Electronic Supplementary Material (ESI) for Organic & Biomolecular Chemistry

Supporting Information

For

Inhibition of Peroxynitrite- and Peroxidase-mediated Protein Tyrosine Nitration by Imidazole-based Thiourea and Selenourea Derivatives

by

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Table S1. Inhibitory activities of selenourea compounds **2**, **6**, **15**, **17**, **19**, **21** and **23** towards PN-mediated nitration of BSA.

Compound	% Nitration of BSA
2	66 ± 4.2
6	82 ± 9.2
15	29 ± 4.9
17	50 ± 6.3
19	56 ± 6.3
21	45 ± 4.3
23	71 ± 4.8

Table S2. Inhibitory activities of thiourea compounds **1**, **5**, **14**, **16**, **18** and **20** towards PN-mediated nitration of BSA.

Compound	% Nitration of BSA
1	32.5 ± 2.1
5	66.5 ± 3.5
14	68.4 ± 2.1
16	64.0 ± 1.1
18	60.0 ± 2.8
20	78.0 ± 1.4

Table S3. Inhibitory activities of selenourea compounds **2**, **6**, **15**, **17**, **19**, **21** and **23** towards LPO-catalyzed nitration of BSA.

Compound	% Nitration of BSA
2	43.0 ± 5.6
6	49.5 ± 4.9
15	52.5 ± 6.3
17	67.0 ± 1.3
19	76.5 ± 7.7
21	79.4 ± 7.7
23	81.5 ± 4.9

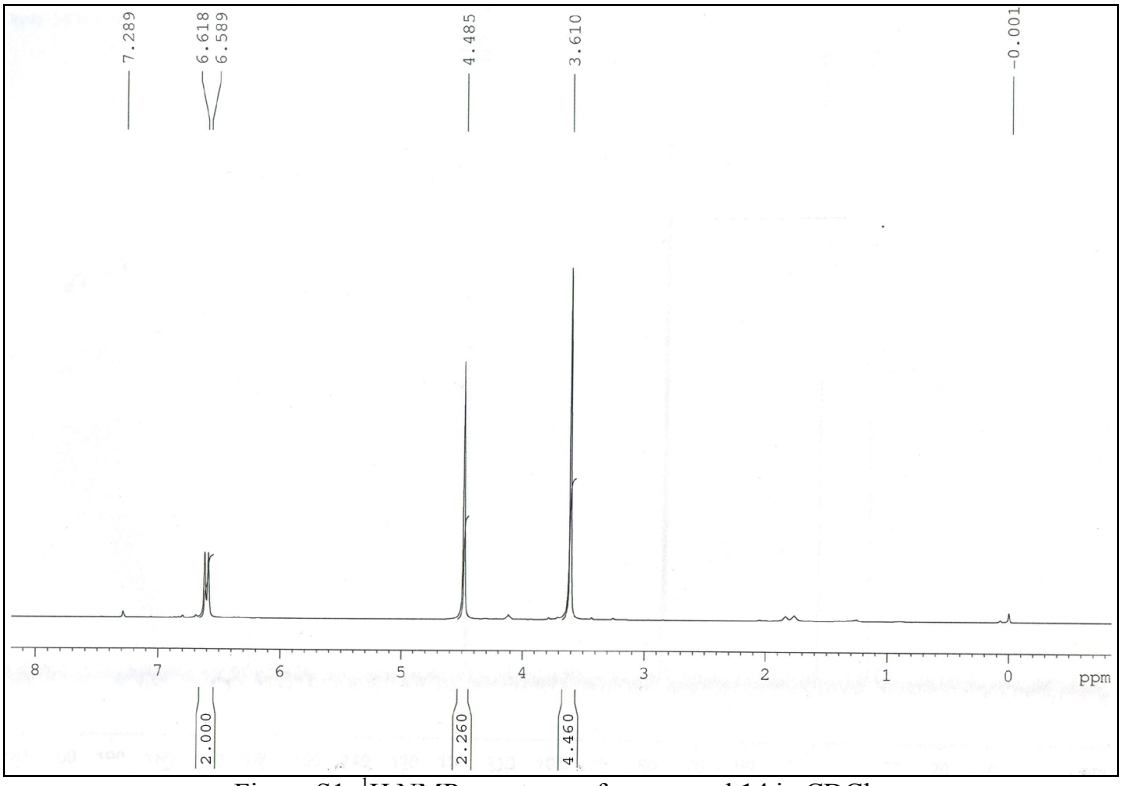

Figure S1. ^{1}H NMR spectrum of compound **14** in $CDCl_3$.

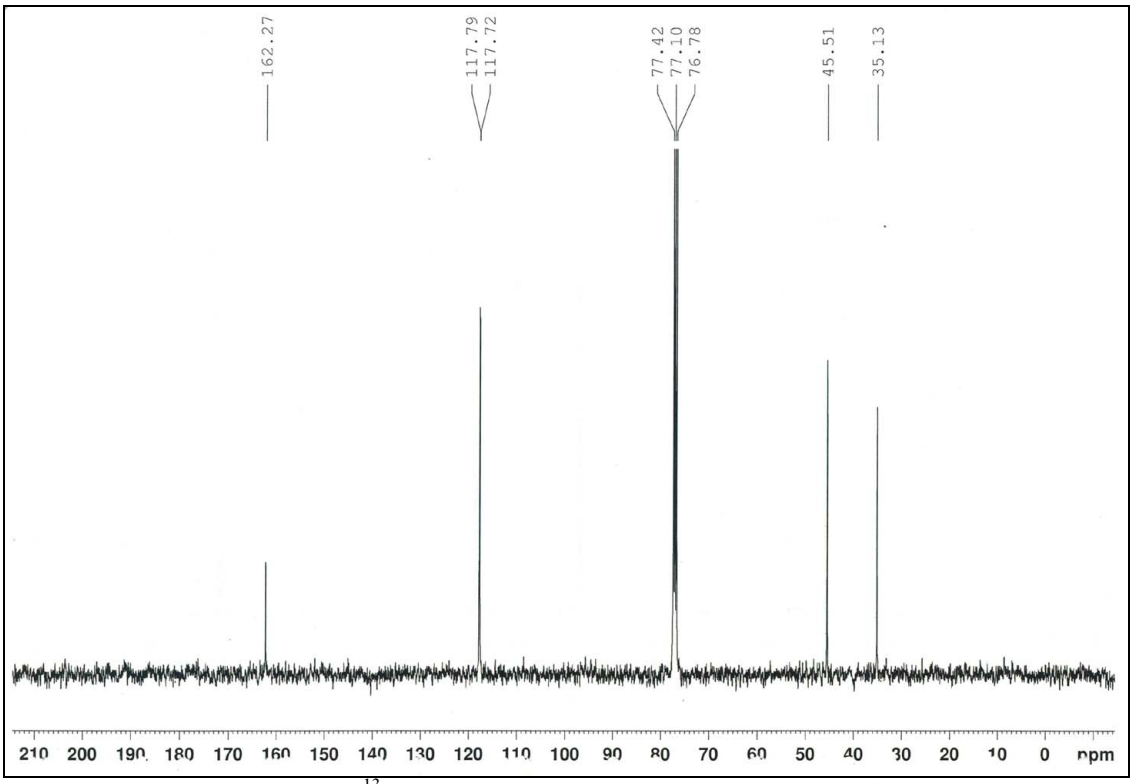

Figure S2. ^{13}C NMR spectrum of compound **14** in $CDCl_3$.

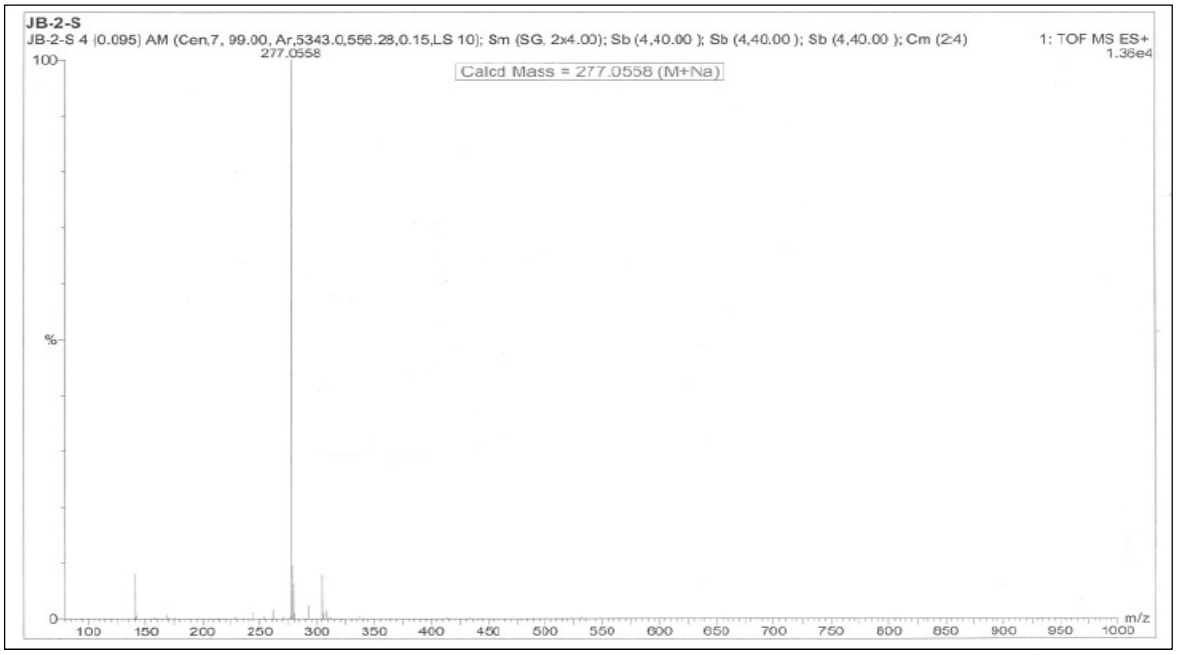

Figure S3. ESI-MS spectrum of compound **14**. Calculated mass $(M+Na)^+$: 277.0558; observed mass: 277.0558.

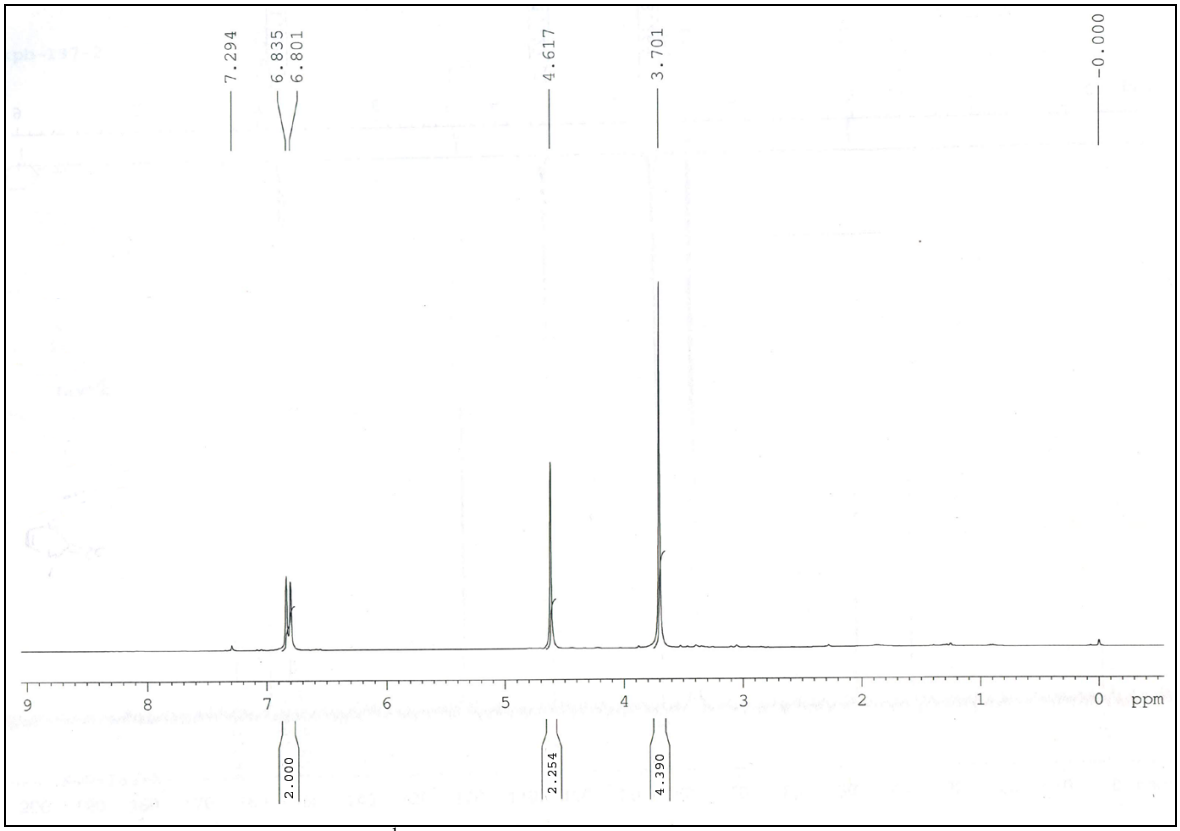

Figure S4. ^{1}H NMR spectrum of compound **15** in $CDCl_3$.

