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Supporting Information

for

Competing electrophilic substitution and oxidative polymerization of arylamines with selenium dioxide

Vishnu Selladurai and Selvakumar Karuthapandi

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

Content page

1. Spectroscopic characterization of polymers 1–3

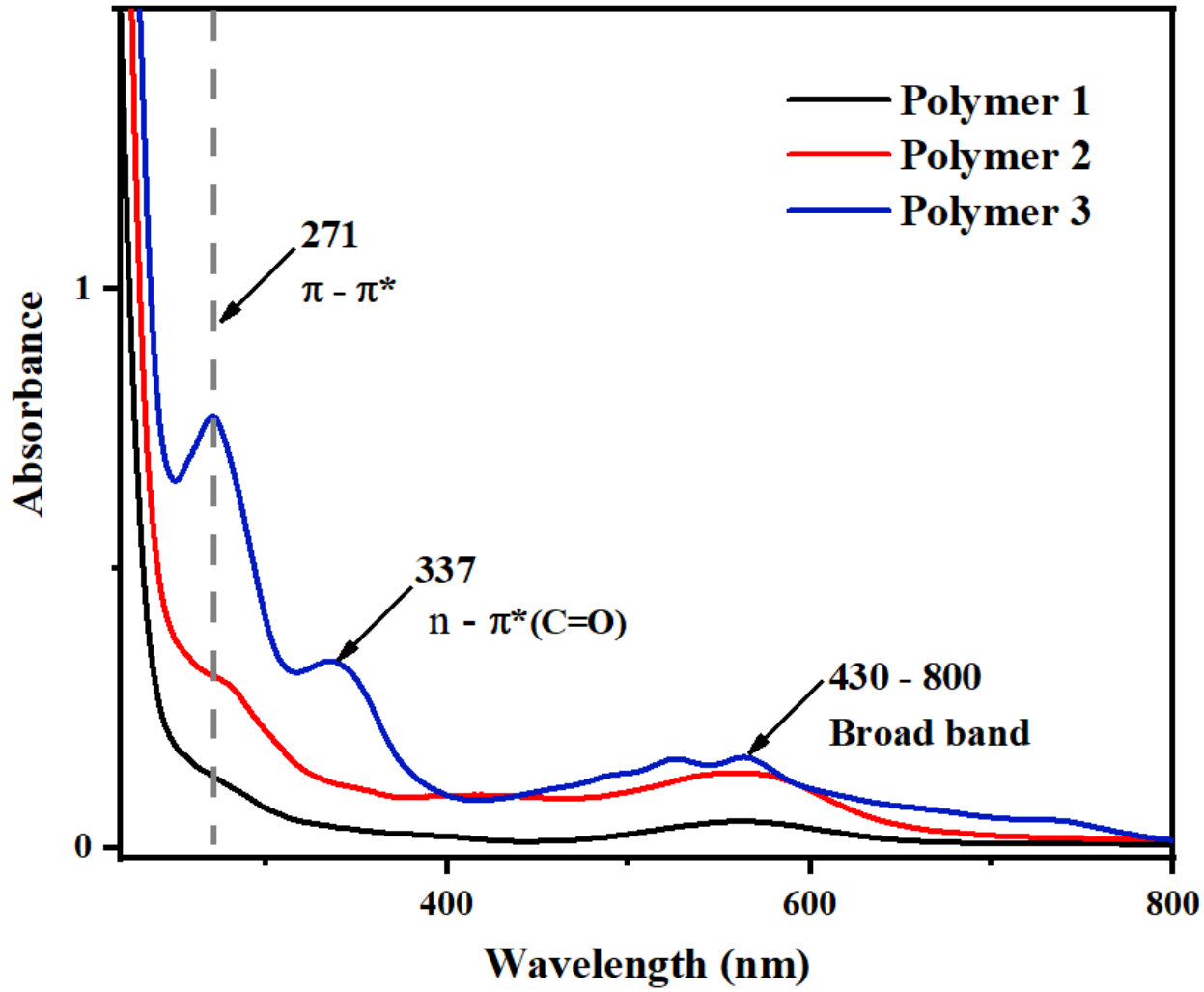


Figure S1. UV–vis spectrum for polymers 1–3.

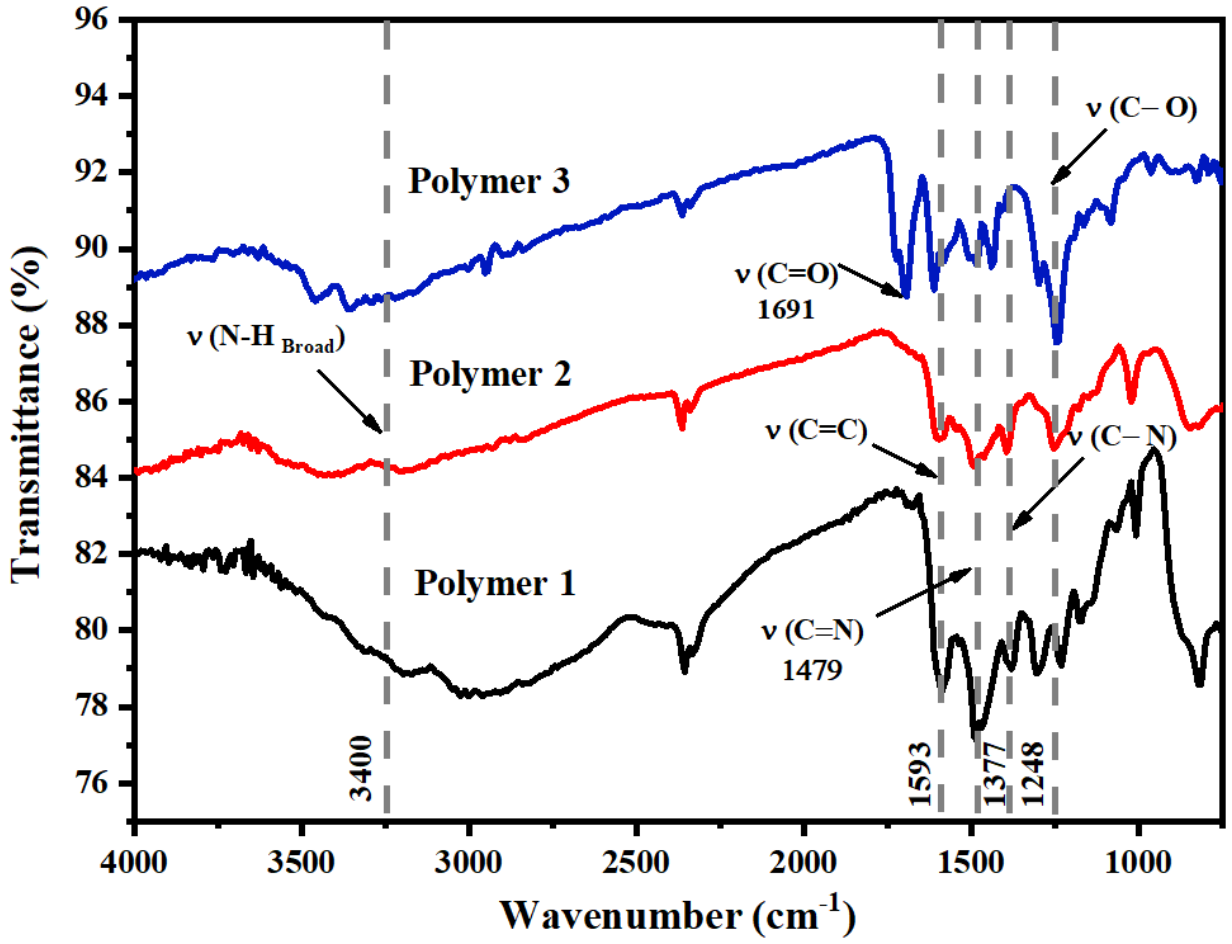


Figure S2. FTIR (KBr) spectrum for polymers 1–3.

2. Spectrometric characterization of products obtained for the reaction of aniline with SeO_2

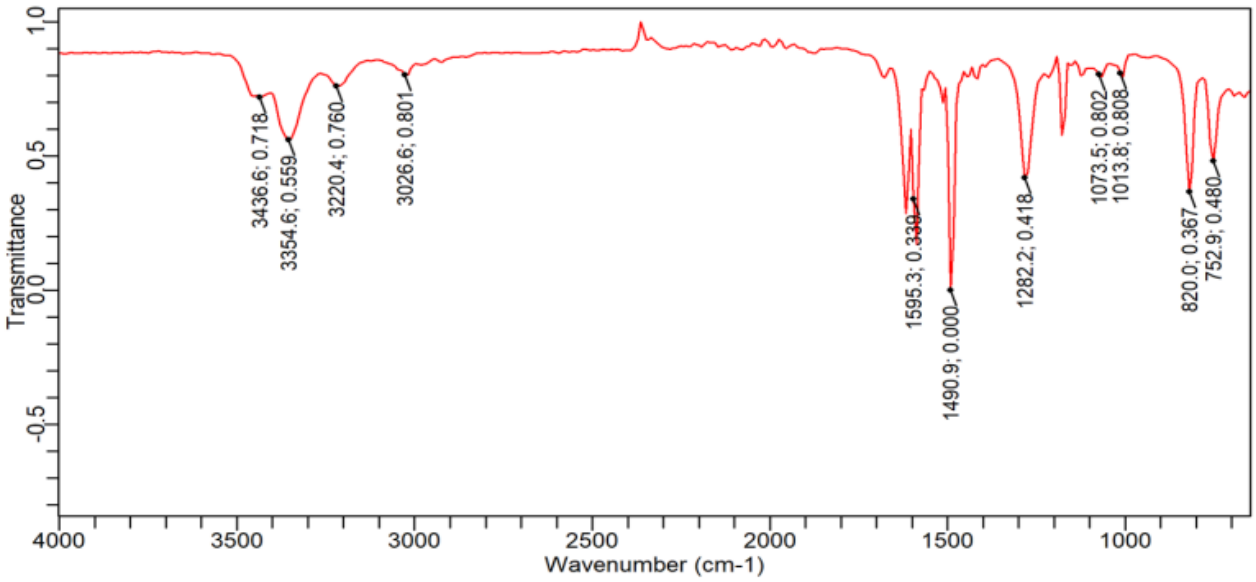


Figure S3. FTIR(KBr) spectrum for mixture of compounds **1** and **2**.

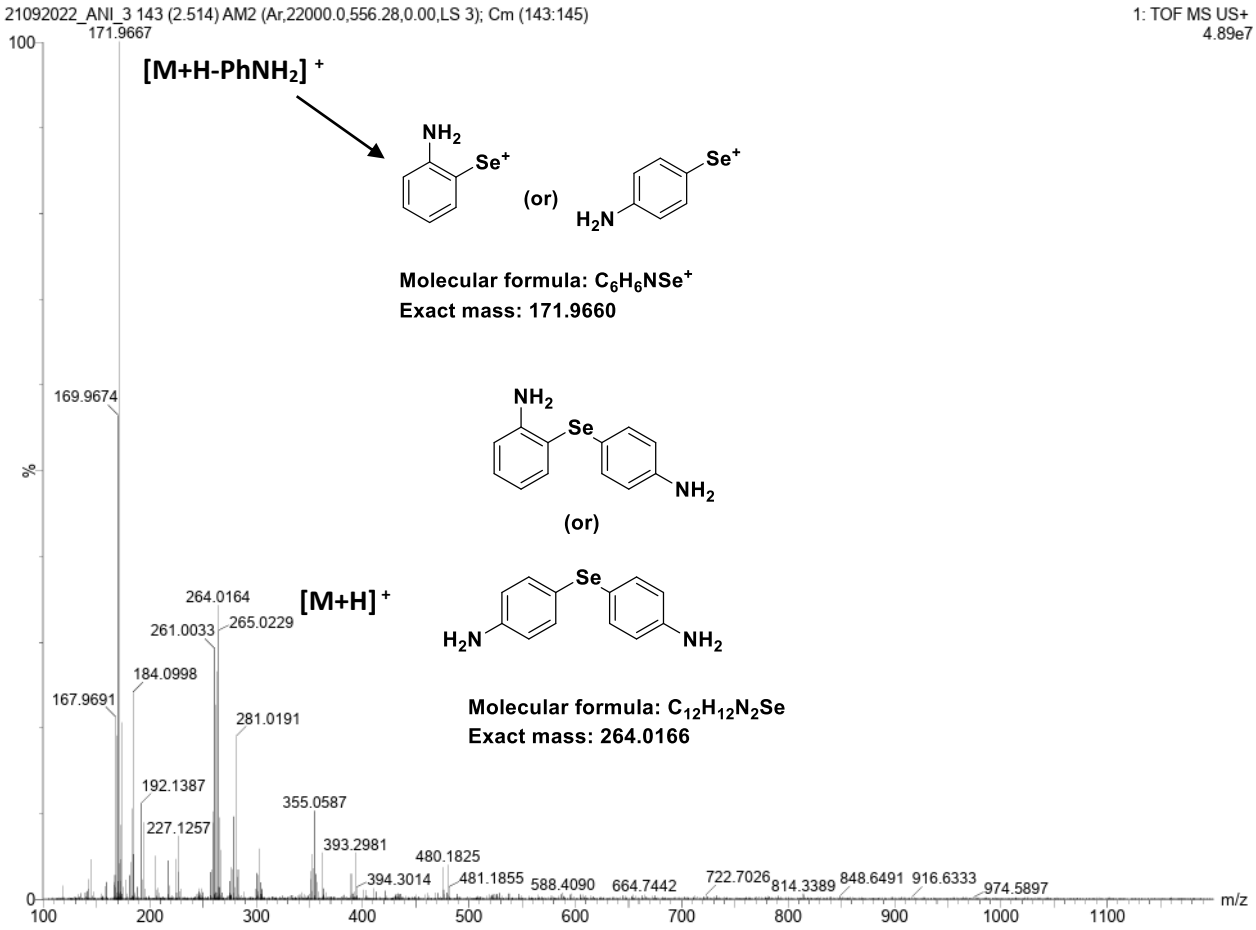


Figure S4. HRMS–ESI spectrum for mixture of compounds **1** and **2**.

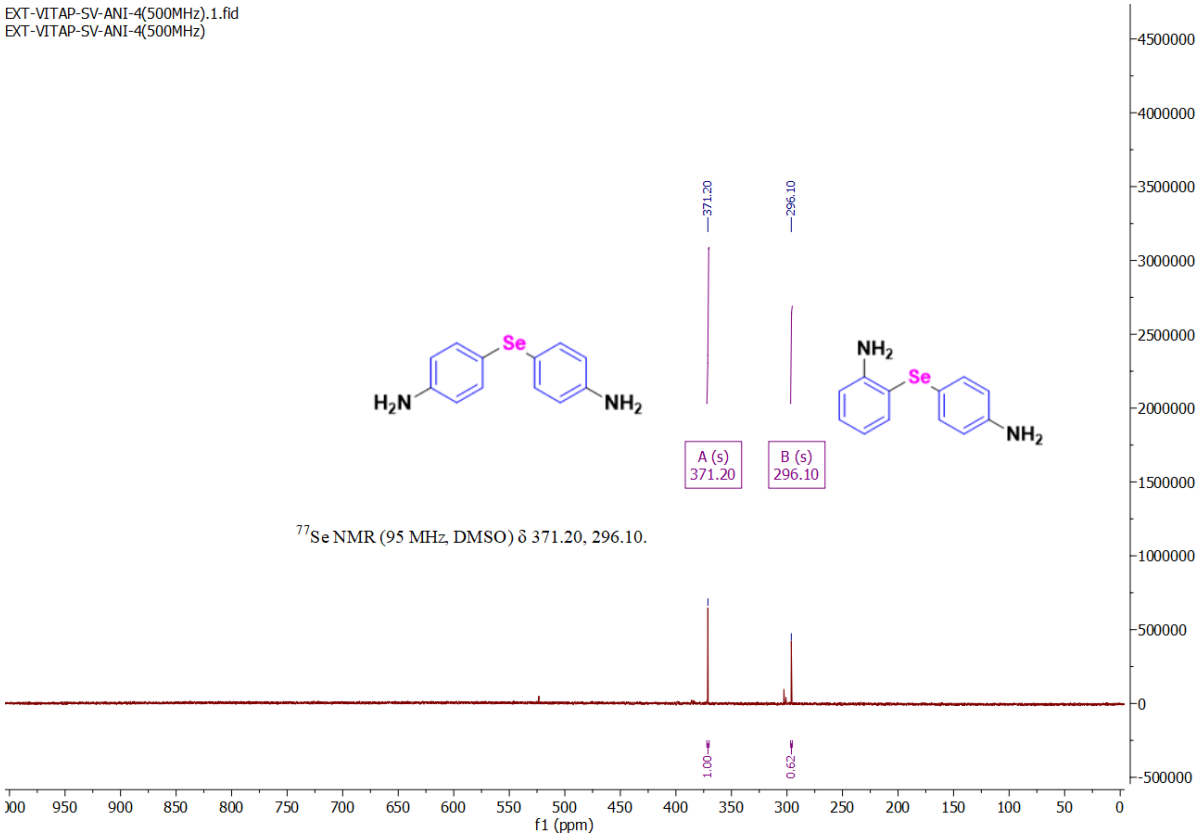


Figure S5. ^{77}Se NMR spectral studies for mixture of compounds **1** and **2**.

