Electronic Supplementary Material (ESI) for Organic & Biomolecular Chemistry

Supporting Information
for

Spirodiazaselenuranes: Synthesis, Structure and Antioxidant Activity

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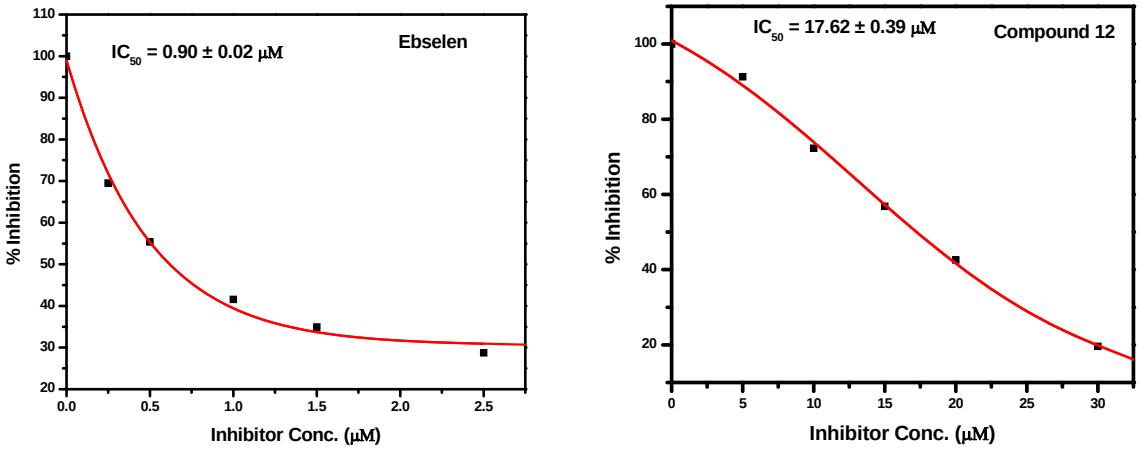


Figure-S1. Plot of inhibition of PN-mediated oxidation of DHR by **ebselen** and compound **12**.

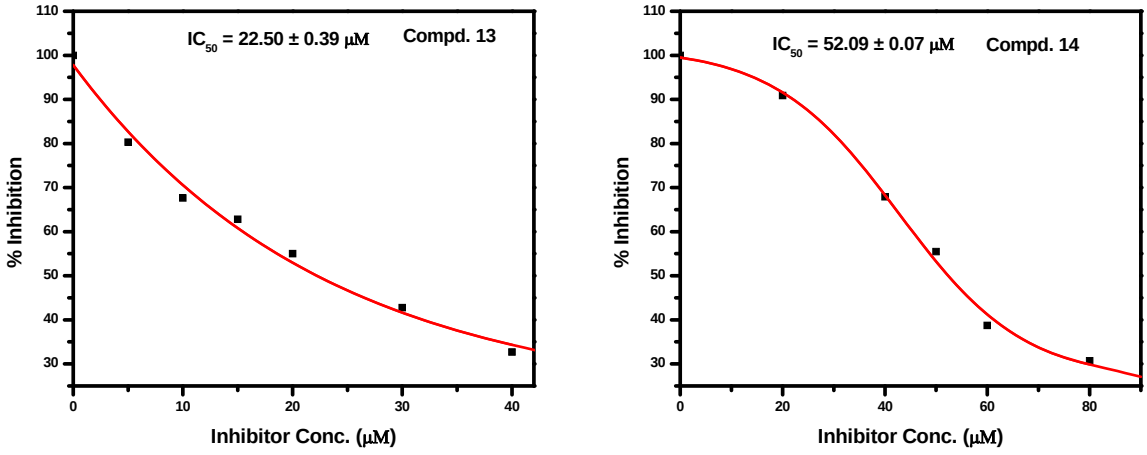


Figure-S2. Plot of inhibition of PN-mediated oxidation of DHR by compound**13** and compound **14**.

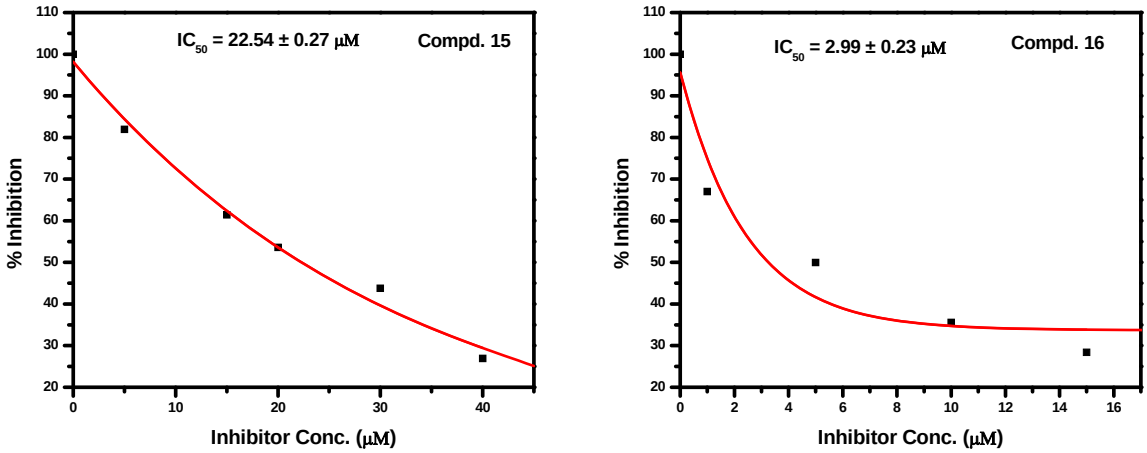


Figure-S3. Plot of inhibition of PN-mediated oxidation of DHR by compound**15** and compound **16**.

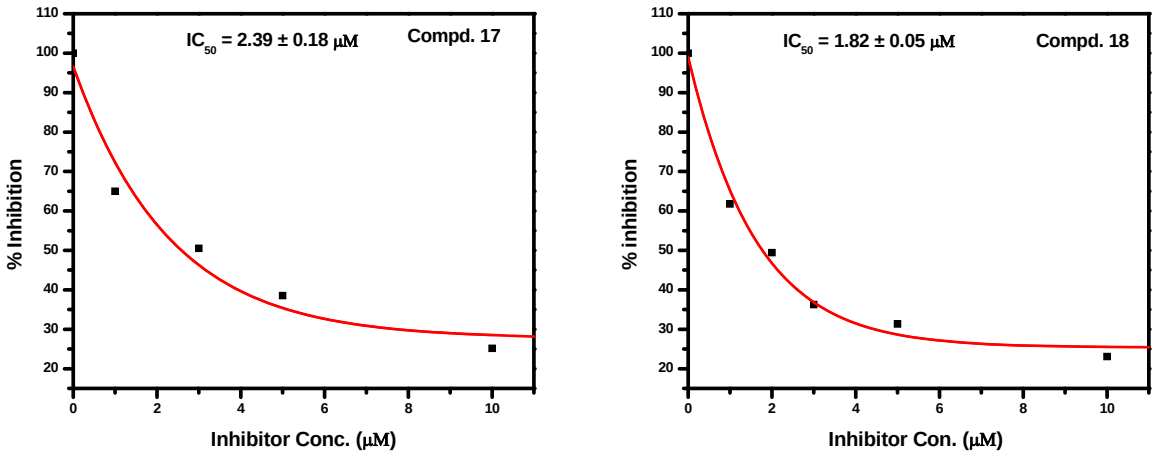


Figure-S4. Plot of inhibition of PN-mediated oxidation of DHR by compound **17** and compound **18**.

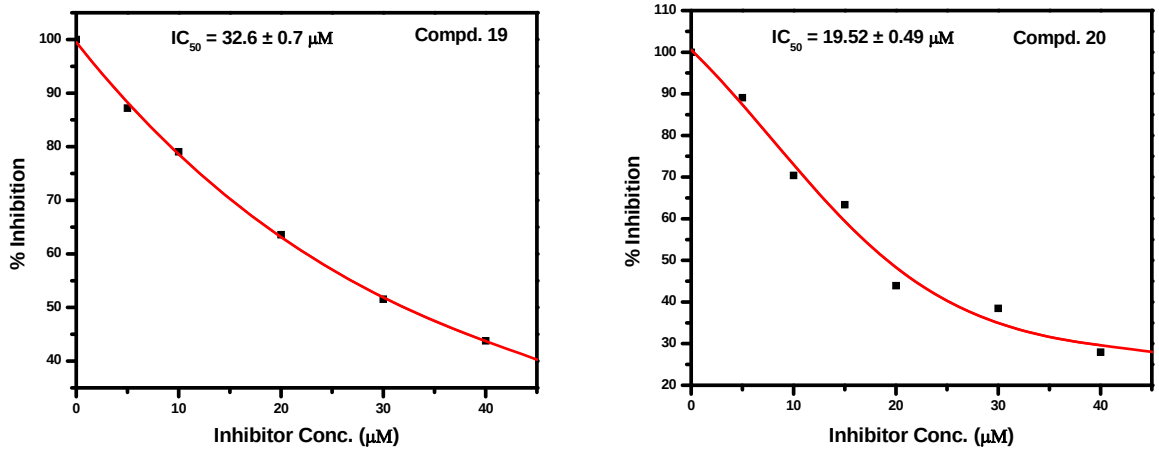


Figure-S5. Plot of inhibition of PN-mediated oxidation of DHR by compound**19** and compound **20**.

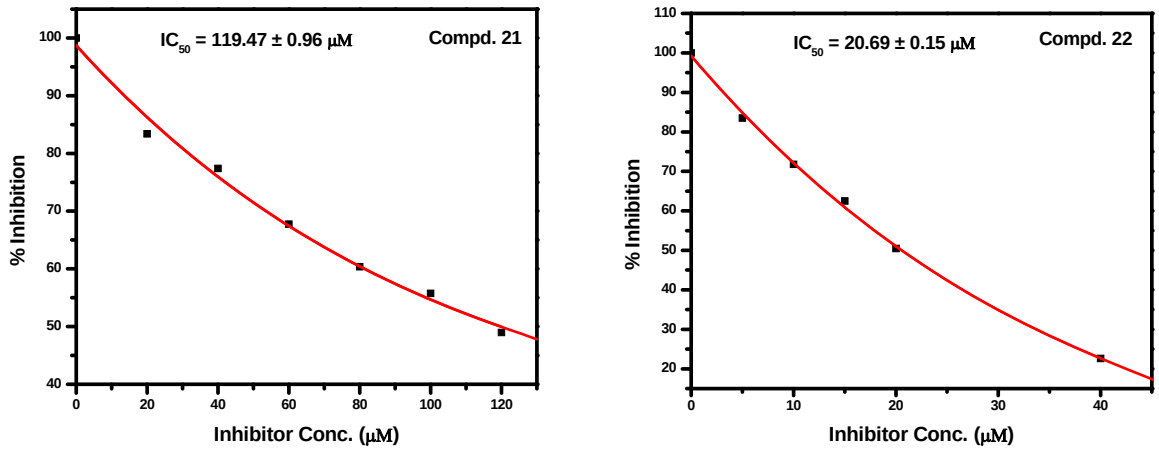


Figure-S6. Plot of inhibition of PN-mediated oxidation of DHR by compound **21** and compound **22**.

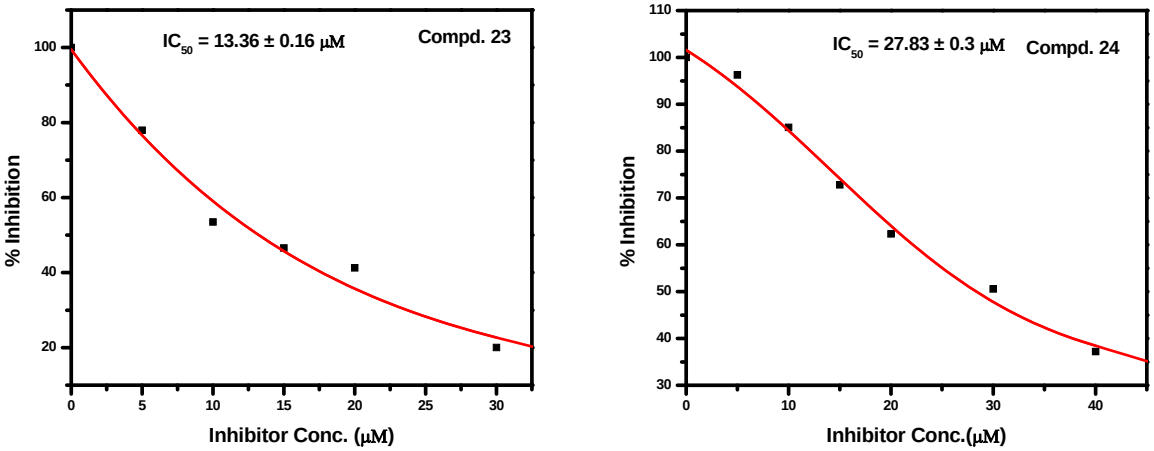


Figure-S7. Plot of inhibition of PN-mediated oxidation of DHR by compound **23** and compound **24**.