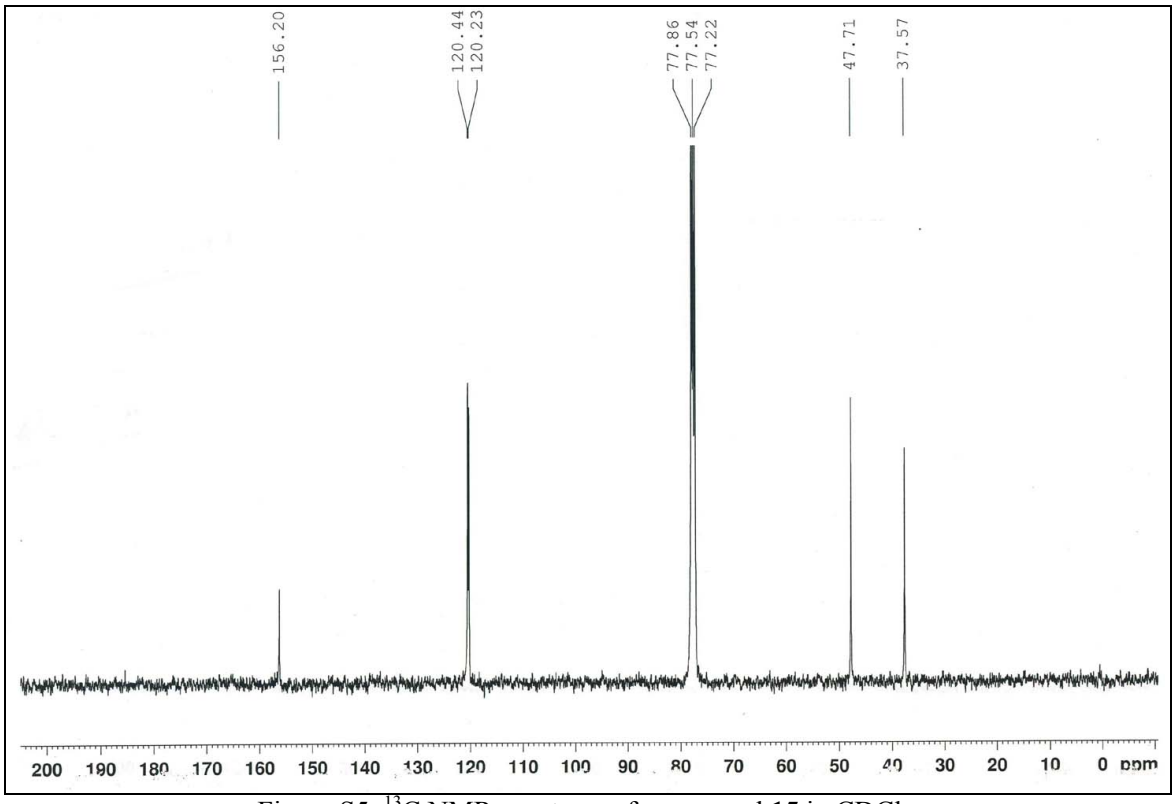

Figure S5. ^{13}C NMR spectrum of compound **15** in $CDCl_3$.

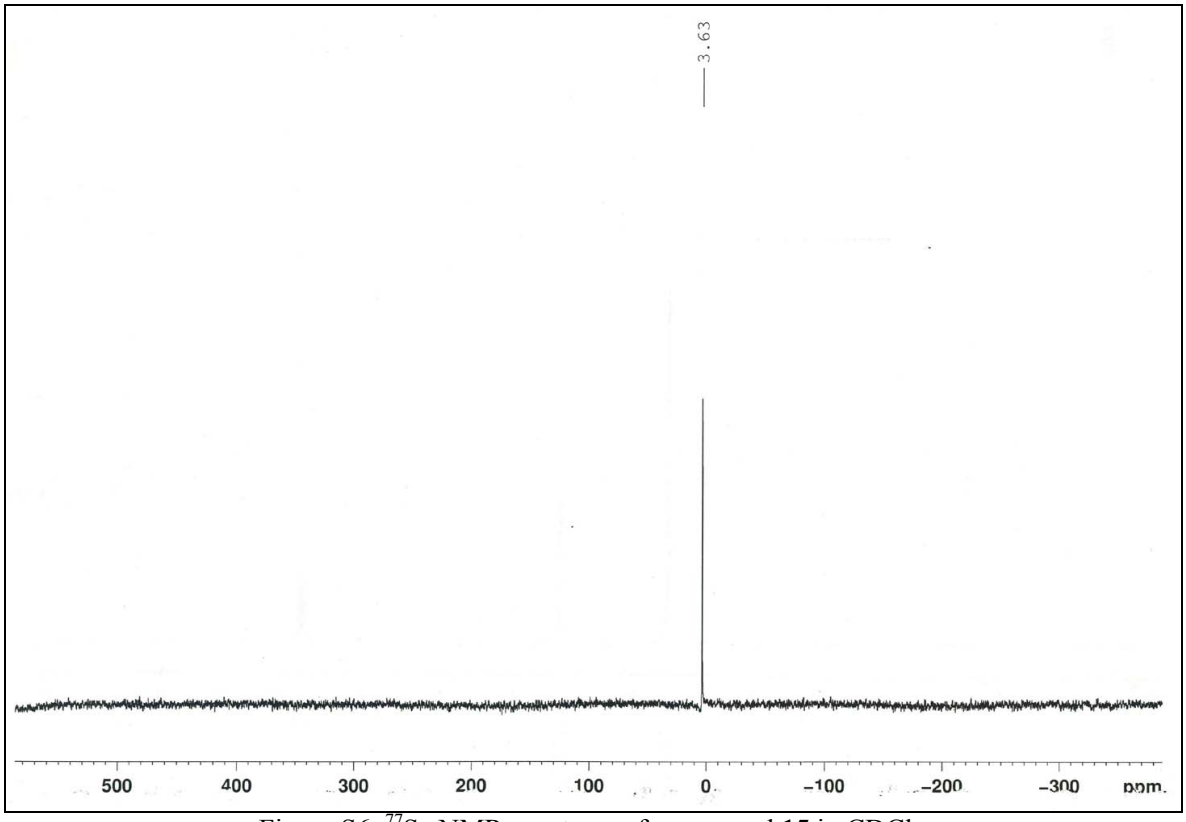

Figure S6. ^{77}Se NMR spectrum of compound **15** in $CDCl_3$.

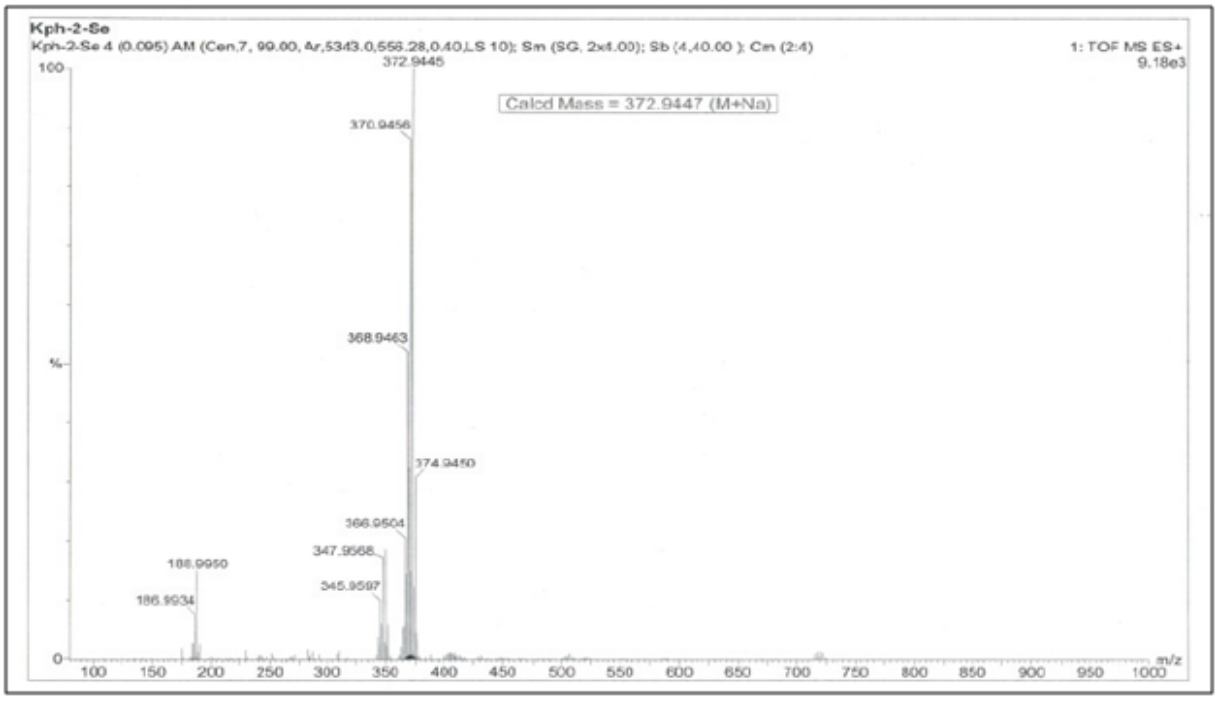

Figure S7. ESI-MS spectrum of compound **15**. Calculated mass $(M+Na)^+$: 372.9447; observed mass: 372.9445.

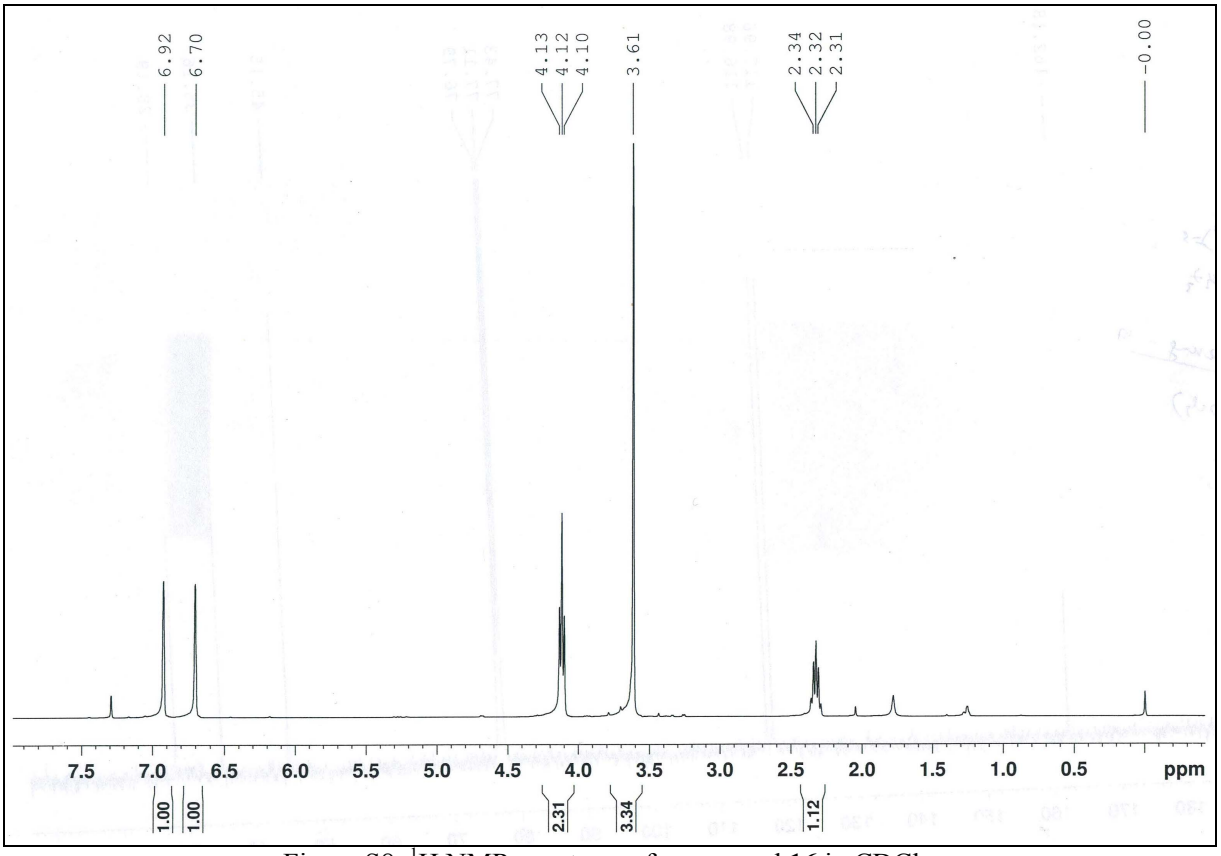

Figure S8. ^{1}H NMR spectrum of compound **16** in $CDCl_3$.

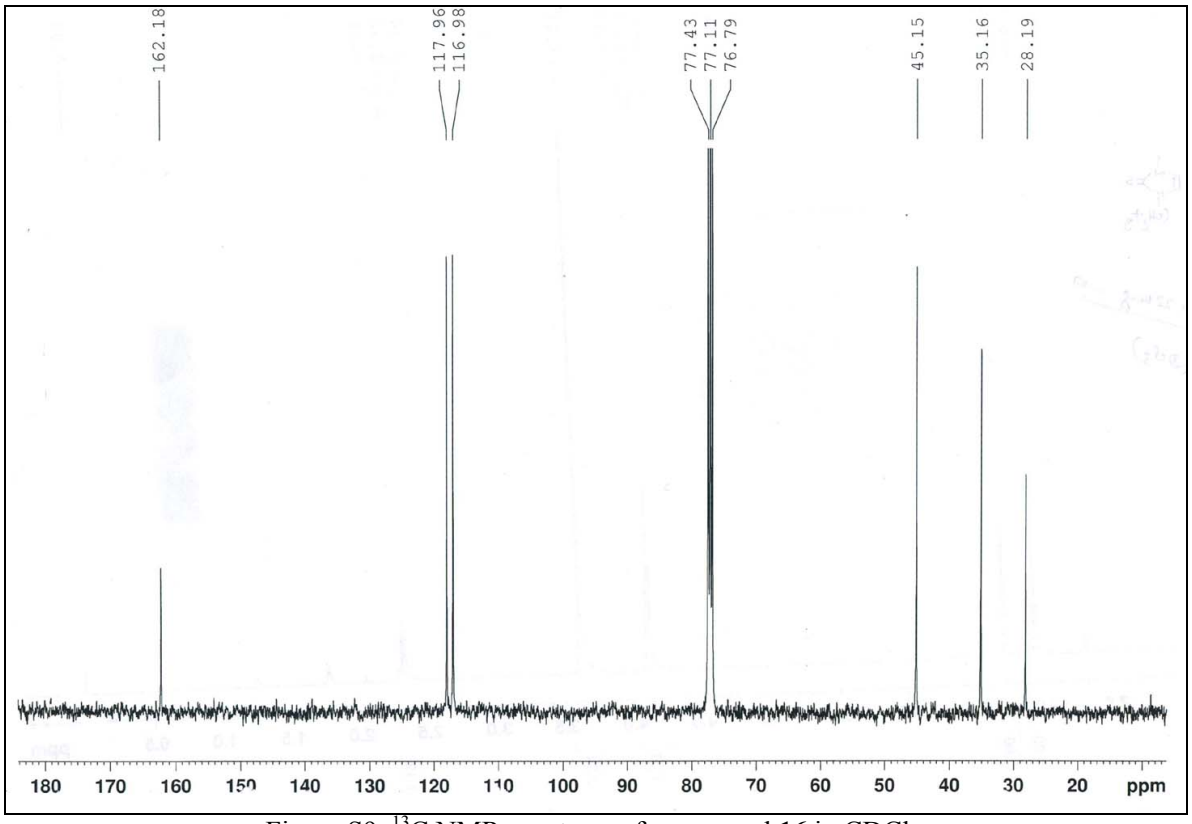

Figure S9. ^{13}C NMR spectrum of compound **16** in $CDCl_3$.