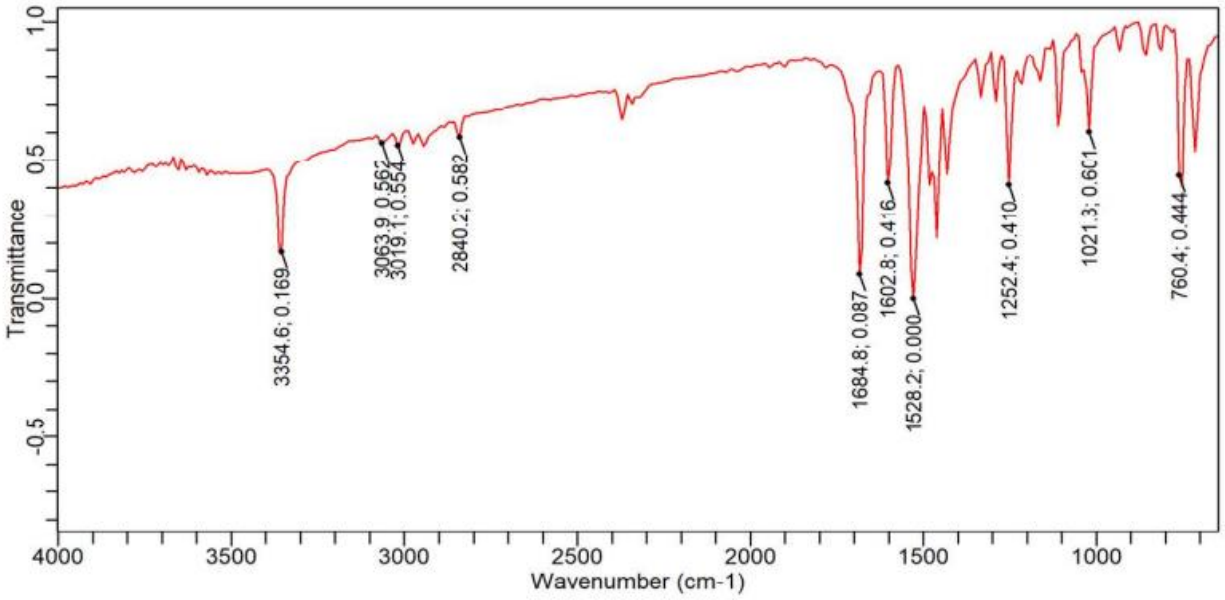


Figure S6. FTIR (KBr) spectrum for compound **3**.

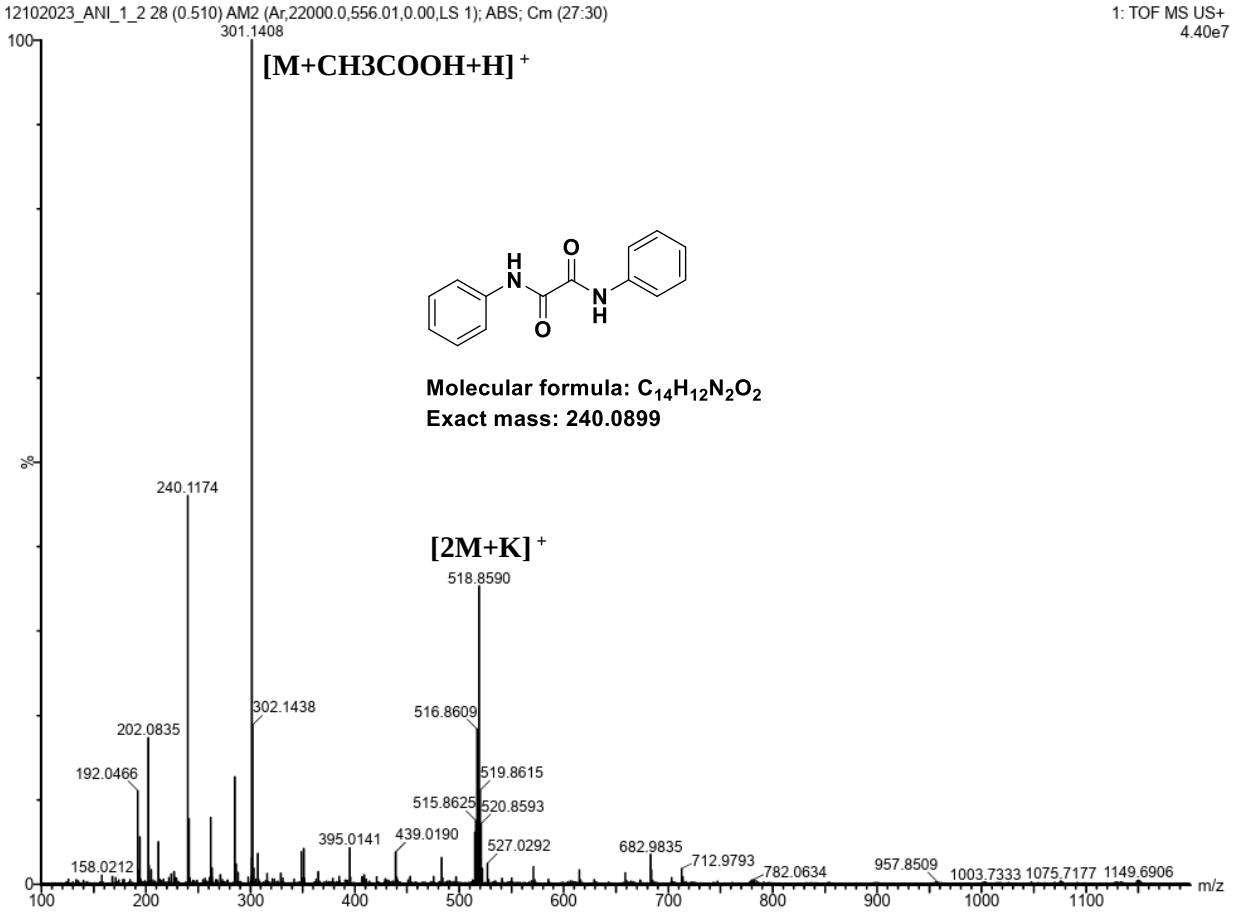


Figure S7. HRMS–ESI spectrum for compound **3**.

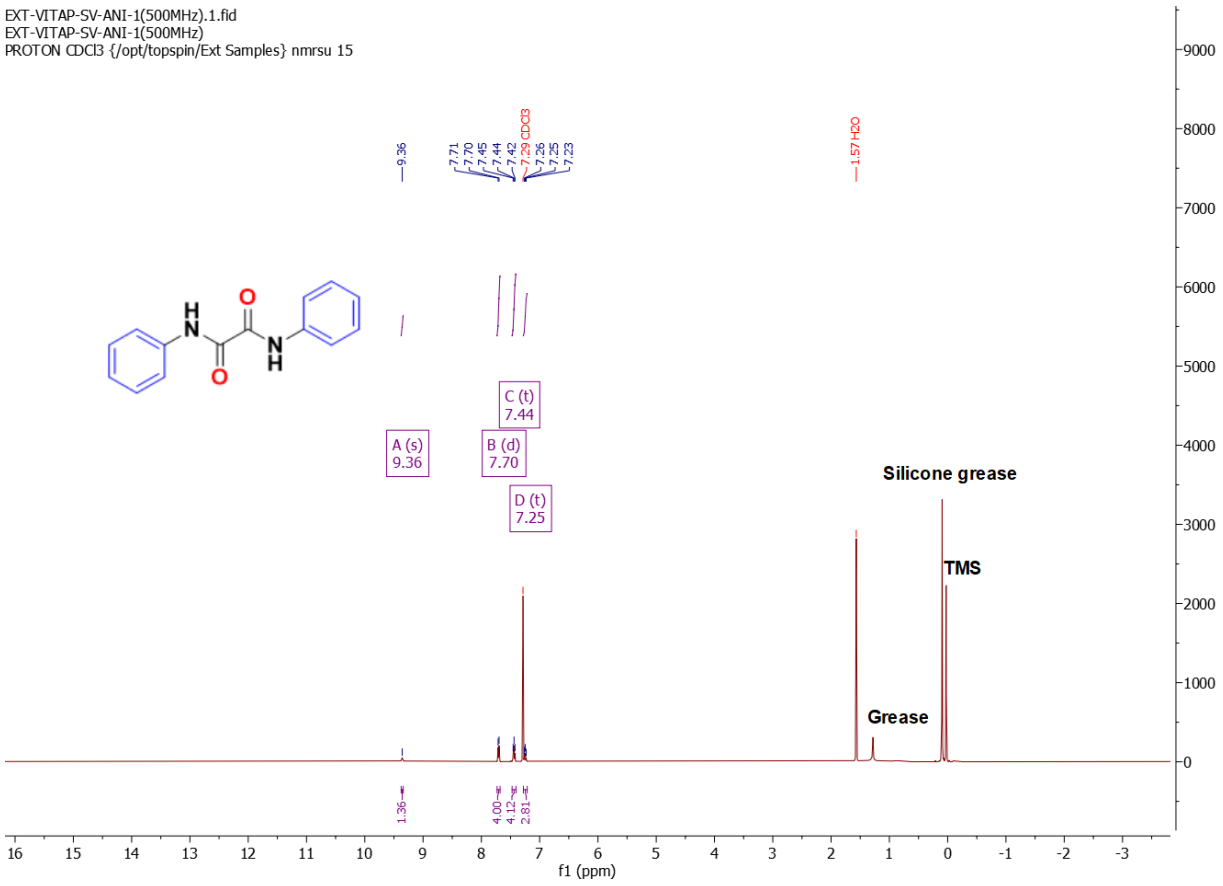


Figure S8. ^{1}H NMR spectral studies for compound **3**.

3. Spectrometric characterization of products obtained from the reaction of *o*-anisidine with SeO_2

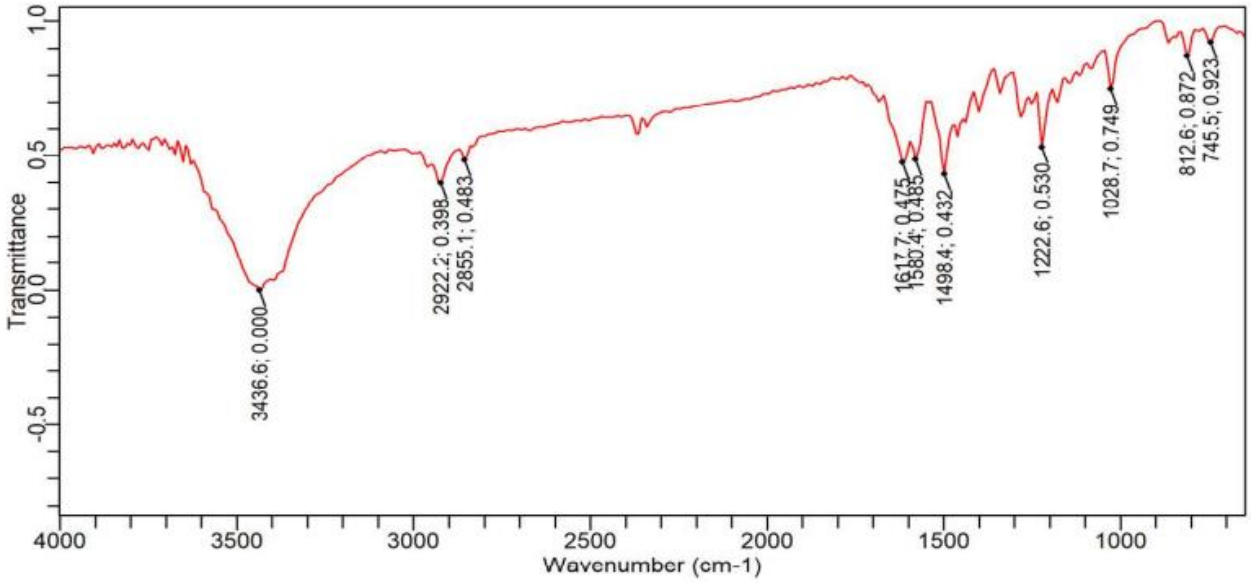


Figure S9. FTIR(KBr) spectrum for mixture of compounds **4**–**8**.

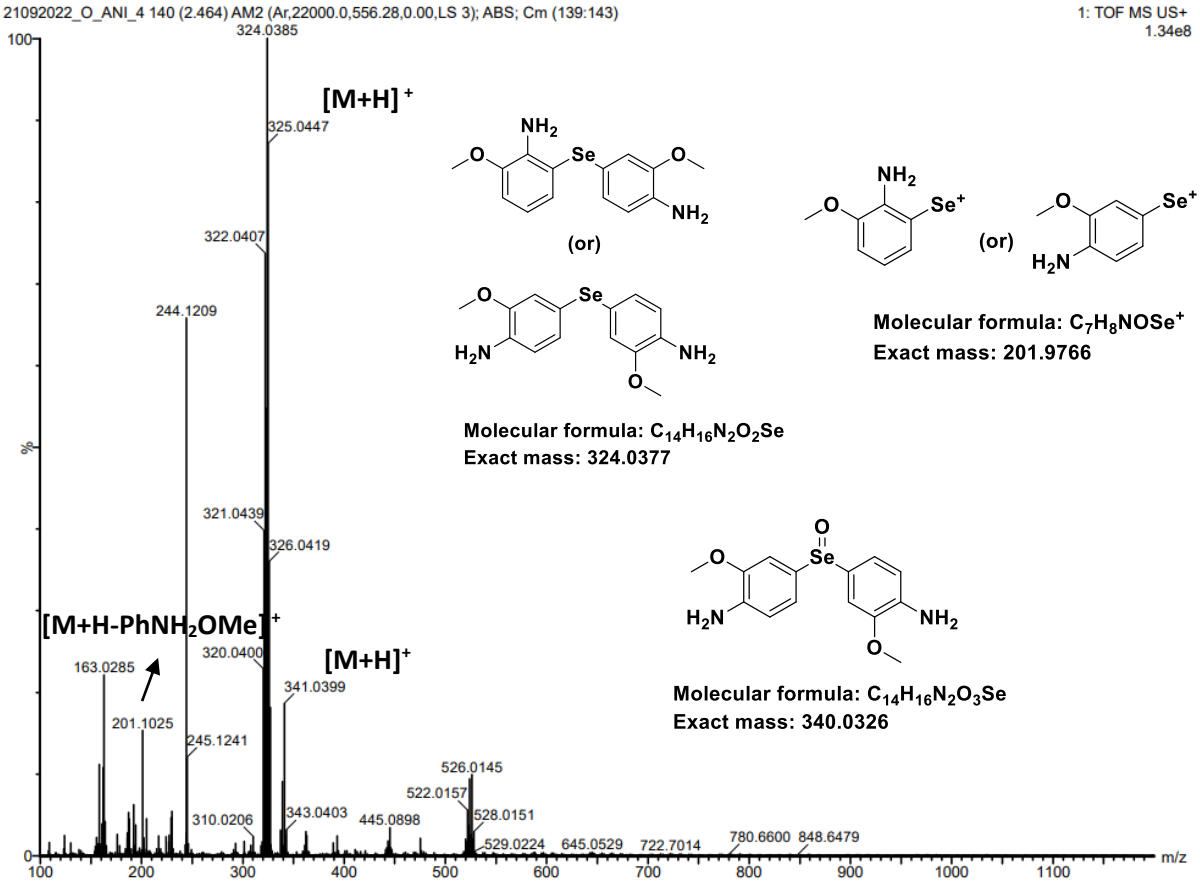


Figure S10. HRMS–ESI spectrum for mixture of compounds **4**–**8**.

