



## Supporting Information

for

### Competing electrophilic substitution and oxidative polymerization of arylamines with selenium dioxide

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**Spectroscopic characterization of products ( $^1\text{H}$ ,  $^{13}\text{C}$  and  $^{77}\text{Se}$  NMR, IR, and HRMS spectra), packing arrangements of compounds and HOMO and LUMO energy values for reactants**

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1. Spectroscopic characterization of polymers 1–3

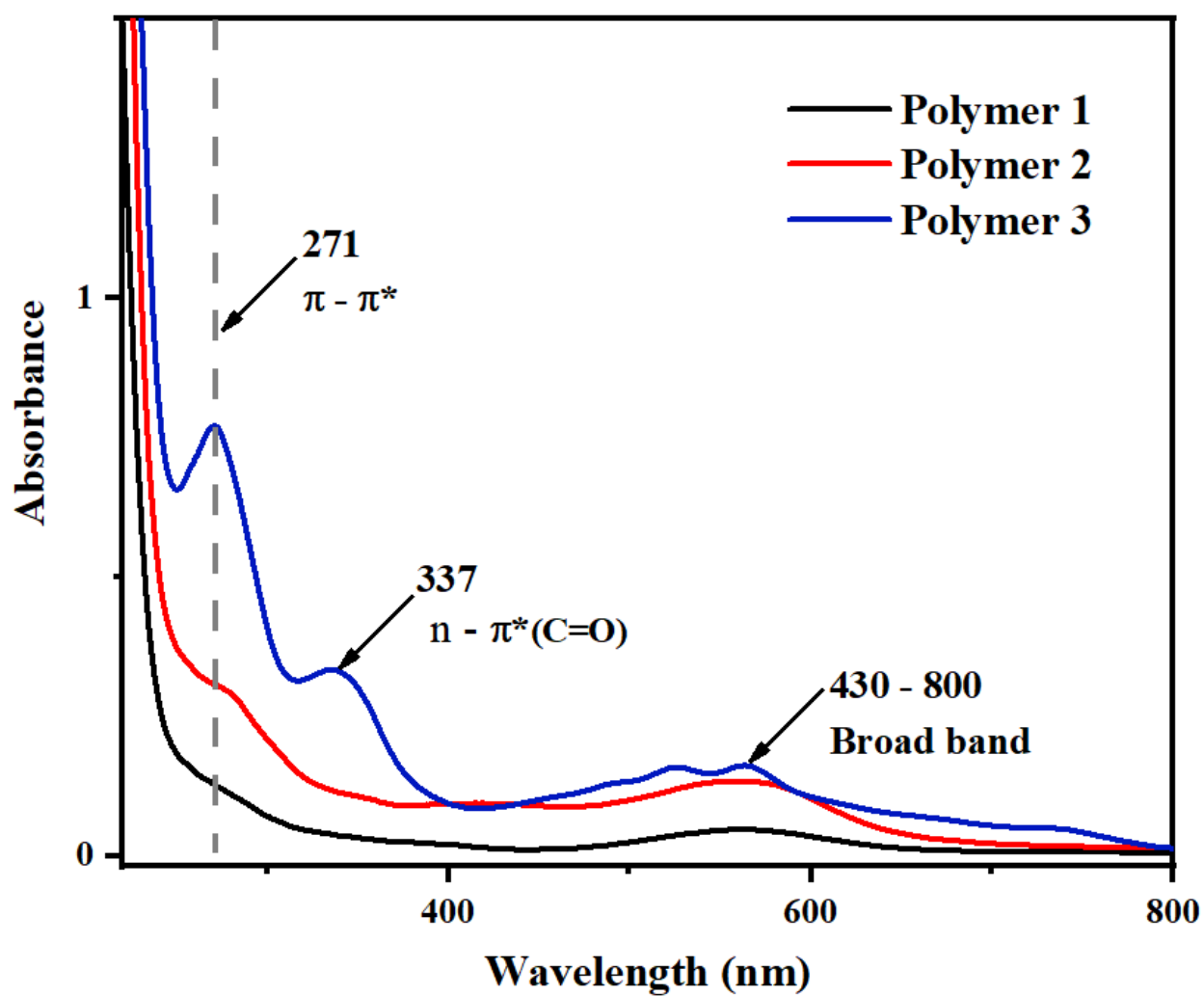


Figure S1. UV-vis spectrum for polymers 1–3.

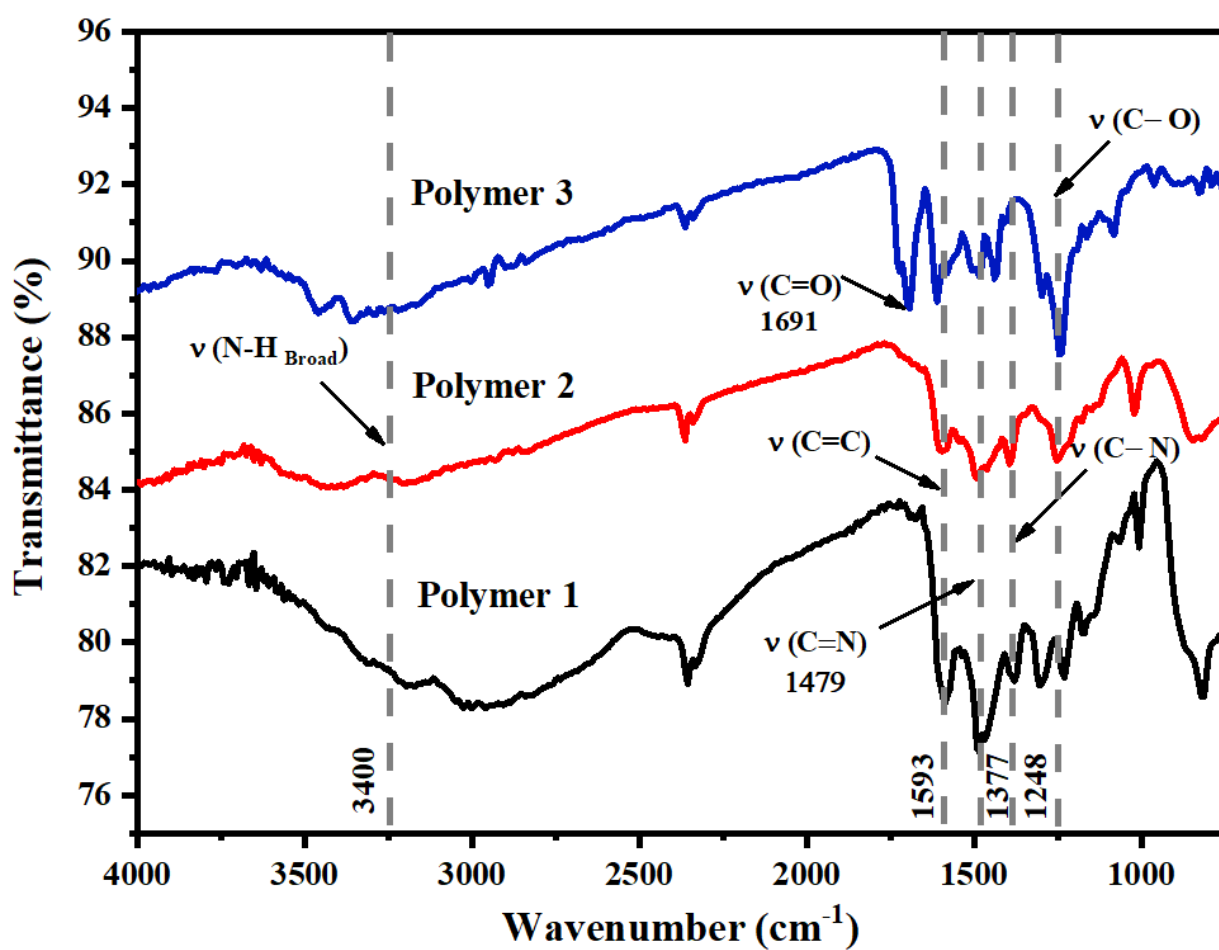
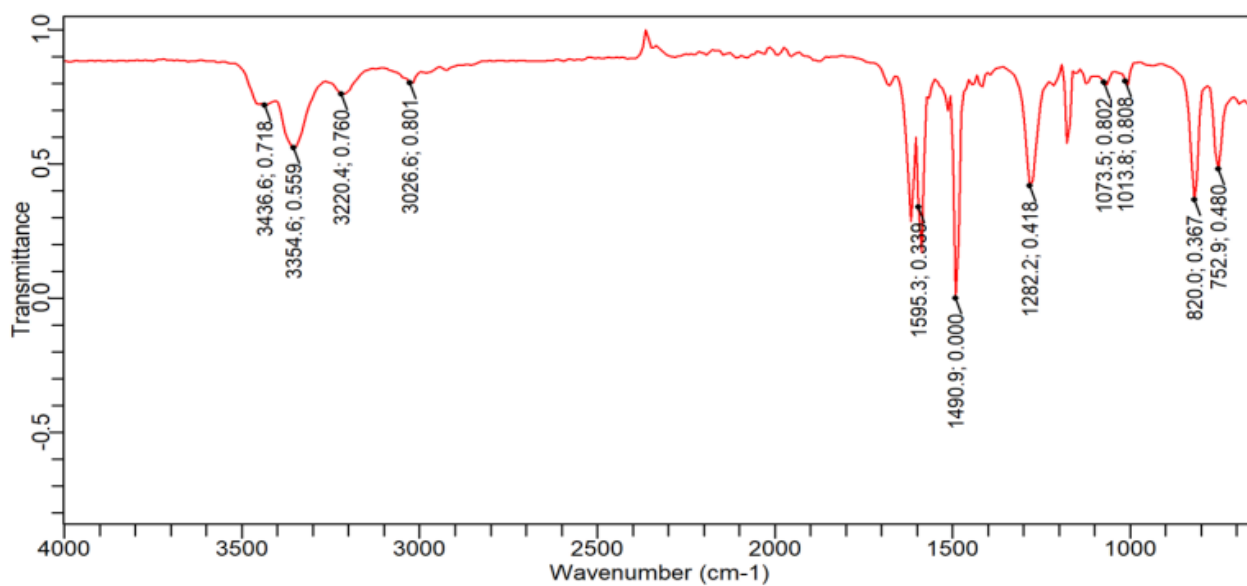
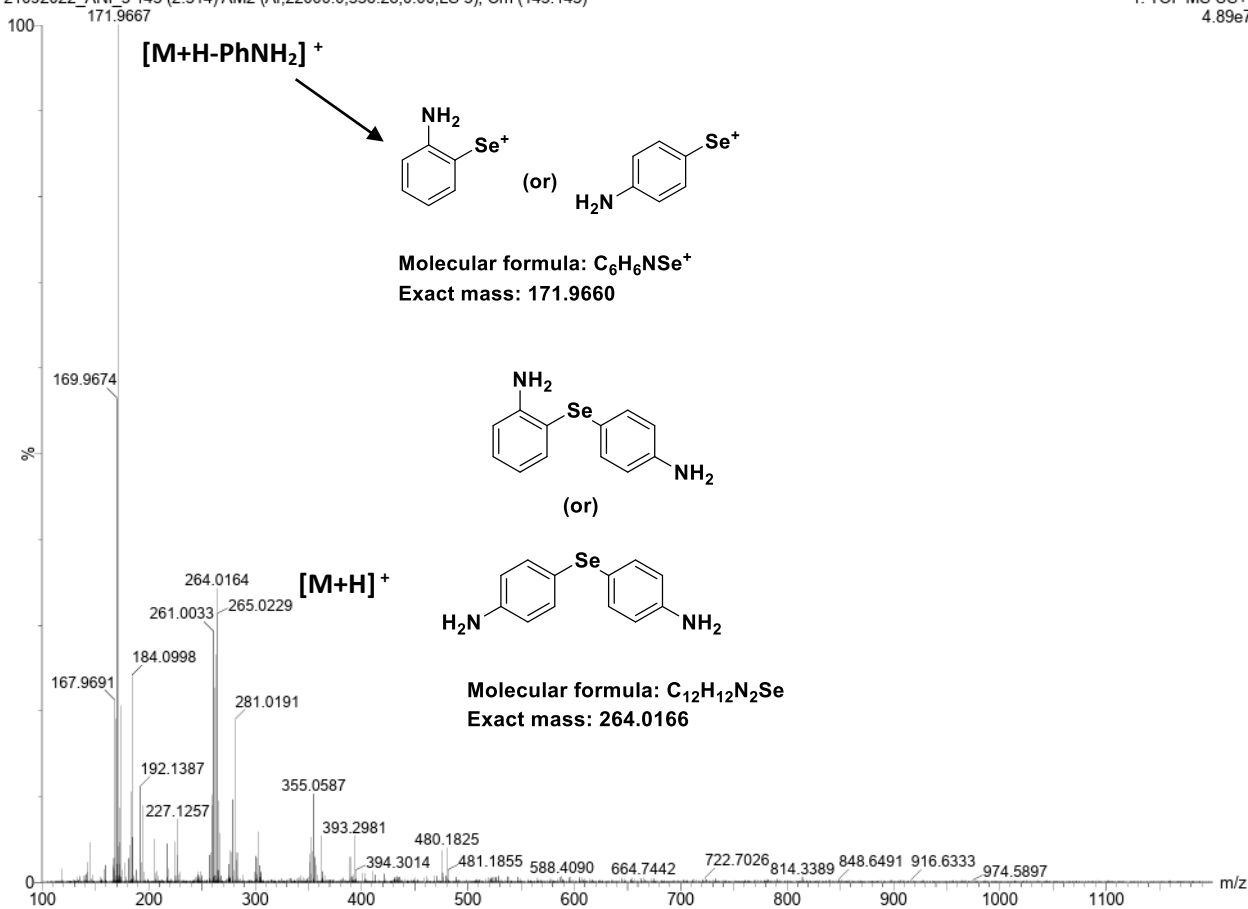


Figure S2. FTIR (KBr) spectrum for polymers 1–3.