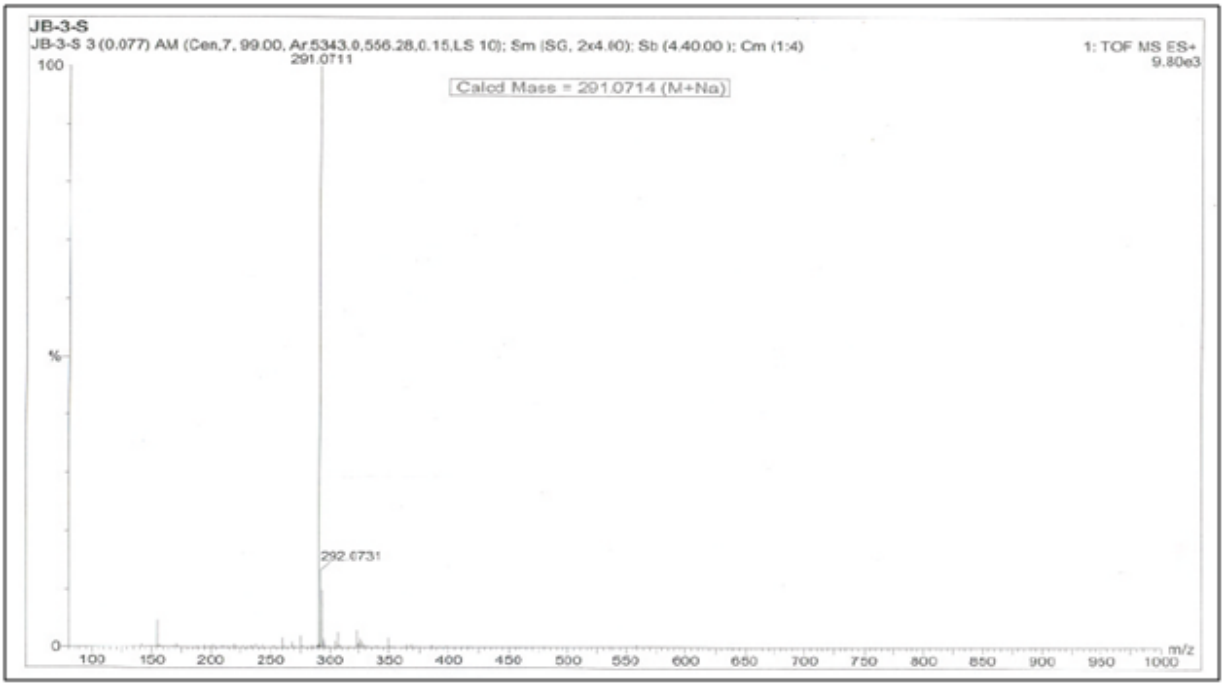

Figure S10. ESI-MS spectrum of compound **16**. Calculated mass $(M+Na)^+$: 291.0714; observed mass: 291.0711.

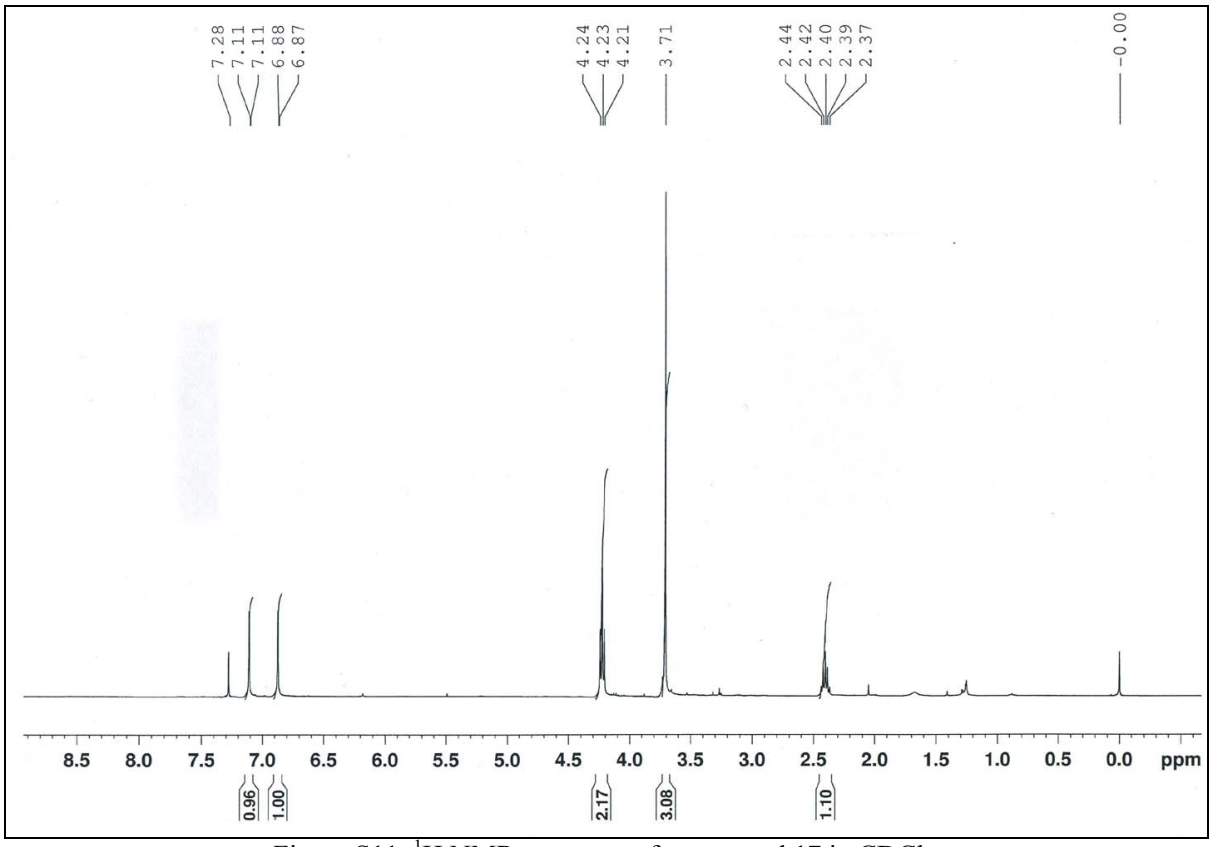

Figure S11. ^{1}H NMR spectrum of compound **17** in $CDCl_3$.

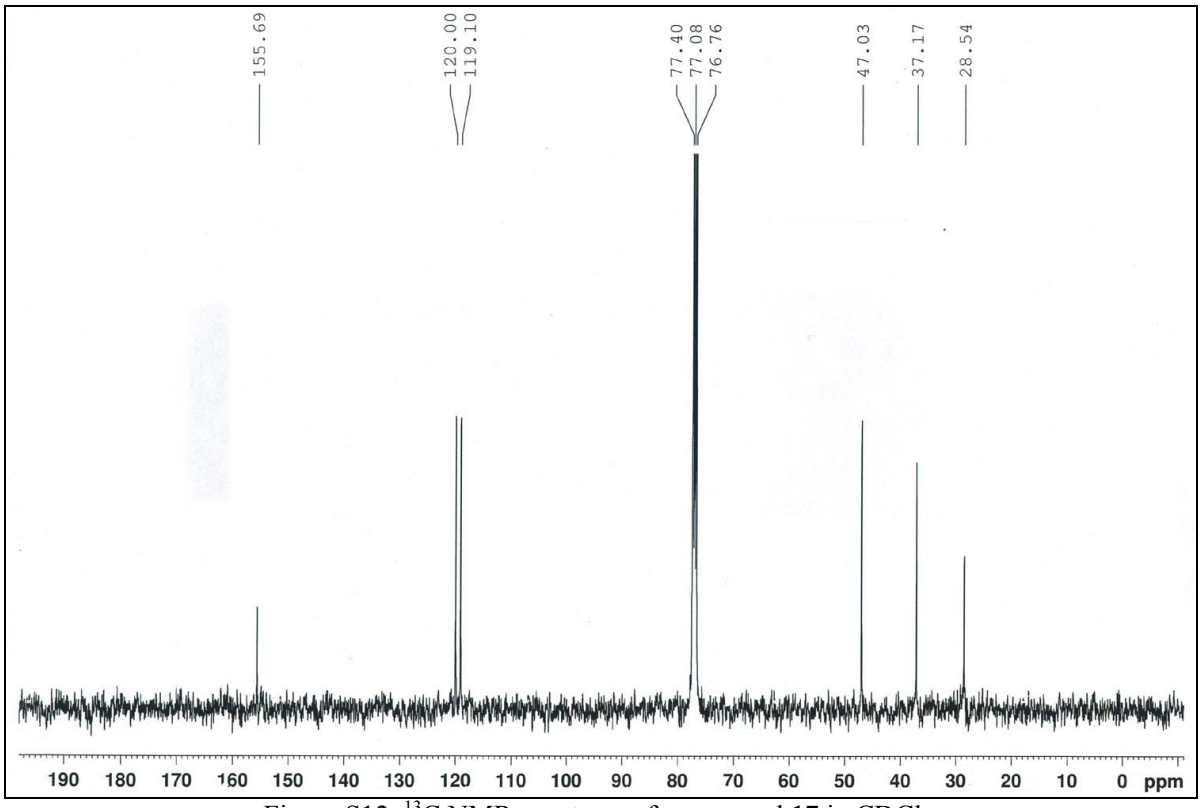

Figure S12. ^{13}C NMR spectrum of compound **17** in $CDCl_3$.

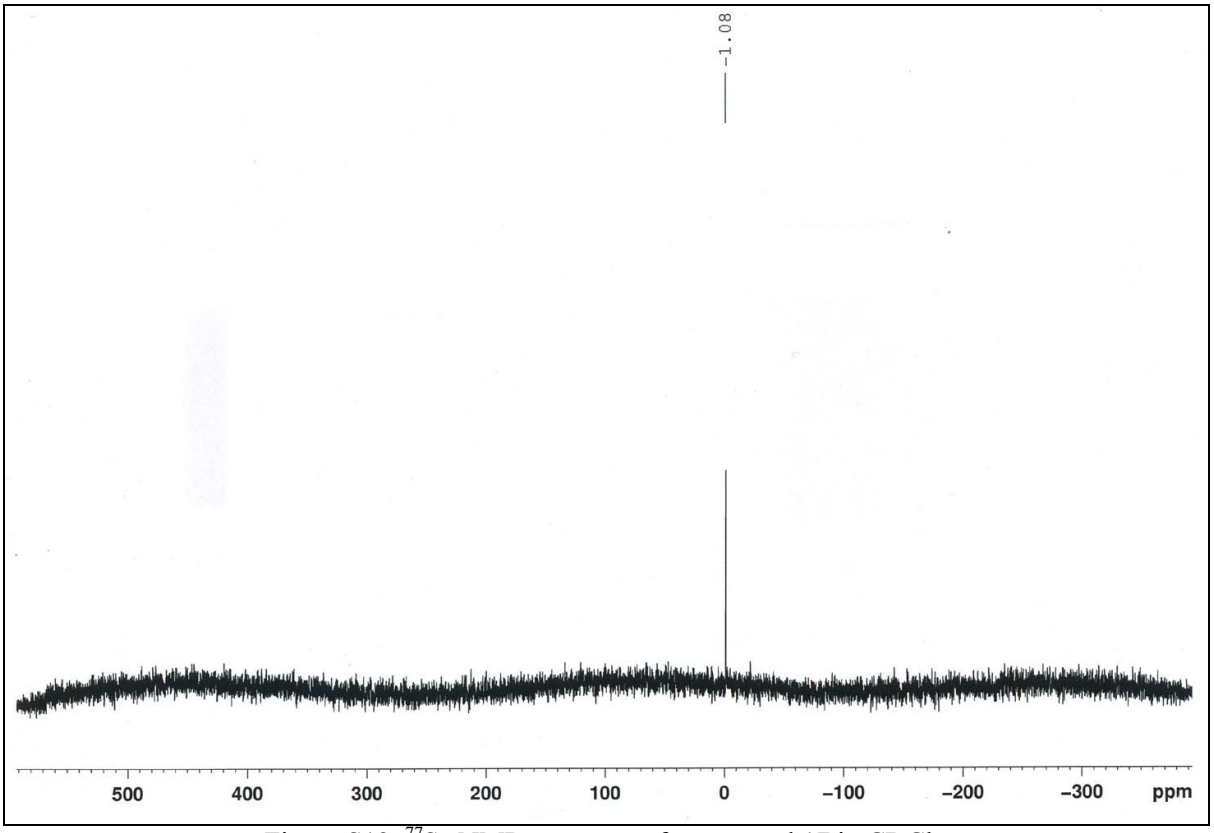

Figure S13. ^{77}Se NMR spectrum of compound **17** in $CDCl_3$.