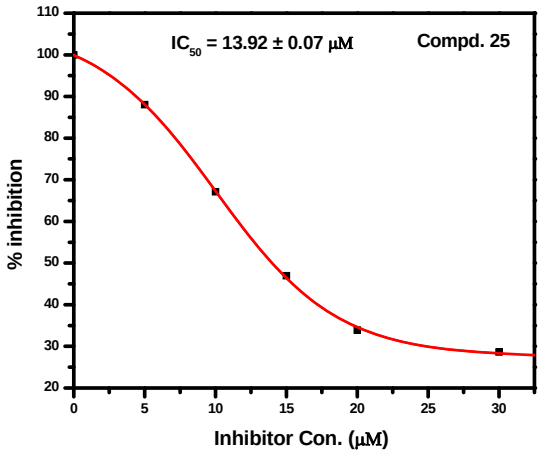


Figure-S8. Plot of inhibition of PN-mediated oxidation of DHR by compound **25**.

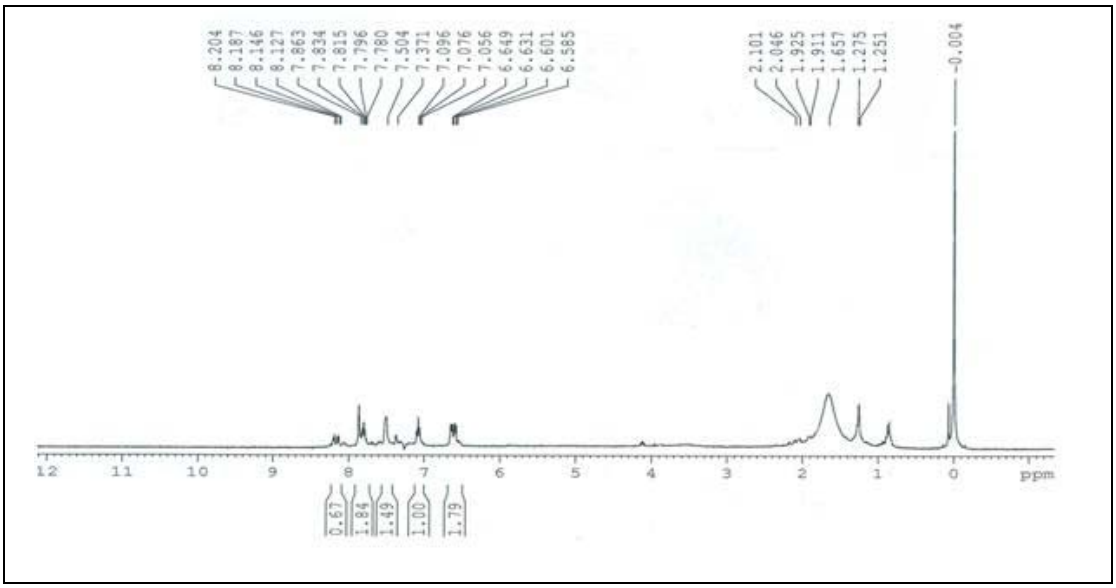


Figure-S9. ^{1}H NMR spectra of pure spirodiazoselenurane **19** in CD_3OD.

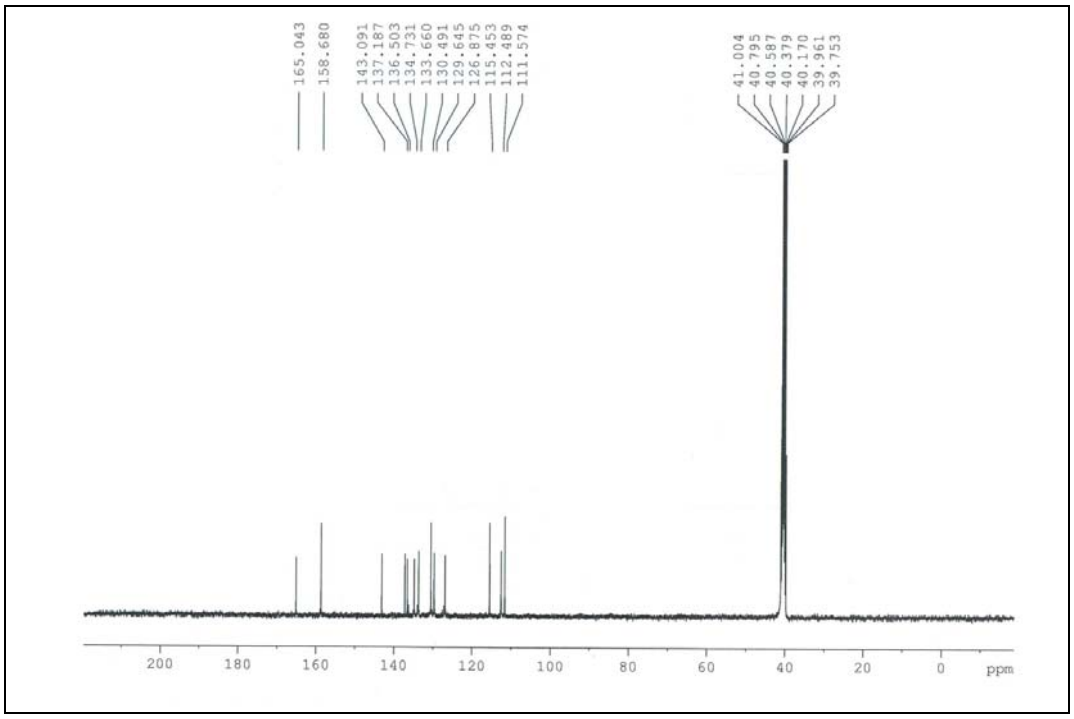


Figure-S10. ^{13}C NMR spectra of pure spirodiazoselenurane **19** in DMSO-d_6.

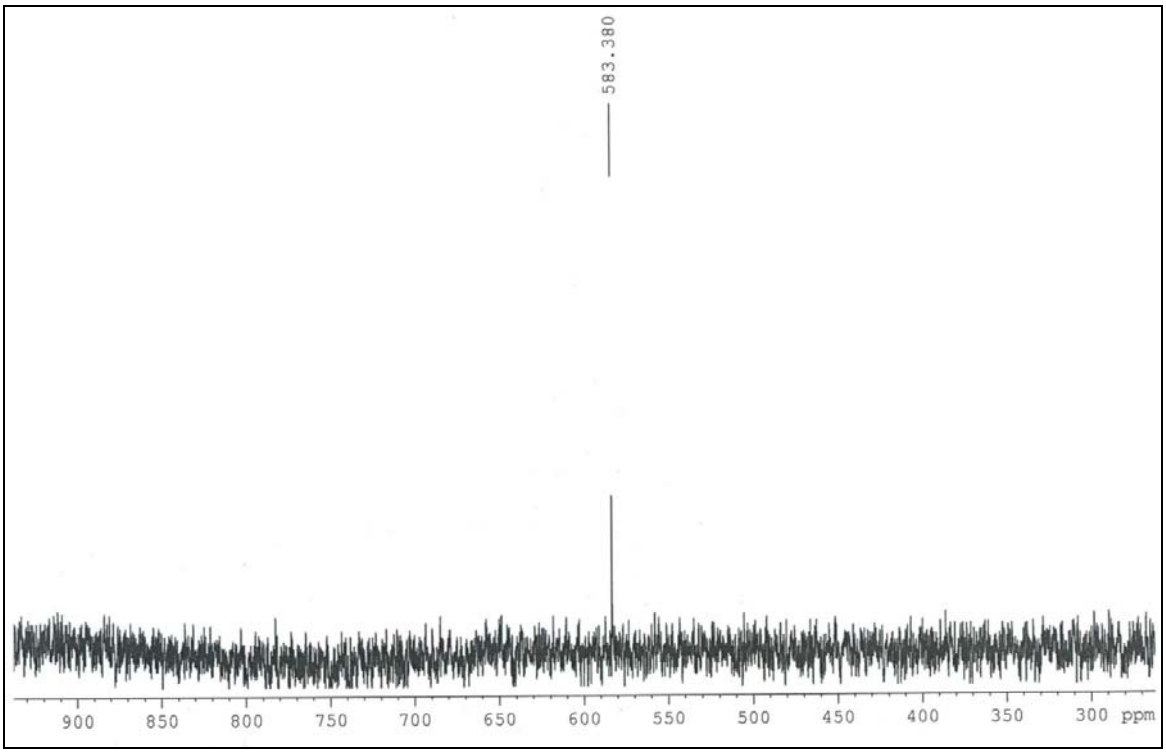


Figure-S11. ^{77}Se NMR spectra of pure spirodiazoselenurane **19** in DMSO-d_6.

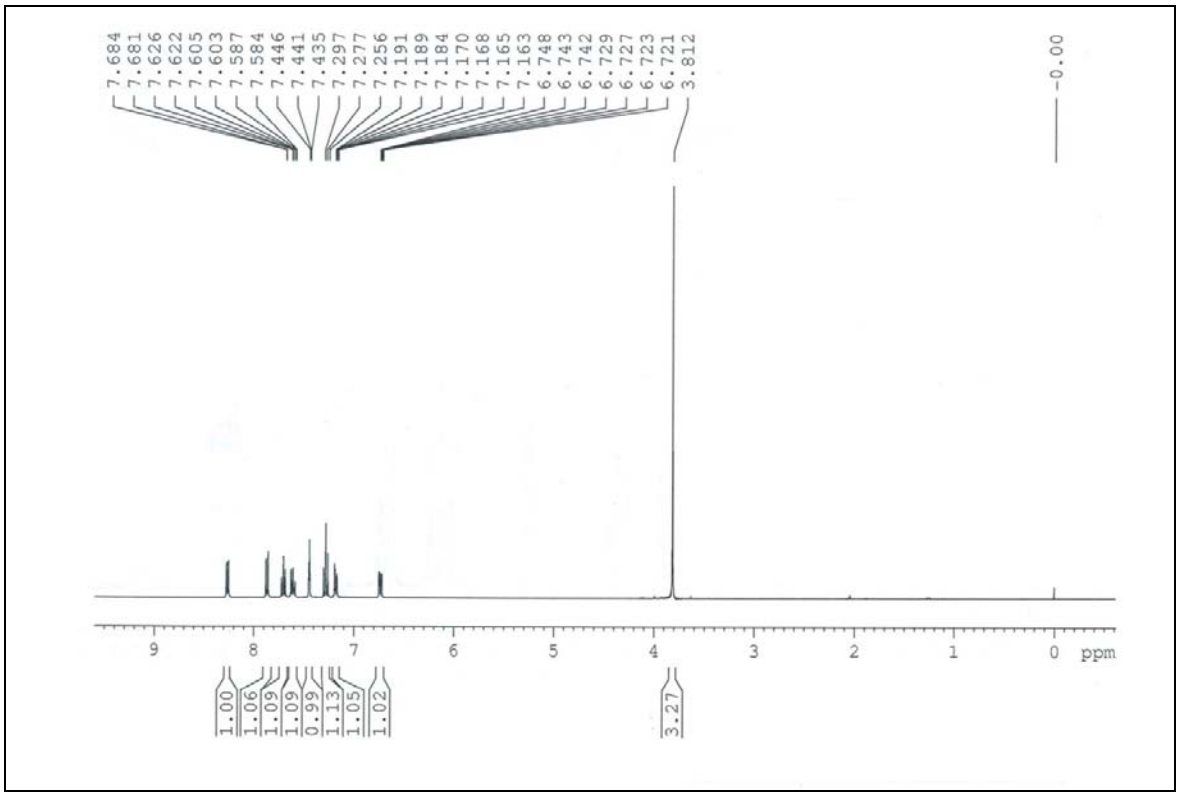


Figure-S12. ^{1}H NMR spectra of pure spirodiazoselenurane **20** in $CDCl_3$.