## 2. Spectrometric characterization of products obtained for the reaction of aniline with $\text{SeO}_2$

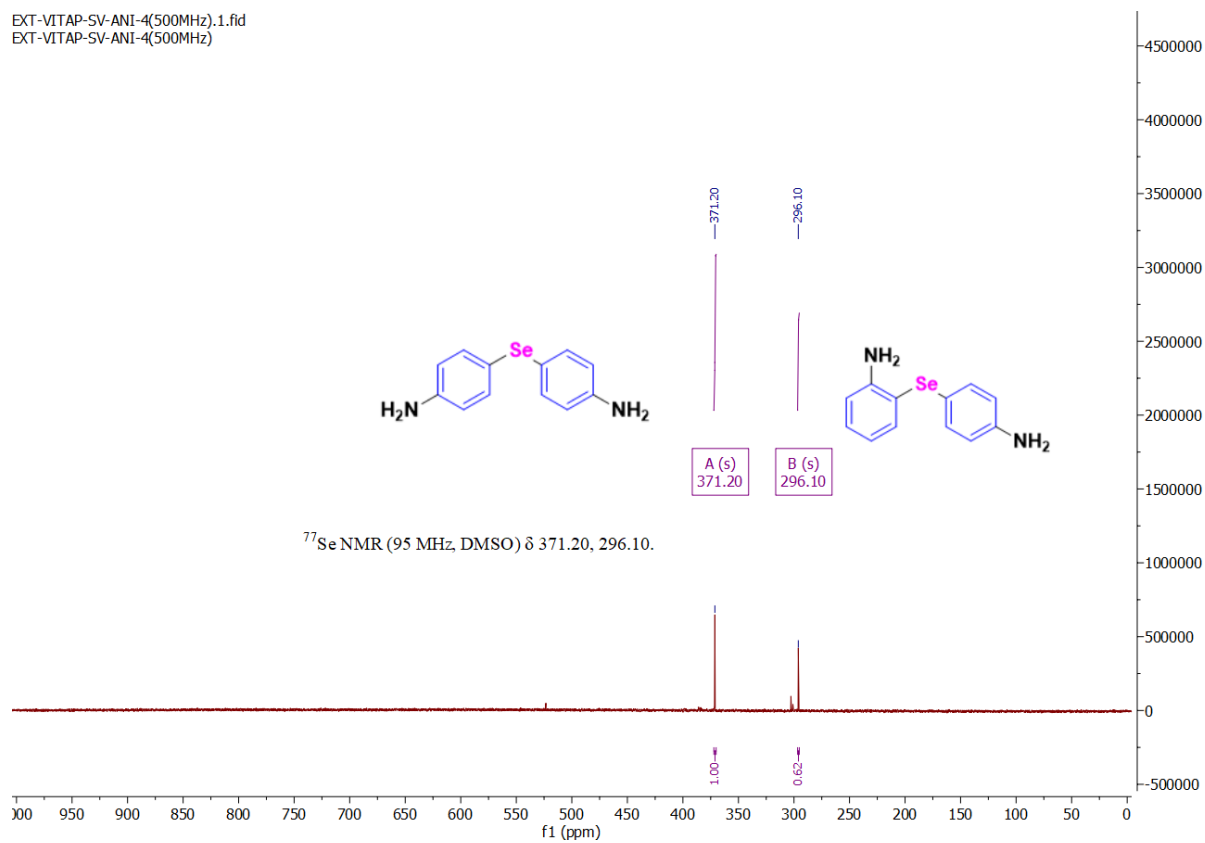


**Figure S3.** FTIR(KBr) spectrum for mixture of compounds **1** and **2**.



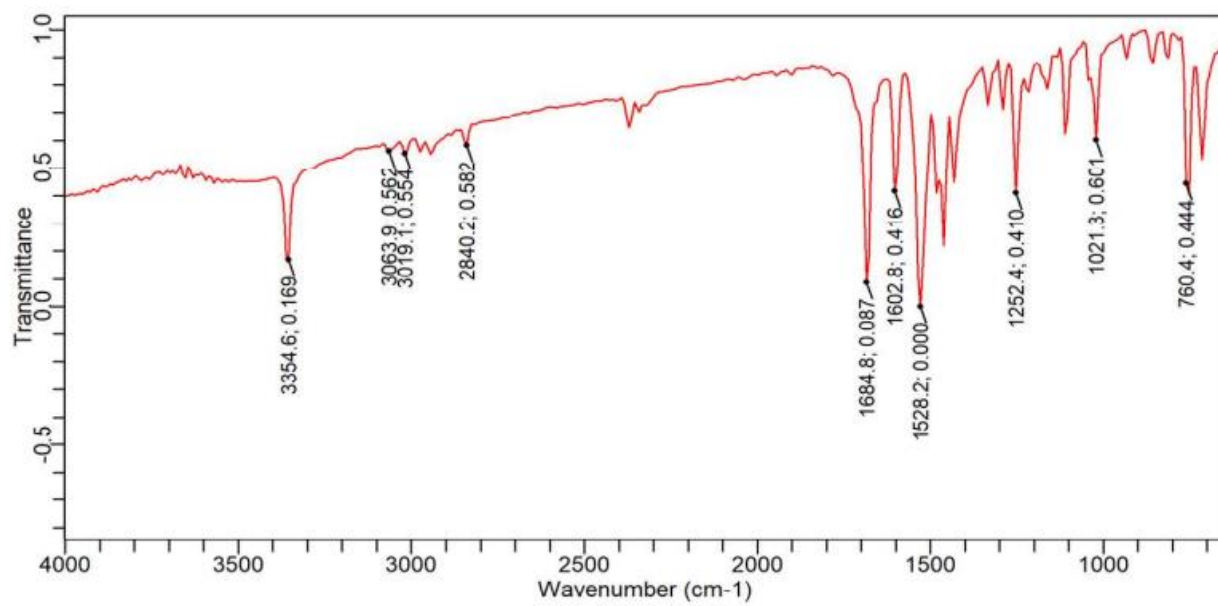
**Figure S4.** HRMS-ESI spectrum for mixture of compounds **1** and **2**.

EXT-VITAP-SV-ANI-4(500MHz).1.fid  
EXT-VITAP-SV-ANI-4(500MHz)

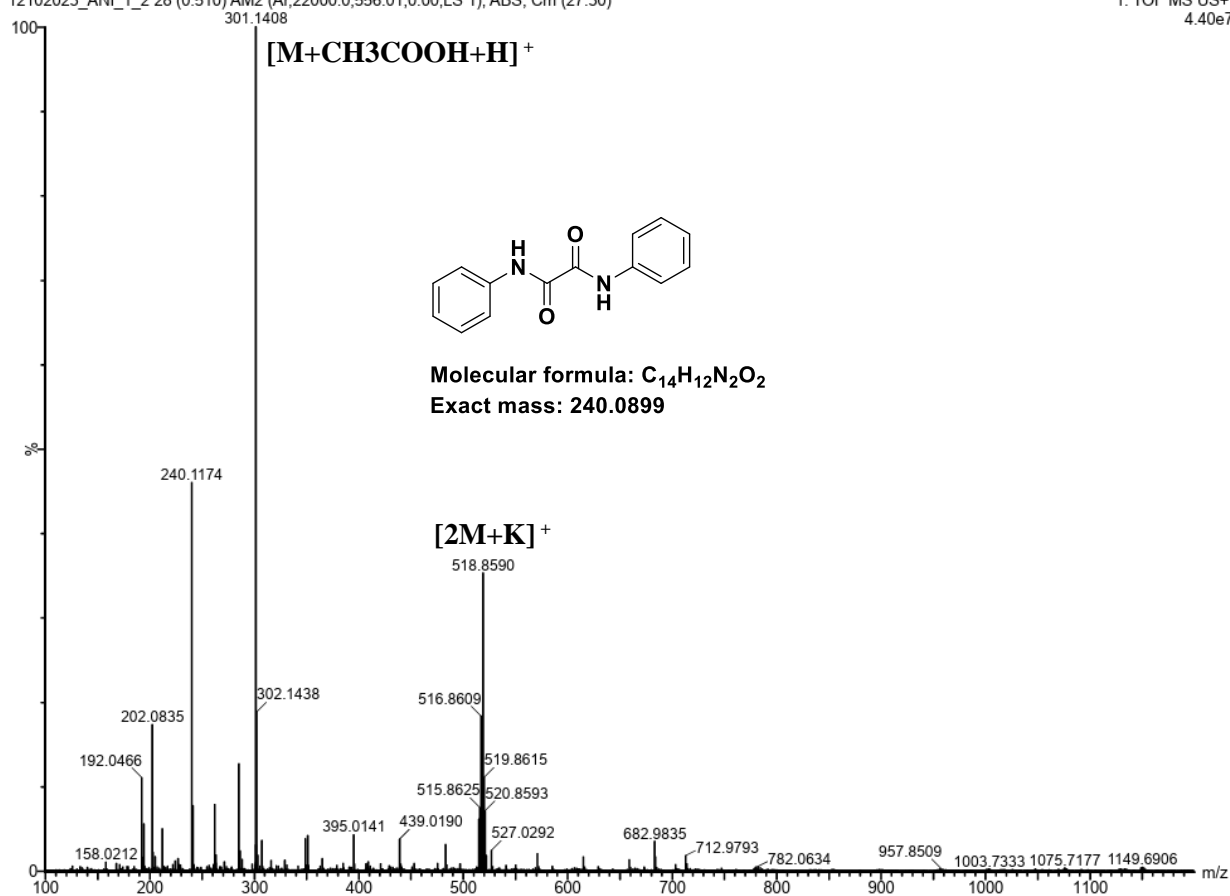


**Figure S5.**  $^{77}\text{Se}$  NMR spectral studies for mixture of compounds **1** and **2**.





**Figure S6.** FTIR (KBr) spectrum for compound 3.



**Figure S7.** HRMS–ESI spectrum for compound **3**.

EXT-VITAP-SV-ANI-1(500MHz).1.fid  
EXT-VITAP-SV-ANI-1(500MHz)  
PROTON CDCl3 {/opt/topspin/Ext Samples} nmrsu 15

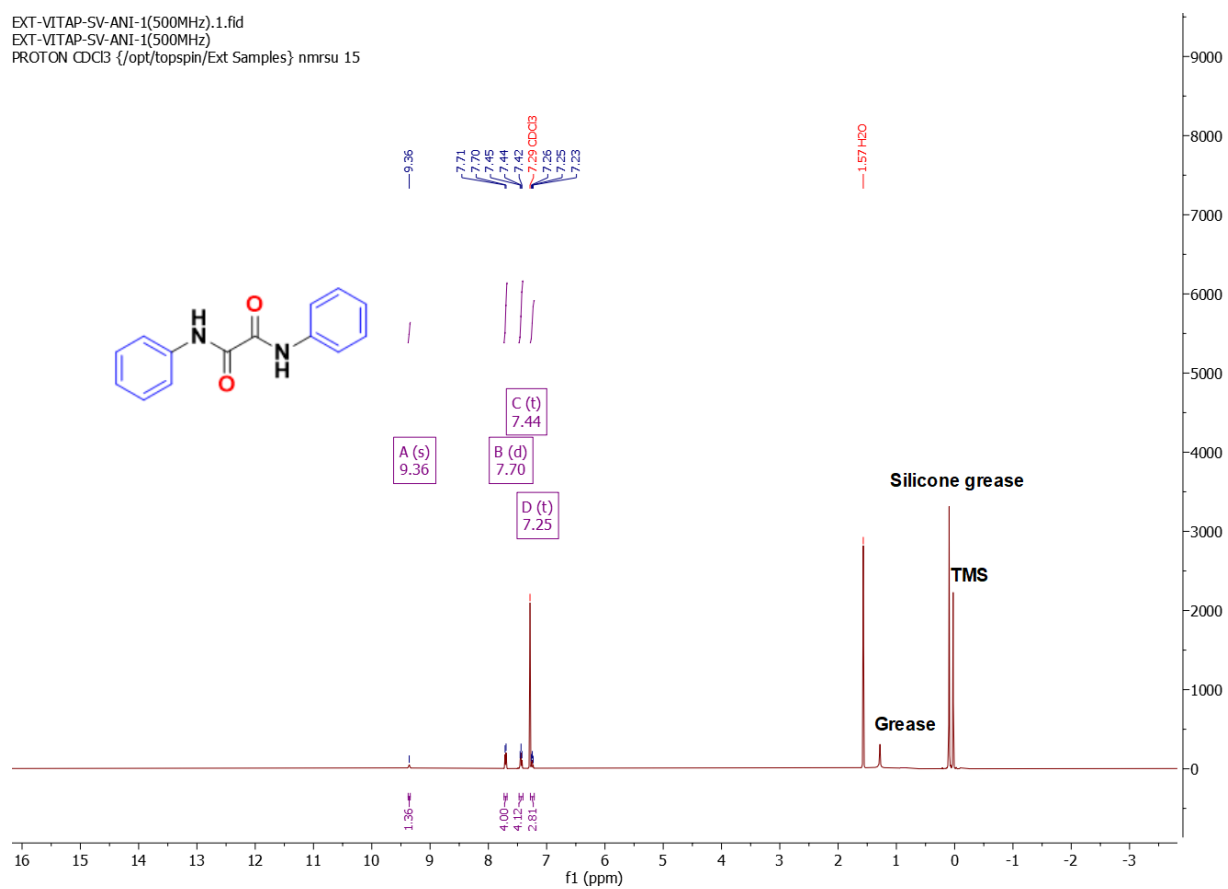
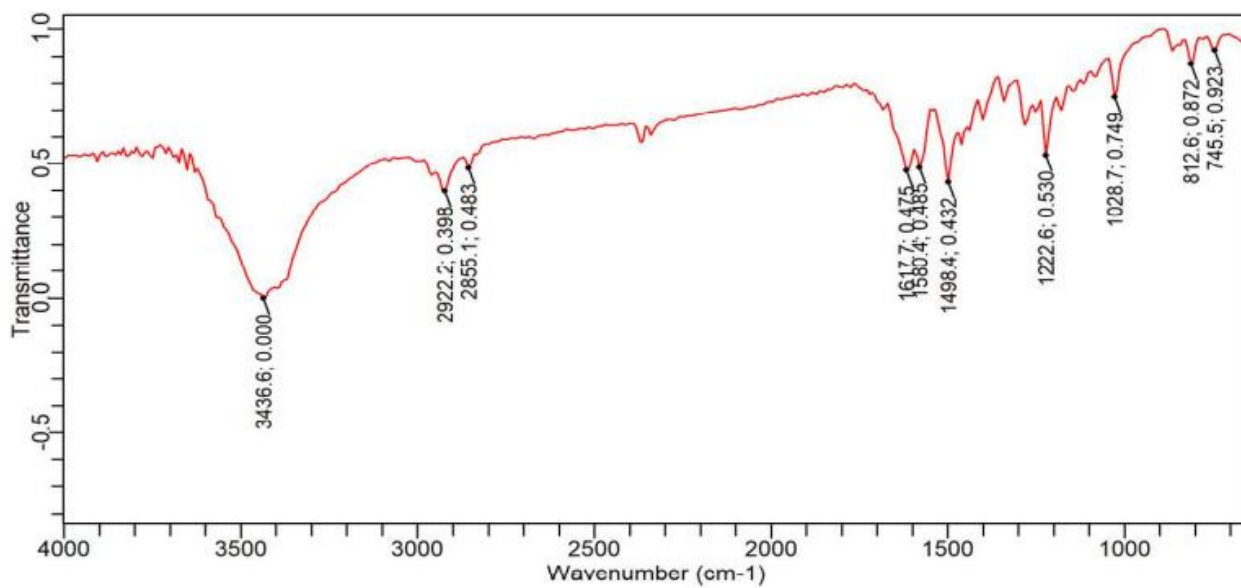
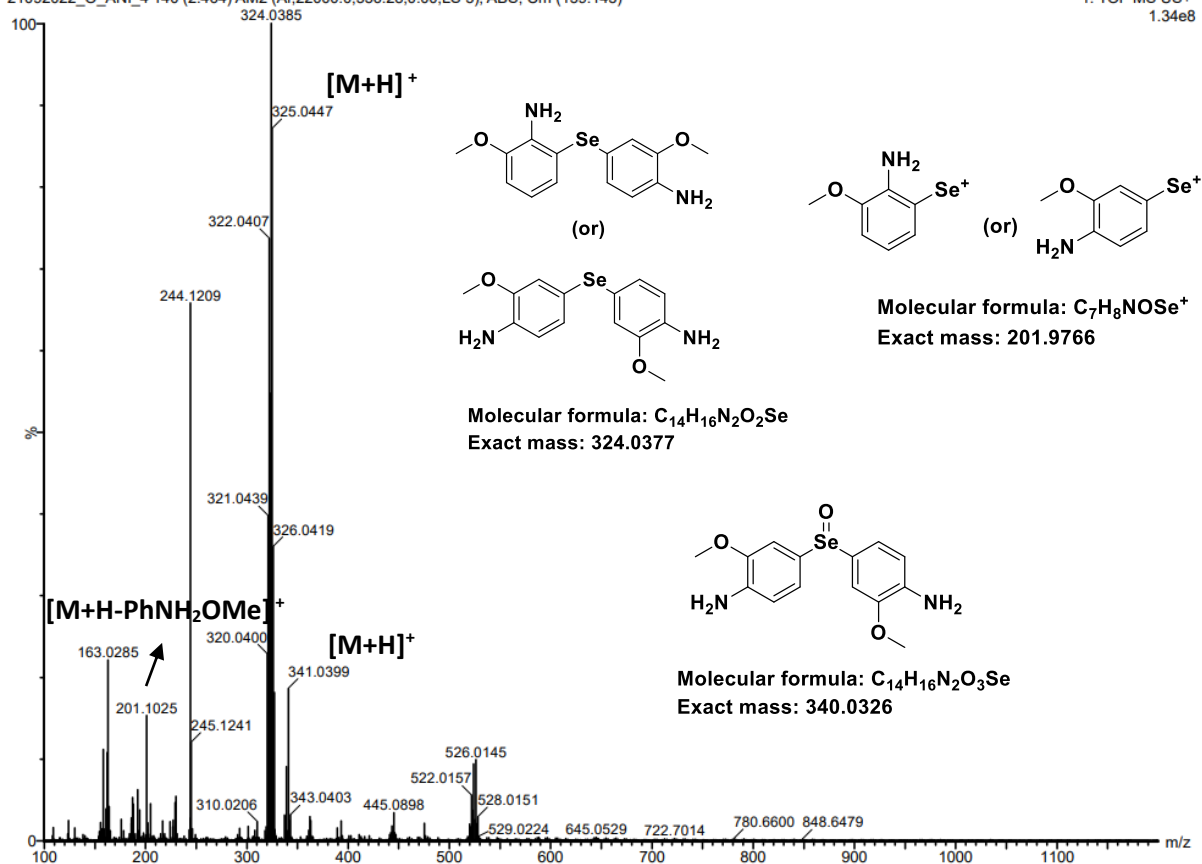


Figure S8. <sup>1</sup>H NMR spectral studies for compound 3.