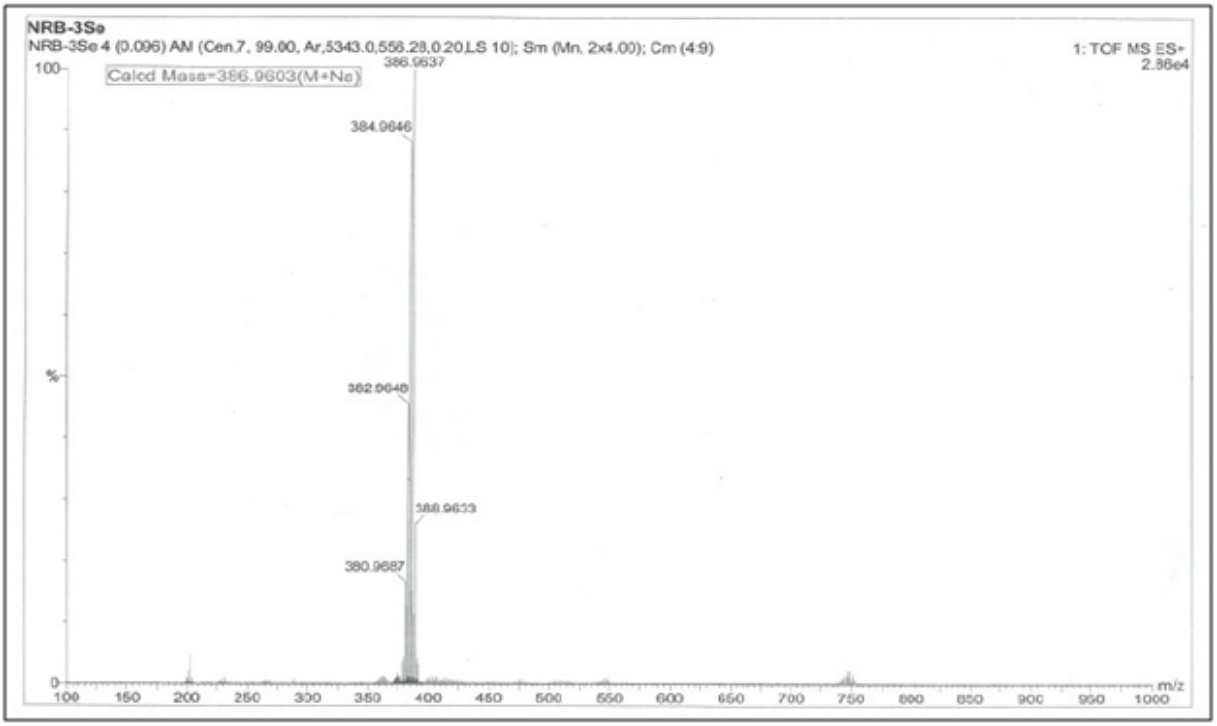

Figure S14. ESI-MS spectrum of compound **17**. Calculated mass $(M+Na)^+$: 386.9603; observed mass: 386.9637.

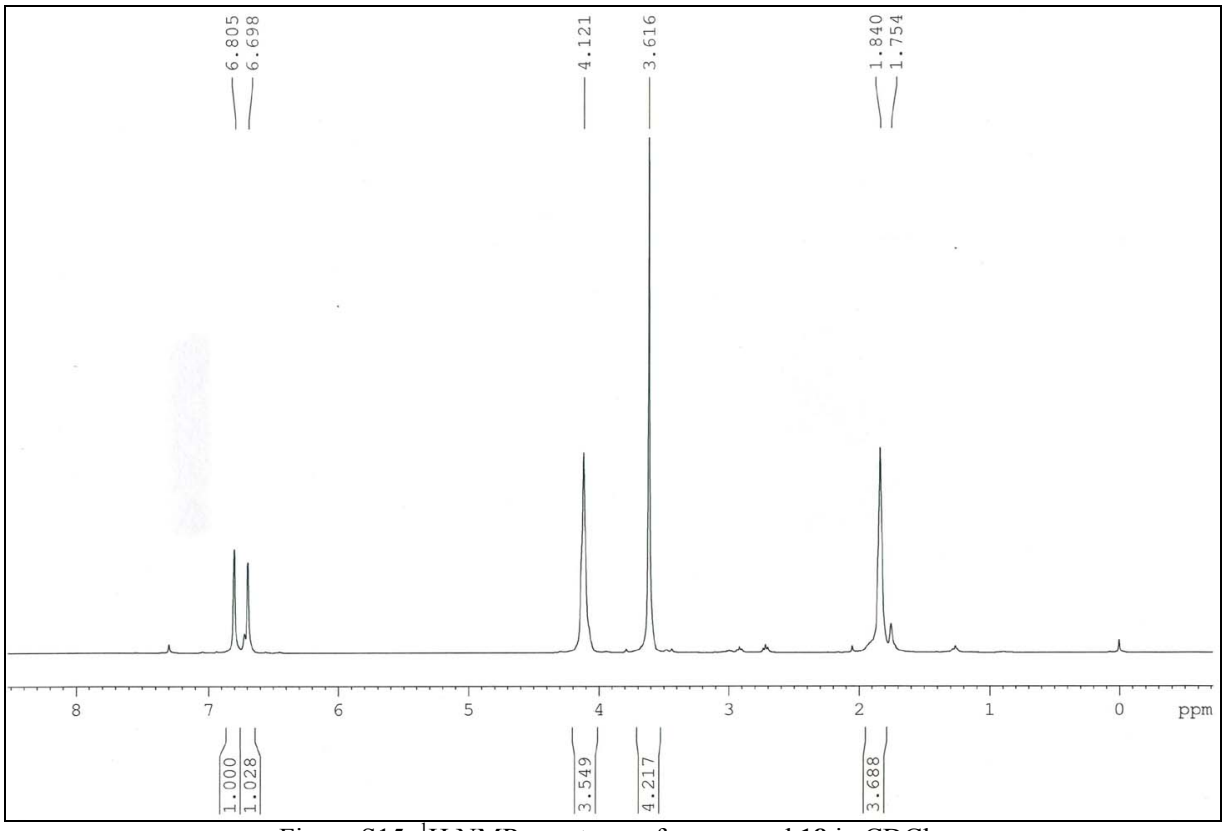

Figure S15. ^{1}H NMR spectrum of compound **18** in $CDCl_3$.

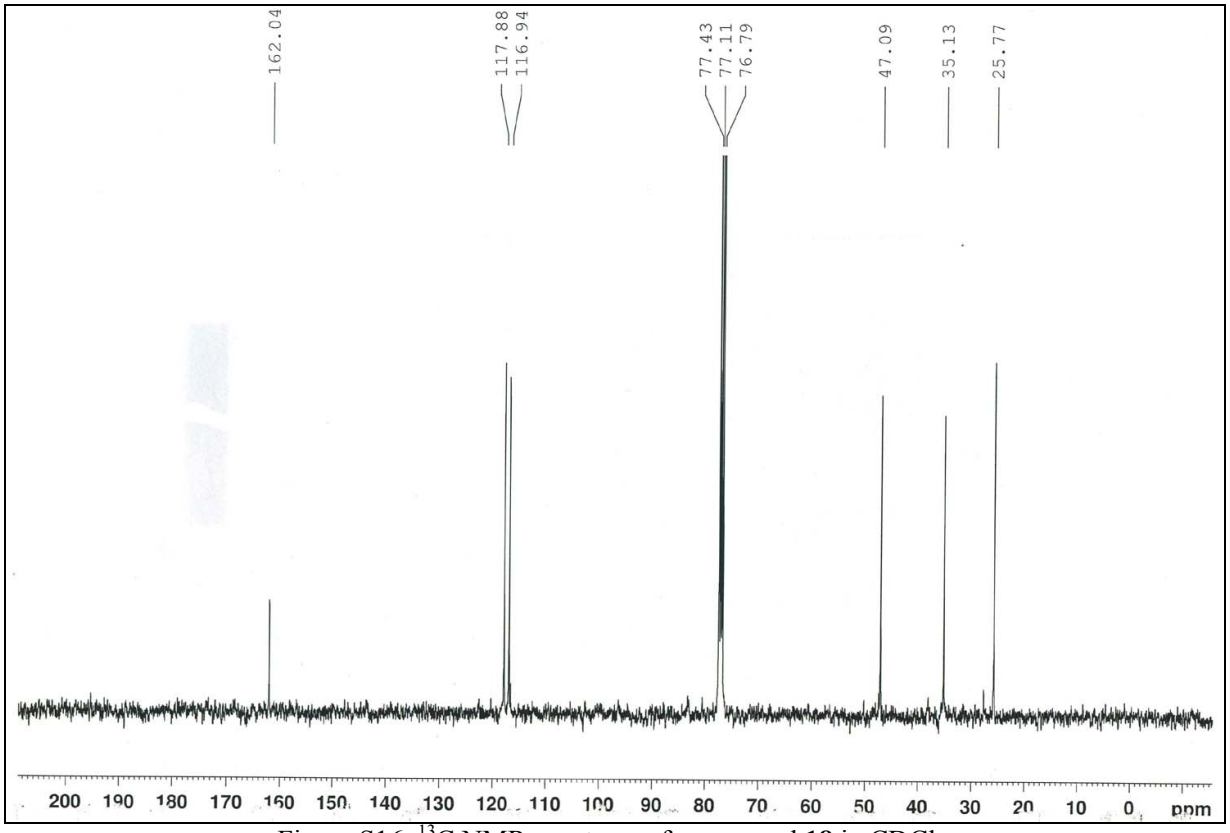

Figure S16. ^{13}C NMR spectrum of compound **18** in $CDCl_3$.

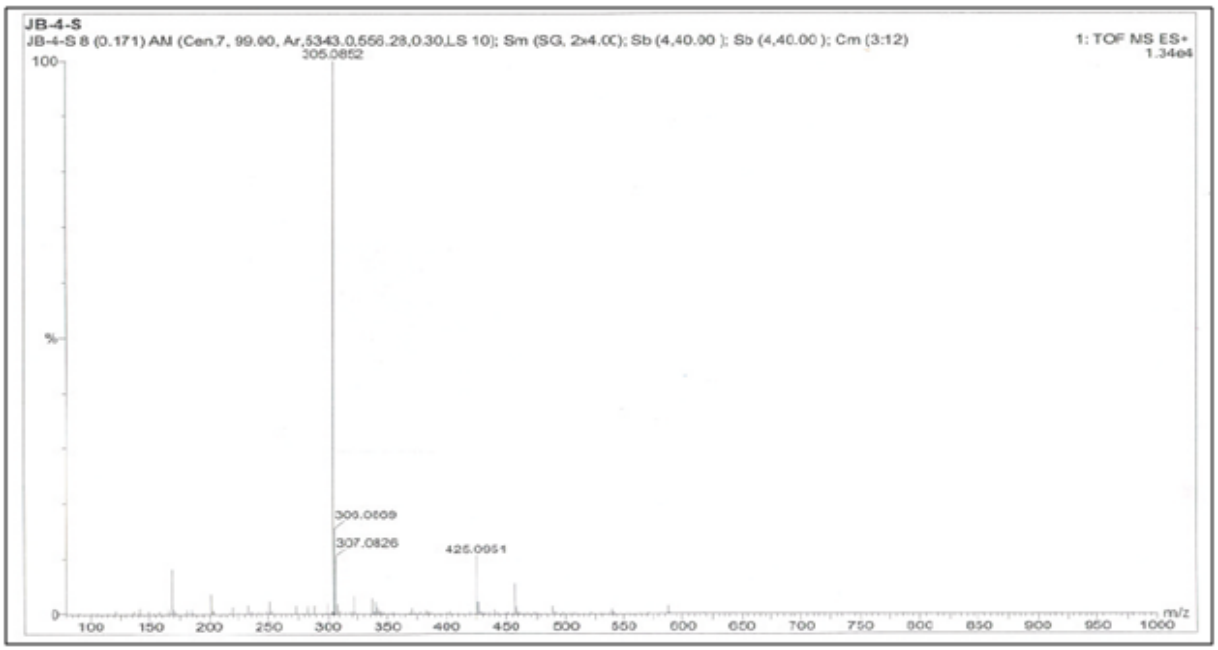

Figure S17. ESI-MS spectrum of compound **18**. Calculated mass $(M+Na)^+$: 305.0851; observed mass: 305.0852.

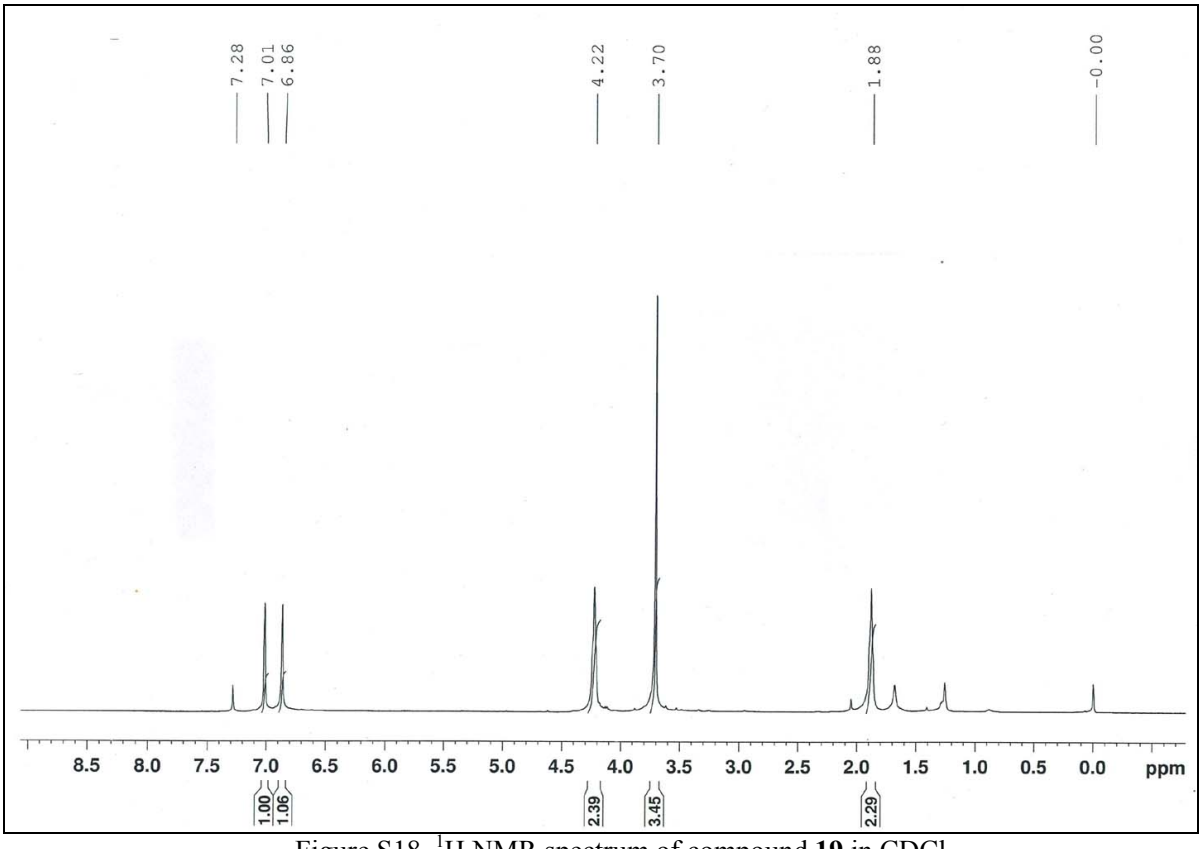

Figure S18. ^{1}H NMR spectrum of compound **19** in $CDCl_3$.

