-j** in water (T=298.15K, P=1atm)

Compound	ZPE (kJ/mol)	S <sup>0</sup> (J/mol*K)	H <sup>0</sup> (au)	G <sup>0</sup> (au)	Cv (J/mol*K)
<b>3a</b>	430.07	440.03	-989.69680	-989.75461	212.66
<b>3b</b>	563.56	487.09	-1181.38310	-1181.44870	271.34
<b>3c</b>	539.80	506.44	-1640.98775	-1641.05501	287.04
<b>3d</b>	537.79	514.86	-3754.67350	-3754.74170	289.10
<b>3e</b>	633.06	512.25	-1220.67390	-1220.74195	296.87
<b>3f</b>	807.55	602.01	-1524.83941	-1524.92254	390.36
<b>3g</b>	534.25	485.47	-1197.43282	-1197.49765	266.40
<b>3h</b>	534.18	484.99	-1197.43505	-1197.50271	266.57
<b>3i</b>	652.69	550.71	-1749.21126	-1749.28236	341.41