### 3. Spectrometric characterization of products obtained from the reaction of *o*-anisidine with SeO<sub>2</sub>

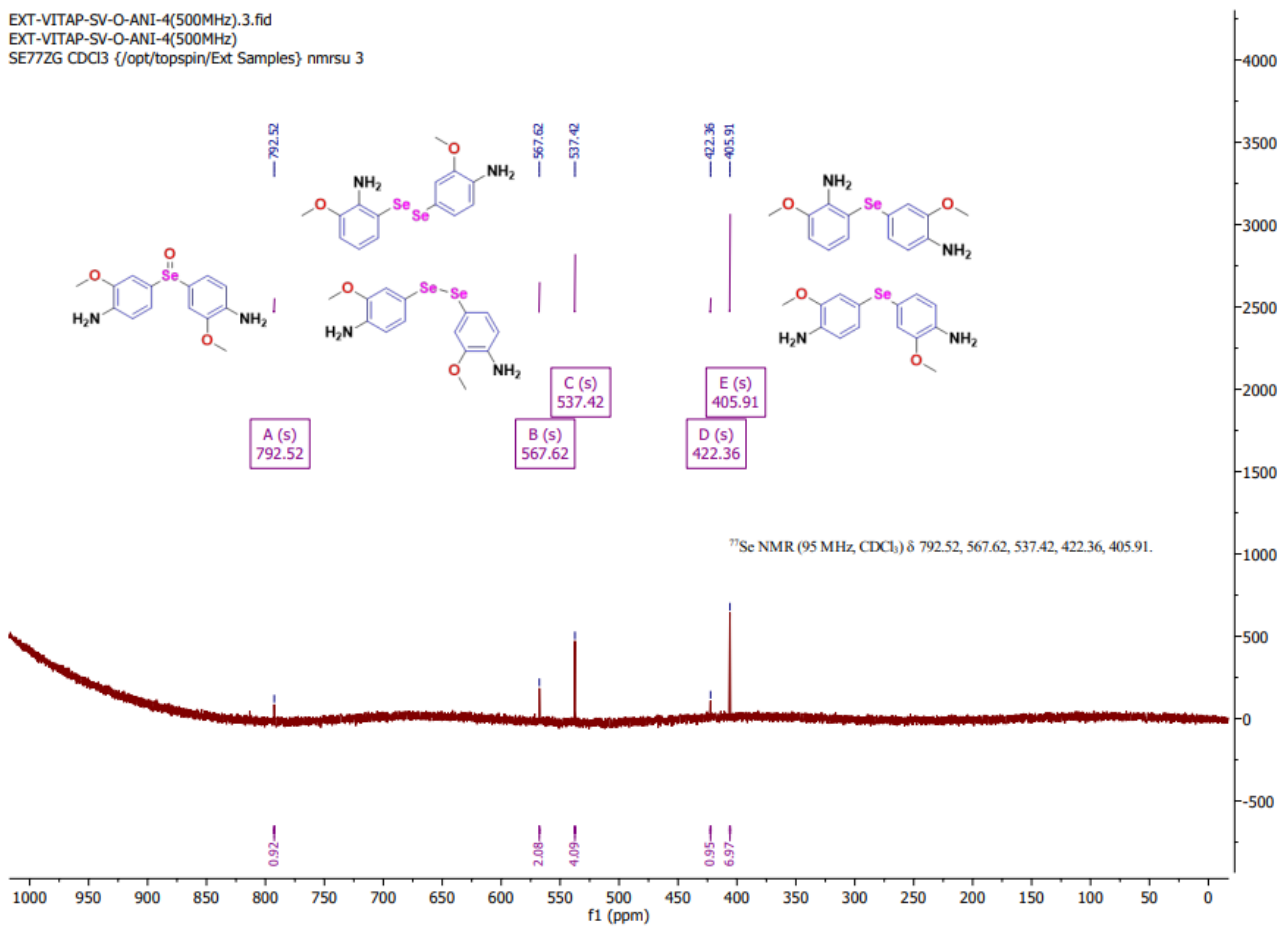


**Figure S9.** FTIR(KBr) spectrum for mixture of compounds 4-8.

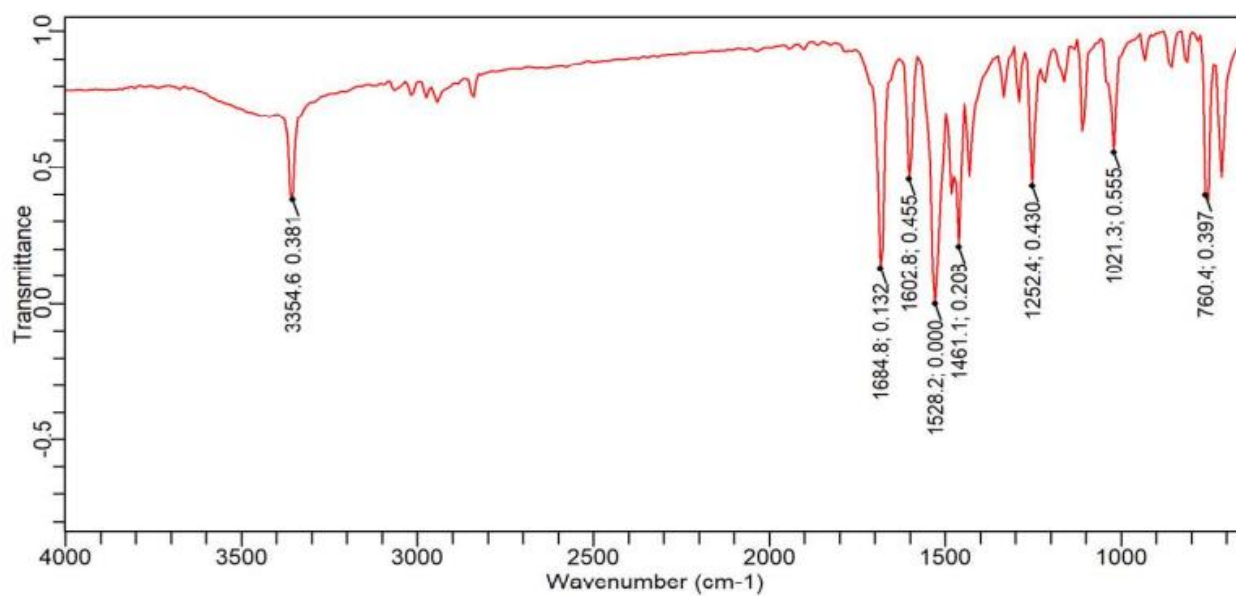


**Figure S10.** HRMS-ESI spectrum for mixture of compounds 4-8.

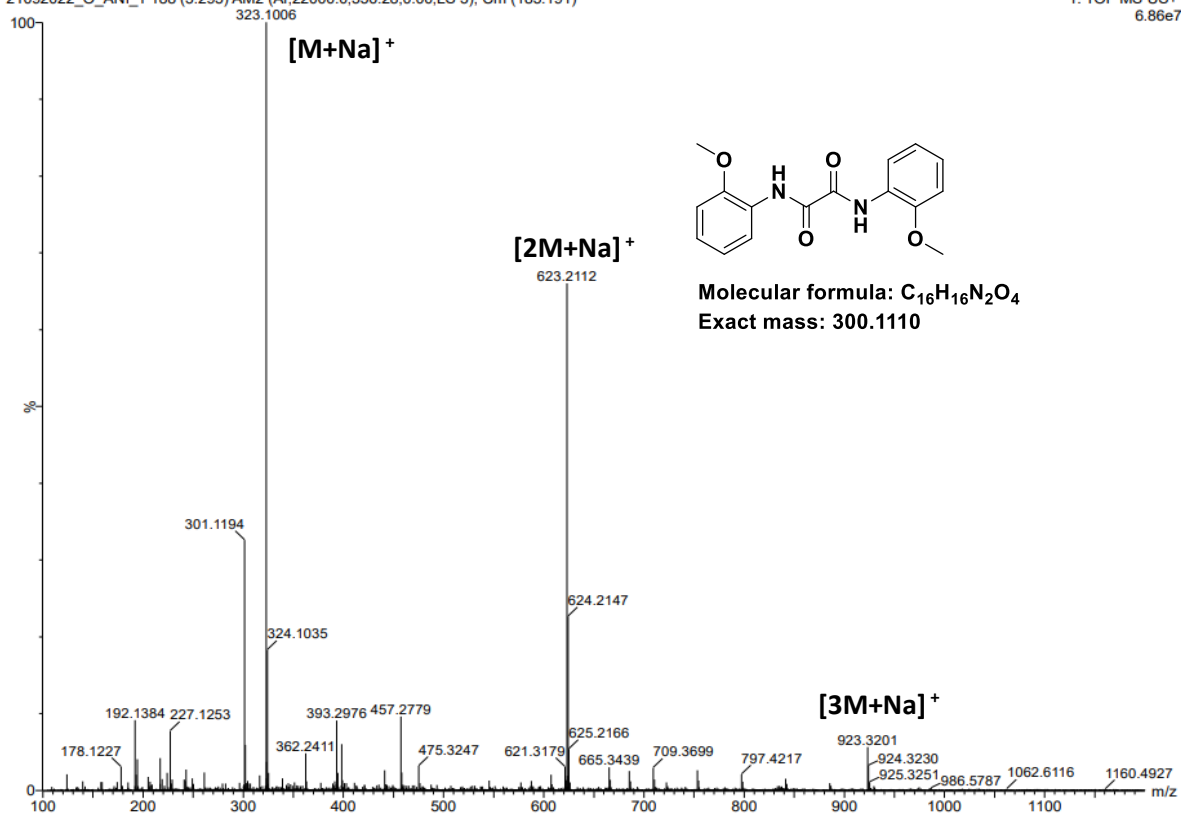
EXT-VITAP-SV-O-ANI-4(500MHz).3.fid  
EXT-VITAP-SV-O-ANI-4(500MHz)  
SE77ZG CDCl3 {/opt/topspin/Ext Samples} nmrsu 3



**Figure S11.** <sup>77</sup>Se NMR spectral studies for mixture of compounds 4–8.



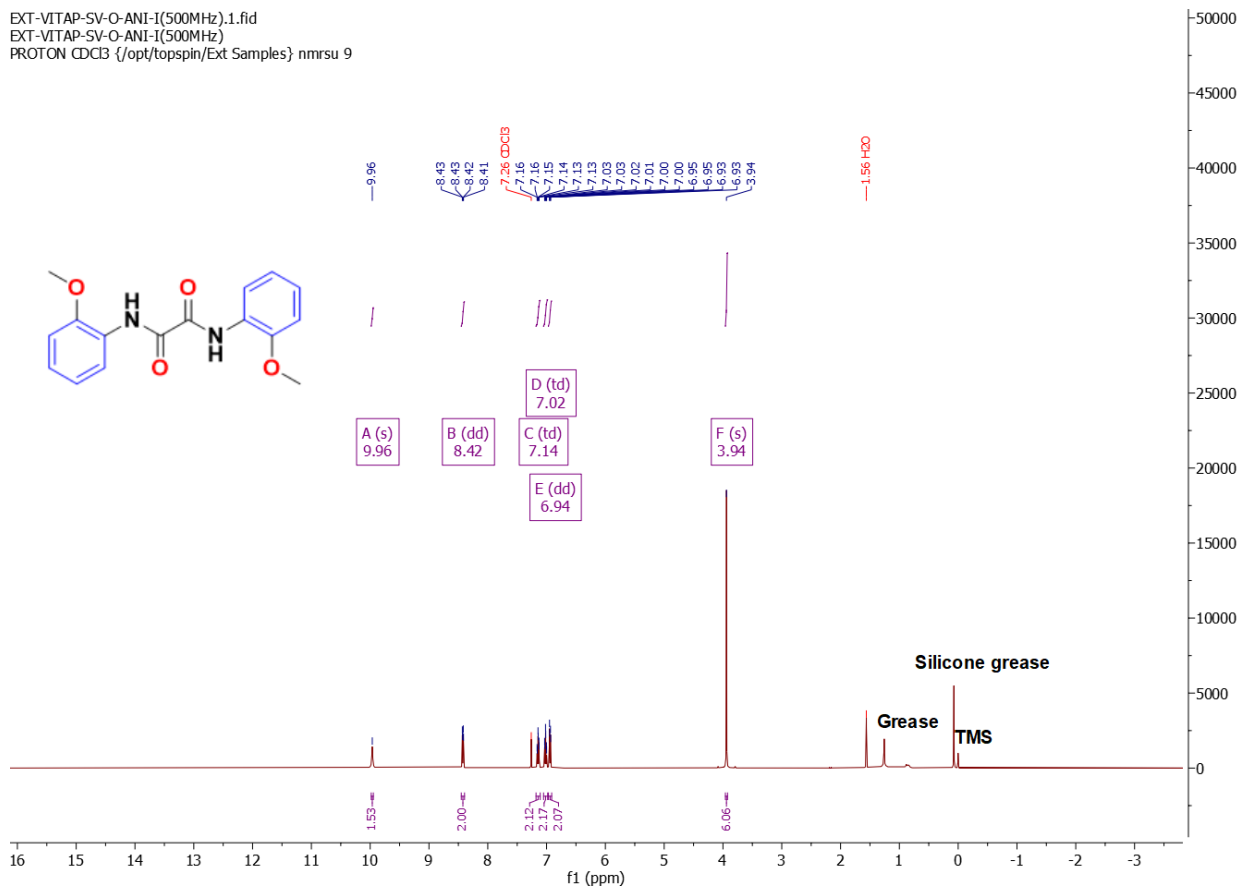
**Figure S12.** FTIR(KBr) spectrum for compound **9**.



**Figure S13.** HRMS–ESI spectrum for compound **9**.



EXT-VITAP-SV-O-ANI-1(500MHz).1.fid  
EXT-VITAP-SV-O-ANI-1(500MHz)  
PROTON CDCl3 {/opt/topspin/Ext Samples} nmrsu 9



**Figure S14.**  $^1\text{H}$  NMR spectral studies for compound **9**.

EXT-VITAP-SV-O-ANI-1(500MHz).2.fid  
EXT-VITAP-SV-O-ANI-1(500MHz)  
C13CPD CDCl3 {/opt/topspin/Ext Samples} nmrso 9