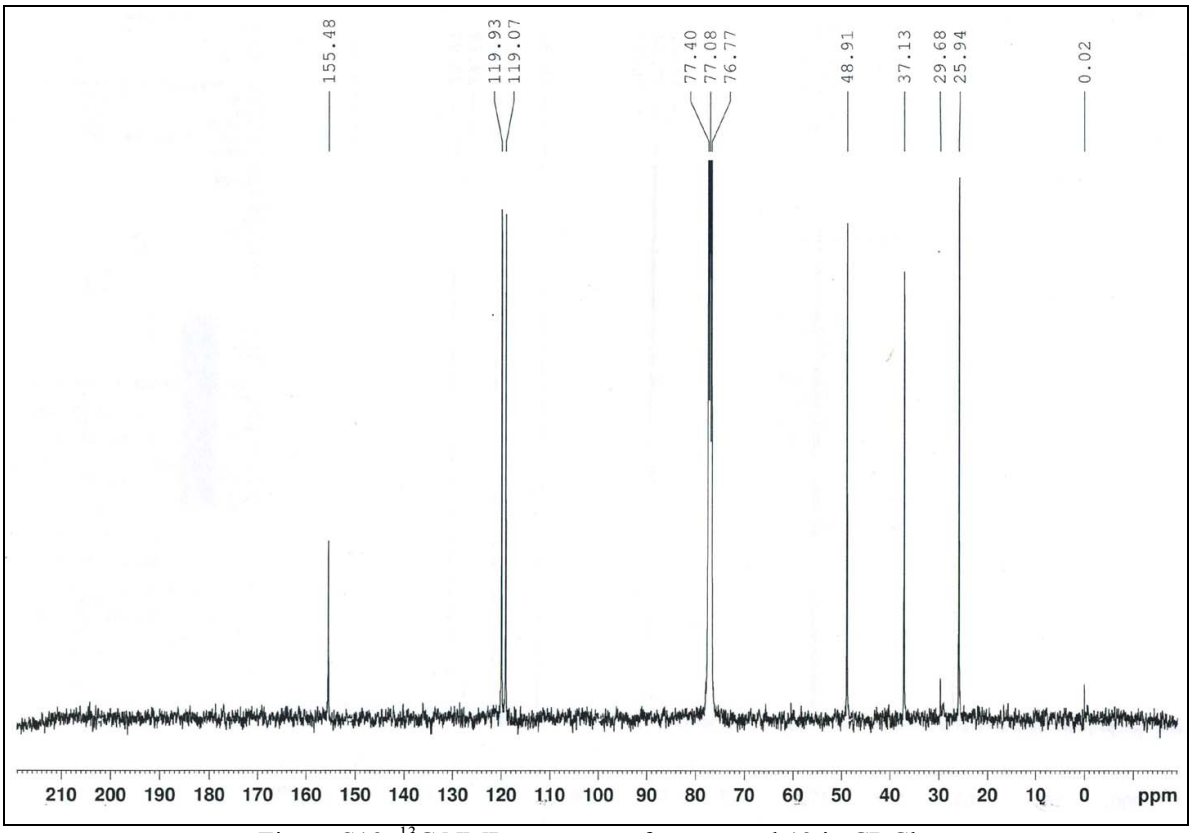

Figure S19. ^{13}C NMR spectrum of compound **19** in $CDCl_3$.

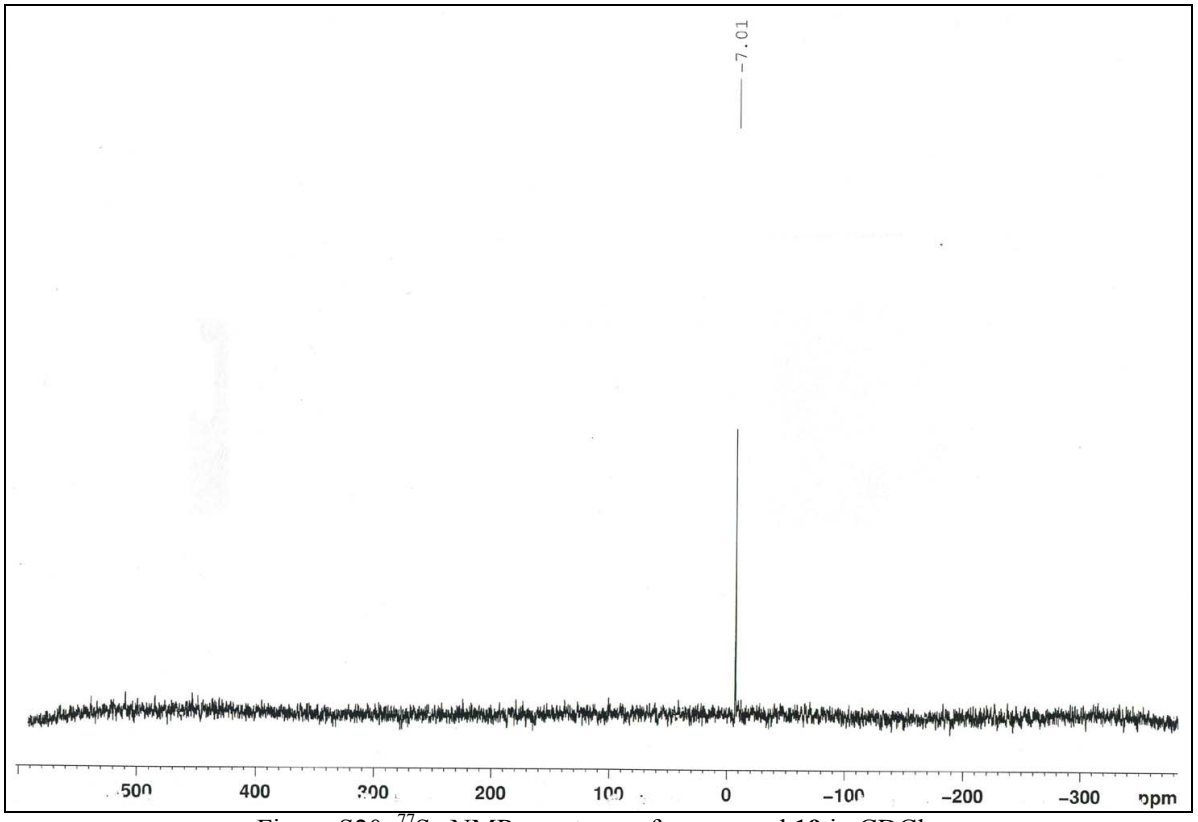

Figure S20. ^{77}Se NMR spectrum of compound **19** in $CDCl_3$.

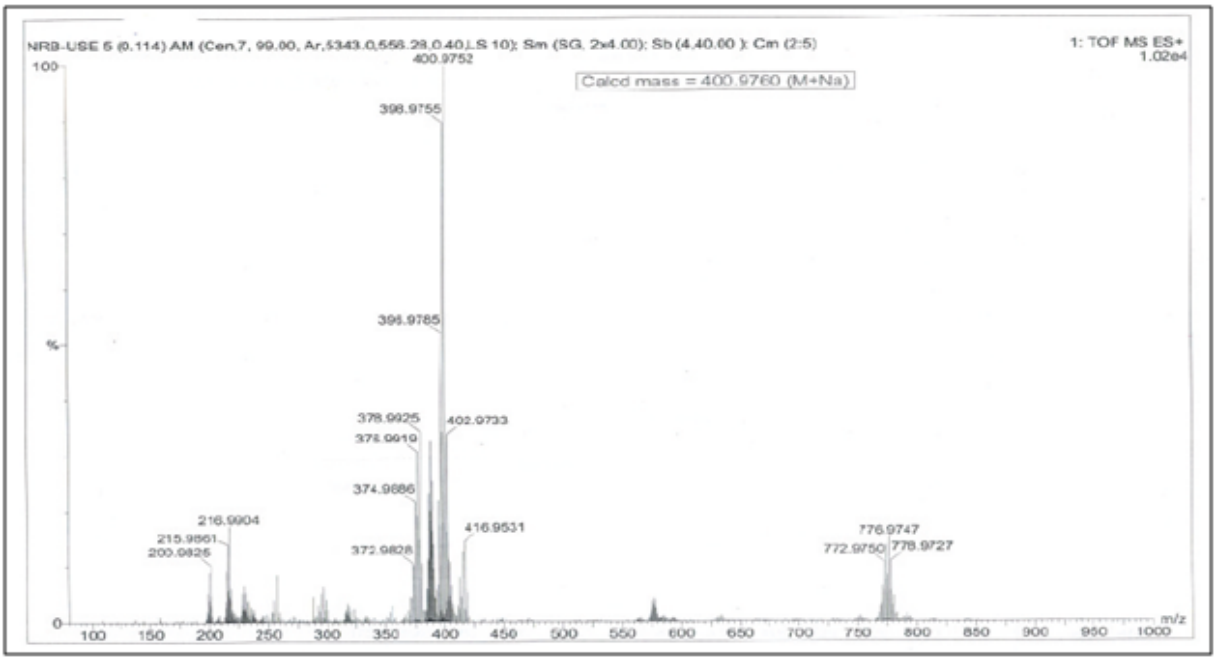

Figure S21. ESI-MS spectrum of compound **19**. Calculated mass $(M+Na)^+$: 400.9760; observed mass: 400.9752.

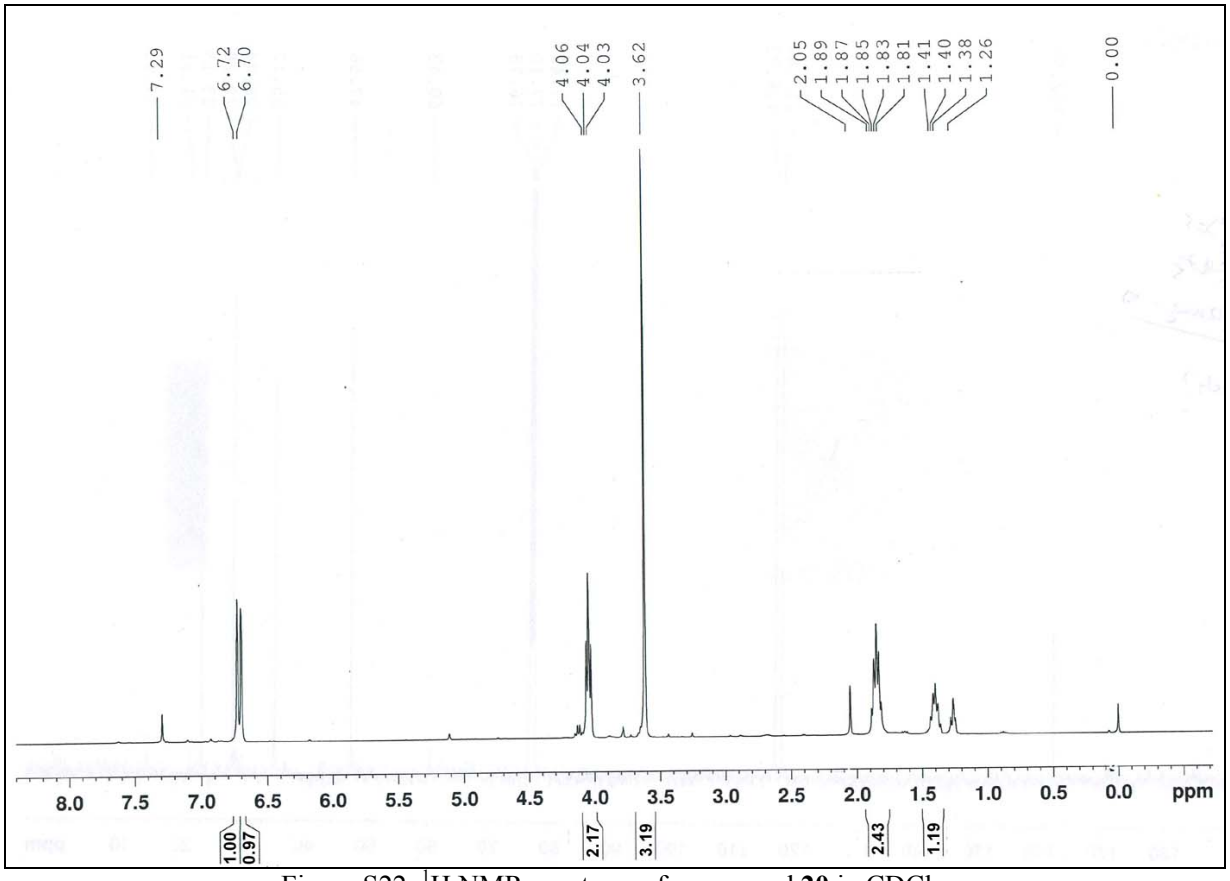

Figure S22. ^{1}H NMR spectrum of compound **20** in $CDCl_3$.