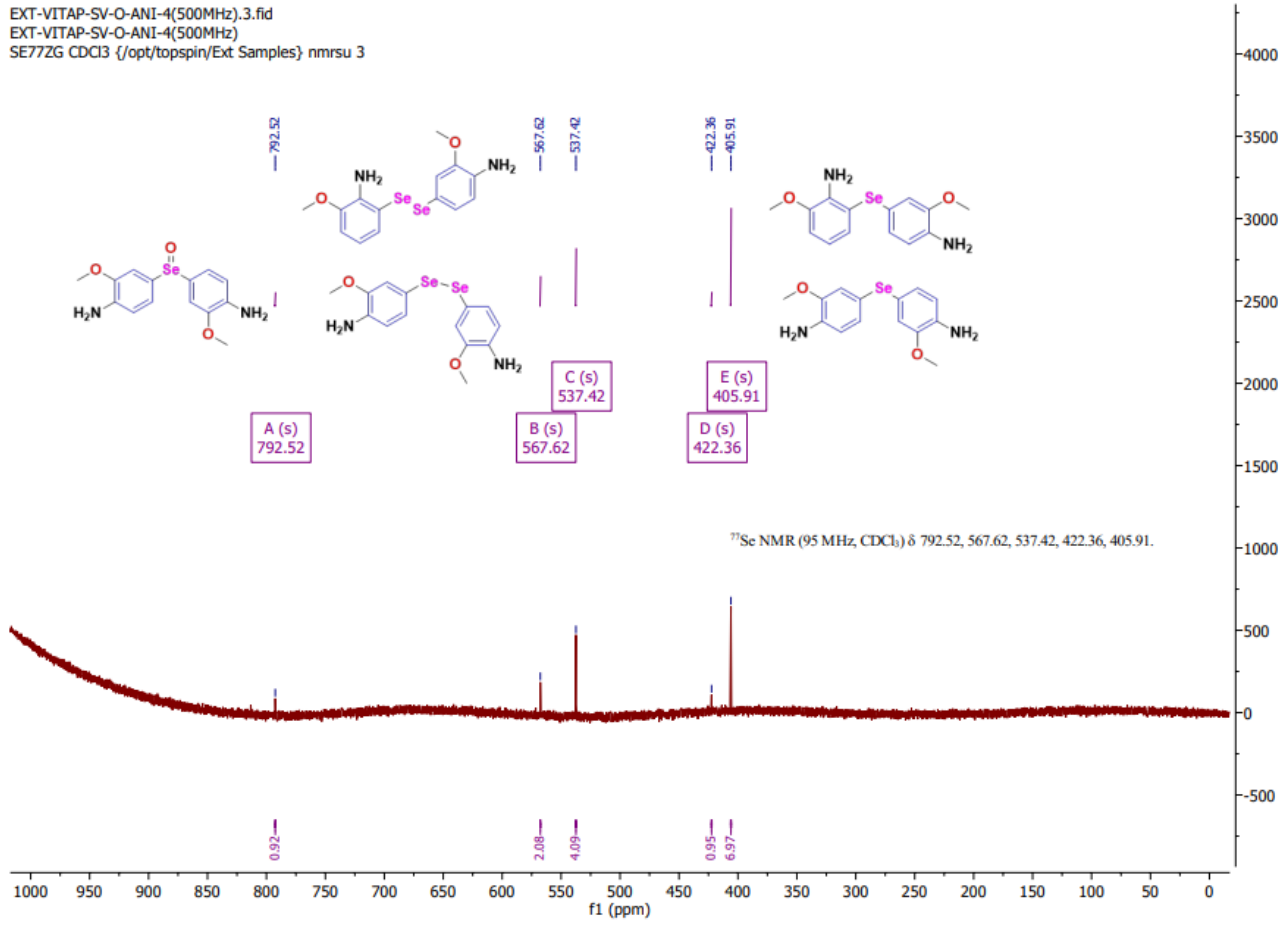


Figure S11. ^{77}Se NMR spectral studies for mixture of compounds **4**–**8**.

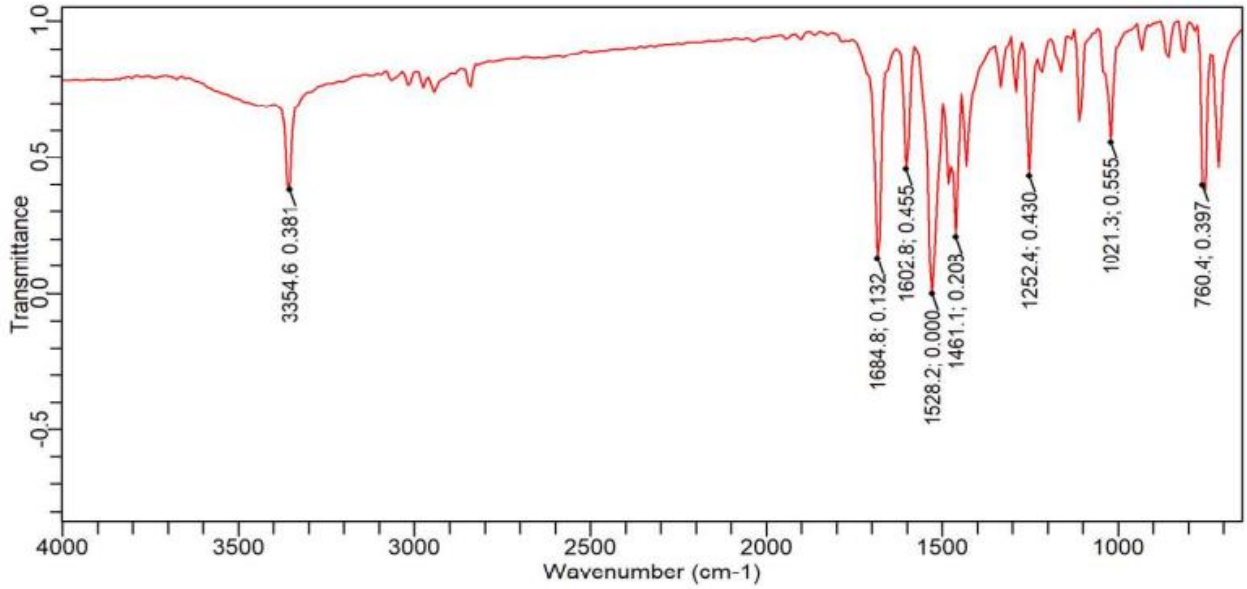


Figure S12. FTIR(KBr) spectrum for compound **9**.

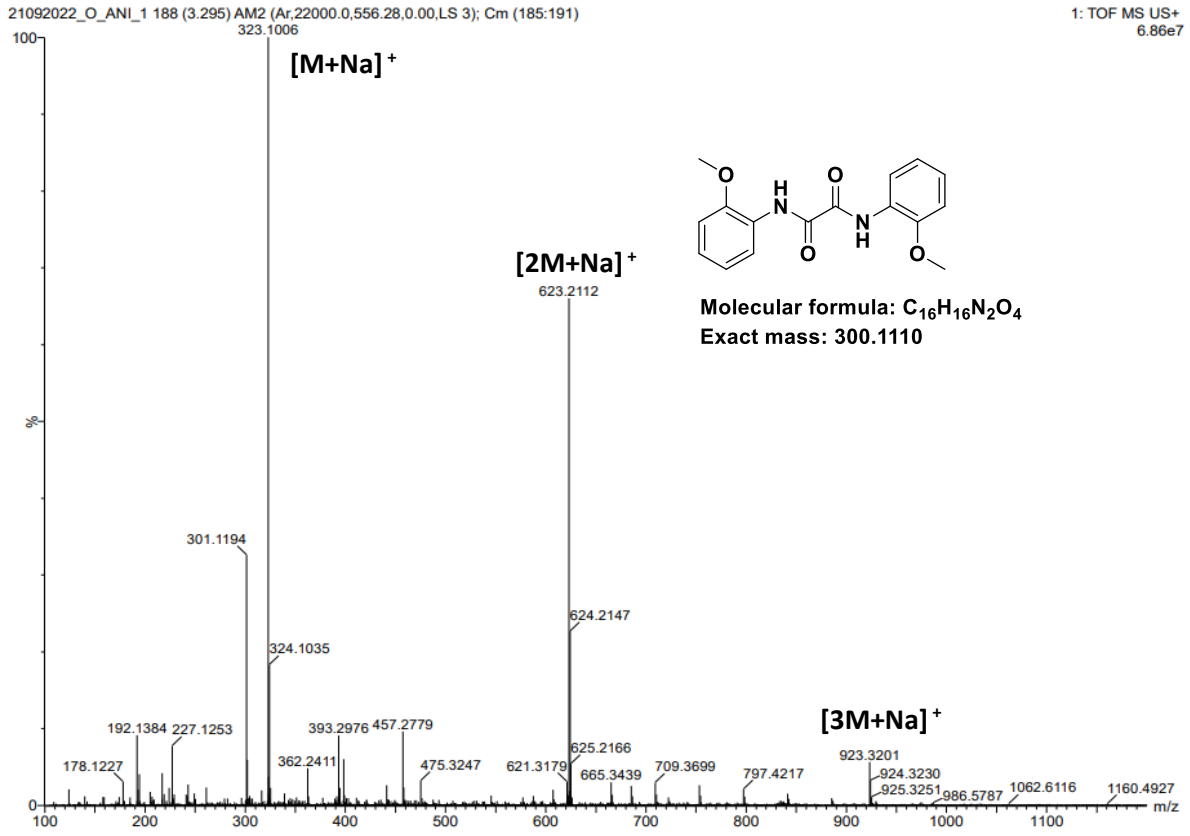


Figure S13. HRMS–ESI spectrum for compound **9**.

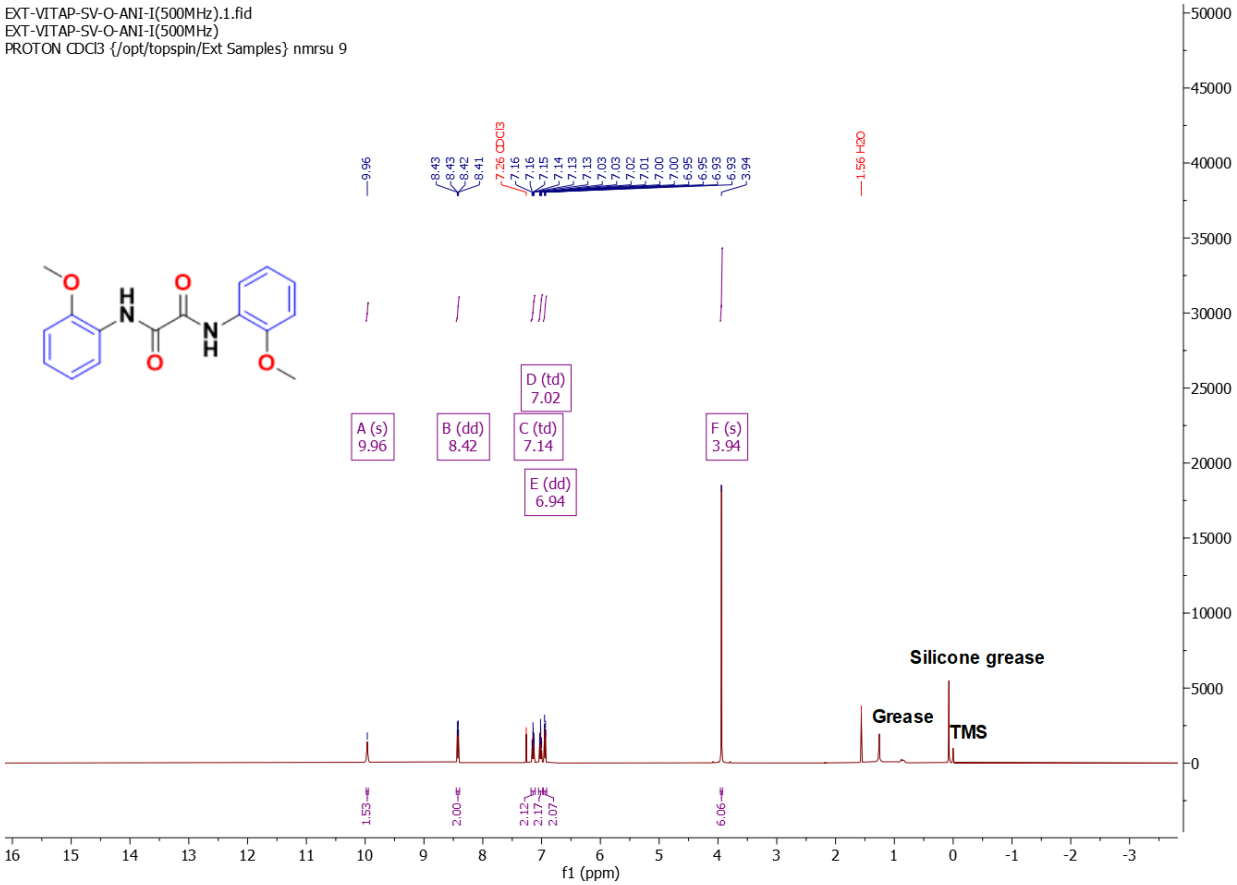


Figure S14. ^{1}H NMR spectral studies for compound **9**.

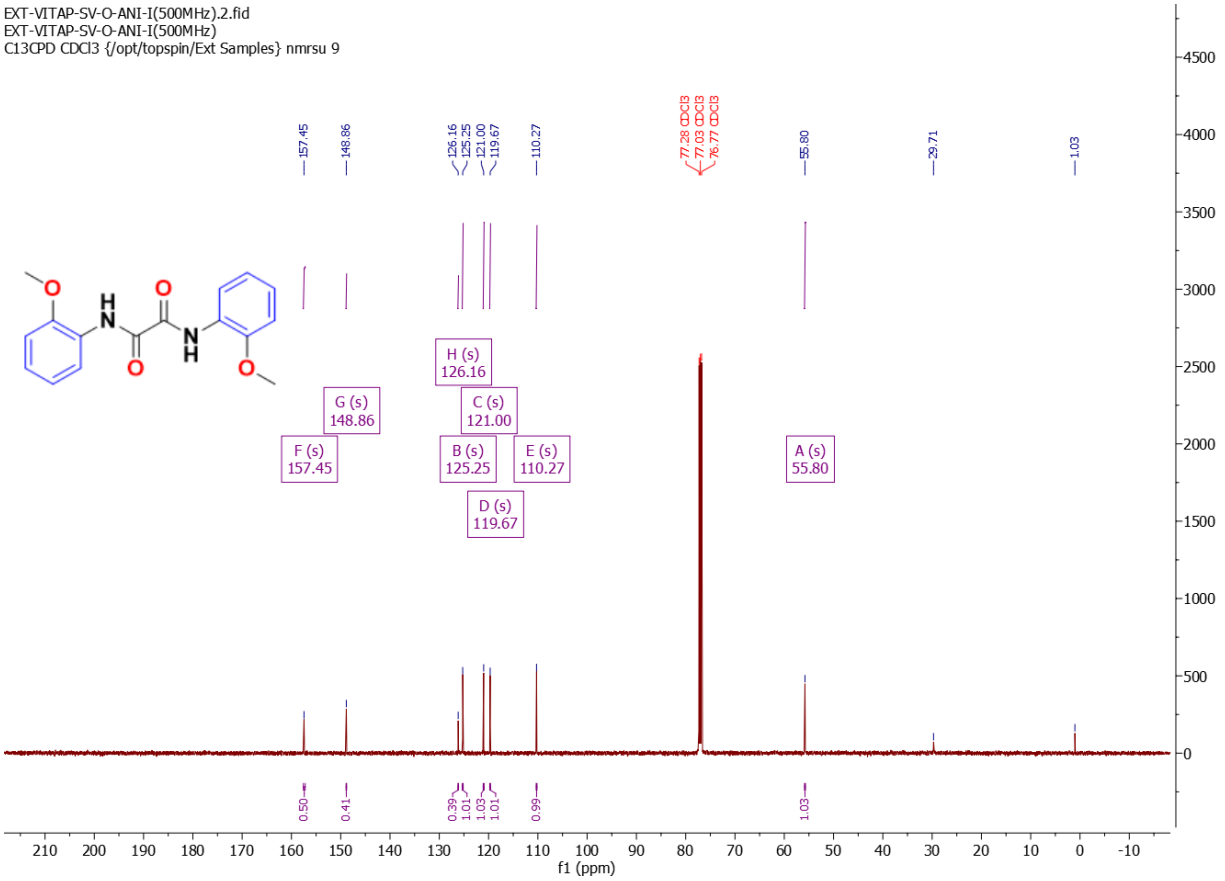


Figure S15. ^{13}C NMR spectral studies for compound **9**.