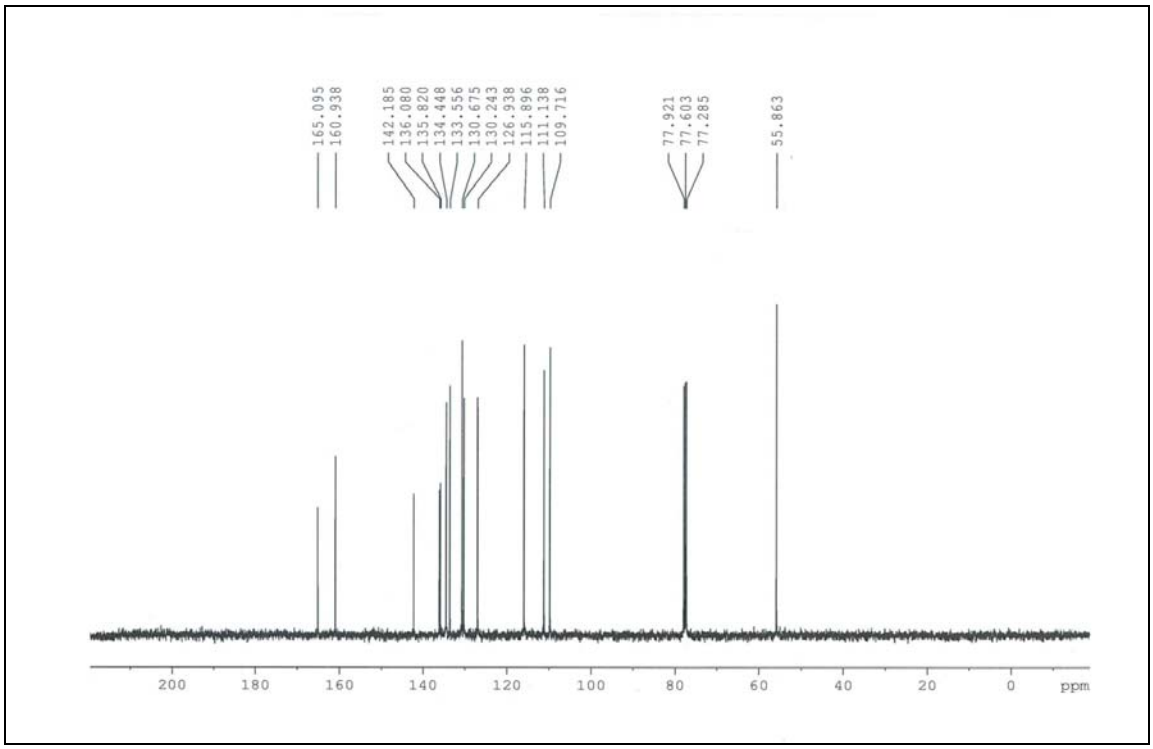


Figure-S13. ^{13}C NMR spectra of pure spirodiazoselenurane **20** in $CDCl_3$.

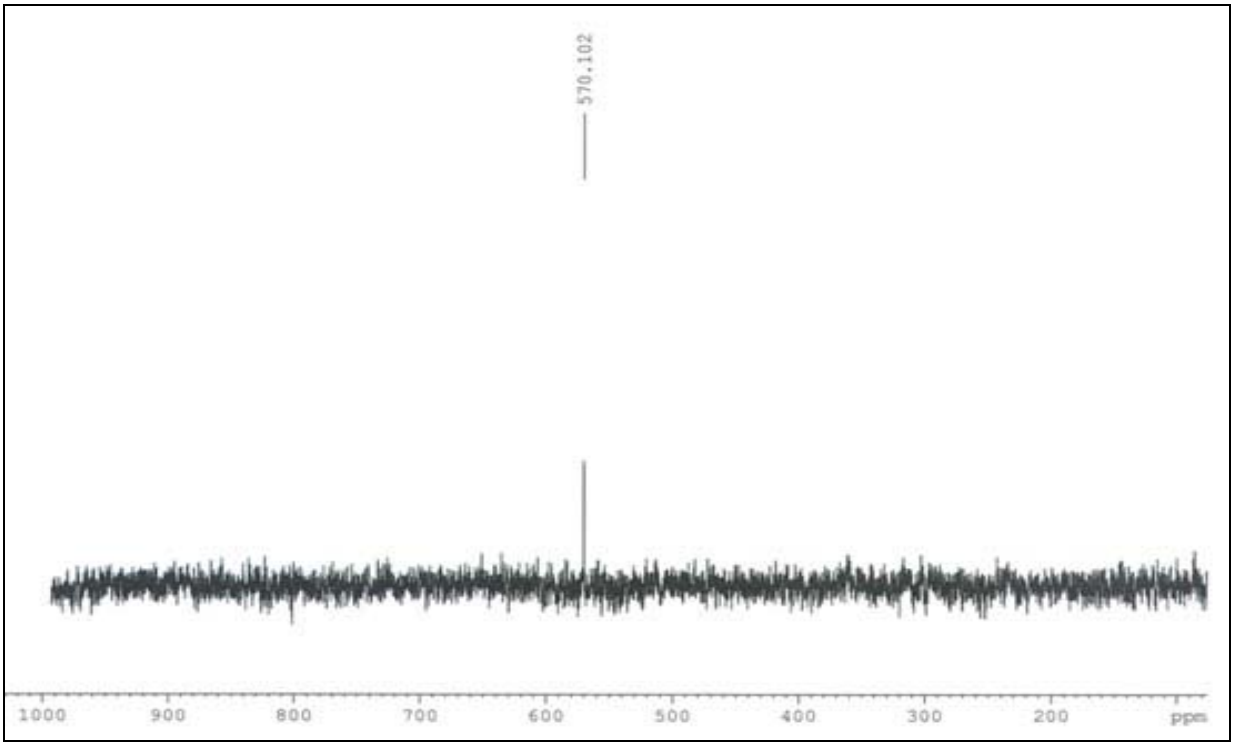


Figure-S14. ^{77}Se NMR spectra of pure spirodiazoselenurane **20** in $CDCl_3$.

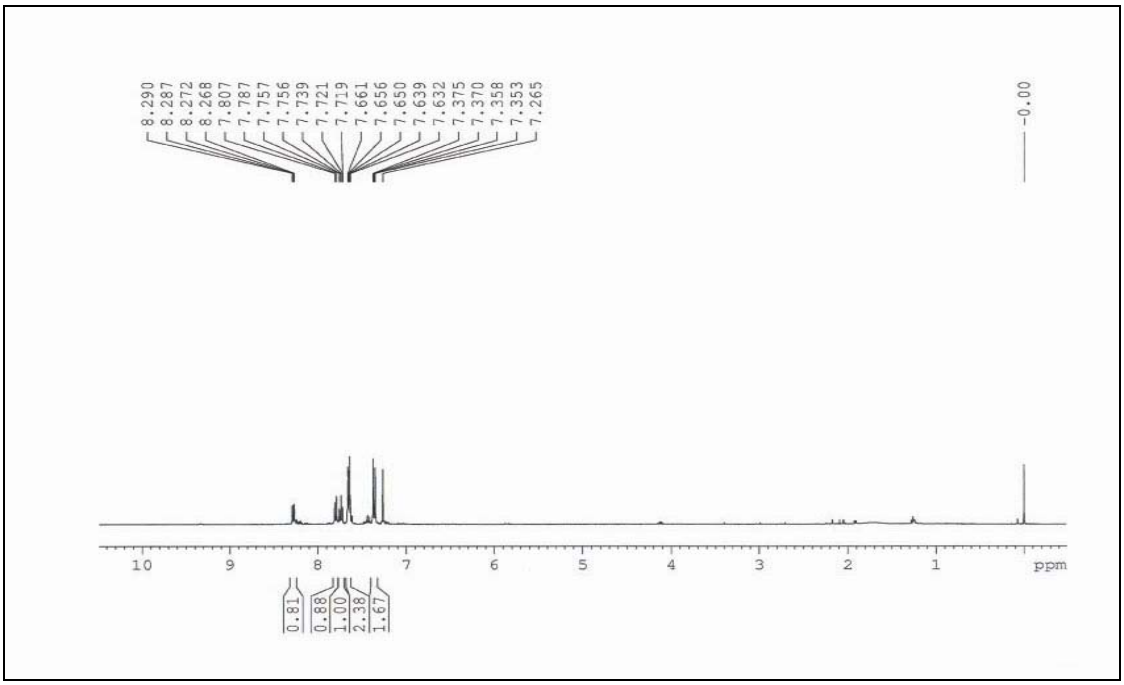


Figure-S15. ^{1}H NMR spectra of pure spirodiazoselenurane **21** in $CDCl_3$.

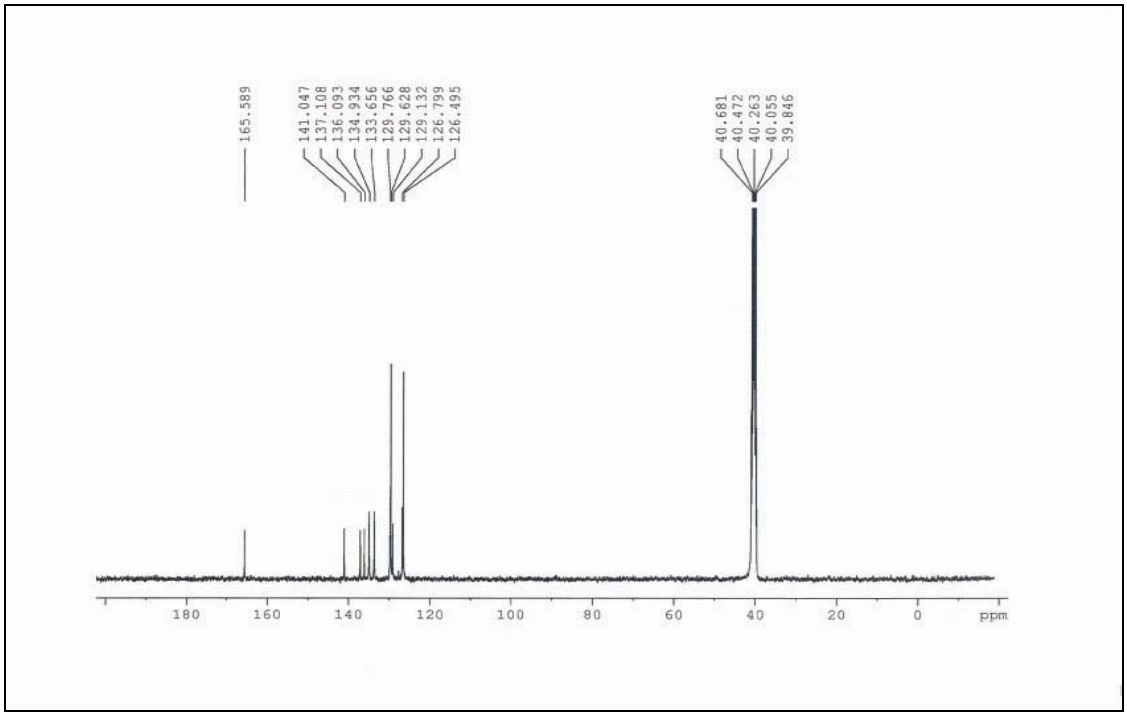


Figure-S16. ^{13}C NMR spectra of pure spirodiazoselenurane **21** in DMSO-d_6.

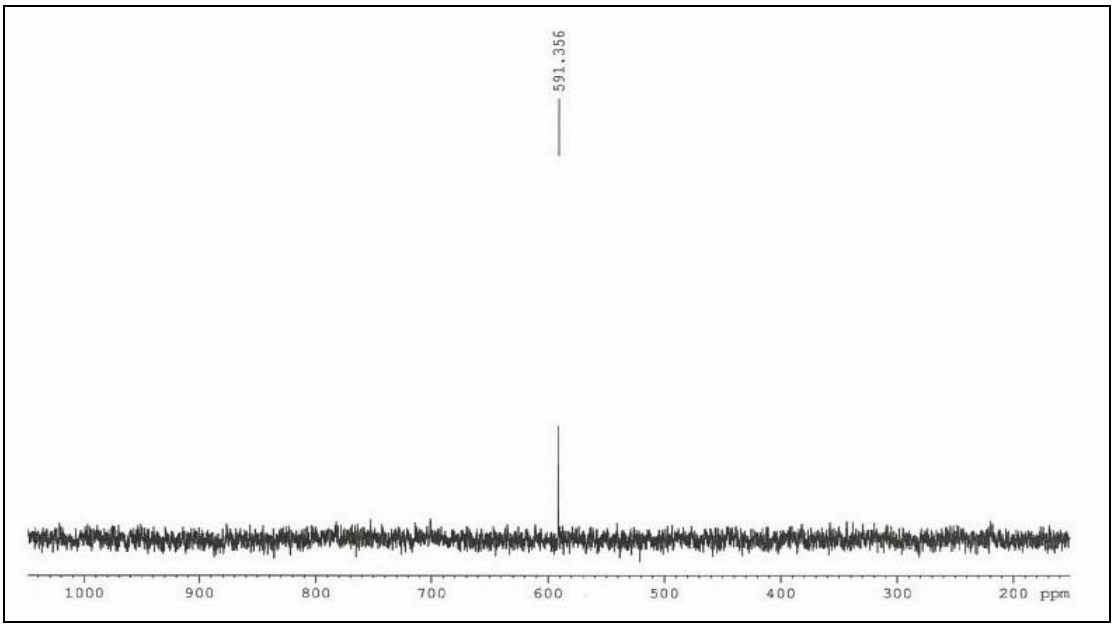


Figure-S17. ^{77}Se NMR spectra of pure spirodiazoselenurane **21** in DMSO-d_6.