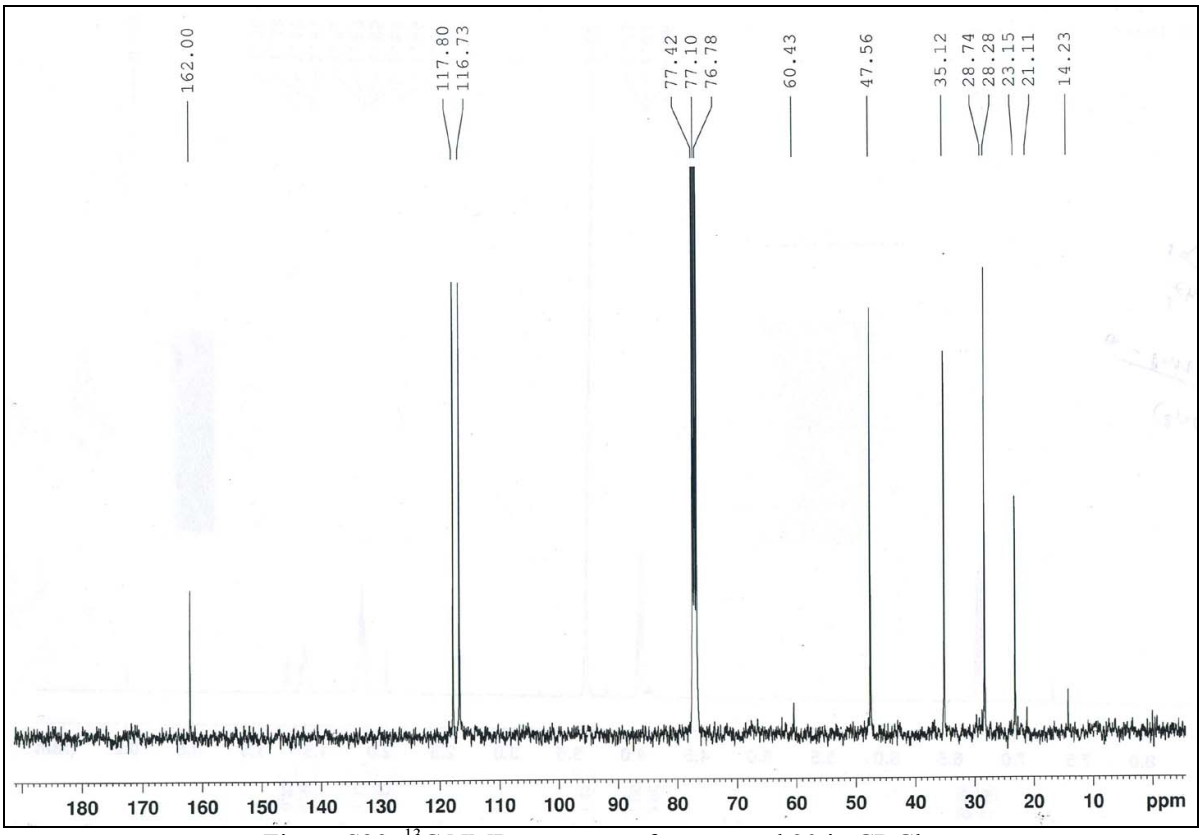

Figure S23. ^{13}C NMR spectrum of compound **20** in $CDCl_3$.

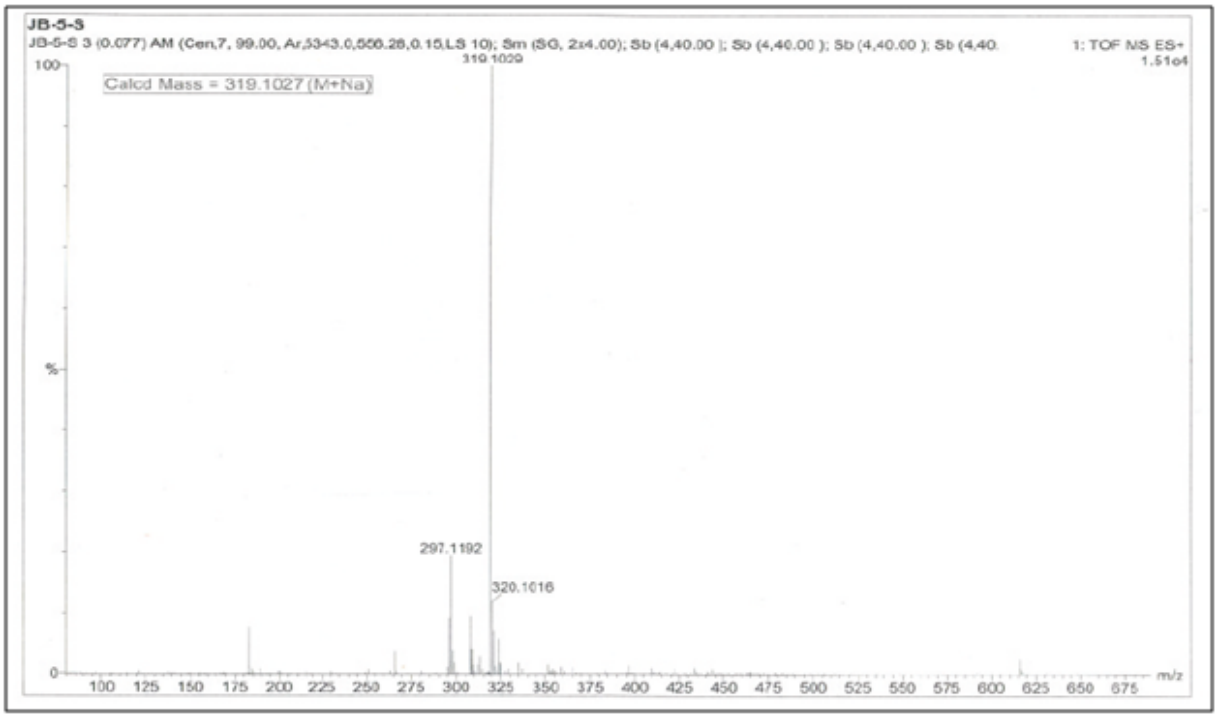

Figure S24. ESI-MS spectrum of compound **20**. Calculated mass $(M+Na)^+$: 319.1027; observed mass: 319.1029.

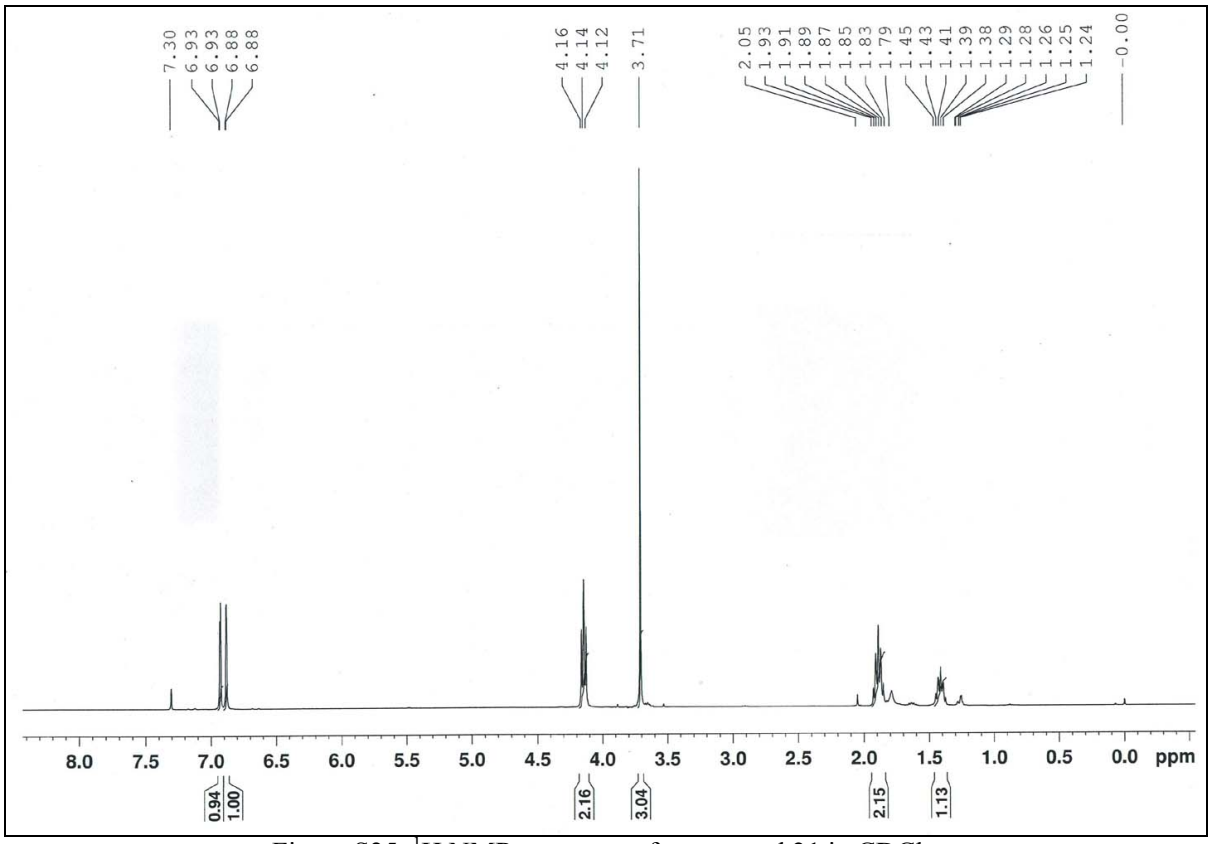

Figure S25. ^{1}H NMR spectrum of compound **21** in $CDCl_3$.

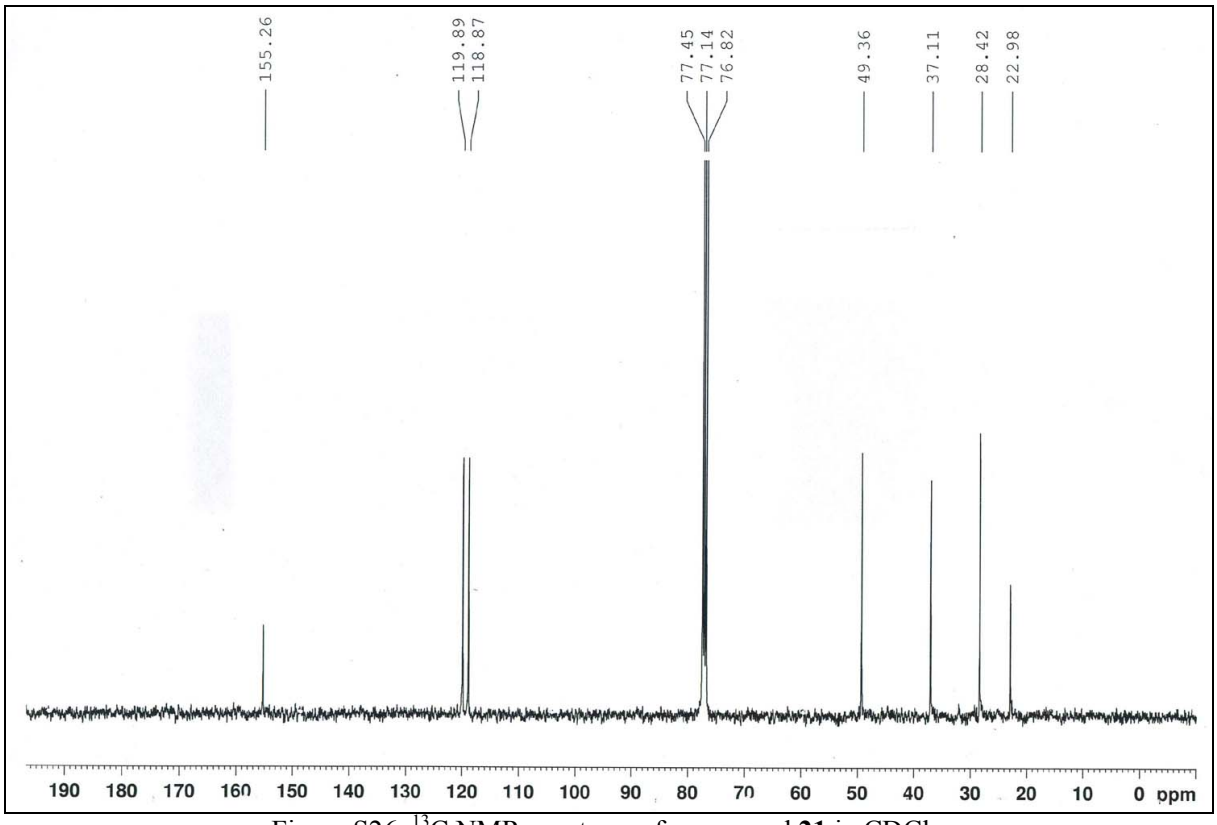

Figure S26. ^{13}C NMR spectrum of compound **21** in $CDCl_3$.

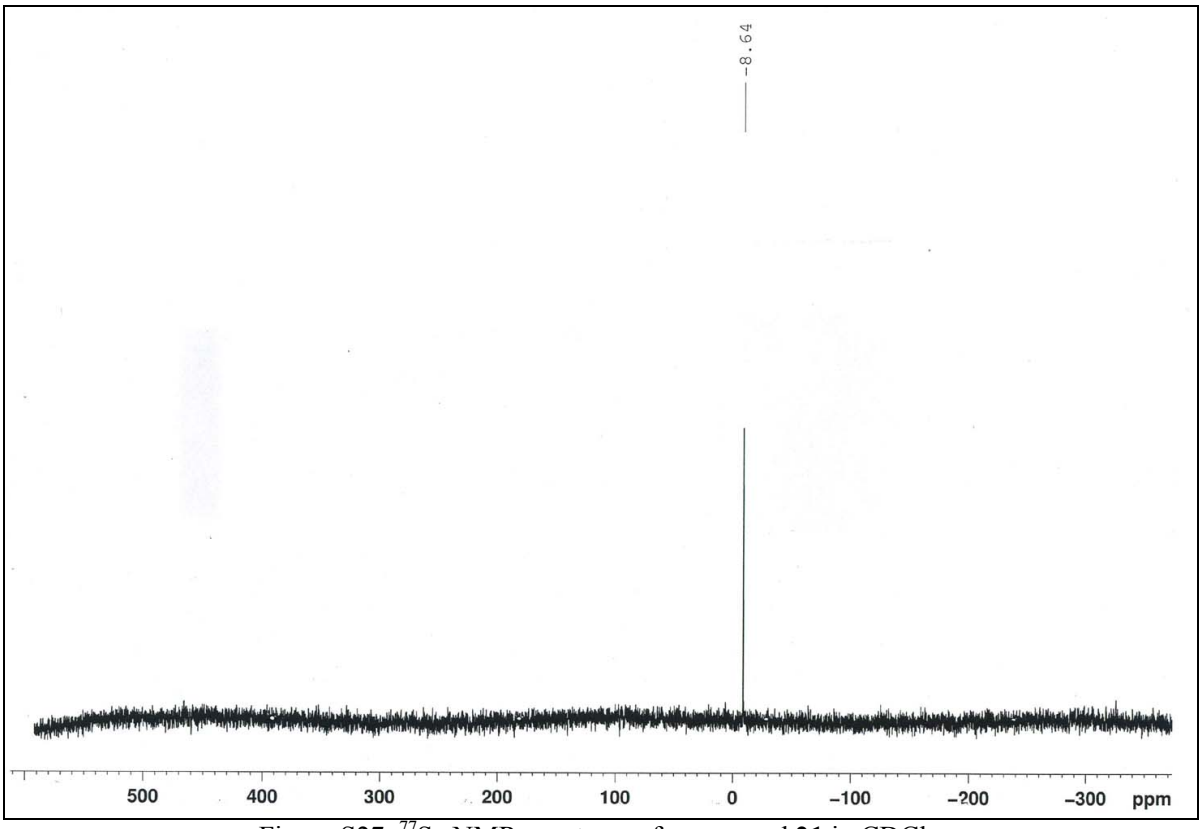

Figure S27. ^{77}Se NMR spectrum of compound **21** in $CDCl_3$.