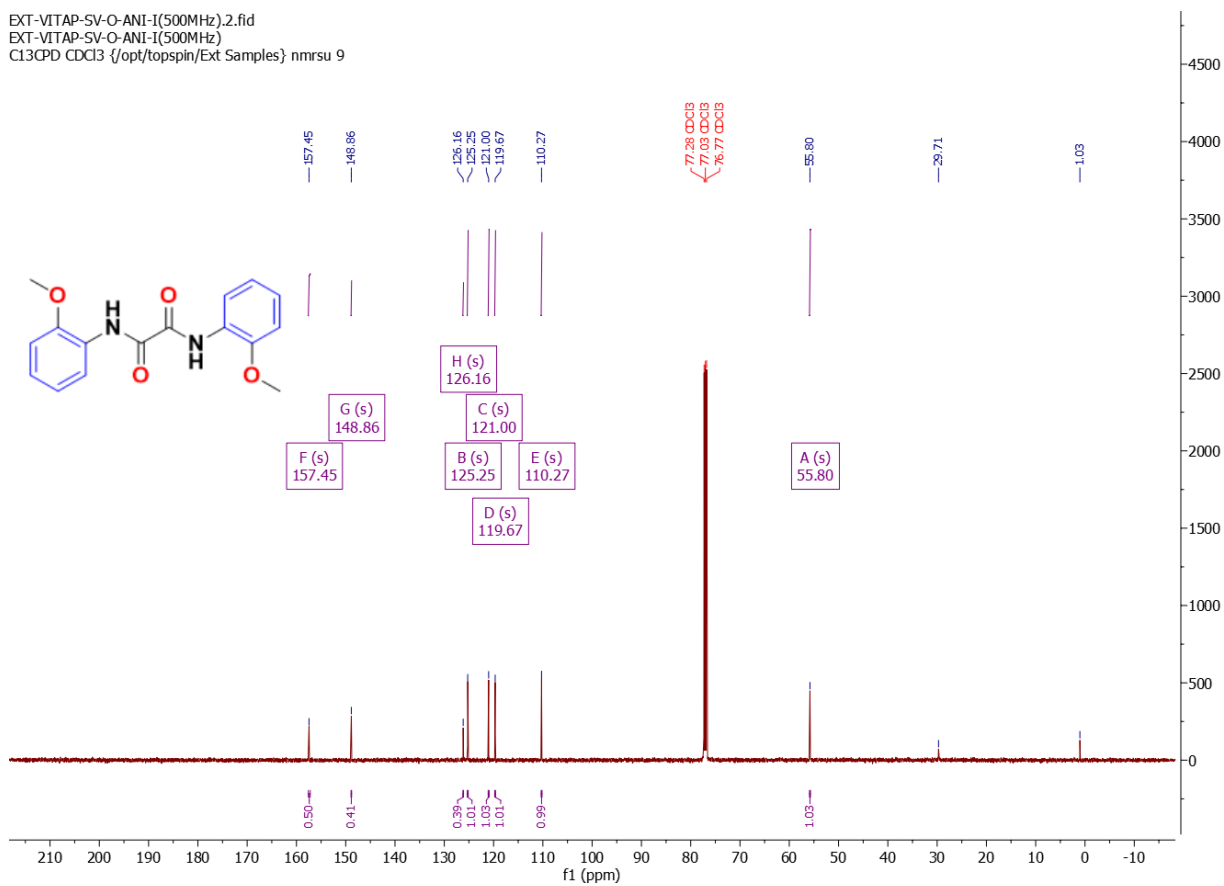
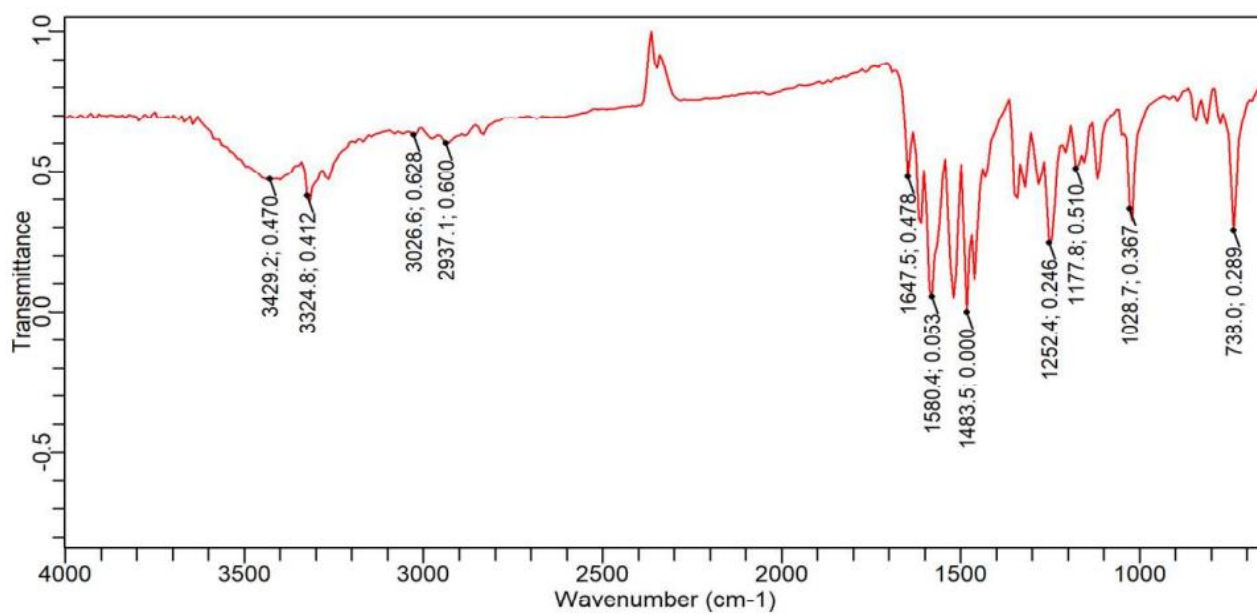
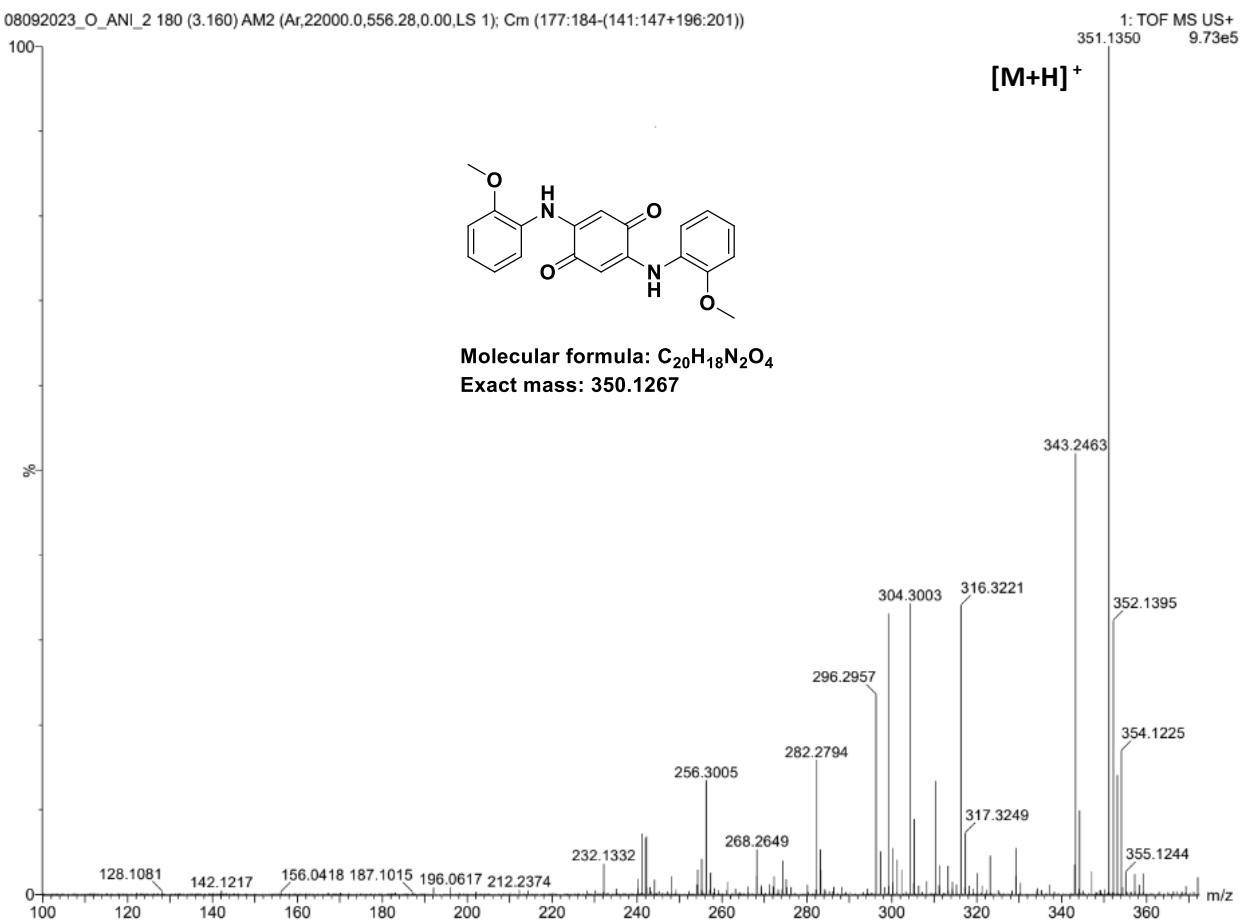


Figure S15. <sup>13</sup>C NMR spectral studies for compound 9.



**Figure S16.** FTIR(KBr) spectrum for compound **10**.



**Figure S17.** HRMS–ESI spectrum for compound **10**.

EXT-VITAP-SV-O-ANI-2(500MHz).1.fid  
EXT-VITAP-SV-O-ANI-2(500MHz)  
PROTON CDCl3 {/opt/topspin/Ext Samples} nmrsu 2

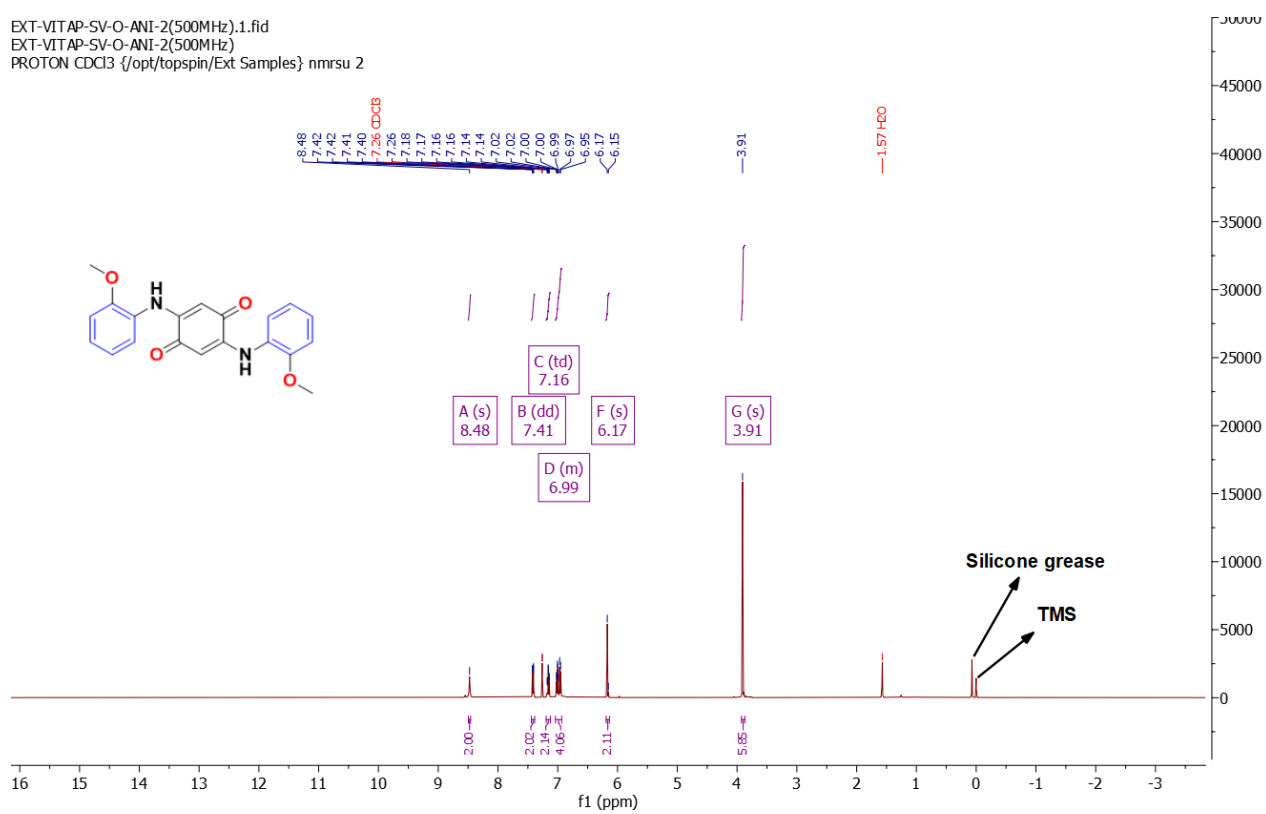
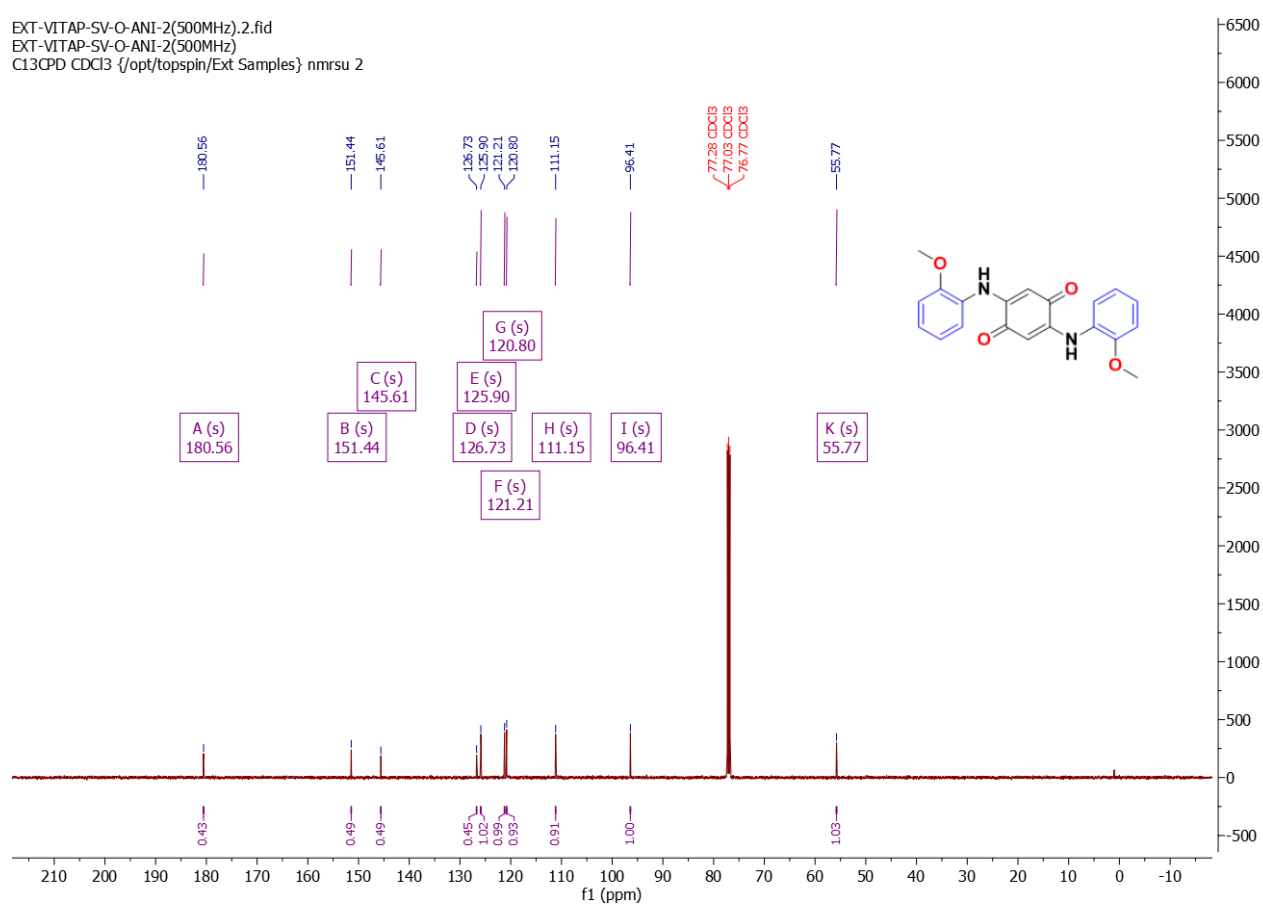


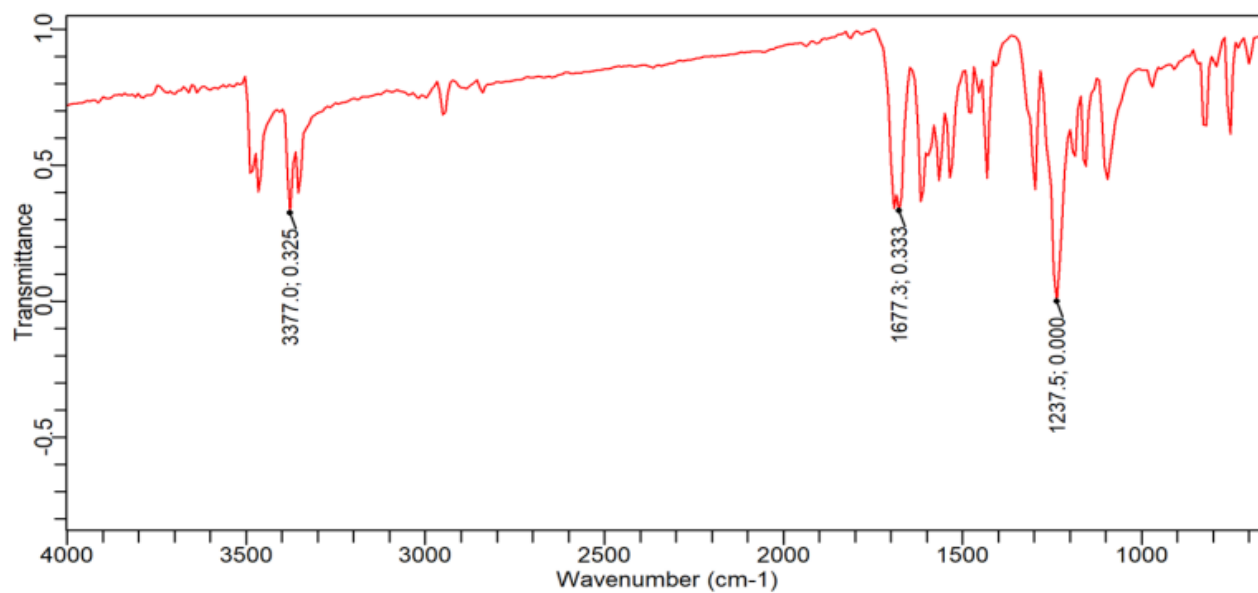
Figure S18. <sup>1</sup>H NMR spectral studies for compound 10,

EXT-VITAP-SV-O-ANI-2(500MHz).2.fid  
EXT-VITAP-SV-O-ANI-2(500MHz)  
C13CPD CDCl3 {/opt/topspin/Ext Samples} nmrsu 2