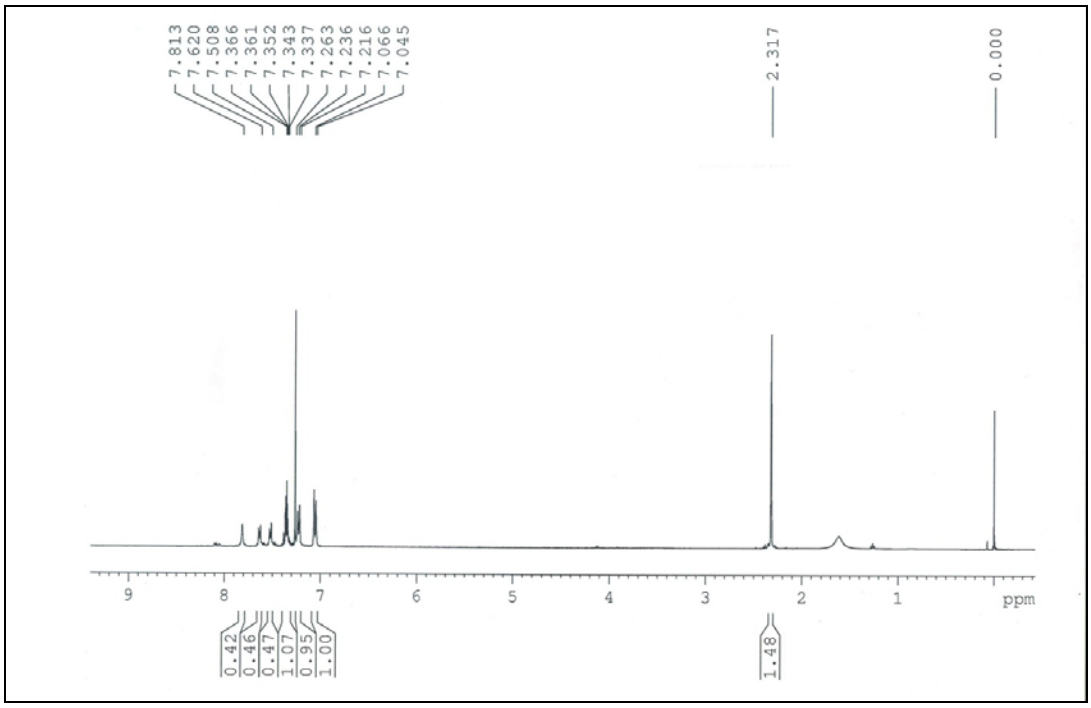


Figure-S18. ^{1}H NMR spectra of pure spirodiazoselenurane **23** in $CDCl_3$.

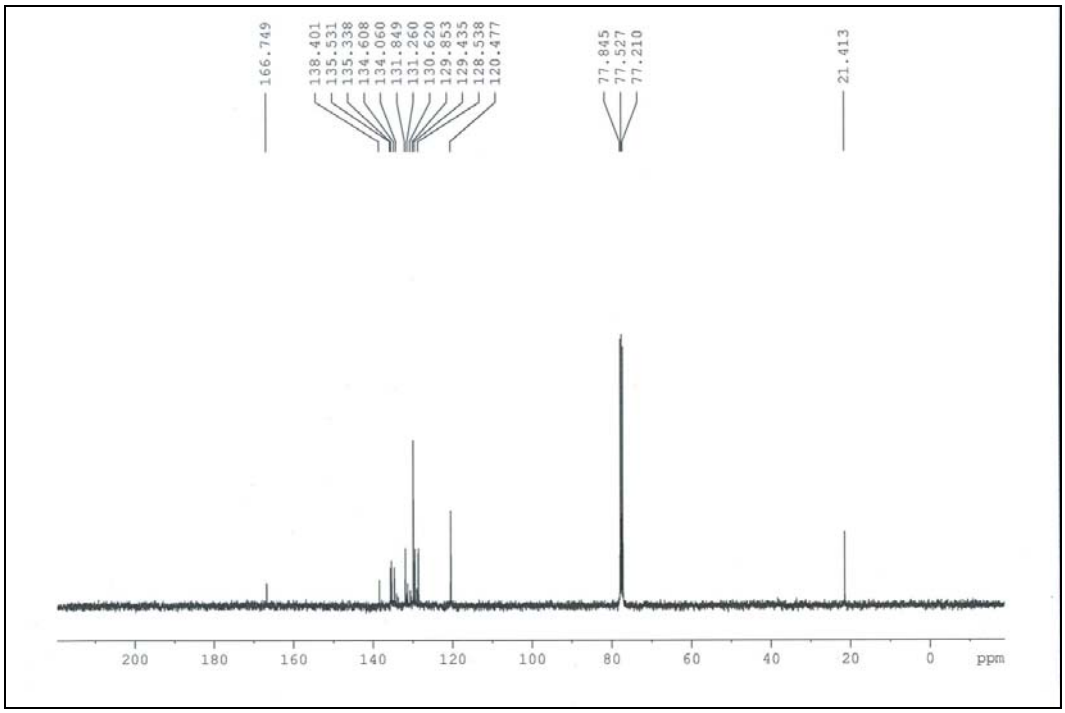


Figure-S19. ^{13}C NMR spectra of pure spirodiazoselenurane **23** in $CDCl_3$.

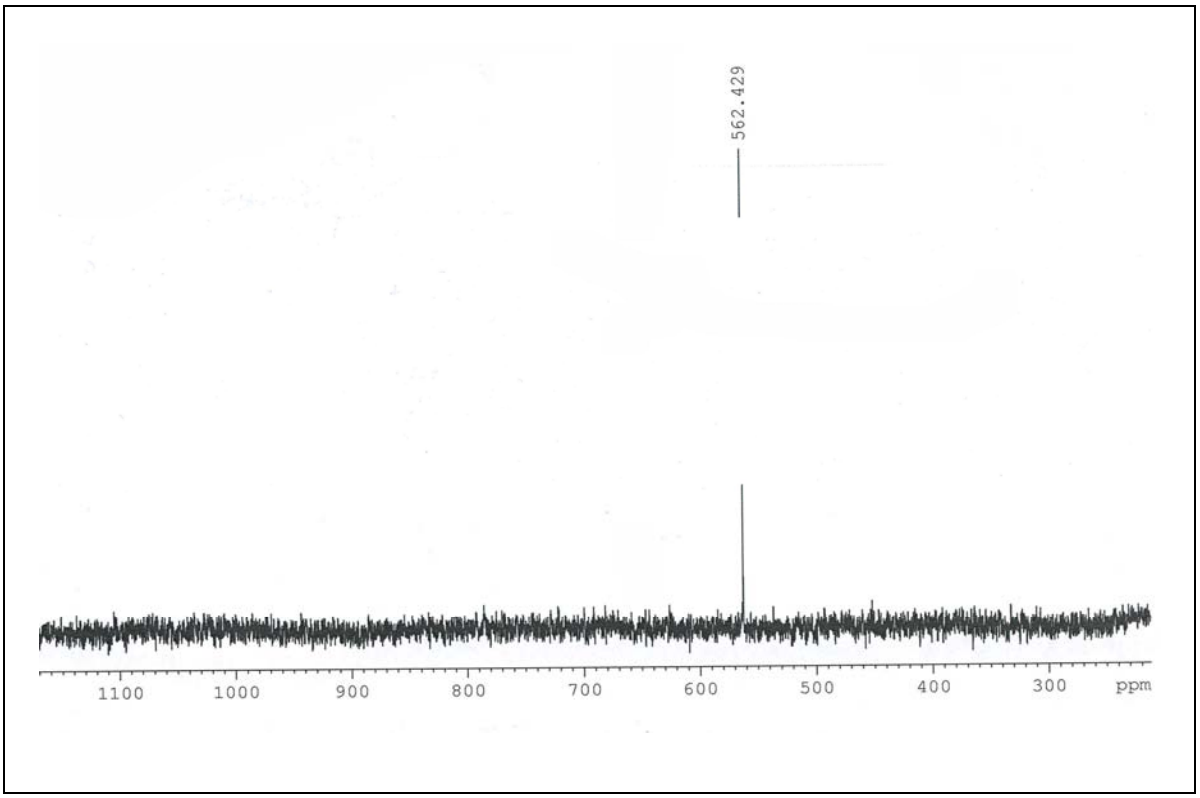


Figure-S20. ^{77}Se NMR spectra of pure spirodiazoselenurane **23** in DMSO-d_6.

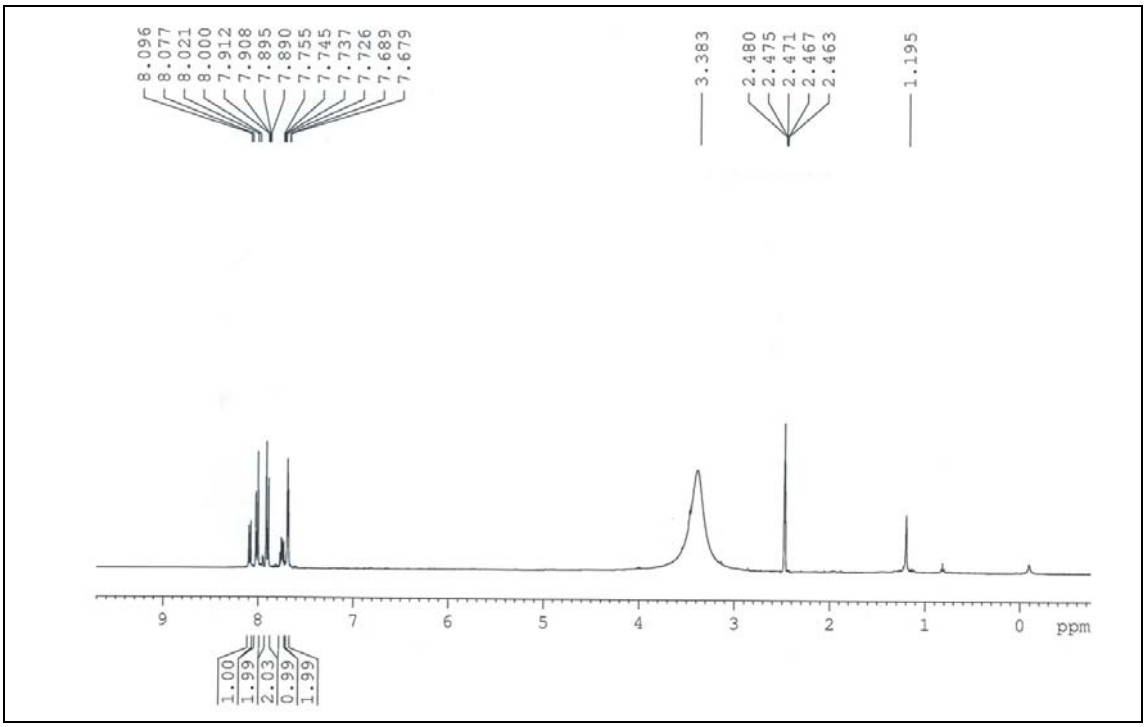


Figure-S21. ^{1}H NMR spectra of pure spirodiazoselenurane **24** in DMSO-d_6.

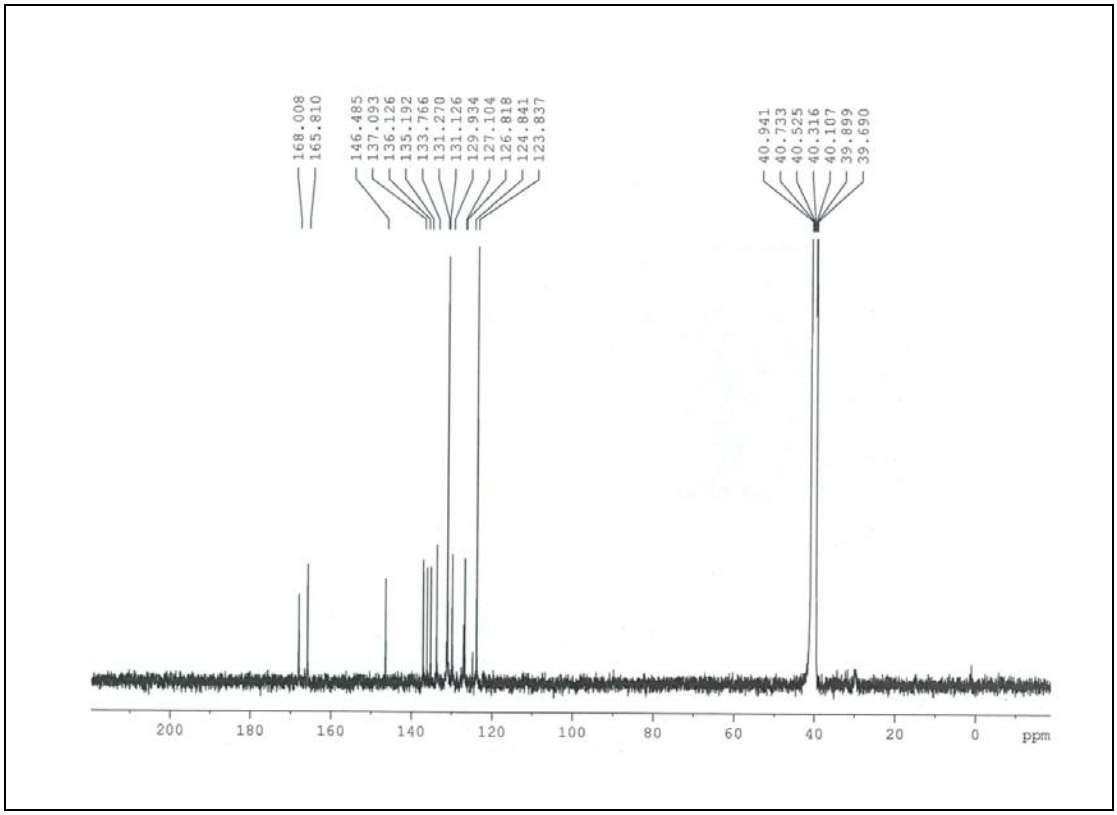


Figure-S22. ^{13}C NMR spectra of pure spirodiazoselenurane **24** in DMSO-d_6.