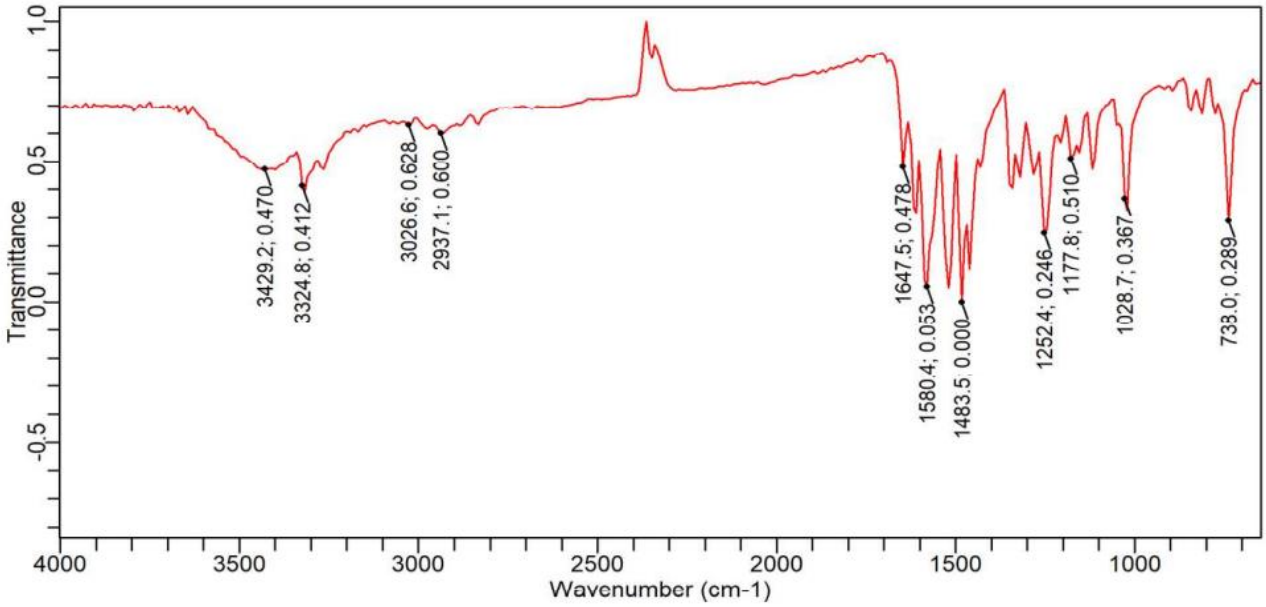


Figure S16. FTIR(KBr) spectrum for compound **10**.

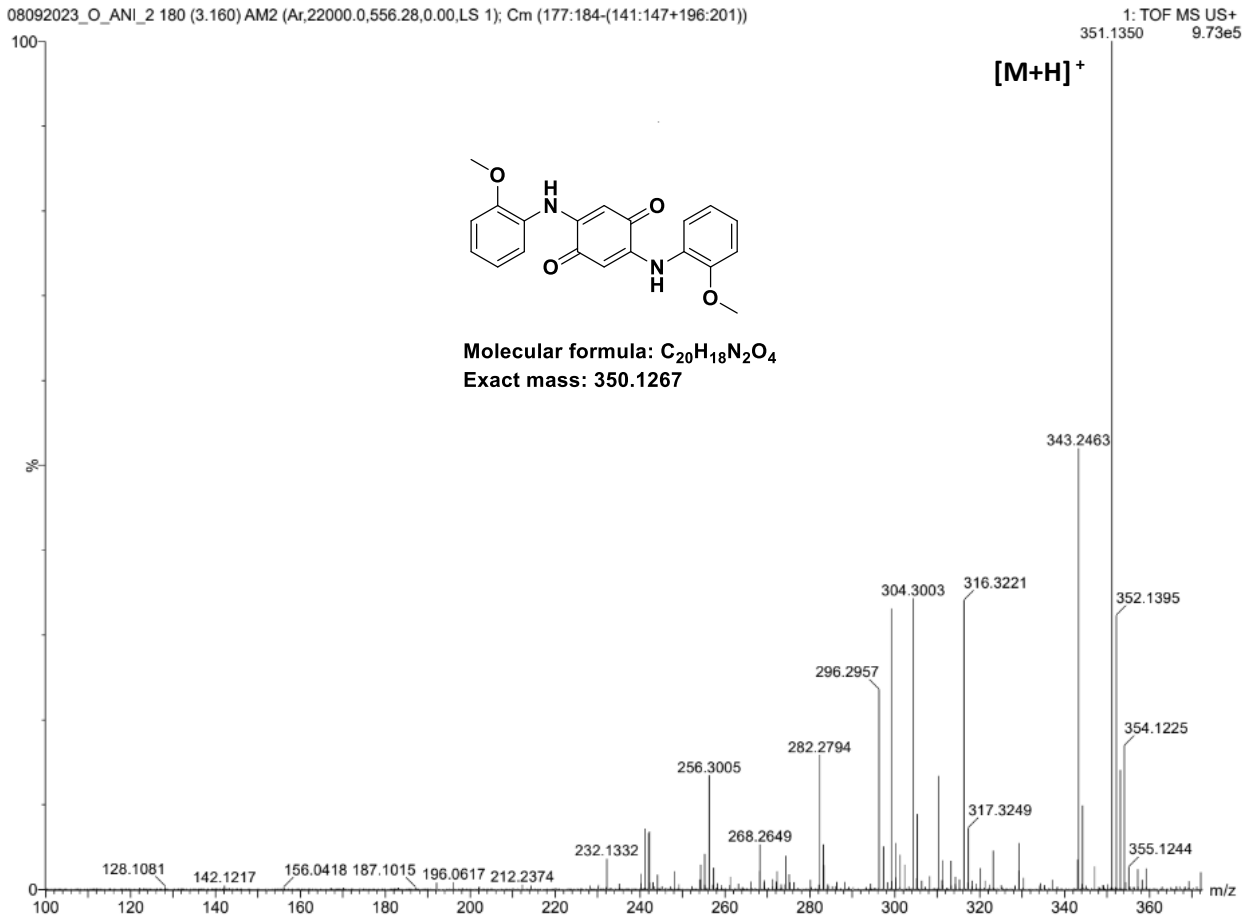


Figure S17. HRMS–ESI spectrum for compound **10**.

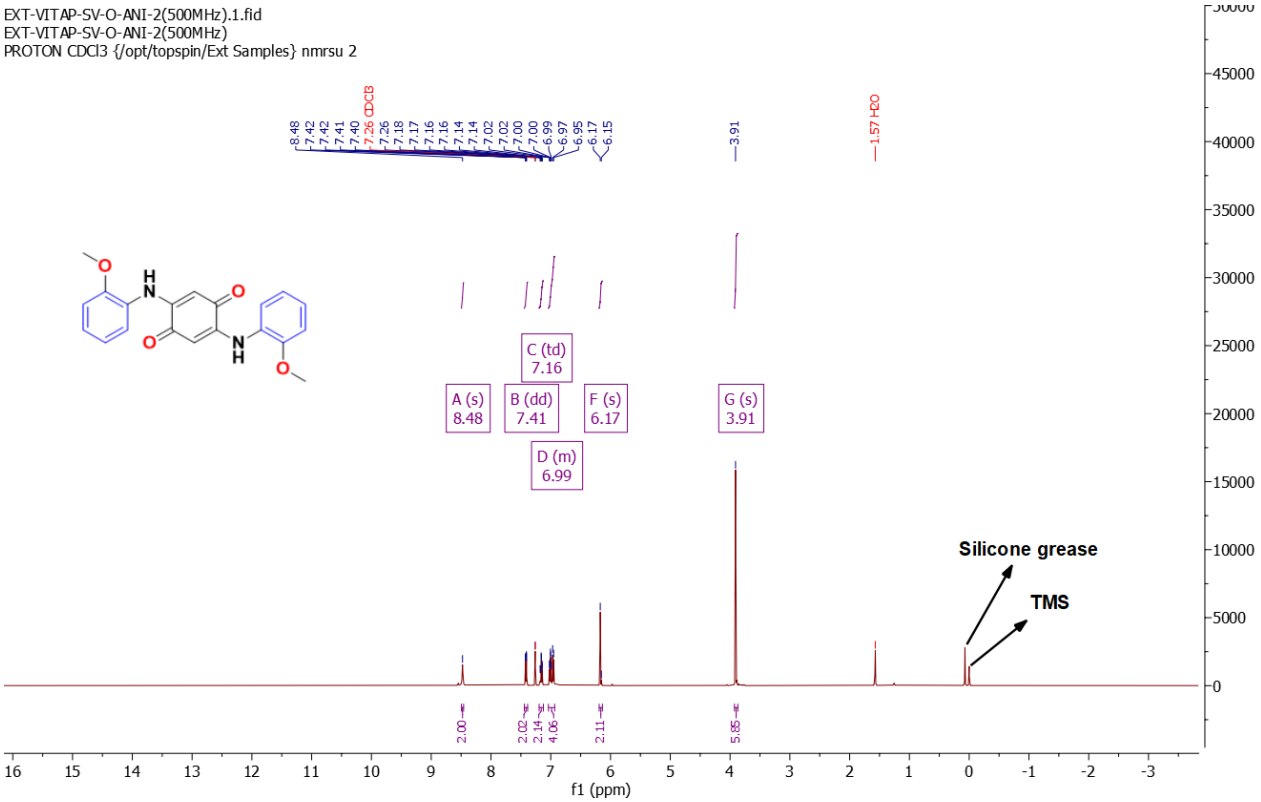


Figure S18. ^{1}H NMR spectral studies for compound **10**,

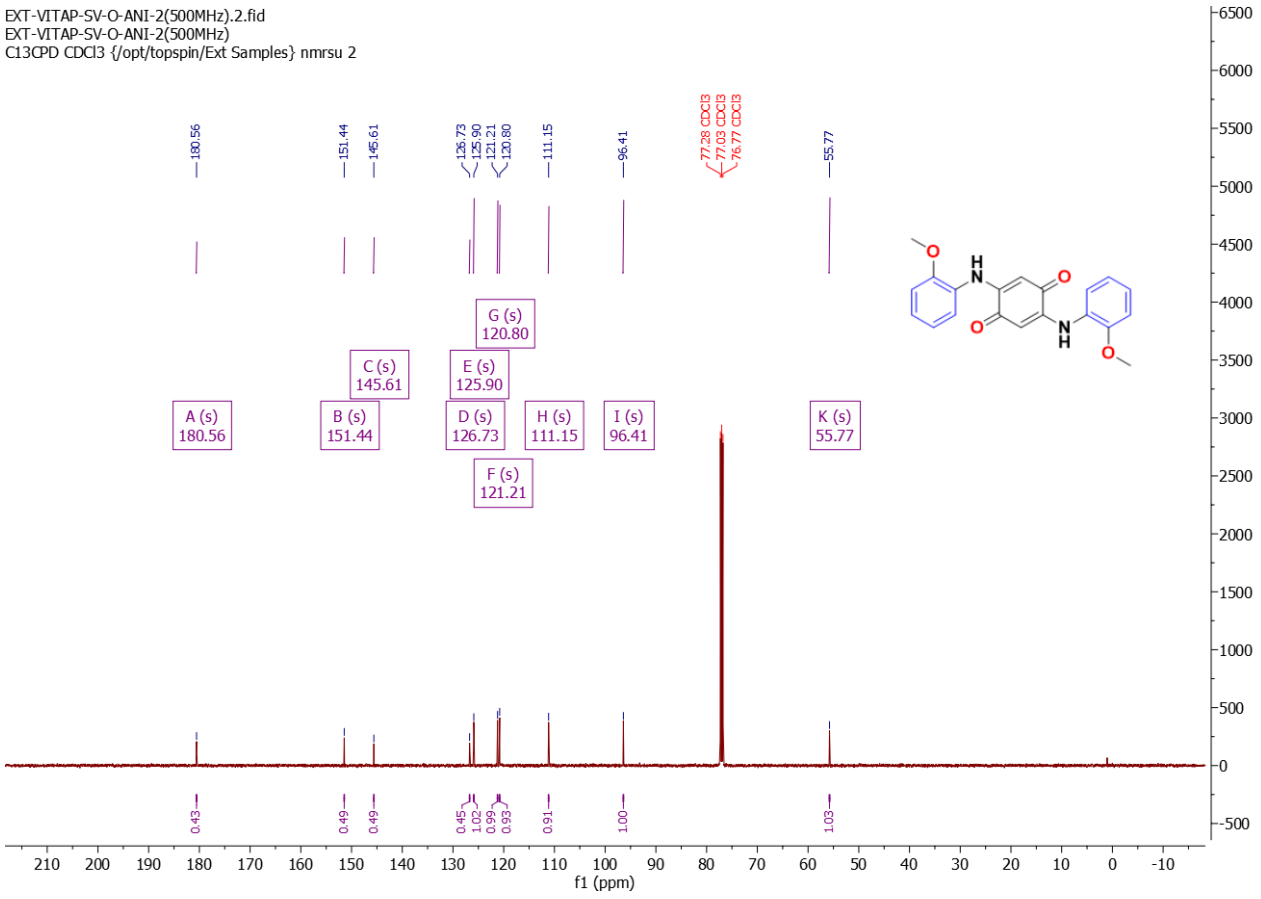


Figure S19. ^{13}C NMR spectral studies for compound **10**.

4. Spectrometric characterization of products obtained from the reaction of methyl anthranilate with SeO_2

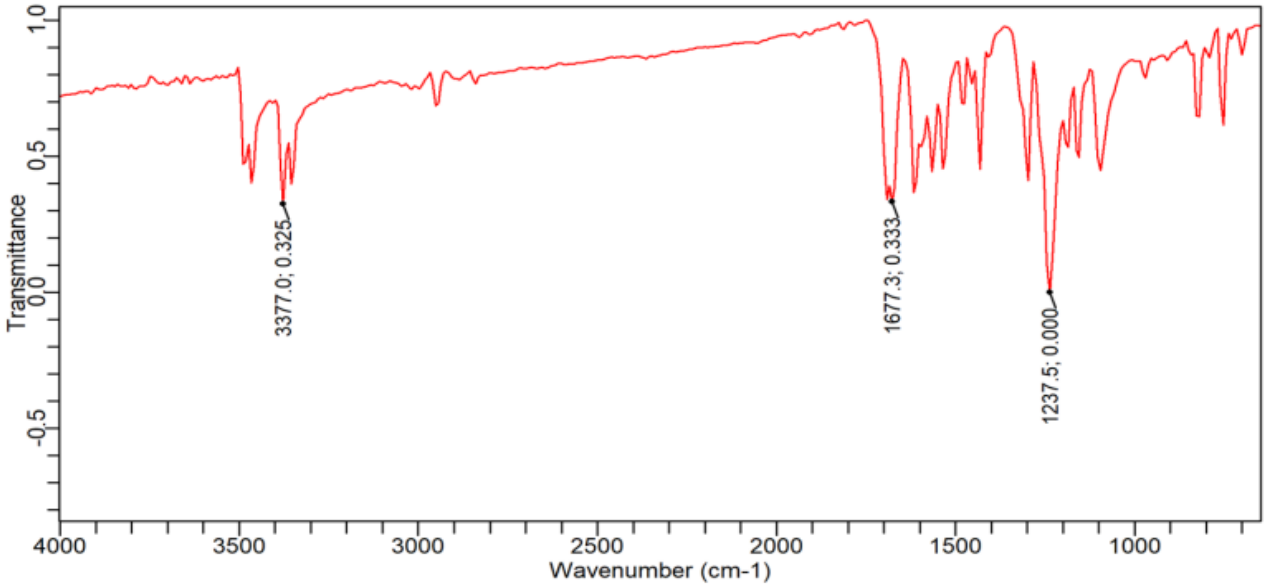


Figure S20. FTIR(KBr) spectrum for compound **11**.