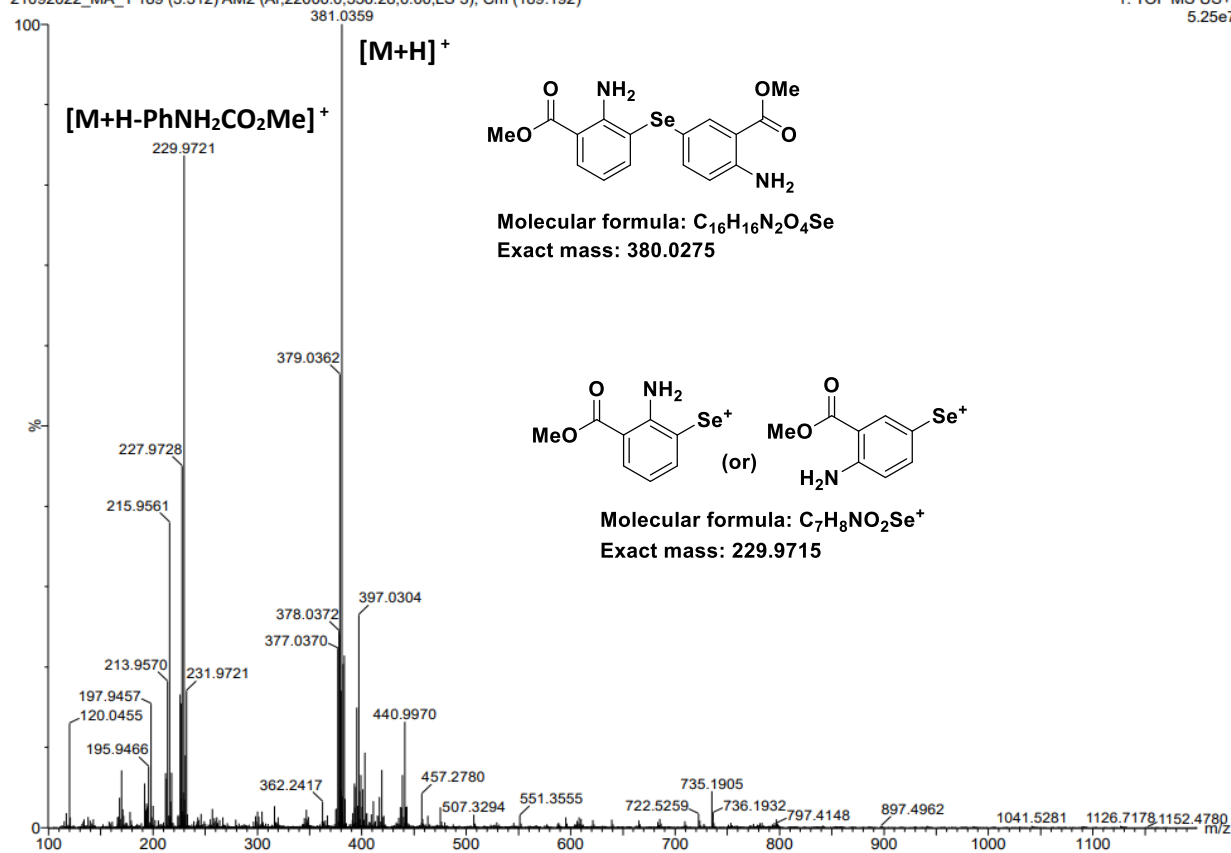


**Figure S19.**  $^{13}\text{C}$  NMR spectral studies for compound 10.

4. Spectrometric characterization of products obtained from the reaction of methyl anthranilate with  $\text{SeO}_2$



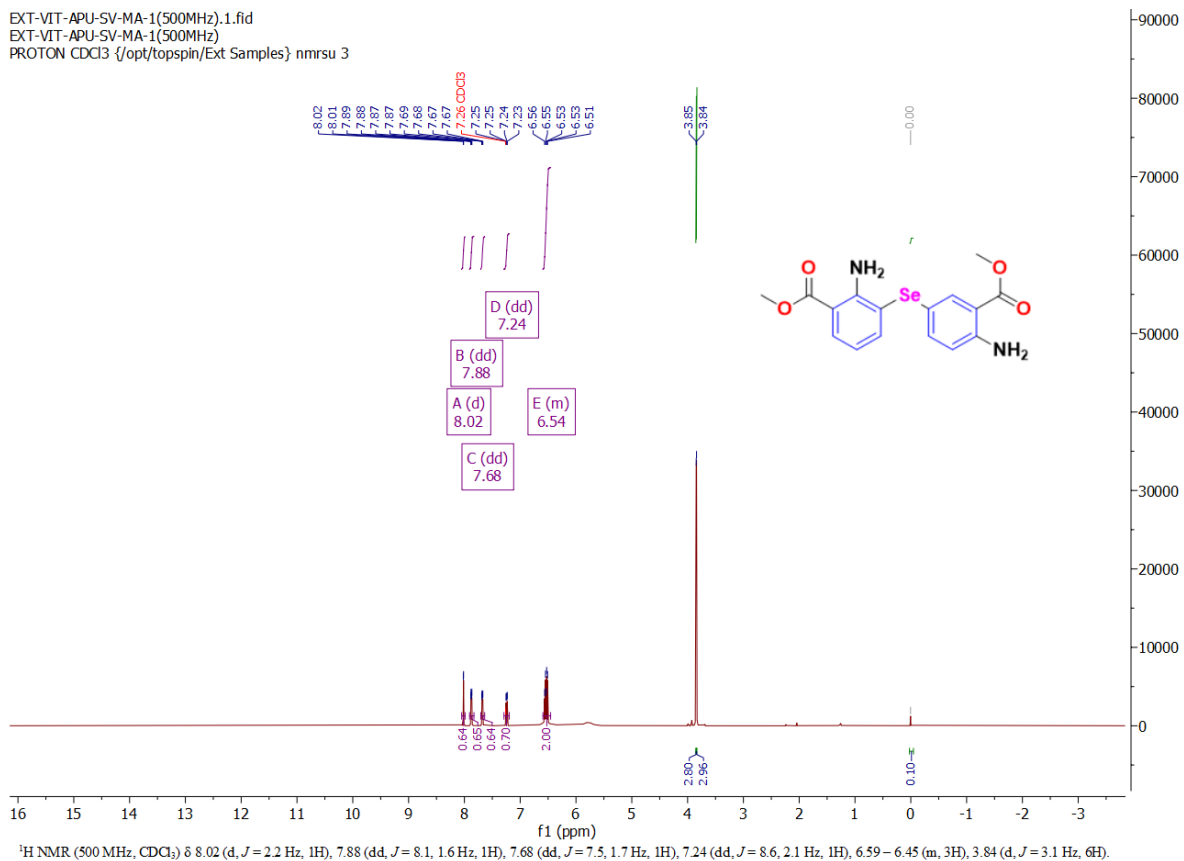
**Figure S20.** FTIR(KBr) spectrum for compound **11**.



**Figure S21.** HRMS–ESI spectrum for compound **11**.



EXT-VIT-APU-SV-MA-1(500MHz).1.fid  
EXT-VIT-APU-SV-MA-1(500MHz)  
PROTON CDCl3 {/opt/topspin/Ext Samples} nmrsu 3



**Figure S22.** <sup>1</sup>H NMR spectral studies for compound 11.

EXT-VIT-APU-SV-MA-1(500MHz).2.fid  
EXT-VIT-APU-SV-MA-1(500MHz)  
C13CPD CDCl3 {/opt/topspin/Ext Samples} nmrsu 3

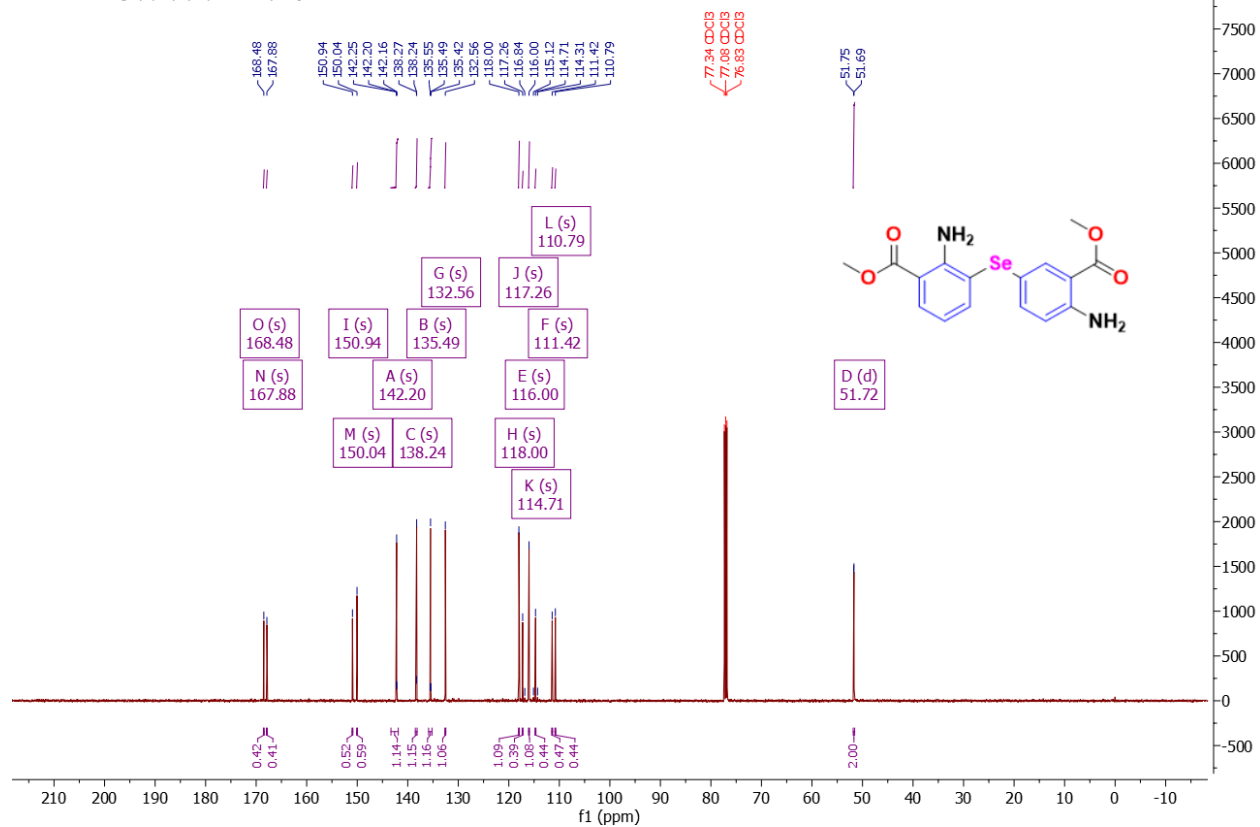
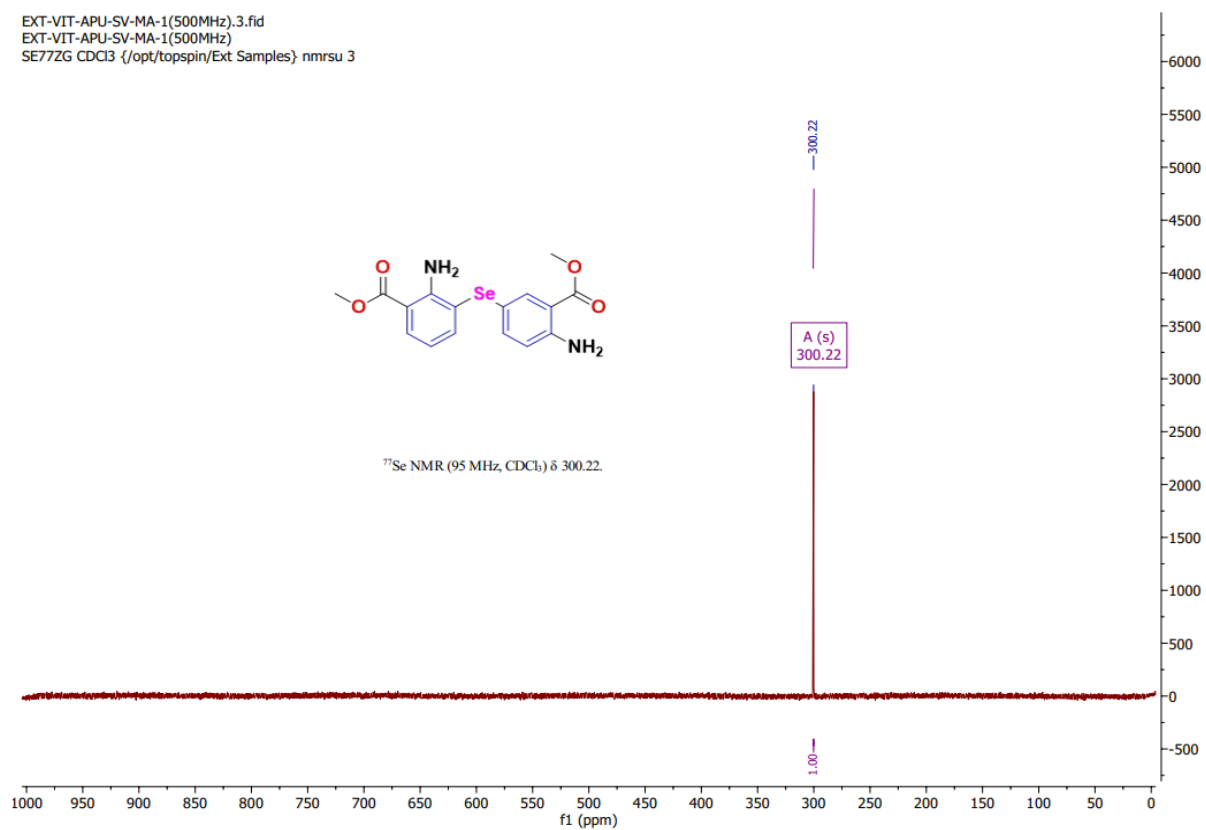
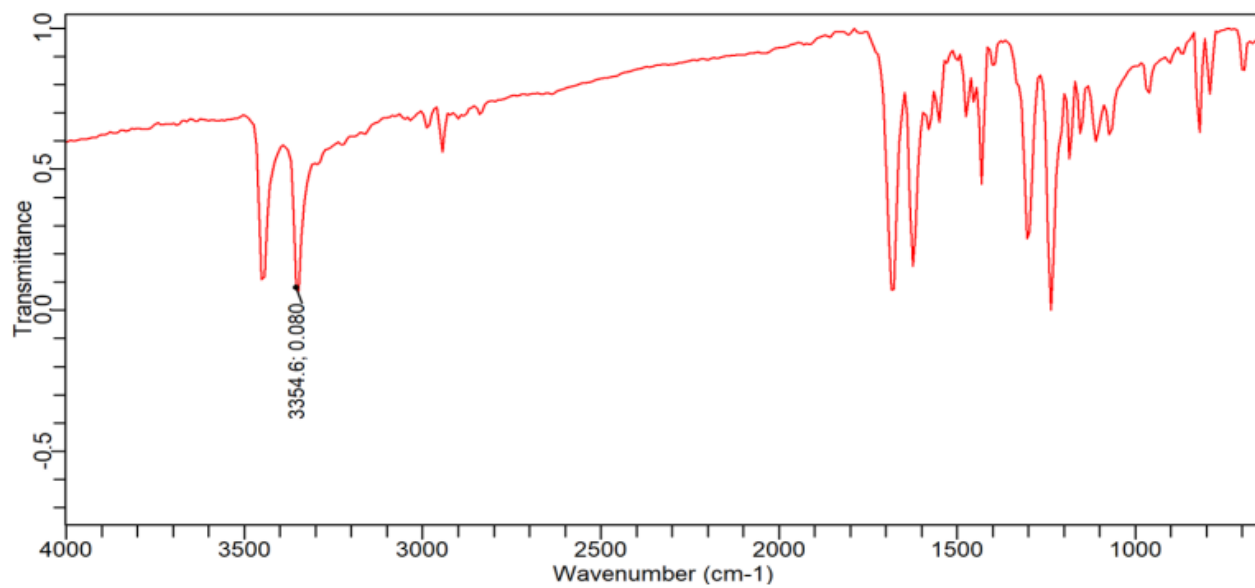


Figure S23.  $^{13}\text{C}$  NMR spectral studies for compound 11.