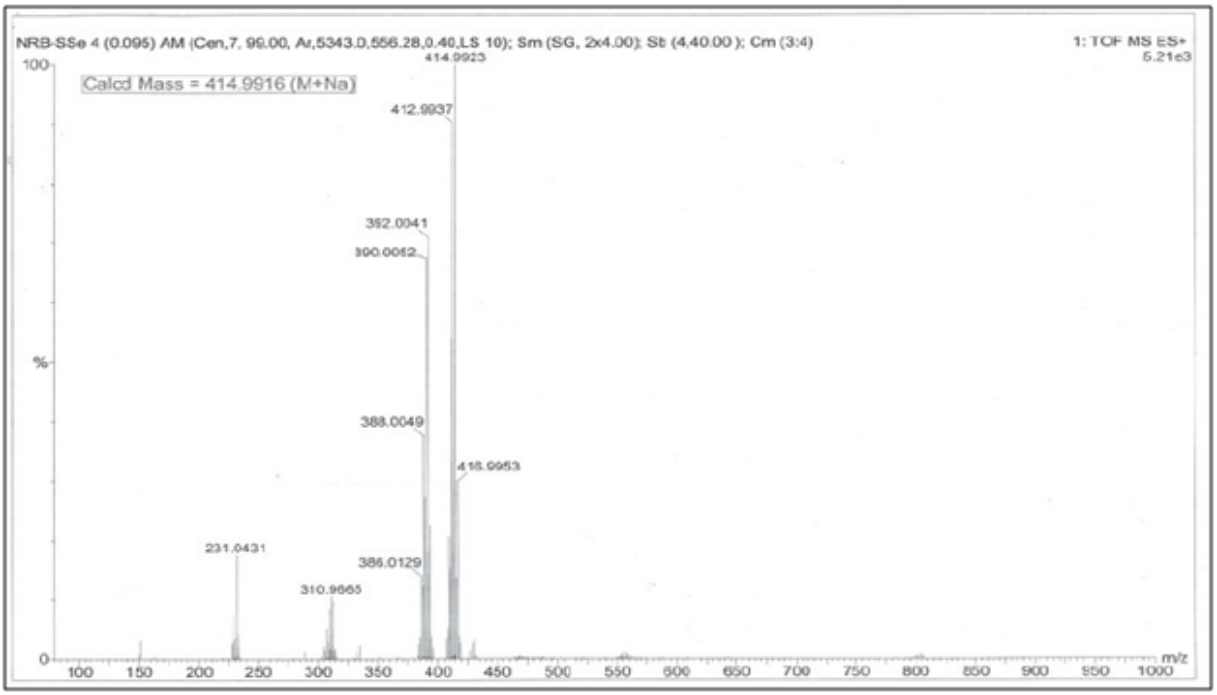

Figure S28. ESI-MS spectrum of compound **21**. Calculated mass $(M+Na)^+$: 414.9916; observed mass: 414.9923.

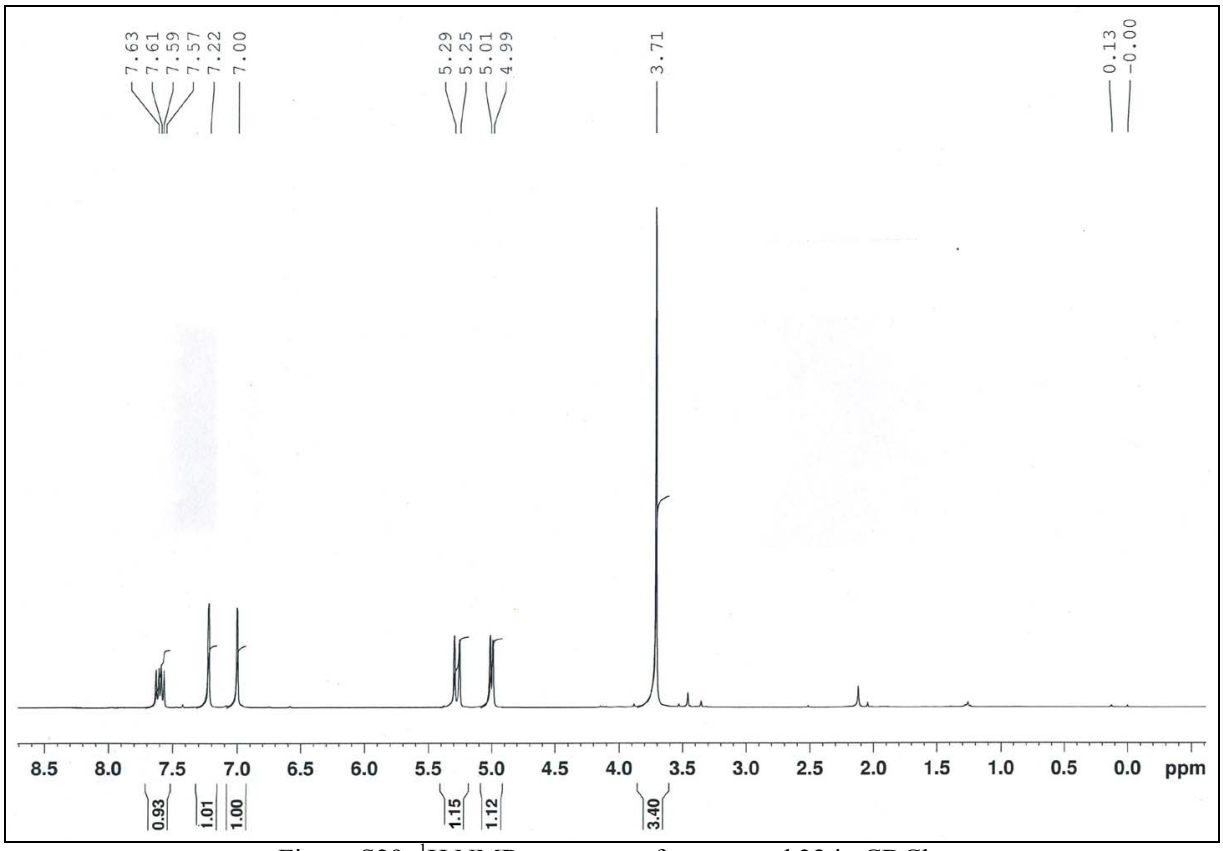

Figure S29. ^{1}H NMR spectrum of compound **23** in $CDCl_3$.

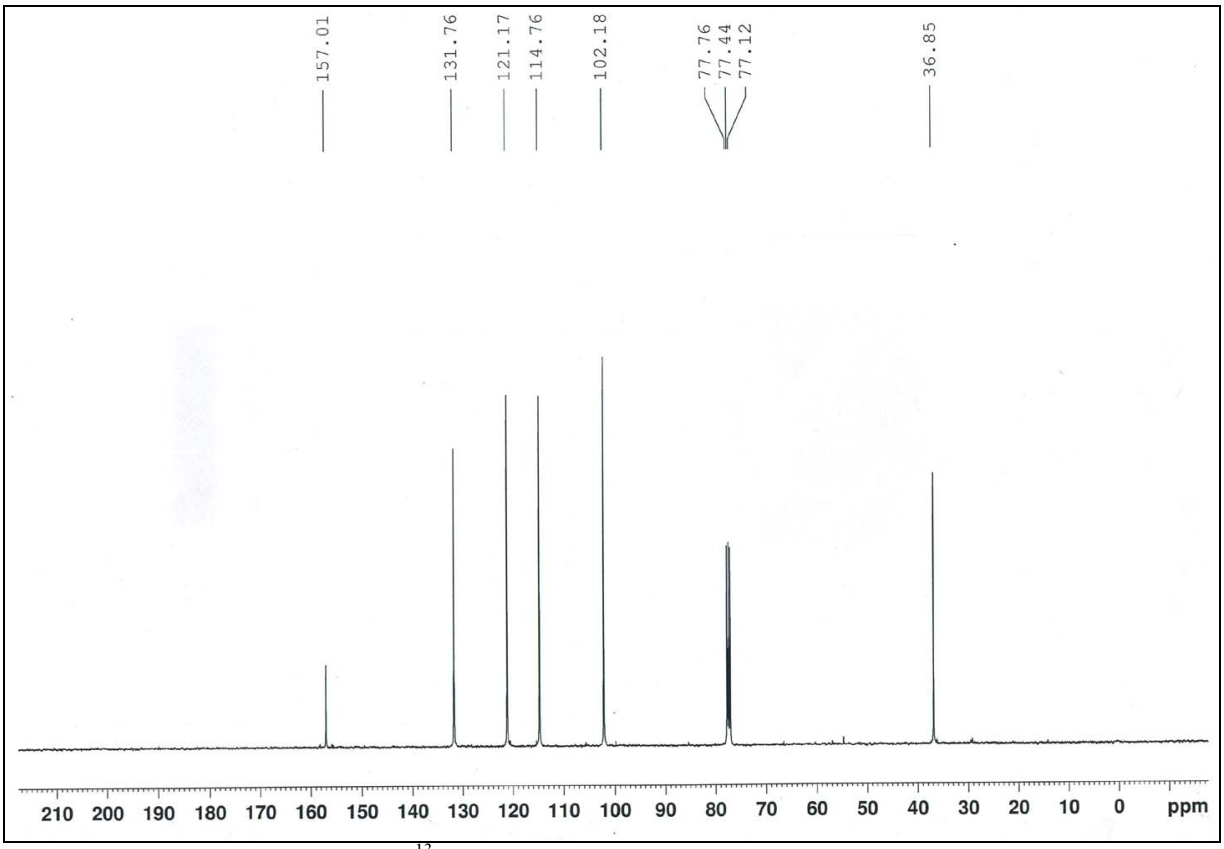

Figure S30. ^{13}C NMR spectrum of compound **23** in $CDCl_3$.

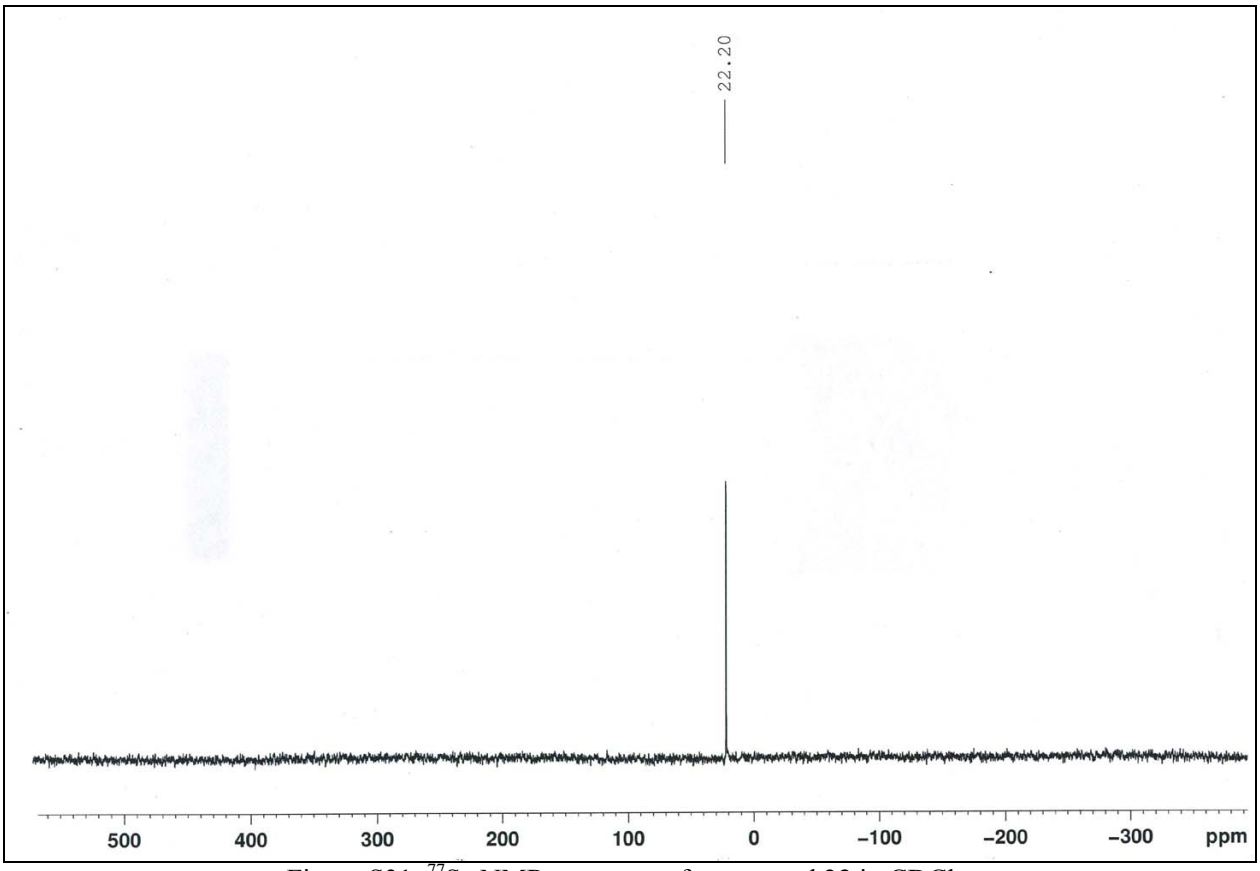

Figure S31. ^{77}Se NMR spectrum of compound **23** in $CDCl_3$.