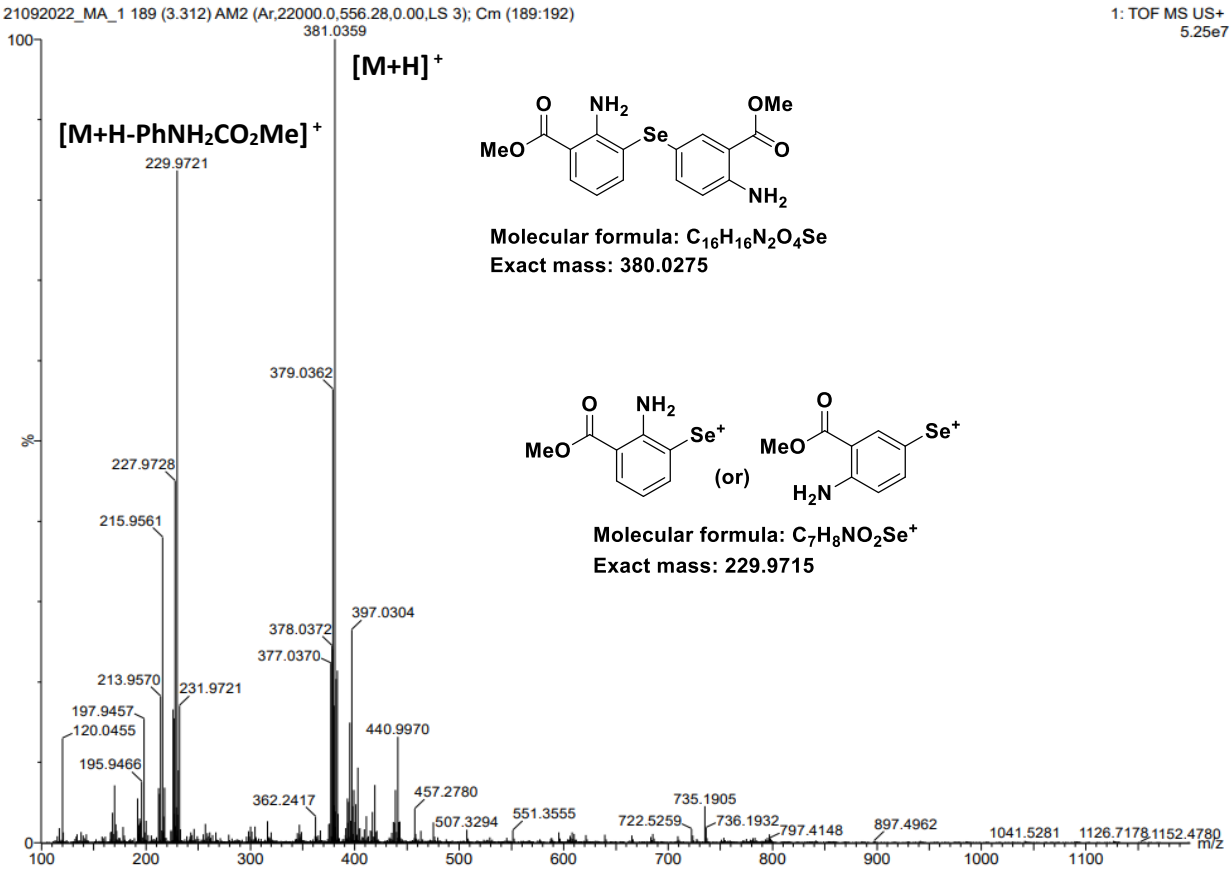
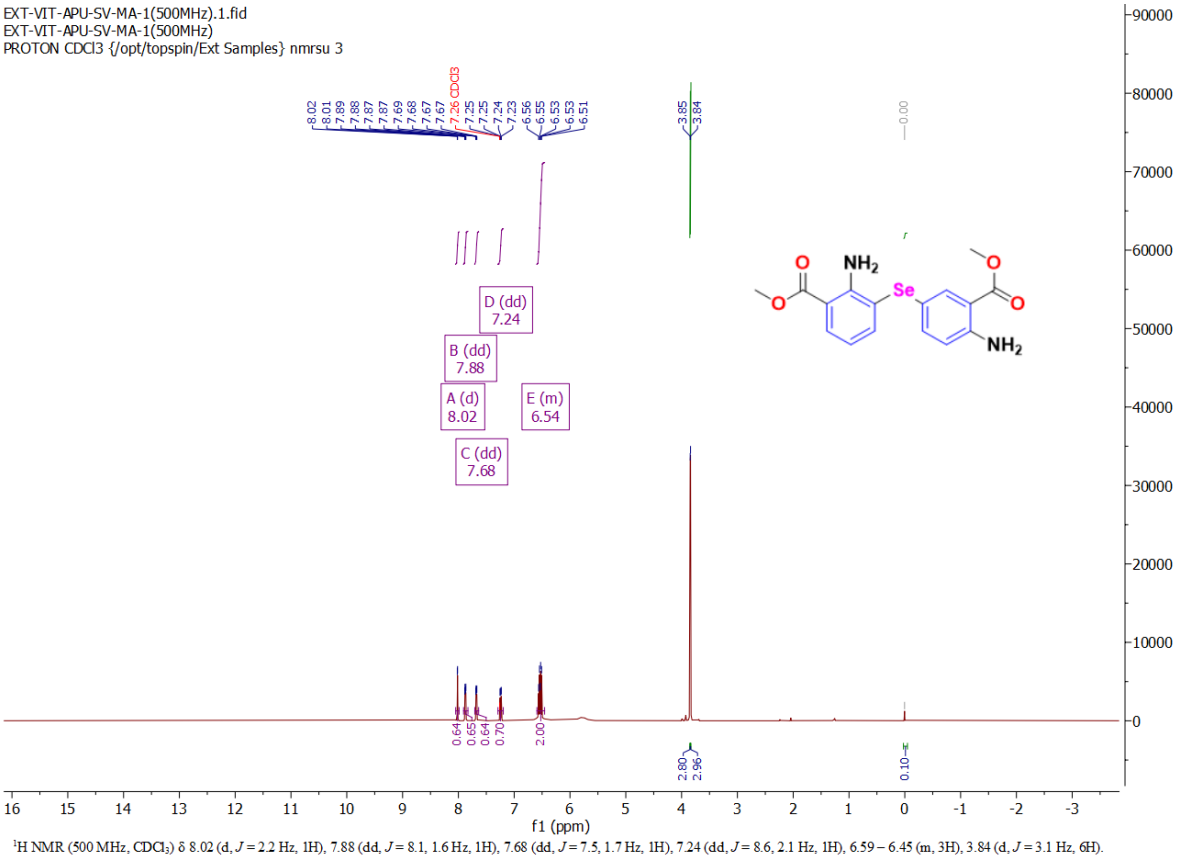


Figure S21. HRMS–ESI spectrum for compound **11**.



^{1}H NMR (500 MHz, $CDCl_3$) δ 8.02 (d, J = 2.2 Hz, 1H), 7.88 (dd, J = 8.1, 1.6 Hz, 1H), 7.68 (dd, J = 7.5, 1.7 Hz, 1H), 7.24 (dd, J = 8.6, 2.1 Hz, 1H), 6.59 – 6.45 (m, 3H), 3.84 (d, J = 3.1 Hz, 6H).

Figure S22. ^{1}H NMR spectral studies for compound **11**.

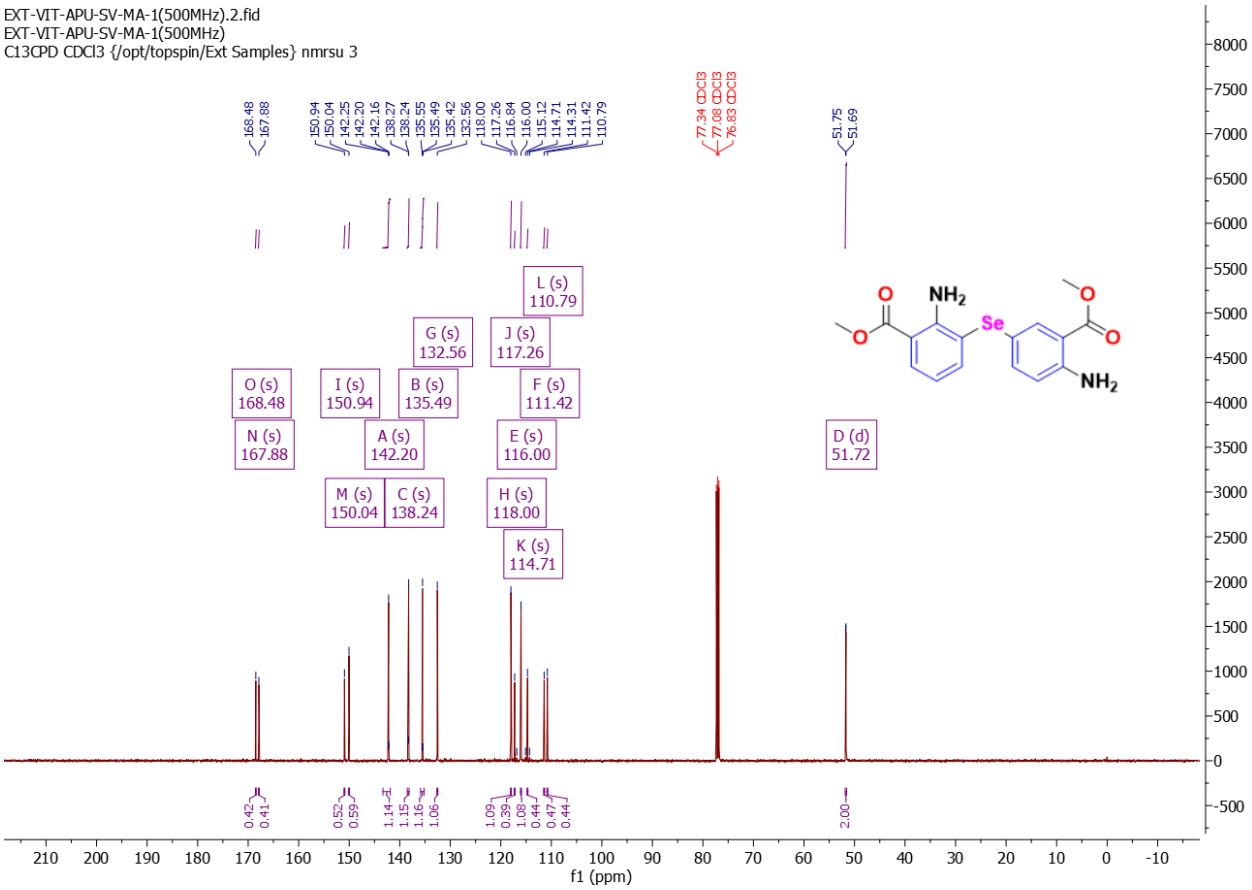


Figure S23. ^{13}C NMR spectral studies for compound **11**.

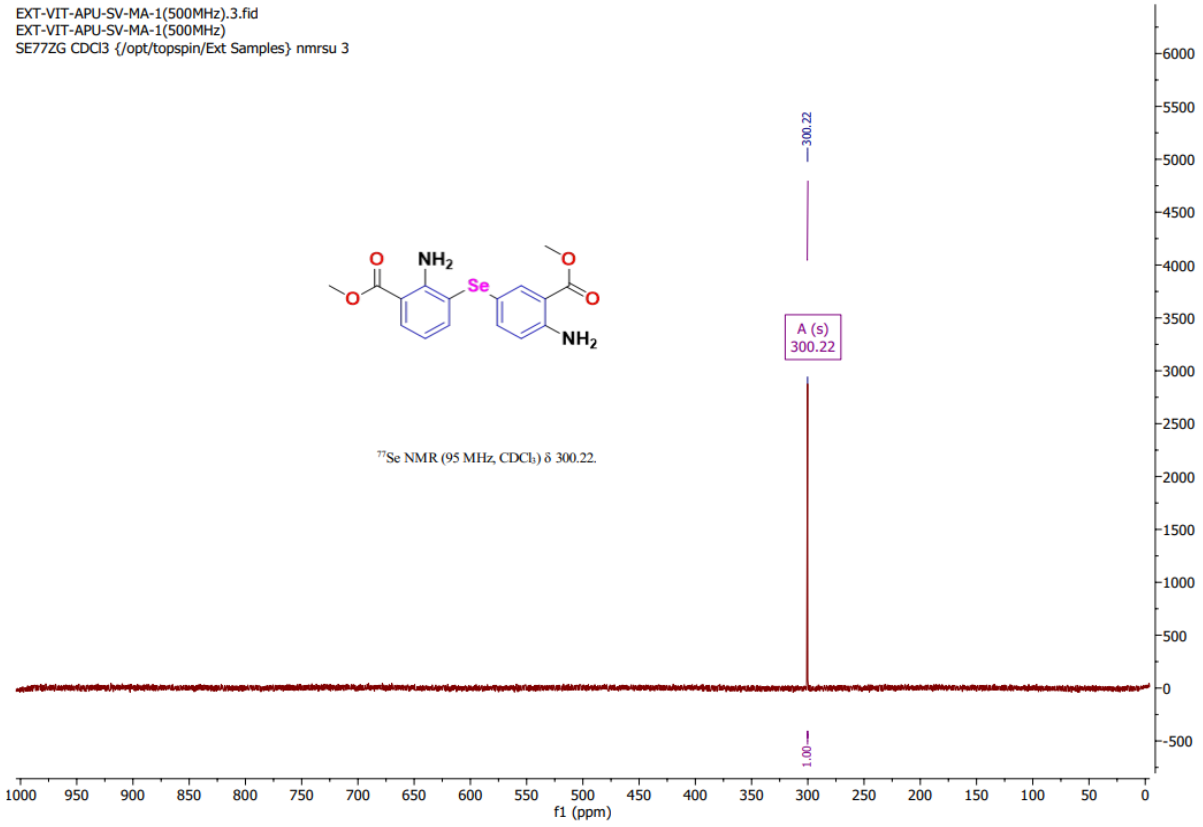


Figure S24. ^{77}Se NMR spectral studies for compound **11**.

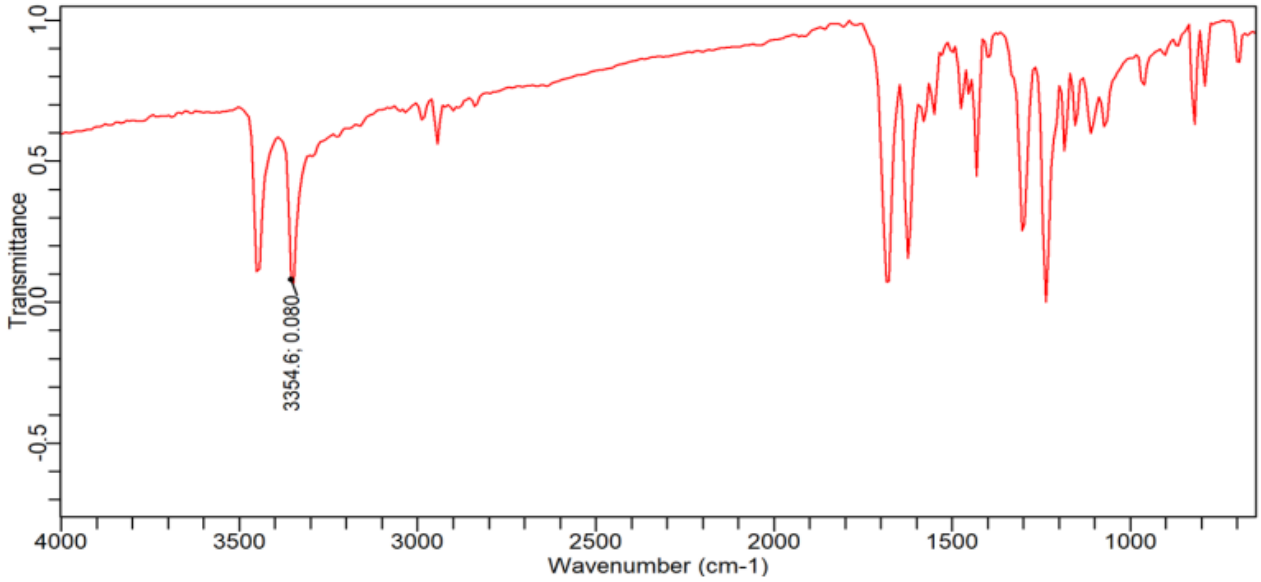


Figure S25. FTIR(KBr) spectrum for compound **12**.