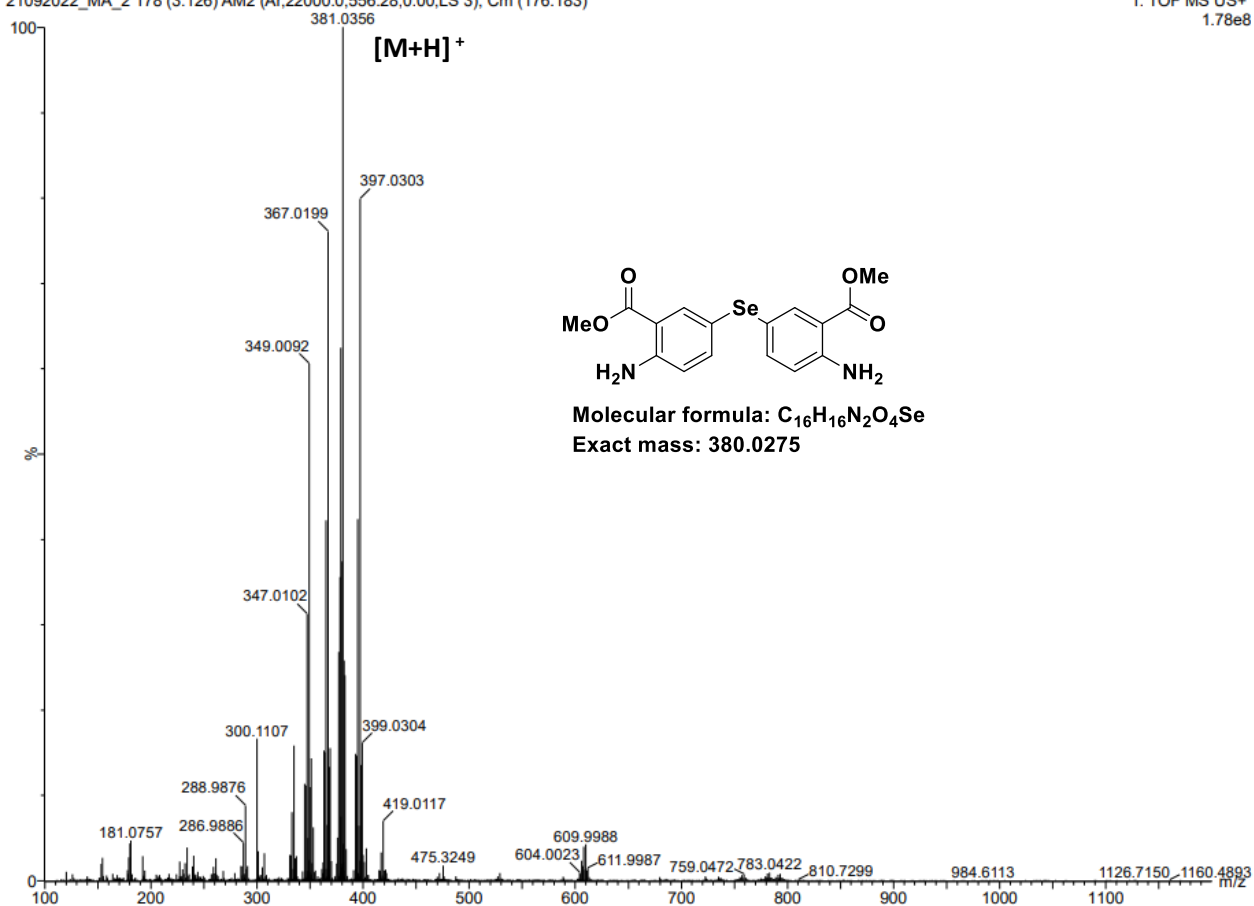
EXT-VIT-APU-SV-MA-1(500MHz).3.fid  
EXT-VIT-APU-SV-MA-1(500MHz)  
SE77ZG CDCl3 {/opt/topspin/Ext Samples} nmrsu 3



**Figure S24.**  $^{77}\text{Se}$  NMR spectral studies for compound **11**.

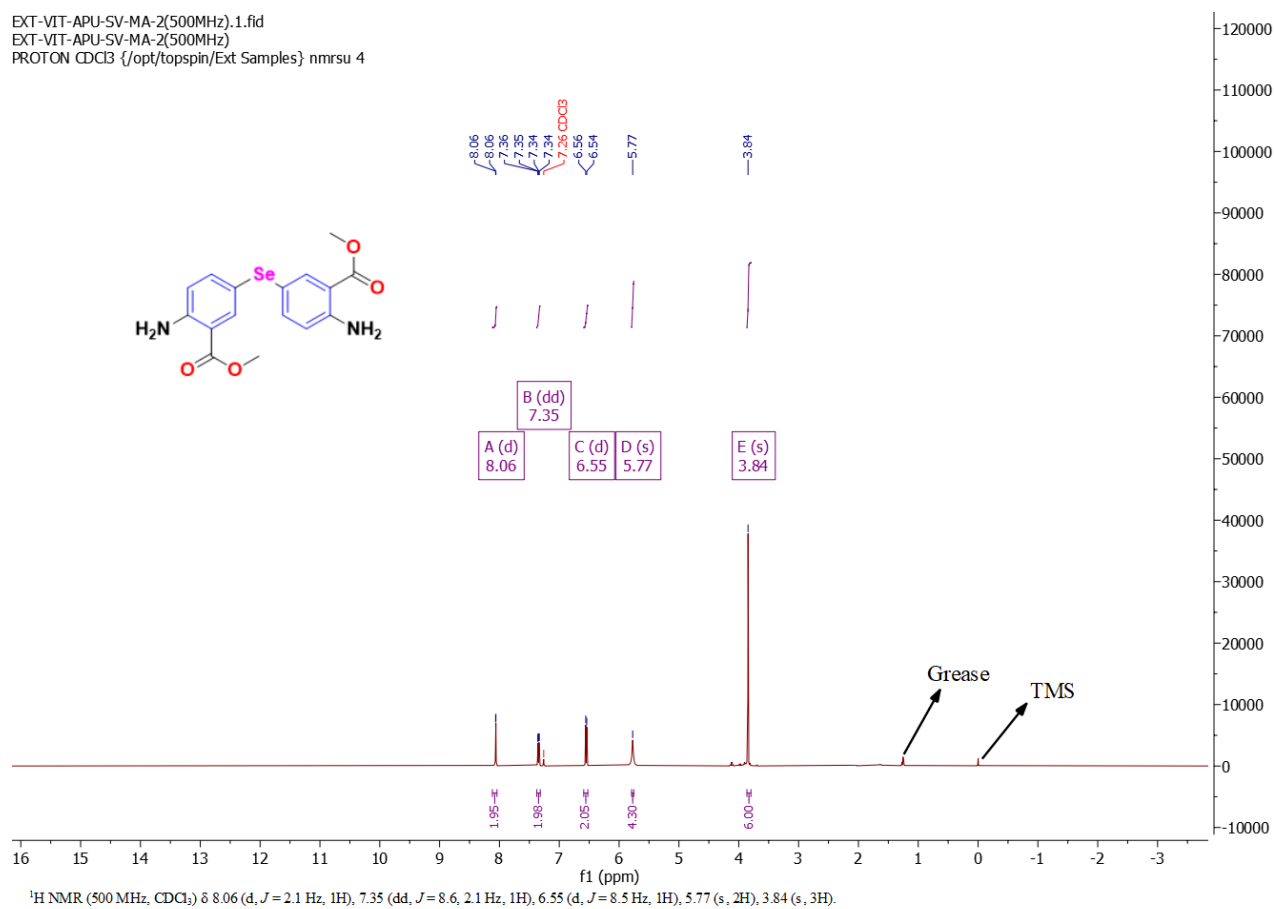


**Figure S25.** FTIR(KBr) spectrum for compound **12**.



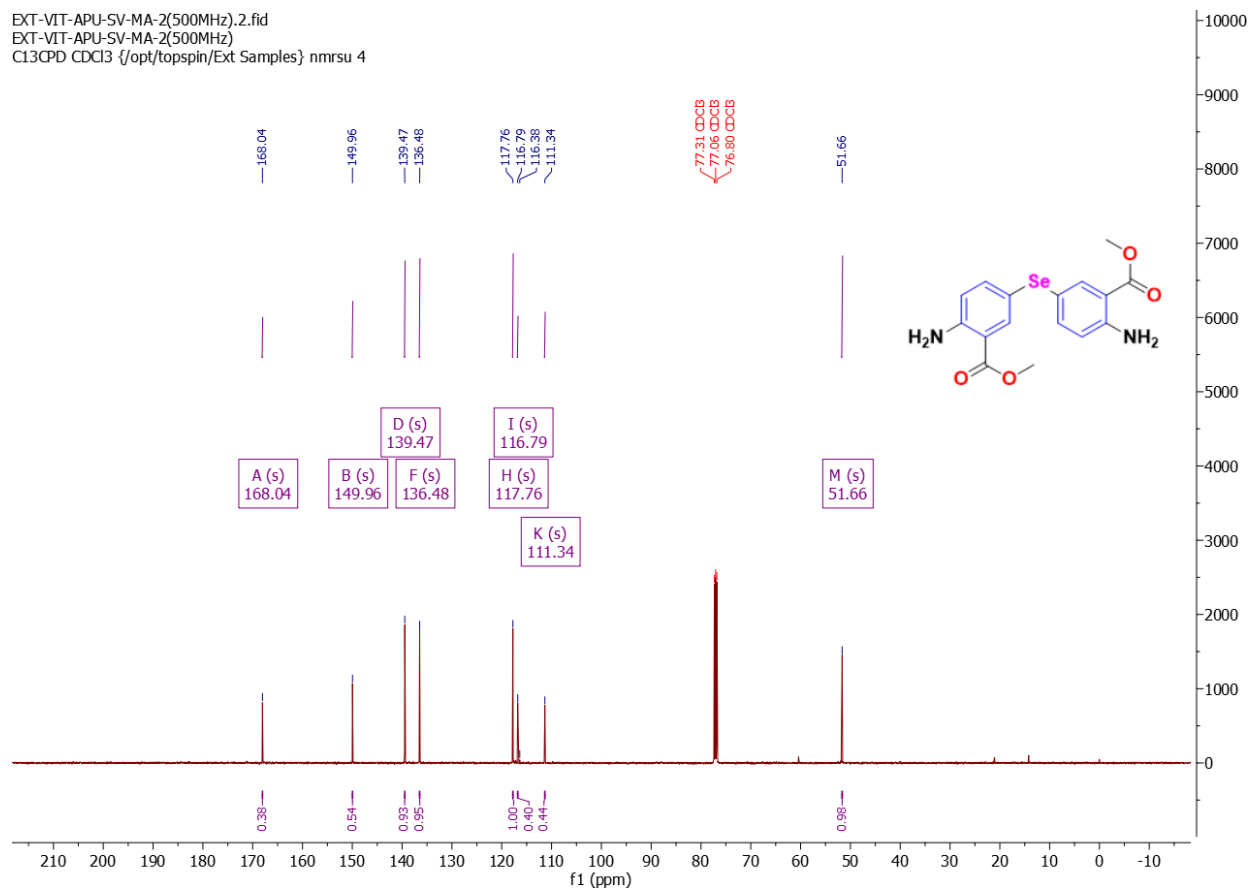
**Figure S26.** HRMS-ESI spectrum for compound **12**.

EXT-VIT-APU-SV-MA-2(500MHz).1.fid  
EXT-VIT-APU-SV-MA-2(500MHz)  
PROTON CDCl3 {/opt/topspin/Ext Samples} nmrsu 4



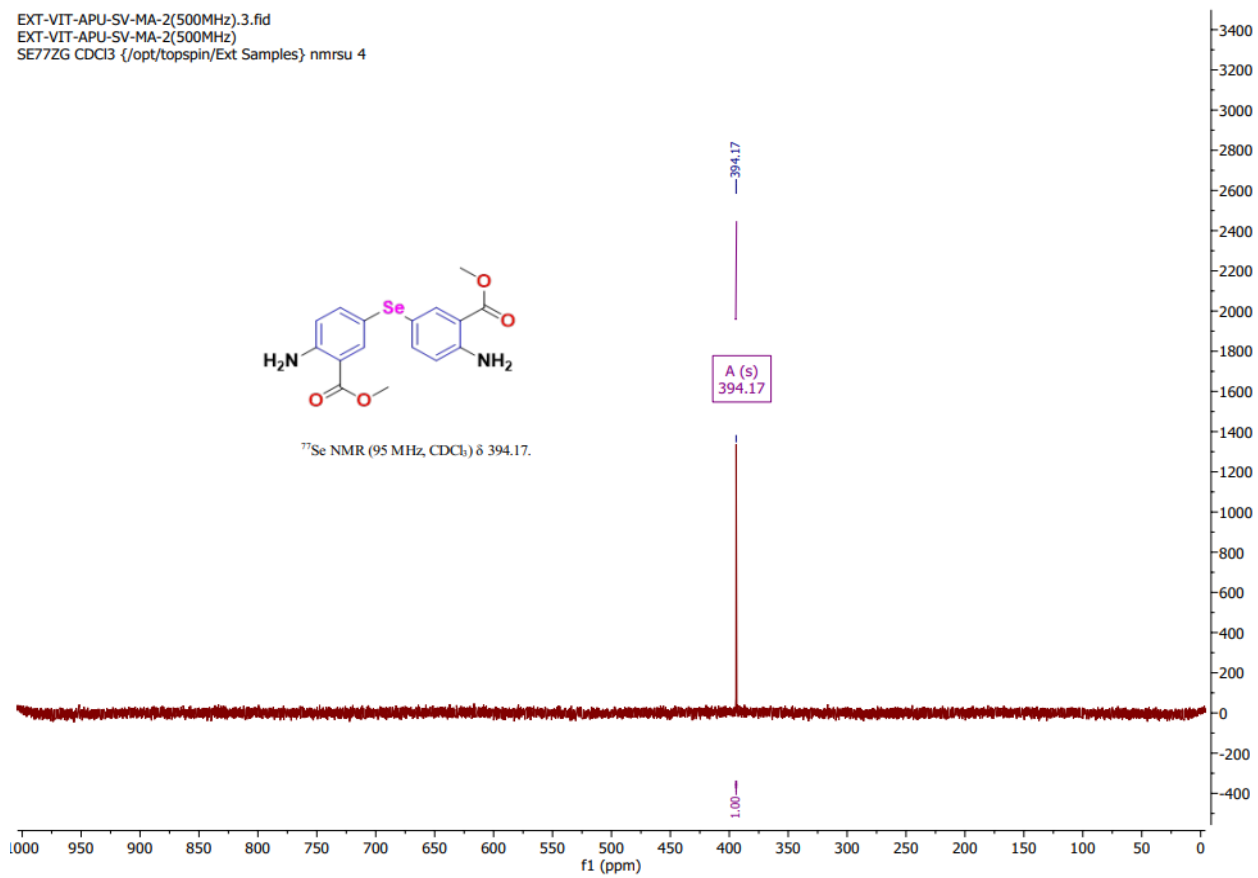
**Figure S27.** <sup>1</sup>H NMR spectral studies for compound **12**.

EXT-VIT-APU-SV-MA-2(500MHz).2.fid  
EXT-VIT-APU-SV-MA-2(500MHz)  
C13CPD CDCl3 {/opt/topspin/Ext Samples} nmr su 4



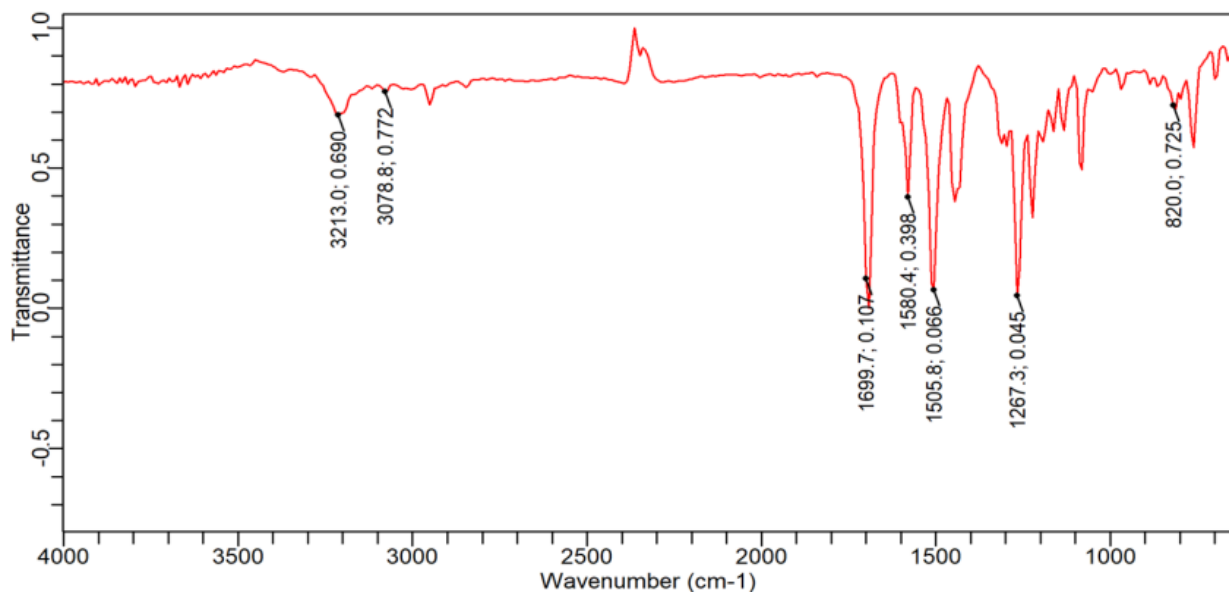
**Figure S28.** <sup>13</sup>C NMR spectral studies for compound 12.