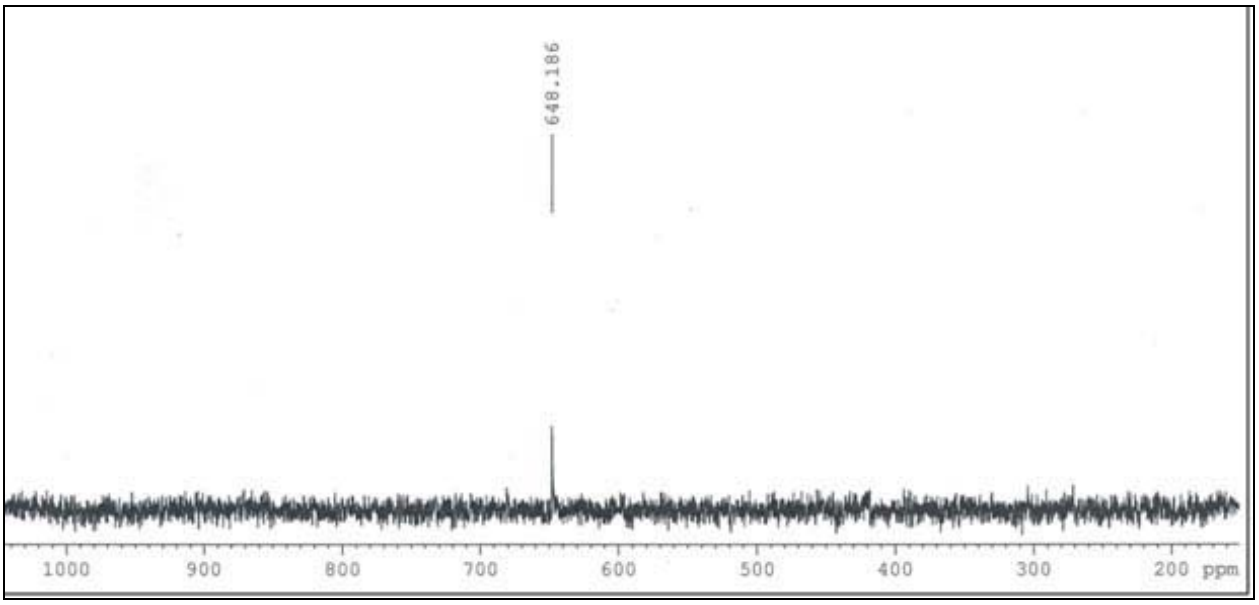
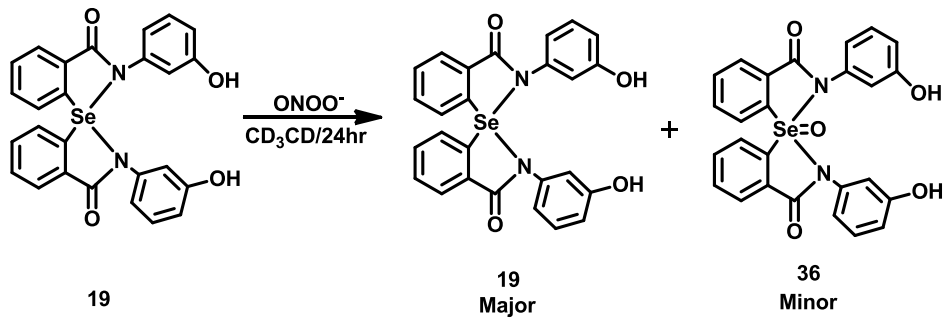


Figure-S23. ^{77}Se NMR spectra of pure spirodiazoselenurane **24** in DMSO-d_6.



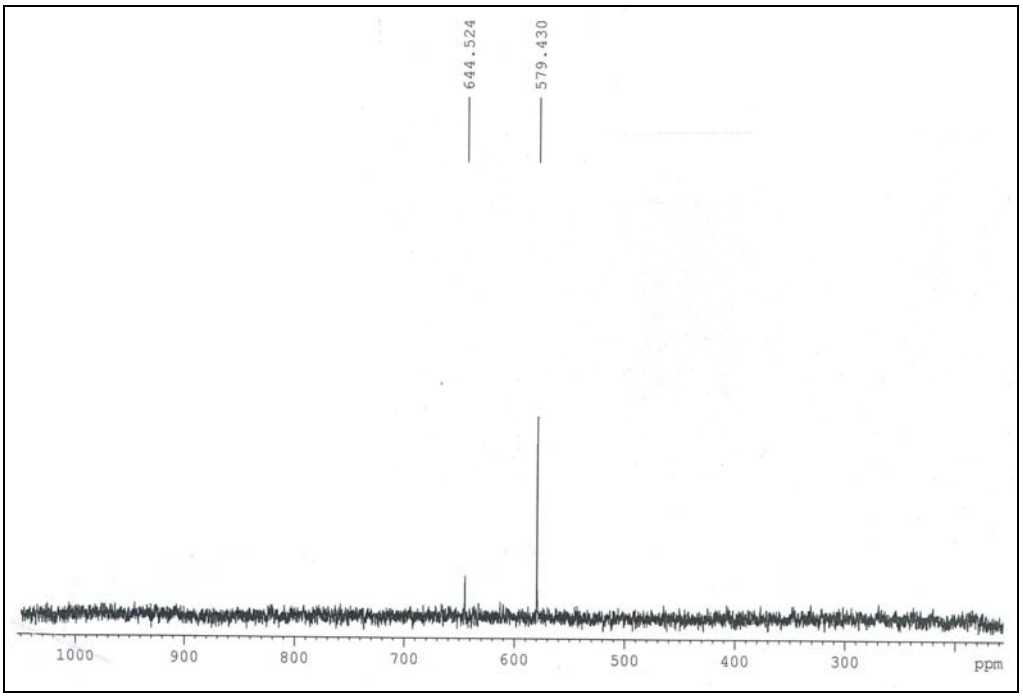
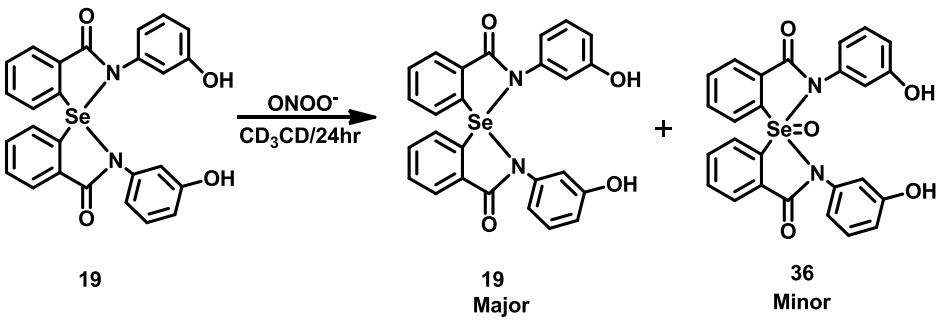


Figure-S24. ^{77}Se NMR spectrum obtained (in CD_3OD) after treatment of the spirodiazaselenurane **19** with 2 equiv of PN, indicating the formation of compounds **19** and **36.**



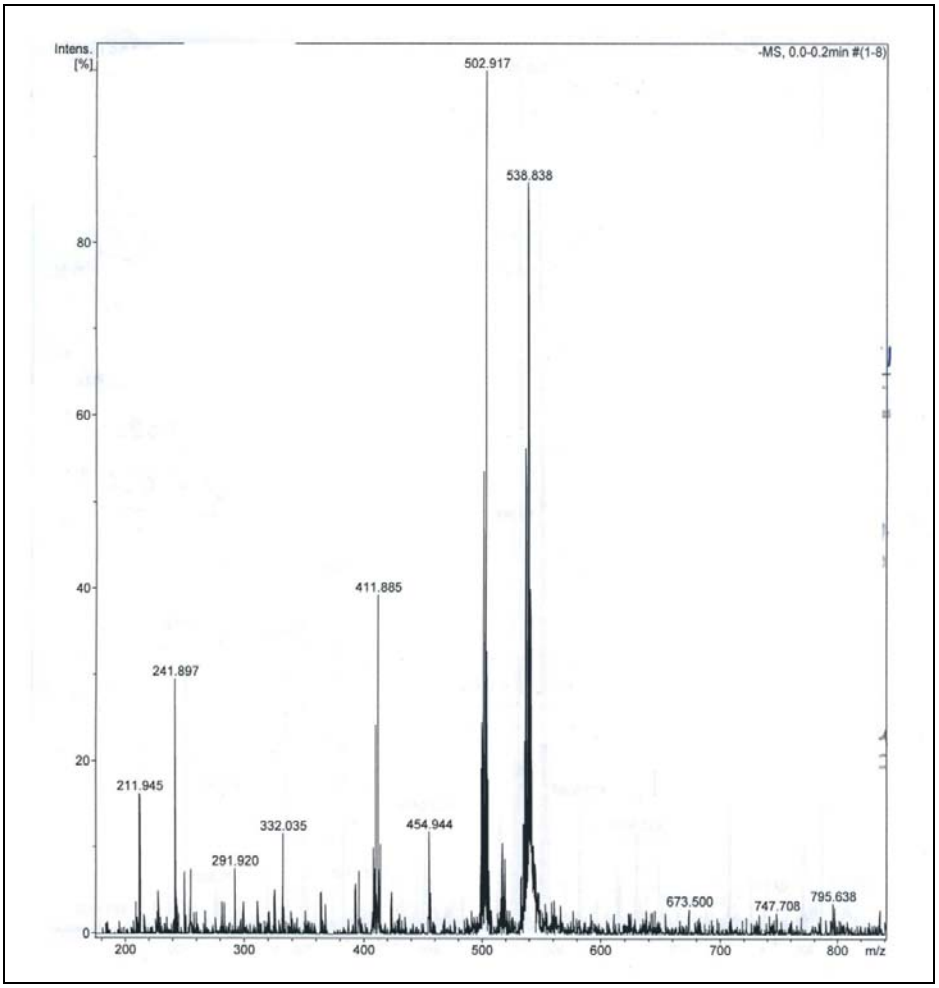
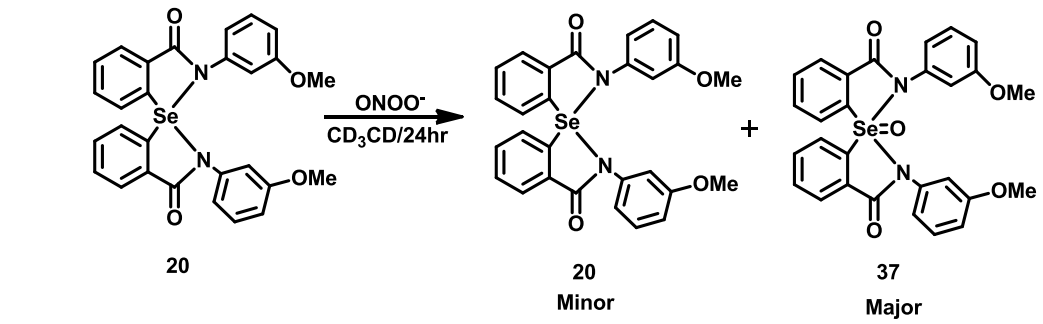


Figure-S25. ESI–Mass spectrum obtained for the reaction of spirodiazaselenurane **19** with 2 equiv of PN, indicating the formation of compounds **19** and **36**. Calculated Mass $(M)^+$: 502.04, Observed Mass:502.91 for the compound **19,** for the compound **36**, Calculated Mass $(M)^+$:518.04, Observed Mass:538.83$(M+Na)^+$