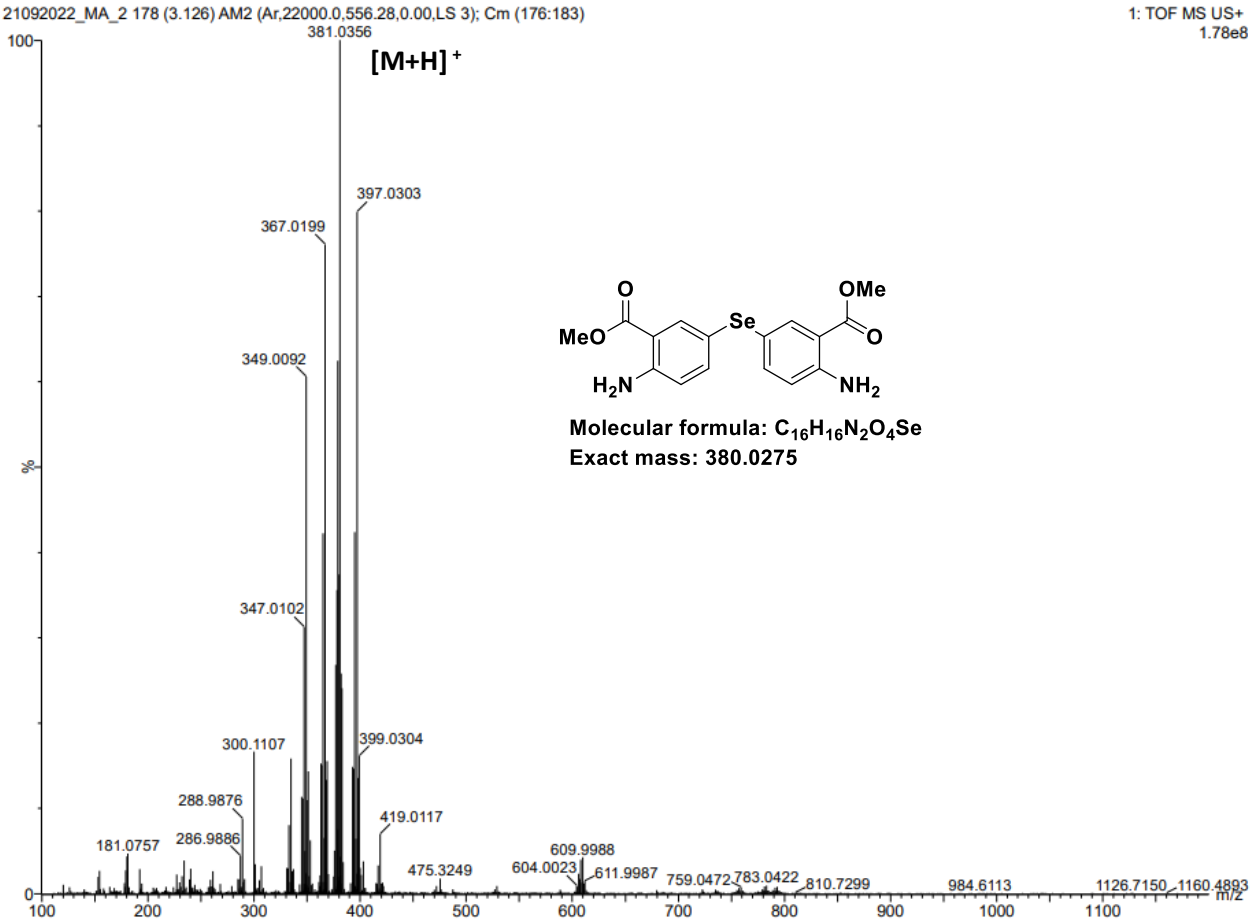
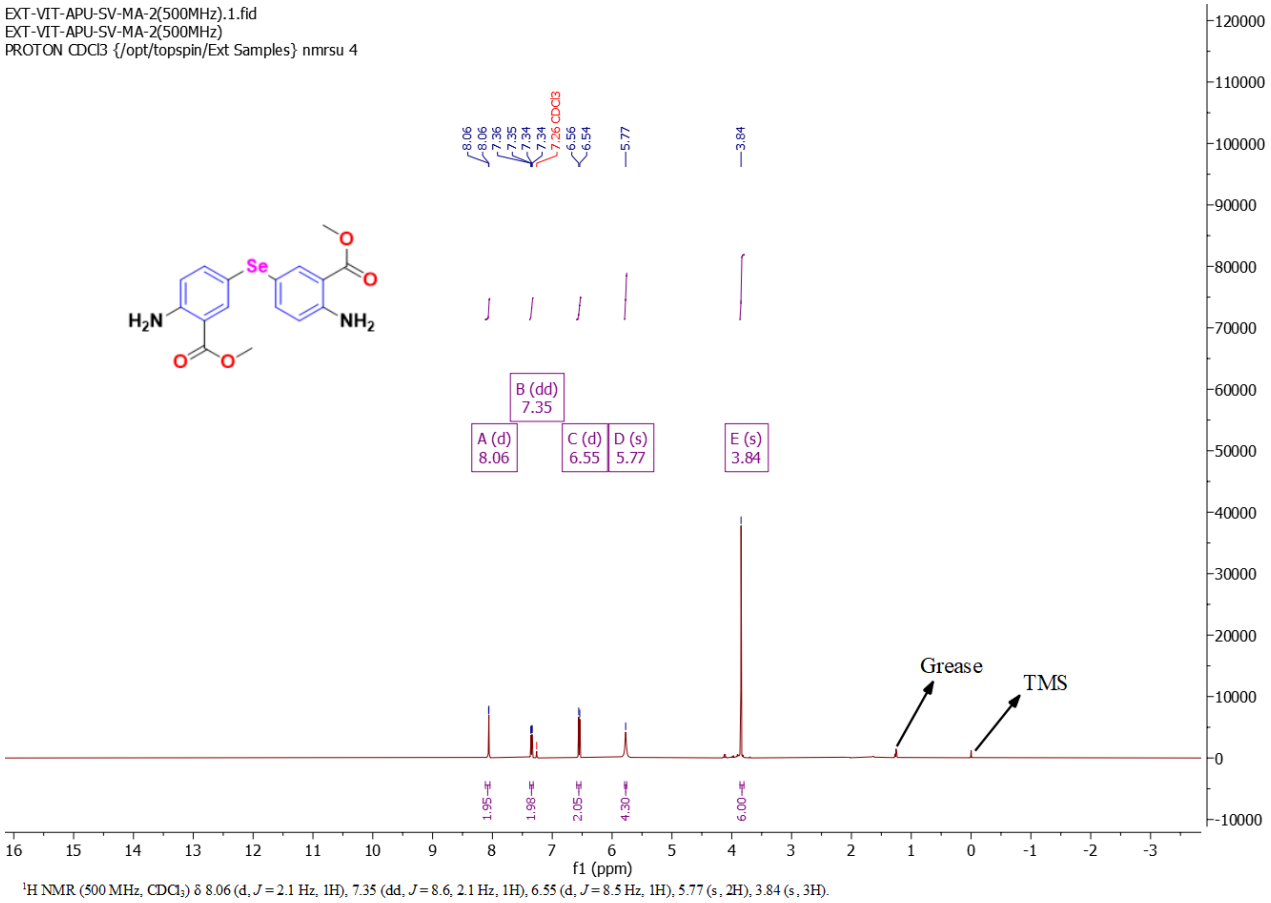


Figure S26. HRMS–ESI spectrum for compound **12**.



^{1}H NMR (500 MHz, $CDCl_3$) δ 8.06 (d, J = 2.1 Hz, 1H), 7.35 (dd, J = 8.6, 2.1 Hz, 1H), 6.55 (d, J = 8.5 Hz, 1H), 5.77 (s, 2H), 3.84 (s, 3H).

Figure S27. ^{1}H NMR spectral studies for compound **12**.

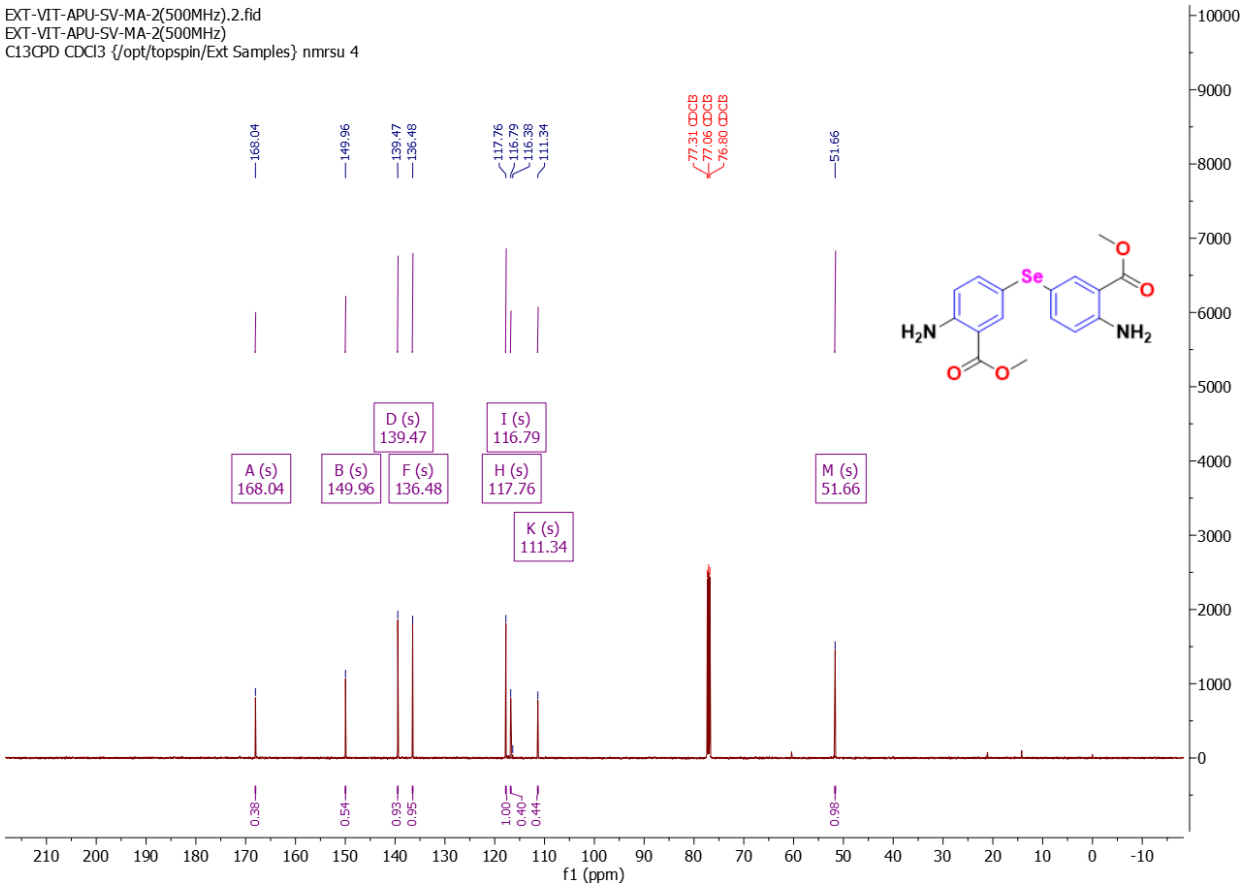


Figure S28. ^{13}C NMR spectral studies for compound **12**.

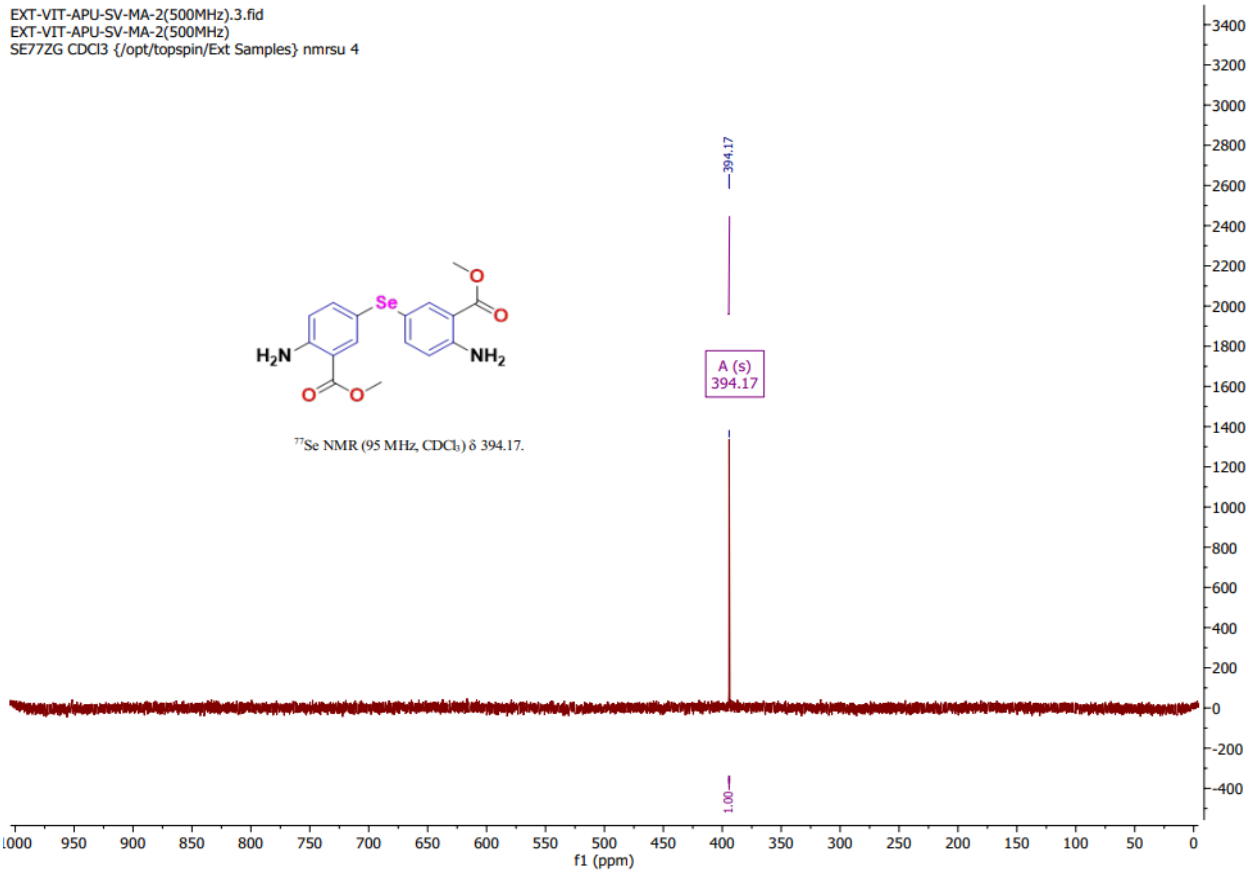


Figure S29. ^{77}Se NMR spectral studies for compound **12**.

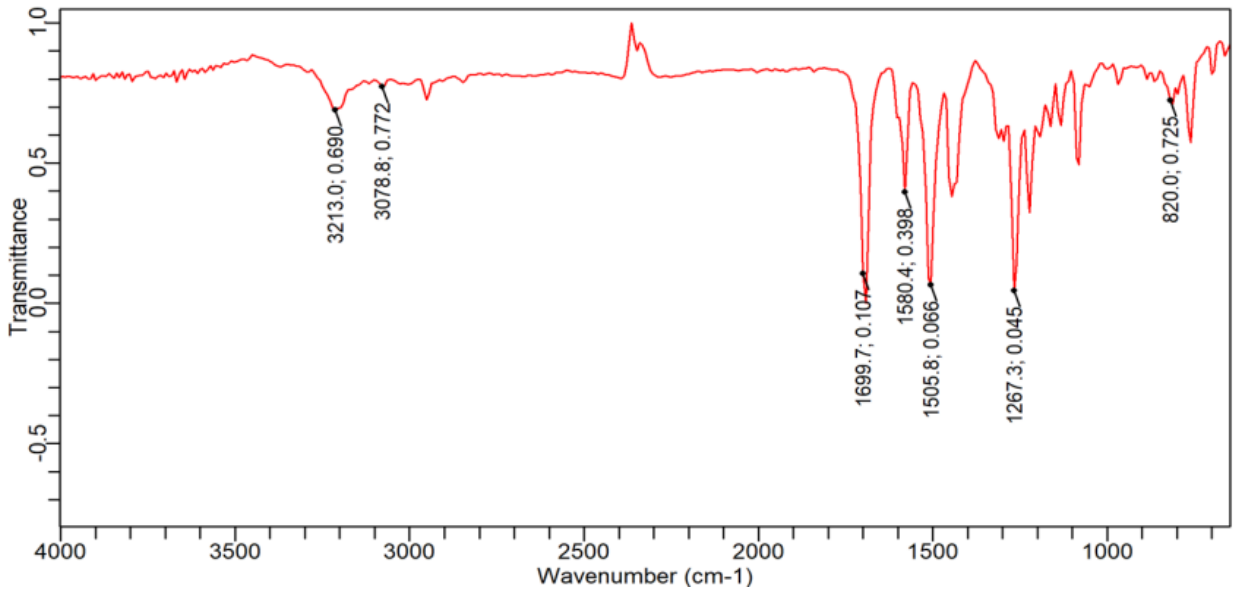


Figure S30. FTIR(KBr) spectrum for compound **13**.