EXT-VIT-APU-SV-MA-2(500MHz).3.fid  
EXT-VIT-APU-SV-MA-2(500MHz)  
SE77ZG CDCl3 {/opt/topspin/Ext Samples} nmr su 4

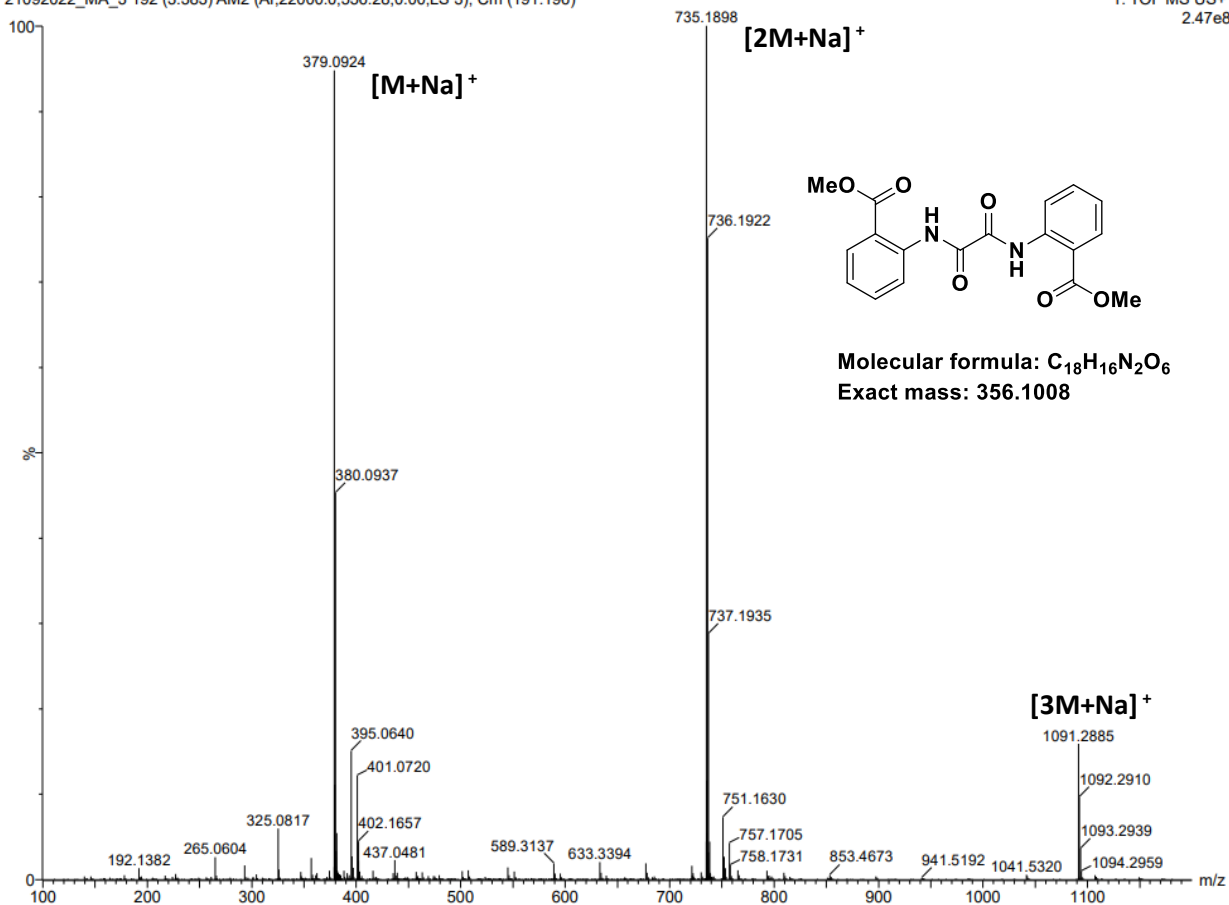


**Figure S29.**  $^{77}\text{Se}$  NMR spectral studies for compound **12**.



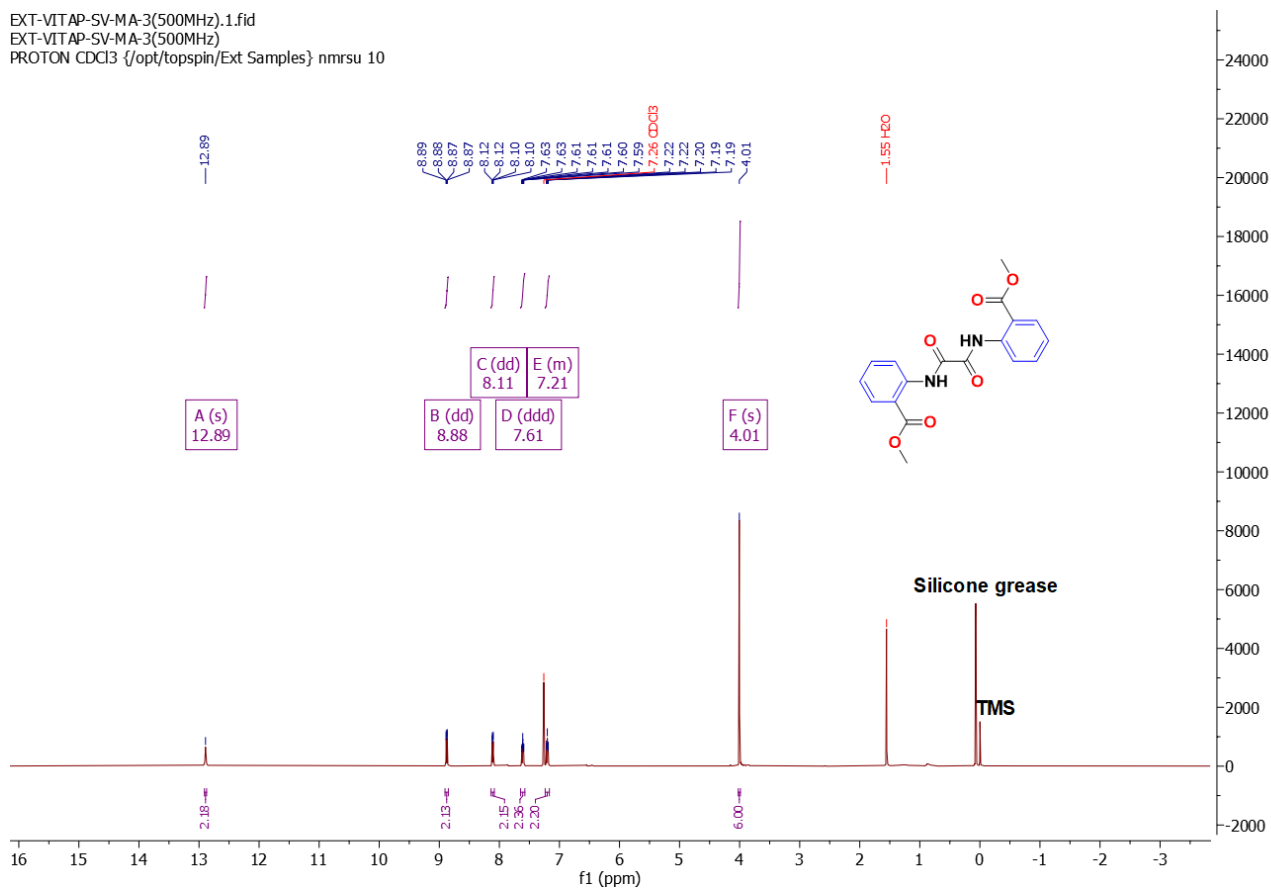


**Figure S30.** FTIR(KBr) spectrum for compound **13**.



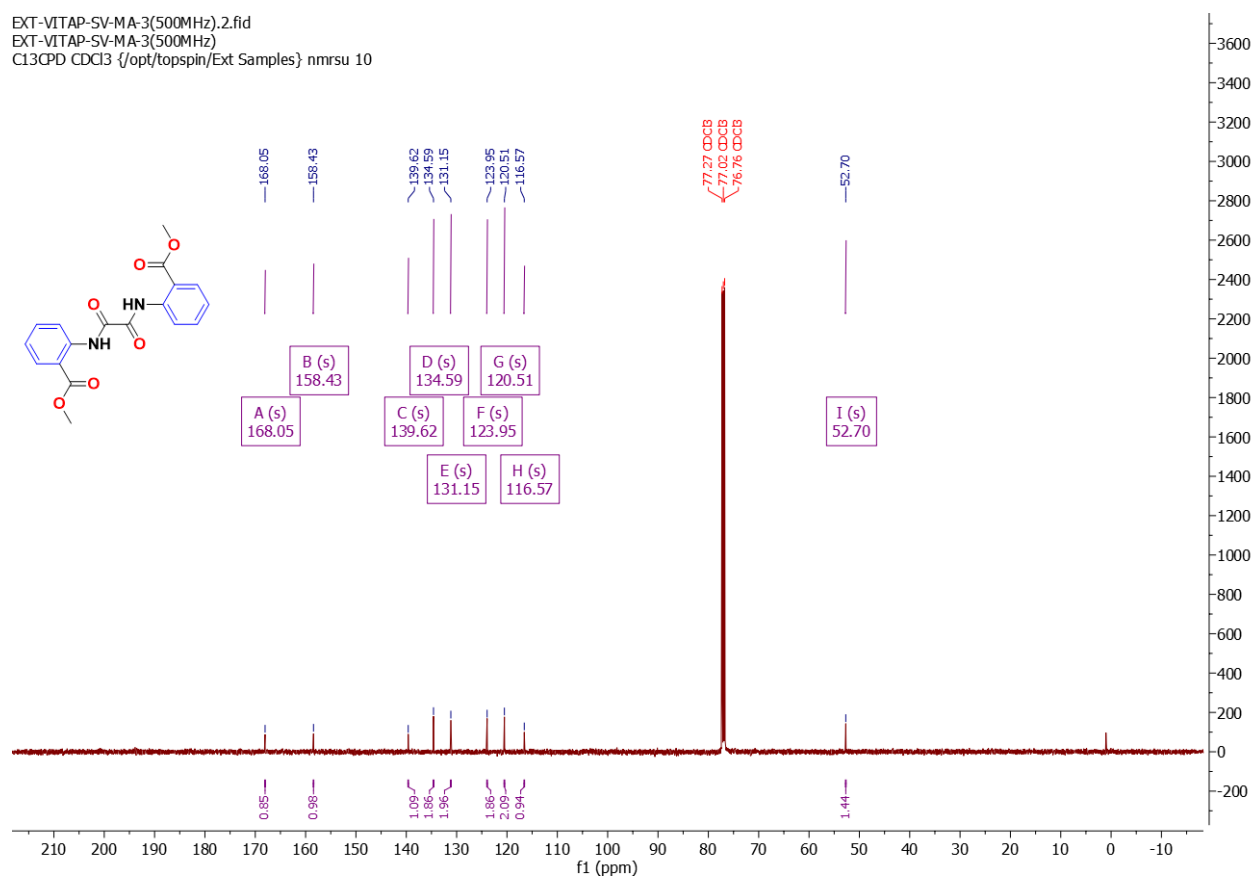
**Figure S31.** HRMS-ESI spectrum for compound 13.

EXT-VITAP-SV-MA-3(500MHz).1.fid  
EXT-VITAP-SV-MA-3(500MHz)  
PROTON CDCl3 {/opt/topspin/Ext Samples} nmrsu 10



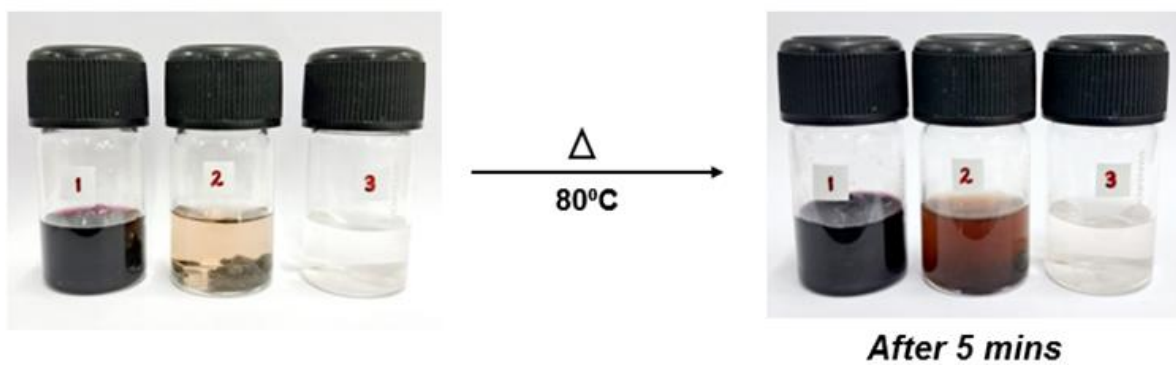
**Figure S32.** <sup>1</sup>H NMR spectral studies for compound **13**.

EXT-VITAP-SV-MA-3(500MHz).2.fid  
EXT-VITAP-SV-MA-3(500MHz)  
C13CPD CDCl3 {/opt/topspin/Ext Samples} nmrsu 10



**Figure S33.**  $^{13}\text{C}$  NMR spectral studies for compound **13**.

5. Relative color change upon addition of  $\text{SeO}_2$  to arylamines in acetonitrile



**Figure S34:** Relative color change upon addition of  $\text{SeO}_2$  to arylamines in acetonitrile: vial 1: *o*-anisidine, vial 2: aniline, vial 3: methyl anthranilate.

6. Packing arrangement for compounds 3 and 9

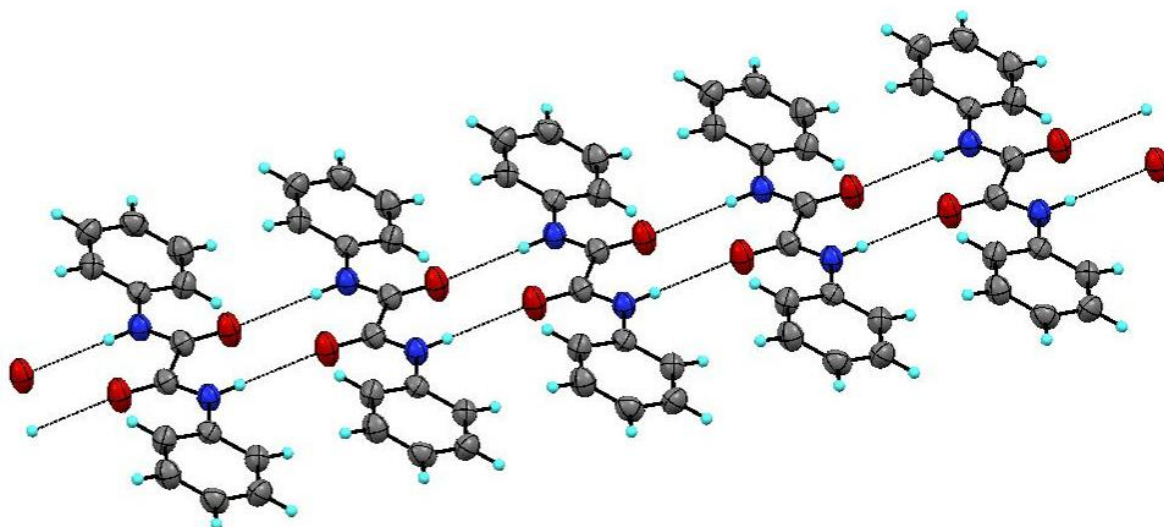


Figure S35. Packing arrangement for compound 3.