20 | 20 Minor | 37 Major

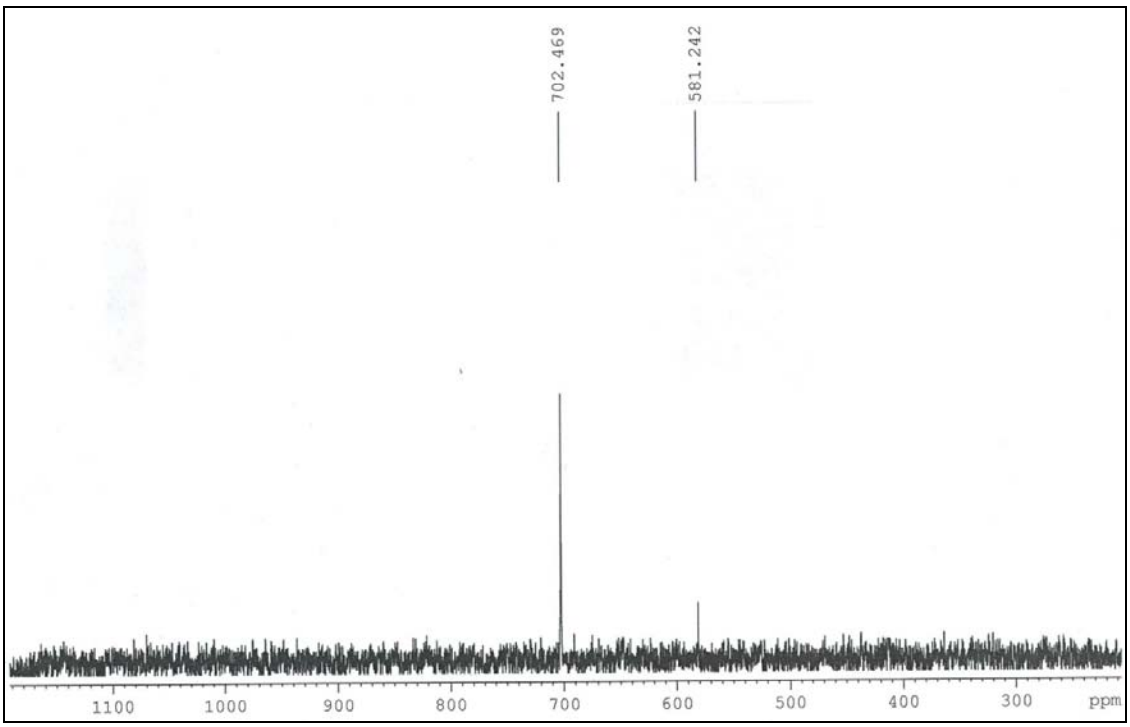
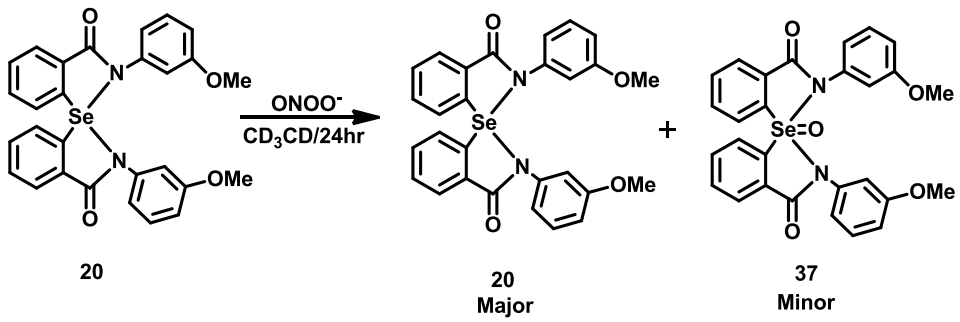


Figure-S26. ^{77}Se NMR spectrum (in CD_3OD) obtained after treating the spirodiazaselenurane **20** with 2 equiv of PN, indicating the formation of compounds **20** and **37**.



20 **20 Major** **37 Minor**

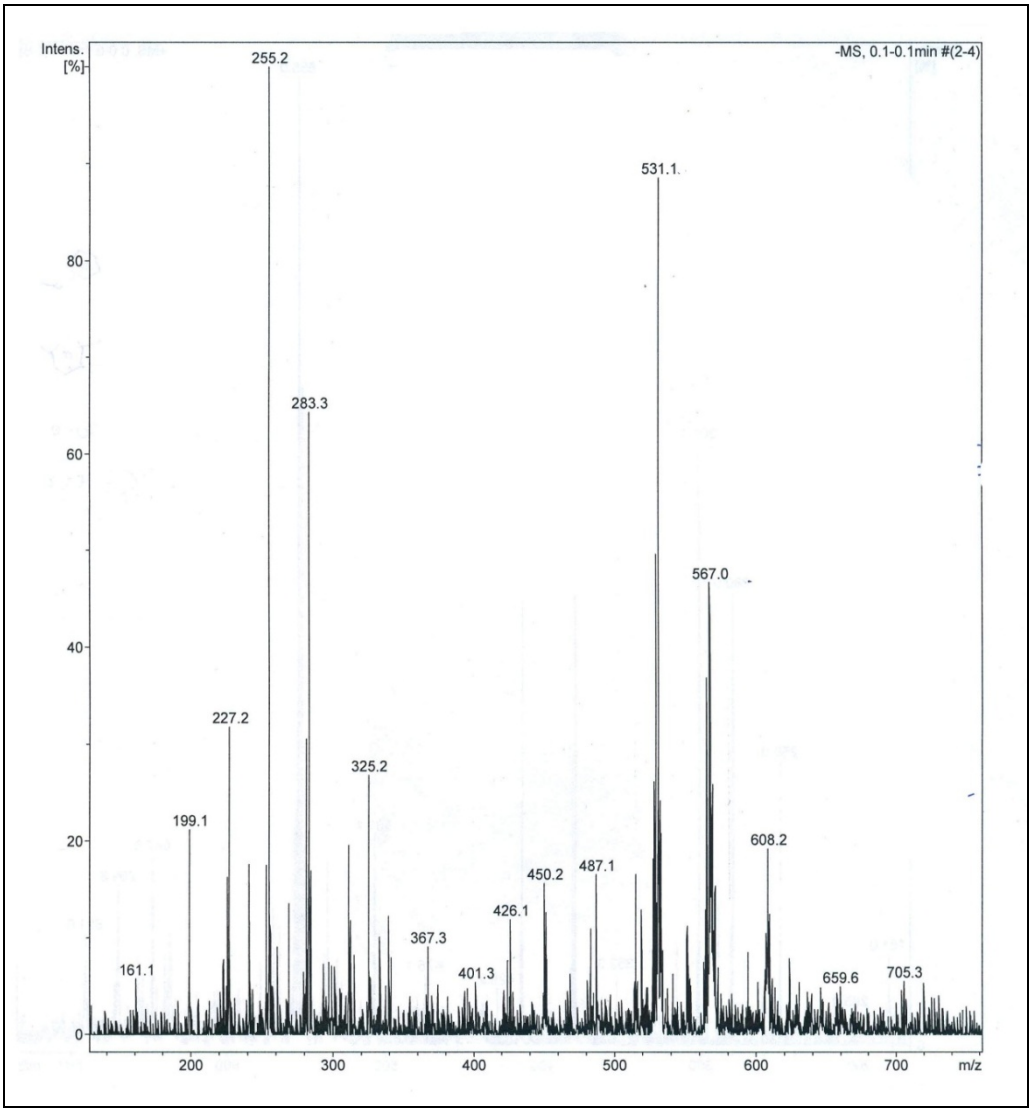
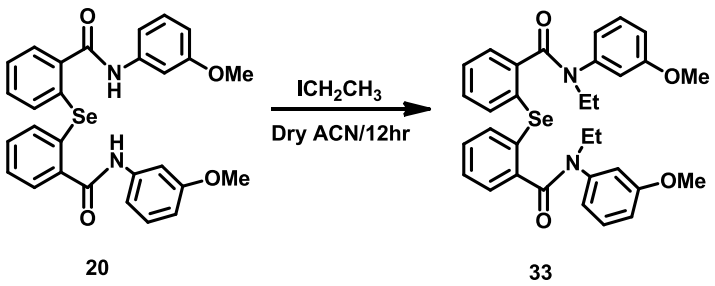


Figure-S27. ESI–Mass spectrum obtained for the reaction of spirodiazaselenurane **20** with 2 equiv of PN, indicating the formation of compounds **20** and **37.** Calculated Mass $(M)^+$: 530.3, Observed Mass:531.1 for the compound **20**, for the compound **37**, Calculated Mass $(M)^+$: 546.0, Observed Mass:567.8 $(M+Na)^+$.



20 **33**

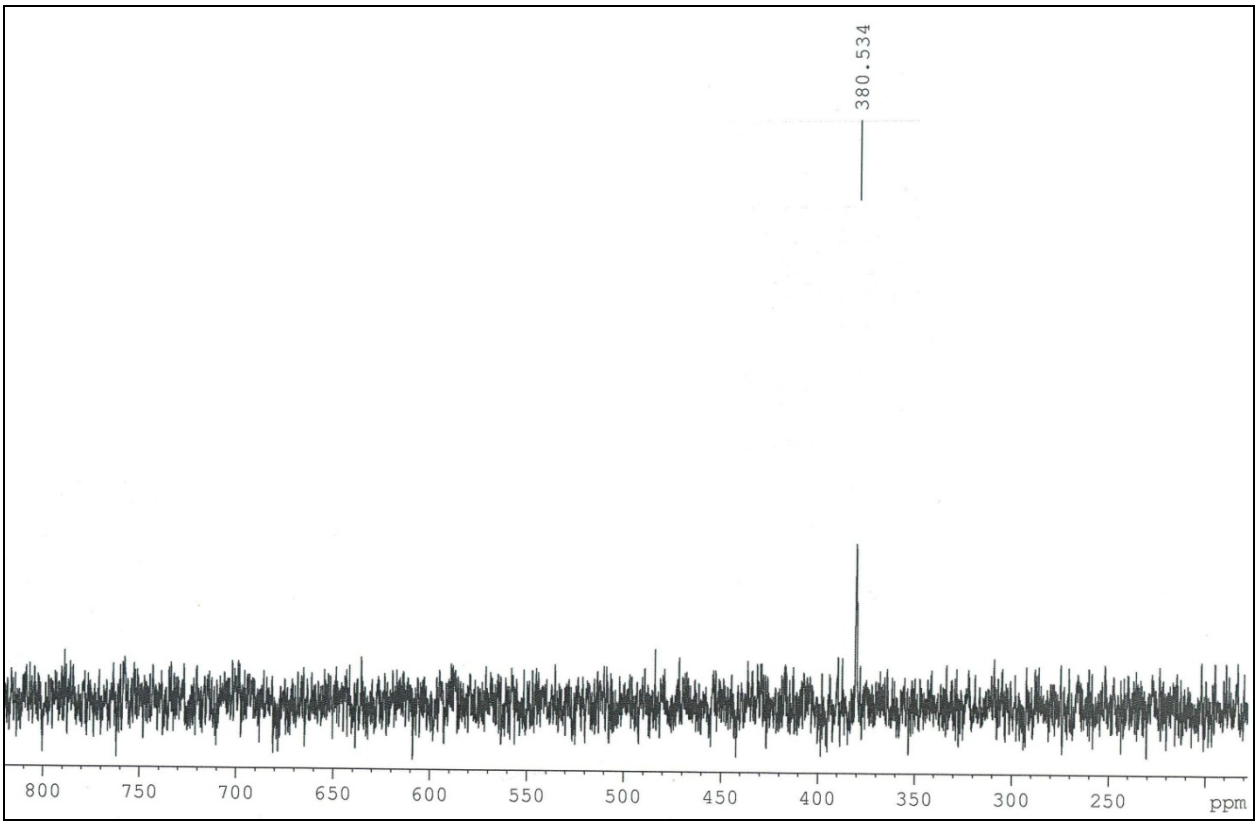


Figure-S28. ^{77}Se NMR spectrum obtained after treating diaryl selenide **20** with 2 eqv ICH_2CH_3 in dry acetonitrile. The spectrum, recorded in $CDCl_3$ after 12 h, indicates the formation of compound **33**.