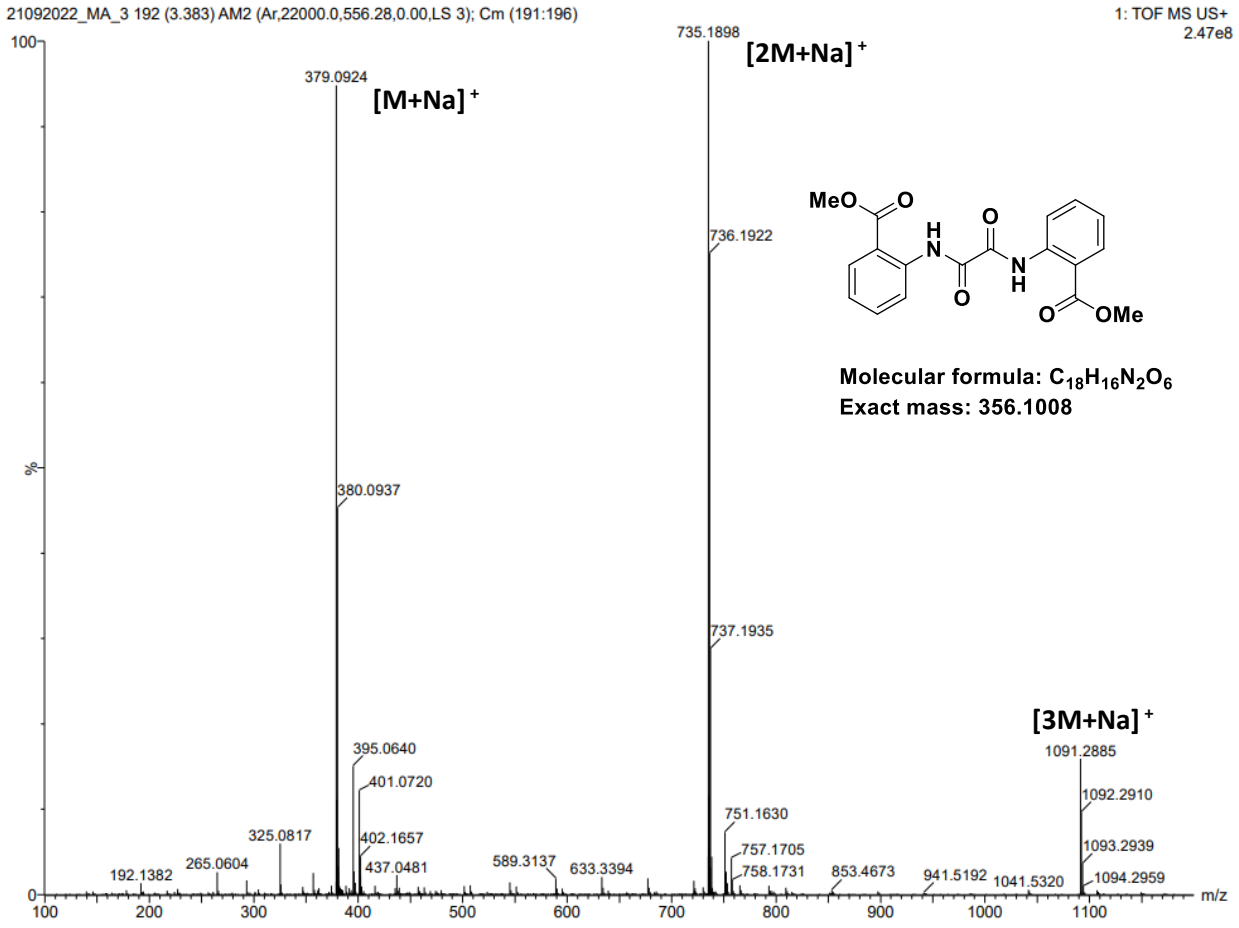


Figure S31. HRMS–ESI spectrum for compound **13**.

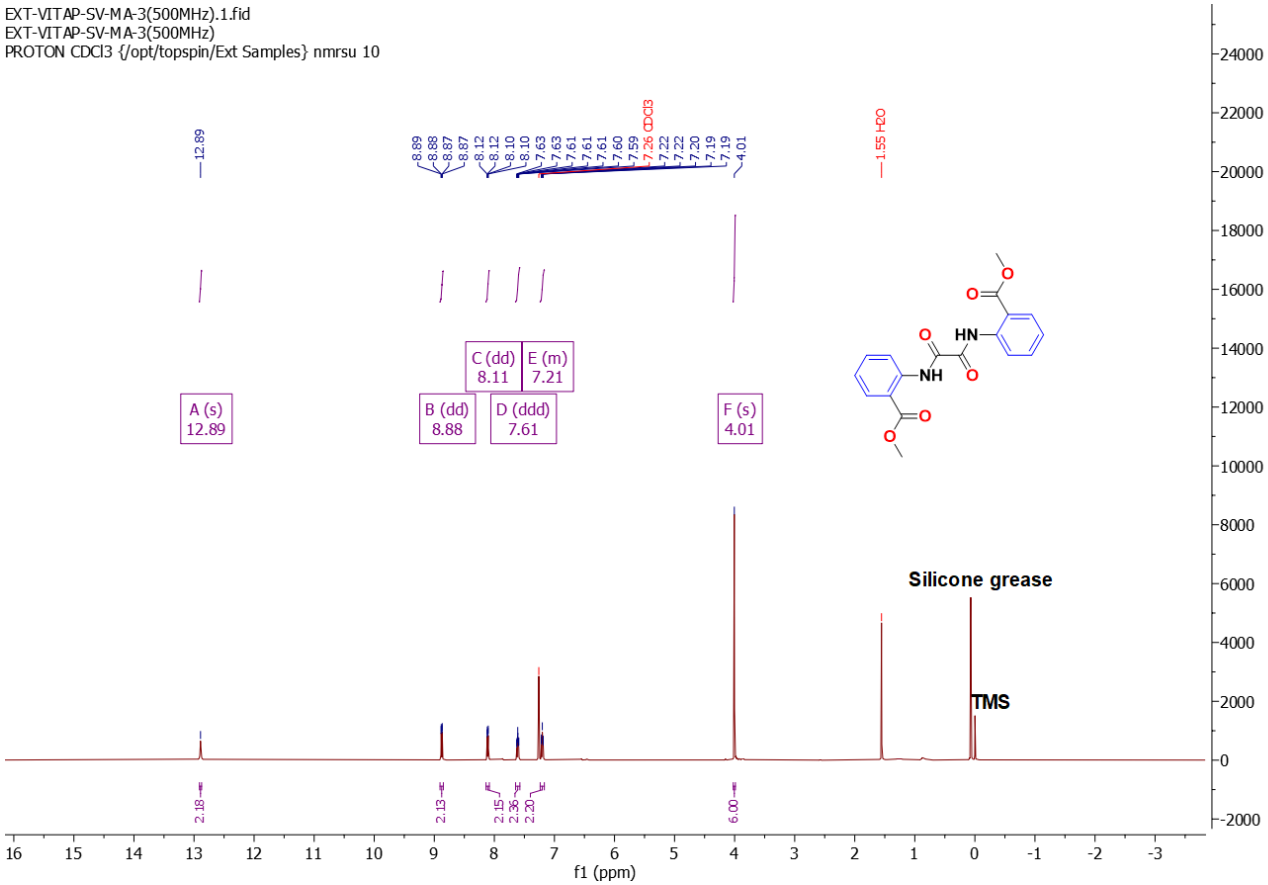


Figure S32. ^{1}H NMR spectral studies for compound **13**.

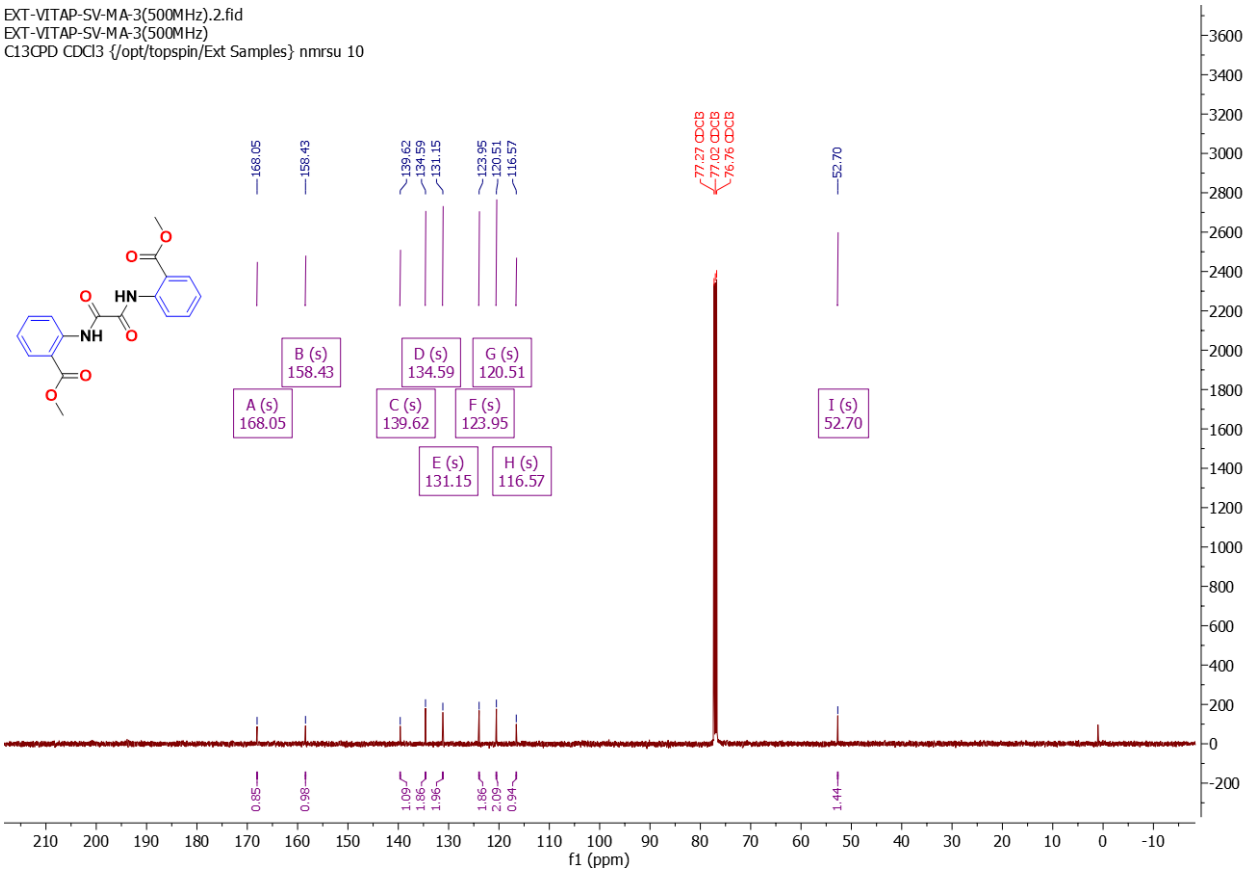


Figure S33. ^{13}C NMR spectral studies for compound **13**.

5. Relative color change upon addition of SeO_2 to arylamines in acetonitrile

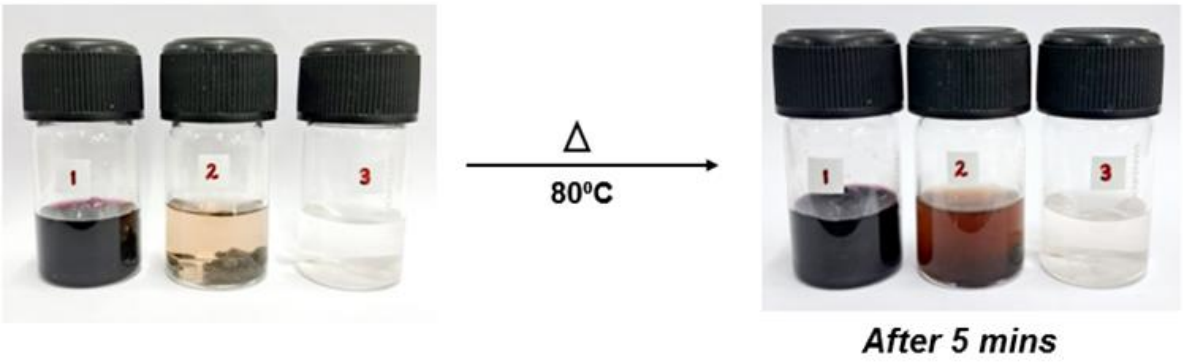


Figure S34: Relative color change upon addition of SeO_2 to arylamines in acetonitrile: vial 1: *o*-anisidine, vial 2: aniline, vial 3: methyl anthranilate.

6. Packing arrangement for compounds 3 and 9

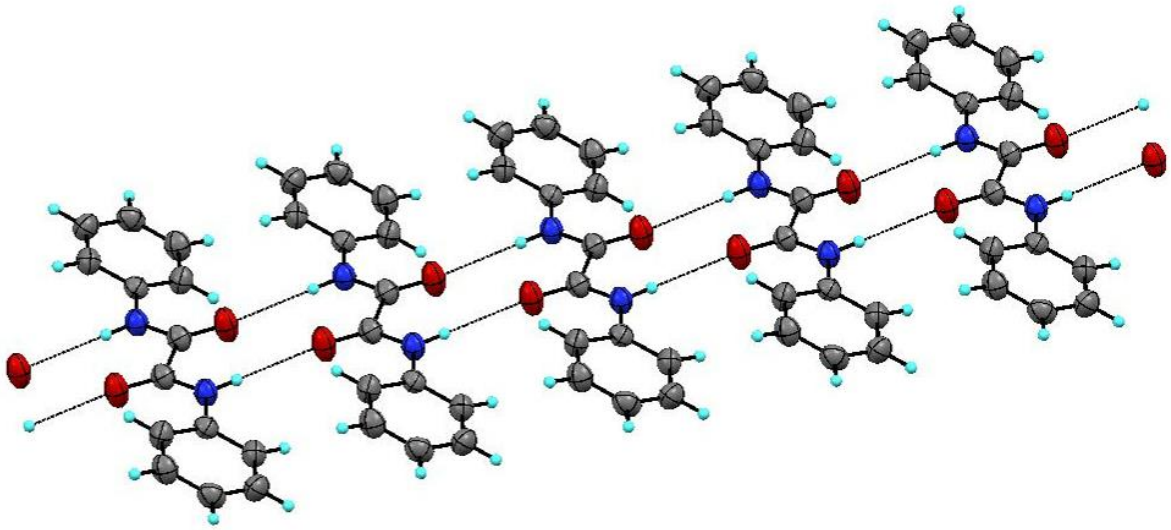


Figure S35. Packing arrangement for compound **3**.