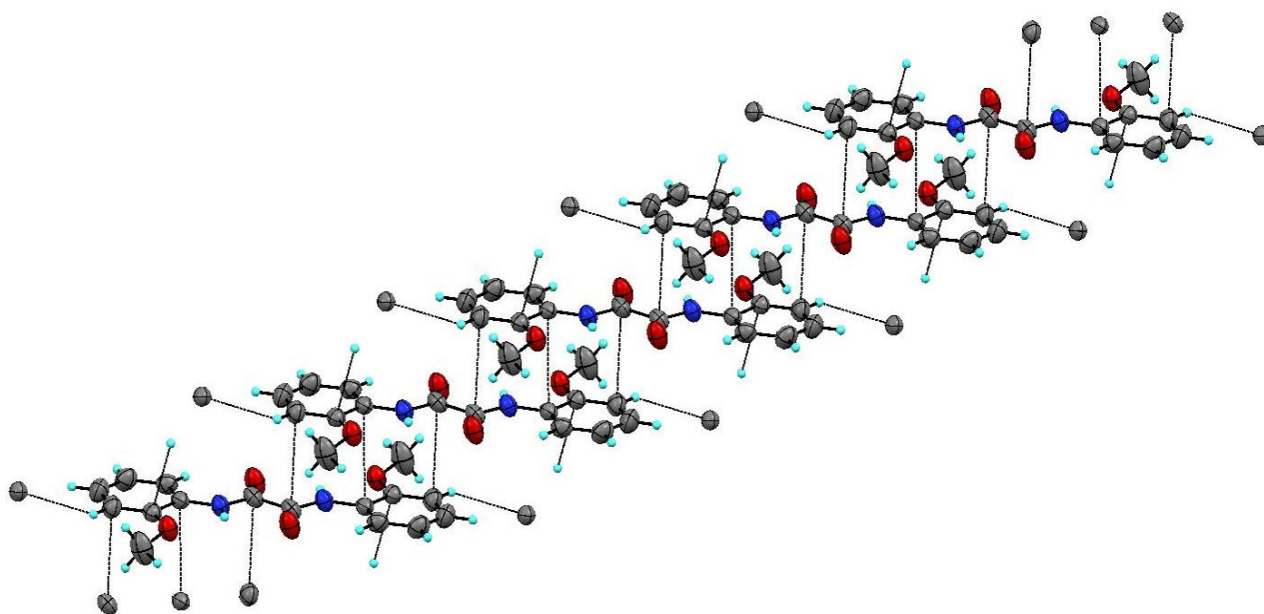
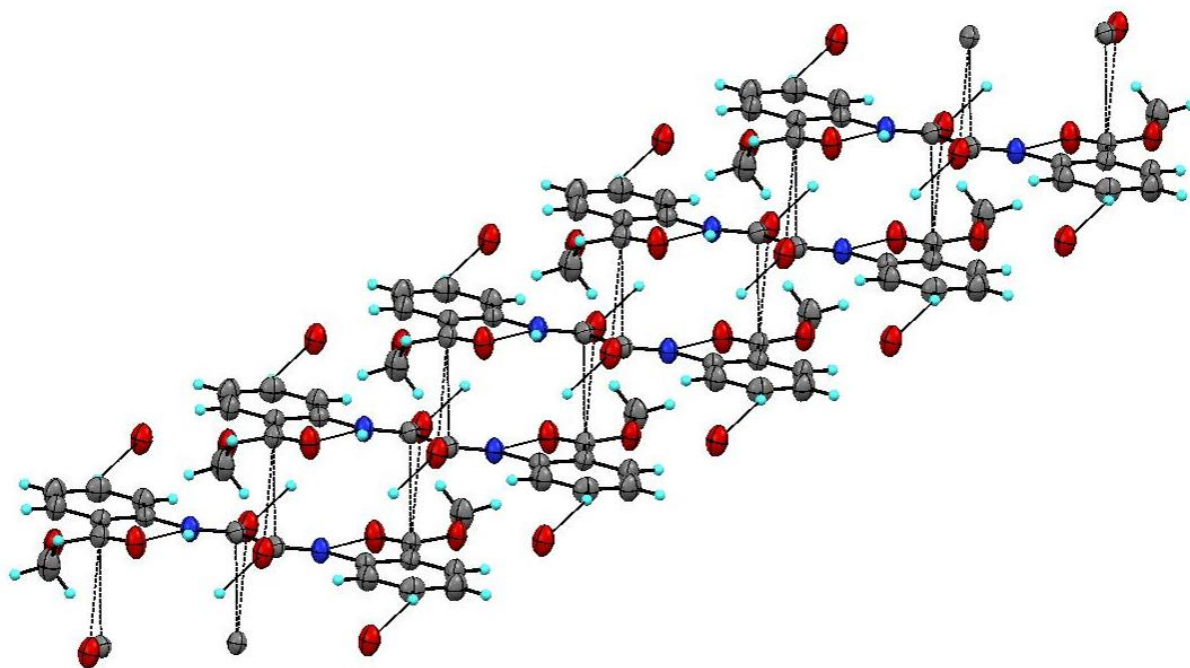
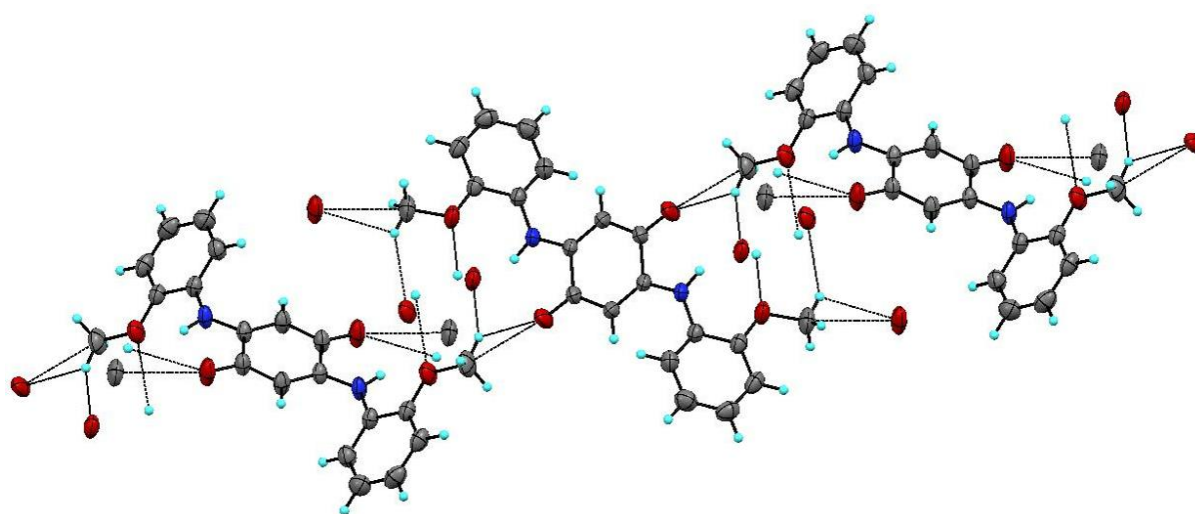


Figure S36. Packing arrangement for compound 9.

## 7. Packing arrangement for compounds 13 and 10

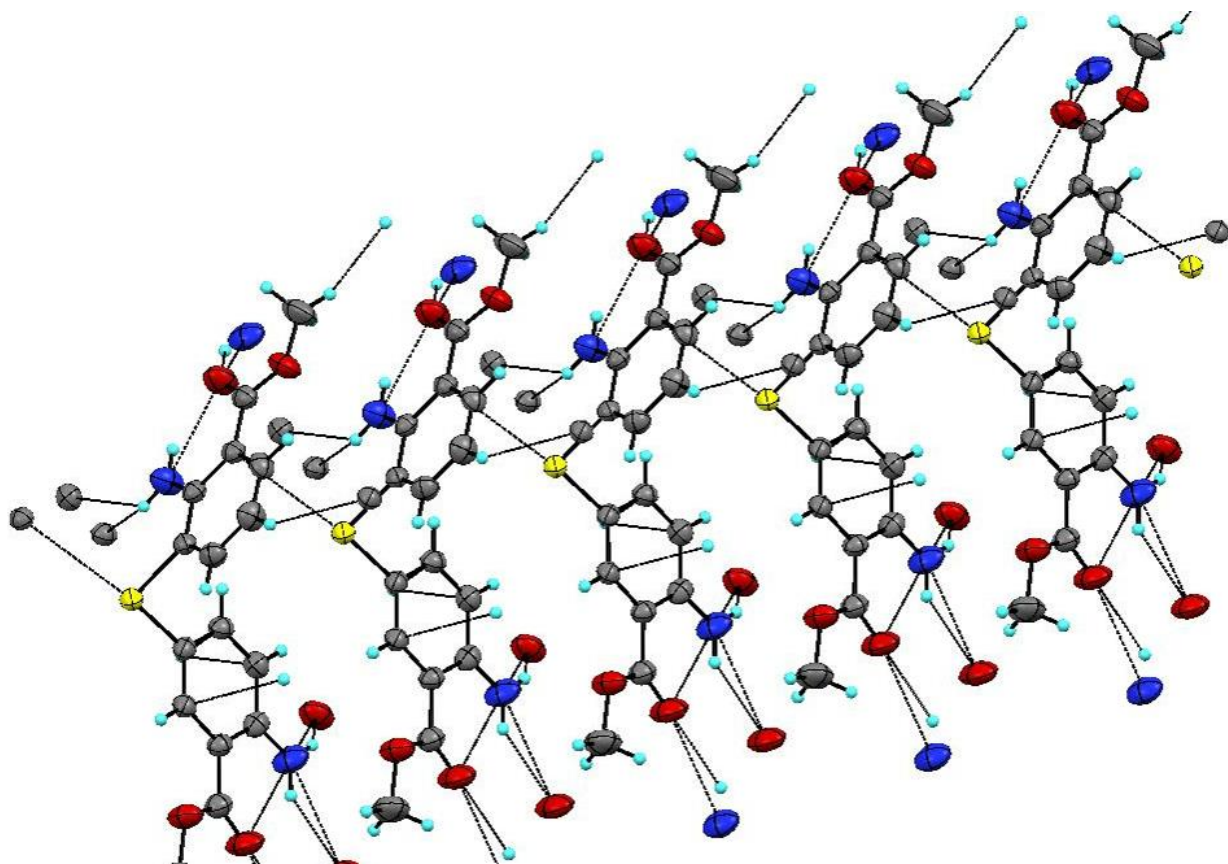


**Figure S37.** Packing arrangement for compound **13**.



**Figure S38.** Packing arrangement for compound **10**.

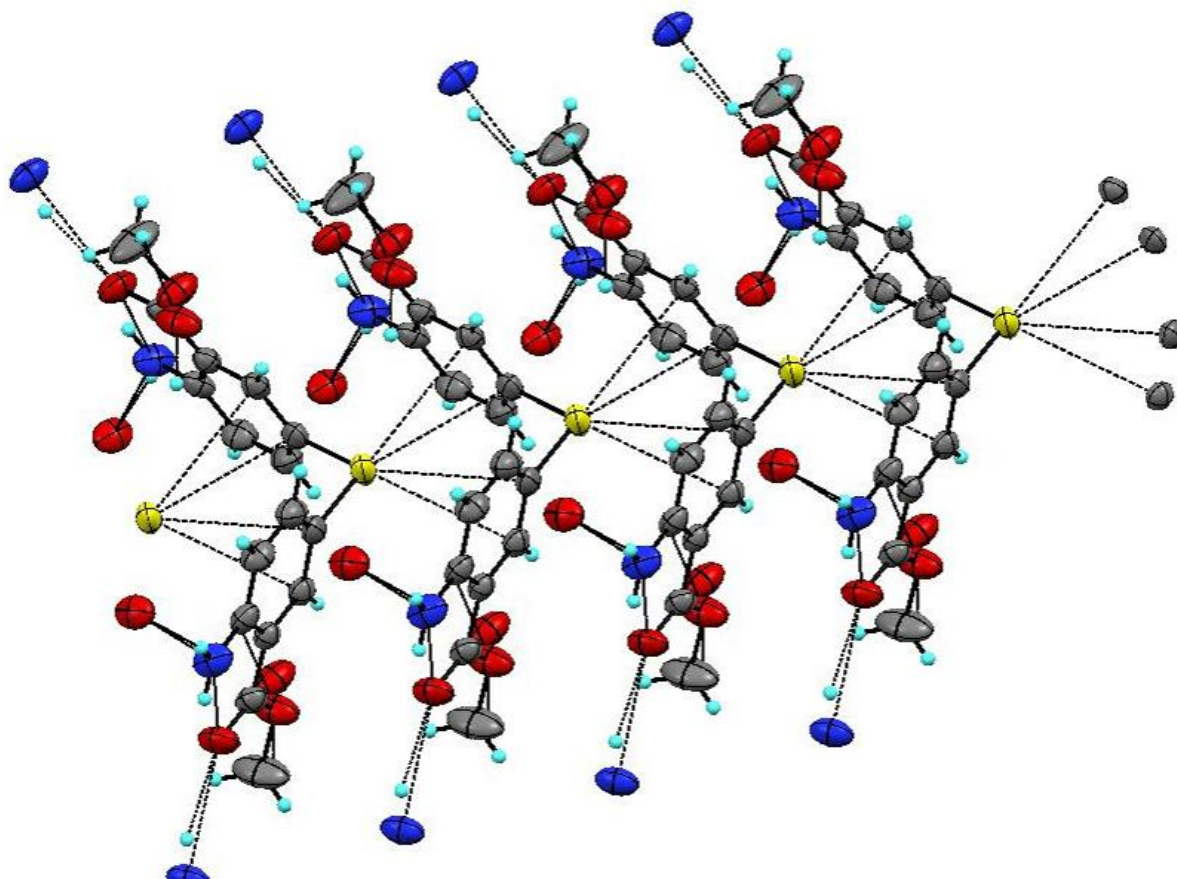
## 8. Packing arrangement for compound 11



**Figure S39.** Packing arrangement for compound 11.

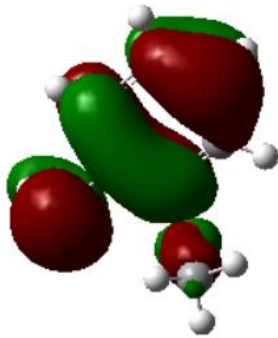
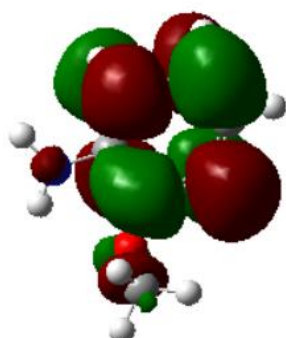
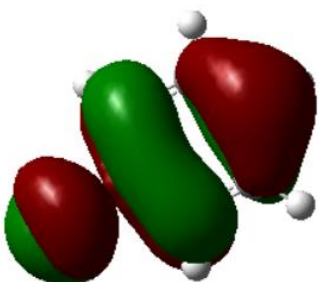
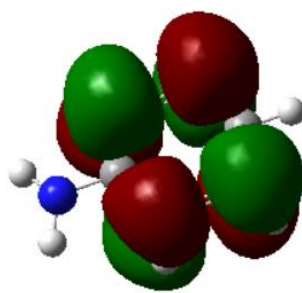
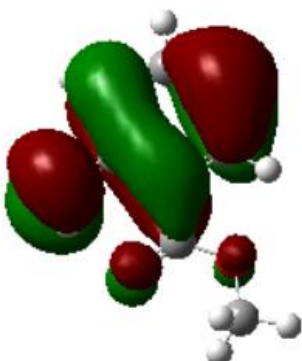
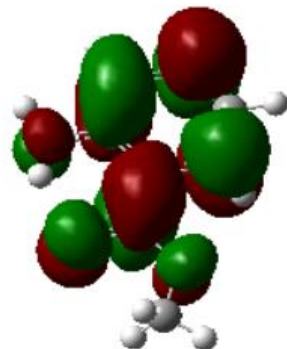


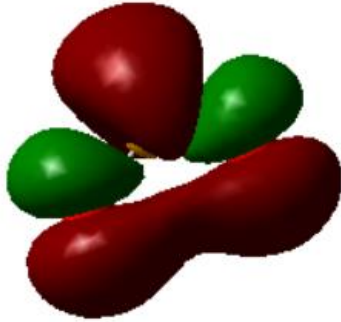
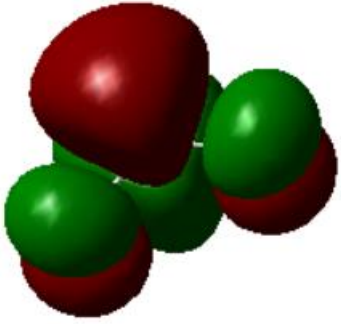
## 9. Packing arrangement for compound 12



**Figure S40.** Packing arrangement for compound 12.

### 10. HOMO and LUMO energy values for reactants

| reactant            | HOMO (donor)<br>kJ/mol   | LUMO (acceptor)<br>kJ/mol   |
|---------------------|--|---|
| <i>o</i> -anisidine | -517.9324<br>   | 24.2334<br>    |
| aniline             | -520.4003<br>  | 22.3955<br>   |
| methyl anthranilate | -526.2552<br> | -91.9450<br> |

|                  |   |  |
|------------------|---|--|
| Selenium dioxide | -820.8101   | -394.4289  |
|                  |  |  |

**Figure S41:** HOMO and LUMO energy values for reactants.