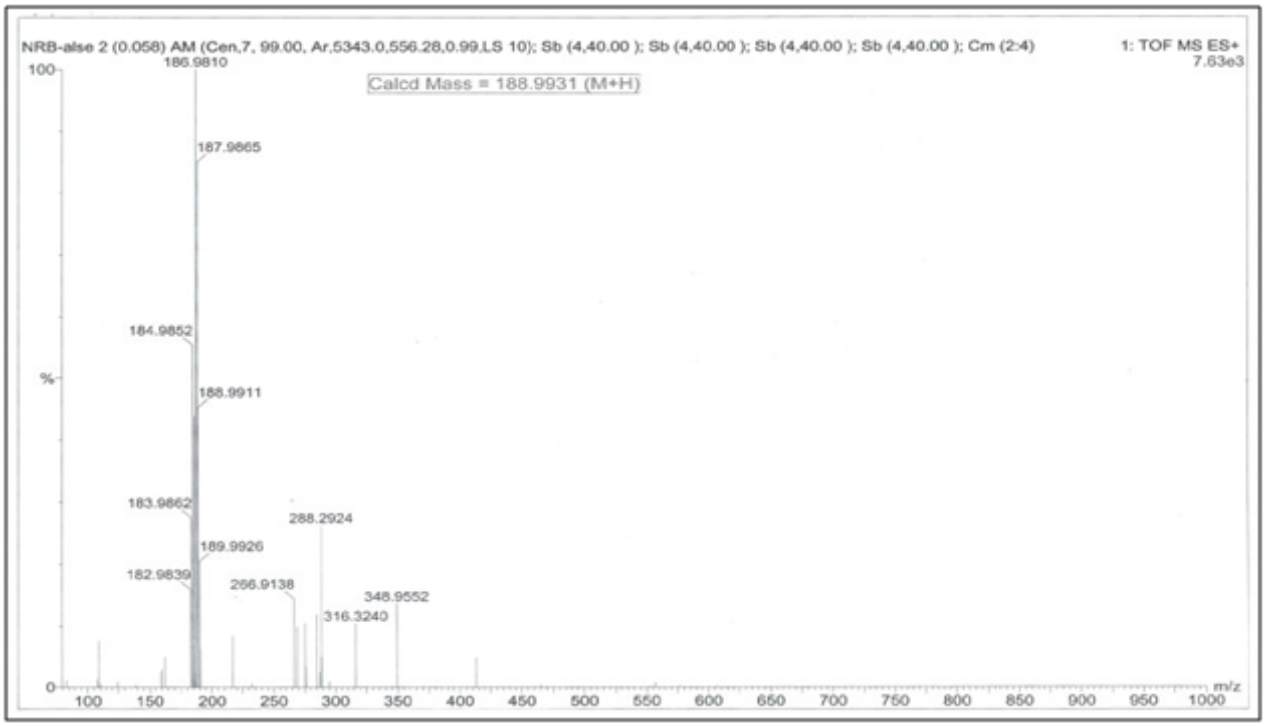

Figure S32. ESI-MS spectrum of compound **23**. Calculated mass $(M+H)^+$: 188.9931; observed mass: 188.9911.

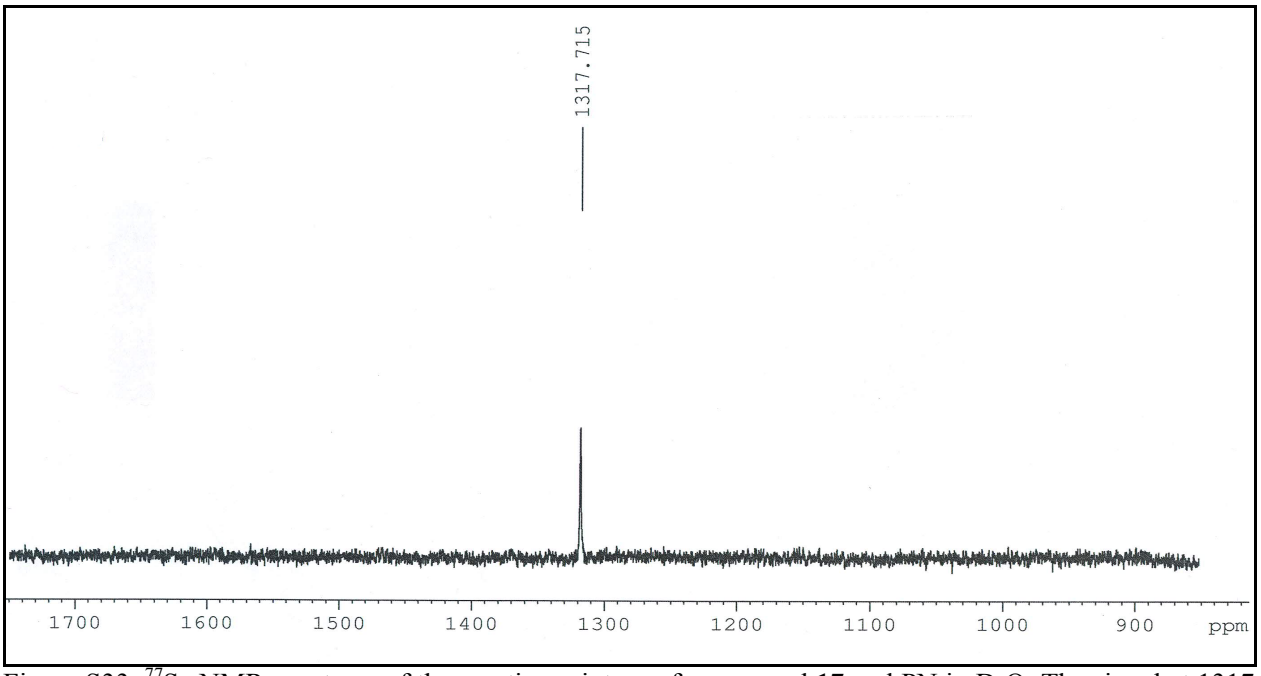

Figure S33. ^{77}Se NMR spectrum of the reaction mixture of compound **17** and PN in D_2O. The signal at 1317 ppm is due to the formation of H_2SeO_3 as the eliminated product.

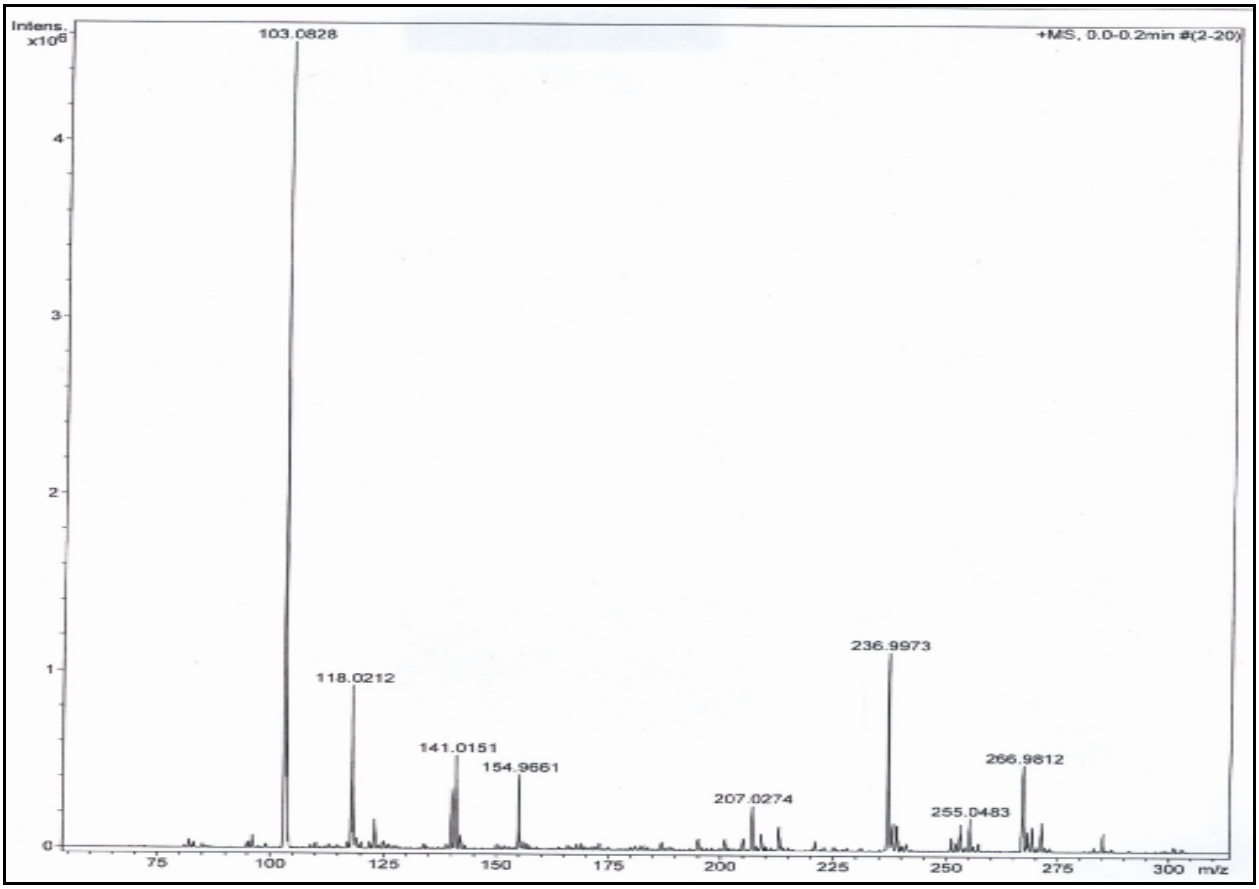

Figure S34. ESI-MS spectrum of the reaction mixture of compound **17** and PN that produces compound **28** as the final metabolite. Calculated mass $(M)^{2+}$ (*m/z*): 103.0760; observed mass: 103.0828.

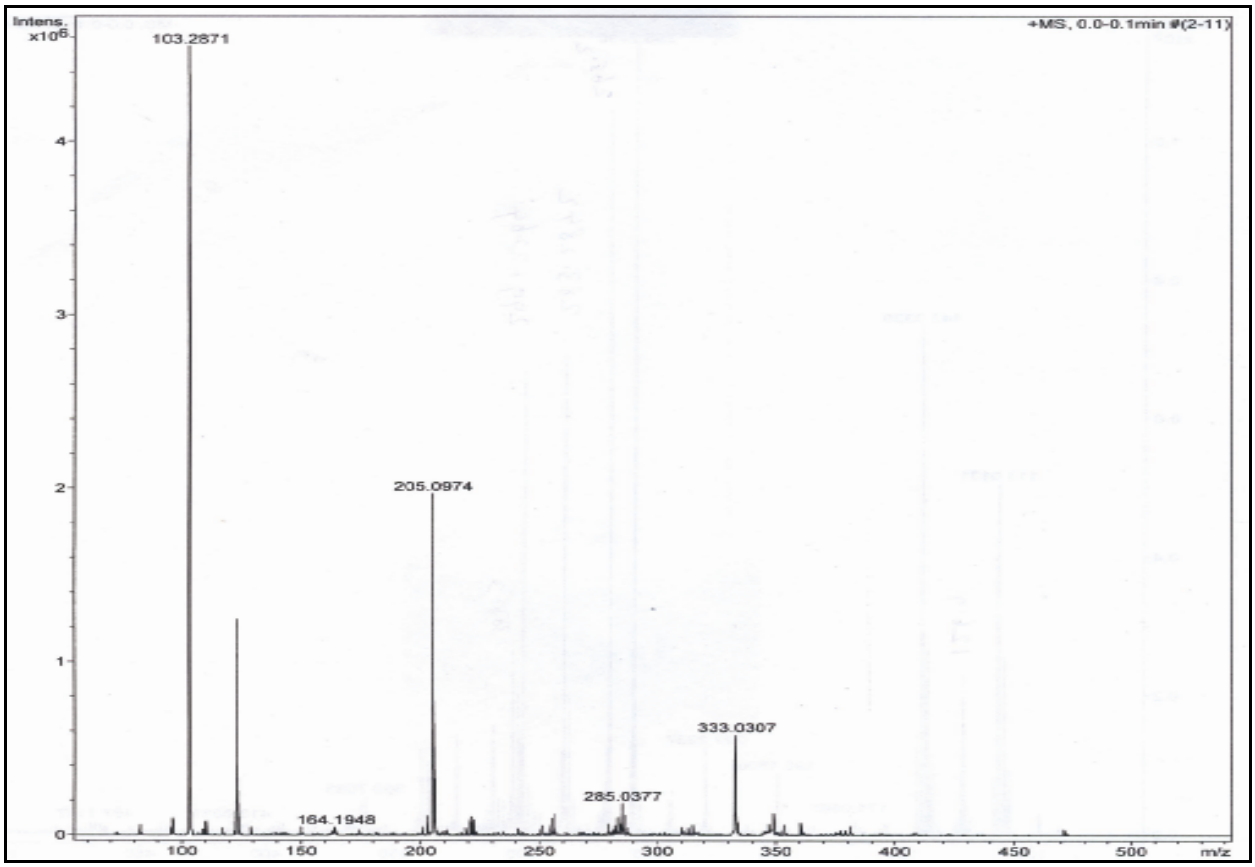

Figure S35. ESI-MS spectrum of the reaction mixture of compound **16** and PN that produces compound **28** as the final metabolite. Calculated mass $(M)^{2+}$ (*m/z*): 103.0760; observed mass: 103.2871.