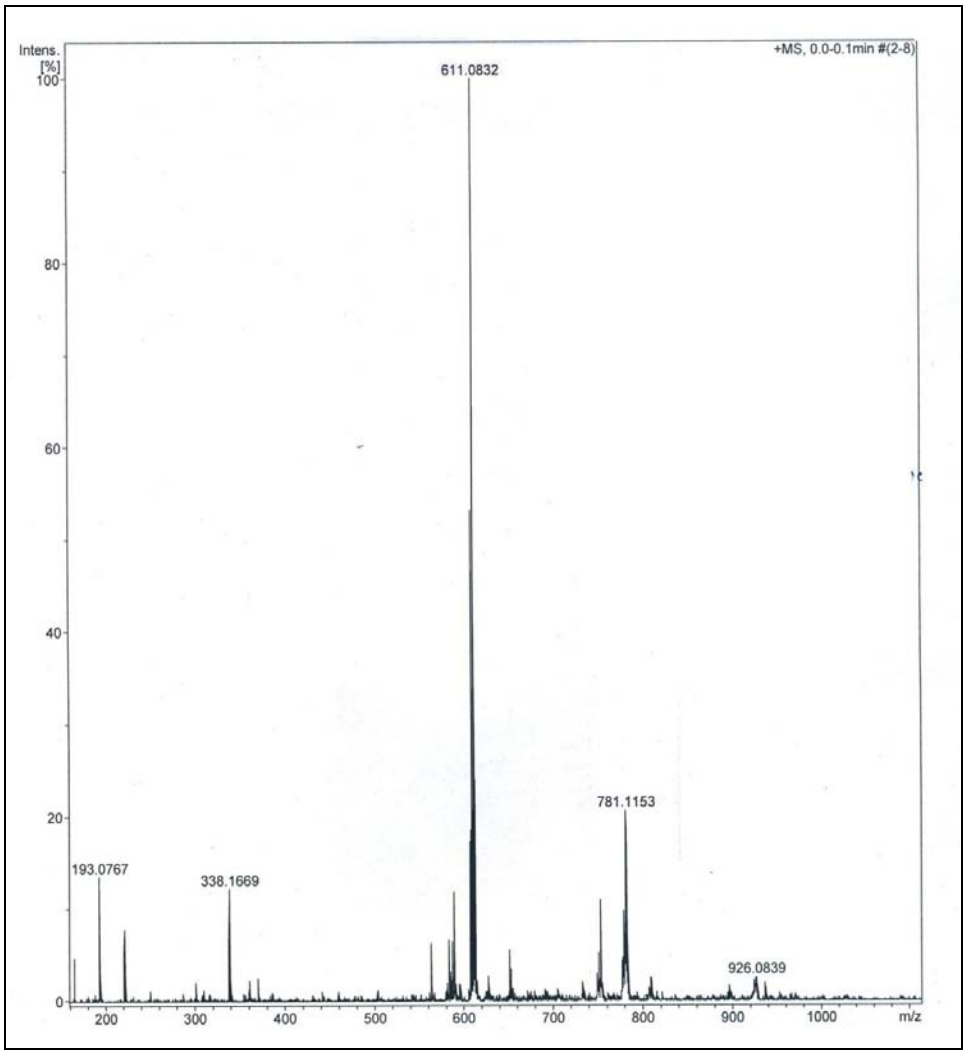
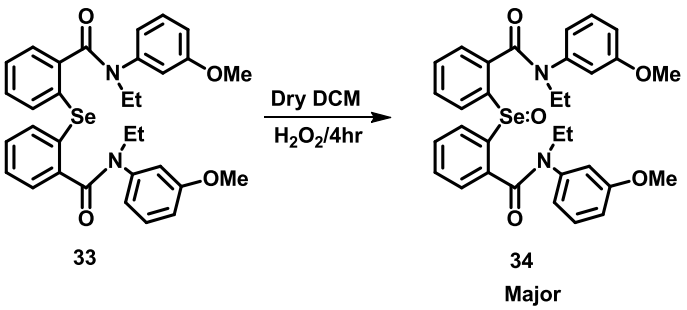


Figure-S29. ESI –Mass spectrum of compound **33.** Calculated Mass $(M)^+$: 588.3, Observed Mass: 611.083 $(M+Na)^+$



33 34 Major

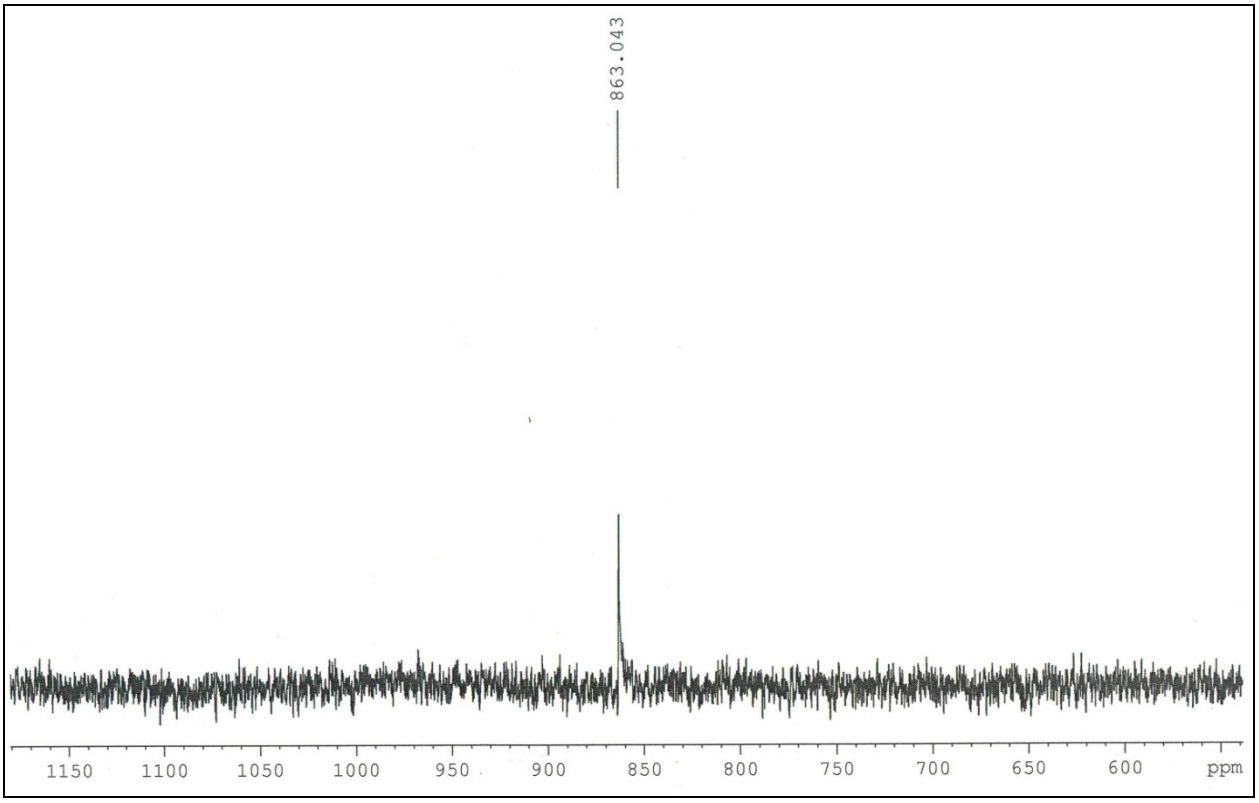


Figure-S30. ^{77}Se NMR spectrum recorded (in $CDCl_3$) after addition of H_2O_2 to **33.** After 4 h, a complete convertion of **33** to **34** was observed.

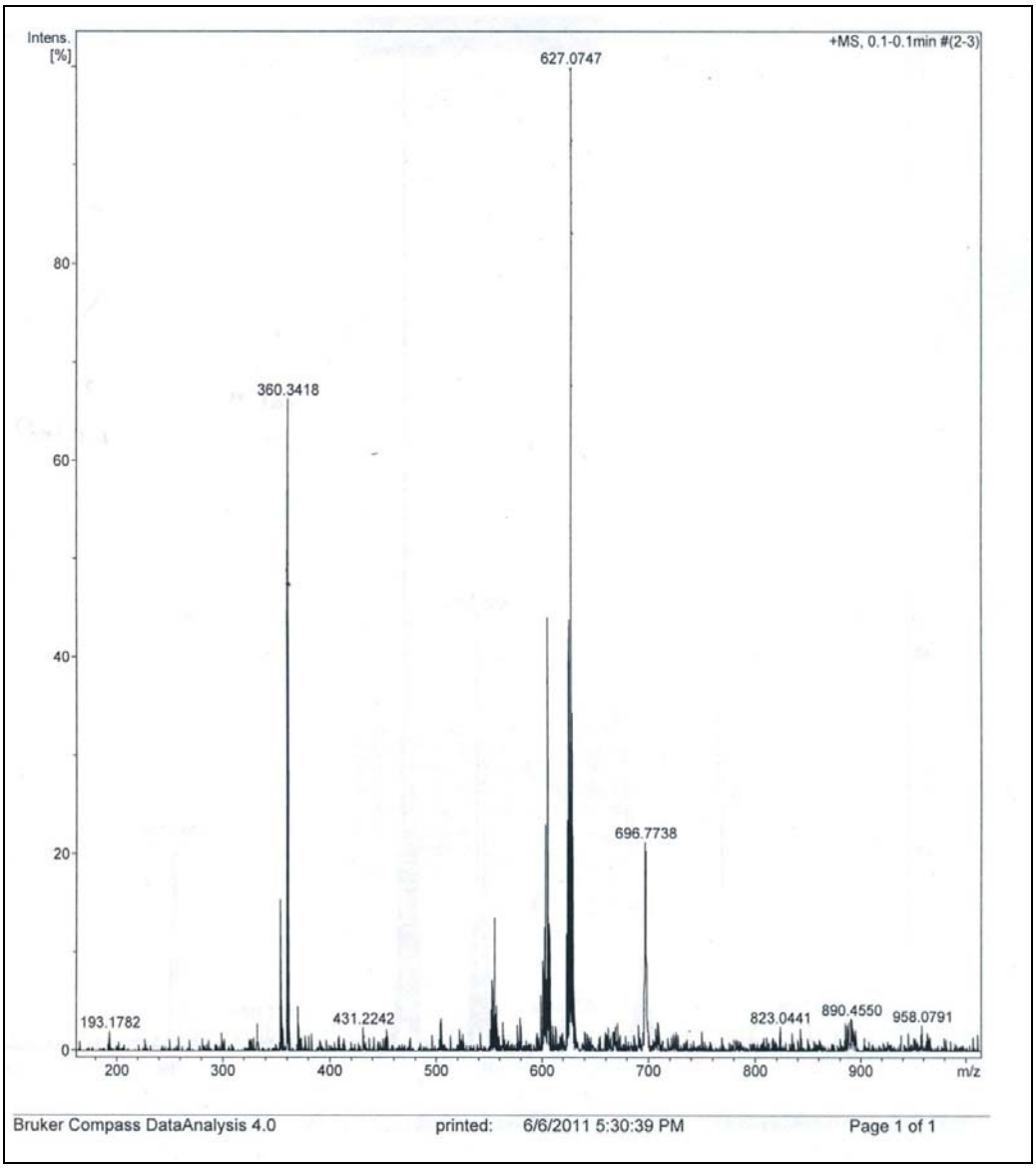


Figure-S31. ESI –Mass spectrum of pure compound **34.** Calculated Mass $(M)^+$: 603.63, observed Mass: 627.074 $(M+Na)^+$

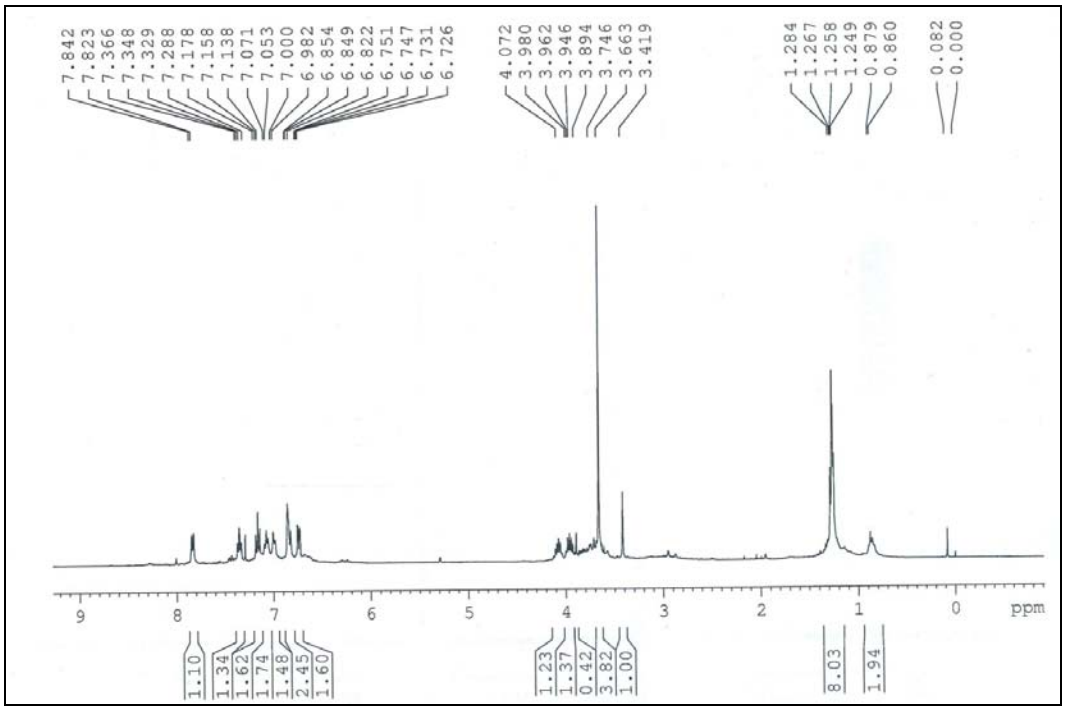


Figure-S32. ^{1}H NMR spectra of pure compound **34** in $CDCl_3$.