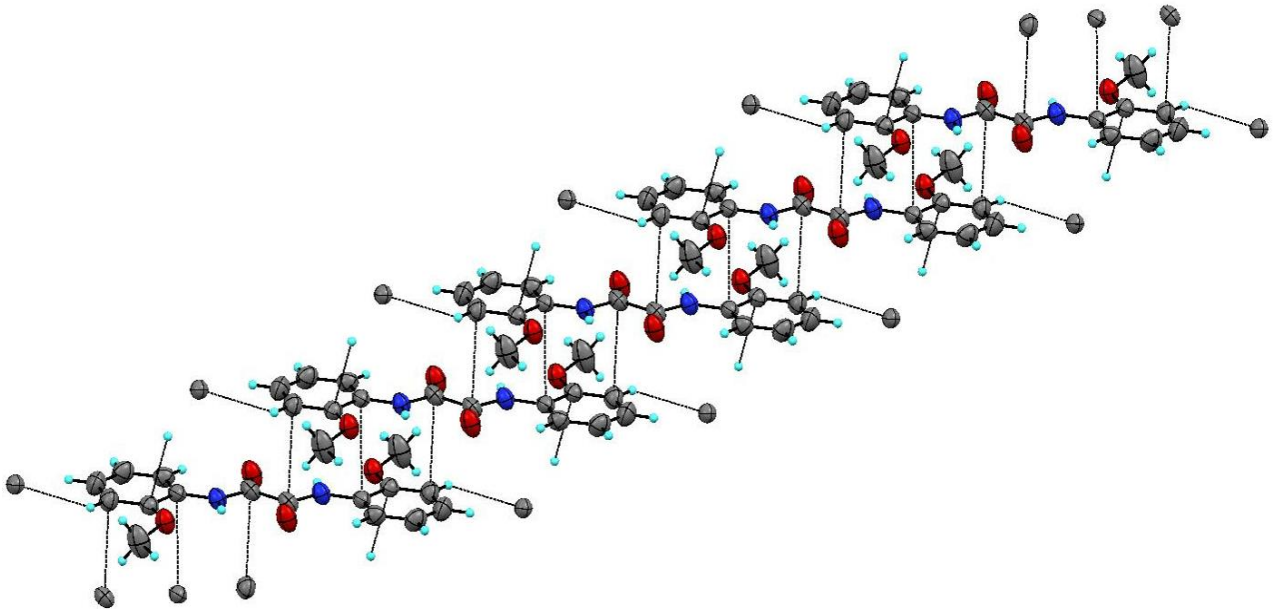


Figure S36. Packing arrangement for compound **9**.

7. Packing arrangement for compounds 13 and 10

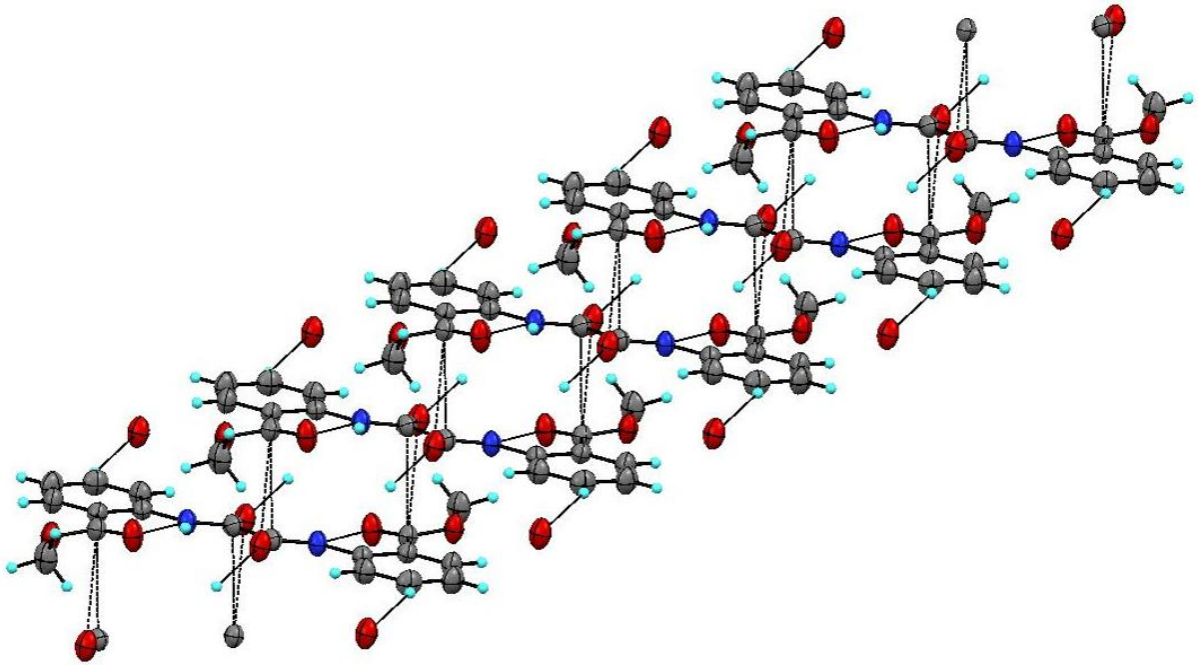


Figure S37. Packing arrangement for compound **13**.

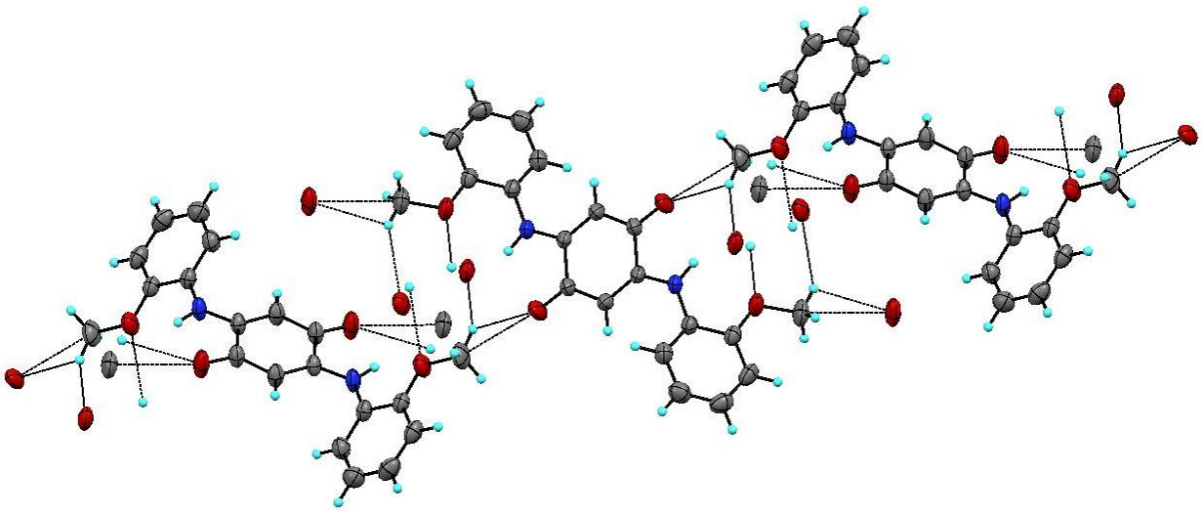


Figure S38. Packing arrangement for compound **10**.

8. Packing arrangement for compound 11

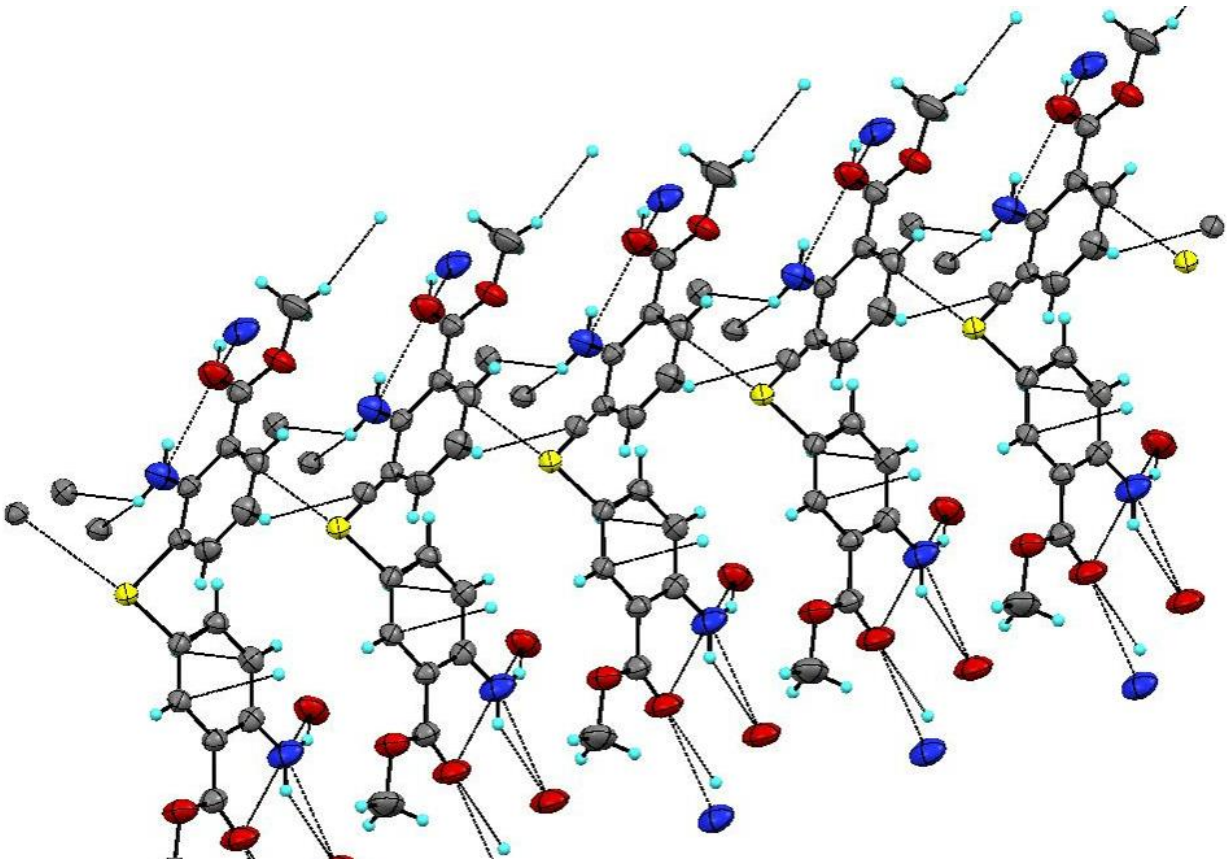


Figure S39. Packing arrangement for compound **11**.

9. Packing arrangement for compound 12

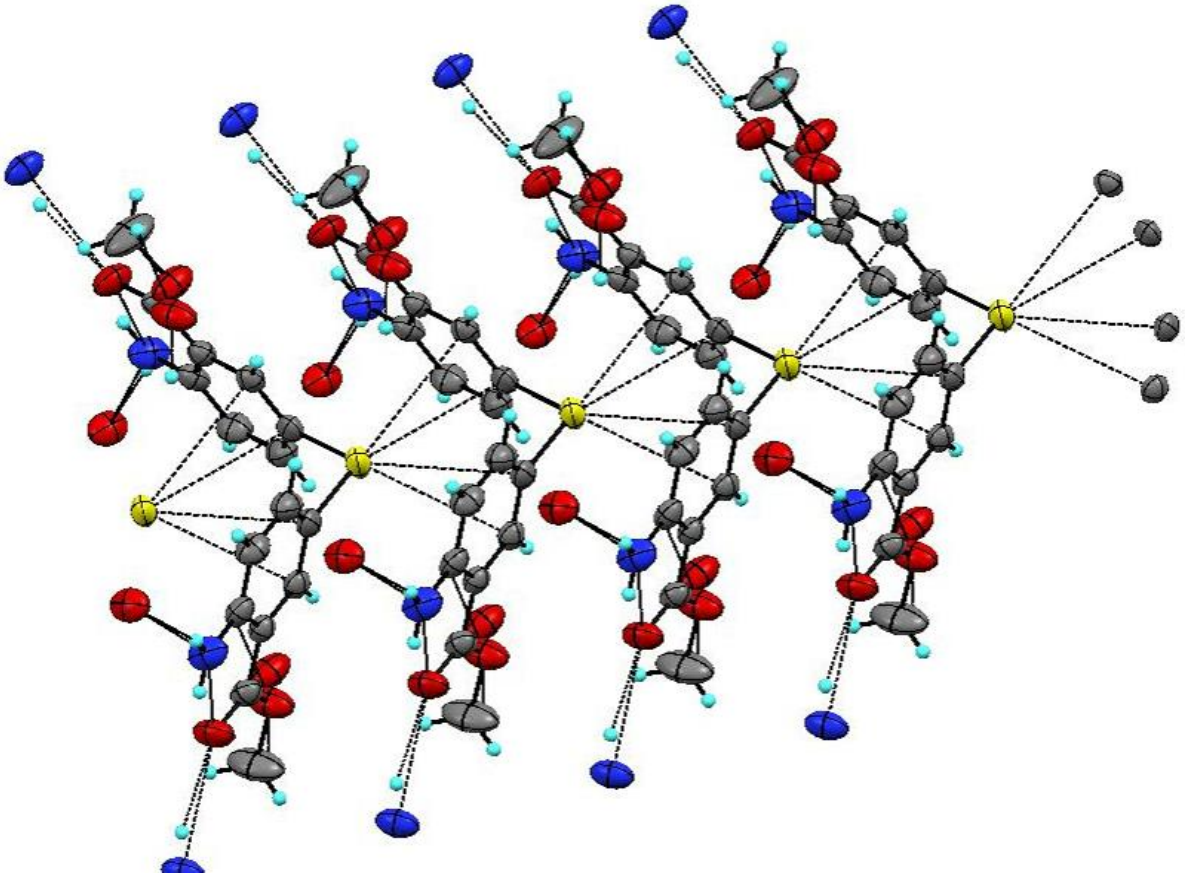
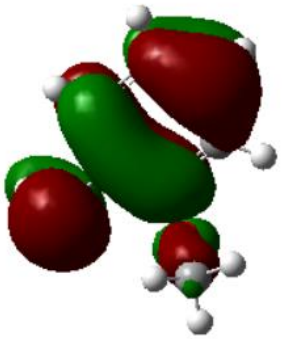
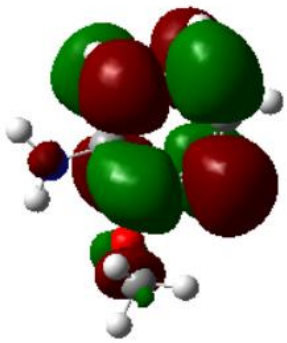
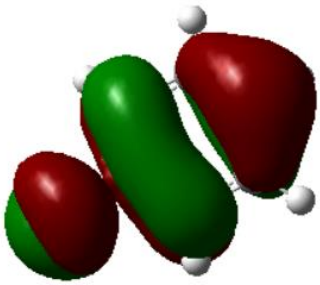
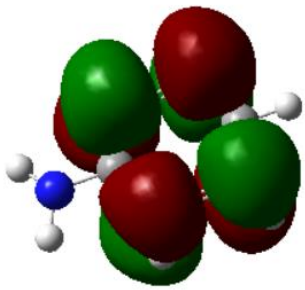
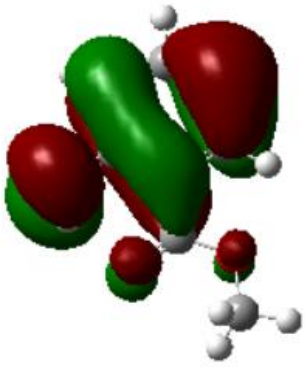
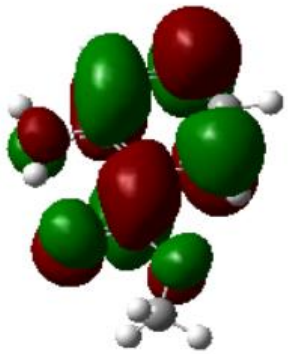


Figure S40. Packing arrangement for compound **12**.

10. HOMO and LUMO energy values for reactants

reactant	HOMO (donor) kJ/mol	LUMO (acceptor) kJ/mol
o–anisidine	-517.9324 	24.2334 
aniline	-520.4003 	22.3955 
methyl anthranilate	-526.2552 	-91.9450 

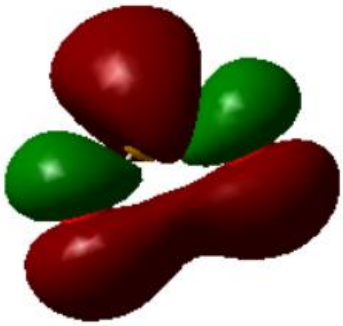
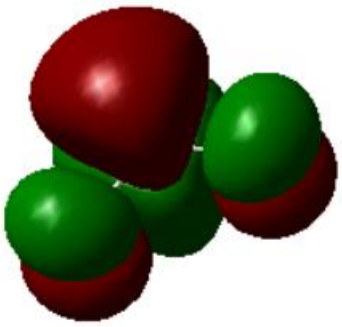
Selenium dioxide	-820.8101 	-394.4289 

Figure S41: HOMO and LUMO energy values for reactants.