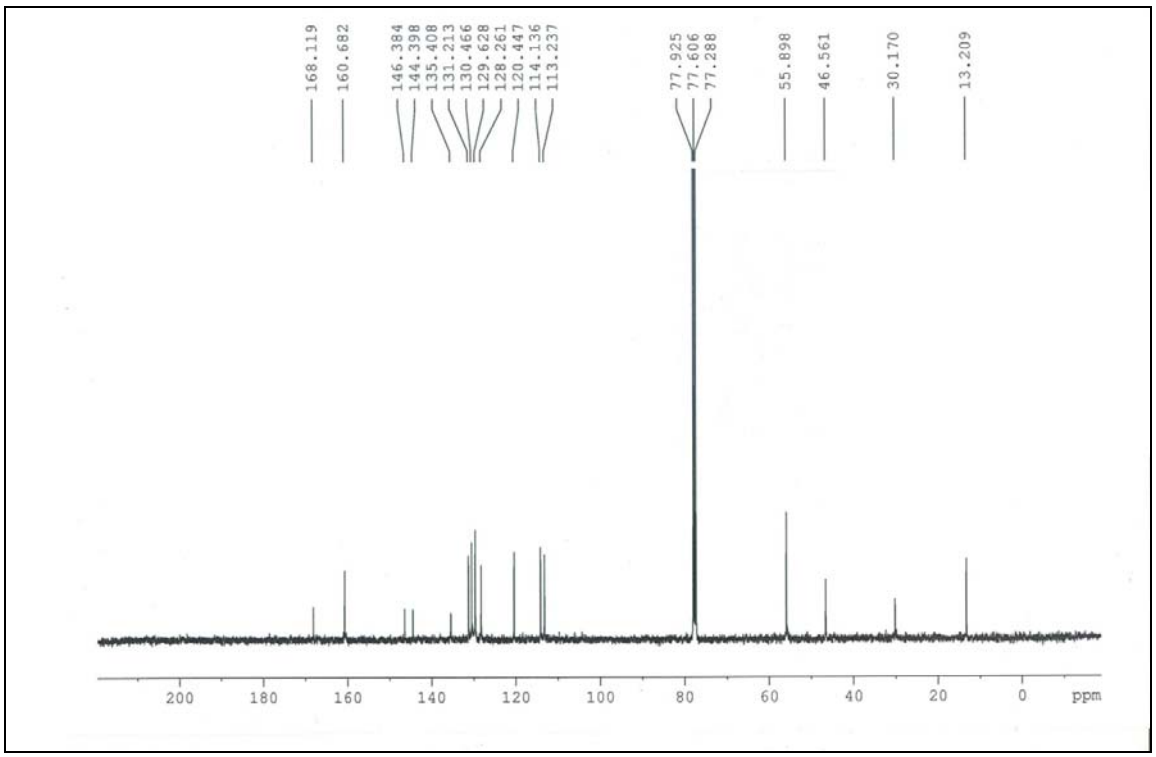
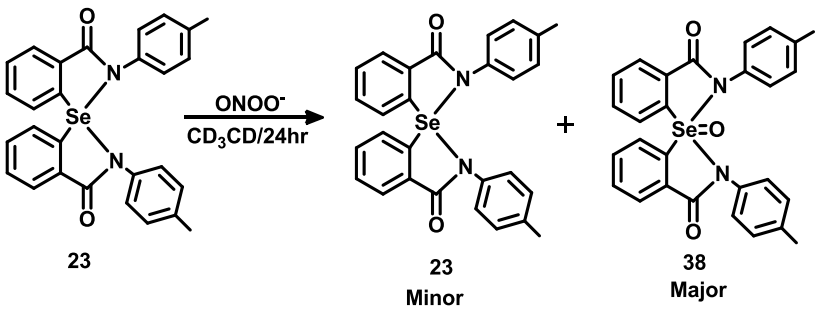


Figure-S33. ^{13}C NMR spectra of pure compound **34** in $CDCl_3$.



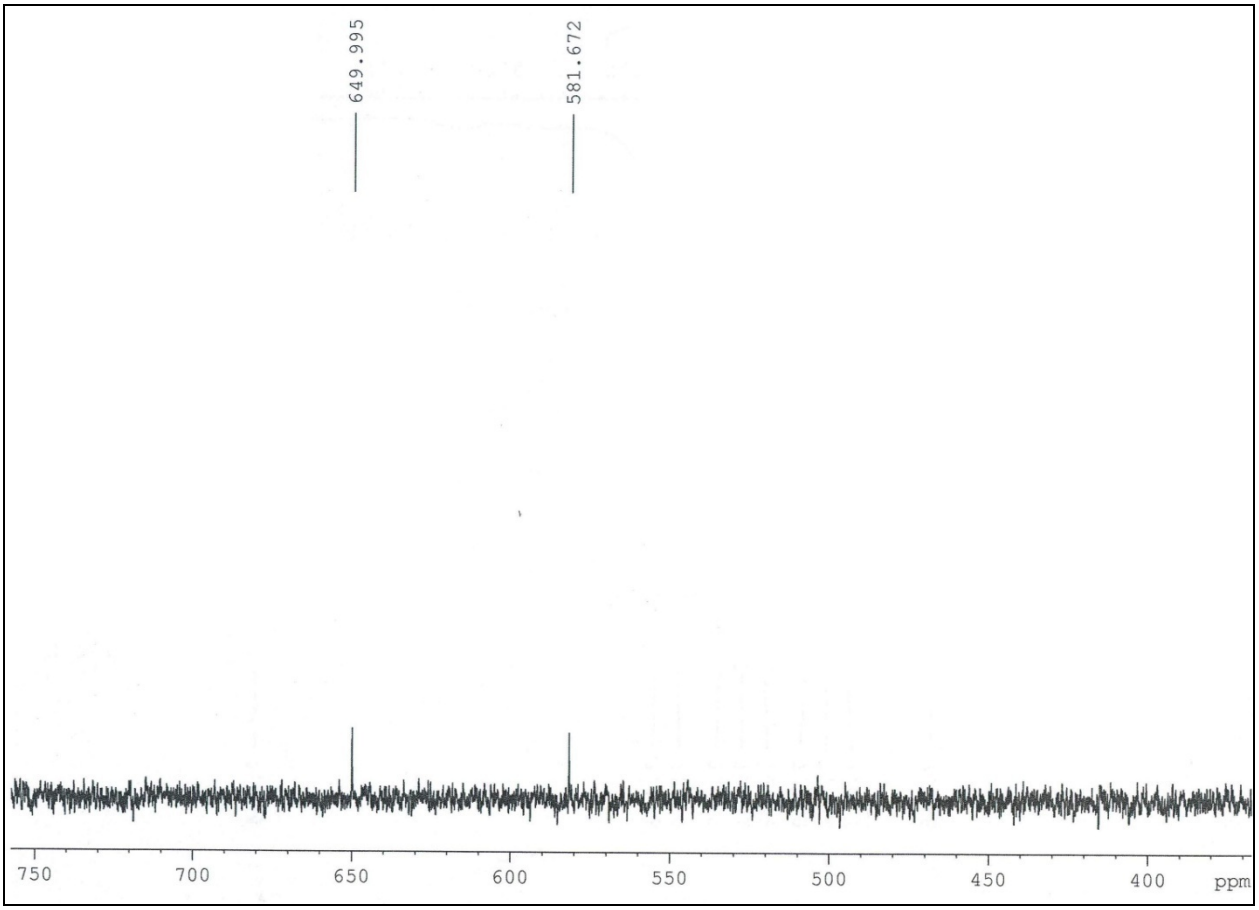
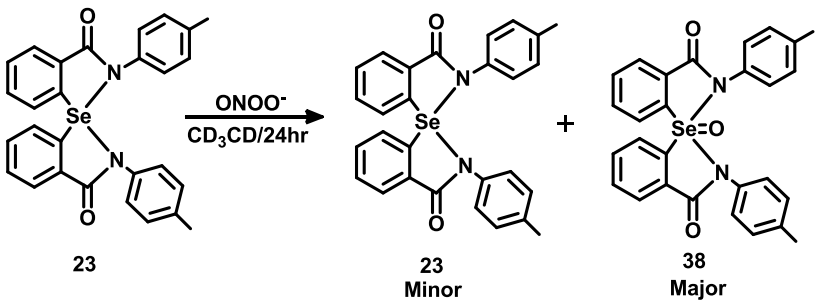


Figure-S34. ^{77}Se NMR spectrum recorded (in CD_3OD) after the addition of 2 equiv of PN to the spirodiazaselenurane **23** indicating the formation of **23** and **38** after 24 h.



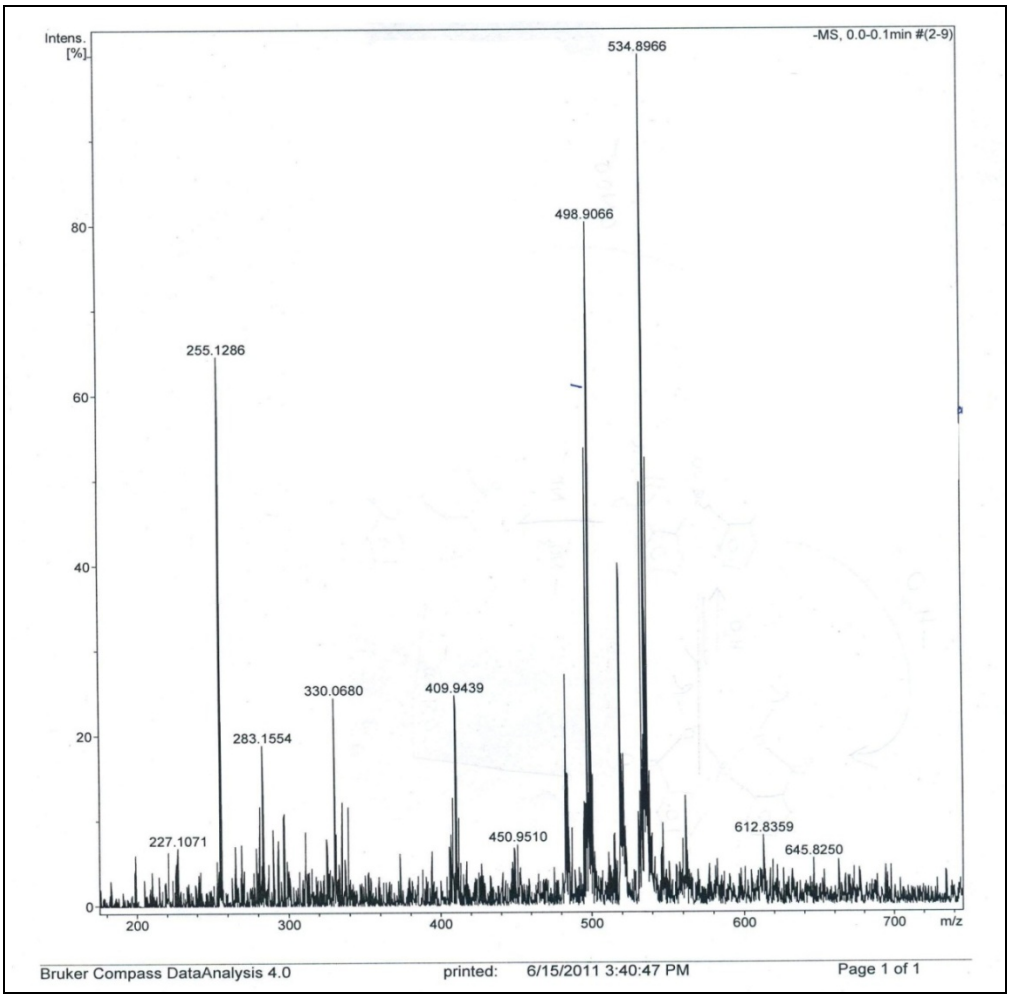


Figure-S35. ESI–Mass spectrum obtained for the reaction of spirodiazaselenurane **23** with 2 equiv of PN, indicating the formation of compounds **23** and **38**. Calculated Mass (M) $^{+}$: 497.47, Observed Mass:498.906 for the compound **23,** for the compound **38**, Calculated Mass (M) $^{+}$: 514.48, Observed Mass:534.895$(M+Na)^{+}$.